

Supplement

Biological activities predicted by the analyzed web-service for the initial and repurposed indications

Designations:

Green cell filling - the target or activity associated with the repurposed and initial indication(s)

Orange cell filling - the target or activity associated with the repurposed indication(s)

Blue cell filling - the target or activity associated with the initial indication(s)

All predicted biological activities are given in the descending order of their probabilities calculated by particular web-service

Supplement 1

Biological activity profile predicted with ChemProt 3.0

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

Predicted Targets

Kappa-type opioid receptor

Mu-type opioid receptor

Cytochrome P450 3A4

Cytochrome P450 3A7

Cytochrome P450 3A5

Alpha-1-acid glycoprotein 1

Serum albumin

Multidrug resistance protein 1

Delta-type opioid receptor

Neuropeptides B/W receptor type 2

Cytochrome c oxidase subunit 3

Proenkephalin-B

Cholinesterase

Cytochrome P450 2C9

E3 ubiquitin-protein ligase HERC2

Prothrombin

Glycogen debranching enzyme

3-hydroxy-3-methylglutaryl-coenzyme A reductase

Opioid growth factor receptor

Non-secretory ribonuclease

Integrin alpha-2

Neuropeptides B/W receptor type 1

Transaldolase

Opioid-binding protein/cell adhesion molecule

Tissue factor

Alpha-1-acid glycoprotein 2
Sigma non-opioid intracellular receptor 1

Alprostadi

Molecular Mechanism (initial) :
prostaglandin E2 receptor agonist
Molecular Mechanism (repurposed) :
prostaglandin E2 receptor agonist

Predicted Targets

Prostaglandin E2 receptor EP4 subtype
Prostaglandin E2 receptor EP2 subtype

Prostacyclin receptor

Amantadine hydrochloride

Molecular Mechanism (initial) :
matrix protein 2 (Influenza virus A) inhibitor
Molecular Mechanism (repurposed) :
dopamine receptor agonists
NMDA receptor antagonists

Predicted Targets

Matrix protein 2
D (UniProtID = P14416 - D(2) dopamine receptor)

Aromatic-L-amino-acid decarboxylase
Amine oxidase B
Solute carrier family 22 member 2
Solute carrier family 22 member 1
Multidrug resistance protein 1
Solute carrier family 22 member 2
Solute carrier family 22 member 1
Multidrug and toxin extrusion protein 1
Carbonic anhydrase 4
Tryptophan--tRNA ligase
Fructose-bisphosphate aldolase C
Hyaluronan synthase 1
Procollagen-lysine
Blood group Rh
Zinc finger and BTB domain-containing protein 32
Alpha-tocopherol transfer protein
Potassium voltage-gated channel subfamily H member 2
Phosphatidylinositol 4-phosphate 5-kinase type-1 beta
Cholinesterase
Orexin
Sigma non-opioid intracellular receptor 1
Solute carrier family 22 member 3
Interferon alpha-1/13
Glutamate receptor ionotropic (NMDA receptor)
Sialidase-1
2'-5'-oligoadenylate synthase 2

Proto-oncogene c-Fos
 Early endosome antigen 1
 Fructose-bisphosphate aldolase A
 Phospholipid hydroperoxide glutathione peroxidase
 Interferon alpha-inducible protein 6
 Tyrosine-protein kinase JAK1
 Catechol O-methyltransferase
 Frataxin
 Epidermal growth factor receptor substrate 15
 Dynamin-1
 Fructose-bisphosphate aldolase B
 Interferon alpha-2
 Epididymal secretory glutathione peroxidase
 Glucagon
 Glutathione peroxidase 1
 Brain-derived neurotrophic factor
 ATP-dependent 6-phosphofructokinase
 Thioredoxin reductase 1
 Prelamin-A/C
 Thyrotropin receptor
 Nuclear factor NF-kappa-B p105 subunit
 Peripheral myelin protein 22
 Signal transducer and activator of transcription 6
 Regulator of G-protein signaling 4
 Nuclear factor erythroid 2-related factor 2
 Os06g0676700 protein
 Histone acetyltransferase KAT2A
 Histone-lysine N-methyltransferase EHMT2
 Matrix protein 2
 Solute carrier organic anion transporter family member 2B1
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 Canalicular multispecific organic anion transporter 1

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

Predicted Targets

Cytochrome P450 2C19
 Cytochrome P450 2C9
 Cytochrome P450 2D6
 Cytochrome P450 3A4
 Cytochrome P450 3A5

Sodium-dependent noradrenaline transporter

Sodium-dependent serotonin transporter
 5-hydroxytryptamine receptor 2A
 5-hydroxytryptamine receptor 1A

Delta-type opioid receptor
Kappa-type opioid receptor
High affinity nerve growth factor receptor
BDNF/NT-3 growth factors receptor
Alpha-1A adrenergic receptor
Alpha-1D adrenergic receptor
Alpha-2A adrenergic receptor
Histamine H1 receptor
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Potassium voltage-gated channel subfamily KQT member 2
Potassium voltage-gated channel subfamily A member 1
Histamine H2 receptor
Sigma non-opioid intracellular receptor 1
5-hydroxytryptamine receptor 2C
Alpha-1B adrenergic receptor
5-hydroxytryptamine receptor 7
5-hydroxytryptamine receptor 1D
Mu-type opioid receptor
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 6
Potassium voltage-gated channel subfamily KQT member 3
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Cytochrome P450 1A2
Cytochrome P450 2B6
Cytochrome P450 2C8
Cytochrome P450 2E1
Serum albumin
Alpha-1-acid glycoprotein 1
Multidrug resistance protein 1
Sodium-dependent serotonin transporter
Potassium voltage-gated channel subfamily H member 2
Histamine H1 receptor
Alpha-1A adrenergic receptor
Solute carrier family 22 member 1

Sodium channel protein type 9 subunit alpha

Sodium channel protein type 5 subunit alpha
Sodium channel protein type 2 subunit alpha
Serine/threonine-protein phosphatase 2A catalytic subunit beta isoform
Serine palmitoyltransferase 2
Asparagine synthetase
Solute carrier family 2
Serine/threonine-protein phosphatase 5
Alpha-1-acid glycoprotein 2
Potassium voltage-gated channel subfamily D member 3

Histamine H4 receptor
Early growth response protein 1
Galactosylgalactosylxylosylprotein 3-beta-glucuronosyltransferase 2
Interleukin-12 subunit beta
Glucocorticoid receptor
UDP-galactose translocator
Serine/threonine-protein phosphatase 2B catalytic subunit gamma isoform
Cyclin-dependent kinase inhibitor 1
Nuclear receptor subfamily 0 group B member 2
2-amino-3-ketobutyrate coenzyme A ligase
Excitatory amino acid transporter 1
5-hydroxytryptamine receptor 2B
Peptidyl-prolyl cis-trans isomerase G
G1/S-specific cyclin-D2
Pro-opiomelanocortin
Serine palmitoyltransferase 1
WD repeat domain phosphoinositide-interacting protein 1
Fibronectin type III domain-containing protein 4
Serine protease hepsin
Phytanoyl-CoA dioxygenase
Glial cell line-derived neurotrophic factor
Sodium- and chloride-dependent GABA transporter 1
Cellular tumor antigen p53
Inhibin beta E chain
Corticoliberin
Sodium-dependent dopamine transporter
Serine/threonine-protein phosphatase with EF-hands 2
Serine/threonine-protein phosphatase 4 catalytic subunit
Transgelin
Sodium channel protein type 3 subunit alpha
Protein DEPP
Fatty acid-binding protein
Orexin
Integrin alpha-2
Serine/threonine-protein phosphatase PP1-beta catalytic subunit
5-aminolevulinate synthase
UDP-glucuronosyltransferase 1-1
Interleukin-12 subunit alpha
UDP-glucuronosyltransferase 2B7
D
Serine/threonine-protein phosphatase 6 catalytic subunit
Hydroxymethylglutaryl-CoA synthase
Protachykinin-1
Serine/threonine-protein phosphatase PP1-alpha catalytic subunit
AP-1 complex subunit sigma-1A
P2X purinoceptor 4
Potassium voltage-gated channel subfamily D member 2
Serine/threonine-protein phosphatase PP1-gamma catalytic subunit
Ryanodine receptor 1
Torsin-1A

Sphingomyelin phosphodiesterase
Biotin--protein ligase
Histamine H3 receptor
Amine oxidase A
5-hydroxytryptamine receptor 3A
Sodium channel protein type 8 subunit alpha
Sterol regulatory element-binding protein 1
Lanosterol synthase
Serine/threonine-protein phosphatase with EF-hands 1
Sterol regulatory element-binding protein 2
Ryanodine receptor 2
UDP-glucuronosyltransferase 1-5
UDP-glucuronosyltransferase 1-4
Amine oxidase B
Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform
Acid ceramidase
Serine/threonine-protein phosphatase 2B catalytic subunit beta isoform
Ryanodine receptor 3
Protein NDRG4
Alpha-2C adrenergic receptor
Corticotropin-releasing factor receptor 1
Nuclear protein 1
Neuropeptide S
Glycerophosphodiester phosphodiesterase domain-containing protein 3
Glutathione S-transferase P
Serine palmitoyltransferase 3
Brain-derived neurotrophic factor
Histone deacetylase 9
UDP-glucuronosyltransferase 1-3
Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform
Arachidonate 15-lipoxygenase B
Thioredoxin reductase 1
Ubiquitin carboxyl-terminal hydrolase 1
Muscarinic acetylcholine receptor M1
Nuclear factor NF-kappa-B p105 subunit
Serine/threonine-protein kinase mTOR
Chromobox protein homolog 1
Ataxin-2
3-hydroxyacyl-CoA dehydrogenase type-2
Alpha-1B adrenergic receptor
Alpha-2B adrenergic receptor
5-hydroxytryptamine receptor 1A
Alpha-1D adrenergic receptor
5-hydroxytryptamine receptor 1B
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
5-hydroxytryptamine receptor 2C
Muscarinic acetylcholine receptor M5
Muscarinic acetylcholine receptor M2
5-hydroxytryptamine receptor 2A

5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 1F
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 6
5-hydroxytryptamine receptor 7
5-hydroxytryptamine receptor 5A
5-hydroxytryptamine receptor 5B
Sodium channel protein type 1 subunit alpha
5-hydroxytryptamine receptor 3A
Histamine H2 receptor
5-hydroxytryptamine receptor 4
5-hydroxytryptamine receptor 3B
Transporter
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Canalicular multispecific organic anion transporter 1
Uncharacterized protein
Sodium-dependent dopamine transporter
5-hydroxytryptamine receptor 6

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

Predicted Targets

Sigma non-opioid intracellular receptor 1

Sigma non-opioid intracellular receptor 1

**D (uniprotID = P14416 D(2) dopamine receptor
uniprotID = P21917 D(4) dopamine receptor)**

Alpha-2C adrenergic receptor

Alpha-2B adrenergic receptor

5-hydroxytryptamine receptor 2C

5-hydroxytryptamine receptor 1A

5-hydroxytryptamine receptor 2A

5-hydroxytryptamine receptor 2B

Alpha-2A adrenergic receptor

5-hydroxytryptamine receptor 1D

5-hydroxytryptamine receptor 1B

Zinc finger protein mex-5 *Caenorhabditis elegans*

Solute carrier family 22 member 1

Potassium voltage-gated channel subfamily H member 2

Lysine-specific demethylase 4E

Menin

Arachidonate 15-lipoxygenase B

ATP-dependent 6-phosphofructokinase

Geminin

Glutaminase kidney isoform

Putative fructose-1
Retinal dehydrogenase 1
Prelamin-A/C
Cellular tumor antigen p53
Luciferin 4-monooxygenase
Cytochrome P450 3A4
Cytochrome P450 2D6
Microtubule-associated protein tau
Vitamin D3 receptor
Cytochrome P450 2C9
15-hydroxyprostaglandin dehydrogenase
Lethal factor Bacillus anthracis
Peripheral myelin protein 22
Mitogen-activated protein kinase 1
Cytochrome P450 2C19
Regulator of G-protein signaling 4
Nuclear receptor ROR-gamma
Histone-lysine N-methyltransferase 2A
Histone-lysine N-methyltransferase EHMT2
3-hydroxyacyl-CoA dehydrogenase type-2
4'-phosphopantetheinyl transferase ffp
Tyrosyl-DNA phosphodiesterase 1
Cytochrome P450 1A2
5-hydroxytryptamine receptor 1A
5-hydroxytryptamine receptor 7
5-hydroxytryptamine receptor 2C
5-hydroxytryptamine receptor 2A
Alpha-1B adrenergic receptor
Alpha-2B adrenergic receptor
Alpha-2C adrenergic receptor
Alpha-2A adrenergic receptor
Alpha-1D adrenergic receptor
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 1F
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 6
Delta-type opioid receptor
Mu-type opioid receptor
Kappa-type opioid receptor
5-hydroxytryptamine receptor 5A
5-hydroxytryptamine receptor 5B
5-hydroxytryptamine receptor 3A
Alpha-1A adrenergic receptor
5-hydroxytryptamine receptor 4
5-hydroxytryptamine receptor 3B

Acetylsalicylic acid

Molecular Mechanism (initial) :
cyclooxygenase inhibitor

**Molecular Mechanism (repurposed) :
cyclooxygenase inhibitor**

Predicted Targets

Multidrug resistance-associated protein 5
Multidrug resistance-associated protein 1
Aldo-keto reductase family 1 member C3
Aldo-keto reductase family 1 member C1
Angiotensinogen
Apoptosis regulator BAX
Apoptosis regulator Bcl-2
BH3-interacting domain death agonist
Baculoviral IAP repeat-containing protein 5
Calmodulin
C-C motif chemokine 2
G2/mitotic-specific cyclin-B1
CD40 ligand
Platelet glycoprotein 4
CD44 antigen
Cyclin-dependent kinase inhibitor 1
CCAAT/enhancer-binding protein beta
Cyclin-dependent kinase inhibitor 1B
Inhibitor of nuclear factor kappa-B kinase subunit alpha
Cocaine esterase
Dermcidin
Growth-regulated alpha protein
Fractalkine
Transcription factor E2F1
Diablo homolog
Tumor necrosis factor receptor superfamily member 6
Fibrinogen gamma chain
Growth arrest-specific protein 6
Glucose-6-phosphate 1-dehydrogenase
Gastrokin-1
Growth/differentiation factor 15
Glycogen synthase kinase-3 beta
Heat shock factor protein 1
Histone deacetylase 3
Interferon gamma
Interleukin-12 subunit beta
Interleukin-12 subunit alpha
Interleukin-1 receptor antagonist protein
Interleukin-1 beta
Interleukin-2
Interleukin-8
Integrin beta-3
Low-density lipoprotein receptor
Transcription factor AP-1
Apolipoprotein
Induced myeloid leukemia cell differentiation protein Mcl-1

NF-kappa-B inhibitor alpha
Tumor necrosis factor receptor superfamily member 16
Nitric oxide synthase
Oncostatin-M
Ornithine carbamoyltransferase
Platelet factor 4 variant
Platelet factor 4
Xaa-Pro dipeptidase
Serum paraoxonase/arylesterase 1
Urokinase plasminogen activator surface receptor
Peroxisome proliferator-activated receptor alpha
Peroxisome proliferator-activated receptor delta
Peroxisome proliferator-activated receptor gamma
Protein kinase C delta type
Protein kinase C beta type
Platelet basic protein
Prostaglandin E synthase
Protein kinase C epsilon type

Prostaglandin G/H synthase 2

Ras-related C3 botulinum toxin substrate 1
Diamine acetyltransferase 1
Renin
Suprabasin
L-selectin
Sucrase-isomaltase
Solute carrier family 22 member 6
Solute carrier family 22 member 11
Signal transducer and activator of transcription 3
SPARC
Stromal membrane-associated protein 2
Solute carrier family 22 member 9
Signal transducer and activator of transcription 6
Sero transferrin
Tumor necrosis factor
Tumor necrosis factor ligand superfamily member 10
Cellular tumor antigen p53
E3 ubiquitin-protein ligase XIAP
VIP peptides
UDP-glucuronosyltransferase 1-7
Merged into Q9HAW8.
14-3-3 protein epsilon
DNA repair protein XRCC3
P2Y purinoceptor 1

Prostaglandin G/H synthase 1

Nuclear receptor subfamily 1 group I member 2
Catechol O-methyltransferase
UDP-glucuronosyltransferase 1-6
Integrin alpha-2
Platelet endothelial aggregation receptor 1
5'-AMP-activated protein kinase catalytic subunit alpha-1

5'-AMP-activated protein kinase catalytic subunit alpha-2
5'-AMP-activated protein kinase subunit beta-2
5'-AMP-activated protein kinase subunit gamma-1
Endothelin-1 receptor
Inhibitor of nuclear factor kappa-B kinase subunit beta
78 kDa glucose-regulated protein
Ribosomal protein S6 kinase alpha-3
Nuclear factor NF-kappa-B p100 subunit
Nuclear factor NF-kappa-B p105 subunit
Cytochrome P450 2C19
Cytochrome P450 2C8
Cytochrome P450 2C9
Serum albumin
Multidrug resistance protein 1
Cytochrome P450 1A2
Cytochrome P450 3A4
Cytochrome P450 2D6
Gamma-glutamyltranspeptidase 1
Carbonic anhydrase 1
Carbonic anhydrase 2
Gamma-secretase subunit APH-1A
Vinculin
Mitogen-activated protein kinase 13
Estrogen receptor
Beta-2-glycoprotein 1
Thrombopoietin
Myeloid leukemia factor 2
Cystic fibrosis transmembrane conductance regulator
T-cell surface glycoprotein CD4
Trafficking protein particle complex subunit 6A
HLA class II histocompatibility antigen gamma chain
Cytochrome b-c1 complex subunit 1
B-cell lymphoma 3 protein
Intercellular adhesion molecule 3
Tumor necrosis factor receptor superfamily member 1A
Integrin beta-4
Dual specificity mitogen-activated protein kinase kinase 5
Cyclin-dependent kinase 19
Tropomodulin-4
Uracil-DNA glycosylase
Tumor necrosis factor receptor superfamily member 10A
Geranylgeranyl transferase type-2 subunit alpha
Heme oxygenase 1
Mitogen-activated protein kinase 12
Mitogen-activated protein kinase 1
Arylsulfatase A
Interleukin-2 receptor subunit beta
Tissue-type plasminogen activator
Metalloproteinase inhibitor 1
Aurora kinase A

Coagulation factor IX
72 kDa type IV collagenase
Phosphoprotein associated with glycosphingolipid-enriched microdomains 1
Probable ATP-dependent RNA helicase DDX5
Protein NKG7
Muellerian-inhibiting factor
Transcription factor RelB
Transforming growth factor beta-1
B-cell antigen receptor complex-associated protein alpha chain
Eosinophil peroxidase
Gamma-secretase subunit PEN-2
Intercellular adhesion molecule 5
Hsp90 co-chaperone Cdc37
Myeloperoxidase
Plasminogen activator inhibitor 1
Aryl hydrocarbon receptor
Interleukin-4
G1/S-specific cyclin-D1
Vitronectin
Voltage-dependent calcium channel gamma-1 subunit
CD82 antigen
Fructose-bisphosphate aldolase C
Protein-lysine 6-oxidase
Glyceraldehyde-3-phosphate dehydrogenase
Baculoviral IAP repeat-containing protein 2
Mitogen-activated protein kinase 14
5'-AMP-activated protein kinase subunit beta-1
Killer cell lectin-like receptor subfamily B member 1
Ornithine decarboxylase
DNA mismatch repair protein Mlh1
Interleukin-5
Lactotransferrin
Receptor expression-enhancing protein 6
Tissue factor pathway inhibitor
Apolipoprotein B-100
Catalase
Apolipoprotein A-I
V-type proton ATPase 21 kDa proteolipid subunit
Protein TFG
14-3-3 protein theta
Breast cancer anti-estrogen resistance protein 3
Proto-oncogene Mas
Apoptosis-associated speck-like protein containing a CARD
Interferon regulatory factor 1
Prostacyclin synthase
Tumor necrosis factor-inducible gene 6 protein
ATP synthase subunit epsilon
Aspartate aminotransferase
Calnexin
Vasodilator-stimulated phosphoprotein

Prostaglandin E2 receptor EP2 subtype
Protein fosB
Allograft inflammatory factor 1-like
Calpain small subunit 1
SUMO-activating enzyme subunit 2
Apolipoprotein E
Leukocyte immunoglobulin-like receptor subfamily A member 2
Ras-related C3 botulinum toxin substrate 2
TNF receptor-associated factor 2
Fibroblast growth factor 1
Fragile X mental retardation syndrome-related protein 2
Mitochondrial-processing peptidase subunit beta
cAMP-regulated phosphoprotein 19
RAF proto-oncogene serine/threonine-protein kinase
40S ribosomal protein S16
Hemoglobin subunit alpha
Ubiquitin conjugation factor E4 A
Thymidine phosphorylase
Elastin
Thrombospondin-1
Erythropoietin
Peroxidase homolog
Glial fibrillary acidic protein
Transcription factor jun-D
Transient receptor potential cation channel subfamily M member 4
GTPase KRas
WW domain-binding protein 2
Coagulation factor XII
E3 ubiquitin-protein ligase TRIM21
Protein BTG1
Vacuolar protein sorting-associated protein 4A
C-reactive protein
POU domain
Calcium-activated potassium channel subunit beta-4
Annexin A1
Serum amyloid A-2 protein
Adenomatous polyposis coli protein
Cyclin-dependent kinase 4
CD63 antigen
Advillin
Toll-like receptor 2
Interleukin-6
Ubiquitin carboxyl-terminal hydrolase 15
Mediator of RNA polymerase II transcription subunit 4
Histone acetyltransferase KAT7
TRAF family member-associated NF-kappa-B activator
Proto-oncogene c-Rel
Tetraspanin-3
Cytosolic Fe-S cluster assembly factor NUBP2
TNF receptor-associated factor 5

Protein phosphatase 1 regulatory subunit 12A
Kinesin-like protein KIF20B
Peptidyl-prolyl cis-trans isomerase G
Ubiquitin-conjugating enzyme E2 K
von Willebrand factor
Lactoperoxidase
Bleomycin hydrolase
Importin subunit alpha-4
Scavenger receptor class B member 1
Cadherin-1
Interleukin-1 alpha
Apoptotic chromatin condensation inducer in the nucleus
E3 ubiquitin-protein ligase SMURF2
Axin-1
Integrin alpha-IIb
Ras-related protein Rab-2A
Potassium-transporting ATPase alpha chain 1
G1/S-specific cyclin-E1
ATP-dependent RNA helicase DDX18
Dual specificity mitogen-activated protein kinase kinase 2
Metalloproteinase inhibitor 2
Actin-related protein 3
Mitogen-activated protein kinase 3
F-actin-capping protein subunit alpha-1
Non-receptor tyrosine-protein kinase TYK2
Phosphatidylinositol 4
Baculoviral IAP repeat-containing protein 3
Potassium channel subfamily K member 6
Bromodomain-containing protein 4
Granulysin
Thromboxane-A synthase
P-selectin
Pro-opiomelanocortin
Cystatin-A
Cell surface glycoprotein MUC18
Histone deacetylase 4
Retinoblastoma-associated protein
Caspase-6
Annexin A3
Intercellular adhesion molecule 1
Lysosome membrane protein 2
Translocon-associated protein subunit gamma
Kininogen-1
Cyclin-dependent kinase 2
V-type proton ATPase 116 kDa subunit a isoform 3
PEST proteolytic signal-containing nuclear protein
Pituitary homeobox 1
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha
Mismatch repair endonuclease PMS2
Calpain-2 catalytic subunit

Serine/threonine-protein phosphatase 4 catalytic subunit
Type-1 angiotensin II receptor
RAC-alpha serine/threonine-protein kinase
Protein Tob1
Furin
Cytochrome b-c1 complex subunit 2
Receptor tyrosine-protein kinase erbB-2
Glucose-6-phosphatase 3
PRA1 family protein 3
Cathepsin K
Protein S100-A11
Ras-related protein Ral-B
Calpain-1 catalytic subunit
Epidermal growth factor receptor
Granzyme A
Ferritin heavy chain
Spermatogenesis-associated protein 5
GDNF family receptor alpha-3
Ras GTPase-activating-like protein IQGAP2
Neurogenic locus notch homolog protein 1
Tumor necrosis factor receptor superfamily member 10B
High affinity immunoglobulin epsilon receptor subunit beta
Serine-protein kinase ATM
Nicastrin
High affinity immunoglobulin epsilon receptor subunit gamma
CCAAT/enhancer-binding protein gamma
Cysteinyl leukotriene receptor 2
Interleukin-18
Tyrosine-protein kinase Fer
T-cell surface glycoprotein CD8 alpha chain
Parathyroid hormone
Heterogeneous nuclear ribonucleoprotein U
3-hydroxy-3-methylglutaryl-coenzyme A reductase
Amyloid beta A4 protein
A disintegrin and metalloproteinase with thrombospondin motifs 1
Wnt inhibitory factor 1
Integrin alpha-M
Vascular cell adhesion protein 1
Prostaglandin E2 receptor EP1 subtype
V-type proton ATPase subunit d 1
Actin
Angiotensin-converting enzyme
ES1 protein homolog
Prostacyclin receptor
Trefoil factor 2
Arachidonate 15-lipoxygenase
Leukotriene C4 synthase
Integrin alpha-5
Signal transducer and activator of transcription 5B
Atrial natriuretic peptide receptor 1

C-C motif chemokine 19
Dual specificity mitogen-activated protein kinase kinase 1
Integrin-linked protein kinase
15-hydroxyprostaglandin dehydrogenase
Alkaline phosphatase
Annexin A5
Melanotransferrin
Amyloid beta A4 precursor protein-binding family B member 1
Granulocyte-macrophage colony-stimulating factor
Interleukin-3
WD repeat and FYVE domain-containing protein 2
Prohibitin
Peptidyl-prolyl cis-trans isomerase B
Plasminogen activator inhibitor 2
PCNA-associated factor
Aminopeptidase N
Ribonuclease K6
Tumor protein p53-inducible protein 13
Tubulin alpha-1A chain
Transcription factor SOX-7
Prepronociceptin
Platelet glycoprotein VI
Insulin receptor substrate 1
Prostaglandin D2 receptor
fMet-Leu-Phe receptor
Bcl-2-like protein 1
Insulin-like growth factor I
Prostaglandin E2 receptor EP4 subtype
Ribonucleoside-diphosphate reductase subunit M2
Platelet glycoprotein IX
Pro-thyrotropin-releasing hormone
M-phase inducer phosphatase 1
Collagen alpha-1 chain
GTP-binding protein 2
Ras-related C3 botulinum toxin substrate 3
Prothrombin
Fibrinogen beta chain
Guanine nucleotide-binding protein G
Poly
Fibrinogen alpha chain
Interleukin-7 receptor subunit alpha
Proto-oncogene c-Fos
Eukaryotic translation initiation factor 2-alpha kinase 3
Elongation of very long chain fatty acids protein 5
Gamma-aminobutyric acid receptor-associated protein
Neuroendocrine convertase 1
P2Y purinoceptor 12
Leukotriene B4 receptor 1
Transforming acidic coiled-coil-containing protein 3
39S ribosomal protein L46

Hematopoietic progenitor cell antigen CD34
Bcl2-associated agonist of cell death
Ubiquitin carboxyl-terminal hydrolase CYLD
Plasminogen
GTPase HRas
Oxidized low-density lipoprotein receptor 1
Telomerase reverse transcriptase
Tensin-3
Fos-related antigen 1
Heat shock 70 kDa protein 6
Protein SEC13 homolog
Caspase-3
ETS-related transcription factor Elf-4
Transcription factor E3
Acyl-CoA dehydrogenase family member 9
RING finger protein 26
CASP8 and FADD-like apoptosis regulator
Leptin
NF-kappa-B inhibitor beta
Ubiquitin-conjugating enzyme E2 N
Cell division control protein 42 homolog
Prostate-specific antigen
Arachidonate 12-lipoxygenase
Hydroperoxide isomerase ALOXE3
Presenilin-1
tRNA dimethylallyltransferase
Hematopoietic lineage cell-specific protein
Histone H4 transcription factor
Guanylate kinase
Cytochrome c oxidase subunit 5A
Choline dehydrogenase
Mucosa-associated lymphoid tissue lymphoma translocation protein 1
Puromycin-sensitive aminopeptidase
Nuclear receptor subfamily 2 group C member 2
Proteinase-activated receptor 1
Protachykinin-1
TNFAIP3-interacting protein 2
Phorbol-12-myristate-13-acetate-induced protein 1
CD151 antigen
Alpha-2-antiplasmin
E3 ubiquitin-protein ligase SIAH2
T-cell differentiation antigen CD6
F-box only protein 11
Proprotein convertase subtilisin/kexin type 7
Cytochrome P450 2B6
Protein flightless-1 homolog
NF-kappa-B inhibitor zeta
Protein tyrosine phosphatase receptor type C-associated protein
Nestin
Dihydrolipoyllysine-residue succinyltransferase component of 2-oxoglutarate dehydrogenase complex

Transcription factor Sp1
DENN domain-containing protein 5A
Homeobox protein TGIF1
Histone-lysine N-methyltransferase NSD2
Translocator protein
Zinc finger protein 37A
Gastrin
Thyroid peroxidase
Platelet glycoprotein Ib alpha chain
Transmembrane emp24 domain-containing protein 9
Caspase-9
Small ubiquitin-related modifier 3
Ectodysplasin-A receptor-associated adapter protein
Anoctamin-9
N-alpha-acetyltransferase 38
E-selectin
Calcitonin
Collagen alpha-1
Tissue factor
Metastasis-associated protein MTA1
Nuclear receptor subfamily 4 group A member 3
85/88 kDa calcium-independent phospholipase A2
Mitogen-activated protein kinase 11
Protein EVI2B
Tyrosine-protein kinase BAZ1B
Interleukin-6 receptor subunit beta
NACHT
Nociceptin receptor
Cyclic AMP-dependent transcription factor ATF-4
Solute carrier family 22 member 8
Fructose-bisphosphate aldolase A
Superoxide dismutase
Biotin--protein ligase
Hypoxia-inducible factor 1-alpha
Tyrosine-protein kinase Lck
Pumilio homolog 2
DNA damage-inducible transcript 3 protein
Zinc finger protein 385A
Ezrin
N-formyl peptide receptor 2
Suppressor of cytokine signaling 2
LIM domain only protein 7
Troponin I
Structural maintenance of chromosomes protein 4
Cathepsin B
Antileukoprotease
Hepatoma-derived growth factor
C-C chemokine receptor type 3
Fibronectin
Insulin-induced gene 1 protein

Intraflagellar transport protein 27 homolog
Phospholipase D1
Catenin beta-1
UDP-glucuronosyltransferase 1-10
Ribonuclease pancreatic
Arf-GAP with coiled-coil
60S acidic ribosomal protein P1
STAM-binding protein
Bcl-2-modifying factor
Phospholipid hydroperoxide glutathione peroxidase
Protein S100-A4
Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
Tryptophan--tRNA ligase
F-box/LRR-repeat protein 3
26S proteasome non-ATPase regulatory subunit 12
DNA repair protein complementing XP-G cells
PDZ and LIM domain protein 7
Cation-independent mannose-6-phosphate receptor
Disintegrin and metalloproteinase domain-containing protein 33
Peroxidasin-like protein
Butyrophilin subfamily 3 member A2
Serum amyloid A-1 protein
Insulin
ETS translocation variant 3
Kinesin-like protein KIF21A
Apoptotic protease-activating factor 1
Breast cancer type 1 susceptibility protein
Caspase-8
MAP kinase-activated protein kinase 3
Proto-oncogene tyrosine-protein kinase Src
Claudin-7
Protein C-ets-2
Coagulation factor VIII
NLR family CARD domain-containing protein 4
CAP-Gly domain-containing linker protein 3
ELKS/Rab6-interacting/CAST family member 1
Antigen-presenting glycoprotein CD1d
Poly synthase 1)
F-actin-capping protein subunit alpha-2
C-X-C motif chemokine 9
TRAF-interacting protein with FHA domain-containing protein A
Conserved oligomeric Golgi complex subunit 2
LIM domain-binding protein 3
Translin-associated protein X
Lysine-specific demethylase 5B
Coagulation factor V
Antithrombin-III
Protocadherin Fat 3
Thrombomodulin
Cysteinyl leukotriene receptor 1

Ubiquitin-conjugating enzyme E2 A
Beta-nerve growth factor
GTPase NRas
Monocarboxylate transporter 1
Glutathione S-transferase omega-1
Growth arrest and DNA damage-inducible protein GADD45 alpha
Protein tyrosine phosphatase type IVA 1
Ubiquitin domain-containing protein 1
Metalloendopeptidase OMA1
UPF0184 protein C9orf16
Growth hormone-inducible transmembrane protein
Type-2 angiotensin II receptor
Prostaglandin-H2 D-isomerase
Mitochondrial-processing peptidase subunit alpha
A disintegrin and metalloproteinase with thrombospondin motifs 13
Phosphatidylinositol 3
G1/S-specific cyclin-D3
Matrix metalloproteinase-9
Tumor necrosis factor receptor superfamily member 5
Pulmonary surfactant-associated protein D
Spectrin alpha chain
Solute carrier family 22 member 7
Syndecan-4
Multidrug resistance-associated protein 4
Fructose-bisphosphate aldolase B
Histone deacetylase 1
UDP-glucuronosyltransferase 1-8
Toll-like receptor 4
Protein SCAI
Peflin
Bcl-2 homologous antagonist/killer
Tyrosine-protein kinase Fgr
Arachidonate 5-lipoxygenase
ATP-binding cassette sub-family A member 1
Tumor necrosis factor receptor superfamily member 27
tRNA pseudouridine synthase A
Isoleucine--tRNA ligase
Thromboxane A2 receptor
Eukaryotic translation initiation factor 2 subunit 2
Advanced glycosylation end product-specific receptor
Coagulation factor VII
Negative elongation factor E
Ninjurin-1
Sperm-associated antigen 6
Tumor necrosis factor receptor superfamily member 1B
Tyrosine-protein kinase SYK
Methylenetetrahydrofolate reductase
Natriuretic peptides B
Mitochondrial import inner membrane translocase subunit Tim17-B
TBC1 domain family member 10B

Neutrophil defensin 1
Arachidonate 15-lipoxygenase B
Reversion-inducing cysteine-rich protein with Kazal motifs
Zinc finger and SCAN domain-containing protein 16
Histamine H2 receptor
Ferritin light chain
Protocadherin-17
Tumor necrosis factor receptor superfamily member 25
6-phosphofructo-2-kinase/fructose-2
Kinesin-like protein KIF3A
Adenine phosphoribosyltransferase
Sushi repeat-containing protein SRPX
Beta-1
Neuronal cell adhesion molecule
Aldo-keto reductase family 1 member C2
Pirin
Arachidonate 5-lipoxygenase-activating protein
Leukocyte elastase inhibitor
BCL2/adenovirus E1B 19 kDa protein-interacting protein 3-like
Thymosin beta-4
Serine/threonine-protein kinase Chk2
Tyrosine 3-monooxygenase
Protein LAP2
Potassium-transporting ATPase alpha chain 2
Programmed cell death 1 ligand 1
Tyrosine-protein kinase JAK2
Gamma-interferon-inducible lysosomal thiol reductase
Myeloid differentiation primary response protein MyD88
Small ubiquitin-related modifier 1
Serpine B5
Otoancorin
RAC-beta serine/threonine-protein kinase
Heterogeneous nuclear ribonucleoprotein U-like protein 1
Myosin-11
Vitamin K-dependent protein S
Hyaluronan mediated motility receptor
Vitamin K epoxide reductase complex subunit 1
60S ribosomal protein L34
Flotillin-2
ICOS ligand
Interferon-induced GTP-binding protein Mx1
Caspase recruitment domain-containing protein 11
Interferon regulatory factor 9
Neuropeptide S
Protein DEK
Calcyphosin-like protein
Transcription factor p65
Mitogen-activated protein kinase kinase kinase 1
Sec1 family domain-containing protein 2
Selenoprotein M

Early growth response protein 4
Epididymal secretory glutathione peroxidase
2'-5'-oligoadenylate synthase 1
Cyclic AMP-responsive element-binding protein 1
Sodium channel subunit beta-1
Basic leucine zipper and W2 domain-containing protein 1
E3 ubiquitin-protein ligase Mdm2
Glutathione peroxidase 1
Cyclin-dependent kinase 3
Serine/threonine-protein kinase/endoribonuclease IRE1
Bcl-2-binding component 3
von Willebrand factor A domain-containing protein 1
Interleukin-10
Caspase-1
Thioredoxin reductase 1
Transformer-2 protein homolog beta
Brain-derived neurotrophic factor
Nucleoside diphosphate kinase 6
Lysine-specific demethylase 4E
Isocitrate dehydrogenase cytoplasmic
Retinal dehydrogenase 1
Glucosylceramidase
Glucocorticoid receptor
Muscarinic acetylcholine receptor M1
Androgen receptor
Lethal factor Bacillus anthracis
Thyrotropin receptor
Nuclear receptor ROR-gamma
Bloom syndrome protein
Putative uncharacterized protein
Histone-lysine N-methyltransferase EHMT2
3-hydroxyacyl-CoA dehydrogenase type-2
Tyrosyl-DNA phosphodiesterase 1
DNA polymerase kappa
DNA polymerase iota
Fatty acid-binding protein
Solute carrier family 22 member 20
Acid-sensing ion channel 3
Solute carrier family 22 member 1
Arachidonate 5-lipoxygenase
Phospholipase A2
Solute carrier organic anion transporter family member 1B3
Glutathione reductase
Histamine H1 receptor
D
Muscarinic acetylcholine receptor M5
Muscarinic acetylcholine receptor M2
Cannabinoid receptor 2
Cannabinoid receptor 1
Alpha-2C adrenergic receptor

Alpha-2B adrenergic receptor
Alpha-2A adrenergic receptor
Alpha-1B adrenergic receptor
Alpha-1A adrenergic receptor
5-hydroxytryptamine receptor 6
5-hydroxytryptamine receptor 5A
5-hydroxytryptamine receptor 3A
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 1A
Kappa-type opioid receptor
Mu-type opioid receptor

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

Predicted Targets

Tumor necrosis factor
Cystic fibrosis transmembrane conductance regulator
Gamma-aminobutyric acid type B receptor subunit 2
Solute carrier family 22 member 8
Glycine receptor subunit beta
Gamma-crystallin D
Glycine receptor subunit alpha-2
Sulfotransferase family cytosolic 2B member 1
CD9 antigen
Vesicular inhibitory amino acid transporter
Rho GTPase-activating protein 4
Proenkephalin-B
Cyclic AMP-dependent transcription factor ATF-2
Neurotensin/neuromedin N
Homeobox protein Hox-B7
Pro-neuropeptide Y
E3 ubiquitin-protein ligase MARCH7
Glutamate decarboxylase 2
Cholecystokinin
Gamma-aminobutyric acid receptor subunit beta-1
Glycine receptor subunit alpha-1
4-aminobutyrate aminotransferase
Pro-opiomelanocortin
Keratin
Gamma-aminobutyric acid receptor subunit beta-2
RAC-alpha serine/threonine-protein kinase
Glycine receptor subunit alpha-3
Gamma-aminobutyric acid receptor subunit gamma-1

Carbonic anhydrase 2
Progonadoliberin-1
Metabotropic glutamate receptor 1
G protein-activated inward rectifier potassium channel 1
Somatostatin
Sodium- and chloride-dependent GABA transporter 1
ATP-sensitive inward rectifier potassium channel 12
Metabotropic glutamate receptor 5
Prolactin
Integrin alpha-2
Prepronociceptin
Homeodomain-interacting protein kinase 3
Pro-thyrotropin-releasing hormone
Substance-P receptor
Protachykinin-1
Adenosine receptor A1
Proto-oncogene c-Fos
Transducin beta-like protein 2
Nitric oxide synthase
5-hydroxytryptamine receptor 1A
Glycoprotein hormones alpha chain
Glutamate decarboxylase 1
Adenylate cyclase type 2
G protein-activated inward rectifier potassium channel 4
Eukaryotic translation initiation factor 4 gamma 2
Metabotropic glutamate receptor 7
Metabotropic glutamate receptor 8
Cannabinoid receptor 1
Voltage-dependent L-type calcium channel subunit alpha-1S
Sodium- and chloride-dependent betaine transporter
D

Relaxin-3 receptor 2
Adenylate cyclase type 10
G protein-activated inward rectifier potassium channel 3

Gamma-aminobutyric acid type B receptor subunit 1

Multidrug resistance-associated protein 4
Glycine receptor subunit alpha-4
Adenosine receptor A3
Fragile X mental retardation protein 1
Growth/differentiation factor 5
Glutamate receptor ionotropic
UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit
Tyrosine 3-monooxygenase
5-hydroxytryptamine receptor 2A
Metabotropic glutamate receptor 2
Neuropeptide S

Gamma-aminobutyric acid receptor subunit gamma-2

Mu-type opioid receptor
Brain-derived neurotrophic factor

Gamma-aminobutyric acid receptor subunit rho-1

ATP-dependent 6-phosphofructokinase
Thioredoxin reductase 1
Prelamin-A/C
Cytochrome P450 3A4
Nuclear factor NF-kappa-B p105 subunit
Regulator of G-protein signaling 4
Bloom syndrome protein
Nuclear factor erythroid 2-related factor 2
Histone acetyltransferase KAT2A
Histone-lysine N-methyltransferase EHMT2
ATPase family AAA domain-containing protein 5
4'-phosphopantetheinyl transferase ffp

Gamma-aminobutyric acid receptor subunit alpha-1
Gamma-aminobutyric acid receptor subunit pi
Gamma-aminobutyric acid receptor subunit delta
Gamma-aminobutyric acid receptor subunit alpha-5
Gamma-aminobutyric acid receptor subunit alpha-3
Gamma-aminobutyric acid receptor subunit alpha-2
Gamma-aminobutyric acid receptor subunit alpha-4
Gamma-aminobutyric acid receptor subunit gamma-3
Gamma-aminobutyric acid receptor subunit alpha-6
Gamma-aminobutyric acid receptor subunit beta-3
GABA theta subunit
Gamma-aminobutyric acid receptor subunit epsilon

Solute carrier family 22 member 1
Sodium channel protein type 1 subunit alpha
Sodium channel protein type 2 subunit alpha
Solute carrier organic anion transporter family member 1B3
Sodium channel protein type 3 subunit alpha
Solute carrier organic anion transporter family member 1B1

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

Predicted Targets

Alpha-2A adrenergic receptor

Alpha-2B adrenergic receptor

Alpha-2C adrenergic receptor

ATP-sensitive inward rectifier potassium channel 1

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Beta-3 adrenergic receptor

Chromatin accessibility complex protein 1

Tyrosine-protein kinase STYK1

UDP-glucuronosyltransferase 1-8

Alpha-1B adrenergic receptor

UDP-glucuronosyltransferase 2B10

Myotubularin-related protein 9
 UDP-glucuronosyltransferase 2A3
 Myosin light chain kinase family member 4
 Receptor tyrosine-protein kinase erbB-3
 UDP-glucuronosyltransferase 3A1
 UDP-glucuronosyltransferase 2B4
 UDP-glucuronosyltransferase 1-6
 UDP-glucuronosyltransferase 3A2
 UDP-glucuronosyltransferase 2A1
 UDP-glucuronosyltransferase 1-1
 UDP-glucuronosyltransferase 2B7
 UDP-glucuronosyltransferase 1-7
 Hairy and enhancer of split-related protein HELT
 UDP-glucuronosyltransferase 2B17
 Cell death regulator Aven
 2-hydroxyacylsphingosine 1-beta-galactosyltransferase
 Receptor tyrosine-protein kinase erbB-4
 UDP-glucuronosyltransferase 2B28
 UDP-glucuronosyltransferase 2B15
 UDP-glucuronosyltransferase 1-5
 Pro-neuregulin-1
 UDP-glucuronosyltransferase 1-10
 UDP-glucuronosyltransferase 1-9
 UDP-glucuronosyltransferase 1-4
 Nuclear transcription factor Y subunit gamma
 Alpha-1A adrenergic receptor
 Myosin light chain kinase 2
 Alpha-1D adrenergic receptor
 Myosin light chain kinase 3
 UDP-glucuronosyltransferase 1-3
 Mitochondrial antiviral-signaling protein
 DNA polymerase epsilon subunit 4

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

Predicted Targets

Bile salt export pump

Endothelin-1 receptor

Endothelin-1

Endothelin B receptor

Cytochrome P450 3A4

Cytochrome P450 2C9

Iroquois-class homeodomain protein IRX-1

Transforming growth factor beta-1

Nitric oxide synthase

Solute carrier organic anion transporter family member 1B3

Hemoglobin subunit alpha
Glucocorticoid receptor
Prostacyclin synthase
Solute carrier organic anion transporter family member 1B1
Collagenase 3
Integrin alpha-2
Renin
Granzyme M
Angiotensin-converting enzyme
Gap junction alpha-1 protein
Coxsackievirus and adenovirus receptor
Glucagon-like peptide 1 receptor
Cathepsin B
Cytochrome P450 2B6
GTPase ERas

Endothelin-3

Endothelin-2

Ephrin type-A receptor 2
cGMP-specific 3'
Integrin alpha-L
EGF
Angiotensinogen
Connective tissue growth factor
Tumor necrosis factor receptor superfamily member 1B
Bone morphogenetic protein receptor type-2
Endothelin-converting enzyme 1
Proliferating cell nuclear antigen
Natriuretic peptides B
Natriuretic peptides A
Vasopressin-neurophysin 2-copeptin
Endothelin-converting enzyme 2

Endothelin B receptor

Endothelin-1 receptor

Bile salt export pump

Endothelin receptor type A

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :

mu-type opioid receptor agonist

Predicted Targets

Mu-type opioid receptor

Kappa-type opioid receptor
Delta-type opioid receptor
Cytochrome P450 3A4
Cytochrome P450 3A5
Cytochrome P450 2C9
Cytochrome P450 2C8

Cytochrome P450 3A7
UDP-glucuronosyltransferase 1-9
Cytochrome P450 2D6
Cytochrome P450 2C18
Cytochrome P450 2C19
Cytochrome P450 1A2
Cytochrome P450 2A6
Multidrug resistance protein 1

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Predicted Targets

Multidrug resistance-associated protein 5
Apoptosis regulator BAX
Apoptosis regulator Bcl-2
Breast cancer anti-estrogen resistance protein 1
BH3-interacting domain death agonist
Baculoviral IAP repeat-containing protein 5
Carbonic anhydrase 3
Carbonic anhydrase 2
Catalase
Cyclin-dependent kinase inhibitor 1
Cyclin-dependent kinase inhibitor 1B
Inhibitor of nuclear factor kappa-B kinase subunit alpha
DNA damage-inducible transcript 3 protein
Cytochrome P450 2C9
Cytochrome P450 1A2
Tumor necrosis factor receptor superfamily member 6
FAS-associated death domain protein
DNA fragmentation factor subunit alpha
Histone H2AX
Glycogen synthase kinase-3 beta
Transcription factor AP-1
Interleukin-1 beta
Dual specificity mitogen-activated protein kinase kinase 2
Induced myeloid leukemia cell differentiation protein Mcl-1
Antigen KI-67
Tumor necrosis factor receptor superfamily member 16
NF-kappa-B inhibitor alpha
Peroxisome proliferator-activated receptor alpha
Peroxisome proliferator-activated receptor delta
Transforming protein RhoA
Rho-related GTP-binding protein RhoB
High affinity copper uptake protein 1
Sequestosome-1
Somatostatin receptor type 2

Steryl-sulfatase
Bile salt sulfotransferase
Tumor necrosis factor
Tumor necrosis factor receptor superfamily member 10A
Tumor necrosis factor receptor superfamily member 11B
Tumor necrosis factor ligand superfamily member 10
Cellular tumor antigen p53
Vascular endothelial growth factor A
Arachidonate 5-lipoxygenase

Prostaglandin G/H synthase 2

Bifunctional epoxide hydrolase 2
Prostaglandin G/H synthase 1
Carbonic anhydrase 1
Cruzipain Trypanosoma cruzi
Quinolone resistance protein NorA
Nuclear receptor subfamily 1 group I member 2
G1/S-specific cyclin-D1
Caspase-3
Transcription factor E2F1
Peroxisome proliferator-activated receptor gamma
Retinoblastoma-associated protein
RAC-alpha serine/threonine-protein kinase
kinase isozyme 1
Cyclin-A1
Cyclin-A2
Matrix metalloproteinase-9
Bcl-2 homologous antagonist/killer
Caspase-8
Caspase-9
Cytochrome P450 3A4
Cytochrome P450 2D6
Catenin beta-1
Prostaglandin G/H synthase 1
Cytosolic phospholipase A2
Prostaglandin E synthase
Aldo-keto reductase family 1 member C3
Prostaglandin-H2 D-isomerase
Prostacyclin synthase
Thromboxane-A synthase
Insulin-like growth factor-binding protein 3
Cytochrome P450 3A5
3-phosphoinositide-dependent protein kinase 1
Serum albumin
Alpha-1-acid glycoprotein 1
Multidrug resistance-associated protein 4
Cytochrome c oxidase subunit 2
Signal transducer and activator of transcription 3
Ras-related C3 botulinum toxin substrate 1
Carbonic anhydrase 4
Carbonic anhydrase 9

Mitogen-activated protein kinase 14
Cytochrome c oxidase subunit 1
Cytochrome c oxidase subunit 2
Nitric oxide synthase
Lactotransferrin
Interleukin-12 subunit beta
Protein-lysine 6-oxidase
Mitogen-activated protein kinase 1
Carbonic anhydrase 12
Estrogen receptor
72 kDa type IV collagenase
Heme oxygenase 1
Proheparin-binding EGF-like growth factor
Fibronectin type III and SPRY domain-containing protein 1
Glyceraldehyde-3-phosphate dehydrogenase
Malate dehydrogenase
Prostaglandin E synthase 3
GTPase KRas
Piwi-like protein 1
Tumor necrosis factor ligand superfamily member 11
Ornithine decarboxylase
ATP-binding cassette sub-family G member 2
Proepiregulin
Prolow-density lipoprotein receptor-related protein 1
C-reactive protein
Prostaglandin E2 receptor EP2 subtype
C-C chemokine receptor type 7
Low-density lipoprotein receptor-related protein 3
Apolipoprotein E
Growth/differentiation factor 15
Cadherin-1
Sortilin-related receptor
Cyclin-dependent kinase 4
Adenomatous polyposis coli protein
Interleukin-6
Interleukin-1 receptor antagonist protein
Sodium-dependent serotonin transporter
Aromatase
Kynurenine--oxoglutarate transaminase 3
Low-density lipoprotein receptor-related protein 6
Histidine ammonia-lyase
G1/S-specific cyclin-D2
Sodium-dependent dopamine transporter
Histone deacetylase 4
Interleukin-1 alpha
Transmembrane emp24 domain-containing protein 2
Potassium-transporting ATPase alpha chain 1
Integral membrane protein DGCR2/IDD
Mitogen-activated protein kinase 3
Glutamate receptor 2

Low-density lipoprotein receptor-related protein 2
P-selectin
Vascular endothelial growth factor receptor 2
Bile salt export pump
Interleukin-7
Death domain-associated protein 6
Intercellular adhesion molecule 1
Multidrug resistance protein 1
Caspase-6
Pro-epidermal growth factor
Superoxide dismutase
1-phosphatidylinositol 4
Cyclin-dependent kinase 2
Receptor tyrosine-protein kinase erbB-2
Insulin-like growth factor 1 receptor
Phorbol-12-myristate-13-acetate-induced protein 1
CD320 antigen
Signal transducer and activator of transcription 5B
Cardiotrophin-1
Tumor necrosis factor receptor superfamily member 10B
Ferritin heavy chain
Epidermal growth factor receptor
Low-density lipoprotein receptor-related protein 12
Perilipin-2
Prostacyclin receptor
Angiotensin-converting enzyme
Choriogonadotropin subunit beta variant 2
15-hydroxyprostaglandin dehydrogenase
Podoplanin
Caseinolytic peptidase B protein homolog
Low-density lipoprotein receptor-related protein 5
Protein S100-P
Melanotransferrin
Transient receptor potential cation channel subfamily V member 3
Integrin alpha-2
Diphosphomevalonate decarboxylase
Arf-GAP domain and FG repeat-containing protein 2
Carbonic anhydrase 4
Kynurenine--oxoglutarate transaminase 1
Prostaglandin E2 receptor EP4 subtype
Dual specificity mitogen-activated protein kinase kinase 1
Bcl-2-like protein 1
GTPase HRas
Fatty acid synthase
Interleukin-12 subunit alpha
Low-density lipoprotein receptor-related protein 8
Carbonic anhydrase 5A
CCAAT/enhancer-binding protein beta
Interleukin-8
78 kDa glucose-regulated protein

Sphingolipid delta
CASP8 and FADD-like apoptosis regulator
Apoptosis-inducing factor 2
Carbonic anhydrase 5B
Ferritin
Interstitial collagenase
Cytochrome c oxidase subunit 5A
Low-density lipoprotein receptor class A domain-containing protein 3
ETS translocation variant 4
Carbonic anhydrase 13
Signal transducer and activator of transcription 5A
Translocator protein
Sodium channel protein type 5 subunit alpha
Transcription factor Sp1
Choline O-acetyltransferase
Cyclic AMP-dependent transcription factor ATF-4
Caveolin-1
Superoxide dismutase
Adenylate cyclase type 2
Beta-3 adrenergic receptor
Endoribonuclease Dicer
Iodotyrosine dehalogenase 1
Insulin
Carbonic anhydrase 7
Prostaglandin E synthase 2
Carbonic anhydrase 14
Low-density lipoprotein receptor-related protein 10
Mitogen-activated protein kinase kinase kinase 5
Kinesin-associated protein 3
Serine/threonine-protein kinase mTOR
Poly synthase 1)
Transforming growth factor beta-2
Tyrosine-protein kinase Fyn
Sugar transporter SWEET1
Low density lipoprotein receptor adapter protein 1
Canalicular multispecific organic anion transporter 1
GTPase NRas
Adenosine receptor A3
Cytochrome P450 2C19
Cytochrome P450 2C8
Phosphatidylinositol 3
Desmin
Urokinase-type plasminogen activator
NADPH oxidase 1
Sodium-dependent noradrenaline transporter
Carbonic anhydrase 6
Tumor necrosis factor receptor superfamily member 1B
Thromboxane A2 receptor
Ferritin light chain
Spermidine synthase

Enhancer of filamentation 1
Proliferating cell nuclear antigen
Low-density lipoprotein receptor-related protein 4
Ferritin heavy polypeptide-like 17
Triosephosphate isomerase
Potassium-transporting ATPase alpha chain 2
Survival motor neuron protein
Vitamin K epoxide reductase complex subunit 1
Very low-density lipoprotein receptor
Low-density lipoprotein receptor-related protein 1B
Transcription factor p65
Glutathione S-transferase P
Multidrug resistance-associated protein 1
Ubiquitin-60S ribosomal protein L40
Dynactin subunit 2
Bcl-2-binding component 3
Alpha-N-acetylgalactosaminide alpha-2
Kinesin light chain 1
Inactive phospholipase C-like protein 1
FSD1-like protein
Prominin-1
Solute carrier family 2
Geminin
Isocitrate dehydrogenase cytoplasmic
Ubiquitin carboxyl-terminal hydrolase 1
Prelamin-A/C
Glucocorticoid receptor
Androgen receptor
Thyroid hormone receptor beta
Thyrotropin receptor
Retinoic acid receptor RXR-alpha
Peripheral myelin protein 22
Glucagon-like peptide 1 receptor
Nuclear receptor ROR-gamma
Mothers against decapentaplegic homolog 3
Potassium voltage-gated channel subfamily H member 2
Nuclear factor erythroid 2-related factor 2
Nuclear receptor subfamily 1 group I member 2
Astrosclerin-3 Astrosclera willeyana
Alpha carbonic anhydrase Stylophora pistillata
Carbonic anhydrase Stylophora pistillata
Alpha-2B adrenergic receptor
D
Carbonic anhydrase
Probable transmembrane carbonic anhydrase
Beta-carbonic anhydrase 1
Carbonic anhydrase 2
Carbonic anhydrase
Delta carbonic anhydrase
Progesterone receptor

Carbonic anhydrase 15
Cyclooxygenase 2
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B1
Solute carrier family 22 member 1
Arachidonate 15-lipoxygenase
Arachidonate 12-lipoxygenase
Solute carrier organic anion transporter family member 1B3
Histamine H2 receptor
Histamine H1 receptor
Muscarinic acetylcholine receptor M5
Muscarinic acetylcholine receptor M2
Cannabinoid receptor 2
Cannabinoid receptor 1
Alpha-2C adrenergic receptor
Alpha-2A adrenergic receptor
Alpha-1B adrenergic receptor
Alpha-1A adrenergic receptor
5-hydroxytryptamine receptor 6
Uncharacterized protein
5-hydroxytryptamine receptor 3A
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 1E
5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 1A
Kappa-type opioid receptor
Mu-type opioid receptor

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

Predicted Targets

Glutathione S-transferase A2
Tumor necrosis factor
Cytochrome P450 3A4
Cytochrome P450 2D6
Cytochrome P450 1A1
Cytochrome P450 2C8
Cytochrome P450 3A5
Multidrug resistance protein 1
Cytochrome P450 1A2
Histidine-rich protein PFHRP-II
Cytochrome P450 2C9
Cytochrome P450 2C19
Chloroquine resistance transporter

Toll-like receptor 9
Toll-like receptor 7
Suppressor of tumorigenicity 14 protein
DNA mismatch repair protein Mlh1
Mitogen-activated protein kinase 14
Toll-like receptor 8
Cation-dependent mannose-6-phosphate receptor
Heme oxygenase 1
Interleukin-1 receptor accessory protein
T-cell surface glycoprotein CD4
Gamma-aminobutyric acid receptor-associated protein-like 2
Beta-2-glycoprotein 1
Carcinoembryonic antigen-related cell adhesion molecule 1
Aquaporin-2
Glutamate--cysteine ligase catalytic subunit
Glutathione reductase
Aquaporin-9
Tissue-type plasminogen activator
Carcinoembryonic antigen-related cell adhesion molecule 5
IgG receptor FcRn large subunit p51
B-cell antigen receptor complex-associated protein alpha chain
L-lactate dehydrogenase B chain
Interleukin-2
Complement C5
C-C motif chemokine 2
Glyceraldehyde-3-phosphate dehydrogenase
Amiloride-sensitive sodium channel subunit alpha
Interferon gamma
Porphobilinogen deaminase
Potassium voltage-gated channel subfamily H member 2
Erythropoietin
Inward rectifier potassium channel 2
Cathepsin D
Malate dehydrogenase
5'-AMP-activated protein kinase subunit gamma-3
Activin receptor type-1C
ATP-binding cassette sub-family G member 2
Copper-transporting ATPase 2
Apolipoprotein E
Complement C3
Carcinoembryonic antigen-related cell adhesion molecule 8
Aspartate aminotransferase
Uroporphyrinogen decarboxylase
Properdin
Aldehyde dehydrogenase
Interleukin-6
ATP-citrate synthase
Cytochrome P450 2E1
Gastrin-releasing peptide
C-reactive protein

Interleukin-1 receptor-associated kinase-like 2
Scavenger receptor class B member 1
Glutamate decarboxylase 2
Toll-like receptor 2
Cyclin-dependent kinase 2-associated protein 1
von Willebrand factor
Tumor necrosis factor receptor superfamily member 13B
Serine-protein kinase ATM
Interleukin-1 beta
E3 ubiquitin-protein ligase RNF167
Lactoperoxidase
Calcium-transporting ATPase type 2C member 2
Interleukin-1 alpha
Mitogen-activated protein kinase 3
Tyrosinase
ATP-binding cassette sub-family B member 6
Ceruloplasmin
Mucolipin-1
Claudin-16
Intercellular adhesion molecule 1
N-terminal kinase-like protein
Furin
Cysteine sulfinic acid decarboxylase
Receptor tyrosine-protein kinase erbB-3
Receptor tyrosine-protein kinase erbB-2
Microtubule-associated proteins 1A/1B light chain 3B
Cellular tumor antigen p53
Interferon alpha-1/13
Ferritin heavy chain
RAC-alpha serine/threonine-protein kinase
Cathepsin K
Suppression of tumorigenicity 18 protein
Epidermal growth factor receptor
Interferon regulatory factor 7
Mas-related G-protein coupled receptor member X1
Serum albumin
Glutamate decarboxylase-like protein 1
L-lactate dehydrogenase C chain
Cardiotrophin-1
Interleukin-18
Parathyroid hormone
L-lactate dehydrogenase A-like 6A
ATP synthase subunit alpha
Alkaline phosphatase
Beta-centractin
Integrin alpha-M
5'-AMP-activated protein kinase subunit gamma-2
Keratin
Toll-like receptor 3
Integrin alpha-2

Complement C2
Granulocyte-macrophage colony-stimulating factor
Aquaporin-3
Insulin receptor
L-lactate dehydrogenase A-like 6B
Peroxiredoxin-2
ATP synthase subunit d
Ubiquitin-conjugating enzyme E2 E1
fMet-Leu-Phe receptor
Beta-defensin 4A
Translocator protein
ATP-dependent zinc metalloprotease YME1L1
Platelet glycoprotein VI
P2Y purinoceptor 12
Interleukin-8
Sodium/hydrogen exchanger 10
Tyrosine-protein kinase BTK
Solute carrier family 22 member 18
Glutamine synthetase
Aquaporin-10
Caspase-3
Vacuolar protein sorting-associated protein 41 homolog
Barrier-to-autointegration factor
Early endosome antigen 1
Hephaestin-like protein 1
Complement C1s subcomponent
Prostatic acid phosphatase
Muscarinic acetylcholine receptor M2
Serine hydroxymethyltransferase
Solute carrier family 2
Sodium/hydrogen exchanger 9
Nitric oxide synthase
Cytochrome P450 2B6
5'-AMP-activated protein kinase subunit gamma-1
Serine/threonine-protein kinase ULK1
ELMO domain-containing protein 2
Sodium/hydrogen exchanger 6
Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
Pre-mRNA 3'-end-processing factor FIP1
T-lymphocyte activation antigen CD86
Interferon lambda-1
Sodium/hydrogen exchanger 7
Heat shock protein HSP 90-alpha
Lysosome-associated membrane glycoprotein 1
Cytochrome b5
Superoxide dismutase
Ribosylidihydronicotinamide dehydrogenase 2)
NADH-cytochrome b5 reductase 3
G protein-activated inward rectifier potassium channel 4
Voltage-dependent calcium channel subunit alpha-2/delta-1

Cathepsin L1
Small nuclear ribonucleoprotein Sm D2
Citrate synthase
Cathepsin B
Tumor necrosis factor ligand superfamily member 13
High mobility group protein B1
Autophagy protein 5
Sodium channel protein type 8 subunit alpha
Copper-transporting ATPase 1
Ubiquitin-like modifier-activating enzyme ATG7
Insulin
Fibronectin
Tyrosine aminotransferase
Lengsin
DNA topoisomerase 1
Sarcoplasmic/endoplasmic reticulum calcium ATPase 3
Enoyl-CoA hydratase domain-containing protein 2
Glutamate decarboxylase 1
Proto-oncogene tyrosine-protein kinase Src
Calcium-transporting ATPase type 2C member 1
DNA repair protein RAD52 homolog
Dynein heavy chain 8
NLR family CARD domain-containing protein 4
Transferrin receptor protein 1
Battenin
Dehydrodolichyl diphosphate synthase
Coagulation factor VIII
Canalicular multispecific organic anion transporter 1
Sodium/hydrogen exchanger 8
Serine/threonine-protein kinase mTOR
Toll-like receptor 1
Complement receptor type 2
Beclin-1
Retinal-specific ATP-binding cassette transporter
Protein S100-A9
Coagulation factor V
Nogo-B receptor
Interleukin-1 receptor-associated kinase 1
Cathepsin S
Alpha-centractin
Ubiquitin-conjugating enzyme E2 variant 3
Ubiquitin-like protein ISG15
Pulmonary surfactant-associated protein D
Tumor necrosis factor receptor superfamily member 5
Putative malate dehydrogenase 1B
Mannose-binding protein C
Toll-like receptor 4
S-formylglutathione hydrolase
Tumor necrosis factor ligand superfamily member 13B
Microtubule-associated proteins 1A/1B light chain 3A

Nuclear cap-binding protein subunit 1
Ferritin light chain
Tumor necrosis factor receptor superfamily member 1B
Frataxin
Calpastatin
Toll-like receptor 6
Interferon alpha-2
Interferon alpha-21
Interferon beta
Complement factor I
Sequestosome-1
Neutrophil defensin 1
Glucose-6-phosphate 1-dehydrogenase
Toll/interleukin-1 receptor domain-containing adapter protein
DNA topoisomerase 2-beta
2'-5'-oligoadenylate synthase 1
Myeloid differentiation primary response protein MyD88
Roundabout homolog 3
Gamma-interferon-inducible lysosomal thiol reductase
Transcription factor p65
Dihydrofolate reductase
L-lactate dehydrogenase A chain
Syncytin-1
HLA class I histocompatibility antigen
Nucleolysin TIA-1 isoform p40
DNA topoisomerase 2-alpha
Lysosome-associated membrane glycoprotein 2
Roundabout homolog 2
Interferon alpha-17
3-beta-hydroxysteroid-Delta
Thioredoxin reductase 1
Flap endonuclease 1
Histone-lysine N-methyltransferase EHMT2
Ataxin-2
Major prion protein
MO15-related protein kinase Pfmrk
Phosphoethanolamine N-methyltransferase
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Solute carrier family 22 member 1
Solute carrier organic anion transporter family member 2B1
Riboflavin-binding protein

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

Predicted Targets

NADPH oxidase 1

D (UniProtID = P14416 - D(2) dopamine receptor)

5-hydroxytryptamine receptor 2A

5-hydroxytryptamine receptor 1A

Alpha-1A adrenergic receptor

Alpha-1B adrenergic receptor

Histamine H1 receptor

Potassium voltage-gated channel subfamily H member 2

5-hydroxytryptamine receptor 2C

5-hydroxytryptamine receptor 2B

Alpha-1D adrenergic receptor

Alpha-2A adrenergic receptor

Alpha-2B adrenergic receptor

Alpha-2C adrenergic receptor

Muscarinic acetylcholine receptor M1

Muscarinic acetylcholine receptor M3

Sphingomyelin phosphodiesterase

Calmodulin

Alpha-1-acid glycoprotein 1

Alpha-1-acid glycoprotein 2

5-hydroxytryptamine receptor 6

5-hydroxytryptamine receptor 7

Cytochrome P450 2D6

Cytochrome P450 1A2

Cytochrome P450 3A4

Cytochrome P450 2E1

Cholinesterase

Serum albumin

Multidrug resistance protein 1

Solute carrier family 22 member 1

Bile salt export pump

Cytochrome P450 2C9

Major prion protein

Trypanothione reductase

Aldehyde oxidase 1

Aldehyde oxidase

Cruzipain Trypanosoma cruzi

Pleiotropic ABC efflux transporter of multiple drugs

Peptidyl-prolyl cis-trans isomerase FKBP4

Oxygen-dependent coproporphyrinogen-III oxidase

Nuclear receptor subfamily 0 group B member 2

Thyroglobulin

Asparagine synthetase

Solute carrier family 2

Heme oxygenase 1

Iron-sulfur cluster co-chaperone protein HscB

Retina-specific copper amine oxidase

Delta-type opioid receptor

DNA mismatch repair protein Msh2

Ornithine decarboxylase

Melanocortin receptor 3
Lathosterol oxidase
Transient receptor potential cation channel subfamily V member 4
Histamine H4 receptor
Sodium-dependent serotonin transporter
WD repeat domain phosphoinositide-interacting protein 1
Phytanoyl-CoA dioxygenase
Transient receptor potential cation channel subfamily A member 1
Serine protease hepsin
Protein DEPP
Insulin-like growth factor-binding protein 1
Pro-opiomelanocortin
Fibronectin type III domain-containing protein 4
Kappa-type opioid receptor
Transient receptor potential cation channel subfamily V member 5
Receptor tyrosine-protein kinase erbB-2
Inhibin beta E chain
Clathrin heavy chain 1
Probable N-acetyltransferase 8
Sodium-dependent dopamine transporter
Integrin alpha-2
G2/mitotic-specific cyclin-B2
Sigma non-opioid intracellular receptor 1
Corticoliberin
5-hydroxytryptamine receptor 5A
Transgelin
Protein S100-B
Fatty acid-binding protein
Arachidonate 15-lipoxygenase
Arginine decarboxylase
Flap endonuclease 1
Transient receptor potential cation channel subfamily V member 3
Melanocortin receptor 4
Cytochrome P450 2A6
Pro-thyrotropin-releasing hormone
Prolactin
Acetylcholinesterase
Fibrinogen alpha chain
Membrane primary amine oxidase
5-hydroxytryptamine receptor 1E
Cytochrome P450 2B6
Repressor of RNA polymerase III transcription MAF1 homolog
Early endosome antigen 1
Melanocortin receptor 5
Hydroxymethylglutaryl-CoA synthase
Muscarinic acetylcholine receptor M2
Antizyme inhibitor 1
Translocator protein
N-acetylaspartate synthetase
AP-1 complex subunit sigma-1A

T-lymphocyte activation antigen CD86
Amine oxidase B
Transient receptor potential cation channel subfamily V member 6
Histamine H3 receptor
Caveolin-1
Amine oxidase A
L-amino-acid oxidase
DNA repair protein XRCC4
Transient receptor potential cation channel subfamily V member 2
Dynein heavy chain 8
5-hydroxytryptamine receptor 3A
Krev interaction trapped protein 1
Lanosterol synthase
Insulin
Histamine H2 receptor
Amiloride-sensitive amine oxidase
Dynamin-2
Carboxypeptidase Z
Sterol regulatory element-binding protein 2
Spermidine synthase
Cytochrome P450 2C19
Tyrosine-protein kinase Fyn
5-hydroxytryptamine receptor 1B
Epidermal growth factor receptor substrate 15
Substance-K receptor
Nuclear protein 1
Phospholipid-transporting ATPase IA
Sodium-dependent noradrenaline transporter
Acid ceramidase
Extracellular superoxide dismutase
Glycerophosphodiester phosphodiesterase domain-containing protein 3
Spermine synthase
Mu-type opioid receptor
Potassium channel subfamily K member 2
Muscarinic acetylcholine receptor M4
Arachidonate 15-lipoxygenase B
Geminin
Isocitrate dehydrogenase cytoplasmic
Thioredoxin reductase 1
Ubiquitin carboxyl-terminal hydrolase 1
Prelamin-A/C
Cellular tumor antigen p53
Microtubule-associated protein tau
Vitamin D3 receptor
Lethal factor Bacillus anthracis
Nuclear factor NF-kappa-B p105 subunit
Peripheral myelin protein 22
Mitogen-activated protein kinase 1
Thrombopoietin
Serine/threonine-protein kinase mTOR

Ras-related protein Rab-9A
 Chromobox protein homolog 1
 Mothers against decapentaplegic homolog 3
 Survival motor neuron protein
 Histone acetyltransferase KAT2A
 Histone-lysine N-methyltransferase EHMT2
 ATPase family AAA domain-containing protein 5
 M-phase phosphoprotein 8
 Ataxin-2
 4'-phosphopantetheinyl transferase ffp
 Tyrosyl-DNA phosphodiesterase 1
 DNA polymerase kappa
 Adenylate cyclase 1
 Transient receptor potential cation channel subfamily V member 1
 Muscarinic acetylcholine receptor M5
 Adenylate cyclase type 3
 Adenylate cyclase type 2
 Adenylate cyclase type 4
 5-hydroxytryptamine receptor 1D
 5-hydroxytryptamine receptor 1F
 Adenylate cyclase type 8
 Adenylate cyclase type 6
 Adenylate cyclase type 5
 Adenylyl cyclase 7
 Glutamate receptor ionotropic
 Epidermal growth factor receptor
 Acetylcholine receptor subunit alpha
 Sodium channel protein type 1 subunit alpha
 Sodium channel protein type 2 subunit alpha
 Sodium channel protein type 3 subunit alpha
 Solute carrier organic anion transporter family member 2B1
 Quinolone resistance protein NorA Staphylococcus aureus
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 Canalicular multispecific organic anion transporter 1
 DRD2 transcript variant 1
 Cannabinoid receptor 1
 Beta-2 adrenergic receptor
 Beta-1 adrenergic receptor
 Adrb2
 Uncharacterized protein
 Prostaglandin E2 receptor EP4 subtype

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :

TNF- α /NF- κ b signaling pathway inhibitor

Predicted Targets

Signal transducer and activator of transcription 1-alpha/beta

Sodium/potassium-transporting ATPase subunit alpha-1

Cytochrome P450 3A4

Cholesterol side-chain cleavage enzyme

Serum albumin

Solute carrier organic anion transporter family member 1A2

Multidrug resistance protein 1

DNA topoisomerase 2-alpha

DNA topoisomerase 2-beta

Niemann-Pick C1 protein

Geminin

Isocitrate dehydrogenase cytoplasmic

Prelamin-A/C

Estrogen receptor

Glucocorticoid receptor

Cellular tumor antigen p53

Androgen receptor

Microtubule-associated protein tau

Thyroid hormone receptor beta

Vitamin D3 receptor

Retinoic acid receptor RXR-alpha

Cruzipain Trypanosoma cruzi

Peroxisome proliferator-activated receptor gamma

Ras-related protein Rab-9A

Nuclear receptor ROR-gamma

Mothers against decapentaplegic homolog 3

Peroxisome proliferator-activated receptor delta

Nuclear factor erythroid 2-related factor 2

ATPase family AAA domain-containing protein 5

Bile acid receptor

Sodium/potassium-transporting ATPase subunit beta-1

Sodium/potassium-transporting ATPase subunit alpha-3

Sodium/potassium-transporting ATPase subunit beta-2

Signal transducer and activator of transcription 3

Sodium/potassium-transporting ATPase subunit alpha-2

Sodium/potassium-transporting ATPase subunit beta-3

Sodium/potassium-transporting ATPase subunit gamma

Sodium/potassium-transporting ATPase subunit alpha-4

Solute carrier organic anion transporter family member 4C1

Acetylcholinesterase

Cholinesterase

Solute carrier organic anion transporter family member 1B3

Solute carrier organic anion transporter family member 1B1

Solute carrier organic anion transporter family member 1A1

Doxepin hydrochloride

Molecular Mechanism (initial) :

5HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

H1 and H2 histamine receptor blocker

Predicted Targets

Histamine H1 receptor

Histamine H2 receptor

Alpha-1A adrenergic receptor

Potassium voltage-gated channel subfamily H member 2

5-hydroxytryptamine receptor 6

Sodium- and chloride-dependent GABA transporter 1

Alpha-1-acid glycoprotein 1

5-hydroxytryptamine receptor 2B

Solute carrier family 2

Histamine H4 receptor

Asparagine synthetase

Muscarinic acetylcholine receptor M3

Alpha-2A adrenergic receptor

Cadherin EGF LAG seven-pass G-type receptor 1

Sodium-dependent serotonin transporter

Intraflagellar transport protein 172 homolog

Cytochrome P450 2C9

ATP synthase subunit beta

Transgelin

Inhibin beta E chain

Intraflagellar transport protein 46 homolog

Multidrug resistance protein 1

Sigma non-opioid intracellular receptor 1

Cadherin EGF LAG seven-pass G-type receptor 2

5-hydroxytryptamine receptor 2C

Dol-P-Man:Man

Telomerase reverse transcriptase

Sonic hedgehog protein

Fatty acid-binding protein

Integrin alpha-2

Alpha-1B adrenergic receptor

Protein DEPP

Muscarinic acetylcholine receptor M1

Cytochrome P450 1A2

5-hydroxytryptamine receptor 1A

Muscarinic acetylcholine receptor M2

Cytochrome P450 3A4

Homeobox protein SIX6

Nuclear protein 1

5-hydroxytryptamine receptor 2A

Lanosterol synthase

Paired box protein Pax-5

D

Cytochrome P450 2C19

Alpha-1D adrenergic receptor

Sodium-dependent noradrenaline transporter

Aldo-keto reductase family 1 member C2

Aldo-keto reductase family 1 member C1

Alpha-2C adrenergic receptor
Glutathione S-transferase P
Glycerophosphodiester phosphodiesterase domain-containing protein 3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Alpha-2B adrenergic receptor
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 1F
5-hydroxytryptamine receptor 7
5-hydroxytryptamine receptor 5A
5-hydroxytryptamine receptor 5B
Sodium channel protein type 1 subunit alpha
5-hydroxytryptamine receptor 3A
Histamine H2 receptor
5-hydroxytryptamine receptor 4
Sodium channel protein type 2 subunit alpha
5-hydroxytryptamine receptor 3B
Sodium channel protein type 3 subunit alpha
Sphingomyelin phosphodiesterase

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

Predicted Targets

Prolactin

Sodium-dependent dopamine transporter

Cytochrome P450 1A2

Cytochrome P450 2D6

Sodium-dependent serotonin transporter

Sodium-dependent noradrenaline transporter

5-hydroxytryptamine receptor 6

Geminin

Thioredoxin reductase 1

Glucosylceramidase

Lysosomal alpha-glucosidase

Peripheral myelin protein 22

Huntingtin

Mothers against decapentaplegic homolog 3

Histone-lysine N-methyltransferase 2A

Histone-lysine N-methyltransferase EHMT2

Muscleblind-like protein 1

DNA polymerase iota

Transporter

Histamine H3 receptor

Histamine H3 receptor

Histamine H1 receptor

Glutamate receptor 3
Muscarinic acetylcholine receptor M2
Adrb2
Beta-1 adrenergic receptor
Adrenergic receptor alpha 2B
Alpha-2A adrenergic receptor
Alpha-1A adrenergic receptor
Adenosine receptor A1
5-hydroxytryptamine receptor 4
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 1F
5-hydroxytryptamine receptor 1E
5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 1A
Substance-P receptor
Neuromedin-K receptor
Delta-type opioid receptor
Uncharacterized protein
Mu-type opioid receptor

Eflornithine hydrochloride

Molecular Mechanism (initial) :

ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

Predicted Targets

Solute carrier family 12 member 5
Rho-associated protein kinase 2
Solute carrier family 12 member 7
DNA mismatch repair protein Msh2
Y+L amino acid transporter 2
Deoxyhypusine synthase
Aquaporin-2
Probable cationic amino acid transporter
Glyceraldehyde-3-phosphate dehydrogenase
Aquaporin-8
Aquaporin-9
Glyceraldehyde-3-phosphate dehydrogenase
Cyclin-dependent kinase inhibitor 1B
Glypican-1
11-cis retinol dehydrogenase
Ras-related C3 botulinum toxin substrate 2
Adenomatous polyposis coli protein 2

Ornithine decarboxylase

Adenomatous polyposis coli protein
Asc-type amino acid transporter 1
G2/mitotic-specific cyclin-B1

Tyrosinase
Neutral and basic amino acid transport protein rBAT
Lens fiber major intrinsic protein
Matrilysin
Large neutral amino acids transporter small subunit 1
Solute carrier family 12 member 2
Nucleophosmin
Cystine/glutamate transporter
Cellular tumor antigen p53
Cyclin-dependent kinase 2
Ras GTPase-activating-like protein IQGAP1
Peroxisomal N
RAC-alpha serine/threonine-protein kinase
Solute carrier family 12 member 9
Glutamate receptor 1
Signal recognition particle 19 kDa protein
Y+L amino acid transporter 1
Arginine decarboxylase
Mitotic checkpoint serine/threonine-protein kinase BUB1 beta
Aquaporin-5
Potassium voltage-gated channel subfamily A member 2
S-adenosylmethionine synthase isoform type-2
Aquaporin-7
Solute carrier family 7 member 13
Lysine-specific histone demethylase 1B
Aquaporin-3
Cationic amino acid transporter 3
Hepatocyte nuclear factor 4-alpha
Ras-related C3 botulinum toxin substrate 3
Catenin alpha-1
Aquaporin-1
Beta-galactosidase
Spermine oxidase
Spermine synthase
Prostaglandin G/H synthase 2
L-amino-acid oxidase
Nitric oxide synthase
Aquaporin-6
Aquaporin-10
Solute carrier family 12 member 4
Antizyme inhibitor 1
Large neutral amino acids transporter small subunit 2
Mothers against decapentaplegic homolog 4
Eukaryotic translation initiation factor 5A-1
Protein-tyrosine kinase 2-beta
Mothers against decapentaplegic homolog 3
Focal adhesion kinase 1
CD59 glycoprotein
Amine oxidase A
Serine/threonine-protein kinase MRCK alpha

Insulin
Phospholipid hydroperoxide glutathione peroxidase
Beta-3 adrenergic receptor
Catenin beta-1
Ras-related C3 botulinum toxin substrate 1
Solute carrier family 12 member 6
Alpha-1-antitrypsin
Serine/threonine-protein kinase MRCK beta
Caspase-8
Lysine-specific histone demethylase 1A
Glutathione peroxidase 7
CAP-Gly domain-containing linker protein 1
Glutathione peroxidase 6
ELAV-like protein 1
Diamine acetyltransferase 1
Dickkopf-related protein 1
Mitotic checkpoint protein BUB3
Arginase-1
Polyamine-modulated factor 1
S-adenosylmethionine synthase isoform type-1
S-adenosylmethionine decarboxylase proenzyme
Tumor-associated calcium signal transducer 2
Amine oxidase B
Casein kinase II subunit beta
Arachidonate 5-lipoxygenase
Phospholipase A2
Myc proto-oncogene protein
Spermidine synthase
Cationic amino acid transporter 4
High affinity cationic amino acid transporter 1
Receptor expression-enhancing protein 5
S-methyl-5'-thioadenosine phosphorylase
Serine/threonine-protein kinase Chk2
Solute carrier family 12 member 1
Homeobox protein CDX-2
Glutathione peroxidase 2
Aquaporin-4
Glutathione peroxidase 3
Rho-associated protein kinase 1
Solute carrier family 12 member 8
Low affinity cationic amino acid transporter 2
Glutathione peroxidase 1
Epididymal secretory glutathione peroxidase
Regulator of G-protein signaling 4
Chromobox protein homolog 1
Nuclear factor erythroid 2-related factor 2
Histone-lysine N-methyltransferase EHMT2
Ornithine decarboxylase
Solute carrier family 22 member 1
Cysteine protease Trypanosoma brucei rhodesiense

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

Predicted Targets

Autophagy protein 5

Amphiregulin

Pro-epidermal growth factor

E3 ubiquitin-protein ligase CHFR

Tyrosine-protein kinase JAK2

Epidermal growth factor receptor

Receptor tyrosine-protein kinase erbB-2

Insulin-like growth factor 1 receptor

Phosphatidylinositol 4

5'-AMP-activated protein kinase catalytic subunit alpha-2

Protein kinase C delta type

Serine/threonine-protein kinase N2

Protein kinase C theta type

cGMP-dependent protein kinase 2

Serine/threonine-protein kinase 3

Serine/threonine-protein kinase 4

Dual specificity testis-specific protein kinase 1

Serine/threonine-protein kinase VRK2

Mitogen-activated protein kinase kinase kinase 12

Serine/threonine-protein kinase 25

Mitogen-activated protein kinase kinase kinase kinase 5

Serine/threonine-protein kinase PLK2

Serine/threonine-protein kinase pim-2

Serine/threonine-protein kinase 38

Serine/threonine-protein kinase Nek1

Serine/threonine-protein kinase tousled-like 1

Cyclin-dependent kinase 14

Phosphatidylinositol 4-phosphate 5-kinase type-1 gamma

STE20/SPS1-related proline-alanine-rich protein kinase

Serine/threonine-protein kinase Sgk3

Inhibitor of nuclear factor kappa-B kinase subunit epsilon

Insulin receptor-related protein

Death-associated protein kinase 2

Serine/threonine-protein kinase Nek6

Eukaryotic translation initiation factor 2-alpha kinase 1

Ribosomal protein S6 kinase alpha-6

Serine/threonine-protein kinase LATS2

Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit beta

Serine/threonine-protein kinase pim-1

Phosphatidylinositol 4-kinase beta

cAMP-dependent protein kinase catalytic subunit alpha

cAMP-dependent protein kinase catalytic subunit beta

Protein kinase C iota type
Serine/threonine-protein kinase D1
Mitogen-activated protein kinase 3
Mitogen-activated protein kinase 6
Mitogen-activated protein kinase 7
Mitogen-activated protein kinase 8
Mitogen-activated protein kinase 11
Mitogen-activated protein kinase 13
Dual specificity mitogen-activated protein kinase kinase 1
Dual specificity mitogen-activated protein kinase kinase 3
Dual specificity mitogen-activated protein kinase kinase 6
RAF proto-oncogene serine/threonine-protein kinase
Rhodopsin kinase
Proto-oncogene tyrosine-protein kinase ROS
Ribosomal protein S6 kinase alpha-1
Dual specificity mitogen-activated protein kinase kinase 4
SRSF protein kinase 1
Serine/threonine-protein kinase Nek4
Serine/threonine-protein kinase PAK 7
Calcium/calmodulin-dependent protein kinase type 1D
Calcium/calmodulin-dependent protein kinase type 1G
Proto-oncogene tyrosine-protein kinase receptor Ret
Dual specificity protein kinase CLK4
Serine/threonine-protein kinase TAO1
Ribosomal protein S6 kinase alpha-2
Casein kinase I isoform gamma-1
Homeodomain-interacting protein kinase 2
Fibroblast growth factor receptor 4
Fibroblast growth factor receptor 2
Fibroblast growth factor receptor 1
Cyclin-dependent kinase-like 5
Ribosomal protein S6 kinase beta-1
Tyrosine-protein kinase SYK
Tyrosine-protein kinase Tec
TGF-beta receptor type-2
Non-receptor tyrosine-protein kinase TYK2
Wee1-like protein kinase
Phosphatidylinositol 5-phosphate 4-kinase type-2 beta
Serine/threonine-protein kinase 24
Serine/threonine-protein kinase MRCK alpha
Calcium/calmodulin-dependent protein kinase type 1
MAP kinase-activated protein kinase 5
Peripheral plasma membrane protein CASK
Cyclin-dependent kinase 13
Receptor-interacting serine/threonine-protein kinase 1
Serine/threonine-protein kinase RIO3
Serine/threonine-protein kinase PRP4 homolog
Cyclin-dependent kinase-like 2
Serine/threonine-protein kinase BRSK2
Dual specificity protein kinase CLK3

Dual specificity protein kinase CLK2
Serine/threonine-protein kinase PLK3
Receptor-type tyrosine-protein kinase FLT3
Cyclin-dependent kinase-like 1
Activin receptor type-1B
Bone morphogenetic protein receptor type-1A
Serine/threonine-protein kinase B-raf
Casein kinase I isoform gamma-3
Ephrin type-A receptor 2
Ephrin type-A receptor 4
Cyclin-dependent kinase 3
Cyclin-dependent kinase 8
Cyclin-dependent kinase 9
Casein kinase I isoform gamma-2
Serine/threonine-protein kinase/endoribonuclease IRE1
Inhibitor of nuclear factor kappa-B kinase subunit beta
Interleukin-1 receptor-associated kinase 1
Activin receptor type-2A
RAC-beta serine/threonine-protein kinase
Cytoplasmic tyrosine-protein kinase BMX
Calcium/calmodulin-dependent protein kinase type IV
Cyclin-dependent kinase 2
Cyclin-dependent kinase 7
Casein kinase I isoform alpha
Casein kinase II subunit alpha
Ephrin type-B receptor 3
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit gamma
Mitogen-activated protein kinase kinase kinase 2
Ribosomal protein S6 kinase alpha-3
TGF-beta receptor type-1
Mitogen-activated protein kinase kinase kinase 6
Serine/threonine-protein kinase LATS1
Dual specificity tyrosine-phosphorylation-regulated kinase 1B
Serine/threonine-protein kinase DCLK1
Ribosomal protein S6 kinase alpha-5
Cyclin-dependent kinase 5
Serine/threonine-protein kinase mTOR
Casein kinase II subunit alpha'
Tyrosine-protein kinase Fes/Fps
Glycogen synthase kinase-3 beta
LIM domain kinase 1
Megakaryocyte-associated tyrosine-protein kinase
Mitogen-activated protein kinase kinase kinase 11
Mitogen-activated protein kinase kinase kinase 10
Serine/threonine-protein kinase Nek2
Serine/threonine-protein kinase Nek3
Serine/threonine-protein kinase PAK 1
Serine/threonine-protein kinase PAK 2
Serine/threonine-protein kinase PAK 3
Cyclin-dependent kinase 18

3-phosphoinositide-dependent protein kinase 1
Serine/threonine-protein kinase PLK1
cAMP-dependent protein kinase catalytic subunit PRKX
Serine/threonine-protein kinase OSR1
RAC-alpha serine/threonine-protein kinase
Macrophage colony-stimulating factor 1 receptor
Tyrosine-protein kinase Fer
Protein kinase C epsilon type
Rho-associated protein kinase 1
RAC-gamma serine/threonine-protein kinase
Tyrosine-protein kinase ITK/TSK
LIM domain kinase 2
Muscle
Homeodomain-interacting protein kinase 3
Serine/threonine-protein kinase D3
Serine/threonine-protein kinase MAK
Mitogen-activated protein kinase kinase kinase 1
Mitogen-activated protein kinase kinase kinase 5
Protein-tyrosine kinase 6
Serine/threonine-protein kinase MRCK beta
BDNF/NT-3 growth factors receptor
Cyclin-dependent kinase 16
Phosphorylase b kinase gamma catalytic chain
Serine/threonine-protein kinase tousled-like 2
5'-AMP-activated protein kinase catalytic subunit alpha-1
Serine/threonine-protein kinase SIK3
Serine/threonine-protein kinase 16
Cyclin-dependent kinase 17
Discoidin domain-containing receptor 2
Serine/threonine-protein kinase receptor R3
Tyrosine-protein kinase BTK
Cyclin-dependent kinase 4
Serine/threonine-protein kinase STK11
Angiopoietin-1 receptor
Mitogen-activated protein kinase kinase kinase 15
Serine/threonine-protein kinase pim-3
Serine/threonine-protein kinase Chk2
Activated CDC42 kinase 1
High affinity nerve growth factor receptor
Myosin light chain kinase family member 4
Serine/threonine-protein kinase PAK 4
Mitogen-activated protein kinase kinase kinase kinase 1
Activin receptor type-1
Activin receptor type-2B
Serine/threonine-protein kinase 32A
Cyclin-dependent kinase-like 3
Phosphatidylinositol 4-phosphate 5-kinase type-1 alpha
Bone morphogenetic protein receptor type-1B
Bone morphogenetic protein receptor type-2
Hormonally up-regulated neu tumor-associated kinase

Maternal embryonic leucine zipper kinase
NUAK family SNF1-like kinase 1
Serine/threonine-protein kinase ICK
Microtubule-associated serine/threonine-protein kinase 1
Serine/threonine-protein kinase 38-like
Cyclin-dependent kinase 19
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase TAO2
Serine/threonine-protein kinase NLK
Serine/threonine-protein kinase TAO3
Serine/threonine-protein kinase MST4
Myosin-IIIa
Ephrin type-B receptor 2
Serine/threonine-protein kinase MARK2
Transient receptor potential cation channel subfamily M member 6
SNF-related serine/threonine-protein kinase
Serine/threonine-protein kinase RIO2
Serine/threonine-protein kinase 32B
Serine/threonine-protein kinase MARK1
Glycogen synthase kinase-3 alpha
Serine/threonine-protein kinase PAK 6
Dual specificity mitogen-activated protein kinase kinase 2
Serine/threonine-protein kinase 33
NUAK family SNF1-like kinase 2
MAP/microtubule affinity-regulating kinase 4
Serine/threonine-protein kinase RIO1
Testis-specific serine/threonine-protein kinase 1
Calcium/calmodulin-dependent protein kinase kinase 1
MAP kinase-activated protein kinase 2
Serine/threonine-protein kinase Nek9
Mitogen-activated protein kinase kinase kinase 9
Serine/threonine-protein kinase DCLK3
Cyclin-dependent kinase 11B
Tyrosine-protein kinase Srms
Serine/threonine-protein kinase 35
Dual specificity tyrosine-phosphorylation-regulated kinase 1A
Serine/threonine-protein kinase Nek7
Mitogen-activated protein kinase 1
Mitogen-activated protein kinase 14
Mitogen-activated protein kinase 15
Cyclin-dependent kinase 15
G protein-coupled receptor kinase 7
Dual specificity mitogen-activated protein kinase kinase 7
Casein kinase I isoform alpha-like
Mitogen-activated protein kinase kinase kinase 7
Mitogen-activated protein kinase kinase kinase kinase 4
Tyrosine-protein kinase Fyn
Serine/threonine-protein kinase NIM1
Focal adhesion kinase 1
Calcium/calmodulin-dependent protein kinase type II subunit gamma

Protein-tyrosine kinase 2-beta
Serine/threonine-protein kinase SIK1
Serine/threonine-protein kinase 32C
Ankyrin repeat and protein kinase domain-containing protein 1
Myosin light chain kinase 3
Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase
Serine/threonine-protein kinase Nek5
Tyrosine-protein kinase ZAP-70
Serine/threonine-protein kinase N1
Wee1-like protein kinase 2
Uncharacterized serine/threonine-protein kinase SBK3
Dual serine/threonine and tyrosine protein kinase
Cell division control protein 2 homolog
Dual specificity protein kinase CLK1
NT-3 growth factor receptor
Mitogen-activated protein kinase 12
Casein kinase I isoform epsilon
TRAF2 and NCK-interacting protein kinase
Death-associated protein kinase 1
Mitogen-activated protein kinase 10
Serine/threonine-protein kinase SIK2
MAP/microtubule affinity-regulating kinase 3
Myosin light chain kinase
Death-associated protein kinase 3
Serine/threonine-protein kinase 36
Tyrosine-protein kinase CSK
Mitogen-activated protein kinase 9
Insulin receptor
Tyrosine-protein kinase receptor UFO
Mitogen-activated protein kinase kinase kinase MLT
Dual specificity protein kinase TTK
Vascular endothelial growth factor receptor 2
Tyrosine-protein kinase Mer
Ephrin type-B receptor 4
MAP kinase-interacting serine/threonine-protein kinase 2
Serine/threonine-protein kinase DCLK2
Tyrosine-protein kinase TXK
Serine/threonine-protein kinase 17B
Ephrin type-A receptor 5
Serine/threonine-protein kinase PLK4
Cytochrome P450 3A4
Nuclear receptor subfamily 1 group I member 2
Cytochrome P450 3A5
Cytochrome P450 1A2
Cytochrome P450 1A1
Cytochrome P450 2D6
Cytochrome P450 2C8
Cytochrome P450 1B1
UDP-glucuronosyltransferase 1-1
Serum albumin

Alpha-1-acid glycoprotein 1
Multidrug resistance protein 1
Receptor tyrosine-protein kinase erbB-4
Platelet-derived growth factor receptor beta
Solute carrier organic anion transporter family member 1B1
Canalicular multispecific organic anion transporter 1
ATP-binding cassette sub-family G member 2
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Ephrin type-A receptor 3
Ephrin type-A receptor 7
Vascular endothelial growth factor receptor 1
Tyrosine-protein kinase FRK
Hepatocyte growth factor receptor
Platelet-derived growth factor receptor alpha
STE20-like serine/threonine-protein kinase
Tyrosine-protein kinase receptor Tie-1
Tyrosine-protein kinase ABL1
Tyrosine-protein kinase Blk
Citron Rho-interacting kinase
Tyrosine-protein kinase Fgr
Tyrosine-protein kinase Lck
Tyrosine-protein kinase Lyn
Serine/threonine-protein kinase TNNI3K
Abelson tyrosine-protein kinase 2
Ephrin type-A receptor 8
Tyrosine-protein kinase HCK
Myosin light chain kinase 2
Interferon-induced
Receptor-interacting serine/threonine-protein kinase 2
Proto-oncogene tyrosine-protein kinase Src
Tyrosine-protein kinase Yes
Serine/threonine-protein kinase MRCK gamma
Mitogen-activated protein kinase 4
Tyrosine-protein kinase receptor TYRO3
Chaperone activity of bc1 complex-like
AarF domain-containing protein kinase 4
Myotonin-protein kinase
BMP-2-inducible protein kinase
Serine/threonine-protein kinase 10
Aurora kinase A
Ephrin type-A receptor 6
Serine/threonine-protein kinase ULK3
Mitogen-activated protein kinase kinase 2
Serine/threonine-protein kinase TBK1
Receptor-interacting serine/threonine-protein kinase 4
Dual specificity tyrosine-phosphorylation-regulated kinase 2
Non-receptor tyrosine-protein kinase TNK1
ALK tyrosine kinase receptor
Ephrin type-B receptor 6

Epithelial discoidin domain-containing receptor 1
Receptor tyrosine-protein kinase erbB-3
Vascular endothelial growth factor receptor 3
Mitogen-activated protein kinase kinase kinase 3
Aurora kinase C
Tyrosine-protein kinase JAK3
Serine/threonine-protein kinase SBK1
Serine/threonine-protein kinase ULK3
MAP kinase-interacting serine/threonine-protein kinase 1
Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma
Mitogen-activated protein kinase kinase kinase 19
Homeodomain-interacting protein kinase 4
Dual specificity mitogen-activated protein kinase kinase 5
G protein-coupled receptor kinase 4
Leucine-rich repeat serine/threonine-protein kinase 2
Leukocyte tyrosine kinase receptor
Tubulin alpha-1A chain
Annexin A5
Plexin-B1
C-C motif chemokine 2
Estrogen receptor
DNA excision repair protein ERCC-1
Heme oxygenase 1
Ankyrin repeat domain-containing protein 54
Hepatocyte growth factor
S-methylmethionine--homocysteine S-methyltransferase BHMT2
Proheparin-binding EGF-like growth factor
G1/S-specific cyclin-D1
Cyclin-dependent kinase inhibitor 1B
tRNA-specific adenosine deaminase 2
Thymidine phosphorylase
Proepiregulin
Cyclin-dependent kinase inhibitor 1
Calumenin
Apelin receptor
GTPase KRas
Guanine nucleotide-binding protein G subunit alpha
Cadherin-1
Protein CIP2A
Signal transducer and activator of transcription 3
DNA repair protein RAD51 homolog 1
Protein LMBR1L
Cellular tumor antigen p53
Clathrin heavy chain 1
Protransforming growth factor alpha
Betaine--homocysteine S-methyltransferase 1
3-hydroxy-3-methylglutaryl-coenzyme A reductase
Mast/stem cell growth factor receptor Kit
Serine/threonine-protein kinase D2
GTPase HRas

Integrin alpha-2
Nucleophosmin
Zinc finger E-box-binding homeobox 2
Carbohydrate sulfotransferase 14
Proprotein convertase subtilisin/kexin type 9
Breakpoint cluster region protein
Eukaryotic translation initiation factor 2-alpha kinase 3
Proto-oncogene c-Fos
Cyclin-G-associated kinase
Glutathione S-transferase Mu 1
Heat shock 70 kDa protein 6
Caspase-3
Aurora kinase B
Cytochrome c oxidase subunit 8A
Zinc fingers and homeoboxes protein 2
Thymidylate synthase
Echinoderm microtubule-associated protein-like 4
Early endosome antigen 1
Zinc finger E-box-binding homeobox 1
Apoptotic protease-activating factor 1
Epigen
Mitochondrial carnitine/acylcarnitine carrier protein
Translocator protein
Probable inactive tRNA-specific adenosine deaminase-like protein 3
Growth factor receptor-bound protein 2
Hypoxia-inducible factor 1-alpha
Single-strand selective monofunctional uracil DNA glycosylase
EGF-containing fibulin-like extracellular matrix protein 1
Metabotropic glutamate receptor 8
Misshapen-like kinase 1
Ubiquitin-like modifier-activating enzyme ATG7
Homeobox protein Nkx-2.1
Midkine
Breast cancer type 1 susceptibility protein
Docking protein 3
DNA repair protein XRCC2
Tumor necrosis factor ligand superfamily member 6
Methionine synthase
Cyclin-dependent kinase inhibitor 2A
Poly synthase 1)
Prostaglandin G/H synthase 2
Antigen KI-67
GTPase NRas
Phosphatidylinositol 3
Pulmonary surfactant-associated protein A2
Heat shock 70 kDa protein 1A/1B
Dynamin-1
Forkhead box protein E1
Fructose-1
Solute carrier family 25 member 45

Enhancer of filamentation 1
Methylenetetrahydrofolate reductase
Proliferating cell nuclear antigen
Low-density lipoprotein receptor-related protein 1B
Sequestosome-1
Solute carrier family 25 member 48
Geminin
Prelamin-A/C
Histone-lysine N-methyltransferase EHMT2
Cell division cycle 7-related protein kinase
Eukaryotic elongation factor 2 kinase
Serine/threonine-protein kinase Chk1
Inhibitor of nuclear factor kappa-B kinase subunit alpha
Dual specificity tyrosine-phosphorylation-regulated kinase 3
Rho-associated protein kinase 2
Protein kinase C gamma type
Cyclin-dependent kinase 1
Fibroblast growth factor receptor 3
G protein-coupled receptor kinase 5
Casein kinase I isoform delta
Macrophage-stimulating protein receptor
Protein kinase C zeta type
Calcium/calmodulin-dependent protein kinase type II subunit beta
Calcium/calmodulin-dependent protein kinase type II subunit delta
cGMP-dependent protein kinase 1
MAP kinase-activated protein kinase 3
Serine/threonine-protein kinase BRSK1
Lymphokine-activated killer T-cell-originated protein kinase
Testis-specific serine/threonine-protein kinase 2
PAS domain-containing serine/threonine-protein kinase
Serine/threonine-protein kinase Sgk2
Dual specificity tyrosine-phosphorylation-regulated kinase 4
Serine/threonine-protein kinase 17A
Calcium/calmodulin-dependent protein kinase type II subunit alpha
Mitogen-activated protein kinase kinase kinase 13
Serine/threonine-protein kinase ULK1
Ribosomal protein S6 kinase alpha-4
Ephrin type-A receptor 1
Tyrosine-protein kinase JAK1
Protein kinase C eta type
Ephrin type-B receptor 1
Calcium-dependent protein kinase 1
SRSF protein kinase 2
Serine/threonine-protein kinase PknB
AP2-associated protein kinase 1
Homeodomain-interacting protein kinase 1
Mitogen-activated protein kinase kinase kinase kinase 3
Serine/threonine-protein kinase ULK2
Serine/threonine-protein kinase Nek1
Myosin-IIIb

Calcium/calmodulin-dependent protein kinase kinase 2
Eukaryotic translation initiation factor 2-alpha kinase 4
SRSF protein kinase 3
Cyclin-dependent kinase 11A
Interleukin-1 receptor-associated kinase 3
Mitogen-activated protein kinase kinase kinase 4
Myelin transcription factor 1

Everolimus

Molecular Mechanism (initial) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Molecular Mechanism (repurposed) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Predicted Targets

No results

Finasteride

Molecular Mechanism (initial) :

**steroid 5alpha reductase inhibitor
androgen receptor antagonist**

Molecular Mechanism (repurposed) :

**steroid 5alpha reductase inhibitor
androgen receptor antagonist**

Predicted Targets

Bile salt export pump

Choriogonadotropin subunit beta

Androgen receptor

3-oxo-5-alpha-steroid 4-dehydrogenase 2 (steroid 5-alpha-reductase)

3-oxo-5-alpha-steroid 4-dehydrogenase 1 (steroid 5-alpha-reductase)

3-oxo-5-beta-steroid 4-dehydrogenase

Cytochrome P450 3A5

Cytochrome P450 3A7

Cytochrome P450 3A4

Cytochrome P450 1A2

Cytochrome P450 2D6

Cytochrome P450 2C9

Cytochrome P450 2C19

Geminin

Prelamin-A/C

Nuclear factor NF-kappa-B p105 subunit

Mitogen-activated protein kinase 1

Thrombopoietin

Nuclear receptor ROR-gamma

Bloom syndrome protein

Histone-lysine N-methyltransferase EHMT2

3 beta-hydroxysteroid dehydrogenase/Delta 5-->4-isomerase type 1

3 beta-hydroxysteroid dehydrogenase/Delta 5-->4-isomerase
3-keto-steroid reductase

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

Predicted Targets

Neuronal acetylcholine receptor subunit beta-2

Acetylcholinesterase

Acetylcholine receptor subunit alpha

Acetylcholine receptor subunit beta

Acetylcholine receptor subunit delta

Acetylcholine receptor subunit gamma

Acetylcholine receptor subunit epsilon

Neuronal acetylcholine receptor subunit alpha-2

Neuronal acetylcholine receptor subunit alpha-3

Neuronal acetylcholine receptor subunit alpha-4

Neuronal acetylcholine receptor subunit alpha-5

Neuronal acetylcholine receptor subunit alpha-6

Neuronal acetylcholine receptor subunit alpha-7

Neuronal acetylcholine receptor subunit beta-3

Neuronal acetylcholine receptor subunit beta-4

Cholinesterase

Cytochrome P450 3A4

Cytochrome P450 2D6

Acetylcholinesterase

Cholinesterase

Retinal dehydrogenase 1

Prelamin-A/C

Vitamin D3 receptor

Glutamate receptor ionotropic

Butyrylcholinesterase

Amyloid beta A4 protein

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

Predicted Targets

Alpha-fetoprotein

Adiponectin

Prostatic acid phosphatase

Alpha-2-macroglobulin

Beta-2-glycoprotein 1

Serum amyloid P-component

Amphiregulin
Apoptosis regulator BAX
Apoptosis regulator Bcl-2
Baculoviral IAP repeat-containing protein 5
BH3-interacting domain death agonist
Brain-derived neurotrophic factor
G2/mitotic-specific cyclin-B1
C-C motif chemokine 3
C-C motif chemokine 2
Cytidine deaminase
CD40 ligand
Cyclin-dependent kinase inhibitor 1
Endothelin-1
Granulocyte-macrophage colony-stimulating factor
Pro-epidermal growth factor
Fibroblast growth factor 2
Tumor necrosis factor receptor superfamily member 6
Interferon alpha-2
Hypoxia-inducible factor 1-alpha
Glycogen synthase kinase-3 beta
Interleukin-15
Interleukin-13
Interleukin-10
Interferon gamma
Interleukin-4
Interleukin-1 beta
Interleukin-1 alpha
Leptin
Kit ligand
Interleukin-8
Dual specificity mitogen-activated protein kinase kinase 6
Myristoylated alanine-rich C-kinase substrate
Stromelysin-1
Myeloperoxidase
Nuclear factor erythroid 2-related factor 2
NF-kappa-B inhibitor alpha
Neurogenic locus notch homolog protein 1
Pappalysin-1
Proto-oncogene c-Rel
Equilibrative nucleoside transporter 1
Ribonucleoside-diphosphate reductase subunit M2
Serine/threonine-protein kinase SMG1
Equilibrative nucleoside transporter 3
Proto-oncogene tyrosine-protein kinase Src
Telomerase reverse transcriptase
Tumor necrosis factor
Thrombopoietin
Cellular tumor antigen p53
Thymidine phosphorylase
Vascular cell adhesion protein 1

von Willebrand factor
Single-stranded DNA cytosine deaminase
Deoxycytidine kinase
Multidrug resistance protein 1
Protein kinase C alpha type
Protein kinase C beta type
Protein kinase C epsilon type
Deoxycytidylate deaminase

Ribonucleoside-diphosphate reductase large subunit

Equilibrative nucleoside transporter 2
Clusterin
Sodium/nucleoside cotransporter 2
Transcription factor Sp1
Upstream stimulatory factor 1
Upstream stimulatory factor 2
Cell division cycle 5-like protein
Enhancer of polycomb homolog 2
Poly synthase 1
Non-canonical poly
UMP-CMP kinase
Multidrug resistance-associated protein 4
Thymidylate synthase
Sodium/nucleoside cotransporter 1
Geminin
Peripheral myelin protein 22

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

Predicted Targets

Alpha-2A adrenergic receptor

Alpha-2B adrenergic receptor
Cytochrome P450 3A4
Cytochrome P450 2C9
Cytochrome P450 2C19
Alpha-1D adrenergic receptor
D
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 2C
Pro-opiomelanocortin
Renin
5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 1A
Alpha-1B adrenergic receptor
Nischarin
Dopamine beta-hydroxylase
Sodium-dependent noradrenaline transporter

Alpha-1A adrenergic receptor
Poly
Alpha-2C adrenergic receptor
Menin
Geminin
Thioredoxin reductase 1
Prelamin-A/C
Muscarinic acetylcholine receptor M1
Cytochrome P450 2D6
Lethal factor Bacillus anthracis
Mitogen-activated protein kinase 1
Histone-lysine N-methyltransferase 2A
Nuclear factor erythroid 2-related factor 2
Hypoxia-inducible factor 1-alpha
Histone-lysine N-methyltransferase EHMT2
3-hydroxyacyl-CoA dehydrogenase type-2
Adrenergic receptor

Ibuprofen

Molecular Mechanism (initial) :

**prostaglandin G/H synthase 2 inhibitor
prostaglandin G/H synthase 1 inhibitor**

Molecular Mechanism (repurposed) :

**prostaglandin G/H synthase 2 inhibitor
prostaglandin G/H synthase 1 inhibitor**

Predicted Targets

Not results

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

**platelet-derived growth factor receptors (PDGFR) inhibitor
stem cell factor (SCF)
proto-oncogene c-Kit inhibitor**

Predicted Targets

Bile salt export pump
ATP-binding cassette sub-family G member 2
Bcl2-associated agonist of cell death
Baculoviral IAP repeat-containing protein 5
BH3-interacting domain death agonist
Collagen alpha-1
Cyclin-dependent kinase inhibitor 1B
Diablo homolog
Crk-like protein
Docking protein 1
Interferon gamma
Heme oxygenase 1

Histone H2AX
Eukaryotic translation initiation factor 4E
Mast/stem cell growth factor receptor Kit
Transcription factor AP-1
Insulin-like growth factor I
Tyrosine-protein kinase Lyn
Induced myeloid leukemia cell differentiation protein Mcl-1

Platelet-derived growth factor receptor alpha

Platelet-derived growth factor receptor beta
Protein kinase C delta type
Peroxisome proliferator-activated receptor gamma
Phosphatidylinositol 3-kinase regulatory subunit alpha
Tumor necrosis factor
Vascular endothelial growth factor A
Aurora kinase A
Aurora kinase B
Aurora kinase C
Vascular endothelial growth factor receptor 2
Proto-oncogene tyrosine-protein kinase Src
Histone deacetylase 1
Histone deacetylase 6
Epidermal growth factor receptor
Serine/threonine-protein kinase B-raf
Tyrosine-protein kinase SYK
Ephrin type-A receptor 3
Tyrosine-protein kinase Fer
Protein kinase C epsilon type
Rho-associated protein kinase 1
Tyrosine-protein kinase receptor Tie-1
Tyrosine-protein kinase Yes
RAC-gamma serine/threonine-protein kinase
Tyrosine-protein kinase ITK/TSK
LIM domain kinase 2
Homeodomain-interacting protein kinase 3
Serine/threonine-protein kinase D3
Serine/threonine-protein kinase MAK
Mitogen-activated protein kinase kinase kinase 1
Mitogen-activated protein kinase kinase kinase 5
Protein-tyrosine kinase 6
Serine/threonine-protein kinase 10
Serine/threonine-protein kinase MRCK beta
BDNF/NT-3 growth factors receptor
Cyclin-dependent kinase 16
Phosphorylase b kinase gamma catalytic chain
Phosphatidylinositol 4
5'-AMP-activated protein kinase catalytic subunit alpha-2
Serine/threonine-protein kinase N2
Protein kinase C theta type
cGMP-dependent protein kinase 2
Serine/threonine-protein kinase 3

Serine/threonine-protein kinase 4
Dual specificity testis-specific protein kinase 1
Tyrosine-protein kinase receptor TYRO3
Serine/threonine-protein kinase VRK2
Mitogen-activated protein kinase kinase kinase 12
Serine/threonine-protein kinase 25
Mitogen-activated protein kinase kinase kinase 2
Serine/threonine-protein kinase PLK2
Serine/threonine-protein kinase pim-2
Citron Rho-interacting kinase
Serine/threonine-protein kinase 38
Serine/threonine-protein kinase Nek1
Serine/threonine-protein kinase tousled-like 1
Cyclin-dependent kinase 14
Phosphatidylinositol 4-phosphate 5-kinase type-1 gamma
STE20/SPS1-related proline-alanine-rich protein kinase
Serine/threonine-protein kinase TBK1
Serine/threonine-protein kinase Sgk3
Inhibitor of nuclear factor kappa-B kinase subunit epsilon
Insulin receptor-related protein
Death-associated protein kinase 2
Serine/threonine-protein kinase Nek6
Eukaryotic translation initiation factor 2-alpha kinase 1
Ribosomal protein S6 kinase alpha-6
Serine/threonine-protein kinase LATS2
Hormonally up-regulated neu tumor-associated kinase
STE20-like serine/threonine-protein kinase
NUAK family SNF1-like kinase 1
Serine/threonine-protein kinase ICK
Microtubule-associated serine/threonine-protein kinase 1
Serine/threonine-protein kinase 38-like
TRAF2 and NCK-interacting protein kinase
Serine/threonine-protein kinase SIK2
Serine/threonine-protein kinase 36
Cyclin-dependent kinase-like 2
Serine/threonine-protein kinase BRSK2
Non-receptor tyrosine-protein kinase TNK1
Dual specificity protein kinase CLK3
Dual specificity protein kinase CLK2
Serine/threonine-protein kinase PLK3
Receptor-type tyrosine-protein kinase FLT3
Cyclin-dependent kinase-like 1
Serine/threonine-protein kinase 17B
Activin receptor type-1B
ALK tyrosine kinase receptor
Bone morphogenetic protein receptor type-1A
Tyrosine-protein kinase CSK
Casein kinase I isoform gamma-3
Myotonin-protein kinase
Ephrin type-A receptor 2

Ephrin type-A receptor 4
Ephrin type-A receptor 7
Ephrin type-B receptor 3
Ephrin type-B receptor 4
Ephrin type-B receptor 6
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit gamma
Mitogen-activated protein kinase kinase kinase kinase 2
Ribosomal protein S6 kinase alpha-3
TGF-beta receptor type-1
Mitogen-activated protein kinase kinase kinase 6
Serine/threonine-protein kinase LATS1
Dual specificity tyrosine-phosphorylation-regulated kinase 1B
Serine/threonine-protein kinase DCLK1
Ribosomal protein S6 kinase alpha-5
Cyclin-dependent kinase 5
Serine/threonine-protein kinase mTOR
Tyrosine-protein kinase JAK2
Serine/threonine-protein kinase PLK1
cAMP-dependent protein kinase catalytic subunit PRKX
Serine/threonine-protein kinase OSR1

Tyrosine-protein kinase ABL1

RAC-alpha serine/threonine-protein kinase
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase TAO2
Serine/threonine-protein kinase NLK
Serine/threonine-protein kinase TAO3
Serine/threonine-protein kinase MST4
Myosin-IIIa
Ephrin type-B receptor 2
Serine/threonine-protein kinase MARK2
MAP kinase-interacting serine/threonine-protein kinase 2
BMP-2-inducible protein kinase
Transient receptor potential cation channel subfamily M member 6
SNF-related serine/threonine-protein kinase
Serine/threonine-protein kinase RIO2
Serine/threonine-protein kinase 32B
Serine/threonine-protein kinase MARK1
Glycogen synthase kinase-3 alpha
Serine/threonine-protein kinase PAK 6
Chaperone activity of bcl complex-like
NT-3 growth factor receptor
Mitogen-activated protein kinase 12
Tyrosine-protein kinase Mer
Serine/threonine-protein kinase tousled-like 2
5'-AMP-activated protein kinase catalytic subunit alpha-1
Serine/threonine-protein kinase SIK3
Serine/threonine-protein kinase 16
Cyclin-dependent kinase 17
Serine/threonine-protein kinase receptor R3
Tyrosine-protein kinase BTK

Serine/threonine-protein kinase PAK 7
Calcium/calmodulin-dependent protein kinase type 1D
Calcium/calmodulin-dependent protein kinase type 1G
Proto-oncogene tyrosine-protein kinase receptor Ret
Receptor-interacting serine/threonine-protein kinase 4
Serine/threonine-protein kinase TAO1
Ribosomal protein S6 kinase alpha-2
Casein kinase I isoform gamma-1
Homeodomain-interacting protein kinase 2
Fibroblast growth factor receptor 4
Fibroblast growth factor receptor 2
Fibroblast growth factor receptor 1
AarF domain-containing protein kinase 4
Mitogen-activated protein kinase kinase kinase 19
Dual specificity mitogen-activated protein kinase kinase 2
Serine/threonine-protein kinase 33
NUAK family SNF1-like kinase 2
MAP/microtubule affinity-regulating kinase 4
Serine/threonine-protein kinase RIO1
Testis-specific serine/threonine-protein kinase 1
Calcium/calmodulin-dependent protein kinase kinase 1
MAP kinase-activated protein kinase 2
Serine/threonine-protein kinase Nek9
Myosin light chain kinase 2
Mitogen-activated protein kinase kinase kinase 9
Serine/threonine-protein kinase DCLK3
Cyclin-dependent kinase 11B
Tyrosine-protein kinase Srms
Serine/threonine-protein kinase 35
Dual specificity tyrosine-phosphorylation-regulated kinase 1A
Serine/threonine-protein kinase Nek7
Mitogen-activated protein kinase 1
Mitogen-activated protein kinase 14
Mitogen-activated protein kinase 15
Mitogen-activated protein kinase 9
Cyclin-dependent kinase 15
G protein-coupled receptor kinase 7
Dual specificity mitogen-activated protein kinase kinase 5
Dual specificity mitogen-activated protein kinase kinase 7
Casein kinase I isoform alpha-like
Mitogen-activated protein kinase kinase kinase 7
Mitogen-activated protein kinase kinase kinase kinase 4
Serine/threonine-protein kinase NIM1
Focal adhesion kinase 1
Calcium/calmodulin-dependent protein kinase type II subunit gamma
Protein-tyrosine kinase 2-beta
Serine/threonine-protein kinase SIK1
Serine/threonine-protein kinase 32C
Ankyrin repeat and protein kinase domain-containing protein 1
Ephrin type-A receptor 5

Myosin light chain kinase 3
Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase
G protein-coupled receptor kinase 4
Leucine-rich repeat serine/threonine-protein kinase 2
Serine/threonine-protein kinase Nek5
Leukocyte tyrosine kinase receptor
Tyrosine-protein kinase ZAP-70
Serine/threonine-protein kinase N1
Wee1-like protein kinase 2
Uncharacterized serine/threonine-protein kinase SBK3
Dual serine/threonine and tyrosine protein kinase
Cell division control protein 2 homolog
Phosphatidylinositol 5-phosphate 4-kinase type-2 beta
Serine/threonine-protein kinase 24
Dual specificity tyrosine-phosphorylation-regulated kinase 2
Serine/threonine-protein kinase MRCK alpha
Calcium/calmodulin-dependent protein kinase type 1
MAP kinase-activated protein kinase 5
Peripheral plasma membrane protein CASK
Cyclin-dependent kinase 13
Receptor-interacting serine/threonine-protein kinase 1
Receptor-interacting serine/threonine-protein kinase 2
Serine/threonine-protein kinase RIO3
Serine/threonine-protein kinase PRP4 homolog
Cyclin-dependent kinase 4
Tyrosine-protein kinase JAK3
Hepatocyte growth factor receptor
Serine/threonine-protein kinase STK11
Angiopoietin-1 receptor
Insulin-like growth factor 1 receptor
Mitogen-activated protein kinase kinase kinase 15
Serine/threonine-protein kinase pim-3
Serine/threonine-protein kinase Chk2
Receptor tyrosine-protein kinase erbB-2
Activated CDC42 kinase 1
High affinity nerve growth factor receptor
Myosin light chain kinase family member 4
Serine/threonine-protein kinase PAK 4
Serine/threonine-protein kinase SBK1
Receptor tyrosine-protein kinase erbB-4
Mitogen-activated protein kinase kinase kinase kinase 1
Ephrin type-A receptor 6
Serine/threonine-protein kinase ULK3
Activin receptor type-1
Activin receptor type-2B
Serine/threonine-protein kinase 32A
Cyclin-dependent kinase-like 3
MAP kinase-interacting serine/threonine-protein kinase 1
Phosphatidylinositol 4-phosphate 5-kinase type-1 alpha
Bone morphogenetic protein receptor type-1B

Bone morphogenetic protein receptor type-2
Cyclin-dependent kinase 3
Cyclin-dependent kinase 8
Cyclin-dependent kinase 9
Casein kinase I isoform gamma-2
Death-associated protein kinase 3
Serine/threonine-protein kinase/endoribonuclease IRE1
Inhibitor of nuclear factor kappa-B kinase subunit beta
Activin receptor type-2A
RAC-beta serine/threonine-protein kinase
Tyrosine-protein kinase receptor UFO
Cytoplasmic tyrosine-protein kinase BMX
Calcium/calmodulin-dependent protein kinase type IV
Cyclin-dependent kinase 2
Cyclin-dependent kinase 7
Casein kinase I isoform alpha
Casein kinase I isoform epsilon
Casein kinase II subunit alpha
Casein kinase II subunit alpha'
Receptor tyrosine-protein kinase erbB-3
Tyrosine-protein kinase Fes/Fps
Vascular endothelial growth factor receptor 1
Vascular endothelial growth factor receptor 3
Glycogen synthase kinase-3 beta
Tyrosine-protein kinase HCK
LIM domain kinase 1
Megakaryocyte-associated tyrosine-protein kinase
Mitogen-activated protein kinase kinase kinase 3
Mitogen-activated protein kinase kinase kinase 11
Mitogen-activated protein kinase kinase kinase 10
Serine/threonine-protein kinase Nek2
Serine/threonine-protein kinase Nek3
Serine/threonine-protein kinase PAK 1
Serine/threonine-protein kinase PAK 2
Serine/threonine-protein kinase PAK 3
Cyclin-dependent kinase 18
3-phosphoinositide-dependent protein kinase 1
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit beta
Serine/threonine-protein kinase pim-1
Phosphatidylinositol 4-kinase beta
cAMP-dependent protein kinase catalytic subunit alpha
cAMP-dependent protein kinase catalytic subunit beta
Protein kinase C iota type
Serine/threonine-protein kinase D1
Mitogen-activated protein kinase 3
Mitogen-activated protein kinase 4
Mitogen-activated protein kinase 6
Mitogen-activated protein kinase 7
Mitogen-activated protein kinase 11
Mitogen-activated protein kinase 13

Dual specificity mitogen-activated protein kinase kinase 1
Dual specificity mitogen-activated protein kinase kinase 3
Dual specificity mitogen-activated protein kinase kinase 6
Interferon-induced
Rhodopsin kinase
Proto-oncogene tyrosine-protein kinase ROS
Ribosomal protein S6 kinase alpha-1
Dual specificity mitogen-activated protein kinase kinase 4
SRSF protein kinase 1
Serine/threonine-protein kinase Nek4
Cyclin-dependent kinase-like 5
Ribosomal protein S6 kinase beta-1
Tyrosine-protein kinase Tec
TGF-beta receptor type-2
Dual specificity protein kinase TTK
Tyrosine-protein kinase TXK
Non-receptor tyrosine-protein kinase TYK2
Wee1-like protein kinase
Mitogen-activated protein kinase kinase kinase kinase 5
Death-associated protein kinase 1
MAP/microtubule affinity-regulating kinase 3
Myosin light chain kinase
Insulin receptor
Tubulin alpha-1A chain
Serine/threonine-protein kinase DCLK2
Multidrug resistance protein 1
Cytochrome P450 3A5
Solute carrier family 22 member 1
Cytochrome P450 1A2
Cytochrome P450 2C9
Cytochrome P450 2C19
Cytochrome P450 2D6
Cytochrome P450 3A4
Tyrosine-protein kinase Blk
Macrophage colony-stimulating factor 1 receptor
Epithelial discoidin domain-containing receptor 1
Discoidin domain-containing receptor 2
Tyrosine-protein kinase Lck
RET proto-oncogene
Cytochrome P450 3A7
Prostaglandin G/H synthase 1
Serum albumin
Alpha-1-acid glycoprotein 1
Solute carrier family 22 member 2
ATP-binding cassette sub-family A member 3
Breakpoint cluster region protein
Ribosylidihydronicotinamide dehydrogenase 2)
14-3-3 protein sigma
Cruzipain Trypanosoma cruzi
Multidrug and toxin extrusion protein 2

Multidrug and toxin extrusion protein 1
Solute carrier family 22 member 3
Cyclin-dependent kinase 19
Dual specificity protein kinase CLK4
Tyrosine-protein kinase FRK
Tyrosine-protein kinase Fgr
RAF proto-oncogene serine/threonine-protein kinase
Serine/threonine-protein kinase TNNI3K
Abelson tyrosine-protein kinase 2
Ephrin type-A receptor 8
Maternal embryonic leucine zipper kinase
Dual specificity protein kinase CLK1
Serine/threonine-protein kinase PLK4
Tyrosine-protein kinase Fyn
Mitogen-activated protein kinase 8
Mitogen-activated protein kinase 10
Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma
Homeodomain-interacting protein kinase 4
Interleukin-1 receptor-associated kinase 1
Mitogen-activated protein kinase kinase kinase MLT
Nucleolar transcription factor 1
Myeloblastin
Glyceraldehyde-3-phosphate dehydrogenase
Estrogen receptor
Keratin
T-cell surface glycoprotein CD4
Thrombopoietin
Interleukin-4 receptor subunit alpha
Carbonic anhydrase 12
Transcription factor RelB
Solute carrier family 22 member 17
Tumor necrosis factor receptor superfamily member 10A
NF-kappa-B inhibitor alpha
Aminoacyl tRNA synthase complex-interacting multifunctional protein 2
Transforming growth factor beta-1
Granulocyte colony-stimulating factor
tRNA pseudouridine
Fructose-bisphosphate aldolase C
ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1
Zinc finger protein GLI1
G1/S-specific cyclin-D1

Kit ligand (stem cell factor - SCF)

Bcl-2-like protein 1
Pro-epidermal growth factor
Fibroblast growth factor receptor 3
Low-density lipoprotein receptor-related protein 3
Cyclin-dependent kinase inhibitor 1
Tumor necrosis factor ligand superfamily member 10
Transforming growth factor beta-3
Histone H4-like protein type G

Pro-low-density lipoprotein receptor-related protein 1
Homeobox protein Hox-D9
Heat shock protein beta-1
Smoothed homolog
Homeobox protein Hox-D11
Platelet-derived growth factor receptor-like protein
Kinesin-like protein KIF11
GTPase KRas
Retinoic acid receptor alpha
RNA-binding protein FUS
Gamma-secretase-activating protein
Glycophorin-C
TRAF family member-associated NF-kappa-B activator
Sortilin-related receptor
Protein NOV homolog
Intercellular adhesion molecule 1
Aldehyde dehydrogenase
Prospero homeobox protein 1
G1/S-specific cyclin-D2
Low-density lipoprotein receptor-related protein 6
Protoheme IX farnesyltransferase
Sodium-dependent serotonin transporter
Mothers against decapentaplegic homolog 7
Eukaryotic translation initiation factor 4B
Mothers against decapentaplegic homolog 2
Myeloid cell surface antigen CD33
Cysteine-rich hydrophobic domain-containing protein 2
Thromboxane-A synthase
Integral membrane protein DGCR2/IDD
Tyrosinase
Low-density lipoprotein receptor-related protein 2
Tumor protein 63
Nectin-1
Signal transducer and activator of transcription 3
E3 ubiquitin-protein ligase CBL
Carbonic anhydrase 2
Cyclin-A2
Thyroid receptor-interacting protein 11
Choline kinase alpha
Retinoblastoma-associated protein
Fibroblast growth factor 7
DNA repair protein RAD51 homolog 1
Insulin-like growth factor-binding protein 4
Cellular tumor antigen p53
Neurogenic locus notch homolog protein 1
Interferon alpha-1/13
Tumor necrosis factor receptor superfamily member 10B
Low-density lipoprotein receptor-related protein 12
Programmed cell death protein 4
Serine-protein kinase ATM

SET-binding protein
Annexin A5
Zinc finger FYVE domain-containing protein 9
Carbonic anhydrase 3
Beta-centractin
High mobility group protein B2
Signal transducer and activator of transcription 5B
Neuronal acetylcholine receptor subunit beta-3
Apoptosis regulator BAX
Low-density lipoprotein receptor-related protein 5
Src substrate cortactin
Runt-related transcription factor 1
Granulocyte-macrophage colony-stimulating factor
Integrin alpha-2
Interleukin-3
NGFI-A-binding protein 2
T-cell leukemia homeobox protein 3
Nucleophosmin
Adapter molecule crk
Carbonic anhydrase 4
CD320 antigen
Envoplakin
Carbonic anhydrase 13
Ras and Rab interactor 1
Interleukin-8
Low-density lipoprotein receptor-related protein 8
Cytotoxic T-lymphocyte protein 4
CCAAT/enhancer-binding protein beta
Hematopoietic progenitor cell antigen CD34
Eukaryotic translation initiation factor 2-alpha kinase 3
Pyruvate dehydrogenase E1 component subunit beta
GTPase HRas
Carbonic anhydrase 5A
Low-density lipoprotein receptor class A domain-containing protein 3
Carbonic anhydrase 5B
Peptidyl-prolyl cis-trans isomerase FKBP2
Caspase-3
Histone-lysine N-methyltransferase NSD3
B-lymphocyte antigen CD19
Zinc fingers and homeoboxes protein 2
Probable ATP-dependent RNA helicase DDX10
Cyclin-G-associated kinase
Thymidylate synthase
Nuclear pore complex protein Nup98-Nup96
Translocator protein
PHD finger protein 23
Hematopoietic lineage cell-specific protein
Serine/threonine-protein kinase 17A
Regulator of G-protein signaling 5
Echinoderm microtubule-associated protein-like 4

Nitric oxide synthase
Malate dehydrogenase
Transcription factor COE1
Lysine--tRNA ligase
N-acetylaspartate synthetase
Macrophage colony-stimulating factor 1
SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related
PHD finger protein 6
Platelet-derived growth factor subunit B
Protein patched homolog 1
DNA-binding protein Ikaros
Protein tyrosine phosphatase type IVA 3
Heat shock protein HSP 90-alpha
Mothers against decapentaplegic homolog 3
Calcium and integrin-binding protein 1
Rho guanine nucleotide exchange factor 1
Pre-mRNA 3'-end-processing factor FIP1
High mobility group protein 20A
Thymocyte selection-associated high mobility group box protein TOX
High mobility group protein B1
Rap1 GTPase-GDP dissociation stimulator 1
Growth factor receptor-bound protein 2
Hypoxia-inducible factor 1-alpha
Single-strand selective monofunctional uracil DNA glycosylase
Friend leukemia integration 1 transcription factor
Suppressor of cytokine signaling 2
Forkhead box protein O3
Signal transducer and activator of transcription 5A
Eukaryotic translation initiation factor 4E-binding protein 1
Tyrosine-protein phosphatase non-receptor type 11
Mothers against decapentaplegic homolog 4
E3 ubiquitin-protein ligase XIAP
Homeobox protein Hox-A9
Tyrosine-protein kinase JAK1
Carbonic anhydrase 7
Catenin beta-1
TOX high mobility group box family member 2
Anoctamin-1
Fibronectin
Protein numb homolog
Histone H4
Insulin
Gamma-adducin
Breast cancer type 1 susceptibility protein
Paired box protein Pax-5
Caspase-8
Neurofibromin
Midkine
DNA repair protein XRCC2
Low-density lipoprotein receptor-related protein 10

Nuclear pore complex protein Nup214
Poly
DNA topoisomerase 1
Signal transducer and activator of transcription 1-alpha/beta
Neprilysin
CAMPATH-1 antigen
Cyclin-dependent kinase inhibitor 2A
Poly synthase 1)
Prostaglandin G/H synthase 2
Interferon regulatory factor 6
Paired mesoderm homeobox protein 1
Carbonic anhydrase 14
GTPase NRas
Alpha-centractin
High mobility group protein B3
T-cell leukemia homeobox protein 1
Neuronal acetylcholine receptor subunit alpha-4
G1/S-specific cyclin-D3
Phosphatidylinositol 3
mRNA export factor
Matrix metalloproteinase-9
P2Y purinoceptor 8
Carbonic anhydrase 6
Forkhead box protein O4
Stromal cell-derived factor 1
Myelodysplastic syndrome 2 translocation-associated protein
Tumor necrosis factor receptor superfamily member 1B
HLA class I histocompatibility antigen
Histamine H2 receptor
tRNA pseudouridine synthase A
Protein sprouty homolog 2
PC4 and SFRS1-interacting protein
5-hydroxytryptamine receptor 2A
Myc proto-oncogene protein
Low-density lipoprotein receptor-related protein 4
Carbonic anhydrase 9
Interferon alpha-21
tRNA pseudouridine synthase-like 1
Proliferating cell nuclear antigen
Interferon alpha-2
Methylcytosine dioxygenase TET2
Very low-density lipoprotein receptor
Low-density lipoprotein receptor-related protein 1B
Doublesex- and mab-3-related transcription factor 1
THO complex subunit 5 homolog
Platelet-derived growth factor D
Multidrug resistance-associated protein 1
Paired box protein Pax-1
TOX high mobility group box family member 3
Transcription factor p65

Forkhead box protein P2
Neurotrophin receptor-interacting factor homolog
Pre-B-cell leukemia transcription factor 1
Histone deacetylase 9
Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform
Interferon alpha-17
COX assembly mitochondrial protein homolog
Prominin-1
E3 ubiquitin-protein ligase Mdm2
Transcription factor A
Arachidonate 15-lipoxygenase B
Geminin
Prelamin-A/C
Luciferin 4-monooxygenase
Flap endonuclease 1
Nuclear receptor ROR-gamma
DNA polymerase kappa
Cell division cycle 7-related protein kinase
Eukaryotic elongation factor 2 kinase
Serine/threonine-protein kinase Chk1
Inhibitor of nuclear factor kappa-B kinase subunit alpha
Dual specificity tyrosine-phosphorylation-regulated kinase 3
Rho-associated protein kinase 2
Ribosomal protein S6 kinase alpha-4
Carbonic anhydrase 1
Protein kinase C gamma type
Cyclin-dependent kinase 1
G protein-coupled receptor kinase 5
Casein kinase I isoform delta
Macrophage-stimulating protein receptor
Protein kinase C zeta type
Calcium/calmodulin-dependent protein kinase type II subunit beta
Calcium/calmodulin-dependent protein kinase type II subunit delta
cGMP-dependent protein kinase 1
MAP kinase-activated protein kinase 3
Misshapen-like kinase 1
Serine/threonine-protein kinase BRSK1
Lymphokine-activated killer T-cell-originated protein kinase
Testis-specific serine/threonine-protein kinase 2
Calcium/calmodulin-dependent protein kinase kinase 2
Carbonic anhydrase 15
Serine/threonine-protein kinase D2
Serine/threonine-protein kinase Sgk2
Dual specificity tyrosine-phosphorylation-regulated kinase 4
Calcium/calmodulin-dependent protein kinase type II subunit alpha
Protein kinase C alpha type
cAMP-dependent protein kinase catalytic subunit gamma
Serine/threonine-protein kinase Sgk1
G2/mitotic-specific cyclin-B1
5'-AMP-activated protein kinase catalytic subunit alpha-2

Polycystin-2
 Mitogen-activated protein kinase kinase kinase 13
 Serine/threonine-protein kinase ULK1
 Ephrin type-A receptor 1
 Protein kinase C eta type
 Ephrin type-B receptor 1
 Calcium-dependent protein kinase 1
 SRSF protein kinase 2
 Serine/threonine-protein kinase PknB
 AP2-associated protein kinase 1
 Serine/threonine-protein kinase MRCK gamma
 Homeodomain-interacting protein kinase 1
 Mitogen-activated protein kinase kinase kinase kinase 3
 Serine/threonine-protein kinase ULK2
 Serine/threonine-protein kinase Nek11
 Myosin-IIIb
 Eukaryotic translation initiation factor 2-alpha kinase 4
 SRSF protein kinase 3
 Cyclin-dependent kinase 11A
 Interleukin-1 receptor-associated kinase 3
 Mitogen-activated protein kinase kinase kinase 4
 Membrane-associated phosphatidylinositol transfer protein 1
 Myelin transcription factor 1

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of *M. tuberculosis*

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

Predicted Targets

Cytochrome P450 1A2
 Cytochrome P450 3A4
 Cytochrome P450 2D6
 Cytochrome P450 2C9
 Cytochrome P450 2C19

Amine oxidase A

Amine oxidase B

Catechol O-methyltransferase
 ATP-citrate synthase
 Succinyl-CoA ligase subunit alpha
 ATP-dependent 6-phosphofructokinase
 Histone acetyltransferase KAT2A
 ATPase family AAA domain-containing protein 5
 Sodium-dependent serotonin transporter

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14-alpha demethylase

Molecular Mechanism (repurposed) :
smoothened homolog inhibitor
lanosterol 14-alpha demethylase inhibitor

Predicted Targets

14-alpha sterol demethylase

25-dihydroxyvitamin D
Bile salt export pump
C-C chemokine receptor type 4
Cruzipain
C-X-C chemokine receptor type 1
Cytochrome P450 1A1
Cytochrome P450 2B6
Cytochrome P450 2D6
Cytochrome P450 2E1
Cytochrome P450 3A4
Cytochrome P450 3A5
Cytochrome P450 3A7
Interleukin-4
Interleukin-5
Lanosterol 14-alpha demethylase
Lanosterol 14-alpha demethylase
Multidrug resistance protein 1
Multidrug resistance protein 1A
Multidrug resistance protein 1B
Solute carrier organic anion transporter family member 1B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 2B1
Tyrosine-protein kinase Fyn
uniprot_name
Vascular endothelial growth factor receptor 2
Vasopressin V2 receptor

Ketoconazole

Molecular Mechanism (initial) :
fungal cytochrome P450 51 inhibitor
Molecular Mechanism (repurposed) :
cytochrome P450 aromatase (CYP19A1) inhibitor

Predicted Targets

Lanosterol 14-alpha demethylase (Cytochrome P450 51)

Androgen receptor
Steroid 21-hydroxylase

Aromatase (CYP19A1)

Cytochrome P450 3A4
Cytochrome P450 2D6
Cytochrome P450 2C9
Cytochrome P450 2C19
Cytochrome P450 3A5
Cytochrome P450 3A7

Cytochrome P450 2C8
Cytochrome P450 1A2
Cytochrome P450 1A1
Cholesterol side-chain cleavage enzyme
Cytochrome P450 11B1
Cytochrome P450 1B1
Cytochrome P450 26A1
Cytochrome P450 2A6
Cytochrome P450 2B6
Bile salt export pump
Multidrug resistance protein 1
Solute carrier organic anion transporter family member 1A2
Casein kinase I isoform gamma-1
Peptidyl-prolyl cis-trans isomerase FKBP9
Aryl hydrocarbon receptor
Squalene synthase
Fatty acid 2-hydroxylase
T-cell surface glycoprotein CD4
Cytochrome P450 26B1
Mitogen-activated protein kinase 13
Serine/threonine-protein kinase VRK1
Early growth response protein 1
Gonadotropin-releasing hormone receptor
Prenylated Rab acceptor protein 1
Protein argonaute-2
Peptidyl-prolyl cis-trans isomerase FKBP14
ATP-binding cassette sub-family G member 2
Interleukin-4
25-hydroxyvitamin D-1 alpha hydroxylase
Mitogen-activated protein kinase 14
Delta-type opioid receptor
Glucocorticoid receptor
Uridine 5'-monophosphate synthase
UDP-glucuronosyltransferase 1-1
Cytochrome P450 2E1
UDP-galactose translocator
Adenylyltransferase and sulfurtransferase MOCS3
Uroporphyrinogen decarboxylase
Potassium voltage-gated channel subfamily A member 5
26S proteasome complex subunit DSS1
Keratin
Solute carrier organic anion transporter family member 1B1
Casein kinase I isoform gamma-2
Tau-tubulin kinase 1
Gamma-glutamyl hydrolase
Tau-tubulin kinase 2
Vascular endothelial growth factor receptor 2
Peptidyl-prolyl cis-trans isomerase G
Sodium-dependent serotonin transporter
Potassium voltage-gated channel subfamily H member 2

Thromboxane-A synthase
Phosphatidylserine decarboxylase proenzyme
Pro-opiomelanocortin
Methionine synthase reductase
Squalene monooxygenase
UDP-glucuronosyltransferase 2B7
Coxsackievirus and adenovirus receptor
Stimulated by retinoic acid gene 8 protein homolog
Lamin-B receptor
Cerebellar degeneration-related protein 2
Sodium-dependent dopamine transporter
AP-1 complex-associated regulatory protein
Renin
Calmodulin
Alpha-2A adrenergic receptor
Steroidogenic acute regulatory protein
Progonadoliberin-1
Delta
Corticoliberin
Sigma non-opioid intracellular receptor 1
UDP-glucuronosyltransferase 1-6
Serum albumin
3-hydroxy-3-methylglutaryl-coenzyme A reductase
Cytochrome P450 26C1
Cytochrome P450 2C18
Arachidonate 15-lipoxygenase
S-adenosylmethionine synthase isoform type-2
Integrin alpha-2
Endothelin-converting enzyme-like 1
Cholesterol 7-alpha-monooxygenase
Substance-K receptor
Cytochrome b5
Ribosome biogenesis regulatory protein homolog
Cytochrome P450 4A11
Elongation factor 2
Alpha-1B adrenergic receptor
Multidrug resistance-associated protein 9
25-hydroxycholesterol 7-alpha-hydroxylase
Peptidyl-prolyl cis-trans isomerase FKBP2
Muscarinic acetylcholine receptor M2
Prostate-specific antigen
Vigilin
17-beta-hydroxysteroid dehydrogenase type 6
5-hydroxytryptamine receptor 1A
Peptidyl-prolyl cis-trans isomerase FKBP10
Serine/threonine-protein kinase Sgk2
Neuropeptide W
Casein kinase I isoform delta
Inactive serine/threonine-protein kinase VRK3
Nitric oxide synthase

Thiosulfate sulfurtransferase/rhodanese-like domain-containing protein 1
Cytochrome P450 11B2
Mitogen-activated protein kinase 11
Cytochrome P450 2A13
Multidrug resistance-associated protein 5
Nuclear receptor subfamily 1 group I member 2
Protein argonaute-4
Lanosterol synthase
Uridine-cytidine kinase-like 1
Serine/threonine-protein kinase VRK2
Cytochrome P450 20A1
UDP-glucuronosyltransferase 1-9
7-dehydrocholesterol reductase
Death-associated protein kinase 1
TBC1 domain family member 9B
Casein kinase I isoform gamma-3
Casein kinase I isoform epsilon
Protein argonaute-1
Dihydropyrimidine dehydrogenase
Uroporphyrinogen-III synthase
Dimethylaniline monooxygenase 3
Nuclear receptor subfamily 1 group I member 3
5-hydroxytryptamine receptor 1B
Potassium voltage-gated channel subfamily A member 10
Steroid 17-alpha-hydroxylase/17
Protein argonaute-3
Cytochrome P450 2J2
Spectrin alpha chain
NADPH-dependent diflavin oxidoreductase 1
S-adenosylmethionine synthase isoform type-1
TBC1 domain family member 9
Alpha-1A adrenergic receptor
Histamine H2 receptor
Uracil phosphoribosyltransferase homolog
UDP-glucuronosyltransferase 1-4
TBC1 domain family member 8
Bromodomain-containing protein 2
Sex hormone-binding globulin
DNA/RNA-binding protein KIN17
Adenine phosphoribosyltransferase
Alpha-1D adrenergic receptor
Sodium-dependent noradrenaline transporter
Casein kinase I isoform alpha-like
GDP-mannose 4
Neurolysin
Glucose-6-phosphate 1-dehydrogenase
Delta-aminolevulinic acid dehydratase
Peptidyl-prolyl cis-trans isomerase FKBP7
GPI ethanolamine phosphate transferase 2

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

Predicted Targets

Voltage-dependent L-type calcium channel subunit alpha-1C

Multidrug and toxin extrusion protein 1

Cytochrome P450 1A2

Potassium voltage-gated channel subfamily D member 2

Sodium channel protein type 5 subunit alpha

Potassium voltage-gated channel subfamily A member 5

Potassium voltage-gated channel subfamily H member 2

Potassium channel subfamily K member 2

Ryanodine receptor 1

Dynein heavy chain 8

CUGBP Elav-like family member 1

Calmodulin

Sodium channel subunit beta-2

Cytochrome P450 3A43

Intercellular adhesion molecule 5

Serine--tRNA ligase

Intercellular adhesion molecule 3

T-cell surface glycoprotein CD4

Potassium voltage-gated channel subfamily KQT member 1

Tissue-type plasminogen activator

Proenkephalin-B

Neurogenic locus notch homolog protein 1

Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4

Solute carrier family 22 member 5

Arginine--tRNA ligase

Cytochrome P450 3A5

G1/S-specific cyclin-D1

Aspartate aminotransferase

Lactotransferrin

Lipoyl synthase

C-reactive protein

Heat shock protein 75 kDa

Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Cytochrome P450 2C9

Interleukin-6

Alpha-1-acid glycoprotein 1

Corticoliberin

Kininogen-1

Cholinesterase

Monocyte to macrophage differentiation factor

Transient receptor potential cation channel subfamily A member 1

Pro-opiomelanocortin

Intercellular adhesion molecule 1

Epidermal growth factor receptor
Receptor tyrosine-protein kinase erbB-3
Multidrug resistance protein 1
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha
Alpha-2
Renin
Insulin

Sodium channel protein type 11 subunit alpha

15-hydroxyprostaglandin dehydrogenase
Cytochrome P450 2C18
Glycerol-3-phosphate dehydrogenase 1-like protein
Potassium voltage-gated channel subfamily E member 4
Muscleblind-like protein 1

Sodium channel protein type 3 subunit alpha

Sodium channel protein type 2 subunit alpha

Melanotransferrin
Somatostatin
Angiotensin-converting enzyme
Serum albumin
Alkaline phosphatase
Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 1
Cytochrome P450 2A6
WD repeat and FYVE domain-containing protein 2
Integrin alpha-2
Nitric oxide synthase
60S ribosomal protein L10-like
Sodium channel subunit beta-3
Proto-oncogene c-Fos
Substance-P receptor
Potassium channel subfamily K member 9
Non-secretory ribonuclease
Protein kinase C epsilon type
Iroquois-class homeodomain protein IRX-1
5-hydroxytryptamine receptor 3A
Caspase-3
Prothrombin
cAMP-dependent protein kinase catalytic subunit alpha
Cysteine and histidine-rich domain-containing protein 1
Acyl-CoA-binding protein
Leptin
Transient receptor potential cation channel subfamily M member 8
Protachykinin-1

Sodium channel subunit beta-4

Heat shock protein HSP 90-beta
Cytochrome P450 2B6

Sodium channel protein type 8 subunit alpha

Cytochrome P450 3A7
Calcitonin
Translocator protein
Caspase-9

Cholecystokinin
Tissue factor
Heat shock protein HSP 90-alpha
Myotonin-protein kinase
CD59 glycoprotein
Cytochrome P450 3A4
NADH-cytochrome b5 reductase 3
Cytochrome b5
60S ribosomal protein L10
Tumor necrosis factor
Selenoprotein N
Beta-nerve growth factor
Voltage-dependent L-type calcium channel subunit alpha-1S
Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 3
Integrin beta-1-binding protein 2
Transcription factor AP-1
Cytochrome P450 2C8

Sodium channel subunit beta-1

Sodium channel protein type 9 subunit alpha

Trafficking protein particle complex subunit 9
Probable methyltransferase-like protein 15
Iroquois-class homeodomain protein IRX-5
Neuropeptide S

Sodium channel protein type 4 subunit alpha

Gamma-aminobutyric acid type B receptor subunit 1

Sodium channel protein type 7 subunit alpha

Glucagon
Alpha-1-acid glycoprotein 2

Sodium channel protein type 10 subunit alpha

Laminin subunit alpha-2
Geminin
Isocitrate dehydrogenase cytoplasmic
Thioredoxin reductase 1
Retinal dehydrogenase 1
Beta-lactamase
Prelamin-A/C
Muscarinic acetylcholine receptor M1
Microtubule-associated protein tau
Mitogen-activated protein kinase 1
Flap endonuclease 1
Chromobox protein homolog 1
Histone-lysine N-methyltransferase EHMT2

Sodium channel protein type 1 subunit alpha

Sodium channel protein type 2 subunit alpha

Sodium channel protein type 3 subunit alpha

Sodium channel protein type 1 subunit alpha

Solute carrier family 22 member 1

Sodium channel protein type 5 subunit alpha

Malate dehydrogenase
Chymotrypsin-C

Sphingomyelin phosphodiesterase
Solute carrier family 22 member 5

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

Predicted Targets

Glutamate receptor ionotropic (NMDA receptor)

5-hydroxytryptamine receptor 3A

D

Cytochrome P450 2B6

Cytochrome P450 2A6

Cytochrome P450 2C19

Solute carrier family 22 member 2

Metabotropic glutamate receptor 5

Acetylcholinesterase

Heat shock 70 kDa protein 4

Bcl-2-like protein 1

Carbonic anhydrase 4

CHRNA7-FAM7A fusion protein

Homeobox protein engrailed-1

Gamma-enolase

Heat shock cognate 71 kDa protein

Small glutamine-rich tetratricopeptide repeat-containing protein alpha

Glutamate receptor 1

Apolipoprotein E

DNA-directed DNA/RNA polymerase mu

A disintegrin and metalloproteinase with thrombospondin motifs 2

Integrin alpha-V

Transcription initiation factor TFIID subunit 4

Protein phosphatase 1 regulatory subunit 1B

Amyloid beta A4 protein

Excitatory amino acid transporter 1

Cholinesterase

Threonine--tRNA ligase

Solute carrier family 22 member 3

Excitatory amino acid transporter 2

Neuronal acetylcholine receptor subunit alpha-4

Huntingtin-associated protein 1

Mannose-6-phosphate isomerase

Rho-related GTP-binding protein RhoD

Argininosuccinate lyase

Cytochrome c

T-complex protein 1 subunit alpha

cAMP-dependent protein kinase catalytic subunit alpha

Hydroxymethylglutaryl-CoA synthase

Beta-secretase 1

Ribosome biogenesis regulatory protein homolog
 Presenilin-1
 Glycogen synthase kinase-3 beta
 Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex
 Atrophin-1
 DnaJ homolog subfamily B member 2
 Adenosine receptor A2a
 Microtubule-associated protein tau
 Huntingtin
 Ubiquitin-like protein 4A
 Apoptotic protease-activating factor 1
 Dynamin-like 120 kDa protein
 Beta-nerve growth factor
 DnaJ homolog subfamily C member 7
 Ataxin-2
 Carboxypeptidase N catalytic chain
 Tumor necrosis factor receptor superfamily member 1B
 Dynamin-1
 Heat shock 70 kDa protein 1A/1B
 DnaJ homolog subfamily A member 1
 Small glutamine-rich tetratricopeptide repeat-containing protein beta
 Rab GDP dissociation inhibitor alpha
 Brain-derived neurotrophic factor
 Thioredoxin reductase 1
 Prelamin-A/C
 Peripheral myelin protein 22
 Serine/threonine-protein kinase mTOR
 Nuclear factor erythroid 2-related factor 2
 Solute carrier family 22 member 1
 Acetylcholinesterase
 Cholinesterase

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

Predicted Targets

Acetyl-CoA carboxylase 1
 Bcl2-associated agonist of cell death
 Apoptosis regulator Bcl-2
 Apoptosis regulator BAX
 Histamine H2 receptor
 Eukaryotic translation initiation factor 4E-binding protein 1
 Interleukin-1 beta
 Interleukin-8

5'-AMP-activated protein kinase catalytic subunit alpha-2

Solute carrier family 15 member 1
 Solute carrier family 22 member 1

Solute carrier family 22 member 2
Solute carrier family 22 member 3
Solute carrier family 2
Zinc finger protein mex-5 *Caenorhabditis elegans*
Dipeptidyl peptidase 4
Multidrug and toxin extrusion protein 1
Pro-neuropeptide Y
Islet amyloid polypeptide
Tumor necrosis factor ligand superfamily member 11
Bifunctional purine biosynthesis protein PURH
Cystic fibrosis transmembrane conductance regulator
Steroid hormone receptor ERR1
Apolipoprotein A-I
Resistin
NF-kappa-B inhibitor alpha
NAD-dependent protein deacetylase sirtuin-1
Calcium/calmodulin-dependent protein kinase kinase 1
Beta-2-glycoprotein 1
Phosphoenolpyruvate carboxykinase
Heme oxygenase 1
TGF-beta-activated kinase 1 and MAP3K7-binding protein 1
Muellerian-inhibiting factor
Tuberin
Aurora kinase A
72 kDa type IV collagenase
CDP-diacylglycerol--inositol 3-phosphatidyltransferase
Tissue-type plasminogen activator
Sodium/hydrogen exchanger 2
Ribosomal protein S6 kinase beta-1
Nicotinamide phosphoribosyltransferase
Bile salt sulfotransferase
Fibroblast growth factor 21
Glucokinase
Plasminogen activator inhibitor 1
Retinoic acid receptor responder protein 2
Apolipoprotein B-100
Baculoviral IAP repeat-containing protein 2
C-C motif chemokine 2
G1/S-specific cyclin-D1
Glucocorticoid receptor
Glyceraldehyde-3-phosphate dehydrogenase

5'-AMP-activated protein kinase subunit beta-1

Progesterone receptor
Proteasome activator complex subunit 3
Tyrosine-protein kinase receptor TYRO3
Apolipoprotein C-II
Tubulin gamma-2 chain
Hormone-sensitive lipase
Aspartate aminotransferase
Apolipoprotein E

Tubulin gamma-1 chain
Hemoglobin subunit alpha
Fatty acid-binding protein
Retina-specific copper amine oxidase
Transcription factor jun-D
Transcription factor GATA-5
C-reactive protein
Nuclear receptor subfamily 0 group B member 2
Galectin-3
Protein kinase C gamma type
Aromatase
ER degradation-enhancing alpha-mannosidase-like protein 1
AMP deaminase 2
Cathepsin L2
Interleukin-6
Interleukin-1 receptor antagonist protein
Peroxisome proliferator-activated receptor alpha
Cytochrome b-245 light chain
Kinesin-like protein KIF11
Glycogen synthase
GTP-binding protein Rheb
Lipase maturation factor 1
RAC-alpha serine/threonine-protein kinase
Carnitine O-palmitoyltransferase 1
Sodium/hydrogen exchanger 1
Plasma kallikrein
Sodium/hydrogen exchanger 3
Pro-opiomelanocortin
Peroxisome proliferator-activated receptor gamma coactivator 1-alpha
Receptor tyrosine-protein kinase erbB-2
Sorbitol dehydrogenase
Multidrug resistance protein 1
Receptor tyrosine-protein kinase erbB-3
Cellular tumor antigen p53
Insulin-like growth factor 1 receptor
CREB-regulated transcription coactivator 3
Angiotensin-converting enzyme
Progonadoliberein-1
Renin
Myocyte-specific enhancer factor 2D
Insulin-like growth factor-binding protein 1
Threonylcarbamoyladenosine tRNA methylthiotransferase
Peroxisome proliferator-activated receptor gamma
A-kinase anchor protein 6
Glycodelin
6-pyruvoyl tetrahydrobiopterin synthase
Somatostatin
Yorkie homolog
Hematopoietically-expressed homeobox protein HHEX
Serine/threonine-protein kinase STK11

Sodium/hydrogen exchanger 5
Sodium/hydrogen exchanger 9B1
Sodium/hydrogen exchanger 4
Cyclic AMP-dependent transcription factor ATF-6 beta
Vascular cell adhesion protein 1
Hermansky-Pudlak syndrome 3 protein
Serine/threonine-protein kinase 11-interacting protein
Serum albumin
Hepatic triacylglycerol lipase
Integrin alpha-2
Equilibrative nucleoside transporter 4
Tumor necrosis factor receptor superfamily member 11B
Nitric oxide synthase
Plasminogen
Insulin receptor substrate 1
Bcl-2-like protein 1
Prolactin
Fatty acid synthase
Insulin-like growth factor I
Insulin receptor
Prothrombin
Protein kinase C beta type
DNA damage-inducible transcript 4 protein
Serine/threonine-protein kinase SIK2
Regulatory-associated protein of mTOR
Glycogen synthase kinase-3 beta
17-beta-hydroxysteroid dehydrogenase type 6
Calcium/calmodulin-dependent protein kinase kinase 2
Mitochondrial uncoupling protein 2
Lipoprotein lipase
Caspase-3
Leptin
Membrane primary amine oxidase
Beta-secretase 1
Segment polarity protein dishevelled homolog DVL-3
Hepatocyte nuclear factor 4-alpha
Sodium/nucleoside cotransporter 2
ER degradation-enhancing alpha-mannosidase-like protein 3
Ubiquitin-conjugating enzyme E2 N
Cytochrome P450 2B6
Tubulin delta chain
Phosphoenolpyruvate carboxykinase
Carbonic anhydrase 13
Sodium/hydrogen exchanger 9
Adiponectin
Casein kinase I isoform delta
Carbohydrate-responsive element-binding protein
Mitochondrial uncoupling protein 3
Four and a half LIM domains protein 2
ATP-sensitive inward rectifier potassium channel 11

STE20-related kinase adapter protein alpha
Multidrug and toxin extrusion protein 2
T-cell surface glycoprotein CD8 beta chain
Sodium/hydrogen exchanger 7
Leptin receptor
Nuclear receptor subfamily 1 group I member 2
Homeobox protein aristaless-like 4
Receptor-interacting serine/threonine-protein kinase 4
Appetite-regulating hormone
Formin-1
Hemoglobin subunit beta
Cathepsin L1
Hypoxia-inducible factor 1-alpha
Superoxide dismutase
Cytochrome P450 3A4
Transcription factor 7
Caveolin-1
Ubiquitin-conjugating enzyme E2 variant 1
Serpine A12
Adiponectin receptor protein 1
Cytochrome P450 1A2
Exostosin-2
Endoribonuclease Dicer
Steroid 17-alpha-hydroxylase/17
Amiloride-sensitive amine oxidase
Insulin
EGF-containing fibulin-like extracellular matrix protein 1
5'-AMP-activated protein kinase catalytic subunit alpha-1
Myocyte-specific enhancer factor 2A
5-hydroxytryptamine receptor 3A
Sterol regulatory element-binding protein 1
Gastric inhibitory polypeptide
Proline dehydrogenase 1
Adiponectin receptor protein 2
Peptide YY
Caspase-8
Casein kinase I isoform epsilon
STE20-like serine/threonine-protein kinase
Sodium/hydrogen exchanger 8
Serine/threonine-protein kinase mTOR
Mitochondrial sodium/hydrogen exchanger 9B2
Conserved oligomeric Golgi complex subunit 2
Poly synthase 1)
Transcription factor 7-like 2
Cyclic AMP-dependent transcription factor ATF-6 alpha
Prostaglandin G/H synthase 2
Tumor necrosis factor ligand superfamily member 6
Prelamin-A/C
Proto-oncogene tyrosine-protein kinase ROS
NAD-dependent protein deacetylase sirtuin-3

ER degradation-enhancing alpha-mannosidase-like protein 2
Phosphatidylinositol 3
Growth arrest and DNA damage-inducible protein GADD45 alpha
Sodium/hydrogen exchanger 6
Tyrosine-protein phosphatase non-receptor type 1
Retinol-binding protein 4
FERM and PDZ domain-containing protein 2
S-adenosylmethionine synthase isoform type-1
Insulin receptor substrate 4
Gelsolin
Matrix metalloproteinase-9
Glucagon-like peptide 1 receptor
Pancreas/duodenum homeobox protein 1
Receptor-type tyrosine-protein phosphatase H
Fructose-1
Bromodomain-containing protein 2
Insulin receptor substrate 2
Coagulation factor VII
Sex hormone-binding globulin
TBC1 domain family member 4
Methylenetetrahydrofolate reductase
Forkhead box protein O1
Acetyl-CoA carboxylase 2
Cardiolipin synthase
F-box only protein 8
ATP-binding cassette sub-family C member 8
Serine/threonine-protein kinase Nek1
SH3 domain-binding protein 5
RAC-beta serine/threonine-protein kinase
Ladinin-1
Calpain-10
Cyclic AMP-responsive element-binding protein 1
Tax1-binding protein 1
Keratin
GTP cyclohydrolase 1
Glucagon
Hepatocyte nuclear factor 4-gamma
Transcription factor p65
Tyrosine-protein phosphatase non-receptor type 13
Tumor necrosis factor
Myocyte-specific enhancer factor 2C
Protein ACN9 homolog
Interleukin-10
Transcription factor A
Geminin
Ferritin light chain
Histone acetyltransferase KAT2A
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B1
Solute carrier organic anion transporter family member 1B3

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :

dihydrofolate reductase inhibitor

Predicted Targets

Bcl-2-like protein 11

Importin subunit alpha-1

Nuclear receptor coactivator 3

Tegument protein VP16

Nuclear receptor coactivator 1

Protein-arginine deiminase type-4

Bifunctional purine biosynthesis protein PURH

Trifunctional purine biosynthetic protein adenosine-3

Thymidylate synthase

Dihydrofolate reductase

Methylenetetrahydrofolate reductase

Aldehyde oxidase

6-phosphogluconate dehydrogenase

Folypolyglutamate synthase

Gamma-glutamyl hydrolase

Serum albumin

Canalicular multispecific organic anion transporter 2

Multidrug resistance-associated protein 4

Multidrug resistance-associated protein 1

Canalicular multispecific organic anion transporter 1

Multidrug resistance protein 1

Solute carrier organic anion transporter family member 1A2

Monocarboxylate transporter 1

Folate transporter 1

Folate receptor alpha

Cytochrome P450 1A2

Cytochrome P450 3A4

Cytochrome P450 2D6

Cytochrome P450 2C9

Cytochrome P450 2C19

Bifunctional dihydrofolate reductase-thymidylate synthase

Lysine-specific demethylase 4E

Menin

ATP-dependent 6-phosphofructokinase

Geminin

Isocitrate dehydrogenase cytoplasmic

Thioredoxin reductase 1

Ubiquitin carboxyl-terminal hydrolase 1

Retinal dehydrogenase 1

Prelamin-A/C

Ferritin light chain

Cellular tumor antigen p53

Alpha-galactosidase A
DNA polymerase beta
Microtubule-associated protein tau
Transcriptional regulator ERG
Vitamin D3 receptor
15-hydroxyprostaglandin dehydrogenase
Arachidonate 15-lipoxygenase
Sphingomyelin phosphodiesterase
Arachidonate 12-lipoxygenase
Retinoic acid receptor RXR-alpha
D
Peripheral myelin protein 22
Caspase-1
Peroxisome proliferator-activated receptor gamma
Flap endonuclease 1
Bloom syndrome protein
Caspase-7
ATP-dependent Clp protease proteolytic subunit
Chromobox protein homolog 1
Runt-related transcription factor 1
Histone-lysine N-methyltransferase 2A
Peroxisome proliferator-activated receptor delta
TAR DNA-binding protein 43
Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
Core-binding factor subunit beta
Nuclear factor erythroid 2-related factor 2
Survival motor neuron protein
Histone acetyltransferase KAT2A
Histone-lysine N-methyltransferase EHMT2
ATPase family AAA domain-containing protein 5
Bile acid receptor
M-phase phosphoprotein 8
3-hydroxyacyl-CoA dehydrogenase type-2
4'-phosphopantetheinyl transferase ffp
Muscleblind-like protein 1
Tyrosyl-DNA phosphodiesterase 1
DNA polymerase kappa
DNA polymerase iota
DNA polymerase eta
Dihydrofolate reductase
Pteridine reductase 1
Solute carrier family 22 member 20
Solute carrier family 22 member 6
Multidrug resistance associated protein
Thymidylate synthase
Solute carrier organic anion transporter family member 2B1
Solute carrier family 22 member 1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Solute carrier family 22 member 8

Multidrug resistance-associated protein 7

Milnacipran

Molecular Mechanism (initial) :

5-HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

5-HT and norepinephrine reuptake inhibitor

Predicted Targets

Sodium-dependent dopamine transporter

Sodium-dependent serotonin transporter

Sodium-dependent noradrenaline (norepinephrine) transporter

Glutamate receptor ionotropic

Miltefosine

Molecular Mechanism (initial) :

Akt/PKB inhibitor

Molecular Mechanism (repurposed) :

phosphatidyl-choline biosynthesis inhibitor

Predicted Targets

Cyclin-dependent kinase 1

Platelet-activating factor receptor

Phospholipase B

M-phase inducer phosphatase 1

RAC-alpha serine/threonine-protein kinase

Interleukin-12 subunit beta

Phosphatidylinositol-glycan-specific phospholipase D

Hepcidin

T-cell surface glycoprotein CD4

Sphingosine 1-phosphate receptor 3

Kallikrein-1

Multidrug resistance protein 3

Glutamate decarboxylase 2

Sphingosine 1-phosphate receptor 4

ATP-binding cassette sub-family B member 5

Bile salt export pump

Phospholipase D2

Paladin

Cytosolic phospholipase A2 delta

Multidrug resistance protein 1

Cysteine sulfinic acid decarboxylase

Phospholipid-transporting ATPase IC

Probable phospholipid-transporting ATPase VD

Glutamate decarboxylase-like protein 1

Probable phospholipid-transporting ATPase VA

Prostate-specific antigen

Sphingosine 1-phosphate receptor 1

Interleukin-12 subunit alpha

Probable phospholipid-transporting ATPase VB

Phospholipase A2
 Kallikrein-2
 Phospholipase D3
 Sphingosine 1-phosphate receptor 5
 Polycystic kidney disease 2-like 1 protein
 Superoxide dismutase
 Phospholipase D1
 Phospholipase A2
 Cell cycle control protein 50A
 Glutamate decarboxylase 1
 Lysophosphatidic acid receptor 1
 Arachidonate 5-lipoxygenase
 Lysophosphatidic acid receptor 3
 Proteasome subunit beta type-2
 Phospholipid-transporting ATPase IA
 Methylenetetrahydrofolate reductase
 Phospholipid-transporting ATPase IB
 Bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase
 Probable bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase 2
 Geminin
 Prelamin-A/C
 Ferritin light chain
 Luciferin 4-monooxygenase
 Cruzipain Trypanosoma cruzi
 Histone acetyltransferase KAT2A
 Platelet-activating factor receptor
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

Predicted Targets

Interleukin-1 beta
 Arachidonate 5-lipoxygenase
 Matrix metalloproteinase-9
 Vascular endothelial growth factor A

Caspase-1

Caspase-3

Cytochrome c

Cytochrome P450 1A2
 Protein kinase C alpha type
 Cytochrome P450 3A4
 Cytochrome P450 2D6

Cytochrome P450 2C9
Interferon regulatory factor 1
Cytochrome P450 2C19
Proteinase-activated receptor 2
Protein-arginine deiminase type-4
Serum albumin
Beta-2 adrenergic receptor
Beta-1 adrenergic receptor
Beta-3 adrenergic receptor
Multidrug transporter MdfA
Acetylcholinesterase
Cholinesterase

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

Predicted Targets

Cytochrome P450 2C19
Multidrug resistance protein 1

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

**platelet-derived growth factor receptors (PDGFR) inhibitor
proto-oncogene c-Kit inhibitor**

Predicted Targets

Proto-oncogene tyrosine-protein kinase Src
Serine/threonine-protein kinase N2
Protein kinase C theta type
cGMP-dependent protein kinase 2
Serine/threonine-protein kinase 3
Serine/threonine-protein kinase 4
Dual specificity testis-specific protein kinase 1
Tyrosine-protein kinase receptor TYRO3
Serine/threonine-protein kinase VRK2
Mitogen-activated protein kinase kinase kinase 12
Serine/threonine-protein kinase 25
Mitogen-activated protein kinase kinase kinase kinase 5
Mitogen-activated protein kinase kinase kinase 2
Serine/threonine-protein kinase PLK2
Serine/threonine-protein kinase pim-2
Citron Rho-interacting kinase
Serine/threonine-protein kinase 38
Serine/threonine-protein kinase Nek1
Serine/threonine-protein kinase tousled-like 1

Cyclin-dependent kinase 14
Phosphatidylinositol 4-phosphate 5-kinase type-1 gamma
STE20/SPS1-related proline-alanine-rich protein kinase
Serine/threonine-protein kinase TBK1
Serine/threonine-protein kinase Sgk3
Inhibitor of nuclear factor kappa-B kinase subunit epsilon
Insulin receptor-related protein
Serine/threonine-protein kinase PLK4
Death-associated protein kinase 2
Serine/threonine-protein kinase Nek6
Eukaryotic translation initiation factor 2-alpha kinase 1
Ribosomal protein S6 kinase alpha-6
Serine/threonine-protein kinase LATS2
Hormonally up-regulated neu tumor-associated kinase
STE20-like serine/threonine-protein kinase
Maternal embryonic leucine zipper kinase
NUAK family SNF1-like kinase 1
Serine/threonine-protein kinase ICK
Microtubule-associated serine/threonine-protein kinase 1
Serine/threonine-protein kinase 38-like
TRAF2 and NCK-interacting protein kinase
Cyclin-dependent kinase 19
Serine/threonine-protein kinase SIK2
Serine/threonine-protein kinase 36
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase TAO2
Serine/threonine-protein kinase NLK
Serine/threonine-protein kinase MST4
Myosin-IIIa
Serine/threonine-protein kinase MARK2
MAP kinase-interacting serine/threonine-protein kinase 2
BMP-2-inducible protein kinase
Transient receptor potential cation channel subfamily M member 6
SNF-related serine/threonine-protein kinase
Serine/threonine-protein kinase RIO2
Serine/threonine-protein kinase 32B
Serine/threonine-protein kinase MARK1
Glycogen synthase kinase-3 alpha
Serine/threonine-protein kinase PAK 6
Chaperone activity of bcl complex-like
Serine/threonine-protein kinase PAK 7
Calcium/calmodulin-dependent protein kinase type 1D
Calcium/calmodulin-dependent protein kinase type 1G
Proto-oncogene tyrosine-protein kinase receptor Ret
Receptor-interacting serine/threonine-protein kinase 4
Ribosomal protein S6 kinase alpha-2
Casein kinase I isoform gamma-1
Homeodomain-interacting protein kinase 2
Fibroblast growth factor receptor 4
Fibroblast growth factor receptor 2

Fibroblast growth factor receptor 1
AarF domain-containing protein kinase 4
Mitogen-activated protein kinase kinase kinase 19
Dual specificity mitogen-activated protein kinase kinase 2
Serine/threonine-protein kinase 33
NUAK family SNF1-like kinase 2
MAP/microtubule affinity-regulating kinase 4
Serine/threonine-protein kinase RIO1
Testis-specific serine/threonine-protein kinase 1
Calcium/calmodulin-dependent protein kinase kinase 1
Activated CDC42 kinase 1
High affinity nerve growth factor receptor
Myosin light chain kinase family member 4
Serine/threonine-protein kinase PAK 4
Serine/threonine-protein kinase SBK1
Receptor tyrosine-protein kinase erbB-4
Wee1-like protein kinase 2
Uncharacterized serine/threonine-protein kinase SBK3
Dual serine/threonine and tyrosine protein kinase
Cell division control protein 2 homolog
Tyrosine-protein kinase ABL1
RAC-alpha serine/threonine-protein kinase
Epidermal growth factor receptor
Mitogen-activated protein kinase 12
Tyrosine-protein kinase Mer
Aurora kinase C
Serine/threonine-protein kinase tousled-like 2
5'-AMP-activated protein kinase catalytic subunit alpha-1
Serine/threonine-protein kinase SIK3
Serine/threonine-protein kinase 16
Cyclin-dependent kinase 17
Serine/threonine-protein kinase receptor R3
Tyrosine-protein kinase BTK
Cyclin-dependent kinase 4
Tyrosine-protein kinase JAK3
Hepatocyte growth factor receptor
Phosphorylase b kinase gamma catalytic chain
Serine/threonine-protein kinase STK11
Insulin-like growth factor 1 receptor
Mitogen-activated protein kinase kinase kinase 15
Serine/threonine-protein kinase pim-3
Serine/threonine-protein kinase Chk2
Receptor tyrosine-protein kinase erbB-2
Casein kinase I isoform gamma-3
Myotonin-protein kinase
Ephrin type-A receptor 7
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit gamma
Mitogen-activated protein kinase kinase kinase 2
Ribosomal protein S6 kinase alpha-3
TGF-beta receptor type-1

Mitogen-activated protein kinase kinase kinase 6
Serine/threonine-protein kinase LATS1
Dual specificity tyrosine-phosphorylation-regulated kinase 1B
Serine/threonine-protein kinase DCLK1
Ribosomal protein S6 kinase alpha-5
Cyclin-dependent kinase 5
Serine/threonine-protein kinase mTOR
Tyrosine-protein kinase JAK2
Phosphatidylinositol 4
Serine/threonine-protein kinase PLK1
cAMP-dependent protein kinase catalytic subunit PRKX
Serine/threonine-protein kinase OSR1
MAP kinase-activated protein kinase 2
Serine/threonine-protein kinase Nek9
Myosin light chain kinase 2
Mitogen-activated protein kinase kinase kinase 9
Serine/threonine-protein kinase DCLK3
Cyclin-dependent kinase 11B
Tyrosine-protein kinase Srms
Serine/threonine-protein kinase 35
Dual specificity tyrosine-phosphorylation-regulated kinase 1A
Serine/threonine-protein kinase Nek7
Mitogen-activated protein kinase 1
Mitogen-activated protein kinase 15
Cyclin-dependent kinase 15
G protein-coupled receptor kinase 7
Homeodomain-interacting protein kinase 4
Dual specificity mitogen-activated protein kinase kinase 7
Casein kinase I isoform alpha-like
Mitogen-activated protein kinase kinase kinase 7
Mitogen-activated protein kinase kinase kinase kinase 4
Serine/threonine-protein kinase NIM1
Focal adhesion kinase 1
Calcium/calmodulin-dependent protein kinase type II subunit gamma
Protein-tyrosine kinase 2-beta
Serine/threonine-protein kinase SIK1
Serine/threonine-protein kinase 32C
Ankyrin repeat and protein kinase domain-containing protein 1
Myosin light chain kinase 3
Membrane-associated tyrosine- and threonine-specific cdc2-inhibitory kinase
Leucine-rich repeat serine/threonine-protein kinase 2
Serine/threonine-protein kinase Nek5
Leukocyte tyrosine kinase receptor
Tyrosine-protein kinase ZAP-70
Serine/threonine-protein kinase N1
Tyrosine-protein kinase Fer
Protein kinase C epsilon type
Rho-associated protein kinase 1
RAC-gamma serine/threonine-protein kinase
Tyrosine-protein kinase ITK/TSK

LIM domain kinase 2
Muscle
Homeodomain-interacting protein kinase 3
Serine/threonine-protein kinase D3
Serine/threonine-protein kinase MAK
Mitogen-activated protein kinase kinase kinase 1
Mitogen-activated protein kinase kinase kinase 5
Protein-tyrosine kinase 6
Cyclin-dependent kinase 16
5'-AMP-activated protein kinase catalytic subunit alpha-2
Protein kinase C delta type
Serine/threonine-protein kinase ULK3
Activin receptor type-1
Activin receptor type-2B
Serine/threonine-protein kinase 32A
Cyclin-dependent kinase-like 3
MAP kinase-interacting serine/threonine-protein kinase 1
Phosphatidylinositol 4-phosphate 5-kinase type-1 alpha
Bone morphogenetic protein receptor type-1B
Bone morphogenetic protein receptor type-2
Cyclin-dependent kinase 3
Cyclin-dependent kinase 8
Cyclin-dependent kinase 9
Casein kinase I isoform gamma-2
Death-associated protein kinase 3
Serine/threonine-protein kinase/endoribonuclease IRE1
Inhibitor of nuclear factor kappa-B kinase subunit beta
Interleukin-1 receptor-associated kinase 1
Activin receptor type-2A
RAC-beta serine/threonine-protein kinase
Tyrosine-protein kinase receptor UFO
Cytoplasmic tyrosine-protein kinase BMX
Calcium/calmodulin-dependent protein kinase type IV
Cyclin-dependent kinase 2
Cyclin-dependent kinase 7
Casein kinase I isoform alpha
Casein kinase I isoform epsilon
Casein kinase II subunit alpha
Casein kinase II subunit alpha'
Receptor tyrosine-protein kinase erbB-3
Tyrosine-protein kinase Fes/Fps
Vascular endothelial growth factor receptor 1
Vascular endothelial growth factor receptor 3
Glycogen synthase kinase-3 beta
Vascular endothelial growth factor receptor 2
LIM domain kinase 1
Megakaryocyte-associated tyrosine-protein kinase
Mitogen-activated protein kinase kinase kinase 3
Mitogen-activated protein kinase kinase kinase 11
Mitogen-activated protein kinase kinase kinase 10

Serine/threonine-protein kinase Nek2
Serine/threonine-protein kinase Nek3
Serine/threonine-protein kinase PAK 1
Serine/threonine-protein kinase PAK 2
Serine/threonine-protein kinase PAK 3
Cyclin-dependent kinase 18
3-phosphoinositide-dependent protein kinase 1
Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit beta
Serine/threonine-protein kinase pim-1
Phosphatidylinositol 4-kinase beta
cAMP-dependent protein kinase catalytic subunit alpha
cAMP-dependent protein kinase catalytic subunit beta
Protein kinase C iota type
Serine/threonine-protein kinase D1
Mitogen-activated protein kinase 3
Mitogen-activated protein kinase 4
Mitogen-activated protein kinase 6
Mitogen-activated protein kinase 7
Mitogen-activated protein kinase 13
Dual specificity mitogen-activated protein kinase kinase 1
Dual specificity mitogen-activated protein kinase kinase 3
Dual specificity mitogen-activated protein kinase kinase 6
Interferon-induced
Rhodopsin kinase
Proto-oncogene tyrosine-protein kinase ROS
Ribosomal protein S6 kinase alpha-1
Dual specificity mitogen-activated protein kinase kinase 4
SRSF protein kinase 1
Serine/threonine-protein kinase Nek4
Cyclin-dependent kinase-like 5
Ribosomal protein S6 kinase beta-1
Tyrosine-protein kinase SYK
Tyrosine-protein kinase Tec
TGF-beta receptor type-2
Dual specificity protein kinase TTK
Tyrosine-protein kinase TXK
Non-receptor tyrosine-protein kinase TYK2
Wee1-like protein kinase
Phosphatidylinositol 5-phosphate 4-kinase type-2 beta
Serine/threonine-protein kinase 24
Dual specificity tyrosine-phosphorylation-regulated kinase 2
Aurora kinase A
Serine/threonine-protein kinase MRCK alpha
Calcium/calmodulin-dependent protein kinase type 1
MAP kinase-activated protein kinase 5
Peripheral plasma membrane protein CASK
Cyclin-dependent kinase 13
Receptor-interacting serine/threonine-protein kinase 1
Receptor-interacting serine/threonine-protein kinase 2
Serine/threonine-protein kinase RIO3

Serine/threonine-protein kinase PRP4 homolog
Cyclin-dependent kinase-like 2
Serine/threonine-protein kinase BRSK2
Non-receptor tyrosine-protein kinase TNK1
Dual specificity protein kinase CLK3
Dual specificity protein kinase CLK2
Serine/threonine-protein kinase PLK3
Receptor-type tyrosine-protein kinase FLT3
Cyclin-dependent kinase-like 1
Serine/threonine-protein kinase 17B
Activin receptor type-1B
ALK tyrosine kinase receptor
Bone morphogenetic protein receptor type-1A
G protein-coupled receptor kinase 4

Mast/stem cell growth factor receptor Kit

Cytochrome P450 3A4
Cytochrome P450 2C8
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2B6
Multidrug resistance protein 1
UDP-glucuronosyltransferase 1-1

Platelet-derived growth factor receptor alpha

Platelet-derived growth factor receptor beta
Epithelial discoidin domain-containing receptor 1
Discoidin domain-containing receptor 2
Macrophage colony-stimulating factor 1 receptor
RAF proto-oncogene serine/threonine-protein kinase
Tyrosine-protein kinase Lyn
Tyrosine-protein kinase Lck
Serine/threonine-protein kinase TAO3
Ephrin type-B receptor 2
Ephrin type-A receptor 8
Dual specificity protein kinase CLK4
Serine/threonine-protein kinase TAO1
Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma
Mitogen-activated protein kinase kinase kinase 1
Ephrin type-A receptor 6
Abelson tyrosine-protein kinase 2
Dual specificity protein kinase CLK1
NT-3 growth factor receptor
Angiopoietin-1 receptor
Tyrosine-protein kinase CSK
Ephrin type-A receptor 2
Ephrin type-A receptor 4
Ephrin type-B receptor 3
Ephrin type-B receptor 4
Ephrin type-B receptor 6
Mitogen-activated protein kinase 14
Mitogen-activated protein kinase 9

Dual specificity mitogen-activated protein kinase kinase 5
Tyrosine-protein kinase Fyn
Ephrin type-A receptor 5
Ephrin type-A receptor 3
Tyrosine-protein kinase Fgr
Tyrosine-protein kinase receptor Tie-1
Tyrosine-protein kinase Yes
Serine/threonine-protein kinase 10
Serine/threonine-protein kinase MRCK beta
BDNF/NT-3 growth factors receptor
Tyrosine-protein kinase Blk
Tyrosine-protein kinase FRK
Tyrosine-protein kinase HCK
Mitogen-activated protein kinase 8
Mitogen-activated protein kinase 11
Mitogen-activated protein kinase 10
Serine/threonine-protein kinase B-raf
Integral membrane protein DGCR2/IDD
Carbonic anhydrase 12
Low-density lipoprotein receptor-related protein 3
ATP-binding cassette sub-family G member 2
Pro-low-density lipoprotein receptor-related protein 1
Low-density lipoprotein receptor-related protein 6
CDK5 and ABL1 enzyme substrate 1
Sortilin-related receptor
Insulin receptor
Low-density lipoprotein receptor-related protein 2
Cysteine-rich hydrophobic domain-containing protein 2
Pro-epidermal growth factor
Programmed cell death protein 4
Ephrin type-A receptor 1
Low-density lipoprotein receptor-related protein 12
Low-density lipoprotein receptor-related protein 8
Low-density lipoprotein receptor-related protein 5
Carbonic anhydrase 2
Carbonic anhydrase 3
Signal transducer and activator of transcription 5B
Breakpoint cluster region protein
Blood group Rh
Carbonic anhydrase 4
CD320 antigen
Envoplakin
Low-density lipoprotein receptor class A domain-containing protein 3
Carbonic anhydrase 5A
Hematopoietic progenitor cell antigen CD34
Aurora kinase B
Carbonic anhydrase 5B
Serine hydroxymethyltransferase
Carbonic anhydrase 13
Lysine--tRNA ligase

Serine/threonine-protein kinase haspin
Single-strand selective monofunctional uracil DNA glycosylase
Pre-mRNA 3'-end-processing factor FIP1
Carbonic anhydrase 7
Growth factor receptor-bound protein 2
Signal transducer and activator of transcription 5A
Crk-like protein
Low-density lipoprotein receptor-related protein 10
Solute carrier family 22 member 1
Carbonic anhydrase 14
Ephrin type-B receptor 1
Carbonic anhydrase 6
Mitogen-activated protein kinase kinase kinase MLT
Low-density lipoprotein receptor-related protein 4
Carbonic anhydrase 9
Very low-density lipoprotein receptor
Low-density lipoprotein receptor-related protein 1B
Carbonic anhydrase 1
Carbonic anhydrase 15
Carbonic anhydrase 13
Serine/threonine-protein kinase Chk1
Cyclin-G-associated kinase
Inhibitor of nuclear factor kappa-B kinase subunit alpha
Mitogen-activated protein kinase kinase kinase 13
Rho-associated protein kinase 2
Serine/threonine-protein kinase ULK1
Ribosomal protein S6 kinase alpha-4
Fibroblast growth factor receptor 3
Tyrosine-protein kinase JAK1
Protein kinase C eta type
MAP/microtubule affinity-regulating kinase 3
Casein kinase I isoform delta
Death-associated protein kinase 1
Calcium-dependent protein kinase 1
SRSF protein kinase 2
Serine/threonine-protein kinase PknB
Macrophage-stimulating protein receptor
Calcium/calmodulin-dependent protein kinase type II subunit beta
Calcium/calmodulin-dependent protein kinase type II subunit delta
cGMP-dependent protein kinase 1
Myosin light chain kinase
AP2-associated protein kinase 1
Serine/threonine-protein kinase TNNI3K
Serine/threonine-protein kinase MRCK gamma
Homeodomain-interacting protein kinase 1
Mitogen-activated protein kinase kinase kinase kinase 3
Serine/threonine-protein kinase ULK2
Misshapen-like kinase 1
Serine/threonine-protein kinase DCLK2
Serine/threonine-protein kinase Nek1 1

Serine/threonine-protein kinase BRSK1
Myosin-IIIb
Calcium/calmodulin-dependent protein kinase kinase 2
Serine/threonine-protein kinase D2
Eukaryotic translation initiation factor 2-alpha kinase 4
Serine/threonine-protein kinase 17A
SRSF protein kinase 3
Cyclin-dependent kinase 11A
Calcium/calmodulin-dependent protein kinase type II subunit alpha
Interleukin-1 receptor-associated kinase 3
Mitogen-activated protein kinase kinase kinase 4

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Predicted Targets

4-hydroxyphenylpyruvate dioxygenase

DNA ligase 1
Mitogen-activated protein kinase 1
WD repeat-containing protein 59
Copper-transporting ATPase 2
Fumarylacetoacetase
Tryptophan 5-hydroxylase 1
WD repeat-containing protein 73
Tryptophan 5-hydroxylase 2
Homogentisate 1
Sucrase-isomaltase
Hepatocyte nuclear factor 4-alpha
Delta-aminolevulinic acid dehydratase
DDB1- and CUL4-associated factor 10
Copper-transporting ATPase 1
Histone-binding protein RBBP4
Hepatocyte nuclear factor 4-gamma
Histone-binding protein RBBP7
Tyrosine 3-monooxygenase

Paclitaxel

Molecular Mechanism (initial) :

tubulin beta modulator (microtubule-stabilizing agent)

Molecular Mechanism (repurposed) :

tubulin beta modulator (microtubule-stabilizing agent)

Predicted Targets

Apoptosis regulator Bcl-2
Nuclear receptor subfamily 1 group I member 2
Microtubule-associated protein 4
Microtubule-associated protein 2

Microtubule-associated protein tau
Cytochrome P450 2C9
Cytochrome P450 3A5
Cytochrome P450 3A7
Cytochrome P450 2C8
Cytochrome P450 3A4
Aromatase
Cytochrome P450 1B1
Bile salt export pump
Multidrug resistance protein 1
Multidrug resistance-associated protein 1
Canalicular multispecific organic anion transporter 1

Tubulin beta chain

Botulinum neurotoxin type A
Integrin beta-3

Tubulin alpha-1A chain

Tubulin beta-2B chain

Similar to alpha-tubulin isoform 1
Menin
Niemann-Pick C1 protein
Geminin
Ubiquitin carboxyl-terminal hydrolase 2
Isocitrate dehydrogenase cytoplasmic
Thioredoxin reductase 1
Ubiquitin carboxyl-terminal hydrolase 1
Beta-lactamase
Prelamin-A/C
Estrogen receptor
Glucocorticoid receptor
Cellular tumor antigen p53
Luciferin 4-monooxygenase
Androgen receptor
Thyroid hormone receptor beta
Vitamin D3 receptor
Lethal factor Bacillus anthracis
Retinoic acid receptor RXR-alpha
Peripheral myelin protein 22
Cruzipain Trypanosoma cruzi
Peroxisome proliferator-activated receptor gamma
Alpha-synuclein
Thrombopoietin
Serine/threonine-protein kinase mTOR
ATP-dependent DNA helicase Q1
Regulator of G-protein signaling 4
Ras-related protein Rab-9A
Nuclear receptor ROR-gamma
Bloom syndrome protein
Chromobox protein homolog 1
Mothers against decapentaplegic homolog 3
Histone-lysine N-methyltransferase 2A

Peroxisome proliferator-activated receptor delta
Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
Nuclear factor erythroid 2-related factor 2
Survival motor neuron protein
Hypoxia-inducible factor 1-alpha
Nonstructural protein
Neuropeptide S receptor
ATPase family AAA domain-containing protein 5
Ataxin-2
3-hydroxyacyl-CoA dehydrogenase type-2
4'-phosphopantetheinyl transferase ffp
Cytochrome P450 1A2

Tubulin beta-4A chain

Tubulin beta chain

Tubulin alpha-1B chain

Tubulin alpha-4A chain

Tubulin beta-4B chain

Tubulin beta-3 chain

Tubulin alpha-3C/D chain

Tubulin beta-2A chain

Tubulin beta-8 chain

Tubulin alpha-3E chain

Tubulin alpha-1A chain

Tubulin alpha-1C chain

Tubulin beta-6 chain

Tubulin beta-1 chain

Substance-K receptor

Cholecystokinin receptor type A

Melanocortin receptor 5

Delta-type opioid receptor

NS3 Hepatitis C virus

Receptor tyrosine-protein kinase erbB-2

Tyrosine-protein kinase Fyn

Integrin alpha-V

Beta-tubulin Leishmania donovani

Cholinesterase

Solute carrier family 22 member 1

Acetylcholinesterase

Solute carrier organic anion transporter family member 2B1

Solute carrier organic anion transporter family member 1B3

Solute carrier organic anion transporter family member 1B1

Multidrug resistance-associated protein 7

Phentolamine mesilate

Molecular Mechanism (initial) :

alpha-adrenoceptor antagonist

Molecular Mechanism (repurposed) :

alpha-adrenoceptor antagonist

Predicted Targets

Sphingosine 1-phosphate receptor 3

Alpha-2A adrenergic receptor

Alpha-1A adrenergic receptor

5-hydroxytryptamine receptor 1A

5-hydroxytryptamine receptor 1E

Estrogen receptor beta

Histamine H1 receptor

Sigma non-opioid intracellular receptor 1

Amine oxidase A

Nischarin

Fibroblast growth factor 1

Cholecystokinin

Calcitonin

Sulfotransferase 1A1

Protachykinin-1

Renin

Kininogen-1

Pro-neuropeptide Y

kinase isozyme 2

kinase isozyme 4

Glucocorticoid receptor

Pancreatic prohormone

Pro-opiomelanocortin

Transmembrane protein 127

Neurotensin/neuromedin N

5-hydroxytryptamine receptor 2B

Kinesin-like protein KIF1B

Heat-stable enterotoxin receptor

Potassium voltage-gated channel subfamily H member 2

Beta-1 adrenergic receptor

Glial cell line-derived neurotrophic factor

Alpha-1B adrenergic receptor

5-hydroxytryptamine receptor 2C

kinase isozyme 1

Progonadoliberein-1

Corticoliberin

Beta-2 adrenergic receptor

Serum albumin

Somatostatin

Angiotensin-converting enzyme

Pro-thyrotropin-releasing hormone

Integrin alpha-2

Atrial natriuretic peptide receptor 1

Insulin

Adenylate cyclase type 2

Caspase-3

5-hydroxytryptamine receptor 3A

cGMP-specific 3'

Succinate dehydrogenase cytochrome b560 subunit

Catechol O-methyltransferase

Dynein heavy chain 8
Adenylate cyclase type 10
VIP peptides
Osteopontin
Alpha-1D adrenergic receptor
Succinate dehydrogenase cytochrome b small subunit
5-hydroxytryptamine receptor 1B
Succinate dehydrogenase iron-sulfur subunit
5-hydroxytryptamine receptor 2A
Natriuretic peptides A
Amine oxidase B
Dopamine beta-hydroxylase
Vasopressin-neurophysin 2-copeptin
Chorion-specific transcription factor GCMb
Inosine triphosphate pyrophosphatase
Tyrosine 3-monooxygenase
Pirin
Histone-lysine N-methyltransferase EHMT1
Neuropeptide S
Alpha-2C adrenergic receptor
Ubiquitin-60S ribosomal protein L40
kinase isozyme 3
Glucagon
Alpha-2B adrenergic receptor
Lysine-specific demethylase 4A
Glutaminase kidney isoform
Prelamin-A/C
Cytochrome P450 2D6
Regulator of G-protein signaling 4
ATP-dependent Clp protease proteolytic subunit
Chromobox protein homolog 1
Histone-lysine N-methyltransferase EHMT2
ATPase family AAA domain-containing protein 5
Ataxin-2
4'-phosphopantetheinyl transferase ffp Bacillus subtilis
Bromodomain adjacent to zinc finger domain protein 2B
DNA polymerase iota
Cytochrome P450 2C19
Heat shock factor protein 1
Alpha-1A adrenergic receptor
Alpha-2A adrenergic receptor
Sodium channel protein type 1 subunit alpha
Sodium channel protein type 2 subunit alpha
Sodium channel protein type 3 subunit alpha
Uncharacterized protein
5-hydroxytryptamine receptor 2A

Raloxifene hydrochloride

Molecular Mechanism (initial) :
estrogen receptor agonist

Molecular Mechanism (repurposed) :
estrogen receptor agonist

Predicted Targets

Bcl-2-related protein A1

Cruzipain Trypanosoma cruzi

Nuclear receptor subfamily 1 group I member 2

Estrogen sulfotransferase

Estrogen receptor

Estrogen receptor beta

Cytochrome P450 2B6

Cytochrome P450 2C8

Aldehyde oxidase

Aromatase

Cytochrome P450 3A4

Cytochrome P450 1A2

Interleukin-6 receptor subunit alpha

Cytochrome P450 2D6

Cytochrome P450 2C19

Interleukin-6 receptor subunit beta

Ubiquitin-conjugating enzyme E2 N

Aldehyde oxidase 1

Bile acid receptor

Leukotriene A-4 hydrolase

25-hydroxyvitamin D-1 alpha hydroxylase

Carbonic anhydrase 12

Asparagine synthetase

Granulins

Oxysterol-binding protein-related protein 7

Ras-related protein Ral-A

Interferon-related developmental regulator 1

Interleukin-10 receptor subunit alpha

Pro-cathepsin H

Carboxypeptidase B2

HEAT repeat-containing protein 6

60S ribosomal protein L6

Protein phosphatase 1 regulatory subunit 15A

Apoptosis-stimulating of p53 protein 1

Metalloproteinase inhibitor 1

Eukaryotic translation initiation factor 5

Mitogen-activated protein kinase 1

Heme oxygenase 1

Oxytocin-neurophysin 1

NF-kappa-B inhibitor alpha

Aurora kinase A

G1/S-specific cyclin-D1

Plasminogen activator inhibitor 1

Tissue-type plasminogen activator

Vesicular glutamate transporter 1

Syntaxin-1A

Hepcidin
HMG box-containing protein 1
Heat shock cognate 71 kDa protein
Granulocyte colony-stimulating factor
Nuclear respiratory factor 1
Myosin-1
Chromobox protein homolog 1
C-C motif chemokine 2
Ubiquitin carboxyl-terminal hydrolase 32
Tryptophan 5-hydroxylase 1
Transforming growth factor beta-3
Guanine nucleotide-binding protein subunit beta-4
Vitamin D3 receptor
Cyclin-dependent kinase inhibitor 1B
Matrix Gla protein
B-cell lymphoma 6 protein
Phosphatidylinositol-glycan-specific phospholipase D
Growth hormone receptor
Tumor necrosis factor alpha-induced protein 3
Protein GREB1
Tissue factor pathway inhibitor
Vitamin K-dependent protein C
Chloride transport protein 6
Delta-type opioid receptor
Myoblast determination protein 1
Uracil-DNA glycosylase
T-box transcription factor TBX2
Tumor necrosis factor ligand superfamily member 11
Dual specificity protein phosphatase 4
DNA-directed DNA/RNA polymerase mu
Condensin complex subunit 2
UAP56-interacting factor
DnaJ homolog subfamily B member 9
Nuclear receptor subfamily 4 group A member 1
Dynein light chain 1
Kelch-like protein 24
Ras-related protein Rab-40C
Metallothionein-2
Complement C3
Threonine--tRNA ligase
Cytochrome P450 2C9
G2/mitotic-specific cyclin-B1
Coagulation factor XII
Protocadherin gamma-C5
Eukaryotic translation initiation factor 2 subunit 1
DnaJ homolog subfamily B member 1
C-reactive protein
5-hydroxytryptamine receptor 2B
Sodium-coupled neutral amino acid transporter 2
Asparagine--tRNA ligase

Thrombospondin-1
Interleukin-6
Serine/arginine-rich splicing factor 1
Stanniocalcin-2
RNA polymerase II elongation factor ELL
Sodium-dependent serotonin transporter
Activating transcription factor 7-interacting protein 1
von Willebrand factor
Ras-related protein Rab-2A
Transcription elongation factor B polypeptide 2
E3 ubiquitin-protein ligase SMURF2
DNA mismatch repair protein Msh3
Phospholipase D2
Mitogen-activated protein kinase 3
Mitogen-activated protein kinase kinase kinase 8
Activated RNA polymerase II transcriptional coactivator p15
Interleukin-1 alpha
Rho-related GTP-binding protein RhoE
Ribonucleoside-diphosphate reductase large subunit
Parathyroid hormone
Tumor necrosis factor receptor superfamily member 11A
Mismatch repair endonuclease PMS2
Kappa-type opioid receptor
Lymphoid enhancer-binding factor 1
Semaphorin-3A
Disintegrin and metalloproteinase domain-containing protein 22
Galanin peptides
Multidrug resistance protein 1
Zinc transporter ZIP6
Golgi to ER traffic protein 4 homolog
Lamina-associated polypeptide 2
Nuclear receptor corepressor 1
Retinoblastoma-associated protein
Ras GTPase-activating-like protein IQGAP1
Cystine/glutamate transporter
Epidermal growth factor receptor
RAC-alpha serine/threonine-protein kinase
Receptor tyrosine-protein kinase erbB-2
Superoxide dismutase
Platelet-activating factor acetylhydrolase
Sodium-dependent dopamine transporter
Cyclin-A2
Alpha-2A adrenergic receptor
5-hydroxytryptamine receptor 2C
Ephrin type-A receptor 1
Rod outer segment membrane protein 1
Progonadoliberin-1
Sigma non-opioid intracellular receptor 1
Homocysteine-responsive endoplasmic reticulum-resident ubiquitin-like domain member 1 protein
Scaffold attachment factor B1

Dual specificity protein phosphatase 2
Dickkopf-related protein 2
cGMP-inhibited 3'
Heterogeneous nuclear ribonucleoprotein U
Unconventional myosin-Ie
Sulfate transporter
Peroxisome proliferator-activated receptor gamma
Trefoil factor 1
Zinc transporter ZIP14
Pro-neuregulin-2
5-hydroxytryptamine receptor 6
Importin subunit beta-1
Angiotensin-converting enzyme
PCNA-associated factor
Brachyury protein
Alkaline phosphatase
Protransforming growth factor alpha
Nucleophosmin
26S proteasome non-ATPase regulatory subunit 6
Integrin alpha-2
Endoplasmin
Nitric oxide synthase
Tumor necrosis factor receptor superfamily member 11B
G-protein coupled estrogen receptor 1
Plasminogen activator inhibitor 2
Protein DEPP
Creatine kinase B-type
DNA topoisomerase 1
PRKC apoptosis WT1 regulator protein
DNA-directed RNA polymerase II subunit RPB2
Aryl hydrocarbon receptor nuclear translocator 2
Fatty acid synthase
Heat shock 70 kDa protein 4
Prolactin
Insulin-like growth factor I
Acetylcholinesterase
Interleukin-12 subunit alpha
Protein phosphatase 1D
CCAAT/enhancer-binding protein beta
UDP-glucuronosyltransferase 2B7
Zinc finger X-chromosomal protein
Elongation of very long chain fatty acids protein 5
D
Proto-oncogene c-Fos
Leptin
Ubiquitin-protein ligase E3C
Matrix metalloproteinase-14
Calretinin
5-hydroxytryptamine receptor 1E
Bcl2-associated agonist of cell death

Prothrombin
Multiple C2 and transmembrane domain-containing protein 1
Dystroglycan
Rac GTPase-activating protein 1
Telomerase reverse transcriptase
Mitogen-activated protein kinase kinase kinase 11
Prostaglandin reductase 1
Tumor necrosis factor receptor superfamily member 10D
Caspase-3
Interstitial collagenase
Hepatocyte nuclear factor 4-alpha
DNA-dependent protein kinase catalytic subunit
Clusterin
Cyclin-G2
Proteinase-activated receptor 1
Zinc finger E-box-binding homeobox 1
5-hydroxytryptamine receptor 1A
Plexin-D1
Nuclear receptor coactivator 1
CD276 antigen
Solute carrier family 2
Golgin-45
Serine/arginine-rich splicing factor 7
5-hydroxytryptamine receptor 1F
Heat shock protein HSP 90-beta
Progesterone receptor
Protein Wnt-11
Macrophage colony-stimulating factor 1
Nuclear receptor ROR-gamma
Phorbol-12-myristate-13-acetate-induced protein 1
Dual specificity protein kinase CLK1
Biglycan
Transcription factor Maf
Filamin-C
Signal transducer and activator of transcription 1-alpha/beta
Adenosine receptor A2a
Pappalysin-1
Trafficking kinesin-binding protein 2
Coatomer subunit beta'
Suppressor of cytokine signaling 3
Apoptosis regulator Bcl-2
Heat shock protein HSP 90-alpha
Semaphorin-4B
Calcitonin
Growth arrest-specific protein 6
Probable G-protein coupled receptor 125
Importin subunit alpha-1
Metastasis-associated protein MTA1
60 kDa heat shock protein
Serine/threonine-protein kinase PRP4 homolog

Transportin-1
Chromobox protein homolog 3
Eukaryotic translation initiation factor 5A-1
Histone H3-like centromeric protein A
ATP-dependent RNA helicase DDX3Y
Angiogenin
Urokinase plasminogen activator surface receptor
5-hydroxytryptamine receptor 7
Caveolin-1
Mucin-1
Carboxypeptidase M
Matrin-3
Nuclear receptor corepressor 2
Apolipoprotein D
Endoribonuclease Dicer
Acidic mammalian chitinase
Phospholipase D1
Insulin-induced gene 1 protein
Cyclic AMP-dependent transcription factor ATF-3
Ras-related C3 botulinum toxin substrate 1
Heterogeneous nuclear ribonucleoproteins A2/B1
CMP-N-acetylneuraminate-beta-galactosamide-alpha-2
Endothelial transcription factor GATA-2
cGMP-specific 3'
Fibronectin
GA-binding protein alpha chain
Coagulation factor VIII
Breast cancer type 1 susceptibility protein
Protein SON
Ras-related protein Rap-1A
Phospholipase D3
Testican-3
Insulin
Heterogeneous nuclear ribonucleoprotein H
Transferrin receptor protein 1
NKG2-A/NKG2-B type II integral membrane protein
Neurofibromin
Peptide YY
ETS-related transcription factor Elf-3
Unconventional myosin-Ic
NKG2-E type II integral membrane protein
Chloride intracellular channel protein 4
Deleted in malignant brain tumors 1 protein
Thrombospondin-2
Paired box protein Pax-2
Caldesmon
Conserved oligomeric Golgi complex subunit 2
Transcription factor E2F2
Tyrosine-protein kinase Fyn
Osteocalcin

Prostaglandin G/H synthase 2
ATP-dependent RNA helicase A
Antigen KI-67
Nogo-B receptor
Tumor necrosis factor ligand superfamily member 15
DnaJ homolog subfamily B member 4
Ubiquitin-like protein 4A
5-hydroxytryptamine receptor 1B
Delta
Syntaxin-16
Transcription factor AP-1
Uncharacterized protein C6orf106
Matrix metalloproteinase-9
Nuclear receptor coactivator 3
Substance-K receptor
Urokinase-type plasminogen activator
Endoglin
Insulin-like growth factor-binding protein 3
Bcl-2 homologous antagonist/killer
Mitogen-activated protein kinase kinase kinase MLT
Tumor necrosis factor receptor superfamily member 25
Wiskott-Aldrich syndrome protein
Ras and EF-hand domain-containing protein
Methylenetetrahydrofolate reductase
RNA-binding protein 10
Angiopoietin-related protein 7
Calsyntenin-1
Homeobox protein Nkx-3.1
Alpha-1D adrenergic receptor
Nuclear pore complex protein Nup160
Neuroblast differentiation-associated protein AHNAK
Tumor protein p73
Xanthine dehydrogenase/oxidase
5-hydroxytryptamine receptor 2A
Proliferating cell nuclear antigen
Sex hormone-binding globulin
Sodium-dependent noradrenaline transporter
Cytochrome P450 1A1
DnaJ homolog subfamily A member 1
Interferon alpha-2
Histone-binding protein RBBP7
Breast cancer type 2 susceptibility protein
Integrator complex subunit 11
cAMP-specific 3'
Serine/threonine-protein kinase TAO3
Spermatogenesis-associated protein 13
Zinc finger protein 222
Transcription factor p65
Aminoacyl tRNA synthase complex-interacting multifunctional protein 1
Vitamin K-dependent protein S

Proteasome activator complex subunit 4
 Kinesin-like protein KIF20A
 Thioredoxin reductase 1
 Alpha-2C adrenergic receptor
 26S proteasome non-ATPase regulatory subunit 14
 Tyrosine-protein phosphatase non-receptor type 6
 Caspase-4
 DNA topoisomerase 2-alpha
 DNA topoisomerase 2-beta
 Mu-type opioid receptor
 Tyrosine-protein phosphatase non-receptor type 13
 Stathmin
 Integrator complex subunit 9
 Nuclear receptor coactivator 2
 3-beta-hydroxysteroid-Delta
 Transcription factor A
 Menin
 ATP-dependent 6-phosphofructokinase
 Geminin
 Ubiquitin carboxyl-terminal hydrolase 2
 Ubiquitin carboxyl-terminal hydrolase 1
 Retinal dehydrogenase 1
 Prelamin-A/C
 Glucosylceramidase
 Cellular tumor antigen p53
 Muscarinic acetylcholine receptor M1
 Microtubule-associated protein tau
 Lethal factor Bacillus anthracis
 Arachidonate 15-lipoxygenase
 Thyrotropin receptor
 Nuclear factor NF-kappa-B p105 subunit
 Peripheral myelin protein 22
 Thrombopoietin
 Serine/threonine-protein kinase mTOR
 ATP-dependent DNA helicase Q1
 Histone-lysine N-methyltransferase 2A
 Nuclear factor erythroid 2-related factor 2
 Histone-lysine N-methyltransferase EHMT2
 ATPase family AAA domain-containing protein 5
 M-phase phosphoprotein 8
 Ataxin-2
 3-hydroxyacyl-CoA dehydrogenase type-2
 Tyrosyl-DNA phosphodiesterase 1
 Alpha-1B adrenergic receptor
 Alpha-2B adrenergic receptor
 C-8 sterol isomerase

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :
dopamine D2 and D3 receptor agonist

Predicted Targets

D (uniprotID = P35462 D(3) dopamine receptor)

Transcription factor AP-1
Apoptosis regulator Bcl-2
5-hydroxytryptamine receptor 1A
5-hydroxytryptamine receptor 1D
5-hydroxytryptamine receptor 2B
5-hydroxytryptamine receptor 1B
5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 2C
Alpha-2A adrenergic receptor
Alpha-2B adrenergic receptor
Alpha-2C adrenergic receptor
Cytochrome P450 1A2
Cytochrome P450 3A4
Cytochrome P450 2D6
RAC-alpha serine/threonine-protein kinase
Mitogen-activated protein kinase 3
Mitogen-activated protein kinase 1
Protein fosB
Melanin-concentrating hormone receptor 1
Aromatic-L-amino-acid decarboxylase
Orexin
Muscarinic acetylcholine receptor M1
Tyrosine-protein phosphatase non-receptor type 2
Glial cell line-derived neurotrophic factor
5-hydroxytryptamine receptor 7
Magnesium transporter MRS2 homolog
Catechol O-methyltransferase
Amine oxidase B
Tyrosine-protein phosphatase non-receptor type 1
Lysine-specific demethylase 4E
ATP-dependent 6-phosphofructokinase
Geminin
Prelamin-A/C
Cytochrome P450 2C9
Cytochrome P450 2C19
Flap endonuclease 1
Chromobox protein homolog 1
Histone-lysine N-methyltransferase EHMT2
Uncharacterized protein
Beta-2 adrenergic receptor
Beta-1 adrenergic receptor
Alpha-1D adrenergic receptor
Alpha-1B adrenergic receptor
Alpha-1A adrenergic receptor
5-hydroxytryptamine receptor 6

5-hydroxytryptamine receptor 5A
5-hydroxytryptamine receptor 4
5-hydroxytryptamine receptor 3A

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :

phospho-diesterase (PDE5A) inhibitor

Predicted Targets

Renin

Cellular tumor antigen p53

Endothelin-1

High affinity cAMP-specific and IBMX-insensitive 3'

Cystic fibrosis transmembrane conductance regulator

Angiotensinogen

Bcl2-associated agonist of cell death

cGMP-dependent 3',5'-cyclic phosphodiesterase

cAMP and cAMP-inhibited cGMP 3'

High affinity cGMP-specific 3'

Nuclear receptor subfamily 1 group I member 2

Nitric oxide synthase

Cytochrome P450 3A4

Cytochrome P450 3A5

cGMP-specific 3'

Retinal rod rhodopsin-sensitive cGMP 3'

Retinal cone rhodopsin-sensitive cGMP 3'

Cytochrome P450 3A7

Cytochrome P450 2C9

Cytochrome P450 2C19

Cytochrome P450 2D6

Cytochrome P450 1A1

Cytochrome P450 2E1

Multidrug resistance-associated protein 4

Multidrug resistance-associated protein 5

Calcium/calmodulin-dependent 3'

cAMP-specific 3'

Rod cGMP-specific 3'

Potassium voltage-gated channel subfamily H member 2

Cone cGMP-specific 3'

Dual 3'

High affinity cAMP-specific 3'

Indoleamine 2

Integrin alpha-IIb

Glial fibrillary acidic protein

Retinal guanylyl cyclase 2

Multidrug resistance-associated protein 7

Vasodilator-stimulated phosphoprotein

Retinal guanylyl cyclase 1

von Willebrand factor
Heat-stable enterotoxin receptor
RAC-alpha serine/threonine-protein kinase
cAMP-dependent protein kinase type II-alpha regulatory subunit
Tyrosine-protein kinase receptor TYRO3
Nitric oxide-associated protein 1
cAMP-dependent protein kinase type II-beta regulatory subunit
Multidrug resistance protein 1
Integrin alpha-2
cGMP-inhibited 3'
Angiotensin-converting enzyme
Prostate-specific antigen
Interleukin-8
Adenosine receptor A1
Endothelin-1 receptor
Myc box-dependent-interacting protein 1
Adenosine receptor A2a
Complement C1s subcomponent
Receptor-interacting serine/threonine-protein kinase 4
Delta-1-pyrroline-5-carboxylate synthase
cAMP-dependent protein kinase type I-alpha regulatory subunit
Cyclic nucleotide-binding domain-containing protein 2
GTPase ERas
Atrial natriuretic peptide receptor 2
Atrial natriuretic peptide receptor 1
cAMP-dependent protein kinase type I-beta regulatory subunit
Nestin
Purine nucleoside phosphorylase
Arginase-1
S-methyl-5'-thioadenosine phosphorylase
Allograft inflammatory factor 1
Gastricsin
cGMP-dependent protein kinase 1
Bone morphogenetic protein receptor type-2
Natriuretic peptides B
Natriuretic peptides A
Carbonic anhydrase 9
Neuronal-specific septin-3
Protein GUCD1
Geminin
Beta-lactamase
Vitamin D3 receptor
Alpha-1B adrenergic receptor
Uncharacterized protein
Phosphodiesterase 1A
Solute carrier organic anion transporter family member 2B1
Class 1 phosphodiesterase PDEB1 Trypanosoma brucei
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
ATP-binding cassette sub-family C member 11

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Predicted Targets

D

Alpha-2B adrenergic receptor

5-hydroxytryptamine receptor 1A

5-hydroxytryptamine receptor 1D

Alpha-2A adrenergic receptor

5-hydroxytryptamine receptor 1B

5-hydroxytryptamine receptor 2A

5-hydroxytryptamine receptor 2B

5-hydroxytryptamine receptor 2C

Alpha-2C adrenergic receptor

Solute carrier family 22 member 2

Solute carrier family 22 member 1

Peripheral myelin protein 22

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

Predicted Targets

Apoptosis regulator BAX

G2/mitotic-specific cyclin-B1

Baculoviral IAP repeat-containing protein 5

Cyclin-dependent kinase inhibitor 1

Cyclin-dependent kinase 1

Insulin-like growth factor-binding protein 6

DNA-binding protein inhibitor ID-1

Interleukin-4

Cellular tumor antigen p53

Keratin

Tumor protein p73

Retinoic acid receptor beta

Retinoic acid receptor alpha

Retinoic acid receptor gamma

Retinoic acid receptor RXR-alpha

Retinoic acid receptor RXR-beta

Retinoic acid receptor RXR-gamma

Cytochrome P450 3A4

Cytochrome P450 2C9
Oxysterols receptor LXR-alpha
RNA-binding protein PNO1
Scavenger receptor class B member 1
Large neutral amino acids transporter small subunit 1
SPARC
Galectin-2
Estrogen receptor
Asparagine synthetase
Cholesteryl ester transfer protein
Vitamin D3 receptor
Tissue-type plasminogen activator
X-box-binding protein 1
Pro-cathepsin H
Apolipoprotein C-III
Cytochrome P450 26A1
G1/S-specific cyclin-D1
Angiomotin-like protein 2
Arginine--tRNA ligase
Glucocorticoid receptor
Class E basic helix-loop-helix protein 41
Homeobox protein CDX-1
Class E basic helix-loop-helix protein 40
Long-chain fatty acid transport protein 1
Period circadian protein homolog 2
Fatty acid-binding protein
Peroxisome proliferator-activated receptor gamma
Receptor tyrosine-protein kinase erbB-2
Retinoblastoma-associated protein
Vesicle-associated membrane protein 8
Lysosome membrane protein 2
Transcription factor GATA-6
Krueppel-like factor 10
Serine-protein kinase ATM
PRA1 family protein 3
Epidermal growth factor receptor
CCAAT/enhancer-binding protein gamma
Procollagen-lysine
Integrin beta-6
Platelet glycoprotein 4
Interleukin-15
Immediate early response gene 2 protein
Angiopoietin-related protein 4
Protein DEPP
Homocysteine-responsive endoplasmic reticulum-resident ubiquitin-like domain member 1 protein
Cytochrome c
Beta-2 adrenergic receptor
Transmembrane 4 L6 family member 1
DNA damage-inducible transcript 4 protein
Serine protease 27

Integral membrane protein 2A
Urokinase plasminogen activator surface receptor
E3 ubiquitin-protein ligase SIAH2
Neuronal membrane glycoprotein M6-b
Homeobox protein MOX-1
Early growth response protein 3
Calreticulin
Interstitial collagenase
Transcription factor Maf
Proline-rich nuclear receptor coactivator 1
Ubiquitin-like modifier-activating enzyme 7
TSC22 domain family protein 3
Protein-glutamine gamma-glutamyltransferase 2
Transcription factor MafF
Gamma-adducin
Ephrin type-A receptor 2
Runt-related transcription factor 2
Matrix metalloproteinase-9
Apolipoprotein A-II
Prostaglandin G/H synthase 2
UDP-N-acetylhexosamine pyrophosphorylase
Dual specificity protein phosphatase 5
Protein S100-A9
Protein AF1q
Protein CYR61
Interleukin-2 receptor subunit alpha

ATP-binding cassette sub-family A member 1

Dickkopf-related protein 1
Aldo-keto reductase family 1 member C1
Aldo-keto reductase family 1 member C3
High affinity cationic amino acid transporter 1
Bifunctional methylenetetrahydrofolate dehydrogenase/cyclohydrolase
Angiopoietin-4
Lysyl oxidase homolog 2
Eukaryotic translation initiation factor 1
Menin
Ubiquitin carboxyl-terminal hydrolase 1
Luciferin 4-monooxygenase
78 kDa glucose-regulated protein
Peripheral myelin protein 22
ATP-dependent DNA helicase Q1
Nuclear receptor ROR-gamma
Bloom syndrome protein
Histone-lysine N-methyltransferase 2A
Histone acetyltransferase KAT2A

Retinoic acid receptor RXR-alpha

Tetrabenazine

Molecular Mechanism (initial) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :
vesicular monoamine transporter 2 (VMAT2) inhibitor

Predicted Targets

Synaptic vesicular amine transporter

D

Cytochrome P450 2D6
Carbonyl reductase
Dopamine beta-hydroxylase
Sodium-dependent dopamine transporter
Sodium-dependent serotonin transporter
Polycomb protein EED
Sigma non-opioid intracellular receptor 1
MFS-type transporter SLC18B1
Chromaffin granule amine transporter
Tyrosine 3-monooxygenase
Alpha-synuclein
Carnitine O-acetyltransferase
Tyrosine-protein phosphatase non-receptor type 2
Choline O-acetyltransferase
Myc box-dependent-interacting protein 1
5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 4
Amine oxidase A
SLIT and NTRK-like protein 1
Vesicular acetylcholine transporter
Lysine-specific demethylase 4A
Glutaminase kidney isoform
DNA polymerase beta
Vitamin D3 receptor
Peripheral myelin protein 22
Flap endonuclease 1
Serine/threonine-protein kinase mTOR
Glucagon-like peptide 1 receptor
ATPase family AAA domain-containing protein 5
DNA polymerase iota
Synaptic vesicular amine transporter
Sodium channel protein type 1 subunit alpha
Sodium channel protein type 2 subunit alpha
Sodium channel protein type 3 subunit alpha

Thalidomide

Molecular Mechanism (initial) :
TNF-alpha production inhibitor

Molecular Mechanism (repurposed) :
cereblon (CRBN) inhibitor

Predicted Targets

E3 ubiquitin-protein ligase XIAP
Vascular endothelial growth factor A

Tumor necrosis factor ligand superfamily member 10

Tumor necrosis factor ligand superfamily member 11
Tumor necrosis factor
Tumor necrosis factor receptor superfamily member 10A
Transforming growth factor beta-1
Signal transducer and activator of transcription 3
Transcription factor Sp1
L-selectin
Sphingomyelin phosphodiesterase 2
Prostaglandin G/H synthase 2
Urokinase plasminogen activator surface receptor
Phosphatidylinositol 3
Serine/threonine-protein kinase pim-1
NF-kappa-B inhibitor alpha
Transcriptional activator Myb
Induced myeloid leukemia cell differentiation protein Mcl-1
Interleukin-8
Interleukin-12 subunit beta
Interleukin-1 beta
Hepatocyte growth factor
Interleukin-12 subunit alpha
Fibroblast growth factor 2
Tumor necrosis factor receptor superfamily member 6
Tumor necrosis factor ligand superfamily member 6
Cytochrome c
Neutrophil elastase
Granulocyte-macrophage colony-stimulating factor
C-X-C chemokine receptor type 2
Catalase
Apoptosis regulator Bcl-2
Tartrate-resistant acid phosphatase type 5
Caspase-3
Serine/threonine-protein kinase Chk1
5' exonuclease Apollo
DNA excision repair protein ERCC-6
Leptin
DNA ligase 1
Poly synthase 1)
Peroxisome proliferator-activated receptor delta
Tumor necrosis factor receptor superfamily member 17
X-ray repair cross-complementing protein 5
Nuclear factor NF-kappa-B p105 subunit
Fibroblast growth factor receptor 2
Alpha-1-acid glycoprotein 1
Alpha-1-acid glycoprotein 2
Cytochrome P450 2C19
Cytochrome P450 1A1
Cytochrome P450 2E1
Cytochrome P450 2C9
Prostaglandin G/H synthase 1

Cytochrome P450 3A5
Cytochrome P450 1A2
DNA damage-binding protein 1
B-cell CLL/lymphoma 7 protein family member B
B-cell antigen receptor complex-associated protein alpha chain
E3 ubiquitin-protein ligase RBX1
Tumor necrosis factor receptor superfamily member 1A
T-cell surface glycoprotein CD4
Pyrin
Sal-like protein 4
72 kDa type IV collagenase
Receptor-interacting serine/threonine-protein kinase 2
Dickkopf-related protein 4
Bone morphogenetic protein 4
Granulocyte colony-stimulating factor
ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1
Gamma-enolase
Interleukin-2
G1/S-specific cyclin-D1
Receptor-type tyrosine-protein kinase FLT3

Protein cereblon

Natural resistance-associated macrophage protein 1
Probable RNA-binding protein 19
C-reactive protein
Sal-like protein 1
Complement C3
Uroporphyrinogen decarboxylase
Syndecan-1
Glial fibrillary acidic protein
von Willebrand factor
Interleukin-1 receptor antagonist protein
DNA damage-binding protein 2
Interleukin-6
Fibroblast growth factor receptor 3
Thrombospondin-1
DNA replication factor Cdt1
Tumor necrosis factor receptor superfamily member 10B
Multidrug resistance protein 1
Vascular endothelial growth factor receptor 2
Intercellular adhesion molecule 1
Fibroblast growth factor 10
Epidermal growth factor receptor
Cellular tumor antigen p53
General transcription factor II-I repeat domain-containing protein 1
Centromere protein C
Receptor tyrosine-protein kinase erbB-2
RAC-alpha serine/threonine-protein kinase
Plasminogen activator inhibitor 2
Hemoglobin subunit epsilon
Vascular endothelial growth factor receptor 1

Interferon alpha-1/13
Interleukin-18
Peroxisome proliferator-activated receptor gamma
Centromere protein H
A disintegrin and metalloproteinase with thrombospondin motifs 1
Nitric oxide synthase
Integrin alpha-2
C-X-C chemokine receptor type 1
Serum albumin
Angiopoietin-1
TGF-beta receptor type-1
Interleukin-6 receptor subunit beta
Prostate-specific antigen
Olfactory receptor 2AG1
Bcl-2-like protein 1
Insulin-like growth factor I
Transducin beta-like protein 2
Breakpoint cluster region protein
B-lymphocyte antigen CD19
Hematopoietic progenitor cell antigen CD34
T-box transcription factor TBX5
CASP8 and FADD-like apoptosis regulator
Hemoglobin subunit gamma-2
Caspase-9
Proteinase-activated receptor 1
Fibroblast growth factor 8
E3 ubiquitin-protein ligase TRIM50
Cytochrome P450 3A4
Mothers against decapentaplegic homolog 3
Platelet-derived growth factor subunit B
E-selectin
PCI domain-containing protein 2
Histone H3-like centromeric protein A
NACHT
ATP-binding cassette sub-family A member 1
Annexin A2
Growth factor receptor-bound protein 2
Frizzled-9
Serine/threonine-protein kinase mTOR
Insulin
Solute carrier family 12 member 6
Fibronectin
Collagen alpha-1 chain
Caspase-8
CAMPATH-1 antigen
E3 ubiquitin-protein ligase parkin
PDZ and LIM domain protein 1
Growth arrest and DNA damage-inducible protein GADD45 alpha
Transcription factor AP-1
Dickkopf-related protein 1

Tumor necrosis factor receptor superfamily member 5
 Zinc finger protein 79
 Matrix metalloproteinase-9
 Endoglin
 Cullin-4B
 Major centromere autoantigen B
 Cullin-4A
 Insulin receptor substrate 2
 Tumor necrosis factor receptor superfamily member 1B
 Membrane-bound transcription factor site-2 protease
 Angiopoietin-1 receptor
 Tyrosine-protein kinase JAK2
 Interferon alpha-2
 Toll-like receptor 7
 Growth-regulated alpha protein
 Toll/interleukin-1 receptor domain-containing adapter protein
 Caspase-5
 Caspase-1
 Putative methyltransferase NSUN5
 DET1 homolog
 Histone deacetylase 9
 Interleukin-10
 Geminin
 Retinal dehydrogenase 1
 Thyroid hormone receptor beta
 Bloom syndrome protein
 Histone-lysine N-methyltransferase EHMT2
 cAMP-specific 3'
 Fatty-acid amide hydrolase 1
 Beta-lactamase
 Malate dehydrogenase
 Chymotrypsin-C
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1

Topiramate

Molecular Mechanism (initial) :

kainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker

Molecular Mechanism (repurposed) :

ckainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker

Predicted Targets

Carbonic anhydrase 3
 Steroid 17-alpha-hydroxylase/17

Carbonic anhydrase 1

Carbonic anhydrase 2

Gamma-aminobutyric acid receptor subunit alpha-1

Sodium channel protein type 1 subunit alpha

Glutamate receptor ionotropic

Carbonic anhydrase 4

Gamma-aminobutyric acid receptor subunit alpha-2

Gamma-aminobutyric acid receptor subunit alpha-3

Gamma-aminobutyric acid receptor subunit alpha-4

Gamma-aminobutyric acid receptor subunit alpha-5

Gamma-aminobutyric acid receptor subunit alpha-6

Gamma-aminobutyric acid receptor subunit beta-1

Gamma-aminobutyric acid receptor subunit beta-2

Gamma-aminobutyric acid receptor subunit beta-3

Gamma-aminobutyric acid receptor subunit delta

Gamma-aminobutyric acid receptor subunit epsilon

Gamma-aminobutyric acid receptor subunit gamma-2

Gamma-aminobutyric acid receptor subunit gamma-3

Gamma-aminobutyric acid receptor subunit pi

Cytochrome P450 2C19

Cytochrome P450 3A4

Aquaporin-4

Aquaporin-4

Carbonic anhydrase 4

Carbonic anhydrase 2

Sodium channel protein type 2 subunit alpha

Carbonic anhydrase 5A

Astrosclerin-3 Astrosclera willeyana

Alpha carbonic anhydrase Stylophora pistillata

Carbonic anhydrase Stylophora pistillata

Carbonic anhydrase

Carbonic anhydrase 12

Carbonic anhydrase 6

Carbonic anhydrase Methanosarcina thermophila

Carbonic anhydrase 7

Carbonic anhydrase

Probable transmembrane carbonic anhydrase

Beta-carbonic anhydrase 1

Carbonic anhydrase 9

Delta carbonic anhydrase

Carbonic anhydrase 13

Carbonic anhydrase 15

Carbonic anhydrase 13

Carbonic anhydrase 14

Carbonic anhydrase 5B

Solute carrier organic anion transporter family member 1B3

Solute carrier organic anion transporter family member 1B1

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

Predicted Targets

Estrogen receptor

Cytochrome P450 3A4

Cytochrome P450 1A1

Cytochrome P450 1A2

Multidrug resistance protein 1

M1 family aminopeptidase

Perilipin-1

Perilipin-5

Hepatocyte nuclear factor 4-alpha

Geminin

Ubiquitin carboxyl-terminal hydrolase 1

Prelamin-A/C

Peripheral myelin protein 22

Histone-lysine N-methyltransferase EHMT2

5-hydroxytryptamine receptor 6

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

Predicted Targets

14-3-3 protein epsilon

E3 ubiquitin-protein ligase XIAP

X-ray repair cross-complementing protein 5

Vascular endothelial growth factor A

Transitional endoplasmic reticulum ATPase

Thymidylate synthase

Thioredoxin domain-containing protein 12

Thioredoxin domain-containing protein 17

Tuberin

Tumor suppressor candidate 2

Thioredoxin

Trafficking protein particle complex subunit 3

TNF receptor-associated factor 1

TNF receptor-associated factor 2

Heat shock protein 75 kDa

Cellular tumor antigen p53

Tumor necrosis factor receptor type 1-associated DEATH domain protein

Tumor necrosis factor ligand superfamily member 10

Tumor necrosis factor receptor superfamily member 10A

Tumor necrosis factor

Transaldolase

Metalloproteinase inhibitor 2
E3 ubiquitin-protein ligase CHIP
Stathmin
Transcription factor Sp1
Nuclear autoantigen Sp-100
Transcription factor Sp3
Secernin-1
Succinate dehydrogenase flavoprotein subunit
Protein S100-A9
Ras-related protein R-Ras
40S ribosomal protein SA
Receptor-interacting serine/threonine-protein kinase 1
60S ribosomal protein L12
Reticulocalbin-2
Ran-specific GTPase-activating protein
Paxillin
DNA repair protein RAD50
Proteasome subunit beta type-2
Prostaglandin G/H synthase 2
Peroxiredoxin-6
DNA-dependent protein kinase catalytic subunit
Proteasome subunit beta type-1
Peroxiredoxin-1
Thioredoxin-dependent peroxide reductase
Peroxiredoxin-5
Protein PML
Phosphomevalonate kinase
Phosphatidylethanolamine-binding protein 1
Protein DJ-1
NF-kappa-B inhibitor alpha
ADP-sugar pyrophosphatase
Myb-related protein B
Transcriptional activator Myb
Induced myeloid leukemia cell differentiation protein Mcl-1
Leukotriene A-4 hydrolase
Transcription factor AP-1
Keratin
Interleukin-8
Interleukin-1 beta
NF-kappa-B essential modulator
Serine protease HTRA2
78 kDa glucose-regulated protein
Heat shock protein HSP 90-beta
Heat shock protein HSP 90-alpha
Hypoxia-inducible factor 1-alpha
Histone H3.1t

Histone deacetylase 3

Histone deacetylase 7

Histone H2AX

Histone deacetylase 1

Glia maturation factor beta
Tumor necrosis factor ligand superfamily member 6
Fructose-1
Tumor necrosis factor receptor superfamily member 6
FAS-associated death domain protein
Fumarylacetoacetase
Eukaryotic translation initiation factor 2-alpha kinase 3
Alpha-enolase
Histone acetyltransferase p300
Diablo homolog
DnaJ homolog subfamily B member 11
Delta
Cytochrome c
Crk-like protein
C-X-C chemokine receptor type 4
Chloride intracellular channel protein 4
Cytochrome c oxidase subunit 5B
CREB-binding protein
Inhibitor of nuclear factor kappa-B kinase subunit alpha
Charged multivesicular body protein 4b
Cyclin-dependent kinase inhibitor 1B
Cyclin-dependent kinase inhibitor 1
Cyclin-dependent kinase 1
G2/mitotic-specific cyclin-B1
Cyclin-A2
Chromobox protein homolog 3
Chromobox protein homolog 5
Calreticulin
Macrophage-capping protein
Baculoviral IAP repeat-containing protein 5
Bcl-2-modifying factor
Baculoviral IAP repeat-containing protein 3
BH3-interacting domain death agonist
Baculoviral IAP repeat-containing protein 2
Bcl-2-related protein A1
Apoptosis regulator Bcl-2
Apoptosis regulator BAX
Bcl-2-binding component 3
Bcl2-associated agonist of cell death
Autophagy protein 5
Ubiquitin-like protein ATG12
Androgen receptor
Rho GDP-dissociation inhibitor 2
Arachidonate 15-lipoxygenase
Apoptosis-inducing factor 1
Adenosine deaminase
Actin
Protein Wnt-3a
Steroidogenic factor 1
Histone deacetylase 4

Tyrosine-protein kinase ABL1
Potassium voltage-gated channel subfamily H member 2
Cytochrome P450 3A4
Histone deacetylase 5
NAD-dependent protein deacylase sirtuin-5
Histone deacetylase 9
3-hydroxy-3-methylglutaryl-coenzyme A reductase

Histone deacetylase 2

Acetoin utilization protein
Angiotensin-converting enzyme
Cystic fibrosis transmembrane conductance regulator

Histone deacetylase 6

Lysine-specific demethylase 4E
Nuclear receptor subfamily 0 group B member 1
Histone deacetylase 10
Histone deacetylase-like amidohydrolase
Histone deacetylase 11
Zinc transporter ZIP6
C-C motif chemokine 17
LIM and cysteine-rich domains protein 1
Granulins
72 kDa type IV collagenase
Ankyrin repeat domain-containing protein 54
Estrogen receptor
B-cell lymphoma 3 protein
Nuclear factor NF-kappa-B p100 subunit
Mitogen-activated protein kinase 1
NAD-dependent protein deacetylase sirtuin-1
BCL-6 corepressor-like protein 1
Endothelial protein C receptor
Thioredoxin-like protein 1
Sal-like protein 4
NAD-dependent protein deacetylase sirtuin-2
Gamma-enolase
Small glutamine-rich tetratricopeptide repeat-containing protein alpha
Prenylated Rab acceptor protein 1
G1/S-specific cyclin-D1
Nuclear factor NF-kappa-B p105 subunit
Heat shock cognate 71 kDa protein
Zinc finger protein GLI1
Heat shock protein beta-1
Cathepsin D
Peroxisomal NADH pyrophosphatase NUDT12
L-lactate dehydrogenase B chain
L-selectin
UDP-galactose translocator
Receptor-type tyrosine-protein kinase FLT3
Tumor necrosis factor ligand superfamily member 9
Microtubule-associated proteins 1A/1B light chain 3B
Histone H3.3

Retinoic acid receptor alpha
RAF proto-oncogene serine/threonine-protein kinase
Transcription initiation factor TFIID subunit 4
Pigment epithelium-derived factor
Protein phosphatase 1 regulatory subunit 1B
Adenylate cyclase type 7
Histone acetyltransferase KAT7
Cyclin-dependent kinase 4
Interleukin-6
Ankyrin repeat domain-containing protein 12
BRCA1-associated RING domain protein 1
Nucleosome assembly protein 1-like 1
Prostaglandin E synthase 3
Synphilin-1
E3 ubiquitin-protein ligase MIB1
Excitatory amino acid transporter 3
Retinoid-inducible serine carboxypeptidase
Cyclin-dependent kinase 4 inhibitor C
Inversin
Cytochrome b-c1 complex subunit 2
Annexin A3
Ankyrin repeat and SOCS box protein 3
Interleukin-1 alpha
Mitogen-activated protein kinase 3
Flavin reductase
Ankyrin repeat and SOCS box protein 1
Histone acetyltransferase KAT2B
Protein TANC1
Endothelial PAS domain-containing protein 1
Guanylate cyclase soluble subunit beta-1
Ankycorbin
Ankyrin repeat domain-containing protein 7
Excitatory amino acid transporter 1
Ankyrin repeat domain-containing protein 32
Serine/threonine-protein phosphatase 6 regulatory ankyrin repeat subunit C
Receptor tyrosine-protein kinase erbB-3
DNA repair protein RAD51 homolog 1
Retinoblastoma-associated protein
Ankyrin repeat domain-containing protein 10
Ceramide synthase 6
SH3 and multiple ankyrin repeat domains protein 1
Serine-protein kinase ATM
Putative ankyrin repeat domain-containing protein 31
RAC-alpha serine/threonine-protein kinase
Receptor tyrosine-protein kinase erbB-2
Low molecular weight phosphotyrosine protein phosphatase
Protein canopy homolog 2
Ankyrin repeat and SOCS box protein 6
Epidermal growth factor receptor
Fibroblast growth factor 18

NF-kappa-B inhibitor epsilon
Cyclin-dependent kinase 4 inhibitor B
Ankyrin repeat and SOCS box protein 15
Tumor necrosis factor receptor superfamily member 10B
Ankyrin repeat and SOCS box protein 16
Adenosine kinase
Ankyrin repeat and BTB/POZ domain-containing protein BTBD11
Interleukin-18
Ankyrin repeat
Phenylalanine--tRNA ligase beta subunit
Ubiquitin/ISG15-conjugating enzyme E2 L6
Erythrocyte band 7 integral membrane protein
Ankyrin repeat domain-containing protein 9
Ankyrin repeat domain-containing protein 18B
Proteasome subunit beta type-4
Signal transducer and activator of transcription 6
Ankyrin repeat domain-containing protein 33B
Homeobox protein engrailed-1
Hedgehog-interacting protein
Annexin A5
Ankyrin repeat and SOCS box protein 5
Endoplasmin
Ankyrin repeat and SAM domain-containing protein 6
Ankyrin repeat and KH domain-containing protein 1
Stress-70 protein
Isocitrate dehydrogenase subunit alpha
Ankyrin repeat domain-containing protein 2
Dual specificity mitogen-activated protein kinase kinase 1
Ankyrin repeat domain-containing protein 11
Bcl-2-like protein 1
Heat shock 70 kDa protein 4
Breakpoint cluster region protein
Potassium voltage-gated channel subfamily S member 3
Ankyrin repeat and SAM domain-containing protein 3
Beta-2 adrenergic receptor
Ankyrin repeat domain-containing protein 37
Ankyrin repeat and SOCS box protein 8
NF-kappa-B inhibitor beta
Argininosuccinate lyase
Ankyrin repeat and SAM domain-containing protein 4B
Heparanase
Caspase-2
Caspase-3
cAMP-dependent protein kinase catalytic subunit alpha
Hippocalcin-like protein 1
CASP8 and FADD-like apoptosis regulator
Acyl-CoA-binding protein
Thiopurine S-methyltransferase
Acyl-CoA-binding domain-containing protein 4
Kallikrein-2

NADH dehydrogenase iron-sulfur protein 8
Uveal autoantigen with coiled-coil domains and ankyrin repeats
Ankyrin repeat and SOCS box protein 2
T-complex protein 1 subunit alpha
Phenylalanine--tRNA ligase alpha subunit
Histone-lysine N-methyltransferase EZH2
Ankyrin repeat domain-containing protein SOWAHB
DNA
SUMO-conjugating enzyme UBC9
Ankyrin repeat domain-containing protein 23
Ankyrin repeat and SOCS box protein 4
Ankyrin repeat domain-containing protein 29
Ankyrin repeat domain-containing protein 24
Ribosome biogenesis regulatory protein homolog
LIM and SH3 domain protein 1
NF-kappa-B inhibitor zeta
Phorbol-12-myristate-13-acetate-induced protein 1
Caspase-9
NAD-dependent protein deacetylase sirtuin-7
Cell adhesion molecule 1
Huntingtin-associated protein 1
Protein patched homolog 1
Suppressor of cytokine signaling 3
Serine/threonine-protein phosphatase 6 regulatory ankyrin repeat subunit B
Receptor-interacting serine/threonine-protein kinase 4
Histone H3.2
Ankyrin repeat domain-containing protein 20A2
Apoptotic protease-activating factor 1
Superoxide dismutase
Eukaryotic translation initiation factor 5A-1
Adenosine receptor A2a
Cyclin-dependent kinase 4 inhibitor D
Histone H3-like centromeric protein A
Ribosylidihydronicotinamide dehydrogenase 2
Espin-like protein
DnaJ homolog subfamily B member 2
Zinc finger and BTB domain-containing protein 16
Annexin A6
Ankyrin repeat and FYVE domain-containing protein 1
Ankyrin repeat domain-containing protein 55
60 kDa heat shock protein
Fermitin family homolog 2
Ubiquitin-like modifier-activating enzyme ATG7
Runt-related transcription factor 3
Catenin beta-1
Histone H4
Huntingtin
E3 ubiquitin-protein ligase MIB2
Tumor necrosis factor receptor superfamily member 14
Breast cancer type 1 susceptibility protein

Ganglioside GM2 activator
Nuclear receptor corepressor 2
Atrophin-1
Ankyrin repeat domain-containing protein 20A4
Ryanodine receptor 1
Probable helicase with zinc finger domain
Ankyrin repeat and SOCS box protein 13
Ankyrin repeat domain-containing protein 17
Death-associated protein kinase 1
Caspase-8
Ankyrin repeat domain-containing protein 30B
C-C motif chemokine 20
X-ray repair cross-complementing protein 6
Histone H3.1
Serine/threonine-protein kinase mTOR
Protein AHNK2
Ankyrin repeat domain-containing protein 30A
Coiled-coil domain-containing protein 144A
Poly synthase 1)
Ankyrin repeat and SOCS box protein 12
Enoyl-CoA delta isomerase 2
Beclin-1
M-phase phosphoprotein 8
Ubiquitin-fold modifier-conjugating enzyme 1
Acyl-CoA-binding domain-containing protein 6
Fibronectin type 3 and ankyrin repeat domains protein 1
Mannosyl-oligosaccharide 1
Ornithine aminotransferase
GA-binding protein subunit beta-2
Phosphatidylinositol 3
Muscleblind-like protein 3
Ankyrin repeat domain-containing protein 22
Ankyrin repeat domain-containing protein 1
Matrix metalloproteinase-9
Annexin A7
Protein SET
Ankyrin repeat domain-containing protein SOWAHC
Bcl-2 homologous antagonist/killer
Folylpolyglutamate synthase
UDP-glucuronosyltransferase 1-8
Histone deacetylase 8
Gelsolin
Ankyrin repeat domain-containing protein 26
DnaJ homolog subfamily C member 7
Glutathione S-transferase P
E3 ubiquitin-protein ligase TRIM22
PHD finger protein 11
Acyl-CoA-binding domain-containing protein 7
Espin
Myc proto-oncogene protein

DnaJ homolog subfamily A member 1
Sushi repeat-containing protein SRPX
Carbonic anhydrase 9
BCL-6 corepressor
Cytochrome P450 1A1
Peroxisome oxidoreductase-4
Enhancer of filamentation 1
GA-binding protein subunit beta-1
Ankyrin repeat and SOCS box protein 9
Ankyrin repeat domain-containing protein 16
40S ribosomal protein S6
Survival motor neuron protein
Aldo-keto reductase family 1 member C3
BCL2/adenovirus E1B 19 kDa protein-interacting protein 3-like
NF-kappa-B inhibitor delta
Ankyrin repeat domain-containing protein 39
Small glutamine-rich tetratricopeptide repeat-containing protein beta
Triosephosphate isomerase
Parathyroid hormone-related protein
Acyl-CoA-binding domain-containing protein 5
Methyl-CpG-binding protein 2
Tonsoku-like protein
Serine/threonine-protein phosphatase 6 regulatory ankyrin repeat subunit A
Ankyrin repeat domain-containing protein 18A
Transcription factor p65
E3 ubiquitin-protein ligase NEDD4-like
Heat shock 70 kDa protein 1A/1B
Putative ankyrin repeat domain-containing protein 30B-like
Ankyrin repeat and SOCS box protein 18
Protein TANC2
Ankyrin repeat domain-containing protein 6
Dihydrofolate reductase
Ankyrin repeat domain-containing protein 63
Ankyrin repeat domain-containing protein 36C
Ankyrin repeat and SOCS box protein 11
Cyclin-dependent kinase inhibitor 1C
Peptidyl-prolyl cis-trans isomerase A
Ankyrin repeat domain-containing protein 36A
Geminin
Peripheral myelin protein 22
Mothers against decapentaplegic homolog 3
Nuclear factor erythroid 2-related factor 2
DNA dC->dU-editing enzyme APOBEC-3F
DNA polymerase iota
Paired box protein Pax-8
Nuclear receptor corepressor 1
Hdac2 protein
Histone deacetylase 1
Zinc finger protein GLI1
Hdac5 protein

Histone deacetylase 3
Histone deacetylase
HD2 type histone deacetylase HDA106
Histone deacetylase 7
Histone deacetylase 6
Histone deacetylase 4
Cytochrome P450 1A2
Cytochrome P450 2D6
Cytochrome P450 2C9
Cytochrome P450 2C19
Macrophage metalloelastase

Supplement 2

Biological activity profile predicted with SEA

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

Predicted Targets

Mu opioid receptor

Alprostadi

Molecular Mechanism (initial) :

prostaglandin E2 receptor agonist

Molecular Mechanism (repurposed) :

prostaglandin E2 receptor agonist

Predicted Targets

Prostanoid EP1 receptor

Prostanoid EP4 receptor

Prostanoid EP2 receptor

Prostanoid EP3 receptor

Prostanoid IP receptor

Prostanoid FP receptor

Transcriptional activator protein Iα

Solute carrier family 22 member 20

Solute carrier family 22 member 6

Dual specificity phosphatase Cdc25C

Leukotriene B4 receptor 1

Phospholipase A2 group IIC

Fatty acid binding protein epidermal

Fatty acid binding protein intestinal

Seed lipoxygenase-1

Fatty acid-binding protein, liver

Group VII phospholipase A2

Sn1-specific diacylglycerol lipase alpha
Transcriptional activator protein traR
Fatty acid binding protein adipocyte
Fatty acid binding protein muscle
Protein kinase C alpha
Dual specificity phosphatase Cdc25A
Peroxisome proliferator-activated receptor gamma
HMG-CoA reductase
Thromboxane A2 receptor
Arachidonate 5-lipoxygenase
N-acylethanolamine-hydrolyzing acid amidase
Dual specificity phosphatase Cdc25B
DNA polymerase beta
Cannabinoid CB2 receptor
Histone deacetylase-like amidohydrolase
Epoxide hydratase
Sphingosine 1-phosphate receptor Edg-5
Anandamide amidohydrolase
Prostanoid DP receptor

Amantadine hydrochloride

Molecular Mechanism (initial) :

matrix protein 2 (Influenza virus A) inhibitor

Molecular Mechanism (repurposed) :

dopamine receptor agonists

NMDA receptor antagonists

Predicted Targets

Sigma opioid receptor

Glutamate [NMDA] receptor subunit epsilon 3

Glutamate (NMDA) receptor subunit zeta 1

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

Predicted Targets

Histamine H1 receptor

Alpha-1a adrenergic receptor

Muscarinic acetylcholine receptor M5

Muscarinic acetylcholine receptor M4

Alpha-1b adrenergic receptor

Alpha-2b adrenergic receptor

Histamine H2 receptor

Muscarinic acetylcholine receptor M1

Dopamine D5 receptor

Dopamine D1 receptor

Serotonin 2b (5-HT2b) receptor

Mannose-6-phosphate isomerase
Serotonin 2c (5-HT2c) receptor
Envelope glycoprotein gp70
Thymidylate synthase
Pleiotropic ABC efflux transporter of multiple drugs
Alpha-1d adrenergic receptor

Sodium channel protein type II alpha subunit

Alpha-2c adrenergic receptor

Serotonin transporter

Alpha-2a adrenergic receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 1b (5-HT1b) receptor
Muscarinic acetylcholine receptor M3
Sodium channel protein type V alpha subunit
Cytochrome P450 2D6
Norepinephrine transporter
Cytochrome P450 2C19
Dopamine transporter
Transporter
Cytochrome P450 11B2
Muscarinic acetylcholine receptor M2
Dopamine D3 receptor
Serotonin 6 (5-HT6) receptor
Sodium channel protein type IX alpha subunit
HERG
Sigma opioid receptor
Serotonin 1a (5-HT1a) receptor
Dopamine D2 receptor
Serotonin 7 (5-HT7) receptor

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

Predicted Targets

Dopamine D1 receptor
Serotonin 7 (5-HT7) receptor
Dopamine D2 receptor
Serotonin 1a (5-HT1a) receptor
Dopamine D3 receptor
M18 aspartyl aminopeptidase
Dopamine D5 receptor
Poly [ADP-ribose] polymerase-1
Dopamine D4 receptor
HERG
Alpha-1b adrenergic receptor
Serotonin transporter
Alpha-1a adrenergic receptor

Serotonin 2a (5-HT2a) receptor

Acetylsalicylic acid

Molecular Mechanism (initial) :

cyclooxygenase inhibitor

Molecular Mechanism (repurposed) :

cyclooxygenase inhibitor

Predicted Targets

Cyclooxygenase-1

Aldo-keto reductase family 1 member C2
Aldo-keto-reductase family 1 member C3
Fatty acid binding protein epidermal
Beta-ketoacyl-ACP synthase III
Aldo-keto reductase family 1 member C1
UDP-galactose 4-epimerase
Fatty acid binding protein adipocyte
Glutamate carboxypeptidase II
Malate dehydrogenase mitochondrial
Fatty acid binding protein intestinal
17-beta-hydroxysteroid-dehydrogenase
Beta-2 adrenergic receptor
DNA-(apurinic or apyrimidinic site) lyase
Fatty acid-binding protein, liver
DNA ligase 1
Liver glycogen phosphorylase
4-hydroxyphenylpyruvate dioxygenase
Cysteine protease falcipain-3
Interleukin-8
Acrosin
Methionine aminopeptidase
Transthyretin
Cyclooxygenase-2
Acyl coenzyme A:cholesterol acyltransferase
Fatty acid binding protein muscle
Beta-lactamase
Glycogen phosphorylase, muscle form
Peripheral-type benzodiazepine receptor
Nuclear receptor subfamily 4 group A member 1
C-C chemokine receptor type 2
Transforming protein RhoA
Carboxylesterase 2
Toll-like receptor 4
Translocator protein
Alpha-chymotrypsin
Beta amyloid A4 protein
Receptor-type tyrosine-protein phosphatase gamma
Female germline-specific tumor suppressor gld-1
D-alanyl-D-alanine carboxypeptidase
Carbonic anhydrase XII

AICAR transformylase
 Eukaryotic translation initiation factor 4H
 Human immunodeficiency virus type 1 integrase
 Tyrosyl-DNA phosphodiesterase 1
 Lysine-specific demethylase 4A
 Elastase 1
 Ubiquitin carboxyl-terminal hydrolase isozyme L1
 Carbonic anhydrase 3
 Myeloperoxidase
 Hydroxycarboxylic acid receptor 2
 Falcipain 2
 Prostanoid EP1 receptor
 Envelope glycoprotein gp160
 Carbonic anhydrase III
 Arachidonate 5-lipoxygenase
 Carbonic anhydrase 15
 Muscle glycogen phosphorylase
 Poly [ADP-ribose] polymerase-2
 Angiotensin-converting enzyme
 Arachidonate 12-lipoxygenase
 Beta-1 adrenergic receptor
 Telomerase reverse transcriptase
 Carbonic anhydrase VI
 Protein-tyrosine phosphatase 1C
 MAP kinase ERK1
 Acetylcholinesterase
 Carbonic anhydrase VA
 Histamine H1 receptor
 Beta-lactamase L1
 Dihydroorotate dehydrogenase
 Transketolase
 Carbonic anhydrase IX
 Bcl2-antagonist of cell death (BAD)
 Protein tyrosine kinase 2 beta
 Polymerase acidic protein
 Hepatitis C virus NS5B RNA-dependent RNA polymerase

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

Predicted Targets

GABA-B receptor 1

Voltage-gated calcium channel alpha2/delta subunit 1
 Kynurenine 3-monooxygenase
 Voltage-dependent calcium channel alpha2delta subunit
 1-deoxyxylulose-5-phosphate reductoisomerase
 G protein-coupled receptor 44

GABA receptor gamma-1 subunit
Carboxypeptidase A1
Carboxypeptidase G2
Thromboxane A2 receptor
Caspase-9
Scytalone dehydratase
Flap endonuclease 1
DNA excision repair protein ERCC-5
Carboxypeptidase N, catalytic subunit
Excitatory amino acid transporter 2
Glutamate receptor ionotropic kainate 3
Acyl coenzyme A:cholesterol acyltransferase
Cellular tumor antigen p53
Cyclooxygenase-2
Glutamate receptor ionotropic kainate 2
Excitatory amino acid transporter 3
Interleukin-8
Excitatory amino acid transporter 1
Hydroxycarboxylic acid receptor 2
Holo-[acyl-carrier-protein] synthase
Pseudolysin
Carboxypeptidase B
Coagulation factor VII
HMG-CoA reductase
ATP-citrate synthase
Free fatty acid receptor 1
Caspase-3
Alpha-2b adrenergic receptor
Beta-lactamase L1
Purine nucleoside phosphorylase
Beta-2 adrenergic receptor
Carbonic anhydrase 2
Carboxypeptidase B2 isoform A
Amine oxidase, copper containing
Beta-1 adrenergic receptor
Prostanoid DP receptor
Glutamate receptor ionotropic kainate 1
Aldose reductase
Peptide deformylase mitochondrial
Adenosine A3 receptor
Disks large homolog 4
Histone deacetylase 5
D-amino-acid oxidase
Plasma kallikrein

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

Predicted Targets

Zinc aminopeptidase
Glutamate [NMDA] receptor subunit epsilon 2
Aminopeptidase N
Alcohol dehydrogenase gamma chain
Cyclooxygenase-1
40S ribosomal protein S27
Lysine-specific histone demethylase 1
Bradykinin B2 receptor
Alcohol dehydrogenase beta chain
Polyamine oxidase
Fructose-1,6-bisphosphatase
Monoamine oxidase A
Carbonic anhydrase III
Carboxypeptidase A1
Neutral cholesterol ester hydrolase 1
Carbonic anhydrase VA
Carbonic anhydrase VB
Nitric oxide synthase, inducible
Carbonic anhydrase 2
PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBC
Sodium channel protein type II alpha subunit
Beta-chymotrypsin
Alpha-L-fucosidase I
Histone deacetylase 6
Cathepsin B
Acetylcholine receptor protein delta chain
Nitric-oxide synthase, brain
Glutamate receptor ionotropic kainate 1
Amiloride-sensitive sodium channel alpha-subunit
Acyl coenzyme A:cholesterol acyltransferase

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

Predicted Targets

Endothelin receptor ET-A

Endothelin receptor ET-B

Fibroblast growth factor receptor 2

C-C chemokine receptor type 4

Carbonic anhydrase 1

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :
mu-type opioid receptor agonist

Predicted Targets

Delta opioid receptor
Kappa opioid receptor

Mu opioid receptor

Nociceptin receptor
HERG
Cytochrome P450 2D6
C-C chemokine receptor type 5

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Predicted Targets

Cyclooxygenase-1

Cyclooxygenase-2

Carbonic anhydrase
Carbonic anhydrase VA
Carbonic anhydrase VB
Cytochrome c oxidase subunit 2
Carbonic anhydrase 15
Astrosclerin-3
PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBC
Alpha carbonic anhydrase
Protein-tyrosine kinase 2-beta
Histone-arginine methyltransferase CARM1
Mineralocorticoid receptor
Carbonic anhydrase XIII
Carbonic anhydrase VI
Carbonic anhydrase III
Carbonic anhydrase VII
Carbonic anhydrase XIV
Cytochrome P450 2D6
Progesterone receptor
Carbonic anhydrase IV
Carbonic anhydrase IX
Carbonic anhydrase XII
Epoxide hydratase
Carbonic anhydrase II
Uncharacterized protein Rv1284/MT1322
Serine/threonine protein phosphatase PP1-alpha catalytic subunit
Protein tyrosine kinase 2 beta
Neuropeptide Y receptor type 5
Alpha-2b adrenergic receptor
MAP kinase p38 alpha

Norepinephrine transporter
Dopamine transporter
Serotonin transporter
Protein kinase Pfmrk
Carbonic anhydrase I
Arachidonate 5-lipoxygenase
Coagulation factor X
Fructose-1,6-bisphosphatase 1
Carbonic anhydrase 1
Coagulation factor IX

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

Predicted Targets

Histidine-rich protein
Quinone reductase 2
HERG
Histamine N-methyltransferase
C-C chemokine receptor type 4
Botulinum neurotoxin type A
Voltage-gated calcium channel alpha2/delta subunit 1
Zinc aminopeptidase
Trypanothione reductase
Falcipain 2
Histamine H3 receptor
Cytochrome P450 1A2
Aminopeptidase N

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

Predicted Targets

Pleiotropic ABC efflux transporter of multiple drugs
Trypanothione reductase
Calmodulin
Alpha-1b adrenergic receptor
Histamine H1 receptor
Muscarinic acetylcholine receptor M5
Alpha-2b adrenergic receptor
Alpha-1d adrenergic receptor
Muscarinic acetylcholine receptor M4
Histamine H2 receptor
Dopamine D5 receptor

Dopamine D1 receptor
C-X-C chemokine receptor type 3
Cytochrome P450 2D6
Serotonin 2c (5-HT2c) receptor
Voltage-gated L-type calcium channel alpha-1S subunit
Cholinesterase
Serotonin 2b (5-HT2b) receptor
Alpha-2c adrenergic receptor

Dopamine D2 receptor

Alpha-2a adrenergic receptor
Tyrosine-protein kinase FYN
Serotonin 2a (5-HT2a) receptor
Muscarinic acetylcholine receptor M1
Dopamine D3 receptor
Serotonin 1b (5-HT1b) receptor
Alpha-1a adrenergic receptor
Peptide deformylase mitochondrial
Cytochrome P450 1A2
Butyrylcholinesterase
Neuropeptide Y receptor type 5
3-beta-hydroxysteroid-delta(8),delta(7)-isomerase
Sigma opioid receptor
Serotonin transporter
Lanosterol 14-alpha demethylase
Muscarinic acetylcholine receptor M3
P-glycoprotein 1
Muscarinic acetylcholine receptor M2
Serotonin 6 (5-HT6) receptor
Serotonin 7 (5-HT7) receptor
Norepinephrine transporter
Dopamine transporter
Kinesin-like protein 1
C-8 sterol isomerase
Taq polymerase 1
Androgen Receptor
Melanocortin receptor 5
Dopamine D4 receptor
Serotonin 1a (5-HT1a) receptor
Neurokinin 2 receptor
HERG
Vanilloid receptor
Histamine H3 receptor
Voltage-gated L-type calcium channel alpha-1C subunit
Urotensin II receptor
Kappa opioid receptor
Delta opioid receptor
Mu opioid receptor

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :

TNF- α /NF- κ b signaling pathway inhibitor

Predicted Targets

Sodium/potassium-transporting ATPase alpha-1 chain

Signal transducer and activator of transcription 3

Potassium-transporting ATPase alpha chain 2

Doxepin hydrochloride

Molecular Mechanism (initial) :

5HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

H1 and H2 histamine receptor blocker

Predicted Targets

Histamine H1 receptor

Alpha-1a adrenergic receptor

Muscarinic acetylcholine receptor M4

Muscarinic acetylcholine receptor M5

Alpha-1b adrenergic receptor

Alpha-2b adrenergic receptor

Histamine H2 receptor

Serotonin 2b (5-HT_{2b}) receptor

Muscarinic acetylcholine receptor M1

Dopamine D1 receptor

Alpha-1d adrenergic receptor

Thromboxane A2 receptor

Serotonin 2c (5-HT_{2c}) receptor

Dopamine D5 receptor

Pleiotropic ABC efflux transporter of multiple drugs

Alpha-2c adrenergic receptor

Alpha-2a adrenergic receptor

Muscarinic acetylcholine receptor M3

Serotonin 2a (5-HT_{2a}) receptor

Muscarinic acetylcholine receptor M2

Sodium channel protein type II alpha subunit

Cytochrome P450 2D6

Norepinephrine transporter

Serotonin 1b (5-HT_{1b}) receptor

Dopamine transporter

Cytochrome P450 2C19

Estrogen receptor beta

Sodium channel protein type V alpha subunit

Serotonin transporter

Dopamine D3 receptor

Serotonin 6 (5-HT₆) receptor

Sigma opioid receptor

Serotonin 1a (5-HT_{1a}) receptor

HERG

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

Predicted Targets

Transporter

Serotonin transporter

Norepinephrine transporter

Dopamine transporter

Beta-2 adrenergic receptor

Serotonin 1b (5-HT1b) receptor

Inosine-5'-monophosphate dehydrogenase, probable

Beta-1 adrenergic receptor

Cytochrome P450 2D6

Nitric oxide synthase, inducible

Cytochrome P450 1A2

Eflornithine hydrochloride

Molecular Mechanism (initial) :

ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

Predicted Targets

Ornithine decarboxylase

GABA receptor alpha-2 subunit

GABA transporter 4

GABA receptor gamma-1 subunit

Carboxypeptidase B

Aminopeptidase B

Carboxypeptidase B2 isoform A

Farnesyl pyrophosphate synthase

GABA transporter 1

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

Predicted Targets

Epidermal growth factor receptor erbB1

Receptor protein-tyrosine kinase erbB-2

Platelet-derived growth factor receptor beta

Tubulin alpha-1 chain

Mitogen-activated protein kinase 4

Vascular endothelial growth factor receptor 2
ULK3 kinase
Receptor protein-tyrosine kinase erbB-4
MAP kinase-interacting serine/threonine-protein kinase MNK1
Vascular endothelial growth factor receptor 3
Receptor tyrosine-protein kinase erbB-3
Serine/threonine-protein kinase Aurora-A
Vascular endothelial growth factor receptor 1
Serine/threonine-protein kinase GAK
Chaperone activity of bc1 complex-like, mitochondrial
Serine/threonine-protein kinase RIPK2
Serine/threonine-protein kinase Aurora-B
Uncharacterized aarF domain-containing protein kinase 4
Fructose-1,6-bisphosphatase
Ephrin type-A receptor 5
Ephrin type-A receptor 6
Ephrin type-A receptor 8
Serine/threonine-protein kinase MRCK gamma
Fibroblast growth factor receptor 2
MAP kinase signal-integrating kinase 2
Serine/threonine-protein kinase SBK1
Dual specificity mitogen-activated protein kinase kinase 5
Myotonin-protein kinase
Serine/threonine-protein kinase 17B
Serine/threonine-protein kinase SIK2
Citron Rho-interacting kinase
Leukocyte tyrosine kinase receptor
Tyrosine-protein kinase ABL2
Serine/threonine-protein kinase 36
Serine/threonine-protein kinase 10
Ephrin type-B receptor 1
Serine/threonine-protein kinase ULK3
Ephrin type-A receptor 7
Receptor-interacting serine/threonine-protein kinase 4
Tyrosine-protein kinase CSK
Tyrosine-protein kinase SRC
Phosphatidylinositol-5-phosphate 4-kinase type-2 gamma
Serine/threonine-protein kinase TNNI3K
Misshapen-like kinase 1
Casein kinase I epsilon
Mitogen-activated protein kinase kinase kinase 3
Serine/threonine-protein kinase 2
Homeodomain-interacting protein kinase 4
Mitogen-activated protein kinase 6
Ephrin type-B receptor 2
Tyrosine-protein kinase TIE-2
Fibroblast growth factor receptor 1
Serine/threonine-protein kinase 17A
myosin light chain kinase 2
Ephrin type-B receptor 6

Tyrosine-protein kinase TXK
Mitogen-activated protein kinase kinase kinase 2
Tyrosine-protein kinase BLK
Ephrin type-A receptor 3
TRAF2- and NCK-interacting kinase
SPS1/STE20-related protein kinase YSK4
Tyrosine-protein kinase FRK
Tyrosine-protein kinase FGR
Epithelial discoidin domain-containing receptor 1
Tyrosine-protein kinase receptor Tie-1
Ribosomal protein S6 kinase alpha 4
Non-receptor tyrosine-protein kinase TNK1
BMP-2-inducible protein kinase
Serine/threonine-protein kinase SRPK3
G protein-coupled receptor kinase 4
Eukaryotic translation initiation factor 2-alpha kinase 4
Dual specificity mitogen-activated protein kinase kinase 7
Tyrosine-protein kinase receptor RET
Death-associated protein kinase 3
Serine/threonine-protein kinase PLK4
Tyrosine-protein kinase Lyn
Tyrosine-protein kinase receptor FLT3
Serine/threonine-protein kinase Aurora-C
Tyrosine-protein kinase YES
Adaptor-associated kinase
Tyrosine-protein kinase ABL
Casein kinase I delta
Tyrosine-protein kinase receptor UFO
Tyrosine-protein kinase receptor TYRO3
Leucine-rich repeat serine/threonine-protein kinase 2
Tyrosine-protein kinase LCK
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Serine/threonine-protein kinase receptor R3
Serine/threonine-protein kinase SIK3
Ephrin type-A receptor 1
Hormonally up-regulated neu tumor-associated kinase
Tyrosine-protein kinase BMX
Serine/threonine-protein kinase 35
Interleukin-1 receptor-associated kinase 1
Activin receptor type-1
Mitogen-activated protein kinase kinase kinase 4
Tyrosine-protein kinase Srms
Dual specificity testis-specific protein kinase 1
cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A
Phosphorylase kinase gamma subunit 1
Macrophage colony stimulating factor receptor
Interleukin-1 receptor-associated kinase 3
Phosphorylase kinase gamma subunit 2
3-phosphoinositide dependent protein kinase-1
Histone deacetylase 5

Proto-oncogene tyrosine-protein kinase MER
Platelet-derived growth factor receptor alpha
Stem cell growth factor receptor
Interferon-induced, double-stranded RNA-activated protein kinase
Ephrin type-B receptor 4
Tyrosine-protein kinase HCK
Bone morphogenetic protein receptor type-1B
Ephrin type-A receptor 4
Dual specificity mitogen-activated protein kinase kinase 2
Histone deacetylase 9
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing subunit gamma
Mixed lineage kinase 7
Histone deacetylase 7
Serine/threonine-protein kinase 32A
Mitogen-activated protein kinase kinase kinase 5
Tyrosine-protein kinase TEC
Serine/threonine protein kinase NLK
Serine/threonine-protein kinase MRCK beta
Mitogen-activated protein kinase kinase kinase 2
Dual specificity protein kinase CLK4
Ephrin type-A receptor 2
Cell division protein kinase 8
Ribosomal protein S6 kinase alpha 6
Dual specificity protein kinase TTK
ALK tyrosine kinase receptor
CaM kinase II delta
Serine/threonine-protein kinase TBK1
Histone deacetylase 3
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing beta polypeptide
Serine/threonine-protein kinase DCLK3
Histone deacetylase 10
Insulin receptor
Cell division cycle 2-like protein kinase 6
Tyrosine-protein kinase BTK
Serine/threonine-protein kinase Chk2
NUAK family SNF1-like kinase 2
Serine/threonine-protein kinase MRCK-A
AMP-activated protein kinase, alpha-1 subunit
Serine/threonine-protein kinase PIM2
Interleukin-1 receptor-associated kinase 4
Fibroblast growth factor receptor 4
PI4-kinase beta subunit
Ribosomal protein S6 kinase alpha 1
Discoidin domain-containing receptor 2
Serine/threonine-protein kinase SIK1
Histone deacetylase 4
Tyrosine-protein kinase FYN
Cyclin-dependent kinase 7
c-Jun N-terminal kinase 2
Tyrosine-protein kinase TYK2

Tyrosine-protein kinase JAK3
Hepatocyte growth factor receptor
c-Jun N-terminal kinase 3
Tyrosine-protein kinase JAK2
MAP kinase p38 alpha
Histone deacetylase 8
Tyrosine-protein kinase BRK
TGF-beta receptor type II
Mitogen-activated protein kinase kinase kinase kinase 3
Histone deacetylase 6
Mitogen-activated protein kinase kinase kinase kinase 1
Fibroblast growth factor receptor 3
Mitogen-activated protein kinase kinase kinase kinase 4
Histone deacetylase 2
Mitogen-activated protein kinase kinase kinase 7

Everolimus

Molecular Mechanism (initial) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Molecular Mechanism (repurposed) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Predicted Targets

FK506-binding protein 1A

FK506 binding protein 4

Finasteride

Molecular Mechanism (initial) :

**steroid 5alpha reductase inhibitor
androgen receptor antagonist**

Molecular Mechanism (repurposed) :

**steroid 5alpha reductase inhibitor
androgen receptor antagonist**

Predicted Targets

Steroid 5-alpha-reductase 2

Steroid 5-alpha-reductase 1

Cytochrome P450 2C19

Cytochrome P450 2C9

3-beta-hydroxysteroid dehydrogenase/delta 5-->4-isomerase type I

Glucose-6-phosphate 1-dehydrogenase

Fatty acid-binding protein, liver

Androgen Receptor

Testis-specific androgen-binding protein

Progesterone receptor

Mineralocorticoid receptor

C-8 sterol isomerase

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

Predicted Targets

Acetylcholinesterase

Butyrylcholinesterase

Cholinesterase

Glutamate [NMDA] receptor subunit epsilon 2

Mu opioid receptor

Kappa opioid receptor

Delta opioid receptor

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

Predicted Targets

DNA polymerase beta

Ribonuclease pancreatic

Cytidine deaminase

DNA polymerase alpha subunit

Calmodulin-sensitive adenylate cyclase

Thermolysin

Glycogen phosphorylase, muscle form

3-oxoacyl-[acyl-carrier-protein] synthase 3

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

Predicted Targets

Nischarin

Alpha-2b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-1d adrenergic receptor

Alpha-2c adrenergic receptor

Sodium/hydrogen exchanger 1

S-100 protein beta chain

Interleukin-8

P2X purinoceptor 7

Carbonic anhydrase 2

Cyclooxygenase-1

Bcl-2-related protein A1

Fatty acid-binding protein, liver
 Amine oxidase, copper containing
 Beta-secretase 1
 Carbonic anhydrase VA
 Carbonic anhydrase VB
 Fatty acid binding protein muscle
 PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBC
 Acrosin
 Sodium channel protein type II alpha subunit
 Urokinase-type plasminogen activator
 Amiloride-sensitive cation channel 3
 Carbonic anhydrase
 Thrombin
 Acyl coenzyme A:cholesterol acyltransferase
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 2a (5-HT2a) receptor

Ibuprofen

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 inhibitor
 prostaglandin G/H synthase 1 inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 inhibitor
 prostaglandin G/H synthase 1 inhibitor

Predicted Targets

Cyclooxygenase-1

Interleukin-8
 Solute carrier family 22 member 20
 Carboxypeptidase A1
 Neprilysin
 Angiotensin-converting enzyme
 Aminopeptidase N
 Oligopeptide transporter small intestine isoform

Cyclooxygenase-2

Angiotensin-converting enzyme 2
 Zinc aminopeptidase
 Aminopeptidase B
 Tryptophan 5-hydroxylase 1
 Solute carrier family 22 member 6
 NAALADase II
 Leucine aminopeptidase
 Carboxypeptidase B
 Tyrosyl-tRNA synthetase
 Arachidonate 5-lipoxygenase
 Voltage-gated calcium channel alpha2/delta subunit 1
 Glutamate carboxypeptidase II
 Formyl peptide receptor 1
 5-lipoxygenase activating protein

Fatty acid-binding protein, liver
Sphingosine 1-phosphate receptor Edg-8
Sphingosine 1-phosphate receptor Edg-6
Carboxypeptidase B2 isoform A
Sphingosine 1-phosphate receptor Edg-1
Angiotensin-converting enzyme-related carboxypeptidase
Aldo-keto reductase family 1 member C1
Nuclear receptor subfamily 4 group A member 1
Atrial natriuretic factor
Estrogen receptor beta
Leukotriene A-4 hydrolase
Microbial collagenase
Interleukin-8 receptor A
Aldo-keto reductase family 1 member C2
Calpain 1
Peroxisome proliferator-activated receptor gamma
Thermolysin
Carboxypeptidase N, catalytic subunit
Arachidonate 12-lipoxygenase
Beta-chymotrypsin
Serine/threonine-protein kinase Sgk1
Peroxisome proliferator-activated receptor alpha
Peroxisome proliferator-activated receptor delta
Endothelin-converting enzyme 1
Excitatory amino acid transporter 3
Aminopeptidase A
Lysine-specific demethylase 4D-like
Sphingosine 1-phosphate receptor Edg-3
Squalene synthetase
Carbonic anhydrase 2
Leukotriene A4 hydrolase
Seed lipoxygenase-1
Calpain small subunit 1
Serotonin 2b (5-HT2b) receptor
Trypsin
Baculoviral IAP repeat-containing protein 3
Beta-2 adrenergic receptor
Protein-tyrosine phosphatase 1B
Neurokinin 1 receptor
Glutamate receptor ionotropic kainate 1
Arachidonate 15-lipoxygenase
Matrix metalloproteinase-2
Receptor-type tyrosine-protein phosphatase beta
Thyroid hormone receptor alpha

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor
stem cell factor (SCF)
proto-oncogene c-Kit inhibitor

Predicted Targets

Tyrosine-protein kinase ABL

Tyrosine-protein kinase Lyn
Epithelial discoidin domain-containing receptor 1
Tyrosine-protein kinase LCK
Tyrosine-protein kinase ABL2
Discoidin domain-containing receptor 2
Tyrosine-protein kinase BLK
Carbonic anhydrase III
Serine/threonine-protein kinase SMG1
Nucleotide-binding oligomerization domain-containing protein 2
Nucleotide-binding oligomerization domain-containing protein 1
MAP kinase p38 alpha
Tyrosine-protein kinase receptor UFO
Tyrosine-protein kinase JAK2
Glycogen synthase kinase-3 beta
Neuropeptide Y receptor type 2
Histone deacetylase 1
Tyrosine-protein kinase JAK3
Ephrin type-A receptor 8

Platelet-derived growth factor receptor alpha

Mixed lineage kinase 7
Phosphatidylinositol-5-phosphate 4-kinase type-2 gamma
Macrophage colony stimulating factor receptor
Tyrosine-protein kinase FGR

Stem cell growth factor receptor

Serine/threonine-protein kinase TNNI3K
Tyrosine-protein kinase FRK
Lysyl-tRNA synthetase
Serotonin 1b (5-HT1b) receptor
Vascular endothelial growth factor receptor 2
Nicotinamide phosphoribosyltransferase
Tyrosine-protein kinase HCK
Heat shock protein beta-1
Ephrin type-A receptor 3
Ephrin type-A receptor 2
Melanin-concentrating hormone receptor 1
Smoothed homolog
CaM kinase II delta
Insulin receptor
Tyrosine-protein kinase receptor FLT3
Carbonic anhydrase 15
Cell division cycle 2-like protein kinase 6
Serine/threonine-protein kinase B-raf

Tyrosine-protein kinase BMX
Cyclin-dependent kinase 2
Hematopoietic prostaglandin D synthase
Serine/threonine-protein kinase MRCK beta
Macrophage colony-stimulating factor 1 receptor
Cyclin-dependent kinase 4
Ephrin type-B receptor 2
Neuronal acetylcholine receptor protein alpha-7 subunit
Interferon-induced, double-stranded RNA-activated protein kinase
Tyrosine-protein kinase TIE-2
Tyrosine-protein kinase SRC
Ephrin type-A receptor 4
Tyrosine-protein kinase FYN
Serine/threonine-protein kinase Aurora-A
Tyrosine-protein kinase TXK
Homeodomain-interacting protein kinase 4
Platelet-derived growth factor receptor beta
Maternal embryonic leucine zipper kinase
Histone deacetylase 6
Insulin-like growth factor I receptor
Acetylcholinesterase
Ephrin type-A receptor 1
Uncharacterized aarF domain-containing protein kinase 4
Ephrin type-B receptor 3
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase Aurora-B
Ephrin type-A receptor 6
Tyrosine-protein kinase YES
Serine/threonine-protein kinase 17A
ATP-binding cassette sub-family G member 2
Carbonic anhydrase VI
Serine/threonine-protein kinase GAK
Interleukin-1 receptor-associated kinase 1
Carbonic anhydrase XIII
Inhibitor of nuclear factor kappa B kinase alpha subunit
Vascular endothelial growth factor receptor 1
Monoamine oxidase B
P-glycoprotein 1
Tyrosine-protein kinase FES
Ephrin type-A receptor 5
Sonic hedgehog protein
Fibroblast growth factor receptor 3
ALK tyrosine kinase receptor
Rho-associated protein kinase 1
Fibroblast growth factor receptor 2
Calcium-dependent protein kinase 1
Tyrosine-protein kinase CSK
Tyrosine-protein kinase receptor RET
Serine/threonine-protein kinase PLK4
Serine/threonine-protein kinase RAF

Dual specificity protein kinase CLK4
Tyrosine-protein kinase SYK
Serotonin 1d (5-HT1d) receptor
Muscarinic acetylcholine receptor M4
Tyrosine-protein kinase BTK
Ribosomal protein S6 kinase 1
Serotonin 1f (5-HT1f) receptor
Cdc2-related kinase
Cyclin-dependent kinase 1
Protein kinase C alpha
Inhibitor of nuclear factor kappa B kinase beta subunit
Vanilloid receptor
Serine/threonine-protein kinase PAK 1
c-Jun N-terminal kinase 1
Tyrosine-protein kinase TYK2
Dual specificity protein kinase CLK1
c-Jun N-terminal kinase 3
c-Jun N-terminal kinase 2
Serine/threonine-protein kinase RIO2
Serotonin 2c (5-HT2c) receptor
MAP kinase p38 beta
FK506 binding protein 12
Tyrosine-protein kinase receptor Tie-1
Somatostatin receptor 5
Acetylcholine-binding protein
Cyclin-dependent kinase 9
NT-3 growth factor receptor
Receptor protein-tyrosine kinase erbB-4
Mitogen-activated protein kinase kinase kinase 1
Fibroblast growth factor receptor 4
Leukotriene A4 hydrolase
Coagulation factor IX
Ephrin type-B receptor 6
Tyrosine-protein kinase ZAP-70
Histamine H1 receptor
TGF-beta receptor type I
Monoglyceride lipase
Histone deacetylase 3
Vascular endothelial growth factor receptor 3
Mineralocorticoid receptor
Ephrin type-B receptor 4
Apoptosis regulator Bcl-2
Ephrin type-A receptor 7
Dual specificity mitogen-activated protein kinase kinase 5
Tyrosine-protein kinase JAK1
Melanin-concentrating hormone receptor 2
Histone deacetylase 2
Serine/threonine-protein kinase TAO1
Ephrin type-B receptor 1
Serine/threonine-protein kinase TAO3

Diacylglycerol O-acyltransferase 1
Carbonic anhydrase VII
Quinone reductase 2
Carbonic anhydrase XIV
Histone deacetylase 11
Receptor protein-tyrosine kinase erbB-2
Serine/threonine-protein kinase AKT2
Signal transducer and activator of transcription 6
Kallikrein 1
Neurotrophic tyrosine kinase receptor type 2
Epoxide hydratase
Hypoxia-inducible factor prolyl 4-hydroxylase
Vasopressin V2 receptor
Tyrosine-protein kinase BRK
Platelet activating factor receptor
Serine/threonine-protein kinase AKT3
Serine/threonine-protein kinase PLK1
Cholinesterase
Transitional endoplasmic reticulum ATPase
Serine/threonine-protein kinase 10
Beta-2 adrenergic receptor
Carbonic anhydrase IV
Serotonin 2a (5-HT2a) receptor
Histamine H2 receptor
Epidermal growth factor receptor erbB1
Beta-ketoacyl-ACP synthase III
Serine/threonine-protein kinase MST2
Prostanoid EP1 receptor
Trypanothione reductase
Histamine H3 receptor
Voltage-gated T-type calcium channel alpha-1I subunit
Protein kinase C theta
Eukaryotic translation initiation factor 2-alpha kinase 3
Fibroblast growth factor receptor 1
Signal transducer and activator of transcription 3
Urokinase-type plasminogen activator
Carbonic anhydrase XII
Thromboxane-A synthase
Carbonic anhydrase IX
Carbonic anhydrase I
Serotonin transporter
Serine-protein kinase ATR
PI3-kinase p110-alpha subunit
Serotonin 1a (5-HT1a) receptor
Apoptosis regulator Bcl-X
PI3-kinase p110-gamma subunit
Cytochrome P450 11B2
Cathepsin K
Serine/threonine-protein kinase AKT
Beta-1 adrenergic receptor

Serine/threonine-protein kinase RIO1
Cyclin-dependent kinase 7
Coagulation factor X
Carbonic anhydrase II

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of *M. tuberculosis*

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

Predicted Targets

Monoamine oxidase B

Monoamine oxidase A

Protein kinase N2
Cytochrome P450 24A1
Lanosterol 14-alpha demethylase
Sodium channel protein type II alpha subunit
Estrogen-related receptor gamma
Malonyl-CoA decarboxylase
Hypoxia-inducible factor prolyl 4-hydroxylase
Rho-associated protein kinase 1
Signal transducer and activator of transcription 3
Vitronectin receptor alpha
Myeloperoxidase
Peptide deformylase
Protein kinase Pfmrk
Tyrosine-protein kinase ITK/TSK
Epoxide hydrolase 2

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14-alpha demethylase

Molecular Mechanism (repurposed) :

smoothened homolog inhibitor

lanosterol 14-alpha demethylase inhibitor

Predicted Targets

14-alpha sterol demethylase (lanosterol 14-alpha demethylase)

Cytochrome P450 51
Cytochrome P450 3A4
Tyrosine-protein kinase FYN
Cruzipain
Heme oxygenase 1
Heme oxygenase 2
Cytochrome P450 24A1
Arachidonate 15-lipoxygenase
Gonadotropin-releasing hormone receptor
Alpha-1b adrenergic receptor

Ketoconazole

Molecular Mechanism (initial) :

fungal cytochrome P450 51 inhibitor

Molecular Mechanism (repurposed) :

cytochrome P450 aromatase (CYP19A1) inhibitor

Predicted Targets

Cytochrome P450 51

Cytochrome P450 3A4
Cytochrome P450 24A1
Gonadotropin-releasing hormone receptor
Cytochrome P450 17A1
Arachidonate 15-lipoxygenase
Alpha-2b adrenergic receptor
Cytochrome P450 11B1
Heme oxygenase 1
Heme oxygenase 2
Thromboxane-A synthase
14-alpha sterol demethylase
Cytochrome P450 2C19
Indoleamine 2,3-dioxygenase 2
Lanosterol 14-alpha demethylase
Cathepsin S
Cytochrome P450 2C9
Voltage-gated potassium channel subunit Kv1.5
Beta-lactamase
Cytochrome P450 2D6
Progesterone receptor
Cytochrome P450 2J2
Cytochrome P450 1A2
Insulin-like growth factor I receptor
Serotonin 1b (5-HT1b) receptor
Alpha-2a adrenergic receptor

Cytochrome P450 19A1

P-glycoprotein 1
Cytochrome P450 11B2
Muscarinic acetylcholine receptor M2
Neurokinin 2 receptor
Delta opioid receptor
Serotonin transporter
HERG
Tyrosine-protein kinase FYN

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

Predicted Targets

Acyl coenzyme A:cholesterol acyltransferase 1
Formyl peptide receptor 1
Carbonic anhydrase IV
Phosphodiesterase 4A
Poly [ADP-ribose] polymerase 3
Histone deacetylase 3
Carbonic anhydrase II
Carbonic anhydrase I
Cytochrome P450 2D6
Calcium-activated potassium channel subunit alpha-1
Protein-tyrosine phosphatase LC-PTP
Telomerase reverse transcriptase
Tyrosine-protein kinase LCK
Interleukin-8
Sonic hedgehog protein
Angiotensin-converting enzyme
Cyclooxygenase-2
Proteinase-activated receptor 1
Orexin receptor 2
Fructose-1,6-bisphosphatase
Cyclophilin A
Cyclooxygenase-1
Sodium channel protein type II alpha subunit
Palmitoyl-CoA oxidase
Thromboxane A2 receptor

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

Predicted Targets

Glutamate [NMDA] receptor subunit epsilon 3
Glutamate (NMDA) receptor subunit zeta 1

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

Predicted Targets

Diamine oxidase

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :
dihydrofolate reductase inhibitor

Predicted Targets

Dihydrofolate reductase

Folylpoly-gamma-glutamate synthetase
Thymidylate synthase
Pteridine reductase 1
GAR transformylase
Folate receptor alpha
Carboxypeptidase G2
Proton-coupled folate transporter
Glutamate carboxypeptidase II
Thymidylate synthase (EC 2.1.1.45) (TS) (TSase)
NAALADase II
AICAR transformylase
Cholecystokinin B receptor
Carbonic anhydrase II
Cholecystokinin A receptor
Glutathione reductase
Carbonic anhydrase IV
Carbonic anhydrase I
Carbonic anhydrase IX

Milnacipran

Molecular Mechanism (initial) :
5-HT and norepinephrine reuptake inhibitor
Molecular Mechanism (repurposed) :
5-HT and norepinephrine reuptake inhibitor

Predicted Targets

Norepinephrine transporter
Transporter
Serotonin transporter
Dopamine transporter

Neurokinin 3 receptor
Sigma-1 receptor
Delta opioid receptor
Pancreatic alpha-amylase
Muscarinic acetylcholine receptor M1
Mu opioid receptor
Monoamine oxidase B

Miltefosine

Molecular Mechanism (initial) :
Akt/PKB inhibitor
Molecular Mechanism (repurposed) :
phosphatidyl-choline biosynthesis inhibitor

Predicted Targets

Lysophosphatidic acid receptor Edg-7
Dynamin-1
Phospholipase A2 group 1B
Monoglyceride lipase
Lysophosphatidic acid receptor Edg-2
Fibronectin-binding protein C
Phospholipase C
Anandamide amidohydrolase
Group IID secretory phospholipase A2
Carnitine palmitoyltransferase 1A
Group VII phospholipase A2
Acetylcholinesterase
Phospholipase A2 group IIC
Muscarinic acetylcholine receptor M1
Carbonic anhydrase III
Muscarinic acetylcholine receptor M2
Cannabinoid CB1 receptor
Muscarinic acetylcholine receptor M4
Carbonic anhydrase IV
Acetylcholine receptor protein delta chain
Carbonic anhydrase XIII
Carbonic anhydrase VB
Lysophosphatidic acid receptor Edg-4

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

Predicted Targets

Not results

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

Predicted Targets

Human immunodeficiency virus type 1 protease

Cytochrome P450 3A4

Progesterone receptor

Tyrosine-protein kinase FYN

Neurokinin 2 receptor

Dopamine D1 receptor

Mu opioid receptor

Adenosine A3 receptor

Norepinephrine transporter
Human rhinovirus A protease
Angiotensin-converting enzyme
Formyl peptide receptor 1

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor
proto-oncogene c-Kit inhibitor

Predicted Targets

Tyrosine-protein kinase Lyn

Tyrosine-protein kinase ABL

Tyrosine-protein kinase LCK

Epithelial discoidin domain-containing receptor 1

Tyrosine-protein kinase ABL2

Discoidin domain-containing receptor 2

Serine/threonine-protein kinase MRCK beta

Tyrosine-protein kinase HCK

Serine/threonine-protein kinase B-raf

Carbonic anhydrase III

Tyrosine-protein kinase TIE-2

Tyrosine-protein kinase FRK

Ephrin type-A receptor 8

Mixed lineage kinase 7

Ephrin type-B receptor 2

Phosphatidylinositol-5-phosphate 4-kinase type-2 gamma

Ephrin type-A receptor 4

Tyrosine-protein kinase BLK

Ephrin type-A receptor 3

Ephrin type-A receptor 1

ParE

Vascular endothelial growth factor receptor 2

Serine/threonine-protein kinase TNKI3K

Calcium-dependent protein kinase 1

Ephrin type-B receptor 3

Tyrosine-protein kinase FGR

Ephrin type-A receptor 6

Carbonic anhydrase 15

Tyrosine-protein kinase SRC

Stem cell growth factor receptor

Ephrin type-A receptor 5

Ephrin type-A receptor 2

Platelet-derived growth factor receptor alpha

MAP kinase p38 alpha

Tyrosine-protein kinase receptor Tie-1

Neurotrophic tyrosine kinase receptor type 2

Insulin receptor

Tyrosine-protein kinase BMX
DNA gyrase subunit B
Cytoplasmic tyrosine-protein kinase BMX
Serine/threonine-protein kinase SMG1
CaM kinase II delta
NT-3 growth factor receptor
Mitogen-activated protein kinase kinase kinase kinase 1
Ephrin type-B receptor 6
MAP kinase p38 beta
Dual specificity mitogen-activated protein kinase kinase 5
Tyrosine-protein kinase YES
Serine/threonine-protein kinase TAO1
Tyrosine-protein kinase FYN
Platelet-derived growth factor receptor beta
Tyrosine-protein kinase CSK
Ephrin type-B receptor 1
Receptor-type tyrosine-protein kinase FLT3
Mitogen-activated protein kinase 9
Proto-oncogene tyrosine-protein kinase ROS
ALK tyrosine kinase receptor
Proto-oncogene tyrosine-protein kinase receptor Ret

Mast/stem cell growth factor receptor Kit

Tyrosine-protein kinase FES
Uncharacterized aarF domain-containing protein kinase 4
Histone deacetylase 1
Carbonic anhydrase VI
Serine/threonine-protein kinase TAO3
Macrophage colony stimulating factor receptor
Carbonic anhydrase XIII
Serine/threonine-protein kinase 10
Ephrin type-B receptor 4
Dual specificity protein kinase CLK4
Dual specificity protein kinase CLK1
Tyrosine-protein kinase JAK3
Proto-oncogene c-JUN
Tyrosine-protein kinase SYK
Tyrosine-protein kinase ZAP-70
Smoothed homolog
Cell division cycle 2-like protein kinase 6
Lysyl-tRNA synthetase
Interferon-induced, double-stranded RNA-activated protein kinase
Homeodomain-interacting protein kinase 4
Tyrosine-protein kinase BTK
Tyrosine-protein kinase TXK
Protein kinase C alpha
Serine/threonine-protein kinase RAF
c-Jun N-terminal kinase 1
c-Jun N-terminal kinase 2
c-Jun N-terminal kinase 3
Tyrosine-protein kinase receptor RET

Carbonic anhydrase VII
 Maternal embryonic leucine zipper kinase
 Histone deacetylase 6
 Probable low molecular weight protein-tyrosine-phosphatase
 Mitogen-activated protein kinase kinase kinase 5
 Serine/threonine-protein kinase 17A
 Epoxide hydratase
 Metabotropic glutamate receptor 5
 Glycogen synthase kinase-3 beta
 Fibroblast growth factor receptor 3
 Serine/threonine-protein kinase GAK
 Interleukin-1 receptor-associated kinase 1
 Sonic hedgehog protein
 Carbonic anhydrase XIV
 Carbonic anhydrase IV
 Carbonic anhydrase VA
 Cyclin-dependent kinase 2
 Receptor protein-tyrosine kinase erbB-2
 Serine/threonine-protein kinase PLK4
 Insulin-like growth factor 1 receptor
 Beta-ketoacyl-ACP synthase III
 Histone deacetylase 11
 Vascular endothelial growth factor receptor 1
 Tyrosine-protein kinase BRK
 Insulin-like growth factor I receptor
 MAP kinase ERK2
 Cyclin-dependent kinase 4
 Nerve growth factor receptor Trk-A
 Natural resistance-associated macrophage protein 2
 Coagulation factor IX
 Carbonic anhydrase XII
 Carbonic anhydrase IX
 Carbonic anhydrase I
 Carbonic anhydrase II
 Serine-protein kinase ATR

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Predicted Targets

4-hydroxyphenylpyruvate dioxygenase

Plasminogen activator inhibitor-1
 Thioredoxin reductase
 Nuclear factor NF-kappa-B p65 subunit
 Carboxylesterase 2
 Monoacylglycerol lipase ABHD6
 Androgen Receptor

Calcium-activated potassium channel subunit alpha-1
Aldo-keto reductase family 1 member C1
Carbonic anhydrase II
Protoporphyrinogen oxidase
Protein kinase Pfmrk
Myeloperoxidase

Paclitaxel

Molecular Mechanism (initial) :
tubulin beta modulator (microtubule-stabilizing agent)
Molecular Mechanism (repurposed) :
tubulin beta modulator (microtubule-stabilizing agent)

Predicted Targets

Not results

Phentolamine mesilate

Molecular Mechanism (initial) :
alpha-adrenoceptor antagonist
Molecular Mechanism (repurposed) :
alpha-adrenoceptor antagonist

Predicted Targets

Alpha-2a adrenergic receptor

Nischarin

Alpha-2b adrenergic receptor

Cytochrome P450 2D6

Alpha-1b adrenergic receptor

Alpha-2c adrenergic receptor

Alpha-1a adrenergic receptor

Alpha-1d adrenergic receptor

Trace amine-associated receptor 1

Serotonin 1b (5-HT1b) receptor

Serotonin 1d (5-HT1d) receptor

Serotonin 2b (5-HT2b) receptor

Serotonin 2c (5-HT2c) receptor

Serotonin 2a (5-HT2a) receptor

Raloxifene hydrochloride

Molecular Mechanism (initial) :
estrogen receptor agonist
Molecular Mechanism (repurposed) :
estrogen receptor agonist

Predicted Targets

Estrogen receptor alpha

Estrogen receptor beta

3-beta-hydroxysteroid-delta(8),delta(7)-isomerase

C-8 sterol isomerase

Leukotriene A4 hydrolase

Histamine H3 receptor
Solute carrier family 22 member 12
Bone morphogenetic protein 4
Prostaglandin-H2 D-isomerase
Tyrosine kinase non-receptor protein 2
Tyrosine-protein kinase YES
HERG
Cytochrome P450 2C9
Serotonin 3a (5-HT3a) receptor
MAP kinase-interacting serine/threonine-protein kinase MNK1
Transporter
Ephrin type-A receptor 2
Advanced glycosylation end product-specific receptor
Quinolone resistance protein norA
Tyrosine-protein kinase receptor FLT3
Glutamate [NMDA] receptor subunit 3A
Thrombin
Hepatocyte growth factor receptor
Serine/threonine-protein kinase PIM3
Activated CDC42 kinase 1
Ribosomal protein S6 kinase alpha 1
Tyrosine-protein kinase LCK
Phospholipase D2
Phospholipase D1
Tyrosine-protein kinase FYN
Alpha-1b adrenergic receptor
Serine/threonine-protein kinase PIM1
Melanin-concentrating hormone receptor 1
Thyroid hormone receptor alpha
Tyrosine-protein kinase SRC
Multidrug resistance-associated protein 1
Serine/threonine-protein kinase Chk2
Vascular endothelial growth factor receptor 1
Tyrosine-protein kinase CSK
Butyrylcholinesterase
Serine/threonine-protein kinase Chk1
Serine/threonine-protein kinase TBK1
Histamine H1 receptor
Vascular endothelial growth factor receptor 2
Serotonin 4 (5-HT4) receptor
Voltage-gated potassium channel subunit Kv7.1
Tyrosine-protein kinase JAK3
Telomerase reverse transcriptase
Serotonin 1b (5-HT1b) receptor
Serotonin 2b (5-HT2b) receptor
Acetylcholinesterase
Dopamine D1 receptor
Alpha-1d adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor

Sigma opioid receptor
Alpha-2a adrenergic receptor
Neurokinin 2 receptor
Dopamine D3 receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 2a (5-HT2a) receptor
Dopamine D2 receptor
Serotonin 6 (5-HT6) receptor
Norepinephrine transporter
Kappa opioid receptor
Dopamine transporter
Mu opioid receptor
Delta opioid receptor
Serotonin transporter
Matrix metalloproteinase 9
15-hydroxyprostaglandin dehydrogenase [NAD+]
Adenosine A2a receptor

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :

dopamine D2 and D3 receptor agonist

Predicted Targets

Dopamine D2 receptor

Dopamine D3 receptor

Serotonin 1a (5-HT1a) receptor
Chitin synthase 1
Malate dehydrogenase, mitochondrial
Puromycin-sensitive aminopeptidase
Sigma opioid receptor
D-amino-acid oxidase
Cyclin-dependent kinase 1
Serotonin 1d (5-HT1d) receptor
Transcriptional regulator ERG
Glycogen synthase kinase-3 beta

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :

phospho-diesterase (PDE5A) inhibitor

Predicted Targets

Phosphodiesterase 5A

Phosphodiesterase 6C
Rod cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha
Phosphodiesterase 6A
Indoleamine 2,3-dioxygenase 2

Phosphodiesterase 3B
Phosphodiesterase 11A
Phosphodiesterase 9A
Alpha-1b adrenergic receptor
Hypoxia-inducible factor 1 alpha

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Predicted Targets

HMG-CoA reductase

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

Predicted Targets

Retinoid X receptor gamma

Retinoid X receptor beta

Retinoid X receptor alpha

Retinoic acid receptor alpha

Retinoic acid receptor beta

Retinoic acid receptor gamma

Carbonic anhydrase

Gonadotropin-releasing hormone receptor

Ornithine decarboxylase

Glutamate receptor ionotropic kainate 2

Tetrabenazine

Molecular Mechanism (initial) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Predicted Targets

Synaptic vesicular amine transporter

Orexin receptor 2

Orexin receptor 1

Acetylcholinesterase

Melatonin receptor 1B

Putative hydrolase RBBP9

Dipeptidyl peptidase IV

Dopamine D1 receptor
Small conductance calcium-activated potassium channel protein 1
Carbonic anhydrase XIV
Small conductance calcium-activated potassium channel protein 2
Carbonic anhydrase VII
Small conductance calcium-activated potassium channel protein 3
Dopamine D5 receptor
Carbonic anhydrase IX

Thalidomide

Molecular Mechanism (initial) :

TNF-alpha production inhibitor

Molecular Mechanism (repurposed) :

cereblon (CRBN) inhibitor

Predicted Targets

Cyclooxygenase-1
Cyclooxygenase-2
Ribonuclease H1
Flap endonuclease 1
DNA excision repair protein ERCC-5
Transthyretin

Topiramate

Molecular Mechanism (initial) :

kainate receptor antagonist

AMPA receptor antagonists

carbonic anhydrase type II inhibitor

sodium channel blocker

Molecular Mechanism (repurposed) :

ckainate receptor antagonist

AMPA receptor antagonists

carbonic anhydrase type II inhibitor

sodium channel blocker

Predicted Targets

Carbonic anhydrase VII
Carbonic anhydrase
Astrosclerin-3
Carbonic anhydrase VA
Carbonic anhydrase XIII

Carbonic anhydrase 2

Alpha carbonic anhydrase
Carbonic anhydrase XIV
Carbonic anhydrase VB
Carbonic anhydrase 15
Carbonic anhydrase VI
Carbonic anhydrase IV
Carbonic anhydrase 1
Uncharacterized protein Rv1284/MT1322

Carbonic anhydrase IX

PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBC

Carbonic anhydrase I

Carbonic anhydrase XII

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

Predicted Targets

Estrogen-related receptor gamma

Quinolone resistance protein norA

3-beta-hydroxysteroid-delta(8),delta(7)-isomerase

C-8 sterol isomerase

Activated CDC42 kinase 1

Leukotriene A4 hydrolase

Estrogen receptor alpha

Estrogen receptor beta

P-glycoprotein 1

Tyrosine kinase non-receptor protein 2

Cyclooxygenase-2

Serine-threonine protein phosphatase 2A regulatory subunit

Transforming growth factor beta-1

Histamine H1 receptor

Progesterone receptor

Phospholipase D2

Lanosterol synthase

Cytochrome P450 2D6

Muscarinic acetylcholine receptor M4

Arachidonate 12-lipoxygenase

PH domain leucine-rich repeat-containing protein phosphatase 2

Muscarinic acetylcholine receptor M5

Peroxisome proliferator-activated receptor gamma

Tyrosine-protein kinase FYN

Galanin receptor 3

Alpha-2b adrenergic receptor

Sigma opioid receptor

Tyrosine-protein kinase SRC

HERG

Platelet-derived growth factor receptor beta

Thyroid hormone receptor alpha

Serine/threonine-protein kinase B-raf

Histamine H2 receptor

Serotonin 2b (5-HT2b) receptor

Phospholipase D1

Farnesyl pyrophosphate synthase

Arachidonate 5-lipoxygenase

Muscarinic acetylcholine receptor M1

Beta-3 adrenergic receptor
Acetylcholinesterase

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

Predicted Targets

Histone deacetylase 10

Histone deacetylase 3

Histone deacetylase 6

Histone deacetylase HD2

Histone deacetylase 8

Histone deacetylase 1

Histone deacetylase HD1B

Histone deacetylase 2

Histone deacetylase

Histone deacetylase 9

Histone deacetylase 5

Histone deacetylase 7

Histone deacetylase 11

Beta-2 adrenergic receptor

Aminopeptidase N

Leukotriene A4 hydrolase

Neprilysin

Histone deacetylase 4

Histone deacetylase-like amidohydrolase

Autotaxin

Zinc aminopeptidase

Thromboxane A2 receptor

RAC-alpha serine/threonine-protein kinase

Peptide deformylase

N-acylsphingosine-amidohydrolase

Serine-protein kinase ATR

Acyl coenzyme A:cholesterol acyltransferase 2

Matrix metalloproteinase-1

Bone morphogenetic protein 1

Glycogen synthase kinase-3 alpha

Leukocyte common antigen

Voltage-gated T-type calcium channel alpha-1G subunit

Excitatory amino acid transporter 2

Matrix metalloproteinase 8

Matrix metalloproteinase 3

Cyclophilin A

3-oxoacyl-[acyl-carrier-protein] synthase 3

Acyl coenzyme A:cholesterol acyltransferase 1

Transient receptor potential cation channel subfamily M member 8

Receptor-type tyrosine-protein phosphatase F (LAR)

Protein-tyrosine phosphatase 1E
Acyl coenzyme A:cholesterol acyltransferase
Melatonin receptor 1B
Matrix metalloproteinase-2
Lanosterol 14-alpha demethylase
Epoxide hydratase
Excitatory amino acid transporter 3
Transient receptor potential cation channel subfamily A member 1
S-100 protein beta chain
Arachidonate 12-lipoxygenase
Matrix metalloproteinase 10
Anandamide amidohydrolase
Proteinase-activated receptor 1
Neuropeptide Y receptor type 5
Group VII phospholipase A2
Glutathione reductase
Carbonic anhydrase VA
Matrix metalloproteinase 16
Leukocyte adhesion molecule-1
Lysine-specific demethylase 2A
Histone lysine demethylase PHF8
Carbonic anhydrase IX
Carbonic anhydrase VB
Matrix metalloproteinase 7
Cysteine protease falcipain-3
Histamine H1 receptor
Tyrosinase
Serotonin 1b (5-HT1b) receptor
Adenylate cyclase type V
UDP-3-O-acyl-GlcNAc deacetylase
Serine-protein kinase ATM
Matrix metalloproteinase 9
P-selectin
Carbonic anhydrase II
Aldose reductase
Melatonin receptor 1A
Matrix metalloproteinase 12
Carbonic anhydrase IV
Trypanothione reductase
Matrix metalloproteinase 14
Sn1-specific diacylglycerol lipase alpha
Caspase-2
Epidermal growth factor receptor erbB1
Telomerase reverse transcriptase
Thermolysin
Carbonic anhydrase XII
NAD-dependent deacetylase sirtuin 2
Arachidonate 15-lipoxygenase
Arachidonate 5-lipoxygenase
Muscarinic acetylcholine receptor M1

Acrosin
Carbonic anhydrase I
Excitatory amino acid transporter 1
Calmodulin-domain protein kinase 1
Protein-arginine N-methyltransferase 1
Plasminogen activator inhibitor-1
Myeloperoxidase
Lysine-specific demethylase 4D-like
Nicotinamide phosphoribosyltransferase
Hydroxycarboxylic acid receptor 2
Carboxylesterase 2
Glycogen synthase kinase-3 beta
Diacylglycerol O-acyltransferase 1
Human immunodeficiency virus type 1 reverse transcriptase
Dehydrosqualene synthase
Trypsin
T-cell protein-tyrosine phosphatase
Botulinum neurotoxin type A
Receptor protein-tyrosine kinase erbB-2
Furin
Methionyl-tRNA synthetase
Prostanoid FP receptor
Leukotriene B4 receptor 1
Matrix metalloproteinase 13
Dihydroorotate dehydrogenase
Caspase-6
Peptide N-myristoyltransferase 1
N-acylethanolamine-hydrolyzing acid amidase
Hematopoietic cell protein-tyrosine phosphatase 70Z-PEP
Cytochrome P450 2D6
Endothelin-converting enzyme 1
Selectin E
Caspase-3
Carbonic anhydrase VII
Phospholipase A2 group 1B
Sphingosine kinase 1
Cytochrome P450 3A4
Adenosine kinase
Aldo-keto reductase family 1 member C2
Natural resistance-associated macrophage protein 2
PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBC
Undecaprenyl pyrophosphate synthase
Cannabinoid CB2 receptor
Glutamate carboxypeptidase II
Trace amine-associated receptor 1
Vanilloid receptor
Monoglyceride lipase
Phospholipase A2 group IIA
Monoamine oxidase A
Calcium-activated potassium channel subunit alpha-1

Uncharacterized protein Rv1284/MT1322
3C-like protease
Inosine-5'-monophosphate dehydrogenase, probable
Adenosine deaminase
Tryptase beta-1
Serotonin 1d (5-HT1d) receptor
Cannabinoid CB1 receptor

Supplement 3

Biological activity profile predicted with SwissTargetPrediction

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

Predicted Targets

Mu-type opioid receptor

Delta-type opioid receptor
Kappa-type opioid receptor
Nociceptin receptor
Renin
Cathepsin D
Napsin-A
C-C chemokine receptor type 1
C-C chemokine receptor type 2
C-C chemokine receptor type 3
C-C chemokine receptor type 5
Beta-secretase 1
Beta-secretase 2
Neuronal acetylcholine receptor subunit alpha-7
CHRNA7-FAM7A fusion protein

Alprostadi

Molecular Mechanism (initial) :

prostaglandin E2 receptor agonist

Molecular Mechanism (repurposed) :

prostaglandin E2 receptor agonist

Predicted Targets

Prostaglandin E2 receptor EP1 subtype
Prostaglandin E2 receptor EP4 subtype
Prostaglandin E2 receptor EP2 subtype
Prostacyclin receptor
Prostaglandin D2 receptor
Prostaglandin E2 receptor EP3 subtype
Solute carrier family 22 member 6

Solute carrier family 22 member 10
Solute carrier family 22 member 25
Solute carrier family 22 member 9
Solute carrier family 22 member 24
Peroxisome proliferator-activated receptor gamma
Peroxisome proliferator-activated receptor delta
Peroxisome proliferator-activated receptor alpha
Prostaglandin F2-alpha receptor

Amantadine hydrochloride

Molecular Mechanism (initial) :

matrix protein 2 (Influenza virus A) inhibitor

Molecular Mechanism (repurposed) :

dopamine receptor agonists

NMDA receptor antagonists

Predicted Targets

Sigma non-opioid intracellular receptor 1
Alpha-trypsin chain 1
Trypsin-2
Trypsin-3
Glutamate receptor ionotropic
Complex
Complex
Glutamate receptor ionotropic
Nischarin
Tyrosyl-DNA phosphodiesterase 1
Dynamin-1
N-acyl ethanolamine-hydrolyzing acid amidase subunit alpha
Dynamin-2
Dynamin-3
Complex

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

Predicted Targets

Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Alpha-2A adrenergic receptor
Muscarinic acetylcholine receptor M1
D(2) dopamine receptor
Alpha-2B adrenergic receptor
Alpha-2C adrenergic receptor
Muscarinic acetylcholine receptor M3
D(1A) dopamine receptor

D(4) dopamine receptor

D(1B) dopamine receptor

Sodium-dependent noradrenaline transporter

Histamine H2 receptor

Alpha-1D adrenergic receptor

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

Predicted Targets

D(2) dopamine receptor

5-hydroxytryptamine receptor 1A

D(1A) dopamine receptor

D(4) dopamine receptor

D(1B) dopamine receptor

5-hydroxytryptamine receptor 1B

5-hydroxytryptamine receptor 7

D(3) dopamine receptor

Potassium voltage-gated channel subfamily H member 2

Sigma non-opioid intracellular receptor 1

Tyrosyl-DNA phosphodiesterase 1

Potassium voltage-gated channel subfamily H member 6

Potassium voltage-gated channel subfamily H member 7

Microtubule-associated protein tau

FAD-linked sulfhydryl oxidase ALR

Acetylsalicylic acid

Molecular Mechanism (initial) :

cyclooxygenase inhibitor

Molecular Mechanism (repurposed) :

cyclooxygenase inhibitor

Predicted Targets

Prostaglandin G/H synthase 1

Prostaglandin G/H synthase 2

Sodium-dependent noradrenaline transporter

Sodium-dependent serotonin transporter

Sodium- and chloride-dependent glycine transporter 1

Sodium-dependent dopamine transporter

Sodium-dependent proline transporter

Sodium- and chloride-dependent neutral and basic amino acid transporter B(0+)

Sodium- and chloride-dependent glycine transporter 2

Muscleblind-like protein 1

Muscleblind-like protein 2

Muscleblind-like protein 3

Carbonic anhydrase 1

Carbonic anhydrase 2

Carbonic anhydrase 3

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

Predicted Targets

Complex

Adenosine receptor A3

Gamma-aminobutyric acid type B receptor subunit 1

Voltage-dependent calcium channel subunit delta-1

Carbonic anhydrase 12

Carbonic anhydrase 1

Carbonic anhydrase 2

Carbonic anhydrase 5A

Carbonic anhydrase 7

Carbonic anhydrase 9

Carbonic anhydrase 14

Carbonic anhydrase 5B

Carbonic anhydrase 13

Carbonic anhydrase 3

Alkaline phosphatase

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

Predicted Targets

Sigma non-opioid intracellular receptor 1

Nitric oxide synthase

Nitric oxide synthase

Nitric oxide synthase

Tyrosyl-DNA phosphodiesterase 1

Activation peptide fragment 1

Sodium channel protein type 2 subunit alpha

Sodium channel protein type 1 subunit alpha

Sodium channel protein type 9 subunit alpha

Sodium channel protein type 3 subunit alpha

Sodium channel protein type 8 subunit alpha

Glutamate receptor ionotropic

Glutamate receptor ionotropic

Neutrophil elastase

Azurocidin

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

Predicted Targets

Endothelin B receptor

Endothelin-1 receptor

Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Tyrosyl-DNA phosphodiesterase 1

5-hydroxytryptamine receptor 6

FAD-linked sulfhydryl oxidase ALR

Fructose-1

Fructose-1

Phosphatidylinositol 4

Phosphatidylinositol 4

Phosphatidylinositol 4

Phosphatidylinositol 4

Corticotropin-releasing factor receptor 1

Corticotropin-releasing factor receptor 2

Tyrosine-protein kinase Lck

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :

mu-type opioid receptor agonist

Predicted Targets

Mu-type opioid receptor

Delta-type opioid receptor

Kappa-type opioid receptor

Nociceptin receptor

Potassium voltage-gated channel subfamily H member 2

Potassium voltage-gated channel subfamily H member 6

Potassium voltage-gated channel subfamily H member 7

Sigma non-opioid intracellular receptor 1

Muscarinic acetylcholine receptor M2

Muscarinic acetylcholine receptor M4

Muscarinic acetylcholine receptor M5

Muscarinic acetylcholine receptor M1

Muscarinic acetylcholine receptor M3

5-hydroxytryptamine receptor 2A

C-C chemokine receptor type 2

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Predicted Targets

Carbonic anhydrase 12
Carbonic anhydrase 1
Carbonic anhydrase 2
Carbonic anhydrase 3
Cytochrome P450 2D6
Alpha-2B adrenergic receptor
Carbonic anhydrase 4
Prostaglandin G/H synthase 1
Carbonic anhydrase 6
Sodium-dependent noradrenaline transporter
Sodium-dependent serotonin transporter
Lipid-phosphate phosphatase
Carbonic anhydrase 5A
Prostaglandin G/H synthase 2
Carbonic anhydrase 7

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

Predicted Targets

Major prion protein
Microtubule-associated protein tau
NAD(P)H dehydrogenase [quinone] 1
Ribosylidihydronicotinamide dehydrogenase [quinone]
Potassium voltage-gated channel subfamily H member 2
Potassium voltage-gated channel subfamily H member 6
Potassium voltage-gated channel subfamily H member 7
Tyrosyl-DNA phosphodiesterase 1
Histamine N-methyltransferase
Histamine H3 receptor
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M3

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

Predicted Targets

Major prion protein
Tyrosine-protein kinase Fyn

Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M4
Multidrug resistance protein 1
5-hydroxytryptamine receptor 1A
Muscarinic acetylcholine receptor M5
Alpha-2A adrenergic receptor
Muscarinic acetylcholine receptor M1

D(2) dopamine receptor

Alpha-2B adrenergic receptor
Alpha-2C adrenergic receptor
Muscarinic acetylcholine receptor M3
Substance-K receptor
D(1A) dopamine receptor

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :

TNF- α /NF- κ b signaling pathway inhibitor

Predicted Targets

Microtubule-associated protein tau
Signal transducer and activator of transcription 3
Signal transducer and activator of transcription 1-alpha/beta
Signal transducer and activator of transcription 2
Signal transducer and activator of transcription 4
Tyrosine-protein phosphatase non-receptor type 2
Tyrosine-protein phosphatase non-receptor type 1
Protein kinase C gamma type
Protein kinase C beta type
Protein kinase C alpha type
Protein kinase C theta type
Protein kinase C delta type regulatory subunit
Tyrosyl-DNA phosphodiesterase 1
Ribosomal protein S6 kinase alpha-5
Ribosomal protein S6 kinase alpha-1

Doxepin hydrochloride

Molecular Mechanism (initial) :

5HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

H1 and H2 histamine receptor blocker

Predicted Targets

Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Alpha-2A adrenergic receptor
Muscarinic acetylcholine receptor M1
D(2) dopamine receptor

Alpha-2B adrenergic receptor
Alpha-2C adrenergic receptor
Muscarinic acetylcholine receptor M3
D(1A) dopamine receptor
D(4) dopamine receptor
D(1B) dopamine receptor

Sodium-dependent noradrenaline transporter

Histamine H2 receptor

Alpha-1D adrenergic receptor

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

Predicted Targets

Sodium-dependent noradrenaline transporter

Sodium-dependent serotonin transporter

Sodium- and chloride-dependent glycine transporter 1

Sodium-dependent dopamine transporter

Potassium voltage-gated channel subfamily H member 2

Sodium- and chloride-dependent glycine transporter 2

Histamine H3 receptor

Sodium-dependent proline transporter

Sodium- and chloride-dependent neutral and basic amino acid transporter B(0+)

Potassium voltage-gated channel subfamily H member 6

Potassium voltage-gated channel subfamily H member 7

Mu-type opioid receptor

Delta-type opioid receptor

5-hydroxytryptamine receptor 1A

5-hydroxytryptamine receptor 1B

Eflornithine hydrochloride

Molecular Mechanism (initial) :

ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

Predicted Targets

Ornithine decarboxylase

Metabotropic glutamate receptor 8

Metabotropic glutamate receptor 6

Metabotropic glutamate receptor 2

Metabotropic glutamate receptor 3

Metabotropic glutamate receptor 4

Metabotropic glutamate receptor 7

Glutamate receptor ionotropic

Glutamate receptor ionotropic

Glutamate receptor ionotropic

Carboxypeptidase B2
Carboxypeptidase A6
Glutamate receptor 1
Glutamate receptor 2
Glutamate receptor 3

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

Predicted Targets

Serine/threonine-protein kinase PLK4
Citron Rho-interacting kinase
Aurora kinase A
Cyclin-G-associated kinase
Ephrin type-B receptor 6
Death-associated protein kinase 3
Receptor-interacting serine/threonine-protein kinase 2
Tyrosine-protein kinase JAK2
Ribosomal protein S6 kinase alpha-4
Serine/threonine-protein kinase 17B
Serine/threonine-protein kinase 10
Mitogen-activated protein kinase kinase kinase 4
Tyrosine-protein kinase ABL1

Epidermal growth factor receptor

Receptor tyrosine-protein kinase erbB-2

Everolimus

Molecular Mechanism (initial) :

FK506-binding protein 12 inhibitor

mTOR inhibitor

Molecular Mechanism (repurposed) :

FK506-binding protein 12 inhibitor

mTOR inhibitor

Predicted Targets

Serine/threonine-protein kinase mTOR
Peptidyl-prolyl cis-trans isomerase FKBP1A
Peptidyl-prolyl cis-trans isomerase FKBP4
Peptidyl-prolyl cis-trans isomerase FKBP1B
Peptidyl-prolyl cis-trans isomerase FKBP5
Peptidyl-prolyl cis-trans isomerase
Eukaryotic translation initiation factor 4E
Cytochrome P450 3A4
Microtubule-associated protein tau
Cytochrome P450 2C9
Cytochrome P450 2C19
Programmed cell death protein 4

Eukaryotic translation initiation factor 4E type 1B
Cytochrome P450 3A5
Cytochrome P450 3A7

Finasteride

Molecular Mechanism (initial) :

steroid 5alpha reductase inhibitor
androgen receptor antagonist

Molecular Mechanism (repurposed) :

steroid 5alpha reductase inhibitor
androgen receptor antagonist

Predicted Targets

3-oxo-5-alpha-steroid 4-dehydrogenase 1 (steroid-5-alpha-reductase)

3-oxo-5-alpha-steroid 4-dehydrogenase 2 (steroid-5-alpha-reductase)

Cytochrome P450 2C9

Cytochrome P450 2C19

Cytochrome P450 2E1

Cytochrome P450 2C8

Cytochrome P450 2A6

Cytochrome P450 2B6

Cytochrome P450 2A7

Cytochrome P450 2F1

Cytochrome P450 2C18

Cytochrome P450 2A13

Androgen receptor

Potassium voltage-gated channel subfamily H member 2

Potassium voltage-gated channel subfamily H member 6

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

Predicted Targets

Cholinesterase

Acetylcholinesterase

Mu-type opioid receptor

Delta-type opioid receptor

Kappa-type opioid receptor

Nociceptin receptor

Sigma non-opioid intracellular receptor 1

Muscleblind-like protein 1

Muscleblind-like protein 2

Muscleblind-like protein 3

Cannabinoid receptor 1

Cannabinoid receptor 2

5-hydroxytryptamine receptor 2A

Potassium voltage-gated channel subfamily H member 2

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

Predicted Targets

Thymidylate synthase
Mitogen-activated protein kinase 1
Mitogen-activated protein kinase 3
Mitogen-activated protein kinase 4
Mitogen-activated protein kinase 7
Mitogen-activated protein kinase 6
Deoxycytidine kinase
Deoxyguanosine kinase
Microtubule-associated protein tau
Adenosine kinase
S-adenosylmethionine decarboxylase alpha chain
Tyrosyl-DNA phosphodiesterase 1
Dual specificity tyrosine-phosphorylation-regulated kinase 1A
Dihydrofolate reductase
Dihydrofolate reductase

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

Predicted Targets

Alpha-2A adrenergic receptor

Alpha-2B adrenergic receptor

Alpha-2C adrenergic receptor

5-hydroxytryptamine receptor 2A

5-hydroxytryptamine receptor 2C

5-hydroxytryptamine receptor 2B

Nischarin

Complex

Sigma non-opioid intracellular receptor 1

Activation peptide fragment 1

Muscleblind-like protein 1

Muscleblind-like protein 2

Muscleblind-like protein 3

Tyrosyl-DNA phosphodiesterase 1

Alpha-1D adrenergic receptor

Ibuprofen

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

Predicted Targets

IL-8(8-77)

Prostaglandin G/H synthase 1

Prostaglandin G/H synthase 2

Muscleblind-like protein 1

Solute carrier family 22 member 6

Solute carrier family 22 member 10

Solute carrier family 22 member 25

Solute carrier family 22 member 9

Solute carrier family 22 member 24

Serum albumin

Alpha-fetoprotein

Connective tissue-activating peptide III(1-81)

GRO-alpha(4-73)

GRO-beta(5-73)

GRO-gamma(5-73)

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

stem cell factor (SCF)

proto-oncogene c-Kit inhibitor

Predicted Targets

Serine/threonine-protein kinase PLK4

Cyclin-G-associated kinase

Carbonic anhydrase 12

Tyrosine-protein kinase JAK2

Serine/threonine-protein kinase 17B

Tyrosine-protein kinase ABL1

Epidermal growth factor receptor

Carbonic anhydrase 1

Carbonic anhydrase 2

RAF proto-oncogene serine/threonine-protein kinase

Receptor tyrosine-protein kinase erbB-2

Tyrosine-protein kinase Lck

Tyrosine-protein kinase Fyn

Macrophage colony-stimulating factor 1 receptor

Carbonic anhydrase 3

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of *M. tuberculosis*

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

Predicted Targets

Amine oxidase [flavin-containing] A

Amine oxidase [flavin-containing] B

Tyrosyl-DNA phosphodiesterase 1

Muscleblind-like protein 1

Muscleblind-like protein 2

Muscleblind-like protein 3

Microtubule-associated protein tau

Inosine-5'-monophosphate dehydrogenase 2

Inosine-5'-monophosphate dehydrogenase 1

FAD-linked sulfhydryl oxidase ALR

Complex

Prostaglandin G/H synthase 1

Prostaglandin G/H synthase 2

Retina-specific copper amine oxidase

Amiloride-sensitive amine oxidase [copper-containing]

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14- α demethylase

Molecular Mechanism (repurposed) :

smoothened homolog inhibitor

lanosterol 14- α demethylase inhibitor

Predicted Targets

Tyrosine-protein kinase Fyn

Cytochrome P450 3A4

Proto-oncogene tyrosine-protein kinase Src

Lanosterol 14- α demethylase

Tyrosine-protein kinase Yes

Tyrosine-protein kinase Fgr

Tyrosine-protein kinase FRK

Cytochrome P450 3A5

Cytochrome P450 3A7

Cytochrome P450 3A43

Microtubule-associated protein tau

D(2) dopamine receptor

5-hydroxytryptamine receptor 2A

Muscarinic acetylcholine receptor M2

Muscarinic acetylcholine receptor M4

Ketoconazole

Molecular Mechanism (initial) :

fungal cytochrome P450 51 inhibitor

Molecular Mechanism (repurposed) :

cytochrome P450 aromatase (CYP19A1) inhibitor

Predicted Targets

Steroid 21-hydroxylase

Lanosterol 14-alpha demethylase (cytochrome P450 51)

Cholesterol side-chain cleavage enzyme

Cholesterol 7-alpha-monooxygenase

5-hydroxytryptamine receptor 1B

Potassium voltage-gated channel subfamily H member 2

Potassium voltage-gated channel subfamily H member 6

Potassium voltage-gated channel subfamily H member 7

Muscarinic acetylcholine receptor M3

Mu-type opioid receptor

Delta-type opioid receptor

Kappa-type opioid receptor

Nociceptin receptor

Cytochrome P450 19A1

Muscarinic acetylcholine receptor M2

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

Predicted Targets

Microtubule-associated protein tau

5-hydroxytryptamine receptor 1B

Muscleblind-like protein 1

Muscleblind-like protein 2

Muscleblind-like protein 3

D(2) dopamine receptor

5-hydroxytryptamine receptor 1D

D(4) dopamine receptor

Cytochrome P450 2D6

Cytochrome P450 2J2

Sodium channel protein type 4 subunit alpha

Sodium channel protein type 5 subunit alpha

Sodium channel protein type 11 subunit alpha

Sodium channel protein type 10 subunit alpha

FAD-linked sulfhydryl oxidase ALR

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

Predicted Targets

Glutamate receptor ionotropic

Complex

Complex

Glutamate receptor ionotropic

Nischarin

Sigma non-opioid intracellular receptor 1

Alpha-trypsin chain 1

Trypsin-2

Trypsin-3

Tyrosyl-DNA phosphodiesterase 1

Complex

Complex

Dynamin-1

N-acylethanolamine-hydrolyzing acid amidase subunit alpha

Dynamin-2

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

Predicted Targets

Nischarin

Nitric oxide synthase

Nitric oxide synthase

Nitric oxide synthase

Tyrosyl-DNA phosphodiesterase 1

Activation peptide fragment 1

Alpha-trypsin chain 1

Trypsin-2

Trypsin-3

5-hydroxytryptamine receptor 5A

Complex

Microtubule-associated protein tau

5-hydroxytryptamine receptor 3B

Indoleamine 2

Indoleamine 2

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :

dihydrofolate reductase inhibitor

Predicted Targets

Dihydrofolate reductase

Thymidylate synthase

Folate transporter 1
Folypolyglutamate synthase

Dihydrofolate reductase

Muscleblind-like protein 1
Tyrosyl-DNA phosphodiesterase 1
Muscleblind-like protein 2
Muscleblind-like protein 3
Methylated-DNA--protein-cysteine methyltransferase
Carbonic anhydrase 1
Carbonic anhydrase 2
Carbonic anhydrase 3
Carbonic anhydrase 5A
Carbonic anhydrase 7

Milnacipran

Molecular Mechanism (initial) :

5-HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

5-HT and norepinephrine reuptake inhibitor

Predicted Targets

Sodium-dependent noradrenaline transporter

Sodium-dependent serotonin transporter

Sodium- and chloride-dependent glycine transporter 1

Sodium-dependent dopamine transporter

Sodium- and chloride-dependent glycine transporter 2
Sodium-dependent proline transporter
Sodium- and chloride-dependent neutral and basic amino acid transporter B(0+)
Dipeptidyl peptidase 4 membrane form
Seprase
Corticosteroid 11-beta-dehydrogenase isozyme 1
Hydroxysteroid 11-beta-dehydrogenase 1-like protein
Mu-type opioid receptor
Delta-type opioid receptor
Kappa-type opioid receptor
Nociceptin receptor

Miltefosine

Molecular Mechanism (initial) :

Akt/PKB inhibitor

Molecular Mechanism (repurposed) :

phosphatidyl-choline biosynthesis inhibitor

Predicted Targets

Carnitine O-palmitoyltransferase 1
Carnitine O-palmitoyltransferase 1
Carnitine O-palmitoyltransferase 1
Phospholipase A2
Calcium-dependent phospholipase A2
Group IIF secretory phospholipase A2

Group IIE secretory phospholipase A2
Group IID secretory phospholipase A2
Lysophosphatidic acid receptor 1
Lysophosphatidic acid receptor 3
Lysophosphatidic acid receptor 2
Phospholipase A2
M-phase inducer phosphatase 1
M-phase inducer phosphatase 2
Platelet-activating factor receptor

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

Predicted Targets

Microtubule-associated protein tau
Tyrosyl-DNA phosphodiesterase 1
22 kDa interstitial collagenase
PEX
Stromelysin-1
67 kDa matrix metalloproteinase-9
Collagenase 3
Stromelysin-2
Macrophage metalloelastase
Matrix metalloproteinase-27
Matrix metalloproteinase-20
Complex
Estrogen receptor
Estrogen receptor beta
Induced myeloid leukemia cell differentiation protein Mcl-1

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

Predicted Targets

Mu-type opioid receptor
Delta-type opioid receptor
Kappa-type opioid receptor
Nociceptin receptor
Sodium-dependent noradrenaline transporter
Sodium-dependent serotonin transporter
Sodium- and chloride-dependent glycine transporter 1
Sodium-dependent dopamine transporter

Sodium- and chloride-dependent glycine transporter 2
Sodium-dependent proline transporter
Sodium- and chloride-dependent neutral and basic amino acid transporter B(0+)
Substance-K receptor
Substance-P receptor
Neuromedin-K receptor
Tyrosine-protein kinase Fyn

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor
proto-oncogene c-Kit inhibitor

Predicted Targets

Ephrin type-B receptor 6
Carbonic anhydrase 12
Serine/threonine-protein kinase 10

Tyrosine-protein kinase ABL1

Carbonic anhydrase 1
Carbonic anhydrase 2
RAF proto-oncogene serine/threonine-protein kinase
High affinity nerve growth factor receptor
Tyrosine-protein kinase Lck
Tyrosine-protein kinase Fyn
Macrophage colony-stimulating factor 1 receptor
Carbonic anhydrase 3
Tyrosine-protein kinase Yes
Tyrosine-protein kinase Lyn
Soluble RET kinase fragment

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Predicted Targets

Catechol O-methyltransferase
Androgen receptor
Sodium-dependent noradrenaline transporter
Sodium-dependent serotonin transporter
Sodium- and chloride-dependent glycine transporter 1
Sodium-dependent dopamine transporter
Sodium-dependent proline transporter
Sodium- and chloride-dependent neutral and basic amino acid transporter B(0+)
Sodium- and chloride-dependent glycine transporter 2
Microtubule-associated protein tau
Muscleblind-like protein 1

Muscleblind-like protein 2
Muscleblind-like protein 3
Progesterone receptor
Cocaine esterase

Paclitaxel

Molecular Mechanism (initial) :

tubulin beta modulator (microtubule-stabilizing agent)

Molecular Mechanism (repurposed) :

tubulin beta modulator (microtubule-stabilizing agent)

Predicted Targets

Substance-K receptor
Substance-P receptor
Neuromedin-K receptor
Multidrug resistance protein 1
Cholecystokinin receptor type A
Gastrin/cholecystokinin type B receptor
Mu-type opioid receptor
Delta-type opioid receptor
Kappa-type opioid receptor
Nociceptin receptor
Multidrug resistance protein 3
Bile salt export pump
ATP-binding cassette sub-family B member 5
Tyrosyl-DNA phosphodiesterase 1
Epidermal growth factor receptor

Phentolamine mesilate

Molecular Mechanism (initial) :

alpha-adrenoceptor antagonist

Molecular Mechanism (repurposed) :

alpha-adrenoceptor antagonist

Predicted Targets

Alpha-2A adrenergic receptor
Alpha-2B adrenergic receptor
Alpha-2C adrenergic receptor
Alpha-1D adrenergic receptor

5-hydroxytryptamine receptor 2A
5-hydroxytryptamine receptor 2C

Alpha-1A adrenergic receptor
Alpha-1B adrenergic receptor

5-hydroxytryptamine receptor 2B
Nischarin
D(2) dopamine receptor
D(3) dopamine receptor
D(4) dopamine receptor
5-hydroxytryptamine receptor 1A
5-hydroxytryptamine receptor 1B

Raloxifene hydrochloride

Molecular Mechanism (initial) :

estrogen receptor agonist

Molecular Mechanism (repurposed) :

estrogen receptor agonist

Predicted Targets

Phospholipase D2

Estrogen receptor

Tyrosine-protein kinase Fyn

Cholinesterase

Tyrosine-protein kinase Yes

Alpha-2A adrenergic receptor

Tyrosine-protein kinase Fgr

Cytochrome P450 2C9

Proto-oncogene tyrosine-protein kinase Src

D(2) dopamine receptor

Alpha-2B adrenergic receptor

Alpha-2C adrenergic receptor

Substance-K receptor

D(1A) dopamine receptor

D(4) dopamine receptor

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :

dopamine D2 and D3 receptor agonist

Predicted Targets

5-hydroxytryptamine receptor 1A

D(2) dopamine receptor

D(4) dopamine receptor

5-hydroxytryptamine receptor 1B

D(3) dopamine receptor

5-hydroxytryptamine receptor 1D

5-hydroxytryptamine receptor 1E

5-hydroxytryptamine receptor 1F

Mu-type opioid receptor

Delta-type opioid receptor

Kappa-type opioid receptor

Nociceptin receptor

5-hydroxytryptamine receptor 7

5-hydroxytryptamine receptor 2A

5-hydroxytryptamine receptor 2C

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :

phospho-diesterase (PDE5A) inhibitor

Predicted Targets

Multidrug resistance-associated protein 5

cGMP-specific 3',5'-cyclic phosphodiesterase

High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A

Carbonic anhydrase 1

Carbonic anhydrase 2

Carbonic anhydrase 3

Carbonic anhydrase 6

Adenosine receptor A2a

Adenosine receptor A2b

Adenosine receptor A1

Carbonic anhydrase 7

Cone cGMP-specific 3'

Potassium voltage-gated channel subfamily H member 2

High affinity cAMP-specific 3'

Dual 3'

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Predicted Targets

Microtubule-associated protein tau

3-hydroxy-3-methylglutaryl-coenzyme A reductase

Substance-K receptor

Sodium-dependent noradrenaline transporter

Substance-P receptor

Neuromedin-K receptor

Sodium-dependent serotonin transporter

Sodium- and chloride-dependent glycine transporter 1

Sodium-dependent dopamine transporter

Sodium- and chloride-dependent glycine transporter 2

Sodium-dependent proline transporter

Sodium- and chloride-dependent neutral and basic amino acid transporter B(0+)

Androgen receptor

Complex

Tyrosyl-DNA phosphodiesterase 1

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

Predicted Targets

Retinoic acid receptor alpha

Retinoic acid receptor beta

Retinoic acid receptor gamma

Retinoic acid receptor RXR-alpha

Retinoic acid receptor RXR-beta

Retinoic acid receptor RXR-gamma

Ornithine decarboxylase

3-oxo-5-alpha-steroid 4-dehydrogenase 2

Microtubule-associated protein tau

Peroxisome proliferator-activated receptor gamma

Peroxisome proliferator-activated receptor delta

Peroxisome proliferator-activated receptor alpha

3-oxo-5-alpha-steroid 4-dehydrogenase 1

Thromboxane A2 receptor

M-phase inducer phosphatase 1

Tetrabenazine**Molecular Mechanism (initial) :**

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Predicted Targets

Synaptic vesicular amine transporter

Chromaffin granule amine transporter

Microtubule-associated protein tau

Alpha-2A adrenergic receptor

Alpha-2B adrenergic receptor

Alpha-2C adrenergic receptor

Melatonin receptor type 1A

Melatonin receptor type 1B

Melatonin-related receptor

Dipeptidyl peptidase 4 membrane form

Seprase

Mu-type opioid receptor

Delta-type opioid receptor

Kappa-type opioid receptor

Nociceptin receptor

Thalidomide**Molecular Mechanism (initial) :**

TNF-alpha production inhibitor

**Molecular Mechanism (repurposed) :
cereblon (CRBN) inhibitor**

Predicted Targets

Prostaglandin G/H synthase 1
Prostaglandin G/H synthase 2
Poly [ADP-ribose] polymerase 1
Dipeptidyl peptidase 4 membrane form
Seprase
P2X purinoceptor 7
PEX
67 kDa matrix metalloproteinase-9
Dipeptidyl peptidase 8
Dipeptidyl peptidase 9
22 kDa interstitial collagenase
Stromelysin-1
Stromelysin-2
Neutrophil collagenase
Macrophage metalloelastase

Topiramate

Molecular Mechanism (initial) :

**kainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker**

Molecular Mechanism (repurposed) :

**ckainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker**

Predicted Targets

Carbonic anhydrase 12
Carbonic anhydrase-related protein 11
Carbonic anhydrase 1
Carbonic anhydrase 2
Carbonic anhydrase 4
Carbonic anhydrase 6
Carbonic anhydrase 5A
Carbonic anhydrase 7
Carbonic anhydrase 9
Carbonic anhydrase 13
Carbonic anhydrase 14
Carbonic anhydrase 5B
Carbonic anhydrase-related protein 10
Carbonic anhydrase 3
Fibroblast growth factor 1

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

Predicted Targets

5-hydroxytryptamine receptor 6

Estrogen receptor

Estrogen receptor beta

Epidermal growth factor receptor

Receptor tyrosine-protein kinase erbB-2

Tyrosine-protein kinase Lck

Tyrosine-protein kinase Fyn

Beta-2 adrenergic receptor

Tyrosine-protein kinase Lyn

Muscarinic acetylcholine receptor M2

Muscarinic acetylcholine receptor M4

Multidrug resistance protein 1

Beta-1 adrenergic receptor

Tyrosine-protein kinase HCK

Muscarinic acetylcholine receptor M5

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

Predicted Targets

Histone deacetylase 3

Complex

Histone deacetylase 4

Histone deacetylase 1

Histone deacetylase 7

Histone deacetylase 2

Histone deacetylase 10

Histone deacetylase 11

Histone deacetylase 8

Histone deacetylase 6

Histone deacetylase 9

Histone deacetylase 5

Lipid-phosphate phosphatase

FAD-linked sulfhydryl oxidase ALR

22 kDa interstitial collagenase

Supplement 4

Biological activity profile predicted with TarPred

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

Predicted Targets

Delta opioid receptor
Kappa Opioid Receptor
Nociceptin Receptor (ORL1 Receptor)
Dopamine D2 receptor
5-hydroxytryptamine receptor 2A
Serotonin Receptor 7
C-C chemokine receptor type 5
Alpha-1b adrenergic receptor
Sigma opioid receptor
Serotonin Receptor 1A
NK1 Receptor
Sigma-1 receptor
Dopamine D3 receptor
GABA transporter 4
Serotonin Receptor 4
Butyrylcholinesterase (BuChE)
Muscarinic acetylcholine receptor M1
Matrix Metalloproteinase-1 (MMP-1)
Matrix metalloproteinase 9
Voltage-gated T-type calcium channel alpha-1I subunit
Dopamine D1 receptor
Muscarinic acetylcholine receptor M2
Neurokinin 2 receptor
C-C chemokine receptor type 3
Cannabinoid Receptor 2
Angiotensin II type 2 (AT-2) receptor
Histamine H3 Receptor
P-glycoprotein 1
Bradykinin B2 receptor
Histamine H1 receptor

Alprostadi

Molecular Mechanism (initial) :

prostaglandin E2 receptor agonist

Molecular Mechanism (repurposed) :

prostaglandin E2 receptor agonist

Predicted Targets

Prostanoid EP4 Receptor
Prostacyclin (IP) Receptor
Prostanoid EP3 receptor
Prostanoid EP1 receptor

Prostanoid EP2 Receptor

Prostanoid FP receptor
Thromboxane A2 receptor
Peroxisome proliferator-activated receptor delta
Arachidonate 15-lipoxygenase
Prostaglandin D2 Receptor CRTH2
HMG-CoA Reductase
Prostanoid DP receptor
Fatty Acid Amide Hydrolase
Cannabinoid Receptor 2
Cannabinoid Receptor 1
Vanilloid receptor 1
HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B
Fatty acid synthase
Phospholipase A2
Protein kinase C alpha
Neuraminidase B
Matrix Metalloproteinase-1 (MMP-1)
Matrix metalloproteinase 9
Thromboxane-A synthase
G-protein Coupled Receptor 40
Cytosolic phospholipase A2
Histone Deacetylase 1 (HDAC1)
Histone Deacetylase 6 (HDAC6)
Transient receptor potential cation channel subfamily A member 1
Phospholipase A2 group 1VD

Amantadine hydrochloride

Molecular Mechanism (initial) :

matrix protein 2 (Influenza virus A) inhibitor

Molecular Mechanism (repurposed) :

dopamine receptor agonists

NMDA receptor antagonists

Predicted Targets

Sigma opioid receptor
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Dipeptidyl peptidase VI
Metabotropic glutamate receptor 8
Glutamate (NMDA) receptor subunit zeta 1
Carbonic anhydrase II
Glutamate [NMDA] receptor subunit epsilon 3
Aromatase (CYP19)
Steroid 17-alpha-Monooxygenase (CYP17)
Carbonic anhydrase I
Carbonic anhydrase IX
Multidrug resistance-associated protein 1
Butyrylcholinesterase (BuChE)
GABA transporter 4
Catechol O-methyltransferase
Cannabinoid Receptor 1

Dopamine D2 receptor

Carbonic anhydrase VA
Serotonin Receptor 1A
Adenosine A1 receptor
Monoamine oxidase B
Steroid 11-beta-Hydroxylase (CYP11B1)
'Retinoic Acid Receptor
Retinoic acid receptor alpha
Cannabinoid Receptor 2
Calcium sensing receptor
'Retinoic Acid Receptor
Carbonic anhydrase VB
Carbonic Anhydrase XII
Carbonic Anhydrase IV

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

Predicted Targets

Histamine H1 receptor
Histamine H2 Receptor
Alpha-1b adrenergic receptor
GABA transporter 4
Dopamine D1 receptor
Dopamine D3 receptor
Dopamine D2 receptor
hERG Potassium Channel 1
Histamine H3 Receptor
5-hydroxytryptamine receptor 2A
Serotonin 6 (5-HT6) receptor
Serotonin Receptor 7
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Serotonin Receptor 2C
Trypanothione Reductase (TryR)
Cytochrome P450 2D1
Serotonin Receptor 1A
Sigma opioid receptor
Arachidonate 15-lipoxygenase
Aromatase (CYP19)
Steroid 11-beta-Hydroxylase (CYP11B1)
Muscarinic acetylcholine receptor M3
Adenosine A3 Receptor
Trace amine-associated receptor1
Peripheral-Type Benzodiazepine Receptor
Sigma-1 receptor
Butyrylcholinesterase (BuChE)

Serotonin 1d (5-HT1d) receptor
Steroid 5-alpha-reductase 1

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

Predicted Targets

Dopamine D1 receptor

Dopamine D2 receptor

Dopamine D3 receptor

Serotonin Receptor 1A

Serotonin Receptor 7

GABA transporter 4

5-hydroxytryptamine receptor 2A

Dopamine D4 receptor

Tryptophan 5-hydroxylase 1

Alpha-1b adrenergic receptor

alpha-2A adrenergic receptor [Homo sapiens]

Arachidonate 15-lipoxygenase

Delta opioid receptor

Kappa Opioid Receptor

Sigma opioid receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Monoamine oxidase B

Serotonin 1d (5-HT1d) receptor

Serotonin Receptor 2C

Butyrylcholinesterase (BuChE)

Serotonin 5b (5-HT5b) receptor

5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]

Histamine H2 Receptor

Adenosine A3 Receptor

Serotonin 6 (5-HT6) receptor

Histamine H1 receptor

Beta-1 Adrenergic Receptor

Nociceptin Receptor (ORL1 Receptor)

Neuronal acetylcholine receptor protein alpha-7 subunit

Acetylsalicylic acid

Molecular Mechanism (initial) :

cyclooxygenase inhibitor

Molecular Mechanism (repurposed) :

cyclooxygenase inhibitor

Predicted Targets

Carbonic Anhydrase XII

Prostaglandin G/H synthase 2

Carbonic anhydrase IX
Carbonic anhydrase I
Arachidonate 15-lipoxygenase
HSP90AA1 protein
Butyrylcholinesterase (BuChE)
GABA transporter 4
Carbonic anhydrase II
Leukocyte elastase
Carbonic Anhydrase XIV
Androgen Receptor
Carbonic anhydrase VA
Tyrosine Kinase c-Kit Mutant (N822K)
Histamine H1 receptor
Tyrosine-protein kinase FGR
'nuclear receptor subfamily 4
Methionine Aminopeptidase Type 2 (MetAP2)
Apurinic-Apyrimidinic Endonuclease 1 (APE1)
Carbonic Anhydrase IV
Dihydroorotate Dehydrogenase (DHODH) Mutant (H185A)
20-alpha-Hydroxysteroid Dehydrogenase (AKR1C1)
Carbonic anhydrase XIII
Thrombin
Trypsin II
Histamine H2 Receptor
P-glycoprotein 1
HM74 nicotinic acid GPCR
HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B
Protein-tyrosine phosphatase 1B

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

Predicted Targets

Adenosine A3 Receptor

Prostaglandin D2 Receptor CRTH2

Voltage-gated calcium channel alpha2/delta subunit 1

Gamma-Aminobutyric Acid Type B Receptor Subunit 2

Protein kinase B (Akt 2)

Peroxisome proliferator-activated receptor delta

Matrix Metalloproteinase-1 (MMP-1)

Matrix metalloproteinase 9

Thromboxane-A synthase

Cannabinoid Receptor 1

Rho-kinase (ROCK II)

Aldose Reductase (ALR2) Mutant (L300P)

GABA transporter 4

'Glycogen Synthase Kinase-3
'Glutamate receptor ionotropic
Purine Nucleoside Phosphorylase (PNP)
Carbonic anhydrase II
Carbonic anhydrase I
Histone Deacetylase 7 (HDAC7)
Carboxylesterase
Aromatase (CYP19)
Muscle glycogen phosphorylase
Caspase-3
Glutamate (NMDA) receptor subunit zeta 1
G-protein Coupled Receptor 40
Histamine H1 receptor
Cytochrome P450 3A43
Cannabinoid Receptor 2
Thromboxane A2 receptor
Excitatory amino acid transporter 2

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

Predicted Targets

Sigma opioid receptor
 Glutamate [NMDA] receptor subunit epsilon 3
 Matrix Metalloproteinase-1 (MMP-1)
 Vanilloid receptor 1
 Aminopeptidase M
 Carbonic anhydrase II
 Carbonic anhydrase I
 Sodium channel protein type II alpha subunit
 Delta opioid receptor
 Kappa Opioid Receptor
 Butyrylcholinesterase (BuChE)
 Carbonic anhydrase VA
 Monoamine oxidase B
 Carbonic Anhydrase XII
 Carbonic Anhydrase IV
 Carbonic anhydrase IX
 Bradykinin B2 receptor
 HIV-1 Protease chain A
 Tyrosine-protein kinase FGR
 Histone Deacetylase 1 (HDAC1)
 Histone Deacetylase 6 (HDAC6)
 ErbB-4 (HER4) Tyrosine Kinase
 Dopamine D2 receptor
 Dopamine D4 receptor

Peripheral-Type Benzodiazepine Receptor
Acyl Cholesterol Acyltransferase 1 (ACAT-1)
Serotonin Receptor 1A
Carbonic anhydrase VB
Trace amine-associated receptor1
Nitric Oxide Synthase

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

Predicted Targets

Endothelin receptor ET-A

Fibroblast growth factor receptor 1
Vanilloid receptor 1
Tyrosine Kinase c-Kit Mutant (N822K)
Carbonic anhydrase II
VEGFR-2 (KDR)
Serotonin Receptor 1A
Carbonic anhydrase I
Cyclophilin A
GABA transporter 4
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Protein kinase B (Akt 2)
Histamine H3 Receptor
Peroxisome proliferator-activated receptor delta
Tubulin alpha-1 chain
Multidrug resistance-associated protein 1
Dopamine D2 receptor
Histamine H1 receptor
Histone Deacetylase 1 (HDAC1)
Somatostatin receptor 5
Dopamine D3 receptor
Tubulin beta-8 chain
Glucocorticoid receptor
Matrix metalloproteinase 9
Prostanoid EP2 Receptor
ErbB-4 (HER4) Tyrosine Kinase
Dihydrofolate Reductase (DHFR)
Arachidonate 15-lipoxygenase
Matrix Metalloproteinase-1 (MMP-1)
Prostaglandin G/H synthase 2

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :

mu-type opioid receptor agonist

Predicted Targets

Kappa Opioid Receptor
Delta opioid receptor
Nociceptin Receptor (ORL1 Receptor)
Sigma opioid receptor
C-C chemokine receptor type 5
Dopamine D2 receptor
Adenosine A3 Receptor
Serotonin Receptor 1A
Butyrylcholinesterase (BuChE)
Dopamine D1 receptor
Muscarinic acetylcholine receptor M2
Sigma-1 receptor
Cholecystokinin B receptor
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M1
estrogen receptor alpha
alpha-2A adrenergic receptor [Homo sapiens]
Cannabinoid Receptor 1
Cannabinoid Receptor 2
5-hydroxytryptamine receptor 2A
Acyl Cholesterol Acyltransferase 1 (ACAT-1)
Beta-1 Adrenergic Receptor
Beta-3 adrenergic receptor
Beta-2 adrenergic receptor
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Glucocorticoid receptor
Aldose Reductase (ALR2) Mutant (L300P)
Arachidonate 15-lipoxygenase
Cytochrome P450 3A43
Tyrosine-protein kinase FGR

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Predicted Targets

Prostaglandin G/H synthase 2

Carbonic anhydrase II
Carbonic anhydrase VA
Carbonic anhydrase VB
Carbonic Anhydrase XII
Carbonic anhydrase IX
Carbonic anhydrase VII
Carbonic anhydrase VI
Carbonic Anhydrase IV
Carbonic anhydrase XIII

Carbonic Anhydrase XIV
MAP Kinase p38 alpha Mutant (G110A)
Carbonic anhydrase I
Coagulation factor X
Neuronal acetylcholine receptor protein alpha-7 subunit
Arachidonate 15-lipoxygenase
Cannabinoid Receptor 1
Cyclin-Dependent Kinase 2 (CDK2)
Cytochrome P450 2D1
Thrombin
GABA transporter 4
Cytochrome P450 2C11
Trypsin II
Carbonic anhydrase III
Multidrug resistance-associated protein 1
Cyclin-Dependent Kinase 1 (CDK1)
I-kappa-B Kinase 2 (IKK-beta)
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Serotonin Receptor 1E
Sodium channel protein type II alpha subunit

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

Predicted Targets

hERG Potassium Channel 1
Quinone reductase 2
C-C chemokine receptor type 4
Voltage-gated calcium channel alpha2/delta subunit 1
Cytochrome P450 2D1
Histamine N-methyltransferase
Histamine H3 Receptor
Aminopeptidase M
C-C chemokine receptor type 5
Cyclin-Dependent Kinase 1 (CDK1)
Cytochrome P450 1A1
Tyrosine-protein kinase FGR
Methionine Aminopeptidase Type 2 (MetAP2)
Aldehyde oxidase
VEGFR-2 (KDR)
HSP90AA1 protein
ErbB-4 (HER4) Tyrosine Kinase
IGF1R
C-C chemokine receptor type 3
Fibroblast growth factor receptor 1
Tyrosine Kinase c-Kit Mutant (N822K)
Corticotropin-releasing Factor Receptor 1

MAP Kinase p38 alpha Mutant (G110A)
Glutamate (NMDA) receptor subunit zeta 1
Neurotensin receptor 1
Adenosine A3 Receptor
EPHA1
Phosphodiesterase Type 5 (PDE5)
Prostaglandin D2 Receptor CRTH2
Butyrylcholinesterase (BuChE)

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

Predicted Targets

Dopamine D2 receptor

Serotonin Receptor 1A
Trypanothione Reductase (TryR)
Histamine H1 receptor
Serotonin Receptor 7
Dopamine D3 receptor
Dopamine D1 receptor
hERG Potassium Channel 1
Aldehyde oxidase
Serotonin 6 (5-HT6) receptor
P-glycoprotein 1
Calmodulin
GABA transporter 4
5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]
Cytochrome P450 2D1
Alpha-1b adrenergic receptor
Histamine H2 Receptor
5-hydroxytryptamine receptor 2A
Butyrylcholinesterase (BuChE)
Prostaglandin G/H synthase 2
Serotonin Receptor 2C
Histamine H3 Receptor
Sigma opioid receptor
Dopamine D4 receptor
Trace amine-associated receptor1
Adenosine A3 Receptor
Peripheral-Type Benzodiazepine Receptor
Muscarinic acetylcholine receptor M3
Glutamate (NMDA) receptor subunit zeta 1
Voltage-gated R-type calcium channel alpha-1E subunit

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :
TNF- α /NF- κ B signaling pathway inhibitor

Predicted Targets

Sodium/potassium-transporting ATPase alpha-2 chain

Carbonic Anhydrase IV
Carbonic anhydrase II
Carbonic anhydrase I
Estradiol 17-beta-dehydrogenase 3
Androgen Receptor
Farnesoid X-Activated Receptor
Steroid 17-alpha-Monooxygenase (CYP17)
Aromatase (CYP19)
Glucocorticoid receptor
Steroid 5-alpha-reductase 2
estrogen receptor alpha
Tyrosinase
Phospholipase A2 group 1B
Mineralocorticoid Receptor (MR)
Prostaglandin G/H synthase 2
Thrombin
Progesterone Receptor (PR)
Steroid 5-alpha-reductase 1
Protein-tyrosine phosphatase 1B
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Sigma opioid receptor
Histone Deacetylase 1 (HDAC1)
Histone deacetylase 8
DNA topoisomerase II beta
Matrix metalloproteinase 9
Thyroid Hormone Receptor (TR-beta)
HMG-CoA Reductase
Butyrylcholinesterase (BuChE)
11-beta-hydroxysteroid dehydrogenase 2

Doxepin hydrochloride

Molecular Mechanism (initial) :
5HT and norepinephrine reuptake inhibitor
Molecular Mechanism (repurposed) :
H1 and H2 histamine receptor blocker

Predicted Targets

Histamine H1 receptor

Histamine H2 Receptor

Alpha-1b adrenergic receptor
Dopamine D1 receptor
Dopamine D3 receptor
Dopamine D2 receptor
GABA transporter 4
hERG Potassium Channel 1

Arachidonate 15-lipoxygenase
Thromboxane A2 receptor
5-hydroxytryptamine receptor 2A
Thromboxane-A synthase
Histamine H3 Receptor
Serotonin 6 (5-HT6) receptor
Serotonin Receptor 7
Serotonin Receptor 2C
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Sigma opioid receptor
estrogen receptor alpha
Serotonin Receptor 1A
Cytochrome P450 2D1
Muscarinic acetylcholine receptor M3
Trypanothione Reductase (TryR)
Serotonin 1d (5-HT1d) receptor
MAP Kinase p38 alpha Mutant (G110A)
Trace amine-associated receptor1
Monoamine oxidase B
alpha-2A adrenergic receptor [Homo sapiens]
Delta opioid receptor

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

Predicted Targets

GABA transporter 4
Cytochrome P450 2D1
Serotonin Receptor 1A
Serotonin 1d (5-HT1d) receptor
hERG Potassium Channel 1
Kappa Opioid Receptor
Histamine H3 Receptor
Beta-1 Adrenergic Receptor
5-hydroxytryptamine receptor 2A
Dopamine D2 receptor
Beta-2 adrenergic receptor
Butyrylcholinesterase (BuChE)
Arachidonate 15-lipoxygenase
Caspase-6
Caspase-1
Caspase-7
Caspase-3
Coagulation factor X
Factor IXa (fIXa)
Urokinase-type plasminogen activator

Histamine H1 receptor
Beta-3 adrenergic receptor
Dopamine D4 receptor
Acyl Cholesterol Acyltransferase 1 (ACAT-1)
NK1 Receptor
C-C chemokine receptor type 4
Serotonin 6 (5-HT6) receptor
Sigma opioid receptor
Mitogen-Activated Protein Kinase 9 (JNK2) Mutant (C162S)
Serotonin Receptor 2C

Eflornithine hydrochloride

Molecular Mechanism (initial) :

ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

Predicted Targets

Farnesyl Diphosphate Synthase (FPPS)

Ornithine decarboxylase

gamma-Aminobutyric Acid Type B Receptor Subunit 2

'Nitric Oxide Synthase

Glutamate (NMDA) receptor subunit zeta 1

NAALADase II

Metabotropic glutamate receptor 8

GABA transporter 4

Renal dipeptidase precursor

Voltage-gated calcium channel alpha2/delta subunit 1

'Glutamate receptor ionotropic

Polyamine oxidase

Aminopeptidase M

Carbonic Anhydrase IV

Aldose Reductase (ALR2) Mutant (L300P)

Betaine--homocysteine S-methyltransferase 1

Carbonic anhydrase II

Prostaglandin G/H synthase 2

Carbonic anhydrase I

Peroxisome proliferator-activated receptor delta

Dipeptidyl peptidase VI

Thromboxane-A synthase

Carbonic anhydrase IX

Glutamate [NMDA] receptor subunit epsilon 3

Carbonic Anhydrase XIV

PIM-2 Kinase

Carbonic anhydrase VII

GABA receptor alpha-5 subunit

Carbonic anhydrase VA

Carbonic anhydrase VB

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

Predicted Targets

ErbB-4 (HER4) Tyrosine Kinase

Fibroblast growth factor receptor 1

Fructose-1,6-bisphosphatase 1

Tyrosine-protein kinase FGR

Tyrosine Kinase c-Kit Mutant (N822K)

Tie-2

VEGFR-2 (KDR)

Tubulin alpha-1 chain

Mitogen-Activated Protein Kinase 9 (JNK2) Mutant (C162S)

Tyrosine-protein kinase ABL

Mitogen- and Stress-Activated Protein Kinase 2 (MSK2)

Tyrosine Kinase c-Met Mutant (M1250T)

ALK tyrosine kinase receptor

AXL Receptor Tyrosine Kinase

EPHA1

Tyrosine-protein kinase receptor FLT3

MAP Kinase p38 alpha Mutant (G110A)

Tyrosine-protein kinase receptor RET

Metabotropic glutamate receptor 8

Histone Deacetylase 6 (HDAC6)

Histone deacetylase 8

Histone Deacetylase 1 (HDAC1)

IGF1R

Tyrosine-protein kinase (BTK)

Serine/threonine-protein kinase SIK1

3-Phosphoinositide-Dependent Protein Kinase 1 (PDK1) Mutant (T222A)

Phosphodiesterase Type 5 (PDE5)

Serine/threonine-protein kinase MRCK-A

Histone Deacetylase 10 (HDAC10)

Activin receptor type-1B

Everolimus

Molecular Mechanism (initial) :

FK506-binding protein 12 inhibitor

mTOR inhibitor

Molecular Mechanism (repurposed) :

FK506-binding protein 12 inhibitor

mTOR inhibitor

Predicted Targets

Peptidyl-prolyl cis-trans isomerase (FKBP) (FK506-binding protein 12)

Immunophilin FKBP12

mTOR

'Serine/threonine protein phosphatase 2B catalytic subunit

P-glycoprotein 1
 HSP90AA1 protein
 HMG-CoA Reductase
 Histone Deacetylase 1 (HDAC1)
 Voltage-gated potassium channel subunit Kv1.1
 Oxytocin receptor
 Prostaglandin G/H synthase 2
 Protein kinase C alpha
 Matrix metalloproteinase 9
 Delta opioid receptor
 Histamine H3 Receptor
 Protein kinase C delta
 Vasopressin V2 Receptor
 Histone Deacetylase 7 (HDAC7)
 Histone Deacetylase 6 (HDAC6)
 Histone deacetylase 8
 Kappa Opioid Receptor
 Serotonin Receptor 1A
 Vasopressin V1a Receptor
 Butyrylcholinesterase (BuChE)
 Cytochrome P450 3A43
 C-C chemokine receptor type 5
 Tyrosine-protein kinase FGR
 Glucocorticoid receptor
 Dopamine D2 receptor
 Leukocyte elastase

Finasteride

Molecular Mechanism (initial) :

steroid 5alpha reductase inhibitor

androgen receptor antagonist

Molecular Mechanism (repurposed) :

steroid 5alpha reductase inhibitor

androgen receptor antagonist

Predicted Targets

Steroid 5-alpha-reductase 2

Steroid 5-alpha-reductase 1

Androgen Receptor

3-beta-hydroxysteroid dehydrogenase/delta 5-->4-isomerase type II

Progesterone Receptor (PR)

Glucocorticoid receptor

Sigma opioid receptor

Mineralocorticoid Receptor (MR)

hERG Potassium Channel 1

Steroid 17-alpha-Monooxygenase (CYP17)

Aromatase (CYP19)

Farnesoid X-Activated Receptor

Butyrylcholinesterase (BuChE)

estrogen receptor alpha

Kappa Opioid Receptor
Liver X Receptor alpha (LXR-alpha)
Carbonic Anhydrase IV
Carbonic anhydrase II
Carbonic anhydrase I
Protein-tyrosine phosphatase 1B
Estradiol 17-beta-dehydrogenase 3
HIV-1 Protease chain A
Cytochrome P450 2C11
Tubulin beta-8 chain
Delta opioid receptor
NK1 Receptor
Tyrosinase
Matrix Metalloproteinase-1 (MMP-1)
Calcium sensing receptor
Matrix metalloproteinase 9

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

Predicted Targets

Butyrylcholinesterase (BuChE)
Delta opioid receptor
Kappa Opioid Receptor
Dopamine D2 receptor
Dopamine D1 receptor
Sigma opioid receptor
5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]
Nociceptin Receptor (ORL1 Receptor)
Dopamine D4 receptor
Serotonin Receptor 1A
Serotonin 1d (5-HT1d) receptor
Dopamine D3 receptor
Serotonin 6 (5-HT6) receptor
5-hydroxytryptamine receptor 2A
hERG Potassium Channel 1
Muscarinic acetylcholine receptor M1
Sodium/potassium-transporting ATPase alpha-2 chain
NK1 Receptor
Serotonin Receptor 7
GABA transporter 4
Serotonin Receptor 2C
Tubulin beta-8 chain
Alpha-1b adrenergic receptor
Alpha-2b adrenergic receptor
alpha-2A adrenergic receptor [Homo sapiens]
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)

Histamine H3 Receptor
Cytochrome P450 3A43
Peroxisome proliferator-activated receptor delta
Tyrosine-protein kinase FGR

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

Predicted Targets

HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B
HIV-1 Protease chain A
Muscle glycogen phosphorylase
DNA Polymerase beta
Adenosine A1 receptor
Adenosine receptor A2a
Pyrimidinerbic receptor P2Y4
Purinergic receptor P2Y2
Pyrimidinerbic receptor P2Y6
Adenosine deaminase
C-X-C chemokine receptor type 4
Thymidylate synthase
Adenosine A3 Receptor
Purine Nucleoside Phosphorylase (PNP)
Thymidine Kinase
Purinergic receptor P2Y14
DNA polymerase alpha catalytic subunit
Adenosine receptor A2b
Glyceraldehyde-3-phosphate dehydrogenase liver
Adenosine Kinase (AK)
Butyrylcholinesterase (BuChE)
Carbonic anhydrase II
Carbonic anhydrase I
Aldehyde dehydrogenase 1A3
Cyclin-Dependent Kinase 1 (CDK1)
6-O-methylguanine-DNA methyltransferase
Carbonic Anhydrase XII
Nitric Oxide Synthase
Carbonic anhydrase IX
Tyrosine-protein kinase FGR

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

Predicted Targets

Sodium/hydrogen exchanger 1
Trace amine-associated receptor1
Aldose Reductase (ALR2) Mutant (L300P)
Thrombin
Dihydrofolate Reductase (DHFR)
Sigma opioid receptor
Phospholipase A2
Urokinase-type plasminogen activator
Glutamate [NMDA] receptor subunit epsilon 3
Trypsin II
Multidrug resistance-associated protein 1
Cannabinoid Receptor 1
Vanilloid receptor 1
Sodium channel protein type II alpha subunit
Matrix Metalloproteinase-1 (MMP-1)
Prostaglandin G/H synthase 2
Voltage-gated T-type calcium channel alpha-1I subunit
Histone Deacetylase 7 (HDAC7)
Coagulation factor X
Histone Deacetylase 1 (HDAC1)
Dopamine D4 receptor
Dopamine D3 receptor
Dopamine D2 receptor
Adenosine receptor A2a
Subtilisin/kexin type 4
Carbonic anhydrase II
Mitogen-Activated Protein Kinase 9 (JNK2) Mutant (C162S)
Carbonic anhydrase I
Caspase-1
HIV-1 Protease chain A

Ibuprofen

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

Predicted Targets

Arachidonate 15-lipoxygenase

Prostaglandin G/H synthase 2

estrogen receptor alpha

Peroxisome proliferator-activated receptor delta

Endothelin-Converting Enzyme 1

NAALADase II

Angiotensin-Converting Enzyme

Butyrylcholinesterase (BuChE)

20-alpha-Hydroxysteroid Dehydrogenase (AKR1C1)

Tyrosine-protein kinase CTK
 Aldose Reductase (ALR2) Mutant (L300P)
 Aminopeptidase M
 Voltage-gated calcium channel alpha2/delta subunit 1
 Tyrosyl-tRNA synthetase
 Delta opioid receptor
 Formyl Peptide Receptor-Like 1
 Steroid 5-alpha-reductase 1
 Steroid 5-alpha-reductase 2
 Matrix metalloproteinase 9
 Matrix Metalloproteinase-1 (MMP-1)
 Beta-1 Adrenergic Receptor
 Beta-3 adrenergic receptor
 Kappa Opioid Receptor
 Tryptophan 5-hydroxylase 1
 Vanilloid receptor 1
 Thromboxane-A synthase
 Peroxisome Proliferator-Activated Receptor alpha
 Fatty Acid Amide Hydrolase
 G-protein Coupled Receptor 40

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor
stem cell factor (SCF)
proto-oncogene c-Kit inhibitor

Predicted Targets

Tyrosine-protein kinase ABL

Tyrosine-protein kinase FGR

Tyrosine Kinase c-Kit Mutant (N822K)

Tyrosine Kinase DDR1
 RAF-1
 ErbB-4 (HER4) Tyrosine Kinase
 Carbonic anhydrase IX
 Carbonic anhydrase II
 Carbonic Anhydrase IV
 Carbonic anhydrase I
 Carbonic Anhydrase XII
 VEGFR-2 (KDR)
 Mitogen-Activated Protein Kinase 9 (JNK2) Mutant (C162S)
 Carbonic Anhydrase XIV
 Histone Deacetylase 1 (HDAC1)
 Carbonic anhydrase VII
 Carbonic anhydrase XIII
 Carbonic anhydrase VI
 Carbonic anhydrase III

ATP-Binding Cassette Transporter ABCG2
EPHA1
Tyrosine Kinase Syk
MAP Kinase p38 alpha Mutant (G110A)
Protein kinase C alpha
Histone Deacetylase 6 (HDAC6)
Maternal embryonic leucine zipper kinase
BCR/ABL p210 fusion protein
ALK tyrosine kinase receptor
IGF1R
Vanilloid receptor 1

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of M. tuberculosis

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

Predicted Targets

Monoamine oxidase B

Rho-kinase (ROCK II)
Serine/threonine-protein kinase MRCK-A
Steroid 17-alpha-Monooxygenase (CYP17)
Histone Deacetylase 1 (HDAC1)
Matrix Metalloproteinase-1 (MMP-1)
Mitogen- and Stress-Activated Protein Kinase 2 (MSK2)
Butyrylcholinesterase (BuChE)
Tyrosine-protein kinase receptor FLT3
Aromatase (CYP19)
Cytochrome P450 2C11
Matrix metalloproteinase 9
Prostaglandin G/H synthase 2
Vanilloid receptor 1
Metabotropic glutamate receptor 8
GABA transporter 4
Dihydrofolate Reductase-Thymidylate Synthase (DHFR-TS) Mutant V1/S
Adenosine A3 Receptor
Cytochrome P450 51(CYP51)
Carbonic anhydrase II
Multidrug resistance-associated protein 1
Adenosine receptor A2a
PKN1
Leukocyte elastase
HM74 nicotinic acid GPCR
Trypsin I
Serotonin Receptor 1A
Protein kinase C alpha
Steroid 11-beta-Hydroxylase (CYP11B1)
Acyl Cholesterol Acyltransferase 1 (ACAT-1)

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14-alpha demethylase

Molecular Mechanism (repurposed) :

smoothened homolog inhibitor

lanosterol 14-alpha demethylase inhibitor

Predicted Targets

Cytochrome P450 3A43

Cytochrome P450 51

P-glycoprotein 1

Heme oxygenase 1

Steroid 17-alpha-Monooxygenase (CYP17)

Steroid 11-beta-Hydroxylase (CYP11B1)

Heme oxygenase 2

Aromatase (CYP19)

Gonadotropin-releasing hormone receptor

hERG Potassium Channel 1

Cytochrome P450 24A1

Cytochrome P450 51(CYP51)

Cytochrome P450 2C11

Cannabinoid Receptor 1

Melanocortin receptor 4

Alpha-1b adrenergic receptor

Cannabinoid Receptor 2

Melanocortin receptor 3

Melanocortin receptor 5

Melanocortin receptor 1

Metabotropic glutamate receptor 8

Coagulation factor X

Serotonin Receptor 1A

Dopamine D4 receptor

Peroxisome proliferator-activated receptor delta

Renin

GABA transporter 4

Dopamine D2 receptor

Sigma opioid receptor

5-hydroxytryptamine receptor 2A

Ketoconazole

Molecular Mechanism (initial) :

fungal cytochrome P450 51 inhibitor

Molecular Mechanism (repurposed) :

cytochrome P450 aromatase (CYP19A1) inhibitor

Predicted Targets

Cytochrome P450 51

Cytochrome P450 3A43

Steroid 17-alpha-Monooxygenase (CYP17)

P-glycoprotein 1

Steroid 11-beta-Hydroxylase (CYP11B1)

Aromatase (CYP19)

Heme oxygenase 1

Heme oxygenase 2

Gonadotropin-releasing hormone receptor

Cytochrome P450 51(CYP51)

hERG Potassium Channel 1

Cytochrome P450 24A1

Cytochrome P450 2C11

Alpha-1b adrenergic receptor

Thromboxane-A synthase

Metabotropic glutamate receptor 8

Coagulation factor X

Cytochrome P450 2D1

Thrombin

Cytochrome P450 1A1

Cannabinoid Receptor 1

Dopamine D3 receptor

Melanocortin receptor 4

Thyroid Hormone Receptor (TR-beta)

Serotonin Receptor 1A

Dopamine D4 receptor

Cytosolic phospholipase A2

Voltage-gated potassium channel subunit Kv1.1

5-hydroxytryptamine receptor 2A

Histamine H1 receptor

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

Predicted Targets

Acyl Cholesterol Acyltransferase 1 (ACAT-1)

Histone Deacetylase 1 (HDAC1)

Sigma opioid receptor

Dopamine D4 receptor

Butyrylcholinesterase (BuChE)

Carbonic Anhydrase IV

Carbonic anhydrase II

HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B

Tyrosine-protein kinase FGR

MAP Kinase p38 alpha Mutant (G110A)

Vanilloid receptor 1

Carbonic anhydrase I

Carboxylesterase

Peroxisome proliferator-activated receptor delta

Angiotensin-Converting Enzyme
ErbB-4 (HER4) Tyrosine Kinase
Multidrug resistance-associated protein 1
Melatonin receptor 1C

Sodium channel protein type II alpha subunit

Monoamine oxidase B
VEGFR-2 (KDR)
Peripheral-Type Benzodiazepine Receptor
Tyrosine Kinase c-Kit Mutant (N822K)
Adenosine A3 Receptor
Mitogen-Activated Protein Kinase 9 (JNK2) Mutant (C162S)
Beta lactamase TEM-152
Oxytocin receptor
Muscle glycogen phosphorylase
Fibroblast growth factor receptor 1
Interleukin-8 receptor B

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

Predicted Targets

Glutamate (NMDA) receptor subunit zeta 1

Glutamate [NMDA] receptor subunit epsilon 3

Sigma opioid receptor
Cannabinoid Receptor 2
Dipeptidyl peptidase VI
Metabotropic glutamate receptor 8
Cannabinoid Receptor 1
Serotonin Receptor 1A
Voltage-gated calcium channel alpha2/delta subunit 1
Renal dipeptidase precursor
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Delta opioid receptor
Monoamine oxidase B
GABA transporter 4
Kappa Opioid Receptor
Nitric Oxide Synthase
Prostaglandin G/H synthase 2
Muscarinic acetylcholine receptor M1
Vasopressin V1a Receptor
Vasopressin V2 Receptor
5-hydroxytryptamine receptor 2A
Aromatase (CYP19)
Androgen Receptor
Serotonin 6 (5-HT6) receptor
HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B
Butyrylcholinesterase (BuChE)

DNA polymerase alpha catalytic subunit
Carbonic anhydrase II
Steroid 17-alpha-Monooxygenase (CYP17)
Muscarinic acetylcholine receptor M2

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

Predicted Targets

Nitric Oxide Synthase
Dihydrofolate Reductase (DHFR)
Thrombin
Diamine oxidase-like protein 2
Trypsin II
Polyamine oxidase
Sodium/hydrogen exchanger 1
Subtilisin/kexin type 4
Urokinase-type plasminogen activator
Carbonic Anhydrase IV
Carbonic anhydrase II
Carbonic anhydrase I
Sigma opioid receptor
Neuraminidase
Trypsin I
Coagulation factor X
Sodium channel protein type II alpha subunit
Neuraminidase B
Hepatocyte growth factor-like protein
C-C chemokine receptor type 5
Adenosine receptor A2a
Thyroid Hormone Receptor (TR-beta)
S-adenosylmethionine decarboxylase 1
Plasma Kallikrein
Factor VIIa (fVIIa)
Histamine H4 receptor
Tyrosinase
Sigma-1 receptor
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :

dihydrofolate reductase inhibitor

Predicted Targets

Dihydrofolate Reductase (DHFR)

Dihydrofolate Reductase-Thymidylate Synthase (DHFR-TS) Mutant V1/S

Folylpoly-gamma-glutamate synthetase

Thymidylate synthase

NAALADase II

GAR transformylase

Carbonic anhydrase II

Carbonic anhydrase I

LAP4

Carbonic anhydrase IX

AICAR Tfase

Carbonic Anhydrase IV

GAR Tfase

Folate receptor alpha

Cholecystokinin-1 Receptor

Cholecystokinin B receptor

Purinergic receptor P2Y12

Coagulation factor X

Aldose Reductase (ALR2) Mutant (L300P)

Histone Deacetylase 1 (HDAC1)

Matrix metalloproteinase 9

Angiotensin-Converting Enzyme

Beta-3 adrenergic receptor

Matrix Metalloproteinase-1 (MMP-1)

HMG-CoA Reductase

Protein-tyrosine phosphatase 1B

Muscle glycogen phosphorylase

Glucagon Receptor

Peroxisome proliferator-activated receptor delta

I-kappa-B Kinase 2 (IKK-beta)

Milnacipran

Molecular Mechanism (initial) :

5-HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

5-HT and norepinephrine reuptake inhibitor

Predicted Targets

GABA transporter 4

Cytochrome P450 2D1

Monoamine oxidase B

NK1 Receptor

Serotonin Receptor 1A

Sigma-1 receptor

Glutamate [NMDA] receptor subunit epsilon 3

Delta opioid receptor

Kappa Opioid Receptor

Sigma opioid receptor

Butyrylcholinesterase (BuChE)
hERG Potassium Channel 1
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Acyl Cholesterol Acyltransferase 1 (ACAT-1)
Dopamine D2 receptor
5-hydroxytryptamine receptor 2A
Histamine H1 receptor
Voltage-gated potassium channel subunit Kv1.1
Dopamine D3 receptor
Voltage-gated R-type calcium channel alpha-1E subunit
Cannabinoid Receptor 2
Peripheral-Type Benzodiazepine Receptor
Voltage-gated calcium channel alpha2/delta subunit 1
Serotonin Receptor 2C
Melanocortin receptor 4
Neurokinin 2 receptor
C-C chemokine receptor type 5
electroneutral potassium-chloride cotransporter KCC2
Nociceptin Receptor (ORL1 Receptor)

Miltefosine

Molecular Mechanism (initial) :

Akt/PKB inhibitor

Molecular Mechanism (repurposed) :

phosphatidyl-choline biosynthesis inhibitor

Predicted Targets

Phospholipase A2
'Phospholipase A2
Butyrylcholinesterase (BuChE)
Carnitine palmitoyltransferase 1B
Fatty Acid Amide Hydrolase
Cannabinoid Receptor 1
Carbonic anhydrase II
Carbonic anhydrase IX
Carbonic anhydrase I
Muscarinic acetylcholine receptor M1
Phospholipase A2 group 1B
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M2
Ectonucleotide pyrophosphatase/phosphodiesterase family member 3
Farnesyl Diphosphate Synthase (FPPS)
Geranylgeranyl Diphosphate Synthase (GGPPS)
Carbonic anhydrase XIII
Squalene epoxidase
Carbonic Anhydrase IV
Carbonic anhydrase VA
Histamine H3 Receptor
Carbonic Anhydrase XIV

Carbonic Anhydrase XII
Carbonic anhydrase III
Carbonic anhydrase VII
Acetylcholine receptor protein epsilon chain
Carbonic anhydrase VB
Carbonic anhydrase VI
Peroxisome proliferator-activated receptor delta
Phospholipase A2 group 1VD

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

Predicted Targets

Matrix metalloproteinase 9
Matrix Metalloproteinase-1 (MMP-1)
NK1 Receptor
Delta opioid receptor
Protein kinase B (Akt 2)
Kappa Opioid Receptor
Serotonin Receptor 1A
Progesterone Receptor (PR)
Aromatase (CYP19)
Dopamine D2 receptor
HSP90AA1 protein
5-hydroxytryptamine receptor 2A
Glucocorticoid receptor
Thrombin
Ornithine decarboxylase
GABA transporter 4
Sodium/hydrogen exchanger 1
DNA topoisomerase 1
ATP-Binding Cassette Transporter ABCG2
Androgen Receptor
Serotonin Receptor 4
Arachidonate 15-lipoxygenase
DNA topoisomerase II beta
Phospholipase A2 group 1B
Cannabinoid Receptor 2
Trypsin II
estrogen receptor alpha
Serotonin 3a (5-HT3a) receptor
Dopamine D1 receptor
Tyrosine-protein kinase FGR

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

Predicted Targets

HIV-1 Protease chain A

Cytochrome P450 3A43

P-glycoprotein 1

Thyroid Hormone Receptor (TR-beta)

Renin

HAP protein (Putative aspartic proteinase)

Angiotensin-Converting Enzyme

Pepsin

Delta opioid receptor

Cholecystokinin B receptor

Endothelin-Converting Enzyme 1

Cathepsin D

HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B

Alpha-1b adrenergic receptor

Dopamine D4 receptor

Thrombin

Cholecystokinin-1 Receptor

Ecdysone receptor

Leukocyte elastase

Voltage-gated R-type calcium channel alpha-1E subunit

Muscle glycogen phosphorylase

Matrix Metalloproteinase-1 (MMP-1)

C-C chemokine receptor type 3

Matrix metalloproteinase 9

NK1 Receptor

GABA transporter 4

Muscarinic acetylcholine receptor M2

C-C chemokine receptor type 5

Cathepsin E

Purinergic receptor P2Y12

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

proto-oncogene c-Kit inhibitor

Predicted Targets

Tyrosine-protein kinase ABL

Tyrosine Kinase DDR1

Tyrosine Kinase c-Kit Mutant (N822K)

Carbonic Anhydrase XII
 Carbonic anhydrase II
 Carbonic anhydrase IX
 Carbonic anhydrase I
 Carbonic Anhydrase IV
 Carbonic Anhydrase XIV
 Carbonic anhydrase VII
 Carbonic anhydrase XIII
 Carbonic anhydrase VI
 Tyrosine-protein kinase FGR
 Carbonic anhydrase III
 EPHA1
 RAF-1
 VEGFR-2 (KDR)
 MAP Kinase p38 alpha Mutant (G110A)
 Protein kinase C alpha
 Carbonic anhydrase VA
 Histone Deacetylase 1 (HDAC1)
 Tie-2
 IGF1R
 Histone Deacetylase 6 (HDAC6)
 Tyrosine Kinase Syk
 Mitogen-Activated Protein Kinase 9 (JNK2) Mutant (C162S)
 ErbB-4 (HER4) Tyrosine Kinase
 Vanilloid receptor 1
 Metabotropic glutamate receptor 8
 ATP-Binding Cassette Transporter ABCG2

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Predicted Targets

4-hydroxyphenylpyruvate dioxygenase

Plasminogen activator inhibitor-1
 Carboxylesterase
 Androgen Receptor
 Vanilloid receptor 1
 GABA transporter 4
 Peroxisome proliferator-activated receptor delta
 Thioredoxin reductase 2
 Cannabinoid Receptor 1
 Cannabinoid Receptor 2
 Progesterone Receptor (PR)
 Multidrug resistance-associated protein 1
 Dihydroorotate dehydrogenase
 Peroxisome Proliferator-Activated Receptor alpha
 Kappa Opioid Receptor

Delta opioid receptor
Adenosine A1 receptor
Histamine H3 Receptor
BCR/ABL p210 fusion protein
C-C chemokine receptor type 5
Dihydroorotate Dehydrogenase (DHODH) Mutant (H185A)
Dipeptidyl peptidase VI
Fatty Acid Amide Hydrolase
Prostaglandin G/H synthase 2
Arachidonate 15-lipoxygenase
Modulator of drug activity A
Butyrylcholinesterase (BuChE)
5-hydroxytryptamine receptor 2A
Serotonin Receptor 1A
Serotonin Receptor 7

Paclitaxel

Molecular Mechanism (initial) :

tubulin beta modulator (microtubule-stabilizing agent)

Molecular Mechanism (repurposed) :

tubulin beta modulator (microtubule-stabilizing agent)

Predicted Targets

P-glycoprotein 1
Butyrylcholinesterase (BuChE)
Cytochrome P450 3A43
Sarco/endoplasmic Reticulum Ca²⁺ ATPase 1
mTOR
Vanilloid receptor 1
Kappa Opioid Receptor
Protein kinase C alpha
Voltage-gated potassium channel subunit Kv1.1
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Protein kinase C delta
C-C chemokine receptor type 5
Adenosine A1 receptor
Adenosine receptor A2a
Adenosine A3 Receptor
Matrix Metalloproteinase-1 (MMP-1)
Beta-chymotrypsin
Adenylate cyclase type I
Tyrosine aminotransferase
Synaptic vesicular amine transporter
DNA Topoisomerase IV Chain B
Acyl Cholesterol Acyltransferase 1 (ACAT-1)
Glucocorticoid receptor
GABA transporter 4
Trypsin I

Protein-tyrosine phosphatase 1B
Thrombin
Delta opioid receptor

Phentolamine mesilate

Molecular Mechanism (initial) :

alpha-adrenoceptor antagonist

Molecular Mechanism (repurposed) :

alpha-adrenoceptor antagonist

Predicted Targets

alpha-2A adrenergic receptor [Homo sapiens]

Alpha-1b adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Serotonin Receptor 1E

Serotonin 1d (5-HT1d) receptor

Nischarin

Serotonin Receptor 1A

Butyrylcholinesterase (BuChE)

Kappa Opioid Receptor

Delta opioid receptor

GABA transporter 4

5-hydroxytryptamine receptor 2A

Dopamine D3 receptor

Serotonin Receptor 2C

Serotonin 5b (5-HT5b) receptor

Dopamine D2 receptor

17-beta-Hydroxysteroid Dehydrogenase 2 (17-beta-HSD2)

17-beta-Hydroxysteroid Dehydrogenase 1 (17-beta-HSD1)

Monoamine oxidase B

estrogen receptor alpha

Sigma opioid receptor

5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]

Dopamine D1 receptor

Androgen Receptor

Multidrug resistance-associated protein 1

Dopamine D4 receptor

Aromatase (CYP19)

Liver X Receptor alpha (LXR-alpha)

Neuronal acetylcholine receptor protein alpha-7 subunit

Raloxifene hydrochloride

Molecular Mechanism (initial) :

estrogen receptor agonist

Molecular Mechanism (repurposed) :

estrogen receptor agonist

Predicted Targets

estrogen receptor alpha

Thrombin
 Sigma opioid receptor
 5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]
 Phospholipase D2
 Aldehyde oxidase
 Multidrug resistance-associated protein 1
 Adenosine A1 receptor
 Tyrosine-protein kinase receptor FLT3
 Histamine H3 Receptor
 Dopamine D2 receptor
 Histamine H1 receptor
 Tyrosine Kinase c-Kit Mutant (N822K)
 Farnesoid X-Activated Receptor
 Matrix Metalloproteinase-1 (MMP-1)
 Matrix metalloproteinase 9
 Dopamine D1 receptor
 Dopamine D3 receptor
 Adenosine receptor A2a
 VEGFR-2 (KDR)
 Apoptosis Regulator Bcl-2
 hERG Potassium Channel 1
 Butyrylcholinesterase (BuChE)
 Histamine H2 Receptor
 5-hydroxytryptamine receptor 2A
 Alpha-1b adrenergic receptor
 Tyrosine-protein kinase FGR
 Cytosolic phospholipase A2
 Protein-tyrosine phosphatase 1B
 Thyroid Hormone Receptor (TR-beta)

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :

dopamine D2 and D3 receptor agonist

Predicted Targets

Dopamine D2 receptor

Serotonin Receptor 1A

Dopamine D3 receptor

Serotonin 1d (5-HT1d) receptor

Dopamine D4 receptor

Sigma opioid receptor

Glycogen Synthase Kinase-3

Cyclin-Dependent Kinase 1 (CDK1)

Dopamine D1 receptor

CDK5

Serotonin 5b (5-HT5b) receptor

Malate dehydrogenase
Sigma-1 receptor
GABA transporter 4
Serotonin 6 (5-HT₆) receptor
5-hydroxytryptamine receptor 2A
Serotonin Receptor 7
Metabotropic glutamate receptor 8
Butyrylcholinesterase (BuChE)
alpha-2A adrenergic receptor [Homo sapiens]
VEGFR-2 (KDR)
estrogen receptor alpha
Trace amine-associated receptor1
Melatonin receptor 1C
Trypanothione Reductase (TryR)
Cytochrome P450 3A43
Protein kinase C alpha
Progesterone Receptor (PR)
Protein kinase C delta
Alpha-1b adrenergic receptor

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :

phospho-diesterase (PDE5A) inhibitor

Predicted Targets

Phosphodiesterase Type 5 (PDE5)

Phosphodiesterase 10A
Phosphodiesterase Type 1 (PDE1B)
Phosphodiesterase Type 11 (PDE11A)
Phosphodiesterase 6A
Multidrug resistance-associated protein 1
Phosphodiesterase 4C
Adenosine A1 receptor
Adenosine receptor A2a
Adenosine receptor A2b
Phosphodiesterase Type 3 (PDE3B)
Phosphodiesterase Type 2 (PDE2A)
Phosphodiesterase Type 7 (PDE7B)
Adenosine A3 Receptor
Beta-3 adrenergic receptor
VEGFR-2 (KDR)
Caspase-3
Leukocyte elastase
Alkaline phosphatase placental type
VCAM-1
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Caspase-7
Thrombin

Dopamine D1 receptor
Prostaglandin D2 Receptor CRTH2
Tyrosine-protein kinase FGR
Serotonin 6 (5-HT6) receptor
Dopamine D2 receptor
electroneutral potassium-chloride cotransporter KCC2
5-hydroxytryptamine receptor 2A

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Predicted Targets

HMG-CoA Reductase

Protein kinase C alpha
Immunophilin FKBP12
HSP90AA1 protein
Caspase-1
Peroxisome proliferator-activated receptor delta
Transcription factor AP-1
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Carboxylesterase
Glucocorticoid receptor
Protein kinase C delta
Dopamine D2 receptor
Caspase-7
Caspase-3
Cannabinoid Receptor 2
Steroid 17-alpha-Monooxygenase (CYP17)
Butyrylcholinesterase (BuChE)
Caspase-6
Prostaglandin G/H synthase 2
ErbB-4 (HER4) Tyrosine Kinase
Tyrosine-protein kinase FGR
Vitamin D receptor
Muscarinic acetylcholine receptor M3
Renin
mTOR
Androgen Receptor
Alpha-amylase 2B
Cannabinoid Receptor 1
Aromatase (CYP19)

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

Predicted Targets

'Retinoic Acid Receptor

Retinoid X receptor beta

'Retinoic Acid Receptor

Retinoic acid receptor alpha

Peroxisome proliferator-activated receptor delta

Multidrug resistance-associated protein 1

Steroid 5-alpha-reductase 2

Gonadotropin-releasing hormone receptor

20-alpha-Hydroxysteroid Dehydrogenase (AKR1C1)

Carbonic Anhydrase XII

Carbonic anhydrase II

Carbonic anhydrase I

Metabotropic glutamate receptor 8

'nuclear receptor subfamily 4

Cytosolic phospholipase A2

Delta opioid receptor

P-glycoprotein 1

Carbonic anhydrase IX

HSP90AA1 protein

Beta-ketoacyl-ACP synthase III

Steroid 5-alpha-reductase 1

Beta-1 Adrenergic Receptor

Beta-3 adrenergic receptor

Neuraminidase

Carbonic anhydrase VA

Carbonic anhydrase VB

Carbonic anhydrase VI

Muscle glycogen phosphorylase

'Glutamate receptor ionotropic

Tetrabenazine

Molecular Mechanism (initial) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Predicted Targets

Synaptic vesicular amine transporter

Dipeptidyl peptidase VI

Melatonin receptor 1C

Carbonic Anhydrase XIV

Carbonic anhydrase IX
 Carbonic anhydrase I
 Dopamine D1 receptor
 Carbonic anhydrase II
 Dopamine D2 receptor
 Butyrylcholinesterase (BuChE)
 Dopamine D3 receptor
 Dopamine D4 receptor
 GABA transporter 4
 Sigma opioid receptor
 Alpha-1b adrenergic receptor
 Monoamine oxidase B
 hERG Potassium Channel 1
 Muscarinic acetylcholine receptor M2
 5-hydroxytryptamine receptor 2A
 Serotonin Receptor 2C
 5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]
 Serotonin Receptor 1A
 Quinone reductase 2
 Serotonin Receptor 7
 Dihydrofolate Reductase (DHFR)
 Aromatase (CYP19)
 17-beta-Hydroxysteroid Dehydrogenase 1 (17-beta-HSD1)
 Muscarinic acetylcholine receptor M1
 Tubulin beta-8 chain
 Multidrug resistance-associated protein 1

Thalidomide

Molecular Mechanism (initial) :

TNF-alpha production inhibitor

Molecular Mechanism (repurposed) :

cereblon (CRBN) inhibitor

Predicted Targets

Prostaglandin G/H synthase 2

Serotonin Receptor 1A

Tumour necrosis factor alpha

Steroid 5-alpha-reductase 1

Caspase-3

Butyrylcholinesterase (BuChE)

Dopamine D2 receptor

Sigma opioid receptor

Arachidonate 15-lipoxygenase

Carboxylesterase

Protein Tyrosine Phosphatase CD45

Protein-tyrosine phosphatase 1B

5-hydroxytryptamine receptor 2A

Serotonin Receptor 7

Monoamine oxidase B
Delta opioid receptor
Matrix Metalloproteinase-1 (MMP-1)
Aldose Reductase (ALR2) Mutant (L300P)
Serotonin Receptor 2C
5-hydroxytryptamine (serotonin) receptor 2B [Homo sapiens]
Muscarinic acetylcholine receptor M2
HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B
Multidrug resistance-associated protein 1
Matrix metalloproteinase 9
Kappa Opioid Receptor
Nociceptin Receptor (ORL1 Receptor)
Metabotropic glutamate receptor 8
MAP Kinase p38 alpha Mutant (G110A)
Alpha-1b adrenergic receptor
Glutamate (NMDA) receptor subunit zeta 1

Topiramate

Molecular Mechanism (initial) :

kainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker

Molecular Mechanism (repurposed) :

ckainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker

Predicted Targets

Carbonic anhydrase II

Carbonic Anhydrase IV
Carbonic anhydrase I
Carbonic anhydrase VA
Carbonic Anhydrase XIV
Carbonic anhydrase IX
Carbonic anhydrase VII
Carbonic Anhydrase XII
Carbonic anhydrase VB
Carbonic anhydrase XIII
Carbonic anhydrase VI
Matrix metalloproteinase 9
Matrix Metalloproteinase-1 (MMP-1)
Carbonic anhydrase III
Cytochrome P450 3A43
HIV-1 Protease chain A
Arachidonate 15-lipoxygenase
Muscarinic acetylcholine receptor M2
alpha-Glucosidase (alpha-Glu)
Methionine Aminopeptidase Type 2 (MetAP2)

Thromboxane-A synthase
Adenosine A3 Receptor
Peroxisome proliferator-activated receptor delta
Aromatase (CYP19)
11-beta-Hydroxysteroid Dehydrogenase 1 (11-beta-HSD1)
Vasopressin V1a Receptor
estrogen receptor alpha
Farnesoid X-Activated Receptor
Muscarinic acetylcholine receptor M1
Kappa Opioid Receptor

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

Predicted Targets

estrogen receptor alpha

'Estrogen-Related Receptor
Sigma opioid receptor
P-glycoprotein 1
Cytochrome P450 2D1
Histamine H3 Receptor
Serotonin Receptor 1A
Serotonin Receptor 7
ErbB-4 (HER4) Tyrosine Kinase
Prostaglandin G/H synthase 2
Dopamine D2 receptor
Tyrosine Kinase c-Kit Mutant (N822K)
Trace amine-associated receptor1
Thyroid Hormone Receptor (TR-beta)
G-protein Coupled Receptor 40
GABA transporter 4
Serotonin 1d (5-HT1d) receptor
Peroxisome proliferator-activated receptor delta
Interleukin-8 receptor B
Dopamine D4 receptor
Apoptosis Regulator Bcl-2
Arachidonate 15-lipoxygenase
Fibroblast growth factor receptor 1
Dopamine D1 receptor
Butyrylcholinesterase (BuChE)
Dopamine D3 receptor
Protein-tyrosine phosphatase 1B
Histone Deacetylase 1 (HDAC1)
Trypsin I
Neuronal acetylcholine receptor protein alpha-7 subunit

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

Predicted Targets

Histone Deacetylase 1 (HDAC1)

Histone Deacetylase 6 (HDAC6)

Histone deacetylase 8

Histone Deacetylase 7 (HDAC7)

Histone Deacetylase 10 (HDAC10)

Acyl Cholesterol Acyltransferase 1 (ACAT-1)

Arachidonate 15-lipoxygenase

Matrix Metalloproteinase-1 (MMP-1)

Cannabinoid Receptor 1

Melatonin receptor 1C

Voltage-gated T-type calcium channel alpha-1I subunit

Phosphodiesterase Type 5 (PDE5)

Carbonic Anhydrase IV

Carbonic anhydrase II

Protein Tyrosine Phosphatase CD45

Carbonic anhydrase VA

Fatty Acid Amide Hydrolase

Cannabinoid Receptor 2

Carbonic anhydrase IX

Matrix metalloproteinase 9

HIV-1 Protease chain A

HIV-1 Reverse Transcriptase RNase H Mutant (L100I/K103N) Chain B

Carbonic Anhydrase XII

Neuronal acetylcholine receptor protein alpha-7 subunit

Butyrylcholinesterase (BuChE)

Matrix metalloproteinase-24

Aminopeptidase M

Nitric Oxide Synthase

Caspase-3

Aldose Reductase (ALR2) Mutant (L300P)

Supplement 5

Biological activity profile predicted with TargetHunter

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

Predicted Targets

Mu opioid receptor

Kappa opioid receptor

Delta opioid receptor

Opioid receptor
Monoamine oxidase A
Monoamine oxidase B
Phospholipidosis
Cytochrome P450 3A4
P-glycoprotein 1
Chromobox protein homolog 1
Serotonin 5a (5-HT5a) receptor

Opioid receptors; mu & delta

Alprostadi

Molecular Mechanism (initial) :

prostaglandin E2 receptor agonist

Molecular Mechanism (repurposed) :

prostaglandin E2 receptor agonist

Predicted Targets

Prostanoid EP1 receptor

Prostanoid EP2 receptor

Prostanoid EP3 receptor
Prostanoid EP4 receptor
Prostanoid IP receptor
Oryctolagus cuniculus
Monoamine oxidase A
Monoamine oxidase B
Luciferin 4-monooxygenase
Hepatotoxicity
Cytochrome P450 2D6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 1A2
Liver microsomes
Cytochrome P450 3A4
Solute carrier organic anion transporter family member 3A1
Solute carrier organic anion transporter family member 2A1
Solute carrier organic anion transporter family member 2B1
Multidrug resistance-associated protein 5
Multidrug resistance-associated protein 4
Acetylcholinesterase
Cholinesterase
Menin/Histone-lysine N-methyltransferase MLL
Thyroid stimulating hormone receptor
Nuclear receptor ROR-gamma
MAP kinase ERK2
15-hydroxyprostaglandin dehydrogenase [NAD+]
Prelamin-A/C
Hypoxia-inducible factor 1 alpha
4'-phosphopantetheinyl transferase ffp
Vitamin D receptor

Amantadine hydrochloride

Molecular Mechanism (initial) :

matrix protein 2 (Influenza virus A) inhibitor

Molecular Mechanism (repurposed) :

dopamine receptor agonists

NMDA receptor antagonists

Predicted Targets

Sigma opioid receptor

Glutamate [NMDA] receptor

Canalicular multispecific organic anion transporter 1

Monoamine oxidase A

Monoamine oxidase B

Nuclear factor NF-kappa-B p105 subunit

Signal transducer and activator of transcription 6

Thyroid stimulating hormone receptor

Phospholipidosis

Nuclear factor erythroid 2-related factor 2

Histone acetyltransferase GCN5

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

6-phospho-1-fructokinase

Cytochrome P450 2C9

Cytochrome P450 3A4

Cytochrome P450 2C19

Cytochrome P450 1A2

Cytochrome P450 2D6

Solute carrier family 22 member 2

Matrix protein 2

Nitric-oxide synthase, brain

Thioredoxin reductase 1, cytoplasmic

Regulator of G-protein signaling 4

P-glycoprotein 1

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Beta-3 adrenergic receptor

Norepinephrine transporter

Aldose reductase

Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor

Calcitonin receptor

Cannabinoid CB1 receptor

Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystikinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1

Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Peripheral myelin protein 22
Solute carrier family 22 member 1
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Multidrug and toxin extrusion protein 1

Influenza virus A matrix protein M2

Thyroid hormone receptor beta-1
Nonstructural protein 1
Bloom syndrome protein
Newcastle disease virus
Survival motor neuron protein
Beta-lactamase AmpC
DNA polymerase beta
Chromobox protein homolog 1
Geminin
Transcriptional regulator ERG

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

Predicted Targets

Muscarinic acetylcholine receptor

Sodium channel alpha subunits; brain (Types I, II, III)

Monoamine oxidase

Serotonin (5-HT) receptor

Alpha-1a adrenergic receptor

Confidence Score:NAN

Histamine H1 receptor

Histamine H2 receptor

Norepinephrine transporter

Serotonin transporter

UDP-glucuronosyltransferase 1A4

Cytochrome P450 3A4

Sphingomyelin phosphodiesterase

Canalicular multispecific organic anion transporter 1

Solute carrier family 22 member 1

Histamine H3 receptor

Dopamine D1 receptor

Dopamine D5 receptor

Dopamine D2 receptor

Dopamine D3 receptor

Nuclear factor NF-kappa-B p105 subunit

FK506 binding protein 12

Muscarinic acetylcholine receptor M1

Endoplasmic reticulum-associated amyloid beta-peptide-binding protein

Cytochrome P450 2D6

Phospholipidosis

Chromobox protein homolog 1

Arachidonate 15-lipoxygenase, type II

Cytochrome P450 2C9

Cytochrome P450 2C19

Cytochrome P450 1A2

Ataxin-2

Thioredoxin reductase 1, cytoplasmic

Ubiquitin carboxyl-terminal hydrolase 1

UDP-glucuronosyltransferase 1-1

UDP-glucuronosyltransferase 1-10

UDP-glucuronosyltransferase 1-6

UDP-glucuronosyltransferase 1-7

UDP-glucuronosyltransferase 1-9

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G

Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Liver microsomes
P-glycoprotein 1
P-glycoprotein 3
Sodium channel protein type II alpha subunit
Sodium channel protein type V alpha subunit
Sodium channel protein type IX alpha subunit
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Lymphoblastoid cells
Prelamin-A/C
Lysine-specific demethylase 4D-like
Microtubule-associated protein tau
Endonuclease 4
Aldehyde dehydrogenase 1A1
Thioredoxin glutathione reductase
Peripheral myelin protein 22
4'-phosphopantetheinyl transferase ffp
Inositol monophosphatase 1
Menin/Histone-lysine N-methyltransferase MLL
Putative fructose-1,6-bisphosphate aldolase
Anthrax lethal factor

Serine-protein kinase ATM
Cellular tumor antigen p53
M-phase phosphoprotein 8
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Vanilloid receptor
Thyroid hormone receptor beta-1
Bile acid receptor FXR
Peroxisome proliferator-activated receptor delta
Peroxisome proliferator-activated receptor gamma
Mothers against decapentaplegic homolog 3
Retinoid X receptor alpha
Geminin
Glucagon-like peptide 1 receptor
Nuclear receptor ROR-gamma
Isocitrate dehydrogenase [NADP] cytoplasmic

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

Predicted Targets

Dopamine D2 receptor

Dopamine D1 receptor
Dopamine receptors; D1 & D2
Dopamine receptor
Adenylate cyclase
Serotonin 1a (5-HT1a) receptor
Opioid receptor
Dopamine D1 and D2 receptor
Serotonin (5-HT) receptor
Adrenergic receptor alpha-2
Adrenergic receptor alpha-1
Serotonin 7 (5-HT7) receptor
Dopamine D3 receptor

Dopamine D4 receptor

Sigma opioid receptor
Serum albumin
Solute carrier family 22 member 1
Menin/Histone-lysine N-methyltransferase MLL
Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
Lysine-specific demethylase 4D-like
Tyrosyl-DNA phosphodiesterase 1
Microtubule-associated protein tau
Cytochrome P450 2C19
Nuclear receptor ROR-gamma
Aldehyde dehydrogenase 1A1
4'-phosphopantetheinyl transferase ffp
MAP kinase ERK2

Putative fructose-1,6-bisphosphate aldolase
Anthrax lethal factor
15-hydroxyprostaglandin dehydrogenase [NAD+]
Cellular tumor antigen p53
Cytochrome P450 3A4
Cytochrome P450 2D6
Cytochrome P450 2C9
6-phospho-1-fructokinase
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Arachidonate 15-lipoxygenase, type II
Cytochrome P450 1A2
Sulfotransferase 1A1
Vitamin D receptor
Regulator of G-protein signaling 4
Peripheral myelin protein 22
Luciferin 4-monooxygenase
Geminin
Glutaminase kidney isoform, mitochondrial
Dopamine receptor D2 and D3
Nuclear factor NF-kappa-B p105 subunit
Hypoxia-inducible factor 1 alpha
Pyruvate kinase isozymes M1/M2
Arachidonate 15-lipoxygenase
Arachidonate 12-lipoxygenase
Muscarinic acetylcholine receptor M1
Pyruvate kinase
Thioredoxin glutathione reductase
Zinc finger protein mex-5
Fructose-bisphosphate aldolase A
Beta-lactamase AmpC
M18 aspartyl aminopeptidase
Lysosomal alpha-glucosidase
Cathepsin L
Cytoplasmic zinc-finger protein
Lysine-specific demethylase 4A
M-phase phosphoprotein 8
Thioredoxin reductase 1, cytoplasmic
Chromobox protein homolog 1
Bromodomain adjacent to zinc finger domain protein 2B
ATPase family AAA domain-containing protein 5
Flap endonuclease 1
DNA polymerase iota
Mothers against decapentaplegic homolog 3
ATP-dependent Clp protease proteolytic subunit
Isocitrate dehydrogenase [NADP] cytoplasmic
Solute carrier organic anion transporter family member 1B1
Solute carrier organic anion transporter family member 1B3
Mannose-6-phosphate isomerase
Nonstructural protein 1
Induced myeloid leukemia cell differentiation protein Mcl-1

DNA polymerase beta
 Glucose-6-phosphate dehydrogenase-6-phosphogluconolactonase
 Runt-related transcription factor 1/Core-binding factor subunit beta
 Eukaryotic translation initiation factor 4E
 Glucose-6-phosphate 1-dehydrogenase
 Polyadenylate-binding protein 1
 Glucagon-like peptide 1 receptor
 Histone-lysine N-methyltransferase MLL
 Survival motor neuron protein
 Ferritin light chain
 Alpha-galactosidase A
 ATP-dependent DNA helicase Q1
 Lethal(3)malignant brain tumor-like protein 1
 Beta-2 adrenergic receptor
 DNA dC->dU-editing enzyme APOBEC-3G
 Mu opioid receptor
 Breast cancer type 1 susceptibility protein
 Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
 Putative uncharacterized protein
 Serotonin 2a (5-HT2a) receptor
 DNA repair protein RAD52 homolog
 Inositol monophosphatase 1

Acetylsalicylic acid

Molecular Mechanism (initial) :

cyclooxygenase inhibitor

Molecular Mechanism (repurposed) :

cyclooxygenase inhibitor

Predicted Targets

Cyclooxygenase-2

Cyclooxygenase-1

Cyclooxygenase

Integrin alpha-IIb/beta-3
 Thromboxane-A synthase
 Arachidonate 5-lipoxygenase
 Glutathione reductase
 Prostaglandin G/H synthase (cyclooxygenase)
 Aldo-keto-reductase family 1 member C3
 Mycobacterium tuberculosis
 Solute carrier family 22 member 6
 Solute carrier family 22 member 20
 Peroxisome proliferator-activated receptor gamma
 Carbonic anhydrase I
 Carbonic anhydrase II
 Gamma-glutamyltranspeptidase 1
 Solute carrier family 22 member 1
 Fatty acid-binding protein, liver
 Phospholipase A2 group 1B
 Monoamine oxidase A

Monoamine oxidase B
Butyrylcholinesterase
Beta-glucuronidase
Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
Lysine-specific demethylase 4D-like
Thyroid stimulating hormone receptor
Tyrosyl-DNA phosphodiesterase 1
Aldehyde dehydrogenase 1A1
Anthrax lethal factor
Bloom syndrome protein
15-hydroxyprostaglandin dehydrogenase [NAD+]
Muscarinic acetylcholine receptor M1
Phospholipidosis
Amiloride-sensitive cation channel 3
Beta-glucocerebrosidase
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Androgen Receptor
Glucocorticoid receptor
Thioredoxin reductase 1, cytoplasmic
DNA polymerase iota
DNA polymerase kappa
UDP-glucuronosyltransferase 1-1
UDP-glucuronosyltransferase 1-6
UDP-glucuronosyltransferase 1-9
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cytochrome P450 1A2
Cytochrome P450 2A6

Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Cytochrome P450 3A4
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1

Tyrosine-protein kinase FYN
 Receptor protein-tyrosine kinase erbB-2
 Tyrosine-protein kinase LCK
 Leukocyte common antigen
 Serotonin 1a (5-HT1a) receptor
 Serotonin 1b (5-HT1b) receptor
 Serotonin 2a (5-HT2a) receptor
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 P-glycoprotein 1
 Interleukin-8
 Nuclear receptor ROR-gamma
 Putative uncharacterized protein
 Isocitrate dehydrogenase [NADP] cytoplasmic
 Solute carrier organic anion transporter family member 1B3
 Prostaglandin E synthase

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

Predicted Targets

GABA-B receptor

GABA-A receptor; anion channel

Sodium channel alpha subunits; brain (Types I, II, III)
 Adenosine A3 receptor
 Solute carrier family 22 member 1
 Prelamin-A/C
 Nuclear factor NF-kappa-B p105 subunit
 4'-phosphopantetheinyl transferase ffp
 Bloom syndrome protein
 Cytochrome P450 3A4
 Hepatotoxicity
 Nuclear factor erythroid 2-related factor 2
 Histone acetyltransferase GCN5
 Dopamine D1 receptor
 Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
 6-phospho-1-fructokinase
 ATPase family AAA domain-containing protein 5

Thioredoxin reductase 1, cytoplasmic
Regulator of G-protein signaling 4
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase

Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1

Vasoactive intestinal polypeptide receptor 1

Vasopressin V1a receptor

Solute carrier family 22 member 8

GABA-A receptor; alpha-1/beta-2/gamma-2

Solute carrier organic anion transporter family member 1B1

Solute carrier organic anion transporter family member 1B3

GABA-B receptor 1

Ubiquitin carboxyl-terminal hydrolase 1

Menin/Histone-lysine N-methyltransferase MLL

Thyroid stimulating hormone receptor

Thyroid hormone receptor beta-1

Ferritin light chain

Guanine nucleotide-binding protein G(s), subunit alpha

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

Predicted Targets

Phospholipidosis

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

Predicted Targets

Endothelin receptor ET-A

Endothelin receptor

Endothelin receptor ET-B

Cytochrome P450 3A4

Endothelin receptor type A

Bile salt export pump

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :

mu-type opioid receptor agonist

Predicted Targets

Mu opioid receptor

Kappa opioid receptor

Delta opioid receptor

HERG

Nociceptin receptor

Opioid receptor

Monoamine oxidase A
UDP-glucuronosyltransferase 1-10
UDP-glucuronosyltransferase 1A4
UDP-glucuronosyltransferase 1-8
UDP-glucuronosyltransferase 2B15
UDP-glucuronosyltransferase 2B7
UDP-glucuronosyltransferase 1-1
DNA polymerase eta
Mothers against decapentaplegic homolog 3
Geminin
Ataxin-2
Glucagon-like peptide 1 receptor
Isocitrate dehydrogenase [NADP] cytoplasmic

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Predicted Targets

Cyclooxygenase-2
Cyclooxygenase-1
Cyclooxygenase
Prostaglandin G/H synthase (cyclooxygenase)

Carbonic anhydrase I
Carbonic anhydrase II
Carbonic anhydrase IV
Carbonic anhydrase IX
Carbonic anhydrase
MAP kinase p38 alpha
Carbonic anhydrase XII
Arachidonate 5-lipoxygenase
Cytochrome P450 2C9
Carbonic anhydrase III
Arachidonate 12-lipoxygenase
Arachidonate 15-lipoxygenase
Cytochrome c oxidase subunit 2
Canalicular multispecific organic anion transporter 1
Solute carrier family 22 member 1
Carbonic anhydrase VI
Carbonic anhydrase 15
Uncharacterized protein Rv1284/MT1322
Prostaglandin E synthase
Nitric oxide synthase, inducible
Alpha carbonic anhydrase
Carbonic anhydrase VA
Carbonic anhydrase VB
Carbonic anhydrase VII
Carbonic anhydrase XIII

Carbonic anhydrase XIV
Cytochrome c oxidase subunit 1
Prelamin-A/C
Thyroid stimulating hormone receptor
Cytochrome P450 3A4
Nuclear factor erythroid 2-related factor 2
Multidrug resistance-associated protein 4
Epoxide hydratase
Signal transducer and activator of transcription 3
Retinoid X receptor alpha
Estrogen receptor alpha
Plasmodium falciparum
Glucocorticoid receptor
Thyroid hormone receptor beta-1
HERG
Androgen Receptor
Peroxisome proliferator-activated receptor delta
Peroxisome proliferator-activated receptor gamma
Mothers against decapentaplegic homolog 3
Ubiquitin carboxyl-terminal hydrolase 1
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2D6
Cytochrome P450 2E1

Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor beta
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor

Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 3-phosphoinositide dependent protein kinase-1
 Peripheral myelin protein 22
 Quinolone resistance protein norA
 Glucagon-like peptide 1 receptor
 Nuclear receptor subfamily 1 group I member 2
 Nuclear receptor ROR-gamma
 Cadherin-11
 Solute carrier organic anion transporter family member 2B1
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBC
 Isocitrate dehydrogenase [NADP] cytoplasmic
 Delta carbonic anhydrase

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

Predicted Targets

NADH-cytochrome b5 reductase
 Arthroderma benhamiae
 Plasmodium berghei
 Protein kinase Pfmrk
 Canalicular multispecific organic anion transporter 1
 Solute carrier family 22 member 1
 Monoamine oxidase A
 Cytochrome P450 3A4
 Cytochrome P450 2B6
 Cytochrome P450 2C9
 Cytochrome P450 2C19
 Cytochrome P450 2D6
 Toll-like receptor (TLR7/TLR9)
 Toll-like receptor 7
 Toll-like receptor 9
 Quinone reductase 2
 Cysteine protease falcipain-3
 Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chloroquine resistance transporter
Thioredoxin reductase 1, cytoplasmic
Flap endonuclease 1
P-glycoprotein 1
Riboflavin-binding protein
Phosphoethanolamine N-methyltransferase
Cytochrome P450 1A2
Human immunodeficiency virus 1
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Serotonin 2c (5-HT2c) receptor
Plasmodium falciparum 3D7
Plasmodium falciparum D6
Plasmodium falciparum NF54
Botulinum neurotoxin type A
Tyrosyl-DNA phosphodiesterase 1
Lysine-specific demethylase 4D-like
Microtubule-associated protein tau
Endonuclease 4

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

Predicted Targets

Serum albumin
Serotonin 6 (5-HT6) receptor
Serotonin 7 (5-HT7) receptor
Glutamate [NMDA] receptor
Glutamate NMDA receptor
Adenylate cyclase

Dopamine D2 receptor

Dopamine receptor
Serotonin 1a (5-HT1a) receptor
Serotonin 1 (5-HT1) receptor
Serotonin 2 (5-HT2) receptor
Adrenergic receptor alpha-1
HERG
Sodium channel alpha subunits; brain (Types I, II, III)
Cytochrome P450 2D6
Dopamine D1 receptor
Muscarinic acetylcholine receptor
Dopamine D2 receptor/Serotonin 2 (5-HT2) receptor
Dopamine receptors; D1 & D2
Trypanothione reductase
Glutathione reductase
Dopamine D3 receptor

UDP-glucuronosyltransferase 1A4
Dopamine transporter
Alpha-1 adrenergic receptor
P-glycoprotein 1
Dopamine D4 receptor
Vanilloid receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 3 (5-HT3) receptor
Serotonin transporter
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M4
Adrenergic receptor alpha-2
Histamine H1 receptor
Sphingomyelin phosphodiesterase
Canalicular multispecific organic anion transporter 1
Solute carrier family 22 member 1
Quinolone resistance protein norA
Histamine H3 receptor
Dopamine D5 receptor
Calmodulin
Nuclear factor NF-kappa-B p105 subunit
Saccharomyces cerevisiae
Ras-related protein Rab-9A
Pleiotropic ABC efflux transporter of multiple drugs
Histone acetyltransferase GCN5
M-phase phosphoprotein 8
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Chromobox protein homolog 1
Arachidonate 15-lipoxygenase, type II
ATPase family AAA domain-containing protein 5
Cytochrome P450 2C9
Cytochrome P450 1A2
Cytochrome P450 2C19
Constitutive androstane receptor
Nuclear receptor subfamily 1 group I member 3
Vitamin D receptor
Ataxin-2
Thioredoxin reductase 1, cytoplasmic
DNA polymerase kappa
Mothers against decapentaplegic homolog 3
Ubiquitin carboxyl-terminal hydrolase 1
UDP-glucuronosyltransferase 1-3
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1a adrenergic receptor
Alpha-1b adrenergic receptor

Alpha-1d adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Glycine receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A

Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1b (5-HT1b) receptor
Serotonin 4 (5-HT4) receptor
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Peripheral myelin protein 22
Mycobacterium smegmatis str. MC2 155
Bile salt export pump
Geminin
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Acetylcholine receptor protein alpha chain
Isocitrate dehydrogenase [NADP] cytoplasmic
Nuclear factor erythroid 2-related factor 2
Heat shock protein beta-1
Peroxisome proliferator-activated receptor delta
Sodium channel alpha subunit
Cytochrome P450 2J2
Proto-oncogene c-JUN
Lysine-specific demethylase 4D-like
Endonuclease 4
Inositol monophosphatase 1
Menin/Histone-lysine N-methyltransferase MLL
Putative fructose-1,6-bisphosphate aldolase
Neuropeptide S receptor
Lysosomal alpha-glucosidase
DNA polymerase beta

Beta-glucocerebrosidase
 Lysine-specific demethylase 4A
 FAD-linked sulfhydryl oxidase ALR
 Bromodomain adjacent to zinc finger domain protein 2B
 Flap endonuclease 1
 DNA polymerase eta
 Bile acid receptor FXR
 Glutaminase kidney isoform, mitochondrial
 Glucagon-like peptide 1 receptor
 Nuclear receptor subfamily 1 group I member 2
 Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
 TAR DNA-binding protein 43
 DNA repair protein RAD52 homolog
 DNA-(apurinic or apyrimidinic site) lyase
 Intercellular adhesion molecule (ICAM-1), Integrin alpha-L/beta-2
 Thyroid stimulating hormone receptor
 Hypoxia-inducible factor 1 alpha
 6-phospho-1-fructokinase
 DNA polymerase iota
 Regulator of G-protein signaling 4
 Alpha-synuclein
 Cerebroside-sulfatase
 Aldehyde dehydrogenase 1A1
 Runt-related transcription factor 1/Core-binding factor subunit beta
 Rac GTPase-activating protein 1
 Guanine nucleotide-binding protein G(s), subunit alpha
 Glycoprotein hormones alpha chain
 Rap guanine nucleotide exchange factor 4
 Eyes absent homolog 2
 Niemann-Pick C1 protein
 Cholinesterase
 microRNA 21
 Nuclear receptor ROR-gamma
 Nonstructural protein 1
 Induced myeloid leukemia cell differentiation protein Mcl-1
 Bloom syndrome protein
 Alpha-galactosidase A
 Muscleblind-like protein 1
 ATP-dependent DNA helicase Q1
 Ubiquitin carboxyl-terminal hydrolase 2
 Bcl-2-related protein A1
 Ubiquitin-conjugating enzyme E2 N
 78 kDa glucose-regulated protein
 Aberrant vpr protein
 Transcriptional regulator ERG

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :
TNF- α /NF- κ b signaling pathway inhibitor

Predicted Targets

Monoclonal antibody (mAb)

Sodium/potassium-transporting ATPase

Sodium/potassium-transporting ATPase alpha-1 chain

DNA topoisomerase II alpha

DNA topoisomerase II beta

Monoamine oxidase A

Monoamine oxidase B

Ras-related protein Rab-9A

Microtubule-associated protein tau

Signal transducer and activator of transcription 3

Signal transducer and activator of transcription 1-alpha/beta

Niemann-Pick C1 protein

Nuclear receptor ROR-gamma

Cellular tumor antigen p53

Nuclear factor erythroid 2-related factor 2

ATPase family AAA domain-containing protein 5

Retinoid X receptor alpha

Estrogen receptor alpha

Androgen Receptor

Thyroid hormone receptor beta-1

Bile acid receptor FXR

Peroxisome proliferator-activated receptor delta

Peroxisome proliferator-activated receptor gamma

Mothers against decapentaplegic homolog 3

Vitamin D receptor

Glucocorticoid receptor

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Beta-3 adrenergic receptor

Norepinephrine transporter

Aldose reductase

Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor

Calcitonin receptor

Cannabinoid CB1 receptor

Carbonic anhydrase II

C-C chemokine receptor type 2

C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Cytochrome P450 3A4
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor beta
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G

Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
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Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
P-glycoprotein 1
Solute carrier organic anion transporter family member 1A1
Solute carrier organic anion transporter family member 4C1
Geminin
Cholinesterase
Isocitrate dehydrogenase [NADP] cytoplasmic
Rattus norvegicus
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Peripheral myelin protein 22
Survival motor neuron protein
Ubiquitin carboxyl-terminal hydrolase 2
UDP-glucuronosyltransferase 2B7
UDP-glucuronosyltransferase 1-1
UDP-glucuronosyltransferase 2B10
UDP-glucuronosyltransferase 2B15
UDP-glucuronosyltransferase 2B4

Doxepin hydrochloride

Molecular Mechanism (initial) :

5HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :
H1 and H2 histamine receptor blocker

Predicted Targets

Sodium channel alpha subunits; brain (Types I, II, III)

Serotonin (5-HT) receptor

Alpha-1a adrenergic receptor

Histamine H1 receptor

Histamine H2 receptor

No relevant target

Sphingomyelin phosphodiesterase

Phospholipidosis

Hepatotoxicity

UDP-glucuronosyltransferase 1A4

Tyrosine-protein kinase LCK

Leukocyte common antigen

Serotonin 1a (5-HT1a) receptor

Serotonin 1b (5-HT1b) receptor

Serotonin 2a (5-HT2a) receptor

Serotonin 2b (5-HT2b) receptor

Serotonin 2c (5-HT2c) receptor

Serotonin 4 (5-HT4) receptor

Serotonin 6 (5-HT6) receptor

Serotonin transporter

Sigma opioid receptor

Neurokinin 1 receptor

Neurokinin 2 receptor

Androgen Receptor

Thromboxane-A synthase

Vascular endothelial growth factor receptor 1

Vasoactive intestinal polypeptide receptor 1

Vasopressin V1a receptor

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Beta-3 adrenergic receptor

Norepinephrine transporter

Aldose reductase

Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor

Calcitonin receptor

Cannabinoid CB1 receptor

Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Cytochrome P450 3A4
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme

Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
P-glycoprotein 1
Rattus norvegicus
Menin/Histone-lysine N-methyltransferase MLL
Prelamin-A/C
Nuclear factor NF-kappa-B p105 subunit
Saccharomyces cerevisiae
Thyroid stimulating hormone receptor
Aldehyde dehydrogenase 1A1
Inositol monophosphatase 1
6-phospho-1-fructokinase
Arachidonate 15-lipoxygenase, type II
Vitamin D receptor
Ataxin-2
Plasmodium falciparum
Peripheral myelin protein 22
Luciferin 4-monooxygenase
Nuclear receptor ROR-gamma
Thioredoxin glutathione reductase
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Solute carrier organic anion transporter family member 1B3
ATP-dependent DNA helicase Q1
Lysine-specific demethylase 4D-like
Vanilloid receptor
Thioredoxin reductase 1, cytoplasmic
Geminin
Glucagon-like peptide 1 receptor

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

Predicted Targets

Serotonin transporter

Norepinephrine transporter

Dopamine transporter

Cytochrome P450 2D6

Transporter

Cytochrome P450 3A4

HERG

Histamine H3 receptor

Histone-lysine N-methyltransferase MLL

microRNA 21

Lysosomal alpha-glucosidase

Beta-glucocerebrosidase

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Cytochrome P450 1A2

Thioredoxin reductase 1, cytoplasmic

DNA polymerase iota

Mothers against decapentaplegic homolog 3

Peripheral myelin protein 22

Serum albumin

Ataxin-2

Glucagon-like peptide 1 receptor

Isocitrate dehydrogenase [NADP] cytoplasmic

Alpha-synuclein

Eflornithine hydrochloride

Molecular Mechanism (initial) :

ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

Predicted Targets

Ornithine decarboxylase

Solute carrier family 22 member 1

Nuclear factor erythroid 2-related factor 2

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chromobox protein homolog 1

Regulator of G-protein signaling 4

Muscarinic acetylcholine receptor M1

Cytochrome P450 2C9

Cytochrome P450 2C19

Cytochrome P450 1A2

Cytochrome P450 2D6

Cytochrome P450 3A4

Prelamin-A/C

Lysine-specific demethylase 4D-like

Ras-related protein Rab-9A

Survival motor neuron protein

Peripheral myelin protein 22

Microtubule-associated protein tau

Bloom syndrome protein

Bromodomain adjacent to zinc finger domain protein 2B

T-complex protein 1 subunit beta

Geminin

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

Predicted Targets

Epidermal growth factor receptor erbB1

Receptor protein-tyrosine kinase erbB-2

Tyrosine-protein kinase FRK

Tyrosine-protein kinase HCK

Ephrin type-B receptor 4

Serine/threonine-protein kinase 17A

Serine/threonine-protein kinase Aurora-C

Tyrosine-protein kinase CSK

Tyrosine-protein kinase ABL

c-Jun N-terminal kinase 3

Serine/threonine-protein kinase 36

Tyrosine-protein kinase YES

Mitogen-activated protein kinase kinase kinase 4

Tyrosine-protein kinase FGR

BMP-2-inducible protein kinase

Ephrin type-A receptor 7

Ephrin type-B receptor 1

MAP kinase signal-integrating kinase 2

Mitogen-activated protein kinase kinase kinase kinase 5

Tyrosine-protein kinase ABL2

Tyrosine-protein kinase BMX

Tyrosine-protein kinase BRK

c-Jun N-terminal kinase 2

Ephrin type-A receptor 8

Tyrosine-protein kinase Lyn

Tyrosine-protein kinase SRC

Tyrosine-protein kinase BTK

Ephrin type-A receptor 3

Tyrosine-protein kinase LCK

Serine/threonine-protein kinase 2

Serine/threonine-protein kinase 10

Serine/threonine-protein kinase RIPK2

Ephrin type-A receptor 4

Ephrin type-A receptor 5

Ephrin type-A receptor 6

Serine/threonine-protein kinase GAK

AMP-activated protein kinase, alpha-1 subunit

Phosphorylase kinase gamma subunit 2

Phosphorylase kinase gamma subunit 1

Tyrosine-protein kinase FYN

Fibroblast growth factor receptor 2

Fibroblast growth factor receptor 1

TRAF2- and NCK-interacting kinase
Tyrosine-protein kinase TIE-2
Ephrin type-A receptor 2
Casein kinase I epsilon
Serine/threonine-protein kinase PLK4
Tyrosine-protein kinase receptor FLT3
Stem cell growth factor receptor
Vascular endothelial growth factor receptor 2
Vascular endothelial growth factor receptor 3
Platelet-derived growth factor receptor beta
Fibroblast growth factor receptor 3
Adaptor-associated kinase
Serine/threonine-protein kinase Aurora-A
ULK3 kinase
Serine/threonine-protein kinase 17B
Dual specificity protein kinase CLK1
Dual specificity protein kinase CLK4
c-Jun N-terminal kinase 1
CaM-kinase kinase beta
CaM kinase I gamma
CaM kinase I alpha
Casein kinase I gamma 1
Cyclin-dependent kinase 2
MAP kinase p38 gamma
Serine/threonine-protein kinase 38-like
Ribosomal protein S6 kinase alpha 2
Serine/threonine-protein kinase MST1
MAP/microtubule affinity-regulating kinase 2
Ribosomal protein S6 kinase alpha 5
CaM kinase I delta
Death-associated protein kinase 2
Serine/threonine-protein kinase 16
Serine/threonine-protein kinase PIM2
Death-associated protein kinase 3
Dual specificity protein kinase CLK2
Serine/threonine-protein kinase MST2
Serine/threonine-protein kinase PCTAIRE-1
Dual specificity protein kinase TTK
Nerve growth factor receptor Trk-A
Cyclin-dependent kinase 5
MAP kinase p38 beta
MAP kinase p38 alpha
Serine/threonine-protein kinase NEK9
Dual specificity protein kinase CLK3
Casein kinase I gamma 2
Serine/threonine-protein kinase NEK2
LIM domain kinase 1
Mitogen-activated protein kinase kinase kinase 5
myosin light chain kinase 2
Insulin receptor

Focal adhesion kinase 1
Ribosomal protein S6 kinase alpha 3
Protein kinase C alpha
Tyrosine-protein kinase FER
Tyrosine kinase non-receptor protein 2
Serine/threonine-protein kinase PIM1
Tyrosine-protein kinase JAK2
Serine/threonine-protein kinase PAK 4
Tyrosine-protein kinase SYK
Serine/threonine-protein kinase PAK7
CaM kinase II beta
Serine/threonine-protein kinase PAK 1
Serine/threonine-protein kinase PAK 3
CaM kinase II delta
CaM kinase II gamma
Serine/threonine-protein kinase PAK6
CaM kinase II alpha
CaM-kinase kinase alpha
Serine/threonine-protein kinase NEK6
Tyrosine-protein kinase JAK1
Tyrosine- and threonine-specific cdc2-inhibitory kinase
Receptor protein-tyrosine kinase erbB-4
Canalicular multispecific organic anion transporter 1
Serine/threonine-protein kinase PCTAIRE-2
Serine/threonine-protein kinase PCTAIRE-3
3-phosphoinositide dependent protein kinase-1
Serine/threonine-protein kinase PFTAIRE-1
Phosphatidylinositol-4-phosphate 5-kinase type-1 alpha
Ribosomal protein S6 kinase alpha 6
Myosin light chain kinase family member 4
Serine/threonine-protein kinase WEE1
Serine/threonine-protein kinase 32C
Serine/threonine-protein kinase 25
Mixed lineage kinase 7
Tyrosine-protein kinase ZAP-70
Phosphatidylinositol-5-phosphate 4-kinase type-2 beta
cAMP-dependent protein kinase beta-1 catalytic subunit
Serine/threonine-protein kinase PRKX
Protein tyrosine kinase 2 beta
Serine/threonine-protein kinase RIO1
Casein kinase I isoform alpha-like
Casein kinase I delta
Casein kinase I isoform gamma-3
Macrophage colony stimulating factor receptor
Serine/threonine-protein kinase tousled-like 1
Serine/threonine-protein kinase tousled-like 2
Neurotrophic tyrosine kinase receptor type 2
NT-3 growth factor receptor
Tyrosine-protein kinase TXK
Casein kinase II alpha

Casein kinase II alpha (prime)
Dual specificity tyrosine-phosphorylation-regulated kinase 1B
MAP kinase ERK1
MAP kinase ERK2
Glycogen synthase kinase-3 alpha
Glycogen synthase kinase-3 beta
Inhibitor of nuclear factor kappa B kinase epsilon subunit
Tyrosine-protein kinase TYK2
Tyrosine-protein kinase receptor TYRO3
LIM domain kinase 2
Serine/threonine-protein kinase 11
Serine/threonine-protein kinase c-TAK1
Dual specificity mitogen-activated protein kinase kinase 1
Dual specificity mitogen-activated protein kinase kinase 2
Dual specificity mitogen-activated protein kinase kinase 3
Maternal embryonic leucine zipper kinase
MAP kinase-interacting serine/threonine-protein kinase MNK1
Serine/threonine-protein kinase MST4
Serine/threonine-protein kinase NEK7
Serine/threonine protein kinase NLK
Insulin-like growth factor I receptor
Insulin receptor-related protein
Activin receptor type-1
Interleukin-1 receptor-associated kinase 3
Tyrosine-protein kinase ITK/TSK
Tyrosine-protein kinase JAK3
Serine/threonine-protein kinase RIO3
Serine/threonine-protein kinase SIK2
Serine/threonine-protein kinase SRPK1
Serine/threonine-protein kinase SRPK2
Activin receptor type-1B
Activin receptor type-2A
Activin receptor type-2B
Serine/threonine-protein kinase 33
Non-receptor tyrosine-protein kinase TNK1
Serine/threonine-protein kinase TNNI3K
Testis-specific serine/threonine-protein kinase 1
Serine/threonine-protein kinase 32B
Eukaryotic translation initiation factor 2-alpha kinase 4
ALK tyrosine kinase receptor
AMP-activated protein kinase, alpha-2 subunit
Ankyrin repeat and protein kinase domain-containing protein 1
Discoidin domain-containing receptor 2
Myotonin-protein kinase
Serine/threonine-protein kinase receptor R3
Chaperone activity of bc1 complex-like, mitochondrial
Serine/threonine-protein kinase AKT
Serine/threonine-protein kinase AKT2
Serine/threonine-protein kinase AKT3
Serine/threonine-protein kinase MRCK gamma

Serine/threonine-protein kinase LATS1
Serine/threonine-protein kinase LATS2
Leukocyte tyrosine kinase receptor
Mitogen-activated protein kinase kinase kinase 1
NUAK family SNF1-like kinase 1
Platelet-derived growth factor receptor alpha
PI3-kinase p110-alpha subunit
Serine/threonine-protein kinase PIM3
cAMP-dependent protein kinase alpha-catalytic subunit
Mitogen-activated protein kinase kinase kinase 3
Serine/threonine-protein kinase Aurora-B
Tyrosine-protein kinase receptor UFO
Tyrosine-protein kinase BLK
Bone morphogenetic protein receptor type-1A
Bone morphogenetic protein receptor type-2
Serine/threonine-protein kinase B-raf
BR serine/threonine-protein kinase 1
Mitogen-activated protein kinase kinase kinase 4
MAP kinase-activated protein kinase 2
MAP kinase-activated protein kinase 5
Serine/threonine-protein kinase MARK1
MAP/microtubule affinity-regulating kinase 4
Dual specificity mitogen-activated protein kinase kinase 4
Dual specificity mitogen-activated protein kinase kinase 6
Proto-oncogene tyrosine-protein kinase MER
Hepatocyte growth factor receptor
CaM kinase IV
PITSLRE serine/threonine-protein kinase CDC2L1
PITSLRE serine/threonine-protein kinase CDC2L2
Cell division cycle 2-like protein kinase 6
Cell division protein kinase 8
Myosin light chain kinase, smooth muscle
Mitogen-activated protein kinase kinase kinase 9
Mitogen-activated protein kinase kinase kinase 10
Mitogen-activated protein kinase kinase kinase 11
Serine/threonine-protein kinase MRCK-A
Serine/threonine-protein kinase MRCK beta
Serine/threonine-protein kinase 24
Muscle, skeletal receptor tyrosine protein kinase
Serine/threonine-protein kinase Chk1
Citron Rho-interacting kinase
Death-associated protein kinase 1
Serine/threonine-protein kinase DCLK1
Serine/threonine-protein kinase DCLK2
Serine/threonine-protein kinase DCLK3
Myosin IIIA
Myosin-IIIB
Serine/threonine-protein kinase Nek1
Serine/threonine-protein kinase Nek5
Serine/threonine-protein kinase PAK 2

Epithelial discoidin domain-containing receptor 1
Uncharacterized aarF domain-containing protein kinase 4
BR serine/threonine-protein kinase 2
Cyclin-dependent kinase 3
Cyclin-dependent kinase 7
Cyclin-dependent kinase 9
NUAK family SNF1-like kinase 2
Serine/threonine-protein kinase SIK1
Tyrosine-protein kinase Srms
Tyrosine-protein kinase TEC
Dual specificity testis-specific protein kinase 1
TGF-beta receptor type I
Ephrin type-A receptor 1
TGF-beta receptor type II
Tyrosine-protein kinase receptor Tie-1
Protein kinase N1
Protein kinase N2
Serine/threonine-protein kinase PLK1
Serine/threonine-protein kinase PLK3
Protein kinase C delta
Protein kinase C epsilon
Protein kinase C eta
Protein kinase C theta
Ephrin type-B receptor 2
Ephrin type-B receptor 3
Tubulin alpha-1 chain
Mitogen-activated protein kinase 6
Mitogen-activated protein kinase 4
Mitogen-activated protein kinase 7
Mitogen-activated protein kinase 15
Protein kinase C mu
Serine/threonine-protein kinase D2
Protein kinase C nu
cGMP-dependent protein kinase 1 beta
cGMP-dependent protein kinase 2
Interferon-induced, double-stranded RNA-activated protein kinase
Serine/threonine-protein kinase RAF
Tyrosine-protein kinase receptor RET
Receptor-interacting serine/threonine-protein kinase 1
Tyrosine-protein kinase FES
Fibroblast growth factor receptor 4
Vascular endothelial growth factor receptor 1
Proto-oncogene tyrosine-protein kinase ROS
Ribosomal protein S6 kinase alpha 1
Ribosomal protein S6 kinase alpha 4
Prelamin-A/C
Dual-specificity tyrosine-phosphorylation regulated kinase 1A
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Cytochrome P450 3A4
Serine/threonine-protein kinase SIK3

Cyclin-dependent kinase 4
Mitogen-activated protein kinase kinase kinase 15
Serine/threonine-protein kinase Chk2
Serine/threonine-protein kinase SBK1
Misshapen-like kinase 1
Serine/threonine-protein kinase ULK3
Serine/threonine-protein kinase 32A
Cyclin-dependent kinase-like 3
Bone morphogenetic protein receptor type-1B
Inhibitor of nuclear factor kappa B kinase alpha subunit
Serine/threonine-protein kinase/endoribonuclease IRE1
Inhibitor of nuclear factor kappa B kinase beta subunit
Interleukin-1 receptor-associated kinase 1
Casein kinase I alpha
Receptor tyrosine-protein kinase erbB-3
Tyrosine-protein kinase CTK
Mitogen-activated protein kinase kinase kinase 3
Macrophage-stimulating protein receptor
Serine/threonine-protein kinase Nek3
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing beta polypeptide
PI3-kinase p110-gamma subunit
PI4-kinase beta subunit
Protein kinase C iota
MAP kinase p38 delta
Rhodopsin kinase
Serine/threonine-protein kinase Nek4
Cyclin-dependent kinase-like 5
Ribosomal protein S6 kinase 1
Serine/threonine-protein kinase ULK1
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Peripheral plasma membrane protein CASK
Cyclin-dependent kinase 13
Serine/threonine-protein kinase PRP4 homolog
Cyclin-dependent kinase-like 2
Cyclin-dependent kinase-like 1
Ephrin type-B receptor 6
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing subunit gamma
Mitogen-activated protein kinase kinase kinase 2
Mitogen-activated protein kinase kinase kinase 6
Mitogen-activated protein kinase kinase kinase 13
Rho-associated protein kinase 2
FK506 binding protein 12
PI3-kinase p110-delta subunit
Serine/threonine-protein kinase OSR1
Rho-associated protein kinase 1
Homeodomain-interacting protein kinase 3
Serine/threonine-protein kinase MAK
Mitogen-activated protein kinase kinase kinase 1
PI3-kinase p110-beta subunit
Serine/threonine-protein kinase VRK2

Mitogen-activated protein kinase kinase kinase 12
Mitogen-activated protein kinase kinase kinase 2
Serine/threonine-protein kinase PLK2
Serine/threonine-protein kinase 38
Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma
STE20/SPS1-related proline-alanine-rich protein kinase
Serine/threonine-protein kinase TBK1
Serine/threonine-protein kinase Sgk3
Serine/threonine-protein kinase SRPK3
Eukaryotic translation initiation factor 2-alpha kinase 1
Hormonally up-regulated neu tumor-associated kinase
Serine/threonine-protein kinase ULK2
Serine/threonine-protein kinase ICK
Microtubule-associated serine/threonine-protein kinase 1
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase TAO2
Serine/threonine-protein kinase TAO3
Transient receptor potential cation channel subfamily M member 6
SNF-related serine/threonine-protein kinase
Serine/threonine-protein kinase RIO2
Receptor-interacting serine/threonine-protein kinase 4
Serine/threonine-protein kinase TAO1
Homeodomain-interacting protein kinase 2
Phosphatidylinositol-5-phosphate 4-kinase type-2 gamma
SPS1/STE20-related protein kinase YSK4
Serine/threonine-protein kinase pknB
Serine/threonine-protein kinase 35
Serine/threonine-protein kinase PFTAIRE-2
G protein-coupled receptor kinase 7
Homeodomain-interacting protein kinase 4
Dual specificity mitogen-activated protein kinase kinase 5
Dual specificity mitogen-activated protein kinase kinase 7
Mitogen-activated protein kinase kinase kinase 7
Serine/threonine-protein kinase Nek1
Homeodomain-interacting protein kinase 1
Serine/threonine-protein kinase NIM1
Myosin light chain kinase
G protein-coupled receptor kinase 4
Leucine-rich repeat serine/threonine-protein kinase 2
Wee1-like protein kinase 2
Putative uncharacterized serine/threonine-protein kinase SgK110
Dual serine/threonine and tyrosine protein kinase
Calcium-dependent protein kinase 1
Cell division control protein 2 homolog
Serine/threonine-protein kinase EEK2
Protein kinase C zeta
PAS domain-containing serine/threonine-protein kinase
PDZ-binding kinase
Serine/threonine-protein kinase Sgk2
G protein-coupled receptor kinase 5

Cell division cycle 7-related protein kinase
Protein kinase C gamma
Dual-specificity tyrosine-phosphorylation regulated kinase 3
Dual specificity tyrosine-phosphorylation-regulated kinase 4
MAP kinase-activated protein kinase 3
Testis-specific serine/threonine-protein kinase 2
Cyclin-dependent kinase 1
Geminin
ATP-binding cassette sub-family G member 2
P-glycoprotein 1
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Myelin transcription factor 1
Histone deacetylase
Histone deacetylase 1
Histone deacetylase 3
Histone deacetylase 6
Histone deacetylase 8

Everolimus

Molecular Mechanism (initial) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Molecular Mechanism (repurposed) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Predicted Targets

Cytochrome P450 3A4

FK506-binding protein 1A (FKBP-12)

FK506 binding protein 12
RAC-alpha serine/threonine-protein kinase
MAP kinase p38 beta
MAP kinase p38 delta
MAP kinase p38 gamma
Serine/threonine-protein kinase PAK 4
Serine/threonine-protein kinase PAK7
Serine/threonine-protein kinase PAK6
3-phosphoinositide dependent protein kinase-1
Serine/threonine-protein kinase PIM1
Serine/threonine-protein kinase PIM2
Serine/threonine-protein kinase PIM3
cAMP-dependent protein kinase alpha-catalytic subunit
Serine/threonine-protein kinase AKT
Serine/threonine-protein kinase AKT2
Protein kinase C alpha
Protein kinase C zeta
Serine/threonine-protein kinase SRPK1
Ribosomal protein S6 kinase alpha 1

Ribosomal protein S6 kinase alpha 3
Ribosomal protein S6 kinase 1
Serine/threonine-protein kinase Sgk1
Myosin light chain kinase, smooth muscle
Tyrosine-protein kinase SRC
Serine/threonine-protein kinase Aurora-B
Serine/threonine-protein kinase Aurora-C
BR serine/threonine-protein kinase 2
CaM kinase I alpha
CaM-kinase kinase alpha
CaM-kinase kinase beta
Cyclin-dependent kinase 2/cyclin A
Serine/threonine-protein kinase Chk1
Serine/threonine-protein kinase Chk2
Casein kinase I delta
Casein kinase II
Tyrosine-protein kinase CSK
Dual-specificity tyrosine-phosphorylation regulated kinase 1A
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Dual-specificity tyrosine-phosphorylation regulated kinase 3
Serine/threonine-protein kinase EE2K
MAP kinase ERK1
MAP kinase ERK2
Mitogen-activated protein kinase 15
Serine/threonine-protein kinase MST2
Serine/threonine-protein kinase NEK2
Serine/threonine-protein kinase NEK6
Serine/threonine-protein kinase NEK7
MAP kinase p38 alpha
Glycogen synthase kinase-3 beta
Homeodomain-interacting protein kinase 2
Homeodomain-interacting protein kinase 3
Inhibitor of nuclear factor kappa B kinase beta subunit
c-Jun N-terminal kinase 1
c-Jun N-terminal kinase 2
c-Jun N-terminal kinase 3
Tyrosine-protein kinase LCK
MAP kinase-activated protein kinase 2
Serine/threonine-protein kinase c-TAK1
Maternal embryonic leucine zipper kinase
Dual specificity mitogen-activated protein kinase kinase 1
MAP kinase-interacting serine/threonine-protein kinase MNK1
MAP kinase-activated protein kinase 3
MAP kinase signal-integrating kinase 2
Ribosomal protein S6 kinase alpha 5
Protein kinase C mu
Serine/threonine-protein kinase PLK1
MAP kinase-activated protein kinase 5
Protein kinase N2
Pyruvate dehydrogenase kinase isoform 1

Nuclear receptor ROR-gamma
Eukaryotic translation initiation factor
Legionella pneumophila
Absidia corymbifera
Mucor circinelloides
Programmed cell death protein 4
Plasmodium falciparum
Mothers against decapentaplegic homolog 3
Ubiquitin carboxyl-terminal hydrolase 1
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta

Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor

Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
P-glycoprotein 1
Solute carrier organic anion transporter family member 1B1
Geminin
Cholinesterase
Serine/threonine-protein kinase MARK1
Serine/threonine-protein kinase SRPK3
Tyrosine-protein kinase ABL2
Serine/threonine-protein kinase Aurora-A
Cyclin-dependent kinase 2/cyclin E
Casein kinase I isoform gamma-3
Death-associated protein kinase 1
Ephrin type-A receptor 5
Fibroblast growth factor receptor 3
Fibroblast growth factor receptor 4
Tyrosine-protein kinase HCK
Inhibitor of nuclear factor kappa B kinase alpha subunit
Serine/threonine-protein kinase MST1
Serine/threonine protein kinase NLK
Death-associated protein kinase 2
Ephrin type-A receptor 7
Hexokinase type IV
Insulin-like growth factor I receptor
Vascular endothelial growth factor receptor 2
CDK3/cyclin E
Tyrosine-protein kinase FER
G protein-coupled receptor kinase 5
LIM domain kinase 1
Serine/threonine-protein kinase PAK 2
Cyclin-dependent kinase 5/CDK5 activator 1
Casein kinase II alpha (prime)
Serine/threonine-protein kinase DCLK2
Ephrin type-A receptor 8
G protein-coupled receptor kinase 6
Serine/threonine-protein kinase 11
Misshapen-like kinase 1
Serine/threonine-protein kinase 24
Serine/threonine-protein kinase PAK 3
Tyrosine-protein kinase receptor UFO
Dual specificity protein kinase CLK2
Discoidin domain-containing receptor 2
Ephrin type-B receptor 1
Dual specificity mitogen-activated protein kinase kinase 6
Proto-oncogene tyrosine-protein kinase MER
Tyrosine kinase non-receptor protein 2
Dual specificity protein kinase CLK3
Myotonin-protein kinase

G protein-coupled receptor kinase 7
Interleukin-1 receptor-associated kinase 1
Serine/threonine-protein kinase 10
Dual specificity mitogen-activated protein kinase kinase 7
Hepatocyte growth factor receptor
ALK tyrosine kinase receptor
Tyrosine-protein kinase BRK
CDK6/cyclin D3
Ephrin type-B receptor 2
Glycogen synthase kinase-3 alpha
Interleukin-1 receptor-associated kinase 4
Activin receptor type-1B
Tyrosine-protein kinase BTK
Cyclin-dependent kinase 7/ cyclin H
Serine/threonine-protein kinase 17A
Ephrin type-B receptor 3
Tyrosine-protein kinase FES
Insulin receptor-related protein
Tyrosine-protein kinase BLK
CDK9/cyclin T1
Ephrin type-B receptor 4
Mitogen-activated protein kinase kinase kinase 9
Muscle, skeletal receptor tyrosine protein kinase
AMP-activated protein kinase (AMPK) alpha-1/beta-1/gamma-1
CaM kinase II beta
Tyrosine-protein kinase FGR
Homeodomain-interacting protein kinase 1
Tyrosine-protein kinase ITK/TSK
Tyrosine-protein kinase Lyn
Serine/threonine-protein kinase MRCK-A
Serine/threonine-protein kinase Nek1
AMP-activated protein kinase, AMPK
Tyrosine-protein kinase BMX
Receptor protein-tyrosine kinase erbB-4
Tyrosine-protein kinase JAK2
NUAK family SNF1-like kinase 1
BR serine/threonine-protein kinase 1
CaM kinase II gamma
Ephrin type-A receptor 1
Focal adhesion kinase 1
Tyrosine-protein kinase receptor FLT3
Tyrosine-protein kinase JAK3
Serine/threonine-protein kinase MRCK beta
Mitogen-activated protein kinase kinase kinase 5
Casein kinase I gamma 1
CaM kinase II delta
Ephrin type-A receptor 2
Fibroblast growth factor receptor 1
Serine/threonine-protein kinase Nek3
CaM kinase IV

Ephrin type-A receptor 3
Vascular endothelial growth factor receptor 3
Serine/threonine-protein kinase haspin
Ribosomal protein S6 kinase alpha 4
Tyrosine-protein kinase ABL
Cyclin-dependent kinase 1/cyclin B
Casein kinase I gamma 2
Fibroblast growth factor receptor 2
Macrophage colony stimulating factor receptor
CaM kinase I delta
Ephrin type-A receptor 4
Protein kinase C eta
Protein kinase C theta
Tyrosine-protein kinase receptor TYRO3
Serine/threonine-protein kinase SIK1
Serine/threonine-protein kinase tousled-like 2
Serine/threonine-protein kinase WNK3
Testis-specific serine/threonine-protein kinase 1
Tyrosine-protein kinase YES
Protein kinase C iota
Serine/threonine-protein kinase SRPK2
Testis-specific serine/threonine-protein kinase 2
Tyrosine-protein kinase ZAP-70
Serine/threonine-protein kinase PLK3
Ribosomal protein S6 kinase alpha 2
Serine/threonine-protein kinase 33
Tyrosine-protein kinase TEC
Serine/threonine-protein kinase AKT3
Serine/threonine-protein kinase D2
Serine/threonine-protein kinase PRKX
Death-associated protein kinase 3
Ribosomal protein S6 kinase alpha 6
Serine/threonine-protein kinase PLK2
Tyrosine-protein kinase TIE-2
Serine/threonine-protein kinase RAF
cGMP-dependent protein kinase 1 beta
Protein tyrosine kinase 2 beta
Tyrosine-protein kinase SYK
Nerve growth factor receptor Trk-A
Stem cell growth factor receptor
Protein kinase C beta
Serine/threonine-protein kinase RIPK2
Mitogen-activated protein kinase kinase kinase 7
Rho-associated protein kinase 1
Neurotrophic tyrosine kinase receptor type 2
MAP/microtubule affinity-regulating kinase 2
Protein kinase C gamma
Serine/threonine-protein kinase TAO1
Tyrosine-protein kinase TXK
Serine/threonine-protein kinase TAO2

Serine/threonine-protein kinase ULK2
PAS domain-containing serine/threonine-protein kinase
Protein kinase C delta
Tyrosine-protein kinase FRK
Tyrosine-protein kinase receptor RET
Serine/threonine-protein kinase TAO3
Platelet-derived growth factor receptor alpha
Protein kinase C epsilon
Phosphorylase kinase gamma subunit 2
Macrophage-stimulating protein receptor
Serine/threonine-protein kinase ULK3

Mammalian target of Rapamycin (mTORC1)

Platelet-derived growth factor receptor beta
Serine/threonine-protein kinase Sgk2
Serine/threonine-protein kinase TBK1
Serine/threonine-protein kinase VRK2
Proto-oncogene tyrosine-protein kinase ROS
Serine/threonine-protein kinase Sgk3
TGF-beta receptor type I
Serine/threonine-protein kinase WNK2
Peptidyl-prolyl cis-trans isomerase FKBP5
Alpha-synuclein
Microtubule-associated protein tau
Hypoxia-inducible factor 1 alpha
Thioredoxin glutathione reductase
4'-phosphopantetheinyl transferase ffp
Nonstructural protein 1
ATPase family AAA domain-containing protein 5
Aldehyde dehydrogenase 1A1
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Vitamin D receptor
Inositol monophosphatase 1
Peripheral myelin protein 22
Nuclear factor erythroid 2-related factor 2
Thioredoxin reductase 1, cytoplasmic
Flap endonuclease 1

Finasteride

Molecular Mechanism (initial) :

**steroid 5alpha reductase inhibitor
androgen receptor antagonist**

Molecular Mechanism (repurposed) :

**steroid 5alpha reductase inhibitor
androgen receptor antagonist**

Predicted Targets

Steroid 5-alpha-reductase 1

Steroid 5-alpha-reductase 2

3-beta-hydroxysteroid dehydrogenase/delta 5-->4-isomerase type I

Steroid 5-alpha-reductase

Androgen Receptor

Cytochrome P450 17A1
3-keto-steroid reductase
Nuclear factor NF-kappa-B p105 subunit
MAP kinase ERK2
Cytochrome P450 3A4
Nuclear receptor ROR-gamma
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
3 beta-hydroxysteroid dehydrogenase/Delta 5-->4-isomerase
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta

Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor

Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Peripheral myelin protein 22

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

Predicted Targets

Acetylcholinesterase

Butyrylcholinesterase
Cholinesterases; ACHE & BCHE
Beta amyloid A4 protein
Cholinesterase
Cytochrome P450 3A4
Catalase
Glutamate NMDA receptor; GRIN1/GRIN2A
Glutamate NMDA receptor; GRIN1/GRIN2B
Prelamin-A/C
Aldehyde dehydrogenase 1A1
Vitamin D receptor
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1

MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2

Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Beta-secretase 1
Dual specificity protein kinase CLK3
Dual specificity protein kinase CLK1
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Dual-specificity tyrosine-phosphorylation regulated kinase 1A
Glutamate [NMDA] receptor subunit epsilon 2
Menin/Histone-lysine N-methyltransferase MLL
Histone acetyltransferase GCN5
Geminin
Isocitrate dehydrogenase [NADP] cytoplasmic
Putative fructose-1,6-bisphosphate aldolase
DNA polymerase beta
Ferritin light chain

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

Predicted Targets

Deoxycytidine kinase

Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Cytochrome P450 3A4
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1

Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1

Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Cytidine deaminase
Ribonucleoside-diphosphate reductase M1 chain
Histidine triad nucleotide-binding protein 1
Peripheral myelin protein 22
Geminin

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

Predicted Targets

Nischarin
Menin/Histone-lysine N-methyltransferase MLL
Prelamin-A/C
Cytochrome P450 2C19
Hypoxia-inducible factor 1 alpha
MAP kinase ERK2
Anthrax lethal factor
Muscarinic acetylcholine receptor M1
Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
Cytochrome P450 3A4
Cytochrome P450 2D6
Cytochrome P450 2C9
Nuclear factor erythroid 2-related factor 2
Dopamine D1 receptor
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Cytochrome P450 1A2
Thioredoxin reductase 1, cytoplasmic
Plasmodium falciparum
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor

Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G

Leukocyte elastase
 Matrix metalloproteinase-1
 Matrix metalloproteinase 9
 Protein kinase C alpha
 MAP kinase ERK1
 MAP kinase p38 alpha
 Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
 Epidermal growth factor receptor erbB1
 Tyrosine-protein kinase FYN
 Receptor protein-tyrosine kinase erbB-2
 Tyrosine-protein kinase LCK
 Leukocyte common antigen
 Serotonin 1a (5-HT1a) receptor
 Serotonin 1b (5-HT1b) receptor
 Serotonin 2a (5-HT2a) receptor
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Androgen Receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 Geminin
 Nuclear receptor ROR-gamma
 Peripheral myelin protein 22
 4'-phosphopantetheinyl transferase ffp
 Microtubule-associated protein tau
 Beta-lactamase AmpC
 Bloom syndrome protein
 DNA polymerase iota
 Transcriptional regulator ERG
 Isocitrate dehydrogenase [NADP] cytoplasmic

Ibuprofen

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 inhibitor
 prostaglandin G/H synthase 1 inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 inhibitor
 prostaglandin G/H synthase 1 inhibitor

Predicted Targets

Prostaglandin G/H synthase (cyclooxygenase)

Arachidonate 5-lipoxygenase

Cyclooxygenase

Cyclooxygenase-1

Cyclooxygenase-2

Prostaglandin-H2 D-isomerase
Cytochrome P450 2C9
Serum albumin
Aldo-keto-reductase family 1 member C3
Gamma-secretase
Acetylcholinesterase
Dehydrogenase/reductase SDR family member 9
Solute carrier family 22 member 6
Solute carrier family 22 member 20
Peroxisome proliferator-activated receptor gamma
Hepatocyte
Canalicular multispecific organic anion transporter 1
Solute carrier family 22 member 1
Staphylococcus aureus
Escherichia coli
Fatty acid-binding protein, liver
Monoamine oxidase A
Monoamine oxidase B
Anandamide amidohydrolase
Monoglyceride lipase
Prelamin-A/C
Nuclear factor NF-kappa-B p105 subunit
Saccharomyces cerevisiae
Nonstructural protein 1
Amiloride-sensitive cation channel 2, neuronal
Hepatotoxicity
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
UDP-glucuronosyltransferase 1A4
UDP-glucuronosyltransferase 1-6
UDP-glucuronosyltransferase 1-9
UDP-glucuronosyltransferase 2A1
UDP-glucuronosyltransferase 2B7
UDP-glucuronosyltransferase 2B17
Chromobox protein homolog 1
DNA polymerase kappa
Luciferin 4-monooxygenase
UDP-glucuronosyltransferase 2B10
UDP-glucuronosyltransferase 2B4
UDP-glucuronosyltransferase 1-1
UDP-glucuronosyltransferase 1-10
UDP-glucuronosyltransferase 1-7
UDP-glucuronosyltransferase 1-8
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2D6
Cytochrome P450 2E1
Cytochrome P450 3A4
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1

Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Solute carrier organic anion transporter family member 1A3
Multidrug resistance-associated protein 4
Solute carrier family 22 member 11
Multidrug resistance-associated protein 1
Solute carrier family 22 member 8
P-glycoprotein 1
Solute carrier organic anion transporter family member 1A1
Solute carrier organic anion transporter family member 1A4

Solute carrier organic anion transporter family member 2B1
 Transcriptional regulator ERG
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 Prostaglandin E synthase
 Seed lipoxygenase-1
 TAR DNA-binding protein 43
 Isocitrate dehydrogenase [NADP] cytoplasmic
 Oryctolagus cuniculus
 Interleukin-8 receptors, CXCR1/CXCR2
 Thyroid stimulating hormone receptor
 Endonuclease 4
 Peripheral myelin protein 22
 Bloom syndrome protein
 6-phospho-1-fructokinase
 Runt-related transcription factor 1/Core-binding factor subunit beta
 Regulator of G-protein signaling 4
 Aldo-keto reductase family 1 member C2
 Aldo-keto reductase family 1 member C4
 Aldo-keto reductase family 1 member C1

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

stem cell factor (SCF)

proto-oncogene c-Kit inhibitor

Predicted Targets

Tyrosine-protein kinase ABL

Platelet-derived growth factor receptor beta

Stem cell growth factor receptor

Tyrosine-protein kinase receptor FLT3

Macrophage colony stimulating factor receptor

Epidermal growth factor receptor erbB1

Tyrosine-protein kinase SRC

Platelet-derived growth factor receptor

cAMP-dependent protein kinase (PKA)

Protein kinase C alpha

Protein kinase C delta

Tyrosine-protein kinase FRK

Tyrosine-protein kinase HCK

Ephrin type-B receptor 4

Serine/threonine-protein kinase 17A

Serine/threonine-protein kinase Aurora-C

Tyrosine-protein kinase CSK

c-Jun N-terminal kinase 3

Serine/threonine-protein kinase 36

Tyrosine-protein kinase YES

Mitogen-activated protein kinase kinase kinase 4
Tyrosine-protein kinase FGR
BMP-2-inducible protein kinase
Ephrin type-A receptor 7
Ephrin type-B receptor 1
MAP kinase signal-integrating kinase 2
Mitogen-activated protein kinase kinase kinase kinase 5
Tyrosine-protein kinase ABL2
Tyrosine-protein kinase BMX
Tyrosine-protein kinase BRK
c-Jun N-terminal kinase 2
Ephrin type-A receptor 8
Tyrosine-protein kinase Lyn
Tyrosine-protein kinase BTK
Ephrin type-A receptor 3
Tyrosine-protein kinase LCK
Serine/threonine-protein kinase 2
Serine/threonine-protein kinase 10
Serine/threonine-protein kinase RIPK2
Ephrin type-A receptor 4
Ephrin type-A receptor 5
Ephrin type-A receptor 6
Serine/threonine-protein kinase GAK
Receptor protein-tyrosine kinase erbB-2
AMP-activated protein kinase, alpha-1 subunit
Phosphorylase kinase gamma subunit 2
Phosphorylase kinase gamma subunit 1
Tyrosine-protein kinase FYN
Fibroblast growth factor receptor 2
Fibroblast growth factor receptor 1
TRAF2- and NCK-interacting kinase
Tyrosine-protein kinase TIE-2
Ephrin type-A receptor 2
Casein kinase I epsilon
Serine/threonine-protein kinase PLK4
Vascular endothelial growth factor receptor 2
Vascular endothelial growth factor receptor 3
Fibroblast growth factor receptor 3
Adaptor-associated kinase
Serine/threonine-protein kinase Aurora-A
ULK3 kinase
Serine/threonine-protein kinase 17B
Dual specificity protein kinase CLK1
Dual specificity protein kinase CLK4
c-Jun N-terminal kinase 1
CaM-kinase kinase beta
CaM kinase I gamma
CaM kinase I alpha
Casein kinase I gamma 1
Cyclin-dependent kinase 2

MAP kinase p38 gamma
Serine/threonine-protein kinase 38-like
Ribosomal protein S6 kinase alpha 2
Serine/threonine-protein kinase MST1
MAP/microtubule affinity-regulating kinase 2
Ribosomal protein S6 kinase alpha 5
CaM kinase I delta
Death-associated protein kinase 2
Serine/threonine-protein kinase 16
Serine/threonine-protein kinase PIM2
Death-associated protein kinase 3
Dual specificity protein kinase CLK2
Serine/threonine-protein kinase MST2
Serine/threonine-protein kinase PCTAIRE-1
Dual specificity protein kinase TTK
Nerve growth factor receptor Trk-A
Cyclin-dependent kinase 5
MAP kinase p38 beta
MAP kinase p38 alpha
Serine/threonine-protein kinase NEK9
Dual specificity protein kinase CLK3
Casein kinase I gamma 2
Serine/threonine-protein kinase NEK2
LIM domain kinase 1
Mitogen-activated protein kinase kinase kinase 5
myosin light chain kinase 2
Insulin receptor
Focal adhesion kinase 1
Ribosomal protein S6 kinase alpha 3
Tyrosine-protein kinase FER
Tyrosine kinase non-receptor protein 2
Serine/threonine-protein kinase PIM1
Tyrosine-protein kinase JAK2
Serine/threonine-protein kinase PAK 4
Tyrosine-protein kinase SYK
Serine/threonine-protein kinase PAK7
CaM kinase II beta
Serine/threonine-protein kinase PAK 1
Serine/threonine-protein kinase PAK 3
CaM kinase II delta
CaM kinase II gamma
Serine/threonine-protein kinase PAK6
CaM kinase II alpha
CaM-kinase kinase alpha
Serine/threonine-protein kinase NEK6
Tyrosine-protein kinase JAK1
Tyrosine- and threonine-specific cdc2-inhibitory kinase
Platelet-derived growth factor receptor alpha
NPM/ALK (Nucleophosmin/ALK tyrosine kinase receptor)
ATP-binding cassette sub-family G member 2

P-glycoprotein 1
Epithelial discoidin domain-containing receptor 1
Histone deacetylase 1
Histone deacetylase 6
Carbonic anhydrase I
Carbonic anhydrase II
Carbonic anhydrase III
Carbonic anhydrase IV
Carbonic anhydrase VA
Carbonic anhydrase VB
Carbonic anhydrase VI
Carbonic anhydrase VII
Carbonic anhydrase IX
Carbonic anhydrase XII
Carbonic anhydrase XIII
Carbonic anhydrase XIV
Carbonic anhydrase 15
Serine/threonine-protein kinase PCTAIRE-2
Serine/threonine-protein kinase PCTAIRE-3
3-phosphoinositide dependent protein kinase-1
Serine/threonine-protein kinase PFTAIRE-1
Phosphatidylinositol-4-phosphate 5-kinase type-1 alpha
Ribosomal protein S6 kinase alpha 6
Myosin light chain kinase family member 4
Serine/threonine-protein kinase WEE1
Serine/threonine-protein kinase 32C
Serine/threonine-protein kinase 25
Mixed lineage kinase 7
Tyrosine-protein kinase ZAP-70
Phosphatidylinositol-5-phosphate 4-kinase type-2 beta
cAMP-dependent protein kinase beta-1 catalytic subunit
Serine/threonine-protein kinase PRKX
Protein tyrosine kinase 2 beta
Serine/threonine-protein kinase RIO1
Casein kinase I isoform alpha-like
Casein kinase I delta
Casein kinase I isoform gamma-3
Serine/threonine-protein kinase tousled-like 1
Serine/threonine-protein kinase tousled-like 2
Neurotrophic tyrosine kinase receptor type 2
NT-3 growth factor receptor
Tyrosine-protein kinase TXK
Casein kinase II alpha
Casein kinase II alpha (prime)
Dual specificity tyrosine-phosphorylation-regulated kinase 1B
MAP kinase ERK1
MAP kinase ERK2
Glycogen synthase kinase-3 alpha
Glycogen synthase kinase-3 beta
Inhibitor of nuclear factor kappa B kinase epsilon subunit

Tyrosine-protein kinase TYK2
Tyrosine-protein kinase receptor TYRO3
LIM domain kinase 2
Serine/threonine-protein kinase 11
Serine/threonine-protein kinase c-TAK1
Dual specificity mitogen-activated protein kinase kinase 1
Dual specificity mitogen-activated protein kinase kinase 2
Dual specificity mitogen-activated protein kinase kinase 3
Maternal embryonic leucine zipper kinase
MAP kinase-interacting serine/threonine-protein kinase MNK1
Serine/threonine-protein kinase MST4
Serine/threonine-protein kinase NEK7
Serine/threonine protein kinase NLK
Insulin-like growth factor I receptor
Insulin receptor-related protein
Activin receptor type-1
Interleukin-1 receptor-associated kinase 3
Tyrosine-protein kinase ITK/TSK
Tyrosine-protein kinase JAK3
Serine/threonine-protein kinase RIO3
Serine/threonine-protein kinase SIK2
Serine/threonine-protein kinase SRPK1
Serine/threonine-protein kinase SRPK2
Activin receptor type-1B
Activin receptor type-2A
Activin receptor type-2B
Serine/threonine-protein kinase 33
Non-receptor tyrosine-protein kinase TNK1
Serine/threonine-protein kinase TNNI3K
Testis-specific serine/threonine-protein kinase 1
Serine/threonine-protein kinase 32B
Eukaryotic translation initiation factor 2-alpha kinase 4
ALK tyrosine kinase receptor
AMP-activated protein kinase, alpha-2 subunit
Ankyrin repeat and protein kinase domain-containing protein 1
Discoidin domain-containing receptor 2
Myotonin-protein kinase
Serine/threonine-protein kinase receptor R3
Chaperone activity of bc1 complex-like, mitochondrial
Serine/threonine-protein kinase AKT
Serine/threonine-protein kinase AKT2
Serine/threonine-protein kinase AKT3
Serine/threonine-protein kinase LATS1
Serine/threonine-protein kinase LATS2
Leukocyte tyrosine kinase receptor
Serine/threonine-protein kinase MRCK gamma
NUAK family SNF1-like kinase 1
PI3-kinase p110-alpha subunit
Serine/threonine-protein kinase PIM3
cAMP-dependent protein kinase alpha-catalytic subunit

Mitogen-activated protein kinase kinase kinase 1
Mitogen-activated protein kinase kinase kinase 3
Serine/threonine-protein kinase Aurora-B
Tyrosine-protein kinase receptor UFO
Tyrosine-protein kinase BLK
Bone morphogenetic protein receptor type-1A
Bone morphogenetic protein receptor type-2
Serine/threonine-protein kinase B-raf
BR serine/threonine-protein kinase 1
Mitogen-activated protein kinase kinase kinase 4
MAP kinase-activated protein kinase 2
MAP kinase-activated protein kinase 5
Serine/threonine-protein kinase MARK1
MAP/microtubule affinity-regulating kinase 4
Dual specificity mitogen-activated protein kinase kinase 4
Dual specificity mitogen-activated protein kinase kinase 6
Proto-oncogene tyrosine-protein kinase MER
Hepatocyte growth factor receptor
CaM kinase IV
PITSLRE serine/threonine-protein kinase CDC2L1
PITSLRE serine/threonine-protein kinase CDC2L2
Cell division cycle 2-like protein kinase 6
Cell division protein kinase 8
Myosin light chain kinase, smooth muscle
Mitogen-activated protein kinase kinase kinase 9
Mitogen-activated protein kinase kinase kinase 10
Mitogen-activated protein kinase kinase kinase 11
Serine/threonine-protein kinase MRCK-A
Serine/threonine-protein kinase MRCK beta
Serine/threonine-protein kinase 24
Muscle, skeletal receptor tyrosine protein kinase
Serine/threonine-protein kinase Chk1
Citron Rho-interacting kinase
Death-associated protein kinase 1
Serine/threonine-protein kinase DCLK1
Serine/threonine-protein kinase DCLK2
Serine/threonine-protein kinase DCLK3
Myosin IIIA
Myosin-IIIB
Serine/threonine-protein kinase Nek1
Serine/threonine-protein kinase Nek5
Serine/threonine-protein kinase PAK 2
Uncharacterized aarF domain-containing protein kinase 4
BR serine/threonine-protein kinase 2
Cyclin-dependent kinase 3
Cyclin-dependent kinase 7
Cyclin-dependent kinase 9
NUAK family SNF1-like kinase 2
Serine/threonine-protein kinase SIK1
Tyrosine-protein kinase Srms

Tyrosine-protein kinase TEC
Dual specificity testis-specific protein kinase 1
TGF-beta receptor type I
Ephrin type-A receptor 1
TGF-beta receptor type II
Tyrosine-protein kinase receptor Tie-1
Protein kinase N1
Protein kinase N2
Serine/threonine-protein kinase PLK1
Serine/threonine-protein kinase PLK3
Protein kinase C epsilon
Protein kinase C eta
Protein kinase C theta
Ephrin type-B receptor 2
Ephrin type-B receptor 3
Tubulin alpha-1 chain
Mitogen-activated protein kinase 6
Mitogen-activated protein kinase 4
Mitogen-activated protein kinase 7
Mitogen-activated protein kinase 15
Protein kinase C mu
Serine/threonine-protein kinase D2
Protein kinase C nu
cGMP-dependent protein kinase 1 beta
cGMP-dependent protein kinase 2
Interferon-induced, double-stranded RNA-activated protein kinase
Serine/threonine-protein kinase RAF
Tyrosine-protein kinase receptor RET
Receptor-interacting serine/threonine-protein kinase 1
Tyrosine-protein kinase FES
Fibroblast growth factor receptor 4
Vascular endothelial growth factor receptor 1
Proto-oncogene tyrosine-protein kinase ROS
Ribosomal protein S6 kinase alpha 1
Ribosomal protein S6 kinase alpha 4
Bcr/Abl fusion protein
Cyclin-dependent kinase 1/cyclin B1
Serine/threonine-protein kinase Chk2
Inhibitor of nuclear factor kappa B kinase alpha subunit
Inhibitor of nuclear factor kappa B kinase beta subunit
Ribosomal protein S6 kinase 1
Polycystin-2
Rho-associated protein kinase 2
Serine/threonine-protein kinase Sgk1
MAP kinase p38 delta
Prelamin-A/C
Nuclear receptor ROR-gamma
Arachidonate 15-lipoxygenase, type II
Cytochrome P450 3A4
Membrane-associated phosphatidylinositol transfer protein 1

Plasmodium falciparum
Flap endonuclease 1
DNA polymerase kappa
Mothers against decapentaplegic homolog 3
Serine/threonine-protein kinase SIK3
Cyclin-dependent kinase 4
Mitogen-activated protein kinase kinase kinase 15
Serine/threonine-protein kinase SBK1
Misshapen-like kinase 1
Receptor protein-tyrosine kinase erbB-4
Serine/threonine-protein kinase ULK3
Serine/threonine-protein kinase 32A
Cyclin-dependent kinase-like 3
Bone morphogenetic protein receptor type-1B
Serine/threonine-protein kinase/endoribonuclease IRE1
Interleukin-1 receptor-associated kinase 1
Casein kinase I alpha
Receptor tyrosine-protein kinase erbB-3
Tyrosine-protein kinase CTK
Mitogen-activated protein kinase kinase kinase 3
Macrophage-stimulating protein receptor
Serine/threonine-protein kinase Nek3
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing beta polypeptide
PI3-kinase p110-gamma subunit
PI4-kinase beta subunit
Protein kinase C iota
Rhodopsin kinase
Serine/threonine-protein kinase Nek4
Cyclin-dependent kinase-like 5
Serine/threonine-protein kinase ULK1
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Peripheral plasma membrane protein CASK
Cyclin-dependent kinase 13
Serine/threonine-protein kinase PRP4 homolog
Cyclin-dependent kinase-like 2
Cyclin-dependent kinase-like 1
Ephrin type-B receptor 6
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing subunit gamma
Mitogen-activated protein kinase kinase kinase 2
Mitogen-activated protein kinase kinase kinase 6
Mitogen-activated protein kinase kinase kinase 13
FK506 binding protein 12
PI3-kinase p110-delta subunit
Serine/threonine-protein kinase OSR1
Rho-associated protein kinase 1
Homeodomain-interacting protein kinase 3
Serine/threonine-protein kinase MAK
Mitogen-activated protein kinase kinase kinase 1
PI3-kinase p110-beta subunit
Serine/threonine-protein kinase VRK2

Mitogen-activated protein kinase kinase kinase 12
Mitogen-activated protein kinase kinase kinase 2
Serine/threonine-protein kinase PLK2
Serine/threonine-protein kinase 38
Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma
STE20/SPS1-related proline-alanine-rich protein kinase
Serine/threonine-protein kinase TBK1
Serine/threonine-protein kinase Sgk3
Serine/threonine-protein kinase SRPK3
Eukaryotic translation initiation factor 2-alpha kinase 1
Hormonally up-regulated neu tumor-associated kinase
Serine/threonine-protein kinase ULK2
Serine/threonine-protein kinase ICK
Microtubule-associated serine/threonine-protein kinase 1
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase TAO2
Serine/threonine-protein kinase TAO3
Transient receptor potential cation channel subfamily M member 6
SNF-related serine/threonine-protein kinase
Serine/threonine-protein kinase RIO2
Receptor-interacting serine/threonine-protein kinase 4
Serine/threonine-protein kinase TAO1
Homeodomain-interacting protein kinase 2
Phosphatidylinositol-5-phosphate 4-kinase type-2 gamma
SPS1/STE20-related protein kinase YSK4
Serine/threonine-protein kinase pknB
Serine/threonine-protein kinase 35
Dual-specificity tyrosine-phosphorylation regulated kinase 1A
Serine/threonine-protein kinase PFTAIRE-2
G protein-coupled receptor kinase 7
Homeodomain-interacting protein kinase 4
Dual specificity mitogen-activated protein kinase kinase 5
Dual specificity mitogen-activated protein kinase kinase 7
Mitogen-activated protein kinase kinase kinase 7
Serine/threonine-protein kinase Nek11
Homeodomain-interacting protein kinase 1
Serine/threonine-protein kinase NIM1
Myosin light chain kinase
G protein-coupled receptor kinase 4
Leucine-rich repeat serine/threonine-protein kinase 2
Wee1-like protein kinase 2
Putative uncharacterized serine/threonine-protein kinase SgK110
Dual serine/threonine and tyrosine protein kinase
Calcium-dependent protein kinase 1
Cell division control protein 2 homolog
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3

Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Serine/threonine-protein kinase EEF2K
Protein kinase C zeta
PDZ-binding kinase
Serine/threonine-protein kinase Sgk2
G protein-coupled receptor kinase 5
Cell division cycle 7-related protein kinase
Dual-specificity tyrosine-phosphorylation regulated kinase 3
Dual specificity tyrosine-phosphorylation-regulated kinase 4
Protein kinase C gamma
MAP kinase-activated protein kinase 3
Testis-specific serine/threonine-protein kinase 2
Cyclin-dependent kinase 1
Luciferin 4-monooxygenase
Quinone reductase 2
Multidrug and toxin extrusion protein 1

Multidrug and toxin extrusion protein 2
Solute carrier family 22 member 3
Solute carrier family 22 member 1
Solute carrier family 22 member 2
Myelin transcription factor 1
Bile acid receptor FXR
Cyclin-dependent kinase 2/cyclin E1
Canalicular multispecific organic anion transporter 1
Thioredoxin reductase 1, cytoplasmic
DNA polymerase iota
Glucagon-like peptide 1 receptor
Isocitrate dehydrogenase [NADP] cytoplasmic
DNA repair protein RAD52 homolog

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of M. tuberculosis

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

Predicted Targets

Monoamine oxidase B

Monoamine oxidase A

Histone acetyltransferase GCN5
6-phospho-1-fructokinase
ATPase family AAA domain-containing protein 5
Cytochrome P450 2C9
Cytochrome P450 1A2
Cytochrome P450 2D6
Cytochrome P450 3A4
Cytochrome P450 2C19
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II

C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
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Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
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Neuropeptide Y receptor type 2
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Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1

Matrix metalloproteinase 9
 Protein kinase C alpha
 MAP kinase ERK1
 MAP kinase ERK2
 MAP kinase p38 alpha
 Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
 Epidermal growth factor receptor erbB1
 Tyrosine-protein kinase FYN
 Receptor protein-tyrosine kinase erbB-2
 Tyrosine-protein kinase LCK
 Leukocyte common antigen
 Serotonin 1a (5-HT1a) receptor
 Serotonin 1b (5-HT1b) receptor
 Serotonin 2a (5-HT2a) receptor
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Androgen Receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 Prelamin-A/C
 15-hydroxyprostaglandin dehydrogenase [NAD+]
 Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
 Chromobox protein homolog 1
 Inositol monophosphatase 1
 Vitamin D receptor
 Glutaminase kidney isoform, mitochondrial
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14-alpha demethylase

Molecular Mechanism (repurposed) :

smoothened homolog inhibitor

lanosterol 14-alpha demethylase inhibitor

Predicted Targets

Cytochrome P450 51 (Lanosterol 14-alpha demethylase)

Serum albumin
 Cytochrome P450 3A4
 P-glycoprotein 1
 P-glycoprotein 3

14-alpha sterol demethylase Cyp51A (Lanosterol 14-alpha demethylase)

14-alpha sterol demethylase
Vascular endothelial growth factor receptor 2
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase

Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor

Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Vasopressin V2 receptor
Prelamin-A/C
Microtubule-associated protein tau
Hypoxia-inducible factor 1 alpha
Menin/Histone-lysine N-methyltransferase MLL
Lysine-specific demethylase 4A
Nuclear factor erythroid 2-related factor 2
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Bromodomain adjacent to zinc finger domain protein 2B
Arachidonate 15-lipoxygenase, type II
HSP40, subfamily A, putative
DNA polymerase kappa
Plasmodium falciparum
Heat shock protein HSP 90-alpha
HSP90
Peripheral myelin protein 22
Geminin
Glomerella tucumanensis
Setosphaeria rostrata
Isocitrate dehydrogenase [NADP] cytoplasmic
TAR DNA-binding protein 43
Alpha-synuclein

Ketoconazole

Molecular Mechanism (initial) :

fungus cytochrome P450 51 inhibitor

Molecular Mechanism (repurposed) :

cytochrome P450 aromatase (CYP19A1) inhibitor

Predicted Targets

Arthroderma benhamiae
Trichophyton rubrum
Phialophora verrucosa
Cytochrome P450 17A1
Cytochrome P450-cam
Beta-lactamase AmpC
Alpha-chymotrypsin
Malate dehydrogenase cytoplasmic

Cytochrome P450 51

Cytochrome P450 19A1

Clavispora lusitaniae
Gonadotropin-releasing hormone receptor
Follicle stimulating hormone receptor

Phospholipase A2 group 1B
Cyclooxygenase
Arachidonate 5-lipoxygenase
Cytochrome P450 3A4
P-glycoprotein 1
P-glycoprotein 3
Cytochrome P450 7A1
Cytochrome P450 11B1
Cytochrome P450 11A1
Cytochrome P450 2C11
Cytochrome P450 2A2
Cytochrome P450 21
Saccharomyces cerevisiae
Cytochrome P450 11B2
Cytochrome P450 24A1
Steroid 5-alpha-reductase 1
Steroid 5-alpha-reductase 2
Large conductance calcium-activated potassium channel
Cytochrome P450 26A1
Cytochrome P450 1A2
Cytochrome P450 2C9
Cytochrome P450 2C19
Cytochrome P450 2B6
Cytochrome P450 2D6
Solute carrier family 22 member 1
Pregnane X receptor
Arthrodermataceae
Nuclear factor NF-kappa-B p105 subunit
Ras-related protein Rab-9A
Survival motor neuron protein
Thyroid stimulating hormone receptor
Tyrosyl-DNA phosphodiesterase 1
Microtubule-associated protein tau
Hypoxia-inducible factor 1 alpha
Aldehyde dehydrogenase 1A1
Peripheral myelin protein 22
Nonstructural protein 1
MAP kinase ERK2
Menin/Histone-lysine N-methyltransferase MLL
Anthrax lethal factor
Ubiquitin carboxyl-terminal hydrolase 2
Bloom syndrome protein
Muscarinic acetylcholine receptor M1
Thrombopoietin
Nuclear receptor ROR-gamma
Neuropeptide S receptor
Geminin
Phospholipidosis
ATP binding cassette transporter Abc1p
Hepatotoxicity

ATPase family AAA domain-containing protein 5
Nuclear factor erythroid 2-related factor 2
Lysine-specific demethylase 4A
Dopamine D1 receptor
M-phase phosphoprotein 8
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Chromobox protein homolog 1
Bromodomain adjacent to zinc finger domain protein 2B
Arachidonate 15-lipoxygenase, type II
Vanilloid receptor
Runt-related transcription factor 1/Core-binding factor subunit beta
Bacillus megaterium
Retinoid X receptor alpha
Ataxin-2
Bile acid receptor FXR
Thioredoxin reductase 1, cytoplasmic
Flap endonuclease 1
Peroxisome proliferator-activated receptor gamma
Estrogen receptor alpha
DNA polymerase kappa
Regulator of G-protein signaling 4
Mothers against decapentaplegic homolog 3
Vitamin D receptor
Heat shock protein HSP 90-alpha
Ubiquitin carboxyl-terminal hydrolase 1
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor

Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK

Leukocyte common antigen
 Serotonin 1a (5-HT1a) receptor
 Serotonin 1b (5-HT1b) receptor
 Serotonin 2a (5-HT2a) receptor
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Androgen Receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 Leishmania amazonensis
 Solute carrier organic anion transporter family member 1A2
 Cellular tumor antigen p53
 Glucagon-like peptide 1 receptor
 Chlorella fusca
 Solute carrier organic anion transporter family member 2B1
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 Indoleamine 2,3-dioxygenase 2
 TAR DNA-binding protein 43
 Cytochrome P450 3A4/3A5

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

Predicted Targets

Serum albumin
 Voltage-gated L-type calcium channel alpha-1C subunit
 Chymotrypsin C
 Malate dehydrogenase cytoplasmic

Sodium channel alpha subunits; brain (Types I, II, III)

Sodium channel protein type V alpha subunit

Dopamine receptor
 Homo sapiens
 Voltage-gated potassium channel subunit Kv1.5
 Potassium voltage-gated channel subfamily D member 2
 Potassium voltage-gated channel subfamily B member 1
 Sphingomyelin phosphodiesterase
 Solute carrier family 22 member 1
 Monoamine oxidase B

Monoamine oxidase A
Prelamin-A/C
Aldehyde dehydrogenase 1A1
Microtubule-associated protein tau
MAP kinase ERK2
Muscarinic acetylcholine receptor M1
Cytochrome P450 3A4
Phospholipidosis
Hepatotoxicity
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2C19
Cytochrome P450 1A2
Chromobox protein homolog 1
Thioredoxin reductase 1, cytoplasmic
Flap endonuclease 1
P-glycoprotein 1
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor

Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor

Serotonin 4 (5-HT₄) receptor
Serotonin 6 (5-HT₆) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Solute carrier family 22 member 5
Geminin
Multidrug and toxin extrusion protein 1
Potassium channel subfamily K member 2
Isocitrate dehydrogenase [NADP] cytoplasmic
Oryctolagus cuniculus

Sodium channel protein type IX alpha subunit

Sodium channel protein type IV alpha subunit

Sodium channel protein type III alpha subunit

Bloom syndrome protein
Lysosomal alpha-glucosidase
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Nuclear factor erythroid 2-related factor 2

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

Predicted Targets

Glutamate [NMDA] receptor subunit epsilon 3

Glutamate [NMDA] receptor

Glutamate NMDA receptor; GRIN1/GRIN2B

Glutamate NMDA receptor; GRIN1/GRIN2A

Solute carrier family 22 member 1
Glutamate (NMDA) receptor subunit zeta 1
Cholinesterase
Acetylcholinesterase
Prelamin-A/C
FK506 binding protein 12
Phospholipidosis
Nuclear factor erythroid 2-related factor 2
Plasmodium falciparum
Thioredoxin reductase 1, cytoplasmic
Peripheral myelin protein 22
Solute carrier family 22 member 2
Dual specificity protein kinase CLK3

Dual specificity protein kinase CLK1
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Dual-specificity tyrosine-phosphorylation regulated kinase 1A

Glutamate [NMDA] receptor subunit epsilon 2

Nuclear factor NF-kappa-B p105 subunit
Cytochrome P450 2C19
Cytochrome P450 2D6
Cytochrome P450 2C9
Cytochrome P450 3A4
Cytochrome P450 1A2
Beta-lactamase AmpC
Neuropeptide S receptor
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Vanilloid receptor
Chromobox protein homolog 1
Isocitrate dehydrogenase [NADP] cytoplasmic
Solute carrier organic anion transporter family member 1B1
Solute carrier organic anion transporter family member 1B3

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

Predicted Targets

Dipeptidyl peptidase IV
Solute carrier family 22 member 1
Prelamin-A/C
Ferritin light chain
Phospholipidosis
Histone acetyltransferase GCN5
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2C19
Cytochrome P450 3A4
Cytochrome P450 1A2
Solute carrier family 22 member 2
Multidrug and toxin extrusion protein 1
Multidrug and toxin extrusion protein 2
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor

Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor

Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
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Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Protein-tyrosine phosphatase 1B
AICAR transformylase

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :

dihydrofolate reductase inhibitor

Predicted Targets

Dihydrofolate reductase

Prelamin-A/C
Menin/Histone-lysine N-methyltransferase MLL
Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
Lysine-specific demethylase 4D-like
Caspase-7
Survival motor neuron protein
Ferritin light chain
Tyrosyl-DNA phosphodiesterase 1
Microtubule-associated protein tau
Aldehyde dehydrogenase 1A1
4'-phosphopantetheinyl transferase ffp
Arachidonate 15-lipoxygenase
Arachidonate 12-lipoxygenase
DNA-(apurinic or apyrimidinic site) lyase
Bloom syndrome protein
15-hydroxyprostaglandin dehydrogenase [NAD+]
Cellular tumor antigen p53
Alpha-galactosidase A
Caspase-1
DNA polymerase beta
ATPase family AAA domain-containing protein 5
Nuclear factor erythroid 2-related factor 2
Histone acetyltransferase GCN5
M-phase phosphoprotein 8
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
6-phospho-1-fructokinase
Chromobox protein homolog 1
Thioredoxin reductase 1, cytoplasmic
Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
Runt-related transcription factor 1/Core-binding factor subunit beta
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 3A4
Cytochrome P450 2C19
Cytochrome P450 1A2
Solute carrier organic anion transporter family member 1A2
ATP-binding cassette sub-family G member 2
Canalicular multispecific organic anion transporter 2
Multidrug resistance-associated protein 4
Thymidylate synthase (EC 2.1.1.45) (TS) (TSase)
Vitamin D receptor
Bile acid receptor FXR
Flap endonuclease 1
DNA polymerase iota
DNA polymerase eta
Peroxisome proliferator-activated receptor delta
DNA polymerase kappa
Peroxisome proliferator-activated receptor gamma
Retinoid X receptor alpha

Ubiquitin carboxyl-terminal hydrolase 1
P-glycoprotein 1
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A

Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Nuclear receptor coactivator 3
Alpha trans-inducing protein (VP16)
Peripheral myelin protein 22

Nuclear receptor coactivator 1
 Solute carrier organic anion transporter family member 1A3
 Solute carrier family 22 member 8
 Solute carrier organic anion transporter family member 1B1
 Multidrug resistance associated protein
 Solute carrier family 22 member 7
 Multidrug resistance-associated protein 1
 Multidrug resistance-associated protein 7
 Solute carrier family 22 member 11
 Solute carrier organic anion transporter family member 1B3
 ATP-binding cassette sub-family C member 11
 Monocarboxylate transporter 1
 Solute carrier organic anion transporter family member 1C1
 Solute carrier organic anion transporter family member 3A1
 Solute carrier organic anion transporter family member 1A1
 Solute carrier organic anion transporter family member 1A4
 Solute carrier organic anion transporter family member 1A5
 Solute carrier organic anion transporter family member 1B2
 Geminin
 ATP-dependent Clp protease proteolytic subunit
 Sphingomyelin phosphodiesterase
 Transcriptional regulator ERG
 Solute carrier organic anion transporter family member 2B1
 Isocitrate dehydrogenase [NADP] cytoplasmic
 Lysine-specific demethylase 4A
 Latent membrane protein 1
 Thyroid stimulating hormone receptor
 Polyadenylate-binding protein 1
 Glucagon-like peptide 1 receptor
 Werner syndrome ATP-dependent helicase

Milnacipran

Molecular Mechanism (initial) :

5-HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

5-HT and norepinephrine reuptake inhibitor

Predicted Targets

Glutamate NMDA receptor
 Glutamate [NMDA] receptor subunit epsilon 3

Serotonin transporter

Norepinephrine transporter

Dopamine transporter

Transporter
 Cytochrome P450 2D6
 Lysine-specific demethylase 4D-like
 MAP kinase ERK2

Miltefosine

Molecular Mechanism (initial) :

Akt/PKB inhibitor

Molecular Mechanism (repurposed) :

phosphatidyl-choline biosynthesis inhibitor

Predicted Targets

Not results

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

Predicted Targets

Serum albumin

Multidrug translocase mdfA

Adrenergic receptor beta

Protein-arginine deiminase type-4

Signal transducer and activator of transcription 1

Interferon regulatory factor 1

Protein kinase C alpha

Monoamine oxidase A

Cytochrome P450 3A4

Cytochrome P450 2D6

Cytochrome P450 2C19

Cytochrome P450 2C9

Cytochrome P450 1A2

Solute carrier family 22 member 7

Solute carrier family 22 member 8

Solute carrier family 22 member 11

Solute carrier family 22 member 6

Acetylcholinesterase

Cholinesterase

Lysine-specific demethylase 4D-like

Tyrosyl-DNA phosphodiesterase 1

Hypoxia-inducible factor 1 alpha

Ubiquitin carboxyl-terminal hydrolase 2

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Ubiquitin carboxyl-terminal hydrolase 1

Glutaminase kidney isoform, mitochondrial

Solute carrier organic anion transporter family member 1B1

Solute carrier organic anion transporter family member 1B3

ATP-dependent DNA helicase Q1

Microtubule-associated protein tau

15-hydroxyprostaglandin dehydrogenase [NAD+]

Vitamin D receptor

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

Predicted Targets

Human immunodeficiency virus type 1 protease

Cytochrome P450 3A4
P-glycoprotein 1
P-glycoprotein 3
Cytochrome P450 3A5
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter

Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor

Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Solute carrier organic anion transporter family member 1A2
ATP-binding cassette sub-family G member 2
Solute carrier family 22 member 1
Solute carrier organic anion transporter family member 1B1
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Nonstructural protein 1
Ferritin light chain
Menin/Histone-lysine N-methyltransferase MLL
Alpha-galactosidase A
Nuclear receptor ROR-gamma
DNA polymerase beta
Beta-glucocerebrosidase
Nuclear factor erythroid 2-related factor 2
Histone acetyltransferase GCN5
Bromodomain adjacent to zinc finger domain protein 2B
DNA polymerase kappa
Mothers against decapentaplegic homolog 3
Peripheral myelin protein 22
Geminin
Ataxin-2
Glucagon-like peptide 1 receptor
TAR DNA-binding protein 43
Isocitrate dehydrogenase [NADP] cytoplasmic
Hypoxia-inducible factor 1 alpha
Survival motor neuron protein
Aldehyde dehydrogenase 1A1
Anthrax lethal factor
Vitamin D receptor
Retinoid X receptor alpha
Thyroid hormone receptor beta-1
Chromobox protein homolog 1
Bile acid receptor FXR
Thioredoxin reductase 1, cytoplasmic
Peroxisome proliferator-activated receptor delta (PPAR-delta)
Peroxisome proliferator-activated receptor gamma
Nuclear receptor subfamily 1 group I member 2
Interleukin-8

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

proto-oncogene c-Kit inhibitor

Predicted Targets

Tyrosine-protein kinase BTK

Carbonic anhydrase I

Carbonic anhydrase II

Carbonic anhydrase III

Carbonic anhydrase IV

Carbonic anhydrase VA

Carbonic anhydrase VB

Carbonic anhydrase VI

Carbonic anhydrase VII

Carbonic anhydrase IX

Carbonic anhydrase XII

Carbonic anhydrase XIII

Carbonic anhydrase XIV

Carbonic anhydrase 15

Tyrosine-protein kinase ABL

Stem cell growth factor receptor

Bcr/Abl fusion protein

Platelet-derived growth factor receptor alpha

Platelet-derived growth factor receptor beta

Epithelial discoidin domain-containing receptor 1

Discoidin domain-containing receptor 2

Macrophage colony stimulating factor receptor

NT-3 growth factor receptor

MAP kinase p38 gamma

Proto-oncogene tyrosine-protein kinase MER

Serine/threonine-protein kinase SRPK2

Serine/threonine-protein kinase Aurora-C

CaM kinase II delta

Serine/threonine-protein kinase tousel-like 2

Serine/threonine-protein kinase Aurora-B

AMP-activated protein kinase, alpha-1 subunit

Serine/threonine-protein kinase SIK3

Serine/threonine-protein kinase 16

Serine/threonine-protein kinase PCTAIRE-2

Serine/threonine-protein kinase receptor R3

Cyclin-dependent kinase 4

Fibroblast growth factor receptor 3

Insulin receptor

Tyrosine-protein kinase JAK3

Hepatocyte growth factor receptor

Phosphorylase kinase gamma subunit 2

Serine/threonine-protein kinase 11
Tyrosine-protein kinase TIE-2
Insulin-like growth factor I receptor
Mitogen-activated protein kinase kinase kinase 15
Serine/threonine-protein kinase PIM3
Serine/threonine-protein kinase Chk2
Receptor protein-tyrosine kinase erbB-2
Ribosomal protein S6 kinase alpha 2
Ribosomal protein S6 kinase alpha 4
Tyrosine kinase non-receptor protein 2
Nerve growth factor receptor Trk-A
Myosin light chain kinase family member 4
Eukaryotic translation initiation factor 2-alpha kinase 4
Serine/threonine-protein kinase PAK 4
Serine/threonine-protein kinase SBK1
Misshapen-like kinase 1
Serine/threonine-protein kinase DCLK2
Receptor protein-tyrosine kinase erbB-4
Mitogen-activated protein kinase kinase kinase kinase 1
Ephrin type-A receptor 6
Myosin-IIIB
Serine/threonine-protein kinase ULK3
Activin receptor type-1
Activin receptor type-2B
Serine/threonine-protein kinase 32A
Cyclin-dependent kinase-like 3
MAP kinase-interacting serine/threonine-protein kinase MNK1
Phosphatidylinositol-4-phosphate 5-kinase type-1 alpha
Bone morphogenetic protein receptor type-1B
Bone morphogenetic protein receptor type-2
CaM kinase II beta
Cyclin-dependent kinase 3
Cell division protein kinase 8
Cyclin-dependent kinase 9
Serine/threonine-protein kinase Chk1
Inhibitor of nuclear factor kappa B kinase alpha subunit
Casein kinase I gamma 2
Death-associated protein kinase 3
Serine/threonine-protein kinase/endoribonuclease IRE1
Inhibitor of nuclear factor kappa B kinase beta subunit
Interleukin-1 receptor-associated kinase 1
Activin receptor type-2A
Serine/threonine-protein kinase AKT2
Tyrosine-protein kinase receptor UFO
Tyrosine-protein kinase BLK
Tyrosine-protein kinase BMX
CaM kinase IV
Cyclin-dependent kinase 2
Cyclin-dependent kinase 7
Casein kinase I alpha

Casein kinase I epsilon
Casein kinase II alpha
Casein kinase II alpha (prime)
Receptor tyrosine-protein kinase erbB-3
Tyrosine-protein kinase FES
Vascular endothelial growth factor receptor 1
Vascular endothelial growth factor receptor 3
Tyrosine-protein kinase FRK
Glycogen synthase kinase-3 beta
Tyrosine-protein kinase HCK
Tyrosine-protein kinase JAK1
Vascular endothelial growth factor receptor 2
LIM domain kinase 1
Tyrosine-protein kinase Lyn
Serine/threonine-protein kinase c-TAK1
Tyrosine-protein kinase CTK
Mitogen-activated protein kinase kinase kinase 3
Mitogen-activated protein kinase kinase kinase 11
Mitogen-activated protein kinase kinase kinase 10
Macrophage-stimulating protein receptor
Serine/threonine-protein kinase NEK2
Serine/threonine-protein kinase Nek3
Serine/threonine-protein kinase PAK 1
Serine/threonine-protein kinase PAK 2
Serine/threonine-protein kinase PAK 3
Serine/threonine-protein kinase PCTAIRE-3
3-phosphoinositide dependent protein kinase-1
Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing beta polypeptide
Serine/threonine-protein kinase PIM1
PI3-kinase p110-gamma subunit
PI4-kinase beta subunit
cAMP-dependent protein kinase alpha-catalytic subunit
cAMP-dependent protein kinase beta-1 catalytic subunit
Protein kinase C iota
Protein kinase C mu
MAP kinase ERK1
Mitogen-activated protein kinase 4
Mitogen-activated protein kinase 6
Mitogen-activated protein kinase 7
c-Jun N-terminal kinase 1
MAP kinase p38 beta
c-Jun N-terminal kinase 3
MAP kinase p38 delta
Dual specificity mitogen-activated protein kinase kinase 1
Dual specificity mitogen-activated protein kinase kinase 3
Dual specificity mitogen-activated protein kinase kinase 6
Interferon-induced, double-stranded RNA-activated protein kinase
Rhodopsin kinase
Proto-oncogene tyrosine-protein kinase ROS
Ribosomal protein S6 kinase alpha 1

Dual specificity mitogen-activated protein kinase kinase 4
Serine/threonine-protein kinase SRPK1
Serine/threonine-protein kinase Nek4
Cyclin-dependent kinase-like 5
Ribosomal protein S6 kinase 1
Tyrosine-protein kinase SYK
Tyrosine-protein kinase TEC
TGF-beta receptor type II
Dual specificity protein kinase TTK
Tyrosine-protein kinase TXK
Tyrosine-protein kinase TYK2
Serine/threonine-protein kinase WEE1
Phosphatidylinositol-5-phosphate 4-kinase type-2 beta
Serine/threonine-protein kinase ULK1
Serine/threonine-protein kinase 24
Dual-specificity tyrosine-phosphorylation regulated kinase 2
Serine/threonine-protein kinase Aurora-A
Serine/threonine-protein kinase MRCK-A
Mitogen-activated protein kinase kinase kinase kinase 3
CaM kinase I alpha
MAP kinase-activated protein kinase 5
Peripheral plasma membrane protein CASK
Cyclin-dependent kinase 13
Receptor-interacting serine/threonine-protein kinase 1
Serine/threonine-protein kinase RIPK2
Serine/threonine-protein kinase RIO3
Serine/threonine-protein kinase PRP4 homolog
Cyclin-dependent kinase-like 2
BR serine/threonine-protein kinase 2
Non-receptor tyrosine-protein kinase TNK1
Dual specificity protein kinase CLK3
Dual specificity protein kinase CLK2
Serine/threonine-protein kinase PLK3
Tyrosine-protein kinase receptor FLT3
Cyclin-dependent kinase-like 1
Serine/threonine-protein kinase 17B
Activin receptor type-1B
ALK tyrosine kinase receptor
Bone morphogenetic protein receptor type-1A
Serine/threonine-protein kinase B-raf
Tyrosine-protein kinase CSK
Casein kinase I isoform gamma-3
Myotonic-protein kinase
Ephrin type-A receptor 2
Ephrin type-A receptor 4
Ephrin type-A receptor 7
Ephrin type-B receptor 1
Ephrin type-B receptor 3
Ephrin type-B receptor 4
Ephrin type-B receptor 6

Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing subunit gamma
Mitogen-activated protein kinase kinase kinase 2
Ribosomal protein S6 kinase alpha 3
TGF-beta receptor type I
Mitogen-activated protein kinase kinase kinase 6
Serine/threonine-protein kinase LATS1
Dual specificity tyrosine-phosphorylation-regulated kinase 1B
Mitogen-activated protein kinase kinase kinase 13
Serine/threonine-protein kinase DCLK1
Ribosomal protein S6 kinase alpha 5
Serine/threonine-protein kinase 17A
Rho-associated protein kinase 2
Cyclin-dependent kinase 5
Death-associated protein kinase 1
FK506 binding protein 12
Tyrosine-protein kinase JAK2
PI3-kinase p110-delta subunit
Serine/threonine-protein kinase PLK1
Serine/threonine-protein kinase PRKX
Serine/threonine-protein kinase OSR1
Tyrosine-protein kinase ABL2
Serine/threonine-protein kinase AKT
Epidermal growth factor receptor erbB1
Ephrin type-A receptor 1
Ephrin type-A receptor 3
Tyrosine-protein kinase FER
Tyrosine-protein kinase FGR
Serine/threonine-protein kinase GAK
Tyrosine-protein kinase LCK
Protein kinase C epsilon
Rho-associated protein kinase 1
Tyrosine-protein kinase SRC
Tyrosine-protein kinase receptor Tie-1
Tyrosine-protein kinase YES
Serine/threonine-protein kinase AKT3
Tyrosine-protein kinase ITK/TSK
LIM domain kinase 2
Muscle, skeletal receptor tyrosine protein kinase
Homeodomain-interacting protein kinase 3
Protein kinase C nu
Serine/threonine-protein kinase MAK
Mitogen-activated protein kinase kinase kinase 1
Mitogen-activated protein kinase kinase kinase 4
Mitogen-activated protein kinase kinase kinase 5
Tyrosine-protein kinase BRK
Serine/threonine-protein kinase 10
Serine/threonine-protein kinase MRCK beta
Neurotrophic tyrosine kinase receptor type 2
Serine/threonine-protein kinase PCTAIRE-1
Phosphorylase kinase gamma subunit 1

PI3-kinase p110-alpha subunit
PI3-kinase p110-beta subunit
AMP-activated protein kinase, alpha-2 subunit
Protein kinase C delta
Protein kinase C eta
Protein kinase N2
Protein kinase C theta
cGMP-dependent protein kinase 1 beta
cGMP-dependent protein kinase 2
Serine/threonine-protein kinase MST2
Serine/threonine-protein kinase MST1
Dual specificity testis-specific protein kinase 1
Tyrosine-protein kinase receptor TYRO3
Serine/threonine-protein kinase VRK2
Mitogen-activated protein kinase kinase kinase 12
Serine/threonine-protein kinase 25
CaM-kinase kinase beta
Mitogen-activated protein kinase kinase kinase kinase 5
Mitogen-activated protein kinase kinase kinase 2
Serine/threonine-protein kinase PLK2
Serine/threonine-protein kinase PIM2
Citron Rho-interacting kinase
Interleukin-1 receptor-associated kinase 3
Serine/threonine-protein kinase 38
Serine/threonine-protein kinase Nek1
Serine/threonine-protein kinase tousled-like 1
Serine/threonine-protein kinase PFTAIRES-1
Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma
STE20/SPS1-related proline-alanine-rich protein kinase
Serine/threonine-protein kinase TBK1
Serine/threonine-protein kinase Sgk3
Inhibitor of nuclear factor kappa B kinase epsilon subunit
Insulin receptor-related protein
Serine/threonine-protein kinase PLK4
Death-associated protein kinase 2
Serine/threonine-protein kinase SRPK3
Serine/threonine-protein kinase NEK6
Eukaryotic translation initiation factor 2-alpha kinase 1
Ribosomal protein S6 kinase alpha 6
Serine/threonine-protein kinase LATS2
Hormonally up-regulated neu tumor-associated kinase
Serine/threonine-protein kinase ULK2
Serine/threonine-protein kinase 2
Maternal embryonic leucine zipper kinase
NUAK family SNF1-like kinase 1
Adaptor-associated kinase
Serine/threonine-protein kinase ICK
Microtubule-associated serine/threonine-protein kinase 1
Serine/threonine-protein kinase 38-like
TRAF2- and NCK-interacting kinase

Cell division cycle 2-like protein kinase 6
Serine/threonine-protein kinase SIK2
Serine/threonine-protein kinase 36
Serine/threonine-protein kinase TNNT3K
Interleukin-1 receptor-associated kinase 4
Serine/threonine-protein kinase TAO2
Serine/threonine protein kinase NLK
Serine/threonine-protein kinase TAO3
Serine/threonine-protein kinase D2
Serine/threonine-protein kinase MST4
Myosin IIIA
Ephrin type-B receptor 2
MAP/microtubule affinity-regulating kinase 2
Serine/threonine-protein kinase MRCK gamma
MAP kinase signal-integrating kinase 2
BMP-2-inducible protein kinase
Transient receptor potential cation channel subfamily M member 6
SNF-related serine/threonine-protein kinase
Serine/threonine-protein kinase RIO2
Serine/threonine-protein kinase 32B
Serine/threonine-protein kinase MARK1
Glycogen synthase kinase-3 alpha
Serine/threonine-protein kinase PAK6
Chaperone activity of bcl complex-like, mitochondrial
Serine/threonine-protein kinase PAK7
CaM kinase I delta
CaM kinase I gamma
Ephrin type-A receptor 8
Tyrosine-protein kinase receptor RET
Receptor-interacting serine/threonine-protein kinase 4
Dual specificity protein kinase CLK4
Serine/threonine-protein kinase TAO1
Casein kinase I gamma 1
Homeodomain-interacting protein kinase 2
Fibroblast growth factor receptor 4
Fibroblast growth factor receptor 2
Fibroblast growth factor receptor 1
PITSLRE serine/threonine-protein kinase CDC2L2
Phosphatidylinositol-5-phosphate 4-kinase type-2 gamma
Uncharacterized aarF domain-containing protein kinase 4
SPS1/STE20-related protein kinase YSK4
Dual specificity mitogen-activated protein kinase kinase 2
Serine/threonine-protein kinase 33
NUAK family SNF1-like kinase 2
MAP/microtubule affinity-regulating kinase 4
Serine/threonine-protein kinase RIO1
Testis-specific serine/threonine-protein kinase 1
CaM-kinase kinase alpha
BR serine/threonine-protein kinase 1
MAP kinase-activated protein kinase 2

Serine/threonine-protein kinase NEK9
myosin light chain kinase 2
Mitogen-activated protein kinase kinase kinase 9
Serine/threonine-protein kinase DCLK3
Serine/threonine-protein kinase pknB
PITSLRE serine/threonine-protein kinase CDC2L1
Myosin light chain kinase, smooth muscle
Tyrosine-protein kinase Srms
Serine/threonine-protein kinase 35
Dual-specificity tyrosine-phosphorylation regulated kinase 1A
Serine/threonine-protein kinase NEK7
Mixed lineage kinase 7
MAP kinase ERK2
MAP kinase p38 alpha
Mitogen-activated protein kinase 15
Casein kinase I delta
c-Jun N-terminal kinase 2
Serine/threonine-protein kinase PFTAIRE-2
G protein-coupled receptor kinase 7
Homeodomain-interacting protein kinase 4
Dual specificity mitogen-activated protein kinase kinase 5
Dual specificity mitogen-activated protein kinase kinase 7
Casein kinase I isoform alpha-like
Mitogen-activated protein kinase kinase kinase 7
Mitogen-activated protein kinase kinase kinase kinase 4
Serine/threonine-protein kinase Nek1 1
Homeodomain-interacting protein kinase 1
Tyrosine-protein kinase FYN
Serine/threonine-protein kinase NIM1
Focal adhesion kinase 1
CaM kinase II alpha
CaM kinase II gamma
Protein tyrosine kinase 2 beta
Serine/threonine-protein kinase SIK1
Serine/threonine-protein kinase 32C
Ankyrin repeat and protein kinase domain-containing protein 1
Ephrin type-A receptor 5
Myosin light chain kinase
Tyrosine- and threonine-specific cdc2-inhibitory kinase
G protein-coupled receptor kinase 4
Leucine-rich repeat serine/threonine-protein kinase 2
Serine/threonine-protein kinase Nek5
Leukocyte tyrosine kinase receptor
Tyrosine-protein kinase ZAP-70
Protein kinase N1
Wee1-like protein kinase 2
Putative uncharacterized serine/threonine-protein kinase SgK110
Dual serine/threonine and tyrosine protein kinase
Calcium-dependent protein kinase 1
Cell division control protein 2 homolog

ATP-binding cassette sub-family G member 2

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Predicted Targets

Not results

Paclitaxel

Molecular Mechanism (initial) :

tubulin beta modulator (microtubule-stabilizing agent)

Molecular Mechanism (repurposed) :

tubulin beta modulator (microtubule-stabilizing agent)

Predicted Targets

Tubulin beta-1 chain

Tubulin

Tubulin alpha chain

Tubulin beta chain

Cytochrome P450 3A4

P-glycoprotein 1

Thymidine kinase, cytosolic

Apoptosis regulator Bcl-2

Apoptosis regulator Bcl-X

Monoamine oxidase A

Menin/Histone-lysine N-methyltransferase MLL

Prelamin-A/C

ATP-dependent DNA helicase Q1

Ras-related protein Rab-9A

Survival motor neuron protein

FK506 binding protein 12

Luciferin 4-monooxygenase

Thyroid hormone receptor beta-1

Microtubule-associated protein tau

Nuclear receptor ROR-gamma

Hypoxia-inducible factor 1 alpha

Peripheral myelin protein 22

4'-phosphopantetheinyl transferase ffp

Nonstructural protein 1

Anthrax lethal factor

Beta-lactamase AmpC

Niemann-Pick C1 protein

Ubiquitin carboxyl-terminal hydrolase 2

Bloom syndrome protein

Thrombopoietin

Cellular tumor antigen p53

Endoplasmic reticulum-associated amyloid beta-peptide-binding protein

Neuropeptide S receptor
Geminin
Cytochrome P450 2C9
Nuclear factor erythroid 2-related factor 2
ATPase family AAA domain-containing protein 5
Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
Cytochrome P450 2D6
Cytochrome P450 2C19
Cytochrome P450 1A2
Multidrug resistance protein 3
Cytochrome P450 2C8
Chromobox protein homolog 1
Thioredoxin reductase 1, cytoplasmic
Androgen Receptor
Peroxisome proliferator-activated receptor delta
Estrogen receptor alpha
Regulator of G-protein signaling 4
Peroxisome proliferator-activated receptor gamma
Mothers against decapentaplegic homolog 3
Vitamin D receptor
Glucocorticoid receptor
Ubiquitin carboxyl-terminal hydrolase 1
Retinoid X receptor alpha
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2

Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor beta
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK

Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Sigma opioid receptor
Neurokinin 1 receptor
Neurokinin 2 receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
P-glycoprotein 3
Multidrug resistance-associated protein 7
Multidrug resistance-associated protein 1
Bile salt export pump
Nuclear receptor subfamily 1 group I member 2
Solute carrier organic anion transporter family member 2B1
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Cholinesterase
Isocitrate dehydrogenase [NADP] cytoplasmic
Alpha-synuclein
Tubulin beta-3 chain
Fibroblast growth factor receptor 1
Tyrosine-protein kinase ABL
Tyrosine-protein kinase SRC
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
DNA polymerase iota
Tyrosyl-DNA phosphodiesterase 1

Phentolamine mesilate

Molecular Mechanism (initial) :

alpha-adrenoceptor antagonist

Molecular Mechanism (repurposed) :

alpha-adrenoceptor antagonist

Predicted Targets

Adrenergic receptor alpha

Adrenergic receptor alpha-1

Adrenergic receptor alpha-2

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Alpha-1a adrenergic receptor

Serotonin 1a (5-HT1a) receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor**Alpha-2c adrenergic receptor**

Sodium channel alpha subunits; brain (Types I, II, III)

Adrenergic receptor beta

Sigma opioid receptor

Alpha-1b adrenergic receptor**Alpha-1d adrenergic receptor**

Dopamine D1 receptor

Dopamine D2 receptor

Dopamine D3 receptor

Dopamine D4 receptor

Serotonin 1b (5-HT1b) receptor

Serotonin 2a (5-HT2a) receptor

Serotonin 2c (5-HT2c) receptor

Nischarin

Prelamin-A/C

Estrogen receptor beta

Heat shock factor protein 1

4'-phosphopantetheinyl transferase ffp

Cytochrome P450 2D6

Hepatotoxicity

Phospholipidosis

Lysine-specific demethylase 4A

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chromobox protein homolog 1

Bromodomain adjacent to zinc finger domain protein 2B

ATPase family AAA domain-containing protein 5

Cytochrome P450 2C9

Cytochrome P450 3A4

Cytochrome P450 2C19

Cytochrome P450 1A2

Ataxin-2

DNA polymerase iota

Regulator of G-protein signaling 4

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Beta-3 adrenergic receptor

Norepinephrine transporter

Aldose reductase

Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor

Calcitonin receptor

Cannabinoid CB1 receptor

Carbonic anhydrase II

C-C chemokine receptor type 2

C-C chemokine receptor type 4

C-C chemokine receptor type 5

Interleukin-8 receptor A

Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN

Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 2b (5-HT2b) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
ATP-dependent Clp protease proteolytic subunit
Glutaminase kidney isoform, mitochondrial
Microtubule-associated protein tau
Putative fructose-1,6-bisphosphate aldolase
Beta-lactamase AmpC
Glucagon-like peptide 1 receptor
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1
Nuclear factor NF-kappa-B p105 subunit
Lysine-specific demethylase 4D-like
Thyroid stimulating hormone receptor
Peripheral myelin protein 22
Nonstructural protein 1
Bloom syndrome protein
Nuclear factor erythroid 2-related factor 2
M-phase phosphoprotein 8
DNA polymerase eta
Mothers against decapentaplegic homolog 3
Geminin
TAR DNA-binding protein 43

Raloxifene hydrochloride

Molecular Mechanism (initial) :

estrogen receptor agonist

Molecular Mechanism (repurposed) :

estrogen receptor agonist

Predicted Targets

Estrogen receptor alpha

Estrogen receptor beta

Estrogen receptor

3-beta-hydroxysteroid-delta(8),delta(7)-isomerase

Sigma opioid receptor

C-8 sterol isomerase

Phospholipase D1

Phospholipase D2

Serotonin 2b (5-HT2b) receptor
ATP-dependent DNA helicase Q1
Nuclear factor NF-kappa-B p105 subunit
Thyroid stimulating hormone receptor
FK506 binding protein 12
Tyrosyl-DNA phosphodiesterase 1
Microtubule-associated protein tau
Cytochrome P450 2C19
Nuclear receptor ROR-gamma
Aldehyde dehydrogenase 1A1
Arachidonate 15-lipoxygenase
Menin/Histone-lysine N-methyltransferase MLL
Anthrax lethal factor
Ubiquitin carboxyl-terminal hydrolase 2
Muscarinic acetylcholine receptor M1
Thrombopoietin
Cellular tumor antigen p53
Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
Cytochrome P450 2D6
Cytochrome P450 3A4
Cytochrome P450 2C9
Aldehyde oxidase
Beta-glucocerebrosidase
Nuclear factor erythroid 2-related factor 2
Dopamine D1 receptor
M-phase phosphoprotein 8
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
6-phospho-1-fructokinase
Chromobox protein homolog 1
ATPase family AAA domain-containing protein 5
Cytochrome P450 1A2
UDP-glucuronosyltransferase 1-1
UDP-glucuronosyltransferase 1-8
UDP-glucuronosyltransferase 1-10
Ubiquitin carboxyl-terminal hydrolase 1
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 2A6
Cytochrome P450 2E1
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1

Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor
Serotonin 6 (5-HT6) receptor
Serotonin transporter
Neurokinin 1 receptor
Neurokinin 2 receptor
Androgen Receptor
Thromboxane-A synthase
Vascular endothelial growth factor receptor 1
Vasoactive intestinal polypeptide receptor 1
Vasopressin V1a receptor
Peripheral myelin protein 22
Bile acid receptor FXR
Pregnane X receptor
Interleukin-6 receptor subunit beta
Huntingtin
Histone-lysine N-methyltransferase MLL
Ferritin light chain
Endonuclease 4
4'-phosphopantetheinyl transferase ffp
Nonstructural protein 1
Beta-lactamase AmpC
Bloom syndrome protein
Neuropeptide S receptor
Lysine-specific demethylase 4A
Bcl-2-related protein A1
Ubiquitin-conjugating enzyme E2 N
Bromodomain adjacent to zinc finger domain protein 2B
Arachidonate 15-lipoxygenase, type II
Runt-related transcription factor 1/Core-binding factor subunit beta
Retinoid X receptor alpha
Thyroid hormone receptor beta-1
Thioredoxin reductase 1, cytoplasmic
DNA polymerase iota
Peroxisome proliferator-activated receptor gamma
Peroxisome proliferator-activated receptor delta

Mothers against decapentaplegic homolog 3
Vitamin D receptor
DNA dC->dU-editing enzyme APOBEC-3F
Rac GTPase-activating protein 1
DNA dC->dU-editing enzyme APOBEC-3G
Glucagon-like peptide 1 receptor
Nuclear receptor subfamily 1 group I member 2
Protein disulfide-isomerase
Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1
Isocitrate dehydrogenase [NADP] cytoplasmic
Anti-estrogen binding site (AEBS)
Thrombin

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :

dopamine D2 and D3 receptor agonist

Predicted Targets

Dopamine D2 receptor

Dopamine D3 receptor

Serotonin 1a (5-HT1a) receptor
Dopamine receptor
Prelamin-A/C
Lysine-specific demethylase 4D-like
Cytochrome P450 2C19
MAP kinase ERK2
Muscarinic acetylcholine receptor M1
Cytochrome P450 2D6
Cytochrome P450 3A4
Cytochrome P450 2C9
Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
6-phospho-1-fructokinase
Chromobox protein homolog 1
Cytochrome P450 1A2
Flap endonuclease 1
Hepatotoxicity
Geminin
Dopamine receptor D2 and D3
Plasmodium falciparum
DNA-(apurinic or apyrimidinic site) lyase
Bloom syndrome protein
HERG
Solute carrier organic anion transporter family member 1B3
Solute carrier organic anion transporter family member 1B1

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :
phospho-diesterase (PDE5A) inhibitor

Predicted Targets

Phosphodiesterase 1

Phosphodiesterase 3

Phosphodiesterase 5A

Phosphodiesterase 2A

Phosphodiesterase 4

Phosphodiesterase, PDE1/PDE5

Phosphodiesterase 2 and 5 (PDE2 and PDE5)

Phosphodiesterase 3 and 5 (PDE3 and PDE5)

Phosphodiesterase 4 and 5 (PDE4 and PDE5)

HERG

Phosphodiesterases; PDE5 & PDE6

Phosphodiesterase 3B

Phosphodiesterase 6

Phosphodiesterase 10A

Phosphodiesterase 11A

Phosphodiesterase 7

Phosphodiesterase 9A

Phosphodiesterase 6C

Phosphodiesterase 6A

Phosphodiesterase 4D

Beta-lactamase AmpC

Cytochrome P450 3A4

Hepatotoxicity

Vitamin D receptor

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Beta-3 adrenergic receptor

Norepinephrine transporter

Aldose reductase

Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor

Calcitonin receptor

Cannabinoid CB1 receptor

Carbonic anhydrase II

C-C chemokine receptor type 2

C-C chemokine receptor type 4

C-C chemokine receptor type 5

Interleukin-8 receptor A
Interleukin-8 receptor B
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Platelet activating factor receptor
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Matrix metalloproteinase-1
Matrix metalloproteinase 9

Protein kinase C alpha
 MAP kinase ERK1
 MAP kinase ERK2
 MAP kinase p38 alpha
 Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
 Epidermal growth factor receptor erbB1
 Tyrosine-protein kinase FYN
 Receptor protein-tyrosine kinase erbB-2
 Tyrosine-protein kinase LCK
 Leukocyte common antigen
 Serotonin 1a (5-HT1a) receptor
 Serotonin 1b (5-HT1b) receptor
 Serotonin 2a (5-HT2a) receptor
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Androgen Receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 Class 1 phosphodiesterase PDEB1
 Multidrug resistance-associated protein 5
 Multidrug resistance-associated protein 7
 Multidrug resistance-associated protein 4
 ATP-binding cassette sub-family C member 11
 Geminin
 Solute carrier organic anion transporter family member 2B1
 Solute carrier organic anion transporter family member 1B3
 Solute carrier organic anion transporter family member 1B1
 Phosphodiesterase 8A
 Phosphodiesterase 7A
 Tryptophan 2,3-dioxygenase
 Indoleamine 2,3-dioxygenase 2

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Predicted Targets

HMG-CoA reductase

Cytochrome P450 3A4

Canalicular multispecific organic anion transporter 1

Solute carrier family 22 member 1
Plasma
3-hydroxy-3-methylglutaryl-coenzyme A reductase
Lysine-specific demethylase 4A
Nuclear factor erythroid 2-related factor 2
Bromodomain adjacent to zinc finger domain protein 2B
Vitamin D receptor
Regulator of G-protein signaling 4
Mothers against decapentaplegic homolog 3
Acetylcholinesterase
Adenosine A1 receptor
Adenosine A2a receptor
Adenosine A3 receptor
Alpha-1d adrenergic receptor
Alpha-1b adrenergic receptor
Alpha-2a adrenergic receptor
Alpha-2b adrenergic receptor
Alpha-2c adrenergic receptor
Beta-1 adrenergic receptor
Beta-2 adrenergic receptor
Beta-3 adrenergic receptor
Norepinephrine transporter
Aldose reductase
Angiotensin II type 2 (AT-2) receptor
Bradykinin B2 receptor
Calcitonin receptor
Cannabinoid CB1 receptor
Carbonic anhydrase II
C-C chemokine receptor type 2
C-C chemokine receptor type 4
C-C chemokine receptor type 5
Interleukin-8 receptor A
Interleukin-8 receptor B
Confidence Score:NAN
Cholecystokinin A receptor
Cyclooxygenase-1
Cyclooxygenase-2
Cytochrome P450 1A2
Cytochrome P450 2A6
Cytochrome P450 2C19
Cytochrome P450 2C9
Cytochrome P450 2D6
Cytochrome P450 2E1
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha

Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Progesterone receptor
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN
Receptor protein-tyrosine kinase erbB-2
Tyrosine-protein kinase LCK
Leukocyte common antigen
Serotonin 1a (5-HT1a) receptor
Serotonin 1b (5-HT1b) receptor
Serotonin 2a (5-HT2a) receptor
Serotonin 2b (5-HT2b) receptor
Serotonin 2c (5-HT2c) receptor
Serotonin 4 (5-HT4) receptor

Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Androgen Receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 Solute carrier organic anion transporter family member 1B1
 P-glycoprotein 1
 Solute carrier organic anion transporter family member 1A1
 Solute carrier organic anion transporter family member 1A4
 Alpha trans-inducing protein (VP16)
 Geminin
 DNA dC->dU-editing enzyme APOBEC-3G
 Photoreceptor-specific nuclear receptor
 Solute carrier organic anion transporter family member 2B1
 Solute carrier organic anion transporter family member 1B3
 Cholinesterase
 TAR DNA-binding protein 43
 Isocitrate dehydrogenase [NADP] cytoplasmic
 Isoprenylcysteine carboxyl methyltransferase
 Squalene synthetase
 Menin/Histone-lysine N-methyltransferase MLL
 Thyroid stimulating hormone receptor
 Microtubule-associated protein tau
 Nuclear receptor ROR-gamma
 Aldehyde dehydrogenase 1A1
 Anthrax lethal factor
 Cellular tumor antigen p53
 Ubiquitin carboxyl-terminal hydrolase 1
 Alpha-galactosidase A
 Prelamin-A/C
 Ubiquitin carboxyl-terminal hydrolase 2
 Peripheral myelin protein 22
 Lysine-specific demethylase 4D-like
 Survival motor neuron protein

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

Predicted Targets

Retinoic acid receptor beta
Retinoid X receptor gamma
Retinoid X receptor alpha
Retinoic acid receptor alpha
Retinoid X receptor beta
Retinoic acid receptor gamma

Menin/Histone-lysine N-methyltransferase MLL
Nuclear receptor ROR-gamma
ATP-dependent DNA helicase Q1
Peroxisome proliferator-activated receptor gamma
LXR-alpha
Histone acetyltransferase GCN5
Cytochrome P450 3A4
Vitamin D receptor
Plasmodium falciparum
Ubiquitin carboxyl-terminal hydrolase 1
Peripheral myelin protein 22
78 kDa glucose-regulated protein
Luciferin 4-monooxygenase

Tetrabenazine

Molecular Mechanism (initial) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Predicted Targets

Sodium channel alpha subunits; brain (Types I, II, III)

Synaptic vesicular amine transporter

FK506 binding protein 12
DNA polymerase beta
ATPase family AAA domain-containing protein 5
Lysine-specific demethylase 4A
Vitamin D receptor
Flap endonuclease 1
DNA polymerase iota
Peripheral myelin protein 22
Glutaminase kidney isoform, mitochondrial
Glucagon-like peptide 1 receptor
Endoplasmic reticulum-associated amyloid beta-peptide-binding protein
Lysine-specific demethylase 4D-like
Thyroid stimulating hormone receptor
Microtubule-associated protein tau
Aldehyde dehydrogenase 1A1
MAP kinase ERK2
15-hydroxyprostaglandin dehydrogenase [NAD+]
Arachidonate 15-lipoxygenase, type II

Thalidomide

Molecular Mechanism (initial) :

TNF-alpha production inhibitor

Molecular Mechanism (repurposed) :

cereblon (CRBN) inhibitor

Predicted Targets

Phosphodiesterase 4

Beta-lactamase AmpC

Chymotrypsin C

Malate dehydrogenase cytoplasmic

Cyclooxygenase-1

Cyclooxygenase-2

TNF-alpha

Progesterone receptor

Anandamide amidohydrolase

Aldehyde dehydrogenase 1A1

Phospholipidosis

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Thyroid hormone receptor beta-1

Acetylcholinesterase

Adenosine A1 receptor

Adenosine A2a receptor

Adenosine A3 receptor

Alpha-1d adrenergic receptor

Alpha-1b adrenergic receptor

Alpha-2a adrenergic receptor

Alpha-2b adrenergic receptor

Alpha-2c adrenergic receptor

Beta-1 adrenergic receptor

Beta-2 adrenergic receptor

Beta-3 adrenergic receptor

Norepinephrine transporter

Aldose reductase

Angiotensin II type 2 (AT-2) receptor

Bradykinin B2 receptor

Calcitonin receptor

Cannabinoid CB1 receptor

Carbonic anhydrase II

C-C chemokine receptor type 2

C-C chemokine receptor type 4

C-C chemokine receptor type 5

Interleukin-8 receptor A

Interleukin-8 receptor B

Confidence Score:NAN

Cholecystokinin A receptor

Cytochrome P450 1A2

Cytochrome P450 2A6

Cytochrome P450 2C19

Cytochrome P450 2C9

Cytochrome P450 2D6

Cytochrome P450 2E1
Cytochrome P450 3A4
Dopamine D1 receptor
Dopamine D2 receptor
Dopamine D3 receptor
Dopamine D4 receptor
Dopamine transporter
Endothelin receptor ET-A
Estrogen receptor alpha
Estrogen receptor beta
Glucocorticoid receptor
Histamine H1 receptor
Histamine H2 receptor
HMG-CoA reductase
Insulin receptor
Leukotriene C4 synthase
Cysteinyl leukotriene receptor 1
Arachidonate 15-lipoxygenase
Melanocortin receptor 3
Melanocortin receptor 4
Melanocortin receptor 5
Monoamine oxidase A
Muscarinic acetylcholine receptor M1
Muscarinic acetylcholine receptor M2
Muscarinic acetylcholine receptor M3
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Neuropeptide Y receptor type 1
Neuropeptide Y receptor type 2
Nitric-oxide synthase, brain
Nitric oxide synthase, inducible
Delta opioid receptor
Kappa opioid receptor
Mu opioid receptor
Phosphodiesterase 5A
Platelet activating factor receptor
HERG
Angiotensin-converting enzyme
Caspase-1
Cathepsin G
Leukocyte elastase
Matrix metalloproteinase-1
Matrix metalloproteinase 9
Protein kinase C alpha
MAP kinase ERK1
MAP kinase ERK2
MAP kinase p38 alpha
Serine/threonine protein phosphatase 2B catalytic subunit, alpha isoform
Epidermal growth factor receptor erbB1
Tyrosine-protein kinase FYN

Receptor protein-tyrosine kinase erbB-2
 Tyrosine-protein kinase LCK
 Leukocyte common antigen
 Serotonin 1a (5-HT1a) receptor
 Serotonin 1b (5-HT1b) receptor
 Serotonin 2a (5-HT2a) receptor
 Serotonin 2b (5-HT2b) receptor
 Serotonin 2c (5-HT2c) receptor
 Serotonin 4 (5-HT4) receptor
 Serotonin 6 (5-HT6) receptor
 Serotonin transporter
 Sigma opioid receptor
 Neurokinin 1 receptor
 Neurokinin 2 receptor
 Androgen Receptor
 Thromboxane-A synthase
 Vascular endothelial growth factor receptor 1
 Vasoactive intestinal polypeptide receptor 1
 Vasopressin V1a receptor
 Geminin
 Solute carrier organic anion transporter family member 1B1
 Solute carrier organic anion transporter family member 1B3
 Nuclear factor NF-kappa-B complex
 Thyroid stimulating hormone receptor
 Tyrosyl-DNA phosphodiesterase 1

Topiramate

Molecular Mechanism (initial) :

kainate receptor antagonist
 AMPA receptor antagonists
 carbonic anhydrase type II inhibitor
 sodium channel blocker

Molecular Mechanism (repurposed) :

ckainate receptor antagonist
 AMPA receptor antagonists
 carbonic anhydrase type II inhibitor
 sodium channel blocker

Predicted Targets

Carbonic anhydrase I

Carbonic anhydrase II

Carbonic anhydrase IV

Carbonic anhydrase IX

Carbonic anhydrase XII

Carbonic anhydrase XIV

Carbonic anhydrase VII

Carbonic anhydrase XIII

Carbonic anhydrase

Carbonic anhydrase V

Carbonic anhydrase VA

Carbonic anhydrase VB
Carbonic anhydrase 1
Carbonic anhydrase VI
Carbonic anhydrase III
Carbonic anhydrase-related protein 2
Carbonic anhydrase 15
Uncharacterized protein Rv1284/MT1322
Aquaporin-4
Alpha carbonic anhydrase

Sodium channel protein type II alpha subunit

PROBABLE TRANSMEMBRANE CARBONIC ANHYDRASE (CARBONATE DEHYDRATASE) (CARBO
Carbonic anhydrase 2
Astrosclerin-3
Solute carrier organic anion transporter family member 1B1
Solute carrier organic anion transporter family member 1B3
Delta carbonic anhydrase

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

Predicted Targets

Histone-lysine N-methyltransferase, H3 lysine-9 specific 3
Ubiquitin carboxyl-terminal hydrolase 1
Peripheral myelin protein 22
P-glycoprotein 1
Geminin
Serotonin 6 (5-HT6) receptor

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

Predicted Targets

Histone deacetylase
Erythroleukemia cell line

Histone deacetylase 1

Histone deacetylase HD2
Histone deacetylase (HDAC1 and HDAC2)

Histone deacetylase 2

Histone deacetylase 6

Histone deacetylase 8
Histone deacetylase 4
Histone deacetylase HD1B
Cytochrome P450 2D6
Cytochrome P450 3A4

Cytochrome P450 1A2
Cytochrome P450 2C9
Cytochrome P450 2C19

Histone deacetylase 3

Inosine-5'-monophosphate dehydrogenase 2
Inosine-5'-monophosphate dehydrogenase 1
Histone deacetylase 5
Histone deacetylase 7
Histone deacetylase 9
Histone deacetylase 3/Nuclear receptor corepressor 2 (HDAC3/NCoR2)
Tyrosine-protein kinase ABL
Histone deacetylase 10
Histone deacetylase-like amidohydrolase
Serine racemase
Histone deacetylase 11
Vitamin D receptor
Cystic fibrosis transmembrane conductance regulator
Serine/threonine-protein kinase AKT
Lysine-specific demethylase 4D-like
Matrix metalloproteinase-2
DNA polymerase iota
Nuclear receptor subfamily 0 group B member 1
Mothers against decapentaplegic homolog 3
Peripheral myelin protein 22
DNA dC->dU-editing enzyme APOBEC-3F
Epidermal growth factor receptor erbB1
Geminin
Zinc finger protein GLI1
Nuclear factor erythroid 2-related factor 2
NAD-dependent protein deacylase sirtuin-5, mitochondrial
HMG-CoA reductase
Histone deacetylase 1/3/5/8
Histone deacetylase 3/NCoR1
Serotransferrin
Angiotensin-converting enzyme
Carbonic anhydrase II
Matrix metalloproteinase 12
DNA topoisomerase II alpha
Human immunodeficiency virus 1
Bromodomain-containing protein 4
Aminopeptidase N

Supplement 6

Biological activity profile predicted with SuperPred

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

initial indication(s):

anesthesia

Repurposed indication(s):

acute pain treatment

Predicted Targets

Opioid receptors; mu & delta E-value: 2.915E-1

Sigma opioid receptor E-value: 4.859E 0

Kappa opioid receptor E-value: 2.229E 0

Opioid receptors; delta & kappa E-value: 6.807E 0

P-glycoprotein E-value: 1.014E 2

Predicted ATC-classes

Opioid Anesthetics (N01AH)

Alprostadil

Molecular Mechanism (initial) :

prostaglandin E2 receptor agonist

Molecular Mechanism (repurposed) :

prostaglandin E2 receptor agonist

initial indication(s):

hypotension and peripheral obstructive vascular disease

Repurposed indication(s):

erectile dysfunction

Predicted Targets

Prostanoid IP receptor

Prostanoid EP2 receptor

Prostanoid EP1 receptor

Prostanoid EP4 receptor

Predicted ATC-classes

Prostaglandins (C01EA)

Prostaglandine (C04AG)

Drugs Used In Erectile Dysfunction (G04BE)

Amantadine hydrochloride

Molecular Mechanism (initial) :

matrix protein 2 (Influenza virus A) inhibitor

Molecular Mechanism (repurposed) :

dopamine receptor agonists

NMDA receptor antagonists

initial indication(s):

Influenza A virus infection

Repurposed indication(s):

Parkinson's disease

Predicted Targets

Sigma opioid receptor

Predicted ATC-classes

Cyclic Amines (J05AC)

Adamantane Derivatives (N04BB)

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

initial indication(s):

depression

Repurposed indication(s):

fibromyalgia

peripheral neuropathy

Predicted Targets

Cytochrome P450 2D2

Histamine H1 receptor

Histamine H2 receptor

Sodium channel protein type II alpha subunit

Muscarinic acetylcholine receptor M4

Adrenergic receptor alpha-1

Alpha-2b adrenergic receptor

Muscarinic acetylcholine receptor M5

Cytochrome P450 2D6

Alpha-2a adrenergic receptor

Muscarinic acetylcholine receptors; M1 & M2

Muscarinic acetylcholine receptor

Dopamine D1 receptor

Dopamine D5 receptor

Alpha-2c adrenergic receptor

Serotonin 2b (5-HT_{2b}) receptor

Muscarinic acetylcholine receptor M2

Serotonin 4 (5-HT₄) receptor

Alpha adrenergic receptor (1a and 1d)

Serotonin 6 (5-HT₆) receptor

Predicted ATC-classes

Non-selective Monoamine Reuptake Inhibitors (N06AA)

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

initial indication(s):

Parkinson's disease

Repurposed indication(s):
erectile dysfunction

Predicted Targets

Dopamine D1 receptor

Dopamine receptors; D2 & D3

Runt-related transcription factor 1/Core-binding factor subunit beta

Serotonin 1a (5-HT1a) receptor

Serotonin (5-HT3) receptor

Apoptosis regulator Bcl-W

Induced myeloid leukemia cell differentiation protein Mcl-1

Dopamine receptors; D3 & D4

DNA repair protein RAD52 homolog

Serotonin transporter

Serotonin 2a (5-HT2a) receptor

Cytochrome P450 1A2

Alpha-2a adrenergic receptor

Alpha adrenergic receptor (1a and 1d)

Cytochrome P450 2C19

Cytochrome P450 3A4

Predicted ATC-classes

Drugs Used In Erectile Dysfunction (G04BE)

Dopamine Agonists (N04BC)

Antidotes (V03AB)

Acetylsalicylic acid

Molecular Mechanism (initial) :

cyclooxygenase inhibitor

Molecular Mechanism (repurposed) :

cyclooxygenase inhibitor

initial indication(s):

inflammation

pain

Repurposed indication(s):

thrombosis

Predicted Targets

Ras-related C3 botulinum toxin substrate 1

Beta amyloid A4 protein

Carbonic anhydrase 15

Cyclooxygenase

Aldo-keto reductase family 1 member C2

Aldo-keto-reductase family 1 member C3

Integrin alpha-V/beta-3 and alpha-IIb/beta 3

Cyclooxygenase-2

Integrin alpha-V/beta-3

Carbonic anhydrase XII

Leukocyte elastase

Cytochrome P450 2C19

Estrogen receptor beta
Carbonic anhydrase I

Predicted ATC-classes

Other Agents For Local Oral Treatment (A01AD)

Platelet Aggregation Inhibitors Excl. Heparin (B01AC) (thrombosis)

Salicylic Acid And Derivatives (N02BA)

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

initial indication(s):

spasticity

Repurposed indication(s):

alcoholism

Predicted Target

GABA-B receptor 1

Predicted ATC-classes

Other Centrally Acting Agents (M03BX)

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

initial indication(s):

hypertension

Repurposed indication(s):

ventricular fibrillation suppression

Predicted Targets

Carbonic anhydrase XII

Carbonic anhydrases; II & IX

Carbonic anhydrase I

Carbonic anhydrase II

Predicted ATC-classes

Guanidine Derivatives (C02CC)

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

initial indication(s):

pulmonary hypertension

Repurposed indication(s):
digital ulcers in systemic sclerosis

Predicted Targets

Endothelin receptor, ET-A/ET-B

Endothelin receptor ET-B

Bile salt export pump

Predicted ATC-classes

Other Antihypertensives (C02KX)

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :

mu-type opioid receptor agonist

initial indication(s):

pain

Repurposed indication(s):

opioid dependency

Predicted Targets

Kappa opioid receptor

Opioid receptors; mu & delta

Opioid receptors; delta & kappa

Nociceptin receptor

Sigma opioid receptor

Cytochrome P450 2D6

Predicted ATC-classes

Oripavine Derivatives (N02AE)

Drugs Used In Opioid Dependence (N07BC)

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

initial indication(s):

arthritis

osteoarthritis

polyposis coli

rheumatoid arthritis

Repurposed indication(s):

pain

dysmenorrhea

ankylosing spondylitis

Predicted Targets

Cyclooxygenase-2

Cyclooxygenase
Carbonic anhydrase 15
Carbonic anhydrase VB
Progesterone receptor
Carbonic anhydrase V
Carbonic anhydrase
Carbonic anhydrase VI
Carbonic anhydrases; II & IX
Carbonic anhydrase II
Carbonic anhydrase VII
Carbonic anhydrase XIII
Carbonic anhydrase I
Carbonic anhydrase XIV
Carbonic anhydrase XII
Carbonic anhydrase IV
Alpha-2b adrenergic receptor
Cell division control protein 42 homolog
Epoxide hydratase
Cytochrome P450 2D6

Predicted ATC-classes

Coxibs (M01AH)

Other Antineoplastic Agents (L01XX)

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

initial indication(s):

malaria

Repurposed indication(s):

glioma

glioblastoma multiforme

Predicted Targets

Prion protein
Aldehyde oxidase
C-C chemokine receptor type 4
Sodium channel alpha subunits; brain (Types I, II, III)
Galanin receptor 3
Quinone reductase 2
Histamine N-methyltransferase
Cytochrome P450 2C8
Cytochrome P450 2D6
HERG
Histamine H2 receptor
Muscarinic acetylcholine receptor M4
Alpha-2b adrenergic receptor
Muscarinic acetylcholine receptor M5

C-C chemokine receptor type 3
Alpha-2a adrenergic receptor
Cytochrome P450 1A2
Alpha-2c adrenergic receptor
Cytochrome P450 3A4
Muscarinic acetylcholine receptor M2

Predicted ATC-classes

Aminoquinolines (P01BA)

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

initial indication(s):

antipsychotic

Repurposed indication(s):

colorectal cancer

Predicted Targets

Histamine H1 receptor
Calmodulin
Aldehyde oxidase
Prion protein
Sodium channel alpha subunits; brain (Types I, II, III)
Solute carrier family 22 member 2
Cytochrome P450 2D6
Solute carrier family 22 member 1
Dopamine D1 receptor
Adrenergic receptor alpha-1

Dopamine receptors; D2 & D3

Serotonin 2b (5-HT2b) receptor
Alpha-2b adrenergic receptor
Adenylate cyclase type 8
Muscarinic acetylcholine receptor M4
Muscarinic acetylcholine receptor M5
Cytochrome P450 1A2
Histamine H2 receptor
Alpha-2c adrenergic receptor
3-beta-hydroxysteroid-delta(8),delta(7)-isomerase
Serotonin 2 (5-HT2) receptor
Muscarinic acetylcholine receptor
Serotonin and norepinephrine transporters (SERT/NET)
Alpha-2a adrenergic receptor
Serotonin 6 (5-HT6) receptor
Cytochrome P450 2C19
Alpha-synuclein
Serotonin 2a (5-HT2a) receptor

Adrenergic receptors; alpha-1 A & B
Muscarinic acetylcholine receptors; M1 & M2
Dopamine D5 receptor
HERG
Sigma opioid receptor
Serotonin 1a (5-HT1a) receptor
Muscarinic acetylcholine receptor M2
Serotonin transporter
Tyrosine-protein kinase FYN
Dopamine receptors; D3 & D4

Predicted ATC-classes

Phenothiazines With Aliphatic Side-chain (N05AA)

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :

TNF- α /NF- κ b signaling pathway inhibitor

initial indication(s):

heart failure

arrhythmia

Repurposed indication(s):

cystic fibrosis

Predicted Targets

Potassium-transporting ATPase alpha chain 2

Sodium/potassium-transporting ATPase

Paired box protein Pax-8

Predicted ATC-classes

Digitalis Glycosides (C01AA)(C05BZ)

Doxepin hydrochloride

Molecular Mechanism (initial) :

5HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

H1 and H2 histamine receptor blocker

initial indication(s):

depression

Repurposed indication(s):

pruritis

insomnia

Predicted Targets

Histamine H1 receptor

Histamine H2 receptor

Muscarinic acetylcholine receptor M4

Adrenergic receptor alpha-1

Sodium channel protein type II alpha subunit
Alpha-2b adrenergic receptor
Muscarinic acetylcholine receptor M5
Cytochrome P450 2D6
Alpha-2a adrenergic receptor
Muscarinic acetylcholine receptors; M1 & M2
Muscarinic acetylcholine receptor
Serotonin 6 (5-HT6) receptor
Dopamine D1 receptor
Alpha-2c adrenergic receptor
Serotonin 2b (5-HT2b) receptor
Dopamine D5 receptor
Serotonin 4 (5-HT4) receptor
Muscarinic acetylcholine receptor M2
Serotonin 2 (5-HT2) receptor
Sigma opioid receptor

Predicted ATC-classes

Non-selective Monoamine Reuptake Inhibitors (N06AA)

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

initial indication(s):

depression

Repurposed indication(s):

urinary incontinence

generalized anxiety disorder

neuropathic pain

Predicted Targets

Transporter

Serotonin and norepinephrine transporters (SERT/NET)

Serotonin transporter

Cytochrome P450 2D6

Monoamine transporters; serotonin & dopamine

Histamine H3 receptor

Serotonin 1a (5-HT1a) receptor

Cytochrome P450 3A4

Monoamine transporters; Norepinephrine & dopamine

Nociceptin receptor

HERG

Predicted ATC-classes

Other Antidepressants (N06AX)

Eflornithine hydrochloride

Molecular Mechanism (initial) :

ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

initial indication(s):

African trypanosomiasis (sleeping sickness)

Repurposed indication(s):

hair growth abnormality

cancer

Predicted Targets

Not results

Predicted ATC-classes

Other Agents Against Leishmaniasis And Trypanosomiasis (P01CX)

Other Dermatologicals (D11AX)

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

initial indication(s):

non-small cell lung cancer

Repurposed indication(s):

pancreatic and pancreatic metastatic cancer

ependymoma

mouth cancer

head and neck cancer

Predicted Targets

Not results

Predicted ATC-classes

Not results

Everolimus

Molecular Mechanism (initial) :

FK506-binding protein 12 inhibitor

mTOR inhibitor

Molecular Mechanism (repurposed) :

FK506-binding protein 12 inhibitor

mTOR inhibitor

initial indication(s):

transplant rejection

Repurposed indication(s):

cancers

Predicted Targets

Not results

Predicted ATC-classes

Not results

Finasteride

Molecular Mechanism (initial) :

steroid 5alpha reductase inhibitor
androgen receptor antagonist

Molecular Mechanism (repurposed) :

steroid 5alpha reductase inhibitor
androgen receptor antagonist

initial indication(s):

benign prostatic hyperplasia

Repurposed indication(s):

hair loss

Predicted Targets

Steroid 5-alpha-reductase 2

Steroid 5-alpha-reductase 1

Cytochrome P450 2C19

Cytochrome P450 2C9

Predicted ATC-classes

Other Dermatologicals (D11AX)

Testosterone-5-alpha Reductase Inhibitors (G04CB)

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

initial indication(s):

polio

paralysis

anesthesia

Repurposed indication(s):

Alzheimer's type dementia

Predicted Targets

Cholinesterases; ACHE & BCHE

Butyrylcholinesterase

Glutamate [NMDA] receptor subunit epsilon 2

Butyrylcholinesterase

Cytochrome P450 2C19

Cytochrome P450 2C9

Predicted ATC-classes

Anticholinesterases (N06DA)

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

initial indication(s):

antiviral

Repurposed indication(s):

cancers (NSCLC, pancreas, breast, biliary, ovary, bladder, breast, lymphoma)

Predicted Targets

Not results

Predicted ATC-classes

Not results

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

initial indication(s):

hypertension

Repurposed indication(s):

attention-deficit/hyperactivity disorder

Predicted Targets

Alpha-2b adrenergic receptor

Alpha-2a adrenergic receptor

Serotonin 2b (5-HT2b) receptor

Adrenergic receptor alpha-1

Cytochrome P450 2D6

Cytochrome P450 2C19

Serotonin 2 (5-HT2) receptor

Serotonin 2a (5-HT2a) receptor

Aldose reductase

Beta-secretase 1

Predicted ATC-classes

Imidazoline Receptor Agonists (C02AC)

Ibuprofen

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

initial indication(s):

inflammation

Repurposed indication(s):
patent ductus arteriosus

Predicted Targets

Cyclooxygenase-2

Cyclooxygenase

Interleukin-8
Arachidonate 5-lipoxygenase
Interleukin-8 receptors, CXCR1/CXCR2
Protein Wnt-3a
DNA damage-inducible transcript 3 protein
X-box-binding protein 1
Anandamide amidohydrolase
Serotonin 2a (5-HT2a) receptor
Cytochrome P450 2C9

Predicted ATC-classes

Other Cardiac Preparations (C01EB)

Antiinflammatory Products For Vaginal Administration (G02CC)

Propionic Acid Derivatives (M01AE)

Antiinflammatory Preparations, Non-steroids For Topical Use (M02AA)

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

stem cell factor (SCF)

proto-oncogene c-Kit inhibitor

initial indication(s):

chronic myelogenous leukemia

Repurposed indication(s):

gastrointestinal stromal tumor

fibrosarcoma

hypereosinophilic syndrome

acute lymphocytic leukemia

myeloproliferative diseases and systemic mastocytosis

Predicted Targets

Not results

Predicted ATC-classes

Not results

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of M. tuberculosis

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

initial indication(s):

tuberculosis

Repurposed indication(s):

depression

Predicted Targets

Monoamine oxidase A

Monoamine oxidase B

Cytochrome P450 3A4

Predicted ATC-classes

Monoamine Oxidase Inhibitors, Non-selective (N06AF)

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14-alpha demethylase

Molecular Mechanism (repurposed) :

smoothened homolog inhibitor

lanosterol 14-alpha demethylase inhibitor

initial indication(s):

antifungal agent

Repurposed indication(s):

non-small cell lung cancer

Predicted Targets

Cytochrome P450 51 (lanosterol 14-alpha demethylase)

Heme oxygenase 2

Glycosyltransferase-like protein LARGE1

P-glycoprotein 1 and 3 (MDR1a/MDR1b)

P-glycoprotein 3

Heat shock protein HSP90

Heme oxygenase 1

Interleukin-8 receptors, CXCR1/CXCR2

C-C chemokine receptor type 4

Muscarinic acetylcholine receptor M4

Tyrosine-protein kinase FYN

Arachidonate 15-lipoxygenase

Adrenergic receptor alpha-1

P-glycoprotein 1

Alpha-2b adrenergic receptor

Cytochrome P450 3A4

Muscarinic acetylcholine receptor M5

Alpha-2a adrenergic receptor

Vasopressin V2 receptor

Alpha-2c adrenergic receptor

Predicted ATC-classes

Triazole Derivatives (J02AC)

Ketoconazole

Molecular Mechanism (initial) :

fungal cytochrome P450 51 inhibitor

Molecular Mechanism (repurposed) :

cytochrome P450 aromatase (CYP19A1) inhibitor

initial indication(s):

antifungal agent

Repurposed indication(s):

seborrheic dermatitis

Cushing syndrome

Predicted Targets

Cytochrome P450 11A1

Cytochrome P450 51

Heme oxygenase 2

Glycosyltransferase-like protein LARGE1

Cytochrome P450 17A1

P-glycoprotein 1 and 3 (MDR1a/MDR1b)

P-glycoprotein 3

Heme oxygenase 1

Cytochrome P450 11B1

Heat shock protein HSP90

Cytochrome P450 3A4

Muscarinic acetylcholine receptor M4

Arachidonate 15-lipoxygenase

Adrenergic receptor alpha-1

Cytochrome P450 19A1

Interleukin-8 receptors, CXCR1/CXCR2

Alpha-2b adrenergic receptor

Muscarinic acetylcholine receptor M5

C-C chemokine receptor type 4

Alpha-2a adrenergic receptor

Predicted ATC-classes

Imidazole And Triazole Derivatives (D01AC)

Imidazole Derivatives (G01AF)

Imidazole Derivatives (J02AB)

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

initial indication(s):

local anesthesia

Repurposed indication(s):

eye disorders

arrhythmia

pain

Predicted Targets

Microphthalmia-associated transcription factor
Perilipin-5
Cytochrome P450 2D6
Cytochrome P450 2C19
Cytochrome P450 2C9

Predicted ATC-classes

Local Anaesthetics For Local Oral Treatment (A01AE)
Products Containing Local Anesthetics (C05AD)
Anesthetics For Topical Use (D04AB)

Amides (N01BB)

Anesthetics, Local (R02AD)
Local Anesthetics (S01HA)
Analgesics And Anesthetics (S02DA)
Antiarrhythmics, Class Ib (C01BB)

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

initial indication(s):

antiviral

Repurposed indication(s):

spasticity

Alzheimer's type dementia

Predicted Targets

Glutamate NMDA receptor; GRIN1/GRIN2A
Glutamate (NMDA) receptor subunit zeta 1
Glutamate [NMDA] receptor subunit epsilon 2
Glutamate [NMDA] receptor subunit epsilon 3

Cytochrome P450 2D6

Predicted ATC-classes

Other Anti-dementia Drugs (N06DX)

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

initial indication(s):

diabetic

Repurposed indication(s):

non-alcoholic steatohepatitis

breast cancer

prostate cancer

Predicted Targets

Not results

Predicted ATC-classes

Biguanides (A10BA)

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :

dihydrofolate reductase inhibitor

initial indication(s):

cancers (breast, metastatic head and neck cancer, leukemia)

rheumatoid arthritis

Repurposed indication(s):

**cancers (gestational choriocarcinoma, chorioadenoma destruens,
cutaneous T cell lymphoma, lung cancer, non-Hodgkin's lymphomas)**

polyarticular juvenile arthritis

psoriasis

Predicted Targets

Dihydrofolate reductase

Thymidylate synthase

Folypoly-gamma-glutamate synthetase

Nuclear receptor coactivator 3

Glutamate carboxypeptidase II

Predicted ATC-classes

Folic Acid Analogues (L01BA)

Milnacipran

Molecular Mechanism (initial) :

5-HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

5-HT and norepinephrine reuptake inhibitor

initial indication(s):

depression

Repurposed indication(s):

fibromyalgia

Predicted Targets

Glutamate [NMDA] receptor subunit 3A

Serotonin and norepinephrine transporters (SERT/NET)

Serotonin transporter

Glutamate [NMDA] receptor subunit epsilon 3

Monoamine transporters; serotonin & dopamine

Monoamine transporters; Norepinephrine & dopamine

Predicted ATC-classes

Other Antidepressants (N06AX)

Miltefosine

Molecular Mechanism (initial) :

Akt/PKB inhibitor

Molecular Mechanism (repurposed) :

phosphatidyl-choline biosynthesis inhibitor

initial indication(s):

cancer

Repurposed indication(s):

leishmaniasis

Predicted Targets

Serine/threonine-protein kinase AKT

Lysophosphatidic acid receptor Edg-7

Lysophosphatidic acid receptor Edg-4

Lysophosphatidic acid receptor Edg-2

Phospholipase A2 group 1B

Platelet activating factor receptor

Predicted ATC-classes

Other Antineoplastic Agents (L01XX)

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

initial indication(s):

antibacterial

acne treatment

Repurposed indication(s):

amyotrophic lateral sclerosis

Huntington's disease

Predicted Targets

Induced myeloid leukemia cell differentiation protein Mcl-1

Predicted ATC-classes

Tetracyclines (J01AA)

Antiinfectives And Antiseptics For Local Oral Treatment (A01AB)

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

initial indication(s):

HIV (Human immuno-deficiency virus) infection

Repurposed indication(s):

cancers (liposarcoma, glioblastoma multiforme, advanced hematologic cancer, refractory or recurrent solid tumors)

Predicted Targets

Not results

Predicted ATC-classes

Protease Inhibitors (J05AE)

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

proto-oncogene c-Kit inhibitor

initial indication(s):

chronic myeloid leukemia

Repurposed indication(s):

glioma

melanoma

Predicted Targets

Not results

Predicted ATC-classes

Not results

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

initial indication(s):

hereditary tyrosinemia type I

Repurposed indication(s):

alkaptonuria

Predicted Targets

4-hydroxyphenylpyruvate dioxygenase

Predicted ATC-classes

Various Alimentary Tract And Metabolism Products (A16AX)

Paclitaxel

Molecular Mechanism (initial) :

tubulin beta modulator (microtubule-stabilizing agent)

Molecular Mechanism (repurposed) :

tubulin beta modulator (microtubule-stabilizing agent)

initial indication(s):

cancers (breast, ovary, lung non-small cell, AIDS-related Kaposi's sarcoma, stomach, endometrium, angiosarcoma, cervix, head and neck, esophageal carcinoma, germ cells)

Repurposed indication(s):

restenosis

Predicted Targets

Tubulin

Tubulin beta-2B chain

Neurokinin 2 receptor

Integrin alpha-V/beta-3

Cholecystokinin A receptor

Cytochrome P450 3A4

Opioid receptors; delta & kappa

Predicted ATC-classes

Taxanes (L01CD)

Phentolamine mesilate

Molecular Mechanism (initial) :

alpha-adrenoceptor antagonist

Molecular Mechanism (repurposed) :

alpha-adrenoceptor antagonist

initial indication(s):

erectile dysfunction

Repurposed indication(s):

reversal of soft-tissue (dental) anesthesia

Predicted Targets

Serotonin 1e (5-HT1e) receptor

Alpha-2b adrenergic receptor

Cytochrome P450 2D6

Alpha-2c adrenergic receptor

Alpha adrenergic receptor (1a and 1d)

Adrenergic receptor alpha-1

Serotonin 1b (5-HT1b) receptor

Adrenergic receptors; alpha-1 A & B

Predicted ATC-classes

Imidazoline Derivatives (C04AB)

Drugs Used In Erectile Dysfunction (G04BE)

Antidotes (V03AB)

Raloxifene hydrochloride

Molecular Mechanism (initial) :

estrogen receptor agonist

Molecular Mechanism (repurposed) :

estrogen receptor agonist

initial indication(s):

erectile dysfunction

Repurposed indication(s):
reversal of soft-tissue (dental) anesthesia

Predicted Targets

Aldehyde oxidase

Estrogen receptor alpha

Estrogen receptor beta

3-beta-hydroxysteroid-delta(8),delta(7)-isomerase

Adrenergic receptor alpha-1

Alpha-2b adrenergic receptor

Tyrosine-protein kinase FYN

Alpha-2a adrenergic receptor

Phospholipase D2

Phospholipase D1

Alpha-2c adrenergic receptor

Serotonin 2b (5-HT2b) receptor

Perilipin-1

Serotonin 6 (5-HT6) receptor

Neurokinin 2 receptor

Cytochrome P450 2D6

Cytochrome P450 2C19

Serotonin 2 (5-HT2) receptor

Serotonin 1b (5-HT1b) receptor

Sigma opioid receptor

Predicted ATC-classes

Selective Estrogen Receptor Modulators (G03XC)

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :

dopamine D2 and D3 receptor agonist

initial indication(s):

Parkinson's disease

Repurposed indication(s):

restless legs syndrome

Predicted Targets

Dopamine receptors; D2 & D3

Dopamine D1 receptor

Dopamine receptors; D2 & D4

Dopamine receptors; D3 & D4

Cytochrome P450 2D6

Serotonin 1a (5-HT1a) receptor

Predicted ATC-classes

Dopamine Agonists (N04BC)

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :

phospho-diesterase (PDE5A) inhibitor

initial indication(s):

erectile dysfunction

Repurposed indication(s):

hypertension

pulmonary arterial

Predicted Targets

Phosphodiesterase 6C

Phosphodiesterase 5A

Retinal cone rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit gamma

Phosphodiesterase 3B

Phosphodiesterase 1A

Indoleamine 2,3-dioxygenase 2

Phosphodiesterase 1

Phosphodiesterase 6A

Phosphodiesterase 1B

Phosphodiesterase 3

Phosphodiesterase 3 and 5 (PDE3 and PDE5)

Phosphodiesterase 6

Phosphodiesterase 11A

Phosphodiesterase 4

Phosphodiesterase 9A

Phosphodiesterase 4B

Phosphodiesterase 4A

Phosphodiesterase 7

Phosphodiesterase 10A

Perilipin-5

Predicted ATC-classes

Hmg Coa Reductase Inhibitors (C10AA)

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

initial indication(s):

anti-cholesterol

Repurposed indication(s):

colorectal cancer

Predicted Targets

Solute carrier organic anion transporter family member 1B1

Photoreceptor-specific nuclear receptor

HMG-CoA reductase

P-glycoprotein 1

Predicted ATC-classes

Hmg Coa Reductase Inhibitors (C10AA)

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

initial indication(s):

T-cell lymphoma

Repurposed indication(s):

Alzheimer's type dementia

Predicted Targets

Retinoid X receptor beta

Retinoid X receptor gamma

Retinoid X receptor alpha

Retinoic acid receptor gamma

Retinoic acid receptor beta

Retinoic acid receptor alpha

Beta-lactoglobulin

Retinoic acid receptor gamma

Retinoic acid receptor alpha

Peroxisome proliferator-activated receptor gamma/Nuclear receptor coactivator 1

Cytochrome P450 2D6

Cytochrome P450 2C19

Peroxisome proliferator-activated receptor alpha

Predicted ATC-classes

Not results

Tetrabenazine

Molecular Mechanism (initial) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

initial indication(s):

Huntington's disease

Repurposed indication(s):

extrapyramidal disorders

tardive dyskinesia

Predicted Targets

Synaptic vesicular amine transporter

Dipeptidyl peptidase II and dipeptidyl peptidase IV (DPP2 and DPP4)

Dopamine D1 receptor

DNA repair protein RAD52 homolog
Serotonin 1a (5-HT1a) receptor

Predicted ATC-classes

Neuroleptics, In Tardive Dyskinesia (N05AK)

Other Nervous System Drugs (N07XX)

Thalidomide

Molecular Mechanism (initial) :

TNF-alpha production inhibitor

Molecular Mechanism (repurposed) :

cereblon (CRBN) inhibitor

initial indication(s):

sedative

nausea preventing

Repurposed indication(s):

leprosy

multiple myeloma

Predicted Targets

Cyclooxygenase

Cyclooxygenase-2

Predicted ATC-classes

Other Immunosuppressive Agents (L04AX)

Topiramate

Molecular Mechanism (initial) :

kainate receptor antagonist

AMPA receptor antagonists

carbonic anhydrase type II inhibitor

sodium channel blocker

Molecular Mechanism (repurposed) :

ckainate receptor antagonist

AMPA receptor antagonists

carbonic anhydrase type II inhibitor

sodium channel blocker

initial indication(s):

epilepsy

Repurposed indication(s):

migraine

alcoholism

Predicted Targets

Not results

Predicted ATC-classes

Not results

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

initial indication(s):

breast cancer

Repurposed indication(s):

osteoporosis

Predicted Targets

3-beta-hydroxysteroid-delta(8),delta(7)-isomerase

Phosphodiesterase 1A

Phosphodiesterase 1

ATP-binding cassette sub-family G member 2

Estrogen receptor alpha

Estrogen receptor beta

Hepatocyte nuclear factor 4-alpha

Perilipin-1

Muscarinic acetylcholine receptor M4

Alpha-2b adrenergic receptor

Sigma opioid receptor

Muscarinic acetylcholine receptor M5

Phospholipase D2

Phospholipase D1

Tyrosine-protein kinase FYN

Alpha-2a adrenergic receptor

Leukotriene A4 hydrolase

Cyclooxygenase

Androgen Receptor

Alpha-2c adrenergic receptor

Predicted ATC-classes

Anti-estrogens (L02BA)

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

initial indication(s):

cutaneous T-cell lymphoma

Repurposed indication(s):

multiple myeloma

Predicted Targets

Histone deacetylase 1

Histone deacetylase 2

Histone deacetylase

Histone deacetylase 3

Histone deacetylase 10

Histone deacetylase 6

Histone deacetylase 8

Nuclear receptor subfamily 0 group B member 1

Histone deacetylase 9

Histone deacetylase 4

Histone deacetylase 11

Histone deacetylase 5

Peroxisome proliferator-activated receptor gamma/Nuclear receptor corepressor 2

Matrix metalloproteinase-25

Zinc finger protein GLI1

Epidermal growth factor receptor erbB1

Glutamate receptor ionotropic kainate 3

Acyl coenzyme A:cholesterol acyltransferase 2

Autotaxin

Predicted ATC-classes

Other Antineoplastic Agents (L01XX)

Supplement 7

Biological activity profile predicted PASS Online

Alfentanil hydrochloride

Molecular Mechanism (initial) :

Mu-type opioid receptor inhibitor

Molecular Mechanism (repurposed) :

Mu-type opioid receptor inhibitor

initial indication(s):

anesthesia

Repurposed indication(s):

acute pain treatment

Predicted Activities

Anesthetic general

Analgesic (acute pain treatment)

Anesthetic

CYP3A3 substrate

CYP2B6 substrate

Antipyretic

CYP2B substrate

CYP3A4 substrate

Antiinflammatory

CYP3A substrate

CYP3A5 substrate

Proteasome ATPase inhibitor

Fusarinine-C ornithinesterase inhibitor

H⁺-transporting two-sector ATPase inhibitor

HMG CoA synthase inhibitor

ATP-binding cassette A1 stimulant

Raynaud's phenomenon treatment

CYP2C19 inducer

Spasmolytic, urinary
Sigma receptor antagonist
GHS receptor agonist
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Antieczematic atopic
Nociceptin (N/OFQ) receptor antagonist
Protein kinase B beta inhibitor
Prokinetic
Ceramide glucosyltransferase inhibitor
Anesthetic local

Alprostadi

Molecular Mechanism (initial) :

prostaglandin E2 receptor agonist

Molecular Mechanism (repurposed) :

prostaglandin E2 receptor agonist

initial indication(s):

hypotension and peripheral obstructive vascular disease

Repurposed indication(s):

erectile dysfunction

Predicted Activities

Vasoprotector
Antisecretoric
Prostaglandin-E2 9-reductase inhibitor

Vasodilator, peripheral (hypotension and peripheral obstructive vascular disease)

GST A substrate
Mucomembranous protector
UGT2B1 substrate
Glutathione S-transferase substrate
CYP4A11 substrate

Vasodilator (hypotension and peripheral obstructive vascular disease)

Antithrombotic
Morphine 6-dehydrogenase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
CYP4F substrate
Antiulcerative
CYP2E1 substrate
Cytoprotectant
CYP2E substrate
GST M substrate
Gastrin inhibitor
Mucositis treatment
Oxytocic
CYP4A substrate
Antieczematic
TNF expression inhibitor
CYP2J substrate

Platelet aggregation stimulant
CYP4F12 substrate
Hemostatic
CYP2J2 substrate
Alkylacetylgllycerophosphatase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Acylcarnitine hydrolase inhibitor
UGT2B substrate
GST P substrate
Hepatoprotectant
UDP-glucuronosyltransferase substrate
GST P1-1 substrate
Fibrinolytic
Ophthalmic drug
Diuretic inhibitor
Prostaglandin E1 agonist
Cyclooxygenase substrate
Ubiquinol-cytochrome-c reductase inhibitor
Antipruritic
Antiglaucomic
Prostaglandin antagonist
Antiischemic, cerebral
Platelet adhesion inhibitor
Prostaglandin E1 antagonist
Analeptic
Alkenylglycerophosphocholine hydrolase inhibitor
Immunosuppressant
CYP2C8 substrate
Antiviral (Influenza)
Hypolipemic
Lipid metabolism regulator
CYP3A5 substrate
CYP2B6 substrate
CYP3A2 substrate
Muscle relaxant
CYP2C substrate
Antipruritic, allergic
CYP3A substrate
Spasmolytic
Cyclooxygenase 1 substrate
Gestagen antagonist
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
CYP3A4 substrate
Hepatic disorders treatment
Ecdysone 20-monooxygenase inhibitor
Respiratory analeptic
Menopausal disorders treatment
Platelet aggregation inhibitor

Prostaglandin E2 antagonist

Alcohol dehydrogenase (acceptor) inhibitor
Peroxidase substrate
Prostaglandin agonist
Antifungal
Prostaglandin EP12 antagonist
GABA aminotransferase inhibitor
Lipoprotein lipase inhibitor
Prostaglandin EP4 antagonist
Cyclic AMP agonist
HMOX1 expression enhancer
Gluconate 2-dehydrogenase (acceptor) inhibitor
Antimetastatic
Anticarcinogenic
Alcohol O-acetyltransferase inhibitor
Oxidizing agent
Antiviral (Rhinovirus)
Antihypercholesterolemic
Macrophage colony stimulating factor agonist
Antipsoriatic
Prostaglandin EP1 antagonist
Phosphatase inhibitor
Antianginal
APOA1 expression enhancer
Cholesterol antagonist
CYP2A substrate
Hair growth stimulant
UGT2B4 substrate
Interleukin 2 agonist
Uterine stimulant
CYP2C8 inhibitor
BRAF expression inhibitor
Membrane permeability enhancer
CYP2C9 substrate
TP53 expression enhancer
Adenomatous polyposis treatment
Leukotriene-C4 synthase inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Sphinganine kinase inhibitor
CYP2A6 substrate
D-lactaldehyde dehydrogenase inhibitor
Luteolytic
Benzoate-CoA ligase inhibitor
Calcium regulator
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Apoptosis agonist
Contraceptive female
Leukotriene agonist

UGT1A9 substrate
Thromboxane antagonist
Antiinflammatory, intestinal
Polyporopepsin inhibitor
Thromboxane agonist
UGT2B28 substrate
CYP2B substrate
Glucan endo-1,3-beta-D-glucosidase inhibitor
Plasmanylethanolamine desaturase inhibitor
Dermatologic
Restenosis treatment
Reductant
Sugar-phosphatase inhibitor
Dextranase inhibitor
Lactase inhibitor
Antidiabetic symptomatic
Alkenylglycerophosphoethanolamine hydrolase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
CYP2C11 substrate
Gastric antisecretory
Cholesterol synthesis inhibitor
Prostaglandin EP2 antagonist
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Proteasome ATPase inhibitor
Prostaglandin D2 agonist
Lipoxygenase substrate
GST M1-1 substrate
Oxidoreductase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
UGT2B7 substrate
UGT1A10 substrate
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Prostaglandin F2 alpha agonist
Phosphatidylinositol diacylglycerol-lyase inhibitor
CYP2C6 substrate
Mycothiol-S-conjugate amidase inhibitor
UGT1A8 substrate
2-Acylglycerol O-acyltransferase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Biotinidase inhibitor
Antipruritic, non-allergic
UGT2B17 substrate
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Sclerosant
Protein-disulfide reductase (glutathione) inhibitor
Linoleate diol synthase inhibitor
Erythropoiesis stimulant
Prostacyclin antagonist
Peptidoglycan glycosyltransferase inhibitor
RNA-directed RNA polymerase inhibitor

Membrane permeability inhibitor
CYP4F2 substrate
MMP9 expression inhibitor
Prostaglandin E2 agonist
UGT1A substrate
Antitoxic
Phosphatidylglycerophosphatase inhibitor
CYP4F8 substrate
CYP2E1 inducer
Adenylate cyclase inhibitor
Chitinase inhibitor
Angiogenesis stimulant
UGT1A4 substrate
Apyrase inhibitor
Prostaglandin EP3 antagonist
UGT1A5 substrate
Glucan 1,4-alpha-maltotriohydrolase inhibitor
CYP3A3 substrate
(S)-2-hydroxy-acid oxidase inhibitor
CYP2H substrate
Peptide agonist
Proliferative diseases treatment
Radioprotector
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Cholesterol oxidase inhibitor
Contraceptive
UGT1A7 substrate
Wound healing agent
3-Phytase inhibitor
Cystinyl aminopeptidase inhibitor
Phosphatidate phosphatase inhibitor
Exoribonuclease II inhibitor
Antiviral (Herpes)
Antibacterial
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Licheninase inhibitor
Myosin-light-chain-phosphatase inhibitor
Antiinfective
Cyclomaltodextrinase inhibitor
Signal peptidase I inhibitor
Hydroxylamine reductase (NADH) inhibitor
Glyceryl-ether monooxygenase inhibitor
Bilirubin oxidase inhibitor
CYP7 inhibitor
Cycloartenol synthase inhibitor
Antiinflammatory, ophthalmic
CYP4B substrate
Thromboxane synthase stimulant
Histidine kinase inhibitor

Hematopoietic
Ketol-acid reductoisomerase inhibitor
UGT2B10 substrate
Histamine release stimulant
Beta glucuronidase inhibitor
Prostacyclin agonist
CYP1A substrate
1,2-alpha-L-fucosidase inhibitor
Aspartyltransferase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-
N-acetylglucosaminyltransferase inhibitor
Macrophage stimulant
P-glycoprotein substrate
Alcohol dehydrogenase substrate
Fucosterol-epoxide lyase inhibitor
Phospholipase C inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Aspergillus nuclease S1 inhibitor
Eicosanoid agonist
CYP4B1 substrate
Antiinfertility, female
Myc inhibitor
HIF1A expression inhibitor
Levansucrase inhibitor
Fibrinogen receptor antagonist
Lysine 2,3-aminomutase inhibitor
Prenyl-diphosphatase inhibitor
ATPase inhibitor
Antiinflammatory
Antiprotozoal (Leishmania)
Immunostimulant
Retinyl-palmitate esterase inhibitor
Caspase 3 stimulant
Xylan endo-1,3-beta-xylosidase inhibitor
CYP3A1 substrate
Laxative
Thromboxane A2 antagonist
Butyrate-CoA ligase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Thromboxane B2 antagonist
CYP2C12 substrate
Antimycoplasmal
Photosensitizer
Antiviral (Influenza A)
Retinol dehydrogenase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Dry eye syndrome treatment
Hydroxysteroid dehydrogenase inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
Thiosulfate sulfurtransferase inhibitor

Antihypoxic
Phosphatidate cytidyltransferase inhibitor
Antihelminthic (Nematodes)
Choleretic
Antiviral (CMV)
Glycerone-phosphate O-acyltransferase inhibitor
Propionate-CoA ligase inhibitor
Gaucher disease treatment
Platelet antagonist
Systemic lupus erythematosus treatment
Flavin-containing monooxygenase inhibitor
Carminative
Uterine relaxant
Thyroxine 5-deiodinase inhibitor
Fibroblast growth factor agonist
Prostaglandin F2 alpha antagonist
Protein synthesis inhibitor
Cholate-CoA ligase inhibitor
Thrombolytic
Phosphoenolpyruvate mutase inhibitor
Adenylate cyclase stimulant
Phenylacetate-CoA ligase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Leukopoiesis stimulant
Epoxide hydrolase substrate
Caspase 8 stimulant
Interferon antagonist
All-trans-retinyl-palmitate hydrolase inhibitor
Tauropine dehydrogenase inhibitor
3-Dehydroquinone dehydratase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
Cell adhesion molecule inhibitor
H⁺-transporting two-sector ATPase inhibitor
ATPase stimulant
Ethanolaminephosphotransferase inhibitor
UGT1A6 substrate
Intermittent claudication treatment
Methylglutamate dehydrogenase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
L-lysine 6-transaminase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Interferon gamma antagonist
3-Methylbutanal reductase inhibitor
Growth hormone agonist
Carnosine synthase inhibitor
Phospholipase A1 inhibitor
Levanase inhibitor
5 Hydroxytryptamine uptake stimulant
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
General pump inhibitor

UGT1A3 substrate
Antidote
Protein-tyrosine sulfotransferase inhibitor
CYP2C9 inducer
Beta-mannosidase inhibitor
Pediculicide
Fibroblast growth factor 1 agonist
Glutamate-tRNA ligase inhibitor
Immunomodulator
Inflammatory Bowel disease treatment
Pectin lyase inhibitor
Gastrointestinal motility stimulant
Phosphoinositide 5-phosphatase inhibitor
HMG CoA synthase inhibitor
Protein synthesis stimulant
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Xenobiotic-transporting ATPase inhibitor
CYP1A2 substrate
Succinic dehydrogenase inhibitor
CYP4A2 substrate
Aldehyde dehydrogenase substrate
Simian immunodeficiency virus proteinase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Aspergillopepsin I inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
Prostaglandin A1 agonist
Mannose isomerase inhibitor
Neurotrophic factor
Glucosyl transferase inhibitor
4-Coumarate-CoA ligase inhibitor
Microtubule formation inhibitor
Pancreatic disorders treatment
Catalase inhibitor
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Melanin inhibitor
Protein kinase stimulant
Plastoquinol-plastocyanin reductase inhibitor
Ganglioside galactosyltransferase inhibitor
Chemopreventive
1,4-Alpha-glucan branching enzyme inhibitor
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Methane monooxygenase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Fumarate reductase (NADH) inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Cardioprotectant
Phosphatidylcholine-sterol O-acyltransferase inhibitor
L-glucuronate reductase inhibitor

UGT1A1 substrate
RNA synthesis inhibitor
Pancreatic elastase inhibitor
Inorganic diphosphatase inhibitor
NAD(P)H dehydrogenase (quinone) inhibitor
Maleate isomerase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Alpha-N-arabinofuranosidase inhibitor
Antihyperammonemic
CYP2D6 substrate
Antibiotic
Galactolipase inhibitor
3-Hydroxybutyrate dehydrogenase inhibitor
UGT2B11 substrate
Atherosclerosis treatment
Cellulose 1,4-beta-cellobiosidase inhibitor
Rhizopuspepsin inhibitor
Choloylglycine hydrolase inhibitor
Secretase alpha stimulant
Secretase stimulant
Malate dehydrogenase inhibitor
Dynein ATPase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
UGT2B12 substrate
Ceramide glucosyltransferase inhibitor
Membrane integrity antagonist
Long-chain-fatty-acid-CoA ligase inhibitor
Expectorant
Aldehyde dehydrogenase (NADP+) inhibitor
Lipotropic
Galacturan 1,4-alpha-galacturonidase inhibitor
Pullulanase inhibitor
Arachidonic acid antagonist
Skin irritation, inactive
1,4-Lactonase inhibitor
Vitamin
Diacylglycerol cholinephosphotransferase inhibitor
Leukotriene B4 antagonist
Antimutagenic
Preneoplastic conditions treatment
Acyloxyacyl hydrolase inhibitor
Keratosis actinic (solar) treatment
Alpha-pinene-oxide decyclase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
Nucleotidase inhibitor
Cyclic AMP modulator
Membrane integrity agonist
Trimethylamine-oxide aldolase inhibitor
Adenylate kinase inhibitor
Serratia marcescens nuclease inhibitor

Lysozyme inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Reductase inhibitor
Chitin synthase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Pyruvate dehydrogenase inhibitor
CYP2D substrate
Eye irritation, inactive
Carboxypeptidase Taq inhibitor
Growth stimulant
Procollagen C-endopeptidase inhibitor
Glutamate dehydrogenase (NADP+) inhibitor
Mucolytic
Antiviral (Hepatitis B)
Antipyretic
Threonine ammonia-lyase inhibitor
Menstruation disorders treatment
Antioxidant
(S)-carnitine 3-dehydrogenase inhibitor
CYP17 inhibitor
Phosphofructokinase-1 inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
5 Hydroxytryptamine release stimulant
ICAM1 expression inhibitor
Insulin promoter
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Acylesterase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Cerebroside-sulfatase inhibitor
Acylglycerone-phosphate reductase inhibitor
Trimethyllysine dioxygenase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Feruloyl esterase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Histone acetyltransferase inhibitor
Bone formation stimulant
Antispirochetal
Poly(beta-D-mannuronate) lyase inhibitor
Alpha,alpha-trehalase inhibitor
Endoglycosylceramidase inhibitor
Antiviral (Picornavirus)
DNA ligase (ATP) inhibitor
Cytokine release inhibitor
Leukotriene antagonist
Oxoglutarate dehydrogenase (lipoamide) inhibitor
Glycosylceramidase inhibitor
Aspartate kinase inhibitor
2-Methyleneglutarate mutase inhibitor
Interleukin 10 antagonist
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor

Paraoxonase substrate
2-Aminoadipate transaminase inhibitor
Acetate-CoA ligase inhibitor
Pantothenase inhibitor
Aminoacylase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
EIF4E expression inhibitor
Propionate CoA-transferase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Chloride channel blocker
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
CYP2C2 substrate
Antifibrinolytic
Gamma-butyrobetaine dioxygenase inhibitor
Anabolic
[phosphorylase] phosphatase inhibitor
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor
Cellulase inhibitor
Protein kinase C stimulant
4-Hydroxymandelate oxidase inhibitor
Prostaglandin-I synthase inhibitor
Contraceptive male
Anticholelithogenic
Chemoprotective
Glutarate-semialdehyde dehydrogenase inhibitor
CYP26A substrate
2-Enoate reductase inhibitor
CYP1A1 substrate
Raynaud's phenomenon treatment
Alpha-amylase inhibitor
Vascular (periferal) disease treatment
Coproporphyrinogen oxidase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Lymphocytopoiesis inhibitor
CYP2A1 substrate
Alpha-L-rhamnosidase inhibitor
Isocitrate dehydrogenase (NAD+) inhibitor
Sucrose-phosphate synthase inhibitor
Ceramidase inhibitor
Folate antagonist
Endopeptidase inhibitor
Toll-Like receptor antagonist
Estrone sulfotransferase inhibitor
GABA transporter 2 inhibitor
Anticoagulant
Interferon alpha agonist
Diacylglycerol kinase inhibitor
Sulfite dehydrogenase inhibitor

2-Oxoglutarate decarboxylase inhibitor
Penicillopepsin inhibitor
UGT2B9 substrate
Pyruvate decarboxylase inhibitor
Aldehyde dehydrogenase inhibitor
Hyaluronic acid agonist
CYP4A1 substrate
Antihypertensive
Mannan endo-1,4-beta-mannosidase inhibitor
Sphingosine kinase inhibitor
Cytosole dipeptidase inhibitor
CYP3A11 substrate
Protein-synthesizing GTPase inhibitor
Arachidonate-CoA ligase inhibitor
Nicotinic alpha4beta2 receptor antagonist
Glycine-tRNA ligase inhibitor
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
D-lactate dehydrogenase inhibitor
CYP19 substrate
Steroid N-acetylglucosaminyltransferase inhibitor
Malate dehydrogenase (NADP+) inhibitor
Nitric oxide scavenger
Triose-phosphate isomerase inhibitor
Cyanate hydratase inhibitor
CYP2C9 inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Tentoxilysin inhibitor
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Antinephritic
Antitreponemal
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
CDC25A inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
Interleukin 4 antagonist
Mucorpepsin inhibitor
Sedoheptulose-bisphosphatase inhibitor
Peptidyltransferase inhibitor
Anthranilate-CoA ligase inhibitor
Endo-1,4-beta-xylanase inhibitor
Ovulation inhibitor
D-glutamate oxidase inhibitor
Antiviral (Poxvirus)
Bile-salt sulfotransferase inhibitor
Prunasin beta-glucosidase inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Glucose-1,6-bisphosphate synthase inhibitor

AR expression inhibitor
Acyl-CoA oxidase inhibitor
Aconitate decarboxylase inhibitor
Galactosylceramidase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Membrane dipeptidase inhibitor
Beta galactosidase inhibitor
Rotamase (FKBP) inhibitor
Paget's disease treatment
HMG CoA reductase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
Aconitate hydratase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Dethiobiotin synthase inhibitor
Pseudolysin inhibitor
Phenylalanine dehydrogenase inhibitor
Sphingomyelinase inhibitor
Phospholipase A2 inhibitor
Aspartate transaminase inhibitor
Riboflavin phosphotransferase inhibitor
Dextranucrase inhibitor
Insecticide
Oxaloacetate tautomerase inhibitor
Pyruvate carboxylase inhibitor
Acetoin dehydrogenase inhibitor
Ca²⁺-transporting ATPase inhibitor
4-Nitrophenylphosphatase inhibitor
Carnitine 3-dehydrogenase inhibitor
Apoptosis antagonist
CYP26 substrate
Leukotriene B4 receptor 1 antagonist
D-lactate dehydrogenase (cytochrome) inhibitor
DNA polymerase I inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Oryzin inhibitor
Sodium/bile acid cotransporter inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
1-Alkyl-2-acetylgllycerol O-acyltransferase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Alpha-L-fucosidase inhibitor
T cell inhibitor
Radical formation agonist
Glyoxylate reductase (NADP⁺) inhibitor
Citrate (Si)-synthase inhibitor
Pregnane X receptor agonist
Antiasthmatic
Anti-Helicobacter pylori
Hypercalcemia treatment

DNA synthesis inhibitor
Isocitrate lyase inhibitor
Glutamate dehydrogenase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
Vanilloid agonist
Beta-glucosidase inhibitor
Prostaglandin EP2 agonist
Serine 3-dehydrogenase inhibitor
Oxaloacetate decarboxylase inhibitor
Protein-arginine deiminase inhibitor
Uroporphyrinogen decarboxylase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Lactate 2-monooxygenase inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
Aerobactin synthase inhibitor
Carboxy-cis,cis-muconate cyclase inhibitor
Protein 50S ribosomal subunit inhibitor
Malate dehydrogenase (decarboxylating) inhibitor
UGT2B18 substrate
D-lactate-2-sulfatase inhibitor
ATP citrate lysase inhibitor
Pancreatic ribonuclease inhibitor
CYP2C10 substrate
Nitric oxide antagonist
Antiacne
Coccolysin inhibitor
Lysine 2-monooxygenase inhibitor
Isocitrate dehydrogenase (NADP+) inhibitor
Acidifying agent gastric
Nitrile hydratase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Lipoprotein lipase stimulant
Fatty acid synthase inhibitor
D-aspartate oxidase inhibitor
Xylan 1,4-beta-xylosidase inhibitor
Glutamyl endopeptidase II inhibitor
Phospholipase inhibitor
Sterol 24-C-methyltransferase inhibitor
Aryl sulfotransferase inhibitor
Lactose synthase inhibitor
UGT2B15 substrate
Trehalose-phosphatase inhibitor
Antihelminthic
Acid phosphatase inhibitor
Antirickettsial
8-Amino-7-oxononanoate synthase inhibitor
Dolichyl-phosphatase inhibitor

Manganese peroxidase inhibitor
Aspartate 4-decarboxylase inhibitor
Aldehyde dehydrogenase 1A2 inhibitor
H⁺-exporting ATPase inhibitor
Keratolytic
IgA-specific metalloendopeptidase inhibitor
Vanilloid 1 agonist
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Cytochrome-b5 reductase inhibitor
Succinate dehydrogenase inhibitor
Diabetic nephropathy treatment
CYP2A11 substrate
Alanine transaminase inhibitor
Aldose reductase substrate
Urocanate hydratase inhibitor
Glucose-6-phosphate isomerase inhibitor
CYP1B1 substrate
4-Phytase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Lactate-malate transhydrogenase inhibitor
Radiosensitizer
Procollagen N-endopeptidase inhibitor
Myosin ATPase inhibitor
CYP2A4 substrate
Acetylserotonin O-methyltransferase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
Peptidyl-dipeptidase B inhibitor
Tyrosine 2,3-aminomutase inhibitor
Kidney function stimulant
VCAM1 expression inhibitor
Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
2-Nitropropane dioxygenase inhibitor
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Antiprotozoal (Toxoplasma)
Bronchodilator
Antineoplastic antibiotic
Antidiabetic (type 1)
Parathyroid hormone antagonist
Prostaglandin EP4 agonist
Quinoprotein glucose dehydrogenase inhibitor
L-lactate dehydrogenase (cytochrome) inhibitor
Antiprotozoal (Trichomonas)
D-2-hydroxy-acid dehydrogenase inhibitor
Electron transport complex I inhibitor
Bontoxilysin inhibitor
Hydroxylysine kinase inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor

Homoserine dehydrogenase inhibitor
D-Lysine 5,6-aminomutase inhibitor
Indanol dehydrogenase inhibitor
Glycogen (starch) synthase inhibitor
Candidapepsin inhibitor
Endopeptidase So inhibitor
Histamine release inhibitor
NADPH oxidoreductase inhibitor
Creatinase inhibitor
Malate synthase inhibitor
D-proline reductase (dithiol) inhibitor
Testosterone agonist
Rhodotorulapepsin inhibitor
CYP3A inducer
Ornithine-oxo-acid transaminase inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Interleukin 5 antagonist
11-Cis-retinyl-palmitate hydrolase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Peroxisome proliferator-activated receptor gamma agonist
Mannosidase inhibitor
Oxygen scavenger
Endopeptidase La inhibitor
Interleukin 1a antagonist
GDP-mannose 6-dehydrogenase inhibitor
Aminolevulinate transaminase inhibitor
Guanidinopropionase inhibitor
Sphingosine kinase 1 inhibitor
5-Aminolevulinate synthase inhibitor
Transforming growth factor beta 1 agonist
Saccharolysin inhibitor
Trans-octaprenyltranstransferase inhibitor
Retinol O-fatty-acyltransferase inhibitor
Glycine N-choloyltransferase inhibitor
Lysine decarboxylase inhibitor
Alpha glucosidase inhibitor
3-Oxoacid CoA-transferase inhibitor
Isoamylase inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
Oligo-1,6-glucosidase inhibitor
CYP24 substrate
Mevalonate kinase inhibitor
Aspartate-tRNA ligase inhibitor
D-Octopine dehydrogenase inhibitor
Neuraminidase inhibitor
Kexin inhibitor
3'-Nucleotidase inhibitor
Pyruvate kinase inhibitor
Lipocortins synthesis antagonist
N-methyl-2-oxoglutaramate hydrolase inhibitor

Antiprotozoal (Coccidial)
Antihyperlipoproteinemic
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Fumarate hydratase inhibitor
Choline dehydrogenase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Glucan 1,6- α -glucosidase inhibitor
Glutamate dehydrogenase [NAD(P)⁺] inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
Glycopeptide α -N-acetylgalactosaminidase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Homoisocitrate dehydrogenase inhibitor
Sarcosine oxidase inhibitor
Bone diseases treatment
Betaine-homocysteine S-methyltransferase inhibitor
Beta-D-fucosidase inhibitor
Hematinic
Inositol-3-phosphate synthase inhibitor
Thiamine-triphosphatase inhibitor
Lipocortins synthesis agonist
Calcineurin inhibitor
Pyridoxamine-oxaloacetate transaminase inhibitor
Glyoxylate reductase inhibitor
Maleate hydratase inhibitor
Carnitine O-octanoyltransferase inhibitor
Alanine dehydrogenase inhibitor
Cutinase inhibitor
CYP3A4 inducer
Glutamate decarboxylase inhibitor
Leucine transaminase inhibitor
AICAR transformylase inhibitor
Leukotriene C antagonist
Glycine C-acetyltransferase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Endocannabinoid uptake inhibitor
Antineoplastic (bone cancer)
CYP3A5 inducer
Glutamate-cysteine ligase inhibitor
Alopecia treatment
UDP-N-acetylmuramate-L-alanine ligase inhibitor
[Isocitrate dehydrogenase (NADP⁺)] kinase inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Pregnane X receptor antagonist
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Arginine deiminase inhibitor
Homocitrate synthase inhibitor
Glucose oxidase inhibitor

Alanine racemase inhibitor
CYP4F3 substrate
4-Chlorobenzoyl-CoA dehalogenase inhibitor
L(+)-Tartrate dehydratase inhibitor
Bacterial leucyl aminopeptidase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Arylamine N-acetyltransferase inhibitor
Phosphomevalonate kinase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
Deoxyribose-phosphate aldolase inhibitor
L-iduronidase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
Aldosterone antagonist
Linoleate isomerase inhibitor
Inositol oxygenase inhibitor
Homoserine kinase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Protein phosphatase 2A inhibitor
CYP2B10 substrate
Antileprosy
Asparagine-tRNA ligase inhibitor
Benzoylformate decarboxylase inhibitor
GABA transporter 3 inhibitor
2-(acetamidomethylene)succinate hydrolase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Pantoate-beta-alanine ligase inhibitor
ATP deaminase inhibitor
N-formylmethionyl-peptidase inhibitor
Retinoid X alpha receptor agonist
N-acetyllactosamine synthase inhibitor
Fumarylacetoacetase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Antinociceptive
4-Hydroxyphenylpyruvate dioxygenase inhibitor
Beta glucosidase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Pyroglutamyl-peptidase I inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Cholestenone 5alpha-reductase inhibitor
Dipeptidase E inhibitor
Ligase inhibitor
Dihydropyrimidinase inhibitor
ATPase (Vacuolar H+) inhibitor
DNA directed DNA polymerase inhibitor
Glutaminase inhibitor
Formate-dihydrofolate ligase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor

Lipid peroxidase inhibitor
Antiuremic
Glutamine-fructose-6-phosphate transaminase inhibitor
Pyruvate, water dikinase inhibitor
Microtubule stabilization
Imidazoleglycerol-phosphate dehydratase inhibitor
Argininosuccinate synthase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Leukotriene B4 receptor 2 antagonist
Gluconate 5-dehydrogenase inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
HIV-2 reverse transcriptase inhibitor
Choline kinase inhibitor
Chitin deacetylase inhibitor
Carnitine palmitoyltransferase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Glycerol-1-phosphatase inhibitor
Hydroxymethylbilane synthase inhibitor
Alpha galactosidase inhibitor
Ornithine decarboxylase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Aspartate 1-decarboxylase inhibitor
Polyamine biosynthesis inhibitor
Mitochondrial intermediate peptidase inhibitor
DELTA14-sterol reductase inhibitor
CYP27A substrate
NADH oxidase inhibitor
Mannosyl-oligosaccharide glucosidase inhibitor
3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor
Glutamate synthase (NADPH) inhibitor
CYP27 substrate
Guanidinobutyrase inhibitor
Phosphoenolpyruvate carboxylase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Glucosylceramidase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Actin depolymerization stimulant
Dimethylhistidine N-methyltransferase inhibitor
Vasodilator, coronary
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Aspartate carbamoyltransferase inhibitor
Acrosin inhibitor
L-fuconate dehydratase inhibitor
Kainate receptor 1 agonist
Urate-ribonucleotide phosphorylase inhibitor
Strombine dehydrogenase inhibitor
Omptin inhibitor
Sweetener
Phosphoribulokinase inhibitor
N-acetylmuramoyl-L-alanine amidase inhibitor

Acyl-CoA dehydrogenase inhibitor
Glutamate (mGluR8) antagonist
Glutamine synthetase inhibitor
RNA-directed RNA polymerase stimulant
Retinoid X receptor agonist
Anesthetic general
Antihypotensive
Fragilysin inhibitor
ATP citrate synthase inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
GABA B receptor antagonist
Tartrate decarboxylase inhibitor

Amantadine hydrochloride

Molecular Mechanism (initial) :

matrix protein 2 (Influenza virus A) inhibitor

Molecular Mechanism (repurposed) :

dopamine receptor agonists

NMDA receptor antagonists

initial indication(s):

Influenza A virus infection

Repurposed indication(s):

Parkinson's disease

Predicted Activities

Antiischemic, cerebral

Antiviral (Influenza A) (Influenza A virus infection)

Antiparkinsonian (Parkinson's disease)

Neurodegenerative diseases treatment

Phobic disorders treatment

Nicotinic alpha2beta2 receptor antagonist

Testosterone 17beta-dehydrogenase (NADP+) inhibitor

5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor

Antiparkinsonian, rigidity relieving

Nicotinic alpha6beta3beta4alpha5 receptor antagonist

Acylcarnitine hydrolase inhibitor

Nootropic

Albendazole monooxygenase inhibitor

Dopamine release stimulant

CYP2J substrate

Pterin deaminase inhibitor

Antiviral (Influenza)

CYP2J2 substrate

Acrocyllindropepsin inhibitor

Chymosin inhibitor

Saccharopepsin inhibitor

Multiple sclerosis treatment

Aspulvinone dimethylallyltransferase inhibitor

NADPH peroxidase inhibitor

Kidney function stimulant
Ubiquinol-cytochrome-c reductase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Cardiovascular analeptic
Complement factor D inhibitor
Alkylacetylgllycerophosphatase inhibitor
Sugar-phosphatase inhibitor
5 Hydroxytryptamine release stimulant
Dementia treatment
Glutamyl endopeptidase II inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
L-glutamate oxidase inhibitor
Polyamine-transporting ATPase inhibitor
Antiviral (Picornavirus)
Hydrogen dehydrogenase inhibitor
Cognition disorders treatment
Ribulose-phosphate 3-epimerase inhibitor
Analgesic
Fusarinine-C ornithinesterase inhibitor
Antidyskinetic
Limulus clotting factor B inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Alopecia treatment
Omptin inhibitor
Chloride peroxidase inhibitor
Ophthalmic drug
Lysase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Spasmolytic, urinary
Thioredoxin inhibitor
Sigma 1 receptor agonist
Alkenylglycerophosphocholine hydrolase inhibitor
Macrophage colony stimulating factor agonist
Exoribonuclease II inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Antiseborrheic
NADPH-cytochrome-c2 reductase inhibitor
Alzheimer's disease treatment
Electron-transferring-flavoprotein dehydrogenase inhibitor
Pseudolysin inhibitor
Imidazoline receptor agonist
Glucose oxidase inhibitor
Lysine 2,3-aminomutase inhibitor
Polyporopepsin inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Dimethylargininase inhibitor
Adenomatous polyposis treatment
Venombin AB inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Vascular dementia treatment

Limulus clotting factor C inhibitor
Sigma receptor agonist
Platelet aggregation stimulant
Antineurotic
Antiglaucomic
Fibrolase inhibitor
Fatty-acyl-CoA synthase inhibitor
Membrane permeability inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Carboxypeptidase Taq inhibitor
Histidine N-acetyltransferase inhibitor
Phthalate 4,5-dioxygenase inhibitor
CYP2B5 substrate
Styrene-oxide isomerase inhibitor
Leukopoiesis stimulant
Acetylcholine neuromuscular blocking agent
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Antiviral (Adenovirus)
Erythropoiesis stimulant
Antidiabetic symptomatic
Fructan beta-fructosidase inhibitor
CYP2C12 substrate
Yeast ribonuclease inhibitor
CYP2D2 inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Sulfite oxidase inhibitor
Antitoxic
Protein-disulfide reductase (glutathione) inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Phospholipid-translocating ATPase inhibitor
Glucagon-like peptide 1 agonist
3-Hydroxybenzoate 6-monooxygenase inhibitor
ADP-thymidine kinase inhibitor
CYP2D16 substrate
Antiprotozoal
CYP3A1 substrate
Arginine 2-monooxygenase inhibitor
Acylesterase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Gluconate 5-dehydrogenase inhibitor
Sphinganine kinase inhibitor
Antiviral (Poxvirus)
S-alkylcysteine lyase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
CYP3A2 substrate
Na⁺-transporting two-sector ATPase inhibitor

JAK2 expression inhibitor
Calcium channel (voltage-sensitive) activator
Neurotransmitter antagonist
Opioid dependency treatment
Ecdysone 20-monooxygenase inhibitor
Glycolate dehydrogenase inhibitor
Cyclamate sulfohydrolase inhibitor
Ovulation inhibitor
Aspartate-ammonia ligase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Mucomembranous protector
Diabetic neuropathy treatment
Alcohol dehydrogenase (acceptor) inhibitor
Cl--transporting ATPase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Immunosuppressant
Fragilysin inhibitor
GABA C receptor agonist
2-Haloacid dehalogenase inhibitor
Antiparkinsonian, tremor relieving
Platelet adhesion inhibitor
Inulinase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Antidiabetic
Anticonvulsant
1,4-Lactonase inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
N-formylmethionyl-peptidase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Myeloblastin inhibitor
Cyclic AMP agonist
Cytoprotectant
Phosphatidylserine decarboxylase inhibitor
Autoimmune disorders treatment
Acute neurologic disorders treatment
All-trans-retinyl-palmitate hydrolase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Glyoxylate reductase inhibitor
GABA aminotransferase inhibitor
CYP2A4 substrate
Aminobutyraldehyde dehydrogenase inhibitor
Malate oxidase inhibitor
Apyrase inhibitor
Sulfite reductase inhibitor
CYP2D15 substrate
CYP2A8 substrate
2-Dehydropantoate aldolase inhibitor
DNA-3-methyladenine glycosylase I inhibitor

Creatininase inhibitor
Prion diseases treatment
Glyoxylate oxidase inhibitor
Trimethylamine-oxide aldolase inhibitor
DELTA14-sterol reductase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Manganese peroxidase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Octopamine antagonist
Mucinaminyserine mucinaminidase inhibitor
IgA-specific serine endopeptidase inhibitor
Endopeptidase So inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Vascular (periferal) disease treatment
CYP2G1 substrate
Xylan endo-1,3-beta-xylosidase inhibitor
Isopenicillin-N epimerase inhibitor
Antineurogenic pain
MAP kinase stimulant
Chitosanase inhibitor
Cyclohexanone monooxygenase inhibitor
Cutinase inhibitor
Levanase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Superoxide dismutase inhibitor
Biotinidase inhibitor
Carminative
Chenodeoxycholytaurine hydrolase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Phenol O-methyltransferase inhibitor
Antiviral
Oxygen scavenger
Phosphoinositide 5-phosphatase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Linoleoyl-CoA desaturase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Antiischemic
Glycine dehydrogenase (decarboxylating) inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Formaldehyde transketolase inhibitor
Pullulanase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Taurine dehydrogenase inhibitor
Vasoprotector
CYP2A2 substrate
Leukotriene-B4 20-monooxygenase inhibitor
Meprin B inhibitor

Thiol oxidase inhibitor
Nucleoside oxidase (H₂O₂-forming) inhibitor
Nitrite reductase (NO-forming) inhibitor
Procollagen N-endopeptidase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Chlordecone reductase inhibitor
Mucositis treatment
CYP7 inhibitor
Oxidizing agent
3-Chloro-D-alanine dehydrochlorinase inhibitor
Ornithine cyclodeaminase inhibitor
Sulfur reductase inhibitor
Phosphoenolpyruvate mutase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Chaperonin ATPase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Nicotinic alpha₄beta₂ receptor antagonist
Peptide alpha-N-acetyltransferase inhibitor
Lysostaphin inhibitor
CYP2C9 inducer
Methylumbelliferyl-acetate deacetylase inhibitor
Pin1 inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Antidiabetic (type 2)
Membrane integrity agonist
Adenylyl-sulfate reductase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Preneoplastic conditions treatment
Aspergillopepsin I inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
Alanine-tRNA ligase inhibitor
Hematopoietic inhibitor
NADH kinase inhibitor
S-formylglutathione hydrolase inhibitor
Mannose isomerase inhibitor
Enteropeptidase inhibitor
Spasmolytic
Feruloyl esterase inhibitor
Antimyopathies
Ligase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
Lactase inhibitor
Linoleate diol synthase inhibitor
5 Hydroxytryptamine uptake stimulant
GST A substrate
Antiprotozoal (Plasmodium)
tRNA-pseudouridine synthase I inhibitor
Glutathione thiolesterase inhibitor
Allantoin racemase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor

Cyclomaltodextrinase inhibitor
Acetylenecarboxylate hydratase inhibitor
Thymidylate 5'-phosphatase inhibitor
Cytochrome-b5 reductase inhibitor
Dipeptidase E inhibitor
Phenylalanine(histidine) transaminase inhibitor
Para amino benzoic acid antagonist
Prostaglandin-A1 DELTA-isomerase inhibitor
Fibrinogen receptor antagonist
Polygalacturonase inhibitor
Threonine aldolase inhibitor
Fucosterol-epoxide lyase inhibitor
D-xylulose reductase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Arylmalonate decarboxylase inhibitor
Aspergillus nuclease S1 inhibitor
Antinociceptive
Gluconolactonase inhibitor
CYP2A1 substrate
Picornain 3C inhibitor
Neuropeptide Y4 antagonist
RNA-directed RNA polymerase inhibitor
Menopausal disorders treatment
Cathepsin T inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Clavamate synthase inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Fructose 5-dehydrogenase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Arylacetonitrilase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Serine-pyruvate transaminase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Polyneuridine-aldehyde esterase inhibitor
NF-E2-related factor 2 stimulant
Mitochondrial processing peptidase inhibitor
Allantoate deiminase inhibitor
Pancreatic elastase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Antiviral (Herpes)
Amine dehydrogenase inhibitor
Sulfite dehydrogenase inhibitor
CYP2C10 substrate
(S)-3-amino-2-methylpropionate transaminase inhibitor
Membrane permeability enhancer

Gaucher disease treatment
CYP2E1 inducer
Hydroxylamine oxidase inhibitor
Opioid kappa 3 receptor antagonist
Benzaldehyde dehydrogenase (NADP+) inhibitor
CYP4A2 substrate
Glycine amidinotransferase inhibitor
Nicotinic alpha6 receptor agonist
Formate-dihydrofolate ligase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Glutamate-tRNA ligase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Thiamine pyridinylase inhibitor
Acidifying agent non gastric
Dynein ATPase inhibitor
Flavin-containing monooxygenase inhibitor
Antidepressant
D-lactaldehyde dehydrogenase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Pediculicide
Sclerosant
Malate dehydrogenase (acceptor) inhibitor
Alpha-pinene-oxide decyclase inhibitor
Cytochrome P450 stimulant
Antiprotozoal (Trypanosoma)
Dextranase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
UGT2B28 substrate
Acetylnithine deacetylase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Polarisation inhibitor
EIF4E expression inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Alkane 1-monooxygenase inhibitor
CYP2C11 substrate
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
CYP3A7 substrate
Carnitine dehydratase inhibitor
Carbon-monoxide dehydrogenase inhibitor
Mood disorders treatment
2-Hydroxyquinoline 8-monooxygenase inhibitor
Aspartate-tRNA ligase inhibitor
Antiviral (Hepatitis)
Carboxypeptidase D inhibitor
Leukopoiesis inhibitor
Steroid synthesis inhibitor
CYP2B10 substrate
Spermidine dehydrogenase inhibitor

Prunasin beta-glucosidase inhibitor
Amyotrophic lateral sclerosis treatment
Plastoquinol-plastocyanin reductase inhibitor
Galactose oxidase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
N-benzoyloxycarbonylglycine hydrolase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Horrilysin inhibitor
Insulysin inhibitor
Gonadotropin antagonist
CYP2C19 inducer
Gingipain K inhibitor
Diamine N-acetyltransferase inhibitor
Lipoprotein lipase inhibitor
Venom exonuclease inhibitor
CYP2C29 substrate
3-Cyanoalanine hydratase inhibitor
RELA expression inhibitor
Valine decarboxylase inhibitor
Pseudouridylate synthase inhibitor
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Undecaprenyl-diphosphatase inhibitor
Hyaluronic acid agonist
CYP4A11 substrate
N-acylmannosamine kinase inhibitor
Asparagine-tRNA ligase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Antiviral (Hepatitis C)
Oxidoreductase inhibitor
Guanidinoacetate kinase inhibitor
Glutamate release inhibitor
Antiinflammatory, intestinal
Ferredoxin hydrogenase inhibitor
Deoxyribonuclease I inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
CYP2B11 substrate
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
CYP2A5 substrate
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Acetylcholine release stimulant
3-Phytase inhibitor
Analgesic stimulant
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
CYP2C18 substrate
Phosphatidylinositol diacylglycerol-lyase inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Nicotine dehydrogenase inhibitor
Glutamate receptor antagonist
Sodium channel blocker class Ib
Lipid metabolism regulator

Glycerol 2-dehydrogenase (NADP+) inhibitor
Gamma-glutamyltransferase inhibitor
Carnosine synthase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Dependence treatment
Maltose-transporting ATPase inhibitor
Mannitol-1-phosphatase inhibitor
BRAF expression inhibitor
5 Hydroxytryptamine release inhibitor
CYP2C8 inhibitor
Antisecretoric
Sphinganine-1-phosphate aldolase inhibitor
Oryzin inhibitor
Thiamine-triphosphatase inhibitor
Morphine 6-dehydrogenase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Antismoking
X-methyl-His dipeptidase inhibitor
Alpha-glucuronidase inhibitor
H⁺-exporting ATPase inhibitor
Glutamate 5-kinase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Adrenaline release stimulant
Dimethylmaleate hydratase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Galactolipase inhibitor
CYP2C6 substrate
Insulin promoter
Cellulose 1,4-beta-cellobiosidase inhibitor
Methionine decarboxylase inhibitor
Bisphosphoglycerate mutase inhibitor
Tyrosine 3 hydroxylase inhibitor
Endothelial growth factor antagonist
Arylesterase inhibitor
Tryptophan transaminase inhibitor
Cyanoalanine nitrilase inhibitor
Phosphatase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
CYP3A4 inducer
Lipotropic
N-acetylneuraminate synthase inhibitor
DNA synthesis inhibitor
Centromere associated protein inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Granzyme A inhibitor
Arylsulfate sulfotransferase inhibitor
Deoxyribonuclease X inhibitor
Aspartoacylase inhibitor
Glucuronate isomerase inhibitor

Glutamate (mGluR5) agonist
Gallate decarboxylase inhibitor
D-amino-acid dehydrogenase inhibitor
TP53 expression enhancer
Serine 3-dehydrogenase inhibitor
CYP3A inducer
UGT1A5 substrate
CYP2C3 substrate
Calcium-sensing receptor agonist
GABA B receptor agonist
Trans-pentaprenyltranstransferase inhibitor
Leukotriene-C4 synthase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Fibrinolytic
Anesthetic general
Renal tissue kallikrein inhibitor
Saccharolysin inhibitor
Bile-salt sulfotransferase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Phosphatidylglycerophosphatase inhibitor
Coccolysin inhibitor
Thiopurine S-methyltransferase inhibitor
Cocain dependency treatment
DNA-(apurinic or apyrimidinic site) lyase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Carnitinamidase inhibitor
CYP2D1 substrate
Peroxidase inhibitor
Chitinase inhibitor
Cysteine transaminase inhibitor
Histamine release stimulant
Stroke treatment
Thiosulfate dehydrogenase inhibitor
Bothrolysin inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
UGT1A4 substrate
Lysyl oxidase inhibitor
Mitochondrial intermediate peptidase inhibitor
Methanol dehydrogenase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Cyclooxygenase substrate
Leucine dehydrogenase inhibitor
Prostaglandin-E2 9-reductase inhibitor
Salicylate 1-monooxygenase inhibitor
ATP phosphoribosyltransferase inhibitor
UGT2B17 substrate
3-Methylbutanal reductase inhibitor
4-Hydroxymandelate oxidase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor

Snapalysin inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Opine dehydrogenase inhibitor
Glutaminase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Antipruritic, allergic
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Retinoic acid metabolism inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Valine-tRNA ligase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Antihelminthic (Fasciola)
Respiratory analeptic
Narcolepsy treatment
Ubiquitin thiolesterase inhibitor
Pitrilysin inhibitor
3'-Nucleotidase inhibitor
Cancer associated disorders treatment
11-Beta-hydroxysteroid dehydrogenase 1 inhibitor
Inflammatory Bowel disease treatment
Antiviral (CMV)
Galacturan 1,4-alpha-galacturonidase inhibitor

NMDA receptor antagonist

Penicillin amidase inhibitor
Oxytocic
Antiperistaltic
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Glutamin-(asparagin-)ase inhibitor
Pappalysin-1 inhibitor
11-Beta-hydroxysteroid dehydrogenase inhibitor
MAP kinase kinase 4 inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
CYP2A3 substrate
Monoamine uptake inhibitor
Trimethylamine dehydrogenase inhibitor
Phospholipase C inhibitor
Cell wall biosynthesis inhibitor
Serratia marcescens nuclease inhibitor
DNA ligase (ATP) inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
UGT1A9 substrate
Monodehydroascorbate reductase (NADH) inhibitor
Anthranilate-CoA ligase inhibitor
MMP9 expression inhibitor
Hydroxysteroid dehydrogenase inhibitor
Transcription factor NF kappa A inhibitor
Transketolase inhibitor
4-Hydroxyproline epimerase inhibitor
GST T substrate
GST T1-1 substrate

Neurotrophic factor enhancer
Nitrate reductase (cytochrome) inhibitor
Licheninase inhibitor
Glycerol-1-phosphatase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Orotate reductase (NADH) inhibitor
Indoleacetaldoxime dehydratase inhibitor
4-Nitrophenylphosphatase inhibitor
Aldosterone antagonist
Fumarate reductase (NADH) inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Iron-cytochrome-c reductase inhibitor
DOPA decarboxylase inhibitor
Hyponitrite reductase inhibitor
Galactokinase inhibitor
CYP2B2 substrate
N-acetylneuraminate 4-O-acetyltransferase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Tropinesterase inhibitor
Selenocysteine lyase inhibitor
Loop diuretic
N-acetyllactosamine synthase inhibitor
Antifibrinolytic
Alternansucrase inhibitor
Myosin ATPase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
Signal peptidase I inhibitor
Isopenicillin-N synthase inhibitor
Cycloartenol synthase inhibitor
Histidinol dehydrogenase inhibitor
tRNA nucleotidyltransferase inhibitor
Antialcoholic
Beta-mannosidase inhibitor
Ceramide glucosyltransferase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Gingipain R inhibitor
Glucuronolactone reductase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Histidinol-phosphatase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Aspergillopepsin II inhibitor
CYP2F1 substrate
Creatinase inhibitor
Peroxidase substrate
Radioprotector
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Valine dehydrogenase (NADP+) inhibitor

P-glycoprotein 1 inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Immunostimulant
FMO1 substrate
Glutamine-pyruvate transaminase inhibitor
Camphor 1,2-monooxygenase inhibitor
Laminaribiose phosphorylase inhibitor
Substance P antagonist
Spasmolytic, Papaverin-like
Pulmonary hypertension treatment
L-threonine 3-dehydrogenase inhibitor
Antiprotozoal (Leishmania)
Brachyurin inhibitor
Glutaminyl-peptide cyclotransferase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Glutathione peroxidase inhibitor
Melanin inhibitor
Antiinflammatory, ophthalmic
Glycine C-acetyltransferase inhibitor
UGT1A6 substrate
Alpha-N-acetylgalactosaminidase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Lipocortins synthesis antagonist
Alpha-Methylacyl-CoA racemase inhibitor
Hydroxymethylbilane synthase inhibitor
Trehalose-phosphatase inhibitor
Uroporphyrinogen-III synthase inhibitor
UGT2B4 substrate
AR expression inhibitor
Urethanase inhibitor
Mandelate 4-monooxygenase inhibitor
Lysine decarboxylase inhibitor
4-Coumarate-CoA ligase inhibitor
Xylose isomerase inhibitor
Pyruvate decarboxylase inhibitor
Gastrointestinal motility stimulant
Aureolysin inhibitor
Acetylserotonin O-methyltransferase inhibitor
Acyl-lysine deacylase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Farnesyltranstransferase inhibitor
Choline-phosphate cytidylyltransferase inhibitor
Metalloproteinase D inhibitor
8-Amino-7-oxononanoate synthase inhibitor

Corticosteroid side-chain-isomerase inhibitor
Diuretic
Bontoxilysin inhibitor
Protein synthesis stimulant
Nardilysin inhibitor
TRPA1 agonist
GST M substrate
O-aminophenol oxidase inhibitor
Analeptic
Indanol dehydrogenase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Rhizopuspepsin inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Cyclic AMP modulator
Antibacterial
CYP19A1 expression inhibitor
Antirickettsial
Tauropine dehydrogenase inhibitor
Mannan endo-1,6- α -mannosidase inhibitor
3-Oxoadipate enol-lactonase inhibitor
Aryldialkylphosphatase inhibitor
Antidiarrheal
Saluretic
Nicotinate dehydrogenase inhibitor
Pancreatic endopeptidase E inhibitor
RNA synthesis inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
Homoserine dehydrogenase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Sweetener
Dolichol kinase inhibitor
4- α -glucanotransferase inhibitor
Thiamine-phosphate kinase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
CYP4B substrate
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Choline-sulfatase inhibitor
Cysteine desulfurase inhibitor
Methyltransferase substrate
Glutamate N-acetyltransferase inhibitor
Aryl-alcohol dehydrogenase (NADP⁺) inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Ferredoxin-NADP⁺ reductase inhibitor
Thromboxane B2 antagonist
Tyrosine kinase stimulant
Hydroxylamine reductase (NADH) inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
3-Hydroxyanthranilate oxidase inhibitor

Cholinergic
Arylalkyl acylamidase inhibitor
Aldehyde dehydrogenase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
Pyroglutamyl-peptidase II inhibitor
Lactate 2-monooxygenase inhibitor
Aldehyde dehydrogenase 2 substrate
Sterol 3-beta-glucosyltransferase inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Leucolysin inhibitor
Peptidyl-dipeptidase B inhibitor
Antiinfective
L-iduronidase inhibitor
Arabinose isomerase inhibitor
Pectin lyase inhibitor
UGT2B15 substrate
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Tankyrase inhibitor
Omega-amidase inhibitor
D-cysteine desulhydrase inhibitor
ATP adenylyltransferase inhibitor
Creatinine deaminase inhibitor
Acyl-CoA oxidase inhibitor
Phosphoinositide phospholipase C inhibitor
Tentoxilysin inhibitor
Carboxymethylenebutenolidase inhibitor
Lactose synthase inhibitor
Vasculitis treatment
Urate-ribonucleotide phosphorylase inhibitor
Mucolytic
Diisopropyl-fluorophosphatase inhibitor
Oligopeptidase B inhibitor
5 Hydroxytryptamine 2B agonist
Thermitase inhibitor
Calcium channel activator
Cytochrome-b5 reductase substrate
Lactaldehyde reductase inhibitor
Beta-glucosidase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Phosphate acetyltransferase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Antihelminthic (Nematodes)
Alkylglycerone-phosphate synthase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Nitric oxide scavenger
CYP4A substrate
Allantoinase inhibitor
P-glycoprotein inhibitor
NMDA 2 receptor antagonist

Acetylcholine nicotinic antagonist
DNA nucleotidylexotransferase inhibitor
Glycerol dehydrogenase (NADP⁺) inhibitor
Deoxyribose-phosphate aldolase inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Antibacterial, ophthalmic
Antihematotoxic
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
H⁺-transporting two-sector ATPase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Uterine relaxant
Plasmanyethanolamine desaturase inhibitor
Methane monooxygenase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
CYP2B18 substrate
CYP3A3 substrate
Caspase 8 stimulant
Riboflavin phosphotransferase inhibitor
Skin whitener
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Arylamine N-acetyltransferase inhibitor
Aconitate decarboxylase inhibitor

NMDA receptor polyamine site agonist

Aldehyde dehydrogenase (NADP⁺) inhibitor
Isomaltulose synthase inhibitor
UGT2B10 substrate
3-Aminobutyryl-CoA ammonia-lyase inhibitor
3-Isopropylmalate dehydratase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Trimethyllysine dioxygenase inhibitor
N6-methyl-lysine oxidase inhibitor
Alcohol dehydrogenase [NAD(P)⁺] inhibitor
CYP4F2 substrate
2-Acylglycerol O-acyltransferase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
CYP1A2 inducer
Diuretic inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Alpha-amylase inhibitor
2-Enoate reductase inhibitor
Aminopeptidase Y inhibitor
2-Aminoadipate transaminase inhibitor
Pantothenase inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Cysteine synthase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
Antihypoxic
Lysozyme inhibitor

SMN2 expression enhancer
Serine-phosphoethanolamine synthase inhibitor
Guanidinoacetase inhibitor
Retinal dehydrogenase inhibitor
Antipruritic
FMO3 substrate
Antispirochetal
3-Ketovalidoxylamine C-N-lyase inhibitor
CYP4B1 substrate
Aldehyde ferredoxin oxidoreductase inhibitor
Gluconate dehydratase inhibitor
Amino-acid racemase inhibitor
Choloylglycine hydrolase inhibitor
Aspartate transaminase inhibitor
Biotin carboxylase inhibitor
Choline kinase inhibitor
Phosphonoacetate hydrolase inhibitor
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Lysyl endopeptidase inhibitor
Reductant
Ferrochelataase inhibitor
Acetoin dehydrogenase inhibitor
Cellulase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Antipruritic, non-allergic
Phenylpyruvate decarboxylase inhibitor
Vasodilator, peripheral
Hydroxymethylglutaryl-CoA lyase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Intermittent claudication treatment
Botulin neurotoxin A light chain inhibitor
Neuropsin inhibitor
D-alanine transaminase inhibitor
Skin irritation, inactive
Antihypotensive
L-lysine 6-transaminase inhibitor
Phenylalanine decarboxylase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Glucarate dehydratase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor
Expectorant
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Aryl hydrocarbon receptor agonist
Anthranilate 3-monooxygenase (deaminating) inhibitor
Beta-D-fucosidase inhibitor
Envelysin inhibitor
Dihydroxy-acid dehydratase inhibitor

Leucine transaminase inhibitor
2-Oxoglutarate decarboxylase inhibitor
Homospermidine synthase inhibitor
CYP2E1 inhibitor
Cholesterol oxidase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Allantoicase inhibitor
Dethiobiotin synthase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Dolichyl-phosphatase inhibitor
Glutamate (mGluR6) antagonist
Rhodotorulapepsin inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Sulfur dioxygenase inhibitor
Glycine hydroxymethyltransferase inhibitor
Atrolysin A inhibitor
Cerebroside-sulfatase inhibitor
Pyruvate carboxylase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Procollagen C-endopeptidase inhibitor
Farnesoid X receptor antagonist
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Acetylspermidine deacetylase inhibitor
Homoserine O-succinyltransferase inhibitor
IgA-specific metalloendopeptidase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Cyclopentanone monooxygenase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Choline acetyltransferase stimulant
D-glutamate oxidase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Cholate-CoA ligase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Gly-X carboxypeptidase inhibitor
Nicotinamide-nucleotide adenyltransferase inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
CYP2B4 substrate
Urease inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Cerebrovascular disorders treatment
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Dactylisin inhibitor
Ribonucleoside triphosphate reductase inhibitor
Histamine agonist

2-Aminohexano-6-lactam racemase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Acylglycerone-phosphate reductase inhibitor
Viral entry inhibitor
CYP3A5 inducer
Allophanate hydrolase inhibitor
D-proline reductase (dithiol) inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
Agmatinase inhibitor
Alpha,alpha-trehalase inhibitor
Glutamine-tRNA ligase inhibitor
CYP3C substrate
NMDA 2A receptor antagonist
Pantoate 4-dehydrogenase inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
UGT2B9 substrate
(R,R)-butanediol dehydrogenase inhibitor
Mevalonate kinase inhibitor
D-lactate dehydrogenase inhibitor

NMDA receptor polyamine site antagonist

Pyridoxine 4-oxidase inhibitor
Acetate kinase inhibitor
Sulfate adenylyltransferase inhibitor
Proline dehydrogenase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
HIV-2 reverse transcriptase inhibitor
Phosphatidate cytidylyltransferase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Homocysteine desulfhydrase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Antiprotozoal (Coccidial)
Membrane integrity antagonist
Protein kinase B alpha inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
GABA C receptor antagonist
Formyltetrahydrofolate dehydrogenase inhibitor
Cytochrome-c3 hydrogenase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Aldehyde oxidase inhibitor
Lombricine kinase inhibitor
Retinyl-palmitate esterase inhibitor
L-lysine oxidase inhibitor
Adenine deaminase inhibitor
HMOX1 expression enhancer
Glucose 1-dehydrogenase inhibitor
Uterine stimulant

Protein-tyrosine sulfotransferase inhibitor
Gametolysin inhibitor
Hypoxia inducible factor 1 alpha inhibitor
Thermomycolin inhibitor
Polyamine oxidase inhibitor
Arachidonic acid antagonist
UGT2B7 substrate
3-Isopropylmalate dehydrogenase inhibitor
Malate-CoA ligase inhibitor
Iduronate-2-sulfatase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Glutamate (mGluR3) agonist
Prostaglandin E1 antagonist
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Histamine release inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
Inorganic diphosphatase inhibitor
Tryptophanamidase inhibitor
Adenylate kinase inhibitor
Endopeptidase La inhibitor
Ribosomal protein S6 kinase 1, 70-kDa inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Antiprotozoal (Babesia)
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
Dichloromuconate cycloisomerase inhibitor
Aerobactin synthase inhibitor
Alpha-N-arabinofuranosidase inhibitor
Alkene monooxygenase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Benzoylformate decarboxylase inhibitor
Phosphoserine phosphatase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Adenylate cyclase stimulant
Muscular dystrophy treatment
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Glycine transaminase inhibitor
Tardive dyskinesia treatment
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Saccharopine dehydrogenase (NAD+, L-glutamate-forming) inhibitor
Testosterone 17beta-dehydrogenase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
2-Methylcitrate dehydratase inhibitor
Clostripain inhibitor
Vascular adhesion protein 1 inhibitor
CYP17 inhibitor

NAD⁺ kinase inhibitor
Prolyl aminopeptidase inhibitor
Adenylyl-sulfate kinase inhibitor
Immunomodulator
Thiol S-methyltransferase inhibitor
Beta-ureidopropionase inhibitor
Prostate disorders treatment
Serine-glyoxylate transaminase inhibitor
Antiprotozoal (Trichomonas)
L-glucuronate reductase inhibitor
Quisqualate antagonist
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Aldehyde dehydrogenase [NAD(P)⁺] inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
Acrosin inhibitor
Diaminopimelate dehydrogenase inhibitor
Acetylcholine M3 receptor agonist
Ribonuclease U2 inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Pregnane X receptor agonist
Lysosomal Pro-X carboxypeptidase inhibitor
Alanine transaminase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
D-Octopine dehydrogenase inhibitor
Sickle-cell anemia treatment
Glutamate uptake inhibitor
Ganglioside galactosyltransferase inhibitor
Agaritine gamma-glutamyltransferase inhibitor
D-stereospecific aminopeptidase inhibitor
DELTA24-sterol reductase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Tripeptidyl-peptidase I inhibitor
Subtilisin inhibitor
Acetoacetate decarboxylase inhibitor
Orotate reductase (NADPH) inhibitor
Nitric-oxide synthase stimulant
Diguanidinobutanase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Putrescine oxidase inhibitor
Phosphofructokinase-1 inhibitor
Picornain 2A inhibitor
Hydroxylamine reductase inhibitor
Methylaspartate ammonia-lyase inhibitor
Glutaminyl-tRNA synthase (glutamine-hydrolysing) inhibitor
Restless leg syndrome treatment
Tryptophan dimethylallyltransferase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Photosensitizer
NOS2 expression inhibitor

Antileprosy
Diiodophenylpyruvate reductase inhibitor
Tryptophanyl aminopeptidase inhibitor
Skeletal muscle relaxant
Laccase inhibitor
Malyl-CoA lyase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
ICAM1 expression inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Gastrin inhibitor
Antiepileptic
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Phosphatidylinositol 3-kinase stimulant
UGT1A3 substrate
Acid-sensing ion channel blocker
Nucleoside-diphosphatase inhibitor
Guanidinopropionase inhibitor
Phenylacetate-CoA ligase inhibitor
5 Hydroxytryptamine 4A antagonist
Vasodilator, coronary
Membrane dipeptidase inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
Peptidyl-glycinamidase inhibitor
Choline dehydrogenase inhibitor
Mycodextranase inhibitor
Catechol oxidase inhibitor
Sorbitol dehydrogenase inhibitor
Nitrile hydratase inhibitor
Aminolevulinate transaminase inhibitor
Alpha,alpha-trehalose phosphorylase inhibitor
Lysine 2-monooxygenase inhibitor
Cytosol dipeptidase inhibitor
Age-related macular degeneration treatment
Peptidylamidoglycolate lyase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Dihydropyrimidinase inhibitor
Antidepressant, Imipramine-like
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Antitussive
Galactoside O-acetyltransferase inhibitor
CYP2B substrate
Glutamate (mGluR1) agonist
Peptidyl-Lys metalloendopeptidase inhibitor
CYP19 substrate
Sepsis treatment
Poly(ADP-ribose) glycohydrolase inhibitor
NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
Vomilenine glucosyltransferase inhibitor
Catalase inhibitor

Antiprotozoal (Amoeba)
Formate dehydrogenase inhibitor
Gluconokinase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Glucan 1,3-beta-glucosidase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
Cathepsin H inhibitor
2-Methyleneglutarate mutase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Aspartate kinase inhibitor
Eye irritation, inactive
2,4-Dichlorophenol 6-monooxygenase inhibitor
Chitin synthase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Arginyltransferase inhibitor
Aminopeptidase B inhibitor
Osmotic diuretic
D-Serine ammonia-lyase inhibitor
Cerevisin inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Glutamate (mGluR8) agonist
Glycogen (starch) synthase inhibitor
Cystathionine beta-lyase inhibitor
Prephenate dehydrogenase inhibitor
Dipeptidyl peptidase inhibitor
Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Xanthommatin reductase inhibitor
D-2-hydroxy-acid dehydrogenase inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
CYP2A13 substrate
Deoxycytidine deaminase inhibitor
3-Oxosteroid 1-dehydrogenase inhibitor
UGT2B substrate
Deoxyribonuclease (pyrimidine dimer) inhibitor
Adenylate cyclase V inhibitor
Antianorexic
Glucosyl transferase inhibitor
Glutamate (mGluR4) agonist
Homogentisate 1,2-dioxygenase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminyltransferase inhibitor
Anesthetic inhalation
Ribosomal protein S6 kinase, 70-kDa inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
CTP synthase inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
Glutamate (mGluR group II) agonist

Pancreatic ribonuclease inhibitor
Interferon alpha agonist
Stromelysin 2 inhibitor
Polyamine biosynthesis inhibitor
Maleate hydratase inhibitor
Secretase alpha stimulant
Secretase stimulant
Ornithine-oxo-acid transaminase inhibitor
tRNA adenylyltransferase inhibitor
Serine protease unspecified inhibitor
Penicillopepsin inhibitor
Ferredoxin-nitrite reductase inhibitor
Carboxypeptidase M inhibitor
Arginine deiminase inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor
Aspartate 1-decarboxylase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
Arylformamidase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Glutamate (mGluR1) antagonist
Acylaminoacyl-peptidase inhibitor
TNF expression inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Tetrahydroxynaphthalene reductase inhibitor
Coagulant
Isocitrate dehydrogenase (NAD⁺) inhibitor
Beta-cyclopiazonate dehydrogenase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Galactosylceramide sulfotransferase inhibitor
Threonine ammonia-lyase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
HCV IRES inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Interleukin 10 agonist
Ribonuclease inhibitor
Retinol O-fatty-acyltransferase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Malate dehydrogenase (NADP⁺) inhibitor
Uridine nucleosidase inhibitor
Cellobiose phosphorylase inhibitor
Acetolactate synthase inhibitor
Lipoxygenase substrate
Corticosteroid antagonist
D-arabinonolactone oxidase inhibitor
Narcotic antagonist
Dihydrouracil oxidase inhibitor
Rhodopsin kinase inhibitor

Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Ca²⁺-transporting ATPase inhibitor
Carnitine 3-dehydrogenase inhibitor
Flavin-containing monooxygenase substrate
Chemoprotective
Pyrroline-5-carboxylate reductase inhibitor
CYP1B substrate
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
UGT1A1 substrate
Acyloxyacyl hydrolase inhibitor
Diacylglycerol kinase inhibitor
L-amino-acid oxidase inhibitor
UGT1A7 substrate
Nicotinic receptor alpha7 subunit antagonist
UGT2B11 substrate
FMN reductase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Succinic dehydrogenase inhibitor
Glutamate dehydrogenase inhibitor
TH expression enhancer
tRNA cytidyltransferase inhibitor
Nuclease inhibitor
Heat shock protein agonist
Fibromyalgia syndrome treatment
Iodide peroxidase inhibitor
NADH dehydrogenase inhibitor
Heme oxygenase inhibitor
Venombin A inhibitor
Chitin deacetylase inhibitor
Leucine-tRNA ligase inhibitor
Sulfinoalanine decarboxylase inhibitor
Phosphatidate phosphatase inhibitor
3C-like protease (Human coronavirus) inhibitor
CYP2B1 substrate
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Argininosuccinate lyase inhibitor
Nitrate reductase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
Alpha-L-fucosidase inhibitor
Glutamate formimidoyltransferase inhibitor
CYP26A substrate
HIV-1 integrase (Overall Integration) inhibitor
Protein-tyrosine phosphatase 2C inhibitor
Oligo-1,6-glucosidase inhibitor
VCAM1 expression inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
Asparaginase inhibitor
Cancer procoagulant inhibitor
CYP19 inhibitor

Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Aryl-acylamidase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Nucleotide metabolism regulator
Antinaupathic
Gastritis treatment
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Aspartate racemase inhibitor
Decylcitrate synthase inhibitor
2-Methylcitrate synthase inhibitor
Succinate dehydrogenase inhibitor
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor
Mannonate dehydratase inhibitor
UGT1A substrate
Shock treatment
Immunoglobulin E antagonist
Paget's disease treatment
Contraceptive female
Urolithiasis treatment
Guanylate kinase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
Sphingosine kinase inhibitor
Anabolic
Isoquinoline 1-oxidoreductase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor
Formimidoylglutamase inhibitor
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Amylo-alpha-1,6-glucosidase inhibitor
Nicotinic alpha3beta4 receptor agonist
Purinergic P2X antagonist
Hippurate hydrolase inhibitor
Antibiotic
Antineoplastic, alkylator
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Adenylylsulphatase inhibitor
S-methyl-5-thioribose kinase inhibitor
Cytosine deaminase inhibitor
CYP2A6 inhibitor
Acidifying agent gastric
Nucleoside deoxyribosyltransferase inhibitor
Argininosuccinate synthase inhibitor
L-ascorbate peroxidase inhibitor
Thioredoxin reductase inhibitor
Phenylalanine-tRNA ligase inhibitor
Acaricide
Glycerophosphocholine cholinephosphodiesterase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Amylosucrase inhibitor

Cytostatic
Phosphoribulokinase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Glutamate (mGluR2) agonist
Deoxyhypusine synthase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Ethanolaminephosphotransferase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
UGT1A8 substrate
X-Pro dipeptidase inhibitor
Glutathione synthase inhibitor
Histamine H1 receptor agonist
Liver X receptor antagonist
CYP3A5 substrate
ATP deaminase inhibitor
Glutamate-cysteine ligase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
UDP-N-acetylglucosamine 2-epimerase inhibitor
GABA A inverse agonist
GABA inverse agonist
SULT1A3 substrate
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Ribosomal protein S6 kinase inhibitor
Diphosphomevalonate decarboxylase inhibitor
Ketoheokinase inhibitor
UDP-glucuronosyltransferase substrate
Pectate lyase inhibitor
Cyanate hydratase inhibitor
Homocitrate synthase inhibitor
Beta-amylase inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor
Hematopoietic
Metabolic disease treatment
Anthranilate synthase inhibitor
4-Phytase inhibitor
Luteinizing hormone-releasing hormone agonist
Oxalate oxidase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
Polynucleotide adenylyltransferase inhibitor
Shab potassium channel blocker
Histamine H2 receptor agonist
Acetolactate decarboxylase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor

2-Nitrophenol 2-monooxygenase inhibitor
11-Cis-retinyl-palmitate hydrolase inhibitor
Urticaria treatment
Carboxylate reductase inhibitor
Sarcosine oxidase inhibitor
Purinergic receptor antagonist
Furin inhibitor
Muconate cycloisomerase inhibitor
Anthrax lethal factor inhibitor
Serralysin inhibitor
Inotropic
Dextranucrase inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
Caspase 3 stimulant
Ribitol 2-dehydrogenase inhibitor
Inositol 1,4,5-triphosphate receptor antagonist
CYP4F substrate
Asparagine-oxo-acid transaminase inhibitor
Acylphosphatase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Nitric-oxide synthase inhibitor
Arylsulfatase inhibitor
6-Methylsalicylate decarboxylase inhibitor
6-Phosphofructo-2-kinase inhibitor
Saccharopine dehydrogenase (NADP⁺, L-lysine-forming) inhibitor
Antineoplastic antimetabolite
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Granulocyte macrophage colony stimulating factor agonist
Thioether S-methyltransferase inhibitor
Alpha, alpha-phosphotrehalase inhibitor
Trimereylsin II inhibitor
CMP-KDO synthase inhibitor
Estrone sulfotransferase inhibitor
Heat shock protein 70 agonist
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
p21-activated kinase inhibitor
Cardioprotectant
Sigma receptor antagonist
Glycine N-acyltransferase inhibitor
CYP4F12 substrate
Microtubule formation inhibitor
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
CYP2B6 substrate
CNS active muscle relaxant
Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Haloalkane dehalogenase inhibitor
CYP2C2 substrate
Adenylate cyclase inhibitor

1-Pyrroline-5-carboxylate dehydrogenase inhibitor
5 Hydroxytryptamine 7 agonist
L-galactonolactone oxidase inhibitor
Aromatic-amino-acid transaminase inhibitor
(R)-aminopropanol dehydrogenase inhibitor
Creatine kinase inhibitor
CYP2A6 substrate
Branched-chain-amino-acid transaminase inhibitor
ACK1 kinase inhibitor
2-Ethylmalate synthase inhibitor
Serine-tRNA ligase inhibitor
Acyl-CoA dehydrogenase (NADP+) inhibitor
Protein-glutamate methylesterase inhibitor
Malate dehydrogenase inhibitor
D-lactate-2-sulfatase inhibitor
Alpha-mannosidase inhibitor
X-His dipeptidase inhibitor
Hydroxylysine kinase inhibitor
Sucrose synthase inhibitor
Thimet oligopeptidase inhibitor
Cholesterol antagonist
Glucan 1,4-alpha-glucosidase inhibitor
Thiosulfate sulfurtransferase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Octadecanal decarbonylase inhibitor
Cystathionine gamma-lyase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Methionine adenosyltransferase inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
Epoxide hydrolase inhibitor
Pyruvate dehydrogenase inhibitor
GABA transporter 3 inhibitor
CYP2C8 substrate
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
Glutamate decarboxylase inhibitor
3'(2'),5'-Bisphosphate nucleotidase inhibitor
Sphingosine 1-phosphate receptor 5 agonist
Mannosyl-oligosaccharide glucosidase inhibitor
3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor
Guanidinobutyrase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
SULT2A1 substrate
dUTP diphosphatase inhibitor
Phosphoglycolate phosphatase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Astringent
Carboxypeptidase U inhibitor
Peristaltic stimulant

Calcium-sensing receptor antagonist
Carboxypeptidase E inhibitor
Urocanate hydratase inhibitor
Endo-1,4-beta-xylanase inhibitor
Interferon antagonist
Interferon gamma antagonist
Aminoacylase inhibitor
CMP-N-acylneuraminate phosphodiesterase inhibitor
4,5-Dihydroxyphthalate decarboxylase inhibitor
Steroid sulfotransferase inhibitor
Lactate-malate transhydrogenase inhibitor
Aryl-alcohol dehydrogenase inhibitor
3-Hydroxybutyrate dehydrogenase inhibitor
Dipeptidyl peptidase IV inhibitor
Methylaspartate mutase inhibitor
Adrenaline uptake inhibitor
Isoamylase inhibitor
Arginine decarboxylase inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
Necroptosis inhibitor
Gentisate 1,2-dioxygenase inhibitor
Cysteine-tRNA ligase inhibitor
Psychosexual dysfunction treatment
Ribulose-bisphosphate carboxylase inhibitor
Analgesic, non-opioid
Anhydrotetracycline monooxygenase inhibitor
5-Aminolevulinate synthase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Pyridoxal kinase inhibitor
ATP diphosphatase inhibitor
Prolactin inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Arabinogalactan endo-1,4-beta-galactosidase inhibitor
CYP2C19 substrate
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Methylthioadenosine nucleosidase inhibitor
Isocitrate lyase inhibitor
Phosphoglucomutase inhibitor
Diamine oxidase inhibitor
Ethanolamine kinase inhibitor
Potassium channel (ATP-sensitive) activator
Potassium channel (Inward rectifier) activator
Inositol-3-phosphate synthase inhibitor
Tripeptide aminopeptidase inhibitor
CYP1A inducer
Dimethylallyltranstransferase inhibitor
Phenylalanine 4-hydroxylase inhibitor
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Alpha, alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
Deoxycytidine kinase inhibitor

Glycerol kinase inhibitor
Nicotinic alpha4beta4 receptor agonist
[citrate-(pro-3S)-lyase] thiolesterase inhibitor
Glutamate dehydrogenase (NADP+) inhibitor
Lipid peroxidase inhibitor
Sucrose alpha-glucosidase inhibitor
Transcription factor STAT6 inhibitor
Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor
3-Deoxy-8-phosphooctulonate synthase inhibitor
Shikimate 5-dehydrogenase inhibitor
Betaine-aldehyde dehydrogenase inhibitor
Mannosidase inhibitor
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Atrolysin C inhibitor
Phenylalanine dehydrogenase inhibitor
Sodium/hydrogen exchanger 5 inhibitor
D-Lysine 5,6-aminomutase inhibitor
Dermatologic
N-acetylneuraminate lyase inhibitor
Malate synthase inhibitor
Glutamine synthetase inhibitor
2-Pyrocatechuate decarboxylase inhibitor
Inositol oxygenase inhibitor
Meprin A inhibitor
Isocitrate dehydrogenase (NADP+) inhibitor
Candidapepsin inhibitor
5-Aminovalerate transaminase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
Formaldehyde dehydrogenase inhibitor
Aldehyde oxidase substrate
Tocolytic
[acyl-carrier-protein] S-malonyltransferase inhibitor
Arginine racemase inhibitor
Glycine N-benzoyltransferase inhibitor
L-Serine ammonia-lyase inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Spermidine synthase inhibitor
Alpha glucosidase inhibitor
Propanediol dehydratase inhibitor
Peptidyltransferase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
D(-)-tartrate dehydratase inhibitor
Nucleotide diphosphatase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Ribose-5-phosphate isomerase inhibitor
Tyrosine 2,3-aminomutase inhibitor
Somatostatin agonist
Beta galactosidase inhibitor
Kexin inhibitor
Purine biosynthesis inhibitor

UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
NAT2 substrate
Histidine decarboxylase inhibitor
Streptopain inhibitor
Laxative
Contraceptive
Aralkylamine dehydrogenase inhibitor
Autophagy inducer
Myc inhibitor
Tryptophan 2-monooxygenase inhibitor
Aspartyl aminopeptidase inhibitor
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
3-Dehydroquinase synthase inhibitor
Sleep apnea treatment
UGT1A10 substrate
Chloride channel activator
CYP2D substrate
Plus-end-directed kinesin ATPase inhibitor
Colony stimulating factor agonist
5 Hydroxytryptamine 3 agonist
Electrolyte absorption antagonist
Alcohol oxidase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
CYP26 substrate
Dihydrodipicolinate synthase inhibitor
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
PRL phosphatase inhibitor
Glutamate (mGluR group III) antagonist
Hemostatic
L-fuconate dehydratase inhibitor
Lanosterol 14 alpha demethylase inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
Arginine kinase inhibitor
Tyrosine-protein kinase TYRO 10 inhibitor
Aspartate ammonia-lyase inhibitor
Choline sulfotransferase inhibitor
Long-chain-acyl-CoA dehydrogenase inhibitor
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Sepiapterin deaminase inhibitor
Apoptosis antagonist
CYP24 substrate
Beta-Lysine 5,6-aminomutase inhibitor
Chorismate mutase inhibitor
Propionate CoA-transferase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
1-Alkyl-2-acetyl-glycerol O-acyltransferase inhibitor
Deoxyadenosine kinase inhibitor

NMN nucleosidase inhibitor
Pyruvate, phosphate dikinase inhibitor
Protein C (activated) inhibitor
Glycine N-methyltransferase inhibitor
Cholinergic antagonist
Cushing's syndrome treatment
Phospholipase D inhibitor
Biliverdin reductase inhibitor
Sepiapterin reductase inhibitor
Quinate 5-dehydrogenase inhibitor
Glutathione reductase inhibitor
Transaldolase inhibitor
Maleylacetoacetate isomerase inhibitor
CYP2C8 inducer
CYP2A substrate
p21-activated kinase 4 inhibitor
Cytokine production stimulant
L-3-cyanoalanine synthase inhibitor
Glycerol dehydratase inhibitor
Antiacne
UDP-N-acetylmuramate dehydrogenase inhibitor
Glutamate (mGluR) antagonist
Phosphoserine transaminase inhibitor
N-acetylglucosamine kinase inhibitor
Lactaldehyde dehydrogenase inhibitor
Phenol 2-monooxygenase inhibitor
UDP-glucose 4-epimerase inhibitor
Glutamate (mGluR3) antagonist
UDP-N-acetylglucosamine diphosphorylase inhibitor
Oxaloacetate decarboxylase inhibitor
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Cell wall synthesis inhibitor
Acetylcholine antagonist
CYP4F8 substrate
CYP24 inhibitor
Nitrilase inhibitor
Protein kinase B inhibitor
Epoxide hydrolase 2 inhibitor
Enoyl-CoA hydratase inhibitor
L-lactate dehydrogenase (cytochrome) inhibitor
Cellulose synthase (UDP-forming) inhibitor
Heat shock protein 70 antagonist
Severe acute respiratory syndrome treatment
Phloroglucinol reductase inhibitor
CYP2D6 substrate
Uracil phosphoribosyltransferase inhibitor
Carnitine O-octanoyltransferase inhibitor
Fumarylacetoacetase inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Beta-fructofuranosidase inhibitor

Alpha-L-rhamnosidase inhibitor
Glutathione S-transferase substrate
Anticholelithogenic
Protein-glutamate O-methyltransferase inhibitor
Thymidine-triphosphatase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Hair growth stimulant
Alanine dehydrogenase inhibitor
Glycine N-choloyltransferase inhibitor
Scytalone dehydratase inhibitor
Dipeptidyl peptidase II inhibitor
Prokinetic
NAT1 substrate
N-acetylglucosaminyldiphosphoundecaprenol N-acetyl-beta-D-mannosaminytransferase inhibitor
N-acylneuraminate cytidyltransferase inhibitor
Proline racemase inhibitor
Diphosphate-serine phosphotransferase inhibitor
Oxaloacetate tautomerase inhibitor
Vitamin
Cytosol alanyl aminopeptidase inhibitor
Benzoate 4-monooxygenase inhibitor
Ornithine carbamoyltransferase inhibitor
Glutamate carboxypeptidase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Urotensin II antagonist
Pyruvate, water dikinase inhibitor
Acetylcholine agonist
UDP-glucose 6-dehydrogenase inhibitor
UGT2B19 substrate
UGT2B23 substrate
UGT2B30 substrate
UGT2B4D substrate
UGT2B4E substrate
Histidine ammonia-lyase inhibitor
5 Hydroxytryptamine 2A agonist
Butyryl-CoA dehydrogenase inhibitor
Adenylate cyclase I inhibitor
Tubulin GTPase inhibitor
Long-chain-fatty-acid-CoA ligase inhibitor
Arginase inhibitor
dCTP deaminase inhibitor
Squalene-hopene cyclase inhibitor
CTGF expression inhibitor
Melanocortin agonist
Orotidylate decarboxylase inhibitor
Glutamate (mGluR8) antagonist
N-formylglutamate deformylase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Endopeptidase inhibitor
Putrescine carbamoyltransferase inhibitor

Glucosylceramidase inhibitor
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Coproporphyrinogen oxidase inhibitor
Antidote
SULT1A1 substrate
Sucrose-phosphate phosphatase inhibitor
Raynaud's phenomenon treatment
Proliferative diseases treatment
1-Phosphofructokinase inhibitor
Endonuclease (influenza) inhibitor
Phosphoribosylformylglycinamide synthase inhibitor
Pantoate-beta-alanine ligase inhibitor
[Isocitrate dehydrogenase (NADP+)] kinase inhibitor
3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
Deoxyguanosine kinase inhibitor
Sucrose phosphorylase inhibitor
Aspartate carbamoyltransferase inhibitor
CYP3A11 substrate
GTP cyclohydrolase I inhibitor
Quercetin 2,3-dioxygenase inhibitor
Glutamate (mGluR) agonist
Dihydrofolate synthase inhibitor
Antihelmintic
Protein N-acetylglucosaminyltransferase inhibitor
Aminopeptidase I inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
Spermine synthase inhibitor
Alpha 3 adrenoceptor agonist
Linoleate isomerase inhibitor
Adrenergic
Asemlin inhibitor
MO15-related protein kinase Pmrk inhibitor
CYP17 substrate
Mycolysin inhibitor
3-Dehydroquinate dehydratase inhibitor
MDM2 inhibitor
GMP synthase inhibitor
Polyphosphate kinase inhibitor
Movement disorders treatment
Citrate (Si)-synthase inhibitor
Phosphoglycerate phosphatase inhibitor
Homoisocitrate dehydrogenase inhibitor
Tartrate decarboxylase inhibitor
Corticotropin releasing factor antagonist
Glutamate (mGluR1a) agonist
Glutamate (mGluR5a) agonist
Valine-pyruvate transaminase inhibitor
Fibroblast activation protein alpha inhibitor
Antifungal (Pneumocystis)
NAD⁺ diphosphatase inhibitor

Glutamate-5-semialdehyde dehydrogenase inhibitor
Calcium antagonist
Cystathionine beta-synthase inhibitor
MAO A substrate
Antidiabetic (type 1)
Acyl-CoA dehydrogenase inhibitor
Proteasome endopeptidase complex inhibitor
Hydroxyquinol 1,2-dioxygenase inhibitor
Cytidylate kinase inhibitor
Histidine-tRNA ligase inhibitor
Triose-phosphate isomerase inhibitor
Strombine dehydrogenase inhibitor
Xylan 1,4-beta-xylosidase inhibitor
Malate dehydrogenase (decarboxylating) inhibitor
Mannitol-1-phosphate 5-dehydrogenase inhibitor
CYP2C18 inhibitor
Tubuliny-Tyr carboxypeptidase inhibitor
Hydroperoxide dehydratase inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Antinephritic
CYP1A3 substrate
4-Hydroxy-2-oxoglutarate aldolase inhibitor
Retinoic acid beta receptor agonist
Nicotinic alpha4beta2 receptor agonist
Dichloromethane dehalogenase inhibitor
Glucose-1-phosphatase inhibitor
Oxytocin agonist
Bacterial leucyl aminopeptidase inhibitor
Potassium channel (ATP-sensitive) blocker
Granzyme B inhibitor
Antimitotic, Podophyllotoxin-like
Acetate-CoA ligase inhibitor
Antineoplastic (bladder cancer)
NMDA receptor phencyclidine site antagonist
Potassium channel small-conductance Ca-activated 3 activator
Nucleoside-triphosphate-adenylate kinase inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
Nociceptin (N/OFQ) receptor agonist
Aralkylamine N-acetyltransferase inhibitor
Acetylcholine muscarinic agonist
Porphobilinogen synthase inhibitor
Glutamate synthase (NADPH) inhibitor
Radiosensitizer
Pyridoxamine-phosphate oxidase inhibitor
Tryptophan-tRNA ligase inhibitor
Fructose 5-dehydrogenase (NADP⁺) inhibitor
Glycolaldehyde dehydrogenase inhibitor
Phosphoglycerate mutase inhibitor
Androst-4-ene-3,17-dione monooxygenase inhibitor

Potassium channel Kv4.3 blocker
Shal potassium channel blocker
AMP nucleosidase inhibitor
Dual specificity phosphatase 1 inhibitor
X-Trp aminopeptidase inhibitor
HDL-cholesterol increasing
3-Oxoacid CoA-transferase inhibitor
Inducible nitric-oxide synthase inhibitor
Glutamate (mGluR4) antagonist
DNA methyltransferase I inhibitor
Nicotinic alpha4 receptor agonist
2-Aminohexanoate transaminase inhibitor
Kynureninase inhibitor
6,7-Dihydropteridine reductase inhibitor
Histone-arginine N-methyltransferase inhibitor
Aldose 1-epimerase inhibitor
GABA B receptor antagonist
Bis(5'-nucleosyl)-tetrphosphatase (symmetrical) inhibitor
FAD diphosphatase inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Protein kinase B stimulant
Acetylcholine nicotinic agonist
Alcohol dehydrogenase inhibitor
Prostaglandin-I synthase inhibitor
DNA methylase inhibitor
Extrapyrmidal disorders treatment
Trypanothione-disulfide reductase inhibitor
CYP2C substrate
Choleretic
Aryl sulfotransferase inhibitor
Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor
5-Alpha-reductase inhibitor
Pyridoxamine-oxaloacetate transaminase inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
Interleukin 1a antagonist
Purinergic P2 antagonist
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Alkylator
Riboflavin synthase inhibitor
Sphingosine 1-phosphate receptor 1 antagonist
Purinergic P2X7 antagonist
NAD⁺ nucleosidase inhibitor
Acetylcholine M4 receptor agonist
tRNA methyltransferase inhibitor
Carboxypeptidase B inhibitor
dCMP deaminase inhibitor
Pyruvate kinase inhibitor
Protein-synthesizing GTPase inhibitor
Bronchodilator

Methylcrotonoyl-CoA carboxylase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor
Bacterial efflux pump inhibitor
3-Deoxy-7-phosphoheptulonate synthase inhibitor
Small monomeric GTPase inhibitor
Dihydropteroate synthase inhibitor
Tubulin-tyrosine ligase inhibitor
2-(acetamidomethylene)succinate hydrolase inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
MAO B substrate
Glucose-1-phosphate adenylyltransferase inhibitor
Anticataract
S-methyl-5-thioadenosine phosphorylase inhibitor
Phosphoketolase inhibitor
Bacillus subtilis ribonuclease inhibitor
Antithyroid
Cytokine modulator
Bis(5'-nucleosyl)-tetraphosphatase (asymmetrical) inhibitor
Sigma 3 receptor antagonist
Oxytocin antagonist
Ribose-5-phosphate adenylyltransferase inhibitor
Nucleoside phosphoacylhydrolase inhibitor
UDP-glucuronate decarboxylase inhibitor
DNA directed DNA polymerase inhibitor
Nav1.5 sodium channel blocker
Uridine kinase inhibitor
5-Alpha-reductase 2 inhibitor
Glycolipid 2-alpha-mannosyltransferase inhibitor
Histamine H4 receptor antagonist
Endo-beta-N-acetylglucosaminidase inhibitor
UDP-sugar diphosphatase inhibitor
CXC chemokine 4 receptor antagonist
GABA transporter inhibitor
Fructokinase inhibitor
Neuronal nicotinic receptor antagonist
UGT2B7H substrate
UGT2B7Y substrate
Acid phosphatase inhibitor
Formate C-acetyltransferase inhibitor
Arginine-tRNA ligase inhibitor
Cortisone alpha-reductase inhibitor
Dopamine D2B antagonist
Hepatoprotectant
Glycogenin glucosyltransferase inhibitor
Hypoxanthine phosphoribosyltransferase inhibitor
Altronate dehydratase inhibitor
Androgen agonist
Procollagen glucosyltransferase inhibitor
Hydroxypyruvate reductase inhibitor
Tryptophan synthase inhibitor

Excitatory amino acid transporter 2 inhibitor
Gentamicin 3'-N-acetyltransferase inhibitor
Antidote, organophosphates
Adenylosuccinate lyase inhibitor
Dopamine D2 agonist inducer
Alpha-N-acetylgalactosaminide alpha-2,6-sialyltransferase inhibitor
Histamine H3 receptor agonist
Phenylalanine 2-monooxygenase inhibitor
Potassium channel (Inward rectifier) blocker
Insecticide
Prolyl endopeptidase inhibitor
Theanine hydrolase inhibitor
Adenylosuccinate synthase inhibitor
Obsessive-compulsive disorder treatment
Amino-acid N-acetyltransferase inhibitor
CPB protease inhibitor
Gastric antisecretory
Prephenate dehydratase inhibitor
Polarisation stimulant
Phospholipase D1 inhibitor
5-Alpha-reductase 1 inhibitor
Glutamate (mGluR2) antagonist
Peptidyl-prolyl cis-trans isomerase inhibitor
5'-Nucleotidase inhibitor
Adenine phosphoribosyltransferase inhibitor
Dopachrome isomerase inhibitor
Carboxy-cis,cis-muconate cyclase inhibitor
Polypeptide N-acetylgalactosaminyltransferase inhibitor
Gamma-glutamyl hydrolase inhibitor
Vasodilator
MARK1 protein inhibitor
Oligonucleotidase inhibitor
NADPH oxidoreductase inhibitor
Kainate receptor agonist
Tryptophan 5 hydroxylase inhibitor
Muscle relaxant
Thymine dioxygenase inhibitor
VEGF expression inhibitor
Deoxyhypusine monooxygenase inhibitor
ATPase inhibitor
Endothelial nitric-oxide synthase inhibitor
CYP26 inhibitor
Histone acetyltransferase inhibitor
Transplant rejection treatment
Calcitonin stimulant
[Skp1-protein]-hydroxyproline N-acetylglucosaminyltransferase inhibitor
GMP reductase inhibitor
Diabetic nephropathy treatment
Antiparasitic
CYP1A1 inhibitor

Antitreponemal
2-Nitropropane dioxygenase inhibitor
Fucokinase inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
4-Pyridoxolactonase inhibitor
Gastricsin inhibitor
Alpha glucosidase I inhibitor
Ribosylpyrimidine nucleosidase inhibitor
Testosterone agonist
Membrane-oligosaccharide glycerophosphotransferase inhibitor
Tartrate dehydrogenase inhibitor
Methenyltetrahydrofolate cyclohydrolase inhibitor
Protein 30S ribosomal subunit inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
Kallikrein 3 inhibitor
Guanylate cyclase 1 inhibitor
CYP1A1 inducer
Phosphorylase kinase inhibitor
Keratolytic
Glutaryl-CoA dehydrogenase inhibitor
MAP-kinase-activated kinase 1 inhibitor
4-Hydroxybenzoate 1-hydroxylase inhibitor
Fumarate hydratase inhibitor
Antiuremic
Kanamycin kinase inhibitor
GABA transporter 1 inhibitor
tRNA (guanine-N7-)-methyltransferase inhibitor
N-acetylglucosaminyldiphosphodolichol N-acetylglucosaminyltransferase inhibitor
Antibiotic Quinolone-like
Dipeptidyl peptidase VIII inhibitor
Protein synthesis inhibitor
UDP-N-acetylglucosamine-lysosomal-enzyme N-acetylglucosaminephosphotransferase inhibitor
Potassium channel activator
Secretase beta inhibitor
Adenosine A1 receptor agonist enhancer
Neurotransmitter uptake inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
2-Isopropylmalate synthase inhibitor
Cortisol sulfotransferase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor
Lysophosphatidic acid receptor agonist
Chitobiosyldiphosphodolichol beta-mannosyltransferase inhibitor
Sphingosine 1-phosphate receptor 4 agonist
Aryl hydrocarbon receptor antagonist
Dolichyldiphosphatase inhibitor
Protein kinase stimulant
Cysteine dioxygenase inhibitor
Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor
Antibiotic Tetracycline-like
Tyrosine-ester sulfotransferase inhibitor

Antihyperaldosteronism
Dipeptidyl peptidase I inhibitor
Prostatic (benign) hyperplasia treatment
Astacin inhibitor
Glutamate (mGluR group I) agonist
Cardiac myosin stimulant
Mental retardation treatment
Alpha 2 adrenoreceptor agonist
Sphingosine 1-phosphate receptor antagonist
Nicotinamidase inhibitor
Amidophosphoribosyltransferase inhibitor
Ribose-phosphate diphosphokinase inhibitor
Beta-N-acetylhexosaminidase inhibitor
Phosphopyruvate hydratase inhibitor
Parathyroid hormone secretion stimulant
Orotate phosphoribosyltransferase inhibitor
Sphingosine 1-phosphate receptor 3 antagonist
Glycerol dehydrogenase inhibitor
Vanillyl-alcohol oxidase inhibitor
Alanine carboxypeptidase inhibitor
2-Methylacetyl-CoA dehydrogenase inhibitor
Potassium channel KCNQ blocker
Glutamate (mGluR group II) antagonist
Tyrosine phenol-lyase inhibitor
Antihyperlipoproteinemic
Thyrotropin releasing hormone agonist
Hydroxyacylglutathione hydrolase inhibitor
Kallikrein 13 inhibitor
Thromboxane A2 antagonist
Secretase beta 2 inhibitor
Glycolipid 3-alpha-mannosyltransferase inhibitor
Tyrosine 3 hydroxylase stimulant
Nicotinate phosphoribosyltransferase inhibitor
TTK protein kinase inhibitor
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Chelator
Stipitatonate decarboxylase inhibitor
Nav1.7 sodium channel blocker
Toll-Like receptor 8 agonist
Tyrosine transaminase inhibitor
Squalene epoxidase inhibitor
Cholestenone 5alpha-reductase inhibitor
MAP3K8 inhibitor
11-Beta-hydroxysteroid dehydrogenase 2 inhibitor
N-acetyllactosaminide beta-1,6-N-acetylglucosaminyl-transferase inhibitor
Nav1.1 sodium channel blocker
CYP1B1 inducer
Potassium channel Kv1.1 blocker
Inosine-adenosine-guanosine-nucleoside hydrolase inhibitor
Streptomycin 6-kinase inhibitor

Glucose-6-phosphate isomerase inhibitor
Sphingosine kinase stimulant
Phosphoglycerate dehydrogenase inhibitor
Secretase beta 1 inhibitor
Diiodotyrosine transaminase inhibitor
Alpha-N-acetylneuraminate alpha-2,8-sialyltransferase inhibitor
Sodium-dependent vitamin C transporter 2 inhibitor
Alpha 1 adrenoreceptor agonist
Puromycin-sensitive aminopeptidase inhibitor
CYP19 inducer
Carbonic anhydrase XIV inhibitor
Phosphoenolpyruvate carboxykinase (GTP) inhibitor
HCV NS3/NS4A protease inhibitor
CC chemokine receptor agonist
Chemokine receptor agonist
Opioid delta 2 receptor antagonist
GRP78 expression inhibitor
Geranyltranstransferase inhibitor
Procollagen galactosyltransferase inhibitor
Pyroglutamyl-peptidase I inhibitor
Dynamin GTPase inhibitor
Formimidoyltetrahydrofolate cyclodeaminase inhibitor
Acetoacetyl-CoA reductase inhibitor
Formyl peptide receptor antagonist
Interferon agonist
3 Beta-hydroxy-delta 5-steroid dehydrogenase inhibitor
CYP17A substrate
Histamine N-methyltransferase inhibitor
Antiprotozoal activity enhancer
CYP4A1 substrate
Pregnane X receptor antagonist
Carboxylesterase inhibitor
Calpain inhibitor
8-oxodGTPase stimulant
Queuine tRNA-ribosyltransferase inhibitor
Transforming growth factor beta 3 antagonist
Thymidine kinase 1 inhibitor
HIV fusion inhibitor
ADAM10 endopeptidase inhibitor
Endothelin-converting enzyme inhibitor
Synaptic vesicle protein SV2, levetiracetam binding site antagonist
Bombesin 2 receptor antagonist
3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor
Folate transporter 1 inhibitor
CYP11B1 substrate
dTMP kinase (Mycobacterium tuberculosis) inhibitor
Neuraminidase inhibitor
Ketosteroid monooxygenase inhibitor
ATP citrate synthase inhibitor
Purine nucleosidase inhibitor

CYP27A substrate
Dipeptidyl peptidase IX inhibitor
CC chemokine 10 receptor antagonist
3(or 17)beta-hydroxysteroid dehydrogenase inhibitor
Anesthetic local
Phosphogluconate dehydrogenase (decarboxylating) inhibitor
Glutamate (mGluR group I) antagonist
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
Sphingosine 1-phosphate receptor 3 agonist
Phosphodiesterase VII inhibitor
Adenosine A1 receptor antagonist
Phytanoyl-CoA dioxygenase inhibitor
Lysine carboxypeptidase inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
Asparaginyl endopeptidase inhibitor
Alpha-1,3-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Thymidine phosphorylase inhibitor
Thyrotropin releasing hormone antagonist
MAP kinase kinase inhibitor
Tannase inhibitor
Vanilloid 4 agonist
CDK4/cyclin D3 inhibitor
Antimutagenic
Cholesterol monooxygenase (side-chain-cleaving) inhibitor
CYP2A11 substrate
Glucosamine N-acetyltransferase inhibitor
CYP19A1 substrate
P3 purinoceptor-like protein antagonist
Neurolysin inhibitor
P2 nucleoside transporter inhibitor
CYP27 substrate
[protein-PII] uridylyltransferase inhibitor
5 Hydroxytryptamine uptake inhibitor
Epoxide hydrolase substrate
Tankyrase 2 inhibitor
CDP-glycerol diphosphatase inhibitor
Methylmalonyl-CoA mutase inhibitor
4-Hydroxyphenylacetate 1-monooxygenase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor
Methionyl-tRNA formyltransferase inhibitor
Necrosis treatment
Trimethylamine-N-oxide reductase inhibitor
Purine nucleoside phosphorylase inhibitor
Pantothenate kinase inhibitor
Ether-a-go-go potassium channel 1 blocker
Ether-a-go-go potassium channel blocker
Transcription factor rho inhibitor

Amitriptyline hydrochloride

Molecular Mechanism (initial) :

norepinephrine and 5-HT reuptake inhibitor

Molecular Mechanism (repurposed) :

sodium channel blocker

initial indication(s):

depression

Repurposed indication(s):

fibromyalgia

peripheral neuropathy

Predicted Activities

Neurotransmitter uptake inhibitor

CYP2E1 inhibitor

Antiparkinsonian, rigidity relieving

Antidepressant

Antidepressant, Imipramin-like

Monoamine uptake inhibitor

Mood disorders treatment

CYP2D substrate

CYP2D6 substrate

Glycosylphosphatidylinositol phospholipase D inhibitor

Membrane integrity agonist

CYP1A2 substrate

P-glycoprotein substrate

CYP1A substrate

CYP3A1 substrate

CYP2B6 substrate

HERG 1 channel blocker

CYP2C substrate

CYP2C9 substrate

CYP2C11 substrate

CYP2C19 substrate

CYP2C12 substrate

Antisecretoric

CYP3A3 substrate

Muscle relaxant

CYP2D2 inhibitor

Phobic disorders treatment

2-Haloacid dehalogenase inhibitor

CYP3A2 substrate

Skeletal muscle relaxant

Anticonvulsant

CYP2B substrate

CYP3A4 substrate

CYP2E substrate

CYP2E1 substrate

Fibrinolytic

CYP2C8 inhibitor

Spasmolytic

CYP3A substrate

Anesthetic general
UGT1A4 substrate
5 Hydroxytryptamine 5 antagonist
Antitoxic
Taurine dehydrogenase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Antiparkinsonian, tremor relieving
CYP2D16 substrate
CYP2A2 substrate
Antipruritic
CYP2J substrate
Mucomembranous protector
Alpha 2b adrenoreceptor antagonist
CYP2H substrate
CNS active muscle relaxant
Ovulation inhibitor
Membrane permeability inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Ubiquinol-cytochrome-c reductase inhibitor
Anxiolytic
Aldehyde oxidase inhibitor
Platelet aggregation stimulant
Carboxypeptidase Taq inhibitor
Trimethylamine-oxide aldolase inhibitor
Antineurotic
Aspulvinone dimethylallyltransferase inhibitor
X-methyl-His dipeptidase inhibitor
Lipid metabolism regulator
Thiamine-triphosphatase inhibitor
Sigma receptor agonist
JAK2 expression inhibitor
Spasmolytic, urinary
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Phosphoenolpyruvate mutase inhibitor
Phospholipid-translocating ATPase inhibitor
CYP2C18 substrate
MAP kinase stimulant
Antipruritic, allergic
5 Hydroxytryptamine 1F antagonist
Antiulcerative
Gluconate 2-dehydrogenase (acceptor) inhibitor
Antipsychotic
FMO1 substrate
Radioprotector
Antiinflammatory
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
CYP2J2 substrate
Oxygen scavenger

Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Fusarinine-C ornithinesterase inhibitor
Macrophage colony stimulating factor agonist
Fibrinogen receptor antagonist
Acylcarnitine hydrolase inhibitor
1,4-Lactonase inhibitor
UGT1A3 substrate
Alpha 2c adrenoreceptor antagonist
Nicotinic alpha2beta2 receptor antagonist

Antineurogenic pain (peripheral neuropathy)

Polyamine-transporting ATPase inhibitor
Phthalate 4,5-dioxygenase inhibitor
CYP2A1 substrate
Histamine release inhibitor
Histamine H1 receptor antagonist
Antihistaminic
Choline-phosphate cytidyltransferase inhibitor
Calcium channel (voltage-sensitive) activator
Methylamine-glutamate N-methyltransferase inhibitor
Rhinitis treatment
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Mucositis treatment
4-Nitrophenol 2-monooxygenase inhibitor
Aryl-acylamidase inhibitor
UGT1A substrate
All-trans-retinyl-palmitate hydrolase inhibitor
CYP2C8 substrate
Ribulose-phosphate 3-epimerase inhibitor
Neurodegenerative diseases treatment
UGT1A9 substrate
CYP2C19 inhibitor
Octopamine antagonist
Albendazole monooxygenase inhibitor
Alpha 2a adrenoreceptor antagonist
Histamine release stimulant
Histamine antagonist
Pseudolysin inhibitor
Antinociceptive
CYP2D1 substrate
Analgesic
5 Hydroxytryptamine 5A antagonist
Antiparkinsonian
Peptide-tryptophan 2,3-dioxygenase inhibitor
Antihypoxic
Flavin-containing monooxygenase substrate
Anesthetic
Steroid synthesis inhibitor
Phenol O-methyltransferase inhibitor
Gonadotropin antagonist

CYP3A7 substrate
Fructose 5-dehydrogenase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Nicotinic alpha4beta4 receptor agonist
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
CYP2A6 substrate
Methyltransferase substrate
CYP2D6 inhibitor
Alopecia treatment
Trimethylamine dehydrogenase inhibitor
CYP2F1 substrate
(R)-6-hydroxynicotine oxidase inhibitor
Venombin AB inhibitor
CYP2G1 substrate
Apyrase inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
Dimethylargininase inhibitor
Sugar-phosphatase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
CYP2A8 substrate
Omptin inhibitor
Retinoic acid metabolism inhibitor
Vasoprotector
Complement factor D inhibitor
Thioredoxin inhibitor
5 Hydroxytryptamine uptake stimulant
Antipruritic, non-allergic
Vasodilator, peripheral
2-Hydroxyquinoline 8-monooxygenase inhibitor
CYP2A substrate
Flavin-containing monooxygenase inhibitor
Cytochrome P450 inhibitor
N-formylmethionyl-peptidase inhibitor
Gluconate 5-dehydrogenase inhibitor
Membrane integrity antagonist
Fibrolase inhibitor
CYP3A5 substrate
Carnitinamidase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Antiemetic
Fatty-acyl-CoA synthase inhibitor
CYP2A3 substrate
Cyclic AMP agonist
Phosphatidylinositol diacylglycerol-lyase inhibitor
Limulus clotting factor B inhibitor
4-Hydroxyproline epimerase inhibitor

Sodium channel blocker

Glutamyl endopeptidase II inhibitor
Chloride peroxidase inhibitor
MAO B substrate

FMO3 substrate
Pullulanase inhibitor
Alkylacetylgllycerophosphatase inhibitor
Prion diseases treatment
Neurotransmitter antagonist
Peptide alpha-N-acetyltransferase inhibitor
Mediator release inhibitor
Leukopoiesis inhibitor
Signal peptidase I inhibitor
Exoribonuclease II inhibitor
Respiratory analeptic
Calcium regulator
5 Hydroxytryptamine 2A antagonist
Alkane 1-monooxygenase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
5-O-(4-coumaroyl)-D-quinatate 3'-monooxygenase inhibitor
Sulfur reductase inhibitor
Amine dehydrogenase inhibitor
Platelet adhesion inhibitor
5 Hydroxytryptamine release stimulant
NADPH peroxidase inhibitor
Nucleoside-diphosphatase inhibitor
Histamine H1 receptor agonist
Hydroxylamine oxidase inhibitor
Nav1.4 sodium channel blocker
CYP2D15 substrate
P-glycoprotein inhibitor
Glycolate dehydrogenase inhibitor
MMP9 expression inhibitor
Nitrite reductase (NO-forming) inhibitor
Oxidoreductase inhibitor
Spermidine dehydrogenase inhibitor
Diabetic neuropathy treatment
Anaphylatoxin receptor antagonist
P-glycoprotein 1 inhibitor
Farnesyltranstransferase inhibitor
Hydrogen dehydrogenase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
N-acylmannosamine kinase inhibitor
Antiseborrheic
Sodium channel (voltage-gated) blocker
GABA transporter 2 inhibitor
Lysostaphin inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Antiprotozoal (Leishmania)
Nicotine dehydrogenase inhibitor
Menopausal disorders treatment
Endopeptidase So inhibitor
Membrane permeability enhancer
Antiinfertility, female

Antitussive, narcotic
Lysase inhibitor
Antimyopathies
Spasmolytic, Papaverin-like
Alcohol dehydrogenase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Lysine 2,3-aminomutase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Sigma 1 receptor agonist
Photosensitizer
Aminobutyraldehyde dehydrogenase inhibitor
Opioid kappa 3 receptor antagonist
IgA-specific serine endopeptidase inhibitor
Cholinergic antagonist
Antiviral (Poxvirus)
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Antidyskinetic
Antiperistaltic
Fragilysin inhibitor
Acetylcholine neuromuscular blocking agent
CYP4A11 substrate
Adenylate cyclase inhibitor
Acylaminoacyl-peptidase inhibitor
Glyoxylate reductase inhibitor
CYP2B5 substrate
Glutathione thiolesterase inhibitor
CYP2A4 substrate
Phosphopantothenoylcysteine decarboxylase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Cyclohexanone monooxygenase inhibitor
5 Hydroxytryptamine 2 antagonist
Chenodeoxycholytaurine hydrolase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Manganese peroxidase inhibitor
Isopenicillin-N epimerase inhibitor
Arginine 2-monooxygenase inhibitor
Formaldehyde transketolase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Glycine amidinotransferase inhibitor
Carnitine 3-dehydrogenase inhibitor
CYP2E1 inducer
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
TP53 expression enhancer
Transforming growth factor beta 1 agonist
Acetylgalactosaminyl-O-glycosyl-glycoprotein
beta-1,3-N-acetylglucosaminyltransferase inhibitor
Limulus clotting factor C inhibitor
Alpha 2 adrenoreceptor antagonist

Peroxidase substrate
Thromboxane B2 antagonist
DNA-3-methyladenine glycosylase I inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
L-glutamate oxidase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Guanylate cyclase 1 stimulant
Glucose oxidase inhibitor
5 Hydroxytryptamine 7 antagonist
Nucleotide metabolism regulator
Analeptic
Loop diuretic
Salicylate 1-monooxygenase inhibitor
Antieczematic atopic
CYP2B11 substrate
Vasodilator, coronary
5 Hydroxytryptamine uptake inhibitor
NF-E2-related factor 2 stimulant
Cytochrome P450 stimulant
5 Hydroxytryptamine 2C antagonist
Pin1 inhibitor
GABA aminotransferase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Reductant
CYP2C3 substrate
Kidney function stimulant
Choline-sulfatase inhibitor
CYP3A inducer
MAO A substrate
Adrenaline release stimulant
Dolichol kinase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
UDP-glucuronosyltransferase substrate
Xylan endo-1,3-beta-xylosidase inhibitor
Yeast ribonuclease inhibitor
Antiviral (Adenovirus)
Creatininase inhibitor
Carnosine synthase inhibitor
Choline dehydrogenase inhibitor
Leukopoiesis stimulant
Antiinflammatory, ophthalmic
Intermittent claudication treatment
Methanol dehydrogenase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Adrenaline uptake inhibitor
Neuropeptide Y2 antagonist
CYP3A4 inducer
Arylmalonate decarboxylase inhibitor
Cell wall biosynthesis inhibitor

Protein-disulfide reductase (glutathione) inhibitor
Lysyl oxidase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Horrisysin inhibitor
Polarisation inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Acidifying agent non gastric
Antimutagenic
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Nav1.5 sodium channel blocker
Radiosensitizer
Morphine 6-dehydrogenase inhibitor
Hematopoietic inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Acetylcholinesterase inhibitor
Acetylspermidine deacetylase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Dementia treatment
Retinal dehydrogenase inhibitor
Antitussive
Feruloyl esterase inhibitor
Alpha 1b adrenoreceptor antagonist
Pappalysin-1 inhibitor
HERG channel blocker
2-Hydroxy-3-oxoadipate synthase inhibitor
Nicotinate dehydrogenase inhibitor
5 Hydroxytryptamine 1D antagonist
Guanidinoacetate kinase inhibitor
Bothrolysin inhibitor
Imidazoline receptor agonist
HCV IRES inhibitor
Cycloartenol synthase inhibitor
Meprin B inhibitor
CYP2C9 inducer
Acetylcholine antagonist
Phosphoserine phosphatase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Gluconolactonase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Sulfotransferase substrate
Antihematotoxic
Glycerol-3-phosphate oxidase inhibitor

ATPase inhibitor
Poly(alpha-L-gulonate) lyase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Acetylnornithine deacetylase inhibitor
Adenomatous polyposis treatment
Acetylcholine muscarinic antagonist
Thymidylate 5'-phosphatase inhibitor
GST A substrate
Cytoprotectant
UGT2B4 substrate
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Gallate decarboxylase inhibitor
Aspartate-ammonia ligase inhibitor
CYP4A substrate
6-Pyruvoyltetrahydropterin synthase inhibitor
Nootropic
Para amino benzoic acid antagonist
3-Phytase inhibitor
Cyanoalanine nitrilase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
CYP1A1 substrate
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Ecdysone 20-monooxygenase inhibitor
TRPA1 agonist
3-Cyanoalanine hydratase inhibitor
Cl--transporting ATPase inhibitor
5 Hydroxytryptamine 7 agonist
Sphinganine kinase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Caspase 8 stimulant
Antiinflammatory, intestinal
Histidinol dehydrogenase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide
beta-N-acetylglucosaminyltransferase inhibitor
Antiprotozoal (Amoeba)
TNF expression inhibitor
Dimethylmaleate hydratase inhibitor
N-acetylneuraminate synthase inhibitor
Antinaupathic
Superoxide dismutase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
5 Hydroxytryptamine 2B antagonist
Sulfite oxidase inhibitor
Sodium channel blocker class Ib
Peptidyl-dipeptidase Dcp inhibitor
Cyclamate sulfohydrolase inhibitor
GABA B receptor agonist
Leukotriene-C4 synthase inhibitor

5 Hydroxytryptamine 2B agonist
5 Hydroxytryptamine 1B antagonist
Cyclooxygenase substrate
Preneoplastic conditions treatment
Na⁺-transporting two-sector ATPase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
CYP2B1 substrate
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Camphor 1,2-monooxygenase inhibitor
Tetrahydroxynaphthalene reductase inhibitor
UGT2B28 substrate
Phospholipase C inhibitor
Erythropoiesis stimulant
Monoamine oxidase substrate
Prostaglandin-A1 DELTA-isomerase inhibitor
Sulfite dehydrogenase inhibitor
CYP7 inhibitor
Cancer associated disorders treatment
Prolactin inhibitor
Gastrin inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
4-Hydroxymandelate oxidase inhibitor
AR expression inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Mitochondrial processing peptidase inhibitor
Carnitine dehydratase inhibitor
Nitrate reductase (cytochrome) inhibitor
Adenosine regulator
Phosphatidate phosphatase inhibitor
HMOX1 expression enhancer
Botulin neurotoxin A light chain inhibitor
Adrenergic
Thiosulfate dehydrogenase inhibitor
Pediculicide
Putrescine oxidase inhibitor
Fructan beta-fructosidase inhibitor
Glyoxylate oxidase inhibitor
Beta 3 adrenoreceptor antagonist
Histidine N-acetyltransferase inhibitor
Lipoxygenase substrate
Cytochrome-b5 reductase inhibitor
Antipyretic
Antihelminthic (Nematodes)
Blasticidin-S deaminase inhibitor
L-lysine 6-transaminase inhibitor
Dopamine D1A antagonist
Nav1.1 sodium channel blocker

NADH kinase inhibitor
Alpha adrenoreceptor antagonist
EIF4E expression inhibitor
Polyporopepsin inhibitor
Creatinine deaminase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Nav1.3 sodium channel blocker
CYP2B2 substrate
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Dopamine release stimulant
Dipeptidase E inhibitor
Corticosteroid side-chain-isomerase inhibitor
Vascular dementia treatment
Creatinase inhibitor
GABA C receptor agonist
Muscular dystrophy treatment
Tyrosine 3 hydroxylase inhibitor
CYP2A6 inhibitor
RNA-directed RNA polymerase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Inulinase inhibitor
UGT1A1 substrate
Mucinaminyserine mucinaminidase inhibitor
Fucosterol-epoxide lyase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Snapalysin inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Arylsulfate sulfotransferase inhibitor
Choline sulfotransferase inhibitor
Oxytocic
D-Octopine dehydrogenase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Biotinidase inhibitor
Acyl-lysine deacylase inhibitor
GST M substrate
Psychosexual dysfunction treatment
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Aureolysin inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Tryptophanamidase inhibitor
Arylesterase inhibitor
Cardiovascular analeptic
Pancreatic elastase inhibitor
Ornithine cyclodeaminase inhibitor
Mannitol-1-phosphatase inhibitor
Cyclopentanone monooxygenase inhibitor
DELTA24-sterol reductase inhibitor
Urethanase inhibitor
Apoptosis antagonist

tRNA nucleotidyltransferase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Glutamate-tRNA ligase inhibitor
Heat shock protein agonist
Acetylcholine M4 receptor antagonist
NOS2 expression inhibitor
Cyclic AMP phosphodiesterase inhibitor
Acetylcholine M1 receptor antagonist
Phosphatidylserine decarboxylase inhibitor
Adenylyl-sulfate reductase inhibitor
ADP-thymidine kinase inhibitor
S-formylglutathione hydrolase inhibitor
Bisphosphoglycerate phosphatase inhibitor
UGT1A5 substrate
Antimitotic
Mannose isomerase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Aldosterone antagonist
Carboxymethylenebutenolidase inhibitor
Amyotrophic lateral sclerosis treatment
Rubredoxin-NAD⁺ reductase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Insulysin inhibitor
Antimigraine
5 Hydroxytryptamine antagonist
Adenylate cyclase V inhibitor
Indolepyruvate C-methyltransferase inhibitor
Nav1.2 sodium channel blocker
Adenylate cyclase stimulant
TH expression enhancer
Lysine decarboxylase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
CYP2C6 substrate
Cathepsin T inhibitor
Cyclomaltodextrinase inhibitor
Aldehyde dehydrogenase 2 substrate
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
IgA-specific metalloendopeptidase inhibitor
Antiadrenergic
N-Acyl-D-aspartate deacylase inhibitor
Transketolase inhibitor
Gastric antisecretory
Calcium antagonist
Antiprotozoal (Trypanosoma)
Potassium channel blocker
Caspase 3 stimulant
Chlordecone reductase inhibitor
UGT2B10 substrate
Pyruvate decarboxylase inhibitor

RNA synthesis inhibitor
Betaine-aldehyde dehydrogenase inhibitor
Antiviral (Influenza)
Ribonucleoside triphosphate reductase inhibitor
Obsessive-compulsive disorder treatment
Cyclic AMP modulator
L-amino-acid oxidase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Trans-pentaprenyltranstransferase inhibitor
Opioid dependency treatment
CYP19A1 expression inhibitor
Liver X receptor antagonist
Clavamate synthase inhibitor
CYP4A2 substrate
Chloride channel activator
Malate dehydrogenase (acceptor) inhibitor
Antiprotozoal (Trichomonas)
Asparagine-tRNA ligase inhibitor
Malate oxidase inhibitor
Tankyrase inhibitor
Acetylcholine M3 receptor antagonist
Oxidizing agent
CYP1A1 inducer
GABA receptor agonist
Myeloblastin inhibitor
tRNA-pseudouridine synthase I inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Sulfite reductase inhibitor
CYP2C29 substrate
Oryzin inhibitor
Mandelate 4-monooxygenase inhibitor
Glycerol-1-phosphatase inhibitor
Ophthalmic drug
Nitrite reductase [NAD(P)H] inhibitor
Histamine agonist
Alpha-glucuronidase inhibitor
Protein kinase C inhibitor
Fumarate reductase (NADH) inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Polyneuridine-aldehyde esterase inhibitor
Smooth muscle myosin light chain kinase inhibitor
Heat shock protein 70 agonist
Linoleoyl-CoA desaturase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Gastrointestinal motility stimulant
Hydroxylamine reductase inhibitor
Ferrochelataase inhibitor
Argininosuccinate lyase inhibitor
Hyponitrite reductase inhibitor

Bontoxilysin inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Histamine H2 receptor antagonist
Guanidinoacetase inhibitor
Acetylcholine M2 receptor antagonist
Gingipain K inhibitor
Procollagen N-endorpeptidase inhibitor
Alpha 1d adrenoreceptor antagonist
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Glutaminase inhibitor
Antidote
Aspartoacylase inhibitor
Shab potassium channel blocker
BRAF expression inhibitor
Gly-X carboxypeptidase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Glutathione reductase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
CYP2B10 substrate
Tropinesterase inhibitor
Hematopoietic
N-Acyl-D-amino-acid deacylase inhibitor
Choline kinase inhibitor
Adrenaline antagonist
Estradiol 17alpha-dehydrogenase inhibitor
Diphosphomevalonate decarboxylase inhibitor
Antineoplastic, alkylator
Squalene epoxidase inhibitor
Insulin promoter
Guanylate cyclase stimulant
Anesthetic local
Aspergillus nuclease S1 inhibitor
Histamine N-methyltransferase inhibitor
2-Enoate reductase inhibitor
Lipocortins synthesis antagonist
2,3-Oxidosqualene-lanosterol cyclase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
CYP1B substrate
Calcium-sensing receptor agonist
Undecaprenyl-diphosphatase inhibitor
Peptidyl-dipeptidase B inhibitor
5 Hydroxytryptamine 1 antagonist
Diuretic inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
RELA expression inhibitor
Galactolipase inhibitor
Nav1.8 sodium channel blocker
Dihydrouracil dehydrogenase (NAD+) inhibitor
Restless leg syndrome treatment

Peptidylamidoglycolate lyase inhibitor
Mannan endo-1,6- α -mannosidase inhibitor
Squalene-hopene cyclase inhibitor
Antiviral (Herpes)
Carbon-monoxide dehydrogenase inhibitor
S-alkylcysteine lyase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Prunasin beta-glucosidase inhibitor
Cytochrome-b5 reductase substrate
Cutinase inhibitor
Deoxyribonuclease I inhibitor
Phosphonoacetate hydrolase inhibitor
Platelet aggregation inhibitor
Metallo-carboxypeptidase D inhibitor
Chaperonin ATPase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Carminative
5 Hydroxytryptamine 6 antagonist
H⁺-exporting ATPase inhibitor
Trypanothione-disulfide reductase inhibitor
UGT2B17 substrate
Sclerosant
4-Coumarate-CoA ligase inhibitor
Aspartate-tRNA ligase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Prostaglandin E1 antagonist
Dolichyl-phosphatase inhibitor
Trehalose-phosphatase inhibitor
MAO inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Sleep disorders treatment
Tryptophanyl aminopeptidase inhibitor
Nucleoside oxidase (H₂O₂-forming) inhibitor
Antialcoholic
Alanine-tRNA ligase inhibitor
Aryl sulfotransferase inhibitor
Dextranase inhibitor
Uterine stimulant
Menstruation disorders treatment
Ubiquitin thiolesterase inhibitor
Phosphatidylglycerophosphatase inhibitor
Antianorexic
Transcription factor NF kappa A inhibitor
Antithrombotic
Carboxypeptidase D inhibitor
Alkylglycerone-phosphate synthase inhibitor
CYP3C substrate

Galacturan 1,4-alpha-galacturonidase inhibitor
Antineoplastic (multiple myeloma)
Urticaria treatment
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Glucuronate isomerase inhibitor
Choline acetyltransferase stimulant
Enteropeptidase inhibitor
Lipotropic
CYP2A5 substrate
Aminomuconate-semialdehyde dehydrogenase inhibitor
Pyroglutamyl-peptidase II inhibitor
CYP2A13 substrate
Kinesin antagonist
Kinesin-like protein 1 inhibitor
Acetylcholine M5 receptor antagonist
Histone deacetylase SIRT1 inhibitor
Beta-D-fucosidase inhibitor
Antiviral (Picornavirus)
Pterin deaminase inhibitor
Hippurate hydrolase inhibitor
Glutamine-tRNA ligase inhibitor
Licheninase inhibitor
Phenylpyruvate decarboxylase inhibitor
Catenin beta inhibitor
Dermatologic
Antineoplastic alkaloid
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Acetoacetate decarboxylase inhibitor
Urolithiasis treatment
Interleukin 10 agonist
4-Nitrophenylphosphatase inhibitor
2-Dehydropantoate 2-reductase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Nardilysin inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Nitric oxide scavenger
4-Hydroxyglutamate transaminase inhibitor
Metabolic disease treatment
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Pseudouridylate synthase inhibitor
Thiamine pyridinylase inhibitor
Dichloromuconate cycloisomerase inhibitor
Bisphosphoglycerate mutase inhibitor
CYP4B substrate
Protein kinase C alpha inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Opine dehydrogenase inhibitor
Bile-salt sulfotransferase inhibitor

Allyl-alcohol dehydrogenase inhibitor
Cytochrome-c3 hydrogenase inhibitor
Guanylate cyclase inhibitor
CYP19 substrate
Potassium channel (Voltage-sensitive) blocker
Chitosanase inhibitor
DNA ligase (ATP) inhibitor
Huntington's disease treatment
Threonine aldolase inhibitor
CYP1A inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Trimethyllysine dioxygenase inhibitor
Nitrile hydratase inhibitor
D-xylulose reductase inhibitor
Acetylenecarboxylate hydratase inhibitor
Dihydroxy-acid dehydratase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Plasmanyethanolamine desaturase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
GST T substrate
GST T1-1 substrate
Methane monooxygenase inhibitor
Venom exonuclease inhibitor
Granzyme A inhibitor
2-Oxoglutarate decarboxylase inhibitor
CYP1A inducer
Tauropine dehydrogenase inhibitor
Hyperprolactinemia treatment
SULT2A1 substrate
Ferredoxin hydrogenase inhibitor
Centromere associated protein inhibitor
5 Hydroxytryptamine 1A antagonist
Fibromyalgia syndrome treatment
Candidapepsin inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Calcium channel blocker
Polyamine oxidase inhibitor
Pregnane X receptor agonist
Ferredoxin-nitrite reductase inhibitor
Pectin lyase inhibitor
Sodium/calcium exchanger 1 inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Cholinergic
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Dynein ATPase inhibitor
Prolyl aminopeptidase inhibitor
Antineoplastic (lymphocytic leukemia)
Antiallergic
D-lactate dehydrogenase (cytochrome) inhibitor
CYP19 inhibitor

Antineoplastic (small cell lung cancer)
CYP26 inhibitor
Homospermidine synthase inhibitor
Narcotic antagonist
CYP1A2 inhibitor
LDLR expression enhancer
Tentoxilysin inhibitor
L-threonine 3-dehydrogenase inhibitor
CYP4A1 substrate
CDC25C inhibitor
Glutamate synthase (ferredoxin) inhibitor
3-Aminobutaryl-CoA ammonia-lyase inhibitor
Hot flush treatment
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Vasodilator
Aldehyde ferredoxin oxidoreductase inhibitor
Pyridoxine 4-oxidase inhibitor
Glycine receptor antagonist
Acetylcholine nicotinic antagonist
D-2-hydroxy-acid dehydrogenase inhibitor
Diisopropyl-fluorophosphatase inhibitor
Polygalacturonase inhibitor
Antineoplastic (brain cancer)
Arylalkyl acylamidase inhibitor
Coccolysin inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Hydroxylamine reductase (NADH) inhibitor
5 Hydroxytryptamine 1E antagonist
Diamine N-acetyltransferase inhibitor
Antineoplastic (lymphoma)
Aspartate-ammonia ligase (ADP-forming) inhibitor
3-Methylbutanal reductase inhibitor
5 Hydroxytryptamine 2A agonist
Cholestanetriol 26-monooxygenase inhibitor
Antineoplastic (ovarian cancer)
MAP kinase kinase 4 inhibitor
Farnesoid X receptor antagonist
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
CYP2C10 substrate
Glutamate 5-kinase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Uroporphyrinogen-III synthase inhibitor
Aerobactin synthase inhibitor
Raynaud's phenomenon treatment
Urease inhibitor
NADPH-ferrihemoprotein reductase inhibitor
CYP2B18 substrate
Myosin ATPase inhibitor
Antiarrhythmic
Acute neurologic disorders treatment

Alpha 1 adrenoreceptor antagonist
Sorbose dehydrogenase inhibitor
Quisqualate antagonist
Allophanate hydrolase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Acaricide
Membrane dipeptidase inhibitor
Pantothenase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Glucarate dehydratase inhibitor
Tyrosine kinase stimulant
Shock treatment
Interferon agonist
CYP1B1 substrate
Pitrilysin inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Glycerol dehydrogenase inhibitor
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
Valine decarboxylase inhibitor
Styrene-oxide isomerase inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
Arachidonic acid antagonist
CDC25 phosphatase inhibitor
Alcohol dehydrogenase (NADP⁺) inhibitor
Histamine H2 receptor agonist
Dynamin GTPase inhibitor
O-aminophenol oxidase inhibitor
Cytokine modulator
Hydroxymethylglutaryl-CoA lyase inhibitor
Mitochondrial intermediate peptidase inhibitor
Allantoate deiminase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Antipsoriatic
Iron-cytochrome-c reductase inhibitor
Leucolysin inhibitor
Aryldialkylphosphatase inhibitor
Telomerase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Phosphatidylinositol 3-kinase stimulant
Levanase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Chitinase inhibitor
Ethanolamine kinase inhibitor
Saluretic
Tryptophan alpha,beta-oxidase inhibitor
Thiol oxidase inhibitor
Benzoylformate decarboxylase inhibitor

Beta 1 adrenoreceptor agonist
NMDA receptor polyamine site antagonist
Stromelysin 2 inhibitor
Lipid peroxidase inhibitor
Eye irritation, inactive
Endo-1,3(4)-beta-glucanase inhibitor
Creatine kinase inhibitor
Glutamin-(asparagin-)ase inhibitor
Allantoinase inhibitor
Gingipain R inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
Testosterone 17beta-dehydrogenase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Aryl hydrocarbon receptor agonist
Lassitude treatment
11-Cis-retinyl-palmitate hydrolase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Prostaglandin-E2 9-reductase inhibitor
Glucuronolactone reductase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Maltose-transporting ATPase inhibitor
Aspergillopepsin I inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
L-lysine oxidase inhibitor
Ca2+/calmodulin-dependent protein kinase inhibitor
VEGF expression inhibitor
ICAM1 expression inhibitor
Bcl2 antagonist
3-Oxoadipate enol-lactonase inhibitor
Isopenicillin-N synthase inhibitor
Gentisate 1,2-dioxygenase inhibitor
Skin irritation, inactive
Bcl-xL inhibitor
Glutaminy-peptide cyclotransferase inhibitor
Carnitine O-octanoyltransferase inhibitor
Cocain dependency treatment
Alpha 1a adrenoreceptor antagonist
Nuclease inhibitor
Tocolytic
3'-Nucleotidase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
CYP4B1 substrate
Anthranilate 3-monooxygenase (deaminating) inhibitor

Bacterial efflux pump inhibitor
Saccharolysin inhibitor
Iduronate-2-sulfatase inhibitor
Protein kinase stimulant
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
DNA nucleotidylexotransferase inhibitor
Deoxyribose-phosphate aldolase inhibitor
Allantoin racemase inhibitor
Riboflavin phosphotransferase inhibitor
Phosphoinositide phospholipase C inhibitor
Pancreatic endopeptidase E inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Penicillin amidase inhibitor
Ribitol 2-dehydrogenase inhibitor
Benzoate 4-monooxygenase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Vomilenine glucosyltransferase inhibitor
Glucan 1,4-beta-glucosidase inhibitor
NMDA receptor polyamine site agonist
Serratia marcescens nuclease inhibitor
Diabetic nephropathy treatment
Prostaglandin D2 agonist
Agmatinase inhibitor
ADP-ribosylarginine hydrolase inhibitor
MO15-related protein kinase Pfmrk inhibitor
Indanol dehydrogenase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Anthranilate-CoA ligase inhibitor
DNA synthesis inhibitor
Antifibrinolytic
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Butyrylcholinesterase inhibitor
Neurotrophic factor
Sigma 3 receptor antagonist
Alkene monooxygenase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
N-acetyllactosamine synthase inhibitor
Protein synthesis stimulant
Prostacyclin agonist
Histone deacetylase SIRT2 inhibitor
SMN2 expression enhancer
Leucine transaminase inhibitor
Guanidinopropionase inhibitor

Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
CYP3A5 inducer
Dopamine D2S antagonist
Calcium channel (voltage-sensitive) blocker
Pim-3 kinase inhibitor
Arylsulfatase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Lombricine kinase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
GABA A receptor agonist
Adenylate cyclase I inhibitor
L-ascorbate peroxidase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
D-proline reductase (dithiol) inhibitor
Phenol 2-monooxygenase inhibitor
Gluconate dehydratase inhibitor
CTGF expression inhibitor
Glutamate N-acetyltransferase inhibitor
Aldehyde oxidase substrate
Anthranilate synthase inhibitor
2-Dehydropantoate aldolase inhibitor
Antineoplastic (non-small cell lung cancer)
Immunosuppressant
Histone deacetylase class III inhibitor
Endopeptidase La inhibitor
Alkylator
Cytostatic
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Anticarcinogenic
Muconate cycloisomerase inhibitor
Secretase alpha stimulant
Secretase stimulant
UGT2B11 substrate
5 Hydroxytryptamine 4 antagonist
Alpha-N-acetylglucosaminidase inhibitor
Antihypotensive
Histamine H3 receptor antagonist
(R)-limonene 6-monooxygenase inhibitor
Anthrax lethal factor inhibitor
Gamma-glutamyltransferase inhibitor
Acidifying agent gastric
Picornain 3C inhibitor
CYP24 inhibitor
Protein-tyrosine sulfotransferase inhibitor
Cyanate hydratase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Age-related macular degeneration treatment

Cysteine desulfurase inhibitor
Homoserine dehydrogenase inhibitor
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
Aminopeptidase Y inhibitor
CYP1A2 inducer
NAD(P)H dehydrogenase (quinone) inhibitor
Chitin deacetylase inhibitor
Glutamate release inhibitor
Retinopathy treatment
Leucine dehydrogenase inhibitor
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Sterol 24-C-methyltransferase inhibitor
Contraceptive female
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
5 Hydroxytryptamine 1B agonist
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
HIV-2 reverse transcriptase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Brachyurin inhibitor
Aconitate decarboxylase inhibitor
Choleretic
Acyl-CoA oxidase inhibitor
Beta 2 adrenoreceptor antagonist
Isoquinoline 1-oxidoreductase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Acyl-CoA dehydrogenase inhibitor
Formate-dihydrofolate ligase inhibitor
Diguanidinobutanase inhibitor
Deoxyhypusine synthase inhibitor
Lysine 2-monooxygenase inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Nav1.7 sodium channel blocker
Antiamyloidogenic
Epoxide hydrolase substrate
Pantoate 4-dehydrogenase inhibitor
Beta-amylase inhibitor
Catechol oxidase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Selenocysteine lyase inhibitor
Oxytocin agonist
Beta 1 adrenoreceptor antagonist
Analgesic, non-opioid
Lactaldehyde reductase inhibitor
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Tyrosine-protein kinase TYRO 10 inhibitor
5 Hydroxytryptamine 4A antagonist
Beta adrenoreceptor antagonist

Thioredoxin reductase inhibitor
CYP2C19 inducer
Interleukin 6 antagonist
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
Thromboxane agonist
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
Guanylate cyclase 1 inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Hydroxymethylbilane synthase inhibitor
Peroxidase inhibitor
Anabolic
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Cancer procoagulant inhibitor
Bone formation stimulant
Protein kinase B stimulant
Pyridoxal kinase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Phenylalanine(histidine) transaminase inhibitor
Calcium channel activator
Serine-pyruvate transaminase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Mevalonate kinase inhibitor
Analgesic stimulant
Antirickettsial
Haloalkane dehalogenase inhibitor
Hepatoprotectant
Fibroblast growth factor 1 agonist
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Atrolysin A inhibitor
Antihelminthic (Fasciola)
Glycerol dehydrogenase (NADP⁺) inhibitor
Galactoside O-acetyltransferase inhibitor
Aspergillopepsin II inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Phospholipase D1 inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Neuropsin inhibitor
Maleate hydratase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Cardioprotectant
Alpha-N-arabinofuranosidase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor

5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Cytosole dipeptidase inhibitor
Premenstrual syndrome treatment
Dopamine D2A antagonist
Cerebroside-sulfatase inhibitor
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Thermomycin inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Urotensin II agonist
Tryptophan transaminase inhibitor
Arylacetonitrilase inhibitor
Succinic dehydrogenase inhibitor
Anticataract
Glycine C-acetyltransferase inhibitor
Thiamine-phosphate kinase inhibitor
Sedoheptulose-bisphosphatase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Estrogen antagonist
D-threo-aldose 1-dehydrogenase inhibitor
Sigma receptor antagonist
SULT1A3 substrate
Sulfur dioxygenase inhibitor
Protein kinase C stimulant
Serine 3-dehydrogenase inhibitor
Extrapyramidal disorders treatment
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Sepsis treatment
Aspartyl aminopeptidase inhibitor
Acetate kinase inhibitor
2-Methylcitrate dehydratase inhibitor
CXC chemokine 4 receptor antagonist
Tryptophan 2-monooxygenase inhibitor
Ca²⁺-transporting ATPase inhibitor
DELTA14-sterol reductase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Carboxypeptidase M inhibitor
Inotropic
Neuronal nicotinic receptor antagonist
Oligopeptidase B inhibitor
3-Isopropylmalate dehydratase inhibitor
Formaldehyde dehydrogenase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
Gametolysin inhibitor
Hyperparathyroidism treatment
Glycerol dehydratase inhibitor
3-Oxosteroid 1-dehydrogenase inhibitor
Aldehyde dehydrogenase (NADP⁺) inhibitor

Dimethylallyltranstransferase inhibitor
Potassium channel Kv4.3 blocker
Shal potassium channel blocker
2-Hydroxy-3-oxopropionate reductase inhibitor
Glycine transporter 2 inhibitor
Autophagy inducer
DNA intercalator
Arginyltransferase inhibitor
CYP4F2 substrate
Aspartate racemase inhibitor
Pyroglutamyl-peptidase I inhibitor
GABA C receptor antagonist
CYP26A substrate
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
CYP2A11 substrate
Phenylacetate-CoA ligase inhibitor
Coagulant
Asparaginase inhibitor
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Acylglycerone-phosphate reductase inhibitor
Pectate lyase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
GABA transporter inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Retinyl-palmitate esterase inhibitor
2-Methyleneglutarate mutase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Azobenzene reductase inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Hydroxylysine kinase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Formimidoylglutamase inhibitor
Diuretic
Mental retardation treatment
Chondroitin 6-sulfotransferase inhibitor
Cholesterol antagonist
Sleep apnea treatment
CYP1A1 inhibitor
Anhydrotetracycline monooxygenase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
GABA uptake inhibitor
Asparaginyl endopeptidase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
UGT1A8 substrate
Picornain 2A inhibitor
Dopamine D5 antagonist

Opioid delta 2 receptor antagonist
Oxalate oxidase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Methionyl aminopeptidase 2 inhibitor
NMDA receptor phencyclidine site antagonist
Thiol S-methyltransferase inhibitor
Thermitase inhibitor
CYP2B4 substrate
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Lactoylglutathione lyase inhibitor
Mannonate dehydratase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Acetylcholine muscarinic agonist
3-Dehydroquinate dehydratase inhibitor
Sodium/calcium exchanger inhibitor
UGT1A6 substrate
Decylcitrate synthase inhibitor
Deacetoxycephalosporin-C synthase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Antiprotozoal (Babesia)
Ganglioside galactosyltransferase inhibitor
Nerve growth factor antagonist
Alpha-amylase inhibitor
Omega-amidase inhibitor
Phospholipase D inhibitor
GABA transporter 1 inhibitor
Benzaldehyde dehydrogenase (NAD+) inhibitor
NAD(P)H dehydrogenase (quinone) 1 inhibitor
Acetylcholine M4 receptor agonist
Betaine-homocysteine S-methyltransferase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Ribonuclease U2 inhibitor
Puromycin-sensitive aminopeptidase inhibitor
Allantoicase inhibitor
SULT1E1 substrate
Dactylysin inhibitor
Premature ejaculation treatment
Cellulase inhibitor
Glutathione S-transferase substrate
Delayed rectifier potassium channel blocker
CMP-N-acetylneuraminate monooxygenase inhibitor
Propanediol dehydratase inhibitor
CYP4F12 substrate
Choloylglycine hydrolase inhibitor
Acid-sensing ion channel blocker
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Acylphosphatase inhibitor

Heme oxygenase inhibitor
Narcolepsy treatment
Prolyl endopeptidase inhibitor
D(-)-tartrate dehydratase inhibitor
Galactose oxidase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Fibroblast growth factor agonist
3-Deoxy-8-phosphooctulonate synthase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Cholesterol synthesis inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
Guanidinobutyrase inhibitor
Carnitine palmitoyltransferase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Phosphorylase kinase inhibitor
UGT2B15 substrate
Sarcosine oxidase inhibitor
UGT2B7 substrate
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Tyrosine 2,3-aminomutase inhibitor
UGT1A7 substrate
Luteinizing hormone-releasing hormone agonist
3(or 17)beta-hydroxysteroid dehydrogenase inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Aldehyde dehydrogenase inhibitor
Dethiobiotin synthase inhibitor
Octadecanal decarbonylase inhibitor
CYP2C2 substrate
Dihydropyrimidinase inhibitor
Procollagen C-endopeptidase inhibitor
D-lactate dehydrogenase inhibitor
Bipolar disorder treatment
Atrolysin C inhibitor
ATP deaminase inhibitor
Prostaglandin H2 antagonist
Methionyl aminopeptidase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Postcoital contraceptive
Aryl-alcohol dehydrogenase (NADP⁺) inhibitor
Altronate dehydratase inhibitor
CYP1B1 inducer
Dopamine D2L antagonist
5 Hydroxytryptamine 6 agonist
Tryptophan 5 hydroxylase inhibitor
Lanosterol 14 alpha demethylase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
2-Aminoadipate transaminase inhibitor
Alcohol dehydrogenase [NAD(P)⁺] inhibitor
Assemblin inhibitor
Urotensin II antagonist

Beta-ureidopropionase inhibitor
Ca²⁺/calmodulin-dependent kinase II inhibitor
Chemokine receptor antagonist
Arginine deiminase inhibitor
MAO A inhibitor
Free radical scavenger
Antinephritic
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
UGT1A10 substrate
Sirtuin 2 inhibitor
Vascular adhesion protein 1 inhibitor
tRNA cytidyltransferase inhibitor
Isomaltulose synthase inhibitor
Histone-lysine N-methyltransferase inhibitor
Adenine deaminase inhibitor
Trimereylisin II inhibitor
Nicotinic receptor alpha7 subunit antagonist
Transcription factor STAT6 inhibitor
Glyceryl-ether monooxygenase inhibitor
Mycolysin inhibitor
(R)-aminopropanol dehydrogenase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
Heat shock protein 70 antagonist
Biotin carboxylase inhibitor
Cholesterol esterase inhibitor
Antineoplastic (bladder cancer)
Carboxy-cis,cis-muconate cyclase inhibitor
Protein-arginine deiminase inhibitor
Geranyltranstransferase inhibitor
D-arabinonolactone oxidase inhibitor
Tyrosine-ester sulfotransferase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Adenylate kinase inhibitor
ATP adenylyltransferase inhibitor
Nociceptin (N/OFQ) receptor agonist
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Cardiotonic
Acetylserotonin O-methyltransferase inhibitor
CYP2C18 inhibitor
Aspartate transaminase inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
CpG-Oligodeoxynucleotides inhibitor
Mycodextranase inhibitor
Tartrate decarboxylase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
CYP17 substrate
DNA methyltransferase I inhibitor
Preterm labor treatment
Integrin alpha2beta1 antagonist

Histidinol-phosphatase inhibitor
Hyaluronic acid agonist
Lysyl endopeptidase inhibitor
Sirtuin inhibitor
Malate-CoA ligase inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor
Pyruvate carboxylase inhibitor

Apomorphine hydrochloride

Molecular Mechanism (initial) :

dopamine D2 agonist

Molecular Mechanism (repurposed) :

dopamine D4 agonist

initial indication(s):

Parkinson's disease

Repurposed indication(s):

erectile dysfunction

Predicted Activities

5 Hydroxytryptamine release stimulant

Tyrosine 3 hydroxylase inhibitor

Dopamine D2A antagonist

Anaphylatoxin receptor antagonist

Antitussive

UGT1A9 substrate

Antihypoxic

Dopamine D5 antagonist

Nicotinic alpha6beta3beta4alpha5 receptor antagonist

Membrane permeability inhibitor

Nicotinic alpha4beta4 receptor agonist

Histamine release stimulant

Octopamine antagonist

UGT1A substrate

(S)-6-hydroxynicotine oxidase inhibitor

(R)-6-hydroxynicotine oxidase inhibitor

Oxygen scavenger

Neurotransmitter antagonist

MAP kinase stimulant

Nicotinic alpha2beta2 receptor antagonist

Respiratory analeptic

Nucleotide metabolism regulator

Antineurotic

Aryl-acylamidase inhibitor

General pump inhibitor

Muscle relaxant

Cyclic AMP phosphodiesterase inhibitor

CYP2D2 inhibitor

Leukopoiesis stimulant

Antinociceptive

Opioid kappa 3 receptor antagonist
Ovulation inhibitor
Antidyskinetic
Antineoplastic alkaloid
UDP-glucuronosyltransferase substrate
CYP2H substrate
Analeptic
CYP3A2 substrate
UGT1A3 substrate
CYP2E1 inducer
Sigma receptor agonist
CYP2C8 substrate
Skeletal muscle relaxant
CYP2D15 substrate
Peroxidase substrate
UGT2B12 substrate
Antidote
Spasmolytic
CYP2B6 substrate
JAK2 expression inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Antialcoholic
CYP3A3 substrate
CYP2C11 substrate
Antiischemic, cerebral
CYP3A4 substrate
Antiparkinsonian
5 Hydroxytryptamine uptake stimulant
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
CYP2D6 substrate
Prolactin inhibitor

Antiparkinsonian, rigidity relieving

CYP2C19 substrate
CYP2D substrate
Vasodilator, peripheral
CYP1A substrate
Antisecretoric
Alopecia treatment
Aldehyde oxidase inhibitor
CYP2D1 substrate
CYP3A5 substrate
CYP3A substrate
Acute neurologic disorders treatment
CYP2C12 substrate
Cardioprotectant
CYP2A6 substrate
Fibrinogen receptor antagonist
Antiperistaltic
Neurodegenerative diseases treatment
CYP3A1 substrate

Laxative
Antitussive, narcotic
TP53 expression enhancer
Flavin-containing monooxygenase substrate
Acetylcholine neuromuscular blocking agent
Antiparkinsonian, tremor relieving
Tetrahydroxynaphthalene reductase inhibitor
5 Hydroxytryptamine 7L antagonist
N-methylhydantoinase (ATP-hydrolysing) inhibitor
CYP2C substrate
CYP3A7 substrate
FMO3 substrate
Polarisation stimulant
CYP1A1 substrate
CYP2A8 substrate
Platelet adhesion inhibitor
Leukopoiesis inhibitor
CYP2C9 substrate
Nootropic
Antiviral (Adenovirus)
CYP2A substrate
CYP2D16 substrate
Sigma 1 receptor agonist
1,4-Lactonase inhibitor
Menopausal disorders treatment
5 Hydroxytryptamine 1 antagonist
CYP2C18 substrate
Histamine release inhibitor
Calcium channel activator
4-Nitrophenol 2-monooxygenase inhibitor
5 Hydroxytryptamine 7 agonist
5 Hydroxytryptamine 1A antagonist
Methyltransferase substrate
Dementia treatment
Monoamine uptake inhibitor
Apoptosis agonist
N-hydroxyarylamine O-acetyltransferase inhibitor
Gonadotropin antagonist
P-glycoprotein substrate
Neurotransmitter uptake inhibitor
Platelet aggregation stimulant
Oxytocic
UGT1A4 substrate
Psychosexual dysfunction treatment
CYP3A4 inducer
5 Hydroxytryptamine 5A antagonist
Adrenaline release stimulant
Uterine relaxant
Opioid dependency treatment
UGT2B7 substrate

Glutathione thiolesterase inhibitor
Vasoprotector
CYP1A2 substrate
UGT1A1 substrate
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Expectorant
CYP3A inducer
Hemostatic
Amyotrophic lateral sclerosis treatment
Albendazole monooxygenase inhibitor
Kidney function stimulant
5 Hydroxytryptamine 7 antagonist
NADPH-cytochrome-c2 reductase inhibitor
Adenylate cyclase V inhibitor
CYP2E1 substrate
CYP2E substrate
CYP2A3 substrate
Hyperprolactinemia treatment
Dopamine D2S antagonist
UGT2B9 substrate
P-glycoprotein inhibitor

Erectile dysfunction treatment

Choleretic
5 Hydroxytryptamine 5 antagonist
CYP2C9 inducer
Xenobiotic-transporting ATPase inhibitor
AR expression inhibitor
Antiinfertility, female
Aminobutyraldehyde dehydrogenase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
P-glycoprotein 1 inhibitor
Alpha 2b adrenoreceptor antagonist
Diuretic inhibitor
MAO B substrate
Steroid N-acetylglucosaminyltransferase inhibitor
Alkane 1-monooxygenase inhibitor
Neuropeptide Y4 antagonist
CYP2C19 inducer
Arylacetonitrilase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
MMP9 expression inhibitor
5 Hydroxytryptamine 7S antagonist
Anesthetic
Uterine stimulant
5 Hydroxytryptamine 2B agonist
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Membrane integrity agonist
2-Enoate reductase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor

HCV IRES inhibitor
UGT2B substrate
EIF4E expression inhibitor
Dopamine D2L antagonist
Lymphocytopoiesis inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Prunasin beta-glucosidase inhibitor
5 Hydroxytryptamine 1F antagonist
Vascular dementia treatment
Antipyretic
Cocain dependency treatment
Thioredoxin inhibitor
Pin1 inhibitor
Analgesic
Cytochrome P450 stimulant
Dopamine release stimulant
Calcium channel (voltage-sensitive) activator
UGT2B18 substrate
Chlordecone reductase inhibitor
CYP2A1 substrate
CYP2B substrate
CYP2A2 substrate
UGT2B4 substrate
UGT1A6 substrate
Immunosuppressant
Antitoxic
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
NADPH peroxidase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Linoleoyl-CoA desaturase inhibitor
5 Hydroxytryptamine antagonist
UGT1A8 substrate
Apoptosis antagonist
Trimethylamine-oxide aldolase inhibitor
Alpha 2 adrenoreceptor antagonist
Anesthetic local
Tropinesterase inhibitor
Fibrinolytic
UGT1A10 substrate
Raynaud's phenomenon treatment
Apyrase inhibitor
Restless leg syndrome treatment
CYP2B11 substrate
Male reproductive dysfunction treatment
Sigma receptor antagonist
Alpha 2c adrenoreceptor antagonist
Lipid peroxidase inhibitor
NOS2 expression inhibitor
Feruloyl esterase inhibitor

Nicotine dehydrogenase inhibitor
CYP1B1 substrate
Huntington's disease treatment
5 Hydroxytryptamine 2 antagonist
Stroke treatment
UGT2B1 substrate
Antiulcerative
Gastritis treatment
NADPH-ferrihemoprotein reductase inhibitor
Thiamine-triphosphatase inhibitor
Antiprotozoal (Trypanosoma)
Cyclic AMP agonist
Kinase inhibitor
Phosphoenolpyruvate mutase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
RELA expression inhibitor
27-Hydroxycholesterol 7 α -monooxygenase inhibitor
Alpha 2a adrenoreceptor antagonist
Creatine kinase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Antiinflammatory
Antineoplastic enhancer
5-O-(4-coumaroyl)-D-quinic acid 3'-monooxygenase inhibitor
Free radical scavenger
Narcotic antagonist
Nav1.1 sodium channel blocker
Hydroxylamine oxidase inhibitor
SULT1E1 substrate
Aspartate-phenylpyruvate transaminase inhibitor
Sodium channel blocker
Histamine H1 receptor agonist
Spasmolytic, Papaverin-like
CYP2C6 substrate
Vasodilator
Retinoic acid metabolism inhibitor
Peptidoglycan glycosyltransferase inhibitor
Neurotrophic factor enhancer
Taurine dehydrogenase inhibitor
Glyoxylate oxidase inhibitor
Glutamyl endopeptidase II inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Monoamine oxidase substrate
5 Hydroxytryptamine 1E antagonist
UDP-N-acetylglucosamine 4-epimerase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Fibromyalgia syndrome treatment
Alkylator
UGT2B10 substrate
5 Hydroxytryptamine 2B antagonist
CYP1A1 inhibitor

Cell wall biosynthesis inhibitor
Phosphatase inhibitor
Catenin beta inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Phobic disorders treatment
UGT2B15 substrate
Nicotinic alpha4beta2 receptor antagonist
Loop diuretic
Steroid synthesis inhibitor
Transcription factor NF kappa A inhibitor
VEGF expression inhibitor
Antiinflammatory, intestinal
CYP1B substrate
FMO1 substrate
Opioid mu 2 receptor antagonist
CYP2C8 inducer
CYP2A4 substrate
Acetylcholine nicotinic antagonist
Antimyopathies
Diuretic
MAP kinase kinase 4 inhibitor
Macrophage colony stimulating factor agonist
Caspase 8 stimulant
Antiprotozoal (Amoeba)
Cancer associated disorders treatment
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Antihypotensive
HIF1A expression inhibitor
Vascular (periferal) disease treatment
Protein-disulfide reductase (glutathione) inhibitor
Antituberculosic
Glycosylphosphatidylinositol phospholipase D inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Acid-sensing ion channel blocker
Tankyrase inhibitor
Acidifying agent non gastric
Gluconate 2-dehydrogenase (acceptor) inhibitor
Antithrombotic
APOA1 expression enhancer
Alpha adrenoreceptor antagonist
5 Hydroxytryptamine 2C antagonist
Adenylate cyclase inhibitor
Antineoplastic (multiple myeloma)
Alcohol dehydrogenase (acceptor) inhibitor
Antiadrenergic
Antidepressant
Testosterone 17beta-dehydrogenase (NADP⁺) inhibitor
CYP19A1 expression inhibitor
Diabetic neuropathy treatment

Mood disorders treatment
Salicylate 1-monooxygenase inhibitor
Thyroxine 5-deiodinase inhibitor
Protein kinase stimulant
Morphine 6-dehydrogenase inhibitor
CYP2A5 substrate
Radiosensitizer
CYP2B2 substrate
Menstruation disorders treatment
Insulysin inhibitor
Iron antagonist
4-Hydroxymandelate oxidase inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Fusarinine-C ornithinesterase inhibitor
Antipruritic
Polarisation inhibitor
Prolactin release inhibitor
Anesthetic general
3-Phytase inhibitor
UGT1A5 substrate
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Prion diseases treatment
5 Hydroxytryptamine 2A antagonist
Fatty-acyl-CoA synthase inhibitor
GST M substrate
Adrenergic, ophthalmic
Alpha 3 adrenoreceptor agonist
Arylsulfate sulfotransferase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Nicotinic receptor alpha7 subunit antagonist
Tryptophan 2,3-dioxygenase inhibitor
Sugar-phosphatase inhibitor
Acylcarnitine hydrolase inhibitor
Manganese peroxidase inhibitor
Phthalate 4,5-dioxygenase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Radioprotector
4-Coumarate-CoA ligase inhibitor
UGT2B7H substrate
UGT2B7Y substrate
Adrenaline antagonist
MAO A substrate
NMDA receptor glutamate site antagonist
DOPA decarboxylase inhibitor
Cardiovascular analeptic
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Thromboxane B2 antagonist
Antimigraine
Taurine-2-oxoglutarate transaminase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor

Antimutagenic
Pseudolysin inhibitor
Opioid mu 1 receptor antagonist
Glutathione reductase inhibitor
Antihypertensive
Hyponitrite reductase inhibitor
Gentisate 1,2-dioxygenase inhibitor
Superoxide dismutase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Caspase 3 stimulant
CF transmembrane conductance regulator agonist
Histidine kinase inhibitor
RNA synthesis inhibitor
Antiseborrheic
CYP2J2 substrate
Antihelminthic (Nematodes)
Antioxidant
Nitric oxide antagonist
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
CYP2G1 substrate
Tardive dyskinesia treatment
Glycerol 2-dehydrogenase (NADP+) inhibitor
Venom exonuclease inhibitor
Formate-dihydrofolate ligase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Peptidyl-dipeptidase B inhibitor
TNF expression inhibitor
Cytochrome-b5 reductase substrate
TH expression enhancer
Nitrite reductase (NO-forming) inhibitor
Dopamine D1A antagonist
Carboxypeptidase Taq inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Nav1.3 sodium channel blocker
Methylamine-glutamate N-methyltransferase inhibitor
Glucose oxidase inhibitor
SULT1A1 substrate
Antipsychotic
Alpha adrenoreceptor agonist
Glycolate dehydrogenase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Cholinergic antagonist
Flavin-containing monooxygenase inhibitor
Preneoplastic conditions treatment
Iduronate-2-sulfatase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Alkylacetylglycerophosphatase inhibitor
Antismoking
Neuronal nicotinic receptor antagonist
Antidepressant, Imipramin-like

UGT1A7 substrate
Phosphopantothienoylcysteine decarboxylase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Liver X receptor antagonist
Sulfite oxidase inhibitor
HMOX1 expression enhancer
Opioid kappa 1 receptor antagonist
Phenylpyruvate decarboxylase inhibitor
CYP19 inhibitor
Clavamate synthase inhibitor
Carnosine synthase inhibitor
Alpha 1 adrenoreceptor agonist
Alpha 1 adrenoreceptor antagonist
Acetylcholine antagonist
Complement factor D inhibitor
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
Muscular dystrophy treatment
GABA C receptor agonist
HIV-1 integrase inhibitor
Estrogen receptor beta antagonist
CYP7 inhibitor
Fructose 5-dehydrogenase inhibitor
Threonine aldolase inhibitor
Ferredoxin-nitrite reductase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Dependence treatment
DNA-3-methyladenine glycosylase I inhibitor
Estrogen antagonist
Iodide peroxidase inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
Sulfur reductase inhibitor
UGT2B28 substrate
Ferredoxin hydrogenase inhibitor
DNA polymerase I inhibitor
Glyoxylate reductase inhibitor
Nicotinic alpha3beta4 receptor agonist
Testosterone 17beta-dehydrogenase inhibitor
CYP2C10 substrate
Quisqualate antagonist
Antiviral (Poxvirus)
5 Hydroxytryptamine 1B antagonist
Hippurate hydrolase inhibitor
Estradiol 17 beta dehydrogenase 2 inhibitor
DNA ligase (ATP) inhibitor
Sulfotransferase substrate
Histamine agonist
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Cyclin-dependent kinase 6 inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor

Antineoplastic (gastric cancer)
Inotropic
Nucleoside oxidase (H₂O₂-forming) inhibitor
Endometriosis treatment
Trimethylamine dehydrogenase inhibitor
CYP2J substrate
CYP1A inducer
SULT1A3 substrate
Succinate-semialdehyde dehydrogenase [NAD(P)⁺] inhibitor
Indanol dehydrogenase inhibitor
Antimycobacterial
5-Hydroxytryptamine 2A agonist
HIV-1 integrase (3'-Processing) inhibitor
Antiviral (Herpes)
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
Squalene epoxidase inhibitor
Phospholipid-translocating ATPase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Acetylcholinesterase inhibitor
CC chemokine receptor 2B antagonist
RNA directed DNA polymerase inhibitor
Azobenzene reductase inhibitor
Dimethylargininase inhibitor
Ornithine cyclodeaminase inhibitor
Amine dehydrogenase inhibitor
Glycerol dehydrogenase (NADP⁺) inhibitor
Histidinol dehydrogenase inhibitor
Antiviral (Influenza)
Ca²⁺/calmodulin-dependent kinase I inhibitor
HIV-1 integrase (Strand Transfer) inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Alpha-glucosidase inhibitor
Shikimate 5-dehydrogenase inhibitor
Protein kinase C beta inhibitor
Histamine N-methyltransferase inhibitor
CYP2E1 inhibitor
Gout treatment
Anti-amyloidogenic
Alpha-N-acetylglucosaminidase inhibitor
Nitrate reductase (cytochrome) inhibitor
Hydrogen dehydrogenase inhibitor
UGT2B11 substrate
NMDA receptor antagonist
Sulfite reductase inhibitor
Bcl2 antagonist
Dihydroxy-acid dehydratase inhibitor
Antiviral (Picornavirus)
Wee-1 tyrosine kinase inhibitor
Alkene monooxygenase inhibitor

Pyroglutamyl-peptidase II inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
2-Haloacid dehalogenase inhibitor
Leukotriene-C4 synthase inhibitor
Venombin AB inhibitor
Quinoprotein glucose dehydrogenase inhibitor
CTGF expression inhibitor
Breast cancer-resistant protein inhibitor
Glucose-6-phosphate translocase inhibitor
Protein kinase C mu inhibitor
Cyclooxygenase substrate
NMDA receptor polyamine site antagonist
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
GST A substrate
Phloroglucinol reductase inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
CYP19 substrate
Nitric oxide scavenger
GABA transporter 3 inhibitor
Hot flush treatment
Phenol 2-monooxygenase inhibitor
Mediator release inhibitor
Protein kinase C zeta inhibitor
Microtubule formation inhibitor
5 Hydroxytryptamine 1D antagonist
Cytostatic
Antinaupathic
5 Hydroxytryptamine 6 antagonist
Botulin neurotoxin A light chain inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Histidine decarboxylase inhibitor
CDC25A inhibitor
Isopenicillin-N epimerase inhibitor
Cholinergic
UGT2B17 substrate
Mucositis treatment
Smooth muscle myosin light chain kinase inhibitor
Linoleate diol synthase inhibitor
GABA aminotransferase inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Antihelminthic (*Fasciola*)
CYP4A2 substrate
Gynecological disorders treatment
Polyribonucleotide nucleotidyltransferase inhibitor
NMDA receptor phencyclidine site antagonist
Anthranilate synthase inhibitor
Opioid delta 1 receptor antagonist
Limulus clotting factor B inhibitor

Hydroxyquinol 1,2-dioxygenase inhibitor
12-Lipoxygenase inhibitor
Osmotin inhibitor
Antiacromegalic
Phosphatidylserine decarboxylase inhibitor
Ca²⁺-transporting ATPase inhibitor
Protein kinase C η inhibitor
Pectate lyase inhibitor
CYP1A2 inducer
Anthranilate 3-monooxygenase (deaminating) inhibitor
Neurotrophic factor
Glycogen synthase stimulant
Isoquinoline 1-oxidoreductase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Antiviral (Rhinovirus)
Glycerol-3-phosphate oxidase inhibitor
Opioid delta 2 receptor antagonist
Tubulin antagonist
Protein kinase C η inhibitor
Lactose synthase inhibitor
Cystathionine beta-synthase inhibitor
Analgesic stimulant
Homogentisate 1,2-dioxygenase inhibitor
Penicillin amidase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Protein kinase C γ inhibitor
Diphosphomevalonate decarboxylase inhibitor
CYP2C8 inhibitor
Chitosanase inhibitor
Bcl-xL inhibitor
Heat shock protein antagonist
Urolithiasis treatment
Antiinflammatory, ophthalmic
Dopamine transporter inhibitor
Oligo-1,6-glucosidase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Viral entry inhibitor
Antidote, heavy metal
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Nitrite reductase [NAD(P)H] inhibitor
N-acylmannosamine kinase inhibitor
Protein kinase C ϵ inhibitor
Interleukin 10 agonist
Succinic dehydrogenase inhibitor
H⁺-exporting ATPase inhibitor
Vesicle monoamine transporter inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Heat shock protein agonist

Di-trans,poly-cis-decaprenylcistransferase inhibitor
Heat shock protein 90 antagonist
Thymidylate 5'-phosphatase inhibitor
Fibrolase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Dopamine D2B antagonist
Glutaminase inhibitor
3-Methylbutanal reductase inhibitor
Dopachrome isomerase inhibitor
CDC25B inhibitor
CYP2B1 substrate
5 Hydroxytryptamine 4 antagonist
Protein kinase A inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Glutathione S-transferase substrate
Arginine 2-monooxygenase inhibitor
N-formylmethionyl-peptidase inhibitor
Glutamate decarboxylase inhibitor
Antineurogenic pain
Matrix metalloproteinase 2 (membrane-type) inhibitor
Gluconate 5-dehydrogenase inhibitor
Poly(ADP-ribose) polymerase 2 inhibitor
Alpha 1d adrenoreceptor antagonist
Antibiotic
Phenylalanine 4-hydroxylase inhibitor
N-acetylneuraminate synthase inhibitor
Topoisomerase II inhibitor
Nav1.5 sodium channel blocker
Intermittent claudication treatment
Gamma-butyrobetaine dioxygenase inhibitor
Aldehyde oxidase substrate
DELTA24-sterol reductase inhibitor
3-Cyanoalanine hydratase inhibitor
Mucomembranous protector
Transforming growth factor beta 1 agonist
Meprin B inhibitor
Aldehyde dehydrogenase 2 substrate
Cyclic AMP modulator
Pyruvate decarboxylase inhibitor
Vomilenine glucosyltransferase inhibitor
Histone deacetylase SIRT2 inhibitor
Phenylalanine decarboxylase inhibitor
Adrenergic
4,5-Dihydroxyphthalate decarboxylase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Lysine 2,3-aminomutase inhibitor
Sphinganine kinase inhibitor
Tauropine dehydrogenase inhibitor
Cyclohexanone monooxygenase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor

Phenol O-methyltransferase inhibitor
5 Hydroxytryptamine 4A antagonist
Histone deacetylase SIRT2 stimulant
Chitinase inhibitor
Peroxidase inhibitor
Acetylcholine nicotinic agonist
CYP1A1 inducer
Histone deacetylase class III inhibitor
NADH kinase inhibitor
SULT2A1 substrate
Stipitatonate decarboxylase inhibitor
Age-related macular degeneration treatment
Poly(beta-D-mannuronate) lyase inhibitor
Histidinol-phosphatase inhibitor
Estrogen alpha receptor agonist
Sigma 2 receptor antagonist
Nav1.2 sodium channel blocker
Antiprotozoal (Leishmania)
Cysteine-S-conjugate beta-lyase inhibitor
Glycerol-1-phosphatase inhibitor
Guanidinoacetase inhibitor
Arylmalonate decarboxylase inhibitor
Catechol O methyltransferase inhibitor
Anhydrotetracycline monooxygenase inhibitor
4-Hydroxyproline epimerase inhibitor
Antibacterial
CDC25C inhibitor
Cerebroside-sulfatase inhibitor
Beta tubulin antagonist
CYP2C29 substrate
Nociceptin (N/OFQ) receptor agonist
Capillary fragility treatment
Kinesin antagonist
Kinesin-like protein 1 inhibitor
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
Antineoplastic (non-small cell lung cancer)
2-Nitropropane dioxygenase inhibitor
Vanilloid 1 agonist
Chenodeoxycholoyltaurine hydrolase inhibitor
Oxytocin agonist
L-ascorbate peroxidase inhibitor
Pim-1 kinase inhibitor
GABA C receptor antagonist
Tannase inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
Sickle-cell anemia treatment
Valine-tRNA ligase inhibitor
S-formylglutathione hydrolase inhibitor
Glutamin-(asparagin-)ase inhibitor
Antiemetic

X-methyl-His dipeptidase inhibitor
 Acylphosphatase inhibitor
 CYP2F1 substrate
 LDLR expression enhancer
 3-Hydroxybenzoate 4-monooxygenase inhibitor
 Cyclamate sulfohydrolase inhibitor
 Beta-fructofuranosidase inhibitor
 Dolichol kinase inhibitor
 L lactate dehydrogenase inhibitor
 Phosphatidylinositol 3-kinase stimulant
 Topoisomerase I inhibitor
 Fatty acid synthase inhibitor
 Prostaglandin-A1 DELTA-isomerase inhibitor
 Formaldehyde transketolase inhibitor
 5 Hydroxytryptamine 6 agonist
 Fructan beta-fructosidase inhibitor
 Cyclomaltodextrinase inhibitor
 Antitreponemal
 4-Hydroxybenzoate 3-monooxygenase inhibitor
 Antipruritic, allergic
 Sigma 1 receptor antagonist
 Hepatoprotectant
 Antihemorrhagic
 Cyclohexyl-isocyanide hydratase inhibitor
 Vesicle monoamine transporter 2 inhibitor
 Sodium/bile acid cotransporter inhibitor
 Antidiarrheal
 N-benzyloxycarbonylglycine hydrolase inhibitor
 D-amino-acid dehydrogenase inhibitor
 Beta 1 adrenoreceptor agonist
 Obsessive-compulsive disorder treatment
 Opioid kappa 2 receptor antagonist
 Opioid kappa 2b receptor antagonist

Acetylsalicylic acid

Molecular Mechanism (initial) :

cyclooxygenase inhibitor

Molecular Mechanism (repurposed) :

cyclooxygenase inhibitor

initial indication(s):

inflammation

pain

Repurposed indication(s):

thrombosis

Predicted Activities

Fibrinolytic (thrombosis)

N-hydroxyarylamine O-acetyltransferase inhibitor

Antipyretic (pain)

Antiseborrheic

Prolyl aminopeptidase inhibitor
Prostaglandin-E2 9-reductase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Chlordecone reductase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Arginine 2-monooxygenase inhibitor
Glucose oxidase inhibitor

Antiseptic (inflammation)

Methylenetetrahydrofolate reductase (NADPH) inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Glutathione thiolesterase inhibitor
Glutamyl endopeptidase II inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Sugar-phosphatase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Dextranase inhibitor
Arylsulfate sulfotransferase inhibitor
Aryl-acylamidase inhibitor
Arylacetonitrilase inhibitor
Benzoate 4-monooxygenase inhibitor
Pullulanase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
5-O-(4-coumaroyl)-D-quininate 3'-monooxygenase inhibitor
Sphinganine kinase inhibitor
Fusarinine-C ornithinesterase inhibitor
Alkane 1-monooxygenase inhibitor
NADH kinase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Glycerol dehydratase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Creatininase inhibitor
Centromere associated protein inhibitor
Fragilysin inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Phenol O-methyltransferase inhibitor
Dimethylargininase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Sulfite reductase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
1,4-Lactonase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
5 Hydroxytryptamine release inhibitor

Chenodeoxycholytaurine hydrolase inhibitor
Superoxide dismutase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Lipid metabolism regulator
Allyl-alcohol dehydrogenase inhibitor
Tryptophanamidase inhibitor
Taurine dehydrogenase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Corticosteroid side-chain-isomerase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
tRNA-pseudouridine synthase I inhibitor
Fatty-acyl-CoA synthase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Aryldialkylphosphatase inhibitor
Threonine aldolase inhibitor
Adenomatous polyposis treatment
Spermidine dehydrogenase inhibitor
Polygalacturonase inhibitor
Aspartate-ammonia ligase inhibitor
Gluconate 5-dehydrogenase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Oxidoreductase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Mucomembranous protector
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Mannitol-1-phosphatase inhibitor
Polyamine-transporting ATPase inhibitor
Alcohol oxidase inhibitor
Acetylerase inhibitor
Pectate lyase inhibitor
Feruloyl esterase inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
2-Enoate reductase inhibitor
Sarcosine oxidase inhibitor
N-acetylneuraminate synthase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
S-alkylcysteine lyase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
ADP-thymidine kinase inhibitor
Membrane permeability inhibitor
4-Hydroxyglutamate transaminase inhibitor
Exoribonuclease II inhibitor
N-Acyl-D-aspartate deacylase inhibitor

3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
Poly(alpha-L-gulonate) lyase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Fructose 5-dehydrogenase inhibitor
Formaldehyde transketolase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Mucinamylserine mucinaminidase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Carbon-monoxide dehydrogenase inhibitor
Limulus clotting factor B inhibitor
Glyoxylate reductase inhibitor
Opine dehydrogenase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Lombricine kinase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Diiodophenylpyruvate reductase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Uroporphyrinogen-III synthase inhibitor
CYP2J substrate
Benzoate-CoA ligase inhibitor
Lysine 2,3-aminomutase inhibitor
Ferredoxin-nitrite reductase inhibitor
Mitochondrial processing peptidase inhibitor
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
Gluconolactonase inhibitor
Transketolase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Urethanase inhibitor
Leukotriene-B₄ 20-monooxygenase inhibitor
Phosphatidylserine decarboxylase inhibitor
CYP2J2 substrate
Peptide-N₄-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
N-acylmannosamine kinase inhibitor
4-Hydroxyproline epimerase inhibitor
Respiratory analeptic
Complement factor D inhibitor
Arylesterase inhibitor
Ecdysone 20-monooxygenase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor

Glyoxylate oxidase inhibitor
Nitrate reductase (cytochrome) inhibitor
Membrane integrity agonist
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Cyanoalanine nitrilase inhibitor
Phobic disorders treatment
Arylalkyl acylamidase inhibitor
Pterin deaminase inhibitor
Antiinflammatory
Hydroxylamine reductase inhibitor
L-glucuronate reductase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Pyruvate decarboxylase inhibitor
L-glutamate oxidase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Lactaldehyde reductase inhibitor
Antieczematic
Phospholipid-translocating ATPase inhibitor
3-Cyanoalanine hydratase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Leucolysin inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Trans-pentaprenyltranstransferase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Sulfite oxidase inhibitor
tRNA nucleotidyltransferase inhibitor
UGT2B1 substrate
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Histidinol-phosphatase inhibitor
Hydroxylamine reductase (NADH) inhibitor
Ornithine cyclodeaminase inhibitor
Cytoprotectant
Platelet adhesion inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Venombin AB inhibitor
Myosin ATPase inhibitor
Phosphatidylglycerophosphatase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Nicotinate dehydrogenase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
TP53 expression enhancer
Fructan beta-fructosidase inhibitor
Astringent
Carnitinamidase inhibitor
Arylmalonate decarboxylase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Hydrogen dehydrogenase inhibitor

Methylumbelliferyl-acetate deacetylase inhibitor
N-formylmethionyl-peptidase inhibitor
Lysostaphin inhibitor
Anthranilate-CoA ligase inhibitor
Phenylacetate-CoA ligase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Dimethylmaleate hydratase inhibitor
Lipoprotein lipase inhibitor
D-xylulose reductase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Nucleotide metabolism regulator
Glucan endo-1,3-alpha-glucosidase inhibitor
Amine dehydrogenase inhibitor
Carboxypeptidase Taq inhibitor
Penicillin amidase inhibitor
Nitrilase inhibitor
Glycolate dehydrogenase inhibitor
Guanidinoacetase inhibitor
Cyclomaltodextrinase inhibitor
Hyponitrite reductase inhibitor
Skin irritation, inactive
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Sulfite dehydrogenase inhibitor
Biotinidase inhibitor
L-3-cyanoalanine synthase inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Glutaminase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Phenylpyruvate decarboxylase inhibitor
Camphor 1,2-monooxygenase inhibitor
CYP2C12 substrate
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Aldehyde dehydrogenase (NADP+) inhibitor
Antiinflammatory, intestinal
Polyporopepsin inhibitor
Malate dehydrogenase (acceptor) inhibitor
Preneoplastic conditions treatment
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Protein-glutamate methylesterase inhibitor

Oryzin inhibitor
Creatinine deaminase inhibitor
Aspartyl aminopeptidase inhibitor
Nitrite reductase (NO-forming) inhibitor
Indanol dehydrogenase inhibitor
Membrane integrity antagonist
Macrophage colony stimulating factor agonist
Bothrolysin inhibitor
Antiinfective
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Gly-X carboxypeptidase inhibitor
L-threonine 3-dehydrogenase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Lysase inhibitor
Acetate kinase inhibitor
Ompin inhibitor
Protein-disulfide reductase (glutathione) inhibitor
3-Oxoadipate enol-lactonase inhibitor
Histidine N-acetyltransferase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Isopenicillin-N epimerase inhibitor
Cyclooxygenase 3 inhibitor
Thymidylate 5'-phosphatase inhibitor
Analeptic
Cl--transporting ATPase inhibitor
NADPH peroxidase inhibitor
4-Hydroxy-2-oxoglutarate aldolase inhibitor
2-Oxoglutarate decarboxylase inhibitor
Cholesterol antagonist
Gentisate 1,2-dioxygenase inhibitor
Beta glucuronidase inhibitor
H⁺-exporting ATPase inhibitor
Oxalate oxidase inhibitor
Beta-amylase inhibitor
S-formylglutathione hydrolase inhibitor
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Histamine release inhibitor
Kidney function stimulant
Salicylate 1-monooxygenase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Levanase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Inulinase inhibitor
GABA C receptor agonist
Acetylornithine deacetylase inhibitor
Acylcarnitine hydrolase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor

Glycerol 2-dehydrogenase (NADP+) inhibitor
Butyrate-CoA ligase inhibitor
Nicotine dehydrogenase inhibitor
Coccolysin inhibitor
Pantoate 4-dehydrogenase inhibitor
Fucosterol-epoxide lyase inhibitor
Nicotinic $\alpha_6\beta_3\beta_4\alpha_5$ receptor antagonist
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Insulin promoter
X-methyl-His dipeptidase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Antiuremic
Erythropoiesis stimulant
Expectorant
Keratolytic
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Styrene-oxide isomerase inhibitor
Aldehyde oxidase inhibitor
Benzoylformate decarboxylase inhibitor
Licheninase inhibitor
Cathepsin T inhibitor
Shikimate 5-dehydrogenase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Anaphylatoxin receptor antagonist
Cyclohexanone monooxygenase inhibitor
Phosphoglycerate mutase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Glucan 1,4- α -maltotetraohydrolase inhibitor
Acetoacetate decarboxylase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Alanine-tRNA ligase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Gastrin inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Creatinase inhibitor
Glyceryl-ether monooxygenase inhibitor
Acetoin dehydrogenase inhibitor
Glucuronate isomerase inhibitor
Mucositis treatment
Methylaspartate ammonia-lyase inhibitor
Trimethylamine-oxide aldolase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Lactate 2-monooxygenase inhibitor
Catechol oxidase inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
Pseudolysin inhibitor
Diisopropyl-fluorophosphatase inhibitor
Antiviral (Picornavirus)

Alkylacetylgllycerophosphatase inhibitor
Fumarate reductase (NADH) inhibitor
GST A substrate
Glycerol-1-phosphatase inhibitor
Thiosulfate dehydrogenase inhibitor
Plasmanyethanolamine desaturase inhibitor
Cyclopentanone monooxygenase inhibitor
Mediator release inhibitor
Chitosanase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Aspergillus nuclease S1 inhibitor
Antithrombotic
Arylformamidase inhibitor
CYP2C9 substrate
Ubiquitin thiolesterase inhibitor
Reductant
Antihypoxic
Acylaminoacyl-peptidase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Porphobilinogen synthase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Eye irritation, inactive
Peroxidase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Loop diuretic
Inorganic diphosphatase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Aspartate-tRNA ligase inhibitor
Alpha-N-arabinofuranosidase inhibitor
Gestagen antagonist
Peptidyl-dipeptidase Dcp inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Valine dehydrogenase (NADP+) inhibitor
Platelet aggregation stimulant
Mannose isomerase inhibitor
Mandelate racemase inhibitor
Aminoacylase inhibitor
Formate-dihydrofolate ligase inhibitor
4-Coumarate-CoA ligase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Vomilenine glucosyltransferase inhibitor
CYP2C8 substrate
Acetylcholine neuromuscular blocking agent
Shikimate O-hydroxycinnamoyltransferase inhibitor
Diiodotyrosine transaminase inhibitor
Hippurate hydrolase inhibitor
Paraoxonase substrate
NAD+ synthase (glutamine-hydrolysing) inhibitor
CYP2B5 substrate
Phloroglucinol reductase inhibitor

Muramoyltetrapeptide carboxypeptidase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Antihelminthic (Nematodes)
Pitrilysin inhibitor
Carboxypeptidase D inhibitor
Thiamine pyridinylase inhibitor
Procollagen N-endorpeptidase inhibitor
Aspartyltransferase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
3-Phytase inhibitor
Serine 3-dehydrogenase inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Sphinganine-1-phosphate aldolase inhibitor
IgA-specific metalloendorpeptidase inhibitor
Phosphatidate phosphatase inhibitor
Methanol dehydrogenase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Dihydroxy-acid dehydratase inhibitor
Endopeptidase So inhibitor
Gallate decarboxylase inhibitor
Thromboxane B2 antagonist
CYP2D16 substrate
Glucan 1,6-alpha-glucosidase inhibitor
Ovulation inhibitor
Thiopurine S-methyltransferase inhibitor
Thioredoxin inhibitor
Choline dehydrogenase inhibitor
Antihypercholesterolemic
D-2-hydroxy-acid dehydrogenase inhibitor
APOA1 expression enhancer
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Endo-1,4-beta-xylanase inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
Peptidoglycan glycosyltransferase inhibitor
D-amino-acid dehydrogenase inhibitor
Haloalkane dehalogenase inhibitor
Sulfur dioxygenase inhibitor
Phenylalanine dehydrogenase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Linoleate diol synthase inhibitor
Acylphosphatase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Aryl-alcohol dehydrogenase inhibitor
Glycerol dehydrogenase (NADP+) inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Manganese peroxidase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor

Non-steroidal antiinflammatory agent
Carboxylate reductase inhibitor
Procollagen glucosyltransferase inhibitor
CYP2A4 substrate
Cyclamate sulfohydrolase inhibitor
Acute neurologic disorders treatment
Acid phosphatase inhibitor
Tryptophan transaminase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Leucine dehydrogenase inhibitor
Choline-phosphate cytidyltransferase inhibitor
Ferrochelataase inhibitor
Hydroxylamine oxidase inhibitor
Allantoinase inhibitor
Calcium channel (voltage-sensitive) activator
Gingipain K inhibitor
Nicotinamidase inhibitor
Cytochrome-b5 reductase inhibitor
Adenylyl-sulfate reductase inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Alopecia treatment
Glucan 1,4-beta-glucosidase inhibitor
Dolichyl-phosphatase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
4-Hydroxybenzoate-CoA ligase inhibitor
L-amino-acid oxidase inhibitor
Urease inhibitor
Farnesyltranstransferase inhibitor
D-cysteine desulfhydrase inhibitor
CYP2F1 substrate
Mandelate 4-monooxygenase inhibitor
Nitrile hydratase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
GABA aminotransferase inhibitor
Valine decarboxylase inhibitor
L-iduronidase inhibitor
2-Nitropropane dioxygenase inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Proteasome ATPase inhibitor
Alcohol O-acetyltransferase inhibitor
CYP4A11 substrate
Phosphoinositide phospholipase C inhibitor
Tyrosine-ester sulfotransferase inhibitor
Aspartoacylase inhibitor
HMOX1 expression enhancer
Clavamate synthase inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Carboxylesterase inhibitor

FMO1 substrate
N-methyl-2-oxoglutaramate hydrolase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Gonadotropin antagonist
Glycerol-3-phosphate oxidase inhibitor
Acyl-lysine deacylase inhibitor
Tauropine dehydrogenase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Vasodilator, peripheral
5 Hydroxytryptamine uptake stimulant
N-acetyllactosamine synthase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Branched-chain-amino-acid transaminase inhibitor
Trimethylamine dehydrogenase inhibitor
Leukotriene-C4 synthase inhibitor
JAK2 expression inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Ribitol 2-dehydrogenase inhibitor
UGT2B substrate
Leukopoiesis stimulant
Sickle-cell anemia treatment
Alpha-glucuronidase inhibitor
Malate oxidase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Cytochrome-c3 hydrogenase inhibitor
CYP2C8 inhibitor
Oxygen scavenger
Antinociceptive
Antipruritic, allergic
L-ascorbate peroxidase inhibitor
Cyclic AMP agonist
Hydroxymethylbilane synthase inhibitor
Enteropeptidase inhibitor
ICAM1 expression inhibitor
Diamine N-acetyltransferase inhibitor
Caspase 8 stimulant
Alpha-Methylacyl-CoA racemase inhibitor
Glucose 1-dehydrogenase inhibitor
Membrane permeability enhancer
Mucolytic
Galactose oxidase inhibitor
Trimethylamine-N-oxide reductase inhibitor
Free radical scavenger
Glycine amidinotransferase inhibitor
Cutinase inhibitor
Guanidinoacetate kinase inhibitor
Phosphatase inhibitor

Insulysin inhibitor
HIF1A expression inhibitor
Formate dehydrogenase inhibitor
Antipsoriatic
Glutamate-tRNA ligase inhibitor
Acaricide
Guanidinoacetate N-methyltransferase inhibitor
Choleretic
Nicotinic alpha2beta2 receptor antagonist
L-galactonolactone oxidase inhibitor
O-aminophenol oxidase inhibitor
CYP2H substrate
Peptidylamidoglycolate lyase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
RNA-directed RNA polymerase inhibitor
TRPA1 agonist
Glucosamine-6-phosphate deaminase inhibitor
Fibrolase inhibitor
Antiviral (Influenza)
Rheumatoid arthritis treatment
L-lactate dehydrogenase (cytochrome) inhibitor
Antiviral (Adenovirus)
Glycine dehydrogenase (decarboxylating) inhibitor
Cyclic AMP phosphodiesterase inhibitor
Dihydrodipicolinate reductase inhibitor
Antisecretoric
Propanediol dehydratase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Rhodotorulapepsin inhibitor
Prephenate dehydrogenase inhibitor
Snapalysin inhibitor
Antiviral (Rhinovirus)
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Para amino benzoic acid antagonist
Monophenol monooxygenase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
Catalase inhibitor
Omega-amidase inhibitor
CYP2C substrate
Formaldehyde dehydrogenase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Antiulcerative
Maillard reaction inhibitor
Venom exonuclease inhibitor
Beta-mannosidase inhibitor
Retinal dehydrogenase inhibitor
Alpha-amylase inhibitor
Undecaprenyl-diphosphatase inhibitor
Pseudouridylate synthase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor

27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Hyaluronic acid agonist
Antiischemic, cerebral
Arylsulfatase inhibitor
Carboxymethylenebutenolidase inhibitor
Pancreatic elastase inhibitor
Mitochondrial intermediate peptidase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
Histamine release stimulant
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
4-Alpha-glucanotransferase inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Acylglycerone-phosphate reductase inhibitor
Muscular dystrophy treatment
Dopachrome isomerase inhibitor
Diuretic inhibitor
Antitussive
Dermatologic
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
AR expression inhibitor
CYP3A1 substrate
Ferredoxin hydrogenase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Laccase inhibitor
Adenylyl-sulfate kinase inhibitor
Antiamyloidogenic
Aminopeptidase Y inhibitor
Diaminopropionate ammonia-lyase inhibitor
Sulfur reductase inhibitor
Pyroglutamyl-peptidase II inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
CYP2C9 inducer
Phenol 2-monooxygenase inhibitor
Antimyopathies
Deoxyribose-phosphate aldolase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Menopausal disorders treatment
6-Methylsalicylate decarboxylase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
4-Phytase inhibitor
N-acetylneuraminase lyase inhibitor
Anesthetic general
Diphosphomevalonate decarboxylase inhibitor
Malate dehydrogenase inhibitor
Carminative
Bile-salt sulfotransferase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor

Serine-phosphoethanolamine synthase inhibitor
Neurotransmitter antagonist
Antineurogenic pain
TNF expression inhibitor
CYP19A1 expression inhibitor
Gamma-glutamyltransferase inhibitor
Xylan 1,4-beta-xylosidase inhibitor
Immunosuppressant
Phosphoenolpyruvate mutase inhibitor
Lipid peroxidase inhibitor
Chitinase inhibitor
2-Pyrocatechuate decarboxylase inhibitor
Pyruvate dehydrogenase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
CYP1A2 inducer
Hypolipemic
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
CYP2E1 inducer
Horriylsin inhibitor
Orotate reductase (NADH) inhibitor
NOS2 expression inhibitor
Aryl sulfotransferase inhibitor
Propionate-CoA ligase inhibitor
Dipeptidase E inhibitor
Apyrase inhibitor
Pyroglutamyl-peptidase I inhibitor
Antianginal
Pediculicide
Polyneuridine-aldehyde esterase inhibitor
Arylamine N-acetyltransferase inhibitor
Metalloprotease D inhibitor
Antidiabetic symptomatic
Aconitate decarboxylase inhibitor
Acetylenecarboxylate hydratase inhibitor
Thiol oxidase inhibitor
Prunasin beta-glucosidase inhibitor
UDP-glucuronosyltransferase substrate
Pin1 inhibitor
Antiparkinsonian, rigidity relieving
Plastoquinol-plastocyanin reductase inhibitor
Fibrinogen receptor antagonist
EIF4E expression inhibitor
Catechol 1,2-dioxygenase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
Glutathione peroxidase inhibitor
Carnitine 3-dehydrogenase inhibitor
CYP4A substrate
D-stereospecific aminopeptidase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor

3'-Nucleotidase inhibitor
Sclerosant
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Myeloblastin inhibitor
Thiosulfate sulfurtransferase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Morphine 6-dehydrogenase inhibitor
CYP3A4 inducer
Caspase 3 stimulant
Glycogen synthase stimulant
Renal tissue kallikrein inhibitor
Antimutagenic
Allophanate hydrolase inhibitor
Histone acetyltransferase inhibitor
L-fuconate dehydratase inhibitor
D-lactate dehydrogenase inhibitor
Carnosine synthase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
CYP2D15 substrate
4,5-Dihydroxyphthalate decarboxylase inhibitor
CYP2A5 substrate
Meprin B inhibitor
CYP3A inducer
Deoxyribonuclease (pyrimidine dimer) inhibitor
Vasodilator, coronary
Allantoate deiminase inhibitor
Choline kinase inhibitor
Ferredoxin-NADP+ reductase inhibitor
Asparagine-tRNA ligase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Aspergillopepsin I inhibitor
Glycine transaminase inhibitor
Aureolysin inhibitor
Bontoxilysin inhibitor
Antidote
Alcohol dehydrogenase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Cysteine desulfurase inhibitor
Protocatechuate 3,4-dioxygenase inhibitor
tRNA adenylyltransferase inhibitor
Leukopoiesis inhibitor
UGT1A substrate
Acetolactate decarboxylase inhibitor
Proline dehydrogenase inhibitor
MAP kinase stimulant
4-Hydroxymandelate oxidase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
D-glutamate oxidase inhibitor
ATP phosphoribosyltransferase inhibitor

Thiamine-phosphate kinase inhibitor
Catechol 2,3-dioxygenase inhibitor
Choline-sulfatase inhibitor
Carnitine dehydratase inhibitor
Laxative
Leucine transaminase inhibitor
UGT1A6 substrate
Serine-glyoxylate transaminase inhibitor
Antituberculosic
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Calcium-sensing receptor agonist
Poly(3-hydroxybutyrate) depolymerase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
CYP3A5 substrate
Glutamate 5-kinase inhibitor
Vasodilator
Antitoxic
CYP2B10 substrate
Pyridoxine 4-oxidase inhibitor
Phenylalanine decarboxylase inhibitor
Isoamylase inhibitor
Pyruvate carboxylase inhibitor
Sweetener
Antiparkinsonian, tremor relieving
Cell wall biosynthesis inhibitor
CYP2A2 substrate
Lactose synthase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
CYP2A1 substrate
Radioprotector
Alpha-pinene-oxide decyclase inhibitor
Fumarylacetoacetase inhibitor
Hemostatic
Retinoic acid metabolism inhibitor
MMP9 expression inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Pappalysin-1 inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Antimycobacterial
Isoquinoline 1-oxidoreductase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
Sorbitol dehydrogenase inhibitor
Lipocortins synthesis antagonist
Glycine-tRNA ligase inhibitor
Bisphosphoglycerate mutase inhibitor
Acyl-CoA oxidase inhibitor
Alkylglycerone-phosphate synthase inhibitor
Glucarate dehydratase inhibitor

Glutamate dehydrogenase [NAD(P)+] inhibitor
Interleukin 10 agonist
Iron-cytochrome-c reductase inhibitor
Xylose isomerase inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Diaminopimelate dehydrogenase inhibitor
Cerebroside-sulfatase inhibitor
Nitrate reductase inhibitor
UGT1A4 substrate
Serine-pyruvate transaminase inhibitor
Cytostatic
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
4-Nitrophenylphosphatase inhibitor
CYP2A6 substrate
Tyrosine 3 hydroxylase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Cysteine synthase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Antiparasitic
UGT1A1 substrate
(S)-2-hydroxy-acid oxidase inhibitor
Galactokinase inhibitor
Antipruritic, non-allergic
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
CYP4A2 substrate
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Linoleoyl-CoA desaturase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
IgA-specific serine endopeptidase inhibitor
Antidiabetic
Pyridoxine 5-dehydrogenase inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Gametolysin inhibitor
Tropinesterase inhibitor
Antibacterial
Electrolyte absorption antagonist
Hepatoprotectant
Envelysin inhibitor
Guanidinobutyrase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
CYP2C10 substrate
Lipoprotein lipase stimulant
Glutamin-(asparagin-)ase inhibitor
Serratia marcescens nuclease inhibitor
Antispirochetal
Antipruritic
Aspartate transaminase inhibitor
CYP3A3 substrate

1,2-alpha-L-fucosidase inhibitor
DOPA decarboxylase inhibitor
Aspartate racemase inhibitor
Antiinflammatory, ophthalmic
Gluconate dehydratase inhibitor
Steroid synthesis inhibitor
Malate-CoA ligase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Triose-phosphate isomerase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Guanidinodeoxy-scyllo-inositol-4-phosphatase inhibitor
RELA expression inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Antifungal
3-Chloro-D-alanine dehydrochlorinase inhibitor
Flavin-containing monooxygenase inhibitor
Inflammatory Bowel disease treatment
Prion diseases treatment
Blasticidin-S deaminase inhibitor
Oxidizing agent
Anticarcinogenic
Octopamine antagonist
Cellulase inhibitor
Chemopreventive
Antiviral (CMV)
Thioredoxin reductase inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Phosphoserine phosphatase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Antihyperlipoproteinemic
NF-E2-related factor 2 stimulant
Histidinol dehydrogenase inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor
Acetate-CoA ligase inhibitor
Apoptosis antagonist
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Dichloromuconate cycloisomerase inhibitor
Uric acid excretion stimulant
Orotate reductase (NADPH) inhibitor
CYP2C19 inducer
Pim-1 kinase inhibitor
CYP7 inhibitor
BRAF expression inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Oxaloacetate decarboxylase inhibitor
Glycine N-acyltransferase inhibitor

2-Haloacid dehalogenase inhibitor
Dihydroorotase inhibitor
ATP adenylyltransferase inhibitor
Cystathionine gamma-lyase inhibitor
Iduronate-2-sulfatase inhibitor
Radiosensitizer
Oxoglutarate dehydrogenase (lipoamide) inhibitor
CYP2C18 substrate
3-Isopropylmalate dehydratase inhibitor
Phosphatidate cytidyltransferase inhibitor
Antifibrinolytic
Saluretic
D-arabinonolactone oxidase inhibitor
HIV-2 reverse transcriptase inhibitor
Tetrahydroxynaphthalene reductase inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Glycine C-acetyltransferase inhibitor
Adrenaline release stimulant
Dementia treatment
Leukotriene synthesis inhibitor
CYP2B6 substrate
Nucleoside oxidase (H₂O₂-forming) inhibitor
Vanillyl-alcohol oxidase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
DNA ligase (ATP) inhibitor
CYP3A2 substrate
Glutamine-tRNA ligase inhibitor
Cerevisin inhibitor
Antinephritic
Glycerol dehydrogenase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
3-Oxosteroid 1-dehydrogenase inhibitor
UGT1A7 substrate
CYP2B11 substrate
Fibroblast growth factor agonist
DNA synthesis inhibitor
GST M substrate
Antidyskinetic
Muconate cycloisomerase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Nardilysin inhibitor
Cytochrome P450 stimulant
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Alanine transaminase inhibitor
Nootropic
Choloylglycine hydrolase inhibitor
Protein phosphatase inhibitor
Isopenicillin-N synthase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor

Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Proline racemase inhibitor
CYP2A substrate
Tryptophan dimethylallyltransferase inhibitor
Vasoprotector
Lysine 2-monooxygenase inhibitor
Methane monooxygenase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Phosphoglycolate phosphatase inhibitor
CF transmembrane conductance regulator agonist
Acrosin inhibitor
Aldehyde dehydrogenase inhibitor
Deoxyribonuclease I inhibitor
Dihydropyrimidinase inhibitor
Pectin lyase inhibitor
Glutamate N-acetyltransferase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Thiol S-methyltransferase inhibitor
Ganglioside galactosyltransferase inhibitor
Opioid kappa 3 receptor antagonist
Antiperistaltic
Cancer associated disorders treatment
Glycogen (starch) synthase inhibitor
ATP deaminase inhibitor
Protein synthesis stimulant
4-Hydroxybenzoate 1-hydroxylase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
Tripeptide aminopeptidase inhibitor
Chloride peroxidase inhibitor
CYP1A inducer
Acidifying agent non gastric
Mevalonate kinase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Autoimmune disorders treatment
Beta-ureidopropionase inhibitor
NAD⁺ kinase inhibitor
Sulfate adenylyltransferase inhibitor
Anthranilate phosphoribosyltransferase inhibitor
Serralysin inhibitor
Alpha-L-rhamnosidase inhibitor
X-Pro dipeptidase inhibitor
Antiprotozoal (Amoeba)
CYP4A1 substrate
Homogentisate 1,2-dioxygenase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Protein-tyrosine phosphatase inhibitor
Anesthetic
CYP2C29 substrate

Lactaldehyde dehydrogenase inhibitor
Guanidinopropionase inhibitor
Succinate dehydrogenase inhibitor
CYP3A7 substrate
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor
Anti-Helicobacter pylori
Beta-D-fucosidase inhibitor
Allantoicase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Clostripain inhibitor
Agaritine gamma-glutamyltransferase inhibitor
Iodide peroxidase inhibitor
Galactolipase inhibitor
Protein-arginine deiminase inhibitor
Transcription factor NF kappa A inhibitor
Inositol oxygenase inhibitor
Aldehyde dehydrogenase 2 substrate
Testosterone 17beta-dehydrogenase inhibitor
Quinate 5-dehydrogenase inhibitor
Trimethyllysine dioxygenase inhibitor
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
Atherosclerosis treatment
UGT2B7 substrate
Immunostimulant
Cholesterol oxidase inhibitor
Antiinfertility, female
Histidine kinase inhibitor
Laminaribiose phosphorylase inhibitor
Peptidyl-dipeptidase B inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Antiprotozoal (Trypanosoma)
Acetylserotonin O-methyltransferase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Antidiabetic (type 2)
3-Oxoacid CoA-transferase inhibitor
Apoptosis agonist
Aspergillopepsin II inhibitor
Cholesterol synthesis inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
Spasmolytic, urinary
L-lysine 6-transaminase inhibitor
UGT2B4 substrate
Endopeptidase La inhibitor
Thimet oligopeptidase inhibitor
CYP2D2 inhibitor
Imidazoleacetate 4-monooxygenase inhibitor
CYP4F2 substrate
FMO3 substrate

Coproporphyrinogen oxidase inhibitor
UGT1A9 substrate
Gastritis treatment
Maleate isomerase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor
Intermittent claudication treatment
Antiprotozoal (Leishmania)
UGT2B9 substrate
Phospholipase A2 inhibitor
Betaine-aldehyde dehydrogenase inhibitor
Hepatocyte nuclear factor 4 alpha agonist
Hepatocyte nuclear factor agonist
Tentoxilysin inhibitor
Glycine hydroxymethyltransferase inhibitor
Wound healing agent
3-Hydroxybutyrate dehydrogenase inhibitor
4-Hydroxybenzoate 3-monooxygenase [NAD(P)H] inhibitor
Glutamate decarboxylase inhibitor
Mannonate dehydratase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Picornain 3C inhibitor
Farnesoid X receptor antagonist
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Chelator
Cystathionine beta-lyase inhibitor
CYP3A substrate
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Interleukin 4 antagonist
Glutathione-disulfide reductase inhibitor
UGT2B17 substrate
Chaperonin ATPase inhibitor
Glucan 1,3-beta-glucosidase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Protein-tyrosine sulfotransferase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Uroporphyrinogen decarboxylase inhibitor
Gout treatment
CYP2C6 substrate
Adenine deaminase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Pantothenase inhibitor
VCAM1 expression inhibitor
Succinic dehydrogenase inhibitor
UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
Antiprotozoal (Toxoplasma)
UGT2B28 substrate
Methylglutamate dehydrogenase inhibitor
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Photosensitizer
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor

UGT1A10 substrate
Pyridoxamine-phosphate oxidase inhibitor
Signal peptidase I inhibitor
Adenylate kinase inhibitor
2-Aminoadipate transaminase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
CYP3A4 substrate
Diuretic
Retinol O-fatty-acyltransferase inhibitor
Levansucrase inhibitor
Penicillopepsin inhibitor
Antialcoholic
Quercetin 2,3-dioxygenase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Interferon antagonist
Phenylalanine 4-hydroxylase inhibitor
Antirickettsial
D-Octopine dehydrogenase inhibitor
Neurotrophic factor enhancer
Microtubule formation inhibitor
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Selenocysteine lyase inhibitor
Valine-tRNA ligase inhibitor
Phosphate acetyltransferase inhibitor
Orcinol 2-monooxygenase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
2-Methylcitrate dehydratase inhibitor
Lactate-malate transhydrogenase inhibitor
Antidiarrheal
Coagulant
Proteasome endopeptidase complex inhibitor
Phospholipase C inhibitor
CYP2B18 substrate
Diabetic retinopathy treatment
Transactivator transcription protein inhibitor
Interferon gamma antagonist
Glutamate (mGluR5) agonist
Acetolactate synthase inhibitor
ATPase inhibitor
Histidine decarboxylase inhibitor
Limulus clotting factor C inhibitor
3-Deoxy-8-phosphooctulonate synthase inhibitor
Saccharolysin inhibitor
Retinyl-palmitate esterase inhibitor
Thermitase inhibitor
Lysyl oxidase inhibitor
Potassium channel (Ca-activated) activator
Peptidyl-Lys metalloendopeptidase inhibitor
Analgesic stimulant
Antimycoplasmal

Oxaloacetate tautomerase inhibitor
3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor
Anthrax lethal factor inhibitor
Cyclooxygenase substrate
Rhizopuspepsin inhibitor
Maleate hydratase inhibitor
Isocitrate dehydrogenase (NADP+) inhibitor
CYP2E1 substrate
FMN reductase inhibitor
Maltose-transporting ATPase inhibitor
Cardiovascular analeptic
CYP2C3 substrate
CYP2G1 substrate
Vascular (periferal) disease treatment
Phospholipase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Anesthetic local
Amyloid beta precursor protein antagonist
Homoserine dehydrogenase inhibitor
Dactylisin inhibitor
Antihelmintic
Transcription factor NF kappa B inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
GST T substrate
GST T1-1 substrate
Diabetic neuropathy treatment
RNA synthesis inhibitor
Ethanolaminephosphotransferase inhibitor
Channel-conductance-controlling ATPase inhibitor
Bilirubin oxidase inhibitor
CYP2E substrate
Cystathionine beta-synthase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Tyrosine 2,3-aminomutase inhibitor
Skin whitener
Tripeptidyl-peptidase I inhibitor
Dynein ATPase inhibitor
Cyclooxygenase 1 inhibitor
3C-like protease (Human coronavirus) inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
Gingipain R inhibitor
UGT1A3 substrate
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Protein-tyrosine phosphatase 1B inhibitor
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
UDP-glucose 4-epimerase inhibitor
Oligo-1,6-glucosidase inhibitor
Xanthine oxidase inhibitor
Transcription factor NF kappa B stimulant

Transcription factor stimulant
Hydroxysteroid dehydrogenase inhibitor
Yeast ribonuclease inhibitor
Asparaginase inhibitor
Tannase inhibitor
Arachidonic acid antagonist
Alanine dehydrogenase inhibitor
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Antileprosy
Urate-ribonucleotide phosphorylase inhibitor
NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
UGT1A5 substrate
3-Methylbutanal reductase inhibitor
Lactase inhibitor
Cellobiose phosphorylase inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Lipoxygenase substrate
Age-related macular degeneration treatment
NADH dehydrogenase inhibitor
Anthranilate synthase inhibitor
Dopamine release stimulant
Antiprotozoal (Coccidial)
Cystic fibrosis treatment
Aminopeptidase B inhibitor
Peptidyl-glycinamidase inhibitor
Glutamate dehydrogenase (NADP⁺) inhibitor
Riboflavin phosphotransferase inhibitor
Antithyroid
P-glycoprotein substrate
Methionine decarboxylase inhibitor
Beta lactamase inhibitor
Thromboxane synthase stimulant
Adenine nucleotide translocase inhibitor
Threonine ammonia-lyase inhibitor
CYP2C19 substrate
HDL-cholesterol increasing
Chondroitin 6-sulfotransferase inhibitor
Nitric-oxide synthase stimulant
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Glutamate (mGluR6) antagonist
Nucleoside-diphosphatase inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Ligase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Lysine decarboxylase inhibitor
Lipoprotein disorders treatment
Protein kinase stimulant
NAD⁺ nucleosidase inhibitor

CYP2A3 substrate
Proliferative diseases treatment
Creatine kinase inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
2-Dehydropantoate aldolase inhibitor
Cytosine deaminase inhibitor
DELTA14-sterol reductase inhibitor
Antihemorrhagic
8-Amino-7-oxononanoate synthase inhibitor
Peroxidase substrate
Agmatinase inhibitor
Transthyretin amyloid fibril formation inhibitor
Cytosol alanyl aminopeptidase inhibitor
2-Aminohexano-6-lactam racemase inhibitor
Ribose-5-phosphate isomerase inhibitor
Serine-sulfate ammonia-lyase inhibitor
Alkene monooxygenase inhibitor
Hematopoietic inhibitor
Metabolic disease treatment
Cathepsin G inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Stromelysin 2 inhibitor
Growth hormone agonist
Thyroxine 5-deiodinase inhibitor
D-alanine transaminase inhibitor
Cardioprotectant
Antiviral (Influenza A)
Nuclease inhibitor
Acetylspermidine deacetylase inhibitor
Homocitrate synthase inhibitor
Dolichol kinase inhibitor
Platelet aggregation inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Glutamate dehydrogenase inhibitor
Retinoic acid beta receptor agonist
Aerobactin synthase inhibitor
CYP2B4 substrate
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Alanine carboxypeptidase inhibitor
N6-methyl-lysine oxidase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Trimerelysin II inhibitor
Severe acute respiratory syndrome treatment
Cyclooxygenase inhibitor
SMN2 expression enhancer
Ketol-acid reductoisomerase inhibitor
Nitric oxide scavenger
Altronate dehydratase inhibitor
Antioxidant
Albendazole monooxygenase inhibitor

5-Aminolevulinate synthase inhibitor
Glucuronolactone reductase inhibitor
Acyloxyacyl hydrolase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Glutathione synthase inhibitor
Thiamine-triphosphatase inhibitor
Alkaline phosphatase inhibitor
Cell adhesion molecule inhibitor
Ulcerative colitis treatment
Antiviral (Herpes)
Nicotinamide-nucleotide adenylyltransferase inhibitor
Subtilisin inhibitor
Glycine receptor agonist
Beta-cyclopiazone dehydrogenase inhibitor
Cycloartenol synthase inhibitor
Phosphofructokinase-1 inhibitor
5 Hydroxytryptamine 4C antagonist
5 Hydroxytryptamine 4D antagonist
Prenyl-diphosphatase inhibitor
Anticataract
Antibacterial, ophthalmic
Sepiapterin reductase inhibitor
Atrolysin A inhibitor
X-His dipeptidase inhibitor
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Spasmolytic
Choline sulfotransferase inhibitor
Galactoside O-acetyltransferase inhibitor
Urocanate hydratase inhibitor
tRNA (guanine-N1-)-methyltransferase inhibitor
Insulin sensitizer
Furin inhibitor
Antineoplastic, alkylator
Kexin inhibitor
Biliverdin reductase inhibitor
Alpha,alpha-trehalase inhibitor
3-Deoxy-7-phosphoheptulonate synthase inhibitor
Caspase 3 inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Keratoses actinic (solar) treatment
Serum-glucocorticoid regulated kinase 1 inhibitor
2-Methyleneglutarate mutase inhibitor
Aldosterone antagonist
Antiprotozoal (Trichomonas)
Transcription factor inhibitor
L-lysine oxidase inhibitor
Macrophage migration inhibitory factor inhibitor
Arginine deiminase inhibitor
CYP2A8 substrate

Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Pim kinase inhibitor
UGT2B10 substrate
Growth stimulant
Endopeptidase inhibitor
Aspartate kinase inhibitor
UGT2B12 substrate
Na⁺-transporting two-sector ATPase inhibitor
Trehalose-phosphatase inhibitor
Stipitatonate decarboxylase inhibitor
Opioid dependency treatment
3-Dehydroquinone dehydratase inhibitor
Aromatic-amino-acid transaminase inhibitor
Sucrose synthase inhibitor
Osteoarthritis treatment
Tryptophan alpha,beta-oxidase inhibitor
5 Hydroxytryptamine release stimulant
Cysteine transaminase inhibitor
Acid-sensing ion channel blocker
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Antiviral (Poxvirus)
HIV-1 integrase (3'-Processing) inhibitor
Brachyurin inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor
Nitric oxide antagonist
Glutamate (mGluR8) agonist
5 Hydroxytryptamine 7 agonist
Aminolevulinate transaminase inhibitor
GABA B receptor agonist
GABA C receptor antagonist
CYP26A substrate
CYP4B substrate
3-Dehydroquinone synthase inhibitor
Deoxycytidine deaminase inhibitor
NADPH oxidase inhibitor
Mycodextranase inhibitor
D-proline reductase (dithiol) inhibitor
CYP2B substrate
NAD(P)H dehydrogenase (quinone) inhibitor
HIV-1 integrase (Strand Transfer) inhibitor
Prolactin inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Lipotropic
Urticaria treatment
Antianorexic
Guanylate kinase inhibitor
Poly(ADP-ribose) glycohydrolase inhibitor
Procollagen C-endopeptidase inhibitor
Antibiotic
Diacylglycerol cholinephosphotransferase inhibitor

L lactate dehydrogenase inhibitor
Putrescine oxidase inhibitor
Sphingosine 1-phosphate receptor antagonist
Aspartate-semialdehyde dehydrogenase inhibitor
Flavin-containing monooxygenase substrate
Analgesic
Undecaprenyl-phosphate mannosyltransferase inhibitor
SULT1A1 substrate
Aconitate hydratase inhibitor
Sphingosine 1-phosphate receptor 1 antagonist
Isocitrate lyase inhibitor
UGT1A8 substrate
Peptidylglycine monooxygenase inhibitor
Argininosuccinate synthase inhibitor
Histamine agonist
Tyrosine kinase stimulant
NAT1 substrate
Phosphonoacetate hydrolase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Luteinizing hormone-releasing hormone agonist
tRNA cytidyltransferase inhibitor
Sulfinioalanine decarboxylase inhibitor
Pyrroline-5-carboxylate reductase inhibitor
Decylcitrate synthase inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Cholate-CoA ligase inhibitor
Menstruation disorders treatment
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Xanthommatin reductase inhibitor
Diguanidinobutanase inhibitor
Factor XIIIa stimulant
Hepatic disorders treatment
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
Prephenate dehydratase inhibitor
Gaucher disease treatment
Interleukin agonist
L-Serine ammonia-lyase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
Hematopoietic
Nucleotidase inhibitor
HIV-1 integrase inhibitor
Thrombolytic
Antineoplastic (thyroid cancer)
Amino-acid racemase inhibitor
Phosphomevalonate kinase inhibitor
GABA transporter 3 inhibitor
CTGF expression inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Thiamine-phosphate diphosphorylase inhibitor

Calcium regulator
Taurine-2-oxoglutarate transaminase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
Antieczematic atopic
Antiemphysemic
Adenylylsulphatase inhibitor
Phosphoribulokinase inhibitor
Ornithine-oxo-acid transaminase inhibitor
CYP4B1 substrate
CTP synthase inhibitor
Pregnane X receptor agonist
Glycine N-benzoyltransferase inhibitor
Diabetic nephropathy treatment
Amyloid beta aggregation inhibitor
Ophthalmic drug
Malyl-CoA lyase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Antihypertriglyceridemic
Uridine nucleosidase inhibitor
Vitamin
Polynucleotide adenylyltransferase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
Beta-glucosidase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Estrone sulfotransferase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Glutamine-pyruvate transaminase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Antihelminthic (Fasciola)
Sigma receptor agonist
ADP-ribosylarginine hydrolase inhibitor
Adenylate cyclase stimulant
Adrenergic, ophthalmic
Gluconokinase inhibitor
4-Pyridoxolactonase inhibitor
Dihydrouracil oxidase inhibitor
Urolithiasis treatment
Membrane dipeptidase inhibitor
Deoxyhypusine monooxygenase inhibitor
Histidine ammonia-lyase inhibitor
Vascular dementia treatment
Contraceptive female
Melanin inhibitor
Pyridoxal kinase inhibitor
Endothelial growth factor antagonist
Glycerone-phosphate O-acyltransferase inhibitor
Homocysteine desulfhydrase inhibitor
Cyclohexadienyl dehydrogenase inhibitor

CYP1A1 inhibitor
P-glycoprotein inhibitor
Insulin secretagogues
Antihypertensive
Xenobiotic-transporting ATPase inhibitor
Picornain 2A inhibitor
Inositol-3-phosphate synthase inhibitor
P-glycoprotein 1 inhibitor
Myc inhibitor
Phenylalanine-tRNA ligase inhibitor
Botulin neurotoxin A light chain inhibitor
Beta-N-acetylhexosaminidase inhibitor
Cyclic AMP modulator
Phosphorylase b inhibitor
Orsellinate decarboxylase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
GDP-mannose 6-dehydrogenase inhibitor
Interferon alpha agonist
Capillary fragility treatment
Heat shock protein 70 antagonist
Oligopeptidase B inhibitor
Insecticide
Ca²⁺-transporting ATPase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Granzyme A inhibitor
Falcipain 3 inhibitor
UGT2B15 substrate
Gastrointestinal motility stimulant
NMDA receptor agonist
Cysteine-tRNA ligase inhibitor
Ethanolamine kinase inhibitor
RNA directed DNA polymerase inhibitor
Dihydrodipicolinate synthase inhibitor
Tryptophan 2-monooxygenase inhibitor
Polyamine oxidase inhibitor
Immunomodulator
(R)-aminopropanol dehydrogenase inhibitor
Malate dehydrogenase (decarboxylating) inhibitor
Cell wall synthesis inhibitor
Pyruvate, phosphate dikinase inhibitor
HIV-1 integrase (Overall Integration) inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Antinaupathic
Antidiabetic (type 1)
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Photinus-luciferin 4-monooxygenase (ATP-hydrolysing) inhibitor
Oxytocic
UDP-glucuronate decarboxylase inhibitor
Ketoheokinase inhibitor
CYP1B substrate

Arylamine N-Acetyltransferase substrate
Glucosyl transferase inhibitor
Antiischemic
Glutathione reductase inhibitor
Alkylator
Chitin synthase inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Cyclooxygenase 2 inhibitor
S-methyl-5-thioribose kinase inhibitor
Aspartate ammonia-lyase inhibitor
CMP-N-acylneuramate phosphodiesterase inhibitor
Antineoplastic (lung cancer)
N-acetylglucosamine kinase inhibitor
Cystinyl aminopeptidase inhibitor
Antidote, heavy metal
Antineoplastic (small cell lung cancer)
ATPase stimulant
5 Hydroxytryptamine 2B agonist
Neurosin inhibitor
Sodium channel blocker class Ib
Dihydropteroate synthase inhibitor
Atrolysin C inhibitor
Heat shock protein antagonist
CYP1A1 substrate
Tryptophan synthase inhibitor
Shikimate kinase inhibitor
Acyl-CoA dehydrogenase (NADP+) inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor
NAT2 substrate
Kynureninase inhibitor
Antianemic
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Antiviral (Trachoma)
Glycerol kinase inhibitor
2-Methylcitrate synthase inhibitor
Calcium channel activator
Long-chain-acyl-CoA dehydrogenase inhibitor
CYP3A5 inducer
Arginine decarboxylase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Antihematotoxic
Retinol dehydrogenase inhibitor
Aldose reductase substrate
Peroxisome proliferator-activated receptor gamma antagonist
Glycine N-methyltransferase inhibitor
Thromboxane antagonist
CYP19 substrate

Indoleamine-pyrrole 2,3-dioxygenase inhibitor
D-Ala-D-Ala ligase inhibitor
Cytochrome-b5 reductase substrate
Anabolic
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
CYP1A1 inducer
Hypoxia inducible factor 1 alpha inhibitor
Leishmanolysin inhibitor
Cancer procoagulant inhibitor
Lactoylglutathione lyase inhibitor
6,7-Dihydropteridine reductase inhibitor
CYP1A3 substrate
Malate dehydrogenase (NADP+) inhibitor
Antihyperammonemic
Phosphoglucomutase inhibitor
Cytosole dipeptidase inhibitor
Cyanate hydratase inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
CYP4F substrate
Spasmolytic, Papaverin-like
Asparagine-oxo-acid transaminase inhibitor
Quisqualate antagonist
Candidapepsin inhibitor
CYP2C8 inducer
Retinoic acid alpha receptor agonist
L-iditol 2-dehydrogenase inhibitor
Aspartate carbamoyltransferase inhibitor
Pancreatic endopeptidase E inhibitor
Linoleate isomerase inhibitor
Potassium channel large-conductance Ca-activated activator
Argininosuccinate lyase inhibitor
Arabinose isomerase inhibitor
Cathepsin H inhibitor
Glucose-6-phosphate translocase inhibitor
Sucrose-phosphate synthase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Serine O-acetyltransferase inhibitor
Streptopain inhibitor
Antineoplastic (endocrine cancer)
Hematinic
Calcium antagonist
3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor
Interleukin 1a antagonist
Calcium channel blocker
Peroxisome proliferator-activated receptor antagonist
LDLR expression enhancer
Lassitude treatment
CYP2E1 inhibitor
Endothelin-converting enzyme inhibitor
Glutamate carboxypeptidase inhibitor

Biliary tract disorders treatment
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Hydroperoxide dehydratase inhibitor
Gamma-glutamyl hydrolase inhibitor
Chalcone isomerase inhibitor
Interleukin 2 agonist
CYP26 substrate
Colony stimulating factor agonist
D-benzoylarginine-4-nitroanilide amidase inhibitor
5-Aminovalerate transaminase inhibitor
Adenylate cyclase inhibitor
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Protein-tyrosine phosphatase epsilon inhibitor
1-Alkyl-2-acetylgllycerol O-acyltransferase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Enoyl-CoA hydratase inhibitor
Hydroxyquinol 1,2-dioxygenase inhibitor
Beta amyloid protein antagonist
Dethiobiotin synthase inhibitor
Glycerate kinase inhibitor
Cholestenone 5alpha-reductase inhibitor
Liver X receptor antagonist
Elastase 1 inhibitor
UDP-N-acetylmuramate-L-alanine ligase inhibitor
Endonuclease (influenza) inhibitor
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Glutamate synthase (NADPH) inhibitor
Hydroxyacylglutathione hydrolase inhibitor
Amino-acid N-acetyltransferase inhibitor
Leukotriene antagonist
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Leucine-tRNA ligase inhibitor
Phenylalanine 2-monooxygenase inhibitor
Amylo-alpha-1,6-glucosidase inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Protocatechuate 4,5-dioxygenase inhibitor
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
Octadecanal decarbonylase inhibitor
Citrate (Si)-synthase inhibitor
NMDA receptor glycine site agonist
Mannose-6-phosphate isomerase inhibitor
Hexokinase inhibitor
Sulfotransferase substrate
CC chemokine receptor 2B antagonist
Guanylate cyclase stimulant
Antitreponemal
Contraceptive
Sphingosine 1-phosphate receptor 5 agonist
Antineoplastic (uterine cancer)
Nicotinate phosphoribosyltransferase inhibitor

Glutamate (mGluR1) agonist
Topoisomerase II inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
Thromboxane A2 antagonist
Dihydropyrimidine dehydrogenase inhibitor
PfA-M1 aminopeptidase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Amyotrophic lateral sclerosis treatment
Antiallergic
Granulocyte macrophage colony stimulating factor agonist
Ethanolamine oxidase inhibitor
Venombin A inhibitor
Antineoplastic (breast cancer)
Xanthine dehydrogenase inhibitor
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor
Ribonucleoside triphosphate reductase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Calcium channel (voltage-sensitive) blocker
Phosphoketolase inhibitor
Anticholelithogenic
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Imidazoline receptor agonist
Protein-synthesizing GTPase inhibitor
Serine-tRNA ligase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
Carboxypeptidase E inhibitor
Fumarate hydratase inhibitor
Tryptophanyl aminopeptidase inhibitor
Dextranucrase inhibitor
Secretase alpha stimulant
Secretase stimulant
Peptide agonist
Diacylglycerol O-acyltransferase inhibitor
Vitamin K-like
Chelator, Iron
Thermomycolin inhibitor
Propionate CoA-transferase inhibitor
Aldose 1-epimerase inhibitor
Phosphoglycerate dehydrogenase inhibitor
SULT1A3 substrate
CYP2C2 substrate
Caspase 2 inhibitor
5 Hydroxytryptamine 4A antagonist
Galactosylgalactosylglucosylceramidase inhibitor
Amidase inhibitor
Beta-fructofuranosidase inhibitor
4-Hydroxyphenylacetate 1-monooxygenase inhibitor

Ribonuclease inhibitor
Pantoate-beta-alanine ligase inhibitor
Aminopeptidase I inhibitor
Hair growth stimulant
Renilla-luciferin 2-monooxygenase inhibitor
Gastric antisecretory
Narcotic antagonist
Formimidoylglutamase inhibitor
Glutamate release inhibitor
GABA transporter 2 inhibitor
Leukotriene B4 antagonist
CYP2D6 substrate
Chitin deacetylase inhibitor
CYP2B1 substrate
Aspartate 1-decarboxylase inhibitor
Glucan 1,4-alpha-glucosidase inhibitor
Alpha-L-fucosidase inhibitor
Neurolysin inhibitor
UGT2B11 substrate
Alanine racemase inhibitor
Aldose reductase inhibitor
Corticosteroid antagonist
UDP-N-acetylmuramate dehydrogenase inhibitor
Butyryl-CoA dehydrogenase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Leukocyte elastase inhibitor
Antiacne
Cytosolic phospholipase A2 inhibitor
CYP4F12 substrate
Vascular adhesion protein 1 inhibitor
Meprin A inhibitor
Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor
N-acylneuraminate cytidyltransferase inhibitor
6-Phosphofructo-2-kinase inhibitor
Aldehyde oxidase substrate
Raynaud's phenomenon treatment
Cerebrovascular disorders treatment
Dimethylallyltranstransferase inhibitor
Glutamate (mGluR group III) antagonist
Skeletal muscle relaxant
5 Hydroxytryptamine 2A agonist
Protein synthesis inhibitor
Pancreatic ribonuclease inhibitor
Protein kinase C stimulant
Arginyltransferase inhibitor
Chorismate mutase inhibitor
PRL phosphatase inhibitor
Phosphogluconate dehydrogenase (decarboxylating) inhibitor
Pancreatic disorders treatment
Nucleotide diphosphatase inhibitor

CYP1B1 inhibitor
CYP2A11 substrate
Lysozyme inhibitor
Beta galactosidase inhibitor
Biotin carboxylase inhibitor
Steroid sulfotransferase inhibitor
Bacterial efflux pump inhibitor
D-Serine ammonia-lyase inhibitor
Protein-glutamate O-methyltransferase inhibitor
Chymase inhibitor
Isomaltulose synthase inhibitor
Long-chain-fatty-acid-CoA ligase inhibitor
5 Hydroxytryptamine 4B antagonist
CYP17 inhibitor
Folate antagonist
Methylthioadenosine nucleosidase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
Glycolaldehyde dehydrogenase inhibitor
CYP2A10 substrate
ABCA1 expression enhancer
Methionyl aminopeptidase inhibitor
X-Trp aminopeptidase inhibitor
Glutamine synthetase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
JNK mitogen-activated protein kinase inhibitor
Benzoin aldolase inhibitor
N-acetylglucosaminyl diphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor
Glutamate (mGluR4) agonist
dCTP deaminase inhibitor
Immunoglobulin E antagonist
11-Cis-retinyl-palmitate hydrolase inhibitor
Arginine kinase inhibitor
Dihydrofolate synthase inhibitor
Pyruvate, water dikinase inhibitor
Mycolysin inhibitor
Contraceptive male
Antifungal (Pneumocystis)
D-lactate-2-sulfatase inhibitor
Guanylate cyclase inhibitor
Arabinogalactan endo-1,4-beta-galactosidase inhibitor
Antihypertensive
Peroxisome proliferator-activated receptor gamma agonist
Homoserine O-succinyltransferase inhibitor
[phosphorylase] phosphatase inhibitor
CYP19 inhibitor
Prostaglandin agonist
CYP2B2 substrate
Heme oxygenase inhibitor
Glutaminy-peptide cyclotransferase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor

Nicotinamide-nucleotide amidase inhibitor
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
L lactate dehydrogenase A inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
CYP26 inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Breast cancer-resistant protein inhibitor
Glutamate (mGluR1) antagonist
Rhodopsin kinase inhibitor
Urate transporter 1 inhibitor
DNA methyltransferase I inhibitor
CYP2D substrate
Peptidoglycan beta-N-acetylmuramidase inhibitor
Iron antagonist
SULT2A1 substrate
NMN nucleosidase inhibitor
CYP2C11 substrate
Methionine adenosyltransferase inhibitor
Beta 1 adrenoreceptor agonist
MAP kinase kinase 4 inhibitor
Antiprotozoal (Babesia)
Imidazoleglycerol-phosphate dehydratase inhibitor
Glutamate uptake inhibitor
Interleukin antagonist
Antiarthritic
Procollagen-proline 3-dioxygenase inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Muscle relaxant
Hydroxypyruvate reductase inhibitor
Carboxy-cis,cis-muconate cyclase inhibitor
MO15-related protein kinase Pfmrk inhibitor
Pregnane X receptor antagonist
Transforming growth factor beta 1 agonist
Necroptosis inhibitor
NMDA receptor polyamine site antagonist
Glutamate-cysteine ligase inhibitor
Chymotrypsin inhibitor
Plasminogen activator stimulant
Thiol protease inhibitor
Glycine N-choloyltransferase inhibitor
Methylaspartate mutase inhibitor
Glutathione S-transferase substrate
Viral entry inhibitor
Nicotinic acid receptor 2 agonist
Prostaglandin-I synthase inhibitor
AICAR transformylase inhibitor
Leukotriene C antagonist

HMG CoA synthase inhibitor
Sucrose alpha-glucosidase inhibitor
DNA methylase inhibitor
CYP1A2 substrate
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Peroxisome proliferator-activated receptor agonist
Leukotriene E4 antagonist
Estrogen agonist
Squalene epoxidase inhibitor
Diacylglycerol kinase inhibitor
Lipoxygenase inhibitor
Saccharopine dehydrogenase (NADP+, L-lysine-forming) inhibitor
Glutamate (mGluR3) agonist
Carboxypeptidase M inhibitor
Plasminogen activator inhibitor antagonist
Alpha,alpha-phosphotrehalase inhibitor
Lysyl endopeptidase inhibitor
1,3-Beta-glucan synthase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
D-aspartate oxidase inhibitor
UDP-glucose 6-dehydrogenase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Acidifying agent gastric
Elastase inhibitor
CMP-KDO synthase inhibitor
Antineoplastic (glioblastoma multiforme)
Antineurotic
Diamine oxidase inhibitor
3(or 17)beta-hydroxysteroid dehydrogenase inhibitor
Maleylacetoacetate isomerase inhibitor
Tubulin-tyrosine ligase inhibitor
Retinoid X alpha receptor agonist
Glutamate (mGluR group II) agonist
Kallikrein 3 inhibitor
Thromboxane synthase inhibitor
Alpha-amino-acid esterase inhibitor
Sphingosine 1-phosphate receptor 3 antagonist
tRNA (guanine-N2-)-methyltransferase inhibitor
Acyl-CoA dehydrogenase inhibitor
Alternansucrase inhibitor
Antineoplastic antimetabolite
Nuclear receptor subfamily 4, group A, member 2 agonist
Nitric oxide donor
Tubuliny-Tyr carboxypeptidase inhibitor
Neuropeptide Y2 antagonist
Glutathione S-transferase inhibitor

Histidine-tRNA ligase inhibitor
Inotropic
Ornithine carbamoyltransferase inhibitor
Phosphoenolpyruvate carboxykinase (GTP) inhibitor
GABA uptake inhibitor
Psychosexual dysfunction treatment
Antineoplastic (multiple myeloma)
Glutamate (mGluR group I) agonist
Ribose-5-phosphate-ammonia ligase inhibitor
Antiviral (Parainfluenza)
Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Complement inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
CYP24 substrate
Calcium channel L-type blocker
Bacterial leucyl aminopeptidase inhibitor
Astacin inhibitor
GTP cyclohydrolase I inhibitor
Sepiapterin deaminase inhibitor
Hydroxylysine kinase inhibitor
Protein-tyrosine phosphatase beta inhibitor
Sodium-dependent vitamin C transporter 2 inhibitor
Benzodiazepine antagonist
Adenosine deaminase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Lysosomal Pro-X carboxypeptidase inhibitor
Phosphoenolpyruvate carboxylase inhibitor
Antiglaucomic
Elastase 2 inhibitor
Uterine relaxant
Glutamine-fructose-6-phosphate transaminase inhibitor
Chloride channel blocker
Nucleoside-triphosphate-adenylate kinase inhibitor
D-Lysine 5,6-aminomutase inhibitor
Peroxisome proliferator-activated receptor alpha agonist
Tryptophan-tRNA ligase inhibitor
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Potassium channel Kv1.3 blocker
Deoxycytidine kinase inhibitor
Oleamide hydrolase inhibitor
15-Lipoxygenase inhibitor
Neuraminidase inhibitor
Tyrosine transaminase inhibitor
Azobenzene reductase inhibitor
Cytidylate kinase inhibitor
Chemoprotective
Malate synthase inhibitor
Pantetheine-phosphate adenylyltransferase inhibitor
Protocollagen prolyl hydroxylase inhibitor

Glutamate receptor agonist
Methylcrotonoyl-CoA carboxylase inhibitor
Aminoacyl-tRNA hydrolase inhibitor
Retinoic acid receptor agonist
5-Alpha-reductase inhibitor
D(-)-tartrate dehydratase inhibitor
CYP3A11 substrate
Lysophosphatidic acid receptor antagonist
tRNA methyltransferase inhibitor
Glutamate (mGluR4) antagonist
Pyridoxamine-oxaloacetate transaminase inhibitor
Aryl hydrocarbon receptor agonist
Autotaxin inhibitor
Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor
Cocaine dependency treatment
Vanilloid 1 agonist
Thyroid hormone antagonist
Carbamoyl-phosphate synthase (ammonia) inhibitor
Leukotriene agonist
Cyclooxygenase 1 substrate
Thioether S-methyltransferase inhibitor
Arabinose-5-phosphate isomerase inhibitor
12-Lipoxygenase inhibitor
Strombine dehydrogenase inhibitor
DELTA24-sterol reductase inhibitor
Phosphorylase inhibitor
Aldehyde dehydrogenase substrate
DNA nucleotidyltransferase inhibitor
Tyrosine phenol-lyase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Restenosis treatment
Sodium/bile acid cotransporter inhibitor
Adenine phosphoribosyltransferase inhibitor
Methyltransferase substrate
Deoxyribonuclease X inhibitor
Serum-glucocorticoid regulated kinase inhibitor
Glutamyl-tRNA synthase (glutamine-hydrolysing) inhibitor
NADPH oxidoreductase inhibitor
Pyruvate kinase inhibitor
Glutamate (mGluR8) antagonist
Dihydroorotate oxidase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
Glutamate (mGluR2) agonist
Histone-arginine N-methyltransferase inhibitor
5'-Nucleotidase inhibitor
Dihydroorotate dehydrogenase inhibitor
Riboflavin synthase inhibitor
Histone deacetylase SIRT1 inhibitor
Vanilloid 4 antagonist

Glutaryl-CoA dehydrogenase inhibitor
Sucrose-phosphate phosphatase inhibitor
Prostaglandin antagonist
Hypoxanthine phosphoribosyltransferase inhibitor
3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor
Alcohol dehydrogenase substrate
Phenylpyruvate tautomerase inhibitor
Epoxide hydrolase substrate
Cysteine dioxygenase inhibitor
Nicotinic acid receptor 1 agonist
Catechol O methyltransferase inhibitor
2-Ethylmalate synthase inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
AMP nucleosidase inhibitor
Serine-type D-Ala-D-Ala carboxypeptidase inhibitor
Androst-4-ene-3,17-dione monooxygenase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Magnolysin inhibitor
GST P1-1 substrate
Lactamase C inhibitor
Uterine stimulant
Mannosidase inhibitor
Reductase inhibitor
Farnesoid X receptor agonist
Interleukin 6 antagonist
Aldose reductase 2 inhibitor
Alpha-N-acetylgalactosaminide alpha-2,6-sialyltransferase inhibitor
Carboxypeptidase U inhibitor
Arginine racemase inhibitor
Methenyltetrahydrofolate cyclohydrolase inhibitor
Nucleotidyltransferase inhibitor
Uridine phosphorylase inhibitor
Aldehyde dehydrogenase 1A2 inhibitor
Osmotic diuretic
Carbonic anhydrase XIV inhibitor
Riboflavin kinase inhibitor
Antineoplastic alkaloid
Uridine kinase inhibitor
MAP-kinase-activated kinase 1 inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
Kainate receptor agonist
Interferon agonist
Procollagen galactosyltransferase inhibitor
TH expression enhancer
Cholesterol absorption inhibitor
Cysteamine dioxygenase inhibitor
Bis(5'-nucleosyl)-tetrphosphatase (asymmetrical) inhibitor
Ornithine decarboxylase inhibitor
Malonyl-CoA decarboxylase inhibitor
Steroid DELTA-isomerase inhibitor

Heparanase inhibitor
Antitussive, narcotic
Leukotriene C4 antagonist
Arginase inhibitor
Phosphorylase kinase inhibitor
Adrenaline agonist
Lanosterol 14 alpha demethylase inhibitor
DNA helicase inhibitor
Alpha glucosidase inhibitor
Monoamine uptake inhibitor
GMP synthase inhibitor
Deoxyadenosine kinase inhibitor
Adenylate cyclase I inhibitor
Vesicular glutamate transport inhibitor
Antiviral
Guanine deaminase inhibitor
Movement disorders treatment
Adenylosuccinate synthase inhibitor
Dihydrofolate reductase (Mycobacterium avium) inhibitor
Dopamine precursors
N-acetylmuramoyl-L-alanine amidase inhibitor
Hyperparathyroidism treatment
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
Oligonucleotidase inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
Orotate phosphoribosyltransferase inhibitor
Heat shock protein 90 antagonist
3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor
Phosphomannomutase inhibitor
Dihydrofolate reductase (Toxoplasma gondii) inhibitor
Tartrate decarboxylase inhibitor
CYP3C substrate
Hirsutism treatment
Ribonuclease U2 inhibitor
5-Lipoxygenase inhibitor
Tankyrase inhibitor
Deoxyguanosine kinase inhibitor
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Antithrombocytopenic
Liver X receptor beta agonist
Coactivator-associated arginine methyltransferase 1 inhibitor
Beta lactamase TEM-1 inhibitor
Amylosucrase inhibitor
Protein-tyrosine phosphatase yopH inhibitor
CPB protease inhibitor
5 Hydroxytryptamine 4E antagonist
Glutamate (mGluR3) antagonist
Homoisocitrate dehydrogenase inhibitor
Kallikrein inhibitor

tRNA (guanine-N7-)-methyltransferase inhibitor
Methionyl aminopeptidase 1 inhibitor
Squalene synthetase inhibitor
Androgen agonist
AMP deaminase inhibitor
Dihydrofolate reductase (*Pneumocystis carinii*) inhibitor
Lipocortins synthesis agonist
GST P substrate
Inositol 1,4,5-triphosphate receptor antagonist
1-Phosphofructokinase inhibitor
2-(acetamidomethylene)succinate hydrolase inhibitor
Phosphoglycerate phosphatase inhibitor
Methionine-tRNA ligase inhibitor
Radical formation agonist
Granzyme B inhibitor
Glutamate (mGluR) antagonist
Protein N-acetylglucosaminyltransferase inhibitor
Retinoid X receptor agonist
CYP4F8 substrate
2-Methylacyl-CoA dehydrogenase inhibitor
Glutamate formimidoyltransferase inhibitor
Shab potassium channel blocker
Leukotriene B4 receptor 1 antagonist
GMP reductase inhibitor
DNA directed DNA polymerase inhibitor
Homoserine O-acetyltransferase inhibitor
Ribose-5-phosphate adenylyltransferase inhibitor
Steroid 9alpha-monooxygenase inhibitor
Benzodiazepine receptor peripheral-type antagonist
CYP1A substrate
Antiviral (HIV)
Tryptophan 5 hydroxylase inhibitor
Spermine synthase inhibitor
Opioid delta 2 receptor antagonist
Antineoplastic (squamous cell carcinoma)
Uracil phosphoribosyltransferase inhibitor
Retinoprotector
Glucose-1-phosphate adenylyltransferase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
NAD⁺ diphosphatase inhibitor
[Isocitrate dehydrogenase (NADP⁺)] kinase inhibitor
DNA directed RNA polymerase stimulant
H⁺-transporting two-sector ATPase inhibitor
N-acetylglucosaminyl diphosphodolichol N-acetylglucosaminyltransferase inhibitor
Tartrate dehydrogenase inhibitor
Carboxycyclohexadienyl dehydratase inhibitor
Paget's disease treatment
Valine-pyruvate transaminase inhibitor
Thymidine-triphosphatase inhibitor
Sigma 1 receptor agonist

Alpha,alpha-trehalose phosphorylase inhibitor
Spermidine synthase inhibitor
ATPase (Vacuolar H⁺) inhibitor
Thyroid hormone alpha 1 antagonist
Aralkylamine dehydrogenase inhibitor
Phosphopyruvate hydratase inhibitor
Estrogen-related receptor alpha antagonist
Beta adrenoreceptor agonist
GABA transporter inhibitor
Progesterone receptor B1 antagonist
Antineoplastic (lymphoma)
Methionyl aminopeptidase 2 inhibitor
Antineoplastic (carcinoma)
Antiprotozoal activity enhancer
Phosphoserine transaminase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Scytalone dehydratase inhibitor
Membrane-oligosaccharide glycerophosphotransferase inhibitor
Andropause treatment
CDC25A inhibitor
Chloride channel activator
Retinoic acid receptor gamma antagonist
Dichloromethane dehalogenase inhibitor
UGT2B19 substrate
UGT2B23 substrate
UGT2B30 substrate
UGT2B4D substrate
UGT2B4E substrate
Maleylacetate reductase inhibitor
[citrate-(pro-3S)-lyase] thiolesterase inhibitor
Alpha-mannosidase inhibitor
T-cell protein-tyrosine phosphatase inhibitor
Protein-tyrosine phosphatase 2C inhibitor
Caspase 8 inhibitor
Prostaglandin E2 antagonist
Carnitine O-octanoyltransferase inhibitor
Retinoic acid receptor antagonist
Cell adhesion inhibitor
Thyroid hormone agonist
Prostaglandin A1 agonist
Glucose-6-phosphate isomerase inhibitor
Heat shock protein agonist
Anhydrotetracycline monooxygenase inhibitor
CYP17 substrate
Diphosphate-serine phosphotransferase inhibitor
Restless leg syndrome treatment
Formimidoyltetrahydrofolate cyclodeaminase inhibitor
NMDA receptor glycine site B antagonist
CYP2A13 substrate
Nicotinic acid receptor agonist

AMP deaminase 3 inhibitor
Serine carboxypeptidase inhibitor
NOS3 expression enhancer
Topoisomerase I inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase (T. brucei) inhibitor
VEGF expression inhibitor
Anesthetic inhalation
CC chemokine 9 receptor antagonist
Galactosylceramide sulfotransferase inhibitor
Arachidonate-CoA ligase inhibitor
Mucorpepsin inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor
Leukotriene A4 hydrolase inhibitor
Leukotriene D4 antagonist
dUTP diphosphatase inhibitor
UDP-N-acetylglucosamine-lysosomal-enzyme N-acetylglucosaminophosphotransferase inhibitor
1-Alkyl-2-acetyl glycerophosphocholine esterase inhibitor
Phosphoglycerate kinase inhibitor
Ketosteroid monooxygenase inhibitor
Aminopeptidase N inhibitor
Glutamate racemase inhibitor
Glutamate (mGluR) agonist
Asparaginyl endopeptidase inhibitor
Arginine-tRNA ligase inhibitor
2-Aminohexanoate transaminase inhibitor
Postcoital contraceptive
Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor
Oxytocin agonist
5-Alpha-reductase 1 inhibitor
Phosphatidylinositol 3-kinase stimulant
Free fatty acid receptor 1 agonist
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
DNA repair enzyme inhibitor
Lactamase A inhibitor
Kainate receptor antagonist
Protein glycation inhibitor
Diaminopimelate decarboxylase inhibitor
Retinoic acid alpha receptor antagonist
Plasmin inhibitor
CF transmembrane conductance regulator antagonist
Beta adrenoreceptor antagonist
Aminoacyl-tRNA synthetase inhibitor
GABA transporter 1 inhibitor
Mannitol-1-phosphate 5-dehydrogenase inhibitor
tRNA (uracil-5-)-methyltransferase inhibitor
Kainate receptor 1 agonist
Purinergic P2X2 antagonist
Putrescine carbamoyltransferase inhibitor
Vibriolysin inhibitor
Retinoid X gamma receptor antagonist

L lactate dehydrogenase B inhibitor
L lactate dehydrogenase B4 inhibitor
Thymine dioxygenase inhibitor
Antibiotic Quinolone-like
Peroxisome proliferator-activated receptor alpha antagonist
Glutamate (mGluR2) antagonist
Sphingosine kinase inhibitor
L lactate dehydrogenase A4 inhibitor
Plus-end-directed kinesin ATPase inhibitor
Antineoplastic (non-small cell lung cancer)
Aminopeptidase microsomal inhibitor
Acid phosphatase 1 inhibitor
Prostaglandin D2 agonist
Leukotriene B4 receptor 2 antagonist
Dual specificity phosphatase inhibitor
L lactate dehydrogenase C inhibitor
L lactate dehydrogenase C4 inhibitor
Glutamate (mGluR1a) agonist
Glutamate (mGluR5a) agonist
Protein-tyrosine phosphatase mu inhibitor
Myocardial ischemia treatment
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Glutamate receptor antagonist
Amidophosphoribosyltransferase inhibitor
Mannosyl-oligosaccharide glucosidase inhibitor
FAD diphosphatase inhibitor
Excitatory amino acid transporter 2 inhibitor
Purinergic P2X1 antagonist
Histamine H2 receptor antagonist
4-Hydroxyphenylpyruvate dioxygenase inhibitor
Homospermidine synthase inhibitor
Protein phosphatase 2A inhibitor
Helicase E1 (Human papillomavirus) inhibitor
Polyphosphate kinase inhibitor
Phospholipase A1 inhibitor
Endo-beta-N-acetylglucosaminidase inhibitor
Theanine hydrolase inhibitor
Ubiquitin-protein ligase inhibitor
CDC25B inhibitor
Nicotinic alpha4beta2 receptor antagonist
GABA B receptor antagonist
Methylmalonyl-CoA mutase inhibitor
Prostaglandin EP4 agonist
CYP24 inhibitor
Antibiotic Carbapenem-like
HIV-1 reverse transcriptase inhibitor
5 Lipoxygenase activating protein inhibitor
Retinoic acid beta receptor antagonist
[Skp1-protein]-hydroxyproline N-acetylglucosaminyltransferase inhibitor
Aryl hydrocarbon receptor antagonist

Myelin associated glycoprotein antagonist
Phospholipase D inhibitor
Angiotensin-converting enzyme inhibitor
Thymidine kinase 1 inhibitor
Aralkylamine N-acetyltransferase inhibitor
Thermolysin inhibitor
Mannitol 2-dehydrogenase inhibitor
Gestagen-like
Antibiotic Naphthyridine-like
Beta lactamase Imi-1 inhibitor
Angiotensin AT1 receptor antagonist
Glucose-1-phosphatase inhibitor
Dolichyldiphosphatase inhibitor
Retinoid X receptor antagonist
Retinoid X beta receptor antagonist
Myosin-light-chain-phosphatase inhibitor
Galectin 3 antagonist
Transaldolase inhibitor
Erythropoietin receptor agonist
Antineoplastic antibiotic
CYP1B1 substrate
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
Sphingosine 1-phosphate receptor 4 agonist
Cyclomaltodextrin glucanotransferase inhibitor
Small monomeric GTPase inhibitor
Glutamate (mGluR group II) antagonist
Retinoid X alpha receptor antagonist
Glutamate (mGluR group III) agonist
Platelet antagonist
Thyroid hormone beta 1 antagonist
Inducible nitric-oxide synthase inhibitor
RNA-directed RNA polymerase (Influenza A) inhibitor
Thrombopoietin agonist
Prolyl endopeptidase inhibitor
Beta lactamase II inhibitor
2-Isopropylmalate synthase inhibitor

Baclofen

Molecular Mechanism (initial) :

GABA(B) receptor agonist

Molecular Mechanism (repurposed) :

GABA(B) receptor agonist

initial indication(s):

spasticity

Repurposed indication(s):

alcoholism

Predicted Activities

Phobic disorders treatment

Antihypoxic

Antiseborrheic
CYP2J2 substrate
Mucositis treatment
CYP2J substrate
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Mucomembranous protector
Acylcarnitine hydrolase inhibitor
Membrane integrity agonist
Arylsulfate sulfotransferase inhibitor
Exoribonuclease II inhibitor
Chlordecone reductase inhibitor
Fibrinolytic
Venombin AB inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
Anticonvulsant
Polyamine-transporting ATPase inhibitor

GABA B receptor agonist

Protein-disulfide reductase (glutathione) inhibitor
Dimethylargininase inhibitor
Aspartate-ammonia ligase inhibitor
Lipoprotein lipase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Arginine 2-monooxygenase inhibitor
NADPH peroxidase inhibitor
Antinaupathic
Phthalate 4,5-dioxygenase inhibitor
Fructose 5-dehydrogenase inhibitor
Preneoplastic conditions treatment
N-benzyloxycarbonylglycine hydrolase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Pseudolysin inhibitor
Skeletal muscle relaxant
Fibrolase inhibitor
Fusarinine-C ornithinesterase inhibitor
Lysine 2,3-aminomutase inhibitor
GST A substrate
Glucose oxidase inhibitor
Prostaglandin-E2 9-reductase inhibitor
X-methyl-His dipeptidase inhibitor
Ompin inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Insulin promoter
Glutamine-phenylpyruvate transaminase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Hydrogen dehydrogenase inhibitor
Acetylornithine deacetylase inhibitor
Ubiquitin thiolesterase inhibitor
Sulfur reductase inhibitor

Membrane permeability inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Oxidoreductase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Carnosine synthase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Macrophage colony stimulating factor agonist
NADPH-cytochrome-c2 reductase inhibitor
Adenomatous polyposis treatment
Sphinganine kinase inhibitor
Superoxide dismutase inhibitor
GABA C receptor agonist
N-formylmethionyl-peptidase inhibitor
Antieczematic
L-glutamate oxidase inhibitor
Carboxypeptidase Taq inhibitor
Phosphatidylglycerophosphatase inhibitor
Muscle relaxant
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Acidifying agent non gastric
Alkenylglycerophosphocholine hydrolase inhibitor
Valine decarboxylase inhibitor
CYP2C10 substrate
Glucan endo-1,3-beta-D-glucosidase inhibitor
Fragilysin inhibitor
Creatininase inhibitor
Alkylacetyl glycerophosphatase inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
5 Hydroxytryptamine uptake stimulant
Enteropeptidase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Carboxypeptidase D inhibitor
Cytochrome-b5 reductase inhibitor
Lipid metabolism regulator
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Phosphatase inhibitor
Dextranase inhibitor
Formaldehyde transketolase inhibitor
Gastrin inhibitor
Coccolysin inhibitor
Limulus clotting factor B inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Platelet aggregation stimulant
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Peroxidase substrate
Calcium channel (voltage-sensitive) activator

Ethanolamine-phosphate cytidyltransferase inhibitor
Dipeptidase E inhibitor
Arylesterase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Aspartoacylase inhibitor
1,4-Lactonase inhibitor
Fructan beta-fructosidase inhibitor
Antineurotic

Antialcoholic

Endopeptidase So inhibitor
Phosphoinositide 5-phosphatase inhibitor
Aspartyltransferase inhibitor
Proteasome ATPase inhibitor
CYP4A11 substrate
Cytoprotectant
Cyclamate sulfohydrolase inhibitor
3-Phytase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Inulinase inhibitor
Carnitinamidase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Guanidinoacetate kinase inhibitor
Cathepsin T inhibitor
Mucinaminyserine mucinaminidase inhibitor
S-alkylcysteine lyase inhibitor
CNS active muscle relaxant
Manganese peroxidase inhibitor
4-Hydroxyproline epimerase inhibitor
Tryptophan transaminase inhibitor
Cl--transporting ATPase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Gingipain K inhibitor
Biotinidase inhibitor
Phosphoenolpyruvate mutase inhibitor
Methane monooxygenase inhibitor
Meprin B inhibitor
Polyporopepsin inhibitor
Yeast ribonuclease inhibitor
Acetylcholine neuromuscular blocking agent
Pyruvate decarboxylase inhibitor
Glutamate uptake inhibitor
Taurine dehydrogenase inhibitor
Protein-tyrosine sulfotransferase inhibitor
Acetylgalactosaminy-O-glycosyl-glycoprotein
beta-1,3-N-acetylglucosaminyltransferase inhibitor
D-xylulose reductase inhibitor
Cholesterol antagonist
N-Acyl-D-amino-acid deacylase inhibitor
Phosphatidate phosphatase inhibitor
Levanase inhibitor

Leukotriene-C4 synthase inhibitor
Pitrilysin inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Glycine amidinotransferase inhibitor
Cell adhesion molecule inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Transketolase inhibitor
Acetylspermidine deacetylase inhibitor
Muramoyltetrapeptide carboxypeptidase inhibitor
GABA B receptor antagonist
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Leukopoiesis stimulant
Glyoxylate reductase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Antidyskinetic
Complement factor D inhibitor
Fibroblast growth factor agonist
Linoleate diol synthase inhibitor
Anesthetic general
Sulfite reductase inhibitor
Oxygen scavenger
Sugar-phosphatase inhibitor
Spermidine dehydrogenase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Glutamyl endopeptidase II inhibitor
GABA aminotransferase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Membrane permeability enhancer
Peptide agonist
Nitrite reductase (NO-forming) inhibitor
Hydroxylamine oxidase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Guanidinoacetase inhibitor
CYP3A1 substrate
Prostaglandin-A1 DELTA-isomerase inhibitor
Phospholipase C inhibitor
Glycerol-3-phosphate oxidase inhibitor
4-Hydroxymandelate oxidase inhibitor
Aminoacylase inhibitor
Ecdysone 20-monooxygenase inhibitor
CYP2C18 substrate
Flavin-containing monooxygenase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
S-formylglutathione hydrolase inhibitor
Eye irritation, inactive
Phenol O-methyltransferase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Fucosterol-epoxide lyase inhibitor
Omega-amidase inhibitor

Pancreatic elastase inhibitor
Antihypercholesterolemic
Thiol oxidase inhibitor
Thiosulfate dehydrogenase inhibitor
Platelet adhesion inhibitor
Interferon alpha agonist
Serine 3-dehydrogenase inhibitor
Antimyopathies
Urease inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Erythropoiesis stimulant
Antisecretoric
Rubredoxin-NAD⁺ reductase inhibitor
Apyrase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
L-lysine 6-transaminase inhibitor

Spasmolytic

GABA receptor agonist

Methylenetetrahydrofolate reductase (NADPH) inhibitor
ADP-thymidine kinase inhibitor
Cyclohexanone monooxygenase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP⁺) inhibitor
Glutamate-tRNA ligase inhibitor
Procollagen N-endopeptidase inhibitor
Antiviral (Picornavirus)
Mitochondrial intermediate peptidase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Threonine aldolase inhibitor
Catalase inhibitor
Oxidizing agent
CYP3A2 substrate
CYP2C8 inhibitor
IgA-specific serine endopeptidase inhibitor
Glucuronate isomerase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Aspergillus nuclease S1 inhibitor
Thymidylate 5'-phosphatase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Fatty-acyl-CoA synthase inhibitor
Phenylalanine(histidine) transaminase inhibitor
CYP7 inhibitor
Mannose isomerase inhibitor
Alopecia treatment
Alanine-tRNA ligase inhibitor
Sulfite dehydrogenase inhibitor
Antiallergic
Gluconolactonase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
2-Oxoglutarate decarboxylase inhibitor

Biliary tract disorders treatment
CYP4A substrate
Choline-phosphate cytidyltransferase inhibitor
RNA-directed RNA polymerase inhibitor
Antitoxic
Phospholipid-translocating ATPase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Cyclic AMP agonist
Acyl-lysine deacylase inhibitor
Interleukin 2 agonist
Glutaminase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Chitosanase inhibitor
Nardilysin inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Chaperonin ATPase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Acylaminoacyl-peptidase inhibitor
L-amino-acid oxidase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Renal tissue kallikrein inhibitor
4-Nitrophenylphosphatase inhibitor
Phosphoserine phosphatase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
TNF expression inhibitor
2-Dehydropantoate aldolase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
FMO3 substrate
Indanol dehydrogenase inhibitor
Aminopeptidase Y inhibitor
Gametolysin inhibitor
Fibroblast growth factor 1 agonist
Membrane integrity antagonist
D-amino-acid dehydrogenase inhibitor
Leucolysin inhibitor
CYP2E1 inhibitor
Metallo-carboxypeptidase D inhibitor
Pullulanase inhibitor
Lysostaphin inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Alcohol O-acetyltransferase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Nicotine dehydrogenase inhibitor
NADH kinase inhibitor
Plasmanylethanolamine desaturase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Carboxymethylenebutenolidase inhibitor
Multiple sclerosis treatment

Guanidinobutyrase inhibitor
Gluconate 5-dehydrogenase inhibitor
EIF4E expression inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Polygalacturonase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
DELTA14-sterol reductase inhibitor
IgA-specific metalloendopeptidase inhibitor
Menopausal disorders treatment
Poly(alpha-L-guluronate) lyase inhibitor
Arylmalonate decarboxylase inhibitor
Phosphatidylserine decarboxylase inhibitor
Aryl-acylamidase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Adenylyl-sulfate reductase inhibitor
Antithrombotic
CYP2C8 substrate
D-Ornithine 4,5-aminomutase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Lysyl oxidase inhibitor
Beta-ureidopropionase inhibitor
Bontoxilysin inhibitor
Lipotropic
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Aspulvinone dimethylallyltransferase inhibitor
Mannitol-1-phosphatase inhibitor
Antipruritic, allergic
NADPH-ferrihemoprotein reductase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Glutamin-(asparagin-)ase inhibitor
Vasoprotector
CYP19A1 expression inhibitor
O-aminophenol oxidase inhibitor
UGT1A6 substrate
Photosensitizer
Mannan endo-1,4-beta-mannosidase inhibitor
Gamma-glutamyltransferase inhibitor
Isopenicillin-N synthase inhibitor
Fibrinogen receptor antagonist
CYP2B6 substrate
Tyrosine 3 hydroxylase inhibitor
Procollagen C-endopeptidase inhibitor
UGT1A9 substrate
Antihyperlipoproteinemic
HMOX1 expression enhancer
2-Hydroxy-3-oxoadipate synthase inhibitor
Arylsulfatase inhibitor

Hematopoietic inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Antianorexic
Nucleotide metabolism regulator
Histidinol dehydrogenase inhibitor
Botulin neurotoxin A light chain inhibitor
Carnitine dehydratase inhibitor
Gingipain R inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Hyaluronic acid agonist
Retinoic acid metabolism inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Mitochondrial processing peptidase inhibitor
Acrosin inhibitor
Diabetic neuropathy treatment
Glycine-tRNA ligase inhibitor
Benzoate-CoA ligase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Calcium-sensing receptor agonist
Diacylglycerol cholinephosphotransferase inhibitor
Dihydropyrimidinase inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
Serine-pyruvate transaminase inhibitor
Antiinflammatory, ophthalmic
Homocysteine desulfhydrase inhibitor
3-Isopropylmalate dehydratase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Iron-cytochrome-c reductase inhibitor
Acute neurologic disorders treatment
Glutamate N-acetyltransferase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Antiinfective
Thiamine-triphosphatase inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Dimethylmaleate hydratase inhibitor
Neurotransmitter antagonist
Antifibrinolytic
Guanidinopropionase inhibitor
Diuretic inhibitor
Clostripain inhibitor
Prunasin beta-glucosidase inhibitor
Thromboxane B2 antagonist
3-Oxadipate enol-lactonase inhibitor
Allantoate deiminase inhibitor
Horrilysin inhibitor
Hydroxylamine reductase inhibitor
tRNA nucleotidyltransferase inhibitor

Trimethylamine-oxide aldolase inhibitor
Saccharolysin inhibitor
Pancreatic ribonuclease inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Asparaginase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Antineoplastic (liver cancer)
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Nicotinate dehydrogenase inhibitor
Cancer associated disorders treatment
Antihelmintic (Nematodes)
Thiopurine S-methyltransferase inhibitor
Saluretic
Branched-chain-amino-acid transaminase inhibitor
Asparagine-tRNA ligase inhibitor
L-threonine 3-dehydrogenase inhibitor
Centromere associated protein inhibitor
CYP3A3 substrate
UGT2B4 substrate
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
L-lysine oxidase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
TP53 expression enhancer
Acetylserotonin O-methyltransferase inhibitor
Protein-glutamate methylesterase inhibitor
Histamine release stimulant
Sphinganine-1-phosphate aldolase inhibitor
Histidine N-acetyltransferase inhibitor
Antiviral (Rhinovirus)
Bothrolysin inhibitor
Tripeptidyl-peptidase I inhibitor
Inorganic diphosphatase inhibitor
Loop diuretic
Bile-salt sulfotransferase inhibitor
3-Cyanoalanine hydratase inhibitor
Glutamate 5-kinase inhibitor
Benzoate 4-monooxygenase inhibitor
Pterin deaminase inhibitor
Arylamine N-acetyltransferase inhibitor
Brachyurin inhibitor
Lysine 2-monooxygenase inhibitor
Antipruritic, non-allergic
UGT1A4 substrate
Creatinine deaminase inhibitor
APOA1 expression enhancer
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Leucine dehydrogenase inhibitor
Sulfite oxidase inhibitor

1,2-alpha-L-fucosidase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Glycine hydroxymethyltransferase inhibitor
Agmatinase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Methanol dehydrogenase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
Leukopoiesis inhibitor
Sickle-cell anemia treatment
Tryptophan 2,3-dioxygenase inhibitor
D-proline reductase (dithiol) inhibitor
N-acetylneuraminate synthase inhibitor
Autoimmune disorders treatment
6-Pyruvoyltetrahydropterin synthase inhibitor
Malate dehydrogenase (acceptor) inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Creatinase inhibitor
Pappalysin-1 inhibitor
CYP2C9 substrate
Kidney function stimulant
3-Chloro-D-alanine dehydrochlorinase inhibitor
Alpha-amylase inhibitor
Antiperistaltic
Lysine decarboxylase inhibitor
Antineurogenic pain
Dolichol kinase inhibitor
CYP4A2 substrate
Tentoxilysin inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Venom exonuclease inhibitor
CYP2E1 substrate
Diamine N-acetyltransferase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Glycine C-acetyltransferase inhibitor
Pyroglutamyl-peptidase II inhibitor
Choline-sulfatase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
HIF1A expression inhibitor
Lactase inhibitor
Antiseptic
Styrene-oxide isomerase inhibitor
Glycerol-1-phosphatase inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Phenylalanine 4-hydroxylase inhibitor
ICAM1 expression inhibitor
Thiamine pyridinylase inhibitor
Hydroxymethylbilane synthase inhibitor
Phosphonoacetate hydrolase inhibitor

Fumarate reductase (NADH) inhibitor
CYP2E substrate
Antiparkinsonian, rigidity relieving
Prion diseases treatment
Calcium regulator
Acetylenecarboxylate hydratase inhibitor
Tryptophan 2-monooxygenase inhibitor
Antihyperammonemic
Aspartate-tRNA ligase inhibitor
CYP4B substrate
Ferredoxin hydrogenase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Guanidinodeoxy-scyllo-inositol-4-phosphatase inhibitor
Prostaglandin E1 antagonist
Homoserine dehydrogenase inhibitor
Antinociceptive
DOPA decarboxylase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Phenylpyruvate decarboxylase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Glutamate (mGluR5) agonist
Trimethyllysine dioxygenase inhibitor
Glutathione peroxidase inhibitor
Lipoxygenase substrate
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Dihydroxy-acid dehydratase inhibitor
JAK2 expression inhibitor
Signal peptidase I inhibitor
Envelysin inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Alanine transaminase inhibitor
Analgesic stimulant
Bone diseases treatment
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Antipruritic
4-Phytase inhibitor
Glyceryl-ether monooxygenase inhibitor
Arginyltransferase inhibitor
Flavin-containing monooxygenase substrate
GST M substrate
Long-chain-aldehyde dehydrogenase inhibitor
Cysteine desulfurase inhibitor
D-Octopine dehydrogenase inhibitor
4-Hydroxyglutamate transaminase inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
Trehalose-phosphatase inhibitor
Phenylalanine dehydrogenase inhibitor
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Urticaria treatment
Antimutagenic

3'-Demethylstaurosporine O-methyltransferase inhibitor
Shikimate 5-dehydrogenase inhibitor
Dichloromuconate cycloisomerase inhibitor
Deoxyribonuclease I inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Selenocysteine lyase inhibitor
Macrophage stimulant
Aconitate decarboxylase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
Morphine 6-dehydrogenase inhibitor
Antianginal
D-glutamate oxidase inhibitor
Intermittent claudication treatment
Urethanase inhibitor
Hematopoietic
Beta-carotene 15,15'-monooxygenase inhibitor
Aspartate transaminase inhibitor
Antiasthmatic
Tripeptide aminopeptidase inhibitor
Ethanolamine oxidase inhibitor
Hydroxylamine reductase (NADH) inhibitor
Histidine kinase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Tauropine dehydrogenase inhibitor
5 Hydroxytryptamine 7S antagonist
CYP17 inhibitor
HIV-1 integrase (Overall Integration) inhibitor
MAP kinase stimulant
Opine dehydrogenase inhibitor
Pediculicide
Cysteine transaminase inhibitor
Radioprotector
Antiinflammatory, intestinal
Gallate decarboxylase inhibitor
2-Aminohexano-6-lactam racemase inhibitor
Antiuremic
Peptidyl-dipeptidase B inhibitor
Corticosteroid side-chain-isomerase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Diguanidinobutanase inhibitor
Chloride peroxidase inhibitor
Cytosol alanyl aminopeptidase inhibitor
L-3-cyanoalanine synthase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Sclerosant
Cyanoalanine nitrilase inhibitor
UGT1A5 substrate
Nitrate reductase (cytochrome) inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Analeptic

2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Antiviral (CMV)
CYP2E1 inducer
2-Enoate reductase inhibitor
Galactolipase inhibitor
Glucan endo-1,3- α -glucosidase inhibitor
Aldehyde oxidase inhibitor
Inflammatory Bowel disease treatment
Peptide α -N-acetyltransferase inhibitor
H⁺-exporting ATPase inhibitor
3'-Nucleotidase inhibitor
Antiviral (Poxvirus)
D-2-hydroxy-acid dehydrogenase inhibitor
Malate oxidase inhibitor
X-Pro dipeptidase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Maleate isomerase inhibitor
Leucine transaminase inhibitor
Uroporphyrinogen decarboxylase inhibitor
Gluconate dehydratase inhibitor
Glycolate dehydrogenase inhibitor
Antileprosy
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Choline kinase inhibitor
Mandelate 4-monooxygenase inhibitor
Limulus clotting factor C inhibitor
Pantothenase inhibitor
Glycopeptide α -N-acetylgalactosaminidase inhibitor
CYP2C29 substrate
Nitrile hydratase inhibitor
Serine protease unspecified inhibitor
Ferrochelataase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Gastrointestinal disorders treatment
UGT1A substrate
Endopeptidase La inhibitor
X-His dipeptidase inhibitor
Benzaldehyde dehydrogenase (NADP⁺) inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Pectin lyase inhibitor
Licheninase inhibitor
Phenylalanine decarboxylase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Aldehyde dehydrogenase (NADP⁺) inhibitor
Tyrosine-ester sulfotransferase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Diisopropyl-fluorophosphatase inhibitor

Acid phosphatase inhibitor
(R)-aminopropanol dehydrogenase inhibitor
Atrolysin A inhibitor
Picornain 2A inhibitor
Chitinase inhibitor
CYP2A8 substrate
Cysteine-S-conjugate beta-lyase inhibitor
Dactylisin inhibitor
Myosin ATPase inhibitor
Nucleoside-diphosphatase inhibitor
Opioid dependency treatment
Aryl-alcohol dehydrogenase inhibitor
Acetolactate synthase inhibitor
Prenyl-diphosphatase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
2-Aminoadipate transaminase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Lactate 2-monooxygenase inhibitor
Muscular dystrophy treatment
Choline dehydrogenase inhibitor
Oxytocic
Cyclooxygenase substrate
Aspartate kinase inhibitor
Apoptosis antagonist
Antipyretic
Feruloyl esterase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Uric acid excretion stimulant
Hypolipemic
Analgesic
CYP2A5 substrate
UGT1A3 substrate
Tryptophanamidase inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Dynein ATPase inhibitor
Lipoprotein lipase stimulant
Protein-arginine deiminase inhibitor
Beta glucuronidase inhibitor
CYP2C9 inducer
Aminopeptidase B inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Chloride channel activator
Uroporphyrinogen-III synthase inhibitor
Methylglutamate dehydrogenase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Peptidyl-glycinamidase inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Phenylacetate-CoA ligase inhibitor
Ligase inhibitor

ATP phosphoribosyltransferase inhibitor
CYP4B1 substrate
Farnesoid X receptor antagonist
Phosphoinositide phospholipase C inhibitor
Serratia marcescens nuclease inhibitor
Glutamine-tRNA ligase inhibitor
Amine dehydrogenase inhibitor
Thermitase inhibitor
Catechol oxidase inhibitor
Growth hormone agonist
Retinal dehydrogenase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
UDP-glucuronosyltransferase substrate
Phenol 2-monooxygenase inhibitor
Allantoicase inhibitor
Ketol-acid reductoisomerase inhibitor
Histidinol-phosphatase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Snapalysin inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Sedoheptulose-bisphosphatase inhibitor
Aureolysin inhibitor
Homogentisate 1,2-dioxygenase inhibitor
Serralysin inhibitor
Antihematotoxic
Bilirubin oxidase inhibitor
Integrin antagonist
Allophanate hydrolase inhibitor
Tubuliny-Tyr carboxypeptidase inhibitor
Antiosteoporotic
Ribonucleoside triphosphate reductase inhibitor
Lysase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Saccharopine dehydrogenase (NADP⁺, L-lysine-forming) inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Saccharopine dehydrogenase (NADP⁺, L-glutamate-forming) inhibitor
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Peptidyltransferase inhibitor
Folate antagonist
Oxalate oxidase inhibitor
Aminolevulinate transaminase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Cysteine synthase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Uterine stimulant
DNA ligase (ATP) inhibitor
Mycothiol-S-conjugate amidase inhibitor
Dethiobiotin synthase inhibitor
Monoamine uptake inhibitor

2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Antidiabetic symptomatic
Skin irritation, inactive
UGT1A1 substrate
Bone formation stimulant
Glycine receptor agonist
Endothelial growth factor antagonist
Blasticidin-S deaminase inhibitor
HCV IRES inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
CYP2C substrate
Aspartate-semialdehyde dehydrogenase inhibitor
Diaminopimelate dehydrogenase inhibitor
8-Amino-7-oxononanoate synthase inhibitor
Thiosulfate sulfurtransferase inhibitor
Arginine deiminase inhibitor
CYP4F2 substrate
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Transcription factor NF kappa A inhibitor
Glyoxylate oxidase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
D-cysteine desulfhydrase inhibitor
CYP2D16 substrate
Dihydrodipicolinate reductase inhibitor
CYP3A4 inducer
Oligopeptidase B inhibitor
Threonine ammonia-lyase inhibitor
Glucagon-like peptide 1 agonist
Vanilloid 1 agonist
Histone acetyltransferase inhibitor
Anthrax lethal factor inhibitor
Lymphocytopoiesis inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Glucosyl transferase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
Benzoylformate decarboxylase inhibitor
Cystathionine gamma-lyase inhibitor
Spasmolytic, urinary
5-Aminolevulinate synthase inhibitor
CYP2B18 substrate
Choleretic
Chenodeoxycholytaurine hydrolase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
GABA transporter 3 inhibitor
Ornithine-oxo-acid transaminase inhibitor
Methionine decarboxylase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Ethanolaminephosphotransferase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor

N-acetyllactosamine synthase inhibitor
Maleate hydratase inhibitor
Glutamate dehydrogenase inhibitor
Cerevisin inhibitor
Acetylesterase inhibitor
Kexin inhibitor
D-alanine transaminase inhibitor
Cycloartenol synthase inhibitor
CYP3A inducer
NMDA receptor agonist
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Electrolyte absorption antagonist
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Aerobactin synthase inhibitor
Lysyl endopeptidase inhibitor
Polyamine oxidase inhibitor
Antiprotozoal (Coccidial)
2-Nitropropane dioxygenase inhibitor
Antifungal
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Glycine transaminase inhibitor
Furin inhibitor
Porphobilinogen synthase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Immunomodulator
Mevalonate kinase inhibitor
Acylglycerone-phosphate reductase inhibitor
Anticoagulant
Phosphoglycolate phosphatase inhibitor
Dolichyl-phosphate beta-glucosyltransferase inhibitor
5 Hydroxytryptamine release inhibitor
Rhodotorulapepsin inhibitor
Anthranilate synthase inhibitor
Picornain 3C inhibitor
Glutamate decarboxylase inhibitor
3-Methylbutanal reductase inhibitor
Malate dehydrogenase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Pyruvate carboxylase inhibitor
Choloylglycine hydrolase inhibitor
Fibromyalgia syndrome treatment
Argininosuccinate lyase inhibitor
Histamine agonist
CYP2A6 substrate
Mucolytic
Lysozyme inhibitor
Vascular adhesion protein 1 inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Acetate kinase inhibitor
2-Methylcitrate dehydratase inhibitor

Cyclohexyl-isocyanide hydratase inhibitor
Glutamate dehydrogenase [NAD(P)+] inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Propionate-CoA ligase inhibitor
Cholate-CoA ligase inhibitor
Aryldialkylphosphatase inhibitor
Histamine release inhibitor
Transactivator transcription protein inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Opioid kappa 3 receptor antagonist
4-Coumarate-CoA ligase inhibitor
UGT2B28 substrate
CYP2C3 substrate
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
UGT2B9 substrate
Poly(3-hydroxybutyrate) depolymerase inhibitor
CYP2B11 substrate
SMN2 expression enhancer
Coagulant
Aspergillopepsin I inhibitor
UGT2B7 substrate
Integrin alphaVbeta5 antagonist
Cystathionine beta-synthase inhibitor
Carboxypeptidase M inhibitor
Homocitrate synthase inhibitor
5 Hydroxytryptamine 2B agonist
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Urocanate hydratase inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
UGT2B17 substrate
Gly-X carboxypeptidase inhibitor
Ornithine cyclodeaminase inhibitor
Retinoprotector
Lysosomal Pro-X carboxypeptidase inhibitor
Valine dehydrogenase (NADP+) inhibitor
Antidote
Aryl sulfotransferase inhibitor
Granzyme A inhibitor
Albendazole monooxygenase inhibitor
Sorbitol dehydrogenase inhibitor
Thimet oligopeptidase inhibitor
Antiprotozoal (Trypanosoma)
Thiol S-methyltransferase inhibitor
Acidifying agent gastric
Peptidylamidoglycolate lyase inhibitor
Arginine decarboxylase inhibitor
Thyroxine 5-deiodinase inhibitor
Antiparkinsonian, tremor relieving
Dihydrodipicolinate synthase inhibitor
Subtilisin inhibitor

Glucarate dehydratase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Rhinitis treatment
Sulfinioalanine decarboxylase inhibitor
Pyruvate dehydrogenase inhibitor
Diabetic nephropathy treatment
Thiamine-phosphate kinase inhibitor
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
Cell wall biosynthesis inhibitor
Myeloblastin inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
D-lactate dehydrogenase inhibitor
Alcohol dehydrogenase [NAD(P)⁺] inhibitor
Alcohol dehydrogenase (NADP⁺) inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Anticataract
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
[phosphorylase] phosphatase inhibitor
UGT2B1 substrate
CYP2C6 substrate
Glutathione reductase inhibitor
Cystathionine beta-lyase inhibitor
Antiviral (Adenovirus)
N-Acyl-D-aspartate deacylase inhibitor
Glutamine-pyruvate transaminase inhibitor
Antithyroid
Menstruation disorders treatment
Deoxyribonuclease (pyrimidine dimer) inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Carboxypeptidase U inhibitor
Potassium channel (Ca-activated) activator
Antiulcerative
Nicotinic alpha2beta2 receptor antagonist
UGT2B substrate
Glutamate (mGluR6) antagonist
Aspartate ammonia-lyase inhibitor
Nicotinamidase inhibitor
Histamine H1 receptor agonist
Orotate reductase (NADH) inhibitor
Anaphylatoxin receptor antagonist
Iduronate-2-sulfatase inhibitor
Laccase inhibitor
Chitin synthase inhibitor
Age-related macular degeneration treatment
Angiogenesis stimulant
Arylacetonitrilase inhibitor
Tropinesterase inhibitor
Propanediol dehydratase inhibitor
Cytosole dipeptidase inhibitor

Serine-glyoxylate transaminase inhibitor
Gastroesophageal reflux disease treatment
CYP2B substrate
Rhizopuspepsin inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Neuropsin inhibitor
Cytochrome P450 stimulant
3-Ketovalidoxylamine C-N-lyase inhibitor
Antihypertensive
Prephenate dehydratase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Maillard reaction inhibitor
Cysteamine dioxygenase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
GST P substrate
Acaricide
Carbamoyl-serine ammonia-lyase inhibitor
GST P1-1 substrate
Glutathione thiolesterase inhibitor
Formate-dihydrofolate ligase inhibitor
Sepiapterin reductase inhibitor
Arachidonic acid antagonist
tRNA cytidyltransferase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Complement inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
5-Aminovalerate transaminase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Carnitine 3-dehydrogenase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
CTGF expression inhibitor
3-Hydroxyanthranilate oxidase inhibitor
MMP9 expression inhibitor
Expectorant
Valine-tRNA ligase inhibitor
Alpha-glucuronidase inhibitor
Cystinyl aminopeptidase inhibitor
Hippurate hydrolase inhibitor
Proteasome endopeptidase complex inhibitor
Dyspepsia treatment
Alpha-N-arabinofuranosidase inhibitor
ATPase inhibitor
Penicillopepsin inhibitor
Mannonate dehydratase inhibitor
CYP3A5 substrate
Prephenate dehydrogenase inhibitor
Nucleotidase inhibitor

CXC chemokine receptor antagonist
Putrescine oxidase inhibitor
CYP2A1 substrate
All-trans-retinyl-palmitate hydrolase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Cytochrome-c3 hydrogenase inhibitor
Alkane 1-monooxygenase inhibitor
Trimereysin II inhibitor
Glutamate (mGluR8) agonist
Phosphatidate cytidyltransferase inhibitor
Glutamate carboxypeptidase inhibitor
Aspartate 1-decarboxylase inhibitor
Vomilenine glucosyltransferase inhibitor
Prolyl aminopeptidase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Proline racemase inhibitor
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Carboxypeptidase E inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
CYP1A inducer
Chitin deacetylase inhibitor
Metabolic disease treatment
Platelet antagonist
Glutamate-cysteine ligase inhibitor
Pregnane X receptor agonist
Galactose oxidase inhibitor
MDM2 inhibitor
GABA transporter 2 inhibitor
Methylaspartate ammonia-lyase inhibitor
Acid-sensing ion channel blocker
Succinate dehydrogenase inhibitor
CYP2A substrate
Stromelysin 2 inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Pantoate-beta-alanine ligase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
4-Alpha-glucanotransferase inhibitor
Sulfur dioxygenase inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
L-glucuronate reductase inhibitor
Bisphosphoglycerate mutase inhibitor
2-Haloacid dehalogenase inhibitor
Aromatic-amino-acid transaminase inhibitor
Muconate cycloisomerase inhibitor
Histidine decarboxylase inhibitor
Hepatoprotectant
Transforming growth factor beta 1 agonist
Sarcosine oxidase inhibitor

ATP deaminase inhibitor
Sodium channel blocker class Ib
Cutinase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Neurokinin 2 antagonist
2-Hydroxy-3-oxopropionate reductase inhibitor
Aldehyde dehydrogenase [NAD(P)⁺] inhibitor
Gaucher disease treatment
Dehydro-L-gulonate decarboxylase inhibitor
CYP2G1 substrate
Beta-cyclopiazionate dehydrogenase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
DNA polymerase I inhibitor
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
Venombin A inhibitor
2-Methyleneglutarate mutase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
CYP3C substrate
(S)-2-Methylmalate dehydratase inhibitor
Serine-phosphoethanolamine synthase inhibitor
Heme oxygenase inhibitor
Imidazoline receptor agonist
Cyclomaltodextrinase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Pin1 inhibitor
Antihelminthic (Fasciola)
Adenylate cyclase stimulant
Sphingosine 1-phosphate receptor 1 antagonist
Interleukin 6 antagonist
Glucan 1,4-beta-glucosidase inhibitor
6,7-Dihydropteridine reductase inhibitor
Kynureninase inhibitor
Cardioprotectant
UGT1A7 substrate
Formimidoylglutamase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
NMDA receptor polyamine site antagonist
NAD⁺ kinase inhibitor
Purine biosynthesis inhibitor
UGT1A8 substrate
L-Serine ammonia-lyase inhibitor
Xylose isomerase inhibitor
Riboflavin phosphotransferase inhibitor
Cyclooxygenase 1 substrate
Atrolysin C inhibitor
Hepatic disorders treatment
Hydroxyquinol 1,2-dioxygenase inhibitor
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor

Glucose 1-dehydrogenase inhibitor
DELTA24-sterol reductase inhibitor
Diphosphomevalonate decarboxylase inhibitor
CYP2C11 substrate
Nuclease inhibitor
Arginase inhibitor
5 Hydroxytryptamine 7L antagonist
Pyridoxal kinase inhibitor
Cell adhesion inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Pancreatic disorders treatment
ATP adenylyltransferase inhibitor
Oryzin inhibitor
Malate-CoA ligase inhibitor
Membrane dipeptidase inhibitor
AICAR transformylase inhibitor
Polyamine biosynthesis inhibitor
Peroxidase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Ribitol 2-dehydrogenase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Gentisate 1,2-dioxygenase inhibitor
Carboxypeptidase B inhibitor
Diiodophenylpyruvate reductase inhibitor
Hydroxylysine kinase inhibitor
BRAF expression inhibitor
Octopamine antagonist
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Arginine kinase inhibitor
Immunostimulant
Glutamate synthase (NADPH) inhibitor
Iodide peroxidase inhibitor
Vanilloid agonist
Acylphosphatase inhibitor
Cellulase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
Arabinose isomerase inhibitor
Sweetener
Septic shock treatment
L-iduronidase inhibitor
Malate dehydrogenase (NADP⁺) inhibitor
Penicillin amidase inhibitor
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
CYP1A1 inducer
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
[citrate-(pro-3S)-lyase] thiolesterase inhibitor
Homocysteine S-methyltransferase inhibitor
Inositol oxygenase inhibitor
HDL-cholesterol increasing

Antirickettsial
N-acylmannosamine kinase inhibitor
CYP2C19 substrate
Coproporphyrinogen oxidase inhibitor
Agaritine gamma-glutamyltransferase inhibitor
UGT1A10 substrate
ADP-ribosylarginine hydrolase inhibitor
Acetoin dehydrogenase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Sucrose-phosphate synthase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Cyanate hydratase inhibitor
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Linoleate isomerase inhibitor
Oxaloacetate decarboxylase inhibitor
Alanine racemase inhibitor
Cancer procoagulant inhibitor
Hemostatic
Levansucrase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Ornithine decarboxylase inhibitor
Alcohol dehydrogenase inhibitor
Anticholelithogenic
Tyrosine transaminase inhibitor
Amino-acid N-acetyltransferase inhibitor
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Restenosis treatment
UGT2B15 substrate
Aldehyde dehydrogenase 2 substrate
Antiprotozoal (Toxoplasma)
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Triose-phosphate isomerase inhibitor
Glutamate dehydrogenase (NADP⁺) inhibitor
Gastritis treatment
Integrin alphaVbeta3 antagonist
Antimetastatic
Lanosterol 14 alpha demethylase inhibitor
3-Deoxy-7-phosphoheptulonate synthase inhibitor
tRNA-pseudouridine synthase I inhibitor
D-Serine ammonia-lyase inhibitor
L-ascorbate peroxidase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Tyrosine 2,3-aminomutase inhibitor
Retinol O-fatty-acyltransferase inhibitor
X-Trp aminopeptidase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Non-steroidal antiinflammatory agent

Asparagine-oxo-acid transaminase inhibitor
Glutamate (mGluR4) agonist
Deoxyhypusine monooxygenase inhibitor
Gout treatment
Aldose reductase substrate
Glutamate receptor agonist
Isocitrate lyase inhibitor
Thromboxane synthase stimulant
Homoserine O-succinyltransferase inhibitor
Adenylate kinase inhibitor
Corticotropin-like
D-Lysine 5,6-aminomutase inhibitor
Cholesterol synthesis inhibitor
Dolichyl-phosphatase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Retinol dehydrogenase inhibitor
Diabetic retinopathy treatment
NADH dehydrogenase inhibitor
Antiviral (Herpes)
CYP2D6 substrate
4-Hydroxybenzoate decarboxylase inhibitor
Putrescine carbamoyltransferase inhibitor
FMO1 substrate
Arginine racemase inhibitor
Glutamate formimidoyltransferase inhibitor
Long-chain-fatty-acid-CoA ligase inhibitor
Amino-acid racemase inhibitor
Glutamate (mGluR1) agonist
Phenylalanine 2-monooxygenase inhibitor
Mediator release inhibitor
Glutathione S-transferase inhibitor
Urolithiasis treatment
Protein-synthesizing GTPase inhibitor
Argininosuccinate synthase inhibitor
Lysine carboxypeptidase inhibitor
Endopeptidase inhibitor
Aryl hydrocarbon receptor agonist
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Meprin A inhibitor
Caspase 8 stimulant
Cyclooxygenase 3 inhibitor
Antiviral (Influenza)
Farnesyltransferase inhibitor
Paget's disease treatment
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Thromboxane antagonist
CMP-N-acetylneuraminate monooxygenase inhibitor
Antihelmintic
Serine O-acetyltransferase inhibitor
UDP-N-acetylmuramate-L-alanine ligase inhibitor

Alanine dehydrogenase inhibitor
Succinic dehydrogenase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
Betaine-aldehyde dehydrogenase inhibitor
CYP1A substrate
Carbon-monoxide dehydrogenase inhibitor
VEGF expression inhibitor
GABA C receptor antagonist
Wound healing agent
Carnitine O-octanoyltransferase inhibitor
Fumarylacetoacetase inhibitor
Aminopeptidase I inhibitor
Histidine ammonia-lyase inhibitor
Antineoplastic, alkylator
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Alpha,alpha-trehalase inhibitor
Myosin-light-chain-phosphatase inhibitor
Vitronectin receptor antagonist
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Glycine N-methyltransferase inhibitor
Dopamine release stimulant
Restless leg syndrome treatment
Chemokine receptor antagonist
Polynucleotide adenylyltransferase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Aspartate 4-decarboxylase inhibitor
Lactate-malate transhydrogenase inhibitor
Dimethylhistidine N-methyltransferase inhibitor
DNA nucleotidylexotransferase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Liver X receptor antagonist
Ferredoxin-nitrite reductase inhibitor
Proliferative diseases treatment
Glyceraldehyde-3-phosphate dehydrogenase (NADP⁺) inhibitor
Thyroid hormone agonist
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Xenobiotic-transporting ATPase inhibitor
Glutamine-fructose-6-phosphate transaminase inhibitor
4-Hydroxy-2-oxoglutarate aldolase inhibitor
Respiratory analeptic
Galactosylgalactosylglucosylceramidase inhibitor
Glutathione synthase inhibitor
UDP-N-acetylmuramate dehydrogenase inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
Antibacterial, ophthalmic
DNA methyltransferase I inhibitor
Homospermidine synthase inhibitor
Tyrosine kinase stimulant

4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
Anthranilate-CoA ligase inhibitor
Raynaud's phenomenon treatment
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Glycine N-acyltransferase inhibitor
GST T substrate
GST T1-1 substrate
Malyl-CoA lyase inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Chemoprotective
Glycerol dehydratase inhibitor
L-lactate dehydrogenase (cytochrome) inhibitor
Phosphofructokinase-1 inhibitor
Isocitrate dehydrogenase (NADP+) inhibitor
Phospholipase A1 inhibitor
Neurotrophic factor enhancer
Glutamine synthetase inhibitor
Serine-sulfate ammonia-lyase inhibitor
Deoxyribose-phosphate aldolase inhibitor
Thrombolytic
D-threo-aldose 1-dehydrogenase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Antiprotozoal (Leishmania)
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
Phospholipase inhibitor
CYP2D substrate
Antianemic
Granzyme B inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Arylamine N-Acetyltransferase substrate
Phosphoribulokinase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
Antidiabetic (type 1)
Nitric oxide scavenger
Gastrointestinal motility stimulant
Antineoplastic antimetabolite
Hydroperoxide dehydratase inhibitor
TRPA1 agonist
Bisphosphoglycerate phosphatase inhibitor
CYP1A2 substrate
CYP4A1 substrate
Acyl-CoA oxidase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor

Falcipain 3 inhibitor
Ribonuclease inhibitor
Sulfate adenylyltransferase inhibitor
Phospholipase D inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Methionine adenosyltransferase inhibitor
Methylaspartate mutase inhibitor
Choline acetyltransferase stimulant
D(-)-tartrate dehydratase inhibitor
Nav1.5 sodium channel blocker
Phosphopantothenoylcysteine decarboxylase inhibitor
L-fuconate dehydratase inhibitor
Oxaloacetate tautomerase inhibitor
TH expression enhancer
Histamine H2 receptor agonist
Tryptophan synthase inhibitor
Lombricine kinase inhibitor
Tubulin-tyrosine ligase inhibitor
Aconitate hydratase inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
Glutathione S-transferase substrate
Arylformamidase inhibitor
Cystic fibrosis treatment
Transthyretin amyloid fibril formation inhibitor
Gelatinase inhibitor
Alanine carboxypeptidase inhibitor
Maleylacetoacetate isomerase inhibitor
Aspartate carbamoyltransferase inhibitor
Adenylyl-sulfate kinase inhibitor
Protein synthesis stimulant
Pyroglutamyl-peptidase I inhibitor
Thromboxane synthase inhibitor
Alpha-L-rhamnosidase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Aspartyl aminopeptidase inhibitor
Aminopeptidase microsomal inhibitor
(R)-limonene 6-monooxygenase inhibitor
Antiamyloidogenic
Insulin secretagogues
Aminopeptidase N inhibitor
Glycogen synthase stimulant
Lactose synthase inhibitor
Alpha 1L adrenoreceptor agonist
D-Alanine-poly(phosphoribitol) ligase inhibitor
Leukotriene agonist
Clavamate synthase inhibitor
Homoserine kinase inhibitor
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Monoamine oxidase substrate
NMDA receptor glycine site agonist

Mycolysin inhibitor
Glutamate racemase inhibitor
Insulysin inhibitor
Anticarcinogenic
CYP3A4 substrate
Prostaglandin D2 agonist
Acyl-CoA dehydrogenase (NADP+) inhibitor
3-Hydroxybutyrate dehydrogenase inhibitor
Theanine hydrolase inhibitor
Dopachrome isomerase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor
6-Phosphofructo-2-kinase inhibitor
Thromboxane A2 antagonist
Coenzyme-B sulfoethylthiotransferase inhibitor
MAO B substrate
Antinephritic
Carboxy-cis,cis-muconate cyclase inhibitor
Antiparasitic
DNA-3-methyladenine glycosylase II inhibitor
Glutamate (mGluR group III) antagonist
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
CYP4F substrate
Acyloxyacyl hydrolase inhibitor
D-lactate-2-sulfatase inhibitor
Guanylate cyclase inhibitor
Camphor 1,2-monooxygenase inhibitor
Macrophage elastase inhibitor
CC chemokine 4 receptor antagonist
CYP2C2 substrate
Growth stimulant
Sulfotransferase substrate
Astacin inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Radiosensitizer
Kainate receptor 1 agonist
Nitrate reductase inhibitor
Glutamate (mGluR group I) agonist
Sodium/bile acid cotransporter inhibitor
Streptopain inhibitor
Stroke treatment
4-Hydroxybenzoate 3-monooxygenase inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD+) inhibitor
Beta-amylase inhibitor
N6-methyl-lysine oxidase inhibitor
Proline dehydrogenase inhibitor
Histidine-tRNA ligase inhibitor
Ornithine carbamoyltransferase inhibitor

2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Adenylylsulphatase inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
MAO A substrate
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Indoleamine-pyrrole 2,3-dioxygenase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Ganglioside galactosyltransferase inhibitor
Thioredoxin reductase inhibitor
Thioredoxin inhibitor
Corticotropin releasing factor antagonist
Gamma-glutamyl hydrolase inhibitor
Neurolysin inhibitor
Allantoinase inhibitor
Interleukin 1a antagonist
Antiepileptic
Phosphoglycerate dehydrogenase inhibitor
Serine carboxypeptidase inhibitor
Sepsis treatment
p21-activated kinase 1 inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
HIV-2 reverse transcriptase inhibitor
Candidapepsin inhibitor
Undecaprenyl-diphosphatase inhibitor
Histone deacetylase SIRT1 inhibitor
DNA methylase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Glutaminyl-peptide cyclotransferase inhibitor
2-Ethylmalate synthase inhibitor
Systemic lupus erythematosus treatment
Vasculitis treatment
Tryptophan 5 hydroxylase inhibitor
Glutamate receptor antagonist
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Cysteine dioxygenase inhibitor
Antidepressant, Imipramine-like
UGT2B10 substrate
Cholestanetriol 26-monooxygenase inhibitor
3-Oxoacid CoA-transferase inhibitor
Rhodopsin kinase inhibitor
Estrone sulfotransferase inhibitor
Urate transporter 1 inhibitor
Glutamate (mGluR3) agonist
Anthranilate phosphoribosyltransferase inhibitor
Adrenergic, ophthalmic
Leishmanolysin inhibitor
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor

Peptidylglycine monooxygenase inhibitor
SULT2A1 substrate
Glycine N-benzoyltransferase inhibitor
Arachidonate-CoA ligase inhibitor
Pyridoxamine-oxaloacetate transaminase inhibitor
Toll-Like receptor antagonist
Linoleoyl-CoA desaturase inhibitor
Methylthioadenosine nucleosidase inhibitor
Isomaltulose synthase inhibitor
Integrin α V β 1 antagonist
Autophagy inducer
NMDA receptor antagonist
Nitric-oxide synthase stimulant
Antifungal (Pneumocystis)
Hyponitrite reductase inhibitor
Phosphoserine transaminase inhibitor
D-aspartate oxidase inhibitor
Antispirochetal
SULT1A3 substrate
Tartrate decarboxylase inhibitor
NMDA 2A receptor antagonist
CYP4F12 substrate
Cerebroside-sulfatase inhibitor
ATPase stimulant
Fumarate hydratase inhibitor
Strombine dehydrogenase inhibitor
CYP3A substrate
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Pantoate 4-dehydrogenase inhibitor
Butyrate-CoA ligase inhibitor
Necroptosis inhibitor
Alpha-L-fucosidase inhibitor
Aminoacyl-tRNA synthetase inhibitor
Dextranucrase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP⁺) inhibitor
Glycine N-choloyltransferase inhibitor
Amylo-alpha-1,6-glucosidase inhibitor
Propionate CoA-transferase inhibitor
Sodium-dependent vitamin C transporter 2 inhibitor
Malate dehydrogenase (decarboxylating) inhibitor
Haloalkane dehalogenase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Channel-conductance-controlling ATPase inhibitor
Cysteine-tRNA ligase inhibitor
Trimethylamine dehydrogenase inhibitor
Nitrilase inhibitor
Phosphoinositide dependent kinase 1 inhibitor
Nav1.4 sodium channel blocker

Excitatory amino acid transporter 2 inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor
3C-like protease (Human coronavirus) inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
Adenylate cyclase inhibitor
CYP2A4 substrate
Diphosphate-serine phosphotransferase inhibitor
Phosphoribosylformylglycinamide synthase inhibitor
Biliverdin reductase inhibitor
Glutamyl-tRNA synthase (glutamine-hydrolysing) inhibitor
Antiprotozoal (Amoeba)
Huntington's disease treatment
Gestagen antagonist
Galactoside 2- α -L-fucosyltransferase inhibitor
Diaminopimelate decarboxylase inhibitor
Glutamate (mGluR8) antagonist
Arginine N-succinyltransferase inhibitor
Magnolysin inhibitor
CYP26A substrate
Acetolactate decarboxylase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Reductase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Dihydrofolate synthase inhibitor
Prostaglandin antagonist
5 Hydroxytryptamine release stimulant
Aldehyde dehydrogenase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Lactaldehyde reductase inhibitor
Tryptophan-tRNA ligase inhibitor
Cytokine modulator
Trans-pentaprenyltransferase inhibitor
Altronate dehydratase inhibitor
CMP-KDO synthase inhibitor
Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor
Ribonuclease U2 inhibitor
Cell wall synthesis inhibitor
Bacterial leucyl aminopeptidase inhibitor
Glucose-1,6-bisphosphate synthase inhibitor
CYP2D15 substrate
Pantetheine-phosphate adenylyltransferase inhibitor
G-protein-coupled bile acid receptor 1 agonist
Octadecanal decarbonylase inhibitor
NMDA receptor polyamine site agonist
Cyclopentanone monooxygenase inhibitor
Prolactin inhibitor
Beta-Lysine 5,6-aminomutase inhibitor
AMPA receptor agonist
Imidazoleacetate 4-monooxygenase inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor

Formaldehyde dehydrogenase inhibitor
Glucagon-like peptide 1 receptor antagonist
Isovaleryl-CoA dehydrogenase inhibitor
Malate synthase inhibitor
Somatostatin agonist
Phospholipase A2 inhibitor
Kainate receptor agonist
Salicylate 1-monooxygenase inhibitor
Aminoacyl-tRNA hydrolase inhibitor
Phloroglucinol reductase inhibitor
Glycogen (starch) synthase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor
2-Oxoaldehyde dehydrogenase (NAD+) inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
ATP citrate lysase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
tRNA methyltransferase inhibitor
2-(acetamidomethylene)succinate hydrolase inhibitor
Antiprotozoal (Trichomonas)
Laminaribiose phosphorylase inhibitor
Ethanolamine kinase inhibitor
Trypanothione-disulfide reductase inhibitor
D-stereospecific aminopeptidase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor
Prostaglandin-I synthase inhibitor
tRNA (adenine-N1-)-methyltransferase inhibitor
Phosphomevalonate kinase inhibitor
Diaminopimelate epimerase inhibitor
Lassitude treatment
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
CYP2B4 substrate
Protein-glutamate O-methyltransferase inhibitor
Tyrosine phenol-lyase inhibitor
Homoserine O-acetyltransferase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
3-Dehydroquinate dehydratase inhibitor
Factor XIIIa inhibitor
Gonadotropin antagonist
AR expression inhibitor
6-Methylsalicylate decarboxylase inhibitor
Severe acute respiratory syndrome treatment
Substance P antagonist
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
Kinesin antagonist
Kinesin-like protein 1 inhibitor
4-Hydroxyphenylacetate 1-monooxygenase inhibitor
CYP2B1 substrate

Citrate (Si)-synthase inhibitor
Protein kinase stimulant
Pectate lyase inhibitor
GABA receptor antagonist
Antibiotic Glycopeptide-like
Diuretic
Dimethylallyltranstransferase inhibitor
N-formylglutamate deformylase inhibitor
Oxytocin agonist
tRNA adenylyltransferase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Spermine synthase inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Caspase 9 inhibitor
Phosphoglycerate phosphatase inhibitor
L(+)-Tartrate dehydratase inhibitor
2-Isopropylmalate synthase inhibitor
CDC25C inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Ethanolamine ammonia-lyase inhibitor
Pyruvate kinase inhibitor
Beta-D-fucosidase inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
Vascular dementia treatment
Tetrahydroxynaphthalene reductase inhibitor
tRNA (uracil-5-)-methyltransferase inhibitor
Glucan 1,3-beta-glucosidase inhibitor
SULT1A1 substrate
Stipitatonate decarboxylase inhibitor
Homoisocitrate dehydrogenase inhibitor
Ribose-5-phosphate isomerase inhibitor
Secretase alpha stimulant
Secretase stimulant
CYP2A6 inhibitor
Adrenaline release stimulant
Decylcitrate synthase inhibitor
Ceramide glucosyltransferase inhibitor
Urotensin II agonist
Hydroxysteroid dehydrogenase inhibitor
Chelator
Thyroid hormone antagonist
Arabinogalactan endo-1,4-beta-galactosidase inhibitor
Glycosylceramidase inhibitor
Phosphoglycerate mutase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Kallikrein 13 inhibitor

1,5-Anhydro-D-fructose reductase inhibitor
3-Deoxy-8-phosphooctulonate synthase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Glutamate (mGluR4) antagonist
CYP1A1 substrate
UDP-N-acetylglucosamine diphosphorylase inhibitor
4-Hydroxybenzoate 1-hydroxylase inhibitor
Spermidine synthase inhibitor
Phenylalanine-tRNA ligase inhibitor
Valine-pyruvate transaminase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Vibriolysin inhibitor
Prostaglandin H2 antagonist
Galactoside O-acetyltransferase inhibitor
Spermine antagonist
L lactate dehydrogenase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Somatostatin 2 agonist
2-Dehydropantolactone reductase (A-specific) inhibitor
Leucyltransferase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Isopenicillin-N epimerase inhibitor
HMG CoA synthase inhibitor
Bombesin 2 receptor antagonist
Pseudouridylate synthase inhibitor
Chloride channel blocker
Phenylacetaldehyde dehydrogenase inhibitor
Retinoid X alpha receptor agonist
Beta galactosidase inhibitor
S-methyl-5-thioribose kinase inhibitor
Kallikrein inhibitor
Aspartate racemase inhibitor
Pyruvate, water dikinase inhibitor
2-Pyrocatechuate decarboxylase inhibitor
Cholesterol oxidase inhibitor
Deoxyhypusine synthase inhibitor
Glutamate (mGluR group II) agonist
Hyperprolactinemia treatment
Leukocyte elastase inhibitor
Arginine-tRNA ligase inhibitor
Cytostatic
Beta amyloid protein antagonist
Diacylglycerol kinase inhibitor
Kainate receptor antagonist
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
DNA synthesis inhibitor
2-Aminohexanoate transaminase inhibitor
CYP3A7 substrate
Antitussive
Factor XIa inhibitor

Glutamate (mGluR1a) agonist
Glutamate (mGluR5a) agonist
Excitatory amino acid transporter 1 inhibitor
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
Phosphoketolase inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Myc inhibitor
Thyroid hormone beta agonist
Assemblin inhibitor
Glutamate release inhibitor
Dihydropteroate synthase inhibitor
Oligo-1,6-glucosidase inhibitor
Adenylate cyclase I inhibitor
Endothelin-converting enzyme inhibitor
Antidiarrheal
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Melanocortin agonist
Neurokinin 3 antagonist
Glycerol dehydrogenase (NADP+) inhibitor
Aldehyde dehydrogenase substrate
CYP2B2 substrate
Lactoylglutathione lyase inhibitor
Interferon agonist
Creatine kinase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
CPB protease inhibitor
GP IIb/IIIa receptor antagonist
VCAM-1 antagonist
Potassium channel large-conductance Ca-activated activator
VCAM antagonist
Dementia treatment
Phosphorylase a inhibitor
Sphingosine 1-phosphate receptor antagonist
CYP24 substrate
Glutamate (mGluR6) agonist
GABA transporter inhibitor
Caspase 3 inhibitor
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
Thioether S-methyltransferase inhibitor
Phosphorylase kinase inhibitor
Methenyltetrahydrofolate cyclohydrolase inhibitor
Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor
L-galactonolactone oxidase inhibitor
Thermolysin inhibitor
Parathyroid hormone antagonist
Pyridoxine 4-oxidase inhibitor
Histone deacetylase class III inhibitor
[Isocitrate dehydrogenase (NADP+)] kinase inhibitor
Lactamase C inhibitor
Adamalysin inhibitor

Dihydrouracil oxidase inhibitor
Acetoacetate decarboxylase inhibitor
Glucan 1,4-alpha-glucosidase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Hypercalcemia treatment
Insecticide
Ribonucleoside diphosphate reductase inhibitor
Hydroxypyruvate reductase inhibitor
Integrin alpha5beta6 antagonist
Protocatechuate 3,4-dioxygenase inhibitor
Adenylate cyclase V inhibitor
NMDA receptor glycine site B antagonist
MAP-kinase-activated kinase 1 inhibitor
Catechol 1,2-dioxygenase inhibitor
Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Dichloromethane dehalogenase inhibitor
Carboxycyclohexadienyl dehydratase inhibitor
Ceramidase inhibitor
Protein kinase B alpha inhibitor
Glutamate (mGluR3) antagonist
tRNA (guanine-N1-)-methyltransferase inhibitor
Pyruvate, phosphate dikinase inhibitor
Eicosanoid agonist
Procollagen galactosyltransferase inhibitor
Endo-1,4-beta-xylanase inhibitor
[glutamate-ammonia-ligase] adenylyltransferase inhibitor
N-acetylmuramoyl-L-alanine amidase inhibitor
AMPA 3 receptor antagonist
Serine-type D-Ala-D-Ala carboxypeptidase inhibitor
Integrin alphaVbeta6 antagonist
Calcium channel activator
Thyroid hormone alpha 1 agonist
Thyroid hormone alpha agonist
Thyroid hormone beta 1 agonist
2-Methylcitrate synthase inhibitor
Amidase inhibitor
CTP synthase inhibitor
Erythropoietin receptor agonist
GABA transporter 1 inhibitor
Tartrate dehydrogenase inhibitor
Antiacromegalic
Methionine-tRNA ligase inhibitor
Phosphopyruvate hydratase inhibitor
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
AMPA 2 receptor antagonist
Peroxisome proliferator-activated receptor gamma antagonist
Hydroxyacylglutathione hydrolase inhibitor
Poly(ADP-ribose) glycohydrolase inhibitor
CYP26 substrate

Glucose-1-phosphatase inhibitor
CYP2A5 inhibitor
Cyclohexadienyl dehydrogenase inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
Thyroid hormone alpha 1 antagonist
Spasmolytic, Papaverin-like
Protein kinase B stimulant
CC chemokine 5 receptor antagonist
Prostaglandin agonist
1-Phosphofructokinase inhibitor
Aralkylamine dehydrogenase inhibitor
Dipeptidyl peptidase II inhibitor
Aldose reductase 2 inhibitor
Carbonic anhydrase XIV inhibitor
Antihypertriglyceridemic
Antiviral (Hepatitis B)
Adenine nucleotide translocase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Phosphoenolpyruvate carboxykinase (GTP) inhibitor
Uridine nucleosidase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Carminative
3-Dehydroquinase synthase inhibitor
Cellobiose phosphorylase inhibitor
Galactokinase inhibitor
Cathepsin H inhibitor
Lysine-tRNA ligase inhibitor
D-arabinonolactone oxidase inhibitor
Adenylosuccinate lyase inhibitor
Choline sulfotransferase inhibitor
CMP-N-acylneuraminate phosphodiesterase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
Adenylosuccinate synthase inhibitor
Integrin alpha2beta1 antagonist
Ulcerative colitis treatment
CYP4F8 substrate
Alkylglycerone-phosphate synthase inhibitor
Glutathione-disulfide reductase inhibitor
1-Alkyl-2-acetyl glycerophosphocholine esterase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Vanilloid 4 agonist
Mucorpepsin inhibitor
CYP3A11 substrate
Peroxisome proliferator-activated receptor antagonist
Hematinic
Ribonucleotide reductase inhibitor
Thymidine-triphosphatase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Glucagon receptor antagonist
Carnitine palmitoyltransferase inhibitor

Prostaglandin F2 alpha antagonist
Glutamate (mGluR) agonist
Anhydrotetracycline monooxygenase inhibitor
Kynurenine 3 monooxygenase inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Steroid synthesis inhibitor
Carboxylate reductase inhibitor
Dihydrofolate reductase inhibitor
Malonyl-CoA decarboxylase inhibitor
Maltose-transporting ATPase inhibitor
Glutaryl-CoA dehydrogenase inhibitor
D-Ala-D-Ala ligase inhibitor
Serine-tRNA ligase inhibitor
Guanylate kinase inhibitor
Formimidoyltetrahydrofolate cyclodeaminase inhibitor
Carboxylesterase inhibitor
Histamine N-methyltransferase inhibitor
Macular degeneration treatment
Glutamate (mGluR group III) agonist
Integrin alpha5beta1 antagonist
Glucose-6-phosphate translocase inhibitor
Kallikrein 3 inhibitor
Tannase inhibitor
Diacylglycerol O-acyltransferase inhibitor
Cytochrome-b5 reductase substrate
AMP deaminase inhibitor
Procollagen-proline 3-dioxygenase inhibitor
5 Lipoxygenase activating protein inhibitor
3-Mercaptopyruvate sulfurtransferase inhibitor
Aldosterone antagonist
Maleylacetate reductase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Endonuclease (influenza) inhibitor
Laxative
Folypolyglutamate synthase inhibitor
Glutamate (mGluR2) antagonist
Acetate-CoA ligase inhibitor
NF-E2-related factor 2 stimulant
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Dipeptidyl peptidase I inhibitor
Folate transporter 1 inhibitor
Butyryl-CoA dehydrogenase inhibitor
ICAM 1 antagonist
Diiodotyrosine transaminase inhibitor
Alternansucrase inhibitor
Dihydrofolate reductase (Mycobacterium avium) inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Somatostatin 5 antagonist
Chorismate mutase inhibitor
Antiviral (Influenza A)

Serum-glucocorticoid regulated kinase 1 inhibitor
Antituberculosic
Keratosis actinic (solar) treatment
CC chemokine 9 receptor antagonist

Bethanidine sulfate

Molecular Mechanism (initial) :

alpha-2a adrenergic receptors agonist

Molecular Mechanism (repurposed) :

potassium channel blocker

initial indication(s):

hypertension

Repurposed indication(s):

ventricular fibrillation suppression

Predicted Activities

Cardiotonic

General pump inhibitor

Antiarrhythmic (ventricular fibrillation suppression)

Phobic disorders treatment

CYP2D16 substrate

Methylamine-glutamate N-methyltransferase inhibitor

Mucomembranous protector

Calcium channel (voltage-sensitive) activator

CYP2H substrate

Nicotinic alpha6beta3beta4alpha5 receptor antagonist

Sodium channel blocker

CYP2C3 substrate

Glycosylphosphatidylinositol phospholipase D inhibitor

Antiulcerative

Ompin inhibitor

Threonine aldolase inhibitor

Antihypertensive

Limulus clotting factor B inhibitor

Nicotinic alpha2beta2 receptor antagonist

Trimethylamine dehydrogenase inhibitor

Macrophage colony stimulating factor agonist

Protein-arginine deiminase inhibitor

Antisecretoric

Oxygen scavenger

Antimyopathies

Polyamine-transporting ATPase inhibitor

Taurine dehydrogenase inhibitor

Phospholipid-translocating ATPase inhibitor

1,4-Lactonase inhibitor

Chloride peroxidase inhibitor

Septic shock treatment

Pro-opiomelanocortin converting enzyme inhibitor

NADPH peroxidase inhibitor

Arginine 2-monooxygenase inhibitor

Glutamyl endopeptidase II inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Albendazole monooxygenase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Kidney function stimulant
CYP2E1 inhibitor
Gastrin inhibitor
Ovulation inhibitor
Pterin deaminase inhibitor
4-Hydroxyproline epimerase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Dimethylargininase inhibitor
CYP2J substrate
Trimethylamine-oxide aldolase inhibitor
Limulus clotting factor C inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
2-Haloacid dehalogenase inhibitor
Fusarinine-C ornithinesterase inhibitor
Complement factor D inhibitor
FMO1 substrate
Hydrogen dehydrogenase inhibitor
Fibrolase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
CYP2J2 substrate
Chenodeoxycholytaurine hydrolase inhibitor
Nav1.5 sodium channel blocker
Pseudolysin inhibitor
Alopecia treatment
Octopamine antagonist
UDP-N-acetylglucosamine 4-epimerase inhibitor
Venombin AB inhibitor
Sugar-phosphatase inhibitor
Antihistaminic
Erythropoiesis stimulant
Methylumbelliferyl-acetate deacetylase inhibitor
Platelet adhesion inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Thioredoxin inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
CYP2D2 inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Dopamine release stimulant
Aminobutyraldehyde dehydrogenase inhibitor
IgA-specific serine endopeptidase inhibitor
Sodium channel (voltage-gated) blocker
Aspartate-phenylpyruvate transaminase inhibitor
Polyporopepsin inhibitor

Ubiquinol-cytochrome-c reductase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Maillard reaction inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Imidazoline receptor agonist
DNA-3-methyladenine glycosylase I inhibitor
Glutathione thiolesterase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Histamine antagonist
N-methylhydantoinase (ATP-hydrolysing) inhibitor
CYP3A2 substrate
Acylcarnitine hydrolase inhibitor
Flavin-containing monooxygenase inhibitor
Carnitinamidase inhibitor
Exoribonuclease II inhibitor
Phosphopantothienoylcysteine decarboxylase inhibitor
Antiprotozoal
Histamine release stimulant
(R)-6-hydroxynicotine oxidase inhibitor
Carboxypeptidase Taq inhibitor
Biotinidase inhibitor
N-formylmethionyl-peptidase inhibitor
Fibrinolytic
Rhinitis treatment
Cathepsin T inhibitor
CYP2F1 substrate
Diabetic neuropathy treatment
CYP2B11 substrate
Arylmalonate decarboxylase inhibitor
Antiperistaltic
Thiamine pyridinylase inhibitor
Membrane integrity agonist
Taurine-2-oxoglutarate transaminase inhibitor
N-acylmannosamine kinase inhibitor
Phenol O-methyltransferase inhibitor
Glyoxylate reductase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Antianorexic
S-formylglutathione hydrolase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
CYP2D15 substrate
L-glutamate oxidase inhibitor
Gluconate 5-dehydrogenase inhibitor
Cyanoalanine nitrilase inhibitor
CYP2A8 substrate
Glucan 1,4- α -maltotetraohydrolase inhibitor
5-Hydroxytryptamine uptake stimulant
Antidiarrheal

Mannan endo-1,4-beta-mannosidase inhibitor
Cl--transporting ATPase inhibitor
Fragilysin inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Polyneuridine-aldehyde esterase inhibitor
CYP2C19 inhibitor
Glycine amidinotransferase inhibitor
Platelet aggregation stimulant
ADP-thymidine kinase inhibitor
Alkane 1-monooxygenase inhibitor
3-Cyanoalanine hydratase inhibitor
FMO3 substrate
4-Nitrophenol 2-monooxygenase inhibitor
Fructose 5-dehydrogenase inhibitor
MAP kinase stimulant
Adrenaline release stimulant
Para amino benzoic acid antagonist
Manganese peroxidase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Formaldehyde transketolase inhibitor
Leukopoiesis inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Hematopoietic inhibitor
Leukopoiesis stimulant
Loop diuretic
Centromere associated protein inhibitor
Camphor 1,2-monooxygenase inhibitor
CYP2A3 substrate
Fatty-acyl-CoA synthase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Antiparkinsonian, rigidity relieving
S-alkylcysteine lyase inhibitor
Mucositis treatment
ICAM1 expression inhibitor
Ethanolamine oxidase inhibitor
Thymidylate 5'-phosphatase inhibitor
Mandelate 4-monooxygenase inhibitor
CYP2C29 substrate
Fibrinogen receptor antagonist
Guanidinoacetate kinase inhibitor
Nitric-oxide synthase inhibitor
Steroid synthesis inhibitor
Acetylcholinesterase inhibitor
Antidepressant
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Histamine H1 receptor agonist
Spermidine dehydrogenase inhibitor
Mitochondrial processing peptidase inhibitor
Histidine N-acetyltransferase inhibitor

CYP2G1 substrate
Acidifying agent non gastric
Nicotine dehydrogenase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Feruloyl esterase inhibitor
Mood disorders treatment
CYP2C12 substrate
Lysine 2,3-aminomutase inhibitor
Phosphatidylserine decarboxylase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Pancreatic elastase inhibitor
GABA C receptor agonist
tRNA-pseudouridine synthase I inhibitor
Ferredoxin hydrogenase inhibitor
Gluconolactonase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Simian immunodeficiency virus proteinase inhibitor
Analgesic
Intermittent claudication treatment
Interleukin 10 agonist
Opine dehydrogenase inhibitor
Gonadotropin antagonist
Prion diseases treatment
Endopeptidase So inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
Glucose oxidase inhibitor
Yeast ribonuclease inhibitor
Antiviral (Adenovirus)
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Antineurotic
Pin1 inhibitor
Acetylcholine neuromuscular blocking agent
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Glycolate dehydrogenase inhibitor
Monoamine uptake inhibitor
Sulfite oxidase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Bisphosphoglycerate phosphatase inhibitor
Gingipain K inhibitor
Sulfur reductase inhibitor
Acetylenecarboxylate hydratase inhibitor
NADH kinase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
CYP2D6 inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Vasoprotector
Choline-phosphate cytidyltransferase inhibitor
X-methyl-His dipeptidase inhibitor

2-Dehydropantoate 2-reductase inhibitor
Adenylyl-sulfate reductase inhibitor
Adrenergic, ophthalmic
Picornain 3C inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Superoxide dismutase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
CYP2B5 substrate
Hyponitrite reductase inhibitor
Fucosterol-epoxide lyase inhibitor
Lysostaphin inhibitor
Transcription factor NF kappa A inhibitor
Mannose isomerase inhibitor
Carbon-monoxide dehydrogenase inhibitor
Endothelial nitric-oxide synthase inhibitor
Enteropeptidase inhibitor
Antinociceptive
HIV attachment inhibitor
Spasmolytic
EIF4E expression inhibitor
Myeloblastin inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Acetylspermidine deacetylase inhibitor
Cyclooxygenase substrate
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Fructan beta-fructosidase inhibitor
Hydroxylamine oxidase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Mucinaminyserine mucinaminidase inhibitor
GABA B receptor agonist
Antiprotozoal (Trypanosoma)
Flavin-containing monooxygenase substrate
CYP2A1 substrate
Diamine N-acetyltransferase inhibitor
Glutamate-tRNA ligase inhibitor
Carboxypeptidase D inhibitor
Meprin B inhibitor
Ethanamine-phosphate cytidyltransferase inhibitor
Acetylgalactosaminy-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminytransferase inhibitor
Ornithine cyclodeaminase inhibitor
Apyrase inhibitor
Nitrite reductase (NO-forming) inhibitor
Indolepyruvate C-methyltransferase inhibitor
Histamine agonist
CYP1A2 inhibitor
Alkylacetylgllycerophosphatase inhibitor
Aspartate-ammonia ligase inhibitor
Nicotinate dehydrogenase inhibitor
Malate oxidase inhibitor
Antiprotozoal (Plasmodium)

Penicillin amidase inhibitor
CYP2B10 substrate
Thiamine-triphosphatase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Glyoxylate oxidase inhibitor
Granzyme A inhibitor
3C-like protease (Human coronavirus) inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
JAK2 expression inhibitor
Antiviral (Poxvirus)
Corticosteroid side-chain-isomerase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Retinoic acid metabolism inhibitor
CYP1A inhibitor
CYP3A7 substrate
CYP2D1 substrate
Botulin neurotoxin A light chain inhibitor
CYP3C substrate
Vanilloid 1 agonist
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Pitrilysin inhibitor
CYP4A11 substrate
Isopenicillin-N epimerase inhibitor
Complement inhibitor
Horrilysin inhibitor
GABA C receptor antagonist
Analgesic, non-opioid
Pseudouridylate synthase inhibitor
Styrene-oxide isomerase inhibitor
Neurotransmitter uptake inhibitor
4-Hydroxyglutamate transaminase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Creatinase inhibitor
Dipeptidase E inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Cyclic AMP modulator
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Transketolase inhibitor
Membrane permeability enhancer
Prostaglandin-A1 DELTA-isomerase inhibitor
5 Hydroxytryptamine 7 agonist
Creatininase inhibitor
Alpha-N-acetylglucosaminidase inhibitor

Gastric antisecretory
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Neuropeptide Y1 antagonist
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Antinaupathic
Alkenylglycerophosphocholine hydrolase inhibitor
GABA aminotransferase inhibitor
HCV IRES inhibitor
Neuronal nitric-oxide synthase inhibitor
Opioid kappa 3 receptor antagonist
Histamine H2 receptor agonist
Urticaria treatment
Nucleoside oxidase (H2O2-forming) inhibitor
Tyrosine kinase stimulant
Pullulanase inhibitor
Antihypotensive
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Myosin ATPase inhibitor
Putrescine oxidase inhibitor
Cytochrome-b5 reductase substrate
Gallate decarboxylase inhibitor
Inducible nitric-oxide synthase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Cardioprotectant
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Alpha adrenoreceptor agonist
Methanol dehydrogenase inhibitor
Metallocoarboxypeptidase D inhibitor
Urethanase inhibitor
N-acetyllactosamine synthase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Carnitine dehydratase inhibitor
Choline-sulfatase inhibitor
Bothrolysin inhibitor
Creatinine deaminase inhibitor
Insulin promoter
Calcium channel activator
Allantoin racemase inhibitor
Glucuronate isomerase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD+) inhibitor
Cyclic AMP agonist
6-Pyruvoyltetrahydropterin synthase inhibitor
Histamine H2 receptor antagonist
Chitinase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor

Undecaprenyldiphospho-muramoylpentapeptide
beta-N-acetylglucosaminyltransferase inhibitor
Oxidizing agent
Antihelminthic (Nematodes)
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Thiosulfate dehydrogenase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
CC chemokine receptor 2B antagonist
Poly(beta-D-mannuronate) lyase inhibitor
Cyclopentanone monooxygenase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Glycerol 2-dehydrogenase (NADP⁺) inhibitor
Tryptophanamidase inhibitor
CYP2A4 substrate
Rubredoxin-NAD⁺ reductase inhibitor
Sphinganine kinase inhibitor
Prunasin beta-glucosidase inhibitor
Reductant
Pyridoxine 4-oxidase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Anti-Helicobacter pylori
CYP2B18 substrate
Proteasome endopeptidase complex inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Chitosanase inhibitor
Vasodilator, peripheral
Acetylnornithine deacetylase inhibitor
Antiviral (Picornavirus)
Viral entry inhibitor
CDK9/cyclin T1 inhibitor
CYP2B2 substrate
Polygalacturonase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Arylesterase inhibitor
Mannitol-1-phosphatase inhibitor
2-Dehydropantoate aldolase inhibitor
Neuropeptide antagonist
Neurotransmitter antagonist
CYP2A2 substrate
Clavamate synthase inhibitor
Aspartoacylase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Amyotrophic lateral sclerosis treatment
Methyltransferase substrate
Sulfite dehydrogenase inhibitor
RNA-directed RNA polymerase inhibitor

Pancreatic endopeptidase E inhibitor
Antifibrinolytic
Salicylate 1-monooxygenase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Acylphosphatase inhibitor
Glycine N-methyltransferase inhibitor
Neuropeptide Y antagonist
Nitric-oxide synthase stimulant
Serine-pyruvate transaminase inhibitor
Quisqualate antagonist
Alkenylglycerophosphoethanolamine hydrolase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Dimethylmaleate hydratase inhibitor
Arginine decarboxylase inhibitor
Oxidoreductase inhibitor
tRNA nucleotidyltransferase inhibitor
Cystic fibrosis treatment
Ferrochelataase inhibitor
Sulfite reductase inhibitor
Cytochrome P450 stimulant
Antihypoxic
Gly-X carboxypeptidase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Fibromyalgia syndrome treatment
TRPA1 agonist
Antiischemic
Formyltetrahydrofolate dehydrogenase inhibitor
MAO B substrate
Venom exonuclease inhibitor
Choline kinase inhibitor
Iron-cytochrome-c reductase inhibitor
Heat shock protein agonist
Alanine-tRNA ligase inhibitor
MMP9 expression inhibitor
(R,R)-butanediol dehydrogenase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Antiprotozoal (Babesia)
Nitrate reductase (cytochrome) inhibitor
Aldehyde dehydrogenase 2 substrate
Caspase 8 stimulant
Aspergillopepsin II inhibitor
D-amino-acid dehydrogenase inhibitor
Cyclomaltodextrinase inhibitor
Analgesic stimulant
MAO A substrate

Procollagen N-endopeptidase inhibitor
Thromboxane B2 antagonist
Farnesyltranstransferase inhibitor
Sodium channel blocker class Ib
Leukotriene-C4 synthase inhibitor
Maltose-transporting ATPase inhibitor
Cancer associated disorders treatment
Antihematotoxic
Glycerol-1-phosphatase inhibitor
Mitochondrial intermediate peptidase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Allantoate deiminase inhibitor
Tryptophanyl aminopeptidase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Sigma receptor agonist
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Thiopurine S-methyltransferase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Bontoxilysin inhibitor
Amine dehydrogenase inhibitor
Uroporphyrinogen-III synthase inhibitor
Inotropic
Nitrilase inhibitor
Glutaminy-peptide cyclotransferase inhibitor
Snapalysin inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Brachyurin inhibitor
Tropinesterase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Lysase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Dolichol kinase inhibitor
Formate-dihydrofolate ligase inhibitor
Thiol oxidase inhibitor
Aldehyde oxidase substrate
Renal tissue kallikrein inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
Signal peptidase I inhibitor
Pyroglutamyl-peptidase II inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Thermitase inhibitor
Oligopeptidase B inhibitor
Glutathione synthase inhibitor

Pappalysin-1 inhibitor
Folate antagonist
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Preneoplastic conditions treatment
NADPH-ferrihemoprotein reductase inhibitor
Prolyl aminopeptidase inhibitor
N-acetylneuraminate synthase inhibitor
Trans-pentaprenyltranstransferase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Neuropsin inhibitor
Histidinol dehydrogenase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Galactolipase inhibitor
Aspergillopepsin I inhibitor
3-Phytase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Alpha 2 adrenoreceptor agonist
Pyruvate decarboxylase inhibitor
Phosphoenolpyruvate mutase inhibitor
4-Hydroxymandelate oxidase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Cutinase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
4-Nitrophenylphosphatase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Dementia treatment
Alpha-Methylacyl-CoA racemase inhibitor
NMDA receptor polyamine site antagonist
(R)-limonene 6-monooxygenase inhibitor
Pantoate 4-dehydrogenase inhibitor
Insecticide
CYP2A13 substrate
N-acetylneuraminate 4-O-acetyltransferase inhibitor
L-threonine 3-dehydrogenase inhibitor
Restless leg syndrome treatment
Polyamine oxidase inhibitor
Linoleoyl-CoA desaturase inhibitor
Antibacterial, ophthalmic
Heat shock protein 70 agonist
NF-E2-related factor 2 stimulant
Aureolysin inhibitor
D-xylulose reductase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Antihelminthic (Fasciola)
CYP4A2 substrate
Xylan endo-1,3-beta-xylosidase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Hyaluronic acid agonist

N-hydroxyarylamine O-acetyltransferase inhibitor
Platelet derived growth factor receptor kinase inhibitor
Anticataract
Antifungal
Inulinase inhibitor
Retinal dehydrogenase inhibitor
Glutamate release inhibitor
Transcription factor STAT6 inhibitor
Glucuronolactone reductase inhibitor
Nardilysin inhibitor
Bisphosphoglycerate mutase inhibitor
Arylsulfate sulfotransferase inhibitor
Lombricine kinase inhibitor
Acyl-CoA oxidase inhibitor
Hydroxylamine reductase inhibitor
Adrenergic
Peptidylamidoglycolate lyase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Alpha-glucuronidase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Amyloid beta precursor protein antagonist
Carnitine 3-dehydrogenase inhibitor
Choline acetyltransferase stimulant
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Phosphonoacetate hydrolase inhibitor
Adenylate cyclase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Membrane permeability inhibitor
Antiprotozoal (Amoeba)
Antibacterial
Carnosine synthase inhibitor
Biotin carboxylase inhibitor
Aminopeptidase Y inhibitor
RELA expression inhibitor
CYP3A1 substrate
Diamine oxidase inhibitor
Glycerol dehydrogenase (NADP⁺) inhibitor
Neuropeptide S antagonist
Allantoinase inhibitor
TNF expression inhibitor
CYP2C11 substrate
Diguanidinobutanase inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Cyclamate sulfohydrolase inhibitor
GST A substrate
Coactivator-associated arginine methyltransferase 1 inhibitor
Dactylisin inhibitor
Cardiovascular analeptic
Dynein ATPase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor

Betaine-aldehyde dehydrogenase inhibitor
Histidinol-phosphatase inhibitor
Hippurate hydrolase inhibitor
Severe acute respiratory syndrome treatment
Adenine deaminase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Isoquinoline 1-oxidoreductase inhibitor
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Immunostimulant
Kallikrein inhibitor
Chlordecone reductase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
CYP2D substrate
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Menopausal disorders treatment
Antiinflammatory, intestinal
Ubiquitin thiolesterase inhibitor
Oryzin inhibitor
Acyl-lysine deacylase inhibitor
Insulysin inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Diaminopropionate ammonia-lyase inhibitor
3,4-Dihydroxy-9,10-secoandrost-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Monoamine oxidase substrate
Methane monooxygenase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Sclerosant
Choline dehydrogenase inhibitor
Alkene monooxygenase inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
O-aminophenol oxidase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Hydroxymethylbilane synthase inhibitor
Antiprotozoal (Trichomonas)
Antidyskinetic
Glutaminase inhibitor
Ferredoxin-nitrite reductase inhibitor
Aryl-acylamidase inhibitor
Deoxyhypusine synthase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Bile-salt sulfotransferase inhibitor
Tyrosine 3 hydroxylase inhibitor
HMGCS2 expression enhancer
Lysine 2-monooxygenase inhibitor
CYP19A1 expression inhibitor
Glutathione peroxidase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Cholestanetriol 26-monooxygenase inhibitor

CYP2C18 substrate
Atrolysin C inhibitor
Malate dehydrogenase (acceptor) inhibitor
5 Hydroxytryptamine 2B agonist
DNA-3-methyladenine glycosylase II inhibitor
GABA A inverse agonist
GABA inverse agonist
Ribonucleoside triphosphate reductase inhibitor
Alkylglycerone-phosphate synthase inhibitor
Homospermidine synthase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
Adenylate cyclase stimulant
CYP2D6 substrate
Diisopropyl-fluorophosphatase inhibitor
Carboxymethylenebutenolidase inhibitor
Lassitude treatment
Hematopoietic
Arylalkyl acylamidase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
Acaricide
Acylaminoacyl-peptidase inhibitor
Potassium channel (ATP-sensitive) blocker
Movement disorders treatment
Sedoheptulose-bisphosphatase inhibitor
JNK mitogen-activated protein kinase inhibitor
L-iduronidase inhibitor
Antineoplastic, alkylator
Thermomycin inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Aspergillus nuclease S1 inhibitor
Carboxypeptidase M inhibitor
H⁺-exporting ATPase inhibitor
Vascular (peripheral) disease treatment
Methylenetetrahydrofolate dehydrogenase (NADP⁺) inhibitor
Radiosensitizer
Phenylpyruvate decarboxylase inhibitor
Leucine dehydrogenase inhibitor
Phosphoinositide phospholipase C inhibitor
Glutamate 5-kinase inhibitor
Peptidyl-dipeptidase B inhibitor
Ca²⁺/calmodulin-dependent kinase I inhibitor
Leukotriene-B₄ 20-monooxygenase inhibitor
Calcium-sensing receptor agonist
Cancer procoagulant inhibitor
Antiviral (Herpes)
Cerevisin inhibitor
5 Hydroxytryptamine 5A antagonist
Lipoxygenase substrate
Rhodotorulapepsin inhibitor
P-glycoprotein 1 inhibitor

Guanidinoacetase inhibitor
Carboxylesterase inhibitor
Narcolepsy treatment
SMN2 expression enhancer
IgA-specific metalloendopeptidase inhibitor
Chloride channel activator
Amino-acid racemase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Venombin A inhibitor
Tentoxilysin inhibitor
2-Enoate reductase inhibitor
Anesthetic general
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Ecdysone 20-monooxygenase inhibitor
Leucolysin inhibitor
Lactaldehyde reductase inhibitor
CYP4A substrate
Acetylcholine nicotinic antagonist
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Vascular dementia treatment
tRNA (cytosine-5-)-methyltransferase inhibitor
H⁺/K⁺-transporting ATPase inhibitor
Argininosuccinate lyase inhibitor
Isopenicillin-N synthase inhibitor
ATP phosphoribosyltransferase inhibitor
Imidazoline I1 receptor agonist
Glutamate N-acetyltransferase inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Gentisate 1,2-dioxygenase inhibitor
Alpha 1L adrenoreceptor agonist
Trimethyllysine dioxygenase inhibitor
Methylaspartate ammonia-lyase inhibitor
Sphingosine kinase inhibitor
Selenocysteine lyase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
Orotate reductase (NADH) inhibitor
Protein kinase B stimulant
Aspartate transaminase inhibitor
Beta-ureidopropionase inhibitor
MAP kinase kinase 4 inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Gastrointestinal motility stimulant
Nav1.8 sodium channel blocker
Valine decarboxylase inhibitor
Saccharopine dehydrogenase (NADP⁺, L-glutamate-forming) inhibitor
Myocardial ischemia treatment
Anthranilate 3-monooxygenase (deaminating) inhibitor
Lysyl oxidase inhibitor
Ethanolamine kinase inhibitor
Phosphatidylinositol 3-kinase stimulant

Sleep apnea treatment
Benzoylformate decarboxylase inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Allantoicase inhibitor
Tryptophan transaminase inhibitor
CYP2C8 substrate
Sorbitol dehydrogenase inhibitor
Tauropine dehydrogenase inhibitor
Sphingomyelinase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Poly(alpha-L-gulonate) lyase inhibitor
5 Hydroxytryptamine release inhibitor
CYP2A6 substrate
Endopeptidase La inhibitor
Galactoside O-acetyltransferase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
Age-related macular degeneration treatment
5 Hydroxytryptamine 5 antagonist
Beta-N-acetylgalactosaminidase inhibitor
CYP2C10 substrate
4-Coumarate-CoA ligase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
Haloalkane dehalogenase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
CYP2C9 inhibitor
TTK protein kinase inhibitor
3-Oxoadipate enol-lactonase inhibitor
Gluconate dehydratase inhibitor
Picornain 2A inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Cyclohexanone monooxygenase inhibitor
Aryldialkylphosphatase inhibitor
Cysteine desulfurase inhibitor
Histamine H4 receptor antagonist
Acrosin inhibitor
Benzaldehyde dehydrogenase (NAD+) inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Rhizopuspepsin inhibitor
Leucine transaminase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Urolithiasis treatment
Fumarate reductase (NADH) inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Muscular dystrophy treatment
Liver X receptor antagonist
Diuretic inhibitor
Chaperonin ATPase inhibitor
Alcohol dehydrogenase inhibitor
Glutathione reductase (NADPH) stimulant

Glutathione reductase stimulant
Xanthommatin reductase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
NMDA receptor polyamine site agonist
Gentamicin 2"-nucleotidyltransferase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Antirickettsial
P-benzoquinone reductase (NADPH) inhibitor
Phenylalanine-tRNA ligase inhibitor
Potassium channel KCNQ blocker
Nucleoside-diphosphatase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Lipoprotein lipase inhibitor
Indanol dehydrogenase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
D-cysteine desulfhydrase inhibitor
Dihydrofolate synthase inhibitor
Tankyrase inhibitor
Arylacetonitrilase inhibitor
CC chemokine receptor agonist
Chemokine receptor agonist
Agmatinase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Antidepressant, Imipramin-like
Glycine N-acyltransferase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Vanilloid 4 antagonist
Acetylserotonin O-methyltransferase inhibitor
Shock treatment
Arginine deiminase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
D-Octopine dehydrogenase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Vomilenine glucosyltransferase inhibitor
Adrenaline agonist
3'-Nucleotidase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Immunoglobulin Fc receptor antagonist
3-Methylbutanal reductase inhibitor
Candidapepsin inhibitor
Ribitol 2-dehydrogenase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Nav1.7 sodium channel blocker
Cell wall biosynthesis inhibitor
Oxytocin agonist
Carminative
MO15-related protein kinase Pfmrk inhibitor
Stromelysin 2 inhibitor
L-lysine oxidase inhibitor

Dihydrouracil oxidase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Thiamine-phosphate kinase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Glucarate dehydratase inhibitor
Atrolysin A inhibitor
Benzoate 4-monooxygenase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Aspartate racemase inhibitor
Histamine N-methyltransferase inhibitor
Integrin alpha2beta1 antagonist
Diphosphomevalonate decarboxylase inhibitor
Galactokinase inhibitor
Autophagy inducer
UGT2B28 substrate
Glutamate formimidoyltransferase inhibitor
Vascular adhesion protein 1 inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Squalene epoxidase inhibitor
Cardiac myosin stimulant
HIV-2 reverse transcriptase inhibitor
Polyamine biosynthesis inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Serralysin inhibitor
Calcium channel N-type blocker
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Nitric oxide scavenger
Anthranilate-CoA ligase inhibitor
Sulfur dioxygenase inhibitor
Potassium channel (Inward rectifier) blocker
CYP2C8 inhibitor
Acetate kinase inhibitor
CYP1A1 inducer
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
CYP7 inhibitor
Levanase inhibitor
Deoxyribose-phosphate aldolase inhibitor
Serratia marcescens nuclease inhibitor
Neurotensin 1 receptor antagonist
Beta 1 adrenoreceptor agonist
CYP4A1 substrate
Methionine decarboxylase inhibitor
Lactate 2-monooxygenase inhibitor
Decylcitrate synthase inhibitor
Cytoprotectant
Neuronal nicotinic receptor antagonist
Isovaleryl-CoA dehydrogenase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Antiviral (CMV)

Antineoplastic (endocrine cancer)
Procollagen C-endopeptidase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Aldosterone antagonist
Plastoquinol-plastocyanin reductase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Glycine C-acetyltransferase inhibitor
Antiinfective
Lipotropic
Acetyl-CoA C-acyltransferase inhibitor
2-Nitropropane dioxygenase inhibitor
Peroxidase substrate
5 Hydroxytryptamine release stimulant
Dichloromuconate cycloisomerase inhibitor
Licheninase inhibitor
Potassium channel activator
Caspase 3 stimulant
Phenylalanine decarboxylase inhibitor
Respiratory distress syndrome treatment
Ribonuclease inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
Neurotensin receptor antagonist
Glycogen (starch) synthase inhibitor
Sepiapterin deaminase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Luteinizing hormone-releasing hormone antagonist
Phosphorylase a inhibitor
Diuretic
Tyrosine-protein kinase TYRO 10 inhibitor
Hyperparathyroidism treatment
Sodium/calcium exchanger inhibitor
Cerebroside-sulfatase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
GST T substrate
GST T1-1 substrate
Ligase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Phosphoserine phosphatase inhibitor
L-galactonolactone oxidase inhibitor
TGF beta receptor type II kinase inhibitor
Subtilisin inhibitor
Aryl-alcohol dehydrogenase inhibitor
Necroptosis inhibitor
Glutamate synthase (ferredoxin) inhibitor
Luteinizing hormone-releasing hormone agonist
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
DELTA24-sterol reductase inhibitor
Tryptophan 5 hydroxylase inhibitor
Sickle-cell anemia treatment
CYP2B6 substrate

Glycine N-benzoyltransferase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
CDC25C inhibitor
Succinic dehydrogenase inhibitor
Asparaginyl endopeptidase inhibitor
Orotate reductase (NADPH) inhibitor
Antibiotic
NMDA 2 receptor antagonist
Octopamine agonist
TH expression enhancer
Muconate cycloisomerase inhibitor
Laminaribiose phosphorylase inhibitor
Insulin sensitizer
Steroid N-acetylglucosaminyltransferase inhibitor
Bacterial efflux pump inhibitor
Alpha adrenoreceptor antagonist
Butyrylcholinesterase inhibitor
Dolichyl-phosphatase inhibitor
Dihydropteroate synthase inhibitor
Photosensitizer
Malate-CoA ligase inhibitor
Proline racemase inhibitor
Opioid dependency treatment
Gamma-glutamyl hydrolase inhibitor
Homoserine dehydrogenase inhibitor
Nav1.3 sodium channel blocker
Phenylalanine 4-hydroxylase inhibitor
Alpha 1 adrenoreceptor agonist
Antiinflammatory, ophthalmic
Malyl-CoA lyase inhibitor
Riboflavin phosphotransferase inhibitor
Homogentisate 1,2-dioxygenase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
GABA transporter 3 inhibitor
Aralkylamine dehydrogenase inhibitor
Phosphorylase kinase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Trehalose-phosphatase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Protein synthesis stimulant
CYP2E1 inducer
Glycine transaminase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate
N-acetylglucosaminephosphotransferase inhibitor
6,7-Dihydropteridine reductase inhibitor
Glutamine-tRNA ligase inhibitor
Oxalate oxidase inhibitor
Undecaprenyl-diphosphatase inhibitor
Fructuronate reductase inhibitor

Tagaturonate reductase inhibitor
DNA nucleotidylexotransferase inhibitor
Assemblin inhibitor
Aconitate decarboxylase inhibitor
Lactose synthase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
CF transmembrane conductance regulator antagonist
Methenyltetrahydrofolate cyclohydrolase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Envelysin inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Tetrahydroxynaphthalene reductase inhibitor
Neurotensin 2 receptor antagonist
MAP3K8 inhibitor
DNA polymerase I inhibitor
Adenylate kinase inhibitor
D-arabinonolactone oxidase inhibitor
Squalene-hopene cyclase inhibitor
Sulfate adenylyltransferase inhibitor
Dihydroxy-acid dehydratase inhibitor
Carboxypeptidase E inhibitor
Pediculicide
CXC chemokine 4 receptor antagonist
D-lactate dehydrogenase inhibitor
Aspartate-tRNA ligase inhibitor
D-2-hydroxy-acid dehydrogenase inhibitor
CYP3A3 substrate
Protein C (activated) inhibitor
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Delayed rectifier potassium channel blocker
Shab potassium channel blocker
Arginyltransferase inhibitor
Ribonuclease U2 inhibitor
Saccharolysin inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
CDK4/cyclin D3 inhibitor
Thromboxane synthase inhibitor
Dextranucrase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Aspartyl aminopeptidase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Dextranase inhibitor
Pim-3 kinase inhibitor
Carboxylate reductase inhibitor
Pantothenase inhibitor
4,5-Dihydroxyphthalate decarboxylase inhibitor

Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Phosphatidate phosphatase inhibitor
Linoleate diol synthase inhibitor
ATP adenylyltransferase inhibitor
Indoleamine-pyrrole 2,3-dioxygenase inhibitor
Omega-amidase inhibitor
Mannonate dehydratase inhibitor
ACK1 kinase inhibitor
Coccolysin inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Potassium channel Kv1.1 blocker
Scytalone dehydratase inhibitor
Formimidoyltetrahydrofolate cyclodeaminase inhibitor
Aerobactin synthase inhibitor
Colony stimulating factor agonist
Antineurogenic pain
Alcohol dehydrogenase [NAD(P)+] inhibitor
Lysyl endopeptidase inhibitor
Calcitonin stimulant
Morphine 6-dehydrogenase inhibitor
Lysine decarboxylase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Potassium channel small-conductance Ca-activated 3 activator
Streptopain inhibitor
Asparagine-tRNA ligase inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Deoxycytidine deaminase inhibitor
Glycine hydroxymethyltransferase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Antiseptic
D-proline reductase (dithiol) inhibitor
Vasodilator, coronary
BRAF expression inhibitor
N6-methyl-lysine oxidase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Gluconokinase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Arginine kinase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
CYP2A6 inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Glycine transporter 2 inhibitor
Collagenase inhibitor
Formimidoylglutamase inhibitor
Guanidinobutyrase inhibitor
Glycerol dehydratase inhibitor
GST M substrate
Thimet oligopeptidase inhibitor

Sphingosine kinase 1 inhibitor
Shikimate 5-dehydrogenase inhibitor
TP53 expression enhancer
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Diaminopimelate dehydrogenase inhibitor
L-amino-acid oxidase inhibitor
Adrenaline uptake inhibitor
Arylformamidase inhibitor
Gamma-glutamyltransferase inhibitor
CYP2A substrate
Nerve growth factor antagonist
Alpha-mannosidase inhibitor
Polarisation inhibitor
Acidifying agent gastric
Dynamin GTPase inhibitor
Alpha,alpha-trehalose phosphorylase inhibitor
Antiparkinsonian, tremor relieving
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
Obsessive-compulsive disorder treatment
Galactosylceramide sulfotransferase inhibitor
Focal adhesion kinase 2 inhibitor
Phosphatidylglycerophosphatase inhibitor
L-lysine 6-transaminase inhibitor
Cytosole dipeptidase inhibitor
NMDA 2A receptor antagonist
Gametolysin inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Antileprosy
Helicase E1 (Human papillomavirus) inhibitor
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Tripeptidyl-peptidase I inhibitor
3-Isopropylmalate dehydratase inhibitor
UGT2B10 substrate
Glucan 1,3-beta-glucosidase inhibitor
2-Methylcitrate dehydratase inhibitor
Thymidine kinase 1 inhibitor
Thiol S-methyltransferase inhibitor
Mycolysin inhibitor
Baculoviral IAP repeat-containing protein inhibitor
Glutamate dehydrogenase inhibitor
Trypanothione-disulfide reductase inhibitor
Serine 3-dehydrogenase inhibitor
CYP1A inducer
Cathepsin H inhibitor
Chloride/bicarbonate exchanger inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
Gaucher disease treatment
Protease (Human cytomegalovirus) inhibitor
Purine biosynthesis inhibitor

Trimereylisin II inhibitor
Dopamine D2B antagonist
Hydroxylamine reductase (NADH) inhibitor
Histamine H3 receptor antagonist
Methionyl-tRNA formyltransferase inhibitor
Choline sulfotransferase inhibitor
Antiadrenergic
Antianginal
Farnesoid X receptor antagonist
NAT2 substrate
Potassium channel Kv1.5 blocker
Neuropeptide Y1 agonist
Diabetic nephropathy treatment
Nav1.2 sodium channel blocker
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Allophanate hydrolase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
Glycolaldehyde dehydrogenase inhibitor
Acylglycerone-phosphate reductase inhibitor
CYP26A substrate
Adenosine A3 receptor agonist
Glutamate (mGluR8) agonist
Epithelial sodium channel blocker
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Alpha 2b adrenoreceptor agonist
Spermine synthase inhibitor
Sigma 3 receptor antagonist
N-acetylglucosamine kinase inhibitor
tRNA adenylyltransferase inhibitor
Guanidinopropionase inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Peptidyl-glycinamidase inhibitor
Aryl hydrocarbon receptor agonist
Iduronate-2-sulfatase inhibitor
Antineoplastic antimetabolite
Guanylate kinase inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Interferon agonist
CYP2C18 inhibitor
Anthrax lethal factor inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Carnitine O-octanoyltransferase inhibitor
Cytochrome-c3 hydrogenase inhibitor
Phosphoglycerate mutase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
SULT1A3 substrate
Carbamoyl-serine ammonia-lyase inhibitor
Folate transporter 1 inhibitor
2-Methylcitrate synthase inhibitor

N-(5-amino-5-carboxypentanoyl)-L-cysteiny-D-valine synthase inhibitor
 Arabinose isomerase inhibitor
 4-Alpha-glucanotransferase inhibitor
 Adrenaline antagonist
 Beta-amylase inhibitor
 UDP-N-acetylglucosamine 2-epimerase inhibitor
 Quercetin 2,3-dioxygenase inhibitor
 (S)-2-Methylmalate dehydratase inhibitor
 Catechol oxidase inhibitor
 Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
 Antiviral (Influenza)
 ATP diphosphatase inhibitor
 D-stereospecific aminopeptidase inhibitor
 Alpha-N-arabinofuranosidase inhibitor
 5-Oxoprolinase (ATP-hydrolysing) inhibitor
 Hedgehog signaling activator
 Shaker potassium channel blocker
 Cerebrovascular disorders treatment
 Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
 3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
 P2 nucleoside transporter inhibitor
 Proline dehydrogenase inhibitor
 Kallikrein 13 inhibitor
 Cycloartenol synthase inhibitor
 Poly(ADP-ribose) glycohydrolase inhibitor
 CYP19 inducer
 CYP2A5 substrate
 Kallikrein 3 inhibitor
 Antibiotic Tribactam-like
 Melanocortin agonist

Bosentan

Molecular Mechanism (initial) :

endothelin (ETA/ETB) receptor antagonist

Molecular Mechanism (repurposed) :

endothelin (ETA/ETB) receptor antagonist

initial indication(s):

pulmonary hypertension

Repurposed indication(s):

digital ulcers in systemic sclerosis

Predicted Activities

CYP2C9 inducer

CYP3A4 inducer

Antihypertensive

CYP3A inducer

CYP2C9 substrate

Endothelin receptor antagonist

Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor

Diabetic nephropathy treatment

Endothelin B receptor antagonist

Vasodilator, peripheral
CYP2C substrate
Glyceryl-ether monooxygenase inhibitor
Endothelin A receptor antagonist
Linoleate diol synthase inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Heart failure treatment

Pulmonary hypertension treatment

Antianginal
CYP3A substrate
Antidiabetic symptomatic
CYP2C8 inhibitor
Cardiotonic
CYP3A4 substrate
Retinol dehydrogenase inhibitor
Antiulcerative
Anaphylatoxin receptor antagonist
MAP3K5 inhibitor
Antiasthmatic
Alcohol O-acetyltransferase inhibitor
Methylglutamate dehydrogenase inhibitor
Antiischemic
Endoglycosylceramidase inhibitor
Atherosclerosis treatment
Para amino benzoic acid antagonist
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Aldehyde oxidase inhibitor
VCAM1 expression inhibitor
Vanilloid 1 agonist
Septic shock treatment
Antidiabetic
Antiprotozoal (Toxoplasma)
Vanilloid agonist
Antiviral (Trachoma)
Myocardial ischemia treatment
Catenin beta inhibitor
Guanylate cyclase 1 stimulant
Restenosis treatment
Phospholipase A1 inhibitor
Guanylate cyclase stimulant
Antineoplastic (small cell lung cancer)
Ceramide glucosyltransferase inhibitor
Glycine receptor agonist
Arylesterase inhibitor
Lactase inhibitor
Celiac disease treatment
Purinergic P2X2 antagonist
Angiotensin II receptor agonist

Phosphodiesterase IV inhibitor
Vasodilator
Ulcerative colitis treatment
CC chemokine 9 receptor antagonist
Hepatic disorders treatment
Antieczematic atopic
Purinergic P2X3 antagonist
Alcohol dehydrogenase substrate
Interleukin agonist
Inflammatory Bowel disease treatment
Trans-octaprenyltransferase inhibitor
JNK mitogen-activated protein kinase inhibitor
Channel-conductance-controlling ATPase inhibitor
Renal failure treatment
Non-steroidal antiinflammatory agent
Interleukin 12 agonist
K(Ca) 3.1 channel blocker
Phosphodiesterase inhibitor
Thrombolytic

Endothelin receptor agonist

Cyclin-dependent kinase 7 inhibitor
Phosphodiesterase 4B inhibitor
Angiotensin agonist
Parathyroid hormone secretion stimulant
Steroid 9alpha-monooxygenase inhibitor
Hepatoprotectant
Cytokine production inhibitor

Buprenorphine hydrochloride

Molecular Mechanism (initial) :

mu-type opioid receptor agonist

Molecular Mechanism (repurposed) :

mu-type opioid receptor agonist

initial indication(s):

pain

Repurposed indication(s):

opioid dependency

Predicted Activities

Analgesic (pain)

UGT1A substrate
UGT1A3 substrate
UGT1A1 substrate
UGT1A10 substrate
UGT2B1 substrate
UGT1A8 substrate
Antinociceptive
Antitussive

Opioid dependency treatment

Narcotic antagonist

UGT2B substrate
UGT2B7 substrate
Opioid kappa 3 receptor antagonist
UGT2B9 substrate
UDP-glucuronosyltransferase substrate
Anesthetic
Dependence treatment
Antipyretic
UGT2B7H substrate
UGT2B7Y substrate
CYP3A4 substrate
CYP3A substrate
Diuretic inhibitor
Sigma receptor antagonist
Histamine release stimulant
Antitussive, narcotic
Non-steroidal antiinflammatory agent
Antiinflammatory
Respiratory analeptic
Neurotransmitter antagonist
Opioid kappa 1 receptor antagonist
Cytochrome P450 inhibitor
Antineoplastic alkaloid
P-glycoprotein substrate
Dementia treatment
Neurotransmitter uptake inhibitor
Immunosuppressant
Analeptic
Imidazoline I1 receptor agonist
UGT2B18 substrate
Laxative
MAP kinase stimulant
CYP2H substrate
Phosphatase inhibitor
Antiviral (Rhinovirus)
Antipruritic
Opioid mu 2 receptor antagonist
Spasmolytic, urinary
Nicotinic alpha4beta4 receptor agonist
Antiperistaltic
Cocain dependency treatment
Antipruritic, non-allergic
Opioid mu 1 receptor antagonist
Opioid delta 1 receptor antagonist
Sigma 1 receptor agonist
UGT2B12 substrate
Tardive dyskinesia treatment
Uterine relaxant
CYP3A2 substrate
MAP3K5 inhibitor

APOA1 expression enhancer
Opioid delta 2 receptor antagonist
Polarisation stimulant
Gestagen antagonist
Antialcoholic
Antidyskinetic
Cytokine release inhibitor
Alpha 3 adrenoreceptor agonist
Opioid kappa 2 receptor antagonist
Opioid kappa 2b receptor antagonist
Corticosteroid antagonist
Thyroxine 5-deiodinase inhibitor

Celecoxib

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 (COX-2) inhibitor

initial indication(s):

arthritis

osteoarthritis

polyposis coli

rheumatoid arthritis

Repurposed indication(s):

pain

dysmenorrhea

ankylosing spondylitis

Predicted Activities

Cyclooxygenase 1 inhibitor

Cyclooxygenase inhibitor

Cyclooxygenase 2 inhibitor

CYP2D15 substrate

Caspase 3 stimulant

Adenomatous polyposis treatment

Non-steroidal antiinflammatory agent

Antiarthritic

CYP19A1 expression inhibitor

CYP2C9 substrate

Antipyretic

Antiinflammatory

Nitrate reductase (cytochrome) inhibitor

Age-related macular degeneration treatment

Phthalate 4,5-dioxygenase inhibitor

Glutamyl endopeptidase II inhibitor

Phospholipid-translocating ATPase inhibitor

Cl⁻-transporting ATPase inhibitor

Cancer associated disorders treatment

Menopausal disorders treatment

Chloride peroxidase inhibitor

NADPH peroxidase inhibitor
CYP2D substrate
Ompin inhibitor
Interleukin antagonist
Endopeptidase So inhibitor
CYP2C9 inhibitor
CYP2C substrate
Rheumatoid arthritis treatment
Analgesic, non-opioid
Diuretic inhibitor
Autoimmune disorders treatment
Interleukin 2 antagonist
Venombin AB inhibitor
CYP2C19 inhibitor
Analgesic
Coactivator-associated arginine methyltransferase 1 inhibitor
Hydroxylamine oxidase inhibitor
Creatininase inhibitor
Osteoarthritis treatment
Anthrax lethal factor inhibitor
PfA-M1 aminopeptidase inhibitor
Interleukin 5 antagonist
CYP2C10 substrate
HMGCS2 expression enhancer
MAP3K5 inhibitor
Polyporopepsin inhibitor
Loop diuretic
Saluretic
Chronic obstructive pulmonary disease treatment
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Transplant rejection treatment
Analgesic stimulant
Cystic fibrosis treatment
N-benzyloxycarbonylglycine hydrolase inhibitor
CYP4A11 substrate
Electrolyte absorption antagonist
Glycerol-3-phosphate oxidase inhibitor
Thiosulfate dehydrogenase inhibitor
Aspergillopepsin II inhibitor
Kallikrein inhibitor
Interleukin 4 antagonist
CYP2B2 substrate
CYP3A2 substrate
Apoptosis agonist
CDK2/cyclin A inhibitor
Diabetic neuropathy treatment
Insulysin inhibitor
Premenstrual syndrome treatment
Alkaline phosphatase inhibitor
Gout treatment

Transcription factor inhibitor
Thioredoxin inhibitor
Antiviral (Trachoma)
Antiobesity
Menstruation disorders treatment
Factor Xa inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Guanylate cyclase 1 stimulant
Na⁺-transporting two-sector ATPase inhibitor
Allergic rhinitis treatment
Antiallergic
Chemopreventive
Antiprotozoal (Toxoplasma)
Antineoplastic (pancreatic cancer)
Aspergillopepsin I inhibitor
K(ir) 6.2 channel activator
CYP2C6 substrate
Antiepileptic
Antihelminthic (Fasciola)
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Keratosis actinic (solar) treatment
Chitinase inhibitor
Purinergic P2X2 antagonist
Sphingosine 1-phosphate receptor antagonist
Protein kinase (CK1) epsilon inhibitor
Antiasthmatic
Oxidoreductase inhibitor
AMPA receptor agonist
Gingipain K inhibitor
Para amino benzoic acid antagonist
Amyloid beta precursor protein antagonist
Carbonic anhydrase VII inhibitor
Epoxide hydrolase inhibitor
Arylsulfate sulfotransferase inhibitor
Potassium channel (Ca-activated) activator
Cyclin-dependent kinase 6 inhibitor
Amyotrophic lateral sclerosis treatment
Diuretic
Antihypertensive
Uric acid excretion stimulant
Myosin ATPase inhibitor
Creatine kinase inhibitor
Channel-conductance-controlling ATPase inhibitor
Sphingosine 1-phosphate receptor 1 antagonist
Dyspepsia treatment
Carbonic anhydrase IX inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Ophthalmic drug
CYP2C8 inhibitor
Phosphoinositide dependent kinase 1 inhibitor

Macular degeneration treatment
Cannabinoid receptor antagonist
Hedgehog signaling inhibitor
Transcription factor NF kappa B inhibitor
Dual specificity phosphatase 1 inhibitor
Posttraumatic stress disorder treatment
Thermomycin inhibitor
Cyclin-dependent kinase 1 inhibitor
Obsessive-compulsive disorder treatment
Ubiquitin-protein ligase inhibitor
Dihydropteroyl synthase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Protein kinase (CK1) inhibitor
Dependence treatment
Cyclin-dependent kinase 2 inhibitor
Heat shock protein agonist
Antineoplastic (bladder cancer)
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Nav1.7 sodium channel blocker
Sulfonylureas
Biliary tract disorders treatment
Nitrate reductase inhibitor
Prostaglandin-E2 synthase 1 inhibitor
Carbonic anhydrase inhibitor
Calcium channel N-type blocker
Premature ejaculation treatment
CYP2C18 substrate
Arylamine N-Acetyltransferase substrate
Fibromyalgia syndrome treatment
Alcohol dehydrogenase substrate
Carbonic anhydrase II inhibitor
3-Phytase inhibitor
Guanylate cyclase stimulant
Heat shock protein 70 agonist
Movement disorders treatment
Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor
Carbonic anhydrase XII inhibitor
Aldehyde oxidase inhibitor
Thrombin inhibitor
I kappa B kinase inhibitor
Antiprotozoal (Coccidial)
Thiol oxidase inhibitor
Pancreatic elastase inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
Purinergic P2X3 antagonist
Mannose-6-phosphate isomerase inhibitor
Cyclin-dependent kinase inhibitor
Cathepsin T inhibitor
Carbonic anhydrase XIV inhibitor
Antiemphemic

Rhinitis treatment
Laccase inhibitor
Calcium release-activated channel blocker
HIV attachment inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
Pancreatic disorders treatment
Orexin receptor antagonist
Liver X receptor antagonist
CC chemokine 9 receptor antagonist
Carbonic anhydrase V inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Lipoxygenase inhibitor
Antiglaucomic
Nardilysin inhibitor
Cytidine deaminase inhibitor
Antituberculosic
I kappa B kinase 2 inhibitor
Arylesterase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Bombesin agonist
Bombesin 3 receptor agonist
Potassium channel large-conductance Ca-activated activator
Carbonic anhydrase XV inhibitor
Cyclin-dependent kinase 7 inhibitor
Nitric oxide donor
Smo receptor antagonist
K(Ca) 3.1 channel blocker
Janus tyrosine kinase 2 inhibitor
Oxalate oxidase inhibitor
Glutamate receptor agonist
Chloride/bicarbonate exchanger inhibitor
Nicotinic alpha6 receptor agonist
CC chemokine receptor agonist
Chemokine receptor agonist
Carbonic anhydrase I inhibitor
Nootropic
Pyruvate dehydrogenase kinase inhibitor
Brachyurin inhibitor
MO15-related protein kinase Pfmrk inhibitor
Trypsin inhibitor
Heme oxygenase stimulant
Gingipain R inhibitor
Mineralocorticoid antagonist
Tyrosine kinase stimulant
CYP2C18 inhibitor
Angiotensin II receptor agonist
Nicotine dehydrogenase inhibitor
CDK/Cyclin complex inhibitor
Diabetic nephropathy treatment
CC chemokine 10 receptor antagonist

Carbonic anhydrase II stimulant
O-aminophenol oxidase inhibitor
JNK mitogen-activated protein kinase inhibitor
Calpain inhibitor
Hexokinase inhibitor
Polo-like kinase-1 inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
Guanylate cyclase inhibitor
Renal disease treatment
Heat shock protein 27 antagonist
Eye irritation, inactive
Phosphodiesterase 10A inhibitor
Phosphodiesterase X inhibitor
Antithrombocytopenic
5-Lipoxygenase inhibitor
Phosphate transporter inhibitor
Carbonic anhydrase IV inhibitor
Protein kinase (CK1) delta inhibitor
Fatty acid elongase inhibitor
Sphingosine 1-phosphate receptor 3 agonist
Phenylethanolamine N methyltransferase inhibitor
Estrone sulfatase inhibitor
Integrin-linked kinase inhibitor
Atherosclerosis treatment
Peroxisome proliferator-activated receptor delta agonist
Diacylglycerol O-acyltransferase 1 inhibitor
Shikimate kinase inhibitor

Chloroquine phosphate

Molecular Mechanism (initial) :

haem polymerase inhibitor

Molecular Mechanism (repurposed) :

TGF beta suppression

initial indication(s):

malaria

Repurposed indication(s):

glioma

glioblastoma multiforme

Predicted Activities

Taurine dehydrogenase inhibitor
Fructose 5-dehydrogenase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Amine dehydrogenase inhibitor
Nicotinate dehydrogenase inhibitor
4-Hydroxyproline epimerase inhibitor
Nitrate reductase (cytochrome) inhibitor
Spermidine dehydrogenase inhibitor
Sulfur reductase inhibitor

Prion diseases treatment
Nicotine dehydrogenase inhibitor
Antiprotozoal (Plasmodium)
Hydroxylamine reductase inhibitor
Antiprotozoal (Amoeba)
(R)-Pantolactone dehydrogenase (flavin) inhibitor
4-Hydroxymandelate oxidase inhibitor
Retinal dehydrogenase inhibitor
Benzoate 4-monooxygenase inhibitor
Aldehyde oxidase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Cyclohexanone monooxygenase inhibitor
Malate dehydrogenase (acceptor) inhibitor
CYP2D6 substrate
CYP2D substrate
Acetylspermidine deacetylase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Antiprotozoal (Leishmania)
Membrane integrity antagonist

Antiprotozoal (malaria)

Glycerol-3-phosphate oxidase inhibitor
Cytochrome-b5 reductase inhibitor
Ethanolamine oxidase inhibitor
Acidifying agent non gastric
Spasmolytic, urinary
CYP2C8 inhibitor
Polyamine oxidase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
L-amino-acid oxidase inhibitor
Pseudolysin inhibitor
Hydroxylamine oxidase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Botulin neurotoxin A light chain inhibitor
Skeletal muscle relaxant
Antialcoholic
Loop diuretic
Acid phosphatase inhibitor
Fibrolase inhibitor
Antiprotozoal (Trichomonas)
Antituberculosic
Antiseborrheic
Acetylcholine neuromuscular blocking agent
Muscle relaxant
O-aminophenol oxidase inhibitor
Choline-phosphate cytidyltransferase inhibitor
CYP2E1 inhibitor
CYP1A2 substrate

Nucleotide metabolism regulator
CYP2A6 substrate
Systemic lupus erythematosus treatment
5 Hydroxytryptamine 2B agonist
General pump inhibitor
Inositol oxygenase inhibitor
Nitrate reductase inhibitor
Antimycobacterial
Thiol oxidase inhibitor
Antiparasitic
Aryl-acylamidase inhibitor
CYP3A substrate
Diuretic inhibitor
Carboxypeptidase Taq inhibitor
Phobic disorders treatment
Mucositis treatment
Immunosuppressant
Proteasome ATPase inhibitor
CYP2D6 inhibitor
Antiprotozoal (Toxoplasma)
Endopeptidase So inhibitor
CYP2A substrate
Tryptophan 2-monooxygenase inhibitor
Antihelminthic
Spasmolytic
Vanilloid 1 agonist
Monoamine uptake inhibitor
CYP1A substrate
Antihypoxic
CYP2B6 substrate
FMO3 substrate
CYP3A4 substrate
Potassium channel blocker
X-methyl-His dipeptidase inhibitor
Antisecretoric
Nav1.8 sodium channel blocker
Sodium channel blocker class Ib
Glutamate synthase (ferredoxin) inhibitor
Nucleoside-diphosphatase inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
CYP2C8 substrate
HERG 1 channel blocker
Flavin-containing monooxygenase substrate
Glyceryl-ether monooxygenase inhibitor
Neuropeptide Y2 antagonist
Peptidyl-dipeptidase Dcp inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Thiosulfate dehydrogenase inhibitor
Antischistosomal
Antiprotozoal (Coccidial)

Mandelate 4-monooxygenase inhibitor
 Cytochrome P450 inhibitor
 Antiparkinsonian, rigidity relieving
 Sodium channel blocker
 Cardiotonic
 Phosphatidylinositol diacylglycerol-lyase inhibitor
 CYP2C18 substrate
 Radiosensitizer
 Platelet derived growth factor receptor kinase inhibitor
 Spasmolytic, Papaverin-like
 Methane monooxygenase inhibitor
 Saluretic
 Fragilysin inhibitor
 Chemosensitizer
 Superoxide dismutase inhibitor
 Acetylornithine deacetylase inhibitor
 Formaldehyde transketolase inhibitor
 Creatininase inhibitor
 5 Hydroxytryptamine uptake stimulant
 CYP1A2 inhibitor
 Antitoxic
 CYP1A inhibitor
 Anticonvulsant
Antineoplastic (multiple myeloma)
 Antidyskinetic
 CYP2A8 substrate
 Histamine release inhibitor
 Fibrinolytic
 Myc inhibitor
 Antineurotic
 Cyclic AMP agonist
 Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
 Fibroblast growth factor agonist
 27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
 Fusarinine-C ornithinesterase inhibitor
 Diabetic neuropathy treatment
 CDP-glycerol glycerophosphotransferase inhibitor
 Gastrin inhibitor
 Octopamine antagonist
 Anaphylatoxin receptor antagonist
 Acute neurologic disorders treatment
 Chloride peroxidase inhibitor
 Omptin inhibitor
 Calcium channel (voltage-sensitive) activator
 Antiischemic, cerebral
 Nicotinic alpha4beta4 receptor agonist
 Nootropic

Chlorpromazine

Molecular Mechanism (initial) :

dopamine D2 antagonists

Molecular Mechanism (repurposed) :

sirtuin 1 inhibitor

initial indication(s):

antipsychotic

Repurposed indication(s):

colorectal cancer

Predicted Activities

Glycosylphosphatidylinositol phospholipase D inhibitor

CYP2E1 inhibitor

Antidepressant, Imipramin-like

Antiparkinsonian, rigidity relieving

Flavin-containing monooxygenase substrate

CYP2C18 substrate

Aldehyde oxidase inhibitor

CYP2D substrate

Prion diseases treatment

Anaphylatoxin receptor antagonist

CYP2D6 substrate

X-methyl-His dipeptidase inhibitor

Beta-adrenergic receptor kinase inhibitor

G-protein-coupled receptor kinase inhibitor

FMO3 substrate

Choline-phosphate cytidylyltransferase inhibitor

CYP2C19 substrate

Antinaupathic

Thiamine-triphosphatase inhibitor

CYP1A2 substrate

Monoamine uptake inhibitor

Aryl-acylamidase inhibitor

CYP2C9 substrate

Phosphatidylcholine-sterol O-acyltransferase inhibitor

CYP1A substrate

CYP2C substrate

CYP2C8 substrate

Antitoxic

Carnosine synthase inhibitor

Anticonvulsant

Skeletal muscle relaxant

Nucleoside-diphosphatase inhibitor

Phobic disorders treatment

CYP2B6 substrate

Phosphatidylinositol diacylglycerol-lyase inhibitor

Neurotransmitter uptake inhibitor

Antineurotic

HERG 1 channel blocker

Antimutagenic

Phosphatidate phosphatase inhibitor

Antisecretoric
CYP3A4 substrate
Muscle relaxant
Spasmolytic, Papaverin-like
Nucleotide metabolism regulator
CYP2B substrate
CYP3A substrate
Phosphoserine phosphatase inhibitor
Taurine dehydrogenase inhibitor
Spasmolytic
Antiparkinsonian, tremor relieving
CYP2D1 substrate
Cyclic AMP phosphodiesterase inhibitor
Leukopoiesis inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
UGT1A4 substrate
L-amino-acid oxidase inhibitor
Antipruritic
Antiischemic, cerebral
Apyrase inhibitor
Phospholipid-translocating ATPase inhibitor
2-Haloacid dehalogenase inhibitor
Dolichol kinase inhibitor
Photosensitizer
Nav1.2 sodium channel blocker
Histamine H1 receptor antagonist
CYP2A6 substrate

Antipsychotic

Antiprotozoal (Leishmania)
Nav1.3 sodium channel blocker
Acute neurologic disorders treatment
Insulysin inhibitor
Antihistaminic
CYP3A7 substrate
Histamine release stimulant
Lipid metabolism regulator
Nav1.8 sodium channel blocker

Antineoplastic (multiple myeloma)

CYP2A substrate
Fibrinolytic
Antitussive
Spermidine dehydrogenase inhibitor
Histamine antagonist
Antiprotozoal (Trypanosoma)
2-Hydroxyquinoline 8-monooxygenase inhibitor
CNS active muscle relaxant
NADPH peroxidase inhibitor
CYP2C19 inhibitor
CYP3A5 substrate
5 Hydroxytryptamine 2B agonist

Caspase 8 stimulant
Membrane integrity agonist
Alcohol dehydrogenase (NADP+) inhibitor
Anesthetic
Adenosine regulator
Histamine N-methyltransferase inhibitor
Antihematotoxic
Phthalate 4,5-dioxygenase inhibitor
Histamine release inhibitor
Sodium channel blocker
CYP2D6 inhibitor
Anesthetic local
Protein-tyrosine kinase p55(blk) inhibitor
Beta glucuronidase inhibitor
Anxiolytic
Fructose 5-dehydrogenase inhibitor
CYP2E1 substrate
Taurine-2-oxoglutarate transaminase inhibitor
Cardiotonic
CYP2E substrate
CYP2A8 substrate
HIF1A expression inhibitor
Antiarrhythmic
Antidepressant
Sulfur reductase inhibitor
Mood disorders treatment
Antianginal
Cl--transporting ATPase inhibitor
Aryl sulfotransferase inhibitor
Oxidoreductase inhibitor
Mediator release inhibitor
CYP1A1 substrate
Diabetic neuropathy treatment
CYP2C8 inhibitor
Calcium channel blocker
Adenylate cyclase V inhibitor
Mucomembranous protector
CYP3A1 substrate
Sigma receptor agonist
Caspase 3 stimulant
Calcium channel (voltage-sensitive) activator
Mucositis treatment
4-Hydroxyproline epimerase inhibitor
Antihelmintic
Complement factor D inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
FMO1 substrate
5 Hydroxytryptamine uptake stimulant
Nav1.1 sodium channel blocker
Nicotine dehydrogenase inhibitor

Radioprotector
ATPase inhibitor
Vasodilator, coronary
Trypanothione-disulfide reductase inhibitor
Antihelminthic (Nematodes)
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
5 Hydroxytryptamine antagonist
Sodium channel (voltage-gated) blocker
Chloride peroxidase inhibitor
Membrane integrity antagonist
Antiparasitic
IgA-specific serine endopeptidase inhibitor
CYP2B2 substrate
Antiischemic
Na⁺-transporting two-sector ATPase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Antiemetic
Trimethylamine-oxide aldolase inhibitor
Antineoplastic (pancreatic cancer)
5 Hydroxytryptamine 7S antagonist
CYP3A3 substrate
DELTA24-sterol reductase inhibitor
Antiparkinsonian
Loop diuretic
Antidote
Intermittent claudication treatment
Calcium channel (voltage-sensitive) blocker
5 Hydroxytryptamine 2 antagonist
CYP2A1 substrate
P-glycoprotein 1 inhibitor
UGT1A3 substrate
Amyotrophic lateral sclerosis treatment
UGT1A substrate
Antiprotozoal
Neuropeptide Y2 antagonist
Nicotinate dehydrogenase inhibitor
Saluretic
CYP2C11 substrate
Adenylate cyclase inhibitor
Alpha adrenoreceptor antagonist
P-glycoprotein inhibitor
CYP2C10 substrate
Apoptosis antagonist
Nav1.5 sodium channel blocker
Analgesic
Stroke treatment
CYP3A2 substrate
2-Haloacid dehalogenase (configuration-inverting) inhibitor
GABA B receptor agonist
Neurodegenerative diseases treatment

Antiperistaltic
LDLR expression enhancer
5 Hydroxytryptamine 2A antagonist
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Hydroxylamine oxidase inhibitor
CYP1A2 inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Lipid peroxidase inhibitor
Guanylate cyclase 1 stimulant
UGT1A9 substrate
Sigma 1 receptor agonist
CYP2D16 substrate
Tetrahydroxynaphthalene reductase inhibitor
Botulin neurotoxin A light chain inhibitor
CYP4A11 substrate
Ubiquinol-cytochrome-c reductase inhibitor
Antimyopathies
Cell wall biosynthesis inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Retinoic acid metabolism inhibitor
Antineurogenic pain
Cyclohexanone monooxygenase inhibitor
Carnitine O-octanoyltransferase inhibitor
5 Hydroxytryptamine 7 antagonist
Thromboxane B2 antagonist
Chemosensitizer
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Alpha 1 adrenoreceptor antagonist
Acaricide
Alcohol dehydrogenase inhibitor
Gastrin inhibitor
Antipruritic, allergic
Smooth muscle myosin light chain kinase inhibitor
Antiadrenergic
Antiprotozoal (Plasmodium)
GABA receptor agonist
Cancer associated disorders treatment
Anesthetic general
Acidifying agent non gastric
CYP4A substrate
CYP1A inhibitor
4-Nitrophenylphosphatase inhibitor
Obsessive-compulsive disorder treatment
Nitrate reductase (cytochrome) inhibitor
Fusarinine-C ornithinesterase inhibitor
Leukotriene-C4 synthase inhibitor
HERG channel blocker
Kinesin antagonist
Kinesin-like protein 1 inhibitor
5 Hydroxytryptamine 2B antagonist

Adrenaline antagonist
Amine dehydrogenase inhibitor
Antihypertensive
Cocain dependency treatment
Rhinitis treatment
CYP2C3 substrate
Diuretic inhibitor
Butyrylcholinesterase inhibitor
CYP2J2 substrate
Ca²⁺/calmodulin-dependent protein kinase inhibitor
Cytochrome P450 inhibitor
Spasmolytic, urinary
Acetylcholine neuromuscular blocking agent
Alpha-Methylacyl-CoA racemase inhibitor
Alpha 1d adrenoreceptor antagonist
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Gastrointestinal motility stimulant
Anticataract
Chloride channel activator
5 Hydroxytryptamine 1F antagonist
Octopamine antagonist
Antipyretic
Adenylate cyclase stimulant
Membrane permeability inhibitor
p21-activated kinase 1 inhibitor
Muscular dystrophy treatment
Antitussive, narcotic
MAO inhibitor
Thiosulfate dehydrogenase inhibitor
Catenin beta inhibitor
5 Hydroxytryptamine 1E antagonist
CYP2H substrate
Alpha 1b adrenoreceptor antagonist
(S)-6-hydroxynicotine oxidase inhibitor
Retinal dehydrogenase inhibitor
Fibromyalgia syndrome treatment
Antihypoxic
Transforming growth factor beta 1 agonist
Antineoplastic enhancer
Ethanolamine-phosphate cytidyltransferase inhibitor
Calcium antagonist
Calpain inhibitor
3-Phytase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
Hematopoietic
5 Hydroxytryptamine 5 antagonist
5 Hydroxytryptamine 2C antagonist
Tryptophan 2,3-dioxygenase inhibitor
Antidiarrheal

Peroxidase substrate
Calcium regulator
Cytochrome P450 stimulant
Antieczematic atopic
Cerebrovascular disorders treatment
Huntington's disease treatment
Antianorexic
Homoserine dehydrogenase inhibitor
Protein kinase C inhibitor
Neuropeptide Y antagonist
L-glutamate oxidase inhibitor
Myocardial ischemia treatment
PfA-M1 aminopeptidase inhibitor
Alpha 1a adrenoreceptor antagonist
Acetylspermidine deacetylase inhibitor
Calcium channel activator
5 Hydroxytryptamine 5A antagonist
1,4-Lactonase inhibitor
Antihelminthic (Fasciola)
Alpha 2b adrenoreceptor antagonist
Diuretic
Gamma-butyrobetaine dioxygenase inhibitor
Antituberculosic
Dopamine D2S antagonist
Antiseborrheic
Choline-sulfatase inhibitor
Neuropeptide antagonist
Respiratory analeptic
Anthrax lethal factor inhibitor
Dopamine D5 antagonist
Aspulvinone dimethylallyltransferase inhibitor
Adrenaline release stimulant
Vascular (peripheral) disease treatment
Electron-transferring-flavoprotein dehydrogenase inhibitor
Lanosterol 14 alpha demethylase inhibitor
Arylacetonitrilase inhibitor
5 Hydroxytryptamine 6 antagonist
CYP2J substrate
Cachexia treatment
Ovulation inhibitor
Trimethylamine dehydrogenase inhibitor
Glyoxylate reductase inhibitor
Dependence treatment
Glutamate synthase (ferredoxin) inhibitor
Analgesic, non-opioid
D-lactaldehyde dehydrogenase inhibitor
N-acylmannosamine kinase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Cholinergic antagonist
4-Hydroxymandelate oxidase inhibitor

Acetylcholine nicotinic antagonist
Sodium/calcium exchanger 1 inhibitor
Antimycobacterial
Lysyl oxidase inhibitor
Ca²⁺/calmodulin-dependent kinase II inhibitor
P-glycoprotein substrate
Urticaria treatment
TH expression enhancer
5 Hydroxytryptamine 7L antagonist
Protein kinase C mu inhibitor
O-aminophenol oxidase inhibitor
Antiprotozoal (Amoeba)
Histamine H1 receptor agonist
p21-activated kinase inhibitor
Protein kinase C theta inhibitor
CYP3A4 inducer
Cycloartenol synthase inhibitor
Protein kinase C beta inhibitor
Aryl hydrocarbon receptor agonist
Antidyskinetic
Methylamine-glutamate N-methyltransferase inhibitor
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
Ubiquitin thiolesterase inhibitor
CYP3A inducer
Protein kinase C epsilon inhibitor
Polyamine-transporting ATPase inhibitor
Calcium channel L-type blocker
Creatininase inhibitor
Membrane permeability enhancer
Immunomodulator
Insulin promoter
Sulfite oxidase inhibitor
Blasticidin-S deaminase inhibitor
Platelet aggregation stimulant
GABA A receptor agonist
NAD⁺ kinase inhibitor
Antiinfertility, female
CYP3C substrate
Protein kinase C gamma inhibitor
Glutamate release inhibitor
Sodium channel blocker class Ib
Acetylcholine muscarinic antagonist
Thioredoxin inhibitor
Hydroxylamine reductase inhibitor
Acetylcholine antagonist
Camphor 1,2-monooxygenase inhibitor
Antialcoholic
CDC25C inhibitor
Chlordecone reductase inhibitor
Restless leg syndrome treatment

MAO A substrate
Guanylate cyclase stimulant
Chaperonin ATPase inhibitor
Bipolar disorder treatment
Phenol O-methyltransferase inhibitor
Antiulcerative
Glutaminy-peptide cyclotransferase inhibitor
5 Hydroxytryptamine 1B antagonist
Macrophage colony stimulating factor agonist
Interferon agonist
Dopamine D2L antagonist
Antiepileptic
Peristaltic stimulant
Protein kinase C zeta inhibitor
Protein kinase C eta inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Pseudolysin inhibitor
Venombin AB inhibitor
5 Hydroxytryptamine uptake inhibitor
Antischistosomal
Chemokine receptor antagonist
Insulin antagonist
Potassium channel Kv4.3 blocker
Shal potassium channel blocker
Gonadotropin antagonist
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Glycine receptor antagonist
Ribonucleoside triphosphate reductase inhibitor
Telomerase inhibitor
Scytalone dehydratase inhibitor
Adenylate cyclase I inhibitor
Lysine 2,3-aminomutase inhibitor
Antiviral (CMV)
Omptin inhibitor
Carboxypeptidase Taq inhibitor
Antiallergic
Cholinergic
Aminobutyraldehyde dehydrogenase inhibitor
Carnitine 3-dehydrogenase inhibitor
Ca²⁺/calmodulin-dependent kinase I inhibitor
Acylcarnitine hydrolase inhibitor
Potassium channel blocker
Insecticide
Protein kinase C nu inhibitor
(R)-limonene 6-monooxygenase inhibitor
Protein kinase C alpha inhibitor
Liver X receptor antagonist
2,4-Dichlorophenol 6-monooxygenase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
DNA intercalator

CYP2B11 substrate
p21-activated kinase 4 inhibitor
Adrenergic
5 Hydroxytryptamine 3 agonist
MDM2 inhibitor
Glucagon-like peptide 1 agonist
Phosphorylase kinase inhibitor
CYP2C29 substrate
Neuropeptide Y1 antagonist
Lassitude treatment
Dimethylargininase inhibitor
Uric acid excretion stimulant
Hyperprolactinemia treatment
Methyltransferase substrate
Adrenaline uptake inhibitor
Squalene-hopene cyclase inhibitor
Aldose reductase substrate
Ribulose-phosphate 3-epimerase inhibitor
UDP-glucuronosyltransferase substrate
Methylumbelliferyl-acetate deacetylase inhibitor
Antiobesity
Guanylate cyclase inhibitor
Dimethylallyltranstransferase inhibitor
Beta 3 adrenoreceptor antagonist
Dual specificity phosphatase inhibitor
Flavin-containing monooxygenase inhibitor
Nicotinic alpha4beta4 receptor agonist
Lipoxygenase substrate
Photinus-luciferin 4-monooxygenase (ATP-hydrolysing) inhibitor
Phospholipase D inhibitor
Ca²⁺-transporting ATPase inhibitor
Retinopathy treatment
Nootropic
5 Hydroxytryptamine 1A antagonist
Malate dehydrogenase (acceptor) inhibitor
Alpha 2c adrenoreceptor antagonist
Glutamyl endopeptidase II inhibitor
Phospholipase D1 inhibitor
Acetylcholine release stimulant
Benzodiazepine antagonist
Arylsulfate sulfotransferase inhibitor
Cytochrome-b5 reductase inhibitor
Dimethylmaleate hydratase inhibitor
Choline dehydrogenase inhibitor
5 Hydroxytryptamine 3A antagonist
Antineoplastic (renal cancer)
Polyamine oxidase inhibitor
CXC chemokine receptor antagonist
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Pyruvate decarboxylase inhibitor

(R)-6-hydroxynicotine oxidase inhibitor
NADPH oxidase inhibitor
MAO B substrate
Sigma receptor antagonist
5 Hydroxytryptamine 1 antagonist
Pantetheine-phosphate adenylyltransferase inhibitor
Guanidinoacetate kinase inhibitor
Glycine amidinotransferase inhibitor
Antinociceptive
GST A substrate
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Antineoplastic (liver cancer)
Skin irritation, inactive
5 Hydroxytryptamine 6 agonist
NMDA receptor glycine site B antagonist
CYP2G1 substrate
Antiviral (Poxvirus)
Potassium channel (Ca-activated) activator
Cutinase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Alkylacetyl-glycerophosphatase inhibitor
Urologic disorders treatment
Nitrite reductase [NAD(P)H] inhibitor
Antineoplastic (small cell lung cancer)
Premature ejaculation treatment
Sigma 2 receptor antagonist
Glycerol-3-phosphate dehydrogenase inhibitor
MAP3K8 inhibitor
Alpha 2a adrenoreceptor antagonist
Beta 1 adrenoreceptor agonist
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Acylaminoacyl-peptidase inhibitor
Monoamine oxidase substrate
Phosphodiesterase VII inhibitor
Squalene epoxidase inhibitor
Gluconate 5-dehydrogenase inhibitor
Ethanolamine oxidase inhibitor
ATM kinase inhibitor
Vascular endothelial growth factor 3 antagonist
GABA transporter 2 inhibitor
Analeptic
N-formylmethionyl-peptidase inhibitor
Cardioprotectant
TP53 expression enhancer
Alpha 1L adrenoreceptor agonist
Antiprotozoal (Trichomonas)
Diabetic nephropathy treatment
Renal failure treatment
Choline acetyltransferase stimulant
Immunosuppressant

5 Hydroxytryptamine 1D antagonist
5 Hydroxytryptamine 2A agonist
CDC25 phosphatase inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Reductant
Neuropeptide Y5 antagonist
Putrescine oxidase inhibitor
Heme oxygenase inhibitor
Eye irritation, inactive
Acetylcholine M5 receptor antagonist
Pim-3 kinase inhibitor
Antineoplastic, alkylator
DNA-3-methyladenine glycosylase I inhibitor
Hydroxyquinol 1,2-dioxygenase inhibitor
2,3-Oxidosqualene-lanosterol cyclase inhibitor
p53 inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Sodium/calcium exchanger inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Sleep apnea treatment
MAO A inhibitor
SULT2A1 substrate
5 Hydroxytryptamine 3 antagonist
5 Hydroxytryptamine 4A antagonist
Farnesyltransferase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Acetylcholine M1 receptor antagonist
Transketolase inhibitor
Anti-Helicobacter pylori
Dopamine transporter inhibitor
SMN2 expression enhancer
GABA transporter inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Aldehyde dehydrogenase substrate
Urinary incontinence treatment
CC chemokine 4 receptor antagonist
Bcl2 antagonist
Benzodiazepine receptor peripheral-type antagonist
Potassium channel (Voltage-sensitive) blocker
Acetylcholinesterase inhibitor
Histamine H2 receptor antagonist
Acetylcholine M4 receptor antagonist
Hematopoietic inhibitor
Benzaldehyde dehydrogenase (NADP⁺) inhibitor
Psychosexual dysfunction treatment
CC chemokine receptor antagonist
CC chemokine 2 receptor antagonist
Carnitinamidase inhibitor
Complement inhibitor
Neuropeptide FF agonist

Neuropeptide FF2 agonist
Apoptosis agonist
Glutathione reductase inhibitor
TNF expression inhibitor
Calcium channel T-type blocker
Viral entry inhibitor
JAK2 expression inhibitor
Electrolyte absorption antagonist
CC chemokine 1 receptor antagonist
GABA transporter 1 inhibitor
Antineoplastic (lymphocytic leukemia)
Histamine H4 receptor antagonist
Check point kinase 1 inhibitor
Glutaminase inhibitor
Peptide deformylase inhibitor
Wee-1 tyrosine kinase inhibitor
CYP2A2 substrate
Orexin receptor 1 antagonist
Autophagy inducer
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Bcl-xL inhibitor
Homocysteine desulfhydrase inhibitor
5 Hydroxytryptamine 7 agonist
Histamine H2 receptor agonist
All-trans-retinyl-palmitate hydrolase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
CYP2A13 substrate
Urotensin II agonist
Opioid kappa 3 receptor antagonist
DNA repair enzyme inhibitor
Shab potassium channel blocker
CYP3A4 inhibitor
3-Cyanoalanine hydratase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Phospholipase C inhibitor
Cell adhesion molecule inhibitor
Sigma 1 receptor antagonist
CF transmembrane conductance regulator agonist
D-alanine transaminase inhibitor
Bradykinin B2 receptor agonist
Laccase inhibitor
Heat shock protein agonist
Polarisation inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Dyspepsia treatment
NMDA receptor antagonist
Choline sulfotransferase inhibitor
Nitrite reductase (NO-forming) inhibitor
Nociceptin (N/OFQ) receptor antagonist
Heat shock protein 90 antagonist

5 Hydroxytryptamine 4 antagonist
 Kidney function stimulant
 Mannose-6-phosphate isomerase inhibitor
 Aminoacyl-tRNA hydrolase inhibitor
 Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
 CDK4/cyclin D inhibitor
 DNA-(apurinic or apyrimidinic site) lyase inhibitor
 Aspartate-phenylpyruvate transaminase inhibitor
 CYP2B1 substrate
 Deoxyhypusine synthase inhibitor
 MAP kinase kinase kinase inhibitor
 Cholestenol delta-isomerase inhibitor
 Nav1.4 sodium channel blocker
 Phospholipase D2 inhibitor
 Sepsis treatment
 Histidinol dehydrogenase inhibitor
 Protease activated receptor antagonist
 Endopeptidase So inhibitor
 Prostaglandin-A1 DELTA-isomerase inhibitor
 CXC chemokine 4 receptor antagonist
 Potassium channel (Inward rectifier) blocker
 Acyl-CoA hydrolase inhibitor
 Palmitoyl-CoA hydrolase inhibitor
 Coccolysin inhibitor
 Acetylcholine agonist

Digitoxin

Molecular Mechanism (initial) :

sodium-potassium ATPase inhibitor

Molecular Mechanism (repurposed) :

TNF- α /NF- κ B signaling pathway inhibitor

initial indication(s):

heart failure

arrhythmia

Repurposed indication(s):

cystic fibrosis

Predicted Activities

Anesthetic general
 UDP-glucuronosyltransferase substrate
 CYP3A2 substrate
 Caspase 3 stimulant
 Cardiotonic
 CYP3A substrate
 CYP3A4 substrate
 Proliferative diseases treatment

Na⁺ K⁺ transporting ATPase inhibitor

Diuretic
 Antineoplastic
 Chemopreventive

Membrane integrity antagonist
CYP2H substrate
Antiprotozoal (Leishmania)
P-glycoprotein substrate
UGT1A1 substrate
UGT1A substrate
Apoptosis agonist
Alkenylglycerophosphocholine hydrolase inhibitor
General pump inhibitor
Glyceryl-ether monooxygenase inhibitor
4-Nitrophenylphosphatase inhibitor
Immunosuppressant
CDP-glycerol glycerophosphotransferase inhibitor
Cholesterol antagonist
Antineoplastic (lung cancer)
Respiratory analeptic
Transcription factor STAT3 inhibitor
Hypoxia inducible factor 1 alpha inhibitor
Caspase 8 stimulant
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Dementia treatment
CYP3A1 substrate
CYP3A5 substrate
Antifungal
Antineoplastic (breast cancer)

Transcription factor NF kappa B stimulant

Transcription factor stimulant
Analeptic
CYP2B6 substrate
Transcription factor STAT inhibitor
Anticarcinogenic
ATPase inhibitor
Antiviral (Influenza)
Bilirubin oxidase inhibitor
Vascular dementia treatment
Membrane permeability inhibitor
Transcription factor NF kappa B inhibitor
CYP3A4 inducer
Chloride channel blocker
CYP3A inducer
Oxidoreductase inhibitor
Antineoplastic (colon cancer)
Antineoplastic (colorectal cancer)
Transcription factor inhibitor
RNA synthesis inhibitor
Hepatoprotectant
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Membrane permeability enhancer
Glucan endo-1,3-beta-D-glucosidase inhibitor
CYP2A11 substrate

Phosphatase inhibitor
Antiparasitic
H⁺-exporting ATPase inhibitor
Antimetastatic
Beta glucuronidase inhibitor
Antibacterial
Prostate disorders treatment
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Cholesterol synthesis inhibitor
Phosphoinositide 5-phosphatase inhibitor
TP53 expression enhancer
Interleukin 6 antagonist
Myc inhibitor
Gestagen antagonist
UGT2B7 substrate
Aspartyltransferase inhibitor
Antinociceptive
Antiprotozoal (Amoeba)
Protein synthesis inhibitor
Prostate cancer treatment
Phospholipase A1 inhibitor
Immunostimulant
CYP17 inhibitor
Morphine 6-dehydrogenase inhibitor
Antihelmintic
Antiviral (Herpes)
Anesthetic
Dermatologic
CYP2B substrate
CYP2C8 substrate
Antihelmintic (Nematodes)
Hypolipemic
Ecdysone 20-monooxygenase inhibitor
Contraceptive
Antieczematic
GDP-mannose 6-dehydrogenase inhibitor
Antineoplastic antibiotic
Antiinflammatory
Lactase inhibitor
DNA ligase (ATP) inhibitor
Antineoplastic (glioma)
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Peptidyltransferase inhibitor
Antileukemic
1,2-alpha-L-fucosidase inhibitor
Antineoplastic (non-small cell lung cancer)
Antineoplastic enhancer
CYP3A7 substrate
Antineoplastic (brain cancer)

Antineoplastic (glioblastoma multiforme)
ICAM1 expression inhibitor
Ceramide glucosyltransferase inhibitor
Antimycoplasmal
Xenobiotic-transporting ATPase inhibitor
Topoisomerase I inhibitor
Acylcarnitine hydrolase inhibitor
Transactivator transcription protein inhibitor
UGT2B18 substrate
Adenylate cyclase inhibitor
Nitric oxide antagonist
Beta-glucosidase inhibitor
Benzoate-CoA ligase inhibitor
CYP2A10 substrate
CYP1A1 substrate
Acetylgalactosaminyl-O-glycosyl-glycoprotein
beta-1,3-N-acetylglucosaminyltransferase inhibitor
Antineoplastic (squamous cell carcinoma)
UGT2B substrate
Alkylacetylgllycerophosphatase inhibitor
Mycothiol-S-conjugate amidase inhibitor
Antineoplastic (cervical cancer)
Spasmolytic, urinary
Antitoxic
HIF1A expression inhibitor
Antibiotic Anthracycline-like
Alcohol O-acetyltransferase inhibitor
Choleretic
Protein-synthesizing GTPase inhibitor
Anaphylatoxin receptor antagonist
Antineoplastic (solid tumors)
Cholesterol oxidase inhibitor
Radical formation agonist
Antirickettsial
Maleate isomerase inhibitor
CYP2A4 substrate
CYP2C9 inducer
Antiprotozoal
Alkylator
Cytostatic
Insecticide
Retinol dehydrogenase inhibitor
Antineoplastic (lymphoma)
Endoglycosylceramidase inhibitor
Antineoplastic (sarcoma)
Menopausal disorders treatment
Sterol 3-beta-glucosyltransferase inhibitor
Antibiotic
Aldose reductase substrate
H⁺-transporting two-sector ATPase inhibitor

Levansucrase inhibitor
Antipruritic
Glycerol-3-phosphate dehydrogenase inhibitor
Cytokine release inhibitor
UGT2B28 substrate
Peptidoglycan glycosyltransferase inhibitor
Antineoplastic (endocrine cancer)
ATPase stimulant
Antineoplastic (carcinoma)
Hyaluronic acid agonist
Antineoplastic (thyroid cancer)
Interleukin 2 agonist
Hepatic disorders treatment
CYP7 inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
Antioxidant
Antineoplastic (ovarian cancer)
UGT1A8 substrate
Interferon antagonist
CYP1A substrate
Vasoprotector
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Galactolipase inhibitor
Calcium regulator
Glycosylceramidase inhibitor
UGT2B15 substrate
Antiacne
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Galactosylceramidase inhibitor
Sodium/bile acid cotransporter inhibitor
Apyrase inhibitor
Antineoplastic, alkylator
[phosphorylase] phosphatase inhibitor
CYP2C9 substrate
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Antihypercholesterolemic
Protein 50S ribosomal subunit inhibitor
Glycine receptor agonist
Estrogen agonist
Lipocortins synthesis antagonist
Topoisomerase II inhibitor
Laxative
Prostatic (benign) hyperplasia treatment
Sterol 24-C-methyltransferase inhibitor
Alpha glucosidase inhibitor
Chitinase inhibitor
Aldose 1-epimerase inhibitor
Acaricide
Methylglutamate dehydrogenase inhibitor

CYP2C substrate
Pyruvate carboxylase inhibitor
Corticosteroid antagonist
Antitreponemal
Dolichyl-phosphate beta-glucosyltransferase inhibitor
RNA directed DNA polymerase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
Sucrose-phosphate synthase inhibitor
DNA synthesis inhibitor
Antineoplastic (liver cancer)
Hydroxysteroid dehydrogenase inhibitor
UGT2B9 substrate
Peristaltic stimulant
Antineoplastic alkaloid
Dextranase inhibitor
Alpha-L-fucosidase inhibitor
Cholestenone 5alpha-reductase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Interferon gamma antagonist
Interleukin agonist
UGT1A4 substrate
Testosterone agonist
Opioid mu 2 receptor antagonist
Biliary tract disorders treatment
RNA agonist
RNA-directed RNA polymerase stimulant
CYP2A6 substrate
(N-acetylneuraminy)-galactosylglucosylceramide
N-acetylgalactosaminyltransferase inhibitor
CYP3A3 substrate
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
CYP2A substrate
2-Acylglycerol O-acyltransferase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
1,3-Beta-glucan synthase inhibitor
Anabolic
Glycine receptor antagonist
Contraceptive female
UGT1A10 substrate
UGT2B4 substrate
CYP2C11 substrate
Hypercalcemia treatment
Protein 30S ribosomal subunit inhibitor
Galectin 3 antagonist
Antiprotozoal (Toxoplasma)
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Antineoplastic (pancreatic cancer)
Steroid DELTA-isomerase inhibitor
Rhodopsin kinase inhibitor
SULT1E1 substrate

Antiviral (Trachoma)
DNA directed RNA polymerase stimulant
UGT2B17 substrate
Trans-octaprenyltranstransferase inhibitor
Sulfite dehydrogenase inhibitor
Neurotrophic factor enhancer
Opioid mu 1 receptor antagonist
Growth stimulant
Angiogenesis stimulant
Rubredoxin-NAD⁺ reductase inhibitor
Interleukin 10 antagonist
UGT1A3 substrate
mRNA (guanine-N7-)-methyltransferase inhibitor
Antibiotic Aminoglycoside-like
G-protein-coupled bile acid receptor 1 agonist
Antiarrhythmic
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
UGT1A7 substrate
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Protein kinase C stimulant
Protein kinase stimulant
Hydroxylamine reductase (NADH) inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
ATPase (Mitochondrial F1F0) inhibitor
Antihemorrhagic
H⁺/K⁺-transporting ATPase inhibitor
Expectorant
Beta-N-acetylhexosaminidase inhibitor
Antifungal enhancer
DNA intercalator
Steroid-like
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
CYP19 substrate
UGT2B19 substrate
UGT2B23 substrate
UGT2B30 substrate
UGT2B4D substrate
UGT2B4E substrate
CYP7B substrate
CYP7B1 substrate
Thyroxine 5-deiodinase inhibitor
CDC25A inhibitor
Estradiol 17 beta dehydrogenase 3 inhibitor
Androgen agonist
Melanin inhibitor
Lipocortins synthesis agonist
Choloylglycine hydrolase inhibitor
Antineoplastic (small cell lung cancer)
Free radical scavenger
Aldosterone antagonist

Diacylglycerol cholinephosphotransferase inhibitor
Mannose isomerase inhibitor
Antiprotozoal (Trichomonas)
Antipsoriatic
UGT1A6 substrate
Antibiotic Macrolide-like
Microtubule formation inhibitor
Ca²⁺-transporting ATPase inhibitor
Macrophage stimulant
UGT2B7H substrate
UGT2B7Y substrate
GRP78 expression inhibitor
Maltose-transporting ATPase inhibitor
CYP2C8 inducer
Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Mucolytic
2-Hydroxyacylsphingosine 1-beta-galactosyltransferase inhibitor
Myosin-light-chain-phosphatase inhibitor
T-cell protein-tyrosine phosphatase inhibitor
Chemoprotective
Antineoplastic (renal cancer)
Adenosine regulator
Diacylglycerol kinase inhibitor
Progesterone agonist
Cholesterol absorption inhibitor
UGT2B11 substrate
Glucosyl transferase inhibitor
Antispirochetal
UGT2B20 substrate
Cortisone beta-reductase inhibitor
Translation initiation factor IF-2 antagonist
Motilin receptor agonist
Selectin antagonist
Dihydropyrimidine dehydrogenase inhibitor
DNA polymerase I inhibitor
Licheninase inhibitor
UGT2B10 substrate
Sodium/glucose cotransporter 1 inhibitor
Arylamine N-acetyltransferase inhibitor
Sugar-phosphatase inhibitor
Estradiol 17 beta dehydrogenase stimulant
Severe acute respiratory syndrome treatment
Keratolytic
CYP27A1 substrate
Glycerone-phosphate O-acyltransferase inhibitor
Estradiol 17 beta dehydrogenase inhibitor
Microtubule stabilization
Undecaprenyl-phosphate mannosyltransferase inhibitor
Selectin P antagonist

UGT2B1 substrate
Antiviral (Hepatitis B)
Antiprotozoal (Plasmodium)
Antiinfertility, female
Reductase inhibitor
Spasmolytic
CYP4B1 substrate
Interleukin 2 antagonist
Chemosensitizer
Sodium/glucose cotransporter inhibitor
Mineralocorticoid
Eicosanoid agonist
CYP17 substrate
Anticholelithogenic
Adenomatous polyposis treatment
Sodium/hydrogen exchanger 1 inhibitor
Antipruritic, non-allergic
Glycolipid 2-alpha-mannosyltransferase inhibitor
Corticosteroid-like
Bile-salt sulfotransferase inhibitor

Doxepin hydrochloride

Molecular Mechanism (initial) :

5HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

H1 and H2 histamine receptor blocker

initial indication(s):

depression

Repurposed indication(s):

pruritis

insomnia

Predicted Activities

Neurotransmitter uptake inhibitor

CYP2D substrate
CYP2D6 substrate
CYP1A2 substrate
CYP2E1 inhibitor
CYP2C9 substrate

Antidepressant

Mood disorders treatment
Membrane integrity agonist
CYP1A substrate
CYP2E substrate
CYP2E1 substrate
CYP2C19 substrate
Spasmolytic
CYP2C substrate
Antidepressant, Imipramin-like
Glycosylphosphatidylinositol phospholipase D inhibitor

CYP3A4 substrate
HERG 1 channel blocker
Antitoxic
P-glycoprotein substrate
CYP3A substrate
Antipruritic
UGT1A4 substrate
CYP2B6 substrate
Monoamine uptake inhibitor
Anticonvulsant

Histamine H1 receptor antagonist

Histamine release inhibitor
CYP3A1 substrate
Muscle relaxant
CYP2C11 substrate
Fibrinolytic
CYP2C19 inhibitor
CYP3A2 substrate
Antipruritic, allergic
Antihistaminic
Spasmolytic, urinary
Phobic disorders treatment
Antiinflammatory
CYP2B substrate
Histamine antagonist
Antiparkinsonian, rigidity relieving
CYP2C8 inhibitor
CYP3A3 substrate
CYP2D2 inhibitor
Mediator release inhibitor
Skeletal muscle relaxant
CYP2D6 inhibitor
Antineurotic
5 Hydroxytryptamine 5 antagonist
UGT1A3 substrate
CYP2C12 substrate
2-Haloacid dehalogenase inhibitor
Antisecretoric
UGT1A substrate
Membrane permeability inhibitor
CYP2C18 substrate
Antineurogenic pain
Lipid metabolism regulator
Platelet aggregation stimulant
CYP2D16 substrate
Spasmolytic, Papaverin-like
CNS active muscle relaxant
Anesthetic general
Anxiolytic
Rhinitis treatment

Trimethylamine-oxide aldolase inhibitor
Antipruritic, non-allergic
Antiparkinsonian, tremor relieving
CYP2A2 substrate
Antiulcerative
Alpha 2b adrenoreceptor antagonist
Cytochrome P450 inhibitor
CYP2F1 substrate
4-Nitrophenol 2-monooxygenase inhibitor
Radioprotector
Antipsychotic
Radiosensitizer
Platelet adhesion inhibitor
Alpha 2c adrenoreceptor antagonist
Ovulation inhibitor
CYP2H substrate
Imidazoline receptor agonist
P-glycoprotein inhibitor
FMO1 substrate
Aspulvinone dimethylallyltransferase inhibitor
5 Hydroxytryptamine 1F antagonist
CYP2A1 substrate
Mucositis treatment
P-glycoprotein 1 inhibitor
Neuropeptide Y2 antagonist
Alpha 2a adrenoreceptor antagonist
MAP kinase stimulant
Photosensitizer
Phosphatidylinositol diacylglycerol-lyase inhibitor
Antiemetic
5 Hydroxytryptamine 5A antagonist
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Vasodilator, coronary
UGT1A9 substrate
TP53 expression enhancer
Gluconate 2-dehydrogenase (acceptor) inhibitor
UDP-glucuronosyltransferase substrate
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Macrophage colony stimulating factor agonist
Flavin-containing monooxygenase substrate
1,4-Lactonase inhibitor
Neurodegenerative diseases treatment
Imidazoline I1 receptor agonist
Antiparkinsonian
Histamine release stimulant
CYP3A7 substrate
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Taurine dehydrogenase inhibitor
MAO B substrate
Antiallergic

Choline-phosphate cytidylyltransferase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
5 Hydroxytryptamine uptake inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Calcium regulator
Gastrin inhibitor
Carboxypeptidase Taq inhibitor
Oxygen scavenger
CYP2C8 substrate
Respiratory analeptic
Thiamine-triphosphatase inhibitor
MAO inhibitor
Antieczematic atopic
Nav1.4 sodium channel blocker
Polarisation inhibitor
HERG channel blocker
Transforming growth factor beta 1 agonist
Guanylate cyclase 1 stimulant
Membrane integrity antagonist
Caspase 8 stimulant
Apyrase inhibitor
Vasodilator, peripheral
Analgesic
CYP2A4 substrate
Antiprotozoal (Leishmania)
MAO A substrate
MMP9 expression inhibitor
HCV IRES inhibitor
Antipyretic
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Diabetic nephropathy treatment
Anesthetic
5 Hydroxytryptamine uptake stimulant
Alpha 2 adrenoreceptor antagonist
Phospholipid-translocating ATPase inhibitor
Gonadotropin antagonist
Steroid synthesis inhibitor
Pin1 inhibitor
Sodium channel blocker
CYP2A6 substrate
Antitussive, narcotic
All-trans-retinyl-palmitate hydrolase inhibitor
Ethanolamine-phosphate cytidylyltransferase inhibitor
Venombin AB inhibitor
Methyltransferase substrate
Aldehyde oxidase inhibitor
Fusarinine-C ornithinesterase inhibitor
Cardiotonic
Antihypoxic

ATPase inhibitor
Phenol O-methyltransferase inhibitor
Antihelminthic (Nematodes)
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
CYP2A6 inhibitor
Adenylate cyclase inhibitor
Antineoplastic (small cell lung cancer)
CYP2A substrate
GABA transporter 2 inhibitor
Topoisomerase I inhibitor
Anaphylatoxin receptor antagonist
GABA aminotransferase inhibitor
Nitrite reductase (NO-forming) inhibitor
Sigma receptor agonist
Farnesyltranstransferase inhibitor
CYP1A inhibitor
Potassium channel blocker
Cell wall biosynthesis inhibitor
Aldosterone antagonist
CYP1A2 inhibitor
Flavin-containing monooxygenase inhibitor
Histidinol dehydrogenase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Apoptosis antagonist
5 Hydroxytryptamine 1B antagonist
Calcium channel (voltage-sensitive) activator
Alcohol dehydrogenase inhibitor
Sugar-phosphatase inhibitor
Fumarate reductase (NADH) inhibitor
Malate dehydrogenase (acceptor) inhibitor
Antimutagenic
HMOX1 expression enhancer
Signal peptidase I inhibitor
Nav1.5 sodium channel blocker
JAK2 expression inhibitor
Complement factor D inhibitor
Glyoxylate reductase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Cholinergic antagonist
HIF1A expression inhibitor
Fructose 5-dehydrogenase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Adrenergic
TRPA1 agonist
5 Hydroxytryptamine 1D antagonist
Vasodilator
Acylcarnitine hydrolase inhibitor
Trimethylamine dehydrogenase inhibitor
Antihematotoxic
X-methyl-His dipeptidase inhibitor

Dementia treatment
Beta 3 adrenoreceptor antagonist
Insulysin inhibitor
Dolichol kinase inhibitor
Arginine 2-monooxygenase inhibitor
Sodium channel (voltage-gated) blocker
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Ecdysone 20-monooxygenase inhibitor
Nitrate reductase (cytochrome) inhibitor
Mucomembranous protector
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Nucleoside-diphosphatase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
Muscular dystrophy treatment
Caspase 3 stimulant
Antiviral (Herpes)
Thromboxane B2 antagonist
Monoamine oxidase substrate
Analeptic
Phthalate 4,5-dioxygenase inhibitor
CYP2J substrate
Retinoic acid metabolism inhibitor
Adenosine regulator
Antiviral (Poxvirus)
Antidyskinetic
Potassium channel (Voltage-sensitive) blocker
Acetylgalactosaminyl-O-glycosyl-glycoprotein
beta-1,3-N-acetylglucosaminyltransferase inhibitor
FMO3 substrate
CYP2B5 substrate
Obsessive-compulsive disorder treatment
CYP2D1 substrate
Antineoplastic alkaloid
NOS2 expression inhibitor
Antimyopathies
Nitrite reductase [NAD(P)H] inhibitor
Formaldehyde transketolase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Guanylate cyclase stimulant
Adrenaline uptake inhibitor
NADPH peroxidase inhibitor
RELA expression inhibitor
Octopamine antagonist
CYP1A1 substrate
Neurotransmitter antagonist
UGT1A1 substrate
Nicotinic alpha2beta2 receptor antagonist
5 Hydroxytryptamine 2B antagonist

5 Hydroxytryptamine 2A agonist
Squalene-hopene cyclase inhibitor
Fatty-acyl-CoA synthase inhibitor
CYP3A inducer
Phosphoenolpyruvate mutase inhibitor
CYP2A3 substrate
CYP3A4 inducer
Alpha adrenoreceptor antagonist
Hydroxylamine oxidase inhibitor
CYP3A5 substrate
CYP2C3 substrate
Vasoprotector
Pseudolysin inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Chemosensitizer
5 Hydroxytryptamine 2A antagonist
Prion diseases treatment
Exoribonuclease II inhibitor
Vascular dementia treatment
Ophthalmic drug
(S)-6-hydroxynicotine oxidase inhibitor
Cyclohexanone monooxygenase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Lysostaphin inhibitor
Glycerol-3-phosphate oxidase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Choline dehydrogenase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Acaricide
Sleep disorders treatment
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Polyamine-transporting ATPase inhibitor
Cytochrome-b5 reductase substrate
N-acylmannosamine kinase inhibitor
Huntington's disease treatment
Hydrogen dehydrogenase inhibitor
Choline-sulfatase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Histamine H2 receptor antagonist
Uric acid excretion stimulant
CYP2A11 substrate
Antiarrhythmic
Antihypertensive
Hematopoietic inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Pappalysin-1 inhibitor
Hydroxylamine reductase (NADH) inhibitor
Acetylcholine neuromuscular blocking agent
2-Hydroxyquinoline 8-monooxygenase inhibitor

5 Hydroxytryptamine antagonist
Cytoprotectant
Fibrinogen receptor antagonist
Gluconate 5-dehydrogenase inhibitor
Manganese peroxidase inhibitor
Albendazole monooxygenase inhibitor
DNA intercalator
Lysyl oxidase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Nicotine dehydrogenase inhibitor
CYP2D15 substrate
Antitussive
CYP2B1 substrate
CYP4A11 substrate
Membrane permeability enhancer
Phosphopantothienoylcysteine decarboxylase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Adrenaline release stimulant
Dermatologic
Antineoplastic (non-small cell lung cancer)
5 Hydroxytryptamine 2 antagonist
Rubredoxin-NAD⁺ reductase inhibitor
Alpha 1b adrenoreceptor antagonist
GST M substrate
Aldose reductase substrate
Antiadrenergic
Antipsoriatic
Peroxidase substrate
5 Hydroxytryptamine release stimulant
2,3-Oxidosqualene-lanosterol cyclase inhibitor
Chloride peroxidase inhibitor
Putrescine oxidase inhibitor
Blasticidin-S deaminase inhibitor
Omptin inhibitor
Lipoxygenase substrate
Azobenzene reductase inhibitor
CYP2J2 substrate
Protein kinase C inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Telomerase inhibitor
Shab potassium channel blocker
5 Hydroxytryptamine 1 antagonist
Sigma 1 receptor agonist
Squalene epoxidase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
5 Hydroxytryptamine 2C antagonist
Aldehyde oxidase substrate
Carnitine 3-dehydrogenase inhibitor
CYP4A substrate

UDP-N-acetylglucosamine 4-epimerase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Fragilysin inhibitor
Anthrax lethal factor inhibitor
5 Hydroxytryptamine 7 antagonist
Tetrahydroxynaphthalene reductase inhibitor
TNF expression inhibitor
2-Enoate reductase inhibitor
CYP2G1 substrate
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Cytochrome P450 stimulant
Systemic lupus erythematosus treatment
CYP2E1 inducer
Male reproductive dysfunction treatment
Glycine amidinotransferase inhibitor
Antineoplastic (uterine cancer)
CYP19A1 expression inhibitor
NADPH-cytochrome-c2 reductase inhibitor
IgA-specific serine endopeptidase inhibitor
CYP2C9 inducer
TH expression enhancer
NF-E2-related factor 2 stimulant
Sulfur reductase inhibitor
Chlordecone reductase inhibitor
Prostaglandin H2 antagonist
Psychosexual dysfunction treatment
General pump inhibitor
Estrogen antagonist
Dimethylargininase inhibitor
Spermidine dehydrogenase inhibitor
5 Hydroxytryptamine 1A antagonist
Fibrolase inhibitor
Limulus clotting factor B inhibitor
Feruloyl esterase inhibitor
Adrenaline antagonist
Dopamine D1A antagonist
Choline sulfotransferase inhibitor
UGT2B28 substrate
MAO B inhibitor
Glucose oxidase inhibitor
Carnosine synthase inhibitor
Acetylspermidine deacetylase inhibitor
Alkylacetylgllycerophosphatase inhibitor
Loop diuretic
5-O-(4-coumaroyl)-D-quinat 3'-monooxygenase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Opioid kappa 3 receptor antagonist
Glutamyl endopeptidase II inhibitor
Smooth muscle myosin light chain kinase inhibitor
Lysine 2,3-aminomutase inhibitor

Antidiabetic symptomatic
Carnitine dehydratase inhibitor
Sodium/calcium exchanger 1 inhibitor
MAO A inhibitor
Phosphatidate phosphatase inhibitor
CYP2C6 substrate
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Apoptosis agonist
Acetylcholine antagonist
5 Hydroxytryptamine release inhibitor
Cyclooxygenase substrate
Adenylate cyclase stimulant
Heat shock protein agonist
Alpha 1 adrenoreceptor antagonist
Acetylcholine muscarinic antagonist
Amyotrophic lateral sclerosis treatment
Retinal dehydrogenase inhibitor
GABA B receptor agonist
CYP2A10 substrate
Antimitotic
Alpha 1d adrenoreceptor antagonist
Antineoplastic (lung cancer)
Anticarcinogenic
CYP2B2 substrate
Alpha 1a adrenoreceptor antagonist
(S)-carnitine 3-dehydrogenase inhibitor
N-formylmethionyl-peptidase inhibitor
Intermittent claudication treatment
Sulfotransferase substrate
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Clavamate synthase inhibitor
Antineoplastic (ovarian cancer)
Antineoplastic, alkylator
Carnitinamidase inhibitor
DELTA24-sterol reductase inhibitor
Protein kinase C alpha inhibitor
Phosphoserine phosphatase inhibitor
5 Hydroxytryptamine 4 antagonist
Nucleotide metabolism regulator
Sphinganine kinase inhibitor
Antiperistaltic
Alkane 1-monooxygenase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Cycloartenol synthase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Insecticide
Restless leg syndrome treatment
Acetylcholine M3 receptor antagonist
Histidine kinase inhibitor
Polyporopepsin inhibitor

Estrogen receptor beta antagonist
Histone deacetylase SIRT2 inhibitor
Argininosuccinate lyase inhibitor
3-Cyanoalanine hydratase inhibitor
Deoxyribonuclease I inhibitor
CYP2C8 inducer
Calcium channel blocker
Hepatoprotectant
Antiprotozoal (Trypanosoma)
Pullulanase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Acylaminoacyl-peptidase inhibitor
Arylsulfate sulfotransferase inhibitor
Heat shock protein 70 agonist
Fructan beta-fructosidase inhibitor
Antiprotozoal (Trichomonas)
Quinoprotein glucose dehydrogenase inhibitor
Gastric antisecretory
Methylumbelliferyl-acetate deacetylase inhibitor
Aldehyde dehydrogenase 2 substrate
CYP2B11 substrate
Sodium/hydrogen exchanger 5 inhibitor
Thioredoxin inhibitor
Acetylcholine M5 receptor antagonist
Acetylcholine M4 receptor antagonist
CYP1B substrate
MAP kinase kinase 4 inhibitor
Phospholipase C inhibitor
Pediculicide
P-benzoquinone reductase (NADPH) inhibitor
Antifibrinolytic
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Antimigraine
Gastrointestinal motility stimulant
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
CDC25 phosphatase inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Mannitol-1-phosphatase inhibitor
Calcium antagonist
CDC25C inhibitor
Antiinflammatory, ophthalmic
5 Hydroxytryptamine 1B agonist
Undecaprenyldiphospho-muramoylpentapeptide
beta-N-acetylglucosaminyltransferase inhibitor
Butyrylcholinesterase inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
5 Hydroxytryptamine 6 antagonist
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
D-Octopine dehydrogenase inhibitor

Antineoplastic (lymphoma)
Thromboxane synthase inhibitor
CYP1A1 inducer
Metabolic disease treatment
Alkene monooxygenase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Peptidylamidoglycolate lyase inhibitor
Kinesin antagonist
Kinesin-like protein 1 inhibitor
Antithrombotic
Diphosphomevalonate decarboxylase inhibitor
Lassitude treatment
Andropause treatment
GST T substrate
GST T1-1 substrate
Dynamin GTPase inhibitor
HIV-2 reverse transcriptase inhibitor
Phosphatidylserine decarboxylase inhibitor
Sodium channel blocker class Ib
Para amino benzoic acid antagonist
Bipolar disorder treatment
4-Coumarate-CoA ligase inhibitor
Preneoplastic conditions treatment
CYP4A1 substrate
Undecaprenyl-diphosphatase inhibitor
CYP1B1 substrate
Histone deacetylase SIRT1 inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Tropinesterase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Licheninase inhibitor
Menopausal disorders treatment
Neurotrophic factor
Benzaldehyde dehydrogenase (NADP+) inhibitor
CYP1A1 inhibitor
Amine dehydrogenase inhibitor
Carnitine O-octanoyltransferase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
Nav1.7 sodium channel blocker
Prolactin inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
Thioredoxin reductase inhibitor
CTGF expression inhibitor
Candidapepsin inhibitor
Cardioprotectant
Alcohol dehydrogenase (NADP+) inhibitor
Leukopoiesis stimulant

Aryl-acylamidase inhibitor
Aureolysin inhibitor
Glycerol dehydrogenase inhibitor
4-Hydroxyproline epimerase inhibitor
RNA synthesis inhibitor
Beta adrenoreceptor antagonist
5 Hydroxytryptamine 2B agonist
Guanylate cyclase inhibitor
Guanylate cyclase 1 inhibitor
5 Hydroxytryptamine 4A antagonist
Choleretic
Postmenopausal disorders treatment
Leukotriene-C4 synthase inhibitor
Acetylcholine M2 receptor antagonist
(R)-6-hydroxynicotine oxidase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Guanidinoacetate kinase inhibitor
Bcl-xL inhibitor
Bulimia treatment
Antiviral (Adenovirus)
Free radical scavenger
N-benzyloxycarbonylglycine hydrolase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Non-steroidal antiinflammatory agent
Keratosis actinic (solar) treatment
Antinaupathic
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Antihemorrhagic
Melanin inhibitor
Hot flush treatment
Interleukin 6 antagonist
Leukotriene-B4 20-monooxygenase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Histamine H2 receptor agonist
Beta 1 adrenoreceptor antagonist
Beta-D-fucosidase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Glutaminase inhibitor
Inotropic
CYP2A8 substrate
Xylan endo-1,3-beta-xylosidase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
4-Hydroxymandelate oxidase inhibitor
Histone deacetylase class III inhibitor
UGT1A5 substrate
Alkenylglycerophosphocholine hydrolase inhibitor
Acylesterase inhibitor
Prostaglandin D2 agonist
Betaine-aldehyde dehydrogenase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor

Succinate dehydrogenase inhibitor
Antineoplastic (breast cancer)
Sulfite oxidase inhibitor
Thromboxane agonist
Adrenergic, ophthalmic
GST A substrate
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
Cyanoalanine nitrilase inhibitor
3-Phytase inhibitor
Melatonin 1 agonist
Antineoplastic (brain cancer)
Capillary fragility treatment
Trehalose-phosphatase inhibitor
Creatininase inhibitor
Catenin beta inhibitor
CYP2B10 substrate
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Sigma receptor antagonist
Antineoplastic (cervical cancer)
5 Hydroxytryptamine 7 agonist
Nootropic
Gynecological disorders treatment
Phosphatidylinositol 3-kinase stimulant
Acyl-lysine deacylase inhibitor
Melatonin 2 agonist
Antinociceptive
Antihelminthic
Horriylsin inhibitor
Isopenicillin-N epimerase inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
Acetylcholine M1 receptor antagonist
Amyloid beta aggregation inhibitor
Cytochrome-b5 reductase inhibitor
Polyneuridine-aldehyde esterase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Thromboxane antagonist
Galacturan 1,4-alpha-galacturonidase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Yeast ribonuclease inhibitor
Carboxymethylenebutenolidase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Prostaglandin antagonist
Gentamicin 2"-nucleotidyltransferase inhibitor
ICAM1 expression inhibitor
Leukotriene B4 antagonist
Galactolipase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor

Cyclic AMP phosphodiesterase inhibitor
Histamine agonist
Beta 2 adrenoreceptor antagonist
4-Nitrophenylphosphatase inhibitor
CYP2A13 substrate
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Antidote
Sclerosant
Dolichyl-phosphatase inhibitor
Thrombolytic
Calcium channel (voltage-sensitive) blocker
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Antiprotozoal (Amoeba)
Mannose isomerase inhibitor
Carnitine palmitoyltransferase inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Cyclic AMP agonist
Thymidylate 5'-phosphatase inhibitor
Urotensin II agonist
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Sphingosine kinase inhibitor
Menstruation disorders treatment
Thyroid hormone alpha antagonist
Nicotinate dehydrogenase inhibitor
SULT2A1 substrate

Duloxetine hydrochloride

Molecular Mechanism (initial) :

5HT, norepinephrine and dopamine reuptake inhibitor

Molecular Mechanism (repurposed) :

5HT, norepinephrine and dopamine reuptake inhibitor

initial indication(s):

depression

Repurposed indication(s):

urinary incontinence

generalized anxiety disorder

neuropathic pain

Predicted Activities

Antineurotic
CYP2D6 substrate
CYP2D substrate
Diabetic neuropathy treatment
Complement factor D inhibitor
Adrenergic
Mucomembranous protector
CYP1A substrate

CYP1A2 substrate
Adrenaline release stimulant
Mood disorders treatment

Antidepressant

Posttraumatic stress disorder treatment
Analgesic
CYP2D2 inhibitor
5 Hydroxytryptamine uptake inhibitor
Antiischemic, cerebral
Urologic disorders treatment
Calcium channel (voltage-sensitive) activator

Urinary incontinence treatment

Stroke treatment
CYP2C9 substrate
Antineurogenic pain
Antinociceptive
Fibromyalgia syndrome treatment
CYP2E1 inhibitor
Antidiabetic symptomatic
Reductant
Nitric-oxide synthase inhibitor
CYP2C18 substrate
Analgesic, non-opioid
CYP2D16 substrate
Neurotransmitter uptake inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Adrenaline uptake inhibitor
CYP2C10 substrate
CYP2C substrate
CDP-glycerol glycerophosphotransferase inhibitor
CYP2D15 substrate
Antidiabetic
Dopamine release stimulant
Monoamine uptake inhibitor
Anaphylatoxin receptor antagonist
Oxygen scavenger
Antidepressant, Imipramin-like
Adrenergic, ophthalmic
CYP2D6 inhibitor
Malate oxidase inhibitor
Spasmolytic, urinary
Prostaglandin E1 antagonist
Obsessive-compulsive disorder treatment
Ovulation inhibitor
Antihelmintic
Amyotrophic lateral sclerosis treatment
Thiamine-triphosphatase inhibitor
Histamine H1 receptor agonist
Acute neurologic disorders treatment
Antiamyloidogenic

5 Hydroxytryptamine 2B agonist
Antiparasitic
5 Hydroxytryptamine release inhibitor
CYP2C12 substrate
Cytochrome P450 inhibitor
CYP2E1 substrate
Antianorexic
Ubiquinol-cytochrome-c reductase inhibitor
Lassitude treatment
CYP2C8 substrate
CYP2C19 substrate
CYP2E substrate
Anti-Helicobacter pylori
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
CYP3A2 substrate
Gonadotropin antagonist
Monodehydroascorbate reductase (NADH) inhibitor
Cancer associated disorders treatment
CYP2B6 substrate
1,4-Lactonase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Lipoprotein disorders treatment
Ompin inhibitor
Opioid dependency treatment
Glycerol-3-phosphate dehydrogenase inhibitor
Proline racemase inhibitor
Antiinflammatory, ophthalmic
Prion diseases treatment
Glycogen synthase stimulant
Mucolytic
Macrophage colony stimulating factor agonist
Caspase 3 stimulant
CYP2A6 inhibitor
Calcium channel blocker
Hemostatic
Aspulvinone dimethylallyltransferase inhibitor
P-glycoprotein substrate
Cytochrome-b5 reductase inhibitor
Antiinfective
Inflammatory Bowel disease treatment
Peptidyltransferase inhibitor
PfA-M1 aminopeptidase inhibitor
Follicle-stimulating hormone agonist
Nav1.5 sodium channel blocker
Trimethylamine-oxide aldolase inhibitor
Imidazoline receptor agonist
Glutamate release inhibitor
Anxiolytic
Alpha adrenoreceptor agonist
MAO inhibitor

Glycosylphosphatidylinositol phospholipase D inhibitor
Expectorant
Free radical scavenger
Dependence treatment
Dopamine transporter inhibitor
Platelet aggregation stimulant
Complement inhibitor
Choline-phosphate cytidylyltransferase inhibitor
CYP2C19 inhibitor
ATPase inhibitor
Radical formation agonist
Beta adrenoreceptor antagonist
CYP1A2 inhibitor
Antimigraine
Alpha 2b adrenoreceptor antagonist
IgA-specific serine endopeptidase inhibitor
CYP3A4 substrate
Anesthetic
Histamine agonist
Calcium channel activator
Antiviral (Influenza)
CYP3A5 substrate
Menopausal disorders treatment
UGT2B12 substrate
Protein kinase C beta inhibitor
Cell wall biosynthesis inhibitor
CYP1A inhibitor
Dyrk kinase inhibitor
Antimyopathies
CYP2J2 substrate
Squalene epoxidase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
CYP2A2 substrate
Vasodilator, coronary
CYP2C9 inhibitor
Antihypotensive
Methane monooxygenase inhibitor
CYP2D1 substrate
Adrenaline agonist
Histone deacetylase SIRT1 inhibitor
HMOX1 expression enhancer
Antiparkinsonian, tremor relieving
4-Hydroxyproline epimerase inhibitor
Transcription factor STAT3 inhibitor
Ophthalmic drug
Hot flush treatment
Glycine transporter 1 inhibitor
Protein kinase C theta inhibitor
Transforming growth factor beta 1 agonist

Transglutaminase 2 inhibitor
Vasoprotector
Aryl-acylamidase inhibitor
Phobic disorders treatment
ICAM1 expression inhibitor
Diabetic retinopathy treatment
Alpha 2 adrenoreceptor antagonist
Antiviral (Picornavirus)
MAO B substrate
Limulus clotting factor B inhibitor
Movement disorders treatment
HCV IRES inhibitor
Phenylalanine-tRNA ligase inhibitor
MAO B inhibitor
Bradykinin B2 receptor agonist
Stearoyl-CoA desaturase inhibitor
Alpha 2c adrenoreceptor antagonist
Acidifying agent non gastric
Attention deficit/hyperactivity disorder treatment
CYP3A substrate
Antiviral (Adenovirus)
5 Hydroxytryptamine uptake stimulant
Sarcosine oxidase inhibitor
Vasodilator, peripheral
Histamine H2 receptor antagonist
Lactamase C inhibitor
Shock treatment
Adenylate cyclase stimulant
Alpha 2d adrenoreceptor antagonist
Inducible nitric-oxide synthase inhibitor
Antiadrenergic
Pancreatic ribonuclease inhibitor
Antibiotic Anthracycline-like
Pin1 inhibitor
Celiac disease treatment
Antihematotoxic
Thioredoxin inhibitor
Azobenzene reductase inhibitor
Alpha 2 adrenoreceptor agonist
2-Nitropropane dioxygenase inhibitor
5 Hydroxytryptamine antagonist
Adrenaline antagonist
Antitussive
Neuropeptide agonist
Glycine transporter inhibitor
Deoxyhypusine synthase inhibitor
Antiuremic
5 Hydroxytryptamine 1A antagonist
Photosensitizer
CYP2B substrate

Protein-arginine deiminase inhibitor
Anthrax lethal factor inhibitor
Bradykinin agonist
Beta amyloid protein antagonist
Urotensin II antagonist
Acaricide
Uterine stimulant
Antineoplastic (uterine cancer)
Beta 3 adrenoreceptor antagonist
NMDA receptor polyamine site antagonist
Histidine kinase inhibitor
GABA A receptor agonist
Neuronal nitric-oxide synthase inhibitor
Carboxycyclohexadienyl dehydratase inhibitor
Protein kinase C gamma inhibitor
Potassium channel Kv1.3 blocker
Anesthetic general
Cognition disorders treatment
Nicotinic alpha4beta4 receptor agonist
Anesthetic local
Polyamine-transporting ATPase inhibitor
Endothelial nitric-oxide synthase inhibitor
Protein kinase C eta inhibitor
DNA repair enzyme inhibitor
Beta 1 adrenoreceptor agonist
CYP1A1 inhibitor
Peroxidase substrate
Antihypertensive
Dipeptidyl peptidase I inhibitor
Beta 2 adrenoreceptor agonist
Preterm labor treatment
CYP2F1 substrate
5 Hydroxytryptamine 1 antagonist
Kallikrein inhibitor
Imidazoline receptor antagonist
CYP4A11 substrate
Antineoplastic (bladder cancer)
GABA transporter 2 inhibitor
Carnitine palmitoyltransferase inhibitor
Peroxisome proliferator-activated receptor agonist
Nicotinic alpha2beta4 receptor agonist
VEGF expression inhibitor
Phosphatidate phosphatase inhibitor
Tyrosine-protein kinase EMT inhibitor
Nicotinic alpha2beta2 receptor antagonist
CYP1A1 inducer

Eflornithine hydrochloride

Molecular Mechanism (initial) :
ornithine decarboxylase inhibitor

Molecular Mechanism (repurposed) :

ornithine decarboxylase inhibitor

initial indication(s):

African trypanosomiasis (sleeping sickness)

Repurposed indication(s):

hair growth abnormality

cancer

Predicted Activities

Antineoplastic (solid tumors)

Lysine decarboxylase inhibitor

Adenomatous polyposis treatment

Arginine decarboxylase inhibitor

Exoribonuclease II inhibitor

Phobic disorders treatment

CDP-glycerol glycerophosphotransferase inhibitor

Antiprotozoal (Trypanosoma)

Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor

Polyamine-transporting ATPase inhibitor

Antiprotozoal

Glucose oxidase inhibitor

Venombin AB inhibitor

Dermatologic

Acylcarnitine hydrolase inhibitor

Dimethylargininase inhibitor

Ornithine decarboxylase inhibitor

Carnosine synthase inhibitor

Antipsoriatic

N-benzyloxycarbonylglycine hydrolase inhibitor

Hydrogen dehydrogenase inhibitor

Acetylornithine deacetylase inhibitor

Lactase inhibitor

Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor

Yeast ribonuclease inhibitor

Fructan beta-fructosidase inhibitor

Fusarinine-C ornithinesterase inhibitor

Glutamate N-acetyltransferase inhibitor

Sulfite reductase inhibitor

Arylsulfate sulfotransferase inhibitor

Apoptosis antagonist

Fibrolase inhibitor

Lysine 2,3-aminomutase inhibitor

Protein-disulfide reductase (glutathione) inhibitor

Phosphatidylglycerophosphatase inhibitor

2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor

Arginine 2-monooxygenase inhibitor

Omptin inhibitor

Levanase inhibitor

Antibiotic Glycopeptide-like

Beta-adrenergic receptor kinase inhibitor

G-protein-coupled receptor kinase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
2-Dehydropantoate aldolase inhibitor
Pseudolysin inhibitor
GABA C receptor agonist
CYP2J substrate
Carboxypeptidase Taq inhibitor
Mucositis treatment
Guanidinoacetase inhibitor
Dipeptidase E inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Macrophage colony stimulating factor agonist
Aspartate-ammonia ligase inhibitor
CYP2J2 substrate
Proteasome ATPase inhibitor
Procollagen N-endopeptidase inhibitor
NADPH peroxidase inhibitor
Sphinganine kinase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Glycine amidinotransferase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Fibroblast growth factor agonist
Angiogenesis inhibitor
Polygalacturonase inhibitor
Arylesterase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Superoxide dismutase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Carboxypeptidase D inhibitor
Sulfur reductase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Ethanolamine-phosphate cytidylyltransferase inhibitor
Peptide agonist
Glycosylphosphatidylinositol phospholipase D inhibitor
Fragilysin inhibitor
Manganese peroxidase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Oxygen scavenger
Glutamate decarboxylase inhibitor
Inulinase inhibitor
Protein-tyrosine sulfotransferase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Limulus clotting factor B inhibitor
Formaldehyde transketolase inhibitor
1,4-Lactonase inhibitor
Cathepsin T inhibitor
Guanidinoacetate kinase inhibitor
Growth hormone agonist

Antiparasitic
Lipotropic
Gingipain K inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Carnitine dehydratase inhibitor
Aspartate ammonia-lyase inhibitor
D-xylulose reductase inhibitor
Meprin B inhibitor
Antiseborrheic
Cysteine transaminase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Lipoprotein lipase inhibitor
L-lysine 6-transaminase inhibitor
Gamma-glutamyltransferase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Fibroblast growth factor 1 agonist
Glutarate-semialdehyde dehydrogenase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Homoserine dehydrogenase inhibitor
Pitrilysin inhibitor
Ecdysone 20-monooxygenase inhibitor
Antineoplastic antimetabolite
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Fibrinolytic
Poly(beta-D-mannuronate) lyase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Enteropeptidase inhibitor
Fructose 5-dehydrogenase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Glycine hydroxymethyltransferase inhibitor
Interferon alpha agonist
Nitrite reductase (NO-forming) inhibitor
Protein-glutamate methylesterase inhibitor
Acetylspermidine deacetylase inhibitor
Aspartyltransferase inhibitor
Preneoplastic conditions treatment
Allantoate deiminase inhibitor
Oxidoreductase inhibitor
Aspartoacylase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Platelet aggregation stimulant
Histidine N-acetyltransferase inhibitor
Galactolipase inhibitor
Clostripain inhibitor
Acidifying agent non gastric
Cyclamate sulfohydrolase inhibitor
Cytoprotectant

Valine decarboxylase inhibitor
Alkylacetyl glycerophosphatase inhibitor
S-alkylcysteine lyase inhibitor
Fucosterol-epoxide lyase inhibitor
Branched-chain-amino-acid transaminase inhibitor
Mycothiol-S-conjugate amidase inhibitor
Ubiquitin thiolesterase inhibitor
Testosterone 17 β -dehydrogenase (NADP⁺) inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Glyoxylate reductase inhibitor
Carnitinamidase inhibitor
Sugar-phosphatase inhibitor
Calcium-sensing receptor agonist
Styrene-oxide isomerase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Pancreatic ribonuclease inhibitor
Guanidinobutyrase inhibitor
Endopeptidase So inhibitor
Alanine-tRNA ligase inhibitor
Diamine N-acetyltransferase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Septic shock treatment
ADP-thymidine kinase inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
Xylan endo-1,3- β -xylosidase inhibitor
Phosphatidylserine decarboxylase inhibitor
Macrophage stimulant
Electron-transferring-flavoprotein dehydrogenase inhibitor
Peptidoglycan glycosyltransferase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Aminoacylase inhibitor
Mannose isomerase inhibitor
Muramoyltetrapeptide carboxypeptidase inhibitor
Platelet adhesion inhibitor
Glutamate 5-kinase inhibitor
Renal tissue kallikrein inhibitor
Spasmolytic, urinary
N-Acyl-D-amino-acid deacylase inhibitor
Oxidizing agent
Cyclic AMP agonist
Interleukin 2 agonist
Undecaprenyldiphospho-muramoylpentapeptide
 β -N-acetylglucosaminyltransferase inhibitor
Omega-amidase inhibitor
Lysostaphin inhibitor
X-methyl-His dipeptidase inhibitor
Cytochrome-b5 reductase inhibitor
Guanidinopropionase inhibitor
Diaminopropionate ammonia-lyase inhibitor

Glycine-tRNA ligase inhibitor
Ferredoxin hydrogenase inhibitor
D-proline reductase (dithiol) inhibitor
Gluconolactonase inhibitor
Leukopoiesis stimulant
D-Ornithine 4,5-aminomutase inhibitor
Gingipain R inhibitor
Anesthetic general
Fatty-acyl-CoA synthase inhibitor
Aminolevulinate transaminase inhibitor
Acetylenecarboxylate hydratase inhibitor
4-Hydroxymandelate oxidase inhibitor
Mitochondrial intermediate peptidase inhibitor
Aspergillus nuclease S1 inhibitor
Phenylalanine(histidine) transaminase inhibitor
Agmatinase inhibitor
Phosphoenolpyruvate mutase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
Glucuronate isomerase inhibitor
Procollagen C-endopeptidase inhibitor
Beta-Lysine 5,6-aminomutase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Glutaminase inhibitor
Gametolysin inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
4-Nitrophenylphosphatase inhibitor
Antiviral
Histidine decarboxylase inhibitor
Phenol O-methyltransferase inhibitor
Asparagine-tRNA ligase inhibitor
Dihydropyrimidinase inhibitor
L-lysine oxidase inhibitor
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Peptidyltransferase inhibitor
5 Hydroxytryptamine uptake stimulant
Alpha-amylase inhibitor
Threonine aldolase inhibitor
S-formylglutathione hydrolase inhibitor
Tyrosine 3 hydroxylase inhibitor
Isopenicillin-N synthase inhibitor
Acrosin inhibitor
Chitosanase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Apyrase inhibitor
UDP-N-acetylmuramate-L-alanine ligase inhibitor

GABA aminotransferase inhibitor
Trimethylamine-oxide aldolase inhibitor
Serine-pyruvate transaminase inhibitor
Alopecia treatment
HCV IRES inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Cancer associated disorders treatment
Glutamyl endopeptidase II inhibitor
Adenylyl-sulfate reductase inhibitor
N-formylmethionyl-peptidase inhibitor
Thymidylate 5'-phosphatase inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Beta-ureidopropionase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Glucagon-like peptide 1 agonist
Arylmalonate decarboxylase inhibitor
GABA B receptor agonist
D-Octopine dehydrogenase inhibitor
Peroxidase substrate
Sulfite oxidase inhibitor
Mannitol-1-phosphatase inhibitor
Phosphatidate phosphatase inhibitor
Tryptophan transaminase inhibitor
Horriylsin inhibitor
Lysine 2-monooxygenase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein
beta-1,3-N-acetylglucosaminyltransferase inhibitor
Polyporopepsin inhibitor
Metallocoarboxypeptidase D inhibitor
Phenylalanine decarboxylase inhibitor
D-Lysine 5,6-aminomutase inhibitor
Thiol oxidase inhibitor
Dimethylmaleate hydratase inhibitor
Glutamate-tRNA ligase inhibitor
Hydroxylamine oxidase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
Arginyltransferase inhibitor
Phospholipase C inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Saccharolysin inhibitor
Chemopreventive
GST A substrate
Erythropoiesis stimulant
N-methyl-2-oxoglutaramate hydrolase inhibitor
Pullulanase inhibitor

Serine 3-dehydrogenase inhibitor
2-Aminoheptano-6-lactam racemase inhibitor
Dynein ATPase inhibitor
Leucolysin inhibitor
Coccolysin inhibitor
NADH kinase inhibitor
4-Alpha-glucanotransferase inhibitor
Antihypoxic
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Antifibrinolytic
Aminopeptidase Y inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Gluconate 5-dehydrogenase inhibitor
Acyl-lysine deacylase inhibitor
Trehalose-phosphatase inhibitor
Venom exonuclease inhibitor
Saccharopine dehydrogenase (NADP⁺, L-lysine-forming) inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Iron-cytochrome-c reductase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Pappalysin-1 inhibitor
Glutamate-cysteine ligase inhibitor
Creatininase inhibitor
FMO3 substrate
Maleate hydratase inhibitor
Acetylcholine neuromuscular blocking agent
Glycerol-3-phosphate oxidase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP⁺) inhibitor
3-Phytase inhibitor
Leukotriene-C4 synthase inhibitor
Biotinidase inhibitor
Membrane integrity agonist
Deoxyribonuclease I inhibitor
Glutamin-(asparagin-)ase inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Menopausal disorders treatment
D-Serine ammonia-lyase inhibitor
Lipid metabolism regulator
Acetylserotonin O-methyltransferase inhibitor
Bothrolysin inhibitor
DOPA decarboxylase inhibitor
Cyclohexanone monooxygenase inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Pyroglutamyl-peptidase II inhibitor
Immunostimulant
Carboxymethylenebutenolidase inhibitor

Amylo-alpha-1,6-glucosidase inhibitor
Benzoate-CoA ligase inhibitor
Homocitrate synthase inhibitor
Glycine C-acetyltransferase inhibitor
Mitochondrial processing peptidase inhibitor
Diguanidinobutanase inhibitor
Methanol dehydrogenase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Flavin-containing monooxygenase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Membrane permeability enhancer
Ceramide glucosyltransferase inhibitor
L-threonine 3-dehydrogenase inhibitor
Antineurogenic pain
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Arabinose isomerase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Tripeptidyl-peptidase I inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
tRNA cytidyltransferase inhibitor
Glycerol-1-phosphatase inhibitor
tRNA nucleotidyltransferase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Xylose isomerase inhibitor
Creatinase inhibitor
4-Hydroxyproline epimerase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Licheninase inhibitor
Prunasin beta-glucosidase inhibitor
Chlordecone reductase inhibitor
Tubulysin-Tyr carboxypeptidase inhibitor
Radioprotector
Phosphatase inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Argininosuccinate lyase inhibitor
Cl--transporting ATPase inhibitor
Kidney function stimulant
Lactaldehyde reductase (NADPH) inhibitor
Phosphoserine phosphatase inhibitor
Trimethyllysine dioxygenase inhibitor
Nardilysin inhibitor
Antiviral (Adenovirus)
DNA ligase (ATP) inhibitor
Antinaupathic
Pterin deaminase inhibitor
CYP4A2 substrate
Beta-carotene 15,15'-monooxygenase inhibitor

Chitinase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Choline-sulfatase inhibitor
Histidine-tRNA ligase inhibitor
Dextranase inhibitor
D-alanine transaminase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Antineoplastic (colorectal cancer)
Dactylisin inhibitor
Complement factor D inhibitor
Phosphonoacetate hydrolase inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
3-Cyanoalanine hydratase inhibitor
Antitoxic
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
Imidazoline receptor agonist
Selenocysteine lyase inhibitor
Fibrinogen receptor antagonist
Arginine racemase inhibitor
L-glutamate oxidase inhibitor
Urease inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Malate oxidase inhibitor
Cysteine desulfurase inhibitor
N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor
Prenyl-diphosphatase inhibitor
Aspartate kinase inhibitor
Protein-arginine deiminase inhibitor
Choline-phosphate cytidyltransferase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Bontoxilysin inhibitor
Snapalysin inhibitor
Immunosuppressant
Tauropine dehydrogenase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Gluconate dehydratase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Allantoicase inhibitor
Chaperonin ATPase inhibitor
Opioid dependency treatment
Sedoheptulose-bisphosphatase inhibitor
Dihydroxy-acid dehydratase inhibitor
Arginine deiminase inhibitor

Sclerosant
Brachyurin inhibitor
Hydroxylysine kinase inhibitor
X-His dipeptidase inhibitor
Furin inhibitor
Methane monooxygenase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Aureolysin inhibitor
Dihydrodipicolinate synthase inhibitor
Sulfite dehydrogenase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Antidote
Peptidyl-dipeptidase B inhibitor
Ornithine carbamoyltransferase inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Aminopeptidase B inhibitor
L-3-cyanoalanine synthase inhibitor
Aspartate-tRNA ligase inhibitor
Serratia marcescens nuclease inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Aspartate transaminase inhibitor
Prephenate dehydrogenase inhibitor
Atherosclerosis treatment
(S)-carnitine 3-dehydrogenase inhibitor
Tentoxilysin inhibitor
Leucine dehydrogenase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Creatinine deaminase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Phosphoinositide phospholipase C inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor
N-acetylneuraminate synthase inhibitor
Pyruvate decarboxylase inhibitor
Acetylesterase inhibitor
Diisopropyl-fluorophosphatase inhibitor
GHS receptor agonist
Analgesic stimulant
Hematopoietic inhibitor
Lysyl endopeptidase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Histidinol dehydrogenase inhibitor
Glutathione peroxidase inhibitor
Phospholipid-translocating ATPase inhibitor
Thiopurine S-methyltransferase inhibitor
CYP4F2 substrate
Methionine decarboxylase inhibitor
Ornithine-oxo-acid transaminase inhibitor
Asparaginase inhibitor

Tripeptide aminopeptidase inhibitor
2-Oxoglutarate decarboxylase inhibitor
CYP2C10 substrate
Sulfinioalanine decarboxylase inhibitor
Lysozyme inhibitor
O-aminophenol oxidase inhibitor
Cytosol alanyl aminopeptidase inhibitor
Phenylpyruvate decarboxylase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Transketolase inhibitor
Carnitine 3-dehydrogenase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Glutamine-tRNA ligase inhibitor
Thimet oligopeptidase inhibitor
Envelysin inhibitor
Phenylalanine 4-hydroxylase inhibitor
Dichloromuconate cycloisomerase inhibitor
Spermidine dehydrogenase inhibitor
Bile-salt sulfotransferase inhibitor
Antineoplastic (bladder cancer)
Cyclooxygenase substrate
Glyoxylate reductase (NADP+) inhibitor
D-glutamate oxidase inhibitor
N-acetyllactosamine synthase inhibitor
Methionine adenosyltransferase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
GABA transporter 3 inhibitor
Cysteine synthase inhibitor
Gallate decarboxylase inhibitor
Antimetabolite
Catalase inhibitor
CYP4A11 substrate
Thermitase inhibitor
Membrane integrity antagonist
Tryptophan dimethylallyltransferase inhibitor
DNA nucleotidylexotransferase inhibitor
3-Isopropylmalate dehydratase inhibitor
Putrescine oxidase inhibitor
4-Phytase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Polyamine oxidase inhibitor
Antidyskinetic
Limulus clotting factor C inhibitor
Cystathionine gamma-lyase inhibitor
Antimyopathies
3'-Nucleotidase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor

Peptide alpha-N-acetyltransferase inhibitor
Pantothenase inhibitor
Serralysin inhibitor
Botulin neurotoxin A light chain inhibitor
Protein synthesis inhibitor
Riboflavin phosphotransferase inhibitor
5-Aminovalerate transaminase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Lactate 2-monooxygenase inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Glycolate dehydrogenase inhibitor
Putrescine carbamoyltransferase inhibitor
Acylaminoacyl-peptidase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Sucrose-phosphate synthase inhibitor
2-Aminoadipate transaminase inhibitor
3-Oxoadipate enol-lactonase inhibitor
Kexin inhibitor
Histidine ammonia-lyase inhibitor
Glucarate dehydratase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Neurotransmitter antagonist
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Antiviral (HIV)
Cystathionine beta-lyase inhibitor
Thiamine pyridinylase inhibitor
Galactose oxidase inhibitor
Corticosteroid side-chain-isomerase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Aconitate decarboxylase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
D-cysteine desulfhydrase inhibitor
Beta-D-fucosidase inhibitor
Dethiobiotin synthase inhibitor
Aryldialkylphosphatase inhibitor
Pyruvate carboxylase inhibitor
3-Methylbutanal reductase inhibitor
Choline dehydrogenase inhibitor
Arginase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Glutamate (mGluR5) agonist
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
CYP2D16 substrate
Calcium channel (voltage-sensitive) activator
Prostaglandin-E2 9-reductase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Catechol oxidase inhibitor
Endopeptidase La inhibitor

GABA transporter 2 inhibitor
Cyanoalanine nitrilase inhibitor
Antiparkinsonian, rigidity relieving
1,2-alpha-L-fucosidase inhibitor
Pancreatic elastase inhibitor
Acidifying agent gastric
Diaminopimelate dehydrogenase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Thiosulfate dehydrogenase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
8-Amino-7-oxononanoate synthase inhibitor
2-Haloacid dehalogenase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Allophanate hydrolase inhibitor
Pin1 inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Smooth muscle myosin light chain kinase inhibitor
Alanine transaminase inhibitor
Prion diseases treatment
Pyridoxal kinase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Glutamine-pyruvate transaminase inhibitor
Acylglycerone-phosphate reductase inhibitor
Histidinol-phosphatase inhibitor
Opine dehydrogenase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
Bisphosphoglycerate mutase inhibitor
5-Aminolevulinate synthase inhibitor
Ketol-acid reductoisomerase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Peptidyl-glycinamidase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Amino-acid N-acetyltransferase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Fumarate reductase (NADH) inhibitor
Hydroxymethylbilane synthase inhibitor
D-amino-acid dehydrogenase inhibitor
Choline kinase inhibitor
Dopamine release stimulant
Arylsulfatase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Corticotropin-like
Leucine transaminase inhibitor
(R)-aminopropanol dehydrogenase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
D-2-hydroxy-acid dehydrogenase inhibitor
[citrate-(pro-3S)-lyase] thiolesterase inhibitor
Aerobactin synthase inhibitor

Hematopoietic
Arginine N-succinyltransferase inhibitor
Homospermidine synthase inhibitor
Tryptophan 2-monooxygenase inhibitor
Chitin deacetylase inhibitor
NMDA receptor polyamine site antagonist
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Chemoprotective
Oligo-1,6-glucosidase inhibitor
Gaucher disease treatment
Antiviral (Picornavirus)
Acetyl-CoA C-acyltransferase inhibitor
Ethanolamine oxidase inhibitor
Glutamate (mGluR6) antagonist
Glucan 1,4-beta-glucosidase inhibitor
Oligopeptidase B inhibitor
Dolichol kinase inhibitor
Steroid synthesis inhibitor
Amino-acid racemase inhibitor
Arginine kinase inhibitor
Antipruritic, non-allergic
Antianorexic
Feruloyl esterase inhibitor
Hydroxylamine reductase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Antihyperammonemic
Urocanate hydratase inhibitor
Dextranucrase inhibitor
Acetoin dehydrogenase inhibitor
Alternansucrase inhibitor
Glutamate dehydrogenase inhibitor
Thiamine-phosphate kinase inhibitor
Arylacetonitrilase inhibitor
Dihydrodipicolinate reductase inhibitor
Pectin lyase inhibitor
Venombin A inhibitor
Antiviral (Poxvirus)
Sorbose dehydrogenase inhibitor
Diphosphate-serine phosphotransferase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Myosin ATPase inhibitor
BRAF expression inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Kynureninase inhibitor
Alpha-N-arabinofuranosidase inhibitor
Deoxyhypusine monooxygenase inhibitor
Isomaltulose synthase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
Flavin-containing monooxygenase substrate
2-Oxoisovalerate dehydrogenase (acylating) inhibitor

4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Cancer procoagulant inhibitor
Formimidoylglutamase inhibitor
Atrolysin A inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
Taurine dehydrogenase inhibitor
Antihypotensive
Phosphofructokinase-1 inhibitor
Valine-tRNA ligase inhibitor
Neuropsin inhibitor
Nitrile hydratase inhibitor
Alpha, alpha-trehalase inhibitor
TNF expression inhibitor
Antibacterial, ophthalmic
Phosphoglycolate phosphatase inhibitor
Antifungal
Mannonate dehydratase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Thiol S-methyltransferase inhibitor
Carboxypeptidase E inhibitor
Homoserine O-succinyltransferase inhibitor
NMDA receptor polyamine site agonist
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Allyl-alcohol dehydrogenase inhibitor
tRNA (adenine-N1-)-methyltransferase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Glutamate formimidoyltransferase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Cycloartenol synthase inhibitor
Cachexia treatment
Rhamnulose-1-phosphate aldolase inhibitor
Maleate isomerase inhibitor
2-Methylcitrate dehydratase inhibitor
Ethanolamine ammonia-lyase inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Homocysteine S-methyltransferase inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
Nicotine dehydrogenase inhibitor
Serine-phosphoethanolamine synthase inhibitor
Somatostatin 2 agonist
Protein-synthesizing GTPase inhibitor
Aspartate 1-decarboxylase inhibitor
Tryptophanamidase inhibitor
Phenylalanine dehydrogenase inhibitor
Linoleate isomerase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Cytochrome-c3 hydrogenase inhibitor

Orotate reductase (NADH) inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Cellulase inhibitor
Glutamate (mGluR8) agonist
Glycine transaminase inhibitor
Propanediol dehydratase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Glyoxylate oxidase inhibitor
Mandelate 4-monooxygenase inhibitor
ATP adenylyltransferase inhibitor
Acetolactate synthase inhibitor
Urethanase inhibitor
Homogentisate 1,2-dioxygenase inhibitor
Ligase inhibitor
Peptidylamidoglycolate lyase inhibitor
Indoleacetaldoxime dehydratase inhibitor
L-iduronidase inhibitor
Picornain 2A inhibitor
Clavamate synthase inhibitor
Oxalate oxidase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Pantoate-beta-alanine ligase inhibitor
6,7-Dihydropteridine reductase inhibitor
Membrane permeability inhibitor
3-Deoxy-7-phosphoheptulonate synthase inhibitor
DELTA14-sterol reductase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Endo-1,3(4)-beta-glucanase inhibitor
Ornithine cyclodeaminase inhibitor
Chenodeoxycholytaurine hydrolase inhibitor
Malyl-CoA lyase inhibitor
Ribonuclease U2 inhibitor
Cerevisin inhibitor
Uterine stimulant
Anthranilate synthase inhibitor
Glycine receptor agonist
2-Hydroxy-3-oxopropionate reductase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Isocitrate dehydrogenase (NAD+) inhibitor
X-Pro dipeptidase inhibitor
Carboxypeptidase U inhibitor
Sulfur dioxygenase inhibitor
Ferrochelataase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Mevalonate kinase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Rhizopuspepsin inhibitor

Estradiol 17alpha-dehydrogenase inhibitor
[phosphorylase] phosphatase inhibitor
L-Serine ammonia-lyase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Thyroxine 5-deiodinase inhibitor
Glycosylceramidase inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Malate dehydrogenase (acceptor) inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
Cysteamine dioxygenase inhibitor
Cyanate hydratase inhibitor
Glutamate (mGluR4) agonist
Astacin inhibitor
Blasticidin-S deaminase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Carboxypeptidase M inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
4-Coumarate-CoA ligase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Iduronate-2-sulfatase inhibitor
Antiinflammatory, intestinal
Hyaluronic acid agonist
Antiviral (Hepatitis)
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Cyclomaltodextrinase inhibitor
Serine-glyoxylate transaminase inhibitor
Glutamate synthase (NADPH) inhibitor
Valine dehydrogenase (NADP+) inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
IgA-specific serine endopeptidase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Antimutagenic
MAP kinase stimulant
Cytosole dipeptidase inhibitor
Glutamate dehydrogenase [NAD(P)+] inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Histone acetyltransferase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Antipruritic
CYP4A substrate
tRNA methyltransferase inhibitor
Ethanolaminephosphotransferase inhibitor
Photosensitizer
Magnesium-protoporphyrin IX methyltransferase inhibitor
Alpha-glucuronidase inhibitor
Glucose 1-dehydrogenase inhibitor
Gly-X carboxypeptidase inhibitor

D-Alanine-poly(phosphoribitol) ligase inhibitor
CYP7 inhibitor
Growth hormone releasing factor agonist
Sulfate adenylyltransferase inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Muconate cycloisomerase inhibitor
Chondroitin 6-sulfotransferase inhibitor
D-lactate dehydrogenase inhibitor
Oxytocic
Vomilenine glucosyltransferase inhibitor
Glutamine synthetase inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
CYP2D15 substrate
Antiviral (Hepatitis C)
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Alanine racemase inhibitor
Membrane dipeptidase inhibitor
Serine protease unspecified inhibitor
Adenylate kinase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
Growth stimulant
Shock treatment
NAD⁺ kinase inhibitor
Diiodophenylpyruvate reductase inhibitor
Spermine antagonist
Levansucrase inhibitor
Uroporphyrinogen-III synthase inhibitor
Deoxyribonuclease X inhibitor
Nitric-oxide synthase inhibitor
Coagulant
Maleylacetoacetate isomerase inhibitor
Porphobilinogen synthase inhibitor
Thioredoxin inhibitor
Pyroglutamyl-peptidase I inhibitor
UGT1A5 substrate
Phosphate acetyltransferase inhibitor
Homocysteine desulfhydrase inhibitor
Proline dehydrogenase inhibitor
Growth hormone release promoting
X-Trp aminopeptidase inhibitor
Threonine ammonia-lyase inhibitor
Polynucleotide adenylyltransferase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Ganglioside galactosyltransferase inhibitor
Theanine hydrolase inhibitor
Pyruvate dehydrogenase inhibitor
Trimerelysin II inhibitor
Releasing hormone agonist
Ribose-5-phosphate-ammonia ligase inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor

Prephenate dehydratase inhibitor
Agaritin gamma-glutamyltransferase inhibitor
Ribonuclease inhibitor
Alcohol O-acetyltransferase inhibitor
Glutamate carboxypeptidase inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
Oryzin inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Hippurate hydrolase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Meprin A inhibitor
GST M substrate
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Loop diuretic
Retinoid X alpha receptor agonist
Uridine nucleosidase inhibitor
Polyamine biosynthesis inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Retinoprotector
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Chelator
2-Enoate reductase inhibitor
Anthrax lethal factor inhibitor
RNA-directed RNA polymerase inhibitor
GlutaminytRNA synthase (glutamine-hydrolysing) inhibitor
Cystinyl aminopeptidase inhibitor
Plasmanylethanolamine desaturase inhibitor
Undecaprenyl-diphosphatase inhibitor
Serine O-acetyltransferase inhibitor
Lysyl oxidase inhibitor
2-Methyleneglutarate mutase inhibitor
Glutamine-fructose-6-phosphate transaminase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Benzoylformate decarboxylase inhibitor
ATP deaminase inhibitor
Sphingosine 1-phosphate receptor antagonist
Rhodopsin kinase inhibitor
Phenylacetate-CoA ligase inhibitor
CYP2E1 substrate
D(-)-tartrate dehydratase inhibitor
Thiosulfate sulfurtransferase inhibitor
tRNA (uracil-5-)-methyltransferase inhibitor
ATP phosphoribosyltransferase inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Tyrosine transaminase inhibitor
Acylphosphatase inhibitor

CYP4B substrate
L-amino-acid oxidase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
HDL-cholesterol increasing
Diabetic nephropathy treatment
EIF4E expression inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Adenylate cyclase stimulant
Spermidine synthase inhibitor
Aspartate 4-decarboxylase inhibitor
Argininosuccinate synthase inhibitor
N-acylmannosamine kinase inhibitor
Homoserine kinase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
Antibacterial
D-lactate-2-sulfatase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Chloride peroxidase inhibitor
IgA-specific metalloendopeptidase inhibitor
Proline racemase inhibitor
Propionate-CoA ligase inhibitor
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
L-glucuronate reductase inhibitor
2-Nitropropane dioxygenase inhibitor
Deoxyhypusine synthase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Malate dehydrogenase (NADP+) inhibitor
Laccase inhibitor
Isocitrate lyase inhibitor
Sickle-cell anemia treatment
D-malate dehydrogenase (decarboxylating) inhibitor
Nicotinate dehydrogenase inhibitor
Aldehyde dehydrogenase (NADP+) inhibitor
Ribitol 2-dehydrogenase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Hemostatic
Nucleotidase inhibitor
Mucolytic
5 Hydroxytryptamine 7L antagonist
Antiacromegalic
Poly(ADP-ribose) glycohydrolase inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
CYP2E substrate
CMP-KDO synthase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Asparagine-oxo-acid transaminase inhibitor
Peroxidase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
Methylaspartate ammonia-lyase inhibitor

Alkane 1-monooxygenase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
Lysase inhibitor
Dolichyl-phosphatase inhibitor
FMO1 substrate
4-Nitrophenol 2-monooxygenase inhibitor
Cell wall synthesis inhibitor
Pim-2 kinase inhibitor
Dimethylhistidine N-methyltransferase inhibitor
Acetate kinase inhibitor
Paget's disease treatment
Mannosyl-oligosaccharide 1,2- α -mannosidase inhibitor
Rhodotorulapepsin inhibitor
CYP2E1 inducer
Deoxyribose-phosphate aldolase inhibitor
Diaminopimelate decarboxylase inhibitor
Magnolysin inhibitor
Neurolysin inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Spermine synthase inhibitor
Glutamate (mGluR1) agonist
Dehydro-L-gulonate decarboxylase inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Leukopoiesis inhibitor
UGT2B28 substrate
Glycogen (starch) synthase inhibitor
Adamalysin inhibitor
GST T substrate
GST T1-1 substrate
Glucan 1,4- α -glucosidase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Methylaspartate mutase inhibitor
CYP4F substrate
Anthranilate 3-monooxygenase (deaminating) inhibitor
Lactose synthase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Methylglutamate dehydrogenase inhibitor
Signal peptidase I inhibitor
Penicillopepsin inhibitor
Sarcosine oxidase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Bombesin agonist
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Antiviral (Influenza A)
Cerebroside-sulfatase inhibitor
2-Ethylmalate synthase inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Glutamate dehydrogenase (NADP⁺) inhibitor

Antidote, heavy metal
3-Oxoacid CoA-transferase inhibitor
L-ascorbate peroxidase inhibitor
Phosphoribulokinase inhibitor
Farnesyltransferase inhibitor
Alpha-L-fucosidase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
5 Hydroxytryptamine 7S antagonist
Lipoxygenase substrate
Inorganic diphosphatase inhibitor
Atrolysin C inhibitor
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Glutamate (mGluR3) agonist
Glutathione thiolesterase inhibitor
Picornain 3C inhibitor
Antialcoholic
Cysteine-tRNA ligase inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Choloylglycine hydrolase inhibitor
Anthranilate-CoA ligase inhibitor
Linoleate diol synthase inhibitor
Succinate dehydrogenase inhibitor
Acyl-CoA oxidase inhibitor
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor
Retinal dehydrogenase inhibitor
Lactate-malate transhydrogenase inhibitor
5 Hydroxytryptamine release stimulant
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor
Lysine-tRNA ligase inhibitor
Aldose reductase substrate
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Aspergillopepsin I inhibitor
Arabinogalactan endo-1,4-beta-galactosidase inhibitor
Cholate-CoA ligase inhibitor
Antithyroid
Lombricine kinase inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
Leucyltransferase inhibitor
Histamine agonist
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Renal failure treatment
3-Deoxy-8-phosphooctulonate synthase inhibitor
Phosphoserine transaminase inhibitor
Alpha-L-rhamnosidase inhibitor
Carboxypeptidase B inhibitor
Strombine dehydrogenase inhibitor

L-lactate dehydrogenase (cytochrome) inhibitor
Succinic dehydrogenase inhibitor
L-fuconate dehydratase inhibitor
Cutinase inhibitor
Phosphoglycerate dehydrogenase inhibitor
Neurotensin 1 receptor agonist
GABA B receptor antagonist
Antiprotozoal (Coccidial)
GABA C receptor antagonist
Oxaloacetate decarboxylase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Mannosyl-oligosaccharide glucosidase inhibitor
Osmotic diuretic
Tartrate decarboxylase inhibitor
Gentisate 1,2-dioxygenase inhibitor
Opioid kappa 3 receptor antagonist
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Hydroxylamine reductase (NADH) inhibitor
Melanocortin MC-4 agonist
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Benzoate 4-monooxygenase inhibitor
Alanine dehydrogenase inhibitor
Aromatic-amino-acid transaminase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Bombesin 3 receptor agonist
Streptopain inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Penicillin amidase inhibitor
Laminaribiose phosphorylase inhibitor
Cyclooxygenase 1 substrate
Methylthioadenosine nucleosidase inhibitor
Glutamate uptake inhibitor
Sepiapterin reductase inhibitor
Glycerol dehydratase inhibitor
Phosphoglycerate phosphatase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Malate-CoA ligase inhibitor
Acid phosphatase inhibitor
Assemblin inhibitor
3-Dehydroquinase synthase inhibitor
Endopeptidase inhibitor
Glutamate (mGluR group III) antagonist
Amylosucrase inhibitor
Sweetener
Thiamine-phosphate diphosphorylase inhibitor
Oxaloacetate tautomerase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Pseudouridylate synthase inhibitor

Propionate CoA-transferase inhibitor
Glucan 1,3-beta-glucosidase inhibitor
Ethanolamine kinase inhibitor
4-Hydroxy-2-oxoglutarate aldolase inhibitor
Glycine N-acyltransferase inhibitor
Beta galactosidase inhibitor
Fumarylacetoacetase inhibitor
6-Phosphofructo-2-kinase inhibitor
Bilirubin oxidase inhibitor
Arginine-tRNA ligase inhibitor
Neurotensin 1 receptor antagonist
Malate dehydrogenase inhibitor
Diaminopimelate epimerase inhibitor
Iodide peroxidase inhibitor
Adenylylsulphatase inhibitor
Aspartyl aminopeptidase inhibitor
Antipruritic, allergic
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Stromelysin 2 inhibitor
Antiulcerative
Glutathione synthase inhibitor
Sucrose alpha-glucosidase inhibitor
Maltose-transporting ATPase inhibitor
Kainate receptor 1 agonist
Thioether S-methyltransferase inhibitor
N-formylglutamate deformylase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Lysine carboxypeptidase inhibitor
Octadecanal decarbonylase inhibitor
Phosphoribosylformylglycinamide synthase inhibitor
Alpha-mannosidase inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
DNA methyltransferase I inhibitor
Acetolactate decarboxylase inhibitor
DNA synthesis inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Triose-phosphate isomerase inhibitor
Sphingosine 1-phosphate receptor 5 agonist
Melanocortin agonist
Ferredoxin-nitrite reductase inhibitor
Monoamine oxidase substrate
Mycolysin inhibitor
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Tyrosine 2,3-aminomutase inhibitor
Aminopeptidase I inhibitor
tRNA-pseudouridine synthase I inhibitor
SMN2 expression enhancer

2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Alcohol dehydrogenase inhibitor
Prolyl aminopeptidase inhibitor
Cysteine dioxygenase inhibitor
Lactamase C inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
Pectate lyase inhibitor
Linoleoyl-CoA desaturase inhibitor
Glycine N-methyltransferase inhibitor
Dopachrome isomerase inhibitor
Expectorant
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Ribonucleoside triphosphate reductase inhibitor
CYP4F12 substrate
Urolithiasis treatment
Glutamate (mGluR group I) agonist
CYP26A substrate
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Lysosomal Pro-X carboxypeptidase inhibitor
CYP2C2 substrate
3-Hydroxybutyrate dehydrogenase inhibitor
Albendazole monooxygenase inhibitor
Tubulin-tyrosine ligase inhibitor
Adenylyl-sulfate kinase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
Beta-amylase inhibitor
Acyloxyacyl hydrolase inhibitor
Glutamate (mGluR1a) agonist
Glutamate (mGluR5a) agonist
Cathepsin F inhibitor
Tyrosine kinase stimulant
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
TRPA1 agonist
Carnitine O-octanoyltransferase inhibitor
Vasoprotector
Aminoacyl-tRNA synthetase inhibitor
Diphosphomevalonate decarboxylase inhibitor
NMDA receptor agonist
Neurotensin receptor antagonist
Carbon-monoxide dehydrogenase inhibitor
Allantoinase inhibitor
Glycine N-benzoyltransferase inhibitor
Antihematotoxic
NADH dehydrogenase inhibitor
Acetoacetate decarboxylase inhibitor
Alanine carboxypeptidase inhibitor
Formaldehyde dehydrogenase inhibitor
CYP2C9 inducer
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor

Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor
Kinesin antagonist
Kinesin-like protein 1 inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Nucleoside-diphosphatase inhibitor
Nicotinamidase inhibitor
Biliary tract disorders treatment
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor
2-(acetamidomethylene)succinate hydrolase inhibitor
Mannosidase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Betaine-aldehyde dehydrogenase inhibitor
NAD(P)+ transhydrogenase (B-specific) inhibitor
Tryptophan synthase inhibitor
Homoserine O-acetyltransferase inhibitor
Beta-glucosidase inhibitor
Altronate dehydratase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Anesthetic inhalation
Antineoplastic, alkylator
Luteinizing hormone-releasing hormone agonist
SULT2A1 substrate
Pyridoxamine-oxaloacetate transaminase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Valine-pyruvate transaminase inhibitor
Glutamate (mGluR8) antagonist
Metabolic disease treatment
Antiviral (CMV)
Malate dehydrogenase (decarboxylating) inhibitor
CYP2B18 substrate
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Transactivator transcription protein inhibitor
DNA methylase inhibitor
Granzyme A inhibitor
Centromere associated protein inhibitor
3-Dehydroquinate dehydratase inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
Mucomembranous protector
Lactaldehyde reductase inhibitor
CPB protease inhibitor
S-methyl-5-thioribose kinase inhibitor
Thiamine-triphosphatase inhibitor
Glucuronolactone reductase inhibitor
Lanosterol 14 alpha demethylase inhibitor
Malate synthase inhibitor
Na+-transporting two-sector ATPase inhibitor
Protein-glutamate O-methyltransferase inhibitor

UDP-N-acetylglucosamine diphosphorylase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Aldehyde dehydrogenase inhibitor
Endo-1,4-beta-xylanase inhibitor
Hepatocyte nuclear factor 4 alpha agonist
Hepatocyte nuclear factor agonist
Isocitrate dehydrogenase (NADP+) inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
Cellobiose phosphorylase inhibitor
Nitric oxide scavenger
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
Sucrose-phosphate phosphatase inhibitor
Arachidonate-CoA ligase inhibitor
Phenylalanine 2-monooxygenase inhibitor
Glutathione S-transferase inhibitor
2-Aminohexanoate transaminase inhibitor
Protein synthesis stimulant
2-Isopropylmalate synthase inhibitor
Secretase beta 1 inhibitor
Aspartate carbamoyltransferase inhibitor
CMP-N-acylneuraminate phosphodiesterase inhibitor
Arylamine N-Acetyltransferase substrate
Camphor 1,2-monooxygenase inhibitor
Phosphoglucomutase inhibitor
L(+)-Tartrate dehydratase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
CYP4A1 substrate
Amine dehydrogenase inhibitor
Pyruvate kinase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
Phosphatidate cytidyltransferase inhibitor
Inositol oxygenase inhibitor
Inositol-3-phosphate synthase inhibitor
Antileprosy
Phosphoglycerate mutase inhibitor
Lymphocytopoiesis inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Glycerol dehydrogenase (NADP+) inhibitor
Carbonic anhydrase XIV inhibitor
Beta-N-acetylgalactosaminidase inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor
Transaldolase inhibitor
Homoisocitrate dehydrogenase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Corneal wound healing stimulator

Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Choline sulfotransferase inhibitor
Periodontitis treatment
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Thymidine-triphosphatase inhibitor
Citrate (Si)-synthase inhibitor
Purine biosynthesis inhibitor
MAO B substrate
Nucleoside phosphoacylhydrolase inhibitor
Secretase beta inhibitor
Thromboxane synthase stimulant
Polyphosphate kinase inhibitor
Beta-fructofuranosidase inhibitor
Tryptophan 5 hydroxylase inhibitor
CTP synthase inhibitor
Gentamicin 3'-N-acetyltransferase inhibitor
1-Alkyl-2-acetyl glycerol O-acyltransferase inhibitor
tRNA adenylyltransferase inhibitor
Antihypertriglyceridemic
Creatine kinase inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Chelator, Iron
Formate-dihydrofolate ligase inhibitor
CYP4B1 substrate
Glyceryl-ether monooxygenase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Galactokinase inhibitor
Trimethylamine dehydrogenase inhibitor
Glucosyl transferase inhibitor
Decylcitrate synthase inhibitor
Long-chain-fatty-acid-CoA ligase inhibitor
D-stereospecific aminopeptidase inhibitor
Pyruvate, water dikinase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Gamma-glutamyl hydrolase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Adenylosuccinate lyase inhibitor
Cathepsin D inhibitor
D-aspartate oxidase inhibitor
Candidapepsin inhibitor
Ribose-5-phosphate isomerase inhibitor
Vascular dementia treatment
Haloalkane dehalogenase inhibitor
Sphingosine 1-phosphate receptor 5 antagonist
N-acetylmuramoyl-L-alanine amidase inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Nucleotide diphosphatase inhibitor
Dipeptidyl peptidase II inhibitor

Anthranilate phosphoribosyltransferase inhibitor
Glucose-1-phosphatase inhibitor
Phosphopyruvate hydratase inhibitor
Guanylate kinase inhibitor
Tartrate dehydrogenase inhibitor
Alkylglycerone-phosphate synthase inhibitor
Small monomeric GTPase inhibitor
Phosphorylase kinase inhibitor
Tropinesterase inhibitor
Hypercalcemia treatment
[Isocitrate dehydrogenase (NADP+)] kinase inhibitor
Adenylosuccinate synthase inhibitor
Aconitate hydratase inhibitor
Nitrate reductase (cytochrome) inhibitor
Procollagen galactosyltransferase inhibitor
Adrenergic, ophthalmic
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD+) inhibitor
Tryptophan-tRNA ligase inhibitor
Retinoic acid metabolism inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Subtilisin inhibitor
Glutamate (mGluR group II) antagonist
Carboxy-cis,cis-muconate cyclase inhibitor
Ca²⁺-transporting ATPase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Fumarate hydratase inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
Hydroxypyruvate reductase inhibitor
CYP2C18 substrate
N-acetylneuraminate lyase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
Serine-tRNA ligase inhibitor
CYP26 substrate
Stipitatonate decarboxylase inhibitor
Protein N-acetylglucosaminyltransferase inhibitor
Carboxycyclohexadienyl dehydratase inhibitor
Kainate receptor agonist
Membrane-oligosaccharide glycerophosphotransferase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
Ceramidase inhibitor
Antibiotic Aminoglycoside-like
Phloroglucinol reductase inhibitor
CYP4F8 substrate
Retinoid X beta receptor antagonist
UDP-sugar diphosphatase inhibitor
Lactamase A inhibitor
GRP78 expression inhibitor

Glycine N-choloyltransferase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
D-arabinonolactone oxidase inhibitor
Dipeptidyl peptidase I inhibitor
UGT1A1 substrate
Growth hormone release inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
NF-E2-related factor 2 stimulant
Nucleotide metabolism regulator
L-galactonolactone oxidase inhibitor
Antineoplastic
Granzyme B inhibitor
Trans-pentaprenyltranstransferase inhibitor
Somatostatin agonist
Ferredoxin-NADP⁺ reductase inhibitor
Dihydrofolate synthase inhibitor
Carbonic anhydrase stimulant
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Phosphoketolase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Sphingosine 1-phosphate receptor 3 antagonist
Galactoside O-acetyltransferase inhibitor
Diacylglycerol kinase inhibitor
Glucose-1,6-bisphosphate synthase inhibitor
Amino acid-polyamine-organocation (APC) transporter antagonist
Nucleoside deoxyribosyltransferase inhibitor
Shikimate 5-dehydrogenase inhibitor
Glutamate (mGluR3) antagonist
Cyclopentanone monooxygenase inhibitor
Histone-arginine N-methyltransferase inhibitor
Dementia treatment
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
Aryl hydrocarbon receptor agonist
NMN nucleosidase inhibitor
CYP19A1 expression inhibitor
Cholesterol antagonist
Neurotensin receptor agonist
Bacterial leucyl aminopeptidase inhibitor
Pyruvate, phosphate dikinase inhibitor
Retinoid X receptor agonist
HIV-2 reverse transcriptase inhibitor
Beta-cyclopiazotate dehydrogenase inhibitor
Phenol 2-monooxygenase inhibitor
Iron antagonist
N-acetylglucosaminyldiphosphodolichol N-acetylglucosaminyltransferase inhibitor
MAO A substrate

NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
Hydroxyquinol 1,2-dioxygenase inhibitor
Glutathionylspermidine synthase inhibitor
Aldehyde dehydrogenase 1A2 inhibitor
Leishmanolysin inhibitor
Glutamate (mGluR6) agonist
5-Guanidino-2-oxopentanoate decarboxylase inhibitor
Aryl-aldehyde dehydrogenase (NADP⁺) inhibitor
2-Methylcitrate synthase inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Aminopeptidase N inhibitor
Adrenaline release stimulant
N-carbamoyl-L-amino-acid hydrolase inhibitor
[Skp1-protein]-hydroxyproline N-acetylglucosaminyltransferase inhibitor
Phosphoenolpyruvate carboxykinase (GTP) inhibitor
UGT2B10 substrate
Bacillus subtilis ribonuclease inhibitor
Secretase beta 2 inhibitor
Alpha, alpha-phosphotrehalase inhibitor
Xylan 1,4-beta-xylosidase inhibitor
Pyrroline-5-carboxylate reductase inhibitor
Antiviral (Hepatitis B)
Aryl-acylamidase inhibitor
Pantoate 4-dehydrogenase inhibitor
Proliferative diseases treatment
NAD⁺ diphosphatase inhibitor
8-oxodGTPase stimulant
Aspartyl protease inhibitor
Vibriolysin inhibitor
Bis(5'-nucleosyl)-tetraphosphatase (symmetrical) inhibitor
Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor
Antiinflammatory, ophthalmic
Aralkylamine N-acetyltransferase inhibitor
Glutamate (mGluR group III) agonist
Formate dehydrogenase inhibitor
[glutamate-ammonia-ligase] adenylyltransferase inhibitor
Serine-sulfate ammonia-lyase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Astringent
Mycodextranase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Anticataract
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Phospholipase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Serine carboxypeptidase inhibitor
3-Mercaptopyruvate sulfurtransferase inhibitor
1-Phosphofructokinase inhibitor
Folylpolyglutamate synthase inhibitor
Proteasome endopeptidase complex inhibitor

Streptomycin 6-kinase inhibitor
Hyponitrite reductase inhibitor
Cyclohexadienyl dehydrogenase inhibitor
dCTP deaminase inhibitor
Aspartate racemase inhibitor
Butyrate-CoA ligase inhibitor
CYP2A4 substrate
tRNA (guanine-N7-)-methyltransferase inhibitor
N-Acetylated alpha-linked acidic dipeptidase inhibitor
Aminopeptidase microsomal inhibitor
Protein 30S ribosomal subunit inhibitor
Adenylate cyclase inhibitor
Biliverdin reductase inhibitor
Formate C-acetyltransferase inhibitor
Sodium channel blocker class Ib
AMP nucleosidase inhibitor
Amyloid beta aggregation inhibitor
Thromboxane B2 antagonist
Dopamine precursors
Complement C5a convertase stimulant
Complement stimulant
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Glycogenin glucosyltransferase inhibitor

Erlotinib hydrochloride

Molecular Mechanism (initial) :

epidermal growth factor receptor (EGFR) inhibitor

Molecular Mechanism (repurposed) :

epidermal growth factor receptor (EGFR) inhibitor

initial indication(s):

non-small cell lung cancer

Repurposed indication(s):

pancreatic and pancreatic metastatic cancer

ependymoma

mouth cancer

head and neck cancer

Predicted Activities

Endothelial growth factor antagonist

ErbB-1 antagonist

Epidermal growth factor receptor kinase inhibitor

Tyrosine kinase inhibitor

Signal transduction pathways inhibitor

Antineoplastic

Growth factor antagonist

Antineoplastic (solid tumors)

ErbB antagonist

Protein kinase inhibitor

ErbB-2 antagonist

Vascular endothelial growth factor antagonist

Vascular endothelial growth factor 2 antagonist
Angiogenesis inhibitor
MAP kinase kinase inhibitor
Platelet aggregation inhibitor
Vanilloid 1 agonist
Antipsoriatic
Antineoplastic (carcinoma)
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Antineoplastic (gastric cancer)
RET inhibitor
Epidermal growth factor antagonist
Antineoplastic (bladder cancer)

Antineoplastic (pancreatic cancer)

Protein-serine-threonine kinase inhibitor
Antineoplastic (squamous cell carcinoma)
5 Hydroxytryptamine release inhibitor
Src kinase inhibitor
Aldehyde oxidase substrate
ErbB-4 antagonist
Aldehyde oxidase inhibitor
Vascular endothelial growth factor 3 antagonist
Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor
Dihydropyrimidine dehydrogenase inhibitor
Abl kinase inhibitor
Platelet activating factor beta antagonist
Undecaprenyl-phosphate mannosyltransferase inhibitor
Antineoplastic (small cell lung cancer)
Platelet activating factor antagonist
Antineoplastic (breast cancer)
Restenosis treatment
Antineoplastic (lymphocytic leukemia)
Lck kinase inhibitor
Janus tyrosine kinase 2 inhibitor
Wound healing agent
Tyrosine-protein kinase receptor FLT3 inhibitor
Fibroblast growth factor 2 antagonist
Vanilloid agonist
Vascular endothelial growth factor 1 antagonist
TIE antagonist
TIE-2 antagonist
Antineoplastic (liver cancer)
Gestagen antagonist
CDK2/cyclin A inhibitor
Catenin beta inhibitor
Transplant rejection treatment
c-Src kinase inhibitor
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
Aurora-B kinase inhibitor
Antiinflammatory, ophthalmic
Protein-tyrosine kinase Lyn inhibitor

CDK9/cyclin T1 inhibitor
Antineoplastic (brain cancer)
Growth factor agonist
Platelet growth factor antagonist
Dermatologic
Antineoplastic (multiple myeloma)
Antimitotic
Pulmonary hypertension treatment
SULT1E1 substrate
Antineoplastic (sarcoma)
Antineoplastic (cervical cancer)
Protein-tyrosine kinase p55(blk) inhibitor
Janus tyrosine kinase inhibitor
Antileukemic
Ephrin antagonist
Preneoplastic conditions treatment
ALK inhibitor
Adenosine regulator
Gastritis treatment
Bcr-Abl kinase inhibitor
Protein kinase (CK2) inhibitor
Proto-oncogene tyrosine-protein kinase Kit inhibitor
Dihydroorotase inhibitor
MAP kinase kinase 1 inhibitor
Glutamate (mGluR1) antagonist
Antineoplastic (non-small cell lung cancer)
Antiviral (Hepatitis B)
CYP1A2 inhibitor
CC chemokine 4 receptor antagonist
Antineoplastic antimetabolite
Transcription factor NF kappa A inhibitor
Channel-conductance-controlling ATPase inhibitor
CYP1A2 substrate
Glutamate (mGluR group I) antagonist
Fructose-1,6-bisphosphatase inhibitor
Insulin antagonist
Janus tyrosine kinase 1 inhibitor
Fibroblast growth factor antagonist
Serum-glucocorticoid regulated kinase 1 inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
Mediator release inhibitor
CYP1A inhibitor
Aurora kinase inhibitor
Cyclic GMP phosphodiesterase inhibitor
Dyrk kinase inhibitor
Antiprotozoal (Coccidial)
Pim-1 kinase inhibitor
Immunosuppressant
Insulin like growth factor 1 antagonist
Fibroblast growth factor 3 antagonist

Inosine nucleosidase inhibitor
Antineoplastic (colorectal cancer)
Bruton tyrosine kinase inhibitor
Cyclin-dependent kinase 6 inhibitor
Platelet derived growth factor receptor kinase inhibitor
Insulin growth factor antagonist
Focal adhesion kinase 1 inhibitor
Retinopathy treatment
Antineoplastic (non-Hodgkin's lymphoma)
Purinergic P2X3 antagonist
Glutamate (mGluR5) antagonist
Janus tyrosine kinase 3 inhibitor
EphB4 antagonist
Inotropic
Antieczematic
Aurora-C kinase inhibitor
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
RNA directed DNA polymerase inhibitor
Platelet activating factor alpha antagonist
DNA directed DNA polymerase inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Bone diseases treatment
Phosphodiesterase VII inhibitor
MAP-kinase-activated kinase inhibitor
Anticarcinogenic
Antiischemic
Formate-dihydrofolate ligase inhibitor
MAP-kinase-activated kinase 2 inhibitor
Antineoplastic (glioblastoma multiforme)
Purinergic P2X2 antagonist
Aurora-A kinase inhibitor
Apoptosis agonist
Antineoplastic (lung cancer)
Phosphodiesterase II inhibitor
Fibroblast growth factor 1 antagonist
MAP kinase 8 inhibitor
Glyceraldehyde-3-phosphate dehydrogenase inhibitor
Antineoplastic (renal cancer)
NAD⁺-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
H⁺/K⁺-transporting ATPase inhibitor
Glutamate (mGluR) antagonist
Antineoplastic (colon cancer)
Fibrosis treatment
DNA directed RNA polymerase inhibitor
Adenosine A2a receptor antagonist
CDK/Cyclin complex inhibitor
Interleukin 8 antagonist
ZAP-70 protein tyrosine kinase inhibitor
CYP3A4 substrate
CYP1A1 substrate

Serum-glucocorticoid regulated kinase inhibitor
Adenosine receptor antagonist
Cyclin-dependent kinase 1 inhibitor
Hepatocyte growth factor antagonist
p21-activated kinase inhibitor
Pim kinase inhibitor
Guanylate cyclase 1 stimulant
Phosphodiesterase V inhibitor
Focal adhesion kinase 2 inhibitor
Polo-like kinase inhibitor
Potassium channel small-conductance Ca-activated activator
Histone-lysine N-methyltransferase inhibitor
Platelet growth factor beta antagonist
Phosphodiesterase I inhibitor
DNA directed RNA polymerase stimulant
Protein kinase (Mos, Mil/Raf, MEKK, RIPK, TESK, LIMK, IRAK, ILK, Activin/TGF-beta) inhibitor
Phosphodiesterase inhibitor
Ribosomal protein S6 kinase 1, 70-kDa inhibitor
Raf kinase inhibitor
Antineoplastic (thyroid cancer)
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Phosphatidylinositol 3-kinase delta inhibitor
Parathyroid hormone secretion stimulant
Endoglycosylceramidase inhibitor
NADPH oxidase inhibitor
Lysine-tRNA ligase inhibitor
Acetylcholine M2 receptor agonist
Cyclin-dependent kinase 9 inhibitor
TEC kinase inhibitor
Retinol dehydrogenase inhibitor
Raf kinase B inhibitor
GABA A receptor agonist
Focal adhesion kinase inhibitor
TRKB antagonist
Estrogen-related receptor alpha antagonist
Ferredoxin hydrogenase inhibitor
Adenosine A2 receptor antagonist
Ribosomal protein S6 kinase, 70-kDa inhibitor
ACK1 kinase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Female sexual dysfunction treatment
Hepatocyte growth factor agonist
Colony stimulating factor antagonist
Vanilloid antagonist
Antiosteoporotic
DNA polymerase III inhibitor
T cell inhibitor
H⁺-transporting two-sector ATPase inhibitor
MDM2 inhibitor
Threonine-tRNA ligase inhibitor

Cyclic AMP agonist
Vanilloid 1 antagonist
Phosphodiesterase 1B inhibitor
Transforming growth factor beta 3 antagonist
Tubulin antagonist
p21-activated kinase 1 inhibitor
Guanine deaminase inhibitor
Myocardial ischemia treatment
Raf kinase C inhibitor
Transforming growth factor antagonist
Apyrase inhibitor
Adenosine receptor agonist

Everolimus

Molecular Mechanism (initial) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

Molecular Mechanism (repurposed) :

**FK506-binding protein 12 inhibitor
mTOR inhibitor**

initial indication(s):

transplant rejection

Repurposed indication(s):

cancers

Predicted Activities

CYP3A4 substrate

Peptidyl-prolyl cis-trans isomerase inhibitor (FK506-binding protein 12 inhibitorFK506-binding protein 12 inhibitor)

Immunosuppressant

CYP3A substrate

HIF1A expression inhibitor

Antifungal

Antieczematic

Proliferative diseases treatment

Antidote

Anticarcinogenic

P-glycoprotein substrate

Immunomodulator

Antineoplastic (non-Hodgkin's lymphoma)

T cell inhibitor

Antibacterial

CYP3A5 substrate

Restenosis treatment

Antineoplastic (multiple myeloma)

Antipruritic

Antibiotic

Antineoplastic

Antipruritic, allergic

CYP2H substrate

Phosphatase inhibitor
CYP3A3 substrate
Systemic lupus erythematosus treatment
Antineoplastic (small cell lung cancer)

mTOR inhibitor

Interleukin 2 antagonist
Interleukin 2 agonist

Antineoplastic (pancreatic cancer)
Antineoplastic (sarcoma)
Antineoplastic (bladder cancer)

Antipsoriatic
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
H⁺-transporting two-sector ATPase inhibitor

Antineoplastic (brain cancer)

General pump inhibitor

Antineoplastic (solid tumors)

Antimitotic
CYP3A2 substrate
Dermatologic
Macular degeneration treatment

Antineoplastic (renal cancer)

Antineoplastic (endocrine cancer)

Antimetastatic
Protein synthesis inhibitor
Neurotrophic factor
CYP2C8 substrate
Transplant rejection treatment

Antineoplastic (thyroid cancer)

Antineoplastic (breast cancer)

Interleukin 10 antagonist
Rotamase (FKBP12) inhibitor
Antiviral (Rhinovirus)
Interleukin antagonist

Antineoplastic (liver cancer)

Ribosomal protein S6 kinase inhibitor
Membrane permeability enhancer

Antineoplastic (non-small cell lung cancer)

Antineoplastic (bone cancer)
Antineoplastic (melanoma)

Cytokine release inhibitor
Prostate cancer treatment
Antiinflammatory
Antimycoplasmal
Antidiabetic symptomatic
Acute neurologic disorders treatment

Antineoplastic (lymphoma)

Antineoplastic (glioblastoma multiforme)

Antineoplastic (ovarian cancer)

APOA1 expression enhancer
Multiple sclerosis treatment

Antineoplastic (glioma)
Rotamase (FKBP) inhibitor
ATPase inhibitor
Antineoplastic (lung cancer)
Ribosomal protein S6 kinase, 70-kDa inhibitor
CYP2A substrate
Apoptosis agonist
Alcohol O-acetyltransferase inhibitor
Antineoplastic (gastric cancer)
Glyceryl-ether monooxygenase inhibitor
Antineoplastic (uterine cancer)
Antieczematic atopic
Dry eye syndrome treatment
Diabetic retinopathy treatment
Endoglycosylceramidase inhibitor
ATPase stimulant
Interleukin 5 antagonist
Antineoplastic antibiotic
Undecaprenyl-phosphate mannosyltransferase inhibitor
Interferon antagonist
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Myc inhibitor
CYP2B6 substrate
CYP2C substrate
Interleukin agonist
Thyroxine 5-deiodinase inhibitor
Interleukin 8 antagonist
CYP2C19 inducer
Antineoplastic (colorectal cancer)
Myosin-light-chain-phosphatase inhibitor
Retinol dehydrogenase inhibitor
Reductase inhibitor
Interferon gamma antagonist
Ophthalmic drug
P-glycoprotein inhibitor
Sucrose-phosphate synthase inhibitor
Chloride channel blocker
Microtubule formation inhibitor
Calcineurin inhibitor
Calcium regulator
CYP2D1 substrate
Autoimmune disorders treatment
Antiparasitic
Actin depolymerization stimulant
Phospholipase A1 inhibitor
Rheumatoid arthritis treatment
Protein 50S ribosomal subunit inhibitor
Interleukin 4 antagonist
Ceramide glucosyltransferase inhibitor
Antineoplastic (squamous cell carcinoma)

Antitreponemal
Growth stimulant
Antineoplastic (colon cancer)
Protein kinase C stimulant
Glycine receptor agonist
CYP2A6 substrate
Peptidyltransferase inhibitor
Antibiotic Macrolide-like
GDP-mannose 6-dehydrogenase inhibitor
Antineoplastic (carcinoma)
CYP3A4 inhibitor
Polarisation stimulant
Polyribonucleotide nucleotidyltransferase inhibitor
Antihelminthic
Bilirubin oxidase inhibitor
Osteoclast antagonist
Antifungal enhancer
Microtubule stabilization
UGT2B18 substrate
CYP1A1 substrate
Nitric oxide donor
Angiogenesis stimulant
Methylglutamate dehydrogenase inhibitor
Galactosylceramidase inhibitor
1,3-Beta-glucan synthase inhibitor
HMG CoA synthase inhibitor
Protein 30S ribosomal subunit inhibitor
Prostaglandin D2 agonist
[phosphorylase] phosphatase inhibitor
Protein phosphatase 2A inhibitor
HMG CoA reductase inhibitor
Trans-octaprenyltranstransferase inhibitor
Sterol 24-C-methyltransferase inhibitor
CYP2C9 substrate
Levansucrase inhibitor
ATPase (Mitochondrial F1F0) inhibitor
Antiacne

Finasteride

Molecular Mechanism (initial) :

steroid 5alpha reductase inhibitor

androgen receptor antagonist

Molecular Mechanism (repurposed) :

steroid 5alpha reductase inhibitor

androgen receptor antagonist

initial indication(s):

benign prostatic hyperplasia

Repurposed indication(s):

hair loss

Predicted Activities

Prostate disorders treatment

Prostatic (benign) hyperplasia treatment

Antiacne

Dermatologic

Androgen antagonist

5-Alpha-reductase inhibitor

5-Alpha-reductase 2 inhibitor

CYP2C substrate

Hair growth stimulant

5-Alpha-reductase 1 inhibitor

CYP2B substrate

CYP3A4 substrate

CYP3A substrate

Antiosteoporotic

Testosterone agonist

Bone diseases treatment

Testosterone 17beta-dehydrogenase (NADP+) inhibitor

CYP2J substrate

CYP2J2 substrate

Membrane permeability inhibitor

Alkylacetylglucophosphatase inhibitor

Phosphatase inhibitor

Erythropoiesis stimulant

CYP17 inhibitor

Spasmolytic, urinary

Proteasome ATPase inhibitor

Antieczematic

CYP3A2 substrate

Male reproductive dysfunction treatment

CYP2A1 substrate

Gestagen antagonist

Menopausal disorders treatment

Acetylcholine neuromuscular blocking agent

Antipruritic

Glycerol-ether monooxygenase inhibitor

Protein-disulfide reductase (glutathione) inhibitor

Acylcarnitine hydrolase inhibitor

Antiinfertility, female

P-glycoprotein substrate

CYP2C11 substrate

Contraceptive

DELTA14-sterol reductase inhibitor

Retinoprotector

CYP7 inhibitor

CYP2C9 inducer

Transcription factor NF kappa B stimulant

Transcription factor stimulant

Antinociceptive

Uterine relaxant

Myc inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
CYP2C12 substrate
Ovulation inhibitor
Vasoprotector
CYP2C19 inducer
Acetylgalactosaminy-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
CYP2C19 substrate
Membrane integrity antagonist
CYP3A4 inducer
Antipruritic, allergic
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Aldosterone antagonist
CYP2A11 substrate
Morphine 6-dehydrogenase inhibitor
CYP3A inducer
CYP3A5 substrate
General pump inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Oxytocic
Adenomatous polyposis treatment
Growth stimulant
Peptidoglycan glycosyltransferase inhibitor
CYP2C8 inducer
Transactivator transcription protein inhibitor
CYP2C6 substrate
Muscular dystrophy treatment
Calcium regulator
Diuretic
Lipocortins synthesis antagonist
CYP2C9 substrate
Interleukin 2 agonist
Bilirubin oxidase inhibitor
Respiratory analeptic
RELA expression inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
CYP3A1 substrate
Bile-salt sulfotransferase inhibitor
CYP2A5 substrate
Cycloartenol synthase inhibitor
Maleate isomerase inhibitor
CYP2A substrate
Chemopreventive
UGT2B18 substrate
Cholestenone 5alpha-reductase inhibitor
Ophthalmic drug
Hirsutism treatment
Phospholipase A1 inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Steroid-like

1,2-alpha-L-fucosidase inhibitor
Signal peptidase I inhibitor
Protein synthesis stimulant
Sodium/bile acid cotransporter inhibitor
CYP2G1 substrate
Alopecia treatment
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Antiinflammatory, ophthalmic
Muramoyltetrapeptide carboxypeptidase inhibitor
ATP-binding cassette A1 stimulant
Raynaud's phenomenon treatment
CYP2B6 substrate
Antipsoriatic
Corticosteroid antagonist
Nicotinic alpha4beta2 receptor antagonist
H⁺-transporting two-sector ATPase inhibitor
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
RNA-directed RNA polymerase inhibitor
Antineoplastic (thyroid cancer)
Dementia treatment
Apyrase inhibitor
CYP2B5 substrate
Steroid synthesis inhibitor
CYP2A4 substrate
Retinyl-palmitate esterase inhibitor
Retinol dehydrogenase inhibitor
Pregnane X receptor agonist
Analeptic
Luteinizing hormone-releasing hormone agonist
Nicotinic alpha4beta4 receptor agonist
CYP2A6 substrate
CYP2A10 substrate
Antineoplastic alkaloid
Sterol 3-beta-glucosyltransferase inhibitor
Antisecretoric
Antineoplastic (endocrine cancer)
DNA polymerase I inhibitor
TNF expression inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Interleukin 10 agonist
CYP3A5 inducer
Indanol dehydrogenase inhibitor
Sterol 24-C-methyltransferase inhibitor
Thyroxine 5-deiodinase inhibitor
CYP19 substrate
Rubredoxin-NAD⁺ reductase inhibitor
Anabolic
Antimetastatic
Kidney function stimulant

Arachidonic acid antagonist
Vascular dementia treatment
Endoglycosylceramidase inhibitor
CYP2D2 inhibitor
Protein-synthesizing GTPase inhibitor
Steroid DELTA-isomerase inhibitor
Antihypotensive
CYP2H substrate
CYP2A2 substrate
Sulfite dehydrogenase inhibitor
UGT2B28 substrate
Hyaluronic acid agonist
Cholesterol oxidase inhibitor
Steroid 17-alpha-hydroxylase/17,20 lyase inhibitor
CYP2B11 substrate
Melanocortin MC-4 agonist
Tocolytic
Cardiovascular analeptic
Microtubule formation inhibitor
Endometriosis treatment
Melanocortin agonist
Contraceptive female
Secretase alpha stimulant
Secretase stimulant
Antipruritic, non-allergic
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Cytoprotectant
3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor
Lipocortins synthesis agonist
Cushing's syndrome treatment
Glucagon-like peptide 1 agonist
Interferon gamma antagonist
Interferon antagonist
Glycine N-choloyltransferase inhibitor
Threonine ammonia-lyase inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Releasing hormone agonist
HIV attachment inhibitor
Thiosulfate dehydrogenase inhibitor
Menstruation disorders treatment
Lysase inhibitor
Proliferative diseases treatment
Cholate-CoA ligase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
DELTA24-sterol reductase inhibitor
Acetylcholinesterase inhibitor
RNA-directed RNA polymerase stimulant
RNA synthesis inhibitor
Nicotinic alpha2beta2 receptor antagonist
UGT2B7 substrate

Hepatoprotectant
UGT2B17 substrate
CYP2B2 substrate
Plasmanylethanolamine desaturase inhibitor
SULT1E1 substrate
Retinol O-fatty-acyltransferase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Progesterone agonist
CYP2D15 substrate
Galactolipase inhibitor
CYP4A11 substrate
RNA agonist
CYP7B substrate
CYP7B1 substrate
Cholestanetriol 26-monooxygenase inhibitor
CYP17 substrate
Gynecological disorders treatment
DNA directed RNA polymerase stimulant
Androgen agonist
Mineralocorticoid antagonist
Phospholipase D inhibitor
Growth hormone agonist
3 Beta-hydroxy-delta 5-steroid dehydrogenase inhibitor
Corticosteroid-like
CYP4B substrate
Nicotinic alpha3beta4 receptor agonist
CYP4B1 substrate
Choloylglycine hydrolase inhibitor
Cortisone beta-reductase inhibitor
Opioid dependency treatment
2-Acylglycerol O-acyltransferase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
CYP2C2 substrate
Parathyroid hormone antagonist
Antiparkinsonian, rigidity relieving
Phosphoinositide 5-phosphatase inhibitor
Alcohol O-acetyltransferase inhibitor
Female sexual dysfunction treatment
Antiviral (Influenza)
Hypercalcemia treatment
UGT2B11 substrate
Cholesterol antagonist
Dopamine release stimulant
Neurotransmitter uptake inhibitor
Steroid sulfotransferase inhibitor
Prostaglandin-E2 9-reductase inhibitor
17-Beta-hydroxysteroid dehydrogenase 1 inhibitor
HIV-2 retropepsin inhibitor
Prolactin inhibitor
Vitamin D3 hydroxylase inhibitor

Estrone sulfotransferase stimulant
Contraceptive male
Gonadotropin antagonist
Trans-octaprenyltranstransferase inhibitor
Glucocorticoid agonist
UGT2B10 substrate
Androst-4-ene-3,17-dione monooxygenase inhibitor
Estradiol 17 beta dehydrogenase stimulant
Cortisone alpha-reductase inhibitor
UGT2B4 substrate
2-Hydroxyacylsphingosine 1-beta-galactosyltransferase inhibitor
Imidazoline I1 receptor agonist
Heme oxygenase stimulant
Opioid kappa 3 receptor antagonist
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Methylglutamate dehydrogenase inhibitor
Antiviral (Influenza A)
Mannan endo-1,4-beta-mannosidase inhibitor
Restless leg syndrome treatment
CYP27A1 substrate
D-lactaldehyde dehydrogenase inhibitor
1,3-Beta-glucan synthase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Hypogonadism treatment

Galantamine hydrobromide

Molecular Mechanism (initial) :

acetylcholinesterase inhibitor

Molecular Mechanism (repurposed) :

acetylcholinesterase inhibitor

initial indication(s):

polio

paralysis

anesthesia

Repurposed indication(s):

Alzheimer's type dementia

Predicted Activities

CYP2D substrate

CYP2D6 substrate

Respiratory analeptic

Dementia treatment

Nootropic (Alzheimer's type dementia)

Analeptic

CYP3A4 substrate

CYP3A substrate

Histamine release stimulant

Neurotransmitter antagonist

Antitussive

CYP2D1 substrate

Polarisation stimulant

CYP3A2 substrate

Antinociceptive (anesthesia)

CYP3A1 substrate

Antitussive, narcotic

Butyrylcholinesterase inhibitor

Analgesic (anesthesia)

Opioid kappa 3 receptor antagonist

CYP3A5 substrate

CYP2H substrate

HIF1A expression inhibitor

CYP3A7 substrate

Antineurogenic pain

CYP2C11 substrate

CYP2C8 substrate

CYP2B6 substrate

H⁺-transporting two-sector ATPase inhibitor

Platelet adhesion inhibitor

Nicotinic alpha4beta4 receptor agonist

Alzheimer's disease treatment

UGT1A substrate

P-glycoprotein substrate

Myc inhibitor

Cholinergic

Antiperistaltic

UGT2B9 substrate

Antiviral (Rhinovirus)

Antimetastatic

TP53 expression enhancer

Opioid dependency treatment

Neurodegenerative diseases treatment

CYP2A6 substrate

Anaphylatoxin receptor antagonist

Antineoplastic alkaloid

Dependence treatment

Octopamine antagonist

Peroxidase substrate

UGT2B7 substrate

CYP2A substrate

UGT1A3 substrate

MAP kinase stimulant

UDP-glucuronosyltransferase substrate

Membrane integrity antagonist

UGT1A9 substrate

CYP3A3 substrate

Antineoplastic (breast cancer)

CYP2C substrate

Antineoplastic (pancreatic cancer)

UGT2B18 substrate

Vascular dementia treatment

CYP2D15 substrate
Imidazoline I1 receptor agonist
JAK2 expression inhibitor
Anesthetic general
Antipruritic
CYP2D2 inhibitor
General pump inhibitor
P-glycoprotein inhibitor
Ovulation inhibitor
Gastrin inhibitor
Antihelmintic (Nematodes)
Vasodilator, peripheral
Caspase 3 stimulant
UGT1A1 substrate
CYP2C19 substrate
Narcotic antagonist
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
P-glycoprotein 1 inhibitor
Cognition disorders treatment
Uterine relaxant
Protein kinase stimulant
CYP1A2 substrate
UGT2B substrate
Acetylcholine neuromuscular blocking agent
UGT2B12 substrate
Beta glucuronidase inhibitor
CYP3A4 inducer
Opioid mu 2 receptor antagonist
Kinase inhibitor
Laxative
Antidote
UGT1A10 substrate
CYP3A inducer
CYP1B1 substrate
Membrane permeability inhibitor
Antineoplastic (thyroid cancer)
Spasmolytic
CYP1A substrate
MMP9 expression inhibitor
Antineoplastic
Vasodilator, coronary
Antimitotic
Antimycoplasmal
CDP-glycerol glycerophosphotransferase inhibitor
Adenosine regulator
4-Coumarate-CoA ligase inhibitor
Spasmolytic, urinary
Aspulinone dimethylallyltransferase inhibitor
Glucagon-like peptide 1 agonist
Antineoplastic (multiple myeloma)

Peptidyltransferase inhibitor
Antineoplastic (lung cancer)
Antitoxic
Phosphatase inhibitor
CYP2C6 substrate
Opioid mu 1 receptor antagonist
CYP2B2 substrate
Xenobiotic-transporting ATPase inhibitor
RELA expression inhibitor
UGT2B7H substrate
UGT2B7Y substrate
APOA1 expression enhancer
Membrane integrity agonist
Melanin inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Apoptosis agonist
Dry eye syndrome treatment
AR expression inhibitor
Reductase inhibitor
CYP2A11 substrate
Microtubule formation inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Protein synthesis inhibitor
Antiinfertility, female
Cytochrome P450 stimulant
Antiviral (Hepatitis B)
Histidine kinase inhibitor
CYP2A4 substrate
UGT1A8 substrate
CYP2B substrate
Antineoplastic (non-Hodgkin's lymphoma)
Antineoplastic (ovarian cancer)
1,4-Lactonase inhibitor
Gonadotropin antagonist
Anesthetic
Glycine receptor antagonist
Oxygen scavenger
Antialcoholic
Radical formation agonist
Antineoplastic (bone cancer)
Niemann-Pick C1-like 1 protein antagonist
Immunosuppressant
Antineoplastic (small cell lung cancer)
Antiviral (Herpes)
5 Hydroxytryptamine 7S antagonist
Nicotinic alpha4beta2 receptor antagonist
UGT2B1 substrate
Chemopreventive
Antineoplastic (endocrine cancer)

4-Nitrophenol 2-monooxygenase inhibitor
Opioid kappa 1 receptor antagonist
Cytostatic
Antioxidant
CYP1B substrate
CYP2C9 substrate
Bilirubin oxidase inhibitor
Antipruritic, non-allergic
UGT2B15 substrate
Cocain dependency treatment
HMOX1 expression enhancer
Antineoplastic (carcinoma)
Cytokine release inhibitor
Interleukin 10 antagonist
Antihemorrhagic
Antimutagenic
Anticarcinogenic
EIF4E expression inhibitor
Antipyretic
Opioid delta 1 receptor antagonist
Neurotrophic factor enhancer
Monoamine uptake inhibitor
CYP2A1 substrate
Carminative
Alpha 3 adrenoreceptor agonist
Corticosteroid antagonist
CYP1A1 inhibitor
Antiprotozoal (Amoeba)
GST M1-1 substrate
5 Hydroxytryptamine 7L antagonist
2-Enoate reductase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Caspase 8 stimulant
Thyroxine 5-deiodinase inhibitor
CYP2C8 inducer
Contraceptive female
Antineoplastic (non-small cell lung cancer)
Diuretic inhibitor
Proliferative diseases treatment
Hepatoprotectant
Cyclooxygenase 1 substrate
Galactosylceramidase inhibitor
UGT2B10 substrate
CYP19A1 expression inhibitor
Hydroxysteroid dehydrogenase inhibitor
Antitreponemal
Nitric oxide scavenger
CYP2C12 substrate
UGT1A7 substrate
Angiogenesis stimulant

Prostate cancer treatment
Sigma receptor antagonist
Capillary fragility treatment
5 Hydroxytryptamine uptake stimulant
UGT2B4 substrate
Acetylcholine agonist
Membrane permeability enhancer
CYP2A10 substrate
DNA ligase (ATP) inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Estrogen antagonist
Antineoplastic (brain cancer)
Antineoplastic antibiotic
CYP1A1 substrate
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
MAO B substrate
CYP2C19 inducer
Premenstrual syndrome treatment
Antineoplastic (lymphoma)
Neurotransmitter uptake inhibitor
Platelet aggregation stimulant
Leukopoiesis inhibitor
Antihypoxic
Antileukemic
Acetylcholine M2 receptor agonist
CYP1B1 inhibitor
Protein kinase C stimulant
Skin whitener
Antipruritic, allergic
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Estrogen beta receptor agonist
Cyclooxygenase substrate
Antidiuretic hormone antagonist
5 Hydroxytryptamine release stimulant
Acetylcholine M4 receptor agonist
Microtubule stabilization
CYP19 substrate
Secretase gamma inhibitor
CYP2A2 substrate
Transforming growth factor beta 1 agonist
Vasopressin 2 antagonist
(R)-6-hydroxynicotine oxidase inhibitor
Prostacyclin agonist
Para amino benzoic acid antagonist
Polyribonucleotide nucleotidyltransferase inhibitor
Estrogen receptor beta antagonist

Gemcitabine hydrochloride

Molecular Mechanism (initial) :

ribonucleoside-diphosphate reductase inhibitor

Molecular Mechanism (repurposed) :

ribonucleoside-diphosphate reductase inhibitor

initial indication(s):

antiviral

Repurposed indication(s):

cancers (NSCLC, pancreas, breast, biliary, ovary, bladder, breast, lymphoma)

Predicted Activities

TP53 expression enhancer

Ribonucleoside triphosphate reductase inhibitor

CDP-glycerol glycerophosphotransferase inhibitor

DNA synthesis inhibitor

Pyrimidine antagonist

Cytostatic

Antineoplastic antimetabolite

Radiosensitizer

Antineoplastic

Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor

Nucleoside oxidase (H₂O₂-forming) inhibitor

Antiviral (Poxvirus)

Antimetabolite

Anticarcinogenic

Phosphatidate phosphatase inhibitor

Antineoplastic (non-Hodgkin's lymphoma)

NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor

Ethanolamine-phosphate cytidyltransferase inhibitor

Proliferative diseases treatment

tRNA adenylyltransferase inhibitor

Antineoplastic (solid tumors)

DNA repair enzyme inhibitor

Antiviral

Nucleotide metabolism regulator

Antineoplastic (pancreatic cancer)

Benzoate-CoA ligase inhibitor

Serine-phosphoethanolamine synthase inhibitor

Thiamine-triphosphatase inhibitor

Ethanolamine kinase inhibitor

Glutamate-5-semialdehyde dehydrogenase inhibitor

Inositol oxygenase inhibitor

CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor

tRNA cytidyltransferase inhibitor

Pancreatic ribonuclease inhibitor

Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor

Ribonucleoside diphosphate reductase inhibitor

Undecaprenyldiphospho-muramoylpentapeptide

beta-N-acetylglucosaminyltransferase inhibitor

4-Nitrophenylphosphatase inhibitor

Antileukemic

Glucose oxidase inhibitor

Ethanolaminephosphotransferase inhibitor

CMP-N-acetylneuraminate monooxygenase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Antiviral (Adenovirus)
Glutamine synthetase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
DNA polymerase I inhibitor
Blasticidin-S deaminase inhibitor
Choline-phosphate cytidyltransferase inhibitor
Cytidine deaminase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Adenosine regulator
Dolichol kinase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Antiviral (Picornavirus)
Diacylglycerol cholinephosphotransferase inhibitor
Phosphatidate cytidyltransferase inhibitor
Nucleoside deoxyribosyltransferase inhibitor
Antineoplastic (small cell lung cancer)
ADP-thymidine kinase inhibitor
Cytochrome-b5 reductase inhibitor
Uridine nucleosidase inhibitor
dUTP diphosphatase inhibitor
RNA directed DNA polymerase inhibitor
Lysase inhibitor
Antiviral (Herpes)
Adenylyl-sulfate kinase inhibitor
Heat shock protein 27 antagonist
3-Hydroxyanthranilate oxidase inhibitor
Glucose 1-dehydrogenase inhibitor
Beta-fructofuranosidase inhibitor
Chitinase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Malate oxidase inhibitor
Phosphofructokinase-1 inhibitor
Pyruvate carboxylase inhibitor
Mannitol-1-phosphate 5-dehydrogenase inhibitor
Deoxyribonuclease X inhibitor
Apoptosis agonist
Antineoplastic (sarcoma)
Aspartate carbamoyltransferase inhibitor
Malate dehydrogenase (acceptor) inhibitor
Membrane permeability enhancer
Antineoplastic (lymphoma)
Antineoplastic (brain cancer)
N-acetyllactosamine synthase inhibitor
(N-acetylneuraminyl)-galactosylglucosylceramide
N-acetylgalactosaminyltransferase inhibitor
Antiviral (Hepatitis B)
Histidine N-acetyltransferase inhibitor
N-acetylglucosamine kinase inhibitor

N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Adenylylsulphatase inhibitor
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Antineoplastic (bladder cancer)
DNA nucleotidylexotransferase inhibitor
Lactoylglutathione lyase inhibitor
H⁺-transporting two-sector ATPase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
DNA directed DNA polymerase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
Pyrroline-5-carboxylate reductase inhibitor
Sphinganine kinase inhibitor
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Lactase inhibitor
Orotate phosphoribosyltransferase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Peptidyltransferase inhibitor
Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor
DNA directed RNA polymerase inhibitor
RNA synthesis inhibitor
Venom exonuclease inhibitor
Cytosine deaminase inhibitor
Glycogen (starch) synthase inhibitor
Sugar-phosphatase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein
beta-1,3-N-acetylglucosaminyltransferase inhibitor
UDP-glucuronate decarboxylase inhibitor
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Thymidylate 5'-phosphatase inhibitor
Immunostimulant
Beta-galactoside alpha-2,3-sialyltransferase inhibitor
Procollagen glucosyltransferase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Mycothiols-S-conjugate amidase inhibitor
Hydroxyacylglutathione hydrolase inhibitor
Lactose synthase inhibitor
3'-Nucleotidase inhibitor
FMN reductase inhibitor
Apyrase inhibitor
CTP synthase inhibitor
FAD diphosphatase inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
Adenylyl-sulfate reductase inhibitor
Hypoxanthine phosphoribosyltransferase inhibitor
Glutathione peroxidase inhibitor
CDK9/cyclin T1 inhibitor
Manganese peroxidase inhibitor
Glucosamine-6-phosphate deaminase inhibitor

Antineoplastic (glioma)
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Laminaribiose phosphorylase inhibitor
Antineoplastic (melanoma)
Rubredoxin-NAD⁺ reductase inhibitor
Adenine phosphoribosyltransferase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Serratia marcescens nuclease inhibitor
Galactokinase inhibitor
Pyruvate, phosphate dikinase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Cyclohexanone monooxygenase inhibitor
Glucosyl transferase inhibitor
CMP-N-acylneuraminate phosphodiesterase inhibitor
Nitrate reductase inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
Antineoplastic (renal cancer)
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Methionine adenosyltransferase inhibitor
Ribose-5-phosphate isomerase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Dihydropyrimidine dehydrogenase inhibitor
Ecdysone 20-monooxygenase inhibitor
Ceramide glucosyltransferase inhibitor
Adenylosuccinate synthase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Antineoplastic (non-small cell lung cancer)
Guanylate cyclase inhibitor
Aspartyltransferase inhibitor
Dynein ATPase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
CYP3A7 substrate
UDP-glucose 4-epimerase inhibitor
Fumarate hydratase inhibitor
Bilirubin oxidase inhibitor
Phosphoglucomutase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Glutamate dehydrogenase inhibitor
Chitin synthase inhibitor
Dethiobiotin synthase inhibitor
S-methyl-5-thioribose kinase inhibitor
Biotinidase inhibitor
Chaperonin ATPase inhibitor
Lipotropic
Sucrose-phosphate synthase inhibitor
Sucrose synthase inhibitor
Lysine 2,3-aminomutase inhibitor
NADH dehydrogenase inhibitor
Phosphogluconate dehydrogenase (decarboxylating) inhibitor

Sulfite dehydrogenase inhibitor
ATP phosphoribosyltransferase inhibitor
Xanthine phosphoribosyltransferase inhibitor
NAD⁺ kinase inhibitor
Argininosuccinate synthase inhibitor
Channel-conductance-controlling ATPase inhibitor
Adenylate cyclase inhibitor
Antimetastatic
Chemosensitizer
3'-Demethylstaurosporine O-methyltransferase inhibitor
Malate dehydrogenase inhibitor
Mitochondrial processing peptidase inhibitor
Fructan beta-fructosidase inhibitor
N6-methyl-lysine oxidase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
ATP adenylyltransferase inhibitor
Formate-dihydrofolate ligase inhibitor
Aspergillus nuclease S1 inhibitor
GDP-mannose 6-dehydrogenase inhibitor
Citrate (Si)-synthase inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
Nucleotide diphosphatase inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
ATP citrate synthase inhibitor
Exoribonuclease II inhibitor
Ribonucleotide reductase inhibitor
Formate dehydrogenase inhibitor
Deoxycytidine deaminase inhibitor
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Glucan endo-1,6-beta-glucosidase inhibitor
Levansucrase inhibitor
Ganglioside galactosyltransferase inhibitor
Ligase inhibitor
Diuretic inhibitor
Antineoplastic (lung cancer)
Glycine-tRNA ligase inhibitor
Fructokinase inhibitor
Nucleoside-diphosphatase inhibitor
Antineoplastic (cervical cancer)
Pyruvate kinase inhibitor
AMP nucleosidase inhibitor
Nicotinate phosphoribosyltransferase inhibitor
5'-Nucleotidase inhibitor
Diacylglycerol kinase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Glycogenin glucosyltransferase inhibitor
Antineoplastic (lymphocytic leukemia)

Hydroxypyruvate reductase inhibitor
4-Coumarate-CoA ligase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Glutathione synthase inhibitor
Thiamine-phosphate kinase inhibitor
DNA ligase (ATP) inhibitor
Protein-synthesizing GTPase inhibitor
NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Adenine deaminase inhibitor
Antineoplastic (glioblastoma multiforme)
Procollagen galactosyltransferase inhibitor
HIF1A expression inhibitor
Phenylalanine-tRNA ligase inhibitor
N-acylneuraminate cytidyltransferase inhibitor
Isopenicillin-N epimerase inhibitor
Antineoplastic (uterine cancer)
Deoxynucleoside kinase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate
N-acetylglucosaminephosphotransferase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Ribonuclease inhibitor
NAD⁺ nucleosidase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Sedoheptulose-bisphosphatase inhibitor
[phosphorylase] phosphatase inhibitor
Uracil phosphoribosyltransferase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
Sulfate adenylyltransferase inhibitor
Antiviral (Hepatitis)
Thymidine-triphosphatase inhibitor
Aryl-aldehyde dehydrogenase (NADP⁺) inhibitor
RELA expression inhibitor
Biotin carboxylase inhibitor
dCMP deaminase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Myosin-light-chain-phosphatase inhibitor
Inosine nucleosidase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Dihydrodipicolinate reductase inhibitor
[acyl-carrier-protein] S-acyltransferase inhibitor
Acylglycerone-phosphate reductase inhibitor
Glutamate synthase (NADPH) inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP⁺) inhibitor
Immunosuppressant
Protein N-acetylglucosaminyltransferase inhibitor
Phosphoenolpyruvate carboxylase inhibitor
Polynucleotide adenylyltransferase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
P-benzoquinone reductase (NADPH) inhibitor

Ribosylpyrimidine nucleosidase inhibitor
Ornithine carbamoyltransferase inhibitor
dCTP deaminase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Fucosterol-epoxide lyase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
NMN nucleosidase inhibitor
Phosphoglycerate kinase inhibitor
GTP cyclohydrolase I inhibitor
Ferredoxin-NADP+ reductase inhibitor
Acyl-CoA oxidase inhibitor
NAD+-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Nicotinamide-nucleotide adenylyltransferase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Alcohol O-acetyltransferase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Nicotinamide phosphoribosyltransferase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Phosphate acetyltransferase inhibitor
tRNA (guanine-N1-)-methyltransferase inhibitor
Acetate-CoA ligase inhibitor
DELTA14-sterol reductase inhibitor
DNA methylase inhibitor
Metabolic disease treatment
UDP-sugar diphosphatase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Uric acid excretion stimulant
Glucose-1-phosphate adenylyltransferase inhibitor
Alkylator
Choline kinase inhibitor
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
RNA-directed RNA polymerase inhibitor
Glutamate-tRNA ligase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
NAD+ diphosphatase inhibitor
2-Oxoaldehyde dehydrogenase (NAD+) inhibitor
Nucleotidase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Vasculitis treatment
Antiviral (HIV)
Deoxycytidine kinase inhibitor
Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Antineoplastic (bone cancer)
1-Phosphofructokinase inhibitor

Maltose-transporting ATPase inhibitor
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Glutaminyl-peptide cyclotransferase inhibitor
Phospholipase A1 inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
N-acylmannosamine kinase inhibitor
UDP-N-acetylmuramate dehydrogenase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Xanthommatin reductase inhibitor
UDP-N-acetylglucosamine-lysosomal-enzyme
N-acetylglucosaminephosphotransferase inhibitor
Alpha,alpha-trehalase inhibitor
Cell wall biosynthesis inhibitor
Macrophage stimulant
Gout treatment
Uridine kinase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Octadecanal decarboxylase inhibitor
Pteridine reductase inhibitor
Sulfur dioxygenase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Diamine N-acetyltransferase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Glycerol dehydrogenase inhibitor
Arylamine N-acetyltransferase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
Glyoxylate reductase (NADP⁺) inhibitor
Antineoplastic (gastric cancer)
Aldose reductase substrate
Phosphorylase b inhibitor
NADPH-ferrihemoprotein reductase inhibitor
L-threonine 3-dehydrogenase inhibitor
Ribonuclease U2 inhibitor
Glyceryl-ether monooxygenase inhibitor
Antineoplastic (ovarian cancer)
6-Phospho-beta-glucosidase inhibitor
Deoxyadenosine kinase inhibitor
MAP3K5 inhibitor
GMP synthase inhibitor
Adenylate kinase inhibitor
Aldehyde dehydrogenase (NADP⁺) inhibitor
Galactoside O-acetyltransferase inhibitor
D-lactaldehyde dehydrogenase inhibitor

Rhodopsin kinase inhibitor
Prostate cancer treatment
Purine nucleosidase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Deoxyguanosine kinase inhibitor
Prenyl-diphosphatase inhibitor
Thymidine phosphorylase inhibitor
2-Methylcitrate synthase inhibitor
Arginase inhibitor
Antiviral (Hepatitis C)
Amidophosphoribosyltransferase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
[glutamate-ammonia-ligase] adenylyltransferase inhibitor
Alpha, alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
Interleukin 2 agonist
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Beta glucuronidase inhibitor
Immunomodulator
Cytidylate kinase inhibitor
[Skp1-protein]-hydroxyproline N-acetylglucosaminyltransferase inhibitor
UGT2B17 substrate
Thiol S-methyltransferase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Valine-tRNA ligase inhibitor
Methylthioadenosine nucleosidase inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
Ketoheokinase inhibitor
Arginine deiminase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Adenylate cyclase V inhibitor
Gluconokinase inhibitor
Biliverdin reductase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
Ribose-phosphate diphosphokinase inhibitor
Thymidine kinase inhibitor
Hexokinase inhibitor
Antimitotic
Acyl-CoA dehydrogenase (NADP⁺) inhibitor
Hematopoietic inhibitor
Guanine deaminase inhibitor
Antineoplastic (liver cancer)
UDP-glucose 6-dehydrogenase inhibitor
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Antineoplastic enhancer
Cardioprotectant
Glyceraldehyde-3-phosphate dehydrogenase (NADP⁺) inhibitor
GlutaminytRNA synthase (glutamine-hydrolysing) inhibitor
Ketol-acid reductoisomerase inhibitor
6-Phosphofructo-2-kinase inhibitor

Alpha-N-acetylglucosaminidase inhibitor
N-acetylglucosaminyldiphosphoundecaprenol
N-acetyl-beta-D-mannosaminyltransferase inhibitor
Orotidylate decarboxylase inhibitor
Transactivator transcription protein inhibitor
D-Octopine dehydrogenase inhibitor
Leucine-tRNA ligase inhibitor
Isomaltulose synthase inhibitor
Tryptophan-tRNA ligase inhibitor
UDP-glucuronate 5'-epimerase inhibitor
Leukopoiesis stimulant
Acetolactate decarboxylase inhibitor
Malate-CoA ligase inhibitor
Guanylate kinase inhibitor
Xylose isomerase inhibitor
Poly(ADP-ribose) glycohydrolase inhibitor
Threonine-tRNA ligase inhibitor
3-Methylbutanal reductase inhibitor
Fucokinase inhibitor
Chitosanase inhibitor
Alpha-amylase inhibitor
CDP-glycerol diphosphatase inhibitor
Pullulanase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
UGT2B10 substrate
L-iduronidase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Analgesic stimulant
Malyl-CoA lyase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase inhibitor
Licheninase inhibitor
Riboflavin phosphotransferase inhibitor
CDP-diacylglycerol diphosphatase inhibitor
Cysteine-tRNA ligase inhibitor
Acyloxyacyl hydrolase inhibitor
Beta-D-fucosidase inhibitor
Glucan 1,3-beta-glucosidase inhibitor
T2-induced deoxynucleotide kinase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Glutamate 5-kinase inhibitor
N-acetylglucosaminyldiphosphodolichol N-acetylglucosaminyltransferase inhibitor
Xanthine dehydrogenase inhibitor
ATP diphosphatase inhibitor
Malate dehydrogenase (NADP⁺) inhibitor
D-lactate dehydrogenase inhibitor
Cellobiose phosphorylase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
Acetoin dehydrogenase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor

Pseudouridylate synthase inhibitor
Antiviral (Influenza)
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Choline sulfotransferase inhibitor
Antineoplastic (breast cancer)
Purinergic P2Y agonist
Decylcitrate synthase inhibitor
Levanase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Prostaglandin-E2 9-reductase inhibitor
Phosphoribulokinase inhibitor
Homoserine dehydrogenase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Polypeptide N-acetylgalactosaminyltransferase inhibitor
Alpha-N-acetylgalactosaminide alpha-2,6-sialyltransferase inhibitor
Glycosylceramidase inhibitor
Dementia treatment
Antiprotozoal (Trypanosoma)
D-arabinonolactone oxidase inhibitor
Galactosylceramidase inhibitor
Topoisomerase I inhibitor
N-acetylglucosaminide beta-1,6-N-acetylglucosaminyl-transferase inhibitor
Cyclic AMP phosphodiesterase inhibitor
ATPase stimulant
Antiviral (Influenza A)
Serine-tRNA ligase inhibitor
Galactose oxidase inhibitor
Undecaprenyl-phosphate galactose phosphotransferase inhibitor
Cellulose synthase (UDP-forming) inhibitor
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Oligonucleotidase inhibitor
X-methyl-His dipeptidase inhibitor
Protein synthesis inhibitor
Endopeptidase La inhibitor
Myosin ATPase inhibitor
Sweetener
Sepiapterin reductase inhibitor
tRNA methyltransferase inhibitor
4-Alpha-glucanotransferase inhibitor
Thiopurine S-methyltransferase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Gaucher disease treatment
Bis(5'-nucleosyl)-tetraphosphatase (asymmetrical) inhibitor
Benzoylformate decarboxylase inhibitor
Ribonuclease T2 inhibitor
HCV NS5B polymerase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor

Glucosamine 6-phosphate N-acetyltransferase inhibitor
Glycolipid 2-alpha-mannosyltransferase inhibitor
S-methyl-5-thioadenosine phosphorylase inhibitor
GABA aminotransferase inhibitor
Growth stimulant
mRNA (guanine-N7-)-methyltransferase inhibitor
Pyruvate, water dikinase inhibitor
Histone-arginine N-methyltransferase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
Phosphorylase inhibitor
Phloroglucinol reductase inhibitor
Pyruvate dehydrogenase inhibitor
3'(2'),5'-Bisphosphate nucleotidase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Galactosylceramide sulfotransferase inhibitor
ADP-ribose diphosphatase inhibitor
Alpha-N-acetylneuraminate alpha-2,8-sialyltransferase inhibitor
Dimethylhistidine N-methyltransferase inhibitor
Glycolipid 3-alpha-mannosyltransferase inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Homocysteine S-methyltransferase inhibitor
Aminoacyl-tRNA synthetase inhibitor
Adenosine A2a receptor antagonist
Bacillus subtilis ribonuclease inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Arginine-tRNA ligase inhibitor
Acid phosphatase inhibitor
Plus-end-directed kinesin ATPase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Inositol 1,4,5-triphosphate receptor antagonist
Vascular dementia treatment
Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
Lysozyme inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Phosphoketolase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Phosphoadenylylsulfatase inhibitor
N-formylglutamate deformylase inhibitor
NTPase/helicase (JEV) inhibitor
Alpha-N-arabinofuranosidase inhibitor
GMP reductase inhibitor
Adenosine deaminase inhibitor
[protein-PII] uridylyltransferase inhibitor
Thymidine kinase 1 inhibitor
Butyrate-CoA ligase inhibitor
Purinergic P2 agonist

Purinergic receptor agonist
Glycerone-phosphate O-acyltransferase inhibitor
Fructose 5-dehydrogenase (NADP+) inhibitor
Antibacterial
Protein-L-isoaspartate (D-aspartate) O-methyltransferase inhibitor
Mevalonate kinase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Glutathione-disulfide reductase inhibitor
Alternansucrase inhibitor
5-Hydroxypentanoate CoA-transferase inhibitor
Interferon inducer
Alpha-1,3-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Purine biosynthesis inhibitor
Bis(5'-nucleosyl)-tetrphosphatase (symmetrical) inhibitor
AICAR transformylase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
Purinergic P2T antagonist
Enoyl-CoA hydratase inhibitor
Angiogenesis stimulant
Glycine N-benzoyltransferase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Trimethylamine-N-oxide reductase inhibitor
Anthranilate phosphoribosyltransferase inhibitor
Hyaluronic acid agonist
Long-chain-acyl-CoA dehydrogenase inhibitor
2-Amino-4-hydroxy-6-hydroxymethyldihydropteridine diphosphokinase inhibitor
CYP3A5 substrate
Polyphosphate kinase inhibitor
Adenosine A2 receptor antagonist
tRNA (guanine-N2-)-methyltransferase inhibitor
Amylo-alpha-1,6-glucosidase inhibitor
Cerebroside-sulfatase inhibitor
Adenosine A1 receptor antagonist
Acetate kinase inhibitor
Anthranilate-CoA ligase inhibitor
Nucleoside-triphosphate-adenylate kinase inhibitor
[Isocitrate dehydrogenase (NADP+)] kinase inhibitor
Galectin 3 antagonist
Dextranucrase inhibitor
Galactolipase inhibitor
Lysine-tRNA ligase inhibitor
Adenine nucleotide translocase inhibitor
UGT2B4 substrate
Antibiotic Aminoglycoside-like
Multiple inositol-polyphosphate phosphatase inhibitor
Cholate-CoA ligase inhibitor
Adenosine receptor antagonist

GDP-L-fucose synthase inhibitor
Phosphoribosylformylglycinamide synthase inhibitor
Cellulase inhibitor
Purinergic receptor antagonist
Methenyltetrahydrofolate cyclohydrolase inhibitor
UGT1A9 substrate
Malate synthase inhibitor
HIV-1 reverse transcriptase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Alanine racemase inhibitor
Nucleoside transporters inhibitor
3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
Adenosine A2b receptor agonist
Protein 30S ribosomal subunit inhibitor
Adenylosuccinate lyase inhibitor
Uridine phosphorylase inhibitor
rRNA (adenosine-2'-O-)-methyltransferase inhibitor
IgA-specific metalloendopeptidase inhibitor
Tubulin GTPase inhibitor
Glycine N-acyltransferase inhibitor
Homocitrate synthase inhibitor
Aralkylamine N-acetyltransferase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Amylosucrase inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Estrone sulfotransferase inhibitor
Isocitrate dehydrogenase (NADP⁺) inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Glycine N-methyltransferase inhibitor
Coactivator-associated arginine methyltransferase 1 inhibitor
Vasodilator, coronary
UDP-N-acetylmuramate-L-alanine ligase inhibitor
Caspase 8 stimulant
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Glycerol kinase inhibitor
Phosphoinositide phospholipase C inhibitor
Spermine synthase inhibitor
Inorganic diphosphatase inhibitor
Keratan sulfotransferase inhibitor
Isocitrate lyase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Adenosine receptor agonist
Purine antagonist
Acyl-CoA dehydrogenase inhibitor
Cysteine synthase inhibitor
Antiviral (Trachoma)
Toll-Like receptor agonist
Antineoplastic (colorectal cancer)
Antiprotozoal (Amoeba)
Glycerol-3-phosphate dehydrogenase [NAD(P)⁺] inhibitor

Osmotic diuretic
Caspase 3 stimulant
Glutamate dehydrogenase [NAD(P)+] inhibitor
Antineoplastic (squamous cell carcinoma)
SMN2 expression enhancer
Carnitine O-octanoyltransferase inhibitor
Thioether S-methyltransferase inhibitor
UTP-glucose-1-phosphate uridylyltransferase inhibitor
Butyryl-CoA dehydrogenase inhibitor
Arabinogalactan endo-1,4-beta-galactosidase inhibitor
Glucose-1-phosphate cytidylyltransferase inhibitor
Ribose-5-phosphate adenylyltransferase inhibitor
Antifungal
Acetylserotonin O-methyltransferase inhibitor
Thymidylate synthase inhibitor
Methylcrotonoyl-CoA carboxylase inhibitor
Beta-Phosphoglucomutase inhibitor
Protein-glutamate O-methyltransferase inhibitor
Streptomycin 6-kinase inhibitor
CYP17 inhibitor
Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor
Glucose-1-phosphatase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Small monomeric GTPase inhibitor
Mycodextranase inhibitor
Alpha,alpha-phosphotrehalase inhibitor
Formate C-acetyltransferase inhibitor
3-Oxoacid CoA-transferase inhibitor
Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor
Cyclomaltodextrinase inhibitor
Guanidinoacetate kinase inhibitor
Pyroglutamyl-peptidase II inhibitor
Antiprotozoal (Coccidial)
Cell wall synthesis inhibitor
Antitoxic
Chitobiosyldiphosphodolichol beta-mannosyltransferase inhibitor
Pterin deaminase inhibitor
dCTP diphosphatase inhibitor
Beta-mannosidase inhibitor
Gentamicin 3'-N-acetyltransferase inhibitor
tRNA (adenine-N1-)-methyltransferase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Antibiotic
Glucan 1,4-beta-glucosidase inhibitor
Interleukin agonist
5-Aminolevulinate synthase inhibitor
Adenosylmethionine cyclotransferase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor

Betaine-aldehyde dehydrogenase inhibitor
UDP-glucuronate 4-epimerase inhibitor
Phosphatase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Antihemorrhagic
3-Hydroxybutyrate dehydrogenase inhibitor
Diphosphomevalonate decarboxylase inhibitor
dTMP kinase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Adenosine A3 receptor antagonist
Acetoacetyl-CoA reductase inhibitor
Purinergetic P2Y antagonist
Cholestenone 5alpha-reductase inhibitor
Alpha,alpha-trehalose phosphorylase inhibitor
Nucleoside phosphoacylhydrolase inhibitor
Toll-Like receptor 7 agonist
Sucrose-phosphate phosphatase inhibitor
dTMP kinase (Mycobacterium tuberculosis) inhibitor
Sucrose alpha-glucosidase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
dTDP-glucose 4,6-dehydratase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
Purinergetic P2X agonist
Antiviral (Herpesvirus 3, Human)
Glutamate dehydrogenase (NADP+) inhibitor
Shikimate kinase inhibitor
Inositol-3-phosphate synthase inhibitor
Phosphoglycerate dehydrogenase inhibitor
Adenosine A2a receptor agonist
Polyphosphate-glucose phosphotransferase inhibitor
Sodium/glucose cotransporter inhibitor
Xanthine oxidase substrate
Phosphatidylglycerophosphatase inhibitor
Spermidine synthase inhibitor
Mannosyl-oligosaccharide glucosidase inhibitor
Sodium/glucose cotransporter 1 inhibitor
NTPase/helicase (WNF) inhibitor
N-acetylgalactosamine-4-sulfatase inhibitor
AMP deaminase inhibitor
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Thymidine kinase 2 inhibitor
Respiratory distress syndrome treatment
Mannokinase inhibitor
3-Phytase inhibitor
2-Methylacyl-CoA dehydrogenase inhibitor
Mannosidase inhibitor
ATP-dependent RNA helicase inhibitor
Antineoplastic (carcinoma)
Adenosine A2 receptor agonist

Diabetes insipidus treatment
Alpha-mannosidase inhibitor
Adenosine kinase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
HMG CoA synthase inhibitor
Antihematotoxic
Threonine synthase inhibitor
Phospho-N-acetylmuramoyl-pentapeptide-transferase inhibitor
Glucosamine N-acetyltransferase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
M7G(5')pppN diphosphatase inhibitor
Neutropenia treatment
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)]-phosphatase inhibitor
mRNA (nucleoside-2'-O-)-methyltransferase inhibitor
Adenosine A3 receptor agonist
CYP4A substrate
Histidine-tRNA ligase inhibitor
Methylglyoxal synthase inhibitor
tRNA (guanine-N7-)-methyltransferase inhibitor
Isoleucine-tRNA ligase inhibitor
Purinergic P2Y1 antagonist
Queuine tRNA-ribosyltransferase inhibitor
Sodium/glucose cotransporter 2 inhibitor
Glutaryl-CoA dehydrogenase inhibitor
GDP-mannose 4,6-dehydratase inhibitor
Erythropoiesis stimulant
Endo-1,4-beta-xylanase inhibitor
Pyruvate synthase inhibitor
IMP cyclohydrolase inhibitor
Antifibrinolytic
Glucan 1,4-alpha-glucosidase inhibitor
Chemoprotective
Aspartate kinase inhibitor
Interferon agonist
UDP-N-acetylmuramoylalanyl-D-glutamate-2,6-diaminopimelate ligase inhibitor
Endo-beta-N-acetylglucosaminidase inhibitor
Sterol 24-C-methyltransferase inhibitor
1,3-Beta-glucan synthase inhibitor
Membrane-oligosaccharide glycerophosphotransferase inhibitor
Equilibrative nucleoside transport protein inhibitor
Inosine kinase inhibitor
S-adenosyl-L-homocysteine hydrolase inhibitor
Phytanoyl-CoA dioxygenase inhibitor
Phosphoribosylformylglycinamide cyclo-ligase inhibitor
Isoamylase inhibitor
N-acetylmuramoyl-L-alanine amidase inhibitor

Guanfacine hydrochloride

Molecular Mechanism (initial) :

alpha-2 adrenergic receptor agonist

Molecular Mechanism (repurposed) :

alpha-2 adrenergic receptor agonist

initial indication(s):

hypertension

Repurposed indication(s):

attention-deficit/hyperactivity disorder

Predicted Activities

Omptin inhibitor

Limulus clotting factor C inhibitor

Pro-opiomelanocortin converting enzyme inhibitor

Arginine 2-monooxygenase inhibitor

Limulus clotting factor B inhibitor

Mucositis treatment

Phobic disorders treatment

CDP-glycerol glycerophosphotransferase inhibitor

IgA-specific serine endopeptidase inhibitor

Antidyskinetic

Enteropeptidase inhibitor

Complement factor D inhibitor

CYP2C3 substrate

Imidazoline receptor agonist

Methylumbelliferyl-acetate deacetylase inhibitor

Cathepsin T inhibitor

Peptide agonist

Peptidyl-dipeptidase Dcp inhibitor

Pin1 inhibitor

Neuropeptide Y2 antagonist

Antimyopathies

Gingipain K inhibitor

Protein-glutamate methylesterase inhibitor

Renal tissue kallikrein inhibitor

Pitrilysin inhibitor

Guanidinoacetate kinase inhibitor

Interleukin 2 agonist

Carboxypeptidase D inhibitor

Insulysin inhibitor

Neuropeptide Y4 antagonist

Macrophage colony stimulating factor agonist

CYP2J substrate

Botulin neurotoxin A light chain inhibitor

CYP2J2 substrate

Antianginal

Dipeptidase E inhibitor

Interferon alpha agonist

Aspartyltransferase inhibitor

Protein-arginine deiminase inhibitor

L-glutamate oxidase inhibitor

Granzyme A inhibitor
Antiviral (Picornavirus)
Antidiarrheal
Bradykinin inhibitor
Fibrinogen receptor antagonist
Venombin AB inhibitor
Sodium channel blocker
Calcium channel (voltage-sensitive) activator
Subtilisin inhibitor
Polyporopepsin inhibitor
Chloride peroxidase inhibitor
Mitochondrial intermediate peptidase inhibitor
Antiischemic
Anticoagulant
Polyamine-transporting ATPase inhibitor
Pseudolysin inhibitor
Macrophage stimulant
CYP2C29 substrate
Hydrogen dehydrogenase inhibitor
5-O-(4-coumaroyl)-D-quinic acid 3'-monooxygenase inhibitor
Beta glucuronidase inhibitor
Maillard reaction inhibitor
Antianorexic
Platelet antagonist
GST A substrate
Membrane integrity antagonist
Diuretic inhibitor
Antiarrhythmic
Cardiotonic
Acute neurologic disorders treatment
CYP2A8 substrate
Aminopeptidase Y inhibitor
Nav1.5 sodium channel blocker
Blasticidin-S deaminase inhibitor
Glycine amidinotransferase inhibitor
Cardioprotectant
Polyamine oxidase inhibitor
Serine protease unspecified inhibitor
Antiperistaltic
TNF expression inhibitor
Sulfur reductase inhibitor
Anesthetic general
Metalloprotease inhibitor
Biliary tract disorders treatment
Opioid dependency treatment
Membrane permeability inhibitor
Antiinflammatory, ophthalmic
Acrosin inhibitor
Rhinitis treatment
Analgesic stimulant

Clostripain inhibitor
Antiviral (Poxvirus)
Neuropsin inhibitor
Sodium channel blocker class Ib
NMDA receptor polyamine site antagonist
Monoamine uptake inhibitor
Muscular dystrophy treatment
Antiprotozoal (Trypanosoma)
Prostaglandin-E2 9-reductase inhibitor
Leukopoiesis inhibitor
Fibrolase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Mycothiols-S-conjugate amidase inhibitor
Sigma receptor agonist
Envelysin inhibitor
Oligopeptidase B inhibitor
Membrane permeability enhancer
Ubiquinol-cytochrome-c reductase inhibitor
Cytosol alanyl aminopeptidase inhibitor
NADPH peroxidase inhibitor
Glutamyl endopeptidase II inhibitor
Cancer associated disorders treatment
Picornain 2A inhibitor
Antiischemic, cerebral
Dimethylargininase inhibitor
Alopecia treatment
Tripeptidyl-peptidase I inhibitor
Pancreatic elastase inhibitor
Diabetic neuropathy treatment
Dactylisin inhibitor
HCV IRES inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Procollagen C-endopeptidase inhibitor
5 Hydroxytryptamine uptake stimulant
Fusarinine-C ornithinesterase inhibitor
Vascular adhesion protein 1 inhibitor
Thermitase inhibitor
Cl--transporting ATPase inhibitor
Yeast ribonuclease inhibitor
Proteasome endopeptidase complex inhibitor
Pterin deaminase inhibitor
Antialcoholic
Cerevisin inhibitor
Leukotriene-C4 synthase inhibitor
Diamine N-acetyltransferase inhibitor
Endopeptidase La inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Kallikrein inhibitor
Acrocylindropepsin inhibitor

Chymosin inhibitor
Saccharopepsin inhibitor
Fibrinolytic
Protein-disulfide reductase (glutathione) inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Myocardial ischemia treatment
Systemic lupus erythematosus treatment
Antieczematic atopic
Nicotinic $\alpha 6\beta 3\beta 4\alpha 5$ receptor antagonist
Antiprotozoal
Venombin A inhibitor
Prion diseases treatment
Phospholipid-translocating ATPase inhibitor
Insulin promoter
Cytoprotectant
Sodium/hydrogen exchanger 5 inhibitor
HIV attachment inhibitor
Picornain 3C inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
Antiviral (Influenza)
Pyroglutamyl-peptidase II inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Beta-ureidopropionase inhibitor
Cell adhesion molecule inhibitor
Antiviral (Influenza A)

Alpha adrenoreceptor agonist

Serralysin inhibitor
Transactivator transcription protein inhibitor
Chitinase inhibitor
CYP2A5 substrate
Phthalate 4,5-dioxygenase inhibitor
Integrin antagonist
RNA-directed RNA polymerase inhibitor
Peptidyl-glycinamidase inhibitor
Pancreatic disorders treatment
Neuropeptide agonist
Cancer procoagulant inhibitor
Lysyl oxidase inhibitor
Hyaluronic acid agonist
Linoleate diol synthase inhibitor
Complement inhibitor
Thimet oligopeptidase inhibitor
Gastrin inhibitor
Furin inhibitor
Diuretic
Aminomuconate-semialdehyde dehydrogenase inhibitor
Falcipain 3 inhibitor
Agmatinase inhibitor
Acetylserotonin O-methyltransferase inhibitor
 Na^+ -transporting two-sector ATPase inhibitor

Kexin inhibitor
Sickle-cell anemia treatment
Aminopeptidase B inhibitor
Membrane integrity agonist
Antiprotozoal (Plasmodium)
4-Nitrophenylphosphatase inhibitor
Antithrombotic
3-Hydroxybenzoate 6-monooxygenase inhibitor
Peptidyl-dipeptidase B inhibitor
Diguandinobutanase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Lysyl endopeptidase inhibitor
Alpha 2 adrenoreceptor agonist
Kallikrein 3 inhibitor
Biotinidase inhibitor
Arylesterase inhibitor
D-Octopine dehydrogenase inhibitor
Follicle-stimulating hormone agonist
CYP2D16 substrate
Adenosine regulator
Antibacterial, ophthalmic
Melanocortin MC-4 agonist
Tripeptide aminopeptidase inhibitor
Antiallergic
Wound healing agent
Glutamate synthase (ferredoxin) inhibitor
Endopeptidase So inhibitor
Albendazole monooxygenase inhibitor
Cystic fibrosis treatment
Muramoyltetrapeptide carboxypeptidase inhibitor
Cytochrome P450 stimulant
Chlordecone reductase inhibitor
CYP2B18 substrate
Myeloblastin inhibitor
Antiasthmatic
Arginine N-succinyltransferase inhibitor
Corticotropin-like
EIF4E expression inhibitor
Histamine agonist
Radioprotector
GABA B receptor agonist
Angiogenesis inhibitor
Angiogenesis stimulant
Factor VIIa inhibitor
Trypanothione-disulfide reductase inhibitor
Opioid kappa 3 receptor antagonist
2-Aminohexano-6-lactam racemase inhibitor
Streptopain inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor

CYP2G1 substrate
Octopamine antagonist
Sodium/hydrogen exchanger inhibitor
Homocitrate synthase inhibitor
Exoribonuclease II inhibitor
Para amino benzoic acid antagonist
Erythropoiesis stimulant
Preneoplastic conditions treatment
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Neuropeptide Y agonist
Gonadotropin antagonist
DNA-3-methyladenine glycosylase I inhibitor
Carboxypeptidase M inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Guanidinobutyrase inhibitor
Septic shock treatment
Cachexia treatment
Neurotensin 1 receptor agonist
Arginine deiminase inhibitor
Cathepsin H inhibitor
Histamine H2 receptor agonist
Nicotinic alpha2beta2 receptor antagonist
Peptidyltransferase inhibitor
Glutamate receptor antagonist
Astacin inhibitor
Arginine decarboxylase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Spermidine dehydrogenase inhibitor
Ribonucleoside triphosphate reductase inhibitor
S-formylglutathione hydrolase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
JAK2 expression inhibitor
Mannose isomerase inhibitor
5 Hydroxytryptamine release inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Anti-Helicobacter pylori
Vasculitis treatment
D-amino-acid dehydrogenase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
Retinoprotector
Antineurogenic pain
Luteinizing hormone-releasing hormone agonist
Carboxypeptidase E inhibitor
Antiprotozoal (Toxoplasma)
Thrombin inhibitor
Fatty-acyl-CoA synthase inhibitor
NMDA receptor antagonist
Cerebrovascular disorders treatment
X-methyl-His dipeptidase inhibitor

Taurine-2-oxoglutarate transaminase inhibitor
Skeletal muscle relaxant
Nitric-oxide synthase stimulant
Antiprotozoal (Coccidial)
Acidifying agent non gastric
Argininosuccinate lyase inhibitor
5 Hydroxytryptamine 2B agonist
Neurotensin receptor antagonist
Streptogrisin A inhibitor
ATP phosphoribosyltransferase inhibitor
Granzyme B inhibitor
Aspartoacylase inhibitor
Thrombolytic
Corneal wound healing stimulator
Ribulose-phosphate 3-epimerase inhibitor
Interleukin 6 antagonist
S-alkylcysteine lyase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Taurine dehydrogenase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Hematopoietic inhibitor
Sulfite oxidase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Meprin A inhibitor
Hyperprolactinemia treatment
CYP2B11 substrate
2-Dehydropantoate aldolase inhibitor
Adenylyl-sulfate reductase inhibitor
Sodium/hydrogen exchanger 3 inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
GABA C receptor agonist
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Candidapepsin inhibitor
Methane monooxygenase inhibitor
Coccolysin inhibitor
DNA polymerase I inhibitor
Antiviral (Hepatitis B)
Thiol oxidase inhibitor
Bone formation stimulant
Leukopoiesis stimulant
Oxygen scavenger
Protein C (activated) inhibitor
Phospholipase C inhibitor
Thymidylate 5'-phosphatase inhibitor
Hematopoietic
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
Folate antagonist
Glycerol-3-phosphate oxidase inhibitor
Manganese peroxidase inhibitor

Thiamine pyridinylase inhibitor
Autophagy inducer
Mucomembranous protector
Cyclic AMP modulator
3C-like protease (Human coronavirus) inhibitor
Deoxyhypusine synthase inhibitor
X-Trp aminopeptidase inhibitor
Choline acetyltransferase stimulant
Kallikrein 13 inhibitor
Neuropeptide Y1 antagonist
Diamine oxidase inhibitor
Antinephritic
GP IIb/IIIa receptor antagonist
Lipid metabolism regulator
Aspartate-ammonia ligase inhibitor
Aldehyde dehydrogenase 2 substrate
Antiviral (Herpes)
Protease activated receptor antagonist
Ubiquitin thiolesterase inhibitor
N-formylmethionyl-peptidase inhibitor
Non-steroidal antiinflammatory agent
Cell adhesion inhibitor
O-aminophenol oxidase inhibitor
Releasing hormone agonist
Amyotrophic lateral sclerosis treatment
Histidine N-acetyltransferase inhibitor
Fragilysin inhibitor
Nuclease inhibitor
Tyrosine kinase stimulant
Monoamine oxidase substrate
Phenylalanine(histidine) transaminase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Iron-cytochrome-c reductase inhibitor
Muscle relaxant
p21-activated kinase 1 inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Alanine-tRNA ligase inhibitor
Acetylenecarboxylate hydratase inhibitor
Ethanolamine oxidase inhibitor
Fructose 5-dehydrogenase inhibitor
Angiotensin II receptor agonist
HIV-1 integrase (Overall Integration) inhibitor
Lysine 2,3-aminomutase inhibitor
Chitosanase inhibitor
PfA-M1 aminopeptidase inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Calpain inhibitor
Thiopurine S-methyltransferase inhibitor
Antiseborrheic
Lipoprotein lipase inhibitor

Polyamine biosynthesis inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Plasminogen activator inhibitor
Protein-synthesizing GTPase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Histidinol dehydrogenase inhibitor
CMP-KDO synthase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Acylcarnitine hydrolase inhibitor
Pancreatic endopeptidase E inhibitor
Formaldehyde transketolase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Glutamate (mGluR5) agonist
Serine-pyruvate transaminase inhibitor
Smooth muscle myosin light chain kinase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Arginine kinase inhibitor
Sodium channel (voltage-gated) blocker
Toll-Like receptor antagonist
DELTA14-sterol reductase inhibitor
Neurolysin inhibitor
Arylsulfate sulfotransferase inhibitor
Leucyltransferase inhibitor
Factor XIa inhibitor
Nitric-oxide synthase inhibitor
CYP3A1 substrate
Antinaupathic
Argininosuccinate synthase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Centromere associated protein inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
K(Ca) 3.1 channel blocker
4-Hydroxymandelate oxidase inhibitor
Factor Xa inhibitor
Aspergillopepsin II inhibitor
Tryptophan 2-monooxygenase inhibitor
Gingipain R inhibitor
Atrolysin A inhibitor
Urokinase inhibitor
CPB protease inhibitor
Ornithine-oxo-acid transaminase inhibitor
Dipeptidyl peptidase I inhibitor
Glutamate-tRNA ligase inhibitor
Neuropeptide FF antagonist
Putrescine carbamoyltransferase inhibitor
Antiprotozoal (Babesia)
Sugar-phosphatase inhibitor
Adrenaline agonist

Endothelial growth factor antagonist
Sleep apnea treatment
CYP3C substrate
Prunasin beta-glucosidase inhibitor
Melanocortin agonist
Inducible nitric-oxide synthase inhibitor
Endopeptidase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Complement C5a chemotactic receptor antagonist
1,4-Alpha-glucan branching enzyme inhibitor
Acetylspermidine deacetylase inhibitor
Carboxypeptidase U inhibitor
Allantoin racemase inhibitor
Neuropeptide FF1 antagonist
Rubredoxin-NAD⁺ reductase inhibitor
[citrate-(pro-3S)-lyase] thiolesterase inhibitor
Sporulation kinase A inhibitor
Cytochrome-b5 reductase substrate
Antihelminthic (Fasciola)
5-Guanidino-2-oxopentanoate decarboxylase inhibitor
Glycine receptor antagonist
Cystinyl aminopeptidase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Thioredoxin inhibitor
Tentoxilysin inhibitor
Nicotine dehydrogenase inhibitor
Arginase inhibitor
Bradykinin agonist
Nardilysin inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
CYP3A2 substrate
Homocysteine desulfhydrase inhibitor
Malate oxidase inhibitor
Transketolase inhibitor
Neuropeptide antagonist
Glucuronolactone reductase inhibitor
Styrene-oxide isomerase inhibitor
Interleukin 2 antagonist
Tryptase inhibitor
Dihydrodipicolinate synthase inhibitor
Loop diuretic
Superoxide dismutase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Phosphorylase kinase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Protease activated receptor 1 antagonist
Histamine release stimulant
Adrenergic
Oxidizing agent
Bradykinin B2 receptor agonist

N-hydroxyarylamine O-acetyltransferase inhibitor
5 Hydroxytryptamine 3 agonist
CYP2C10 substrate
Histidine kinase inhibitor
Homogentisate 1,2-dioxygenase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Sodium/calcium exchanger 1 inhibitor
Saluretic
Angiotensin agonist
Tyrosine 3 hydroxylase inhibitor
Chaperonin ATPase inhibitor
CYP1A2 inducer
Assemblin inhibitor
Vascular (periferal) disease treatment
Amino-acid N-acetyltransferase inhibitor
Selenocysteine lyase inhibitor
Pediculicide
Choline-phosphate cytidyltransferase inhibitor
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
Bontoxilysin inhibitor
Homospermidine synthase inhibitor
5 Hydroxytryptamine 7S antagonist
Antiprotozoal (Trichomonas)
Free radical scavenger
Thiol protease inhibitor
Cell wall synthesis inhibitor
Antiviral (CMV)
Fructan beta-fructosidase inhibitor
Gelatinase inhibitor
Pyroglutamyl-peptidase I inhibitor
HMGCS2 expression enhancer
Glucuronate isomerase inhibitor
3-Cyanoalanine hydratase inhibitor
Beta-cyclopiazonate dehydrogenase inhibitor
Chloride channel activator
Carboxypeptidase B inhibitor
VLA-4 antagonist
N-Acyl-D-amino-acid deacylase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Immunostimulant
Lactaldehyde reductase (NADPH) inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Bradykinin antagonist
Platelet aggregation stimulant
Opine dehydrogenase inhibitor
Aminopeptidase microsomal inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP⁺) inhibitor
Kynureninase inhibitor

Vitronectin receptor antagonist
Uterine stimulant
Gamma-glutamyltransferase inhibitor
Bradykinin B2 receptor antagonist
Kidney function stimulant
Cutinase inhibitor
Mucolytic
CYP2C19 inducer
Anticholelithogenic
Glutamate N-acetyltransferase inhibitor
Nicotinate dehydrogenase inhibitor
Neurotensin 1 receptor antagonist
GST M substrate
Calcium-sensing receptor agonist
DOPA decarboxylase inhibitor
Magnolysin inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Carnosine synthase inhibitor
Asparagine-tRNA ligase inhibitor
Heart failure treatment
Aminopeptidase N inhibitor
Uric acid excretion stimulant
Arginyltransferase inhibitor
Matriptase inhibitor
Histidine ammonia-lyase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Neurotensin receptor agonist
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Cytochrome-b5 reductase inhibitor
Factor VII inhibitor
Creatininase inhibitor
Antiseptic
Cystathionine beta-synthase inhibitor
Inulinase inhibitor
Thymidine kinase 1 inhibitor
Secretase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Radiosensitizer
Glutamine synthetase inhibitor
Insulin secretagogues
Excitatory amino acid transporter EAAC1 inhibitor
Melatonin 3 antagonist
MAP-kinase-activated kinase 1 inhibitor
Platelet adhesion inhibitor
Aspergillopepsin I inhibitor
Urease inhibitor
Lysine carboxypeptidase inhibitor
Trypsin inhibitor
CYP2D1 substrate

HDL-cholesterol increasing
Thiamine-triphosphatase inhibitor
Spasmolytic
Neurotensin 2 receptor antagonist
Glucose oxidase inhibitor
Melanocortin antagonist
3-Hydroxyanthranilate oxidase inhibitor
Melanocortin 4 antagonist
Glutamate release inhibitor
Neuropeptide Y1 agonist
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Allantoicase inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
Threonine ammonia-lyase inhibitor
Vasoprotector
Acid-sensing ion channel blocker
Mitochondrial processing peptidase inhibitor
Neuronal nitric-oxide synthase inhibitor
Glycolate dehydrogenase inhibitor
Dihydropteroate synthase inhibitor
Ornithine carbamoyltransferase inhibitor
Aryl hydrocarbon receptor agonist
Metabolic disease treatment
Aspartate-ammonia ligase (ADP-forming) inhibitor
Omega-amidase inhibitor
Tryptophan transaminase inhibitor
Anticonvulsant
CYP1A inducer
Sodium/hydrogen exchanger 1 inhibitor
Glyoxylate reductase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Asparaginyl endopeptidase inhibitor
Spermidine synthase inhibitor
Allantoate deiminase inhibitor
Transcription factor NF kappa A inhibitor
Isopenicillin-N synthase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Flavin-containing monooxygenase substrate
Tpr proteinase (Porphyromonas gingivalis) inhibitor
CTGF expression inhibitor
Antibiotic Glycopeptide-like
Glutamine-tRNA ligase inhibitor
Gluconate 5-dehydrogenase inhibitor
Choline-sulfatase inhibitor
Complement factor 1 inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Chenodeoxycholytaurine hydrolase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor

NMDA receptor polyamine site agonist
Gastrointestinal motility stimulant
All-trans-retinyl-palmitate hydrolase inhibitor
Anthrax lethal factor inhibitor
[phosphorylase] phosphatase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Aldehyde oxidase inhibitor
CYP4A11 substrate
Tumour necrosis factor antagonist
Plasmin inhibitor
DELTA24-sterol reductase inhibitor
Polygalacturonase inhibitor
Bombesin 2 receptor antagonist
GST T substrate
GST T1-1 substrate
Carnitinamidase inhibitor
Amine dehydrogenase inhibitor
Menstruation disorders treatment
8-oxodGTPase stimulant
2-Haloacid dehalogenase inhibitor
Phenol O-methyltransferase inhibitor
Glucagon-like peptide 1 agonist
Cellulose 1,4-beta-cellobiosidase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
H⁺-exporting ATPase inhibitor
Glutamate synthase (NADPH) inhibitor
Vanilloid 1 agonist
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Protein kinase B gamma inhibitor
Asparaginase inhibitor
Protease inhibitor
3-Methylbutanal reductase inhibitor
Endothelial nitric-oxide synthase inhibitor
Arginine-tRNA ligase inhibitor
Farnesoid X receptor antagonist
Oxytocin antagonist
Potassium channel small-conductance Ca-activated 3 activator
Sodium/calcium exchanger inhibitor
Acetylcholinesterase inhibitor
VCAM-1 antagonist
D-stereospecific aminopeptidase inhibitor
Glutathione peroxidase inhibitor
Uterine relaxant
VCAM antagonist
CYP7 inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
MO15-related protein kinase Pfmrk inhibitor
Fucosterol-epoxide lyase inhibitor
Histamine H1 receptor agonist
GRP78 expression inhibitor

Arylmalonate decarboxylase inhibitor
Integrin alpha2beta1 antagonist
N-acetylneuraminate 4-O-acetyltransferase inhibitor
NMDA 2A receptor antagonist
Phosphoinositide 5-phosphatase inhibitor
Oryzin inhibitor
Prephenate dehydratase inhibitor
Cytosole dipeptidase inhibitor
Nav1.7 sodium channel blocker
CYP19A1 expression inhibitor
3-Phytase inhibitor
Meprin B inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Neuropeptide Y antagonist
Melatonin 5 antagonist
Chitin synthase inhibitor
Cathepsin L inhibitor
Falcipain 2 inhibitor
Falcipain inhibitor
NMDA receptor glycine site agonist
Saccharolysin inhibitor
Integrin alphaVbeta5 antagonist
Glucosyl transferase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Epithelial sodium channel blocker
Antihypercholesterolemic
Cyclomaltodextrinase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Pyruvate decarboxylase inhibitor
Acylaminoacyl-peptidase inhibitor
Urolithiasis treatment
Prokineticin receptor 1 antagonist
Procollagen N-endopeptidase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Glutamin-(asparagin-)ase inhibitor
Glycine C-acetyltransferase inhibitor
Integrin alpha5beta1 antagonist

Attention deficit/hyperactivity disorder treatment

Ferredoxin hydrogenase inhibitor
Nav1.2 sodium channel blocker
Purinergic P2X antagonist
Dihydrouracil oxidase inhibitor
CYP4A2 substrate
Neuraminidase inhibitor
Interleukin 10 antagonist
Thymidine kinase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Dipeptidyl peptidase II inhibitor
Potassium channel KCNQ blocker

CYP1A1 inducer
Macrophage scavenger receptor antagonist
Vasopressin 1B antagonist
Amiloride-sensitive cation channel 3 blocker
Beta-N-acetylgalactosaminidase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Methionine decarboxylase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Putrescine oxidase inhibitor
UDP-N-acetylmuramate dehydrogenase inhibitor
Glutamate (mGluR6) antagonist
TRPA1 antagonist
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Neuraminidase (influenza) inhibitor
Integrin alphaVbeta1 antagonist
4-Hydroxyproline epimerase inhibitor
Scytalone dehydratase inhibitor
Phosphorylase a inhibitor
Glutaminy-peptide cyclotransferase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Dopamine release stimulant
p21-activated kinase inhibitor
Homoserine O-succinyltransferase inhibitor
Antirickettsial
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
NMDA 2 receptor antagonist
Stroke treatment
Antiviral (Adenovirus)
Cysteine desulfurase inhibitor
Adamalysin inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Tryptase 1 inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Rhizopuspepsin inhibitor
Heme oxygenase inhibitor
Fibrosis treatment
Integrin alpha5beta6 antagonist
Potassium channel intermediate-conductance Ca-activated blocker
Shikimate O-hydroxycinnamoyltransferase inhibitor
NMDA receptor agonist
Tubuliny-Tyr carboxypeptidase inhibitor
Carnitine O-octanoyltransferase inhibitor
Sodium/hydrogen exchanger 2 inhibitor
Neuraminidase (Influenza B) inhibitor
ADP-thymidine kinase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Amino-acid racemase inhibitor
Somatostatin agonist
1,4-Lactonase inhibitor

SMN2 expression enhancer
 Hydroxylamine oxidase inhibitor
 S-adenosyl-L-methionine decarboxylase inhibitor
 Histidine-tRNA ligase inhibitor
 Lysosomal Pro-X carboxypeptidase inhibitor
 Sedoheptulose-bisphosphatase inhibitor
 Carnitine dehydratase inhibitor
 Integrin alphaVbeta6 antagonist
 Transthyretin amyloid fibril formation inhibitor
 CC chemokine 4 receptor antagonist
 Aryl-alcohol dehydrogenase inhibitor
 Antineurotic
 Xylose isomerase inhibitor
 GABA aminotransferase inhibitor
 Antidiuretic hormone agonist
 Queuine tRNA-ribosyltransferase inhibitor
 Check point kinase 2 inhibitor
 Glycerol dehydrogenase (NADP+) inhibitor
 KiSS-1 receptor agonist
 Transcription factor STAT3 inhibitor
 Ethanolamine-phosphate cytidyltransferase inhibitor
 Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor

Ibuprofen

Molecular Mechanism (initial) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

Molecular Mechanism (repurposed) :

prostaglandin G/H synthase 2 inhibitor

prostaglandin G/H synthase 1 inhibitor

initial indication(s):

inflammation

Repurposed indication(s):

patent ductus arteriosus

Predicted Activities

HIF1A expression inhibitor

Antiinflammatory

Cyclooxygenase 3 inhibitor

Anesthetic general

N-formylmethionyl-peptidase inhibitor

Fibrinolytic

Testosterone 17beta-dehydrogenase (NADP+) inhibitor

Linoleate diol synthase inhibitor

Phobic disorders treatment

Antipyretic

Ubiquinol-cytochrome-c reductase inhibitor

Alkenylglycerophosphocholine hydrolase inhibitor

Oxidoreductase inhibitor

Mucomembranous protector

UGT2B1 substrate
Polyporopepsin inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
CYP2J substrate
Insulin promoter
Antieczematic
Acylcarnitine hydrolase inhibitor
Fragilysin inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
CYP2J2 substrate
Alkylacetylgllycerophosphatase inhibitor
Glutamyl endopeptidase II inhibitor
CYP2C8 substrate
Pseudolysin inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
Antiseborrheic
Lipoprotein lipase inhibitor
Chlordecone reductase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Carboxypeptidase Taq inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Lipid metabolism regulator
5-O-(4-coumaroyl)-D-quinat 3'-monooxygenase inhibitor
Proteasome ATPase inhibitor
Dimethylargininase inhibitor
Sugar-phosphatase inhibitor
Omptin inhibitor
Biotinidase inhibitor
NADH kinase inhibitor
Preneoplastic conditions treatment
CYP2C9 substrate
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Opine dehydrogenase inhibitor
Fusarinine-C ornithinesterase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Arginine 2-monooxygenase inhibitor
Limulus clotting factor B inhibitor
Adenomatous polyposis treatment
Electron-transferring-flavoprotein dehydrogenase inhibitor
Aspartate-ammonia ligase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
Antisecretoric
Prostaglandin-E2 9-reductase inhibitor
Dextranase inhibitor
Platelet aggregation stimulant

Aspulvinone dimethylallyltransferase inhibitor
Antihypoxic
CYP2C substrate
Arylmalonate decarboxylase inhibitor
Fibrinogen receptor antagonist
N-Acyl-D-amino-acid deacylase inhibitor
Carminative
Fibrolase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Macrophage colony stimulating factor agonist
Glutarate-semialdehyde dehydrogenase inhibitor
Pullulanase inhibitor
Lysostaphin inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
UGT2B substrate
Creatininase inhibitor
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
1,4-Lactonase inhibitor
Acetylesterase inhibitor
Protein-glutamate methylesterase inhibitor
Mucositis treatment
UGT1A4 substrate
Exoribonuclease II inhibitor
Non-steroidal antiinflammatory agent
Indoleacetaldoxime dehydratase inhibitor
Sphinganine kinase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Gluconate 5-dehydrogenase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Tryptophan transaminase inhibitor
Phenol O-methyltransferase inhibitor
CYP2E1 inducer
Venombin AB inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Lysine 2,3-aminomutase inhibitor
Antipruritic, allergic
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
X-methyl-His dipeptidase inhibitor
Acylaminoacyl-peptidase inhibitor
UGT1A substrate
Gastrin inhibitor
Aminoacylase inhibitor
L-glucuronate reductase inhibitor
Feruloyl esterase inhibitor
Endopeptidase So inhibitor
Cathepsin T inhibitor

CYP19A1 expression inhibitor
Pitrilysin inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Antihypercholesterolemic
Polyamine-transporting ATPase inhibitor
Nootropic
Gluconolactonase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Membrane permeability inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Formaldehyde transketolase inhibitor
Nitrite reductase (NO-forming) inhibitor
D-lactaldehyde dehydrogenase inhibitor
Cholesterol antagonist
Pancreatic elastase inhibitor
Serine 3-dehydrogenase inhibitor
Mannitol-1-phosphatase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)l asparagine amidase inhibitor
Antipruritic
Phosphoinositide 5-phosphatase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Acetylgalactosaminy-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminytransferase inhibitor
Carboxylate reductase inhibitor
UGT1A3 substrate
Cholestanetriol 26-monooxygenase inhibitor
Coccolysin inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Urethanase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
CYP2C10 substrate
N-(long-chain-acyl)ethanolamine deacylase inhibitor
GST A substrate
UDP-glucuronosyltransferase substrate
4-Hydroxyglutamate transaminase inhibitor
Tryptophanamidase inhibitor
DELTA14-sterol reductase inhibitor
Hydrogen dehydrogenase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Taurine dehydrogenase inhibitor
Valine decarboxylase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminytransferase inhibitor
CYP2C19 substrate
Antinociceptive
5 Hydroxytryptamine release stimulant
ADP-thymidine kinase inhibitor
Glyoxylate reductase inhibitor

6-Pyruvoyltetrahydropterin synthase inhibitor
NADPH peroxidase inhibitor
CYP2C8 inhibitor
2-Dehydropantoate 2-reductase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Methanol dehydrogenase inhibitor
Arylesterase inhibitor
CYP3A1 substrate
Glutathione thiolesterase inhibitor
Sclerosant
Fructose 5-dehydrogenase inhibitor
Mitochondrial processing peptidase inhibitor
Arylformamidase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Cl--transporting ATPase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Plasmanyethanolamine desaturase inhibitor
Gingipain K inhibitor
Amyloid beta precursor protein antagonist
Pterin deaminase inhibitor
Antiarthritic
Fatty-acyl-CoA synthase inhibitor
Lactate 2-monooxygenase inhibitor
UGT1A9 substrate
S-alkylcysteine lyase inhibitor
Chenodeoxycholoyltaurine hydrolase inhibitor
UGT2B9 substrate
Flavin-containing monooxygenase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Antiinflammatory, ophthalmic
Long-chain-fatty-acid-CoA ligase inhibitor
CYP2D16 substrate
Kidney function stimulant
CYP3A5 substrate
Aspergillopepsin I inhibitor
2-Oxoglutarate decarboxylase inhibitor
Phosphoenolpyruvate mutase inhibitor
Muscular dystrophy treatment
tRNA nucleotidyltransferase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Phenylpyruvate decarboxylase inhibitor
CYP3A substrate
Phosphatase inhibitor
CYP2H substrate
3-Phytase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
CYP3A4 substrate
Sulfite dehydrogenase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor

UGT1A6 substrate
Antiuremic
Leukotriene-B4 20-monooxygenase inhibitor
CYP7 inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
CYP3A2 substrate
Sulfite reductase inhibitor
Dimethylmaleate hydratase inhibitor
Leucine dehydrogenase inhibitor
Glycolate dehydrogenase inhibitor
Carboxypeptidase D inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Nardilysin inhibitor
L-glutamate oxidase inhibitor
Enteropeptidase inhibitor
Mucinaminyserine mucinaminidase inhibitor
tRNA-pseudouridine synthase I inhibitor
Erythropoiesis stimulant
Formate-dihydrofolate ligase inhibitor
Immunosuppressant
Alcohol O-acetyltransferase inhibitor
ICAM1 expression inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
UGT1A1 substrate
H⁺-exporting ATPase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Pectin lyase inhibitor
Fucosterol-epoxide lyase inhibitor
Valine dehydrogenase (NADP⁺) inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Hypolipemic
Shikimate O-hydroxycinnamoyltransferase inhibitor
Aminopeptidase Y inhibitor
Aspartate-tRNA ligase inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Tyrosine-ester sulfotransferase inhibitor
Catalase inhibitor
Expectorant
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Thiosulfate dehydrogenase inhibitor
Bontoxilysin inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Glutamate-tRNA ligase inhibitor
Mitochondrial intermediate peptidase inhibitor
3-Isopropylmalate dehydratase inhibitor

Alcohol dehydrogenase [NAD(P)+] inhibitor
Dipeptidase E inhibitor
Cytochrome-b5 reductase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
GABA aminotransferase inhibitor
Hydroxylamine reductase (NADH) inhibitor
Malate dehydrogenase (acceptor) inhibitor
Antihyperlipoproteinemic
Phospholipid-translocating ATPase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Acetylcholine neuromuscular blocking agent
CYP4A11 substrate
Alopecia treatment
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Snopalysin inhibitor
UGT2B4 substrate
Uroporphyrinogen-III synthase inhibitor
Aryldialkylphosphatase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Arylsulfate sulfotransferase inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Carbon-monoxide dehydrogenase inhibitor
Thymidylate 5'-phosphatase inhibitor
Cholesterol oxidase inhibitor
Malate oxidase inhibitor
Trimethylamine-oxide aldolase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
N-acetylneuraminase synthase inhibitor
Glycerol-ether monooxygenase inhibitor
Apyrase inhibitor
TP53 expression enhancer
Dermatologic
Antipsoriatic
Bisphosphoglycerate phosphatase inhibitor
Neurotransmitter antagonist
Alkane 1-monooxygenase inhibitor
3-Cyanoalanine hydratase inhibitor
Fructan beta-fructosidase inhibitor
Serine-pyruvate transaminase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Picornain 3C inhibitor
N-benzoyloxycarbonylglycine hydrolase inhibitor
Penicillin amidase inhibitor

D-alanine 2-hydroxymethyltransferase inhibitor
Ecdysone 20-monooxygenase inhibitor
Antipruritic, non-allergic
Leukopoiesis stimulant
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Hydroxylamine oxidase inhibitor
Renal tissue kallikrein inhibitor
S-formylglutathione hydrolase inhibitor
Antiviral (Rhinovirus)
Membrane permeability enhancer
Glucose oxidase inhibitor
Leucolysin inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Complement factor D inhibitor
Mucolytic
Cyclomaltodextrinase inhibitor
RNA-directed RNA polymerase inhibitor
Phosphatidylglycerophosphatase inhibitor
Superoxide dismutase inhibitor
Membrane integrity antagonist
Limulus clotting factor C inhibitor
Cyanoalanine nitrilase inhibitor
L-amino-acid oxidase inhibitor
Peroxidase inhibitor
Inulinase inhibitor
Alanine-tRNA ligase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
IgA-specific metalloendopeptidase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Phosphatidylserine decarboxylase inhibitor
Bile-salt sulfotransferase inhibitor
Threonine aldolase inhibitor
UGT2B7 substrate
Analgesic
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Ornithine cyclodeaminase inhibitor
Cell adhesion molecule inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Phenylalanine dehydrogenase inhibitor
Mannose isomerase inhibitor
Horriylsin inhibitor
UGT2B17 substrate
Signal peptidase I inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
Histamine release inhibitor

Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Platelet aggregation inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Licheninase inhibitor
Phenylacetate-CoA ligase inhibitor
2-Enoate reductase inhibitor
Glucuronate isomerase inhibitor
Sulfur reductase inhibitor
Pyruvate decarboxylase inhibitor
Acetylornithine deacetylase inhibitor
Gly-X carboxypeptidase inhibitor
Transketolase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
APOA1 expression enhancer
Glycine dehydrogenase (decarboxylating) inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Ferrochelataase inhibitor
Bothrolysin inhibitor
Glyoxylate oxidase inhibitor
Aspartyltransferase inhibitor
CYP2C18 substrate
Tyrosine 3 hydroxylase inhibitor
Indanol dehydrogenase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Manganese peroxidase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Histidinol-phosphatase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Calcium-sensing receptor agonist
Antiviral (Picornavirus)
Dolichyl-phosphatase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Chitinase inhibitor
Muramoyltetrapeptide carboxypeptidase inhibitor
Meprin B inhibitor
Lysase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Rubredoxin-NAD+ reductase inhibitor
Carnitinamidase inhibitor
Fibroblast growth factor agonist
Creatinine deaminase inhibitor
5 Hydroxytryptamine release inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Interferon alpha agonist
Aryl sulfotransferase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Urease inhibitor

Cytoprotectant
Aldehyde dehydrogenase (NADP+) inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
3-Oxoadipate enol-lactonase inhibitor
CYP3A3 substrate
Oxygen scavenger
D-xylulose reductase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Levanase inhibitor
EIF4E expression inhibitor
GABA C receptor agonist
Fumarate reductase (NADH) inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
UGT1A10 substrate
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Benzoate-CoA ligase inhibitor
BRAF expression inhibitor
Diisopropyl-fluorophosphatase inhibitor
Aconitate decarboxylase inhibitor
Tentoxilysin inhibitor
Methane monooxygenase inhibitor
General pump inhibitor
5 Hydroxytryptamine uptake stimulant
Glutathione dehydrogenase (ascorbate) inhibitor
Polygalacturonase inhibitor
3,4-Dihydroxy-9,10-secoandrost-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Aspartoacylase inhibitor
Cyclic AMP agonist
Aryl-alcohol dehydrogenase inhibitor
CYP2B11 substrate
Hematopoietic inhibitor
Peptide agonist
Platelet adhesion inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Antimyopathies
Chitosanase inhibitor
Pappalysin-1 inhibitor
Myc inhibitor
Dactylisin inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
Membrane integrity agonist
Peroxidase substrate
4-Hydroxyproline epimerase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Glycine amidinotransferase inhibitor
CYP3A inducer
NAD+ synthase (glutamine-hydrolysing) inhibitor
Envelysin inhibitor
Pyroglutamyl-peptidase II inhibitor

Pyroglutamyl-peptidase I inhibitor
Hyaluronic acid agonist
Procollagen N-endopeptidase inhibitor
Bisphosphoglycerate mutase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Inflammatory Bowel disease treatment
(S)-3-amino-2-methylpropionate transaminase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Metallo-carboxypeptidase D inhibitor
GABA B receptor agonist
Ethanolamine-phosphate cytidyltransferase inhibitor
Calcium regulator
Glycerol-1-phosphatase inhibitor
N-acylmannosamine kinase inhibitor
Adenylyl-sulfate reductase inhibitor
Aureolysin inhibitor
Cyclamate sulfohydrolase inhibitor
Leukotriene-C4 synthase inhibitor
Cerevisin inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Calcium channel (voltage-sensitive) activator
Atrolysin C inhibitor
CYP2C19 inducer
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Nitrile hydratase inhibitor
Transcription factor NF kappa A inhibitor
Oryzin inhibitor
Betaine-aldehyde dehydrogenase inhibitor
Aspergillus nuclease S1 inhibitor
Saccharolysin inhibitor
Immunomodulator
Alcohol dehydrogenase (acceptor) inhibitor
Antihelminthic (Nematodes)
CYP3A4 inducer
Endothelial growth factor antagonist
UGT1A8 substrate
Histidine N-acetyltransferase inhibitor
Spermidine dehydrogenase inhibitor
Cutinase inhibitor
Thermitase inhibitor
Creatinase inhibitor
Peptidylamidoglycolate lyase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Antinaupathic
Gout treatment
Linoleoyl-CoA desaturase inhibitor
Antiamyloidogenic
CYP2A4 substrate

Photosensitizer
Aldehyde ferredoxin oxidoreductase inhibitor
Cancer associated disorders treatment
1,2-alpha-L-fucosidase inhibitor
Thromboxane B2 antagonist
Acyl-lysine deacylase inhibitor
Prunasin beta-glucosidase inhibitor
Clavamate synthase inhibitor
Peptidyl-dipeptidase B inhibitor
Antiinfective
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
CYP2C9 inducer
Allantoate deiminase inhibitor
N-acetyllactosamine synthase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
CYP2C12 substrate
4-Coumarate-CoA ligase inhibitor
Rhodotorulapepsin inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
AR expression inhibitor
Morphine 6-dehydrogenase inhibitor
Prostate disorders treatment
ATPase inhibitor
Atrolysin A inhibitor
CYP4A substrate
Diiodophenylpyruvate reductase inhibitor
CYP4A2 substrate
Anthranilate-CoA ligase inhibitor
Phospholipase C inhibitor
Procollagen C-endopeptidase inhibitor
Proliferative diseases treatment
Spasmolytic, Papaverin-like
Retinoic acid metabolism inhibitor
Pin1 inhibitor
Tropinesterase inhibitor
Anesthetic
Thioredoxin inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
P-glycoprotein substrate
Nicotinic alpha2beta2 receptor antagonist
Atherosclerosis treatment
Tripeptide aminopeptidase inhibitor
Myosin ATPase inhibitor
Prolyl aminopeptidase inhibitor
HMOX1 expression enhancer
Glycerol 2-dehydrogenase (NADP+) inhibitor
Threonine ammonia-lyase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Antithrombotic
Camphor 1,2-monooxygenase inhibitor

Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Gallate decarboxylase inhibitor
4-Nitrophenylphosphatase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Lactaldehyde reductase inhibitor
Hydroxylamine reductase inhibitor
Hepatoprotectant
D-2-hydroxy-acid dehydrogenase inhibitor
Carboxymethylenebutenolidase inhibitor
Acetate kinase inhibitor
Cycloartenol synthase inhibitor
MAP kinase stimulant
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Ketol-acid reductoisomerase inhibitor
Choleretic
Tauropine dehydrogenase inhibitor
Antiviral (Influenza)
Eye irritation, inactive
X-Pro dipeptidase inhibitor
Ubiquitin thiolesterase inhibitor
Brachyurin inhibitor
Fibroblast growth factor 1 agonist
Malate dehydrogenase inhibitor
3-Aminobutaryl-CoA ammonia-lyase inhibitor
Cyclohexanone monooxygenase inhibitor
Alpha-glucuronidase inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Pediculicide
Choloylglycine hydrolase inhibitor
4-Hydroxymandelate oxidase inhibitor
CYP2B5 substrate
Acetylserotonin O-methyltransferase inhibitor
Lombricine kinase inhibitor
Gametolysin inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
2-Aminoadipate transaminase inhibitor
3-Methylbutanal reductase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
D-amino-acid dehydrogenase inhibitor
Hydroxymethylbilane synthase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Antiparkinsonian, tremor relieving
CYP4B substrate
3-Chloro-D-alanine dehydrochlorinase inhibitor
Orotate reductase (NADH) inhibitor

Branched-chain-amino-acid transaminase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Antiprotozoal (Coccidial)
Tryptophan 2,3-dioxygenase inhibitor
Dihydroxy-acid dehydratase inhibitor
Antianorexic
Rhizopuspepsin inhibitor
Subtilisin inhibitor
Guanidinoacetase inhibitor
Trans-pentaprenyltranstransferase inhibitor
MMP9 expression inhibitor
Oxidizing agent
CYP2C9 inhibitor
Acetolactate synthase inhibitor
Neuropsin inhibitor
Beta-ureidopropionase inhibitor
Retinyl-palmitate esterase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Thyroxine 5-deiodinase inhibitor
L-threonine 3-dehydrogenase inhibitor
2-Haloacid dehalogenase inhibitor
AICAR transformylase inhibitor
Styrene-oxide isomerase inhibitor
Uric acid excretion stimulant
Aminomuconate-semialdehyde dehydrogenase inhibitor
Cytosol alanyl aminopeptidase inhibitor
Serralysin inhibitor
Proteasome endopeptidase complex inhibitor
Aminopeptidase B inhibitor
Acidifying agent non gastric
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Antileprosy
D-cysteine desulfhydrase inhibitor
Osteoarthritis treatment
Peptidyl-glycinamidase inhibitor
Benzoylformate decarboxylase inhibitor
Vasoprotector
Thiosulfate sulfurtransferase inhibitor
Oxytocic
Radioprotector
Stromelysin 2 inhibitor
Alpha-pinene-oxide decyclase inhibitor
Mevalonate kinase inhibitor
Glutaminase inhibitor
Anticarcinogenic
Glucan 1,4-beta-glucosidase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Tripeptidyl-peptidase I inhibitor
Choline dehydrogenase inhibitor

Allophanate hydrolase inhibitor
CYP2C29 substrate
Sulfite oxidase inhibitor
Picornain 2A inhibitor
X-His dipeptidase inhibitor
CC chemokine receptor 2B antagonist
Centromere associated protein inhibitor
Antiinflammatory, intestinal
Alpha-N-arabinofuranosidase inhibitor
TNF expression inhibitor
H⁺-transporting two-sector ATPase inhibitor
Maleate isomerase inhibitor
Phenylalanine decarboxylase inhibitor
Protein-arginine deiminase inhibitor
Nitrate reductase (cytochrome) inhibitor
Yeast ribonuclease inhibitor
Gingipain R inhibitor
Trimethyllysine dioxygenase inhibitor
Antidyskinetic
Interleukin 8 antagonist
Cysteine desulfurase inhibitor
Cytosole dipeptidase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Cytochrome-c3 hydrogenase inhibitor
CYP4F2 substrate
Nicotine dehydrogenase inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Chaperonin ATPase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Glutamine-pyruvate transaminase inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Raynaud's phenomenon treatment
Inorganic diphosphatase inhibitor
CYP4B1 substrate
Antihyperammonemic
Thimet oligopeptidase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Spasmolytic
Carnosine synthase inhibitor
Galactolipase inhibitor
Acrosin inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Oligopeptidase B inhibitor
Sulfur dioxygenase inhibitor
Lysine 2-monooxygenase inhibitor
Anticataract
Phenylacetaldehyde dehydrogenase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Thiamine pyridinylase inhibitor
Prenyl-diphosphatase inhibitor

Cyclooxygenase substrate
Isopenicillin-N synthase inhibitor
CYP17 inhibitor
Farnesyltranstransferase inhibitor
Analgesic stimulant
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
UGT1A7 substrate
Antihelmintic
Lysyl oxidase inhibitor
CYP2D15 substrate
Sterol 3-beta-glucosyltransferase inhibitor
Gamma-glutamyltransferase inhibitor
Antitussive
Cholesterol synthesis inhibitor
Nitric oxide scavenger
Tryptophan dimethylallyltransferase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Selenocysteine lyase inhibitor
Adrenaline release stimulant
1,4-Alpha-glucan branching enzyme inhibitor
D-glutamate oxidase inhibitor
Allantoinase inhibitor
Aspartyl aminopeptidase inhibitor
Farnesoid X receptor antagonist
Undecaprenyl-diphosphatase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
Cholate-CoA ligase inhibitor
Clostripain inhibitor
Succinate dehydrogenase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Venom exonuclease inhibitor
DOPA decarboxylase inhibitor
Aldehyde dehydrogenase (NAD+) inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Serum-glucocorticoid regulated kinase 1 inhibitor

Cyclooxygenase 1 inhibitor

Thrombolytic
Formaldehyde dehydrogenase inhibitor
Antiparkinsonian, rigidity relieving
Nitrite reductase [NAD(P)H] inhibitor
Xenobiotic-transporting ATPase inhibitor
Penicillopepsin inhibitor
Intermittent claudication treatment
FMO1 substrate
CYP2E1 substrate
Lipoprotein disorders treatment
Leucine transaminase inhibitor
Phosphopantothenoylecysteine decarboxylase inhibitor

Arylacetonitrilase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Phosphatidate cytidyltransferase inhibitor
Antiviral (Adenovirus)
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Mandelate 4-monooxygenase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor
Deoxyribose-phosphate aldolase inhibitor
4-Phytase inhibitor
JAK2 expression inhibitor
Tyrosine 2,3-aminomutase inhibitor
Salicylate 1-monooxygenase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Antitoxic
Reductant
CYP3C substrate
Uterine relaxant
Hyponitrite reductase inhibitor
2-Methylcitrate dehydratase inhibitor
Antiviral (CMV)
Ribitol 2-dehydrogenase inhibitor
Antifungal
Shikimate 5-dehydrogenase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Iron-cytochrome-c reductase inhibitor
Vomilenine glucosyltransferase inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor
Neurotrophic factor enhancer
Antiprotozoal (Trypanosoma)
Prephenate dehydrogenase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Aerobactin synthase inhibitor
Sarcosine oxidase inhibitor
Benzaldehyde dehydrogenase (NAD+) inhibitor
Lactose synthase inhibitor
Glycerol dehydratase inhibitor
Candidapepsin inhibitor
Choline-sulfatase inhibitor
CYP2E substrate
Nuclease inhibitor
Dihydropyrimidinase inhibitor
Ferredoxin-nitrite reductase inhibitor
Pantothenase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
2-Aminohexano-6-lactam racemase inhibitor
Carnitine 3-dehydrogenase inhibitor
Vasodilator, peripheral
Endopeptidase La inhibitor

Peptide-tryptophan 2,3-dioxygenase inhibitor
Nicotinate dehydrogenase inhibitor
Antineurogenic pain
Thiol oxidase inhibitor
Arachidonic acid antagonist
Cellulose 1,4-beta-cellobiosidase inhibitor
Antineurotic
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Glycine C-acetyltransferase inhibitor
Anthrax lethal factor inhibitor
Antiparasitic
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
UGT2B28 substrate
Antithyroid
Valine-tRNA ligase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
Glucarate dehydratase inhibitor
Arylsulfatase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Methylaspartate ammonia-lyase inhibitor
Antimetastatic
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Menopausal disorders treatment
Lactase inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Omega-amidase inhibitor
Thiamine-phosphate kinase inhibitor
Uterine stimulant
Arginyltransferase inhibitor
Dementia treatment
Guanidinoacetate kinase inhibitor
Bilirubin oxidase inhibitor
Ethanolaminephosphotransferase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Alpha-amylase inhibitor
Retinol O-fatty-acyltransferase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Deoxyribonuclease I inhibitor
Phosphoinositide phospholipase C inhibitor
L-iduronidase inhibitor
Dichloromuconate cycloisomerase inhibitor
Glutamate 5-kinase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
Beta-cyclopiazonate dehydrogenase inhibitor
NF-E2-related factor 2 stimulant
Hippurate hydrolase inhibitor
Multiple sclerosis treatment
D-lactate dehydrogenase inhibitor
8-Amino-7-oxononanoate synthase inhibitor

SULT1A1 substrate
Serratia marcescens nuclease inhibitor
Trehalose-phosphatase inhibitor
Oxaloacetate tautomerase inhibitor
ATPase stimulant
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Acetoacetate decarboxylase inhibitor
Prolactin inhibitor
Antiviral (Herpes)
L-lysine 6-transaminase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Cyclopentanone monooxygenase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Dynein ATPase inhibitor
Acylglycerone-phosphate reductase inhibitor
UGT2B15 substrate
Cysteine transaminase inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Angiogenesis stimulant
Vanilloid 1 agonist
Apoptosis antagonist
Lymphocytopoiesis inhibitor
Retinol dehydrogenase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Interleukin 2 agonist
Paraoxonase substrate
Ovulation inhibitor
Aldehyde oxidase substrate
Proline dehydrogenase inhibitor
Ophthalmic drug
Antidiabetic
Transforming growth factor beta 1 agonist
Cell adhesion inhibitor
Sphingosine 1-phosphate receptor 1 antagonist
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Ferredoxin hydrogenase inhibitor
Thiamine-triphosphatase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
Gentisate 1,2-dioxygenase inhibitor
HMG CoA synthase inhibitor
Phosphatidate phosphatase inhibitor
CYP1A substrate
Ligase inhibitor
2-Dehydropantoate aldolase inhibitor
Carnitine dehydratase inhibitor
Homogentisate 1,2-dioxygenase inhibitor
Phosphonoacetate hydrolase inhibitor
Interleukin 6 antagonist

Neuropeptide Y4 antagonist
Pyruvate dehydrogenase inhibitor
Asparagine-tRNA ligase inhibitor
Glucuronolactone reductase inhibitor
Antifibrinolytic
Alkylglycerone-phosphate synthase inhibitor
Methionine decarboxylase inhibitor
Sorbitol dehydrogenase inhibitor
Isopenicillin-N epimerase inhibitor
Glycerol dehydrogenase (NADP+) inhibitor
Dopamine release stimulant
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Calpain inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Benzoate 4-monooxygenase inhibitor
Cyclooxygenase inhibitor
Methylglutamate dehydrogenase inhibitor
Furin inhibitor
Glycogen (starch) synthase inhibitor
O-aminophenol oxidase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Fumarylacetoacetase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Glutathione peroxidase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
Angiotensin II receptor agonist
CDK9/cyclin T1 inhibitor
Glutamate N-acetyltransferase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
ATP deaminase inhibitor
RELA expression inhibitor
Aspergillopepsin II inhibitor
Acylphosphatase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Guanidinopropionase inhibitor
Iduronate-2-sulfatase inhibitor
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor
Arylamine N-acetyltransferase inhibitor
Glycine transaminase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Pectate lyase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Galactose oxidase inhibitor
DNA ligase (ATP) inhibitor
Endopeptidase inhibitor
Acute neurologic disorders treatment
Hydroxysteroid dehydrogenase inhibitor

Pantoate 4-dehydrogenase inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
FMO3 substrate
Aldehyde dehydrogenase 2 substrate
CYP2D2 inhibitor
Pancreatic disorders treatment
Diaminopimelate dehydrogenase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
GST M substrate
Lactaldehyde reductase (NADPH) inhibitor
Alanine transaminase inhibitor
Lipoxygenase substrate
Antihematotoxic
Glutamate synthase (ferredoxin) inhibitor
Chemopreventive
Haloalkane dehalogenase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
CYP26A substrate
L-galactonolactone oxidase inhibitor
Homoserine O-succinyltransferase inhibitor
Diphosphomevalonate decarboxylase inhibitor
Gluconate dehydratase inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
Beta-amylase inhibitor
CYP2A1 substrate
L-fuconate dehydratase inhibitor
Glutamin-(asparagin-)ase inhibitor
Dihydrodipicolinate reductase inhibitor
Nicotinamidase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
HIV-2 reverse transcriptase inhibitor
IgA-specific serine endopeptidase inhibitor
Myosin-light-chain-phosphatase inhibitor
Glucose 1-dehydrogenase inhibitor
Sodium/bile acid cotransporter inhibitor
Phosphoserine phosphatase inhibitor
D-proline reductase (dithiol) inhibitor
Lysine decarboxylase inhibitor
Opioid kappa 3 receptor antagonist
Acetylenecarboxylate hydratase inhibitor
Amine dehydrogenase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Mycolysin inhibitor
Retinal dehydrogenase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Aldose reductase substrate
Carboxypeptidase U inhibitor
L-lactate dehydrogenase (cytochrome) inhibitor
Histamine release stimulant
Antiseptic

Myeloblastin inhibitor
CYP2F1 substrate
Antiulcerative
Kexin inhibitor
Allantoicase inhibitor
Cystic fibrosis treatment
CYP2C3 substrate
Lysyl endopeptidase inhibitor
CYP2B6 substrate
N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor
VCAM1 expression inhibitor
Pancreatic endopeptidase E inhibitor
Trimereysin II inhibitor
CYP4A1 substrate
Polyneuridine-aldehyde esterase inhibitor
Chemoprotective
2-Methyleneglutarate mutase inhibitor
Antimycoplasmal
ATP adenylyltransferase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
HIV-1 integrase (Overall Integration) inhibitor
5-Aminolevulinate synthase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Monophenol monooxygenase inhibitor
Aspartate transaminase inhibitor
Serine-phosphoethanolamine synthase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Bacterial leucyl aminopeptidase inhibitor
Diabetic nephropathy treatment
Testosterone 17beta-dehydrogenase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Menstruation disorders treatment
Vascular dementia treatment
Triose-phosphate isomerase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Granzyme A inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
GST T substrate
GST T1-1 substrate
Guanidinobutyrase inhibitor
Loop diuretic
Antitreponemal
Chloride channel blocker
Tryptophan 2-monooxygenase inhibitor
SULT1A3 substrate
Glutamate (mGluR5) agonist
Procollagen-lysine 5-dioxygenase inhibitor

Endothelin-converting enzyme inhibitor
Diiodotyrosine transaminase inhibitor
Choline kinase inhibitor
Growth stimulant
Leishmanolysin inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Alanine carboxypeptidase inhibitor
Riboflavin phosphotransferase inhibitor
Steroid synthesis inhibitor
Protein synthesis stimulant
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Secretase alpha stimulant
Secretase stimulant
Pseudouridylate synthase inhibitor
Muconate cycloisomerase inhibitor
Thiopurine S-methyltransferase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Glutamate uptake inhibitor
ATP phosphoribosyltransferase inhibitor
Cysteine synthase inhibitor
Aminopeptidase I inhibitor
X-Trp aminopeptidase inhibitor
Calcium antagonist
Vasodilator, coronary
Urticaria treatment
Coproporphyrinogen oxidase inhibitor
CYP2B10 substrate
Leukopoiesis inhibitor
Cancer procoagulant inhibitor
Agaricine gamma-glutamyltransferase inhibitor
CYP1A2 substrate
Lipotropic
Homoserine dehydrogenase inhibitor
3'-Nucleotidase inhibitor
CYP2C6 substrate
Keratosis actinic (solar) treatment
Protein-tyrosine sulfotransferase inhibitor
Serine-glyoxylate transaminase inhibitor
L-Serine ammonia-lyase inhibitor
Peptidylglycine monooxygenase inhibitor
Aspartate kinase inhibitor
Phosphoglycerate mutase inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Aspartate racemase inhibitor
Albendazole monooxygenase inhibitor
Cystathionine gamma-lyase inhibitor
D-stereospecific aminopeptidase inhibitor
Thiol S-methyltransferase inhibitor
CYP2A5 substrate

Ornithine-oxo-acid transaminase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
2-Nitropropane dioxygenase inhibitor
Acid phosphatase inhibitor
Malate-CoA ligase inhibitor
Lipid peroxidase inhibitor
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor
Membrane dipeptidase inhibitor
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
Oxalate oxidase inhibitor
Antispirochetal
Macrophage elastase inhibitor
Melanin inhibitor
Imidazoleacetate 4-monooxygenase inhibitor
Gaucher disease treatment
Histidine kinase inhibitor
Vascular adhesion protein 1 inhibitor
Acyl-CoA oxidase inhibitor
CYP2C11 substrate
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Insulin sensitizer
Argininosuccinate synthase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Urolithiasis treatment
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Ganglioside galactosyltransferase inhibitor
Nitrilase inhibitor
Glutamate (mGluR6) antagonist
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Meprin A inhibitor
Antineoplastic (bone cancer)
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Acetolactate decarboxylase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Malate dehydrogenase (NADP⁺) inhibitor
Hyperprolactinemia treatment
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Aromatic-amino-acid transaminase inhibitor
Beta-mannosidase inhibitor
Coagulant
Carboxypeptidase B inhibitor
Lipoprotein lipase stimulant
Purine biosynthesis inhibitor
Arylalkyl acylamidase inhibitor
Lactate-malate transhydrogenase inhibitor
Endo-1,4-beta-xylanase inhibitor

Lysosomal Pro-X carboxypeptidase inhibitor
Antibiotic Glycopeptide-like
Acetoin dehydrogenase inhibitor
Catechol oxidase inhibitor
Maltose-transporting ATPase inhibitor
Glutamine-tRNA ligase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Trimethylamine dehydrogenase inhibitor
Protein kinase stimulant
Pregnane X receptor agonist
Thyroid hormone antagonist
UGT2B10 substrate
Antituberculosic
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Maleate hydratase inhibitor
Antidote
Insulin secretagogues
HDL-cholesterol increasing
(S)-2-Methylmalate dehydratase inhibitor
Agmatinase inhibitor
3-Deoxy-7-phosphoheptulonate synthase inhibitor
Dethiobiotin synthase inhibitor
CYP2G1 substrate
Pyridoxine 4-oxidase inhibitor
UGT1A5 substrate
Chloride peroxidase inhibitor
N-acetylneuraminate lyase inhibitor
Aldosterone antagonist
Glycerophosphocholine cholinephosphodiesterase inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Streptopain inhibitor
Transactivator transcription protein inhibitor
Gestagen antagonist
Caspase 3 inhibitor
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Phloroglucinol reductase inhibitor
Aldehyde oxidase inhibitor
Alcohol dehydrogenase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Dry eye syndrome treatment
D-arabinonolactone oxidase inhibitor
Acetylspermidine deacetylase inhibitor
Carboxypeptidase E inhibitor
Antiacne
Peroxisome proliferator-activated receptor gamma antagonist
P-glycoprotein 1 inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
Gonadotropin antagonist
Cellulase inhibitor

3-Hydroxybutyrate dehydrogenase inhibitor
Arabinose isomerase inhibitor
Asparagine-oxo-acid transaminase inhibitor
Caspase 8 stimulant
Antirickettsial
Levansucrase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Glutamate dehydrogenase inhibitor
Diamine N-acetyltransferase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
Thiol protease inhibitor
Aminopeptidase microsomal inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Uroporphyrinogen decarboxylase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Antinephritic
Phenylalanine 2-monooxygenase inhibitor
Cystinyl aminopeptidase inhibitor
Porphobilinogen synthase inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Propanediol dehydratase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
[phosphorylase] phosphatase inhibitor
Laxative
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Glycine receptor agonist
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
D-alanine transaminase inhibitor
Galactokinase inhibitor
Transcription factor NF kappa B inhibitor
Hematopoietic
Pyruvate carboxylase inhibitor
CXC chemokine 1 receptor antagonist
Glycine N-acyltransferase inhibitor
Glutathione reductase inhibitor
Angiotensin agonist
Urocanate hydratase inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
Antihypotensive
Histone acetyltransferase inhibitor
Vanilloid agonist
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Beta glucuronidase inhibitor
Peroxisome proliferator-activated receptor alpha agonist
Serine carboxypeptidase inhibitor
Oxaloacetate decarboxylase inhibitor

Endonuclease (influenza) inhibitor
Dolichol kinase inhibitor
CYP2B4 substrate
Succinic dehydrogenase inhibitor
CNS active muscle relaxant
Hemostatic
Glucan 1,3-beta-glucosidase inhibitor
CYP4F substrate
Iodide peroxidase inhibitor
Phospholipase A2 inhibitor
Isocitrate dehydrogenase (NADP+) inhibitor
Wound healing agent
Phenylalanine 4-hydroxylase inhibitor
Peroxisome proliferator-activated receptor antagonist
Anti-Helicobacter pylori
Reductase inhibitor
Diabetic neuropathy treatment
Leukocyte elastase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Cardioprotectant
L-lysine oxidase inhibitor
DELTA24-sterol reductase inhibitor
Antiviral (Influenza A)
Argininosuccinate lyase inhibitor
Viral entry inhibitor
Propionate-CoA ligase inhibitor
Acaricide
tRNA adenylyltransferase inhibitor
Xylose isomerase inhibitor
Liver X receptor antagonist
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
D-Octopine dehydrogenase inhibitor
Cyanate hydratase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Phospholipase inhibitor
2-Ethylmalate synthase inhibitor
Aminopeptidase N inhibitor
Prostaglandin E1 antagonist
Acyloxyacyl hydrolase inhibitor
Bcl2 antagonist
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
Sickle-cell anemia treatment
Autoimmune disorders treatment
3C-like protease (Human coronavirus) inhibitor
UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
Nucleotidase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
CYP26 substrate

Phospholipase A1 inhibitor
Propionate CoA-transferase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Aldehyde dehydrogenase inhibitor
4-Hydroxyphenylacetate 1-monooxygenase inhibitor
Paget's disease treatment
Sweetener
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Carboxypeptidase M inhibitor
4-Hydroxy-2-oxoglutarate aldolase inhibitor
Thromboxane synthase stimulant
12-Lipoxygenase inhibitor
Toll-Like receptor antagonist
Nucleotide metabolism regulator
CYP2C19 inhibitor
Adenylate kinase inhibitor
Hydroperoxide dehydratase inhibitor
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
Glutamate (mGluR8) agonist
CYP2C2 substrate
Amino-acid racemase inhibitor
Antimycobacterial
Hair growth stimulant
Sphingosine 1-phosphate receptor antagonist
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Glutamate carboxypeptidase inhibitor
Asparaginase inhibitor
Phosphofructokinase-1 inhibitor
Homocysteine desulfhydrase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Formimidoylglutamase inhibitor
Severe acute respiratory syndrome treatment
Folate antagonist
4-Alpha-glucanotransferase inhibitor
Beta amyloid protein antagonist
CYP4F12 substrate
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Peroxisome proliferator-activated receptor gamma agonist
Falcipain 3 inhibitor
NAD⁺ kinase inhibitor
Mannonate dehydratase inhibitor
Adenylate cyclase stimulant
Analeptic
Chitin deacetylase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP⁺) inhibitor
Pyridoxamine-oxaloacetate transaminase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Antiemphysemic
ADP-ribosylarginine hydrolase inhibitor

Methylaspartate mutase inhibitor
Mediator release inhibitor
Immunostimulant
Phosphoglycolate phosphatase inhibitor
Laminaribiose phosphorylase inhibitor
Granzyme B inhibitor
Dihydrodipicolinate synthase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Insecticide
(R)-aminopropanol dehydrogenase inhibitor
3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor
Histidinol dehydrogenase inhibitor
Beta lactamase inhibitor
S-methyl-5-thioribose kinase inhibitor
Lysozyme inhibitor
CYP2E1 inhibitor
Sulfotransferase substrate
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Homocitrate synthase inhibitor
Cathepsin G inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
Alpha-L-rhamnosidase inhibitor
Catechol 1,2-dioxygenase inhibitor
Saccharopine dehydrogenase (NADP+, L-lysine-forming) inhibitor
Sulfate adenylyltransferase inhibitor
Dyspepsia treatment
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Glutamate decarboxylase inhibitor
Arginine deiminase inhibitor
Respiratory distress syndrome treatment
Glutamate dehydrogenase (NADP+) inhibitor
Protocatechuate 3,4-dioxygenase inhibitor
Antibacterial
ABCA1 expression enhancer
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor
Putrescine oxidase inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Cathepsin H inhibitor
Glycine-tRNA ligase inhibitor
Astringent
L-3-cyanoalanine synthase inhibitor
Aminolevulinate transaminase inhibitor
Vanillyl-alcohol oxidase inhibitor
Peroxisome proliferator-activated receptor agonist
L-ascorbate peroxidase inhibitor
Neurolysin inhibitor
Nucleoside-diphosphatase inhibitor
Pyridoxal kinase inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
Skin irritation, inactive

Prion diseases treatment
Sulfinilalanine decarboxylase inhibitor
Antimutagenic
Gelatinase inhibitor
Glycine N-benzoyltransferase inhibitor
Hepatic disorders treatment
Anticholelithogenic
Xylan 1,4-beta-xylosidase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
Laccase inhibitor
5-Alpha-reductase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Anthranilate synthase inhibitor
Malonyl-CoA decarboxylase inhibitor
Lactaldehyde dehydrogenase inhibitor
Cerebroside-sulfatase inhibitor
CYP3A5 inducer
Ferredoxin-NADP+ reductase inhibitor
Mandelate racemase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
Cystathionine beta-lyase inhibitor
Astacin inhibitor
Microtubule formation inhibitor
Diguanidinobutanase inhibitor
6-Methylsalicylate decarboxylase inhibitor
Tyrosine kinase stimulant
Integrin antagonist
Alanine dehydrogenase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Glycine N-choloyltransferase inhibitor
Cellobiose phosphorylase inhibitor
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Mucorpepsin inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Sepsis treatment
SULT1A2 substrate
Antiviral (HIV)
CYP2A2 substrate
Flavin-containing monooxygenase substrate
Caspase 3 stimulant
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
Radiosensitizer
Antiviral
Sucrose-phosphate synthase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor

[myelin basic protein]-arginine N-methyltransferase inhibitor
Opioid dependency treatment
D-lactate-2-sulfatase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Leukotriene agonist
Prostaglandin agonist
Endothiapepsin inhibitor

Cyclooxygenase 2 inhibitor

Prephenate dehydratase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Amyotrophic lateral sclerosis treatment
Glucosyl transferase inhibitor
Cyclooxygenase 1 substrate
Formaldehyde dehydrogenase (glutathione) inhibitor
Orotate reductase (NADPH) inhibitor
Interleukin antagonist
3-Deoxy-8-phosphooctulonate synthase inhibitor
Aconitate hydratase inhibitor
Leukotriene antagonist
Diacylglycerol kinase inhibitor
Integrin alphaVbeta3 antagonist
Retinoid X alpha receptor agonist
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Vitamin
Kainate receptor 1 agonist
CYP2A8 substrate
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Glutamine synthetase inhibitor
Hematinic
Galactoside 2-alpha-L-fucosyltransferase inhibitor
SULT2A1 substrate
Isoquinoline 1-oxidoreductase inhibitor
3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor
TRPA1 agonist
CXC chemokine 2 receptor antagonist
2-Pyrocatechuate decarboxylase inhibitor
Pantoate-beta-alanine ligase inhibitor
Huntington's disease treatment
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Aspartate 1-decarboxylase inhibitor
Vibriolysin inhibitor
Malyl-CoA lyase inhibitor
L lactate dehydrogenase inhibitor
Urate transporter 1 inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
Malate dehydrogenase (decarboxylating) inhibitor
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
Tubuliny-Tyr carboxypeptidase inhibitor
Biliverdin reductase inhibitor
CYP2B18 substrate

DNA helicase inhibitor
Acidifying agent gastric
Protease inhibitor
P-glycoprotein inhibitor
Tyrosine transaminase inhibitor
Venombin A inhibitor
Histidine ammonia-lyase inhibitor
Glycerol dehydrogenase inhibitor
Sepiapterin reductase inhibitor
CYP3A11 substrate
Isocitrate lyase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Alcohol oxidase inhibitor
Antihypertriglyceridemic
Acetyl-CoA C-acyltransferase inhibitor
Heme oxygenase inhibitor
Alpha,alpha-trehalase inhibitor
Antiperistaltic
Angiotensin-converting enzyme inhibitor
Skin whitener
Chitin synthase inhibitor
Antifungal enhancer
Altronate dehydratase inhibitor
4,5-Dihydroxyphthalate decarboxylase inhibitor
Transcription factor inhibitor
Bone formation stimulant
DNA methyltransferase I inhibitor
Serine protease unspecified inhibitor
Carboxy-cis,cis-muconate cyclase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
CYP1A2 inducer
Beta-D-fucosidase inhibitor
Cholestenone 5alpha-reductase inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Thermolysin inhibitor
2-Isopropylmalate synthase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
Decylcitrate synthase inhibitor
Glycine hydroxymethyltransferase inhibitor
Glutamate (mGluR group III) antagonist
Antioxidant
Formate dehydrogenase inhibitor
Renal failure treatment
Acid-sensing ion channel blocker
Glutamate-cysteine ligase inhibitor
Glutamate synthase (NADPH) inhibitor

DNA nucleotidyltransferase inhibitor
3-Dehydroquinate dehydratase inhibitor
Hepatocyte nuclear factor 4 alpha agonist
Hepatocyte nuclear factor agonist
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Valine-pyruvate transaminase inhibitor
UDP-N-acetylmuramate-L-alanine ligase inhibitor
Ca²⁺-transporting ATPase inhibitor
NMDA receptor polyamine site antagonist
Tubulin-tyrosine ligase inhibitor
Necroptosis inhibitor
Linoleate isomerase inhibitor
CYP2A3 substrate
5-Aminovalerate transaminase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
3-Oxosteroid 1-dehydrogenase inhibitor
Galactoside O-acetyltransferase inhibitor
Malate synthase inhibitor
Antihypertensive
Carboxylesterase inhibitor
CPB protease inhibitor
Serine O-acetyltransferase inhibitor
Alpha-L-fucosidase inhibitor
CDC25A inhibitor
Fumarate hydratase inhibitor
D-Serine ammonia-lyase inhibitor
Alzheimer's disease treatment
Endo-beta-N-acetylglucosaminidase inhibitor
Antidiabetic (type 1)
Thyroid hormone agonist
Free fatty acid receptor 1 agonist
Ribonucleoside diphosphate reductase inhibitor
Beta-N-acetylhexosaminidase inhibitor
Gastricsin inhibitor
Protein kinase C stimulant
Urate-ribonucleotide phosphorylase inhibitor
Cyclohexadienyl dehydrogenase inhibitor
D-Lysine 5,6-aminomutase inhibitor
Pyruvate, phosphate dikinase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Inositol oxygenase inhibitor
Biliary tract disorders treatment
Factor XIIIa stimulant
Aryl-alcohol dehydrogenase (NADP⁺) inhibitor
Alcohol dehydrogenase substrate
Glutamate (mGluR4) agonist
Peptidoglycan beta-N-acetylmuramidase inhibitor
1-Alkyl-2-acetyl glycerol O-acyltransferase inhibitor
Maleylacetoacetate isomerase inhibitor

Parathyroid hormone antagonist
Bone diseases treatment
Antineoplastic, alkylator
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Kynureninase inhibitor
Aldose reductase inhibitor
RNA synthesis inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
D(-)-tartrate dehydratase inhibitor
Inositol-3-phosphate synthase inhibitor
Plasminogen activator stimulant
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Leucine-tRNA ligase inhibitor
Respiratory analeptic
Interleukin 10 agonist
Telomerase inhibitor
CYP24 substrate
Mycodextranase inhibitor
Diuretic inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Alanine racemase inhibitor
2-Aminohexanoate transaminase inhibitor
GABA B receptor antagonist
Deoxycytidine deaminase inhibitor
Thromboxane antagonist
UGT2B11 substrate
Pyruvate kinase inhibitor
Chloride channel activator
D-Alanine-poly(phosphoribitol) ligase inhibitor
Guanylate kinase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
Rheumatoid arthritis treatment
Anthranilate phosphoribosyltransferase inhibitor
Acetate-CoA ligase inhibitor
Aryl-acylamidase inhibitor
Neutral endopeptidase inhibitor
Thermomycin inhibitor
Luteinizing hormone-releasing hormone agonist
Free radical scavenger
Phosphoribulokinase inhibitor
Arabinogalactan endo-1,4-beta-galactosidase inhibitor
Ribonucleotide reductase inhibitor
Lysine carboxypeptidase inhibitor
Stipitatonate decarboxylase inhibitor
Interferon agonist
Strombine dehydrogenase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Dopachrome isomerase inhibitor
Prostaglandin antagonist

Homoisocitrate dehydrogenase inhibitor
Trimethylamine-N-oxide reductase inhibitor
Retinoprotector
Liver X receptor alpha agonist
Octopamine antagonist
Tannase inhibitor
CYP19 substrate
Aspartate 4-decarboxylase inhibitor
Oxytocin agonist
Glutamate racemase inhibitor
6-Phosphofructo-2-kinase inhibitor
Sphingosine 1-phosphate receptor 3 antagonist
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Thioether S-methyltransferase inhibitor
Sterol 24-C-methyltransferase inhibitor
Adenylyl-sulfate kinase inhibitor
CYP4F8 substrate
Protein-tyrosine phosphatase yopH inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
Interferon antagonist
Ethanolamine oxidase inhibitor
Endoglycosylceramidase inhibitor
Interferon gamma antagonist
SMN2 expression enhancer
Anticoagulant
Cholesterol esterase inhibitor
Thromboxane synthase inhibitor
Nitrate reductase inhibitor
D-aspartate oxidase inhibitor
Arginine racemase inhibitor
Proline racemase inhibitor
Choline-phosphate cytidyltransferase inhibitor
Antibiotic
Cell wall synthesis inhibitor
Saluretic
Phosphomevalonate kinase inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
Interleukin 1a antagonist
Cardiovascular analeptic
Squalene synthetase inhibitor
6,7-Dihydropteridine reductase inhibitor
Corticotropin releasing factor antagonist
Collagenase inhibitor
D-Ala-D-Ala ligase inhibitor
Ornithine carbamoyltransferase inhibitor
Pantetheine-phosphate adenylyltransferase inhibitor
CYP26 inhibitor
Isoamylase inhibitor
Thyroid hormone alpha 1 agonist

Thyroid hormone alpha agonist
Thyroid hormone beta 1 agonist
Glutathione synthase inhibitor
Aspartate ammonia-lyase inhibitor
Arginine kinase inhibitor
Glutamate (mGluR3) antagonist
GABA transporter 3 inhibitor
3-Dehydroquinate synthase inhibitor
Kainate receptor agonist
Nitric-oxide synthase stimulant
Prostaglandin D2 agonist
Glucan 1,3-alpha-glucosidase inhibitor
Phenol 2-monooxygenase inhibitor
11-Cis-retinyl-palmitate hydrolase inhibitor
Glutamate (mGluR1) agonist
Gluconokinase inhibitor
Quinate 5-dehydrogenase inhibitor
Prostaglandin-I synthase inhibitor
Endothelin receptor antagonist
Arginase inhibitor
Homocysteine S-methyltransferase inhibitor
Tardive dyskinesia treatment
Histidine decarboxylase inhibitor
DNA directed DNA polymerase inhibitor
Poly(ADP-ribose) glycohydrolase inhibitor
Glutamate (mGluR3) agonist
Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
Tryptophan synthase inhibitor
Vesicle monoamine transporter inhibitor
Isomaltulose synthase inhibitor
Methylthioadenosine nucleosidase inhibitor
Ribonuclease inhibitor
Protein N-acetylglucosaminyltransferase inhibitor
CXC chemokine receptor antagonist
Diacylglycerol O-acyltransferase inhibitor
CC chemokine 9 receptor antagonist
Histamine agonist
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Tankyrase inhibitor
Tartrate decarboxylase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Beta-glucosidase inhibitor
NOS2 expression inhibitor
Angiotensin AT2 receptor agonist
Arachidonate-CoA ligase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
Ribose-5-phosphate isomerase inhibitor
Arginine decarboxylase inhibitor
Cathepsin E inhibitor
NADH dehydrogenase inhibitor

Serine-type D-Ala-D-Ala carboxypeptidase inhibitor
Octadecanal decarboxylase inhibitor
CTP synthase inhibitor
Antidiabetic (type 2)
Formyl peptide receptor antagonist
Glutamate (mGluR8) antagonist
Glutamate formimidoyltransferase inhibitor
Asemlin inhibitor
Antianemic
Chorismate mutase inhibitor
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Tryptophan 5 hydroxylase inhibitor
1,3-Beta-glucan synthase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Anabolic
Trans-octaprenyltransferase inhibitor
Age-related macular degeneration treatment
UDP-N-acetylglucosamine 2-epimerase inhibitor
Shock treatment
Homoserine kinase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor
Cysteine-tRNA ligase inhibitor
Neurotensin 1 receptor agonist
Integrin alpha4beta1 antagonist
Aggrecanase 1 inhibitor
DNA methylase inhibitor
Dextranase inhibitor
Cystathionine beta-synthase inhibitor
CDC25C inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Adenylylsulphatase inhibitor
MDM2 inhibitor
3-Oxoacid CoA-transferase inhibitor
Glycosylceramidase inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
AMPA receptor agonist
Ethanolamine kinase inhibitor
Purinergic P2X3 antagonist
Glutamine-fructose-6-phosphate transaminase inhibitor
Peptidyl-prolyl cis-trans isomerase inhibitor
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Sodium-dependent vitamin C transporter 2 inhibitor
Keratolytic
Hypercalcemia treatment
Protein C (activated) inhibitor
Caspase 9 inhibitor
Protein-glutamate O-methyltransferase inhibitor
Corneal wound healing stimulator
Theanine hydrolase inhibitor
Purinergic P2X2 antagonist

Ceramide glucosyltransferase inhibitor
Metabolic disease treatment
Nucleotidyltransferase inhibitor
Tryptophan-tRNA ligase inhibitor
Chymotrypsin inhibitor
Antiviral (Poxvirus)
Adenine deaminase inhibitor
Hydroxylysine kinase inhibitor
Para amino benzoic acid antagonist
Thromboxane A2 antagonist
Phosphate acetyltransferase inhibitor
Hydroxyquinol 1,2-dioxygenase inhibitor
Antiallergic
Hexokinase inhibitor
AMP deaminase inhibitor
[Isocitrate dehydrogenase (NADP+)] kinase inhibitor
Nav1.3 sodium channel blocker
Serine-tRNA ligase inhibitor
Nitric oxide donor
UDP-N-acetylmuramate dehydrogenase inhibitor
Squalene epoxidase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
Celiac disease treatment
Leukotriene B4 antagonist
Dimethylhistidine N-methyltransferase inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
Leukotriene C antagonist
Preterm labor treatment
N6-methyl-lysine oxidase inhibitor
Spasmolytic, urinary
Long-chain-acyl-CoA dehydrogenase inhibitor
Benzoin aldolase inhibitor
[citrate-(pro-3S)-lyase] thioesterase inhibitor
Glucose-1,6-bisphosphate synthase inhibitor
Granulocyte macrophage colony stimulating factor agonist
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
2-(acetamidomethylene)succinate hydrolase inhibitor
Integrin alpha4 antagonist
Tetrahydroxynaphthalene reductase inhibitor
Leukotriene E4 antagonist
Aldose 1-epimerase inhibitor
NAD(P)+ transhydrogenase (AB-specific) inhibitor
Lanosterol 14 alpha demethylase inhibitor
GlutaminyI-tRNA synthase (glutamine-hydrolysing) inhibitor
Nitric-oxide synthase inhibitor
Peroxisome proliferator-activated receptor delta agonist
CYP1A1 inhibitor
4-Hydroxybenzoate 1-hydroxylase inhibitor
2-Methylcitrate synthase inhibitor
Ketoheokinase inhibitor

CYP2B substrate
Pyridoxamine-phosphate oxidase inhibitor
Retinoid X receptor agonist
Protein synthesis inhibitor
PRL phosphatase inhibitor
Liver X receptor beta agonist
Magnolysin inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
Glutamate (mGluR group I) agonist
Protein phosphatase 2A inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
Glucagon-like peptide 1 receptor antagonist
Complement inhibitor
Xanthommatin reductase inhibitor
tRNA cytidyltransferase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
HMG CoA reductase inhibitor
Sucrose-phosphate phosphatase inhibitor
Carboxycyclohexadienyl dehydratase inhibitor
Dihydroorotate oxidase inhibitor
Dihydrouracil oxidase inhibitor
Glutamate receptor agonist
Nicotinamide-nucleotide adenylyltransferase inhibitor
Glutamate (mGluR4) antagonist
5-Alpha-reductase 2 inhibitor
Steroid sulfotransferase inhibitor
Aggrecanase 2 inhibitor
Alternansucrase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Cholesterol absorption inhibitor
CTGF expression inhibitor
Parathyroid hormone secretion stimulant
Aspartate carbamoyltransferase inhibitor
Nav1.1 sodium channel blocker
Dihydrofolate synthase inhibitor
Putrescine carbamoyltransferase inhibitor
CYP27A substrate
Glycerol kinase inhibitor
Cathepsin D inhibitor
Phosphopyruvate hydratase inhibitor
Hyperparathyroidism treatment
Cytochrome P450 inhibitor
Elastase inhibitor
Uridine nucleosidase inhibitor
Polynucleotide adenylyltransferase inhibitor
Citrate (Si)-synthase inhibitor
Thyroid hormone alpha 1 antagonist
Histone deacetylase SIRT1 inhibitor
RNA-directed RNA polymerase (Influenza A) inhibitor

CYP24 inhibitor
Vitamin K-like
Nucleotidyltransferase (FIV) inhibitor
Procollagen-proline 3-dioxygenase inhibitor
Polyamine oxidase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor
Glucose-1-phosphate adenylyltransferase inhibitor
NADPH oxidoreductase inhibitor
Transthyretin amyloid fibril formation inhibitor
Streptogrisin A inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylglactosaminyltransferase inhibitor
GABA uptake inhibitor
Diphosphate-serine phosphotransferase inhibitor
Phosphoserine transaminase inhibitor
CYP2B2 substrate
Glutamate dehydrogenase [NAD(P)+] inhibitor
Contraceptive female
Pyruvate, water dikinase inhibitor
L lactate dehydrogenase A inhibitor
N-acetylglucosaminyldiphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor
TH expression enhancer
Prostaglandin E2 antagonist
Tartrate dehydrogenase inhibitor
Glycerate kinase inhibitor
Postsynaptic density protein 95 inhibitor
Alpha,alpha-phosphotrehalase inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
Neurotensin receptor antagonist
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Glucose-6-phosphate isomerase inhibitor
Sphingosine 1-phosphate receptor 5 antagonist
Cysteine dioxygenase inhibitor
Phosphoglucomutase inhibitor
Histidine-tRNA ligase inhibitor
Pyrroline-5-carboxylate reductase inhibitor
Aralkylamine N-acetyltransferase inhibitor
CYP27 substrate
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Thymidine-triphosphatase inhibitor
Prostaglandin E2 agonist
Butyrate-CoA ligase inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
Protein-tyrosine phosphatase 1B inhibitor
Metalloproteinase inhibitor
Integrin alpha4beta7 antagonist
Amino-acid N-acetyltransferase inhibitor
Prostaglandin EP4 agonist
Quisqualate antagonist
Proteasome inhibitor
Calcitonin stimulant

ICAM 1 antagonist
Phosphoketolase inhibitor
Lipocortins synthesis antagonist
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Glucan 1,4-alpha-glucosidase inhibitor
Phosphoglycerate phosphatase inhibitor
Potassium channel (Ca-activated) activator
15-Lipoxygenase inhibitor
Tocolytic
Glycine N-methyltransferase inhibitor
Cadherin antagonist
Antifungal (Pneumocystis)
Antibacterial, ophthalmic
CMP-N-acylneuraminate phosphodiesterase inhibitor
tRNA methyltransferase inhibitor
Prostaglandin A1 agonist
Hydroxypyruvate reductase inhibitor
Sphingosine kinase inhibitor
4-Pyridoxolactonase inhibitor
Lysophosphatidic acid receptor agonist
Phenylpyruvate tautomerase inhibitor
dCTP deaminase inhibitor
Thyroid hormone beta agonist
DNA synthesis inhibitor
Alkene monooxygenase inhibitor
G-protein-coupled bile acid receptor 1 agonist
L-iditol 2-dehydrogenase inhibitor
Phosphoenolpyruvate carboxykinase (GTP) inhibitor
Capillary fragility treatment
D-benzoylarginine-4-nitroanilide amidase inhibitor
Glucose-6-phosphate translocase inhibitor
ATPase (Vacuolar H⁺) inhibitor
Glutamate (mGluR1a) agonist
Glutamate (mGluR5a) agonist
Glutathione S-transferase inhibitor
Acyl-CoA dehydrogenase (NADP⁺) inhibitor
3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor
Toll-Like receptor 2 antagonist
5 Lipoxygenase activating protein inhibitor
Monoamine uptake inhibitor
Aldose reductase 2 inhibitor
Prostacyclin antagonist
HIV-1 protease inhibitor
Tyrosine phenol-lyase inhibitor
Retinoid X gamma receptor antagonist
Lipoxygenase inhibitor
Beta 1 adrenoreceptor agonist
Aminoacyl-tRNA hydrolase inhibitor
5-Alpha-reductase 1 inhibitor
N-Acetylated alpha-linked acidic dipeptidase inhibitor

Vesicle monoamine transporter 2 inhibitor
Peptide deformylase inhibitor
3(or 17)beta-hydroxysteroid dehydrogenase inhibitor
Growth hormone agonist
Enoyl-CoA hydratase inhibitor
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Eicosanoid agonist
Thioredoxin reductase inhibitor
PfA-M1 aminopeptidase inhibitor
Actin polymerization inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Butyryl-CoA dehydrogenase inhibitor
Sphingosine 1-phosphate receptor 1 agonist
Protein phosphatase inhibitor
Deoxyhypusine monooxygenase inhibitor
Procollagen glucosyltransferase inhibitor
Sphingosine 1-phosphate receptor agonist
Carbonic anhydrase XIV inhibitor
Endothelin A receptor antagonist
Calcium-sensing receptor antagonist
4-Hydroxybenzoate-CoA ligase inhibitor
Cholesterol ester transfer protein antagonist
Androst-4-ene-3,17-dione monooxygenase inhibitor
Oleamide hydrolase inhibitor
HCV IRES inhibitor
1-Phosphofructokinase inhibitor
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Alpha,alpha-trehalose phosphorylase inhibitor
Prostacyclin agonist
Oligo-1,6-glucosidase inhibitor
CYP2A6 substrate
N-acylneuraminate cytidyltransferase inhibitor
Membrane-oligosaccharide glycerophosphotransferase inhibitor
Phosphoglycerate dehydrogenase inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Nav1.5 sodium channel blocker
Helicase E1 (Human papillomavirus) inhibitor
Aralkylamine dehydrogenase inhibitor
N-acetylglucosaminylidiphosphodolichol N-acetylglucosaminyltransferase inhibitor
L lactate dehydrogenase B inhibitor
L lactate dehydrogenase B4 inhibitor
Tryptophanyl aminopeptidase inhibitor
UDP-glucose 4-epimerase inhibitor
Glutamate (mGluR2) antagonist
T cell inhibitor
Leucyltransferase inhibitor
ATP citrate lysase inhibitor
Prostaglandin EP2 antagonist
Calcineurin inhibitor
Erythropoietin receptor agonist

Prolyl endopeptidase inhibitor
Integrin alpha5beta1 antagonist
Antithrombocytopenic
NMN nucleosidase inhibitor
Thyroid hormone beta 1 antagonist
HIV-2 retropepsin inhibitor
Bombesin 2 receptor antagonist
Vesicular glutamate transport inhibitor
FMN reductase inhibitor
Corticosteroid antagonist
Nicotinamide-nucleotide amidase inhibitor
Caspase 8 inhibitor
Cell wall biosynthesis inhibitor
Peroxisome proliferator-activated receptor alpha antagonist
Methylcrotonoyl-CoA carboxylase inhibitor
Glutamate (mGluR group II) antagonist
Leukotriene C4 antagonist
RAS guanyl releasing protein antagonist
Potassium channel Kv1.3 blocker
Peroxisome proliferator-activated receptor delta antagonist
Neurotensin 1 receptor antagonist
Thyroid hormone beta antagonist
LDLR expression enhancer
Glycolaldehyde dehydrogenase inhibitor
Autophagy inducer
Glutaryl-CoA dehydrogenase inhibitor
Glucose-1-phosphatase inhibitor
Glucagon receptor antagonist
3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor
CMP-KDO synthase inhibitor
Nucleoside oxidase (H2O2-forming) inhibitor
Retinoid X beta receptor antagonist
Methyltransferase substrate
1-Alkyl-2-acetylglycerophosphocholine esterase inhibitor
CYP17 substrate
Retinoid X receptor antagonist
5-Lipoxygenase inhibitor
Opioid delta 2 receptor antagonist
Antiviral (Parainfluenza)
Aminopeptidase A inhibitor
Shab potassium channel blocker
Secretase gamma inhibitor
Integrin alpha5beta6 antagonist
Retinoid X alpha receptor antagonist
L(+)-Tartrate dehydratase inhibitor
CYP3A7 substrate
Methylmalonyl-CoA carboxytransferase inhibitor
Rhodopsin kinase inhibitor
Baculoviral IAP repeat-containing protein inhibitor
Aspartyl protease inhibitor

Bombesin 1 receptor antagonist
Urotensin II agonist
Farnesoid X receptor agonist
UGT2B19 substrate
UGT2B23 substrate
UGT2B30 substrate
UGT2B4D substrate
UGT2B4E substrate

Imatinib

Molecular Mechanism (initial) :

proto-oncogene tyrosine-protein kinase ABL inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

stem cell factor (SCF)

proto-oncogene c-Kit inhibitor

initial indication(s):

chronic myelogenous leukemia

Repurposed indication(s):

gastrointestinal stromal tumor

fibrosarcoma

hypereosinophilic syndrome

acute lymphocytic leukemia

myeloproliferative diseases and systemic mastocytosis

Predicted Activities

Tyrosine-protein kinase TYRO 10 inhibitor

Protein kinase inhibitor

Growth factor agonist

Stem cell growth factor agonist

EIF4E expression inhibitor

Janus tyrosine kinase 3 inhibitor

Bcr-Abl kinase inhibitor

Signal transduction pathways inhibitor

Janus tyrosine kinase inhibitor

Tyrosine kinase inhibitor

Angiogenesis inhibitor

Cytokine production inhibitor

Transcription factor STAT inhibitor

Tumour necrosis factor alpha antagonist

Focal adhesion kinase inhibitor

Nootropic

Platelet aggregation inhibitor

Protein-serine-threonine kinase inhibitor

Macrophage colony stimulating factor antagonist

Tumour necrosis factor antagonist

Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor

Abl kinase inhibitor

Janus tyrosine kinase 2 inhibitor

Focal adhesion kinase 2 inhibitor

Lck kinase inhibitor
Syk tyrosine kinase inhibitor

Antineoplastic

Prion diseases treatment
Autoimmune disorders treatment
Histamine release inhibitor
Transplant rejection treatment
Rhinitis treatment
Vascular endothelial growth factor antagonist
Antineoplastic (non-Hodgkin's lymphoma)
Src kinase inhibitor
Vascular endothelial growth factor 2 antagonist
Platelet activating factor alpha antagonist
Platelet derived growth factor receptor kinase inhibitor
Urticaria treatment
Nicotinic alpha4beta4 receptor agonist
CDK9/cyclin T1 inhibitor
p38 MAP kinase inhibitor
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
Platelet activating factor antagonist
Proto-oncogene tyrosine-protein kinase Kit inhibitor
Protein-tyrosine kinase Lyn inhibitor
Bruton tyrosine kinase inhibitor
Colony stimulating factor antagonist
Antiallergic
Transcription factor inhibitor
Platelet activating factor beta antagonist
Focal adhesion kinase 1 inhibitor
Antiasthmatic
Serum-glucocorticoid regulated kinase 1 inhibitor
TRKB antagonist
Polo-like kinase-1 inhibitor
MAP kinase inhibitor
MAP kinase 1 inhibitor
RET inhibitor
MAP3K5 inhibitor
Insulin antagonist
Aurora-C kinase inhibitor
Antiarthritic
Rheumatoid arthritis treatment
Aurora kinase inhibitor
Kinase inhibitor
c-Src kinase inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
Heat shock protein 27 antagonist
Interleukin antagonist
Antineoplastic (solid tumors)
Antieczematous atopic
Immunosuppressant
Aurora-A kinase inhibitor

Pulmonary hypertension treatment
ALK inhibitor
Gastric antisecretory
Cyclin-dependent kinase 6 inhibitor
Glycogen synthase stimulant
Antineoplastic (bone cancer)
Polarisation stimulant
Protein kinase C inhibitor
Antimitotic
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
Protein kinase (CK1) inhibitor
Macular degeneration treatment
Growth factor antagonist
P-glycoprotein substrate
Protein kinase (CK1) epsilon inhibitor
Polo-like kinase inhibitor
Farnesoid X receptor antagonist
Botulin neurotoxin A light chain inhibitor
p21-activated kinase 1 inhibitor
p21-activated kinase inhibitor
Ribosomal protein S6 kinase 1, 70-kDa inhibitor
I kappa B kinase inhibitor
Alzheimer's disease treatment
Protein kinase (Mos, Mil/Raf, MEKK, RIPK, TESK, LIMK, IRAK, ILK, Activin/TGF-beta) inhibitor
Fibroblast growth factor 2 antagonist
Raf kinase inhibitor
Aurora-B kinase inhibitor
Interleukin 6 antagonist
Protein kinase (CK2) inhibitor
Respiratory distress syndrome treatment
MAP kinase 14 inhibitor
Protein kinase B alpha inhibitor
Liver fibrosis treatment
Interleukin agonist
Ephrin antagonist
CDK2/cyclin A inhibitor
Fibroblast growth factor antagonist
AXL receptor tyrosine kinase inhibitor
Ribosomal protein S6 kinase, 70-kDa inhibitor
Ribosomal protein S6 kinase inhibitor
Fibroblast growth factor 3 antagonist
ErbB antagonist
TIE-2 antagonist
Interleukin 2 antagonist
Platelet growth factor antagonist
Cyclin-dependent kinase 7 inhibitor
TIE antagonist
Insulin like growth factor 1 antagonist
T cell inhibitor
Interleukin 1 antagonist

Antineoplastic (multiple myeloma)
Transcription factor STAT6 inhibitor
Antileukemic
ZAP-70 protein tyrosine kinase inhibitor
Antineoplastic (ovarian cancer)
p21-activated kinase 4 inhibitor
Cyclin-dependent kinase inhibitor
Protein kinase C delta inhibitor
Allergic rhinitis treatment
Antineoplastic (colorectal cancer)
Janus tyrosine kinase 1 inhibitor
HIV attachment inhibitor
CYP2C9 inhibitor
Fibroblast growth factor 1 antagonist
MAP-kinase-activated kinase inhibitor
Fibrosis treatment
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Hedgehog signaling inhibitor
Protein kinase (CK1) delta inhibitor
ErbB-2 antagonist
Diabetic retinopathy treatment
MAP kinase 10 inhibitor
Rho-associated kinase inhibitor
Intermittent claudication treatment
Diuretic inhibitor
Raf kinase B inhibitor
MAP kinase 8 inhibitor
Acetylcholine nicotinic agonist
Ribosomal protein S6 kinase, 90-kDa inhibitor
Insulin growth factor antagonist
Ca²⁺/calmodulin-dependent protein kinase inhibitor
Breast cancer-resistant protein inhibitor
Hepatocyte growth factor antagonist
Vascular endothelial growth factor 1 antagonist
Antineoplastic (pancreatic cancer)
Antineoplastic (colon cancer)
Rho-associated kinase II inhibitor
Neurodegenerative diseases treatment
Interleukin 8 antagonist
Inflammatory Bowel disease treatment
Cyclin-dependent kinase 1 inhibitor
Glycogen synthase kinase-3 beta inhibitor
Kidney function stimulant
Rho-associated kinase I inhibitor
Cyclin-dependent kinase 2 inhibitor
Cystic fibrosis treatment
Narcolepsy treatment
Glycogen synthase kinase-3 inhibitor
Antiamyloidogenic
Epidermal growth factor receptor kinase inhibitor

Cell adhesion molecule inhibitor
Cyclic AMP modulator
Pim-1 kinase inhibitor
Wee-1 tyrosine kinase inhibitor
MAP-kinase-activated kinase 2 inhibitor
MAP kinase kinase 1 inhibitor
ErbB-4 antagonist
Tyrosine-protein kinase receptor FLT3 inhibitor
Vascular endothelial growth factor 3 antagonist
I kappa B kinase 2 inhibitor
TTK protein kinase inhibitor
Transcription factor AP-1 inhibitor
Multiple sclerosis treatment
EphB4 antagonist
Interleukin 1b antagonist
Tyrosine-protein kinase receptor antagonist
Cyclin-dependent kinase 4 inhibitor
Antineoplastic (glioma)
Cyclin-dependent kinase 9 inhibitor
Serum-glucocorticoid regulated kinase inhibitor
Protein kinase C alpha inhibitor
Autotaxin inhibitor
Imidazoline I1 receptor agonist
5 Hydroxytryptamine 7S antagonist
Potassium channel KCNQ3 activator
Bone formation stimulant
Proto-oncogene tyrosine-protein kinase c-hck inhibitor
CDK/Cyclin complex inhibitor
Sleep apnea treatment
TRKA antagonist
Antinephritic
Antineoplastic (small cell lung cancer)
Protein kinase B inhibitor
Nicotinic neuronal receptor agonist
Tumour necrosis factor alpha release inhibitor
Dyrk kinase inhibitor
Raf kinase C inhibitor
Cholinergic
TEC kinase inhibitor
Movement disorders treatment
Antineoplastic (sarcoma)
Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor
Ca²⁺/calmodulin-dependent kinase II inhibitor
CC chemokine receptor 2B antagonist
Pyruvate dehydrogenase kinase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Pim kinase inhibitor
Potassium channel small-conductance Ca-activated blocker
Protein kinase C theta inhibitor
Antineoplastic (gastric cancer)

Renal disease treatment
Nicotinic alpha7 receptor agonist
Systemic lupus erythematosus treatment
Interleukin 12 agonist
NAD⁺-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
General pump inhibitor
Protein kinase C epsilon inhibitor
Antineoplastic (endocrine cancer)
CDK4/cyclin D inhibitor
CYP3A4 inhibitor
Platelet growth factor beta antagonist
MAP kinase 9 inhibitor
Pim-2 kinase inhibitor
Retinopathy treatment
Protein kinase C mu inhibitor
CDC7 inhibitor
Phosphoinositide dependent kinase 1 inhibitor
Integrin alphaVbeta1 antagonist
5 Hydroxytryptamine 3 agonist
Protein kinase B beta inhibitor
Catalase stimulant
Adenosine A2b receptor antagonist
Protein kinase C eta inhibitor
Transforming growth factor antagonist
Steroid 9alpha-monooxygenase inhibitor
Histone deacetylase SIRT1 stimulant
Histone deacetylase stimulant
Myt1 kinase inhibitor
Phosphatidylinositol 3-kinase alpha inhibitor
Antiprotozoal (Histomonas)
Cardiac myosin stimulant
Sporulation kinase A inhibitor
H⁺/K⁺-transporting ATPase inhibitor
MAP3K8 inhibitor
Tyrosine-protein kinase EMT inhibitor
5 Hydroxytryptamine release inhibitor
Protein kinase C beta inhibitor
Pteridine reductase inhibitor
ATM kinase inhibitor
Alpha 2a adrenoreceptor antagonist
Ca²⁺/calmodulin-dependent kinase I inhibitor

Iproniazid

Molecular Mechanism (initial) :

generation of reactive metabolites inhibiting biosynthetic enzymes of M. tuberculosis

Molecular Mechanism (repurposed) :

monoamine oxidase inhibitor

initial indication(s):

tuberculosis

Repurposed indication(s):
depression

Predicted Activities

Ethanolamine oxidase inhibitor
Taurine dehydrogenase inhibitor
Isopenicillin-N epimerase inhibitor
Trimethylamine dehydrogenase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor

Amine dehydrogenase inhibitor

Aralkylamine dehydrogenase inhibitor
Threonine aldolase inhibitor
Serine-pyruvate transaminase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Phosphatidylserine decarboxylase inhibitor
Polyamine oxidase inhibitor

Antituberculosic

Serine-glyoxylate transaminase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Antimycobacterial
Nicotinamidase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
Glycine transaminase inhibitor
Alanine transaminase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
8-Amino-7-oxononanoate synthase inhibitor
Pseudolysin inhibitor
Methionine decarboxylase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Antiviral (Picornavirus)
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Fragilysin inhibitor
Oxygen scavenger
Kidney function stimulant
Thromboxane B2 antagonist
Nicotinate dehydrogenase inhibitor
Fibrolase inhibitor
Chenodeoxycholoyltaurine hydrolase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Nicotinic alpha2beta2 receptor antagonist
CYP2E1 inducer
6-Pyruvoyltetrahydropterin synthase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Glutathione thiolesterase inhibitor

Carboxypeptidase Taq inhibitor
CYP2A8 substrate
Glutamyl endopeptidase II inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Putrescine oxidase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Fusarinine-C ornithinesterase inhibitor
Endopeptidase So inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Phobic disorders treatment
CYP2E1 inhibitor
Fructose 5-dehydrogenase inhibitor
Membrane integrity agonist
Beta-Lysine 5,6-aminomutase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Peroxidase inhibitor
Formaldehyde transketolase inhibitor
Glutamine-pyruvate transaminase inhibitor
tRNA-pseudouridine synthase I inhibitor
Cathepsin T inhibitor
Lysostaphin inhibitor
Cystathionine gamma-lyase inhibitor
Sulfur reductase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Pterin deaminase inhibitor
Analeptic
PfA-M1 aminopeptidase inhibitor
Chloride peroxidase inhibitor
Nucleoside oxidase (H₂O₂-forming) inhibitor
Polyporopepsin inhibitor
Formate dehydrogenase inhibitor
Methanol dehydrogenase inhibitor
Manganese peroxidase inhibitor
Polyneuridine-aldehyde esterase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Testosterone 17beta-dehydrogenase (NADP⁺) inhibitor
Fibrinolytic
Ovulation inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Cytoprotectant
Carbon-monoxide dehydrogenase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Cardiovascular analeptic
Dimethylargininase inhibitor
Erythropoiesis stimulant
Antidepressant
Urethanase inhibitor
Spermidine dehydrogenase inhibitor
Anticonvulsant
Methylamine-glutamate N-methyltransferase inhibitor

Fibrinogen receptor antagonist
Glucan endo-1,6-beta-glucosidase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Limulus clotting factor B inhibitor
Nicotine dehydrogenase inhibitor
Platelet derived growth factor receptor kinase inhibitor
Acetylesterase inhibitor
Superoxide dismutase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Biotinidase inhibitor
Glucuronate isomerase inhibitor
Hydroxylamine reductase inhibitor
Serum-glucocorticoid regulated kinase 1 inhibitor
Omptin inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Mood disorders treatment
5-O-(4-coumaroyl)-D-quinic acid 3'-monooxygenase inhibitor
Meprin B inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
4-Hydroxyproline epimerase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Cyanoalanine nitrilase inhibitor
Complement factor D inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Thioredoxin inhibitor
CYP2D16 substrate
Phospholipid-translocating ATPase inhibitor
Creatininase inhibitor
CYP2C3 substrate
CYP2H substrate
Alkane 1-monooxygenase inhibitor
Aspergillopepsin I inhibitor
Botulin neurotoxin A light chain inhibitor
Nitrate reductase (cytochrome) inhibitor
Transcription factor STAT3 inhibitor
Picornain 3C inhibitor
Histidine N-acetyltransferase inhibitor
Nitrilase inhibitor
Leucolysin inhibitor
Fatty-acyl-CoA synthase inhibitor
Lysine 2,3-aminomutase inhibitor
Gallate decarboxylase inhibitor
Arylacetonitrilase inhibitor
ATP phosphoribosyltransferase inhibitor
5 Hydroxytryptamine uptake stimulant
Glutamate-tRNA ligase inhibitor
Catechol oxidase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Transcription factor STAT inhibitor

NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Gluconolactonase inhibitor
Aspartate-ammonia ligase inhibitor
Mandelate 4-monooxygenase inhibitor
Cyclic AMP agonist
NADPH peroxidase inhibitor
Tryptophan 2-monooxygenase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Preneoplastic conditions treatment
Aspulvinone dimethylallyltransferase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Sugar-phosphatase inhibitor
Antinociceptive
Antiviral (Poxvirus)
Glucose oxidase inhibitor
Alopecia treatment
Antithrombotic
Histidinol-phosphatase inhibitor
Acylcarnitine hydrolase inhibitor
Arylalkyl acylamidase inhibitor
Hydroxylamine oxidase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Polyamine-transporting ATPase inhibitor
Venombin AB inhibitor
Macrophage colony stimulating factor agonist
Albendazole monooxygenase inhibitor
Malate dehydrogenase (acceptor) inhibitor
Limulus clotting factor C inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Diabetic neuropathy treatment
S-formylglutathione hydrolase inhibitor
Platelet adhesion inhibitor
Intermittent claudication treatment
Ecdysone 20-monooxygenase inhibitor
Hydrogen dehydrogenase inhibitor
2-Dehydropantoate 2-reductase inhibitor
CYP17 inhibitor
Indolepyruvate C-methyltransferase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
2-Haloacid dehalogenase inhibitor
Opine dehydrogenase inhibitor
Gluconate 5-dehydrogenase inhibitor
4-Hydroxymandelate oxidase inhibitor
Serum-glucocorticoid regulated kinase inhibitor
Methylaspartate ammonia-lyase inhibitor
Loop diuretic
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
FMO1 substrate
Lipoprotein lipase inhibitor

CYP2F1 substrate
Mitochondrial processing peptidase inhibitor
Arginine 2-monooxygenase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
S-alkylcysteine lyase inhibitor
5 Hydroxytryptamine 2B agonist
Pin1 inhibitor
Pyridoxal kinase inhibitor
Heat shock protein 27 antagonist
5 Hydroxytryptamine release inhibitor
EIF4E expression inhibitor
Acetylnornithine deacetylase inhibitor
Cyclooxygenase substrate
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Maillard reaction inhibitor
Cl--transporting ATPase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Antiviral (Adenovirus)
Venom exonuclease inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
ATPase stimulant
MO15-related protein kinase Pfmrk inhibitor
Respiratory analeptic
Threonine ammonia-lyase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Centromere associated protein inhibitor
Antileprosy
N-benzyloxycarbonylglycine hydrolase inhibitor
Cyclohexanone monooxygenase inhibitor
Pullulanase inhibitor
Bontoxilysin inhibitor
N-acetyllactosamine synthase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Nucleotide metabolism regulator
Simian immunodeficiency virus proteinase inhibitor
Aromatic-amino-acid transaminase inhibitor
Mucomembranous protector
Snapalysin inhibitor
Tryptophanamidase inhibitor
Lysase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Pseudouridylate synthase inhibitor
Antiseborrheic
Vasoprotector
Retinoic acid metabolism inhibitor
Antibacterial
Phosphopantothenoylecysteine decarboxylase inhibitor

Phenol O-methyltransferase inhibitor
Indoleacetaldoxime dehydratase inhibitor
MAO inhibitor
Glycerol-3-phosphate oxidase inhibitor
Platelet aggregation stimulant
Fucosterol-epoxide lyase inhibitor
Pitrilysin inhibitor
Spasmolytic
Glycerol 2-dehydrogenase (NADP⁺) inhibitor
Allantoin racemase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
CYP2D2 inhibitor
D-amino-acid dehydrogenase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Horrilysin inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Alkylacetylgllycerophosphatase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Sulfite reductase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Mannan endo-1,4-beta-mannosidase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Pancreatic elastase inhibitor
Nicotinic alpha4beta4 receptor agonist
Antihypoxic
Procollagen N-endopeptidase inhibitor
Thymidylate 5'-phosphatase inhibitor
Sulfite dehydrogenase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
NAT1 substrate
Bothrolysin inhibitor
Retinal dehydrogenase inhibitor
Thiosulfate dehydrogenase inhibitor
Tryptophanyl aminopeptidase inhibitor
Dementia treatment
3C-like protease (Human coronavirus) inhibitor
Neuropeptide Y2 antagonist
Coccolysin inhibitor
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
CYP2C29 substrate
NF-E2-related factor 2 stimulant
Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
3-Cyanoalanine hydratase inhibitor
Monoamine uptake inhibitor
Dipeptidase E inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
3-Isopropylmalate dehydratase inhibitor
L-glutamate oxidase inhibitor

Sphinganine kinase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Arylmalonate decarboxylase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
CYP7 inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Aureolysin inhibitor
Pyroglutamyl-peptidase II inhibitor
Dihydrodipicolinate reductase inhibitor
N-formylmethionyl-peptidase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Alanine-tRNA ligase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Glycolate dehydrogenase inhibitor
NADH kinase inhibitor
Leukopoiesis inhibitor
Nardilysin inhibitor
Diisopropyl-fluorophosphatase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
MAP3K5 inhibitor
Pappalysin-1 inhibitor
Diaminopimelate dehydrogenase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Mucinaminyserine mucinaminidase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Adenylyl-sulfate reductase inhibitor
Opioid kappa 3 receptor antagonist
Antiprotozoal (Coccidial)
Antimyopathies
Linoleoyl-CoA desaturase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Feruloyl esterase inhibitor
Orotate reductase (NADH) inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Enteropeptidase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Glycine hydroxymethyltransferase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Nitric-oxide synthase stimulant
Antiprotozoal (Amoeba)
Procollagen-lysine 5-dioxygenase inhibitor
Pancreatic endopeptidase E inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Focal adhesion kinase 2 inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor

Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Membrane permeability inhibitor
Lysyl oxidase inhibitor
Trimethylamine-oxide aldolase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Mucositis treatment
3-Hydroxybenzoate 4-monooxygenase inhibitor
MAP kinase kinase 4 inhibitor
Nitrite reductase [NAD(P)H] inhibitor
ADP-thymidine kinase inhibitor
Endothelial growth factor antagonist
Quercetin 2,3-dioxygenase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Clavamate synthase inhibitor
Flavin-containing monooxygenase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Crotonyl-[acyl-carrier-protein] hydratase inhibitor
Ornithine cyclodeaminase inhibitor
Leukopoiesis stimulant
Thiol oxidase inhibitor
Cyclopentanone monooxygenase inhibitor
Carnitinamidase inhibitor
Hematopoietic
N-acylmannosamine kinase inhibitor
Peptidyl-dipeptidase B inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Glycine amidinotransferase inhibitor
Saccharopine dehydrogenase (NADP⁺, L-glutamate-forming) inhibitor
Age-related macular degeneration treatment
Cyclic AMP modulator
Catalase stimulant
Glutamate (mGluR5) agonist
Sodium channel blocker class Ib
(S)-3-amino-2-methylpropionate transaminase inhibitor
Inotropic
Gonadotropin antagonist
Prion diseases treatment
Aminolevulinate transaminase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
2-Hydroxy-3-oxoadipate synthase inhibitor
Atrolysin A inhibitor
Formate-dihydrofolate ligase inhibitor
Glyoxylate reductase inhibitor
NAD⁺ nucleosidase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Serine-phosphoethanolamine synthase inhibitor
Creatinine deaminase inhibitor

Monodehydroascorbate reductase (NADH) inhibitor
Antiparkinsonian, rigidity relieving
Aspergillopepsin II inhibitor
Urease inhibitor
Muscular dystrophy treatment
N-Acyl-D-aspartate deacylase inhibitor
Hematopoietic inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
CYP2J substrate
Diaminopimelate epimerase inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
L-threonine 3-dehydrogenase inhibitor
Beta-ureidopropionase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
Tankyrase inhibitor
Falcipain 3 inhibitor
CYP2D15 substrate
Prostaglandin-A1 DELTA-isomerase inhibitor
CDK9/cyclin T1 inhibitor
Peptide alpha-N-acetyltransferase inhibitor
CYP2B11 substrate
Transketolase inhibitor
Gly-X carboxypeptidase inhibitor
Mannose isomerase inhibitor
CYP2J2 substrate
Tryptophan 2,3-dioxygenase inhibitor
Fibroblast growth factor agonist
Yeast ribonuclease inhibitor
Methane monooxygenase inhibitor
Cardioprotectant
Leucine dehydrogenase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
NAT2 substrate
Choline kinase inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
L-galactonolactone oxidase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Methyltransferase substrate
Rhizopuspepsin inhibitor
Aldehyde oxidase substrate
Aspartoacylase inhibitor
Nucleoside-diphosphatase inhibitor
Stromelysin 2 inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Sulfite oxidase inhibitor
Gingipain K inhibitor
Cyclomaltodextrinase inhibitor
NAD+-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor

DNA-3-methyladenine glycosylase I inhibitor
CYP2B5 substrate
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Dimethylmaleate hydratase inhibitor
Pyridoxine 4-oxidase inhibitor
Selenocysteine lyase inhibitor
Valine-tRNA ligase inhibitor
Anti-Helicobacter pylori
5 Hydroxytryptamine release stimulant
Ferredoxin hydrogenase inhibitor
Protein kinase B alpha inhibitor
Acylaminoacyl-peptidase inhibitor
Cysteine synthase inhibitor
Ornithine-oxo-acid transaminase inhibitor
Mitochondrial intermediate peptidase inhibitor
Metallo-carboxypeptidase D inhibitor
Peptidylamidoglycolate lyase inhibitor
Antiprotozoal (Trichomonas)
Procollagen C-endopeptidase inhibitor
TRPA1 agonist
Malate oxidase inhibitor
Ferredoxin-nitrite reductase inhibitor
Steroid 9alpha-monooxygenase inhibitor
Rhodotorulapepsin inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
IgA-specific metalloendopeptidase inhibitor
Oryzin inhibitor
Fibroblast growth factor 1 agonist
Alanine carboxypeptidase inhibitor
1,4-Lactonase inhibitor
Calpain inhibitor
Spasmolytic, urinary
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Acidifying agent non gastric
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
GABA aminotransferase inhibitor
Tripeptidyl-peptidase I inhibitor
X-methyl-His dipeptidase inhibitor
Galactolipase inhibitor
Protein synthesis stimulant
Aminopeptidase Y inhibitor
Choline acetyltransferase stimulant
Linoleate diol synthase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Para amino benzoic acid antagonist
Oxidoreductase inhibitor
D-cysteine desulphydrase inhibitor

N-Acyl-D-amino-acid deacylase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Alkene monooxygenase inhibitor
Indanol dehydrogenase inhibitor
Isoquinoline 1-oxidoreductase inhibitor
Phenylalanine decarboxylase inhibitor
Oxalate oxidase inhibitor
Antidote
Glutaminyl-peptide cyclotransferase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Nitrite reductase (NO-forming) inhibitor
Camphor 1,2-monooxygenase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor
Antinephritic
Chitosanase inhibitor
Leukotriene-C4 synthase inhibitor
Picornain 2A inhibitor
Heat shock protein agonist
Tryptophan transaminase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Benzoate 4-monooxygenase inhibitor
Saluretic
CYP2A6 inhibitor
CYP2A4 substrate
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
D-Lysine 5,6-aminomutase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Biotin carboxylase inhibitor
Salicylate 1-monooxygenase inhibitor
Mycothiols-S-conjugate amidase inhibitor
Acetylspermidine deacetylase inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD+) inhibitor
Guanidinoacetase inhibitor
Thiamine pyridinylase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Focal adhesion kinase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Gamma-glutamyltransferase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
L-iditol 2-dehydrogenase inhibitor
Oxidizing agent
CYP2B10 substrate

Transcription factor NF kappa A inhibitor
HIV attachment inhibitor
Check point kinase 2 inhibitor
Octopamine antagonist
Tauropine dehydrogenase inhibitor
Nitrate reductase inhibitor
Dethiobiotin synthase inhibitor
Histone deacetylase SIRT1 inhibitor
Envelysin inhibitor
HMGCS2 expression enhancer
Tyrosine kinase stimulant
Uroporphyrinogen-III synthase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Anthrax lethal factor inhibitor
CYP2C12 substrate
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Cutinase inhibitor
Diamine oxidase inhibitor
ICAM1 expression inhibitor
Penicillin amidase inhibitor
Myeloblastin inhibitor
FMO3 substrate
Ethanolamine-phosphate cytidyltransferase inhibitor
Glutamate decarboxylase inhibitor
Cysteine desulfurase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Hydroxylamine reductase (NADH) inhibitor
CYP2A3 substrate
tRNA nucleotidyltransferase inhibitor
3-Methylbutanal reductase inhibitor
Chelator
Dihydroxy-acid dehydratase inhibitor
X-His dipeptidase inhibitor
Cancer procoagulant inhibitor
IgA-specific serine endopeptidase inhibitor
RELA expression inhibitor
Vascular adhesion protein 1 inhibitor
GABA A inverse agonist
GABA inverse agonist
MAP kinase stimulant
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Bisphosphoglycerate mutase inhibitor
Streptopain inhibitor
Isopenicillin-N synthase inhibitor
Glycine N-acyltransferase inhibitor
DOPA decarboxylase inhibitor
Serralysin inhibitor

Inulinase inhibitor
Galactose oxidase inhibitor
Antihypotensive
Lysosomal Pro-X carboxypeptidase inhibitor
Insulin promoter
N-Carbamoyl-D-amino acid hydrolase inhibitor
Gametolysin inhibitor
Kinase inhibitor
Viral entry inhibitor
CYP2B18 substrate
D-2-hydroxy-acid dehydrogenase inhibitor
Porphobilinogen synthase inhibitor
Valine decarboxylase inhibitor
Exoribonuclease II inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Alpha-glucuronidase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Glycine C-acetyltransferase inhibitor
Dactylisin inhibitor
Aldosterone antagonist
Atrolysin C inhibitor
Cell wall biosynthesis inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
4-Nitrophenylphosphatase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Peptidoglycan glycosyltransferase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Analgesic stimulant
CYP1A2 inducer
Allantoicase inhibitor
Thimet oligopeptidase inhibitor
CYP2A1 substrate
Glutarate-semialdehyde dehydrogenase inhibitor
Antirickettsial
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Glucuronolactone reductase inhibitor
Thiopurine S-methyltransferase inhibitor
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
O-aminophenol oxidase inhibitor
CYP2C8 inhibitor
Granzyme A inhibitor
Mannitol-1-phosphatase inhibitor
Heat shock protein 70 agonist
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Aspartate-tRNA ligase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Carboxylate reductase inhibitor
Thiol S-methyltransferase inhibitor
Choline-phosphate cytidyltransferase inhibitor

Acrosin inhibitor
CYP2A5 substrate
Thermitase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Vasodilator, coronary
Mannan endo-1,6-alpha-mannosidase inhibitor
Histidine ammonia-lyase inhibitor
D-Octopine dehydrogenase inhibitor
Cytochrome-b5 reductase inhibitor
Caspase 3 inhibitor
Tentoxilysin inhibitor
Acyl-CoA dehydrogenase (NADP+) inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
RNA-directed RNA polymerase inhibitor
Glyoxylate oxidase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Hippurate hydrolase inhibitor
Arylamine N-Acetyltransferase substrate
Beta-cyclopiazotate dehydrogenase inhibitor
CYP1A2 inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Sarcosine oxidase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Trans-pentaprenyltranstransferase inhibitor
Chaperonin ATPase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
JNK mitogen-activated protein kinase inhibitor
Antialcoholic
Cathepsin H inhibitor
Tryptophan alpha,beta-oxidase inhibitor
CYP4A2 substrate
Tyrosine 3 hydroxylase inhibitor
Brachyurin inhibitor
Thioredoxin reductase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Ribitol 2-dehydrogenase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
Acetylserotonin O-methyltransferase inhibitor
Iron-cytochrome-c reductase inhibitor
Antibacterial, ophthalmic
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
CYP1A inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Glutamate 5-kinase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Saccharolysin inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor

Quinoprotein glucose dehydrogenase inhibitor
Diuretic inhibitor
L-Serine ammonia-lyase inhibitor
Antiviral (Influenza)
Alcohol dehydrogenase inhibitor
Arylsulfate sulfotransferase inhibitor
Polygalacturonase inhibitor
Steroid synthesis inhibitor
Aryl-alcohol dehydrogenase inhibitor
Lactose synthase inhibitor
Glyoxylate reductase (NADP+) inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Nitrile hydratase inhibitor
MAO A inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
CF transmembrane conductance regulator agonist
Acetylcholine M2 receptor agonist
Allantoinase inhibitor
2-Oxoglutarate decarboxylase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Pim-3 kinase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Plasmanylethanolamine desaturase inhibitor
Arylesterase inhibitor
Serine 3-dehydrogenase inhibitor
Galactoside O-acetyltransferase inhibitor
Choline-sulfatase inhibitor
Thiol protease inhibitor
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Histamine release inhibitor
Aspergillus nuclease S1 inhibitor
tRNA adenylyltransferase inhibitor
Ferrochelataase inhibitor
Aurora-C kinase inhibitor
Bcr-Abl kinase inhibitor
Narcolepsy treatment
Alkenylglycerophosphocholine hydrolase inhibitor
Phloroglucinol reductase inhibitor
Styrene-oxide isomerase inhibitor
Homoserine dehydrogenase inhibitor
Sweetener
Lysine 2-monooxygenase inhibitor
CYP4A11 substrate
Acetoin dehydrogenase inhibitor
GST A substrate
Lactaldehyde reductase inhibitor

Hydroxymethylglutaryl-CoA lyase inhibitor
Histamine agonist
D-xylulose reductase inhibitor
Scytalone dehydratase inhibitor
H⁺-exporting ATPase inhibitor
Dihydrouracil oxidase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
HCV NS3-helicase inhibitor
Phosphatidate phosphatase inhibitor
Lipid metabolism regulator
Diabetic nephropathy treatment
Antiprotozoal (Histomonas)
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Pregnane X receptor agonist
Phosphoglycerate mutase inhibitor
Neuropeptide Y5 antagonist
Catalase inhibitor
Hyaluronic acid agonist
2,4-Dichlorophenol 6-monooxygenase inhibitor
Protocollagen prolyl hydroxylase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
D-lactaldehyde dehydrogenase inhibitor
2-Aminohexano-6-lactam racemase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Glycine N-benzoyltransferase inhibitor
Tyrosine-protein kinase TYRO 10 inhibitor
Glutathione peroxidase inhibitor
Dihydropteroate synthase inhibitor
Sclerosant
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Fructan beta-fructosidase inhibitor
Adenine deaminase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Phosphonoacetate hydrolase inhibitor
Inositol oxygenase inhibitor
Polarisation inhibitor
Vomilenine glucosyltransferase inhibitor
Maltose-transporting ATPase inhibitor
Cystic fibrosis treatment
Protein-glutamate methylesterase inhibitor
CYP3C substrate
Histone deacetylase class III inhibitor
Phosphoinositide phospholipase C inhibitor
Chitinase inhibitor
Cysteamine dioxygenase inhibitor
Quisqualate antagonist
Polar-amino-acid-transporting ATPase inhibitor
Myosin ATPase inhibitor
Proteasome ATPase inhibitor

NADPH-ferrihemoprotein reductase inhibitor
CYP2C9 inducer
Antifibrinolytic
Aryl-alcohol dehydrogenase (NADP+) inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Aspartate kinase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Mannonate dehydratase inhibitor
Cytosole dipeptidase inhibitor
Caspase 8 stimulant
Antiviral (CMV)
Granulocyte macrophage colony stimulating factor agonist
Neurotransmitter antagonist
Succinic dehydrogenase inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Immunoglobulin E antagonist
Antidyskinetic
Subtilisin inhibitor
Aldehyde dehydrogenase 2 substrate
Carnitine 3-dehydrogenase inhibitor
MAP-kinase-activated kinase 1 inhibitor
CYP2C19 inhibitor
Chlordecone reductase inhibitor
GABA C receptor agonist
Antianemic
Cruzipain inhibitor
CYP2A2 substrate
Sphingosine kinase inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Glutamate N-acetyltransferase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
TH expression enhancer
Shab potassium channel blocker
Valine dehydrogenase (NADP+) inhibitor
Alcohol oxidase inhibitor
Glutaminase inhibitor
Acetylcholine release stimulant
Lipotropic
Prolyl aminopeptidase inhibitor
Interleukin 10 agonist
Proline dehydrogenase inhibitor
Urticaria treatment
Glutamate synthase (ferredoxin) inhibitor
Antiprotozoal (Babesia)
Cysteine transaminase inhibitor
Antineoplastic antimetabolite
Agaritine gamma-glutamyltransferase inhibitor
Antidiarrheal
TTK protein kinase inhibitor
Alpha-amylase inhibitor

Formaldehyde dehydrogenase inhibitor
Phosphoserine phosphatase inhibitor
Nicotinamide phosphoribosyltransferase inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Glutamin-(asparagin-)ase inhibitor
Gaucher disease treatment
Guanidinoacetate kinase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Nuclease inhibitor
Neuropeptide Y antagonist
Alkenylglycerophosphoethanolamine hydrolase inhibitor
L-amino-acid oxidase inhibitor
Monocarboxylic acid transporter 1 inhibitor
Monocarboxylic acid transporter inhibitor
Membrane dipeptidase inhibitor
Signal peptidase I inhibitor
Oxytocic
(S)-2-hydroxy-acid oxidase inhibitor
Histone deacetylase SIRT2 inhibitor
Membrane integrity antagonist
Nootropic
Gastrin inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
Macular degeneration treatment
CYP2G1 substrate
Angiogenesis stimulant
Xylose isomerase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Protein kinase B stimulant
Carboxypeptidase D inhibitor
Ubiquitin thiolesterase inhibitor
Aryl-acylamidase inhibitor
Orotate reductase (NADPH) inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Tropinesterase inhibitor

MAO B inhibitor

Cerevisin inhibitor
CYP26A substrate
Methionyl aminopeptidase inhibitor
Neuropeptide antagonist
Aspartyl aminopeptidase inhibitor
Growth factor agonist
Deoxyribose-phosphate aldolase inhibitor
Tripeptide aminopeptidase inhibitor
Ethanolamine kinase inhibitor
Lactate 2-monooxygenase inhibitor
Meprin A inhibitor
Farnesoid X receptor antagonist
(R)-aminopropanol dehydrogenase inhibitor
2-Aminoadipate transaminase inhibitor

3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Arabinose isomerase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Dynamin GTPase inhibitor
X-Pro dipeptidase inhibitor
UGT2B28 substrate
GST T substrate
GST T1-1 substrate
Allantoate deiminase inhibitor
Sulfate adenylyltransferase inhibitor
Proteasome inhibitor
Folate antagonist
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
UDP-glucuronate decarboxylase inhibitor
Amino-acid racemase inhibitor
Hydroxymethylbilane synthase inhibitor
Hyponitrite reductase inhibitor
Pyruvate carboxylase inhibitor
Acid phosphatase inhibitor
Colony stimulating factor agonist
Histamine H2 receptor agonist
5 Hydroxytryptamine 2A agonist
Histidine decarboxylase inhibitor
Cyclin-dependent kinase 5 inhibitor
Polyamine biosynthesis inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Oligopeptidase B inhibitor
Thermomycin inhibitor
BRAF expression inhibitor
Huntington's disease treatment
Alkylglycerone-phosphate synthase inhibitor
Sepiapterin deaminase inhibitor
Hemostatic
UGT2B10 substrate
Neurosin inhibitor
Arylformamidase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
D-alanine transaminase inhibitor
Glutathione synthase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Phospholipase D inhibitor
Flavin-containing monooxygenase substrate
Penicillopepsin inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Imidazoline receptor agonist
Trimethyllysine dioxygenase inhibitor
Prunasin beta-glucosidase inhibitor
Isomaltulose synthase inhibitor
Asparagine-tRNA ligase inhibitor

Janus tyrosine kinase 2 inhibitor
Laminaribiose phosphorylase inhibitor
HIV-1 integrase (Strand Transfer) inhibitor
Aerobactin synthase inhibitor
Granzyme B inhibitor
Cell wall synthesis inhibitor
Glutamate formimidoyltransferase inhibitor
Aspartate racemase inhibitor
3-Phytase inhibitor
Malonyl-CoA decarboxylase inhibitor
Omega-amidase inhibitor
Leishmanolysin inhibitor
Asparaginase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
Coactivator-associated arginine methyltransferase 1 inhibitor
Thromboxane synthase inhibitor
p21-activated kinase 1 inhibitor
Haloalkane dehalogenase inhibitor
Undecaprenyl-diphosphatase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Pantoate-beta-alanine ligase inhibitor
Levanase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Lysyl endopeptidase inhibitor
Aryldialkylphosphatase inhibitor
Allophanate hydrolase inhibitor
Neuropathy treatment
Antithrombocytopenic
Glycerol dehydrogenase (NADP+) inhibitor
Xanthommatin reductase inhibitor
Acetylenecarboxylate hydratase inhibitor
Potassium channel KCNQ blocker
Cytosol alanyl aminopeptidase inhibitor
Neurotrophic factor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Mcl-1 antagonist
Shock treatment
Glucan endo-1,3-alpha-glucosidase inhibitor
Gentisate 1,2-dioxygenase inhibitor
K(ir) 6.2 channel activator
Diiodophenylpyruvate reductase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Factor XIIIa inhibitor
Gluconate dehydratase inhibitor
Serratia marcescens nuclease inhibitor
Lombricine kinase inhibitor
Ribonucleoside diphosphate reductase inhibitor
Monophenol monooxygenase inhibitor
Methionyl aminopeptidase 1 inhibitor
CTP synthase inhibitor

N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Sphingomyelinase inhibitor
Ribonuclease inhibitor
Thromboxane antagonist
4-Pyridoxolactonase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Leucine-tRNA ligase inhibitor
Phospholipase D1 inhibitor
Branched-chain-amino-acid transaminase inhibitor
Endothelin-converting enzyme inhibitor
Potassium channel Kv1.1 blocker
Protein-arginine deiminase inhibitor
Gingipain R inhibitor
DNA synthesis inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
Linoleate isomerase inhibitor
Pyruvate decarboxylase inhibitor
Apyrase inhibitor
Potassium channel KCNQ3 activator
Caspase 3 stimulant
D-proline reductase (dithiol) inhibitor
D-glutamate oxidase inhibitor
FMN reductase inhibitor
Homospermidine synthase inhibitor
CDK2/cyclin A inhibitor
N-acetylneuraminate lyase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminephosphotransferase inhibitor
Histone deacetylase SIRT1 stimulant
Histone deacetylase stimulant
Glucagon receptor antagonist
Mannose-6-phosphate isomerase inhibitor
Cyclamate sulfohydrolase inhibitor
Homocitrate synthase inhibitor
Vasodilator, peripheral
Acetolactate decarboxylase inhibitor
Aminopeptidase B inhibitor
Deoxyhypusine monooxygenase inhibitor
Aldehyde dehydrogenase (NADP+) inhibitor
Phosphatidylinositol 3-kinase stimulant
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Anthranilate-CoA ligase inhibitor
Alkaline phosphatase inhibitor
Peptidylglycine monooxygenase inhibitor
Acetylcholine neuromuscular blocking agent
Dihydropyrimidinase inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor

Galactokinase inhibitor
Xanthine dehydrogenase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
G-protein-coupled bile acid receptor 1 agonist
5 Hydroxytryptamine 4A antagonist
Calcitonin stimulant
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Interleukin 1 beta converting enzyme inhibitor
Arginine decarboxylase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Nav1.8 sodium channel blocker
Agmatinase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
MAP3K8 inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
HIV-1 integrase (3'-Processing) inhibitor
Thiamine-phosphate kinase inhibitor
Bacterial efflux pump inhibitor
Asparaginyl endopeptidase inhibitor
Radioprotector
Cerebroside-sulfatase inhibitor
MARK1 protein inhibitor
Acylglycerone-phosphate reductase inhibitor
Aminopeptidase I inhibitor
Acetolactate synthase inhibitor
Acyl-CoA oxidase inhibitor
Urocanate hydratase inhibitor
HDL-cholesterol increasing
Laccase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Carminative
Nicotinate phosphoribosyltransferase inhibitor
UGT2B12 substrate
Antianorexic
Aminoacylase inhibitor
D-Serine ammonia-lyase inhibitor
2-Dehydropantoate aldolase inhibitor
Nicotinamide-nucleotide amidase inhibitor
Ligase inhibitor
Liver fibrosis treatment
Endo-1,3(4)-beta-glucanase inhibitor
Formimidoylglutamase inhibitor
JAK2 expression inhibitor
RNA synthesis inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
Cysteine-tRNA ligase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase B inhibitor
Elastase 1 inhibitor
Severe acute respiratory syndrome treatment

Chelator, Iron
Morphine 6-dehydrogenase inhibitor
YAK3 inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Potassium channel (ATP-sensitive) activator
Potassium channel (Inward rectifier) activator
Peptide agonist
Sulfur dioxygenase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Arginyltransferase inhibitor
Carboxypeptidase E inhibitor
Insecticide
Ribosomal protein S6 kinase 1, 70-kDa inhibitor
Octadecanal decarbonylase inhibitor
Endopeptidase La inhibitor
GST P1-1 substrate
Dopachrome isomerase inhibitor
Saccharopine dehydrogenase (NAD+, L-glutamate-forming) inhibitor
Fumarate reductase (NADH) inhibitor
Cytostatic
Antineoplastic (brain cancer)
Arginine kinase inhibitor
Glutamate carboxypeptidase inhibitor
CDK5/p25 inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
DNA nucleotidylexotransferase inhibitor
Antineoplastic (bladder cancer)
Propanediol dehydratase inhibitor
Carboxypeptidase M inhibitor
Renal tissue kallikrein inhibitor
CYP1A inducer
2-Nitrophenol 2-monooxygenase inhibitor
Restless leg syndrome treatment
Urolithiasis treatment
Asparagine-oxo-acid transaminase inhibitor
Glutathione reductase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
Leucine transaminase inhibitor
Dolichyl-phosphatase inhibitor
Maleate hydratase inhibitor
Cysteine dioxygenase inhibitor
Shikimate kinase inhibitor
Ferredoxin-NADP+ reductase inhibitor
Antidote, organophosphates
Nucleotide diphosphatase inhibitor
D-arabinonolactone oxidase inhibitor
Cystathionine beta-lyase inhibitor
Arginine deiminase inhibitor
Movement disorders treatment

Cysteine-S-conjugate beta-lyase inhibitor
5-Aminovalerate transaminase inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
Phenylalanine 2-monooxygenase inhibitor
Glycerol-1-phosphatase inhibitor
Aspartate transaminase inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Deoxycytidine deaminase inhibitor
Aspartate 1-decarboxylase inhibitor
Purine biosynthesis inhibitor
Ornithine decarboxylase inhibitor
Selectin E antagonist
Homocysteine desulfhydrase inhibitor
Glutamate (mGluR8) agonist
4,5-Dihydroxyphthalate decarboxylase inhibitor
Protein kinase (Mos, Mil/Raf, MEKK, RIPK, TESK, LIMK, IRAK, ILK, Activin/TGF-beta) inhibitor
NOS3 expression enhancer
Phenylacetaldehyde dehydrogenase inhibitor
NAD⁺ diphosphatase inhibitor
Alpha-N-arabinofuranosidase inhibitor
Lysozyme inhibitor
HIV-2 reverse transcriptase inhibitor
Raf kinase inhibitor
S-adenosyl-L-methionine decarboxylase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
CYP26 substrate
Pyrroline-5-carboxylate reductase inhibitor
Dopamine release stimulant
Gastricsin inhibitor
L-lysine 6-transaminase inhibitor
Pyruvate dehydrogenase inhibitor
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
Glucose 1-dehydrogenase inhibitor
Protein C (activated) inhibitor
Insulysin inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
Signal transduction pathways inhibitor
Polo-like kinase-1 inhibitor
Guanidinobutyrase inhibitor
Phosphoglycolate phosphatase inhibitor
Histamine release stimulant
Farnesyltranstransferase inhibitor
Thrombopoietin agonist
Endonuclease (influenza) inhibitor
Acetate kinase inhibitor
Geranyltranstransferase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Pyridoxamine-pyruvate transaminase inhibitor
Antihyperlipoproteinemic

Excitatory amino acid transporter EAAC1 inhibitor
N-acetylglucosaminyldiphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Beta 1 adrenoreceptor agonist
Cytochrome-c3 hydrogenase inhibitor
p21-activated kinase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
Acetylcholine M3 receptor agonist
Dynein ATPase inhibitor
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
Pyroglutamyl-peptidase I inhibitor
Somatostatin agonist
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Strombine dehydrogenase inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
Rhodopsin kinase inhibitor
Mevalonate kinase inhibitor
GST P substrate
2-Methylcitrate synthase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
D-stereospecific aminopeptidase inhibitor
Methenyltetrahydrofolate cyclohydrolase inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
Mediator release inhibitor
Antiviral (Parainfluenza)
D-lactate dehydrogenase inhibitor
Kynureninase inhibitor
Glutamine-tRNA ligase inhibitor
Pyridoxamine-phosphate oxidase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Trimethylamine-N-oxide reductase inhibitor
Trimereylsin II inhibitor
Phenylalanine 4-hydroxylase inhibitor
Cardiac myosin stimulant
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Creatinase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Decylcitrate synthase inhibitor
Lactaldehyde dehydrogenase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
4-Hydroxy-2-oxoglutarate aldolase inhibitor
Leukocyte elastase inhibitor
CC chemokine 9 receptor antagonist
Ganglioside galactosyltransferase inhibitor
Adenomatous polyposis treatment
Cytochrome P450 stimulant
11-Cis-retinyl-palmitate hydrolase inhibitor
Plasmepsin inhibitor
N-acetylneuraminate synthase inhibitor

Transcription factor inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Peptidyl-glycinamidase inhibitor
Proline transporter inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Phosphatidylglycerophosphatase inhibitor
DNA methylase inhibitor
Cyclin-dependent kinase 4 inhibitor
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Deoxyribonuclease X inhibitor
CYP26 inhibitor
Altronate dehydratase inhibitor
Plasmepsin II inhibitor
Secretase alpha stimulant
Secretase stimulant
Glutamate synthase (NADPH) inhibitor
Dihydrofolate synthase inhibitor
Argininosuccinate lyase inhibitor
CYP19 inducer
Bacterial leucyl aminopeptidase inhibitor
Thioether S-methyltransferase inhibitor
Maleylacetoacetate isomerase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Cytosine deaminase inhibitor
DELTA14-sterol reductase inhibitor
Tryptophan 5 hydroxylase inhibitor
Valine-pyruvate transaminase inhibitor
Neurolysin inhibitor
Cyclin-dependent kinase 2 inhibitor
Cytidine deaminase inhibitor
CYP1A3 substrate
Sterol 3-beta-glucosyltransferase inhibitor
Posttraumatic stress disorder treatment
Arginine racemase inhibitor
Pantoate 4-dehydrogenase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Antineurotic
tRNA (guanine-N2-)-methyltransferase inhibitor
Xanthine oxidase inhibitor
CMP-KDO synthase inhibitor
Sulfinoalanine decarboxylase inhibitor
Assemblin inhibitor

Itraconazole

Molecular Mechanism (initial) :

lanosterol 14-alpha demethylase

Molecular Mechanism (repurposed) :
smoothened homolog inhibitor
lanosterol 14-alpha demethylase inhibitor

initial indication(s):
antifungal agent

Repurposed indication(s):
non-small cell lung cancer

Predicted Activities

Lanosterol 14 alpha demethylase inhibitor

CYP51 inhibitor
Cytochrome P450 inhibitor
CYP3A4 substrate
Antimycobacterial
CYP3A substrate
Antifungal
CYP17 inhibitor
CYP3A4 inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Hypolipemic
P-glycoprotein 1 inhibitor
Cell wall synthesis inhibitor
CYP2C9 inhibitor
P-glycoprotein inhibitor
Mucorpepsin inhibitor
CYP7 inhibitor
CYP2C19 inhibitor
CYP2C8 inhibitor
Antiinfertility, female
CYP19 inhibitor
Anticonvulsant
Cruzipain inhibitor
CYP1A2 inhibitor
Chemosensitizer
Cyclic GMP phosphodiesterase inhibitor
CYP1A inhibitor

Antineoplastic (sarcoma)

Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
Antimigraine
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Alpha 2c adrenoreceptor antagonist
5 Hydroxytryptamine agonist
Microsomal triglyceride transfer protein inhibitor
Histidine kinase inhibitor
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
Antiprotozoal
Squalene synthetase inhibitor

Ketoconazole

Molecular Mechanism (initial) :

fungal cytochrome P450 51 inhibitor

Molecular Mechanism (repurposed) :

cytochrome P450 aromatase (CYP19A1) inhibitor

initial indication(s):

antifungal agent

Repurposed indication(s):

seborrheic dermatitis

Cushing syndrome

Predicted Activities

27-Hydroxycholesterol 7alpha-monooxygenase inhibitor

CYP17 inhibitor

Lanosterol 14 alpha demethylase inhibitor

Antiprotozoal (Amoeba)

Cytochrome P450 inhibitor

CYP51 inhibitor

CYP2C8 inhibitor

CYP7 inhibitor

CYP2C19 inhibitor

Antiprotozoal (Leishmania)

CYP2A6 inhibitor

Antimycobacterial

CYP1A2 inhibitor

CYP1A inhibitor

Antiprotozoal (Trypanosoma)

Antifungal

CYP3A4 inhibitor

Chemosensitizer

CYP19 inhibitor

CYP2C9 inhibitor

Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor

Antiprotozoal (Coccidial)

Anticonvulsant

CYP3A4 substrate

Aspergillopepsin I inhibitor

Radiosensitizer

Antiprotozoal

CYP3A substrate

Mucorpepsin inhibitor

CYP1A1 inhibitor

Cell wall synthesis inhibitor

P-glycoprotein 1 inhibitor

HERG channel blocker

P-glycoprotein inhibitor

Glucan endo-1,3-beta-D-glucosidase inhibitor

CYP2D6 inhibitor

Trans-acenaphthene-1,2-diol dehydrogenase inhibitor

CYP11B2 inhibitor

CYP24 inhibitor

Lysyl oxidase inhibitor
 Cyclic GMP phosphodiesterase inhibitor
 (R)-limonene 6-monooxygenase inhibitor
 Steroid 17-alpha-hydroxylase/17,20 lyase inhibitor
 CYP11B1 inhibitor
 Dimethylallyltranstransferase inhibitor
 Potassium channel (Voltage-sensitive) blocker
 Antieczematic
 Farnesyltransferase inhibitor
 Polyribonucleotide nucleotidyltransferase inhibitor
 N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
 Retinoprotector
 Heme oxygenase inhibitor
 Anaphylatoxin receptor antagonist
 Glycogen synthase stimulant
 Biliary tract disorders treatment
 Glucan endo-1,6-beta-glucosidase inhibitor
 Transketolase inhibitor
 Cruzipain inhibitor
 Antidiabetic (type 2)
 Lipoprotein lipase stimulant
 (N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
 Squalene synthetase inhibitor
 Uterine relaxant
 Luteinizing hormone-releasing hormone antagonist
 Geranylgeranyltransferase I inhibitor
 Histidine kinase inhibitor
 Hypolipemic
 Geranylgeranyltransferase inhibitor
 LFA antagonist
 LFA-1 antagonist

Lidocaine

Molecular Mechanism (initial) :

sodium channels (voltage-gated) blocker

Molecular Mechanism (repurposed) :

sodium channels (voltage-gated) blocker

initial indication(s):

local anesthesia

Repurposed indication(s):

eye disorders

arrhythmia

pain

Predicted Activities

CYP2C12 substrate

Sodium channel blocker class Ib

Membrane integrity antagonist

Taurine dehydrogenase inhibitor

Gluconate 2-dehydrogenase (acceptor) inhibitor

Anesthetic
Anesthetic general
CYP2A6 substrate
CYP2C11 substrate
Antihypoxic
CYP2A substrate
Anesthetic local
Spermidine dehydrogenase inhibitor
Alkane 1-monooxygenase inhibitor
CYP2C18 substrate
Proteasome ATPase inhibitor
Phenol O-methyltransferase inhibitor
CYP3A2 substrate
CYP2B6 substrate
Spasmolytic, urinary
CYP2B1 substrate
2-Hydroxyquinoline 8-monooxygenase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Amine dehydrogenase inhibitor
CYP2C8 substrate
Phobic disorders treatment
Trimethylamine-oxide aldolase inhibitor
Calcium channel (voltage-sensitive) activator
Sulfite reductase inhibitor
Antiseborrheic
Anticonvulsant
Venombin AB inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Pseudolysin inhibitor
Endopeptidase So inhibitor
Fructose 5-dehydrogenase inhibitor
Polyamine-transporting ATPase inhibitor
Fusarinine-C ornithinesterase inhibitor
Gastrin inhibitor
Membrane integrity agonist
Nicotinate dehydrogenase inhibitor
CYP1A2 substrate
CYP2D substrate
CYP1A substrate
Superoxide dismutase inhibitor
Antidyskinetic
General pump inhibitor
CYP2B substrate
CYP3A5 substrate
Sodium channel blocker
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Cardiotonic
4-Hydroxyproline epimerase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
CYP2J substrate

Glutamyl endopeptidase II inhibitor
CYP2C substrate
Long-chain-aldehyde dehydrogenase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
CYP2B2 substrate
Ompin inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
CYP2D1 substrate
Sulfur reductase inhibitor
Octopamine antagonist
Urethanase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Fragilysin inhibitor
Fibrolase inhibitor
Antiarrhythmic
CYP2F1 substrate
pFOX inhibitor
Thiol oxidase inhibitor
Dimethylargininase inhibitor
Nitrate reductase (cytochrome) inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Nitrite reductase (NO-forming) inhibitor
Carboxypeptidase Taq inhibitor
Formaldehyde transketolase inhibitor
Cl--transporting ATPase inhibitor
Platelet aggregation stimulant
Limulus clotting factor B inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Sigma receptor agonist
Hydroxylamine oxidase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Sulfur dioxygenase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Fatty-acyl-CoA synthase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
1,4-Lactonase inhibitor
Macrophage colony stimulating factor agonist
Phthalate 4,5-dioxygenase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
CYP2C8 inhibitor
Fibrinolytic
Laccase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
2-Haloacid dehalogenase inhibitor
Cyclic AMP agonist
Diamine N-acetyltransferase inhibitor
Thymidylate 5'-phosphatase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor

Fibrinogen receptor antagonist
Neuropeptide Y2 antagonist
FMO1 substrate
Protein-disulfide reductase (glutathione) inhibitor
CYP2J2 substrate
Glutathione thiolesterase inhibitor
ADP-thymidine kinase inhibitor
CYP3A1 substrate
Insulysin inhibitor
Lysostaphin inhibitor
CYP2C9 substrate
NADPH-cytochrome-c2 reductase inhibitor
Methanol dehydrogenase inhibitor
5 Hydroxytryptamine release inhibitor
Polyporopepsin inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Antiparkinsonian, rigidity relieving
CYP3A4 substrate
Thiosulfate dehydrogenase inhibitor
Phospholipid-translocating ATPase inhibitor
Spasmolytic
Oxygen scavenger
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Nicotine dehydrogenase inhibitor
Ecdysone 20-monooxygenase inhibitor
Chenodeoxycholoyltaurine hydrolase inhibitor
Tryptophanamidase inhibitor
Mandelate 4-monooxygenase inhibitor
CYP2D16 substrate
Sigma 1 receptor agonist
Gluconolactonase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
MAP kinase stimulant
Respiratory analeptic
Catechol oxidase inhibitor
Acetylcholine neuromuscular blocking agent
Malate dehydrogenase (acceptor) inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Antineurogenic pain
Kidney function stimulant
Acaricide
Cyclohexanone monooxygenase inhibitor
Gluconate 5-dehydrogenase inhibitor
Aldehyde oxidase inhibitor
Limulus clotting factor C inhibitor
CYP3A substrate
N-formylmethionyl-peptidase inhibitor

Exoribonuclease II inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Trimethylamine dehydrogenase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Retinal dehydrogenase inhibitor
Choline-phosphate cytidyltransferase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Mitochondrial processing peptidase inhibitor
Arylmalonate decarboxylase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Flavin-containing monooxygenase substrate
Prolyl aminopeptidase inhibitor
Alanine-tRNA ligase inhibitor
Cathepsin T inhibitor
Fucosterol-epoxide lyase inhibitor
Antianginal
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Botulin neurotoxin A light chain inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Dimethylmaleate hydratase inhibitor
Ferrodoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Erythropoiesis stimulant
2-Hydroxy-3-oxoadipate synthase inhibitor
Cyclopentanone monooxygenase inhibitor
Antihelminthic (Nematodes)
Acute neurologic disorders treatment
4-Hydroxymandelate oxidase inhibitor
CYP2G1 substrate
Arylacetonitrilase inhibitor
Creatininase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Leukopoiesis stimulant
Chloride peroxidase inhibitor
Gingipain K inhibitor
Prion diseases treatment
Urticaria treatment
Peptidyl-dipeptidase Dcp inhibitor
Complement factor D inhibitor
Sphinganine kinase inhibitor
Manganese peroxidase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
N-acylmannosamine kinase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Mucomembranous protector
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Lysine 2,3-aminomutase inhibitor
Hydrogen dehydrogenase inhibitor

Antileprosy
Benzoate-CoA ligase inhibitor
Glyceryl-ether monooxygenase inhibitor
Cardiovascular analeptic
Aspulvinone dimethylallyltransferase inhibitor
Analeptic
Flavin-containing monooxygenase inhibitor
Diuretic inhibitor
Arginine 2-monooxygenase inhibitor
Peroxidase inhibitor
tRNA nucleotidyltransferase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Cytoprotectant
Poly(beta-D-mannuronate) lyase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
5 Hydroxytryptamine uptake stimulant
Platelet derived growth factor receptor kinase inhibitor
Antisecretoric
IgA-specific serine endopeptidase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Plasmanylethanolamine desaturase inhibitor
Loop diuretic
Acetylspermidine deacetylase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Hematopoietic inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Pterin deaminase inhibitor
Pullulanase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Intermittent claudication treatment
Adrenaline release stimulant
6-Pyruvoyltetrahydropterin synthase inhibitor
Carboxypeptidase D inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
3-Cyanoalanine hydratase inhibitor
FMO3 substrate
Bisphosphoglycerate phosphatase inhibitor
Phosphatidylserine decarboxylase inhibitor
Myc inhibitor
Muramoyltetrapeptide carboxypeptidase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Cyanoalanine nitrilase inhibitor
Oxidoreductase inhibitor
Arylsulfate sulfotransferase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
CYP2D6 substrate

CYP4A substrate
Urease inhibitor
Platelet adhesion inhibitor
Sugar-phosphatase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Antinaupathic
Alkylacetylgllycerophosphatase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
CYP2C10 substrate
NADH kinase inhibitor
Mannitol-1-phosphatase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Muscle relaxant
TRPA1 agonist
Mannan endo-1,4-beta-mannosidase inhibitor
Leukopoiesis inhibitor
Creatinase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Vasodilator, coronary
Nardilysin inhibitor
Gallate decarboxylase inhibitor
Antinociceptive
CYP1A inhibitor
Tryptophan 2,3-dioxygenase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Tyrosine 3 hydroxylase inhibitor
CYP1A1 substrate
CYP1A2 inhibitor
DELTA14-sterol reductase inhibitor
CYP2C29 substrate
Renal tissue kallikrein inhibitor
RNA-directed RNA polymerase inhibitor
CYP2D15 substrate
N-acetyllactosamine synthase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Skeletal muscle relaxant
S-formylglutathione hydrolase inhibitor
Methane monooxygenase inhibitor
Glycolate dehydrogenase inhibitor
Calcium channel activator
Pyruvate decarboxylase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Gonadotropin antagonist
Arylesterase inhibitor
Antischistosomal
Retinoic acid metabolism inhibitor
Transketolase inhibitor
Acetylesterase inhibitor
Saluretic
Histidine N-acetyltransferase inhibitor

Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Thioredoxin inhibitor
Opine dehydrogenase inhibitor
Phosphopantothienoylcysteine decarboxylase inhibitor
Antiperistaltic
Nav1.3 sodium channel blocker
Pancreatic elastase inhibitor
Aryl-acylamidase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Hydroxylamine reductase inhibitor
Sulfite dehydrogenase inhibitor
Aspartate-ammonia ligase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Oxytocic
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Ferrochelataase inhibitor
Alopecia treatment
Adenylyl-sulfate reductase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Ornithine cyclodeaminase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Aminoacylase inhibitor
Thiamine pyridinylase inhibitor
Polarisation inhibitor
Centromere associated protein inhibitor
Antiprotozoal (Trichomonas)
Antimyopathies
Nicotinic alpha2beta2 receptor antagonist
CYP2A8 substrate
NAT1 substrate
Raynaud's phenomenon treatment
[acyl-carrier-protein] S-acetyltransferase inhibitor
Acylcarnitine hydrolase inhibitor
Ethanolamine oxidase inhibitor
CNS active muscle relaxant
Transcription factor STAT3 inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Nootropic
Nav1.8 sodium channel blocker
Nav1.2 sodium channel blocker
Calpain inhibitor
Pitrilysin inhibitor
Immunosuppressant
Aspergillopepsin I inhibitor
TNF expression inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Carnitinamidase inhibitor
Antiprotozoal (Amoeba)
Histamine release stimulant

Mitochondrial intermediate peptidase inhibitor
Aldehyde dehydrogenase 2 substrate
Antiprotozoal (Trypanosoma)
Inotropic
Lysase inhibitor
O-aminophenol oxidase inhibitor
Antipyretic
Poly(alpha-L-gulonate) lyase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Diisopropyl-fluorophosphatase inhibitor
Hemostatic
Cardioprotectant
2-Dehydropantoate 2-reductase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
CYP2A5 substrate
Quinoprotein glucose dehydrogenase inhibitor
Neurotransmitter antagonist
Enteropeptidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Gamma-glutamyltransferase inhibitor
Glucuronate isomerase inhibitor
Dihydroxy-acid dehydratase inhibitor
L-glutamate oxidase inhibitor
Meprin B inhibitor
Leucolysin inhibitor
Biotinidase inhibitor
Antifibrinolytic
Antiviral (Picornavirus)
Fructan beta-fructosidase inhibitor
Membrane permeability enhancer
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Glucose oxidase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
EIF4E expression inhibitor
Apyrase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
Picornain 3C inhibitor
Glyoxylate reductase inhibitor
Antidote
Bontoxilysin inhibitor
Aspergillus nuclease S1 inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
3-Phytase inhibitor
Cyclic AMP modulator
L-threonine 3-dehydrogenase inhibitor

Ubiquitin thiolesterase inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
MMP9 expression inhibitor
Antitussive
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Sodium channel (voltage-gated) blocker
Sphingosine 1-phosphate receptor antagonist
Porphobilinogen synthase inhibitor
Endopeptidase La inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Choline acetyltransferase stimulant
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Benzoate 4-monooxygenase inhibitor
Bile-salt sulfotransferase inhibitor
Oxalate oxidase inhibitor
Aspartoacylase inhibitor
Menopausal disorders treatment
Antiparkinsonian, tremor relieving
Indolepyruvate C-methyltransferase inhibitor
Dipeptidase E inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Snapalysin inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Isopenicillin-N epimerase inhibitor
Peptidylamidoglycolate lyase inhibitor
Clavamate synthase inhibitor
Oxidizing agent
Fibroblast growth factor agonist
Electrolyte absorption antagonist
Coagulant
Polygalacturonase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Aspergillopepsin II inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
CYP2B5 substrate
Deacetoxycephalosporin-C synthase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
CYP2C3 substrate
Interleukin 10 agonist
Mannose isomerase inhibitor
Procollagen N-endopeptidase inhibitor
Aureolysin inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor

Muscular dystrophy treatment
Gly-X carboxypeptidase inhibitor
Cytochrome P450 stimulant
Ribitol 2-dehydrogenase inhibitor
Gingipain R inhibitor
Venom exonuclease inhibitor
Transactivator transcription protein inhibitor
Hyaluronic acid agonist
Aldehyde dehydrogenase (NADP⁺) inhibitor
Glucan endo-1,3- α -glucosidase inhibitor
Alcohol dehydrogenase [NAD(P)⁺] inhibitor
Chitosanase inhibitor
Horrilysin inhibitor
Simian immunodeficiency virus proteinase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Leukotriene-C₄ synthase inhibitor
Pappalysin-1 inhibitor
Yeast ribonuclease inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Aryldialkylphosphatase inhibitor
Bothrolysin inhibitor
Tyrosine kinase stimulant
HCV IRES inhibitor
Histamine release inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Aldehyde dehydrogenase [NAD(P)⁺] inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Transcription factor STAT inhibitor
X-methyl-His dipeptidase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Quercetin 2,3-dioxygenase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
CYP2E1 substrate
Polyamine oxidase inhibitor
Antiparasitic
Camphor 1,2-monooxygenase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
CYP2C19 substrate
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Ovulation inhibitor
Nucleoside oxidase (H₂O₂-forming) inhibitor
Coccolysin inhibitor
CYP2E substrate
Alpha-amylase inhibitor
Creatinine deaminase inhibitor
Nav1.1 sodium channel blocker
NAT2 substrate

Phosphatidylglycerophosphatase inhibitor
N-acetylneuraminate synthase inhibitor
CYP2E1 inducer
Cytidine deaminase inhibitor
tRNA-pseudouridine synthase I inhibitor
Allantoate deiminase inhibitor
Systemic lupus erythematosus treatment
Antihelminthic
Nucleotide metabolism regulator
Spasmolytic, Papaverin-like
Hydroxylamine reductase (NADH) inhibitor
Glycine amidinotransferase inhibitor
Imidazoline receptor agonist
Carbon-monoxide dehydrogenase inhibitor
Lck kinase inhibitor
Uroporphyrinogen-III synthase inhibitor
Chitinase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
Nitrile hydratase inhibitor
Radioprotector
Pyroglutamyl-peptidase II inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Cycloartenol synthase inhibitor
Pancreatic endopeptidase E inhibitor
Calcium antagonist
Envelysin inhibitor
Polyneuridine-aldehyde esterase inhibitor
Ferrodoxin-nitrite reductase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Antiprotozoal (Leishmania)
Inulinase inhibitor
Antinephritic
Feruloyl esterase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Acylaminoacyl-peptidase inhibitor
Cytochrome-b5 reductase inhibitor
CYP2C19 inducer
Alpha-Methylacyl-CoA racemase inhibitor
Lipocortins synthesis antagonist
Monoamine uptake inhibitor
Radiosensitizer
Cysteamine dioxygenase inhibitor
Acetylornithine deacetylase inhibitor
Anticataract
Aminopeptidase Y inhibitor
1,2-alpha-L-fucosidase inhibitor
Hypolipemic
Glucan endo-1,6-beta-glucosidase inhibitor

N-carbamoyl-L-amino-acid hydrolase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Nicotinamidase inhibitor
Nitrate reductase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Arylamine N-acetyltransferase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Glutaminyl-peptide cyclotransferase inhibitor
Antiulcerative
Chaperonin ATPase inhibitor
Albendazole monooxygenase inhibitor
Acyl-CoA oxidase inhibitor
Insecticide
Picornain 2A inhibitor
CYP2B11 substrate
Myeloblastin inhibitor
Myosin ATPase inhibitor
Metallo-carboxypeptidase D inhibitor
Tentoxilysin inhibitor
CYP1A2 inducer
Catenin beta inhibitor
Ferredoxin hydrogenase inhibitor
Mucositis treatment
Peptidyltransferase inhibitor
Malate oxidase inhibitor
Pulmonary hypertension treatment
Hydroxymethylglutaryl-CoA lyase inhibitor
Dactylisin inhibitor
3-Aminobutyl-CoA ammonia-lyase inhibitor
CYP4A2 substrate
Ethanolamine-phosphate cytidyltransferase inhibitor
Antiviral (Adenovirus)
Trans-pentaprenyltransferase inhibitor
Antitoxic
Ribonucleoside triphosphate reductase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Antiischemic
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
S-alkylcysteine lyase inhibitor
Dynein ATPase inhibitor
Thimet oligopeptidase inhibitor
Antiischemic, cerebral
Serine-pyruvate transaminase inhibitor
CYP1A3 substrate
Lysyl oxidase inhibitor
Aryl hydrocarbon receptor agonist
Atrolisin A inhibitor
NF-E2-related factor 2 stimulant
Levanase inhibitor

Granzyme A inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Carboxylesterase inhibitor
Phosphoinositide phospholipase C inhibitor
Antipruritic, allergic
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Maillard reaction inhibitor
Guanidinoacetase inhibitor
Thiamine-phosphate kinase inhibitor
Pin1 inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
CYP2C9 inducer
UGT2B12 substrate
Maleate isomerase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Prenyl-diphosphatase inhibitor
Transcription factor inhibitor
Insulin promoter
Leishmanolysin inhibitor
Bisphosphoglycerate mutase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Gastrointestinal motility stimulant
Galactolipase inhibitor
Phosphoenolpyruvate mutase inhibitor
Glycerol-1-phosphatase inhibitor
Tryptophan 2-monooxygenase inhibitor
Rhodotorulapepsin inhibitor
CYP2A4 substrate
GST A substrate
Cyclic AMP phosphodiesterase inhibitor
Cyclomaltodextrinase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
CYP2A1 substrate
Glucan 1,4-alpha-maltotriohydrolase inhibitor
HIV-2 reverse transcriptase inhibitor
Thiamine-triphosphatase inhibitor
Angiotensin II receptor agonist
HMOX1 expression enhancer
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
ATPase inhibitor
Brachyurin inhibitor
5 Hydroxytryptamine 7L antagonist
Stromelysin 2 inhibitor
Antipruritic
Alcohol dehydrogenase (acceptor) inhibitor
Chlordecone reductase inhibitor
Kinase inhibitor
Tryptophanyl aminopeptidase inhibitor
Thiol S-methyltransferase inhibitor

L-amino-acid oxidase inhibitor
Galactose oxidase inhibitor
CYP2A2 substrate
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Acetolactate decarboxylase inhibitor
Trypanothione-disulfide reductase inhibitor
Acid phosphatase inhibitor
Dextranase inhibitor
CYP26A substrate
CYP2D6 inhibitor
CYP2A3 substrate
Signal peptidase I inhibitor
Peptide agonist
Alkylglycerone-phosphate synthase inhibitor
Clostripain inhibitor
Glutaminase inhibitor
CYP4A11 substrate
Cellulose 1,4-beta-cellobiosidase inhibitor
Inositol oxygenase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
D-stereospecific aminopeptidase inhibitor
Opioid kappa 3 receptor antagonist
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
IgA-specific metalloendopeptidase inhibitor
Phosphoglycerate mutase inhibitor
D-xylulose reductase inhibitor
Antiprotozoal (Plasmodium)
(S)-3-amino-2-methylpropionate transaminase inhibitor
Oryzin inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
GABA C receptor agonist
N-Carbamoyl-D-amino acid hydrolase inhibitor
Orotate reductase (NADH) inhibitor
Aurora-C kinase inhibitor
Lombricine kinase inhibitor
ATP-binding cassette A1 stimulant
Tryptophan dimethylallyltransferase inhibitor
CYP2B10 substrate
Antituberculosic
Telomerase inhibitor
Diuretic
Antialcoholic
Dolichyl-phosphatase inhibitor
CYP2B18 substrate
Anthrax lethal factor inhibitor
Antianorexic
Antineoplastic (multiple myeloma)
Oligopeptidase B inhibitor

Acylglycerone-phosphate reductase inhibitor
Saccharolysin inhibitor
Allantoicase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Gametolysin inhibitor
Procollagen C-endopeptidase inhibitor
Antineoplastic (liver cancer)
D-Octopine dehydrogenase inhibitor
Dopamine release stimulant
Alkylator
Peptidyl-dipeptidase B inhibitor
CYP2E1 inhibitor
NADPH peroxidase inhibitor
Antimutagenic
Tripeptidyl-peptidase I inhibitor
Heat shock protein agonist
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
Transcription factor NF kappa A inhibitor
Phloroglucinol reductase inhibitor
Gastric antisecretory
Skin irritation, inactive
Isopenicillin-N synthase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Pim-3 kinase inhibitor
Cyclamate sulfohydrolase inhibitor
Choline-sulfatase inhibitor
Steroid synthesis inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Adenosine regulator
D-threo-aldose 1-dehydrogenase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Antimycobacterial
Acetylenecarboxylate hydratase inhibitor
Glycerol dehydratase inhibitor
Acyl-lysine deacylase inhibitor
NADH dehydrogenase inhibitor
Allantoinase inhibitor
Lactaldehyde reductase inhibitor
Farnesoid X receptor antagonist
Thermitase inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Prunasin beta-glucosidase inhibitor
Glutamate synthase (ferredoxin) inhibitor
RNA synthesis inhibitor
4-Nitrophenylphosphatase inhibitor
Restless leg syndrome treatment
NADPH oxidase inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
Calcium-sensing receptor agonist

Aryl-alcohol dehydrogenase inhibitor
Cytochrome-c3 hydrogenase inhibitor
Adenomatous polyposis treatment
Antineoplastic, alkylator
Diabetic neuropathy treatment
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
Antiprotozoal
Linoleoyl-CoA desaturase inhibitor
CYP2C9 inhibitor
Photosensitizer
Guanidinoacetate kinase inhibitor
Pseudouridylate synthase inhibitor
Chelator
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Serralysin inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
P-glycoprotein 1 inhibitor
Para amino benzoic acid antagonist
Quisqualate antagonist
Thermomycin inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Caspase 3 stimulant
Glucuronolactone reductase inhibitor
Hippurate hydrolase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Hematopoietic
HDL-cholesterol increasing
Aspartate-ammonia ligase (ADP-forming) inhibitor
Hydroxymethylbilane synthase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Tripeptide aminopeptidase inhibitor
DELTA24-sterol reductase inhibitor
Serum-glucocorticoid regulated kinase 1 inhibitor
CYP2A6 inhibitor
Nucleoside-diphosphatase inhibitor
Heat shock protein 70 agonist
Prolactin inhibitor
Carminative
Guanidinoacetate N-methyltransferase inhibitor
Butyrylcholinesterase stimulant
Glycine transporter 2 inhibitor
Carnitine 3-dehydrogenase inhibitor
Antiamyloidogenic
Aspartyl aminopeptidase inhibitor
Female sexual dysfunction treatment
Carboxymethylenebutenolidase inhibitor
Phenylpyruvate decarboxylase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)⁺] inhibitor
Nuclease inhibitor

Orexin receptor antagonist
ATP adenylyltransferase inhibitor
Preneoplastic conditions treatment
Asparaginase inhibitor
Lipoxygenase substrate
Protein-tyrosine kinase p55(blk) inhibitor
Antiuremic
Arylalkyl acylamidase inhibitor
Alkaline phosphatase inhibitor
Sulfite oxidase inhibitor
CYP3A3 substrate
Acidifying agent non gastric
Sphingosine 1-phosphate receptor 1 antagonist
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Erectile dysfunction treatment
Alkenylglycerophosphoethanolamine hydrolase inhibitor
2-Dehydropantoate aldolase inhibitor
Growth factor agonist
Antiviral (CMV)
D-2-hydroxy-acid dehydrogenase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Pectin lyase inhibitor
Deoxyribonuclease I inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
H⁺-exporting ATPase inhibitor
Interleukin 2 agonist
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Selenocysteine lyase inhibitor
Protein-tyrosine kinase Lyn inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Thromboxane B2 antagonist
Lipid peroxidase inhibitor
Licheninase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Multiple sclerosis treatment
Pyridoxal kinase inhibitor
Pantothenase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Histidinol dehydrogenase inhibitor
2-Oxoglutarate decarboxylase inhibitor
Malate-CoA ligase inhibitor
3C-like protease (Human coronavirus) inhibitor
Venombin A inhibitor
Histidinol-phosphatase inhibitor
Agmatinase inhibitor
Bcr-Abl kinase inhibitor
Acetyl-CoA transferase inhibitor
Serratia marcescens nuclease inhibitor
Mediator release inhibitor

Linoleate diol synthase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Ganglioside galactosyltransferase inhibitor
Protein synthesis stimulant
Cholate-CoA ligase inhibitor
Dementia treatment
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Alcohol dehydrogenase inhibitor
Vasoprotector
UDP-N-acetylglucosamine diphosphorylase inhibitor
Lysosomal Pro-X carboxypeptidase inhibitor
Glutamin-(asparagin-)ase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Glutamate 5-kinase inhibitor
Glutamate-tRNA ligase inhibitor
Iron-cytochrome-c reductase inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Neuropsin inhibitor
Alpha-glucuronidase inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Sorbose dehydrogenase inhibitor
Allantoin racemase inhibitor
CYP3A7 substrate
Aspartate racemase inhibitor
Lysine decarboxylase inhibitor
Narcolepsy treatment
5 Hydroxytryptamine release stimulant
Aldehyde ferredoxin oxidoreductase inhibitor
Reductant
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Aminopeptidase B inhibitor
Vascular adhesion protein 1 inhibitor
CYP7 inhibitor
Homospermidine synthase inhibitor
Antiprotozoal (Coccidial)
Cutinase inhibitor
Antiprotozoal (Babesia)
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Haloalkane dehalogenase inhibitor
Valine decarboxylase inhibitor
Neuropeptide Y4 antagonist
Pyruvate dehydrogenase inhibitor
Endothelial growth factor antagonist
Calcium channel blocker
tRNA adenylyltransferase inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Extrapyrmidal disorders treatment

Nitric-oxide synthase stimulant
Viral entry inhibitor
GABA aminotransferase inhibitor
Antiviral (Poxvirus)
Putrescine oxidase inhibitor
Oxytocin agonist
D-Ornithine 4,5-aminomutase inhibitor
Dihydropyrimidinase inhibitor
DNA methyltransferase I inhibitor
Tropinesterase inhibitor
Antibacterial, ophthalmic
Antiepileptic
CF transmembrane conductance regulator agonist
Endopeptidase inhibitor
Glutathione peroxidase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Trimethylamine-N-oxide reductase inhibitor
Protein-tyrosine sulfotransferase inhibitor
Glutamate N-acetyltransferase inhibitor
Phosphate acetyltransferase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Membrane permeability inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Squalene epoxidase inhibitor
Penicillin amidase inhibitor
Glucarate dehydratase inhibitor
Calcium channel (voltage-sensitive) blocker
DNA ligase (ATP) inhibitor
JAK2 expression inhibitor
Vasodilator, peripheral
Pectate lyase inhibitor
Antineoplastic (bone cancer)
D-alanine 2-hydroxymethyltransferase inhibitor
Respiratory distress syndrome treatment
Mucolytic
Malate dehydrogenase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Gentisate 1,2-dioxygenase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Phosphonoacetate hydrolase inhibitor
Mevalonate kinase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Decylcitrate synthase inhibitor
Formimidoylglutamate inhibitor

Guanidinodeoxy-scyllo-inositol-4-phosphatase inhibitor
Alpha-N-arabinofuranosidase inhibitor
P-glycoprotein inhibitor
ADP-ribosylarginine hydrolase inhibitor
Lipoprotein lipase inhibitor
Glycerol dehydrogenase (NADP+) inhibitor
Trimereysin II inhibitor
CYP26 substrate
MO15-related protein kinase Pfmrk inhibitor
Cyclooxygenase 3 inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Analgesic
Mannonate dehydratase inhibitor
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
4-Coumarate-CoA ligase inhibitor
Bombesin 1 receptor antagonist
Autophagy inducer
Acetolactate synthase inhibitor
CYP2D2 inhibitor
3-Methylbutanal reductase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
Tetrahydroxynaphthalene reductase inhibitor
Arylamine N-Acetyltransferase substrate
X-His dipeptidase inhibitor
Hyponitrite reductase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
Gluconate dehydratase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Beta-amylase inhibitor
Rhizopuspepsin inhibitor
Sodium/calcium exchanger inhibitor
Biotin carboxylase inhibitor
GABA B receptor agonist
Muconate cycloisomerase inhibitor
Arylsulfatase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Glutamine-tRNA ligase inhibitor
Protein-synthesizing GTPase inhibitor
Methionyl aminopeptidase inhibitor
Ribonuclease inhibitor
Glycine N-acyltransferase inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
Peptidyl-glycinamidase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Ophthalmic drug
Analgesic stimulant
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor
Vomilenine glucosyltransferase inhibitor

Leucine dehydrogenase inhibitor
Omega-amidase inhibitor
Interferon agonist
Glycine C-acetyltransferase inhibitor
Cysteine desulfurase inhibitor
Myocardial ischemia treatment
CYP1A1 inhibitor
Chloride channel activator
Src kinase inhibitor
Antidepressant, Imipramin-like
Orotate reductase (NADPH) inhibitor
L-fuconate dehydratase inhibitor
Cellulase inhibitor
Glyoxylate oxidase inhibitor
Hyperprolactinemia treatment
Iron antagonist
Atrolisin C inhibitor
Inorganic diphosphatase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Guanidinopropionase inhibitor
Glucose 1-dehydrogenase inhibitor
Wee-1 tyrosine kinase inhibitor
Aldehyde dehydrogenase inhibitor
Alpha-L-fucosidase inhibitor
Antihematotoxic
Streptopain inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
NMDA receptor polyamine site antagonist
Amyotrophic lateral sclerosis treatment
5 Hydroxytryptamine 7 agonist
Psychosexual dysfunction treatment
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Sarcosine oxidase inhibitor
Arginyltransferase inhibitor
Cancer procoagulant inhibitor
Caspase 8 stimulant
Dolichol kinase inhibitor
Mycolysin inhibitor
Choline sulfotransferase inhibitor
Antiinflammatory, intestinal
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Formate-dihydrofolate ligase inhibitor
TH expression enhancer
Bipolar disorder treatment
Acetate kinase inhibitor
Cytosol alanyl aminopeptidase inhibitor
Cysteine synthase inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor

T cell inhibitor
L-glucuronate reductase inhibitor
Choleretic
Catalase inhibitor
3-Isopropylmalate dehydratase inhibitor
Cerebrovascular disorders treatment
AR expression inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Tankyrase inhibitor
CYP3C substrate
Diamine oxidase inhibitor
BRAF expression inhibitor
Shab potassium channel blocker
Polynucleotide adenylyltransferase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Dihydrouracil oxidase inhibitor
NMDA receptor glycine site agonist
GABA A inverse agonist
GABA inverse agonist
Choline dehydrogenase inhibitor
Lysozyme inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Mallyl-CoA lyase inhibitor
Thiopurine S-methyltransferase inhibitor
Sodium/calcium exchanger 1 inhibitor
Styrene-oxide isomerase inhibitor
Alzheimer's disease treatment
Methylaspartate ammonia-lyase inhibitor
NMDA receptor agonist
Tauropine dehydrogenase inhibitor
Acetylserotonin O-methyltransferase inhibitor
Peptidylglycine monooxygenase inhibitor
Sclerosant
Xanthommatin reductase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Galactoside O-acetyltransferase inhibitor
Dichloromuconate cycloisomerase inhibitor
Lactose synthase inhibitor
CYP1A inducer
Cyclooxygenase substrate
CYP2C6 substrate
Beta-ureidopropionase inhibitor
Antineoplastic alkaloid
Lysyl endopeptidase inhibitor
Allophanate hydrolase inhibitor
CC chemokine 2 receptor antagonist
Formaldehyde dehydrogenase (glutathione) inhibitor
Membrane dipeptidase inhibitor

Gaucher disease treatment
Guanidinobutyrase inhibitor
Pediculicide
Cholinergic
Homocitrate synthase inhibitor
Acylphosphatase inhibitor
11-Cis-retinyl-palmitate hydrolase inhibitor
RET inhibitor
Myt1 kinase inhibitor
Butyrylcholinesterase inhibitor
Xylose isomerase inhibitor
Trehalose-phosphatase inhibitor
Dihydroorotase inhibitor
Acrosin inhibitor
Farnesyltranstransferase inhibitor
CYP1B substrate
2-Acylglycerol O-acyltransferase inhibitor
Dihydroxyacetanilide dehydrogenase inhibitor
Dihydroxyacetanilide epoxidase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Sleep apnea treatment
Acetyl-CoA C-acyltransferase inhibitor
Hepatoprotectant
Interleukin 6 antagonist
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminephosphotransferase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
Antidiarrheal
Cerevisin inhibitor
Antirickettsial
Urolithiasis treatment
4,5-Dihydroxyphthalate decarboxylase inhibitor
Retinopathy treatment
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
Aerobactin synthase inhibitor
CYP19A1 expression inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Phenylalanine 4-hydroxylase inhibitor
D-cysteine desulfhydrase inhibitor
Angiotensin agonist
Glucan 1,4-beta-glucosidase inhibitor
Antiinflammatory, ophthalmic
1,4-Alpha-glucan branching enzyme inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Riboflavin phosphotransferase inhibitor
Pyruvate carboxylase inhibitor
Formate dehydrogenase inhibitor
Galactokinase inhibitor
Furin inhibitor
Glycine receptor antagonist

6-Methylsalicylate decarboxylase inhibitor
Glycine N-benzoyltransferase inhibitor
Vascular (periferal) disease treatment
VEGF expression inhibitor
Huntington's disease treatment
Delayed rectifier potassium channel activator
Potassium channel (Voltage-sensitive) activator
Potassium channel KCNQ activator
Phosphorylase kinase inhibitor
Adenylate kinase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Cysteine dioxygenase inhibitor
Purinergic P2X antagonist
Neuropeptide Y1 antagonist
Glycerophosphocholine phosphodiesterase inhibitor
Age-related macular degeneration treatment
5-Oxoprolinase (ATP-hydrolysing) inhibitor
L-ascorbate peroxidase inhibitor
Phenylalanine decarboxylase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Arabinose isomerase inhibitor
Pyruvate dehydrogenase kinase inhibitor
Adenylyl-sulfate kinase inhibitor
Formaldehyde dehydrogenase inhibitor
Vascular dementia treatment
Sterol 3-beta-glucosyltransferase inhibitor
N6-methyl-lysine oxidase inhibitor
Kexin inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Macrophage scavenger receptor antagonist
Pyridoxine 4-oxidase inhibitor
Proteasome endopeptidase complex inhibitor
Propanediol dehydratase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Interleukin 2 antagonist
Nicotinic alpha2beta4 receptor agonist
Antineoplastic (lymphoma)
Andropause treatment
Galacturan 1,4-alpha-galacturonidase inhibitor
Fibromyalgia syndrome treatment
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Phosphorylase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Chemokine receptor antagonist
5 Hydroxytryptamine 1E antagonist
Amylo-alpha-1,6-glucosidase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
CYP1A1 inducer
Cytochrome-b5 reductase substrate

Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Phenol 2-monooxygenase inhibitor
Sulfate adenylyltransferase inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Antineurotic
FMN reductase inhibitor
RELA expression inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
D-proline reductase (dithiol) inhibitor
Pantoate 4-dehydrogenase inhibitor
Acetyl-CoA transferase 2 inhibitor
ErbB-4 antagonist
Glycine transporter inhibitor
Anthranilate synthase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
DNA nucleotidylexotransferase inhibitor
D-arabinonolactone oxidase inhibitor
Lipid metabolism regulator
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Heat shock protein 90 antagonist
Tryptophan alpha,beta-oxidase inhibitor
Liver X receptor antagonist
CYP24 substrate
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Indanol dehydrogenase inhibitor
Globoside alpha-N-acetylglucosaminyltransferase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Choline kinase inhibitor
Beta-D-fucosidase inhibitor
Fibroblast growth factor 2 antagonist
Serine 3-dehydrogenase inhibitor
Ceramide glucosyltransferase inhibitor
Sphingosine 1-phosphate receptor 3 antagonist
5 Hydroxytryptamine 2B agonist
Cancer associated disorders treatment
UDP-N-acetylglucosamine 2-epimerase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Sphingosine 1-phosphate receptor 5 agonist
(R)-aminopropanol dehydrogenase inhibitor
Dethiobiotin synthase inhibitor
Interferon alpha agonist
Expectorant
CTGF expression inhibitor
Deoxyhypusine synthase inhibitor
Homoserine dehydrogenase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
3'-Nucleotidase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Gastritis treatment
HERG 1 channel blocker

Arginine deiminase inhibitor
Liver cirrhosis treatment
Aminopeptidase I inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Delayed rectifier potassium channel blocker
Carboxypeptidase E inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
CC chemokine receptor agonist
Chemokine receptor agonist
Ribonucleoside diphosphate reductase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Maltose-transporting ATPase inhibitor
Preterm labor treatment
Carnitine dehydratase inhibitor
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
GST T substrate
GST T1-1 substrate
Indole-3-acetaldehyde reductase (NADPH) inhibitor
CYP4A1 substrate
Chymotrypsin inhibitor
Bacterial efflux pump inhibitor
Agaritine gamma-glutamyltransferase inhibitor
Riboflavin kinase inhibitor
Antiviral (Influenza)
Deoxyribose-phosphate aldolase inhibitor
Falcipain 3 inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Cathepsin H inhibitor
Aldosterone antagonist
Heat shock protein antagonist
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
L-3-cyanoalanine synthase inhibitor
Bruton tyrosine kinase inhibitor
Methyltransferase substrate
Fibroblast growth factor 1 agonist
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
Antihypercholesterolemic
Aralkylamine dehydrogenase inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Chymase inhibitor
Antiprotozoal (Toxoplasma)
Angiotensin AT2 receptor agonist
Endonuclease (influenza) inhibitor
CYP2H substrate
Methionyl aminopeptidase 2 inhibitor
Threonine aldolase inhibitor
Cytostatic

Long-chain-acyl-CoA dehydrogenase inhibitor
Tyrosine-protein kinase TYRO 10 inhibitor
Integrin alphaVbeta1 antagonist
Ribulose-bisphosphate carboxylase inhibitor
Alkene monooxygenase inhibitor
I(Ks) voltage-gated potassium channel blocker
Anthranilate-CoA ligase inhibitor
Chelator, Iron
Valine-tRNA ligase inhibitor
Granzyme B inhibitor
Dihydroorotate oxidase inhibitor
HIV attachment inhibitor
Sedoheptulose-bisphosphatase inhibitor
TP53 expression enhancer
Saccharopine dehydrogenase (NADP+, L-lysine-forming) inhibitor
Antihypotensive
Antiinfertility, female
Coproporphyrinogen oxidase inhibitor
Cytosole dipeptidase inhibitor
Hypoxanthine phosphoribosyltransferase inhibitor
Phenylacetate-CoA ligase inhibitor
Antiviral (Herpes)
Antidote, heavy metal
ATP phosphoribosyltransferase inhibitor
Dihydropteroate synthase inhibitor
Luteinizing hormone-releasing hormone agonist
Lipotropic
Bis(5'-adenosyl)-triphosphatase inhibitor
Maleate hydratase inhibitor
Phosphorylase a inhibitor
Neurolysin inhibitor
Caspase 3 inhibitor
Rhinitis treatment
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Maleylacetoacetate isomerase inhibitor
Shikimate 5-dehydrogenase inhibitor
Sporulation kinase A inhibitor
Uterine stimulant
Chitin synthase inhibitor
Alpha 1L adrenoreceptor agonist
Celiac disease treatment
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Guanylate kinase inhibitor
Vanilloid 4 antagonist
Succinic dehydrogenase inhibitor
GABA C receptor antagonist
Fumarate reductase (NADH) inhibitor
Polyamine biosynthesis inhibitor
Glucosamine 6-phosphate N-acetyltransferase inhibitor
4-Alpha-glucanotransferase inhibitor

Steroid N-acetylglucosaminyltransferase inhibitor
Orexin receptor 1 antagonist
Hexokinase inhibitor
4-Phytase inhibitor
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Meprin A inhibitor
Interleukin 10 antagonist
L-Serine ammonia-lyase inhibitor
Protein-glutamate methylesterase inhibitor
Phospholipase D inhibitor
Adenine deaminase inhibitor
X-Pro dipeptidase inhibitor
Lactaldehyde dehydrogenase inhibitor
Cyanate hydratase inhibitor
Cell wall synthesis inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
Fatty acid oxidation inhibitor
Cardiac myosin stimulant
Cerebroside-sulfatase inhibitor
Tyrosine kinase inhibitor
Subtilisin inhibitor
Tubuliny-Tyr carboxypeptidase inhibitor
Endo-1,4-beta-xylanase inhibitor
Neuropeptide Y antagonist
Adenine nucleotide translocase inhibitor
Potassium channel KCNQ2 activator
Peptidoglycan beta-N-acetylmuramidase inhibitor
Amidase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Opioid dependency treatment
5-Aminolevulinate synthase inhibitor
Histamine H2 receptor agonist
Phosphatidate phosphatase inhibitor
Acetyl-CoA transferase 1 inhibitor
Tryptophan transaminase inhibitor
MAO inhibitor
Serine-glyoxylate transaminase inhibitor
Acetylcholinesterase stimulant
Alanine transaminase inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Protein N-acetylglucosaminyltransferase inhibitor
CC chemokine receptor antagonist
N-acylneuramate cytidyltransferase inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Thymidine kinase 1 inhibitor
Pregnane X receptor agonist

Methionine decarboxylase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Glucosyl transferase inhibitor
Phosphoglycolate phosphatase inhibitor
GHS receptor antagonist
Methionyl aminopeptidase 1 inhibitor
MAP3K5 inhibitor
Malonyl-CoA decarboxylase inhibitor
Carnosine synthase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
Acyloxyacyl hydrolase inhibitor
Microtubule formation inhibitor
L-lysine 6-transaminase inhibitor
Nitrilase inhibitor
Acyl-CoA dehydrogenase inhibitor
Protein C (activated) inhibitor
Gamma-glutamyl hydrolase inhibitor
Uridine nucleosidase inhibitor
Cytochrome P450 inhibitor
H⁺-transporting two-sector ATPase inhibitor
Potassium channel activator
Immunomodulator
Carbonic anhydrase inhibitor
L-lysine oxidase inhibitor
ACK1 kinase inhibitor
Enoyl-CoA hydratase inhibitor
Methyltransferase inhibitor
Vanilloid 1 agonist
Spermine antagonist
Phosphoserine phosphatase inhibitor
Scytalone dehydratase inhibitor
Octadecanal decarbonylase inhibitor
dUTP diphosphatase inhibitor
tRNA cytidyltransferase inhibitor
Immunoglobulin E antagonist
Ethanolamine kinase inhibitor
Lysine 2-monooxygenase inhibitor
Alpha adrenoreceptor agonist
CYP2A13 substrate
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Menstruation disorders treatment
Altronate dehydratase inhibitor
Cystic fibrosis treatment
Histone acetyltransferase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
Arginine decarboxylase inhibitor
CDK4/cyclin D1 inhibitor
Carboxylate reductase inhibitor
Stem cell growth factor agonist

Linoleate isomerase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
CMP-N-acylneuramate phosphodiesterase inhibitor
ATPase (Vacuolar H⁺) inhibitor
5-Alpha-reductase 2 inhibitor
Metabolic disease treatment
Phosphatidylinositol 3-kinase stimulant
(R)-limonene 6-monooxygenase inhibitor
Butyryl-CoA dehydrogenase inhibitor
Biliverdin reductase inhibitor
Beta 3 adrenoreceptor antagonist
Diguanidinobutanase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Potassium channel (Inward rectifier) 11 blocker
Sphingosine 1-phosphate receptor 3 agonist
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Platelet activating factor alpha antagonist
Pantoate-beta-alanine ligase inhibitor
CC chemokine 9 receptor antagonist
CXC chemokine 4 receptor antagonist
Glutathione S-transferase substrate
Secretase alpha stimulant
Secretase stimulant
Pyruvate dehydrogenase stimulant
Neuropeptide antagonist
Trimethyllysine dioxygenase inhibitor
Lactate 2-monooxygenase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
CDC25C inhibitor
Fibroblast growth factor 3 antagonist
Protease activated receptor antagonist
DNA helicase inhibitor
Proline dehydrogenase inhibitor
Photinus-luciferin 4-monooxygenase (ATP-hydrolysing) inhibitor
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Argininosuccinate lyase inhibitor
SULT1A3 substrate
Dopachrome isomerase inhibitor
Adenosine uptake inhibitor
Serine-phosphoethanolamine synthase inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor
Free radical scavenger
Epoxide hydrolase inhibitor
Puromycin-sensitive aminopeptidase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Sweetener
Shikimate kinase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Phospholipase C inhibitor

Deoxycytidylate 5-hydroxymethyltransferase inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
CYP3A5 inducer
NAD⁺ kinase inhibitor
Morphine 6-dehydrogenase inhibitor
Glutathione reductase inhibitor
Ribonuclease U2 inhibitor
Purinergic P2X7 antagonist
Hepatocyte nuclear factor 4 alpha agonist
Hepatocyte nuclear factor agonist
PRL phosphatase inhibitor
NAD⁺ diphosphatase inhibitor
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Tocolytic
Collagenase inhibitor
dCTP deaminase inhibitor
D-amino-acid dehydrogenase inhibitor
Glycine N-choloyltransferase inhibitor
Saccharopine dehydrogenase (NADP⁺, L-glutamate-forming) inhibitor
Aminoacyl-tRNA hydrolase inhibitor
ErbB-2 antagonist
Chemosensitizer
Glycerol dehydrogenase inhibitor
Rhodopsin kinase inhibitor
Chitin deacetylase inhibitor
Cytokine modulator
Homocysteine S-methyltransferase inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
DNA methylase inhibitor
UGT2B28 substrate
Alanine carboxypeptidase inhibitor
Salicylate 1-monooxygenase inhibitor
Carbonic anhydrase II inhibitor
Diaminopimelate dehydrogenase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
Monophenol monooxygenase inhibitor
Glycine hydroxymethyltransferase inhibitor
Methylcrotonoyl-CoA carboxylase inhibitor
L-iditol 2-dehydrogenase inhibitor
GST M substrate
Deoxyribonuclease X inhibitor
Undecaprenyl-diphosphatase inhibitor
L-galactonolactone oxidase inhibitor
Potassium channel Kv1.1 blocker
Alpha 2 adrenoreceptor agonist
Acid-sensing ion channel blocker
Beta-cyclopiazonate dehydrogenase inhibitor
Carbonic anhydrase stimulant
Antineoplastic (non-Hodgkin's lymphoma)

Thyroid hormone agonist
Alpha-pinene-oxide decyclase inhibitor
Glycine transaminase inhibitor
Aspartate kinase inhibitor
Pyridoxamine-phosphate oxidase inhibitor
Mannitol-1-phosphate 5-dehydrogenase inhibitor
Hypoxia inducible factor 1 alpha inhibitor
Heat shock protein 27 antagonist
Orexin receptor 2 antagonist
Leucine transaminase inhibitor
Atherosclerosis treatment
Vitamin K-like
Candidapepsin inhibitor
Purinergic P2 antagonist
Potassium channel (Inward rectifier) blocker
Mental retardation treatment
Nitric oxide scavenger
Acetylcholine release stimulant
Plus-end-directed kinesin ATPase inhibitor
Carbonic anhydrase I inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Glutamate carboxypeptidase inhibitor
Dipeptidyl peptidase I inhibitor
3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
Benzoylformate decarboxylase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor
Benzodiazepine antagonist
Proline transporter inhibitor
Alpha-1,3-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Phosphoenolpyruvate carboxylase inhibitor
ErbB antagonist
Glutamate (mGluR6) antagonist
CpG-Oligodeoxynucleotides inhibitor
Excitatory amino acid transporter 1 inhibitor
Purinergic receptor antagonist
CYP19 inducer
Catechol O methyltransferase inhibitor
Urocanate hydratase inhibitor
Penicillopepsin inhibitor
ATM kinase inhibitor
Cholesterol esterase inhibitor
Protein kinase B stimulant
Xanthine dehydrogenase inhibitor
Stipitatonate decarboxylase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor

Memantine hydrochloride

Molecular Mechanism (initial) :

NMDA receptor antagonists

Molecular Mechanism (repurposed) :

NMDA receptor antagonists

initial indication(s):

antiviral

Repurposed indication(s):

spasticity

Alzheimer's type dementia

Predicted Activities

Antiischemic, cerebral

Antiviral (Influenza A)

Antiparkinsonian

Nootropic

Analgesic

Neurodegenerative diseases treatment

Multiple sclerosis treatment

Dopamine release stimulant

Antidepressant

Testosterone 17beta-dehydrogenase (NADP+) inhibitor

Analgesic, non-opioid

Mood disorders treatment

Antidiabetic symptomatic

Dementia treatment

Acylcarnitine hydrolase inhibitor

Alzheimer's disease treatment

CYP2J substrate

Vascular dementia treatment

Ophthalmic drug

Prion diseases treatment

CYP2J2 substrate

Antiviral (Influenza)

Autoimmune disorders treatment

Diabetic neuropathy treatment

Antiglaucomic

Vascular (periferal) disease treatment

Antineurogenic pain

Phobic disorders treatment

Antiparkinsonian, rigidity relieving

Alkylacetylgllycerophosphatase inhibitor

Antidiabetic

Opioid dependency treatment

Alopecia treatment

Pterin deaminase inhibitor

5-O-(4-coumaroyl)-D-quinat 3'-monooxygenase inhibitor

Adenomatous polyposis treatment

Kidney function stimulant

Antidiabetic (type 2)

Albendazole monooxygenase inhibitor

Lysase inhibitor

Spasmolytic

CYP2B5 substrate
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Erythropoiesis stimulant
Cognition disorders treatment
Alkenylglycerophosphocholine hydrolase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Antiviral (Picornavirus)
Antiseborrheic
Acetylcholine neuromuscular blocking agent
Glutamate receptor antagonist
Glutamyl endopeptidase II inhibitor
NMDA receptor antagonist
Cardiovascular analeptic
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Antitoxic
Ovulation inhibitor
Antiviral (Adenovirus)
Spasmolytic, urinary
Sigma 1 receptor agonist
Mannan endo-1,4-beta-mannosidase inhibitor
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Antiischemic
Ompin inhibitor
Amyotrophic lateral sclerosis treatment
Antidyskinetic
Complement factor D inhibitor
Protein-disulfide reductase (glutathione) inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
CYP2A4 substrate
JAK2 expression inhibitor
Ecdysone 20-monooxygenase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Leukopoiesis stimulant
Glucan 1,4-alpha-maltotriohydrolase inhibitor
1,4-Lactonase inhibitor
Limulus clotting factor B inhibitor
Glutamate release inhibitor
NMDA 2 receptor antagonist
DELTA14-sterol reductase inhibitor
Dependence treatment
Platelet aggregation stimulant
Hydrogen dehydrogenase inhibitor
Sugar-phosphatase inhibitor
CYP2G1 substrate
Aspulinone dimethylallyltransferase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Antiepileptic

Fusarinine-C ornithinesterase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Nicotinic alpha2beta2 receptor antagonist
CYP7 inhibitor
Antismoking
ATP-binding cassette A1 stimulant
Membrane permeability inhibitor
Macrophage colony stimulating factor agonist
NMDA 2A receptor antagonist
Sigma receptor agonist
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Antiparkinsonian, tremor relieving
Polyamine-transporting ATPase inhibitor
Neurotransmitter antagonist
CYP3A2 substrate
Antinociceptive
CYP2A2 substrate
CYP2C12 substrate
CYP3A1 substrate
Apyrase inhibitor
Platelet adhesion inhibitor
Acetylgalactosaminy-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Lipocortins synthesis antagonist
Venombin AB inhibitor
CYP2C9 inducer
Fatty-acyl-CoA synthase inhibitor
CYP17 inhibitor
Cocain dependency treatment
Alkenylglycerophosphoethanolamine hydrolase inhibitor
CYP2D15 substrate
Pseudolysin inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Menopausal disorders treatment
Electron-transferring-flavoprotein dehydrogenase inhibitor
Polyporopepsin inhibitor
Malate oxidase inhibitor
Imidazoline receptor agonist
NADPH-cytochrome-c2 reductase inhibitor
Chloride peroxidase inhibitor
Glucagon-like peptide 1 agonist
L-glutamate oxidase inhibitor
Lysine 2,3-aminomutase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
GABA aminotransferase inhibitor
NF-E2-related factor 2 stimulant
2-Dehydropantoate 2-reductase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
NADPH peroxidase inhibitor
Thioredoxin inhibitor

Phosphoinositide 5-phosphatase inhibitor
Histidine N-acetyltransferase inhibitor
Calcium channel (voltage-sensitive) activator
Antiviral
Yeast ribonuclease inhibitor
Trimethylamine-oxide aldolase inhibitor
UGT2B28 substrate
Taurine-2-oxoglutarate transaminase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Fibrolase inhibitor
CYP2A1 substrate
Membrane permeability enhancer
Antiprotozoal
Steroid synthesis inhibitor
Dimethylargininase inhibitor
Phosphatase inhibitor
CYP2D16 substrate
Pediculicide
Limulus clotting factor C inhibitor
HCV IRES inhibitor
RNA-directed RNA polymerase inhibitor
Exoribonuclease II inhibitor
Vasoprotector
Cyclic AMP agonist
5 Hydroxytryptamine release stimulant
Peptide-N4-(N-acetyl-beta-glucosaminy)l)asparagine amidase inhibitor
Glycolate dehydrogenase inhibitor
Morphine 6-dehydrogenase inhibitor
Sulfite dehydrogenase inhibitor
CYP2B11 substrate
Linoleate diol synthase inhibitor
CYP2A5 substrate
Phospholipid-translocating ATPase inhibitor
Flavin-containing monooxygenase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Pulmonary hypertension treatment
Antiviral (Herpes)
UGT1A5 substrate
Sphinganine kinase inhibitor
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Immunosuppressant
CYP2D2 inhibitor
Octopamine antagonist
Oxidizing agent
Gonadotropin antagonist
Calcium regulator
CYP3A4 inducer
UGT2B17 substrate
Fructan beta-fructosidase inhibitor

CYP3A7 substrate
Nitrite reductase (NO-forming) inhibitor
2-Haloacid dehalogenase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Radioprotector
Chitosanase inhibitor
Sulfite oxidase inhibitor
Opioid kappa 3 receptor antagonist
Antiprotozoal (Plasmodium)
CYP3A inducer
Styrene-oxide isomerase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Hyaluronic acid agonist
Dextranase inhibitor
CYP2C19 inducer
Shikimate O-hydroxycinnamoyltransferase inhibitor
Venom exonuclease inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Gluconate 5-dehydrogenase inhibitor
Mannose isomerase inhibitor
Carboxypeptidase Taq inhibitor
Prostatic (benign) hyperplasia treatment
CYP4A11 substrate
Antimyopathies
Tpr proteinase (Porphyromonas gingivalis) inhibitor
UGT1A4 substrate
Prostate disorders treatment
Phenol O-methyltransferase inhibitor
CYP4A2 substrate
Bile-salt sulfotransferase inhibitor
Arginine 2-monooxygenase inhibitor
Phthalate 4,5-dioxygenase inhibitor
CYP2A8 substrate
D-alanine 2-hydroxymethyltransferase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Narcolepsy treatment
D-lactaldehyde dehydrogenase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
CYP2C29 substrate
DNA-3-methyladenine glycosylase I inhibitor
Ligase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
RELA expression inhibitor
Thiamine-triphosphatase inhibitor
Acetylcholinesterase inhibitor
Thiamine pyridinylase inhibitor

Estradiol 17alpha-dehydrogenase inhibitor
Protein-tyrosine phosphatase 2C inhibitor
Cyclamate sulfohydrolase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Cytoprotectant
Analgesic stimulant
Antiviral (Poxvirus)
MAP kinase stimulant
(S)-3-amino-2-methylpropionate transaminase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Gaucher disease treatment
Phosphopantothienoylcysteine decarboxylase inhibitor
Protein synthesis stimulant
Carminative
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Dipeptidase E inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Transcription factor NF kappa A inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Alpha-pinene-oxide decyclase inhibitor
Antiperistaltic
Sodium channel blocker class Ib
Pancreatic elastase inhibitor
Cyclomaltodextrinase inhibitor
MMP9 expression inhibitor
Acute neurologic disorders treatment
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Myeloblastin inhibitor
CYP2E1 inducer
Ceramide glucosyltransferase inhibitor
ADP-thymidine kinase inhibitor
2-Dehydropantoate aldolase inhibitor
Aspartate-ammonia ligase inhibitor
Adenylyl-sulfate reductase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Aldosterone antagonist
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
N-formylmethionyl-peptidase inhibitor
Cytochrome-b5 reductase inhibitor
Cl--transporting ATPase inhibitor
Galactolipase inhibitor
Linoleoyl-CoA desaturase inhibitor
CYP4B substrate
UGT2B4 substrate
Methylamine-glutamate N-methyltransferase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor

TP53 expression enhancer
BRAF expression inhibitor
DNA ligase (ATP) inhibitor
Fragilysin inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Cyclohexanone monooxygenase inhibitor
Dynein ATPase inhibitor
Prostaglandin-E2 9-reductase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Glucose oxidase inhibitor
Aspergillopepsin I inhibitor
Sclerosant
Para amino benzoic acid antagonist
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Enteropeptidase inhibitor
Mucinaminyserine mucinaminidase inhibitor
GABA C receptor agonist
Corticosteroid antagonist
EIF4E expression inhibitor
UGT2B10 substrate
Nitric oxide scavenger
IgA-specific serine endopeptidase inhibitor
Glyoxylate reductase inhibitor
Thiosulfate dehydrogenase inhibitor
Deoxyribonuclease I inhibitor
Chaperonin ATPase inhibitor
S-alkylcysteine lyase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Mucomembranous protector
Leukopoiesis inhibitor
Oxytocic
Indanol dehydrogenase inhibitor
Levanase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
CYP4B1 substrate
Oxidoreductase inhibitor
Choloylglycine hydrolase inhibitor
Cytochrome P450 stimulant
Acetylenecarboxylate hydratase inhibitor
Isopenicillin-N epimerase inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Endopeptidase So inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Thymidylate 5'-phosphatase inhibitor
CYP2A11 substrate
Long-chain-aldehyde dehydrogenase inhibitor
Oxygen scavenger

Lactase inhibitor
Glyoxylate oxidase inhibitor
Fibroblast activation protein alpha inhibitor
Stroke treatment
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Cutinase inhibitor
3-Methylbutanal reductase inhibitor
Alanine-tRNA ligase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Lipoprotein lipase inhibitor
Diamine N-acetyltransferase inhibitor
Glycine amidinotransferase inhibitor
Signal peptidase I inhibitor
Inulinase inhibitor
Gamma-glutamyltransferase inhibitor
Clavamate synthase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
CYP3A5 inducer
Polygalacturonase inhibitor
CYP2C18 substrate
Cycloartenol synthase inhibitor
Leucine dehydrogenase inhibitor
Gingipain K inhibitor
Glutamate-tRNA ligase inhibitor
Cholesterol oxidase inhibitor
CYP2B2 substrate
Valine decarboxylase inhibitor
Antiinflammatory, ophthalmic
S-formylglutathione hydrolase inhibitor
Allantoate deiminase inhibitor
Substance P antagonist
Pin1 inhibitor
Malate dehydrogenase (acceptor) inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Antipruritic, non-allergic
Antiviral (CMV)
Acetylcholine release stimulant
Maltose-transporting ATPase inhibitor
Glucuronolactone reductase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Allantoin racemase inhibitor
Neurotrophic factor enhancer
Retinyl-palmitate esterase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Undecaprenyl-diphosphatase inhibitor
Cyclooxygenase substrate
Aspergillus nuclease S1 inhibitor
Transactivator transcription protein inhibitor
Dipeptidyl peptidase inhibitor
Antirickettsial

4-Nitrophenol 2-monooxygenase inhibitor
Chenodeoxycholytaurine hydrolase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Cell wall biosynthesis inhibitor
Deoxyribonuclease X inhibitor
Arachidonic acid antagonist
Dehydro-L-gulonate decarboxylase inhibitor
Acidifying agent non gastric
Superoxide dismutase inhibitor
Plasmanylethanolamine desaturase inhibitor
GABA B receptor agonist
2-Hydroxy-3-oxoadipate synthase inhibitor
GST T substrate
GST T1-1 substrate
Nicotinic alpha4beta2 receptor antagonist
Prostaglandin-A1 DELTA-isomerase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Arylesterase inhibitor
Valine-tRNA ligase inhibitor
Ornithine cyclodeaminase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Phosphoenolpyruvate mutase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
CYP2C3 substrate
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Hematopoietic inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Cholate-CoA ligase inhibitor
CYP2B10 substrate
Carnitine dehydratase inhibitor
Peroxidase substrate
Dipeptidyl peptidase IV inhibitor
Alpha-glucuronidase inhibitor
11-Beta-hydroxysteroid dehydrogenase 1 inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
DELTA24-sterol reductase inhibitor
11-Beta-hydroxysteroid dehydrogenase inhibitor
Granzyme A inhibitor
CYP2A3 substrate
Sulfur reductase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Creatininase inhibitor
Caspase 8 stimulant
Adenylate cyclase stimulant
Phospholipase C inhibitor
DNA synthesis inhibitor
Phosphatidylserine decarboxylase inhibitor

Cancer associated disorders treatment
CYP2C6 substrate
Pregnane X receptor agonist
Biotinidase inhibitor
Fumarate reductase (NADH) inhibitor
Procollagen N-endorpeptidase inhibitor
CYP19 substrate
Picornain 3C inhibitor
Glutamate (mGluR5) agonist
Fucosterol-epoxide lyase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Testosterone 17beta-dehydrogenase inhibitor
Antipruritic, allergic
Gluconolactonase inhibitor
AR expression inhibitor
Formate-dihydrofolate ligase inhibitor
NADH kinase inhibitor
Aspartate-tRNA ligase inhibitor
CYP2C11 substrate
Polar-amino-acid-transporting ATPase inhibitor
Isopenicillin-N synthase inhibitor
Gestagen antagonist
UGT2B15 substrate
UGT1A9 substrate
Peptidyl-dipeptidase Dcp inhibitor
Sulfite reductase inhibitor
UGT1A6 substrate
Cellulose 1,4-beta-cellobiosidase inhibitor
Amine dehydrogenase inhibitor
Glutaminase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Antiinflammatory, intestinal
1,4-Alpha-glucan branching enzyme inhibitor
P-glycoprotein 1 inhibitor
Meprin B inhibitor
Glutamate 5-kinase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Lysine decarboxylase inhibitor
Antidiarrheal
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Tyrosine kinase stimulant
Cysteine transaminase inhibitor
Endothelial growth factor antagonist
Antiprotozoal (Trypanosoma)
Antiprotozoal (Leishmania)
Antibacterial
3-Cyanoalanine hydratase inhibitor
Polyneuridine-aldehyde esterase inhibitor

ADP-ribosylarginine hydrolase inhibitor
UGT2B7 substrate
Serine-pyruvate transaminase inhibitor
Hydroxylamine reductase (NADH) inhibitor
Acyl-CoA oxidase inhibitor
Polarisation inhibitor
Antisecretoric
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Saccharolysin inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
CYP2C8 inducer
Secretase alpha stimulant
Secretase stimulant
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Tyrosine 3 hydroxylase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Cathepsin T inhibitor
UGT2B11 substrate
tRNA-pseudouridine synthase I inhibitor
Selenocysteine lyase inhibitor
Sodium/bile acid cotransporter inhibitor
Anabolic
Arylmalonate decarboxylase inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
P-glycoprotein inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
5 Hydroxytryptamine uptake stimulant
Asparagine-tRNA ligase inhibitor
3-Oxosteroid 1-dehydrogenase inhibitor
Melanin inhibitor
Chitinase inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
CYP4A substrate
Calcium-sensing receptor agonist
Feruloyl esterase inhibitor
UGT2B18 substrate
Lactose synthase inhibitor
Tropinesterase inhibitor
Alkane 1-monooxygenase inhibitor
Methionine decarboxylase inhibitor
Carboxypeptidase D inhibitor
Oryzin inhibitor
Aldehyde dehydrogenase (NADP+) inhibitor
Leukotriene-C4 synthase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Purinergic P2X antagonist
Cyclohexyl-isocyanide hydratase inhibitor
Formaldehyde transketolase inhibitor

Carbon-monoxide dehydrogenase inhibitor
Choline kinase inhibitor
Sigma receptor antagonist
N-Acyl-D-aspartate deacylase inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Oligopeptidase B inhibitor
Aspergillopepsin II inhibitor
Taurine dehydrogenase inhibitor
Retinal dehydrogenase inhibitor
Cholestenone 5alpha-reductase inhibitor
Aspartoacylase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Myosin ATPase inhibitor
Lysostaphin inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Antifibrinolytic
Antiviral (Hepatitis)
Homoserine dehydrogenase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Nitric-oxide synthase inhibitor
Carnosine synthase inhibitor
Histamine agonist
Gingipain R inhibitor
Skin whitener
Bisphosphoglycerate mutase inhibitor
4-Nitrophenylphosphatase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Antiviral (Hepatitis C)
Arabinose isomerase inhibitor
Psychosexual dysfunction treatment
Retinoic acid metabolism inhibitor
Anticonvulsant
Hydroxymethylglutaryl-CoA lyase inhibitor
Rhizopuspepsin inhibitor
Thermitase inhibitor
Antibacterial, ophthalmic
Lysyl oxidase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Alternansucrase inhibitor
Brachyurin inhibitor
Prunasin beta-glucosidase inhibitor
Hydroxylamine oxidase inhibitor
Acetylserotonin O-methyltransferase inhibitor
Glutamine-pyruvate transaminase inhibitor
Glutamate (mGluR3) agonist
RNA synthesis inhibitor
Serratia marcescens nuclease inhibitor
Narcotic antagonist
Thiol oxidase inhibitor

SMN2 expression enhancer
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Trans-pentaprenyltranstransferase inhibitor
Inducible nitric-oxide synthase inhibitor
Anesthetic inhalation
Glutamate N-acetyltransferase inhibitor
5-Alpha-reductase inhibitor
Manganese peroxidase inhibitor
Retinol O-fatty-acyltransferase inhibitor
Myc inhibitor
ICAM1 expression inhibitor
Mitochondrial processing peptidase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Tankyrase inhibitor
Adrenaline release stimulant
Gentamicin 2"-nucleotidyltransferase inhibitor
Glutamin-(asparagin-)ase inhibitor
Heme oxygenase inhibitor
Antihypotensive
CYP4F2 substrate
Trimethyllysine dioxygenase inhibitor
Mannitol-1-phosphatase inhibitor
CYP2C8 inhibitor
Antihelminthic (Fasciola)
Phosphatidylglycerophosphatase inhibitor
Paget's disease treatment
MAP kinase kinase 4 inhibitor
H⁺-exporting ATPase inhibitor
Homospermidine synthase inhibitor
Antihematotoxic
Urate-ribonucleotide phosphorylase inhibitor
Bilirubin oxidase inhibitor
5 Hydroxytryptamine release inhibitor
CYP3A3 substrate
Arylamine N-acetyltransferase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Glutamate (mGluR6) antagonist
Preneoplastic conditions treatment
UGT2B9 substrate
N-acylmannosamine kinase inhibitor
Chlordecone reductase inhibitor
Farnesyltranstransferase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Dimethylmaleate hydratase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
CYP19 inhibitor
Insulin promoter
HMOX1 expression enhancer
CYP3A5 substrate
Nucleoside oxidase (H₂O₂-forming) inhibitor

Thermomycolin inhibitor
Mucolytic
CYP2B18 substrate
Coagulant
Mallyl-CoA lyase inhibitor
Glycoprotein 3- α -L-fucosyltransferase inhibitor
Tryptophan transaminase inhibitor
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
D-xylulose reductase inhibitor
Cholinergic
Contraceptive female
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Valine dehydrogenase (NADP⁺) inhibitor
Iron-cytochrome-c reductase inhibitor
NMDA receptor polyamine site agonist
Tauropine dehydrogenase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Ferredoxin-NADP⁺ reductase inhibitor
Ca²⁺-transporting ATPase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Polarisation stimulant
Serine 3-dehydrogenase inhibitor
Glycerol dehydrogenase (NADP⁺) inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
3(or 17) α -hydroxysteroid dehydrogenase inhibitor
Agmatinase inhibitor
Testosterone agonist
UGT1A7 substrate
Arylsulfate sulfotransferase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
CYP2C2 substrate
P-glycoprotein substrate
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Mitochondrial intermediate peptidase inhibitor
Hepatocyte nuclear factor 4 α antagonist
Hepatocyte nuclear factor antagonist
2-Aminoadipate transaminase inhibitor
Microtubule formation inhibitor
Tentoxilysin inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Phosphatidylinositol 3-kinase stimulant
Steroid sulfotransferase inhibitor
Pyruvate carboxylase inhibitor
Amino-acid racemase inhibitor
2-Methyleneglutarate mutase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Urolithiasis treatment

Farnesoid X receptor antagonist
Phosphate acetyltransferase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Ribonuclease U2 inhibitor
Hydroxymethylbilane synthase inhibitor
3-Phytase inhibitor
Antibiotic
Diacylglycerol kinase inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Deoxyribose-phosphate aldolase inhibitor
Threonine ammonia-lyase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Immunoglobulin E antagonist
CYP3C substrate
Cysteine desulfurase inhibitor
Phosphatidate cytidyltransferase inhibitor
Aldehyde dehydrogenase 2 substrate
Choline acetyltransferase stimulant
CYP1A2 inducer
Pantothenase inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
Phosphoinositide phospholipase C inhibitor
Trimethylamine dehydrogenase inhibitor
Galactokinase inhibitor
Penicillin amidase inhibitor
Hypoxia inducible factor 1 alpha inhibitor
Glycine C-acetyltransferase inhibitor
Coccolysin inhibitor
Pullulanase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
NMDA receptor polyamine site antagonist
Trehalose-phosphatase inhibitor
Interferon gamma antagonist
Rhodopsin kinase inhibitor
CYP26A substrate
Interferon antagonist
Histidinol dehydrogenase inhibitor
SULT2A1 substrate
Purinergic receptor antagonist
Glycerol-3-phosphate dehydrogenase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Restless leg syndrome treatment
NOS2 expression inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Antineoplastic (thyroid cancer)
Aldehyde dehydrogenase inhibitor

Glutamate (mGluR4) agonist
Retinoprotector
D-glutamate oxidase inhibitor
D-proline reductase (dithiol) inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Fructose 5-dehydrogenase inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
Galacturan 1,4- α -galacturonidase inhibitor
Spermidine dehydrogenase inhibitor
Pappalysin-1 inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
VCAM1 expression inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Globoside α -N-acetylgalactosaminyltransferase inhibitor
Dolichyl-phosphatase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
11-Cis-retinyl-palmitate hydrolase inhibitor
Guanidinoacetate kinase inhibitor
Beta-glucosidase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
mRNA (guanine-N7-)-methyltransferase inhibitor
Dolichol kinase inhibitor
Homoserine O-succinyltransferase inhibitor
Alpha-L-fucosidase inhibitor
Estrone sulfotransferase inhibitor
Phospholipase A1 inhibitor
Anesthetic general
D-amino-acid dehydrogenase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
DNA nucleotidylexotransferase inhibitor
L-lysine oxidase inhibitor
Pseudouridylate synthase inhibitor
GST A substrate
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Mucositis treatment
Biotin carboxylase inhibitor
CYP24 substrate
8-Amino-7-oxononanoate synthase inhibitor
D-cysteine desulhydrase inhibitor
Lactate 2-monooxygenase inhibitor
UGT1A substrate
Neuropsin inhibitor
Isomaltulose synthase inhibitor
Saluretic
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Aldehyde oxidase inhibitor
Antiacne

Ribonuclease inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Snapalysin inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Lysozyme inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Glutathione thiolesterase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Glutamate uptake inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Polyamine biosynthesis inhibitor
Bisphosphoglycerate phosphatase inhibitor
CYP1B substrate
Gastrointestinal motility stimulant
Membrane dipeptidase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
UGT2B substrate
Laminaribiose phosphorylase inhibitor
Peptidyl-dipeptidase B inhibitor
Acetylcholine nicotinic antagonist
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Pectin lyase inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
L-threonine 3-dehydrogenase inhibitor
Orotate reductase (NADH) inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Uroporphyrinogen-III synthase inhibitor
Cytochrome-b5 reductase substrate
Creatinase inhibitor
Antineurotic
Fibrinogen receptor antagonist
Lipotropic
Anthranilate-CoA ligase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
D-alanine transaminase inhibitor
Pyruvate decarboxylase inhibitor
Thiamine-phosphate kinase inhibitor
Urease inhibitor
D-lactate dehydrogenase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
tRNA nucleotidyltransferase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Epoxide hydrolase inhibitor
Aerobactin synthase inhibitor
Steroid DELTA-isomerase inhibitor
Glycine N-choloyltransferase inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
CYP24 inhibitor
Cysteine-S-conjugate beta-lyase inhibitor

Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Methyltransferase substrate
Pancreatic endopeptidase E inhibitor
Nardilysin inhibitor
CYP19A1 expression inhibitor
DOPA decarboxylase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
UGT1A1 substrate
Glutaminyl-peptide cyclotransferase inhibitor
Glycerol-1-phosphatase inhibitor
Lysyl endopeptidase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
4-Hydroxyglutamate transaminase inhibitor
Dethiobiotin synthase inhibitor
Cushing's syndrome treatment
Glyoxylate reductase (NADP+) inhibitor
Thiol S-methyltransferase inhibitor
Riboflavin phosphotransferase inhibitor
Acyl-lysine deacylase inhibitor
Horriylsin inhibitor
Polyamine oxidase inhibitor
Acetylorlithine deacetylase inhibitor
Alkene monooxygenase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Sterol 24-C-methyltransferase inhibitor
UGT2B19 substrate
UGT2B23 substrate
UGT2B30 substrate
UGT2B4D substrate
UGT2B4E substrate
Glutathione peroxidase inhibitor
Dipeptidyl peptidase II inhibitor
Inorganic diphosphatase inhibitor
Alpha, alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
UGT1A8 substrate
Deoxyhypusine synthase inhibitor
Luteinizing hormone-releasing hormone agonist
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Licheninase inhibitor
Adenylate cyclase I inhibitor
H⁺-transporting two-sector ATPase inhibitor
Vitamin
CYP17 substrate
Galactosylceramide sulfotransferase inhibitor
Centromere associated protein inhibitor
Contraceptive
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Protein kinase B alpha inhibitor
Ferrochelataase inhibitor
Beta-D-fucosidase inhibitor

Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Aminolevulinate transaminase inhibitor
Decylcitrate synthase inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Amylosucrase inhibitor
Cyanoalanine nitrilase inhibitor
Cyclic AMP modulator
Allantoicase inhibitor
Choline-sulfatase inhibitor
CYP2D1 substrate
O-aminophenol oxidase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
FMO1 substrate
Glutamate (mGluR group II) agonist
Mannan endo-1,6-alpha-mannosidase inhibitor
Aconitate decarboxylase inhibitor
Membrane integrity antagonist
CYP4F12 substrate
ATP adenylyltransferase inhibitor
Mevalonate kinase inhibitor
Guanidinopropionase inhibitor
Anticholelithogenic
4-Alpha-glucanotransferase inhibitor
N6-methyl-lysine oxidase inhibitor
Carboxymethylenebutenolidase inhibitor
4-Coumarate-CoA ligase inhibitor
Gluconate dehydratase inhibitor
UGT1A3 substrate
Polynucleotide 5'-hydroxy-kinase inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Sphingosine kinase inhibitor
Cysteine synthase inhibitor
Malate synthase inhibitor
Spasmolytic, Papaverin-like
D-Serine ammonia-lyase inhibitor
4-Hydroxymandelate oxidase inhibitor
N-acetylneuraminase synthase inhibitor
Allophanate hydrolase inhibitor
Aryl hydrocarbon receptor agonist
Retinol dehydrogenase inhibitor
Orotate reductase (NADPH) inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Maleate hydratase inhibitor
Proline dehydrogenase inhibitor
Galactoside O-acetyltransferase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor

CYP2A10 substrate
Maleate isomerase inhibitor
Androst-4-ene-3,17-dione monooxygenase inhibitor
2-Methylcitrate dehydratase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Acetylcholine M3 receptor agonist
Gluconokinase inhibitor
Expectorant
D-stereospecific aminopeptidase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminephosphotransferase inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
Homocysteine desulfhydrase inhibitor
Cytosole dipeptidase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
Allantoinase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
CYP2B4 substrate
Thioether S-methyltransferase inhibitor
Deoxyadenosine kinase inhibitor
Glutamate (mGluR2) agonist
Leucine-tRNA ligase inhibitor
Opine dehydrogenase inhibitor
ATP deaminase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Metallo-carboxypeptidase D inhibitor
Atrolysin A inhibitor
Adenylate kinase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Ganglioside galactosyltransferase inhibitor
Aspartate kinase inhibitor
Xylose isomerase inhibitor
Purinergic P2X7 antagonist
Threonine aldolase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
Ubiquitin thiolesterase inhibitor
Xanthommatin reductase inhibitor
Age-related macular degeneration treatment
N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor
SULT1A3 substrate
Guanidinoacetate N-methyltransferase inhibitor
Glutaminyl-tRNA synthase (glutamine-hydrolysing) inhibitor
Glutamate (mGluR1) agonist
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Aryldialkylphosphatase inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
Renal tissue kallikrein inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor

Nicotine dehydrogenase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Putrescine oxidase inhibitor
Serine-phosphoethanolamine synthase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Aureolysin inhibitor
Galactose oxidase inhibitor
Methanol dehydrogenase inhibitor
Diisopropyl-fluorophosphatase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Sulfur dioxygenase inhibitor
CYP26 substrate
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Anhydrotetracycline monooxygenase inhibitor
Clostripain inhibitor
Ferredoxin hydrogenase inhibitor
RNA agonist
Glutamate (mGluR8) agonist
Malate-CoA ligase inhibitor
2-Aminohexano-6-lactam racemase inhibitor
3'-Nucleotidase inhibitor
Loop diuretic
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Alpha,alpha-trehalose phosphorylase inhibitor
Cortisone alpha-reductase inhibitor
Purinergic P2 antagonist
(S)-carnitine 3-dehydrogenase inhibitor
2-Ethylmalate synthase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Acylglycerone-phosphate reductase inhibitor
Sodium/hydrogen exchanger 5 inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
Antiprotozoal (Trichomonas)
Alpha glucosidase inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Urotensin II antagonist
Cyclopentanone monooxygenase inhibitor
Antiinfective
Osmotic diuretic
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Inositol 1,4,5-triphosphate receptor antagonist
L-lysine 6-transaminase inhibitor
Ornithine-oxo-acid transaminase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Glucuronate isomerase inhibitor
HIV-2 reverse transcriptase inhibitor
Adenylate cyclase inhibitor
Alpha-mannosidase inhibitor

Glutamate (mGluR1) antagonist
Arginyltransferase inhibitor
Mycodextranase inhibitor
Viral entry inhibitor
Cellulase inhibitor
Calcium channel activator
Diguanidinobutanase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Histamine release stimulant
Cellobiose phosphorylase inhibitor
Dactylisin inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Indoleacetaldoxime dehydratase inhibitor
Ribosomal protein S6 kinase 1, 70-kDa inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Apoptosis agonist
Carbamoyl-phosphate synthase (ammonia) inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
N-acetyllactosamine synthase inhibitor
S-methyl-5-thioribose kinase inhibitor
5 Hydroxytryptamine 4A antagonist
GST M substrate
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
Nucleoside deoxyribosyltransferase inhibitor
Androgen agonist
Omega-amidase inhibitor
Beta-mannosidase inhibitor
Thiopurine S-methyltransferase inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Bontoxilysin inhibitor
Camphor 1,2-monooxygenase inhibitor
Cytochrome-c3 hydrogenase inhibitor
Alpha,alpha-trehalase inhibitor
CMP-KDO synthase inhibitor
2-Methylcitrate synthase inhibitor
Leucine transaminase inhibitor
Phosphofructokinase-1 inhibitor
Nicotinamide-nucleotide adenyltransferase inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Antipruritic
Aspartate 1-decarboxylase inhibitor
Dichloromuconate cycloisomerase inhibitor
3-Oxadipate enol-lactonase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Lactaldehyde reductase inhibitor
CYP4F substrate
ATP phosphoribosyltransferase inhibitor

Beta-N-acetylgalactosaminidase inhibitor
Arginine deiminase inhibitor
L-glucuronate reductase inhibitor
Transketolase inhibitor
5-Alpha-reductase 2 inhibitor
Pitrilysin inhibitor
X-methyl-His dipeptidase inhibitor
GABA transporter inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
3'(2'),5'-Bisphosphate nucleotidase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Antihelminthic (Nematodes)
Methylaspartate mutase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Melanocortin agonist
Chorismate mutase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Protein-tyrosine sulfotransferase inhibitor
Malate dehydrogenase (NADP+) inhibitor
Dextranucrase inhibitor
D-lactate-2-sulfatase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Dihydrouracil oxidase inhibitor
L-iduronidase inhibitor
Choline dehydrogenase inhibitor
Interleukin 1a antagonist
Cortisol sulfotransferase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
Antibiotic Quinolone-like
Glucarate dehydratase inhibitor
Glycolipid 2-alpha-mannosyltransferase inhibitor
Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor
6-Methylsalicylate decarboxylase inhibitor
Methane monooxygenase inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Formimidoylglutamase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Gallate decarboxylase inhibitor
DNA directed RNA polymerase stimulant
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
D-Lysine 5,6-aminomutase inhibitor
Glucan 1,4-alpha-glucosidase inhibitor
RNA-directed RNA polymerase stimulant
Alpha,alpha-phosphotrehalase inhibitor

Asparagine-oxo-acid transaminase inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
ACK1 kinase inhibitor
Urethanase inhibitor
NMDA receptor phencyclidine site antagonist
Plus-end-directed kinesin ATPase inhibitor
CYP4F8 substrate
Magnesium-protoporphyrin IX methyltransferase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
GABA transporter 1 inhibitor
Acetoin dehydrogenase inhibitor
CYP2A13 substrate
Sigma 3 receptor antagonist
UDP-glucuronosyltransferase substrate
Lipocortins synthesis agonist
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Cathepsin H inhibitor
Chitin deacetylase inhibitor
Long-chain-fatty-acid-CoA ligase inhibitor
Immunostimulant
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Lysosomal Pro-X carboxypeptidase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Histamine H2 receptor agonist
Assemblin inhibitor
3-Hydroxyanthranilate oxidase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
UGT2B7H substrate
UGT2B7Y substrate
Asparaginase inhibitor
Acidifying agent gastric
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Transaldolase inhibitor
5-Alpha-reductase 1 inhibitor
Dihydroxy-acid dehydratase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Nitrate reductase (cytochrome) inhibitor
SULT1A1 substrate
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Cyanate hydratase inhibitor
Acetolactate synthase inhibitor
Antispirochetal
Sulfinioalanine decarboxylase inhibitor
Argininosuccinate lyase inhibitor
Cellulose synthase (UDP-forming) inhibitor

Glutamate formimidoyltransferase inhibitor
Histamine H3 receptor agonist
CYP3A11 substrate
Phosphonoacetate hydrolase inhibitor
5-Aminovalerate transaminase inhibitor
Postcoital contraceptive
Diaminopimelate dehydrogenase inhibitor
Arginine racemase inhibitor
ATP diphosphatase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Valine-pyruvate transaminase inhibitor
Serine-glyoxylate transaminase inhibitor
Ketohehexokinase inhibitor
Sulfate adenylyltransferase inhibitor
CYP17A substrate
Glutathione dehydrogenase (ascorbate) inhibitor
Ribonucleoside triphosphate reductase inhibitor
Ethanolaminephosphotransferase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Phosphoribulokinase inhibitor
Hydroxylysine kinase inhibitor
11-Beta-hydroxysteroid dehydrogenase 2 inhibitor
Membrane integrity agonist
Glucocorticoid antagonist
Deoxycytidine kinase inhibitor
Diuretic inhibitor
Antineoplastic, alkylator
Photosensitizer
Acetoacetate decarboxylase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Glutamate synthase (ferredoxin) inhibitor
UGT1A10 substrate
Acetate kinase inhibitor
Serine-tRNA ligase inhibitor
Adenine deaminase inhibitor
Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor
Peptidyl-glycinamidase inhibitor
Succinate dehydrogenase inhibitor
CYP11B1 substrate
Ketosteroid monooxygenase inhibitor
Inositol polyphosphate-5-phosphatase D stimulant
Glutamate (mGluR) antagonist
Lactate-malate transhydrogenase inhibitor
Hair growth stimulant
CTP synthase inhibitor
3 Beta-hydroxy-delta 5-steroid dehydrogenase inhibitor
Alkylglycerone-phosphate synthase inhibitor
Antiprotozoal activity enhancer
FMO3 substrate
3-Isopropylmalate dehydratase inhibitor

Neuropeptide FF agonist
Neuropeptide FF2 agonist
Sucrose alpha-glucosidase inhibitor
CYP27A substrate
Lysine 2-monooxygenase inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
2-Aminohexanoate transaminase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Aspartate transaminase inhibitor
Glycine transaminase inhibitor
CYP19A1 substrate
Glycerol-3-phosphate dehydrogenase (NAD⁺) inhibitor
Cholesterol monooxygenase (side-chain-cleaving) inhibitor
Mannosidase inhibitor
Diphosphate-serine phosphotransferase inhibitor
Deoxycytidine deaminase inhibitor
Reductant
Galactosylgalactosylglucosylceramidase inhibitor
CYP7B substrate
CYP7B1 substrate
SULT1E1 substrate
Diiodophenylpyruvate reductase inhibitor
Glucosylceramidase inhibitor
TH expression enhancer
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor

Metformin hydrochloride

Molecular Mechanism (initial) :

AMP-activated protein kinase (AMPK) activator

Molecular Mechanism (repurposed) :

AMP-activated protein kinase (AMPK) activator

initial indication(s):

diabetic

Repurposed indication(s):

non-alcoholic steatohepatitis

breast cancer

prostate cancer

Predicted Activities

Protein-arginine deiminase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Arginine 2-monooxygenase inhibitor
Omptin inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Limulus clotting factor C inhibitor
Limulus clotting factor B inhibitor
Anesthetic general
Peptide agonist

Methylumbelliferyl-acetate deacetylase inhibitor
Phobic disorders treatment
Mucositis treatment
Imidazoline receptor agonist
CYP2C3 substrate
Peptidyl-dipeptidase Dcp inhibitor
IgA-specific serine endopeptidase inhibitor
NADPH peroxidase inhibitor
Protein-glutamate methylesterase inhibitor

Antidiabetic

Complement factor D inhibitor
Insulysin inhibitor
Cathepsin T inhibitor
Membrane integrity antagonist
Guanidinoacetate kinase inhibitor
Pitrilysin inhibitor
Antimyopathies
Enteropeptidase inhibitor
Antidyskinetic
Glycine amidinotransferase inhibitor
Polyamine-transporting ATPase inhibitor
Macrophage stimulant
Acylcarnitine hydrolase inhibitor
Carboxypeptidase D inhibitor
Venombin AB inhibitor
Fibrinogen receptor antagonist
Aspartyltransferase inhibitor
Phospholipid-translocating ATPase inhibitor
Pin1 inhibitor
Dipeptidase E inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Macrophage colony stimulating factor agonist
Antiviral (Poxvirus)
Gingipain K inhibitor
Membrane permeability inhibitor
Interferon alpha agonist
Renal tissue kallikrein inhibitor
Neuropeptide Y4 antagonist
Antianginal
Ubiquinol-cytochrome-c reductase inhibitor
Antiischemic
Methylamine-glutamate N-methyltransferase inhibitor
Dimethylargininase inhibitor
Exoribonuclease II inhibitor
Metallo-carboxypeptidase D inhibitor
Interleukin 2 agonist
Fibrolase inhibitor
Mitochondrial intermediate peptidase inhibitor
CYP2D16 substrate
Hydrogen dehydrogenase inhibitor

Fusarinine-C ornithinesterase inhibitor
Trimethylamine-oxide aldolase inhibitor
2-Haloacid dehalogenase inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Argininosuccinate lyase inhibitor
HCV IRES inhibitor
Alopecia treatment
Nicotinic $\alpha 6 \beta 3 \beta 4 \alpha 5$ receptor antagonist
Albendazole monooxygenase inhibitor
Platelet antagonist
Antiviral (Picornavirus)
Pseudolysin inhibitor
Para amino benzoic acid antagonist
Multiple sclerosis treatment
Pterin deaminase inhibitor
Membrane integrity agonist
Chloride peroxidase inhibitor
Myocardial ischemia treatment
Oxygen scavenger
Acrosin inhibitor
Blasticidin-S deaminase inhibitor
Membrane permeability enhancer
NADPH-cytochrome-c2 reductase inhibitor
Cardioprotectant
Anticoagulant
Antiviral (Influenza)
Polyporopepsin inhibitor
Maillard reaction inhibitor
Aminopeptidase Y inhibitor
Testosterone 17 β -dehydrogenase (NADP⁺) inhibitor
Antiarrhythmic
D-Octopine dehydrogenase inhibitor
Chitinase inhibitor
TNF expression inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Beta glucuronidase inhibitor
1,4-Lactonase inhibitor
Hematopoietic inhibitor
Yeast ribonuclease inhibitor
Monoamine uptake inhibitor
Mucomembranous protector
Cardiotonic
Folate antagonist
Kidney function stimulant
Antiprotozoal
DNA-3-methyladenine glycosylase I inhibitor
Antiprotozoal (Trypanosoma)
Fatty-acyl-CoA synthase inhibitor

4-Nitrophenylphosphatase inhibitor
Clostripain inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Glutamyl endopeptidase II inhibitor
N-acylmannosamine kinase inhibitor
Cytoprotectant
Granzyme A inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Polyamine oxidase inhibitor
Sugar-phosphatase inhibitor
Envelysin inhibitor
Diamine N-acetyltransferase inhibitor
Gastrin inhibitor
Pyroglutamyl-peptidase II inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Ovulation inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Platelet aggregation stimulant
Choline-phosphate cytidyltransferase inhibitor
Arginine N-succinyltransferase inhibitor
Antiviral (Adenovirus)
Lysine 2,3-aminomutase inhibitor
Procollagen C-endopeptidase inhibitor
Sigma receptor agonist
Antiperistaltic
(S)-6-hydroxynicotine oxidase inhibitor
Subtilisin inhibitor
Opioid dependency treatment
Allantoate deiminase inhibitor
Botulin neurotoxin A light chain inhibitor
Gonadotropin antagonist
Muscular dystrophy treatment
Antianorexic
Fructan beta-fructosidase inhibitor
Leukopoiesis stimulant
Leukopoiesis inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Guanidinobutyrase inhibitor
CYP2C29 substrate
Pyroglutamyl-peptidase I inhibitor
Nicotinic alpha2beta2 receptor antagonist
Endopeptidase La inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
GP IIb/IIIa receptor antagonist
MAP kinase stimulant
Mycothiol-S-conjugate amidase inhibitor
Antiinflammatory, ophthalmic
Calcium channel (voltage-sensitive) activator

Neuropsin inhibitor
2-Dehydropantoate aldolase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Brachyurin inhibitor
Mucinaminyserine mucinaminidase inhibitor
Trimethylamine dehydrogenase inhibitor
Biotinidase inhibitor
X-methyl-His dipeptidase inhibitor
Manganese peroxidase inhibitor
Prion diseases treatment
Serralysin inhibitor
Fragilysin inhibitor
Sulfite oxidase inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
Antiviral (Influenza A)
Agmatinase inhibitor
Flavin-containing monooxygenase inhibitor
Oligopeptidase B inhibitor
Sodium channel blocker
Electron-transferring-flavoprotein dehydrogenase inhibitor
Sodium/hydrogen exchanger 5 inhibitor
Radioprotector
ADP-thymidine kinase inhibitor
CYP2H substrate
Choline-sulfatase inhibitor
Histidine N-acetyltransferase inhibitor
S-alkylcysteine lyase inhibitor
Nav1.5 sodium channel blocker
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Dactylisin inhibitor
Formaldehyde transketolase inhibitor
Protease activated receptor 1 antagonist
Neuropeptide FF antagonist
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Aspartate-ammonia ligase inhibitor
Sulfur reductase inhibitor
Neuropeptide Y2 antagonist
Beta-ureidopropionase inhibitor
Erythropoiesis stimulant
Threonine aldolase inhibitor
Cancer associated disorders treatment
Glycine dehydrogenase (decarboxylating) inhibitor
FMO1 substrate
Glucan 1,4-alpha-maltotriohydrolase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Cerevisin inhibitor
Radiosensitizer
Cytosol alanyl aminopeptidase inhibitor
Alanine-tRNA ligase inhibitor
NMDA receptor polyamine site antagonist

CYP2J substrate
Serine protease unspecified inhibitor
S-formylglutathione hydrolase inhibitor
Styrene-oxide isomerase inhibitor
Thioredoxin inhibitor
Diguanidinobutanase inhibitor
Fibrinolytic
Nitric-oxide synthase inhibitor
Meprin B inhibitor
Tripeptidyl-peptidase I inhibitor
Platelet adhesion inhibitor
Diuretic inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Mannose isomerase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Diabetic neuropathy treatment
Peptidyl-dipeptidase B inhibitor
Glutamate synthase (ferredoxin) inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Neurotensin 1 receptor agonist
Aminobutyraldehyde dehydrogenase inhibitor
Alkylacetylgllycerophosphatase inhibitor
Picornain 3C inhibitor
Adenylyl-sulfate reductase inhibitor
Octopamine antagonist
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Acetylenecarboxylate hydratase inhibitor
Analgesic stimulant
Phosphopantothenoylcysteine decarboxylase inhibitor
Carboxypeptidase Taq inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Carnitinamidase inhibitor
CYP2J2 substrate
Shikimate O-hydroxycinnamoyltransferase inhibitor
Antiviral (Herpes)
Arylesterase inhibitor
GABA C receptor agonist
Thimet oligopeptidase inhibitor
Furin inhibitor
Anesthetic
Acetylserotonin O-methyltransferase inhibitor
Cl--transporting ATPase inhibitor
Corneal wound healing stimulator
Glucan endo-1,3-beta-D-glucosidase inhibitor
L-glutamate oxidase inhibitor
Apyrase inhibitor
Astacin inhibitor
Antibacterial, ophthalmic
Antineurotic

Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Thermitase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
CYP2D6 substrate
Nucleoside oxidase (H₂O₂-forming) inhibitor
Venombin A inhibitor
Picornain 2A inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Acetylspermidine deacetylase inhibitor
Gluconate 5-dehydrogenase inhibitor
Oxidizing agent
Phosphatidylserine decarboxylase inhibitor
Cyclic AMP modulator
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Glutamate-tRNA ligase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Neurotransmitter uptake inhibitor
Taurine dehydrogenase inhibitor
Serine-pyruvate transaminase inhibitor
Kallikrein inhibitor
Thymidylate 5'-phosphatase inhibitor
Biliary tract disorders treatment
Lysyl endopeptidase inhibitor
Melanocortin MC-4 agonist
CYP2D substrate
Superoxide dismutase inhibitor
2-Aminoheptano-6-lactam racemase inhibitor
Malate oxidase inhibitor
Transactivator transcription protein inhibitor
Peptidyl-glycinamidase inhibitor
Glyoxylate reductase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Fucosterol-epoxide lyase inhibitor
Arginine decarboxylase inhibitor
CYP3A1 substrate
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Arginase inhibitor
[citrate-(pro-3S)-lyase] thioesterase inhibitor
Polygalacturonase inhibitor
Cytochrome-b5 reductase substrate
Carboxypeptidase M inhibitor
Sphinganine kinase inhibitor
Kexin inhibitor
Aminopeptidase B inhibitor
Vascular adhesion protein 1 inhibitor
Antialcoholic
Falcipain 3 inhibitor
Histamine H₂ receptor agonist

Acylaminoacyl-peptidase inhibitor
Lipid metabolism regulator
Cancer procoagulant inhibitor
Acetylesterase inhibitor
D-xylulose reductase inhibitor
Complement inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Arginine deiminase inhibitor
Thiol oxidase inhibitor
Aspartoacylase inhibitor
Rhinitis treatment
Carnosine synthase inhibitor
Levanase inhibitor
GABA aminotransferase inhibitor
5-Guanidino-2-oxopentanoate decarboxylase inhibitor
Tripeptide aminopeptidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Histamine agonist
Endopeptidase So inhibitor
Inulinase inhibitor
Corticotropin-like
3-Cyanoalanine hydratase inhibitor
Homocitrate synthase inhibitor
Peptidyltransferase inhibitor
Chitosanase inhibitor
Carnitine dehydratase inhibitor
Glucose oxidase inhibitor
CYP3A2 substrate
Hyperprolactinemia treatment
FMO3 substrate
Procollagen N-endopeptidase inhibitor
CYP2A8 substrate
Nitrite reductase (NO-forming) inhibitor
Dopamine release stimulant
Chenodeoxycholytaurine hydrolase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
CYP2C12 substrate
Ferredoxin hydrogenase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Antiprotozoal (Trichomonas)
CYP2D15 substrate
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Candidapepsin inhibitor
4-Hydroxyproline epimerase inhibitor
CYP2D1 substrate
Glucuronate isomerase inhibitor
Deoxyhypusine synthase inhibitor
Septic shock treatment
3-Chloro-D-alanine dehydrochlorinase inhibitor

Proteasome endopeptidase complex inhibitor
Galactolipase inhibitor
Antidiarrheal
5 Hydroxytryptamine 2B agonist
D-lactaldehyde dehydrogenase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
CYP2D2 inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Immunostimulant
Amyotrophic lateral sclerosis treatment
Phenylalanine(histidine) transaminase inhibitor
Dynein ATPase inhibitor
Clavamate synthase inhibitor
GABA B receptor agonist
Benzaldehyde dehydrogenase (NADP+) inhibitor
Gluconolactonase inhibitor
Histamine release stimulant
Venom exonuclease inhibitor
Leukotriene-C4 synthase inhibitor
Pancreatic elastase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Glycolate dehydrogenase inhibitor
Camphor 1,2-monooxygenase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Antiprotozoal (Babesia)
Antisecretoric
Phenol O-methyltransferase inhibitor
Meprin A inhibitor
Thiamine-triphosphatase inhibitor
Aspergillus nuclease S1 inhibitor
Streptogrisin A inhibitor
Phospholipase C inhibitor
5 Hydroxytryptamine uptake stimulant
Sulfite reductase inhibitor
Kallikrein 3 inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Aldehyde oxidase inhibitor
NADH kinase inhibitor
Neuropeptide agonist
Alpha-N-acetylglucosaminidase inhibitor
Sodium/hydrogen exchanger inhibitor
Monoamine oxidase substrate
Thiamine pyridinylase inhibitor
CYP1A2 substrate
Acetylcholine neuromuscular blocking agent
Antitoxic

Cellulose 1,4-beta-cellobiosidase inhibitor
4-Hydroxymandelate oxidase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Opioid kappa 3 receptor antagonist
Factor VIIa inhibitor
Mitochondrial processing peptidase inhibitor
Neurotransmitter antagonist
1,4-Alpha-glucan branching enzyme inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Iron-cytochrome-c reductase inhibitor
Choline kinase inhibitor
Prostaglandin-E2 9-reductase inhibitor
Adenosine regulator
Xylose isomerase inhibitor
Phosphoserine phosphatase inhibitor
Argininosuccinate synthase inhibitor
Aldehyde dehydrogenase substrate
NAD(P)+-arginine ADP-ribosyltransferase inhibitor
CYP2B11 substrate
Angiogenesis stimulant
Phosphoinositide 5-phosphatase inhibitor
CYP2A1 substrate
Retinoic acid metabolism inhibitor
CYP4A2 substrate
Thiamine-phosphate diphosphorylase inhibitor
Antithrombotic
Cyanoalanine nitrilase inhibitor
Selenocysteine lyase inhibitor
Fructose 5-dehydrogenase inhibitor
Isopenicillin-N synthase inhibitor
Follicle-stimulating hormone agonist
Steroid synthesis inhibitor
Arylmalonate decarboxylase inhibitor
NAD+ synthase (glutamine-hydrolysing) inhibitor
CMP-KDO synthase inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Antiparkinsonian, rigidity relieving
Lysostaphin inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor
Acetylorbithine deacetylase inhibitor
Protein-synthesizing GTPase inhibitor
Lipotropic
CYP2A2 substrate
Saccharolysin inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Cystic fibrosis treatment

HIV attachment inhibitor
N-acetyllactosamine synthase inhibitor
Dolichol kinase inhibitor
Flavin-containing monooxygenase substrate
Threonine ammonia-lyase inhibitor
Prunasin beta-glucosidase inhibitor
Vasculitis treatment
Glycerol 2-dehydrogenase (NADP+) inhibitor
Streptopain inhibitor
Acid phosphatase inhibitor
Alpha adrenoreceptor agonist
N-formylmethionyl-peptidase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Creatinase inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Putrescine carbamoyltransferase inhibitor
Maltose-transporting ATPase inhibitor
Antiviral (Hepatitis B)
Rheumatoid arthritis treatment
Arginine kinase inhibitor
Ubiquitin thiolesterase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Peptidoglycan glycosyltransferase inhibitor
CYP2G1 substrate
Arylformamidase inhibitor
Interleukin 6 antagonist
Allantoin racemase inhibitor
Loop diuretic
Ornithine-oxo-acid transaminase inhibitor
Smooth muscle myosin light chain kinase inhibitor
Allantoicase inhibitor
Amino-acid racemase inhibitor
Assemblin inhibitor
Carboxypeptidase E inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Ornithine cyclodeaminase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Mucolytic
Myeloblastin inhibitor
Endopeptidase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
Farnesyltranstransferase inhibitor
Cyclamate sulfohydrolase inhibitor
Linoleate diol synthase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Dihydrodipicolinate synthase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor

GST A substrate
N-Carbamoyl-D-amino acid hydrolase inhibitor
Antiprotozoal (Plasmodium)
Luteinizing hormone-releasing hormone agonist
Gingipain R inhibitor
Sedoheptulose-bisphosphatase inhibitor
Cathepsin H inhibitor
Signal peptidase I inhibitor
Diamine oxidase inhibitor
Glutathione peroxidase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Thiopurine S-methyltransferase inhibitor
Adrenaline release stimulant
Anti-Helicobacter pylori
Uterine stimulant
Dimethylmaleate hydratase inhibitor
Horriylsin inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Pancreatic disorders treatment
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Plasminogen activator inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Glycerol-3-phosphate oxidase inhibitor
Cytochrome P450 stimulant
Homospermidine synthase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Acidifying agent non gastric
Putrescine oxidase inhibitor
Opine dehydrogenase inhibitor
CYP2B18 substrate
CYP3C substrate
5 Hydroxytryptamine release inhibitor
Bisphosphoglycerate mutase inhibitor
Mandelate 4-monooxygenase inhibitor
Preneoplastic conditions treatment
Glutarate-semialdehyde dehydrogenase inhibitor
Dihydropteroate synthase inhibitor
ATP phosphoribosyltransferase inhibitor
Choline dehydrogenase inhibitor
Leucyltransferase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Glutathione thiolesterase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Glyoxylate oxidase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Hydroxylamine oxidase inhibitor
DNA polymerase I inhibitor
Diuretic

Neuropeptide FF agonist
Neuropeptide FF2 agonist
Spermidine dehydrogenase inhibitor
Glutamate 5-kinase inhibitor
Sodium channel blocker class Ib
Mannitol-1-phosphatase inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Antibiotic Glycopeptide-like
Arylsulfate sulfotransferase inhibitor
5 Hydroxytryptamine 3 agonist
Sphinganine-1-phosphate aldolase inhibitor
X-Trp aminopeptidase inhibitor
Aspergillopepsin I inhibitor
Nardilysin inhibitor
Deoxyribonuclease X inhibitor
Antinaupathic
DNA ligase (ATP) inhibitor
Methyltransferase substrate
Histidine ammonia-lyase inhibitor
Gastrointestinal motility stimulant
3-Methylbutanal reductase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Cerebroside-sulfatase inhibitor
Glutaminase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Carnitine 3-dehydrogenase inhibitor
Histidinol dehydrogenase inhibitor
Tentoxilysin inhibitor
Antihypoxic

Antineoplastic, alkylator

Trypanothione-disulfide reductase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Pseudouridylate synthase inhibitor
DNA synthesis inhibitor
Spermidine synthase inhibitor
Polyamine biosynthesis inhibitor
Hemostatic
Complement C5a chemotactic receptor antagonist
Tyrosine kinase stimulant
Amino-acid N-acetyltransferase inhibitor
Cysteine desulfurase inhibitor
Tyrosine 3 hydroxylase inhibitor
UGT2B28 substrate
Valine decarboxylase inhibitor
Omega-amidase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Linoleoyl-CoA desaturase inhibitor
NMDA receptor polyamine site agonist

Carboxypeptidase U inhibitor
Feruloyl esterase inhibitor
Antiprotozoal (Amoeba)
Aspartate transaminase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Intermittent claudication treatment
Glutaminyl-peptide cyclotransferase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Polyneuridine-aldehyde esterase inhibitor
Cyclooxygenase substrate
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
DELTA24-sterol reductase inhibitor
Vasoprotector
Phosphorylase kinase inhibitor
Gluconate dehydratase inhibitor
Cyclomaltodextrinase inhibitor
Antiulcerative
tRNA-pseudouridine synthase I inhibitor
Releasing hormone agonist
Methane monooxygenase inhibitor
Glycerol-1-phosphatase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Sulfate adenylyltransferase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Bontoxilysin inhibitor
Trimethyllysine dioxygenase inhibitor
Tryptophan transaminase inhibitor
Angiotensin II receptor agonist
Chaperonin ATPase inhibitor
Bradykinin agonist
CYP1A substrate
Cyclic AMP agonist
Polynucleotide 5'-hydroxy-kinase inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
CYP2A13 substrate
Arylacetonitrilase inhibitor
Histidinol-phosphatase inhibitor
CPB protease inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Magnolysin inhibitor
Membrane dipeptidase inhibitor
Phosphoinositide phospholipase C inhibitor
Wound healing agent
Neurolysin inhibitor
Metabolic disease treatment
L-threonine 3-dehydrogenase inhibitor
Dementia treatment

Antiprotozoal (Toxoplasma)
Ornithine carbamoyltransferase inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Shock treatment
Methionine decarboxylase inhibitor
Glutamate N-acetyltransferase inhibitor
Protein-tyrosine sulfotransferase inhibitor
Serratia marcescens nuclease inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Protein C (activated) inhibitor
Arabinose isomerase inhibitor
Antihelminthic (Nematodes)
D-threo-aldose 1-dehydrogenase inhibitor
Glutamate release inhibitor
Nicotine dehydrogenase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Creatininase inhibitor
Antiseptic
Glutamin-(asparagin-)ase inhibitor
Quisqualate antagonist
Phosphatidylglycerophosphatase inhibitor
Rhizopuspepsin inhibitor
Bothrolysin inhibitor
Methanol dehydrogenase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Homoserine dehydrogenase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Snapalysin inhibitor
tRNA nucleotidyltransferase inhibitor
Sclerosant
Urokinase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Coccolysin inhibitor
Glucuronolactone reductase inhibitor
Photosensitizer
D-amino-acid dehydrogenase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Leucine dehydrogenase inhibitor
Antihematotoxic
O-aminophenol oxidase inhibitor
Antinociceptive
Ethanolamine kinase inhibitor
Neuropeptide FF1 antagonist
Phosphatidate phosphatase inhibitor
Ecdysone 20-monooxygenase inhibitor
CYP3A7 substrate
Carbon-monoxide dehydrogenase inhibitor
[phosphorylase] phosphatase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Adenine deaminase inhibitor

Polar-amino-acid-transporting ATPase inhibitor
D-cysteine desulfhydrase inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Alkane 1-monooxygenase inhibitor
CYP2A4 substrate
Leucolysin inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Antihelminthic (Fasciola)
Glutamine synthetase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
Pappalysin-1 inhibitor
Antirickettsial
Cutinase inhibitor
EIF4E expression inhibitor
Riboflavin phosphotransferase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Biotin carboxylase inhibitor
Transketolase inhibitor
Antihypotensive
Amyloid beta aggregation inhibitor
Retinoprotector
Calcium-sensing receptor agonist
Lysyl oxidase inhibitor
Expectorant
Angiotensin agonist
Aspartate-tRNA ligase inhibitor
Cysteine transaminase inhibitor
Urticaria treatment
Glyoxylate reductase (NADP+) inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Indoleacetaldoxime dehydratase inhibitor
Tropinesterase inhibitor
Matriptase inhibitor
Nucleotide metabolism regulator
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Glutathione synthase inhibitor
Phosphonoacetate hydrolase inhibitor
Trehalose-phosphatase inhibitor
Neurotensin receptor agonist
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Nucleoside-diphosphatase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Choline sulfotransferase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Neuropeptide Y agonist
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Vascular dementia treatment
Ribonuclease U2 inhibitor
Aspergillopepsin II inhibitor

5-Formyltetrahydrofolate cyclo-ligase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Isopenicillin-N epimerase inhibitor
Phosphoenolpyruvate mutase inhibitor
Serine 3-dehydrogenase inhibitor
Aureolysin inhibitor
Pyruvate decarboxylase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Anthranilate synthase inhibitor
Granzyme B inhibitor
Gamma-glutamyltransferase inhibitor
Antipsoriatic
Glutamate (mGluR5) agonist
Alcohol dehydrogenase (acceptor) inhibitor
Melatonin 3 antagonist
Antineoplastic antimetabolite
D-Ornithine 4,5-aminomutase inhibitor
Menopausal disorders treatment
Kallikrein 13 inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Bradykinin B2 receptor agonist
Bile-salt sulfotransferase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
TRPA1 agonist
Homoserine O-succinyltransferase inhibitor
Neuropeptide Y1 antagonist
Deoxyribonuclease I inhibitor
Tauropine dehydrogenase inhibitor
Histamine N-methyltransferase inhibitor
Lipoxygenase substrate
Endothelial nitric-oxide synthase inhibitor
Ligase inhibitor
Glycine C-acetyltransferase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Melanocortin agonist
Laminaribiose phosphorylase inhibitor
Pancreatic endopeptidase E inhibitor
Heat shock protein agonist
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Acyl-lysine deacylase inhibitor
Aryl-acylamidase inhibitor
Asparagine-tRNA ligase inhibitor
Nitrile hydratase inhibitor
Orotate reductase (NADH) inhibitor
Centromere associated protein inhibitor

Arginyltransferase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Antinephritic
Arginine-tRNA ligase inhibitor
Glutamine-tRNA ligase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Glycine N-methyltransferase inhibitor
Lysine 2-monooxygenase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
CYP2F1 substrate
Antimutagenic
Antidote
MAP kinase kinase 4 inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Histamine H1 receptor agonist
Gaucher disease treatment
Factor VII inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Diisopropyl-fluorophosphatase inhibitor
Hyaluronic acid agonist
Lipoprotein lipase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Kynureninase inhibitor
Dipeptidyl peptidase I inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Vasodilator, peripheral
Ferrochelataze inhibitor
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
L-lysine oxidase inhibitor
Valine-tRNA ligase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Lysozyme inhibitor
Atrolysin A inhibitor
Nav1.1 sodium channel blocker
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD+) inhibitor
4-Alpha-glucanotransferase inhibitor
Neurotensin receptor antagonist
Lactose synthase inhibitor
Fibrosis treatment
DNA nucleotidylexotransferase inhibitor
CYP19A1 expression inhibitor
Allantoinase inhibitor
Sodium/calcium exchanger 1 inhibitor
Neurotensin 1 receptor antagonist

Interferon agonist
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Restless leg syndrome treatment
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Acylphosphatase inhibitor
Adenylate cyclase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Galactokinase inhibitor
Antibacterial
Antiviral (CMV)
Alpha-glucuronidase inhibitor
Melanocortin antagonist
Tryptophan alpha,beta-oxidase inhibitor
L-iduronidase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Lysine decarboxylase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Glucarate dehydratase inhibitor
Carboxymethylenebutenolidase inhibitor
Ribonuclease inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
GST T substrate
GST T1-1 substrate
Glycine hydroxymethyltransferase inhibitor
Cytostatic
Acute neurologic disorders treatment
Alternansucrase inhibitor
Carboxypeptidase B inhibitor
Acyl-CoA oxidase inhibitor
Malyl-CoA lyase inhibitor
CYP2B5 substrate
JAK2 expression inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
3'-Nucleotidase inhibitor
CYP2B10 substrate
Thrombin inhibitor
Factor XIa inhibitor
Licheninase inhibitor
Arylsulfatase inhibitor
RELA expression inhibitor
Alpha 2 adrenoreceptor agonist
Creatinine deaminase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor

Narcolepsy treatment
Cyclohexanone monooxygenase inhibitor
Transcription factor NF kappa A inhibitor
Acidifying agent gastric
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Aryldialkylphosphatase inhibitor
Phosphatidylinositol 3-kinase stimulant
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Protease activated receptor antagonist
Adrenergic, ophthalmic
D-proline reductase (dithiol) inhibitor
Galactose oxidase inhibitor
Heat shock protein 70 agonist
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Betaine-aldehyde dehydrogenase inhibitor
Cell wall synthesis inhibitor
Guanidinoacetase inhibitor
Antiprotozoal (Coccidial)
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Lactate 2-monooxygenase inhibitor
Formimidoylglutamase inhibitor
Undecaprenyl-diphosphatase inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
3-Isopropylmalate dehydratase inhibitor
Glutamate synthase (NADPH) inhibitor
Dihydropyrimidinase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
D-glutamate oxidase inhibitor
Hydroxymethylbilane synthase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Neuronal nitric-oxide synthase inhibitor
Autophagy inducer
Sleep apnea treatment
Aldehyde dehydrogenase 2 substrate
Glutamine-pyruvate transaminase inhibitor
Cystinyl aminopeptidase inhibitor
Guanidinopropionase inhibitor
3-Phytase inhibitor
Thiamine-phosphate kinase inhibitor
2-Amino adipate transaminase inhibitor
Glutamate formimidoyltransferase inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Inducible nitric-oxide synthase inhibitor
Cysteine synthase inhibitor
Ferredoxin-NADP⁺ reductase inhibitor
CXC chemokine 4 receptor antagonist
N-acetylglucosamine kinase inhibitor
K(Ca) 3.1 channel activator

Potassium channel intermediate-conductance Ca-activated activator
Chlordecone reductase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
Free radical scavenger
Glucosamine-6-phosphate deaminase inhibitor
Vitronectin receptor antagonist
Asparaginyl endopeptidase inhibitor
Beta-D-fucosidase inhibitor
Acid-sensing ion channel blocker
Rhodopsin kinase inhibitor
Nitric oxide scavenger
Lactaldehyde reductase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
CYP2C19 substrate
MAO A substrate
Carnitine O-octanoyltransferase inhibitor
Tryptase inhibitor
Glycine transaminase inhibitor
Anabolic
Isomaltulose synthase inhibitor
Xanthommatin reductase inhibitor
Diaminopimelate dehydrogenase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Lysine carboxypeptidase inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Plasmin inhibitor
Sodium channel (voltage-gated) blocker
Adenylate kinase inhibitor
Sorbose dehydrogenase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Adenylate cyclase stimulant
Antifibrinolytic
MAO B substrate
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Polarisation inhibitor
Astringent
MMP9 expression inhibitor
Gametolysin inhibitor
Serine-phosphoethanolamine synthase inhibitor
8-Amino-7-oxononanoate synthase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Neuraminidase inhibitor
Sodium/hydrogen exchanger 1 inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor
SMN2 expression enhancer
CYP2C9 inducer
CYP2C19 inducer
Indolepyruvate C-methyltransferase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor

Protein synthesis stimulant
Beta-N-acetylgalactosaminidase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Glutamate (mGluR8) agonist
Urolithiasis treatment
Fibromyalgia syndrome treatment
Histidine-tRNA ligase inhibitor
Stromelysin 2 inhibitor
Asparaginase inhibitor
ATP adenylyltransferase inhibitor
Diphosphomevalonate decarboxylase inhibitor
Pullulanase inhibitor
Oryzin inhibitor
GHS receptor agonist
Dextranucrase inhibitor
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
CYP2C10 substrate
Glycerophosphocholine cholinephosphodiesterase inhibitor
MAP-kinase-activated kinase 1 inhibitor
Atrolysin C inhibitor
D-alanine transaminase inhibitor
Dethiobiotin synthase inhibitor
Sulfite dehydrogenase inhibitor
Thermomycolin inhibitor
Myosin ATPase inhibitor
Mannonate dehydratase inhibitor
Cell wall biosynthesis inhibitor
Melanocortin 4 antagonist
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Hyponitrite reductase inhibitor
Pyruvate carboxylase inhibitor
CYP7 inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
Hydroxylysine kinase inhibitor
Skeletal muscle relaxant
GlutaminytRNA synthase (glutamine-hydrolysing) inhibitor
BRAF expression inhibitor
Formate-dihydrofolate ligase inhibitor
Acylglycerone-phosphate reductase inhibitor
Huntington's disease treatment
Interleukin 2 antagonist
Glycogen (starch) synthase inhibitor
TH expression enhancer
ATP diphosphatase inhibitor
Aerobactin synthase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Nicotinate dehydrogenase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor

GABA C receptor antagonist
Trans-pentaprenyltransferase inhibitor
Saccharopine dehydrogenase (NADP⁺, L-glutamate-forming) inhibitor
DELTA14-sterol reductase inhibitor
N-acetylneuraminate synthase inhibitor
Thiosulfate dehydrogenase inhibitor
Aldosterone antagonist
2-Acylglycerol O-acyltransferase inhibitor
5 Hydroxytryptamine 3 antagonist
Homogentisate 1,2-dioxygenase inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Adenylylsulphatase inhibitor
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Aspartate 1-decarboxylase inhibitor
Dextranase inhibitor
Cachexia treatment
Amylo-alpha-1,6-glucosidase inhibitor
Sodium/hydrogen exchanger 3 inhibitor
Phosphate acetyltransferase inhibitor
Cytosole dipeptidase inhibitor
Uroporphyrinogen-III synthase inhibitor
Thiol S-methyltransferase inhibitor
Cytokine modulator
N6-methyl-lysine oxidase inhibitor
Nitric-oxide synthase stimulant
Homoserine kinase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Dihydrouracil oxidase inhibitor
Gallate decarboxylase inhibitor
Alkylator
Adamalysin inhibitor
Antimycobacterial
Diaminopropionate ammonia-lyase inhibitor
Dihydroxy-acid dehydratase inhibitor
Dichloromuconate cycloisomerase inhibitor
Cellulase inhibitor
Sulfur dioxygenase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
D-Serine ammonia-lyase inhibitor
8-oxodGTPase stimulant
Ornithine decarboxylase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Pantothenase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
D-stereospecific aminopeptidase inhibitor
DNA-3-methyladenine glycosylase II inhibitor

Deoxyribose-phosphate aldolase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Phenylpyruvate decarboxylase inhibitor
Antiseborrheic
Procollagen-lysine 5-dioxygenase inhibitor
Aspartate kinase inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Integrin antagonist
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
Maleylacetoacetate isomerase inhibitor
Deoxycytidine deaminase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Decylcitrate synthase inhibitor
Osmotic diuretic
Oxalate oxidase inhibitor
Ethanolaminephosphotransferase inhibitor
Cystathionine beta-lyase inhibitor
Sickle-cell anemia treatment
S-adenosyl-L-methionine decarboxylase inhibitor
Protein kinase B gamma inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP⁺) inhibitor
Transcription factor STAT6 inhibitor
Guanylate cyclase 1 stimulant
Valine dehydrogenase (NADP⁺) inhibitor
Adenylyl-sulfate kinase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Factor Xa inhibitor
Methylaspartate ammonia-lyase inhibitor
Cellulose synthase (UDP-forming) inhibitor
Adenylosuccinate synthase inhibitor
Tryptophan dimethylallyltransferase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Galactoside O-acetyltransferase inhibitor
Arginine racemase inhibitor
Lysase inhibitor
UGT2B10 substrate
Neuropeptide antagonist
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
Trimereylisin II inhibitor
Allophanate hydrolase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Hematopoietic
Streptomycin 6-kinase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Trypsin inhibitor
Malate dehydrogenase (acceptor) inhibitor

SULT2A1 substrate
Amylosucrase inhibitor
Sepiapterin deaminase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
Chitin synthase inhibitor
Tyrosine-protein kinase TYRO 10 inhibitor
Glutamate dehydrogenase inhibitor
Purine biosynthesis inhibitor
Tryptophanyl aminopeptidase inhibitor
Thioether S-methyltransferase inhibitor
Dynamin GTPase inhibitor
Pyridoxal kinase inhibitor
GRP78 expression inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
Diacylglycerol kinase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Urethanase inhibitor
Adenomatous polyposis treatment
D-lactate dehydrogenase inhibitor
Peptidoglycan beta-N-acetylmuramidase inhibitor
Aminopeptidase microsomal inhibitor
Sucrose alpha-glucosidase inhibitor
2-Methylcitrate synthase inhibitor
Antiinflammatory, intestinal
Homocysteine desulphydrase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
3-Oxoadipate enol-lactonase inhibitor
Malate-CoA ligase inhibitor
Diiodophenylpyruvate reductase inhibitor
Caspase 8 stimulant
Saccharopine dehydrogenase (NADP⁺, L-lysine-forming) inhibitor
Anthranilate-CoA ligase inhibitor
(R)-aminopropanol dehydrogenase inhibitor
Beta amyloid protein antagonist
Gastric antisecretory
Poly(ADP-ribose) glycohydrolase inhibitor
Rhodotorulapepsin inhibitor
Histamine H2 receptor antagonist
Chitin deacetylase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Nucleotide diphosphatase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Protein kinase C mu inhibitor
CYP3A3 substrate
Carbamoyl-phosphate synthase (ammonia) inhibitor
Cyclopentanone monooxygenase inhibitor
Pyridoxine 4-oxidase inhibitor

RNA-directed RNA polymerase inhibitor
Gluconokinase inhibitor
Acetylcholine nicotinic antagonist
Glucosyl transferase inhibitor
Galactosylceramide sulfotransferase inhibitor
Phosphoglycolate phosphatase inhibitor
Gly-X carboxypeptidase inhibitor
Aryl-aldehyde dehydrogenase (NADP⁺) inhibitor
Alpha,alpha-phosphotrehalase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
Anhydrotetracycline monooxygenase inhibitor
Imidazoleglycerol-phosphate dehydratase inhibitor
Deoxyadenosine kinase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Serine-glyoxylate transaminase inhibitor
Peroxidase substrate
Sweetener
Cell adhesion inhibitor
Glutamate (mGluR3) agonist
N-formylglutamate deformylase inhibitor
4-Coumarate-CoA ligase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
H⁺-exporting ATPase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Aminopeptidase N inhibitor
Proline dehydrogenase inhibitor
Choline acetyltransferase stimulant
Guanylate kinase inhibitor
Acyl-CoA dehydrogenase inhibitor
Spermine synthase inhibitor
NF-E2-related factor 2 stimulant
Complement factor 1 inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Oxytocic
mRNA (guanine-N7-)-methyltransferase inhibitor
5-Aminolevulinate synthase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
L-lysine 6-transaminase inhibitor
Glycerol dehydrogenase (NADP⁺) inhibitor
L-Serine ammonia-lyase inhibitor
Oxytocin agonist
D-arabinonolactone oxidase inhibitor
Antibiotic
Leucine transaminase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP⁺) inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Cerebrovascular disorders treatment
Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor
Glutamate decarboxylase inhibitor
Cytochrome-b5 reductase inhibitor

2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Nav1.7 sodium channel blocker
Polynucleotide adenylyltransferase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
5 Hydroxytryptamine 4A antagonist
Uridine nucleosidase inhibitor
Cysteine-tRNA ligase inhibitor
Pantoate 4-dehydrogenase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Gamma-glutamyl hydrolase inhibitor
Serine-tRNA ligase inhibitor
CYP2B2 substrate
Muconate cycloisomerase inhibitor
D-lactate-2-sulfatase inhibitor
Tubuliny-Tyr carboxypeptidase inhibitor
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor
Na⁺ K⁺ transporting ATPase inhibitor
Acetolactate synthase inhibitor
Catechol oxidase inhibitor
Tubulin GTPase inhibitor
Orotidylate decarboxylase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Ketoheokinase inhibitor
Succinic dehydrogenase inhibitor
3'(2'),5'-Bisphosphate nucleotidase inhibitor
Uric acid excretion stimulant
Interleukin 10 agonist
Antibiotic Aminoglycoside-like
Integrin alphaVbeta6 antagonist
Sulfinioalanine decarboxylase inhibitor
Oligo-1,6-glucosidase inhibitor
Nucleoside deoxyribosyltransferase inhibitor
Dipeptidyl peptidase II inhibitor
Muscle relaxant
Leucine-tRNA ligase inhibitor
5 Hydroxytryptamine release stimulant
Leukotriene-B4 20-monooxygenase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
Colony stimulating factor agonist
Radical formation agonist
Protein kinase C nu inhibitor
5-Aminovalerate transaminase inhibitor
Deoxycytidine kinase inhibitor
Aconitate decarboxylase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor

Arabinogalactan endo-1,4-beta-galactosidase inhibitor
Maleate hydratase inhibitor
Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor
Anesthetic inhalation
Alpha,alpha-trehalose phosphorylase inhibitor
5 Hydroxytryptamine 2A agonist
Tryptophanamidase inhibitor
Sodium/calcium exchanger inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Lombricine kinase inhibitor
CYP4F2 substrate
CMP-N-acylneuramate phosphodiesterase inhibitor
Nicotinamide-nucleotide adenyltransferase inhibitor
Aspartate racemase inhibitor
Glucose 1-dehydrogenase inhibitor
S-methyl-5-thioribose kinase inhibitor
Diphosphate-serine phosphotransferase inhibitor
Ganglioside galactosyltransferase inhibitor
Prokineticin receptor 1 antagonist
X-His dipeptidase inhibitor
Neuraminidase (influenza) inhibitor
CTP synthase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Anthrax lethal factor inhibitor
Alpha-N-arabinofuranosidase inhibitor
Phosphoglycerate phosphatase inhibitor
PRL phosphatase inhibitor
4-Phytase inhibitor
Cellobiose phosphorylase inhibitor
UGT2B17 substrate
RNA synthesis inhibitor
tRNA cytidyltransferase inhibitor
Glutamate carboxypeptidase inhibitor
NAD⁺ kinase inhibitor
Epithelial sodium channel blocker
Sepsis treatment
2-Ethylmalate synthase inhibitor
GMP synthase inhibitor
Cathepsin E inhibitor
2-Methylcitrate dehydratase inhibitor
Transaldolase inhibitor
Antifungal
Phenylalanine decarboxylase inhibitor
Cycloartenol synthase inhibitor
Protein 30S ribosomal subunit inhibitor
Bradykinin B2 receptor antagonist
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
CYP2E1 inhibitor
TTK protein kinase inhibitor
Integrin alphaVbeta3 antagonist

Alkylglycerone-phosphate synthase inhibitor
Aminolevulinate transaminase inhibitor
6,7-Dihydropteridine reductase inhibitor
Polyphosphate kinase inhibitor
NMN nucleosidase inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
Methenyltetrahydrofolate cyclohydrolase inhibitor
Pyrroline-5-carboxylate reductase inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
ICAM1 expression inhibitor
Methylthioadenosine nucleosidase inhibitor
Urocanate hydratase inhibitor
Urease inhibitor
Amiloride-sensitive cation channel 3 blocker
Neurotensin 2 receptor antagonist
CYP2A3 substrate
Ethanolamine ammonia-lyase inhibitor
L-amino-acid oxidase inhibitor
Growth hormone release promoting
Neuraminidase (Influenza B) inhibitor
Lactase inhibitor
Insulin sensitizer
Chloride channel activator
D-Lysine 5,6-aminomutase inhibitor
ADAM10 endopeptidase inhibitor
Protease inhibitor
Alkene monooxygenase inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
Phosphoribulokinase inhibitor
Eye irritation, inactive
Plus-end-directed kinesin ATPase inhibitor
Alpha-amylase inhibitor
Glutamate (mGluR1a) agonist
Glutamate (mGluR5a) agonist
CDC25C inhibitor
Proline racemase inhibitor
Glutamate-cysteine ligase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
Phosphoserine transaminase inhibitor
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Phosphoribosylformylglycinamide synthase inhibitor
Small monomeric GTPase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Cardiovascular analeptic
Mannosyl-oligosaccharide glucosidase inhibitor
Asparagine-oxo-acid transaminase inhibitor
Tankyrase inhibitor

Laccase inhibitor
Haloalkane dehalogenase inhibitor
Inositol 1,4,5-triphosphate receptor antagonist
Cyanate hydratase inhibitor
Bombesin 2 receptor antagonist
NMDA 2A receptor antagonist
6-Phosphofructo-2-kinase inhibitor
Glucose-1-phosphatase inhibitor
GTP cyclohydrolase I inhibitor
Nucleoside-triphosphate-adenylate kinase inhibitor
Nuclease inhibitor
Pancreatic ribonuclease inhibitor
Strombine dehydrogenase inhibitor
Ribonucleoside diphosphate reductase inhibitor
Glutamate (mGluR1) agonist
Tryptophan 5 hydroxylase inhibitor
Cytochrome-c3 hydrogenase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Fumarate reductase (NADH) inhibitor
NAD⁺ diphosphatase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Squalene-hopene cyclase inhibitor
Peptidylamidoglycolate lyase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
CYP2A5 substrate
Chloramphenicol O-acetyltransferase inhibitor
Carminative
Vasopressin 1B antagonist
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
UGT1A5 substrate
Alanine transaminase inhibitor
Sodium/hydrogen exchanger 2 inhibitor
Aspartate carbamoyltransferase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Retinal dehydrogenase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
Tryptophan 2-monooxygenase inhibitor
Mycodextranase inhibitor
Gelatinase inhibitor
Iduronate-2-sulfatase inhibitor
Iodide peroxidase inhibitor
Glucan 1,4-alpha-glucosidase inhibitor
Adenylate cyclase I inhibitor
Queuine tRNA-ribosyltransferase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Agaritine gamma-glutamyltransferase inhibitor
Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
Histamine H3 receptor agonist
D(-)-tartrate dehydratase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor

L-3-cyanoalanine synthase inhibitor
Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor
Vasopressin 1B agonist
1-Phosphofructokinase inhibitor
MO15-related protein kinase Pfmrk inhibitor
5 Hydroxytryptamine 7 agonist
Dihydrofolate synthase inhibitor
Ribitol 2-dehydrogenase inhibitor
Luteinizing hormone-releasing hormone antagonist
Methylaspartate mutase inhibitor
Sucrose-phosphate phosphatase inhibitor
CYP4A11 substrate
Protein-glutamate O-methyltransferase inhibitor
Reductant
Glycine N-benzoyltransferase inhibitor
Beta-fructofuranosidase inhibitor
Penicillopepsin inhibitor
Antidote, organophosphates
Prolyl aminopeptidase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Sucrose synthase inhibitor

AMP nucleosidase inhibitor

Bis(5'-nucleosyl)-tetrphosphatase (asymmetrical) inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Imidazoline receptor antagonist
Bacillus subtilis ribonuclease inhibitor
Glucagon receptor antagonist
Vomilenine glucosyltransferase inhibitor
Uridine kinase inhibitor
Methionine adenosyltransferase inhibitor
Benzoylformate decarboxylase inhibitor
Tryptase 1 inhibitor
Kanamycin kinase inhibitor
P2 nucleoside transporter inhibitor
Integrin alpha5beta6 antagonist
Baculoviral IAP repeat-containing protein inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
Glycine N-acyltransferase inhibitor
Histone-lysine N-methyltransferase inhibitor
Formimidoyltetrahydrofolate cyclodeaminase inhibitor
Translation initiation factor IF-2 antagonist
Saluretic
Melatonin 5 antagonist
Beta lactamase TEM-1 inhibitor
CYP2C substrate
Valine-pyruvate transaminase inhibitor
Glycolaldehyde dehydrogenase inhibitor
UDP-sugar diphosphatase inhibitor
N-acylneuraminate cytidyltransferase inhibitor
CYP2C18 substrate

Phosphorylase a inhibitor
Protein N-acetylglucosaminyltransferase inhibitor
Acetate kinase inhibitor
Imidazoline I2 receptor antagonist
Sphingosine 1-phosphate receptor 5 agonist
Polypeptide N-acetylgalactosaminyltransferase inhibitor
Tyrosine 3 hydroxylase stimulant
Integrin alphaVbeta5 antagonist
KiSS-1 receptor agonist
Chitobiosyldiphosphodolichol beta-mannosyltransferase inhibitor
CYP19 inducer
Cholestanetriol 26-monooxygenase inhibitor
2-Methyleneglutarate mutase inhibitor
Cardiac myosin stimulant
HIV-2 reverse transcriptase inhibitor
Uracil phosphoribosyltransferase inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Bone formation stimulant
Oligonucleotidase inhibitor
L-ascorbate peroxidase inhibitor
Orotate reductase (NADPH) inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
Beta-cyclopiazotate dehydrogenase inhibitor
Beta-Lysine 5,6-aminomutase inhibitor
Glucosamine 6-phosphate N-acetyltransferase inhibitor
GST M substrate
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Antibiotic Carbapenem-like
CDK4/cyclin D3 inhibitor
Gentamicin 3'-N-acetyltransferase inhibitor
Phosphofructokinase-1 inhibitor
Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor
Acetylcholine M3 receptor agonist
2-Isopropylmalate synthase inhibitor
Dimethylhistidine N-methyltransferase inhibitor
Transforming growth factor beta 1 agonist
N-acetylglucosaminyldiphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor
D-2-hydroxy-acid dehydrogenase inhibitor
ATP deaminase inhibitor
Malate dehydrogenase (NADP+) inhibitor
Glucan 1,3-beta-glucosidase inhibitor
Antispirochetal
Alpha,alpha-trehalase inhibitor
Mycolysin inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Deoxyhypusine monooxygenase inhibitor
Hydroxyacylglutathione hydrolase inhibitor
Alpha-mannosidase inhibitor
Acyl-CoA dehydrogenase (NADP+) inhibitor

Bis(5'-nucleosyl)-tetrphosphatase (symmetrical) inhibitor
Cathepsin V inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Methionyl-tRNA formyltransferase inhibitor
Histamine H4 receptor antagonist
FAD diphosphatase inhibitor
Baculoviral IAP repeat-containing protein 4 inhibitor
Neuraminidase (Influenza A) inhibitor
Long-chain-acyl-CoA dehydrogenase inhibitor
Fructose 5-dehydrogenase (NADP+) inhibitor
Octadecanal decarbonylase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Glycogenin glucosyltransferase inhibitor

Methotrexate

Molecular Mechanism (initial) :

dihydrofolate reductase inhibitor

Molecular Mechanism (repurposed) :

dihydrofolate reductase inhibitor

initial indication(s):

cancers (breast, metastatic head and neck cancer, leukemia)

rheumatoid arthritis

Repurposed indication(s):

**cancers (gestational choriocarcinoma, chorioadenoma destruens,
cutaneous T cell lymphoma, lung cancer, non-Hodgkin's lymphomas)**

polyarticular juvenile arthritis

psoriasis

Predicted Activities

Mandelate 4-monooxygenase inhibitor
Glycine hydroxymethyltransferase inhibitor
Glutamate formimidoyltransferase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Sepiapterin deaminase inhibitor
Aldehyde oxidase substrate

Dihydrofolate reductase inhibitor

Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Folate antagonist
Glycine N-methyltransferase inhibitor
Antiviral (Poxvirus)
Purine biosynthesis inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Erythropoiesis stimulant
Methenyltetrahydrofolate cyclohydrolase inhibitor
Cytostatic
Glutathione synthase inhibitor
Methionyl-tRNA formyltransferase inhibitor

Antineoplastic antimetabolite

Hematopoietic inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor

Folypolyglutamate synthase inhibitor
Formimidoyltetrahydrofolate cyclodeaminase inhibitor
6,7-Dihydropteridine reductase inhibitor
Antimetabolite
Folate transporter 1 inhibitor
Dihydropteroate synthase inhibitor
RNA-directed RNA polymerase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor
Antineoplastic (lymphocytic leukemia)
S-formylglutathione hydrolase inhibitor
Benzoate 4-monooxygenase inhibitor
Immunostimulant
Glutamate carboxypeptidase inhibitor
Thymidylate synthase inhibitor
AICAR transformylase inhibitor
Arylamine N-acetyltransferase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
DNA synthesis inhibitor
Pteridine reductase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Dihydrofolate synthase inhibitor
Cyclic AMP agonist
Antiprotozoal (Toxoplasma)
Antiviral (Herpes)
Pancreatic ribonuclease inhibitor
Interferon alpha agonist
Aspartyltransferase inhibitor
Antineoplastic
3'-Demethylstaurosporine O-methyltransferase inhibitor
Macrophage stimulant
Peptide agonist
Antineoplastic (multiple myeloma)
HCV IRES inhibitor
Gamma-glutamyl hydrolase inhibitor
Glutamate-tRNA ligase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Antineoplastic (liver cancer)
Protein-arginine deiminase inhibitor
ICAM1 expression inhibitor
Fibroblast growth factor agonist
Antiprotozoal (Trypanosoma)
CDK9/cyclin T1 inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Antineoplastic (sarcoma)
Diuretic inhibitor
Saluretic
Thiopurine S-methyltransferase inhibitor
Formate-dihydrofolate ligase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor

Antihyperammonemic
4-Nitrophenylphosphatase inhibitor
Hematopoietic
Polyribonucleotide nucleotidyltransferase inhibitor
Proteasome ATPase inhibitor
Fibroblast growth factor 1 agonist
Antiviral (Hepatitis B)
Ethanolamine oxidase inhibitor
Growth stimulant
Xanthine oxidase inhibitor
Hydroxyacylglutathione hydrolase inhibitor
Prion diseases treatment
Dimethylhistidine N-methyltransferase inhibitor
Adenosine regulator
Antileukemic
Dihydrodipicolinate reductase inhibitor
Respiratory distress syndrome treatment
Inositol oxygenase inhibitor
Interleukin 2 agonist
Neuropeptide Y4 antagonist
Queuine tRNA-ribosyltransferase inhibitor
Alcohol O-acetyltransferase inhibitor
Alkylator
Maillard reaction inhibitor
Systemic lupus erythematosus treatment
Glycine-tRNA ligase inhibitor
Nucleotide metabolism regulator
Antipsoriatic
Guanidinoacetate kinase inhibitor
Intermittent claudication treatment
Sepiapterin reductase inhibitor
D-Octopine dehydrogenase inhibitor
MAP3K5 inhibitor
Protein-synthesizing GTPase inhibitor
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor
Biliary tract disorders treatment
Chloride channel blocker
Homocysteine S-methyltransferase inhibitor
Pyruvate carboxylase inhibitor
Antineoplastic (glioblastoma multiforme)
Diuretic
Antiviral (Influenza A)
Metabolic disease treatment
Acetylserotonin O-methyltransferase inhibitor
Purinergetic P2X3 antagonist
[phosphorylase] phosphatase inhibitor
Interleukin 4 antagonist
Prenyl-diphosphatase inhibitor
Glutamate dehydrogenase inhibitor
Macular degeneration treatment

Kidney function stimulant
Ketol-acid reductoisomerase inhibitor
Interferon agonist
Antiviral (Picornavirus)
Benzoate-CoA ligase inhibitor
DNA polymerase I inhibitor
Proliferative diseases treatment
Antineoplastic, alkylator
Dihydrofolate reductase (*Toxoplasma gondii*) inhibitor
Lymphocytopoiesis inhibitor
Antineoplastic (pancreatic cancer)
Antiprotozoal
Immunomodulator
Inflammatory Bowel disease treatment
Antiviral
Transcription factor NF kappa B stimulant
Transcription factor stimulant
H⁺-transporting two-sector ATPase inhibitor
GDP-mannose 6-dehydrogenase inhibitor
Endopeptidase La inhibitor
Angiogenesis stimulant
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Antineoplastic (renal cancer)
tRNA (guanine-N1-)-methyltransferase inhibitor
Antineoplastic (bladder cancer)
Guanylate cyclase stimulant
Myosin-light-chain-phosphatase inhibitor

Antineoplastic (lymphoma)

Interferon inducer
Antieczematic atopic
Biotinidase inhibitor
NAD⁺-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
Cell adhesion molecule inhibitor
Channel-conductance-controlling ATPase inhibitor
Sulfate adenylyltransferase inhibitor
Guanine deaminase inhibitor
Radiosensitizer
Rheumatoid arthritis treatment
Acrosin inhibitor
Lysine-tRNA ligase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Antineoplastic (glioma)
Cystinyl aminopeptidase inhibitor
Alanine racemase inhibitor
Serum-glucocorticoid regulated kinase 1 inhibitor
Serine O-acetyltransferase inhibitor
Electrolyte absorption antagonist
Antitoxic
(N-acetylneuraminyl)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
Pancreatic disorders treatment

Coactivator-associated arginine methyltransferase 1 inhibitor
Cyclic AMP modulator
Autoimmune disorders treatment
2-Amino-4-hydroxy-6-hydroxymethyldihydropteridine diphosphokinase inhibitor
Hepatic disorders treatment
Methylglutamate dehydrogenase inhibitor
RNA directed DNA polymerase inhibitor
Antiviral (Hepatitis)
ATP phosphoribosyltransferase inhibitor
N-formylglutamate deformylase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Butyrate-CoA ligase inhibitor
Insulin antagonist
Glutathione peroxidase inhibitor
Propionate-CoA ligase inhibitor
DNA methylase inhibitor
Adenylosuccinate synthase inhibitor
Glutamate dehydrogenase [NAD(P)+] inhibitor
p21-activated kinase inhibitor
Falcipain 3 inhibitor
Nitric-oxide synthase inhibitor
Corticotropin-like
Corneal wound healing stimulator
Leukopoiesis inhibitor
Adenosine deaminase inhibitor
DNA repair enzyme inhibitor
TP53 expression enhancer
Aspartate 4-decarboxylase inhibitor
Purinergic receptor antagonist
Blasticidin-S deaminase inhibitor
Adenylyl-sulfate reductase inhibitor
Homoserine kinase inhibitor
Amino-acid N-acetyltransferase inhibitor
Cyclooxygenase substrate
Glutamine-phenylpyruvate transaminase inhibitor
GMP synthase inhibitor
Multiple sclerosis treatment
Anticarcinogenic
Inosine nucleosidase inhibitor
Glycine N-acyltransferase inhibitor
Mucorpepsin inhibitor
rRNA (adenosine-2'-O-)-methyltransferase inhibitor
Xanthommatin reductase inhibitor
Antiprotozoal (Plasmodium)
Ribonuclease inhibitor
Glutaminyl-peptide cyclotransferase inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
Neurotensin 1 receptor agonist
Fibrosis treatment
Phosphoribosylglycinamide formyltransferase inhibitor

Mucositis treatment
Constipation treatment
Aminoacyl-tRNA synthetase inhibitor
CYP2H substrate
Vasculitis treatment
Diaminopimelate epimerase inhibitor
Xanthine oxidase substrate
Sucrose-phosphate synthase inhibitor
UDP-N-acetylmuramate-L-alanine ligase inhibitor
Dyspepsia treatment
Tryptophan hydroxylase 1 inhibitor
[glutamate-ammonia-ligase] adenylyltransferase inhibitor
Toll-Like receptor agonist
Homoserine O-acetyltransferase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Arginine-tRNA ligase inhibitor
Nicotinamide phosphoribosyltransferase inhibitor
Allergic rhinitis treatment
Choline kinase inhibitor
Antiviral (Hepatitis C)
Argininosuccinate synthase inhibitor
p21-activated kinase 4 inhibitor
Phosphoadenylylsulfatase inhibitor
G-protein-coupled bile acid receptor 1 agonist
Glutamine-fructose-6-phosphate transaminase inhibitor
Dihydroneopterin aldolase inhibitor
Glutamate (mGluR4) agonist
Bilirubin oxidase inhibitor
Purinergic P2 antagonist
Ethanolaminephosphotransferase inhibitor
Immunosuppressant
NAT2 substrate
Glycine N-benzoyltransferase inhibitor
Purinergic P2Y antagonist
Farnesyltransferase inhibitor
Alcohol dehydrogenase inhibitor
Glucagon-like peptide 1 agonist
Purinergic P2X2 antagonist
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Antibiotic Trimethoprim-like
Glycine amidinotransferase inhibitor
Leucyltransferase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase inhibitor
Platelet antagonist
Enteropeptidase inhibitor
Toll-Like receptor 7 agonist
Histidine-tRNA ligase inhibitor
MAP kinase kinase 7 inhibitor
O6-alkylguanine-DNA alkyltransferase inhibitor
tRNA (adenine-N1-)-methyltransferase inhibitor

Protocollagen prolyl hydroxylase inhibitor
Tryptophan 5 hydroxylase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
N-Acetylated alpha-linked acidic dipeptidase inhibitor
tRNA (uracil-5-)-methyltransferase inhibitor
Growth hormone agonist
Neuronal nitric-oxide synthase inhibitor
5-Aminolevulinate synthase inhibitor

Milnacipran

Molecular Mechanism (initial) :

5-HT and norepinephrine reuptake inhibitor

Molecular Mechanism (repurposed) :

5-HT and norepinephrine reuptake inhibitor

initial indication(s):

depression

Repurposed indication(s):

fibromyalgia

Predicted Activities

5 Hydroxytryptamine uptake inhibitor

Phobic disorders treatment
Sigma 1 receptor agonist
Cardiovascular analeptic
Spasmolytic, urinary
Gluconate 2-dehydrogenase (acceptor) inhibitor
Sigma receptor agonist
Antineurogenic pain
Mucomembranous protector
Antiseborrheic
Acetylcholine neuromuscular blocking agent
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Anticonvulsant
Neurotransmitter uptake inhibitor
Platelet aggregation stimulant
Phenol O-methyltransferase inhibitor
Fusarinine-C ornithinesterase inhibitor
Polyamine-transporting ATPase inhibitor
Antidyskinetic

Fibromyalgia syndrome treatment

Acylcarnitine hydrolase inhibitor
CYP2C19 inducer
Antinociceptive
Ecdysone 20-monooxygenase inhibitor
Ovulation inhibitor
Acute neurologic disorders treatment
Octopamine antagonist
Antiparkinsonian, rigidity relieving
MAP kinase stimulant
UGT2B12 substrate

4-Nitrophenol 2-monooxygenase inhibitor
Pseudolysin inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Dopamine transporter inhibitor
Limulus clotting factor B inhibitor
CYP2D6 inhibitor
Superoxide dismutase inhibitor
Dimethylargininase inhibitor
Sulfur reductase inhibitor
Trimethylamine-oxide aldolase inhibitor
Sulfite reductase inhibitor
Flavin-containing monooxygenase inhibitor
Fibrolase inhibitor
Taurine dehydrogenase inhibitor
Macrophage colony stimulating factor agonist
Antialcoholic
Oxidoreductase inhibitor
Platelet adhesion inhibitor
Limulus clotting factor C inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Adrenaline uptake inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Gonadotropin antagonist
Complement factor D inhibitor
Sodium channel blocker class Ib
Neurotransmitter antagonist
CYP2H substrate
Ompin inhibitor
Protein-disulfide reductase (glutathione) inhibitor
CYP2D16 substrate
Venombin AB inhibitor
Nitrite reductase (NO-forming) inhibitor
Alopecia treatment
Antimyopathies
Electron-transferring-flavoprotein dehydrogenase inhibitor
CYP2C12 substrate
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Fatty-acyl-CoA synthase inhibitor
CYP2J substrate
Fibrinolytic
Cyclic AMP agonist
Alkylacetylglucophosphatase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Steroid synthesis inhibitor
Antifibrinolytic
2-Haloacid dehalogenase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Septic shock treatment
N-hydroxy-2-acetamidofluorene reductase inhibitor
Fibrinogen receptor antagonist

Amine dehydrogenase inhibitor
Adrenergic
Phosphatidylcholine-retinol O-acyltransferase inhibitor
CYP2G1 substrate
Albendazole monooxygenase inhibitor
GABA C receptor agonist
Alkane 1-monooxygenase inhibitor
Pin1 inhibitor
Antidepressant
DELTA14-sterol reductase inhibitor
CYP2J2 substrate
Monoamine uptake inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Mood disorders treatment
Diamine N-acetyltransferase inhibitor
Transactivator transcription protein inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Diabetic neuropathy treatment
Lysine 2,3-aminomutase inhibitor
TRPA1 agonist
Gastrin inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Erythropoiesis stimulant
Respiratory analeptic
Antisecretoric
Trimethylamine dehydrogenase inhibitor
Thiosulfate dehydrogenase inhibitor
Spermidine dehydrogenase inhibitor
Analeptic
Dipeptidase E inhibitor
Hydroxylamine oxidase inhibitor
CYP4A substrate
Tyrosine 3 hydroxylase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Endopeptidase So inhibitor
CYP2C19 inhibitor
FMO1 substrate
Fragilysin inhibitor
Thiol oxidase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Kidney function stimulant
Antihypoxic
Peptidoglycan glycosyltransferase inhibitor
Antianorexic
Antinaupathic
CYP2C9 inducer
Anesthetic general
Proteasome ATPase inhibitor

Spasmolytic
CYP3A2 substrate
Oxytocic
Ubiquinol-cytochrome-c reductase inhibitor
Cytochrome P450 inhibitor
Sphinganine kinase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Ethanolamine oxidase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Fructose 5-dehydrogenase inhibitor
Hydrogen dehydrogenase inhibitor
Acylesterase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Botulin neurotoxin A light chain inhibitor
N-formylmethionyl-peptidase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Imidazoline receptor agonist
Aspartate-ammonia ligase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
Lysase inhibitor
Carboxypeptidase Taq inhibitor
Histidine N-acetyltransferase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Signal peptidase I inhibitor
Glycolate dehydrogenase inhibitor
CYP7 inhibitor
Histamine release stimulant
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
Lipocortins synthesis antagonist
DNA-3-methyladenine glycosylase I inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
CYP17 inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Cyclohexanone monooxygenase inhibitor
Exoribonuclease II inhibitor
Arginine 2-monooxygenase inhibitor
Antiparkinsonian, tremor relieving
Mandelate 4-monooxygenase inhibitor
Yeast ribonuclease inhibitor
Antiviral (Picornavirus)
1,4-Lactonase inhibitor
CYP2C10 substrate
4-Hydroxymandelate oxidase inhibitor
Calcium channel (voltage-sensitive) activator
Peptide alpha-N-acetyltransferase inhibitor
Methane monooxygenase inhibitor

Prion diseases treatment
Acetylspermidine deacetylase inhibitor
CYP2A6 inhibitor
NMDA receptor antagonist
Formaldehyde transketolase inhibitor
Irritable Bowel syndrome treatment
Enteropeptidase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
5 Hydroxytryptamine uptake stimulant
Menopausal disorders treatment
Cerebrovascular disorders treatment
Opioid kappa 3 receptor antagonist
5 Hydroxytryptamine 7L antagonist
Cytoprotectant
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Myc inhibitor
Restless leg syndrome treatment
5 Hydroxytryptamine release stimulant
Glutamyl endopeptidase II inhibitor
FMO3 substrate
2-Dehydropantoate 2-reductase inhibitor
Oxygen scavenger
Antiperistaltic
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Opioid dependency treatment
Leukopoiesis stimulant
Choline-phosphate cytidyltransferase inhibitor
Membrane integrity antagonist
Keratosis actinic (solar) treatment
Urologic disorders treatment
Nicotinate dehydrogenase inhibitor
GABA aminotransferase inhibitor
CYP2A4 substrate
Malate dehydrogenase (acceptor) inhibitor
Hemostatic
Gluconate 5-dehydrogenase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Glutamate receptor antagonist
3-Hydroxybenzoate 4-monooxygenase inhibitor
Gingipain K inhibitor
Cysteamine dioxygenase inhibitor
Phospholipid-translocating ATPase inhibitor
NMDA 2 receptor antagonist
Lysyl oxidase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Interleukin 10 agonist
[acyl-carrier-protein] S-acetyltransferase inhibitor
Glucose oxidase inhibitor
NMDA 2A receptor antagonist
Sulfite dehydrogenase inhibitor

Antiviral (Herpes)
Urinary incontinence treatment
3-Cyanoalanine hydratase inhibitor
Retinal dehydrogenase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Serine-pyruvate transaminase inhibitor
Aldosterone antagonist
Antiepileptic
Putrescine oxidase inhibitor
Polyamine oxidase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Lysine decarboxylase inhibitor
Isopenicillin-N epimerase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Oxidizing agent
Poly(beta-D-mannuronate) lyase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
CYP2B5 substrate
Neuropeptide Y4 antagonist
Anthranilate 3-monooxygenase (deaminating) inhibitor
Cathepsin T inhibitor
CYP2A1 substrate
Aspulvinone dimethylallyltransferase inhibitor
Muramoyltetrapeptide carboxypeptidase inhibitor
Chenodeoxycholoyletaurine hydrolase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Stroke treatment
Adenosine regulator
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
S-formylglutathione hydrolase inhibitor
Adrenaline release stimulant
Skeletal muscle relaxant
D-lactaldehyde dehydrogenase inhibitor
Angiotensin II receptor agonist
Arylacetonitrilase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Antiprotozoal (Amoeba)
Phosphoinositide phospholipase C inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Arylesterase inhibitor
Adenylyl-sulfate reductase inhibitor
Membrane permeability enhancer
Protein-synthesizing GTPase inhibitor
Aspartoacylase inhibitor
Polarisation inhibitor
Anesthetic

Peroxidase inhibitor
Diuretic inhibitor
Dementia treatment
Vascular (periferal) disease treatment
Cyclopentanone monooxygenase inhibitor
Meprin B inhibitor
Aldehyde dehydrogenase 2 substrate
Phosphoenolpyruvate mutase inhibitor
CYP3A1 substrate
Cytochrome-b5 reductase inhibitor
Nicotinic alpha2beta2 receptor antagonist
Methanol dehydrogenase inhibitor
Protein synthesis stimulant
Glucuronolactone reductase inhibitor
Inulinase inhibitor
Dopamine release stimulant
Mucinaminyserine mucinaminidase inhibitor
Uterine stimulant
Hydroxylamine reductase (NADH) inhibitor
Anesthetic local
Glycine amidinotransferase inhibitor
Pterin deaminase inhibitor
Arylmalonate decarboxylase inhibitor
GABA C receptor antagonist
Cyanoalanine nitrilase inhibitor
Tankyrase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
CYP2C8 inducer
Thiamine-triphosphatase inhibitor
Adenomatous polyposis treatment
Methylamine-glutamate N-methyltransferase inhibitor
CYP3A5 substrate
CYP2C3 substrate
Diaminopropionate ammonia-lyase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Glutathione thiolesterase inhibitor
HIV attachment inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Creatininase inhibitor
Fucosterol-epoxide lyase inhibitor
4-Hydroxyproline epimerase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Flavin-containing monooxygenase substrate
CYP2D1 substrate
Tryptophan 2,3-dioxygenase inhibitor
Heat shock protein 27 antagonist
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Analgesic
Saluretic
Antiviral (Adenovirus)

Polygalacturonase inhibitor
Phosphatidylglycerophosphatase inhibitor
CNS active muscle relaxant
Apyrase inhibitor
Cytochrome P450 stimulant
Valine decarboxylase inhibitor
Antitoxic
Isopenicillin-N synthase inhibitor
Gamma-glutamyltransferase inhibitor
GABA B receptor agonist
Gluconolactonase inhibitor
Bontoxilysin inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
ATPase stimulant
Dimethylmaleate hydratase inhibitor
HCV IRES inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Inotropic
Nicotine dehydrogenase inhibitor
Aldehyde oxidase inhibitor
Nitrile hydratase inhibitor
Alanine-tRNA ligase inhibitor
Thioredoxin inhibitor
CYP2D15 substrate
CYP2D2 inhibitor
Membrane dipeptidase inhibitor
Antipruritic, non-allergic
Granzyme A inhibitor
Lysostaphin inhibitor
DELTA24-sterol reductase inhibitor
CYP2A5 substrate
Thiamine pyridinylase inhibitor
Thiol S-methyltransferase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Fructan beta-fructosidase inhibitor
Mitochondrial processing peptidase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Mitochondrial intermediate peptidase inhibitor
Tentoxilysin inhibitor
Leukotriene-C4 synthase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Catechol oxidase inhibitor
CYP2B2 substrate
Aldehyde dehydrogenase [NAD(P)⁺] inhibitor
Nardilysin inhibitor
Lipid metabolism regulator
Glucuronate isomerase inhibitor

Venom exonuclease inhibitor
Ubiquitin thiolesterase inhibitor
Cycloartenol synthase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Bile-salt sulfotransferase inhibitor
Galactolipase inhibitor
Sodium/hydrogen exchanger 5 inhibitor
Muscle relaxant
Aldehyde dehydrogenase (NADP+) inhibitor
Malate oxidase inhibitor
Succinic dehydrogenase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Glutamate-tRNA ligase inhibitor
Homospermidine synthase inhibitor
Creatinase inhibitor
CYP2B1 substrate
NAT2 substrate
Hematopoietic
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Manganese peroxidase inhibitor
L-threonine 3-dehydrogenase inhibitor
Peptidyl-dipeptidase B inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
CYP2E1 inducer
Ornithine cyclodeaminase inhibitor
Alpha-L-fucosidase inhibitor
Selenocysteine lyase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
ADP-thymidine kinase inhibitor
3-Methylbutanal reductase inhibitor
Prolactin inhibitor
O-aminophenol oxidase inhibitor
CYP1A2 inducer
Alcohol dehydrogenase [NAD(P)+] inhibitor
Hyperprolactinemia treatment
Oxalate oxidase inhibitor
Calcium-sensing receptor agonist
TH expression enhancer
Deoxyhypusine synthase inhibitor
NF-E2-related factor 2 stimulant
Alkenylglycerophosphocholine hydrolase inhibitor
Narcotic antagonist
CYP2A2 substrate
Allantoate deiminase inhibitor
Carboxypeptidase D inhibitor
Aldehyde dehydrogenase substrate
Immunomodulator
Xaa-Pro dipeptidyl-peptidase inhibitor
CYP2A8 substrate
Sulfur dioxygenase inhibitor

CYP3A5 inducer
Cyclooxygenase substrate
Porphobilinogen synthase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Acidifying agent non gastric
Antiamyloidogenic
Antischistosomal
MMP9 expression inhibitor
D-Ornithine 4,5-aminomutase inhibitor
tRNA nucleotidyltransferase inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Oxytocin agonist
Taurine-2-oxoglutarate transaminase inhibitor
Tryptophan 2-monooxygenase inhibitor
Cytosole dipeptidase inhibitor
Ornithine decarboxylase inhibitor
NMDA receptor polyamine site antagonist
Glutarate-semialdehyde dehydrogenase inhibitor
Phosphatidylserine decarboxylase inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Antitussive, narcotic
Trans-pentaprenyltranstransferase inhibitor
RNA-directed RNA polymerase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Sulfite oxidase inhibitor
Saccharolysin inhibitor
Atrolysin A inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Tyrosine kinase stimulant
NADH kinase inhibitor
Polyamine biosynthesis inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Pyridoxal kinase inhibitor
Antidepressant, Imipramin-like
Gingipain R inhibitor
CYP3A4 inducer
CYP2C8 inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Lysosomal Pro-X carboxypeptidase inhibitor
Sugar-phosphatase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Plasmanylethanolamine desaturase inhibitor
Chloride channel activator
CYP2C11 substrate
Interferon alpha agonist
Electrolyte absorption antagonist
Dactylisin inhibitor
Antibacterial, ophthalmic
Dermatologic
Acetylornithine deacetylase inhibitor

Glucagon-like peptide 1 agonist
Hematopoietic inhibitor
Antihypotensive
Nav1.8 sodium channel blocker
Clavamate synthase inhibitor
Pancreatic ribonuclease inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Antidote
Coccolysin inhibitor
Aspartate-tRNA ligase inhibitor
Anticholelithogenic
UGT2B28 substrate
Aminoacylase inhibitor
D-Octopine dehydrogenase inhibitor
CYP4A2 substrate
Cl--transporting ATPase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Guanidinoacetate kinase inhibitor
Pullulanase inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Vascular dementia treatment
L-glutamate oxidase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Calcium channel activator
Loop diuretic
Biotinidase inhibitor
Leucolysin inhibitor
CYP3A inducer
Cyclic AMP modulator
JAK2 expression inhibitor
Pyroglutamyl-peptidase II inhibitor
Prostate disorders treatment
Leukotriene-B4 20-monooxygenase inhibitor
Trypanothione-disulfide reductase inhibitor
Smooth muscle myosin light chain kinase inhibitor
Pitrilysin inhibitor
L-lysine 6-transaminase inhibitor
Nucleoside oxidase (H₂O₂-forming) inhibitor
Lysyl endopeptidase inhibitor
Neuropsin inhibitor
Protein-arginine deiminase inhibitor
Glutaminase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Antiacne
Guanidinoacetase inhibitor
Hydroxylamine reductase inhibitor
Arylsulfate sulfotransferase inhibitor
Glutamate 5-kinase inhibitor
Acrocylindropepsin inhibitor

Chymosin inhibitor
Saccharopepsin inhibitor
Cysteine desulfurase inhibitor
CYP2B11 substrate
Procollagen N-endopeptidase inhibitor
Metalloprotease inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Gastrointestinal motility stimulant
Renilla-luciferin 2-monooxygenase inhibitor
Preneoplastic conditions treatment
Deoxyribonuclease I inhibitor
Picornain 3C inhibitor
DNA ligase (ATP) inhibitor
Asparaginase inhibitor
Squalene epoxidase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
ATP-binding cassette A1 stimulant
Glycerol dehydrogenase (NADP⁺) inhibitor
CYP2B6 substrate
CYP2B18 substrate
Amyotrophic lateral sclerosis treatment
Mannan endo-1,6- α -mannosidase inhibitor
Phosphatase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Mannose isomerase inhibitor
Cyclamate sulfohydrolase inhibitor
Phosphorylase kinase inhibitor
Nitrilase inhibitor
CYP2B substrate
3-Chloro-D-alanine dehydrochlorinase inhibitor
Arginyltransferase inhibitor
3-Isopropylmalate dehydratase inhibitor
Nicotinamidase inhibitor
Linoleoyl-CoA desaturase inhibitor
CYP2C18 substrate
Chloride peroxidase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Aspergillus nuclease S1 inhibitor
Sepsis treatment
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Coagulant
Butyrylcholinesterase stimulant
Aldehyde dehydrogenase (NAD⁺) inhibitor
3C-like protease (Human coronavirus) inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Catalase inhibitor
Acetylenecarboxylate hydratase inhibitor
Na⁺ K⁺ transporting ATPase inhibitor

4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Myeloblastin inhibitor
Benzoate 4-monooxygenase inhibitor
Pappalysin-1 inhibitor
Oligopeptidase B inhibitor
Analgesic stimulant
Anhydrotetracycline monooxygenase inhibitor
Phenol 2-monooxygenase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Urease inhibitor
Antineoplastic (thyroid cancer)
Galactose oxidase inhibitor
Inositol oxygenase inhibitor
Carnosine synthase inhibitor
Pancreatic elastase inhibitor
Catechol O methyltransferase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Threonine aldolase inhibitor
Glutamate N-acetyltransferase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Maleate isomerase inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
5 Hydroxytryptamine release inhibitor
N-acetylneuraminate synthase inhibitor
Chaperonin ATPase inhibitor
ADAM10 endopeptidase inhibitor
Serine 3-dehydrogenase inhibitor
Tryptophanyl aminopeptidase inhibitor
Pancreatic endopeptidase E inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
S-alkylcysteine lyase inhibitor
IgA-specific serine endopeptidase inhibitor
Angiotensin agonist
Mannitol-1-phosphatase inhibitor
Transcription factor NF kappa A inhibitor
Thymidylate 5'-phosphatase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
Trimerelysin II inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Ribitol 2-dehydrogenase inhibitor
Thermitase inhibitor
Glycine C-acetyltransferase inhibitor
Glutamine-tRNA ligase inhibitor
Leucine dehydrogenase inhibitor
Antineurotic
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Choline-sulfatase inhibitor

CYP2B10 substrate
N-hydroxyarylamine O-acetyltransferase inhibitor
Tryptophanamidase inhibitor
Antileprosy
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Spermine antagonist
Gamma-butyrobetaine dioxygenase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Guanidinopropionase inhibitor
Agmatinase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Brachyurin inhibitor
Spasmolytic, Papaverin-like
Platelet derived growth factor receptor kinase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Psychosexual dysfunction treatment
D-proline reductase (dithiol) inhibitor
CYP4B substrate
Pyridoxine 5-dehydrogenase inhibitor
Angiotensin AT2 receptor agonist
GST A substrate
ADP-ribosylarginine hydrolase inhibitor
CYP3A7 substrate
Insecticide
Fibroblast growth factor 1 agonist
Integrin alphaVbeta3 antagonist
Aralkylamine dehydrogenase inhibitor
Nerve growth factor antagonist
(S)-2-hydroxy-acid oxidase inhibitor
Prunasin beta-glucosidase inhibitor
5-Alpha-reductase inhibitor
Gallate decarboxylase inhibitor
ABCA1 expression enhancer
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Pediculicide
Arginine deiminase inhibitor
Phospholipase A1 inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Antitussive
CYP2C29 substrate
Diisopropyl-fluorophosphatase inhibitor
Beta-ureidopropionase inhibitor
Antiinflammatory, intestinal
Protein kinase B stimulant
Methyltransferase substrate
Choleretic
Cancer procoagulant inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
2-Dehydropantoate aldolase inhibitor

Pectin lyase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Methionine decarboxylase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Malyl-CoA lyase inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Antibiotic Aminoglycoside-like
Hydroxymethylbilane synthase inhibitor
Autophagy inducer
Delayed rectifier potassium channel blocker
Lipoprotein lipase inhibitor
Dextranase inhibitor
Mucositis treatment
Somatostatin agonist
Neuropeptide Y agonist
X-Pro dipeptidase inhibitor
Sphingosine kinase inhibitor
Acylglycerone-phosphate reductase inhibitor
Renal tissue kallikrein inhibitor
Antipruritic
Tryptophan alpha,beta-oxidase inhibitor
L-lysine oxidase inhibitor
Luteinizing hormone-releasing hormone agonist
X-methyl-His dipeptidase inhibitor
3-Phytase inhibitor
CYP24 substrate
Allantoicase inhibitor
Baculoviral IAP repeat-containing protein inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Potassium channel KCNQ blocker
NADPH-ferrihemoprotein reductase inhibitor
Preterm labor treatment
Protein 30S ribosomal subunit inhibitor
Retinoid X receptor agonist
Cholate-CoA ligase inhibitor
Somatostatin 2 agonist
D-xylulose reductase inhibitor
Cyclomaltodextrinase inhibitor
CYP4A11 substrate
Aureolysin inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
H⁺-transporting two-sector ATPase inhibitor
Neuraminidase inhibitor
Picornain 2A inhibitor
Chitosanase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Carnitine dehydratase inhibitor

Liver X receptor antagonist
 Urticaria treatment
 Iron-cytochrome-c reductase inhibitor
 Opine dehydrogenase inhibitor
 Myosin ATPase inhibitor
 Laccase inhibitor
 Pantoate-beta-alanine ligase inhibitor
 GABA transporter 3 inhibitor
 GST T substrate
 GST T1-1 substrate
 Carnitinamidase inhibitor
 Snapalysin inhibitor
 5 Hydroxytryptamine 4A antagonist
 Tryptophan dimethylallyltransferase inhibitor
 H⁺-exporting ATPase inhibitor
 Formate-dihydrofolate ligase inhibitor
 Apoptosis antagonist
 Gaucher disease treatment
 Aminopeptidase Y inhibitor
 Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
 N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
 Valine dehydrogenase (NADP⁺) inhibitor
 MAO B substrate
 ICAM1 expression inhibitor
 Trimethyllysine dioxygenase inhibitor
 Baculoviral IAP repeat-containing protein 4 inhibitor
 Neuraminidase (Influenza B) inhibitor
 DNA-(apurinic or apyrimidinic site) lyase inhibitor
 2,4-Diaminopentanoate dehydrogenase inhibitor
 3-Hydroxybutyryl-CoA dehydrogenase inhibitor
 Lysine 6-dehydrogenase inhibitor

Miltefosine

Molecular Mechanism (initial) :

Akt/PKB inhibitor

Molecular Mechanism (repurposed) :

phosphatidyl-choline biosynthesis inhibitor

initial indication(s):

cancer

Repurposed indication(s):

leishmaniasis

Predicted Activities

Glyceryl-ether monooxygenase inhibitor
 Macrophage colony stimulating factor agonist
 Urticaria treatment
 Vasoprotector
 Choline-phosphate cytidyltransferase inhibitor
 Membrane integrity antagonist

Antiprotozoal (Leishmania)

Protein-tyrosine sulfotransferase inhibitor
Angiogenesis stimulant
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Sugar-phosphatase inhibitor
Phospholipase C inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Benzoate-CoA ligase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Histamine release stimulant
Platelet aggregation stimulant
Trimethylamine-oxide aldolase inhibitor

Antineoplastic (uterine cancer)

Cutinase inhibitor
Acylcarnitine hydrolase inhibitor
Nootropic
Prenyl-diphosphatase inhibitor
Alkylglycerone-phosphate synthase inhibitor
Apoptosis agonist
Sphinganine kinase inhibitor
IgA-specific serine endopeptidase inhibitor
Phospholipase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Antiparasitic
Antihelmintic
Ethanolamine-phosphate cytidyltransferase inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Ceramidase inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Immunostimulant
Multiple sclerosis treatment
Carboxypeptidase Taq inhibitor
Antieczematic atopic
Platelet aggregation inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Antiprotozoal
Phobic disorders treatment
Antithrombotic
D-lactaldehyde dehydrogenase inhibitor
Antiinflammatory
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Antihypercholesterolemic
Farnesyltranstransferase inhibitor
Hypolipemic
Wound healing agent
Ethanolaminephosphotransferase inhibitor
Phospholipase A2 inhibitor
Alkylacetyl glycerophosphatase inhibitor
Gluconate 5-dehydrogenase inhibitor

Glucan 1,4-alpha-maltotriohydrolase inhibitor
Paraoxonase substrate
Urethanase inhibitor
Anesthetic general
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Cerebroside-sulfatase inhibitor
Exoribonuclease II inhibitor
Homoserine O-acetyltransferase inhibitor
Carboxylesterase inhibitor
Phosphatidate phosphatase inhibitor
Acetylesterase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
IgA-specific metalloendopeptidase inhibitor
Antineoplastic
Pancreatic disorders treatment
Membrane permeability enhancer
Antineoplastic (non-Hodgkin's lymphoma)
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Antipruritic, allergic
Antipruritic
Ribulose-phosphate 3-epimerase inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Antipsoriatic
Betaine-aldehyde dehydrogenase inhibitor
Antifungal
Phosphoserine phosphatase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Lysine 2,3-aminomutase inhibitor
Acaricide
Poly(beta-D-mannuronate) lyase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Glycerol dehydrogenase inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
Galactolipase inhibitor
Oxygen scavenger
Dermatologic
Sphinganine-1-phosphate aldolase inhibitor
ADP-thymidine kinase inhibitor
Diamine N-acetyltransferase inhibitor
Aspergillus nuclease S1 inhibitor
Polyporopepsin inhibitor
Alcohol O-acetyltransferase inhibitor
2-Acylglycerol O-acyltransferase inhibitor
Aryldialkylphosphatase inhibitor
Levansucrase inhibitor
Glutamate-5-semialdehyde dehydrogenase inhibitor
Eye irritation, inactive
Diuretic inhibitor

Carnitine 3-dehydrogenase inhibitor
Phosphatidate cytidyltransferase inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Antineoplastic (non-small cell lung cancer)
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Phospholipase A1 inhibitor
GST A substrate
Oryzin inhibitor
Phosphopantothenoylecysteine decarboxylase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Venombin AB inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Channel-conductance-controlling ATPase inhibitor
Platelet activating factor antagonist
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Respiratory distress syndrome treatment
Phosphatidylserine decarboxylase inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Carnitine palmitoyltransferase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
CYP2C12 substrate
Ecdysone 20-monooxygenase inhibitor
FMO1 substrate
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Glucose oxidase inhibitor
Ceramide glucosyltransferase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
Histidine N-acetyltransferase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Lipoprotein lipase inhibitor
Immunosuppressant
Antianginal
H⁺-transporting two-sector ATPase inhibitor
Dynein ATPase inhibitor
Aldehyde dehydrogenase (NADP⁺) inhibitor
Fucosterol-epoxide lyase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Flavin-containing monooxygenase inhibitor
Analeptic
Glycerol-3-phosphate dehydrogenase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Hydroxylamine oxidase inhibitor
Oxidizing agent
CYP4A substrate
Acylglycerone-phosphate reductase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor

Phenol O-methyltransferase inhibitor
Respiratory analeptic
Alkanal monooxygenase (FMN-linked) inhibitor
Bilirubin oxidase inhibitor
Diacylglycerol O-acyltransferase inhibitor
Leukopoiesis stimulant
Glucan endo-1,3-beta-D-glucosidase inhibitor
Endopeptidase So inhibitor
Pancreatic ribonuclease inhibitor
Pullulanase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Dimethylhistidine N-methyltransferase inhibitor
Choline sulfotransferase inhibitor
Ganglioside galactosyltransferase inhibitor
Atherosclerosis treatment
Bisphosphoglycerate mutase inhibitor
2-Haloacid dehalogenase inhibitor
Antineoplastic (multiple myeloma)
CYP2J substrate
Phosphoinositide 5-phosphatase inhibitor
Dolichyl-phosphatase inhibitor
Antihelminthic (Nematodes)
Acylaminoacyl-peptidase inhibitor
Skin irritation, inactive
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Apyrase inhibitor
Glycerone-phosphate O-acyltransferase inhibitor
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Antipyretic
Glycosylphosphatidylinositol phospholipase D inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Cyclomaltodextrinase inhibitor
1,4-Lactonase inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Phosphatidylglycerophosphatase inhibitor
Formaldehyde dehydrogenase inhibitor
Levanase inhibitor
Colony stimulating factor agonist
Transketolase inhibitor
Choline kinase inhibitor
CYP2J2 substrate
Pappalysin-1 inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Inorganic diphosphatase inhibitor
Pin1 inhibitor
Serratia marcescens nuclease inhibitor
2-Dehydropantoate aldolase inhibitor
OmpT inhibitor
Sclerosant

Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Glutamyl endopeptidase II inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Coccolysin inhibitor
Cyclic AMP agonist
DNA polymerase I inhibitor
Taurine dehydrogenase inhibitor
Long-chain-fatty-acid-CoA ligase inhibitor
Dextranase inhibitor
Limulus clotting factor B inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
4-Nitrophenylphosphatase inhibitor
Insecticide
[acyl-carrier-protein] S-acetyltransferase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Licheninase inhibitor
Anthranilate-CoA ligase inhibitor
Carnosine synthase inhibitor
Lipoxygenase substrate
Glycogen (starch) synthase inhibitor
Succinate-hydroxymethylglutarate CoA-transferase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Gonadotropin antagonist
NADH kinase inhibitor
Mevalonate kinase inhibitor
Myosin-light-chain-phosphatase inhibitor
Hepatic disorders treatment
Thymidylate 5'-phosphatase inhibitor
X-methyl-His dipeptidase inhibitor
D-Octopine dehydrogenase inhibitor
Glycerol-3-phosphate oxidase inhibitor
CMP-N-acetylneuraminate monooxygenase inhibitor
Trans-octaprenyltranstransferase inhibitor
Carnitine dehydratase inhibitor
DNA directed RNA polymerase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Cardiotonic
Complement factor D inhibitor
Aspergillopepsin I inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Antidiabetic symptomatic
Nitrite reductase (NO-forming) inhibitor
Prostaglandin-E2 9-reductase inhibitor
Isopenicillin-N synthase inhibitor
Procollagen N-endopeptidase inhibitor
3-Methylbutanal reductase inhibitor
Toll-Like receptor antagonist
Polyribonucleotide nucleotidyltransferase inhibitor
Pyruvate dehydrogenase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor

Malate oxidase inhibitor
Adenylyl-sulfate reductase inhibitor
Arginine 2-monooxygenase inhibitor
Phosphomevalonate kinase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
CYP2A1 substrate
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Lipotropic
Pseudolysin inhibitor
Endoglycosylceramidase inhibitor
Undecaprenyl-diphosphatase inhibitor
Antileukemic
Cyclohexanone monooxygenase inhibitor
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor
Anticataract
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Antiischemic
Adenylate kinase inhibitor
Phenol 2-monooxygenase inhibitor
N-acetyllactosamine synthase inhibitor
Lactase inhibitor
Tropinesterase inhibitor
Acyl-CoA oxidase inhibitor
Lysase inhibitor
Ophthalmic drug
Steroid N-acetylglucosaminyltransferase inhibitor
Glycine-tRNA ligase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Cholate-CoA ligase inhibitor
Sulfite dehydrogenase inhibitor
Anesthetic
Alpha-glucuronidase inhibitor
Signal peptidase I inhibitor
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Sulfur dioxygenase inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Nucleoside-diphosphatase inhibitor
Phenylacetate-CoA ligase inhibitor
Butyrate-CoA ligase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Glycerol-3-phosphate dehydrogenase (NAD+) inhibitor
Deoxyribose-phosphate aldolase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Acetate-CoA ligase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
Secretory phospholipase A2 inhibitor
Thiamine-triphosphatase inhibitor
Clostripain inhibitor

Fusarinine-C ornithinesterase inhibitor
Mucositis treatment
N-methyl-2-oxoglutaramate hydrolase inhibitor
CYP2B10 substrate
Keratolytic
Glucose-1,6-bisphosphate synthase inhibitor
Phosphatidylinositol 3-kinase stimulant
Chaperonin ATPase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Uroporphyrinogen-III synthase inhibitor
Ketol-acid reductoisomerase inhibitor
DELTA14-sterol reductase inhibitor
Glutaminy-peptide cyclotransferase inhibitor
Sucrose-phosphate synthase inhibitor
DNA directed DNA polymerase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
CYP4A11 substrate
Preneoplastic conditions treatment
Vasodilator
N-hydroxyarylamine O-acetyltransferase inhibitor
CYP2D16 substrate
5 Hydroxytryptamine uptake stimulant
Histone acetyltransferase inhibitor
Hydrogen dehydrogenase inhibitor
FAD diphosphatase inhibitor
Lipoprotein lipase stimulant
4-Hydroxymandelate oxidase inhibitor
1,2-alpha-L-fucosidase inhibitor
Malate dehydrogenase (acceptor) inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Nucleotide diphosphatase inhibitor
Procollagen C-endopeptidase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Superoxide dismutase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
Dolichol kinase inhibitor
Glycine amidinotransferase inhibitor
Phospholipid-translocating ATPase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Aspartyl aminopeptidase inhibitor
Peptidoglycan glycosyltransferase inhibitor
CYP2C18 substrate
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Hydroxylamine reductase (NADH) inhibitor
CYP3A1 substrate
Methylumbelliferyl-acetate deacetylase inhibitor
Acyloxyacyl hydrolase inhibitor
Acrosin inhibitor
Antimyopathies
Phosphate acetyltransferase inhibitor

Antitoxic
Diphosphomevalonate decarboxylase inhibitor
Antihypertensive
Protein-synthesizing GTPase inhibitor
Glutamate-tRNA ligase inhibitor
Polyamine-transporting ATPase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Isopenicillin-N epimerase inhibitor
Antiviral (Rhinovirus)
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Limulus clotting factor C inhibitor
Mitochondrial processing peptidase inhibitor
Glycerol kinase inhibitor
Antiprotozoal (Trichomonas)
Methylamine-glutamate N-methyltransferase inhibitor
Macrophage stimulant
Lipid metabolism regulator
Cellulose 1,4-beta-cellobiosidase inhibitor
Cytochrome-c3 hydrogenase inhibitor
Transforming growth factor beta 1 agonist
NAD(P)⁺ transhydrogenase (AB-specific) inhibitor
Feruloyl esterase inhibitor
TP53 expression enhancer
Acetylspermidine deacetylase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Aldehyde dehydrogenase inhibitor
Antimetabolite
Carboxypeptidase D inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Aureolysin inhibitor
DNA synthesis inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Rhodotorulapepsin inhibitor
Mandelate 4-monooxygenase inhibitor
Alzheimer's disease treatment
Carnitinamidase inhibitor
Antiviral (Poxvirus)
Prostaglandin-A1 DELTA-isomerase inhibitor
Alpha-N-arabinofuranosidase inhibitor
Cl⁻-transporting ATPase inhibitor
4-Coumarate-CoA ligase inhibitor
[phosphorylase] phosphatase inhibitor
Creatinase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
3-Hydroxybutyrate dehydrogenase inhibitor
Pediculicide

Guanidinoacetate kinase inhibitor
Aldehyde dehydrogenase substrate
Arylesterase inhibitor
DNA ligase (ATP) inhibitor
Calcium channel (voltage-sensitive) activator
Sphingosine 1-phosphate receptor antagonist
Malate-CoA ligase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Arylsulfatase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Methylglyoxal synthase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
CYP4A2 substrate
Nitrite reductase [NAD(P)H] inhibitor
Endopeptidase La inhibitor
Ethanolamine kinase inhibitor
Carnitine O-octanoyltransferase inhibitor
Dimethylallyltranstransferase inhibitor
Vasodilator, peripheral
Antiinfertility, female
Peroxidase substrate
Lysostaphin inhibitor
Ovulation inhibitor
Platelet adhesion inhibitor
Arylformamidase inhibitor
Endopeptidase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
Leucine dehydrogenase inhibitor
Calcium regulator
Retinol dehydrogenase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
CYP3A2 substrate
Acylphosphatase inhibitor
L-glucuronate reductase inhibitor
Sulfur reductase inhibitor
Alkylator
Retinyl-palmitate esterase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
NADPH peroxidase inhibitor
Acetate kinase inhibitor
GDP-mannose 6-dehydrogenase inhibitor
Cyclooxygenase substrate
Clavamate synthase inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor
Alpha,alpha-trehalase inhibitor

Peptidyl-Lys metalloendopeptidase inhibitor
Decylcitrate synthase inhibitor
Sphingosine 1-phosphate receptor 1 antagonist
Homoserine dehydrogenase inhibitor
Dimethylargininase inhibitor
Fragilysin inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Aspartate kinase inhibitor
Glucosamine-6-phosphate deaminase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
Nicotinamide phosphoribosyltransferase inhibitor
Coproporphyrinogen oxidase inhibitor
Poly(ADP-ribose) glycohydrolase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Galactokinase inhibitor
ADP-ribosylarginine hydrolase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
CYP2A3 substrate
Alternansucrase inhibitor
Chitinase inhibitor
Antisecretoric
Homocitrate synthase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
Acetolactate decarboxylase inhibitor
Biotinidase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Antiviral (Adenovirus)
Membrane permeability inhibitor
Myosin ATPase inhibitor
BRAF expression inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Lactosylceramide alpha-2,3-sialyltransferase inhibitor
Putrescine oxidase inhibitor
Antineoplastic (breast cancer)
Antischistosomal
Glutamate dehydrogenase (NADP⁺) inhibitor
Glycine C-acetyltransferase inhibitor
Antiviral
Pyruvate carboxylase inhibitor
Choline dehydrogenase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Glycerol-1,2-cyclic-phosphate 2-phosphodiesterase inhibitor
Ferredoxin-NADP⁺ reductase inhibitor
N6-methyl-lysine oxidase inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Phospholipase A2 IIa inhibitor
Arylamine N-acetyltransferase inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor

Leukotriene-C4 synthase inhibitor
Mannitol-1-phosphatase inhibitor
Cholesterol antagonist
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Hematopoietic
Ornithine-oxo-acid transaminase inhibitor
Trimethylamine dehydrogenase inhibitor
Sphingosine 1-phosphate receptor 5 agonist
Glutamate 5-kinase inhibitor
Metabolic disease treatment
Glutamate dehydrogenase [NAD(P)⁺] inhibitor
Cycloartenol synthase inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Glyoxylate reductase (NADP⁺) inhibitor
Nitrile hydratase inhibitor
Glycine N-acyltransferase inhibitor
Acyl-CoA dehydrogenase (NADP⁺) inhibitor
Acetylserotonin O-methyltransferase inhibitor
Malyl-CoA lyase inhibitor
Testosterone 17 β -dehydrogenase (NADP⁺) inhibitor
8-Amino-7-oxononanoate synthase inhibitor
Thiamine-phosphate kinase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Cytoprotectant
Antihyperlipoproteinemic
Arginine deiminase inhibitor
Homoserine kinase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
L-threonine 3-dehydrogenase inhibitor
Thromboxane synthase stimulant
Yeast ribonuclease inhibitor
Amidase inhibitor
Enteropeptidase inhibitor
Fructose-2,6-bisphosphate 6-phosphatase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Azobenzene reductase inhibitor
Phosphofructokinase-1 inhibitor
Dethiobiotin synthase inhibitor
Pyroglutamyl-peptidase I inhibitor
CYP4A1 substrate
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Glycine hydroxymethyltransferase inhibitor
UGT2B28 substrate
Renal tissue kallikrein inhibitor
Cyclooxygenase 1 substrate
Polar-amino-acid-transporting ATPase inhibitor
Sulfate adenylyltransferase inhibitor
Long-chain-acyl-CoA dehydrogenase inhibitor
Myeloblastin inhibitor
Alcohol dehydrogenase inhibitor

Ribonuclease U2 inhibitor
Diacylglycerol kinase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Galactoside O-acetyltransferase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
Aldehyde dehydrogenase [NAD(P)⁺] inhibitor
CYP2A2 substrate
Mannose isomerase inhibitor
Phosphogluconate 2-dehydrogenase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
Allantoate deiminase inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Cholinergic
Chelator
Aldehyde dehydrogenase 2 substrate
Adenylyl-sulfate kinase inhibitor
Purinergic P2 antagonist
Sulfate adenylyltransferase (ADP) inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Deoxyhypusine synthase inhibitor
Aspergillopepsin II inhibitor
Phosphoglycolate phosphatase inhibitor
Lysyl endopeptidase inhibitor
Alanine racemase inhibitor
6-Phospho-beta-glucosidase inhibitor
N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor
Alpha-amylase inhibitor
Hematopoietic inhibitor
Snapalysin inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
CYP2C9 inducer
Adrenaline release stimulant
Cysteine synthase inhibitor
Citrate (Si)-synthase inhibitor
Purinergic receptor antagonist
Beta-D-fucosidase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Cellulase inhibitor
CYP4F2 substrate
Cardioprotectant
Laminaribiose phosphorylase inhibitor
ATP adenylyltransferase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Hydroxymethylbilane synthase inhibitor
Estrone sulfotransferase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
CMP-N-acylneuraminate phosphodiesterase inhibitor
Nitrate reductase inhibitor
Hepatoprotectant

Dehydro-L-gulonate decarboxylase inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
Pectin lyase inhibitor
Oxaloacetate decarboxylase inhibitor
Thioredoxin inhibitor
Lysine 2-monooxygenase inhibitor
Caspase 8 stimulant
Flavin-containing monooxygenase substrate
3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor
Proteasome endopeptidase complex inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Lysozyme inhibitor
Squalene-hopene cyclase inhibitor
Rhizopuspepsin inhibitor
Benzaldehyde dehydrogenase (NADP⁺) inhibitor
Antiparkinsonian, rigidity relieving
Malate dehydrogenase inhibitor
Cardiovascular analeptic
Enoyl-CoA hydratase inhibitor
Antineoplastic antimetabolite
Acidifying agent gastric
Inositol-3-phosphate synthase inhibitor
Lactose synthase inhibitor
Loop diuretic
Glyceraldehyde-3-phosphate dehydrogenase (NADP⁺) inhibitor
Threonine-tRNA ligase inhibitor
Cytochrome-b5 reductase inhibitor
Adenylate cyclase stimulant
Bis(5'-adenosyl)-triphosphatase inhibitor
Arginine decarboxylase inhibitor
Sarcosine oxidase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Choline-sulfatase inhibitor
Formate-dihydrofolate ligase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Venom exonuclease inhibitor
Mucinaminyserine mucinaminidase inhibitor
Sulfite oxidase inhibitor
Candidapepsin inhibitor
Sphingosine 1-phosphate receptor 3 antagonist
Triose-phosphate isomerase inhibitor
Antiviral (Herpes)
3-Ketovalidoxylamine C-N-lyase inhibitor
Butyryl-CoA dehydrogenase inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor
Glutamate (mGluR6) antagonist
Trehalose-phosphatase inhibitor
11-Cis-retinyl-palmitate hydrolase inhibitor

Antiviral (CMV)
Diisopropyl-fluorophosphatase inhibitor
Amino-acid N-acetyltransferase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
Arylsulfate sulfotransferase inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Dipeptidase E inhibitor
Beta-mannosidase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Glutathione peroxidase inhibitor
Lysophosphatidic acid receptor antagonist
GABA aminotransferase inhibitor
2-Aminoadipate transaminase inhibitor
CYP2C29 substrate
Nitrate reductase (cytochrome) inhibitor
Fructan beta-fructosidase inhibitor
3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor
Photosensitizer
Pyridoxal kinase inhibitor
3-Dehydroquinate synthase inhibitor
3'-Nucleotidase inhibitor
Arabinose-5-phosphate isomerase inhibitor
NAD⁺ kinase inhibitor
N-acylmannosamine kinase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Serine-phosphoethanolamine synthase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Biotin carboxylase inhibitor
[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor
Glucosyl transferase inhibitor
Ferredoxin-nitrite reductase inhibitor
Aspartate ammonia-lyase inhibitor
Alpha-L-rhamnosidase inhibitor
Acyl-CoA dehydrogenase inhibitor
Fibrolase inhibitor
1-Alkyl-2-acetyl-glycerophosphocholine esterase inhibitor
Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Deoxyribonuclease X inhibitor
Methane monooxygenase inhibitor
3-Cyanoalanine hydratase inhibitor
Trimethyllysine dioxygenase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
[acetyl-CoA carboxylase] kinase inhibitor
CYP2C6 substrate
Acetoin dehydrogenase inhibitor
Leukopoiesis inhibitor

5-Aminolevulinate synthase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Glycogenin glucosyltransferase inhibitor
Beta-Phosphoglucomutase inhibitor
Hydroxylysine kinase inhibitor
6-Phosphofructo-2-kinase inhibitor
Purinergic P2 agonist
Purinergic receptor agonist
Threonine synthase inhibitor
Malate dehydrogenase (NADP+) inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
D-lactate dehydrogenase inhibitor
Membrane dipeptidase inhibitor
RNA directed DNA polymerase inhibitor
Guanylate cyclase inhibitor
Malate synthase inhibitor
Endo-1,4-beta-xylanase inhibitor
Gaucher disease treatment
2-Oxoaldehyde dehydrogenase (NAD+) inhibitor
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Cholesterol synthesis inhibitor
CYP2D2 inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
1-Alkyl-2-acetylgllycerol O-acyltransferase inhibitor
Sphingosine 1-phosphate receptor 5 antagonist
Antihematotoxic
DNA-3-methyladenine glycosylase I inhibitor
Leucine-tRNA ligase inhibitor
Glycine N-benzoyltransferase inhibitor
Phosphorylase kinase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminephosphotransferase inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Creatininase inhibitor
Glycerol-3-phosphate dehydrogenase [NAD(P)+] inhibitor
Ribose-5-phosphate isomerase inhibitor
Alcohol dehydrogenase substrate
Phosphoenolpyruvate-protein phosphotransferase inhibitor
TRPA1 agonist
NADH dehydrogenase inhibitor
Leukotriene agonist
FMO3 substrate
Polyneuridine-aldehyde esterase inhibitor
Homospermidine synthase inhibitor
Ornithine carbamoyltransferase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Isocitrate lyase inhibitor
Beta galactosidase inhibitor
Tauropine dehydrogenase inhibitor
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
Linoleate isomerase inhibitor

Valine-tRNA ligase inhibitor
Hemostatic
GABA B receptor agonist
Antineoplastic (lymphoma)
Glycolate dehydrogenase inhibitor
Sphingosine 1-phosphate receptor 4 agonist
Aryl-acylamidase inhibitor
Phosphoribulokinase inhibitor
Kexin inhibitor
Glutamate-cysteine ligase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Immunomodulator
Aryl sulfotransferase inhibitor
Tryptophan-tRNA ligase inhibitor
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Furin inhibitor
Dextranucrase inhibitor
Aldehyde dehydrogenase 1 substrate
Phenylalanine dehydrogenase inhibitor
Guanidinopropionase inhibitor
Dolichyldiphosphatase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Ribonuclease inhibitor
Xanthommatin reductase inhibitor
Agmatinase inhibitor
NAD⁺-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
Cellobiose phosphorylase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Malonyl-CoA decarboxylase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Uridine nucleosidase inhibitor
Penicillopepsin inhibitor
Purinergic P2Y agonist
CYP2C8 inducer
Fatty-acyl-CoA synthase inhibitor
D-proline reductase (dithiol) inhibitor
Plasminogen activator stimulant
Chitin synthase inhibitor
Pyridoxamine-oxaloacetate transaminase inhibitor
Gluconolactonase inhibitor
Tryptophan synthase inhibitor
Purinergic P2X agonist
Polygalacturonase inhibitor
Rhodopsin kinase inhibitor
CYP2C11 substrate
Glutathione synthase inhibitor
Phosphopyruvate hydratase inhibitor
L-lysine 6-transaminase inhibitor
Beta-fructofuranosidase inhibitor
Antipruritic, non-allergic

Laccase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Nucleoside phosphoacylhydrolase inhibitor
Inositol 1,4,5-triphosphate receptor antagonist
3-Oxoacid CoA-transferase inhibitor
tRNA-pseudouridine synthase I inhibitor
tRNA cytidyltransferase inhibitor
Oligo-1,6-glucosidase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
3-Deoxy-8-phosphooctulonate synthase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
CYP2C3 substrate
Purinergic P2Y antagonist
Glucose 1-dehydrogenase inhibitor
CYP2E1 inducer
Phosphoglycerate dehydrogenase inhibitor
N-acetylglucosaminyl diphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor
Sphingomyelinase inhibitor
Guanidinoacetase inhibitor
Phosphoketolase inhibitor
Interferon agonist
Phosphoadenylylsulfatase inhibitor
Ribose-5-phosphate-ammonia ligase inhibitor
4-Phytase inhibitor
Aerobactin synthase inhibitor
UDP-glucose 4-epimerase inhibitor
Oxaloacetate tautomerase inhibitor
Acid phosphatase inhibitor
Coagulant
Succinate-semialdehyde dehydrogenase inhibitor
Xylan 1,4-beta-xylosidase inhibitor
Aralkylamine N-acetyltransferase inhibitor
Polyamine oxidase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Pancreatic elastase inhibitor
Acetylenecarboxylate hydratase inhibitor
Pantetheine-phosphate adenylyltransferase inhibitor
Methylcrotonoyl-CoA carboxylase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Succinate dehydrogenase inhibitor
Venombin A inhibitor
Ketohekinase inhibitor
Octadecanal decarbonylase inhibitor
Polyphosphate-glucose phosphotransferase inhibitor
Butyrylcholinesterase inhibitor
Antidiabetic (type 1)
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Protein kinase C inhibitor
CYP2A4 substrate
Riboflavin phosphotransferase inhibitor

N-formylmethionyl-peptidase inhibitor
Pancreatic endopeptidase E inhibitor
Arylmalonate decarboxylase inhibitor
Asparaginase inhibitor
Cyclic AMP modulator
CYP2D15 substrate
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Deoxycytidine kinase inhibitor
L-aminoadipate-semialdehyde dehydrogenase inhibitor
D-Ala-D-Ala ligase inhibitor
2-Isopropylmalate synthase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Mannosyl-oligosaccharide glucosidase inhibitor
Antineoplastic, alkylator
Reductant
Guanylate kinase inhibitor
D-lactate-2-sulfatase inhibitor
Glutamate dehydrogenase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
CYP4F substrate
tRNA (guanine-N1-)-methyltransferase inhibitor
AR expression inhibitor
Geranyltranstransferase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Phosphoglycerate phosphatase inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
Carbamoyl-phosphate synthase (ammonia) inhibitor
N-acetylglucosamine kinase inhibitor
Glucose-6-phosphate isomerase inhibitor
Acetolactate synthase inhibitor
Arachidonic acid antagonist
Malate dehydrogenase (decarboxylating) inhibitor
Oxidoreductase inhibitor
Glutamate (mGluR6) agonist
Purinerbic P2Y1 antagonist
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Inositol oxygenase inhibitor
DNA nucleotidylexotransferase inhibitor
Argininosuccinate lyase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Hydroperoxide dehydratase inhibitor
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Polynucleotide adenylyltransferase inhibitor
Cysteine-tRNA ligase inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Lipase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Dichloromethane dehalogenase inhibitor
Neurotensin receptor agonist
[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor

Thermomycolin inhibitor
[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor
Trimethylamine-N-oxide reductase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Argininosuccinate synthase inhibitor
Purinergic P2X1 antagonist
Pyridoxamine-phosphate oxidase inhibitor
Pyruvate synthase inhibitor
Antiviral (Picornavirus)
Phthalate 4,5-dioxygenase inhibitor
Deoxyadenosine kinase inhibitor
Anesthetic inhalation
Isocitrate dehydrogenase (NADP+) inhibitor
Methylglutamate dehydrogenase inhibitor
Dynamin GTPase inhibitor
Dimethylmaleate hydratase inhibitor
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Hydroxyacylglutathione hydrolase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
Protein-glutamate methylesterase inhibitor
2-Amino-4-hydroxy-6-hydroxymethyldihydropteridine diphosphokinase inhibitor
Alpha, alpha-trehalose phosphorylase inhibitor
Alanine dehydrogenase inhibitor
GST T substrate
GST T1-1 substrate
Simian immunodeficiency virus proteinase inhibitor
CYP2G1 substrate
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Quinoprotein glucose dehydrogenase inhibitor
Phosphoglucomutase inhibitor
Valine decarboxylase inhibitor
CYP2B2 substrate
Thymidylate synthase inhibitor
Phytanoyl-CoA dioxygenase inhibitor
Phosphoserine transaminase inhibitor
Assemblin inhibitor
Tripeptidyl-peptidase I inhibitor
ADP-ribose diphosphatase inhibitor
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Cholesterol oxidase inhibitor
Riboflavin kinase inhibitor
2-Methylacyl-CoA dehydrogenase inhibitor
Glutaryl-CoA dehydrogenase inhibitor
Thromboxane B2 antagonist
Radioprotector
Adenylylsulphatase inhibitor
Queuine tRNA-ribosyltransferase inhibitor
Amylo-alpha-1,6-glucosidase inhibitor
HIV-2 reverse transcriptase inhibitor

Serine O-acetyltransferase inhibitor
Benzoylformate decarboxylase inhibitor
Pantothenate kinase inhibitor
Vitamin
Autophagy inducer
Antimutagenic
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Sphingosine 1-phosphate receptor 3 agonist
Tubulin GTPase inhibitor
Formaldehyde transketolase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Transaldolase inhibitor
GDP-L-fucose synthase inhibitor
3-Dehydroquinate dehydratase inhibitor
Phosphoinositide phospholipase C inhibitor
Cytosole dipeptidase inhibitor
Biliverdin reductase inhibitor
Urease inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
FMN adenylyltransferase inhibitor
CYP2B5 substrate
Antiprotozoal (Trypanosoma)
Histidinol dehydrogenase inhibitor
T2-induced deoxynucleotide kinase inhibitor
Purinergic P2X3 antagonist
Arabinose isomerase inhibitor
Glutaminyl-tRNA synthase (glutamine-hydrolysing) inhibitor
NAD⁺ diphosphatase inhibitor
3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor
CYP2C2 substrate
[glutamate-ammonia-ligase] adenylyltransferase inhibitor
Plus-end-directed kinesin ATPase inhibitor
T cell receptor antagonist
T cell receptor gamma-delta antagonist
Threonine ammonia-lyase inhibitor
Alpha glucosidase I inhibitor
Mannitol-1-phosphate 5-dehydrogenase inhibitor
Juvenile-hormone esterase inhibitor
Methylmalonyl-CoA carboxytransferase inhibitor
Polypeptide N-acetylgalactosaminyltransferase inhibitor
Ca²⁺-transporting ATPase inhibitor
Multiple inositol-polyphosphate phosphatase inhibitor
ZAP-70 protein tyrosine kinase inhibitor
CYP4F2 inhibitor
ATP phosphoribosyltransferase inhibitor
Chloride peroxidase inhibitor
Glucan 1,3-alpha-glucosidase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Arachidonate-CoA ligase inhibitor
GST P substrate

Phloroglucinol reductase inhibitor
UGT2B10 substrate
Trypanothione-disulfide reductase inhibitor
Gentamicin 3'-N-acetyltransferase inhibitor
Squalene epoxidase inhibitor
Glycerate kinase inhibitor
Alpha-mannosidase inhibitor
Purinergic P2Y12 antagonist
Pyruvate, phosphate dikinase inhibitor
Pyruvate, water dikinase inhibitor
Anthranilate phosphoribosyltransferase inhibitor
Lactaldehyde reductase inhibitor
L-lysine oxidase inhibitor
S-formylglutathione hydrolase inhibitor
Aspartate-ammonia ligase inhibitor
Cytosol alanyl aminopeptidase inhibitor
Chlordecone reductase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Maleylacetoacetate isomerase inhibitor
CYP2F1 substrate
Laxative
Brachyurin inhibitor
Gluconokinase inhibitor
Keratan sulfotransferase inhibitor
Isoamylase inhibitor
Gametolysin inhibitor
Acetoacetyl-CoA reductase inhibitor
High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
Toll-Like receptor 2 antagonist
Lysophosphatidic acid receptor agonist
Histidine-tRNA ligase inhibitor
Hydroxypyruvate reductase inhibitor
Formate C-acetyltransferase inhibitor
Glyoxylate reductase inhibitor
Gly-X carboxypeptidase inhibitor
Maltose-transporting ATPase inhibitor
S-methyl-5-thioribose kinase inhibitor
Beta-galactoside alpha-2,3-sialyltransferase inhibitor
Cellulose synthase (UDP-forming) inhibitor
Mannitol 2-dehydrogenase inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
Membrane integrity agonist
Imidazoleglycerol-phosphate dehydratase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate-2,6-diaminopimelate ligase inhibitor
Spasmolytic
Eicosanoid agonist
Thioredoxin reductase inhibitor
DNA methylase inhibitor
Pantoate-beta-alanine ligase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor

Neuropsin inhibitor
Styrene-oxide isomerase inhibitor
Glutamine synthetase inhibitor
Betaine-homocysteine S-methyltransferase inhibitor
ADAM inhibitor
Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor
Oligopeptidase B inhibitor
Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor
Aspartate-semialdehyde dehydrogenase inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor
Adenylate cyclase inhibitor
Dactylisin inhibitor
Protein N-acetylglucosaminyltransferase inhibitor
Inositol 1,4,5-triphosphate receptor 1 antagonist
ATP citrate synthase inhibitor
Undecaprenyl-phosphate galactose phosphotransferase inhibitor
Sphingosine kinase stimulant
Potassium channel (Ca-activated) blocker
3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
N-formylglutamate deformylase inhibitor
Acyl-lysine deacylase inhibitor
Purinergic P2T antagonist
Antineoplastic enhancer
ATP diphosphatase inhibitor
Sulfite reductase inhibitor
Phosphoglycerate kinase inhibitor
CYP4F12 substrate
Oxytocic
Pyruvate kinase inhibitor
Oleamide hydrolase inhibitor
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Antineoplastic (sarcoma)
Mannosidase inhibitor
tRNA adenylyltransferase inhibitor
tRNA nucleotidyltransferase inhibitor
CYP3A7 substrate
Steroid synthesis inhibitor
Glutaminase inhibitor
Propionate CoA-transferase inhibitor
3'(2'),5'-Bisphosphate nucleotidase inhibitor
Fibrinogen receptor antagonist
dCMP deaminase inhibitor
Methionine adenosyltransferase inhibitor
Guanidinobutyrase inhibitor
Fumarate reductase (NADH) inhibitor
Carboxymethylenebutenolidase inhibitor
Intermittent claudication treatment
3-Hydroxyisobutyryl-CoA hydrolase inhibitor
Cell wall synthesis inhibitor
Manganese peroxidase inhibitor

Glutamate (mGluR group III) agonist
CYP2A13 substrate
Camphor 1,2-monooxygenase inhibitor
Glutathione S-transferase inhibitor
Tentoxilysin inhibitor
NMDA receptor polyamine site agonist
Fructokinase inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Gingipain K inhibitor
D-xylulose reductase inhibitor
Antibiotic Tribactam-like
Linoleoyl-CoA desaturase inhibitor
Lysine decarboxylase inhibitor
Sphingosine 1-phosphate receptor agonist
Sorbitol dehydrogenase inhibitor
Allantoicase inhibitor
Sphingosine 1-phosphate receptor 1 agonist
D-Lysine 5,6-aminomutase inhibitor
Phosphoribosylformylglycinamide synthase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Glutamate (mGluR group III) antagonist
Cyanate hydratase inhibitor
NMDA receptor polyamine site antagonist
Amino-acid racemase inhibitor
Aminoacyl-tRNA synthetase inhibitor
Methyltransferase substrate
Diabetic neuropathy treatment
UDP-glucose 6-dehydrogenase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Thromboxane agonist
Polyphosphate kinase inhibitor
CYP19 substrate
Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor
IMP cyclohydrolase inhibitor
Antidote, heavy metal
Sucrose alpha-glucosidase inhibitor
5-Hydroxypentanoate CoA-transferase inhibitor
Antihypoxic
NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Glycolaldehyde dehydrogenase inhibitor
CTP synthase inhibitor
Methylmalonyl-CoA mutase inhibitor
Serine-tRNA ligase inhibitor
Glutamate synthase (NADPH) inhibitor
Glucose-1-phosphate adenylyltransferase inhibitor
Shab potassium channel blocker
15-Hydroxyprostaglandin-D dehydrogenase (NADP⁺) inhibitor
UGT1A5 substrate
H⁺-exporting ATPase inhibitor

(S)-6-hydroxynicotine oxidase inhibitor
Aspartate transaminase inhibitor
dUTP diphosphatase inhibitor
Thymidine-triphosphatase inhibitor
CYP2C18 inhibitor
tRNA methyltransferase inhibitor
Phosphoenolpyruvate carboxylase inhibitor
Asparagine synthase (glutamine-hydrolysing) inhibitor
DELTA24-sterol reductase inhibitor
Fumarylacetoacetase inhibitor
Adenylosuccinate lyase inhibitor
Glutamine-fructose-6-phosphate transaminase inhibitor

Minocycline hydrochloride

Molecular Mechanism (initial) :

30S ribosomal protein inhibitor

Molecular Mechanism (repurposed) :

iNOS inhibitor

p38 mitogen-activated protein kinase (MAPK) inhibitor

cytochrome c release inhibitor (downregulation caspase-1 and caspase-3)

initial indication(s):

antibacterial

acne treatment

Repurposed indication(s):

amyotrophic lateral sclerosis

Huntington's disease

Predicted Activities

Respiratory analeptic

Analeptic

Antiviral (Trachoma)

Antispirochetal

Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor

Antibiotic Tetracycline-like

Cytostatic

Polyribonucleotide nucleotidyltransferase inhibitor

Peptidyltransferase inhibitor

Antiparasitic

Antibacterial

Antiprotozoal (Amoeba)

CYP2H substrate

Antirickettsial

Protein synthesis inhibitor

SMN2 expression enhancer

Immunostimulant

Skin irritation, inactive

UGT1A9 substrate

Anhydrotetracycline monooxygenase inhibitor

Eye irritation, inactive

Neuropeptide Y4 antagonist

Antibiotic
UGT1A6 substrate
Glutamate dehydrogenase inhibitor
Antiprotozoal
UGT1A3 substrate
Histidine kinase inhibitor
Protein 30S ribosomal subunit inhibitor
HCV IRES inhibitor
UGT1A4 substrate
UGT2B15 substrate
Antituberculosic
CYP3A4 inhibitor
Tetracycline antiport transporter antagonist
Proliferative diseases treatment
Histamine H1 receptor agonist
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
UGT1A8 substrate
Antimycobacterial
Antineoplastic (glioblastoma multiforme)
UGT1A substrate
UGT1A1 substrate
Angiogenesis inhibitor
Antiviral
Bone formation stimulant
Respiratory distress syndrome treatment
UGT2B7 substrate
UGT2B12 substrate
Dermatologic
Apoptosis agonist
Antineoplastic (glioma)
Antineoplastic
Antineoplastic (brain cancer)
Antifungal
Radical formation agonist
CF transmembrane conductance regulator agonist
CDP-glycerol glycerophosphotransferase inhibitor
Transactivator transcription protein inhibitor
Lipocortins synthesis antagonist
Antibiotic Anthracycline-like
NAD⁺-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
Thromboxane synthase stimulant
UGT1A10 substrate
Xenobiotic-transporting ATPase inhibitor
Azobenzene reductase inhibitor
Glycine receptor agonist
Vanilloid 1 agonist
Antiviral (HIV)
Vanilloid agonist
p21-activated kinase 1 inhibitor
Antimycoplasmal

RNA synthesis inhibitor
Antiviral (Influenza A)
Antineoplastic antibiotic
Glutamate-5-semialdehyde dehydrogenase inhibitor
Protein 50S ribosomal subunit inhibitor
UGT2B substrate
Antiarthritic
HIV-1 reverse transcriptase inhibitor
Antineoplastic (renal cancer)
Antineoplastic (lymphoma)
5 Hydroxytryptamine 7L antagonist
UDP-glucuronosyltransferase substrate
Topoisomerase I inhibitor
Aspartyltransferase inhibitor
Antiosteoporotic
Dual specificity phosphatase 1 inhibitor
Antiacne
Chloride channel blocker
Topoisomerase II inhibitor
p21-activated kinase inhibitor
Cytokine release inhibitor
Dopamine D2A antagonist
SULT1E1 substrate
5 Hydroxytryptamine 7S antagonist
GDP-mannose 6-dehydrogenase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
P-glycoprotein substrate
Antineoplastic (melanoma)
Leukopoiesis inhibitor
Estrogen agonist
Adenosine regulator
Bone diseases treatment
Corticosteroid antagonist

Nelfinavir mesilate

Molecular Mechanism (initial) :

HIV-1 (Human immuno-deficiency virus, type 1) protease inhibitor

Molecular Mechanism (repurposed) :

proteasome inhibitor (caspase 9 activator, PPARgamma affinity)

initial indication(s):

HIV (Human immuno-deficiency virus) infection

Repurposed indication(s):

cancers (liposarcoma, glioblastoma multiforme, advanced hematologic cancer, refractory or recurrent solid tumors)

Predicted Activities

CYP2C19 substrate
CYP2C9 substrate
CYP2D substrate
CYP2C substrate

CYP2D6 substrate
Nicotinic alpha4beta4 receptor agonist
CYP3A substrate
CYP3A4 substrate
P-glycoprotein substrate

Antiviral

Antiviral (HIV)

CYP2C19 inhibitor
Phosphatase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
CYP1A2 substrate
CYP2D6 inhibitor
Acute neurologic disorders treatment
CYP2B6 substrate

HIV-1 protease inhibitor

Retinoprotector
CYP2C9 inhibitor

Proteasome ATPase inhibitor

HIV-2 retropepsin inhibitor
Spasmolytic, urinary
Muramoyltetrapeptide carboxypeptidase inhibitor
Protease inhibitor
Antianginal
CYP1A substrate
Bilirubin oxidase inhibitor
Lactase inhibitor
Antileukemic
P-glycoprotein 1 inhibitor
Fibroblast growth factor agonist
Neuropeptide Y4 antagonist
Uterine relaxant
Fibroblast growth factor 1 agonist
Diuretic
Glucagon-like peptide 1 agonist
CYP3A4 inhibitor
General pump inhibitor
Levansucrase inhibitor
Cardiotonic
Antiviral (Influenza A)
CYP2B substrate
Pancreatic disorders treatment
CYP2A6 substrate
Prostate disorders treatment
Vasodilator
CYP2E1 substrate
Antiarrhythmic
CYP2E substrate
P-glycoprotein inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
Bcl2 antagonist

Protein-arginine deiminase inhibitor
Bcl-xL inhibitor
CYP2A substrate
Ceramide glucosyltransferase inhibitor
Inflammatory Bowel disease treatment
Antithrombotic
Falcipain 3 inhibitor
Tardive dyskinesia treatment
Antihypotensive
Raynaud's phenomenon treatment
CYP2D1 substrate
Transcription factor NF kappa B stimulant
Transcription factor stimulant
pFOX inhibitor
Peptidyltransferase inhibitor
Peptide agonist
Dermatologic
APOA1 expression enhancer
Neurotransmitter uptake inhibitor
Angiogenesis stimulant
Testosterone agonist
Ophthalmic drug
Antioxidant
Calcium-sensing receptor antagonist
Prostatic (benign) hyperplasia treatment
Growth stimulant
Analeptic

Nilotinib hydrochloride monohydrate

Molecular Mechanism (initial) :

Bcr-Abl kinase inhibitor

Molecular Mechanism (repurposed) :

platelet-derived growth factor receptors (PDGFR) inhibitor

proto-oncogene c-Kit inhibitor

initial indication(s):

chronic myeloid leukemia

Repurposed indication(s):

glioma

melanoma

Predicted Activities

Tyrosine-protein kinase TYRO 10 inhibitor

Bcr-Abl kinase inhibitor

Stem cell growth factor agonist

Growth factor agonist

Protein kinase inhibitor

Signal transduction pathways inhibitor

Nootropic

Cytokine production inhibitor

Angiogenesis inhibitor

Janus tyrosine kinase inhibitor
Tyrosine kinase inhibitor
Focal adhesion kinase inhibitor
Protein-serine-threonine kinase inhibitor
Janus tyrosine kinase 3 inhibitor
Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor
Abl kinase inhibitor
Alzheimer's disease treatment
Autoimmune disorders treatment
Antiamyloidogenic
Lck kinase inhibitor

Platelet derived growth factor receptor kinase inhibitor

Focal adhesion kinase 2 inhibitor
Macrophage colony stimulating factor antagonist
Vascular endothelial growth factor antagonist
Janus tyrosine kinase 2 inhibitor
CYP2C19 inhibitor
Vascular endothelial growth factor 2 antagonist
Platelet aggregation inhibitor
CYP2C9 inhibitor
Neurodegenerative diseases treatment
Transplant rejection treatment
CYP1A2 inhibitor
Histamine release inhibitor
Antineoplastic
Cytochrome P450 inhibitor
Antiarthritic
CYP1A inhibitor
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
Proto-oncogene tyrosine-protein kinase Kit inhibitor
Src kinase inhibitor
Protein-tyrosine kinase Lyn inhibitor
p38 MAP kinase inhibitor
Rheumatoid arthritis treatment
EIF4E expression inhibitor
Focal adhesion kinase 1 inhibitor
Respiratory distress syndrome treatment
Colony stimulating factor antagonist
Antiepileptic
Transcription factor inhibitor
Protein kinase (CK1) inhibitor
Polo-like kinase-1 inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Platelet activating factor alpha antagonist
MAP kinase inhibitor
CDK9/cyclin T1 inhibitor
Insulin antagonist
Serum-glucocorticoid regulated kinase 1 inhibitor
Dihydroorotase inhibitor
Tumour necrosis factor antagonist

Pulmonary hypertension treatment
Platelet activating factor beta antagonist
Immunosuppressant
Aurora kinase inhibitor
Raf kinase inhibitor
Protein kinase (Mos, Mil/Raf, MEKK, RIPK, TESK, LIMK, IRAK, ILK, Activin/TGF-beta) inhibitor
MAP kinase 1 inhibitor
Bruton tyrosine kinase inhibitor
Cyclic AMP modulator
Tumour necrosis factor alpha antagonist
Syk tyrosine kinase inhibitor
Prion diseases treatment
TRKB antagonist
Antiasthmatic
CYP3A4 inhibitor
RET inhibitor
Interleukin antagonist
Aurora-C kinase inhibitor
TIE antagonist
Aurora-A kinase inhibitor
Platelet activating factor antagonist
TIE-2 antagonist
MAP3K5 inhibitor
Cystic fibrosis treatment
Heat shock protein 27 antagonist
Growth factor antagonist
Multiple sclerosis treatment
Macular degeneration treatment
Liver fibrosis treatment
Rhinitis treatment
Aurora-B kinase inhibitor
GABA A receptor agonist
Polo-like kinase inhibitor
Antiallergic
Interleukin 6 antagonist
Ephrin antagonist
Renal disease treatment
Cerebrovascular disorders treatment
p21-activated kinase 1 inhibitor
Antimitotic
p21-activated kinase inhibitor
Interleukin agonist
Ribosomal protein S6 kinase 1, 70-kDa inhibitor
c-Src kinase inhibitor
Ribosomal protein S6 kinase inhibitor
Transcription factor AP-1 inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
Protein kinase (CK1) delta inhibitor
Insulin like growth factor 1 antagonist
ALK inhibitor

Antiischemic, cerebral
MAP kinase 14 inhibitor
Protein kinase (CK2) inhibitor
Tyrosine-protein kinase receptor FLT3 inhibitor
Interleukin 2 antagonist
CDK2/cyclin A inhibitor
MAP kinase 10 inhibitor
T cell inhibitor
Ribosomal protein S6 kinase, 70-kDa inhibitor
Insulin growth factor antagonist
Antineoplastic (solid tumors)
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
Protein kinase (CK1) epsilon inhibitor
Heart failure treatment
Atherosclerosis treatment
Interleukin 1 antagonist
p21-activated kinase 4 inhibitor
Botulin neurotoxin A light chain inhibitor
Platelet growth factor antagonist
Fibroblast growth factor 2 antagonist
Ribosomal protein S6 kinase, 90-kDa inhibitor
Transcription factor STAT inhibitor
Antieczematous atopic
Diabetic retinopathy treatment
Tumour necrosis factor alpha release inhibitor
Interleukin 12 agonist
Antileukemic
EphB4 antagonist
Glycogen synthase stimulant
ZAP-70 protein tyrosine kinase inhibitor
Cyclin-dependent kinase 6 inhibitor
I kappa B kinase inhibitor
K(ir) 6.2 channel activator
Fibroblast growth factor antagonist
Hedgehog signaling inhibitor
MAP kinase 8 inhibitor
Protein kinase C inhibitor
Raf kinase B inhibitor
Antineoplastic (endocrine cancer)
Cyclin-dependent kinase inhibitor
NAD+-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor
Vascular endothelial growth factor 1 antagonist
Fibroblast growth factor 3 antagonist
Pim-1 kinase inhibitor
Cyclin-dependent kinase 1 inhibitor
Fibroblast growth factor 1 antagonist
Glycogen synthase kinase-3 beta inhibitor
Serum-glucocorticoid regulated kinase inhibitor
Cyclin-dependent kinase 2 inhibitor
Interleukin 8 antagonist

H⁺/K⁺-transporting ATPase inhibitor
Glycogen synthase kinase-3 inhibitor
Antineoplastic (multiple myeloma)
Analgesic, non-opioid
Hepatocyte growth factor antagonist
Vascular endothelial growth factor 3 antagonist
Raf kinase C inhibitor
Janus tyrosine kinase 1 inhibitor
Fibrosis treatment
Allergic rhinitis treatment
Chronic obstructive pulmonary disease treatment
MAP-kinase-activated kinase inhibitor
Proto-oncogene tyrosine-protein kinase c-hck inhibitor
MAP kinase kinase 1 inhibitor
Dyrk kinase inhibitor
I kappa B kinase 2 inhibitor
GABA receptor agonist
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Epidermal growth factor receptor kinase inhibitor
ErbB-4 antagonist
Glutamate (mGluR5) antagonist
NOS3 expression enhancer
Phosphodiesterase 3A inhibitor
Cyclin-dependent kinase 7 inhibitor
Vanilloid antagonist
Protein kinase B alpha inhibitor
HIV attachment inhibitor
Interleukin 1b antagonist
Sporulation kinase A inhibitor
Antianemic
Catalase stimulant
ErbB antagonist
TEC kinase inhibitor
Cyclin-dependent kinase 4 inhibitor
Tyrosine-protein kinase receptor antagonist
Cyclin-dependent kinase 9 inhibitor
Restenosis treatment
Hepatic disorders treatment
MAP-kinase-activated kinase 2 inhibitor
Antineoplastic (brain cancer)
Renal failure treatment
Cachexia treatment
ErbB-2 antagonist
TRKA antagonist
Pim-3 kinase inhibitor
Potassium channel KCNQ3 activator
Glutamate (mGluR group I) antagonist
MAP kinase 9 inhibitor
Glutamate (mGluR) antagonist
CDK/Cyclin complex inhibitor

Antineoplastic (ovarian cancer)
CYP4F2 inhibitor
Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor
Pim kinase inhibitor
Tyrosine-protein kinase EMT inhibitor
Osteoarthritis treatment
Calcium release-activated channel blocker
Protein kinase C alpha inhibitor
Sodium/hydrogen exchanger 3 inhibitor
Transforming growth factor antagonist
CDC7 inhibitor
AXL receptor tyrosine kinase inhibitor
Protein kinase B inhibitor
Antineoplastic (glioma)
Sodium/hydrogen exchanger inhibitor
Platelet growth factor beta antagonist
Acetylcholine nicotinic agonist

Nitisinone

Molecular Mechanism (initial) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

Molecular Mechanism (repurposed) :

4-hydroxy-phenylpyruvate dioxygenase inhibitor

initial indication(s):

hereditary tyrosinemia type I

Repurposed indication(s):

alkaptonuria

Predicted Activities

Ubiquinol-cytochrome-c reductase inhibitor

4-Hydroxyphenylpyruvate dioxygenase inhibitor

Membrane permeability inhibitor
Chloride channel blocker
Polarisation stimulant
Phobic disorders treatment
P-benzoquinone reductase (NADPH) inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Benzoate-CoA ligase inhibitor
Neurotransmitter antagonist
Prostaglandin-A1 DELTA-isomerase inhibitor
L-glutamate oxidase inhibitor
Acetylcholine neuromuscular blocking agent
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
GST P substrate
Lysase inhibitor
RNA-directed RNA polymerase inhibitor
Gestagen antagonist
Fibrinolytic
Acrocylindropepsin inhibitor
Chymosin inhibitor

Saccharopepsin inhibitor
GST P1-1 substrate
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Alcohol O-acetyltransferase inhibitor
Fusarinine-C ornithinesterase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Apyrase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
3-Phytase inhibitor
Phospholipid-translocating ATPase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Prostaglandin-E2 9-reductase inhibitor
APOA1 expression enhancer
Salicylate 1-monooxygenase inhibitor
Oxidoreductase inhibitor
CYP3A2 substrate
CYP2J substrate
HERG 1 channel blocker
Indanol dehydrogenase inhibitor
GST M substrate
GST A substrate
EIF4E expression inhibitor
Acute neurologic disorders treatment
CYP19A1 expression inhibitor
CYP2C8 substrate
UGT2B12 substrate
Glucan endo-1,3-beta-D-glucosidase inhibitor
HMGCS2 expression enhancer
Metabolic disease treatment
HIF1A expression inhibitor
GST M1-1 substrate
Dermatologic
Alpha-pinene-oxide decyclase inhibitor
Thioredoxin reductase inhibitor
Interleukin 2 agonist
Mannan endo-1,4-beta-mannosidase inhibitor
Platelet aggregation stimulant
Platelet derived growth factor receptor kinase inhibitor
CYP3A5 substrate
Gastrin inhibitor
Vasoprotector
Insecticide
Prostate disorders treatment
Polyporopepsin inhibitor
Thymidylate 5'-phosphatase inhibitor
Antiprotozoal (Coccidial)
Cutinase inhibitor
Antiprotozoal (Trypanosoma)
Antihypoxic
CYP2A1 substrate

Channel-conductance-controlling ATPase inhibitor
Cyclohexanone monooxygenase inhibitor
Choline-phosphate cytidyltransferase inhibitor
CYP2B11 substrate
S-formylglutathione hydrolase inhibitor
Age-related macular degeneration treatment
Spermidine dehydrogenase inhibitor
CYP2A3 substrate
Non-steroidal antiinflammatory agent
Menopausal disorders treatment
TP53 expression enhancer
Bisphosphoglycerate phosphatase inhibitor
CYP2B5 substrate
CYP2J2 substrate
Contraceptive
Photosensitizer
Antiischemic, cerebral
3-Oxoadipate enol-lactonase inhibitor
CYP3A3 substrate
Na⁺-transporting two-sector ATPase inhibitor
Superoxide dismutase inhibitor
Aldosterone antagonist
MO15-related protein kinase Pfmrk inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
3C-like protease (Human coronavirus) inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
CYP1A1 substrate
Hyponitrite reductase inhibitor
Chitosanase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
(R)-Pantolactone dehydrogenase (flavin) inhibitor
N-acylmannosamine kinase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Antileprosy
Pantoate 4-dehydrogenase inhibitor
Mucomembranous protector
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Bothrolysin inhibitor
Acidifying agent non gastric
Androgen antagonist
Phosphoinositide 5-phosphatase inhibitor
Prostatic (benign) hyperplasia treatment
Antihelminthic
Calcium channel activator
Dimethylmaleate hydratase inhibitor
Opine dehydrogenase inhibitor

Simian immunodeficiency virus proteinase inhibitor
Camphor 1,2-monooxygenase inhibitor
Uroporphyrinogen-III synthase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
CYP3A4 substrate
Glycine-tRNA ligase inhibitor
CYP1A2 substrate
Sickle-cell anemia treatment
Thioredoxin inhibitor
Skin irritation, inactive
Alopecia treatment
Antiacne
Alkylglycerone-phosphate synthase inhibitor
Lipid metabolism regulator
Pterin deaminase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Dry eye syndrome treatment
Contraceptive male
Arylsulfate sulfotransferase inhibitor
CYP2B6 substrate
Deoxyribonuclease I inhibitor
Tropinesterase inhibitor
27-Hydroxycholesterol 7 α -monooxygenase inhibitor
Histidinol dehydrogenase inhibitor
Antineoplastic (pancreatic cancer)
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Cholesterol oxidase inhibitor
Undecaprenyl-diphosphatase inhibitor
K(ir) 6.2 channel activator
Apoptosis antagonist
Anthranilate-CoA ligase inhibitor
Pyruvate decarboxylase inhibitor
Vasodilator, peripheral
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
CYP2A11 substrate
Mucorpepsin inhibitor
Antiparasitic
CYP1B1 substrate
Dopamine release stimulant
CYP1B substrate
NADPH-ferrihemoprotein reductase inhibitor
Cytochrome P450 stimulant
CYP2A4 substrate
Acetylcholinesterase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
CYP1A substrate
Poly(α -L-gulonate) lyase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Glyoxylate oxidase inhibitor
AR expression inhibitor

Lombricine kinase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
4-Hydroxybenzoate-CoA ligase inhibitor
Carnitinamidase inhibitor
CYP3A substrate
Trans-pentaprenyltranstransferase inhibitor
Antineoplastic (uterine cancer)
CYP2C9 substrate
Antieczematic
Neurotransmitter uptake inhibitor
Adrenaline release stimulant
Cycloartenol synthase inhibitor
Glutamyl endopeptidase II inhibitor
Retinol O-fatty-acyltransferase inhibitor
Raynaud's phenomenon treatment
Mucinaminyserine mucinaminidase inhibitor
Sphingosine 1-phosphate receptor 1 antagonist
Urethanase inhibitor
Antitoxic
Antischistosomal
Creatine kinase inhibitor
Gonadotropin antagonist
Catalase inhibitor
CYP2B10 substrate
Arylalkyl acylamidase inhibitor
Cyclopentanone monooxygenase inhibitor
CYP2D15 substrate
Androgen agonist
MAP kinase stimulant
Alanine-tRNA ligase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Aspergillopepsin I inhibitor
CYP2A6 substrate
Nicotinic alpha6 receptor agonist
4-Hydroxyproline epimerase inhibitor
5 Hydroxytryptamine release stimulant
Paraoxonase substrate
Antineoplastic (sarcoma)
Glycolate dehydrogenase inhibitor
Antihelmintic (Fasciola)
Vomilenine glucosyltransferase inhibitor
CYP3A1 substrate
Lactose synthase inhibitor
Antidyskinetic
Antipruritic, allergic
Tauropine dehydrogenase inhibitor
Oryzin inhibitor
Hair growth stimulant
CTGF expression inhibitor
UGT1A9 substrate

Tankyrase inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Neuropeptide agonist
CC chemokine receptor 2B antagonist
Prostate cancer treatment
Allophanate hydrolase inhibitor
Acetoacetate decarboxylase inhibitor
Chitinase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Aspergillopepsin II inhibitor
Phosphoenolpyruvate mutase inhibitor
Cerebrovascular disorders treatment
CYP2A substrate
Chaperonin ATPase inhibitor
Antiinflammatory, ophthalmic
Antiviral (Picornavirus)
Pin1 inhibitor
Dihydroorotase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Cholesterol antagonist
Formate-dihydrofolate ligase inhibitor
Glutathione reductase inhibitor
Preneoplastic conditions treatment
Carminative
CYP2E1 inducer
Glutamine-tRNA ligase inhibitor
Bisphosphoglycerate mutase inhibitor
Erythropoiesis stimulant
RNA synthesis inhibitor
Histidinol-phosphatase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
CYP2C substrate
Rubredoxin-NAD⁺ reductase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
GST T substrate
GST T1-1 substrate
Hydroxylamine reductase (NADH) inhibitor
Acetate kinase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Antibacterial, ophthalmic
Aspartate racemase inhibitor
Tardive dyskinesia treatment
Muscular dystrophy treatment
UDP-glucose 4-epimerase inhibitor
Nicotinic alpha2beta2 receptor antagonist
Peptidoglycan glycosyltransferase inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Guanidinoacetase inhibitor

Arachidonic acid antagonist
Lactate 2-monooxygenase inhibitor
CYP2B substrate
UGT1A6 substrate
NAD⁺ kinase inhibitor
Alcohol oxidase inhibitor
Morphine 6-dehydrogenase inhibitor
Prolyl aminopeptidase inhibitor
Glucarate dehydratase inhibitor
CYP7 inhibitor
Eye irritation, inactive
Malate oxidase inhibitor
Antipyretic
Dihydroorotate oxidase inhibitor
Myosin ATPase inhibitor
Sugar-phosphatase inhibitor
Interleukin 10 antagonist
HMOX1 expression enhancer
Hirsutism treatment
Transactivator transcription protein inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Anabolic
Catechol O methyltransferase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP⁺) inhibitor
CYP2B2 substrate
Lipoprotein lipase inhibitor
Respiratory analeptic
Electron-transferring-flavoprotein dehydrogenase inhibitor
Aryldialkylphosphatase inhibitor
Leucolysin inhibitor
Carboxylesterase inhibitor
Thermomycolin inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
CYP4A11 substrate
4-Chlorobenzoyl-CoA dehalogenase inhibitor
T cell inhibitor
Glutathione S-transferase substrate
Antiprotozoal (Leishmania)
Glycerol-3-phosphate dehydrogenase inhibitor
Antiparkinsonian, rigidity relieving
Ligase inhibitor
Transglutaminase 2 inhibitor
Interleukin 6 antagonist
Glutathione peroxidase inhibitor
Antiuremic
NF-E2-related factor 2 stimulant
Andropause treatment
Phenylacetate-CoA ligase inhibitor
Neuropeptide Y agonist
Glutaminyl-peptide cyclotransferase inhibitor

4-Nitrophenol 2-monooxygenase inhibitor
Iduronate-2-sulfatase inhibitor
Antineoplastic (bladder cancer)
Antineoplastic (endocrine cancer)
Phenol 2-monooxygenase inhibitor
Vascular (periferal) disease treatment
Celiac disease treatment
Adenomatous polyposis treatment
Potassium channel (ATP-sensitive) activator
Potassium channel (Inward rectifier) activator
2-Oxoglutarate decarboxylase inhibitor
Adenylate kinase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Guanidinoacetate kinase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Gamma-glutamyltransferase inhibitor
Caspase 8 stimulant
Inducible nitric-oxide synthase inhibitor
Rhizopuspepsin inhibitor
Pyridoxine 5-dehydrogenase inhibitor
Glutamate release inhibitor
Cyclic GMP phosphodiesterase inhibitor
Saluretic
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Antinociceptive
L-amino-acid oxidase inhibitor
Antiprotozoal (Histomonas)
Muconate cycloisomerase inhibitor
Antiischemic
L-ascorbate peroxidase inhibitor
Methylaspartate ammonia-lyase inhibitor
Catalase stimulant
L-threonine 3-dehydrogenase inhibitor
Nuclease inhibitor
Glutamin-(asparagin-)ase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
CYP2B4 substrate
Leukotriene-B4 20-monooxygenase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Calcium-sensing receptor agonist
Potassium channel activator
CYP2E1 substrate
Menstruation disorders treatment
Peptide alpha-N-acetyltransferase inhibitor
Aldehyde dehydrogenase (NAD⁺) inhibitor
Antiinfective
Calcium regulator
UGT1A1 substrate
Hypoxia inducible factor 1 alpha inhibitor
Ferredoxin-NADP⁺ reductase inhibitor

Rhodotorulapepsin inhibitor
CYP2A10 substrate
Cholestenone 5alpha-reductase inhibitor
Liver cirrhosis treatment
3-Ketovalidoxylamine C-N-lyase inhibitor
Focal adhesion kinase 2 inhibitor
Succinate dehydrogenase inhibitor
Subtilisin inhibitor
Complement factor D inhibitor
Histidine kinase inhibitor
K(Ca) 3.1 channel blocker
Antineurotic
Phosphatidylserine decarboxylase inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
Sphingosine 1-phosphate receptor antagonist
Chloride channel activator
Estrogen-related receptor alpha antagonist
Limulus clotting factor B inhibitor
CYP2E substrate
2-Nitrophenol 2-monooxygenase inhibitor
Oxidizing agent
Aldose reductase 2 inhibitor
UDP-glucuronosyltransferase substrate
Triose-phosphate isomerase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Antipruritic, non-allergic
Prostaglandin D2 agonist
Radiosensitizer
Antineoplastic (glioblastoma multiforme)
5-Alpha-reductase 1 inhibitor
Quisqualate antagonist
CYP2D6 substrate
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Ovulation inhibitor
Sweetener
4,5-Dihydroxyphthalate decarboxylase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Antiprotozoal (Babesia)
Interferon gamma antagonist
Albendazole monooxygenase inhibitor
Botulin neurotoxin A light chain inhibitor
Pancreatic ribonuclease inhibitor
Hydroxymethylbilane synthase inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Choloylglycine hydrolase inhibitor
Nicotinamide-nucleotide adenylyltransferase inhibitor
Interferon antagonist
Muscle relaxant
Guanidinoacetate N-methyltransferase inhibitor
UGT2B15 substrate

Protein-glutamate methylesterase inhibitor
Methyltransferase inhibitor
CYP2G1 substrate
N-acetylneuraminate lyase inhibitor
Acaricide
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Diphosphomevalonate decarboxylase inhibitor
CYP2D substrate
4-Hydroxybenzoate 1-hydroxylase inhibitor
Scytalone dehydratase inhibitor
Nerve growth factor antagonist
Hydroxymethylglutaryl-CoA lyase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Endo-1,4-beta-xylanase inhibitor
Secretase alpha stimulant
Secretase stimulant
Interleukin 2 antagonist
Antirickettsial
Alkylacetylgllycerophosphatase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Argininosuccinate synthase inhibitor
Diguanydinobutanase inhibitor
Glutamate receptor antagonist
Transcription factor NF kappa B inhibitor
Transthyretin amyloid fibril formation inhibitor
Dihydroorotate dehydrogenase inhibitor
Potassium channel intermediate-conductance Ca-activated blocker
3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor
Severe acute respiratory syndrome treatment
Bombesin 1 receptor antagonist
TRPA1 agonist
Antimycobacterial
CYP4F2 substrate
Interleukin antagonist
DELTA24-sterol reductase inhibitor
UGT2B28 substrate
Macrophage colony stimulating factor agonist
Calcium channel (voltage-sensitive) activator
5-Alpha-reductase inhibitor
Carnitine 3-dehydrogenase inhibitor
Mannose-6-phosphate isomerase inhibitor
Hypogonadism treatment
Lysine decarboxylase inhibitor
NADPH oxidase inhibitor
Malate-CoA ligase inhibitor
Lipoprotein disorders treatment
Diaminopimelate dehydrogenase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Membrane permeability enhancer
Potassium channel KCNQ blocker

NOS3 expression enhancer
2-Dehydropantolactone reductase (A-specific) inhibitor
CYP4F substrate
CYP2C11 substrate
Progesterone receptor B antagonist
Fumarylacetoacetase inhibitor
Rotamase (FKBP) inhibitor
Focal adhesion kinase inhibitor
ATP phosphoribosyltransferase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Prostaglandin-E2 synthase 1 inhibitor
CYP1A inhibitor
Isoamylase inhibitor
Venombin A inhibitor
CYP1A2 inhibitor
Interleukin agonist
Peroxisome proliferator-activated receptor antagonist
Pregnane X receptor antagonist
Antiinflammatory
Aryl hydrocarbon receptor agonist
Peptide-tryptophan 2,3-dioxygenase inhibitor
Ubiquitin-protein ligase inhibitor
Hematinic
Glutamate (mGluR4) agonist
L-galactonolactone oxidase inhibitor
Endometriosis treatment
CYP3A7 substrate
5 Hydroxytryptamine uptake stimulant
Oxytocic
Heme oxygenase stimulant
Carbon-monoxide dehydrogenase inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
Peroxisome proliferator-activated receptor gamma antagonist
Tyrosine-protein kinase TYRO 10 inhibitor
Prostaglandin-I synthase inhibitor
Hydroxysteroid dehydrogenase inhibitor
5-Alpha-reductase 2 inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
CYP2C9 inducer
Bile-salt sulfotransferase inhibitor
CYP2A2 substrate
Pectate lyase inhibitor
4-Hydroxymandelate oxidase inhibitor
Microbial collagenase inhibitor
CYP2C29 substrate
Transcription factor AP-1 inhibitor
Dihydrouracil oxidase inhibitor
Sphingosine 1-phosphate receptor 4 antagonist
Acylcarnitine hydrolase inhibitor

CC chemokine 9 receptor antagonist
CYP4B substrate
CYP2H substrate
Poly(3-hydroxybutyrate) depolymerase inhibitor
Pancreatic elastase inhibitor
ATPase stimulant
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Polo-like kinase-1 inhibitor
Potassium channel (Inward rectifier) 1 blocker
Arylacetonitrilase inhibitor
JAK2 expression inhibitor
Ca²⁺-transporting ATPase inhibitor
RELA expression inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
Protein synthesis stimulant
Heat shock protein 70 antagonist
Aldehyde dehydrogenase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Potassium channel (Inward rectifier) blocker
Prostaglandin E1 agonist
Histone acetyltransferase inhibitor
Antiulcerative
NMDA receptor glycine site agonist
N-formylmethionyl-peptidase inhibitor
UGT2B18 substrate
Kynurenine 3 monooxygenase inhibitor
Intermittent claudication treatment
CYP19 substrate
Inotropic
Hemostatic
Isopenicillin-N epimerase inhibitor
CYP2C18 substrate
Pyruvate dehydrogenase (lipoamide) inhibitor
SULT1A3 substrate
Thromboxane A2 antagonist
Antiprotozoal (Trichomonas)
Aspartate-phenylpyruvate transaminase inhibitor
UGT1A4 substrate
Hydrogen dehydrogenase inhibitor
D-stereospecific aminopeptidase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Cathepsin H inhibitor
Antiepileptic
Glucose 1-dehydrogenase inhibitor
Xylan 1,4-beta-xylosidase inhibitor
Inositol-3-phosphate synthase inhibitor
Progesterone receptor B1 antagonist
Chemosensitizer
UGT1A7 substrate
Antiprotozoal

Proliferative diseases treatment
 Alanine dehydrogenase inhibitor
 Signal peptidase I inhibitor
 Dihydroxy-acid dehydratase inhibitor
 Steroid DELTA-isomerase inhibitor
 Sporulation kinase A inhibitor
 Deacetoxycephalosporin-C synthase inhibitor
 Antineoplastic (insulinoma)
 CC chemokine 2 receptor antagonist
 Cholestanetriol 26-monooxygenase inhibitor
 Cyclooxygenase substrate
 Acetylgalactosaminy-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
 Glycerophosphocholine cholinephosphodiesterase inhibitor
 Thromboxane antagonist
 Antiviral (Adenovirus)
 Calcitonin stimulant
 Calcium channel blocker
 Porphobilinogen synthase inhibitor
 UGT2B substrate
 Neurotrophic factor enhancer
 Inorganic diphosphatase inhibitor
 Focal adhesion kinase 1 inhibitor
 UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
 3-Dehydroquinate dehydratase inhibitor
 Testosterone agonist
 Trimethylamine-oxide aldolase inhibitor
 UGT2B1 substrate
 Diacylglycerol O-acyltransferase 1 inhibitor
 Adenosine A1 receptor agonist enhancer
 Alkenylglycerophosphoethanolamine hydrolase inhibitor
 Prostaglandin F2 alpha agonist
 Glucan 1,4-alpha-maltotriohydrolase inhibitor
 Lipoxygenase substrate
 Nicotinic acid receptor 2 agonist
 NADPH oxidoreductase inhibitor
 Antisecretoric

Paclitaxel

Molecular Mechanism (initial) :

tubulin beta modulator (microtubule-stabilizing agent)

Molecular Mechanism (repurposed) :

tubulin beta modulator (microtubule-stabilizing agent)

initial indication(s):

cancers (breast, ovary, lung non-small cell, AIDS-related Kaposi's sarcoma, stomach, endometrium, angiosarcoma, cervix, head and neck, esophageal carcinoma, germ cells)

Repurposed indication(s):

restenosis

Predicted Activities

Respiratory analeptic

TP53 expression enhancer

Antineoplastic

Cytostatic

Analeptic

TNF expression inhibitor

Antineoplastic (colorectal cancer)

Antineoplastic (colon cancer)

CYP2C8 substrate

Antineoplastic (breast cancer)

CYP3A3 substrate

CYP3A4 inducer

CYP3A inducer

Tubulin antagonist

Antineoplastic (ovarian cancer)

CYP3A5 substrate

CYP3A substrate

Antimitotic

CYP2C substrate

Anticarcinogenic

CYP19A1 expression inhibitor

CYP3A4 substrate

Proliferative diseases treatment

Microtubule formation inhibitor

P-glycoprotein inhibitor

Antineoplastic (lung cancer)

Radiosensitizer

CYP1B substrate

CYP1B1 inhibitor

Antineoplastic (lymphoma)

P-glycoprotein substrate

Antineoplastic (carcinoma)

Cancer associated disorders treatment

Protein-arginine deiminase inhibitor

Prostate cancer treatment

Immunostimulant

Nootropic

CYP2H substrate

Antineoplastic (squamous cell carcinoma)

Antineoplastic (non-Hodgkin's lymphoma)

Antineoplastic (solid tumors)

Antineoplastic (pancreatic cancer)

Beta glucuronidase inhibitor

Antineoplastic (non-small cell lung cancer)

Phosphatase inhibitor

Chemosensitizer

Antineoplastic (thyroid cancer)

Antineoplastic (endocrine cancer)

Antineoplastic (bone cancer)

Antineoplastic (renal cancer)

CYP1B1 substrate

Gestagen antagonist
Antineoplastic (small cell lung cancer)
Alcohol dehydrogenase substrate
Antineoplastic (liver cancer)
Microtubule stabilization
Antiviral (Rhinovirus)
Antineoplastic (brain cancer)
Transactivator transcription protein inhibitor
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Antineoplastic (melanoma)
Antiemphysemic
Bilirubin oxidase inhibitor
Antineoplastic (glioblastoma multiforme)
Thromboxane synthase stimulant
Myc inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Antineoplastic (uterine cancer)
Antimetastatic
Antineoplastic (sarcoma)
Antimycoplasmal
Growth hormone agonist
CYP2A11 substrate
Levansucrase inhibitor
1,2-alpha-L-fucosidase inhibitor
Antineoplastic (gastric cancer)
CYP17 inhibitor
Antineoplastic (bladder cancer)
Aspartyltransferase inhibitor
Corticosteroid antagonist
Maleate isomerase inhibitor
Lipocortins synthesis antagonist
Antineoplastic (cervical cancer)
Antineoplastic (glioma)
Nitric oxide antagonist
Protein synthesis inhibitor
Protein kinase C stimulant
HIF1A expression inhibitor
Keratosis actinic (solar) treatment
Protein-synthesizing GTPase inhibitor
Cholestanone 5alpha-reductase inhibitor
Galactosylceramidase inhibitor
Protein kinase stimulant
Phospholipase A1 inhibitor
Cyclooxygenase 1 substrate
Antipsoriatic
Keratolytic
Steroid DELTA-isomerase inhibitor
Polyribonucleotide nucleotidyltransferase inhibitor
APOA1 expression enhancer

Alcohol O-acetyltransferase inhibitor
Testosterone agonist
Growth stimulant
HCV NS3/NS4A protease inhibitor
1,3-Beta-glucan synthase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
Retinol dehydrogenase inhibitor
UGT2B18 substrate
CYP2A10 substrate
Glutamate-5-semialdehyde dehydrogenase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Restenosis treatment
Nucleotidase inhibitor
Spasmolytic, urinary
Antineoplastic enhancer
Reductase inhibitor
Antieczematic
CYP2C8 inducer

Phentolamine mesilate

Molecular Mechanism (initial) :

alpha-adrenoceptor antagonist

Molecular Mechanism (repurposed) :

alpha-adrenoceptor antagonist

initial indication(s):

erectile dysfunction

Repurposed indication(s):

reversal of soft-tissue (dental) anesthesia

Predicted Activities

Octopamine antagonist
Male reproductive dysfunction treatment

Alpha 2b adrenoceptor antagonist

Erectile dysfunction treatment
Alpha 1L adrenoceptor agonist
Alpha 2c adrenoceptor antagonist
Rhinitis treatment
Alpha 2a adrenoceptor antagonist
Kidney function stimulant
Alpha 2 adrenoceptor antagonist
Imidazoline I1 receptor agonist
Antiadrenergic
Adrenaline antagonist
Alpha adrenoceptor antagonist
Insulin promoter
Spasmolytic
Calcium channel (voltage-sensitive) activator
Nav1.8 sodium channel blocker
Urologic disorders treatment
Antinociceptive

Cardiotonic
Female sexual dysfunction treatment
Urinary incontinence treatment
APOA1 expression enhancer
UGT1A9 substrate
Membrane permeability inhibitor
Nav1.2 sodium channel blocker
Alkane 1-monooxygenase inhibitor
Imidazoline receptor agonist
Vascular (periferal) disease treatment
Alpha 1 adrenoreceptor agonist
Platelet adhesion inhibitor
Alopecia treatment
Antiarrhythmic
Anthelmintic (Nematodes)
Aminobutyraldehyde dehydrogenase inhibitor
Nav1.3 sodium channel blocker
Fibrinolytic
Sodium channel blocker
MAP kinase stimulant
Opioid dependency treatment
UGT2B12 substrate
Nav1.1 sodium channel blocker
Erythropoiesis stimulant
Aspartate-phenylpyruvate transaminase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Renilla-luciferin 2-monooxygenase inhibitor
Mucomembranous protector
Alpha 1b adrenoreceptor antagonist
N-methylhydantoinase (ATP-hydrolysing) inhibitor
ATPase (Mitochondrial F1F0) inhibitor
FMO1 substrate
Glutathione thiolesterase inhibitor
Glutamyl endopeptidase II inhibitor
Alpha adrenoreceptor agonist
Sodium channel (voltage-gated) blocker
CF transmembrane conductance regulator agonist
Ubiquinol-cytochrome-c reductase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Omptin inhibitor
Trimethylamine-oxide aldolase inhibitor
Kinase inhibitor
Acetylcholine neuromuscular blocking agent
2-Dehydropantoate 2-reductase inhibitor
Mucositis treatment
Aspulinone dimethylallyltransferase inhibitor
Botulin neurotoxin A light chain inhibitor
Histamine agonist
Adrenergic

Centromere associated protein inhibitor
Ophthalmic drug
Adrenergic, ophthalmic
Reductant
CDK9/cyclin T1 inhibitor
Venombin AB inhibitor
Thioredoxin inhibitor
Heat shock protein 27 antagonist
Para amino benzoic acid antagonist
CYP2C12 substrate
Analeptic
Neurotransmitter antagonist
Nucleoside oxidase (H₂O₂-forming) inhibitor
Phosphatase inhibitor
Linoleate diol synthase inhibitor
Antiamyloidogenic
Thiamine pyridinylase inhibitor
ATP-binding cassette A1 stimulant
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Nicotinic alpha4beta4 receptor agonist
Dehydro-L-gulonate decarboxylase inhibitor
Fusarinine-C ornithinesterase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Myosin ATPase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Retinoic acid metabolism inhibitor
Antiseborrheic
CYP19A1 expression inhibitor
Alpha 1a adrenoreceptor agonist
Membrane integrity agonist
Analgesic
Tryptophan 2,3-dioxygenase inhibitor
Testosterone 17beta-dehydrogenase (NADP⁺) inhibitor
Cyclic AMP agonist
Taurine dehydrogenase inhibitor
Beta 3 adrenoreceptor antagonist
CYP2C29 substrate
Arylsulfate sulfotransferase inhibitor
Histidine kinase inhibitor
Insulysin inhibitor
CYP2J substrate
Pyruvate decarboxylase inhibitor
Antidyskinetic
Pancreatic elastase inhibitor
Anesthetic
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
MAP kinase kinase 4 inhibitor
Prion diseases treatment

Thromboxane B2 antagonist
HIF1A expression inhibitor
MMP9 expression inhibitor
5 Hydroxytryptamine 2B agonist
5 Hydroxytryptamine uptake stimulant
Glucose oxidase inhibitor
Preneoplastic conditions treatment
Fatty-acyl-CoA synthase inhibitor
Polarisation inhibitor
Vasodilator, peripheral
Cancer associated disorders treatment
Antineoplastic alkaloid
NADPH-cytochrome-c2 reductase inhibitor
Aldehyde oxidase inhibitor
Cardioprotectant
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
5 Hydroxytryptamine release inhibitor
N6-methyl-lysine oxidase inhibitor
CYP2D15 substrate
Polyporopepsin inhibitor
Steroid synthesis inhibitor
Pterin deaminase inhibitor
Antiglaucomic
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Anesthetic local
CYP2J2 substrate
Quercetin 2,3-dioxygenase inhibitor
Vanilloid 1 agonist
Endothelial growth factor antagonist
Acyl-CoA oxidase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Nicotinic alpha2beta2 receptor antagonist
Thymidylate 5'-phosphatase inhibitor
Antiprotozoal (Babesia)
FMO3 substrate
JAK2 expression inhibitor
UGT1A substrate
NADPH-ferrihemoprotein reductase inhibitor
Insulin secretagogues
Transcription factor NF kappa A inhibitor
Catalase stimulant
ATPase inhibitor
CYP2D16 substrate
Gastritis treatment
Beta 2 adrenoreceptor antagonist
Opioid kappa 3 receptor antagonist
Nicotine dehydrogenase inhibitor
Adrenaline agonist
Leukopoiesis stimulant
Radioprotector

Tyrosine 3 hydroxylase inhibitor
Ribonucleoside triphosphate reductase inhibitor
S-formylglutathione hydrolase inhibitor
Hyponitrite reductase inhibitor
NADPH peroxidase inhibitor
Phosphatidylserine decarboxylase inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
CXC chemokine receptor antagonist
Acid-sensing ion channel blocker
Arylsulfatase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
3-Phytase inhibitor
Apoptosis antagonist
Peroxidase substrate
CYP2A5 substrate
Keratosis actinic (solar) treatment
Antihypotensive
Plastoquinol-plastocyanin reductase inhibitor
5 Hydroxytryptamine 2A agonist
MO15-related protein kinase Pfmrk inhibitor
Caspase 3 stimulant
Indanol dehydrogenase inhibitor
Calcium channel activator
Anthranilate 3-monooxygenase (deaminating) inhibitor
SULT1A3 substrate
Neuropeptide Y4 antagonist
Bone diseases treatment
Beta adrenoreceptor antagonist
Loop diuretic
Oxygen scavenger
Tyrosine kinase stimulant
Chitosanase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Trimethylamine dehydrogenase inhibitor
CYP7 inhibitor
TP53 expression enhancer
CYP2C3 substrate
Nitrate reductase (cytochrome) inhibitor
Hydroxylamine oxidase inhibitor
Chlordecone reductase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Intermittent claudication treatment
Anesthetic general
Corticosteroid antagonist
RELA expression inhibitor
Vasoprotector
EIF4E expression inhibitor
Mandelate 4-monooxygenase inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Beta 1 adrenoreceptor antagonist

CYP2C8 inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Lipid peroxidase inhibitor
Benzoate 4-monooxygenase inhibitor
Dihydroxy-acid dehydratase inhibitor
GABA aminotransferase inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Tetrahydroxynaphthalene reductase inhibitor
CYP3A3 substrate
Antirickettsial
Venom exonuclease inhibitor
Alpha 2 adrenoreceptor agonist
2-Hydroxyquinoline 8-monooxygenase inhibitor
SULT1E1 substrate
CDP-glycerol glycerophosphotransferase inhibitor
Antiparkinsonian, rigidity relieving
Flavin-containing monooxygenase substrate
HCV IRES inhibitor
Histidinol-phosphatase inhibitor
Prunasin beta-glucosidase inhibitor
Octopamine agonist
Dementia treatment
Threonine aldolase inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Narcotic antagonist
Ribulose-phosphate 3-epimerase inhibitor
1,4-Lactonase inhibitor
Amine dehydrogenase inhibitor
Phloroglucinol reductase inhibitor
Orotate reductase (NADPH) inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
HMGCS2 expression enhancer
Rubredoxin-NAD⁺ reductase inhibitor
4,5-Dihydroxyphthalate decarboxylase inhibitor
Formate-dihydrofolate ligase inhibitor
Aldehyde dehydrogenase 2 substrate
CYP2G1 substrate
CYP1A1 inhibitor
Antidiarrheal
Alpha 1d adrenoreceptor antagonist
D-amino-acid dehydrogenase inhibitor
Antiinfective
Manganese peroxidase inhibitor
CYP4A11 substrate
SMN2 expression enhancer
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Glyoxylate reductase inhibitor
4-Hydroxybenzoate-CoA ligase inhibitor
Pseudolysin inhibitor

Muscular dystrophy treatment
Glycine receptor antagonist
Urticaria treatment
Diamine oxidase inhibitor
MAP kinase kinase 7 inhibitor
Hydroxymethylbilane synthase inhibitor
Prolyl aminopeptidase inhibitor
Gastrointestinal motility stimulant
N-benzyloxycarbonylglycine hydrolase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
UDP-glucuronosyltransferase substrate
2-Nitrophenol 2-monooxygenase inhibitor
Limulus clotting factor B inhibitor
CYP3A7 substrate
NOS2 expression inhibitor
Glutaminyl-peptide cyclotransferase inhibitor
GABA C receptor agonist
SULT1A2 substrate
Alkene monooxygenase inhibitor
CYP2F1 substrate
Pyridoxine 5-dehydrogenase inhibitor
Antiprotozoal (Amoeba)
Cyclic AMP modulator
Gonadotropin antagonist
Proto-oncogene tyrosine-protein kinase Fgr inhibitor
NAT2 substrate
Spermidine dehydrogenase inhibitor
Antihemorrhagic
Malate dehydrogenase (acceptor) inhibitor
Quinoprotein glucose dehydrogenase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Creatine kinase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
CYP2B11 substrate
General pump inhibitor
Uroporphyrinogen-III synthase inhibitor
Imidazoline II receptor antagonist
Viral entry inhibitor
Chloride channel blocker
Antiinflammatory, intestinal
Leukopoiesis inhibitor
Apyrase inhibitor
CYP2A3 substrate
Gentisate 1,2-dioxygenase inhibitor
Nitric oxide scavenger
SULT1A1 substrate
Alpha 1a adrenoreceptor antagonist
Alpha 1 adrenoreceptor antagonist
Vomilenine glucosyltransferase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor

CYP3A2 substrate
Platelet derived growth factor receptor kinase inhibitor
Transcription factor STAT6 inhibitor
Cardiovascular analeptic
Glucan endo-1,6-beta-glucosidase inhibitor
Glycerol dehydrogenase (NADP+) inhibitor
Dihydroxyacetanilide dehydrogenase inhibitor
Dihydroxyacetanilide epoxidase inhibitor
Tropinesterase inhibitor
Phenylalanine decarboxylase inhibitor
Chloride peroxidase inhibitor
Antihypoxic
H⁺-exporting ATPase inhibitor
Nicotinate dehydrogenase inhibitor
Lysase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Oxytocic
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
6-Methylsalicylate decarboxylase inhibitor
Sulfite reductase inhibitor
Cytochrome-b5 reductase substrate
Linoleoyl-CoA desaturase inhibitor
Peroxidase inhibitor
Antioxidant
Antihelminthic (Fasciola)
Laccase inhibitor
5 Hydroxytryptamine 7S antagonist
Ferredoxin hydrogenase inhibitor
Phenylpyruvate decarboxylase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Imidazoline receptor antagonist
4-Coumarate-CoA ligase inhibitor
Tyrosine phenol-lyase inhibitor
Phospholipid-translocating ATPase inhibitor
Antidote
Malate oxidase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
CYP1B substrate
Arylesterase inhibitor
4-Hydroxyproline epimerase inhibitor
CYP26A substrate
Laxative
Vascular dementia treatment
Vanillyl-alcohol oxidase inhibitor
RNA synthesis inhibitor
ATP phosphoribosyltransferase inhibitor
Catenin beta inhibitor
CYP2D substrate
Dopamine release stimulant

Endopeptidase So inhibitor
Chemokine receptor antagonist
Alpha 3 adrenoreceptor agonist
Retinoprotector
Antisecretoric
Alpha 2c adrenoreceptor agonist
Alpha 2d adrenoreceptor agonist
Dactylisin inhibitor
Antiperistaltic
Dihydropteroate synthase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Antiprotozoal (Trypanosoma)
Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
Guanidinoacetase inhibitor
Acetylcholine nicotinic antagonist
Bacterial efflux pump inhibitor
Imidazoline I2 receptor antagonist
Hippurate hydrolase inhibitor
Inotropic
Alpha 2d adrenoreceptor antagonist
Antiparkinsonian
O-aminophenol oxidase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
L-ascorbate peroxidase inhibitor
4-Hydroxymandelate oxidase inhibitor
Orcinol 2-monooxygenase inhibitor
HMOX1 expression enhancer
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Antiischemic
Nitrite reductase [NAD(P)H] inhibitor
CXC chemokine 4 receptor antagonist
Mitochondrial processing peptidase inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Anthranilate phosphoribosyltransferase inhibitor
Oxytocin agonist
Cyclic GMP phosphodiesterase inhibitor
Mucinaminyserine mucinaminidase inhibitor
CYP2D6 substrate
Azobenzene reductase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
CYP1A1 inducer
UGT1A6 substrate
Purinergic P2X2 antagonist
Antianorexic
CYP2B2 substrate
Necroptosis inhibitor
Nitric-oxide synthase stimulant
Feruloyl esterase inhibitor

Procollagen-lysine 5-dioxygenase inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Tyrosine 2,3-aminomutase inhibitor
Transforming growth factor beta 1 agonist
Indoleacetaldoxime dehydratase inhibitor
Thiol oxidase inhibitor
NMDA 2 receptor antagonist
Glycerol-3-phosphate oxidase inhibitor
Lactase inhibitor
Alpha 2b adrenoreceptor agonist
Penicillin amidase inhibitor
Serum-glucocorticoid regulated kinase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Nav1.5 sodium channel blocker
Urethanase inhibitor
Attention deficit/hyperactivity disorder treatment
Fructose 5-dehydrogenase inhibitor
Ferrochelataze inhibitor
Beta glucuronidase inhibitor
Histamine release stimulant
NMDA receptor polyamine site antagonist
Acidifying agent non gastric
Adenine nucleotide translocase inhibitor
Choline sulfotransferase inhibitor
Aralkylamine dehydrogenase inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
CC chemokine receptor 2B antagonist
Prostaglandin-A1 DELTA-isomerase inhibitor
Interleukin 12 agonist
Prephenate dehydrogenase inhibitor
Paraoxonase substrate
Nucleotide metabolism regulator
Chenodeoxycholytaurine hydrolase inhibitor
GST M substrate
Gluconate 2-dehydrogenase (acceptor) inhibitor
DELTA24-sterol reductase inhibitor
CYP1A inducer
Tryptophan dimethylallyltransferase inhibitor
Age-related macular degeneration treatment
Pim-3 kinase inhibitor
Antifibrinolytic
Sulfite oxidase inhibitor

Raloxifene hydrochloride

Molecular Mechanism (initial) :

estrogen receptor agonist

Molecular Mechanism (repurposed) :

estrogen receptor agonist

initial indication(s):

erectile dysfunction

Repurposed indication(s):

reversal of soft-tissue (dental) anesthesia

Predicted Activities

Aldehyde oxidase inhibitor

Fibrinolytic

Estrogen antagonist

MMP9 expression inhibitor

Estrogen receptor beta antagonist

Antiosteoporotic

Bone diseases treatment

TNF expression inhibitor

Postmenopausal disorders treatment

AR expression inhibitor

Anaphylatoxin receptor antagonist

Neurotransmitter uptake inhibitor

Antineoplastic (breast cancer)

CYP19 inhibitor

Lipid metabolism regulator

Restenosis treatment

Antineoplastic (uterine cancer)

Inotropic

Nicotinic alpha4beta4 receptor agonist

Spasmolytic, urinary

Calcium channel (voltage-sensitive) activator

Vasodilator, coronary

Histamine release stimulant

Hypolipemic

CYP2D6 substrate

Estrogen agonist

CYP2D substrate

Aspulvinone dimethylallyltransferase inhibitor

Gonadotropin antagonist

APOA1 expression enhancer

Acetylcholine neuromuscular blocking agent

LDLR expression enhancer

p21-activated kinase 1 inhibitor

Estrogen alpha receptor agonist

CYP2C substrate

Lipoprotein disorders treatment

MAP kinase stimulant

CYP2C19 inhibitor

p21-activated kinase inhibitor

Spasmolytic

Calcium channel activator

Caspase 8 stimulant

Spasmolytic, Papaverin-like

Gynecological disorders treatment

CYP2C9 substrate

Antineurogenic pain

Antineurotic
Antihelminthic (Nematodes)
Proliferative diseases treatment
Antitussive
Estrogen beta receptor agonist
Neurotransmitter antagonist
CYP2C19 substrate
Antineoplastic enhancer
Vascular (periferal) disease treatment
Antihypoxic
Lipid peroxidase inhibitor
HIF1A expression inhibitor
FMO3 substrate
Capillary fragility treatment
Cyclic AMP phosphodiesterase inhibitor
p21-activated kinase 4 inhibitor
Thromboxane B2 antagonist
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Cancer associated disorders treatment
Antipyretic
Viral entry inhibitor
Phosphatase inhibitor
Antihyperlipoproteinemic
Antianginal
Heat shock protein 27 antagonist
Platelet aggregation stimulant
UGT2B12 substrate
CYP2D6 inhibitor
Antieczematic
Catenin beta inhibitor
Chlordecone reductase inhibitor
ATPase inhibitor
Opioid kappa 3 receptor antagonist
Antiischemic, cerebral
Caspase 3 stimulant
Estradiol 17 beta dehydrogenase 2 inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
HDL-cholesterol increasing
Prostate disorders treatment
Dopamine D1A antagonist
Antitoxic
Endometriosis treatment
5 Hydroxytryptamine 7S antagonist
Peptidoglycan glycosyltransferase inhibitor
Transforming growth factor beta 1 agonist
Contraceptive female
Antihistaminic
5 Hydroxytryptamine 7L antagonist
P-glycoprotein 1 inhibitor

Anesthetic
Antischistosomal
Histamine H1 receptor antagonist
Sigma 1 receptor agonist
Phospholipase D inhibitor
Amyotrophic lateral sclerosis treatment
Antiparkinsonian, tremor relieving
Antisecretoric
Antineoplastic
Squalene-hopene cyclase inhibitor
Estradiol 17 beta dehydrogenase inhibitor
CYP1A2 inhibitor
Adrenaline release stimulant
Vasoprotector
Muramoyltetrapeptide carboxypeptidase inhibitor
Neuropeptide Y4 antagonist
Psychosexual dysfunction treatment
Antidiarrheal
Radioprotector
Protein-disulfide reductase (glutathione) inhibitor
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Cytochrome P450 inhibitor
CYP1A inhibitor
Histamine antagonist
5 Hydroxytryptamine 1E antagonist
Dual specificity phosphatase 1 inhibitor
Phospholipase D1 inhibitor
Lactase inhibitor
GABA transporter 2 inhibitor
Monoamine uptake inhibitor
CYP2C8 substrate
MAP kinase kinase 4 inhibitor
Gout treatment
Vanilloid agonist
Flavin-containing monooxygenase substrate
Glycine receptor agonist
DELTA14-sterol reductase inhibitor
CYP3A4 substrate
CF transmembrane conductance regulator agonist
Antiinflammatory
Antihemorrhagic
Interleukin 1 antagonist
Glycosylphosphatidylinositol phospholipase D inhibitor
Antimetastatic
CYP2D1 substrate
GABA transporter 3 inhibitor
Bone formation stimulant
Phospholipase inhibitor
CYP2E1 inhibitor
Apyrase inhibitor

Ribulose-phosphate 3-epimerase inhibitor
CYP2C18 substrate
Glyceryl-ether monooxygenase inhibitor
CYP2D15 substrate
Interleukin 2 agonist
Undecaprenyl-phosphate mannosyltransferase inhibitor
Cardiotonic
1,4-Lactonase inhibitor
CYP2A4 substrate
N-methyl-2-oxoglutaramate hydrolase inhibitor
Antinaupathic
5 Hydroxytryptamine 4C antagonist
5 Hydroxytryptamine 4D antagonist
Lipoprotein lipase stimulant
CYP2C12 substrate
Membrane integrity agonist
N-hydroxyarylamine O-acetyltransferase inhibitor
Histidine kinase inhibitor
Uric acid excretion stimulant
Ca²⁺/calmodulin-dependent kinase I inhibitor
Nitrite reductase (NO-forming) inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
Cardiovascular analeptic
Antipruritic
P-glycoprotein inhibitor
Menopausal disorders treatment
Peptide alpha-N-acetyltransferase inhibitor
Protein kinase C beta inhibitor
Antineoplastic (lymphoma)
Contraceptive
Complement factor D inhibitor
Antiseborrheic
Non-steroidal antiinflammatory agent
CYP2D2 inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Tubulin antagonist
Antidiabetic
3-Phytase inhibitor
Keratolytic
Cholestenol delta-isomerase inhibitor
Prion diseases treatment
2,3-Oxidosqualene-lanosterol cyclase inhibitor
Interleukin antagonist
Long-chain-aldehyde dehydrogenase inhibitor
Cyclic AMP modulator
Respiratory analeptic
Antiperistaltic
Alopecia treatment
Sepsis treatment
Beta glucuronidase inhibitor

Histamine H2 receptor antagonist
Acute neurologic disorders treatment
Chloride channel blocker
Interleukin 10 antagonist
Chemosensitizer
Antidote
Linoleoyl-CoA desaturase inhibitor
Anticarcinogenic
Cardioprotectant
Antineoplastic (sarcoma)
Leukotriene A4 hydrolase inhibitor
2-Enoate reductase inhibitor
Retinoic acid metabolism inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
Acetylcholinesterase inhibitor
Dolichol kinase inhibitor
Gestagen antagonist
Protein kinase C ϵ inhibitor
CYP1A2 substrate
Histamine N-methyltransferase inhibitor
Glucan endo-1,6- β -glucosidase inhibitor
Vanilloid 1 agonist
Antitussive, narcotic
Steroid N-acetylglucosaminyltransferase inhibitor
CYP2C10 substrate
3(or 17) β -hydroxysteroid dehydrogenase inhibitor
4-Hydroxyphenylpyruvate dioxygenase inhibitor
Protein kinase C ϵ inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Paraoxonase substrate
Nicotinic $\alpha 6\beta 3\beta 4\alpha 5$ receptor antagonist
Insulin sensitizer
Ubiquinol-cytochrome-c reductase inhibitor
HCV NS3-helicase inhibitor
GABA uptake inhibitor
Antineoplastic (solid tumors)
Antihypertriglyceridemic
Histone acetyltransferase inhibitor
Antiinfertility, female
Glycogen synthase stimulant
Phospholipase D2 inhibitor
Clavamate synthase inhibitor
Antihematotoxic
NADPH-ferrihemoprotein reductase inhibitor
Nav1.3 sodium channel blocker
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Dual specificity protein phosphatase VHR inhibitor
4-Coumarate-CoA ligase inhibitor
Polarisation inhibitor

AXL receptor tyrosine kinase inhibitor
 Plasminogen activator inhibitor antagonist
 Protein kinase C gamma inhibitor
 CDK9/cyclin T1 inhibitor
 Anti-Helicobacter pylori
 Peroxisome proliferator-activated receptor antagonist
 17-Beta-hydroxysteroid dehydrogenase 1 inhibitor
 Sphinganine kinase inhibitor
 Botulin neurotoxin A light chain inhibitor
 Antiarrhythmic
 SULT1E1 substrate
 Protein kinase C delta inhibitor
 Multidrug resistance-associated protein inhibitor
 Antidiabetic (type 2)
 Antidepressant, Imipramine-like
 Kinase inhibitor
 CYP3A substrate
 Corticosteroid antagonist
 Multidrug resistance-associated protein 1 inhibitor
 Peroxisome proliferator-activated receptor gamma agonist
 Narcotic antagonist
 Antimutagenic
 Peroxisome proliferator-activated receptor gamma antagonist
 Protein kinase C beta I inhibitor
 VCAM1 expression inhibitor
 GABA transporter inhibitor
 Sigma receptor agonist
 Peroxisome proliferator-activated receptor agonist
 NADPH-cytochrome-c2 reductase inhibitor

Ropinirole

Molecular Mechanism (initial) :

dopamine D2 and D3 receptor agonist

Molecular Mechanism (repurposed) :

dopamine D2 and D3 receptor agonist

initial indication(s):

Parkinson's disease

Repurposed indication(s):

restless legs syndrome

Predicted Activities

Anticonvulsant
 5 Hydroxytryptamine release stimulant
 Antihypoxic
 Taurine dehydrogenase inhibitor
 Muscle relaxant
 Gluconate 2-dehydrogenase (acceptor) inhibitor
 Antiischemic, cerebral
 Proteasome ATPase inhibitor
 CYP2C12 substrate

HERG 1 channel blocker
CYP1A2 substrate
CYP3A4 substrate
Neurotransmitter uptake inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Aryl-acylamidase inhibitor
CYP3A substrate
Phenol O-methyltransferase inhibitor
Acute neurologic disorders treatment
Antisecretoric
Fibrinolytic
Polyamine-transporting ATPase inhibitor
Pseudolysin inhibitor
CYP1A substrate
Thioredoxin inhibitor
Fusarinine-C ornithinesterase inhibitor
Platelet aggregation stimulant
Ovulation inhibitor
CYP2C19 substrate
Cyclic AMP phosphodiesterase inhibitor
Vasodilator
Fibrinogen receptor antagonist
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Antianginal
Electron-transferring-flavoprotein dehydrogenase inhibitor
Mitochondrial processing peptidase inhibitor
Sulfur reductase inhibitor
Lysase inhibitor
Spermidine dehydrogenase inhibitor
CYP2J substrate
Kidney function stimulant
Antidyskinetic
Trimethylamine dehydrogenase inhibitor
CYP2C18 substrate
CYP2J2 substrate
Trimethylamine-oxide aldolase inhibitor
Macrophage colony stimulating factor agonist
Endopeptidase So inhibitor
Cytoprotectant
Phobic disorders treatment
Oxidoreductase inhibitor
Amine dehydrogenase inhibitor
Skeletal muscle relaxant
Nicotinic alpha2beta2 receptor antagonist
Dimethylargininase inhibitor
Calcium channel (voltage-sensitive) activator
CYP2C8 inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Analeptic
Vasodilator, peripheral

Cyclic AMP agonist
Carboxypeptidase Taq inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Sodium channel blocker class Ib
Cardiotonic
Gluconate 5-dehydrogenase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
2-Haloacid dehalogenase inhibitor
CYP1A2 inhibitor
CYP2C substrate
CYP2C9 substrate
Ribulose-phosphate 3-epimerase inhibitor
N-formylmethionyl-peptidase inhibitor
Pterin deaminase inhibitor

Antiparkinsonian, tremor relieving

CYP1A inhibitor
CYP2D6 substrate
All-trans-retinyl-palmitate hydrolase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
CYP2C8 substrate
CYP2D substrate
1,4-Lactonase inhibitor
Spasmolytic, urinary
Cyclic AMP modulator
Pyroglutamyl-peptidase II inhibitor
4-Hydroxyproline epimerase inhibitor
Glyceryl-ether monooxygenase inhibitor
RNA-directed RNA polymerase inhibitor
CYP2C19 inducer
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Adrenaline release stimulant
FMO3 substrate
Vasodilator, coronary
Protein-disulfide reductase (glutathione) inhibitor
Fucosterol-epoxide lyase inhibitor
5 Hydroxytryptamine uptake stimulant
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Anesthetic general
NADPH-cytochrome-c2 reductase inhibitor
Flavin-containing monooxygenase substrate
Benzoate-CoA ligase inhibitor
Pullulanase inhibitor
Lysine 2,3-aminomutase inhibitor
CYP3A3 substrate
Octopamine antagonist
Platelet adhesion inhibitor
Superoxide dismutase inhibitor

Antiparkinsonian, rigidity relieving
Fructose 5-dehydrogenase inhibitor
Exoribonuclease II inhibitor
Sphinganine kinase inhibitor
Apyrase inhibitor
Platelet derived growth factor receptor kinase inhibitor
Nicotinate dehydrogenase inhibitor
Amyotrophic lateral sclerosis treatment
Ompin inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Venombin AB inhibitor
Respiratory analeptic
Antiprotozoal (Leishmania)
Aminobutyraldehyde dehydrogenase inhibitor
Polarisation inhibitor
Poly(alpha-L-guluronate) lyase inhibitor
Gastrin inhibitor
Xylan endo-1,3-beta-xylosidase inhibitor
Leukopoiesis stimulant
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Alkylacetylgllycerophosphatase inhibitor
CYP2D16 substrate
Cardiovascular analeptic
Inotropic
Mucomembranous protector
Fibrolase inhibitor
Tyrosine 3 hydroxylase inhibitor
Mucositis treatment
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Antiviral (Picornavirus)
Spasmolytic
Cancer associated disorders treatment
CYP2B6 substrate
Acetylcholinesterase inhibitor
Stroke treatment
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Oxytocic
Polyporopepsin inhibitor
Limulus clotting factor B inhibitor
Monoamine uptake inhibitor
D-lactaldehyde dehydrogenase inhibitor
Prolactin inhibitor
Cl--transporting ATPase inhibitor
Glycolate dehydrogenase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Antiarrhythmic
Formaldehyde transketolase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor

Oxygen scavenger
CYP3A5 substrate
Glutarate-semialdehyde dehydrogenase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
Membrane integrity agonist
5 Hydroxytryptamine 1F antagonist
ADP-thymidine kinase inhibitor
5 Hydroxytryptamine 7L antagonist
Systemic lupus erythematosus treatment
Myc inhibitor
Antimigraine
Ornithine cyclodeaminase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
5 Hydroxytryptamine 7S antagonist
Nav1.5 sodium channel blocker
Thymidylate 5'-phosphatase inhibitor
Botulin neurotoxin A light chain inhibitor
Tankyrase inhibitor
Creatininase inhibitor
Preneoplastic conditions treatment
Thromboxane B2 antagonist
GABA aminotransferase inhibitor
Chloride peroxidase inhibitor
Malate dehydrogenase (acceptor) inhibitor
CYP2C9 inducer
Intermittent claudication treatment
Glutamate receptor antagonist
CYP3A1 substrate
Antineurotic
Choline-phosphate cytidyltransferase inhibitor
Glutamyl endopeptidase II inhibitor
Lipocortins synthesis antagonist
Pin1 inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Limulus clotting factor C inhibitor
Antineoplastic alkaloid
Erythropoiesis stimulant
Chloride channel activator
Glycine amidinotransferase inhibitor
Antineoplastic (non-Hodgkin's lymphoma)
Spasmolytic, Papaverin-like
Benzaldehyde dehydrogenase (NADP+) inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Nitrite reductase (NO-forming) inhibitor
Antiparkinsonian
CYP2D1 substrate
CYP4A11 substrate
Long-chain-aldehyde dehydrogenase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor

Diamine N-acetyltransferase inhibitor
3-Phytase inhibitor
Phospholipid-translocating ATPase inhibitor
NMDA receptor antagonist
Sulfite dehydrogenase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Mandelate 4-monooxygenase inhibitor
Dimethylmaleate hydratase inhibitor
Hydroxylamine oxidase inhibitor
Antiischemic
Alcohol dehydrogenase [NAD(P)+] inhibitor
Interleukin 2 agonist
Antihypertensive
Apoptosis antagonist
N-hydroxy-2-acetamidofluorene reductase inhibitor
Tryptophan alpha,beta-oxidase inhibitor
Tryptophan dimethylallyltransferase inhibitor
Gonadotropin antagonist
Antineurogenic pain
Chitinase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
CYP2B10 substrate
Uterine stimulant
Dolichyl-phosphate beta-glucosyltransferase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Thiosulfate dehydrogenase inhibitor
Tryptophan 2-monooxygenase inhibitor
Methanol dehydrogenase inhibitor
Cyclomaltodextrinase inhibitor
Glycine receptor antagonist
Sugar-phosphatase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Fatty-acyl-CoA synthase inhibitor
Bipolar disorder treatment
Maleate isomerase inhibitor
Antiepileptic
FMO1 substrate
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Chenodeoxycholytaurine hydrolase inhibitor
Mediator release inhibitor
Antiamyloidogenic
Fragilysin inhibitor
Polyamine oxidase inhibitor
CYP17 inhibitor
Peptidyl-dipeptidase Dcp inhibitor
1,2-alpha-L-fucosidase inhibitor
Urethanase inhibitor
Acrocylindropepsin inhibitor

Chymosin inhibitor
Saccharopepsin inhibitor
5 Hydroxytryptamine release inhibitor
5 Hydroxytryptamine 1B antagonist
5 Hydroxytryptamine 2B agonist
CYP7 inhibitor
Prenyl-diphosphatase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Aspartate-ammonia ligase inhibitor
Nootropic
Flavin-containing monooxygenase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Yeast ribonuclease inhibitor
Aspergillus nuclease S1 inhibitor
Proto-oncogene tyrosine-protein kinase Yes inhibitor
Oryzin inhibitor
Ecdysone 20-monooxygenase inhibitor
Arylmalonate decarboxylase inhibitor
Kinase inhibitor
Phosphatidylglycerophosphatase inhibitor
TRPA1 agonist
4-Hydroxymandelate oxidase inhibitor
Peptidoglycan glycosyltransferase inhibitor
CYP2C11 substrate
Plastoquinol-plastocyanin reductase inhibitor
Retinal dehydrogenase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Tyrosine kinase stimulant
Leukotriene-C4 synthase inhibitor
3-Cyanoalanine hydratase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Lysyl oxidase inhibitor
5 Hydroxytryptamine 1D antagonist
Cyclohexyl-isocyanide hydratase inhibitor
tRNA nucleotidyltransferase inhibitor
Beta 3 adrenoreceptor antagonist
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Malate oxidase inhibitor
P-glycoprotein 1 inhibitor
CYP3A2 substrate
Opine dehydrogenase inhibitor
Membrane integrity antagonist
Liver X receptor antagonist
MAP kinase stimulant
HMGCS2 expression enhancer
4-Nitrophenol 2-monooxygenase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
5 Hydroxytryptamine 5 antagonist
Kainate receptor 2 antagonist

Na⁺-transporting two-sector ATPase inhibitor
Putrescine oxidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Neurotransmitter antagonist
Aldehyde dehydrogenase 2 substrate
Coccolysin inhibitor
Histamine release stimulant
Glutathione thiolesterase inhibitor
Calcium antagonist
Hematopoietic inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Ferrochelataase inhibitor
MAO A substrate
Gluconolactonase inhibitor
Nicotine dehydrogenase inhibitor
Gingipain K inhibitor
Acylcarnitine hydrolase inhibitor
5 Hydroxytryptamine 1E antagonist
CYP2E1 substrate
RET inhibitor
Antiulcerative
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Cytochrome P450 stimulant
Glutamate 5-kinase inhibitor
Aspergillopepsin I inhibitor
Diuretic inhibitor
Nitrite reductase [NAD(P)H] inhibitor
L-glutamate oxidase inhibitor
CYP2D6 inhibitor
DELTA14-sterol reductase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
Muramoyltetrapeptide carboxypeptidase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Dipeptidase E inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Transketolase inhibitor
Cycloartenol synthase inhibitor
Raynaud's phenomenon treatment
APOA1 expression enhancer
Acidifying agent non gastric
Dry eye syndrome treatment
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Ethanolamine oxidase inhibitor
CYP2E substrate
Nitrate reductase (cytochrome) inhibitor
Follicle-stimulating hormone agonist

CYP2F1 substrate
Allyl-alcohol dehydrogenase inhibitor
Beta-cyclopiazonate dehydrogenase inhibitor
Sigma receptor agonist
Antieczematic
CYP2A8 substrate
Arginine 2-monooxygenase inhibitor
Prion diseases treatment
Alpha 2b adrenoreceptor antagonist
Pappalysin-1 inhibitor
Nardilysin inhibitor
Antidepressant, Imipramin-like
CYP2C29 substrate
CYP4A2 substrate
2-Aminohexano-6-lactam racemase inhibitor
Pectin lyase inhibitor

Dopamine D2S antagonist

Ethanolamine-phosphate cytidyltransferase inhibitor
Pyroglutamyl-peptidase I inhibitor
Antineoplastic (multiple myeloma)
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Quisqualate antagonist
Cytochrome-c3 hydrogenase inhibitor
5 Hydroxytryptamine 7 agonist
Dihydroorotase inhibitor
Histidinol dehydrogenase inhibitor
5 Hydroxytryptamine 5A antagonist
Smooth muscle myosin light chain kinase inhibitor
Adenylyl-sulfate reductase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
5 Hydroxytryptamine 2A agonist
Age-related macular degeneration treatment
Gamma-glutamyltransferase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
N-acetylneuraminase synthase inhibitor
Gallate decarboxylase inhibitor
Atrolysin A inhibitor
Cyclohexanone monooxygenase inhibitor
Calcium channel blocker
Antinaupathic
Antiviral (Poxvirus)
Tryptophanamidase inhibitor
Hydrogen dehydrogenase inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Pitrilysin inhibitor
CYP2A1 substrate
Alpha-glucuronidase inhibitor
Acetylspermidine deacetylase inhibitor

6-Pyruvoyltetrahydropterin synthase inhibitor
Pim-3 kinase inhibitor
Acetylcholine muscarinic antagonist
ATP-binding cassette A1 stimulant
Cachexia treatment
Uroporphyrinogen-III synthase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Gingipain R inhibitor
Cyanoalanine nitrilase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Sulfite reductase inhibitor
Glucuronolactone reductase inhibitor
Antinephritic
Aspartoacylase inhibitor
S-formylglutathione hydrolase inhibitor
Acetylcholine M4 receptor antagonist
CYP2A6 substrate
Shab potassium channel blocker
Nitric-oxide synthase stimulant
N-acetyllactosamine synthase inhibitor
Vascular (periferal) disease treatment
Alkylglycerone-phosphate synthase inhibitor
Insulin promoter
Photosensitizer
Leishmanolysin inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Acetylcholine M3 receptor antagonist
Male reproductive disfunction treatment
Anesthetic
Acetylserotonin O-methyltransferase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Antitussive, narcotic
Oxidizing agent
X-methyl-His dipeptidase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Inulinase inhibitor
Cathepsin T inhibitor
Sigma 1 receptor agonist
Mitochondrial intermediate peptidase inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Aldehyde oxidase inhibitor
Dactylisin inhibitor
Bontoxilysin inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Cyclooxygenase substrate
Arylesterase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Sepiapterin reductase inhibitor
AMPA 4 receptor antagonist
Antinociceptive

Leukopoiesis inhibitor
Tentoxilysin inhibitor
Plasmanyethanolamine desaturase inhibitor
Endothelial growth factor antagonist
Creatinase inhibitor
NADH kinase inhibitor
Glycogen synthase kinase-3 inhibitor
Thiamine-triphosphatase inhibitor
Prolyl aminopeptidase inhibitor
Antiseborrheic
Sodium channel blocker
Serine-pyruvate transaminase inhibitor
H⁺-transporting two-sector ATPase inhibitor
NOS2 expression inhibitor
Dihydropyrimidinase inhibitor
Orotate reductase (NADH) inhibitor
Simian immunodeficiency virus proteinase inhibitor
Cyclin-dependent kinase 1 inhibitor
Antileprosy
Trans-pentaprenyltranstransferase inhibitor
Oxytocin agonist
Monoamine oxidase substrate
Atrolysin C inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
CYP2A2 substrate
5 Hydroxytryptamine antagonist
IgA-specific serine endopeptidase inhibitor
Alpha 2a adrenoreceptor antagonist
Calcium channel activator
5 Hydroxytryptamine 7 antagonist
Cholinergic antagonist
Nuclease inhibitor
Antihypotensive
Urease inhibitor
Anesthetic local
Carnosine synthase inhibitor
Glycogen synthase kinase-3 beta inhibitor
Lysostaphin inhibitor
CYP2C3 substrate
P-glycoprotein substrate
Phenylalanine decarboxylase inhibitor
Pancreatic elastase inhibitor
Diisopropyl-fluorophosphatase inhibitor
Neurodegenerative diseases treatment
Gamma-butyrobetaine dioxygenase inhibitor
Procollagen C-endopeptidase inhibitor
Huntington's disease treatment
Nucleoside-diphosphatase inhibitor
Antidote
Diaminopropionate ammonia-lyase inhibitor

Imidazoline receptor agonist
Steroid synthesis inhibitor
Acetylcholine antagonist
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Kainate receptor 4 antagonist
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
5 Hydroxytryptamine 1 agonist
Sodium/calcium exchanger 1 inhibitor
Galactolipase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Antihematotoxic
Alpha 2c adrenoreceptor antagonist
Adenylate cyclase stimulant
Cyclin-dependent kinase 5 inhibitor
CYP4A substrate
Pro-opiomelanocortin converting enzyme inhibitor
Dolichol kinase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
Phosphoenolpyruvate mutase inhibitor
CYP2D15 substrate
Aspulvinone dimethylallyltransferase inhibitor
Nav1.8 sodium channel blocker
O-aminophenol oxidase inhibitor
Hematopoietic
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
AMPA receptor antagonist
CNS active muscle relaxant
DNA methyltransferase I inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Mucinaminyserine mucinaminidase inhibitor
Urticaria treatment
CYP1A2 inducer
Guanylate cyclase 1 stimulant
Histidine N-acetyltransferase inhibitor
Sulfur dioxygenase inhibitor
Ca²⁺/calmodulin-dependent protein kinase inhibitor
N-acylmannosamine kinase inhibitor
Iron antagonist
Autophagy inducer
Deacetoxycephalosporin-C synthase inhibitor
Antimyopathies
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Camphor 1,2-monooxygenase inhibitor
Acetylcholine M2 receptor antagonist
Antifibrinolytic
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Kainate receptor antagonist
L-threonine 3-dehydrogenase inhibitor

Sigma receptor antagonist
5 Hydroxytryptamine 1 antagonist
Calcium regulator
Kainate receptor 5 antagonist
Chaperonin ATPase inhibitor
Glycogen synthase kinase-3 alpha inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
5 Hydroxytryptamine 1A antagonist
Homospermidine synthase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Sarcosine oxidase inhibitor
Narcotic antagonist
Formyltetrahydrofolate dehydrogenase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
CYP2B substrate
Cerebrovascular disorders treatment
AMPA 2 receptor antagonist
Hydroxylamine reductase inhibitor
Nav1.3 sodium channel blocker
Antidiabetic (type 1)
Tryptophanyl aminopeptidase inhibitor
Nav1.1 sodium channel blocker
AMPA 3 receptor antagonist
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Histamine N-methyltransferase inhibitor
Fibroblast growth factor agonist
Aralkylamine dehydrogenase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Calcium channel (voltage-sensitive) blocker
Cyclin-dependent kinase 9 inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
AMPA 1 receptor antagonist
Methyltransferase substrate
Antiviral (Adenovirus)
Radioprotector
Acylglycerone-phosphate reductase inhibitor
Cholinergic
NMDA 2 receptor antagonist
Guanidinoacetase inhibitor
Mannitol-1-phosphatase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Picornain 2A inhibitor
Aldehyde dehydrogenase (NAD+) inhibitor
(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor

Pancreatic ribonuclease inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
Guanidinoacetate kinase inhibitor
CYP3C substrate
Ferredoxin-nitrite reductase inhibitor
Peroxidase substrate
Alcohol dehydrogenase inhibitor
Allantoin racemase inhibitor
Antihelminthic (Nematodes)
CYP2B1 substrate
N-Carbamoyl-D-amino acid hydrolase inhibitor
P-glycoprotein inhibitor
Antineoplastic (endocrine cancer)
Butyrylcholinesterase inhibitor
Phospholipase D inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Dopamine D2L antagonist
Melatonin 1 agonist
MDM2 inhibitor
Gastric antisecretory
Carnitine 3-dehydrogenase inhibitor
Cyclamate sulfohydrolase inhibitor
Beta adrenoreceptor antagonist
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
Procollagen N-endopeptidase inhibitor
GABA B receptor agonist
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Bile-salt sulfotransferase inhibitor
Interferon agonist
H⁺-exporting ATPase inhibitor
Ophthalmic drug
Hyperprolactinemia treatment
Urate-ribonucleotide phosphorylase inhibitor
CYP2C10 substrate
Puromycin-sensitive aminopeptidase inhibitor
CYP2A substrate
Dopamine release stimulant
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Phosphoinositide phospholipase C inhibitor
Kainate receptor 3 antagonist
Nav1.2 sodium channel blocker
Antiglaucomic
Loop diuretic
Gastrointestinal motility stimulant
Aromatic-hydroxylamine O-acetyltransferase inhibitor
MO15-related protein kinase Pfmrk inhibitor
MAO B substrate
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
Antineoplastic (bone cancer)

Enteropeptidase inhibitor
Fibroblast growth factor antagonist
Peptidyltransferase inhibitor
Interleukin 10 agonist
Xaa-Pro dipeptidyl-peptidase inhibitor
Signal peptidase I inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Irritable Bowel syndrome treatment
[acyl-carrier-protein] S-acetyltransferase inhibitor
Phosphatidylserine decarboxylase inhibitor
Melatonin antagonist
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Antitussive
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Gaucher disease treatment
CDK1/cyclin B inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Alanine-tRNA ligase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Melanocortin MC-4 agonist
Pseudouridylate synthase inhibitor
Anthranilate synthase inhibitor
Beta 2 adrenoreceptor antagonist
Complement factor D inhibitor
Thiol oxidase inhibitor
Picornain 3C inhibitor
Releasing hormone agonist
Antihistaminic
Catenin beta inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Pyridoxal kinase inhibitor
Clostripain inhibitor
Glyoxylate reductase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
5 Hydroxytryptamine 6 agonist
Adrenergic
Ubiquitin thiolesterase inhibitor
Tryptophan transaminase inhibitor
Histamine H1 receptor antagonist
DELTA24-sterol reductase inhibitor
Thimet oligopeptidase inhibitor
TH expression enhancer
Peptidyl-dipeptidase B inhibitor
Reductant
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
Guanidinopropionase inhibitor
Adrenaline agonist
Cytochrome-b5 reductase inhibitor
Farnesyltranstransferase inhibitor

Clavamate synthase inhibitor
Dihydroxy-acid dehydratase inhibitor
Cell wall biosynthesis inhibitor
Fibroblast growth factor 1 antagonist
RNA synthesis inhibitor
Isopenicillin-N epimerase inhibitor
Antischistosomal
Acetylcholine neuromuscular blocking agent
Aspergillopepsin II inhibitor
Gametolysin inhibitor
Manganese peroxidase inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Protein synthesis stimulant
Antineoplastic (pancreatic cancer)
CYP2C8 inducer
Carboxypeptidase D inhibitor
Stromelysin 2 inhibitor
Aurora-C kinase inhibitor
Shock treatment
NMDA 2A receptor antagonist
Glucose oxidase inhibitor
Andropause treatment
Licheninase inhibitor
Melatonin 1b antagonist
Benzodiazepine antagonist
Glycerol dehydrogenase (NADP⁺) inhibitor
5 Hydroxytryptamine agonist
Antidiarrheal
D-Ornithine 4,5-aminomutase inhibitor
Vanilloid 4 antagonist
Hydroxymethylbilane synthase inhibitor
Pancreatic endopeptidase E inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Methane monooxygenase inhibitor
Glucan endo-1,3-alpha-glucosidase inhibitor
Insulysin inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Glucuronate isomerase inhibitor
Plasminogen activator stimulant
Phenylalanine dehydrogenase inhibitor
Neuropeptide Y2 antagonist
Thiol S-methyltransferase inhibitor
Acetylcholine M1 receptor antagonist
Protein-tyrosine sulfotransferase inhibitor
Beta 1 adrenoreceptor agonist
Beta 1 adrenoreceptor antagonist
CF transmembrane conductance regulator agonist
Trypanothione-disulfide reductase inhibitor
CYP2H substrate
Melatonin agonist

Guanidinobutyrase inhibitor
Carboxypeptidase E inhibitor
Phosphoserine phosphatase inhibitor
MAO inhibitor
Platelet aggregation inhibitor
GABA C receptor agonist
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Lysyl endopeptidase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Electrolyte absorption antagonist
Histamine release inhibitor
Cholate-CoA ligase inhibitor
Alpha adrenoreceptor agonist
Ganglioside galactosyltransferase inhibitor
Aralkylamine N-acetyltransferase inhibitor
Leucolysin inhibitor
Retinopathy treatment
Glucan 1,4-beta-glucosidase inhibitor
Renal tissue kallikrein inhibitor
Melatonin 2 agonist
Histidinol-phosphatase inhibitor
Transactivator transcription protein inhibitor
Venom exonuclease inhibitor
Acyl-lysine deacylase inhibitor
Carnitinamidase inhibitor
GABA receptor agonist
Thermitase inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
Protein-synthesizing GTPase inhibitor
Nicotinic alpha6 receptor agonist
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Biotinidase inhibitor
Dextranase inhibitor
Alanine transaminase inhibitor
Glycine C-acetyltransferase inhibitor
Calcium channel L-type blocker
Dyspepsia treatment
Carboxymethylenebutenolidase inhibitor
Adenylate cyclase V inhibitor
Nitrile hydratase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
Ceramide glucosyltransferase inhibitor
Chlordecone reductase inhibitor
Acetylcholine M5 receptor antagonist
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
5 Hydroxytryptamine 1B agonist
Alkanal monooxygenase (FMN-linked) inhibitor
D-Octopine dehydrogenase inhibitor

Glutaminyl-peptide cyclotransferase inhibitor
Lysozyme inhibitor
Endometriosis treatment
Melanocortin agonist
Polynucleotide 5'-hydroxy-kinase inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
GABA C receptor antagonist
Serralysin inhibitor
Antiinfertility, female
Thiamine-phosphate kinase inhibitor
Alpha 2 adrenoreceptor agonist
N-methyl-2-oxoglutaramate hydrolase inhibitor
Cellulase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor
CYP2C6 substrate
Immunoglobulin Fc receptor antagonist
Acetylornithine deacetylase inhibitor
Histamine antagonist
Preterm labor treatment
Arginyltransferase inhibitor
Aerobactin synthase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Antithrombotic
Orotate reductase (NADPH) inhibitor
Candidapepsin inhibitor
CYP3A5 inducer
Dynein ATPase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
CYP2E1 inducer
Fibroblast growth factor 1 agonist
Polygalacturonase inhibitor
2-Nitropropane dioxygenase inhibitor
Decylcitrate synthase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Saccharolysin inhibitor
Pantothenase inhibitor
Ca²⁺/calmodulin-dependent kinase II inhibitor
Hirsutism treatment
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Antianorexic
Kainate receptor 1 antagonist
Arylalkyl acylamidase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Alpha-amylase inhibitor
Levanase inhibitor
Focal adhesion kinase 1 inhibitor
Deoxyribonuclease I inhibitor

CYP2B5 substrate
Alpha 2 adrenoreceptor antagonist
Monodehydroascorbate reductase (NADH) inhibitor
Retinoic acid metabolism inhibitor
Aminopeptidase B inhibitor
NMDA receptor polyamine site antagonist
CYP2E1 inhibitor
Channel-conductance-controlling ATPase inhibitor
Colony stimulating factor agonist
VEGF expression inhibitor
Tankyrase 2 inhibitor
Lassitude treatment
11-Cis-retinyl-palmitate hydrolase inhibitor
Mycolysin inhibitor
Centromere associated protein inhibitor
Alkane 1-monooxygenase inhibitor
Allantoate deiminase inhibitor
Melatonin 1 antagonist
IgA-specific metalloendopeptidase inhibitor
Neuropsin inhibitor
Phosphatidate phosphatase inhibitor
Factor XIIIa inhibitor
Endonuclease (influenza) inhibitor
Neurolysin inhibitor
GST A substrate
Myocardial ischemia treatment
3-Hydroxyanthranilate oxidase inhibitor
CYP3A4 inducer
CYP2D2 inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
3-Methylbutanal reductase inhibitor
Acetolactate synthase inhibitor
2-Oxoglutarate decarboxylase inhibitor
GST T substrate
GST T1-1 substrate
Arylsulfate sulfotransferase inhibitor
Adenomatous polyposis treatment
Arylsulfatase inhibitor
CYP3A inducer
DNA-3-methyladenine glycosylase II inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Glutaminase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Fructan beta-fructosidase inhibitor
ATPase inhibitor
Melatonin 1a antagonist
Benzodiazepine receptor peripheral-type antagonist
Hydroxylamine reductase (NADH) inhibitor
Guanylate kinase inhibitor
Alcohol dehydrogenase (NADP+) inhibitor

Membrane dipeptidase inhibitor
Aminoacylase inhibitor
Cyanate hydratase inhibitor
Luteinizing hormone-releasing hormone antagonist
Acetyl-CoA transferase 2 inhibitor
L-glucuronate reductase inhibitor
Allophanate hydrolase inhibitor
MAO A inhibitor
Nociceptin (N/OFQ) receptor antagonist
Polynucleotide adenylyltransferase inhibitor
Acyl-CoA oxidase inhibitor
Anxiolytic
Beta 2 adrenoreceptor agonist
Granulocyte macrophage colony stimulating factor agonist
Aspartate-ammonia ligase (ADP-forming) inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
SULT1A3 substrate
Skin irritation, inactive
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Adenylate kinase inhibitor
Aldehyde dehydrogenase substrate
Pyruvate dehydrogenase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
D-proline reductase (dithiol) inhibitor
Phosphodiesterase I inhibitor
NADPH oxidase inhibitor
Porphobilinogen synthase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Beta-amylase inhibitor
Isopenicillin-N synthase inhibitor
NMDA 2B receptor antagonist
Propanediol dehydratase inhibitor
Granzyme A inhibitor
Membrane permeability enhancer
Dopamine D2A antagonist
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Sclerosant
Metallo-carboxypeptidase D inhibitor
Asparaginase inhibitor
RAS guanyl releasing protein antagonist
NMDA receptor polyamine site agonist
Glycerol dehydratase inhibitor
(S)-2-hydroxy-acid oxidase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
Homocitrate synthase inhibitor
Adenylate cyclase inhibitor
Sigma 1 receptor antagonist
UDP-N-acetylglucosamine diphosphorylase inhibitor
Myosin ATPase inhibitor
Pancreatic disorders treatment

Sildenafil citrate

Molecular Mechanism (initial) :

phospho-diesterase (PDE5A) inhibitor

Molecular Mechanism (repurposed) :

phospho-diesterase (PDE5A) inhibitor

initial indication(s):

erectile dysfunction

Repurposed indication(s):

hypertension pulmonary arterial

Predicted Activities

Phosphodiesterase I inhibitor

Phosphodiesterase 1B inhibitor

Erectile dysfunction treatment

Male reproductive disfunction treatment

Phosphodiesterase V inhibitor

Phosphodiesterase 5A inhibitor

Cyclic GMP phosphodiesterase inhibitor

Phosphodiesterase inhibitor

CYP2C19 substrate

Antianginal (hypertension pulmonary arterial)

CYP2C9 substrate

Osteoarthritis treatment

Phosphodiesterase 9A inhibitor

Autoimmune disorders treatment

Phosphodiesterase IX inhibitor

Rheumatoid arthritis treatment

Phosphodiesterase VI inhibitor

CYP2D6 substrate

CYP2D substrate

Phosphodiesterase 3A inhibitor

Antiasthmatic

Antidiabetic

Pulmonary hypertension treatment

CYP2C substrate

Kinase inhibitor

Phosphodiesterase II inhibitor

Antiallergic

Phosphodiesterase 6B inhibitor

Antidiabetic (type 2)

Antihypertensive

Sepsis treatment

Lipoprotein disorders treatment

Dual specificity phosphatase 1 inhibitor

Phosphodiesterase 6A inhibitor

Vasodilator

Phosphodiesterase III inhibitor

Cystic fibrosis treatment

Undecaprenyl-phosphate mannosyltransferase inhibitor

CYP3A4 inhibitor
Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
Transcription factor STAT inhibitor
Proto-oncogene tyrosine-protein kinase Fyn inhibitor
Chronic obstructive pulmonary disease treatment
Phosphodiesterase 11A inhibitor
Phosphodiesterase XI inhibitor
Phosphodiesterase 10A inhibitor
Phosphodiesterase X inhibitor
Anaphylatoxin receptor antagonist
Rho-associated kinase I inhibitor
Phosphodiesterase 4A inhibitor
Cyclic AMP phosphodiesterase inhibitor
Transcription factor STAT3 inhibitor
Uterine relaxant
CYP3A4 substrate
Nootropic
Diuretic inhibitor
Phosphodiesterase IV inhibitor
Phosphodiesterase 4D inhibitor
Posttraumatic stress disorder treatment
RET inhibitor
5 Hydroxytryptamine 7S antagonist
Cardiotonic
HERG channel blocker
Phosphodiesterase 4C inhibitor
Phosphodiesterase 4B inhibitor
Calcium channel N-type blocker
Peroxisome proliferator-activated receptor agonist
Amyotrophic lateral sclerosis treatment
TTK protein kinase inhibitor
PfA-M1 aminopeptidase inhibitor
Analgesic, non-opioid
Polo-like kinase inhibitor
5 Hydroxytryptamine 1E antagonist
Ca(v)2.2 blocker
Cytidine deaminase inhibitor
Inosine nucleosidase inhibitor
Ribosomal protein S6 kinase, 90-kDa inhibitor
Antidiabetic symptomatic
Aurora-A kinase inhibitor
11-Beta-hydroxysteroid dehydrogenase 1 inhibitor
Myt1 kinase inhibitor
Analgesic
5 Hydroxytryptamine 7L antagonist
Adenosine A2b receptor antagonist
Adenosine receptor antagonist
11-Beta-hydroxysteroid dehydrogenase inhibitor
Smooth muscle myosin light chain kinase inhibitor
Cognition disorders treatment

Tumour necrosis factor alpha antagonist

Simvastatin

Molecular Mechanism (initial) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

Molecular Mechanism (repurposed) :

3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitor

initial indication(s):

anti-cholesterol

Repurposed indication(s):

colorectal cancer

Predicted Activities

Lipid metabolism regulator

Antihypercholesterolemic

HMOX1 expression enhancer

Hypolipemic

Vasodilator, coronary

APOA1 expression enhancer

CYP3A4 substrate

CYP3A substrate

CYP3A5 substrate

Antihyperlipoproteinemic

CYP2D6 substrate

CYP2D substrate

HMG CoA reductase inhibitor

Reductase inhibitor

Cholesterol synthesis inhibitor

Antifungal

Antieczematic

P-glycoprotein substrate

NOS3 expression enhancer

Nootropic

HDL-cholesterol increasing

Immunosuppressant

Sepsis treatment

CYP2H substrate

Cystic fibrosis treatment

Angiogenesis stimulant

Vasodilator

Antipsoriatic

Phosphatase inhibitor

Chemopreventive

H⁺-transporting two-sector ATPase inhibitor

General pump inhibitor

HIF1A expression inhibitor

CYP2C9 inhibitor

Dermatologic

Atherosclerosis treatment

Antineoplastic (non-Hodgkin's lymphoma)

Antimetastatic
Ubiquinol-cytochrome-c reductase inhibitor
Antibacterial
Pulmonary hypertension treatment
Membrane permeability enhancer
UDP-glucuronosyltransferase substrate
Paraoxonase substrate
Beta glucuronidase inhibitor
Antiparasitic
Antineoplastic (lung cancer)
LDLR expression enhancer
Lipoprotein disorders treatment
H⁺-exporting ATPase inhibitor
Protein synthesis inhibitor
Restenosis treatment
Acute neurologic disorders treatment
Cholesterol antagonist
Chloride channel blocker
HMG CoA synthase inhibitor
CYP2C19 inducer
Multiple sclerosis treatment
Glyceryl-ether monooxygenase inhibitor
Antiprotozoal (Leishmania)
Cholesterol absorption inhibitor
Antimycoplasmal
P-glycoprotein inhibitor
CYP17 inhibitor
Alcohol O-acetyltransferase inhibitor
ATPase stimulant
Alkenylglycerophosphocholine hydrolase inhibitor
Myc inhibitor
Calcium regulator
CYP2D6 inhibitor
Antihelminthic
Proteasome ATPase inhibitor
Lipoprotein lipase stimulant
CYP3A4 inhibitor
Acylcarnitine hydrolase inhibitor
Antiviral (Rhinovirus)
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Hydroxysteroid dehydrogenase inhibitor
Antibiotic
LFA antagonist
LFA-1 antagonist
Transcription factor NF kappa B stimulant
Transcription factor stimulant
ATPase inhibitor
Membrane integrity antagonist
Interleukin 2 agonist
Antiprotozoal

Neurotrophic factor enhancer
Alzheimer's disease treatment
Bilirubin oxidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Interleukin agonist
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Dextranase inhibitor
Antiviral (Herpes)
1,2-alpha-L-fucosidase inhibitor
Retinoprotector
Growth stimulant
Myosin-light-chain-phosphatase inhibitor
CDP-glycerol glycerophosphotransferase inhibitor
Alkylacetyl glycerophosphatase inhibitor
Antipruritic, allergic
CYP2A11 substrate
Polyribonucleotide nucleotidyltransferase inhibitor
Retinol dehydrogenase inhibitor
Proliferative diseases treatment
Antineoplastic (thyroid cancer)
CYP2J2 substrate
Contraceptive
Peptidoglycan glycosyltransferase inhibitor
Antineoplastic (pancreatic cancer)
Protein 50S ribosomal subunit inhibitor
Neurotrophic factor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Benzoate-CoA ligase inhibitor
Phospholipase A1 inhibitor
Undecaprenyl-phosphate mannosyltransferase inhibitor
CYP7 inhibitor
Antieczematic atopic
Thyroxine 5-deiodinase inhibitor
Gestagen antagonist
Microtubule formation inhibitor
UGT2B18 substrate
Actin depolymerization stimulant
Antineoplastic antibiotic
Protein kinase C stimulant
Antifungal enhancer
Thromboxane synthase stimulant
CYP2J substrate
Maleate isomerase inhibitor
Antineoplastic
Sucrose-phosphate synthase inhibitor
Protein kinase stimulant
Cytokine release inhibitor
Antihelminthic (Nematodes)
Ketol-acid reductoisomerase inhibitor
Testosterone 17beta-dehydrogenase (NADP+) inhibitor

GDP-mannose 6-dehydrogenase inhibitor
ICAM1 expression inhibitor
RNA synthesis inhibitor
Sterol 24-C-methyltransferase inhibitor
Endoglycosylceramidase inhibitor
Microtubule stabilization
Interleukin 10 antagonist
Threonine-tRNA ligase inhibitor
CYP2C8 inducer
CDC25A inhibitor
Antineoplastic (endocrine cancer)
Antimitotic
Interferon antagonist
CYP3A inducer
Dolichyl-phosphate beta-glucosyltransferase inhibitor
CYP2A10 substrate
Anabolic
Transforming growth factor beta 1 agonist
Antiprotozoal (Toxoplasma)
Anticarcinogenic
SULT1E1 substrate
Interleukin 12 agonist
Ceramide glucosyltransferase inhibitor
Transplant rejection treatment
Antitreponemal
Antioxidant
Methylglutamate dehydrogenase inhibitor
Dry eye syndrome treatment
Lactase inhibitor
Antirickettsial
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Uterine relaxant
Anesthetic
CYP3A4 inducer
Protein-synthesizing GTPase inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Galactosylceramidase inhibitor
Antidote
Platelet aggregation stimulant
Aspartyltransferase inhibitor
Prostaglandin D2 agonist
UGT2B9 substrate
Apyrase inhibitor
Glycosylceramidase inhibitor
Hydroxymethylglutaryl-CoA reductase inhibitor
ICAM 1 antagonist
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Prostaglandin agonist
Antineoplastic (squamous cell carcinoma)
Rotamase (FKBP) inhibitor

[phosphorylase] phosphatase inhibitor
Hypercalcemia treatment
CYP2A4 substrate
Apoptosis agonist
Antibiotic Macrolide-like
Rotamase (FKBP12) inhibitor
Retinyl-palmitate esterase inhibitor
UGT2B28 substrate
Electron transport complex I inhibitor
Melanin inhibitor
2,3-Oxidosqualene-lanosterol cyclase inhibitor
Antineoplastic (multiple myeloma)
1,3-Beta-glucan synthase inhibitor
Peptidyltransferase inhibitor
Nitric oxide antagonist
Oxidoreductase inhibitor
Antineoplastic (lymphoma)
Antiviral (Influenza)
Polarisation stimulant
Hydroxylamine reductase (NADH) inhibitor
Histidine kinase inhibitor
Antiacne
NADH oxidase inhibitor
Steroid DELTA-isomerase inhibitor
Lipocortins synthesis antagonist
Squalene synthetase inhibitor
Elastase 1 inhibitor
Corticosteroid antagonist
ATPase (Vacuolar H⁺) inhibitor
RNA-directed RNA polymerase stimulant
Antineoplastic (sarcoma)
Antiviral (Trachoma)
RNA agonist
Calcineurin inhibitor
Lipocortins synthesis agonist
Antineoplastic (bone cancer)
T cell inhibitor
Gonadotropin antagonist
ATP citrate lysase inhibitor
Antibiotic Tetracycline-like
Interferon gamma antagonist
Vitamin D3 hydroxylase inhibitor
Estrogen agonist
Adrenergic, ophthalmic
Parathyroid hormone antagonist
Tubulin agonist
Actin polymerization inhibitor
CYP7B substrate
CYP7B1 substrate

Targretin

Molecular Mechanism (initial) :

retinoid X receptor (RXR) agonist

Molecular Mechanism (repurposed) :

retinoid X receptor (RXR) agonist

ATP-binding cassette transporter (ABCA1) expression enhancers

extracellular-regulated kinase (ERK) inhibitor

SAPK1 (JNK) inhibitor

initial indication(s):

T-cell lymphoma

Repurposed indication(s):

Alzheimer's type dementia

Predicted Activities

Antipsoriatic

Phosphatidylcholine-retinol O-acyltransferase inhibitor

Antieczematic

Testosterone 17beta-dehydrogenase (NADP+) inhibitor

Retinoic acid receptor antagonist

Retinoic acid receptor agonist

Retinoic acid beta receptor agonist

Dermatologic

CYP2C9 substrate

CYP2B substrate

CYP2C substrate

Glutamyl endopeptidase II inhibitor

Retinoic acid beta receptor antagonist

Chlordecone reductase inhibitor

Fatty-acyl-CoA synthase inhibitor

Retinoic acid receptor gamma antagonist

Alkenylglycerophosphocholine hydrolase inhibitor

Sugar-phosphatase inhibitor

Ribulose-phosphate 3-epimerase inhibitor

5-O-(4-coumaroyl)-D-quinic acid 3'-monooxygenase inhibitor

NADH kinase inhibitor

CYP2C19 substrate

CYP2J substrate

ABCA1 expression enhancer

CYP3A4 inducer

UDP-glucuronosyltransferase substrate

Electron-transferring-flavoprotein dehydrogenase inhibitor

CYP3A inducer

Retinoic acid alpha receptor antagonist

Beta-adrenergic receptor kinase inhibitor

G-protein-coupled receptor kinase inhibitor

Glutamate-5-semialdehyde dehydrogenase inhibitor

(R)-Pantolactone dehydrogenase (flavin) inhibitor

Mannan endo-1,4-beta-mannosidase inhibitor

Kidney function stimulant

Fusarinine-C ornithinesterase inhibitor

1,4-Lactonase inhibitor
Alkane 1-monooxygenase inhibitor
L-glutamate oxidase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Ecdysone 20-monooxygenase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Gluconate 5-dehydrogenase inhibitor
Phenol O-methyltransferase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Polyamine-transporting ATPase inhibitor
CYP3A4 substrate
Dimethylargininase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Benzoate-CoA ligase inhibitor
Pterin deaminase inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Urease inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
CYP3A substrate
Cyclohexanone monooxygenase inhibitor
Glycolate dehydrogenase inhibitor
Keratolytic
Glutathione thiolesterase inhibitor
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Erythropoiesis stimulant
Glucan endo-1,6-beta-glucosidase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Arginine 2-monooxygenase inhibitor
Glutamine-phenylpyruvate transaminase inhibitor
Mucomembranous protector
Chenodeoxycholytaurine hydrolase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Aspartate-ammonia ligase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
Limulus clotting factor B inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
CYP2C8 inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Pullulanase inhibitor
Alpha-pinene-oxide decyclase inhibitor
Glyoxylate oxidase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Factor XIIIa stimulant
Ornithine cyclodeaminase inhibitor
tRNA-pseudouridine synthase I inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor

Creatininase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Antiacne
N-Acyl-D-aspartate deacylase inhibitor
Sphinganine kinase inhibitor
Hydrogen dehydrogenase inhibitor
Fibrinolytic
Glutarate-semialdehyde dehydrogenase inhibitor
Antineoplastic
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Poly(alpha-L-gulonate) lyase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Exoribonuclease II inhibitor
Ferrochelataase inhibitor
Chemopreventive
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Anticarcinogenic
FMO1 substrate
Thymidylate 5'-phosphatase inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Xylan endo-1,3-beta-xylosidase inhibitor
Lysine 2,3-aminomutase inhibitor
Oxidoreductase inhibitor
Glyoxylate reductase inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Retinal dehydrogenase inhibitor
Gluconolactonase inhibitor
Retinoid X gamma receptor antagonist
Aspartyltransferase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Taurine dehydrogenase inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Carbon-monoxide dehydrogenase inhibitor
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
Prostaglandin-E2 9-reductase inhibitor
Antipruritic, allergic
S-alkylcysteine lyase inhibitor
Transcription factor NF kappa B stimulant
Transcription factor stimulant
Acetylcholinesterase inhibitor
HMOX1 expression enhancer
N-acetylneuraminase synthase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
Arylesterase inhibitor
CYP4A11 substrate
Retinoic acid alpha receptor agonist

2-Dehydropantoate 2-reductase inhibitor
Gluconate 2-dehydrogenase (acceptor) inhibitor
Amine dehydrogenase inhibitor
Histamine release inhibitor
Opine dehydrogenase inhibitor
Fructose 5-dehydrogenase inhibitor
Cytoprotectant
Mannitol-1-phosphatase inhibitor
4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Chitosanase inhibitor
Formaldehyde transketolase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Caspase 8 stimulant
Platelet adhesion inhibitor
Arylsulfate sulfotransferase inhibitor
Adenomatous polyposis treatment
Centromere associated protein inhibitor
Antipruritic
Antieczematic atopic
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Inulinase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Histidine N-acetyltransferase inhibitor
CYP2J2 substrate
Fumarate reductase (NADH) inhibitor
Cyclomaltodextrinase inhibitor
Dextranase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
ADP-thymidine kinase inhibitor
Glycerol-ether monooxygenase inhibitor
Phospholipid-translocating ATPase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Retinoid X receptor agonist
4-Hydroxyglutamate transaminase inhibitor
Mannose isomerase inhibitor
Alcohol O-acetyltransferase inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
5 Hydroxytryptamine release inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Plasmanylethanolamine desaturase inhibitor
Phosphatidylserine decarboxylase inhibitor
N-acylmannosamine kinase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Hydroxymethylbilane synthase inhibitor

N-hydroxyarylamine O-acetyltransferase inhibitor
Isopenicillin-N epimerase inhibitor
Mucinaminyserine mucinaminidase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Corticosteroid side-chain-isomerase inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Salicylate 1-monooxygenase inhibitor
GABA aminotransferase inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
tRNA nucleotidyltransferase inhibitor
Spermidine dehydrogenase inhibitor
Lipid metabolism regulator
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Styrene-oxide isomerase inhibitor
Fructan beta-fructosidase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Alpha-glucuronidase inhibitor
Deoxyribose-phosphate aldolase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
S-formylglutathione hydrolase inhibitor
Phosphatase inhibitor
Uroporphyrinogen-III synthase inhibitor
3-Cyanoalanine hydratase inhibitor
CYP2H substrate
Trans-pentaprenyltranstransferase inhibitor
Sulfite dehydrogenase inhibitor
Antiuremic
Anthranilate-CoA ligase inhibitor
Nitrate reductase (cytochrome) inhibitor
Pyruvate decarboxylase inhibitor
Loop diuretic
Bilirubin oxidase inhibitor
Retinoid X alpha receptor agonist
Malate oxidase inhibitor
Camphor 1,2-monooxygenase inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Hepatocyte nuclear factor 4 alpha agonist
Hepatocyte nuclear factor agonist
Phenylacetate-CoA ligase inhibitor
D-lactaldehyde dehydrogenase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Antinociceptive
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Cyanoalanine nitrilase inhibitor
Antipruritic, non-allergic
4-Chlorophenylacetate 3,4-dioxygenase inhibitor

CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Antiemphysemic
Diuretic inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Chitinase inhibitor
Cathepsin T inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Hydroxylamine reductase (NADH) inhibitor
Cyclamate sulfohydrolase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
3-Aminobutaryl-CoA ammonia-lyase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Lactaldehyde reductase inhibitor
Sulfite oxidase inhibitor
Gingipain K inhibitor
Pediculicide
Cholestanetriol 26-monooxygenase inhibitor
CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
Eye irritation, inactive
Gamma-butyrobetaine dioxygenase inhibitor
CYP4A substrate
Alpha-N-acetylglucosaminidase inhibitor
Hyponitrite reductase inhibitor
Phosphatidylglycerophosphatase inhibitor
Tryptophanamidase inhibitor
Trimethylamine-oxide aldolase inhibitor
3-Oxadipate enol-lactonase inhibitor
Fragilysin inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD+) inhibitor
Alanine-tRNA ligase inhibitor
Creatinine deaminase inhibitor
Thromboxane B2 antagonist
Acylcarnitine hydrolase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Antiviral (Rhinovirus)
BRAF expression inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Thiosulfate dehydrogenase inhibitor
Biotinidase inhibitor
Farnesyltranstransferase inhibitor
Mitochondrial processing peptidase inhibitor
Superoxide dismutase inhibitor
Acetylornithine deacetylase inhibitor
Alkylacetylgllycerophosphatase inhibitor
Sulfur dioxygenase inhibitor
Urethanase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor

Dihydrodipicolinate reductase inhibitor
Nicotine dehydrogenase inhibitor
Insulin promoter
Ompin inhibitor
Orotate reductase (NADH) inhibitor
Threonine aldolase inhibitor
Glucan endo-1,3- α -glucosidase inhibitor
Glycogen synthase stimulant
APOA1 expression enhancer
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Cyclopentanone monooxygenase inhibitor
4-Hydroxyproline epimerase inhibitor
Carnitinamidase inhibitor
NF-E2-related factor 2 stimulant
Methylumbelliferyl-acetate deacetylase inhibitor
Membrane permeability inhibitor
Nitrite reductase [NAD(P)H] inhibitor
1,2- α -L-fucosidase inhibitor
Phenylalanine(histidine) transaminase inhibitor
Lipoprotein lipase inhibitor
Gallate decarboxylase inhibitor
Transketolase inhibitor
Glycerol-1-phosphatase inhibitor
Dimethylmaleate hydratase inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
D-xylulose reductase inhibitor
Bile-salt sulfotransferase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Insulin sensitizer
Keratosis actinic (solar) treatment
Transforming growth factor beta 1 agonist
CYP2A6 substrate
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Sulfite reductase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Retinol dehydrogenase inhibitor
Adenylyl-sulfate reductase inhibitor
Phenylpyruvate decarboxylase inhibitor
DNA ligase (ATP) inhibitor
Cholesterol antagonist
Lombricin kinase inhibitor
Leukotriene-B4 20-monooxygenase inhibitor
EIF4E expression inhibitor
Cysteine desulfurase inhibitor
Blasticidin-S deaminase inhibitor
Carboxypeptidase D inhibitor
MMP9 expression inhibitor
GABA C receptor agonist
Leucine dehydrogenase inhibitor
TP53 expression enhancer

Aryldialkylphosphatase inhibitor
Oxidizing agent
Orotate reductase (NADPH) inhibitor
Pantoate 4-dehydrogenase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
CYP2A substrate
Pseudouridylate synthase inhibitor
Thiamine pyridinylase inhibitor
Acyl-lysine deacylase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
H⁺-exporting ATPase inhibitor
Glycine amidinotransferase inhibitor
Acyl-CoA oxidase inhibitor
Retinoid X beta receptor antagonist
Antineoplastic (renal cancer)
Hypolipemic
Allantoinase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Antihypercholesterolemic
Dihydroxy-acid dehydratase inhibitor
Arylalkyl acylamidase inhibitor
Skin irritation, inactive
4-Coumarate-CoA ligase inhibitor
Glucose oxidase inhibitor
Glucuronate isomerase inhibitor
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Antineoplastic (breast cancer)
Aspartoacylase inhibitor
Glutamate-tRNA ligase inhibitor
Nicotinate dehydrogenase inhibitor
Glycerol 2-dehydrogenase (NADP⁺) inhibitor
Choleretic
Indolepyruvate C-methyltransferase inhibitor
Myosin ATPase inhibitor
Acetylcholine neuromuscular blocking agent
Antidote
Gly-X carboxypeptidase inhibitor
Venombin AB inhibitor
Cholesterol synthesis inhibitor
Macrophage colony stimulating factor agonist
Glucan 1,4-beta-glucosidase inhibitor
Malate dehydrogenase (acceptor) inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Dolichyl-phosphatase inhibitor
Maleate isomerase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Carboxymethylenebutenolidase inhibitor
Licheninase inhibitor
Glycine-tRNA ligase inhibitor

Leucolysin inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Menopausal disorders treatment
Polygalacturonase inhibitor
Antiperistaltic
D-threo-aldose 1-dehydrogenase inhibitor
Aspartate-tRNA ligase inhibitor
Carminative
4-Hydroxybenzoate-CoA ligase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Diisopropyl-fluorophosphatase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
FMO3 substrate
Antidiabetic
D-amino-acid dehydrogenase inhibitor
Tryptophan transaminase inhibitor
Nitrite reductase (NO-forming) inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Glycerol dehydrogenase (NADP+) inhibitor
Acetylenecarboxylate hydratase inhibitor
Prolyl aminopeptidase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Undecaprenyl-diphosphatase inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Antimutagenic
Opioid kappa 3 receptor antagonist
Apyrase inhibitor
Morphine 6-dehydrogenase inhibitor
Procollagen N-endopeptidase inhibitor
Bothrolysin inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Glutaminase inhibitor
Magnesium-protoporphyrin IX methyltransferase inhibitor
Levanase inhibitor
Serine 3-dehydrogenase inhibitor
3C-like protease (Human coronavirus) inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
N-acetyllactosamine synthase inhibitor
Retinoic acid metabolism inhibitor
Protein-arginine deiminase inhibitor
Beta glucuronidase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Histidinol-phosphatase inhibitor

Sigma receptor agonist
Valine decarboxylase inhibitor
Antiviral (Adenovirus)
Retinyl-palmitate esterase inhibitor
Rhamnulose-1-phosphate aldolase inhibitor
Acetate kinase inhibitor
Choloylglycine hydrolase inhibitor
L-glucuronate reductase inhibitor
Hydroxylamine reductase inhibitor
Glycopeptide alpha-N-acetylgalactosaminidase inhibitor
Antiinflammatory, intestinal
Acylphosphatase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
Creatinase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
CYP2C8 substrate
L-amino-acid oxidase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Alcohol dehydrogenase [NAD(P)+] inhibitor
Thiopurine S-methyltransferase inhibitor
Carboxypeptidase Taq inhibitor
Cl--transporting ATPase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
2-Oxoglutarate decarboxylase inhibitor
CYP2E1 inducer
Glutamate 5-kinase inhibitor
Gamma-glutamyltransferase inhibitor
L-threonine 3-dehydrogenase inhibitor
Antiviral (CMV)
Acetate-CoA ligase inhibitor
Glucan 1,6-alpha-glucosidase inhibitor
Carnitine dehydratase inhibitor
N-acetylneuraminate 4-O-acetyltransferase inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Retinoid X receptor antagonist
Mevalonate kinase inhibitor
Coproporphyrinogen oxidase inhibitor
Biliverdin reductase inhibitor
Contraceptive
Fibroblast growth factor agonist
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
2-Enoate reductase inhibitor
Glutamine-tRNA ligase inhibitor
JNK mitogen-activated protein kinase inhibitor
Succinate-CoA ligase (ADP-forming) inhibitor
Porphobilinogen synthase inhibitor

Valine dehydrogenase (NADP+) inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
Aryl-alcohol dehydrogenase inhibitor
Aldehyde dehydrogenase (NADP+) inhibitor
Cytochrome-c3 hydrogenase inhibitor
Electrolyte absorption antagonist
UGT1A substrate
Flavin-containing monooxygenase substrate
Aconitate decarboxylase inhibitor
Skin whitener
CYP2C9 inducer
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Ferredoxin-nitrite reductase inhibitor
Dementia treatment
3-Oxosteroid 1-dehydrogenase inhibitor
Iron-cytochrome-c reductase inhibitor
FMN reductase inhibitor
Pyridoxine 4-oxidase inhibitor
Prephenate dehydrogenase inhibitor
Wound healing agent
UGT2B7 substrate
Cholesterol oxidase inhibitor
N-formylmethionyl-peptidase inhibitor
D-lactate dehydrogenase (cytochrome) inhibitor
D-2-hydroxy-acid dehydrogenase inhibitor
Antisecretoric
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Vanillyl-alcohol oxidase inhibitor
Guanidinoacetase inhibitor
CYP2A4 substrate
Hyaluronic acid agonist
Trimethylamine dehydrogenase inhibitor
Leucine transaminase inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
2-Dehydropantolactone reductase (A-specific) inhibitor
Coccolysin inhibitor
2-Methyleneglutarate mutase inhibitor
Gastrin inhibitor
Retinoid X alpha receptor antagonist
Dihydroorotase inhibitor
L-iduronidase inhibitor
Antileukemic
Severe acute respiratory syndrome treatment
Alpha-N-arabinofuranosidase inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Alopecia treatment
Mitochondrial intermediate peptidase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor

NAD(P)⁺ transhydrogenase (B-specific) inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Histone acetyltransferase inhibitor
UGT2B substrate
X-methyl-His dipeptidase inhibitor
Shikimate 5-dehydrogenase inhibitor
CYP2B6 substrate
AR expression inhibitor
D-cysteine desulfhydrase inhibitor
CYP2C29 substrate
Antiseptic
3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor
Aspartate racemase inhibitor
Complement factor D inhibitor
Glutamin-(asparagin-)ase inhibitor
RNA-directed RNA polymerase inhibitor
Saluretic
Asparagine-tRNA ligase inhibitor
Arylmalonate decarboxylase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
6-Methylsalicylate decarboxylase inhibitor
Preneoplastic conditions treatment
Phthalate 4,5-dioxygenase inhibitor
TRPA1 agonist
Pyridoxine 5-dehydrogenase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Xaa-Pro dipeptidyl-peptidase inhibitor
UGT2B9 substrate
Antirickettsial
CYP2F1 substrate
Aldosterone antagonist
Antifungal
Indanol dehydrogenase inhibitor
Diabetic nephropathy treatment
Dichloromuconate cycloisomerase inhibitor
CYP2A5 substrate
Free radical scavenger
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Choline dehydrogenase inhibitor
3'-Demethylstaurosporine O-methyltransferase inhibitor
Growth hormone agonist
Cell wall biosynthesis inhibitor
Diamine N-acetyltransferase inhibitor
Gentisate 1,2-dioxygenase inhibitor
Guanidinoacetate N-methyltransferase inhibitor
D-glutamate oxidase inhibitor
Hippurate hydrolase inhibitor
Interferon antagonist

Acetolactate decarboxylase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
Membrane permeability enhancer
Triose-phosphate isomerase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Anaphylatoxin receptor antagonist
Metalloproteinase D inhibitor
Nitric oxide scavenger
2,4-Dichlorophenol 6-monooxygenase inhibitor
Haloalkane dehalogenase inhibitor
Ribitol 2-dehydrogenase inhibitor
Tauropine dehydrogenase inhibitor
Cytochrome-b5 reductase inhibitor
Aspergillus nuclease S1 inhibitor
Malate-CoA ligase inhibitor
Methylaspartate ammonia-lyase inhibitor
Sorbitol dehydrogenase inhibitor
Retinol O-fatty-acyltransferase inhibitor
Interferon gamma antagonist
Succinate dehydrogenase inhibitor
Antineoplastic (lung cancer)
Cycloartenol synthase inhibitor
Myc inhibitor
Antineoplastic (thyroid cancer)
ATP deaminase inhibitor
Transcription factor NF kappa B inhibitor
Cysteine-S-conjugate beta-lyase inhibitor
Caspase 3 stimulant
CYP2C6 substrate
Leukotriene-C4 synthase inhibitor
Vascular dementia treatment
Pitrilysin inhibitor
UGT1A1 substrate
D-lactate dehydrogenase inhibitor
Guanidinoacetate kinase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Formate-dihydrofolate ligase inhibitor
Benzoylformate decarboxylase inhibitor
Acyl-CoA hydrolase inhibitor
Palmitoyl-CoA hydrolase inhibitor
Choline-sulfatase inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
CYP2C12 substrate
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Testosterone 17beta-dehydrogenase inhibitor
Phloroglucinol reductase inhibitor
Lactate 2-monooxygenase inhibitor

Uroporphyrinogen decarboxylase inhibitor
4,5-Dihydroxyphthalate decarboxylase inhibitor
Beta-amylase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Cushing's syndrome treatment
O-aminophenol oxidase inhibitor
tRNA (guanine-N1-)-methyltransferase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Serratia marcescens nuclease inhibitor
4-Nitrophenylphosphatase inhibitor
Benzoate 4-monooxygenase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Lysine decarboxylase inhibitor
Trimethyllysine dioxygenase inhibitor
Indoleacetaldoxime dehydratase inhibitor
D-arabinonolactone oxidase inhibitor
Galactokinase inhibitor
Oxaloacetate decarboxylase inhibitor
(S)-3-amino-2-methylpropionate transaminase inhibitor
Allophanate hydrolase inhibitor
Sedoheptulose-bisphosphatase inhibitor
Polyporopepsin inhibitor
Choline kinase inhibitor
Thiamine-phosphate kinase inhibitor
Gluconate dehydratase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Aspartyl aminopeptidase inhibitor
Antineoplastic (lymphoma)
Acetolactate synthase inhibitor
Acylglycerone-phosphate reductase inhibitor
Reductant
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
Anthranilate phosphoribosyltransferase inhibitor
3-Isopropylmalate dehydrogenase inhibitor
2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor
Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Methylglutamate dehydrogenase inhibitor
CYP2B4 substrate
Antiinfective
Antiosteoporotic
Kainate receptor 1 antagonist
Venom exonuclease inhibitor
UGT1A4 substrate
Nitric oxide antagonist
Glycerol dehydratase inhibitor
Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor
Antimyopathies
X-Pro dipeptidase inhibitor

CYP26A substrate
D-stereospecific aminopeptidase inhibitor
HDL-cholesterol increasing
Ornithine decarboxylase inhibitor
UGT2B17 substrate
Glutamate N-acetyltransferase inhibitor
Dipeptidase E inhibitor
Pyroglutamyl-peptidase II inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Pseudolysin inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Carnitine 3-dehydrogenase inhibitor
Farnesoid X receptor antagonist
Antifibrinolytic
Calcium channel (voltage-sensitive) activator
2-Methylcitrate dehydratase inhibitor
Deoxyribonuclease I inhibitor
Protein kinase stimulant
Glyoxylate reductase (NADP+) inhibitor
CYP2B5 substrate
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Alcohol dehydrogenase (NADP+) inhibitor
Muconate cycloisomerase inhibitor
Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor
Anthranilate synthase inhibitor
Asparaginase inhibitor
Phosphoinositide phospholipase C inhibitor
Aldehyde dehydrogenase (NAD+) inhibitor
Gametolysin inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Thiol S-methyltransferase inhibitor
Hemostatic
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Bone diseases treatment
Protein-disulfide reductase (glutathione) inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Fructuronate reductase inhibitor
Tagaturonate reductase inhibitor
Carboxylate reductase inhibitor
Protein synthesis inhibitor
L-galactonolactone oxidase inhibitor
Isoquinoline 1-oxidoreductase inhibitor
Diphosphomevalonate decarboxylase inhibitor
Glutathione peroxidase inhibitor
Thyroid hormone antagonist
Inorganic diphosphatase inhibitor
UGT1A10 substrate
Glucarate dehydratase inhibitor
Guanidinopropionase inhibitor
Xanthommatin reductase inhibitor

Nicotinamide-nucleotide adenylyltransferase inhibitor
Malate dehydrogenase inhibitor
NAD⁺ kinase inhibitor
Sarcosine oxidase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Apoptosis agonist
Mandelate 4-monooxygenase inhibitor
Aryl-aldehyde dehydrogenase (NADP⁺) inhibitor
Hepatoprotectant
Estrone sulfotransferase inhibitor
Rhodotorulapepsin inhibitor
Beta-mannosidase inhibitor
Antiinfertility, female
Antithrombotic
Diaminopimelate dehydrogenase inhibitor
Vitamin
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Phospholipase C inhibitor
Neurotransmitter antagonist
DNA synthesis inhibitor
Antineoplastic (non-small cell lung cancer)
Cyclic AMP agonist
Phospholipase inhibitor
Acid-sensing ion channel blocker
Propionate-CoA ligase inhibitor
Adenylate cyclase stimulant
Adenylate kinase inhibitor
Aminopeptidase Y inhibitor
Arylacetonitrilase inhibitor
Formaldehyde dehydrogenase inhibitor
Histamine release stimulant
Omega-amidase inhibitor
Glucose 1-dehydrogenase inhibitor
Glucan 1,3-beta-glucosidase inhibitor
L-fuconate dehydratase inhibitor
Lysase inhibitor
UGT1A8 substrate
Choline-phosphate cytidylyltransferase inhibitor
Acaricide
(S)-2-hydroxy-acid oxidase inhibitor
Galactoside O-acetyltransferase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Nucleotidase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Gonadotropin antagonist
3'-Nucleotidase inhibitor
5-Aminolevulinate synthase inhibitor
JAK2 expression inhibitor
Threonine ammonia-lyase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor

2-Hydroxy-3-oxoadipate synthase inhibitor
Glycine transaminase inhibitor
Melanin inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
D-alanine transaminase inhibitor
Nuclease inhibitor
Lipocortins synthesis antagonist
Galactose oxidase inhibitor
Glycine receptor agonist
Mycodextranase inhibitor
Cysteine synthase inhibitor
Oxaloacetate tautomerase inhibitor
Glutamate (mGluR1) antagonist
Vomilenine glucosyltransferase inhibitor
Feruloyl esterase inhibitor
Acetylserotonin O-methyltransferase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
GDP-mannose 6-dehydrogenase inhibitor
Penicillin amidase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
CYP4A1 substrate
Antithyroid
Arylamine N-acetyltransferase inhibitor
ATP adenylyltransferase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
CYP7 inhibitor
Uric acid excretion stimulant
Quinate 5-dehydrogenase inhibitor
Deoxycytidine deaminase inhibitor
GST A substrate
L-lactate dehydrogenase (cytochrome) inhibitor
Membrane integrity antagonist
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Platelet aggregation stimulant
Imidazoleacetate 4-monooxygenase inhibitor
Glycine N-acyltransferase inhibitor
Farnesoid X receptor agonist
L-lysine oxidase inhibitor
Histidinol dehydrogenase inhibitor
Maleate hydratase inhibitor
Diaminopropionate ammonia-lyase inhibitor
CYP2E1 substrate
Phospholipase A2 inhibitor
Lactaldehyde dehydrogenase inhibitor
Allantoicase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Leukopoiesis stimulant
3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
Cerebroside-sulfatase inhibitor

Pyruvate carboxylase inhibitor
Decylcitrate synthase inhibitor
Dihydrouracil oxidase inhibitor
VCAM1 expression inhibitor
Phobic disorders treatment
Lactate-malate transhydrogenase inhibitor
Antineoplastic enhancer
Endo-1,4-beta-xylanase inhibitor
Carnosine synthase inhibitor
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Phenylalanine decarboxylase inhibitor
Laminaribiose phosphorylase inhibitor
Heat shock protein 70 antagonist
Cerevisin inhibitor
Sucrose-phosphate synthase inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Muramoyltetrapeptide carboxypeptidase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Phosphoenolpyruvate mutase inhibitor
SMN2 expression enhancer
Sclerosant
Alcohol oxidase inhibitor
Cardioprotectant
Butyrate-CoA ligase inhibitor
Aconitate hydratase inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Erythro-3-hydroxyaspartate ammonia-lyase inhibitor
CDC25A inhibitor
CYP2E substrate
ICAM1 expression inhibitor
Thrombolytic
Trimethylamine-N-oxide reductase inhibitor
UGT2B1 substrate
Sulfinioalanine decarboxylase inhibitor
Pancreatic elastase inhibitor
Serine-sulfate ammonia-lyase inhibitor
Fructose-2,6-bisphosphate 2-phosphatase inhibitor
Estradiol 17alpha-dehydrogenase inhibitor
TNF expression inhibitor
Fumarylacetoacetase inhibitor
Protein phosphatase inhibitor
Phosphoribulokinase inhibitor
Tryptophan 2,3-dioxygenase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Chondroitin 6-sulfotransferase inhibitor
Glutamate decarboxylase inhibitor
Antiseborrheic
Homogentisate 1,2-dioxygenase inhibitor

Homoserine dehydrogenase inhibitor
Thermitase inhibitor
Isocitrate lyase inhibitor
Calcium-sensing receptor agonist
Arachidonic acid antagonist
Glutamate dehydrogenase inhibitor
Diiodophenylpyruvate reductase inhibitor
Aminolevulinate transaminase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Sulfate adenylyltransferase (ADP) inhibitor
Photosensitizer
Cancer associated disorders treatment
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
UDP-N-acetylmuramate-L-alanine ligase inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
Polyamine oxidase inhibitor
CYP26 substrate
Anabolic
CYP2D16 substrate
4-Alpha-glucanotransferase inhibitor
Pyridoxamine-phosphate oxidase inhibitor
Cellulase inhibitor
Antioxidant
Hydroxysteroid dehydrogenase inhibitor
Ovulation inhibitor
N-acetylneuraminate lyase inhibitor
Endopeptidase So inhibitor
Prostate disorders treatment
Gluconokinase inhibitor
Astringent
Lysostaphin inhibitor
UGT2B4 substrate
Valine-tRNA ligase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
3-Phytase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Aryl sulfotransferase inhibitor
Chloride peroxidase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Heme oxygenase inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
2-Acylglycerol O-acyltransferase inhibitor
CYP2D15 substrate
Aminoacylase inhibitor
MAP kinase stimulant
Malyl-CoA lyase inhibitor
CYP3A5 substrate
3(or 17)beta-hydroxysteroid dehydrogenase inhibitor

CYP1B substrate
Alpha-amylase inhibitor
NADH dehydrogenase inhibitor
Proliferative diseases treatment
Ca²⁺-transporting ATPase inhibitor
Diguanidinobutanase inhibitor
4-Hydroxybenzoate 3-monooxygenase [NAD(P)H] inhibitor
Propanediol dehydratase inhibitor
Cytosolic phospholipase A2 inhibitor
Bontoxilysin inhibitor
Membrane dipeptidase inhibitor
Tyrosine-ester sulfotransferase inhibitor
Aldehyde dehydrogenase inhibitor
Antineoplastic (uterine cancer)
Phenol 2-monooxygenase inhibitor
2-Pyrocatechuate decarboxylase inhibitor
Cholestenone 5alpha-reductase inhibitor
Opioid dependency treatment
4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor
Nicotinamidase inhibitor
L-ascorbate peroxidase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor
Laxative
Clavamate synthase inhibitor
Prunasin beta-glucosidase inhibitor
Protein-tyrosine phosphatase inhibitor
Acetoin dehydrogenase inhibitor
GABA transporter 2 inhibitor
Urolithiasis treatment
Alpha-Methylacyl-CoA racemase inhibitor
Isocitrate dehydrogenase (NAD⁺) inhibitor
Insulysin inhibitor
Thimet oligopeptidase inhibitor
Serine-glyoxylate transaminase inhibitor
Antihyperlipoproteinemic
Aldehyde oxidase inhibitor
Thiosulfate sulfurtransferase inhibitor
Inositol oxygenase inhibitor
Adenine nucleotide translocase inhibitor
Mannonate dehydratase inhibitor
Butyryl-CoA dehydrogenase inhibitor
CYP4B substrate
Shikimate O-hydroxycinnamoyltransferase inhibitor
D-malate dehydrogenase (decarboxylating) inhibitor
Sigma 1 receptor agonist
NADPH peroxidase inhibitor
Pyruvate dehydrogenase (lipoamide) inhibitor
Alanine transaminase inhibitor
Serine-phosphoethanolamine synthase inhibitor
Xylan 1,4-beta-xylosidase inhibitor

Guanidinobutyrase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Phosphoserine phosphatase inhibitor
CYP4A2 substrate
NOS2 expression inhibitor
Acylaminoacyl-peptidase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Cellobiose phosphorylase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
Isocitrate dehydrogenase (NADP+) inhibitor
Peptidyl-dipeptidase B inhibitor
Cathepsin H inhibitor
CYP4B1 substrate
Alanine dehydrogenase inhibitor
Glycerol-3-phosphate dehydrogenase (NAD+) inhibitor
Alanine racemase inhibitor
Tentoxilysin inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Proline dehydrogenase inhibitor
Carboxylesterase inhibitor
Lysine 2-monooxygenase inhibitor
3-Deoxy-7-phosphoheptulonate synthase inhibitor
2-Methylcitrate synthase inhibitor
UGT2B10 substrate
Plastoquinol-plastocyanin reductase inhibitor
Pectate lyase inhibitor
K(Ca) 3.1 channel blocker
Fibrolase inhibitor
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Cytosine deaminase inhibitor
Aspartate transaminase inhibitor
11-Cis-retinyl-palmitate hydrolase inhibitor
Phosphate acetyltransferase inhibitor
Contraceptive male
Phosphoglycerate mutase inhibitor
Inositol-polyphosphate 5-phosphatase inhibitor
Glutamate (mGluR6) antagonist
4-Pyridoxolactonase inhibitor
4-Hydroxybenzoate 1-hydroxylase inhibitor
Xylose isomerase inhibitor
4-Hydroxybenzoate decarboxylase inhibitor
Procollagen-lysine 5-dioxygenase inhibitor
Chorismate mutase inhibitor
Glutamate (mGluR8) agonist
Long-chain-acyl-CoA dehydrogenase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Glycosylphosphatidylinositol phospholipase D inhibitor
Acid phosphatase inhibitor

CYP2B10 substrate
Ubiquitin thiolesterase inhibitor
Tripeptide aminopeptidase inhibitor
Arylsulfatase inhibitor
Oxoglutarate dehydrogenase (lipoamide) inhibitor
Arginine deiminase inhibitor
Diiiodotyrosine transaminase inhibitor
GABA uptake inhibitor
UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
Hydroperoxide dehydratase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Peptidyl-glycinamidase inhibitor
Succinic dehydrogenase inhibitor
[myelin basic protein]-arginine N-methyltransferase inhibitor
Steroid sulfotransferase inhibitor
Galactoside 2-alpha-L-fucosyltransferase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Diuretic
Glucosamine-6-phosphate deaminase inhibitor
Thioredoxin reductase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
Agmatinase inhibitor
Para amino benzoic acid antagonist
D-Ala-D-Ala ligase inhibitor
Antimetastatic
3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor
Glycine N-benzoyltransferase inhibitor
Homocitrate synthase inhibitor
Phosphoglucomutase inhibitor
L-3-cyanoalanine synthase inhibitor
Ferredoxin-NADP⁺ reductase inhibitor
Antiviral (Influenza)
Yeast ribonuclease inhibitor
L lactate dehydrogenase inhibitor
Glycerol-3-phosphate O-acyltransferase inhibitor
Antiprotozoal (Amoeba)
Glucosamine 6-phosphate N-acetyltransferase inhibitor
Trimerelysin II inhibitor
Potassium channel intermediate-conductance Ca-activated blocker
Phosphoketolase inhibitor
Antispirochetal
Antidyskinetic
TH expression enhancer
Alpha-L-rhamnosidase inhibitor
Urocanate hydratase inhibitor
UGT1A3 substrate
3-Hydroxyanthranilate 3,4-dioxygenase inhibitor
Hypoxia inducible factor 1 alpha inhibitor
Glycerol-3-phosphate oxidase inhibitor
Phosphatidate cytidyltransferase inhibitor

Agaritrine gamma-glutamyltransferase inhibitor
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Muscular dystrophy treatment
Oryzin inhibitor
Anticholelithogenic
4-Hydroxy-2-oxoglutarate aldolase inhibitor
Antialcoholic
Pyruvate, phosphate dikinase inhibitor
Transthyretin amyloid fibril formation inhibitor (Alzheimer's type dementia)
Gastritis treatment
Isoamylase inhibitor
Phosphomevalonate kinase inhibitor
Flavin-containing monooxygenase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
UGT1A7 substrate
Altronate dehydratase inhibitor
tRNA adenylyltransferase inhibitor
Gestagen antagonist
Horriylsin inhibitor
Envelysin inhibitor
1,3-Beta-glucan synthase inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
CYP19A1 expression inhibitor
Heme oxygenase stimulant
Beta-ureidopropionase inhibitor
Succinate-semialdehyde dehydrogenase inhibitor
Malate dehydrogenase (decarboxylating) inhibitor
Bcl2 antagonist
Nitrate reductase inhibitor
Phosphoglycolate phosphatase inhibitor
Oxygen scavenger
Chelator
Sepiapterin reductase inhibitor
Leukotriene synthesis inhibitor
Dihydropyrimidinase inhibitor
Clostripain inhibitor
CYP2A2 substrate
UGT2B28 substrate
Pappalysin-1 inhibitor
Glycine N-choloyltransferase inhibitor
CYP26 inhibitor
Antiparasitic
Thromboxane synthase stimulant
Proteasome ATPase inhibitor
Tannase inhibitor
2-Aminoheptano-6-lactam racemase inhibitor
2-Aminoadipate transaminase inhibitor
Saccharopine dehydrogenase (NAD⁺, L-lysine-forming) inhibitor
Glucuronolactone reductase inhibitor
CDC25B inhibitor

Arylformamidase inhibitor
4-Phytase inhibitor
Methanol dehydrogenase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
HMG CoA synthase inhibitor
4-Hydroxybenzoate 3-monooxygenase inhibitor
Enoyl-CoA hydratase inhibitor
Expectorant
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
Phenylalanine 4-hydroxylase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Nitrilase inhibitor
Aerobactin synthase inhibitor
Anesthetic local
Aspartate kinase inhibitor
dCTP deaminase inhibitor
Antiinflammatory, ophthalmic
Aspartate-semialdehyde dehydrogenase inhibitor
Mucolytic
Putrescine oxidase inhibitor
Catalase inhibitor
Hair growth stimulant
Phosphatidate phosphatase inhibitor
Prostaglandin antagonist
5-Aminovalerate transaminase inhibitor
CTP synthase inhibitor
Ganglioside galactosyltransferase inhibitor
Lipoprotein disorders treatment
Orcinol 2-monooxygenase inhibitor
Vasodilator, peripheral
Glutamate dehydrogenase [NAD(P)+] inhibitor
Peptidyl-Lys metalloendopeptidase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Pyruvate dehydrogenase inhibitor
Catechol 1,2-dioxygenase inhibitor
Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
Glycolaldehyde dehydrogenase inhibitor
3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor
Interleukin 1a antagonist
Acyl-CoA dehydrogenase inhibitor
Mandelate racemase inhibitor
Tropinesterase inhibitor
Catechol oxidase inhibitor
Orsellinate decarboxylase inhibitor
Secretase alpha stimulant
Secretase stimulant
Fucosterol-epoxide lyase inhibitor
[acyl-carrier-protein] S-malonyltransferase inhibitor
Hydroxymethylglutaryl-CoA lyase inhibitor
Hematinic

UDP-glucose 4-epimerase inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Pyruvate, water dikinase inhibitor
Meprin B inhibitor
ATP phosphoribosyltransferase inhibitor
Respiratory analeptic
Saccharolysin inhibitor
Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
Acrosin inhibitor
Glutamate receptor antagonist
Dihydroorotate oxidase inhibitor
Cystathionine beta-lyase inhibitor
Protein-tyrosine phosphatase 1B inhibitor
Ketoheokinase inhibitor
Protein synthesis stimulant
Cystathionine beta-synthase inhibitor
Phosphofructokinase-1 inhibitor
Coagulant
Indole-3-acetaldehyde reductase (NADPH) inhibitor
N-acetylglucosamine-6-phosphate deacetylase inhibitor
Thioredoxin inhibitor
UGT1A6 substrate
Pyrroline-5-carboxylate reductase inhibitor
Riboflavin synthase inhibitor
Beta-D-fucosidase inhibitor
Glutamate dehydrogenase (NADP+) inhibitor
Penicillopepsin inhibitor
Antitussive
Snapalysin inhibitor
Alcohol dehydrogenase substrate
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Maltose-transporting ATPase inhibitor
Microtubule formation inhibitor
Gingipain R inhibitor
2-Methyl-branched-chain-enoyl-CoA reductase inhibitor
Prostaglandin E1 antagonist
Antineoplastic (endocrine cancer)
Calcium regulator
RELA expression inhibitor
Bisphosphoglycerate mutase inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Sweetener
Methylaspartate mutase inhibitor
Check point kinase 2 inhibitor
Enteropeptidase inhibitor
3-Hydroxybutyrate dehydrogenase inhibitor
Stipitatonate decarboxylase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor
Serine-tRNA ligase inhibitor
Transcription factor NF kappa B inhibitor

Inositol-3-phosphate synthase inhibitor
3-Dehydroquinate synthase inhibitor
2-Oxoaldehyde dehydrogenase (NAD⁺) inhibitor
Propionate CoA-transferase inhibitor
Nicotinamide-nucleotide amidase inhibitor
Dihydroorotate dehydrogenase inhibitor
Phenylalanine dehydrogenase inhibitor
Glutamate (mGluR4) agonist
Plasminogen activator inhibitor antagonist
Pectin lyase inhibitor
Pantoate-beta-alanine ligase inhibitor
Anthrax lethal factor inhibitor
Adenine deaminase inhibitor
CYP3A3 substrate
UDP-N-acetylmuramate dehydrogenase inhibitor
CYP2C2 substrate
Prostaglandin H2 antagonist
3-Ketovalidoxylamine C-N-lyase inhibitor
Cathepsin G inhibitor
Isopenicillin-N synthase inhibitor
Glycerol kinase inhibitor
Antipyretic
CYP24 substrate
CYP19 inhibitor
Mediator release inhibitor
Acidifying agent non gastric
Betaine-aldehyde dehydrogenase inhibitor
Nitrile hydratase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
2-Nitropropane dioxygenase inhibitor
GABA transporter inhibitor
Vasoprotector
Methylenetetrahydrofolate dehydrogenase (NADP⁺) inhibitor
Contraceptive female
Adenylyl-sulfate kinase inhibitor
Trehalose-phosphatase inhibitor
Ornithine-oxo-acid transaminase inhibitor
Protocatechuate 3,4-dioxygenase inhibitor
Nicotinic acid receptor 2 agonist
Endonuclease (influenza) inhibitor
Riboflavin kinase inhibitor
S-methyl-5-thioribose kinase inhibitor
Asparagine-oxo-acid transaminase inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Formate dehydrogenase inhibitor
Arabinose-5-phosphate isomerase inhibitor
Protein-glutamate O-methyltransferase inhibitor
Cyclohexadienyl dehydrogenase inhibitor
Linoleate diol synthase inhibitor
Guanylate kinase inhibitor

3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor
N6-methyl-lysine oxidase inhibitor
Pregnane X receptor antagonist
L lactate dehydrogenase A inhibitor
ATPase stimulant
Thromboxane synthase inhibitor
CYP2C11 substrate
Sulfate adenylyltransferase inhibitor
L lactate dehydrogenase B inhibitor
L lactate dehydrogenase B4 inhibitor
Selenocysteine lyase inhibitor
Aureolysin inhibitor
NAT1 substrate
Lipoprotein lipase stimulant
Proline racemase inhibitor
GABA transporter 1 inhibitor
CYP2B18 substrate
Procollagen glucosyltransferase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
5-Alpha-reductase inhibitor
T-cell protein-tyrosine phosphatase inhibitor
Oxalate oxidase inhibitor
UGT2B15 substrate
Laccase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Antineoplastic antimetabolite
CYP4F2 substrate
Pantothenase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Serine O-acetyltransferase inhibitor
Glutathione reductase inhibitor
Aspergillopepsin I inhibitor
Peroxisome proliferator-activated receptor gamma antagonist
CYP2D2 inhibitor
UGT2B11 substrate
Dihydrofolate synthase inhibitor
Antibacterial, ophthalmic
Antineoplastic (gastric cancer)
Glutamate (mGluR) antagonist
Maleylacetate reductase inhibitor
Allantoate deiminase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Mucositis treatment
Inositol polyphosphate-5-phosphatase D stimulant
Kainate receptor antagonist
Insecticide
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Glutaryl-CoA dehydrogenase inhibitor
Procollagen-proline 3-dioxygenase inhibitor
Glucose-6-phosphate translocase inhibitor

Citrate (Si)-synthase inhibitor
Protein-tyrosine phosphatase epsilon inhibitor
Chemoprotective
CYP1B1 substrate
Antineoplastic (glioblastoma multiforme)
Hyperparathyroidism treatment
Glutathione synthase inhibitor
Ulcerative colitis treatment
Growth stimulant
Chalcone isomerase inhibitor
Leukotriene C antagonist
Cytidylate kinase inhibitor
tRNA cytidyltransferase inhibitor
Adenylylsulphatase inhibitor
3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor
Beta lactamase inhibitor
Arginine kinase inhibitor
Carboxy-cis,cis-muconate cyclase inhibitor
Deoxyhypusine monooxygenase inhibitor
Glutamate (mGluR group III) antagonist
Corticosteroid antagonist
Sickle-cell anemia treatment
2-Haloacid dehalogenase inhibitor
UDP-glucuronate decarboxylase inhibitor
2-Methylacyl-CoA dehydrogenase inhibitor
UGT1A9 substrate
ATPase inhibitor
L-Serine ammonia-lyase inhibitor
UDP-glucose 6-dehydrogenase inhibitor
Argininosuccinate synthase inhibitor
Prostaglandin agonist
Hydroxylamine oxidase inhibitor
L lactate dehydrogenase A4 inhibitor
Leukotriene B4 antagonist
Cysteine transaminase inhibitor
Testosterone agonist
Linoleate isomerase inhibitor
L lactate dehydrogenase C inhibitor
L lactate dehydrogenase C4 inhibitor
Uridine nucleosidase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
Oxytocic
CYP2B11 substrate
Radioprotector
Vesicular glutamate transport inhibitor
Antidote, heavy metal
Aldose 1-epimerase inhibitor
DELTA24-sterol reductase inhibitor
Peroxisome proliferator-activated receptor antagonist
N-acetylglucosamine kinase inhibitor

Glucan 1,4-alpha-glucosidase inhibitor
Antiparkinsonian, tremor relieving
Potassium channel (Ca-activated) activator
CYP19 substrate
Gout treatment
Deoxyadenosine kinase inhibitor
Adenylate cyclase inhibitor
Protocatechuate 4,5-dioxygenase inhibitor
Aldehyde dehydrogenase substrate
Prephenate dehydratase inhibitor
Glycogen (starch) synthase inhibitor
Protein kinase C stimulant
Antibiotic Quinolone-like
Metabolic disease treatment
Adenylate cyclase I inhibitor

Tetrabenazine

Molecular Mechanism (initial) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

Molecular Mechanism (repurposed) :

vesicular monoamine transporter 2 (VMAT2) inhibitor

initial indication(s):

Huntington's disease

Repurposed indication(s):

extrapyramidal disorders

tardive dyskinesia

Predicted Activities

5 Hydroxytryptamine release stimulant
Gluconate 2-dehydrogenase (acceptor) inhibitor
MAP kinase stimulant
UGT2B12 substrate
Nootropic
Antidyskinetic

Vesicle monoamine transporter inhibitor

Acetylcholine neuromuscular blocking agent
Tardive dyskinesia treatment
Vesicle monoamine transporter 2 inhibitor
Antiinflammatory
Antieczematic
CYP2H substrate
General pump inhibitor
Antinociceptive
CYP3A5 substrate
Neurodegenerative diseases treatment
CYP2D2 inhibitor
Sigma receptor agonist
Mucomembranous protector
HIF1A expression inhibitor
CYP3A4 substrate

Fibrinolytic
Antileprosy
Fibrinogen receptor antagonist
Extrapyramidal disorders treatment
Membrane permeability inhibitor
Huntington's disease treatment
CYP2E1 inducer
CYP3A3 substrate
Antipruritic, allergic
CYP3A substrate
Antimycobacterial
CYP2C19 substrate
Spasmolytic
Histamine release stimulant
CYP3A4 inducer
Polarisation stimulant
CYP3A inducer
P-glycoprotein substrate
Antipruritic
Muscle relaxant
Vasodilator, peripheral
Ovulation inhibitor
Opioid dependency treatment
Nicotinic alpha4beta4 receptor agonist
Antitussive
Ubiquinol-cytochrome-c reductase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
CYP2C substrate
Antineurotic
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
CYP3A1 substrate
Platelet aggregation stimulant
Antisecretoric
Oxygen scavenger
Antipsychotic
CYP3A2 substrate
Platelet adhesion inhibitor
5 Hydroxytryptamine 7L antagonist
Octopamine antagonist
CYP2D6 substrate
Antibacterial
Gastrointestinal motility stimulant
Antiprotozoal (Leishmania)
Follicle-stimulating hormone agonist
ATPase stimulant
Uterine stimulant
CYP2D substrate
Immunosuppressant
Antineoplastic alkaloid
Spasmolytic, Papaverin-like

Expectorant
Antiischemic, cerebral
5 Hydroxytryptamine 7S antagonist
5 Hydroxytryptamine 1E antagonist
Steroid N-acetylglucosaminyltransferase inhibitor
Neurotransmitter antagonist
Neurotransmitter uptake inhibitor
Menopausal disorders treatment
CYP2D1 substrate
Opioid kappa 3 receptor antagonist
Xenobiotic-transporting ATPase inhibitor
CYP2C9 inducer
Antineoplastic (non-Hodgkin's lymphoma)
P-glycoprotein inhibitor
Oxidoreductase inhibitor
Sigma 1 receptor agonist
Dopamine release stimulant
Monoamine uptake inhibitor
Antiviral (Rhinovirus)
CYP2C8 substrate
Antiprotozoal (Amoeba)
Oxytocic
Prolactin inhibitor
Carminative
Antimyopathies
Tyrosine 3 hydroxylase inhibitor
Leukopoiesis inhibitor
Antineoplastic (bone cancer)
Cardiovascular analeptic
Ophthalmic drug
TRKB antagonist
Antihypoxic
Plastoquinol-plastocyanin reductase inhibitor
CC chemokine receptor 2B antagonist
CYP2D15 substrate
Neuropeptide Y4 antagonist
P-glycoprotein 1 inhibitor
Gonadotropin antagonist
Anticonvulsant
UGT2B7 substrate
Nav1.3 sodium channel blocker
Antischistosomal
Uterine relaxant
JAK2 expression inhibitor
Microtubule formation inhibitor
Tumour necrosis factor alpha release inhibitor
HCV IRES inhibitor
UGT2B1 substrate
LDLR expression enhancer
Prostate disorders treatment

Antiprotozoal (Plasmodium)
Respiratory analeptic
Anesthetic general
RELA expression inhibitor
Myc inhibitor
AR expression inhibitor
Methyltransferase substrate
Pin1 inhibitor
Spasmolytic, urinary
Anxiolytic
Antiinflammatory, intestinal
Antiparkinsonian, tremor relieving
Lipid peroxidase inhibitor
Apoptosis agonist
Formate-dihydrofolate ligase inhibitor
Vasoprotector
Alpha 2 adrenoreceptor antagonist
Antiglaucomic
Retinoic acid metabolism inhibitor
Phobic disorders treatment
Raynaud's phenomenon treatment
Antimetastatic
Tubulin antagonist
Neurotrophic factor
Antineoplastic (sarcoma)
Anaphylatoxin receptor antagonist
Leukopoiesis stimulant
Antimycoplasmal
Antiinflammatory, ophthalmic
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
UGT2B substrate
Dementia treatment
Cognition disorders treatment
Cytokine release inhibitor
Hyperprolactinemia treatment
Narcotic antagonist
Interleukin 2 agonist
Alopecia treatment
CYP2A11 substrate
Antiinfertility, female
Aldosterone antagonist
Preneoplastic conditions treatment
Matrix metalloproteinase 2 (membrane-type) inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
UGT2B9 substrate
Antitussive, narcotic
Protein kinase stimulant

Laxative
TNF expression inhibitor
Proteasome ATPase inhibitor
CC chemokine 4 receptor antagonist
Interleukin 10 antagonist
CYP2B10 substrate
Dermatologic
Tocolytic
Nicotinic alpha4beta2 receptor antagonist
Imidazoline I1 receptor agonist
Adrenaline release stimulant
Mucolytic
Lymphocytopoiesis inhibitor
Antihypertensive
Prostatic (benign) hyperplasia treatment
UGT2B10 substrate
CYP7 inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Antifungal enhancer
Vasodilator, coronary
Cholinergic
Lysyl oxidase inhibitor
Amyotrophic lateral sclerosis treatment
GST M1-1 substrate
Membrane permeability enhancer
Analeptic
CYP2C6 substrate
Alpha adrenoreceptor antagonist
Prostaglandin D2 agonist
Septic shock treatment
Antituberculosic
HMG CoA synthase inhibitor
Thermitase inhibitor
Acetylcholine M2 receptor agonist
Rotamase (FKBP) inhibitor
Antiamyloidogenic
Antiseborrheic
Thiamine-triphosphatase inhibitor
CYP2B6 substrate
CYP2C8 inhibitor
UGT2B17 substrate
Gastric emptying disorders treatment
Nav1.2 sodium channel blocker
Enteropeptidase inhibitor
Aldehyde oxidase inhibitor
Beta tubulin antagonist
5 Hydroxytryptamine 7 agonist
Peptidyl-prolyl cis-trans isomerase inhibitor
Calcium antagonist
Antiparkinsonian

Amine dehydrogenase inhibitor
Antihypotensive
Immunoglobulin Fc receptor antagonist
Fusarinine-C ornithinesterase inhibitor
Transcription factor NF kappa A inhibitor
Antineoplastic (thyroid cancer)
Nav1.8 sodium channel blocker
NOS2 expression inhibitor
Polyporopepsin inhibitor
Nav1.5 sodium channel blocker
Melatonin 1b antagonist
TP53 expression enhancer
5-O-(4-coumaroyl)-D-quinic acid 3'-monooxygenase inhibitor
Melatonin 1 agonist
CYP19 substrate
Cyclooxygenase 3 inhibitor
Leukocyte elastase inhibitor
Dopamine D2A antagonist
Beta 1 adrenoreceptor agonist
Pantetheine-phosphate adenylyltransferase inhibitor
UGT1A5 substrate
Vasodilator
Bronchodilator
Protein synthesis inhibitor
Opioid kappa 1 receptor antagonist
Antiacne
Cushing's syndrome treatment
Dopamine D5 antagonist
Thrombolytic
GST P1-1 substrate
CYP2A substrate
Antiprotozoal
NMDA receptor glutamate site antagonist
Diabetic neuropathy treatment
Antibiotic Glycopeptide-like
Vanilloid 1 agonist
Dopamine D2S antagonist
Chlordecone reductase inhibitor
Prolactin release inhibitor
Polarisation inhibitor
Vascular dementia treatment
Calcium regulator
Cytochrome P450 stimulant
Shab potassium channel blocker
Inotropic
Beta-carotene 15,15'-monooxygenase inhibitor
Antibiotic
Calcineurin inhibitor
Antineoplastic (small cell lung cancer)
Antihelmintic

Nicotinic receptor alpha7 subunit antagonist
Rotamase (FKBP12) inhibitor
Interferon antagonist
CYP1A1 inhibitor
Alpha 1L adrenoreceptor antagonist
Prostaglandin E1 agonist
Interferon gamma antagonist
GST P substrate
Acetylcholine nicotinic antagonist
Antiadrenergic
CYP2A10 substrate
Nav1.1 sodium channel blocker
CYP2A6 substrate
Melatonin 2 antagonist
Antibacterial, ophthalmic
ALK inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor

Thalidomide

Molecular Mechanism (initial) :

TNF-alpha production inhibitor

Molecular Mechanism (repurposed) :

cereblon (CRBN) inhibitor

initial indication(s):

sedative

nausea preventing

Repurposed indication(s):

leprosy

multiple myeloma

Predicted Activities

CYP2C12 substrate
Nicotinic alpha2beta2 receptor antagonist
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Nootropic
CYP2C11 substrate
CYP2A8 substrate
Mannan endo-1,4-beta-mannosidase inhibitor
Antineoplastic (multiple myeloma)
Antineoplastic (non-Hodgkin's lymphoma)
Pterin deaminase inhibitor
Interleukin 2 agonist
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
CYP2C6 substrate

Tumour necrosis factor alpha release inhibitor

TNF expression inhibitor
Age-related macular degeneration treatment
Electron-transferring-flavoprotein dehydrogenase inhibitor
Antiamyloidogenic
Phobic disorders treatment

CYP2C19 substrate
Lysase inhibitor
L-glutamate oxidase inhibitor
Antiviral (Picornavirus)
Glucan endo-1,6-beta-glucosidase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Antidyskinetic
3-Hydroxybenzoate 6-monooxygenase inhibitor
Fusarinine-C ornithinesterase inhibitor
Chloride peroxidase inhibitor
Membrane integrity antagonist
Interleukin 10 agonist
Ribulose-phosphate 3-epimerase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Nicotinic alpha4beta4 receptor agonist
(R)-6-hydroxynicotine oxidase inhibitor
Antihypoxic
Cholestanetriol 26-monooxygenase inhibitor
Neurotransmitter antagonist
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Immunomodulator
Polyamine-transporting ATPase inhibitor
CYP17 inhibitor
Thioredoxin inhibitor
Chitinase inhibitor
5 Hydroxytryptamine uptake stimulant
(S)-6-hydroxynicotine oxidase inhibitor
Dimethylargininase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
CYP2H substrate
Ovulation inhibitor
Peptide alpha-N-acetyltransferase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
ADP-thymidine kinase inhibitor
NADPH-cytochrome-c2 reductase inhibitor
Sickle-cell anemia treatment
5-O-(4-coumaroyl)-D-quinic acid 3'-monooxygenase inhibitor
Acetylcholine neuromuscular blocking agent
Ornithine cyclodeaminase inhibitor
Interleukin agonist
Kidney function stimulant
Prostate disorders treatment
Antileprosy
Membrane permeability inhibitor
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Pseudolysin inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
CYP2C9 inducer
CYP2C substrate
Leukopoiesis stimulant

Platelet adhesion inhibitor
Albendazole monooxygenase inhibitor
Glutamyl endopeptidase II inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Uterine relaxant
Octopamine antagonist
Macrophage colony stimulating factor agonist
CYP2D16 substrate

Antineurotic

Creatininase inhibitor
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Calcium channel (voltage-sensitive) activator
Pullulanase inhibitor
Oxygen scavenger
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Complement factor D inhibitor
Phospholipid-translocating ATPase inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Yeast ribonuclease inhibitor
Glycolate dehydrogenase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
2-Dehydropantoate 2-reductase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Antineoplastic (small cell lung cancer)
Antineoplastic (pancreatic cancer)
Glutathione thiolesterase inhibitor
Multiple sclerosis treatment
N-formylmethionyl-peptidase inhibitor
Gluconate 5-dehydrogenase inhibitor
Poly(beta-D-mannuronate) lyase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Omptin inhibitor
Antiarthritic
Glucan endo-1,3-beta-D-glucosidase inhibitor
Limulus clotting factor B inhibitor
Antiemetic
Inulinase inhibitor
Phenol O-methyltransferase inhibitor
Cytokine production inhibitor
CYP2J substrate
Chenodeoxycholytaurine hydrolase inhibitor
CYP2C9 substrate
Superoxide dismutase inhibitor
Amyotrophic lateral sclerosis treatment
Orotate reductase (NADH) inhibitor
Interleukin 2 antagonist
Diabetic neuropathy treatment
Erythropoiesis stimulant

Vasodilator, peripheral
Isopenicillin-N epimerase inhibitor
Fibrolase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Histidinol dehydrogenase inhibitor
Aspartate-ammonia ligase inhibitor
Alopecia treatment
Cardiovascular analeptic
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Pseudouridylate synthase inhibitor
Fatty-acyl-CoA synthase inhibitor
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Alkylacetylgllycerophosphatase inhibitor
Hydrogen dehydrogenase inhibitor
Acetylesterase inhibitor
Pyroglutamyl-peptidase II inhibitor
Pancreatic disorders treatment
Glutamate 5-kinase inhibitor
Lysine 2,3-aminomutase inhibitor
CYP7 inhibitor
CYP2J2 substrate
5-Oxoprolinase (ATP-hydrolysing) inhibitor
2-Haloacid dehalogenase inhibitor
Polyporopepsin inhibitor
Aspergillopepsin I inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Antineoplastic (solid tumors)
Arylmalonate decarboxylase inhibitor
GABA aminotransferase inhibitor
Adrenaline release stimulant
Protein-disulfide reductase (glutathione) inhibitor
Cytochrome P450 stimulant
CYP2C19 inducer
Spermidine dehydrogenase inhibitor
CYP2B10 substrate
Cl⁻-transporting ATPase inhibitor
Thymidylate 5'-phosphatase inhibitor
N-acetylneuraminate synthase inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
Inflammatory Bowel disease treatment
Glycosylphosphatidylinositol phospholipase D inhibitor
Arylalkyl acylamidase inhibitor
Tumour necrosis factor antagonist
Nucleoside oxidase (H₂O₂-forming) inhibitor
Allantoin racemase inhibitor
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Mitochondrial processing peptidase inhibitor
Cachexia treatment

MAP kinase stimulant
Dolichyl-phosphate beta-glucosyltransferase inhibitor
Formaldehyde transketolase inhibitor
Antimetastatic
Opioid kappa 3 receptor antagonist
CYP2D2 inhibitor
Antinociceptive
Antineoplastic (liver cancer)
Biotinidase inhibitor
Acute neurologic disorders treatment
Xylan endo-1,3-beta-xylosidase inhibitor
Sulfur reductase inhibitor
Steroid synthesis inhibitor
Venombin AB inhibitor
Sodium channel blocker class Ib
Glutamine-phenylpyruvate transaminase inhibitor
Carboxypeptidase Taq inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Serine-pyruvate transaminase inhibitor
Cyclomaltodextrinase inhibitor
Chitosanase inhibitor
Trimethylamine-oxide aldolase inhibitor
Antineoplastic (sarcoma)
Opioid dependency treatment
Sugar-phosphatase inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Platelet aggregation stimulant
Antineoplastic (non-small cell lung cancer)
Oxidoreductase inhibitor
Anticonvulsant
2-Hydroxyquinoline 8-monooxygenase inhibitor
Analeptic
Taurine dehydrogenase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Venom exonuclease inhibitor
Retinoic acid metabolism inhibitor
Limulus clotting factor C inhibitor
Skeletal muscle relaxant
Antiparkinsonian, tremor relieving
Sulfite oxidase inhibitor
Opine dehydrogenase inhibitor
Pin1 inhibitor
Centromere associated protein inhibitor
Lipocortins synthesis antagonist
4-Hydroxyproline epimerase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Fibrinogen receptor antagonist
Muscular dystrophy treatment
GABA receptor agonist

Cellulose 1,4-beta-cellobiosidase inhibitor
Trimethylamine dehydrogenase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
Poly(alpha-L-gulonate) lyase inhibitor
Tankyrase inhibitor
CYP3A4 inducer
Maleate isomerase inhibitor
Cyanoalanine nitrilase inhibitor
Diuretic inhibitor
3-Cyanoalanine hydratase inhibitor
Amine dehydrogenase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Imidazoline receptor agonist
CYP2E1 inducer
Malate oxidase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
NADPH peroxidase inhibitor
Alpha-N-acetylglucosaminidase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Interleukin 12 agonist
Immunosuppressant
Tumour necrosis factor alpha antagonist
Antineoplastic (brain cancer)
CYP2D15 substrate
NADH kinase inhibitor
Arginine 2-monooxygenase inhibitor
N-acylmannosamine kinase inhibitor
Thyroxine 5-deiodinase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
Vascular (periferal) disease treatment
CYP2A5 substrate
CYP2D1 substrate
Fucosterol-epoxide lyase inhibitor
CYP3A inducer
DNA synthesis inhibitor
GABA C receptor agonist
NAD(P)+-arginine ADP-ribosyltransferase inhibitor
Oryzin inhibitor
S-formylglutathione hydrolase inhibitor
RELA expression inhibitor
Catalase inhibitor
Vasoprotector
Glyoxylate reductase inhibitor
Antineoplastic (endocrine cancer)
Hematopoietic
DNA-3-methyladenine glycosylase I inhibitor
Acylcarnitine hydrolase inhibitor
Antisecretoric
Glucuronolactone reductase inhibitor

Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Phosphopantothencysteine decarboxylase inhibitor
1,4-Lactonase inhibitor
Methanol dehydrogenase inhibitor
N-hydroxy-2-acetamidofluorene reductase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Manganese peroxidase inhibitor
Fructose 5-dehydrogenase inhibitor
Nicotinate dehydrogenase inhibitor
Glycine amidinotransferase inhibitor
Prostatic (benign) hyperplasia treatment
Histidine N-acetyltransferase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor
Alpha-glucuronidase inhibitor
Histidinol-phosphatase inhibitor
Pancreatic elastase inhibitor
Macular degeneration treatment
Endopeptidase So inhibitor
Raynaud's phenomenon treatment
CYP2A1 substrate
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Antiperistaltic
Simian immunodeficiency virus proteinase inhibitor
Peptidyl-dipeptidase Dcp inhibitor
Oxytocic
2-Hydroxy-3-oxoadipate synthase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Alanine-tRNA ligase inhibitor
Thermitase inhibitor
Dipeptidase E inhibitor
Tryptophan 2,3-dioxygenase inhibitor
CYP2A4 substrate
Dopamine release stimulant
Respiratory analeptic
Fragilysin inhibitor
Bisphosphoglycerate phosphatase inhibitor
Pro-opiomelanocortin converting enzyme inhibitor
TP53 expression enhancer
Antidiabetic symptomatic
Prunasin beta-glucosidase inhibitor
Tetrahydroxynaphthalene reductase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Endo-1,3(4)-beta-glucanase inhibitor
S-alkylcysteine lyase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Adenylyl-sulfate reductase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Leukopoiesis inhibitor

Benzoylformate decarboxylase inhibitor
HMGCS2 expression enhancer
JAK2 expression inhibitor
Apyrase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Nicotinic alpha4beta2 receptor antagonist
Sigma receptor agonist
Phosphoenolpyruvate mutase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Penicillin amidase inhibitor
Antineoplastic (glioblastoma multiforme)
Picornain 3C inhibitor
Clavamate synthase inhibitor
Polarisation stimulant
Glucuronate isomerase inhibitor
Quisqualate antagonist
Antinephritic
Trans-pentaprenyltransferase inhibitor
Transketolase inhibitor
Muscle relaxant
Sphinganine kinase inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Meprin B inhibitor
Gingipain K inhibitor
Guanidinoacetate kinase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Aspartoacylase inhibitor
Indolepyruvate C-methyltransferase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Dimethylmaleate hydratase inhibitor
CYP2B5 substrate
Inotropic
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Glycerol dehydrogenase (NADP⁺) inhibitor
Proteasome ATPase inhibitor
Tyrosine 3 hydroxylase inhibitor
N-acetyllactosamine synthase inhibitor
Ca²⁺/calmodulin-dependent protein kinase inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
2-Oxoaldehyde dehydrogenase (NADP⁺) inhibitor
Mucinaminyserine mucinamidase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
(S)-3-amino-2-methylpropionate transaminase inhibitor
Hematopoietic inhibitor
Somatostatin 2 agonist
Cathepsin T inhibitor
DELTA14-sterol reductase inhibitor
Thiol oxidase inhibitor

Cognition disorders treatment
Leukotriene-C4 synthase inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
Glyoxylate oxidase inhibitor
Tropinesterase inhibitor
Antibiotic Glycopeptide-like
Antiviral (Influenza)
Exoribonuclease II inhibitor
Phenylalanine(histidine) transaminase inhibitor
Antineoplastic (lymphoma)
Anticarcinogenic
Membrane integrity agonist
Gallate decarboxylase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Prostate cancer treatment
Gamma-glutamyltransferase inhibitor
CYP2C3 substrate
Nicotine dehydrogenase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Cyclic AMP modulator
Angiogenesis inhibitor
CYP2F1 substrate
Muramoyltetrapeptide carboxypeptidase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Thromboxane B2 antagonist
CYP2C29 substrate
Dehydro-L-gulonate decarboxylase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Excitatory amino acid transporter EAAC1 inhibitor
3-Phytase inhibitor
Methyltransferase substrate
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Ferredoxin-nitrite reductase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Ca²⁺/calmodulin-dependent kinase I inhibitor
Tyrosine kinase stimulant
Focal adhesion kinase 2 inhibitor
Malate dehydrogenase (acceptor) inhibitor
2-Aminohexano-6-lactam racemase inhibitor
Antiviral (Poxvirus)
Anesthetic general
Ferrochelataase inhibitor
Antimycobacterial
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Cytokine modulator
Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor
Alkane 1-monooxygenase inhibitor

Releasing hormone agonist
CYP2A3 substrate
Chaperonin ATPase inhibitor
Uroporphyrinogen-III synthase inhibitor
HIF1A expression inhibitor
Glutamin-(asparagin-)ase inhibitor
CYP4A2 substrate
Melanocortin MC-4 agonist
Antineoplastic (renal cancer)
Orotate reductase (NADPH) inhibitor
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Antimyopathies
Gluconolactonase inhibitor
MO15-related protein kinase Pfmrk inhibitor
Loop diuretic
CYP2A2 substrate
Aryl-acylamidase inhibitor
Polar-amino-acid-transporting ATPase inhibitor
Antineoplastic (glioma)
Cell wall biosynthesis inhibitor
Botulin neurotoxin A light chain inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
tRNA nucleotidyltransferase inhibitor
Glutamate-tRNA ligase inhibitor
Gingipain R inhibitor
Cyclamate sulfohydrolase inhibitor
Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Uterine stimulant
Antiviral (CMV)
Antineoplastic alkaloid
Mannose isomerase inhibitor
Ligase inhibitor
IgA-specific serine endopeptidase inhibitor
Lysostaphin inhibitor
Tryptophanyl aminopeptidase inhibitor
Histamine release inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
Antiviral (Adenovirus)
Monoamine uptake inhibitor
Glucan 1,3-beta-glucosidase inhibitor
CYP2B11 substrate
N-benzyloxycarbonylglycine hydrolase inhibitor
Prolyl aminopeptidase inhibitor
Hydroxylamine oxidase inhibitor
Antismoking
Sulfite dehydrogenase inhibitor
Interleukin antagonist

Thiosulfate dehydrogenase inhibitor
Fibromyalgia syndrome treatment
Myeloblastin inhibitor
Linoleoyl-CoA desaturase inhibitor
Protein-tyrosine kinase p55(blk) inhibitor
Tryptophanamidase inhibitor
VEGF expression inhibitor
Fibrinolytic
Hyaluronic acid agonist
Selenocysteine lyase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Cyclohexanone monooxygenase inhibitor
Bisphosphoglycerate mutase inhibitor
Narcolepsy treatment
Phosphatidylinositol 3-kinase stimulant
5 Hydroxytryptamine release stimulant
Camphor 1,2-monooxygenase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
4-Hydroxyphenylacetate 3-monooxygenase inhibitor
Nitrite reductase (NO-forming) inhibitor
Sulfite reductase inhibitor
Glucan 1,6- α -glucosidase inhibitor
Nardilysin inhibitor
Antineoplastic, alkylator
Caspase 2 inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
3-Aminobutyl-CoA ammonia-lyase inhibitor
Antiulcerative
Glutaminy-peptide cyclotransferase inhibitor
Phosphatidylserine decarboxylase inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Transcription factor inhibitor
Aldosterone antagonist
Creatinase inhibitor
Pectin lyase inhibitor
Alkylator
tRNA-pseudouridine synthase I inhibitor
Liver X receptor antagonist
Histamine release stimulant
Glycopeptide α -N-acetylgalactosaminidase inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)⁺] inhibitor
Cushing's syndrome treatment
Peristaltic stimulant
MDM2 inhibitor
Cytochrome-c3 hydrogenase inhibitor
Diisopropyl-fluorophosphatase inhibitor
Antinaupathic
Dihydroxy-acid dehydratase inhibitor

CYP1A2 inducer
Antineoplastic enhancer
Glucose oxidase inhibitor
Metabolic disease treatment
3C-like protease (Human coronavirus) inhibitor
Horriylsin inhibitor
Acetylornithine deacetylase inhibitor
Tryptophan transaminase inhibitor
Lysyl oxidase inhibitor
Nuclease inhibitor
Deoxyribonuclease I inhibitor
Bontoxilysin inhibitor
Fructan beta-fructosidase inhibitor
Pancreatic endopeptidase E inhibitor
Gonadotropin antagonist
Ca²⁺/calmodulin-dependent kinase II inhibitor
CYP19 inhibitor
Mitochondrial intermediate peptidase inhibitor
Polyneuridine-aldehyde esterase inhibitor
CYP3A3 substrate
Ethanolamine-phosphate cytidyltransferase inhibitor
Membrane dipeptidase inhibitor
Dolichyl-phosphate beta-D-mannosyltransferase inhibitor
Antiviral (Herpes)
Cysteine desulfurase inhibitor
Feruloyl esterase inhibitor
Cardioprotectant
Choline acetyltransferase stimulant
Carnitinamidase inhibitor
Thiopurine S-methyltransferase inhibitor
RNA synthesis inhibitor
Smooth muscle myosin light chain kinase inhibitor
Carbon-monoxide dehydrogenase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Analgesic stimulant
Shab potassium channel blocker
Salicylate 1-monooxygenase inhibitor
Antiinflammatory, intestinal
Antimitotic
L-glucuronate reductase inhibitor
Erectile dysfunction treatment
Enteropeptidase inhibitor
Vascular adhesion protein 1 inhibitor
Galactose oxidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Leucolysin inhibitor
Triose-phosphate isomerase inhibitor
Asparagine-tRNA ligase inhibitor
5 Hydroxytryptamine 7 agonist

Mandelate 4-monooxygenase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Antiviral (Hepatitis)
Aspergillus nuclease S1 inhibitor
Urethanase inhibitor
Mannan endo-1,6- α -mannosidase inhibitor
Granzyme A inhibitor
Thiamine pyridinylase inhibitor
Cyclic AMP agonist
Preneoplastic conditions treatment
H⁺-exporting ATPase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Bothrolysin inhibitor
MAP kinase kinase 4 inhibitor
Hyponitrite reductase inhibitor
Tocolytic
EIF4E expression inhibitor
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
Phosphoinositide 5-phosphatase inhibitor
Anabolic
Chlordecone reductase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
RNA-directed RNA polymerase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
ATP phosphoribosyltransferase inhibitor
Beta-cyclopiazone dehydrogenase inhibitor
Nav1.5 sodium channel blocker
Aspergillopepsin II inhibitor
Alkylglycerone-phosphate synthase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Lysosomal Pro-X carboxypeptidase inhibitor
Allantoinase inhibitor
Focal adhesion kinase inhibitor
Sarcosine oxidase inhibitor
Methionine decarboxylase inhibitor
Ubiquitin thiolesterase inhibitor
Indoleacetaldoxime dehydratase inhibitor
Glycerol 2-dehydrogenase (NADP⁺) inhibitor
Polarisation inhibitor
Glycogen synthase kinase-3 beta inhibitor
Choline-sulfatase inhibitor
Transcription factor STAT3 inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Beta-mannosidase inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
D-threo-aldose 1-dehydrogenase inhibitor
Deoxycytidine deaminase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor
2,6-Dihydropyridine 3-monooxygenase inhibitor
DNA ligase (ATP) inhibitor

D-amino-acid dehydrogenase inhibitor
Isopenicillin-N synthase inhibitor
CYP3C substrate
Valine dehydrogenase (NADP⁺) inhibitor
Thiamine-triphosphatase inhibitor
TRPA1 agonist
CYP3A5 inducer
Lactose synthase inhibitor
Alcohol dehydrogenase [NAD(P)⁺] inhibitor
Stromelysin 2 inhibitor
Alpha-amylase inhibitor
CYP2C10 substrate
Atrolysin C inhibitor
Melanocortin agonist
Tryptophan alpha,beta-oxidase inhibitor
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor
Myocardial infarction treatment
Acidifying agent non gastric
3-Hydroxybenzoate 4-monooxygenase inhibitor
4-Nitrophenylphosphatase inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Iron-cytochrome-c reductase inhibitor
Scytalone dehydratase inhibitor
Lombricine kinase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Transcription factor NF kappa A inhibitor
Cyclin-dependent kinase 6 inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
5 Hydroxytryptamine release inhibitor
Peptidyl-dipeptidase B inhibitor
Radiosensitizer
Pappalysin-1 inhibitor
Aspartate-tRNA ligase inhibitor
Caspase 8 stimulant
Xaa-Pro dipeptidyl-peptidase inhibitor
Dihydrouracil oxidase inhibitor
Styrene-oxide isomerase inhibitor
CYP4A11 substrate
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Antiviral (Hepatitis C)
Biotin carboxylase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Saluretic
ATP-binding cassette A1 stimulant
CYP3A2 substrate

Tyrosine-protein kinase TYRO 10 inhibitor
Tentoxilysin inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Beta-amylase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
Demethylsterigmatocystin 6-O-methyltransferase inhibitor
Electrolyte absorption antagonist
Homospermidine synthase inhibitor
Phenylacetaldehyde dehydrogenase inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Myosin ATPase inhibitor
NADPH-ferrihemoprotein reductase inhibitor
Corticosteroid side-chain-isomerase inhibitor
Glycogen synthase kinase-3 inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Acetylcholine nicotinic antagonist
Antineoplastic
Prolactin inhibitor
NF-E2-related factor 2 stimulant
Methylaspartate ammonia-lyase inhibitor
FMO3 substrate
Phosphodiesterase 11A inhibitor
Phosphodiesterase XI inhibitor
Pitrilysin inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Necroptosis inhibitor
ADP-ribosylarginine hydrolase inhibitor
Aerobactin synthase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Allyl-alcohol dehydrogenase inhibitor
Phosphoinositide phospholipase C inhibitor
Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor
Wee-1 tyrosine kinase inhibitor
Hydroxymethylbilane synthase inhibitor
GST A substrate
L-threonine 3-dehydrogenase inhibitor
(R,R)-butanediol dehydrogenase inhibitor
DNA methyltransferase I inhibitor
Arylesterase inhibitor
Lactaldehyde reductase inhibitor
Maltose-transporting ATPase inhibitor
Nicotinamide-nucleotide adenyltransferase inhibitor
Aldehyde dehydrogenase 2 substrate
Dementia treatment
Protein kinase C beta inhibitor
Mucositis treatment
Cytostatic
Antiviral (Influenza A)

Ecdysone 20-monooxygenase inhibitor
8-Amino-7-oxononanoate synthase inhibitor
Creatinine deaminase inhibitor
Mycodextranase inhibitor
Acetylenecarboxylate hydratase inhibitor
Antiprotozoal (Babesia)
Cyclooxygenase substrate
Dolichyl-phosphatase inhibitor
Cellulase inhibitor
Antibacterial, ophthalmic
Intermittent claudication treatment
ErbB-1 antagonist
Allophanate hydrolase inhibitor
Beta lactamase inhibitor
Movement disorders treatment
Threonine aldolase inhibitor
O-aminophenol oxidase inhibitor
Protein kinase C gamma inhibitor
4-Coumarate-CoA ligase inhibitor
Apoptosis antagonist
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
D-xylulose reductase inhibitor
3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor
Arylacetonitrilase inhibitor
Insulin promoter
Arylsulfate sulfotransferase inhibitor
Neurokinin 2 antagonist
Antineoplastic (ovarian cancer)
Flavin-containing monooxygenase inhibitor
Picornain 2A inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
4-Hydroxymandelate oxidase inhibitor
Serralysin inhibitor
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
3-Hydroxyanthranilate oxidase inhibitor
Aldose reductase substrate
Antineoplastic (melanoma)
Sphingosine 1-phosphate receptor 1 antagonist
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Vasopressin 1 antagonist
Adenylate cyclase V inhibitor
Oxytocin agonist
NAT2 substrate
Protein kinase C epsilon inhibitor
Lysozyme inhibitor
Serine 3-dehydrogenase inhibitor
Antidiuretic hormone antagonist
GST T substrate
GST T1-1 substrate

Endothelial growth factor antagonist
Pyridoxine 4-oxidase inhibitor
CYP2B18 substrate
Polyamine oxidase inhibitor
Acetylserotonin O-methyltransferase inhibitor
Puromycin-sensitive aminopeptidase inhibitor
Protein-synthesizing GTPase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
Rhizopuspepsin inhibitor
Pectate lyase inhibitor
Calcium channel activator
Glycoprotein 3-alpha-L-fucosyltransferase inhibitor
Protein kinase C mu inhibitor
Cutinase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Polynucleotide 5'-hydroxy-kinase inhibitor
Antineoplastic (colorectal cancer)
Guanidinoacetate N-methyltransferase inhibitor
Glycine C-acetyltransferase inhibitor
Dihydropyrimidinase inhibitor
Retinal dehydrogenase inhibitor
Diamine N-acetyltransferase inhibitor
CYP19A1 expression inhibitor
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Procollagen N-endopeptidase inhibitor
Metallo-carboxypeptidase D inhibitor
Antiparkinsonian, rigidity relieving
Dermatologic
Luteinizing hormone-releasing hormone agonist
Brachyurin inhibitor
Sulfur dioxygenase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Gastrointestinal motility stimulant
D-stereospecific aminopeptidase inhibitor
3-Isopropylmalate dehydratase inhibitor
Mannitol-1-phosphatase inhibitor
D-glutamate oxidase inhibitor
UDP-N-acetylglucosamine 2-epimerase inhibitor
Cell wall synthesis inhibitor
Saccharolysin inhibitor
Glutaminase inhibitor
NOS3 expression enhancer
Haloalkane dehalogenase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Cyclopentanone monooxygenase inhibitor
Cyclin-dependent kinase 4 inhibitor
Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor
Carboxypeptidase E inhibitor

Acyl-CoA oxidase inhibitor
Calcium-sensing receptor agonist
Coccolysin inhibitor
Nicotinic receptor alpha7 subunit antagonist
Nitrite reductase [NAD(P)H] inhibitor
Acyl-lysine deacylase inhibitor
Tryptophan 2-monooxygenase inhibitor
Snapalysin inhibitor
Galactolipase inhibitor
Gaucher disease treatment
Cytochrome-b5 reductase substrate
Glutamate-5-semialdehyde dehydrogenase inhibitor
Cytochrome-b5 reductase inhibitor
Atrolysin A inhibitor
Oxytocin antagonist
Phospholipase D inhibitor
Antibacterial
Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor
Alpha glucosidase inhibitor
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Restless leg syndrome treatment
Glucosamine-1-phosphate N-acetyltransferase inhibitor
3-Methylbutanal reductase inhibitor
5 Hydroxytryptamine 7L antagonist
Alpha-N-acetylgalactosaminidase inhibitor
2-Dehydropantoate aldolase inhibitor
Cytoprotectant
Polygalacturonase inhibitor
Glycerol-1-phosphatase inhibitor
Heat shock protein agonist
GABA A inverse agonist
GABA inverse agonist
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Phosphodiesterase I inhibitor
Cellulose synthase (UDP-forming) inhibitor
Kallikrein 3 inhibitor
Carboxypeptidase D inhibitor
Antihelminthic (Fasciola)
Proline dehydrogenase inhibitor
Prion diseases treatment
Aspartate racemase inhibitor
Carboxymethylenebutenolidase inhibitor
Hydroxylamine reductase inhibitor
CTP synthase inhibitor
Tryptophan dimethylallyltransferase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
HIV-2 reverse transcriptase inhibitor
Creatine kinase inhibitor
Tauropine dehydrogenase inhibitor
Cysteine-S-conjugate beta-lyase inhibitor

Aureolysin inhibitor
1-Pyrroline-5-carboxylate dehydrogenase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Monodehydroascorbate reductase (NADH) inhibitor
Nitrile hydratase inhibitor
Glutamine-tRNA ligase inhibitor
Protein kinase C alpha inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Adenine deaminase inhibitor
Arginyltransferase inhibitor
Vasopressin 1A antagonist
Succinic dehydrogenase inhibitor
Prolyl endopeptidase inhibitor
Phosphonoacetate hydrolase inhibitor
TH expression enhancer
Omega-amidase inhibitor
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
N-acetylneuraminase lyase inhibitor
NMDA receptor polyamine site agonist
Cadherin antagonist
Protein kinase C eta inhibitor
Nav1.7 sodium channel blocker
UDP-glucose 4-epimerase inhibitor
Antihematotoxic
Diaminopimelate dehydrogenase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Histone deacetylase 8 inhibitor
L-iduronidase inhibitor
Diaminopropionate ammonia-lyase inhibitor
UDP-N-acetylglucosamine diphosphorylase inhibitor
1,4-Alpha-glucan branching enzyme inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
5 Hydroxytryptamine 2B agonist
Vasodilator
Sclerosant
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Protein kinase C nu inhibitor
Neurosin inhibitor
Nitrate reductase (cytochrome) inhibitor
Bile-salt sulfotransferase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Allantoate deiminase inhibitor
Calcitonin stimulant
Transcription factor STAT inhibitor
Anticataract
Homoserine O-succinyltransferase inhibitor
Kinesin antagonist
Kinesin-like protein 1 inhibitor
Mucomembranous protector
Dopamine D2S antagonist

Undecaprenyl-diphosphatase inhibitor
Glucan endo-1,3- α -glucosidase inhibitor
Penicillopepsin inhibitor
Urticaria treatment
Vascular dementia treatment
Somatostatin agonist
Substance P antagonist
Gametolysin inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Cytosine deaminase inhibitor
Prokinetic
Deacetoxycephalosporin-C synthase inhibitor
Pediculicide
Prephenate dehydrogenase inhibitor
Poly(ADP-ribose) polymerase inhibitor
Aminocarboxymuconate-semialdehyde decarboxylase inhibitor
Niemann-Pick C1-like 1 protein antagonist
Fumarate reductase (NADH) inhibitor
Phosphodiesterase V inhibitor
Chloride channel activator
Histone deacetylase SIRT1 inhibitor
Ferredoxin hydrogenase inhibitor
Xenobiotic-transporting ATPase inhibitor
Leucine dehydrogenase inhibitor
Methylenetetrahydrofolate dehydrogenase (NADP⁺) inhibitor
Plasmanylethanolamine desaturase inhibitor
Antiinflammatory, ophthalmic
Antiseborrheic
Protein kinase C zeta inhibitor
3-Isopropylmalate dehydrogenase inhibitor
NMDA receptor polyamine site antagonist
Phospholipase D1 inhibitor
CYP3A7 substrate
11-Cis-retinyl-palmitate hydrolase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Formate-dihydrofolate ligase inhibitor
Dactylisin inhibitor
X-methyl-His dipeptidase inhibitor
Potassium channel small-conductance Ca-activated 3 activator
Heat shock protein 70 agonist
DNA nucleotidylexotransferase inhibitor
Benzaldehyde dehydrogenase (NAD⁺) inhibitor
TRKB antagonist
Kinase inhibitor
Gastrin inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Transglutaminase 2 inhibitor
Lipotropic
Acetylcholine release stimulant
L-lysine 6-transaminase inhibitor

4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
Tryptophan 5 hydroxylase inhibitor
Site-specific DNA-methyltransferase (adenine-specific) inhibitor
Caspase 3 stimulant
Pyruvate decarboxylase inhibitor
Antirickettsial
Melanocortin 4 antagonist
Antithrombotic
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
GABA C receptor antagonist
Septic shock treatment
Vasopressin 2 antagonist
Glutamate N-acetyltransferase inhibitor
Acetylspermidine deacetylase inhibitor
Granzyme B inhibitor
Alanine transaminase inhibitor
Nociceptin (N/OFQ) receptor agonist
CYP2C8 inducer
Aldehyde dehydrogenase [NAD(P)+] inhibitor
1,5-Anhydro-D-fructose reductase inhibitor
Phosphorylase kinase inhibitor
Thiol S-methyltransferase inhibitor
Leucine transaminase inhibitor
Spasmolytic
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Testosterone 17beta-dehydrogenase inhibitor
Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor
Nerve growth factor antagonist
Morphine 6-dehydrogenase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
4-Carboxymethyl-4-methylbutenolide mutase inhibitor
Melanocortin antagonist
Poly(ADP-ribose) polymerase 2 inhibitor
Antieczematic
Cysteine synthase inhibitor
Gly-X carboxypeptidase inhibitor
TTK protein kinase inhibitor
Pantoate 4-dehydrogenase inhibitor
Sleep apnea treatment
Antifungal
3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
Phosphatidylglycerophosphatase inhibitor
Gluconate dehydratase inhibitor
CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor
Growth hormone release inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Glutamine-pyruvate transaminase inhibitor
Aryl-aldehyde dehydrogenase (NADP+) inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Topoisomerase I inhibitor

Alpha 3 adrenoreceptor agonist
mRNA (guanine-N7-)-methyltransferase inhibitor
Xanthommatin reductase inhibitor
Procollagen C-endopeptidase inhibitor
Aromatic-amino-acid transaminase inhibitor
Gastritis treatment
Endonuclease (influenza) inhibitor
N4-(beta-N-acetylglucosaminy)-L-asparaginase inhibitor
UGT2B28 substrate
Acetylcholine M3 receptor agonist
N-acetylglucosaminyldiphosphoundecaprenol N-acetyl-beta-D-mannosaminytransferase inhibitor
3'-Nucleotidase inhibitor
Allantoicase inhibitor
Histone deacetylase 4 inhibitor
D-arabinonolactone oxidase inhibitor
Thyrotropin releasing hormone agonist
Microtubule formation inhibitor
H⁺-transporting two-sector ATPase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Alpha,alpha-trehalose phosphorylase inhibitor
Acetate kinase inhibitor
N6-methyl-lysine oxidase inhibitor
Histone deacetylase class IIa inhibitor
Immunoglobulin E antagonist
Nicotinic alpha3beta4 receptor agonist
Phenylalanine decarboxylase inhibitor
Antialcoholic
GABA B receptor agonist
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
Anthranilate synthase inhibitor
Choline-phosphate cytidylyltransferase inhibitor
Bacterial efflux pump inhibitor
Galactokinase inhibitor
Hyperprolactinemia treatment
Choline kinase inhibitor
CYP1A1 inhibitor
Thiamine-phosphate kinase inhibitor
Indole-3-acetaldehyde reductase (NADPH) inhibitor
Formimidoylglutamase inhibitor
Neurokinin antagonist
CYP26 inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
D-cysteine desulfhydrase inhibitor
Ribosomal protein S6 kinase, 90-kDa inhibitor
Valine decarboxylase inhibitor
Phenylpyruvate decarboxylase inhibitor
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Anhydrotetracycline monooxygenase inhibitor
BRAF expression inhibitor

Hair growth stimulant
Plasminogen activator stimulant
Malonate-semialdehyde dehydrogenase inhibitor
Para amino benzoic acid antagonist
Hydroxylamine reductase (NADH) inhibitor
Heart failure treatment
Neuropeptide S antagonist
5 Hydroxytryptamine 3 agonist
Trehalose-phosphatase inhibitor
N-acetylglucosaminylidiphosphodolichol N-acetylglucosaminyltransferase inhibitor
Female sexual dysfunction treatment
2-Oxoglutarate decarboxylase inhibitor
CYP19 substrate
Arginine deiminase inhibitor
CYP2A13 substrate
Galactoside 2-alpha-L-fucosyltransferase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
2-Enoate reductase inhibitor
Cyanate hydratase inhibitor
Glucan 1,4-alpha-glucosidase inhibitor
CYP2G1 substrate
Diabetic retinopathy treatment
Serine-phosphoethanolamine synthase inhibitor
Trypanothione-disulfide reductase inhibitor
N-carbamoyl-L-amino-acid hydrolase inhibitor
Farnesoid X receptor antagonist
MAP3K8 inhibitor
Decylcitrate synthase inhibitor
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Hydroxysteroid dehydrogenase inhibitor
5 Hydroxytryptamine 4A antagonist
Ryanodine receptor 1 antagonist
Ryanodine receptor antagonist
Nitric-oxide synthase stimulant
Amino-acid racemase inhibitor
Protein kinase C theta inhibitor
FMO1 substrate
N-acetylneuraminate 4-O-acetyltransferase inhibitor
Phosphodiesterase 5A inhibitor
Oxalate oxidase inhibitor
Complement C5a chemotactic receptor antagonist
Melanin inhibitor
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
DNA gyrase inhibitor
Dichloromuconate cycloisomerase inhibitor
Alcohol dehydrogenase inhibitor
Neurotensin receptor antagonist
3-Oxadipate enol-lactonase inhibitor
Isoquinoline 1-oxidoreductase inhibitor
Carminative

Dimethylallyltranstransferase inhibitor
Peptidylamidoglycolate lyase inhibitor
Phosphodiesterase 9A inhibitor
N-(long-chain-acyl)ethanolamine deacylase inhibitor
Deoxyribose-phosphate aldolase inhibitor
Inositol 1,4,5-trisphosphate 3-kinase B inhibitor
Dynein ATPase inhibitor
Iduronate-2-sulfatase inhibitor
Hippurate hydrolase inhibitor
Aralkylamine dehydrogenase inhibitor
Laminaribiose phosphorylase inhibitor
Antibiotic
Sedoheptulose-bisphosphatase inhibitor
Deoxyribonuclease X inhibitor
Cocain dependency treatment
Oligopeptidase B inhibitor
Carnitine dehydratase inhibitor
Alpha 1 adrenoreceptor antagonist
Serine-glyoxylate transaminase inhibitor
Aryl hydrocarbon receptor agonist
Glutamate (mGluR5) agonist
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Flavin-containing monooxygenase substrate
Pyruvate carboxylase inhibitor
Antifibrinolytic
Estradiol 17alpha-dehydrogenase inhibitor
Antihypotensive
Polo-like kinase inhibitor
Ganglioside galactosyltransferase inhibitor
Histone deacetylase 6 inhibitor
Quinoline-4-carboxylate 2-oxidoreductase inhibitor
Histone deacetylase 3 inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Glutathione peroxidase inhibitor
Carnitine 3-dehydrogenase inhibitor
Isovaleryl-CoA dehydrogenase inhibitor
dUTP diphosphatase inhibitor
Sucrose-phosphate synthase inhibitor
Histone deacetylase class IIb inhibitor
Envelysin inhibitor
Beta-ureidopropionase inhibitor
Cysteine transaminase inhibitor
Immunostimulant
Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Somatostatin 5 antagonist
Glucarate dehydratase inhibitor
Acetyl-CoA C-acyltransferase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor
Lysine decarboxylase inhibitor

Globoside alpha-N-acetylgalactosaminyltransferase inhibitor
CYP2C18 substrate
Agmatinase inhibitor
Alpha 1a adrenoreceptor antagonist
Endo-1,4-beta-xylanase inhibitor
Antihyperaldosteronism
Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor
Somatostatin 1 antagonist
Trimethyllysine dioxygenase inhibitor
Sorbose dehydrogenase inhibitor
2-Pyrocatechuate decarboxylase inhibitor
P-glycoprotein 1 inhibitor
Histone deacetylase class II inhibitor
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Ca²⁺-transporting ATPase inhibitor
Aminopeptidase Y inhibitor
Homoserine dehydrogenase inhibitor
Glycerol dehydratase inhibitor
Guanylate kinase inhibitor
Antineoplastic (bladder cancer)
Cytosole dipeptidase inhibitor
2-Aminoadipate transaminase inhibitor
5 Hydroxytryptamine 3 antagonist
D-alanine transaminase inhibitor
Polynucleotide adenylyltransferase inhibitor
Dopachrome isomerase inhibitor
Deoxycytidine kinase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Tyrosine 3 hydroxylase stimulant
N-acetylglucosamine-6-phosphate deacetylase inhibitor
DNA intercalator
Imidazoline II receptor agonist
Methane monooxygenase inhibitor
Oxidizing agent
Dipeptidyl peptidase inhibitor
Glutamate (mGluR8) agonist
CYP2B6 substrate
Cancer associated disorders treatment
Leukotriene-B4 20-monooxygenase inhibitor
Astringent
Antibiotic Carbapenem-like
Glycine transaminase inhibitor
(R)-limonene 6-monooxygenase inhibitor
Dopamine D2 agonist inducer
Potassium channel (Inward rectifier) 1 blocker
Melatonin 3 antagonist
Homocysteine desulfhydrase inhibitor
Somatostatin 5 agonist
Galacturan 1,4-alpha-galacturonidase inhibitor
Pyrroline-5-carboxylate reductase inhibitor

Transcription factor AP-1 inhibitor
Gentamicin 2"-nucleotidyltransferase inhibitor
Breast cancer-resistant protein inhibitor
Maleylacetoacetate isomerase inhibitor
Antimigraine
Sulfate adenylyltransferase (ADP) inhibitor
Transplant rejection treatment
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Poly(3-hydroxybutyrate) depolymerase inhibitor
Tankyrase 2 inhibitor
Protein kinase C inhibitor
Urocanate hydratase inhibitor
Cerevisin inhibitor
Galactosylceramide sulfotransferase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
Nucleoside-diphosphatase inhibitor
Arylamine N-acetyltransferase inhibitor
Deoxyribonuclease (pyrimidine dimer) inhibitor
3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor
SULT2A1 substrate
Neurotransmitter uptake inhibitor
Phosphoserine phosphatase inhibitor
Cellobiose phosphorylase inhibitor
Thiosulfate sulfurtransferase inhibitor
Cholinergic antagonist
Alkene monooxygenase inhibitor
Homocitrate synthase inhibitor
Thimet oligopeptidase inhibitor
Protein synthesis stimulant
Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor
5 Hydroxytryptamine 7S antagonist
5 Hydroxytryptamine 2 agonist
Aspartate transaminase inhibitor
Aconitate decarboxylase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Streptopain inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
Radioprotector
Acetylcholine antagonist
Cerebroside-sulfatase inhibitor
Malate-CoA ligase inhibitor
Glycerophosphocholine phosphodiesterase inhibitor
Guanidinoacetase inhibitor
Thyrotropin releasing hormone antagonist
Urease inhibitor
Dethiobiotin synthase inhibitor
CDC25C inhibitor
Malyl-CoA lyase inhibitor
Melatonin 5 antagonist

Uracil phosphoribosyltransferase inhibitor
Queuine tRNA-ribosyltransferase inhibitor
Iodide peroxidase inhibitor
Anxiolytic
Phospholipase D2 inhibitor
p53 inhibitor
Antineoplastic antimetabolite
L-aminoadipate-semialdehyde dehydrogenase inhibitor
Phosphodiesterase IX inhibitor
N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
Deoxyhypusine synthase inhibitor
Premature ejaculation treatment
Shikimate 5-dehydrogenase inhibitor
MAP-kinase-activated kinase 1 inhibitor
Nucleotidyltransferase (FIV) inhibitor
L-lysine oxidase inhibitor
Formate dehydrogenase inhibitor
Protein N-acetylglucosaminyltransferase inhibitor
X-Pro dipeptidase inhibitor
Baculoviral IAP repeat-containing protein inhibitor
Somatostatin 3 antagonist
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Transcription factor NF kappa B inhibitor
Histone deacetylase inhibitor
Levanase inhibitor
Thymidine-triphosphatase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Phenylacetate-CoA ligase inhibitor
Mycolysin inhibitor
ICAM1 expression inhibitor
Histone deacetylase 2 inhibitor
Nucleoside deoxyribosyltransferase inhibitor
DNA polymerase I inhibitor
Pim-3 kinase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
CYP26A substrate
HIV fusion inhibitor
Thiamine-phosphate diphosphorylase inhibitor
Pyroglutamyl-peptidase I inhibitor
Acetylcholine M2 receptor agonist
Trimerelysin II inhibitor
Pantothenase inhibitor
Cycloartenol synthase inhibitor
Somatostatin antagonist
Ribonuclease inhibitor

Topiramate

Molecular Mechanism (initial) :

kainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker

Molecular Mechanism (repurposed) :

ckainate receptor antagonist
AMPA receptor antagonists
carbonic anhydrase type II inhibitor
sodium channel blocker

initial indication(s):

epilepsy

Repurposed indication(s):

migraine
alcoholism

Predicted Activities

Anticonvulsant
Carbonic anhydrase II stimulant

Antialcoholic

Bipolar disorder treatment
CYP2C19 inhibitor
CYP3A4 inducer
CYP3A inducer
Growth stimulant
Ophthalmic drug
CYP3A4 substrate
Antineurogenic pain
CYP3A substrate
Antiglaucomic
Antismoking
Carbonic anhydrase V inhibitor
Obsessive-compulsive disorder treatment
GABA receptor agonist

Antiepileptic

Carbonic anhydrase IX inhibitor
Sodium channel blocker
Imidazoline II receptor agonist

Antimigraine

Carbonic anhydrase inhibitor
Carbonic anhydrase II inhibitor
Gastric antisecretory
Antiobesity
Antiallergic
CYP17 inhibitor
Dependence treatment
Carbonic anhydrase I inhibitor
Analgesic
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Prenyl-diphosphatase inhibitor
Sugar-phosphatase inhibitor

Integrin alpha4beta1 antagonist
DNA synthesis inhibitor
Antiviral (Herpes)
Antineoplastic
Antihypercholesterolemic
Bilirubin oxidase inhibitor
Antineoplastic, alkylator
Cytochrome P450 inhibitor
Estrone sulfatase inhibitor
Carbonic anhydrase stimulant
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Chloride peroxidase inhibitor
Polyporopepsin inhibitor
Hypolipemic
Carbonic anhydrase IV inhibitor
HMG CoA synthase inhibitor
Alkylator
Immunomodulator
Glycerol-3-phosphate oxidase inhibitor
Acrocylindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Exoribonuclease II inhibitor
Carbonic anhydrase XII inhibitor
NADPH peroxidase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
RELA expression inhibitor
Biliary tract disorders treatment
Antiasthmatic
Maltose-transporting ATPase inhibitor
Xenobiotic-transporting ATPase inhibitor
Antiprotozoal (Leishmania)
Alkylacetylgllycerophosphatase inhibitor
Microtubule formation inhibitor
Antineoplastic (solid tumors)
Sweetener
Glutamyl endopeptidase II inhibitor
Protein kinase C mu inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Endoglycosylceramidase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
CYP2D15 substrate
Sclerosant
CYP51 inhibitor
Imidazoline receptor agonist
Protein kinase C nu inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
Antiinflammatory
Cyclomaltodextrinase inhibitor
P-glycoprotein substrate

Ribulose-phosphate 3-epimerase inhibitor
Rhodopsin kinase inhibitor
TNF expression inhibitor
Isoleucine-tRNA ligase inhibitor
Galactolipase inhibitor
UDP-N-acetylglucosamine 4-epimerase inhibitor
Aspergillopepsin I inhibitor
Lipocortins synthesis agonist
Pregnane X receptor agonist
Antineoplastic (breast cancer)
GST T substrate
GST T1-1 substrate
Fructan beta-fructosidase inhibitor
Complement factor D inhibitor
Licheninase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
H⁺-transporting two-sector ATPase inhibitor
Hirsutism treatment
Antineoplastic antibiotic
Cl⁻-transporting ATPase inhibitor
Levanase inhibitor
Lactamase C inhibitor
Phospholipid-translocating ATPase inhibitor
Levansucrase inhibitor
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Antimycobacterial
Venombin AB inhibitor
Electron transport complex I inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Aspergillopepsin II inhibitor
Glyoxylate reductase inhibitor
IgA-specific serine endopeptidase inhibitor
Protein kinase C zeta inhibitor
Chemopreventive
Acylcarnitine hydrolase inhibitor
Ganglioside galactosyltransferase inhibitor
Alternansucrase inhibitor
Osmotic diuretic
Phosphogluconate 2-dehydrogenase inhibitor
6-Phospho-beta-glucosidase inhibitor
Leucine-tRNA ligase inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
L-iduronidase inhibitor
Protein kinase C gamma inhibitor
Keratan sulfotransferase inhibitor
Estrone sulfotransferase inhibitor
Serine-tRNA ligase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Phthalate 4,5-dioxygenase inhibitor
Benzoate-CoA ligase inhibitor

Protein kinase C eta inhibitor
Cell wall synthesis inhibitor
CYP2A4 substrate

Toremifene

Molecular Mechanism (initial) :

selective estrogen receptor modulator

Molecular Mechanism (repurposed) :

selective estrogen receptor modulator

initial indication(s):

breast cancer

Repurposed indication(s):

osteoporosis

Predicted Activities

CYP1A2 substrate
CYP1A substrate
CYP2C12 substrate
CYP2D substrate
CYP2D6 substrate
CYP1A1 substrate
CYP2A6 substrate
CYP2A substrate
CYP2E substrate
CYP2E1 substrate
CYP2B6 substrate
CYP2B substrate
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor

Antineoplastic (breast cancer)

CYP3A4 substrate
CYP3A1 substrate
CYP3A substrate
Antiestrogenic
CYP2A2 substrate
CYP2C19 substrate
Antineoplastic

Bone diseases treatment (osteoporosis)

CYP2C substrate
CYP2C9 substrate
Antiinfertility, female
CYP2C11 substrate
Chemosensitizer
Estrogen antagonist
CYP2A1 substrate
CYP3A2 substrate
TP53 expression enhancer
Glycosylphosphatidylinositol phospholipase D inhibitor
Transforming growth factor beta 1 agonist
Peroxidase substrate

CYP2C6 substrate
Flavin-containing monooxygenase substrate
Gonadotropin antagonist
Cytostatic
CYP3A5 substrate
Venombin AB inhibitor
Spasmolytic
Membrane integrity agonist
Antisecretoric
CYP3A4 inducer
CYP3A inducer
Neurotransmitter uptake inhibitor
CYP2C8 inhibitor
Menopausal disorders treatment
CYP2C8 substrate
Arginine 2-monooxygenase inhibitor
CYP2C18 substrate
Monoamine uptake inhibitor
FMO1 substrate
TNF expression inhibitor
Phobic disorders treatment
Trimethylamine-oxide aldolase inhibitor
Oxidoreductase inhibitor
Anticarcinogenic
Gynecological disorders treatment
Antihypoxic
Respiratory analeptic
Choline-phosphate cytidyltransferase inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Polyporopepsin inhibitor
Estrogen agonist
Aldehyde oxidase inhibitor
Ubiquinol-cytochrome-c reductase inhibitor
Anesthetic
Platelet aggregation stimulant
Spasmolytic, Papaverin-like
Postmenopausal disorders treatment
Alzheimer's disease treatment
1,4-Lactonase inhibitor
Osteoarthritis treatment
Caspase 8 stimulant
Anesthetic general
Spasmolytic, urinary
Lymphocytopoiesis inhibitor
CYP2H substrate
Omptin inhibitor
Nitrite reductase (NO-forming) inhibitor
Bone formation stimulant
Glutamyl endopeptidase II inhibitor

CYP3A7 substrate
GST A substrate
Calcium channel (voltage-sensitive) activator
Phosphatidylinositol diacylglycerol-lyase inhibitor
Arylesterase inhibitor
Analeptic
CYP2D16 substrate
Proliferative diseases treatment
Farnesyltranstransferase inhibitor
Arylsulfate sulfotransferase inhibitor
Vasodilator, coronary
Antiparkinsonian, tremor relieving
Nucleotide metabolism regulator
Hematopoietic inhibitor
Cancer associated disorders treatment
Acetylgalactosaminy-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminytransferase inhibitor
Macrophage colony stimulating factor agonist
Long-chain-aldehyde dehydrogenase inhibitor
2-Haloacid dehalogenase inhibitor
Phenol O-methyltransferase inhibitor
Antianorexic
Membrane integrity antagonist
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
GABA aminotransferase inhibitor
Apyrase inhibitor
FMO3 substrate
Estrogen receptor beta antagonist
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Menstruation disorders treatment
Tpr proteinase (Porphyromonas gingivalis) inhibitor
Hypolipemic
Antiviral (Poxvirus)
Pseudolysin inhibitor
Ethanolamine-phosphate cytidyltransferase inhibitor
CYP2C8 inducer
CYP2D2 inhibitor
Acylaminoacyl-peptidase inhibitor
Antinaupathic
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Peptidoglycan glycosyltransferase inhibitor
P-glycoprotein 1 inhibitor
Betaine-aldehyde dehydrogenase inhibitor
CYP19 inhibitor
Aldehyde oxidase substrate
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
Chlordecone reductase inhibitor
Urticaria treatment
Flavin-containing monooxygenase inhibitor
Lipid metabolism regulator

Oryzin inhibitor
Anesthetic local
P-glycoprotein inhibitor
Lysase inhibitor
2-Haloacid dehalogenase (configuration-inverting) inhibitor
Pancreatic elastase inhibitor
Alkylator
Linoleate diol synthase inhibitor
CYP2B5 substrate
Carboxypeptidase D inhibitor
Antipruritic
Adrenaline release stimulant
Antipruritic, allergic
Radiosensitizer
CYP2F1 substrate
Antitussive
HMG CoA synthase inhibitor
Aspergillopepsin I inhibitor
Leukopoiesis inhibitor
Dolichol kinase inhibitor
Sphinganine kinase inhibitor
Limulus clotting factor C inhibitor
CYP2D15 substrate
Alkenylglycerophosphocholine hydrolase inhibitor
Antiinflammatory, ophthalmic
Methylumbelliferyl-acetate deacetylase inhibitor
Antiseborrheic
Phosphatidylcholine-sterol O-acyltransferase inhibitor
Fibrinolytic
Aspergillopepsin II inhibitor
Antihypercholesterolemic
MAP kinase stimulant
CYP2C3 substrate
Guanylate cyclase 1 stimulant
Antitussive, narcotic
Caspase 3 stimulant
Antipruritic, non-allergic
CYP2B10 substrate
Antimyopathies
CYP2D1 substrate
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Complement factor D inhibitor
Antidepressant, Imipramin-like
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
Renal tissue kallikrein inhibitor
Choline-sulfatase inhibitor
Catenin beta inhibitor
Guanidinoacetate kinase inhibitor
Sugar-phosphatase inhibitor
CYP2A4 substrate

Endopeptidase La inhibitor
Nardilysin inhibitor
Retinoic acid metabolism inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Antiparkinsonian, rigidity relieving
Neurodegenerative diseases treatment
Endopeptidase So inhibitor
Antineoplastic (uterine cancer)
Nucleoside-diphosphatase inhibitor
DELTA14-sterol reductase inhibitor
Antiprotozoal (Amoeba)
Gingipain R inhibitor
Intermittent claudication treatment
CYP2B1 substrate
CYP2B11 substrate
Membrane permeability inhibitor
Choline dehydrogenase inhibitor
Antineoplastic (solid tumors)
CYP2B18 substrate
Chemopreventive
Phospholipid-translocating ATPase inhibitor
5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
Antineoplastic (multiple myeloma)
Anthelmintic (Nematodes)
Lipoxygenase substrate
Phosphatidylcholine-retinol O-acyltransferase inhibitor
CYP2B2 substrate
Undecaprenyl-phosphate mannosyltransferase inhibitor
Andropause treatment
Trimethylamine dehydrogenase inhibitor
Fucosterol-epoxide lyase inhibitor
Phosphodiesterase 4A inhibitor
Adenosine regulator
CYP2G1 substrate
Antineoplastic, alkylator
Ovulation inhibitor
Antiischemic, cerebral
Methane monooxygenase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
DELTA24-sterol reductase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
5 Hydroxytryptamine uptake stimulant
Prostate cancer treatment
Steroid synthesis inhibitor
CYP4A substrate
NADPH peroxidase inhibitor
Taurine dehydrogenase inhibitor
CYP19A1 expression inhibitor
Cl--transporting ATPase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor

Cytoprotectant
Carboxypeptidase Taq inhibitor
Diamine N-acetyltransferase inhibitor
3-Cyanoalanine hydratase inhibitor
Antineoplastic (small cell lung cancer)
Proteasome endopeptidase complex inhibitor
Fusarinine-C ornithinesterase inhibitor
Polarisation inhibitor
CYP4A1 substrate
Thiamine-triphosphatase inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
Methyltransferase substrate
Hydrogen dehydrogenase inhibitor
Gingipain K inhibitor
NOS2 expression inhibitor
Dextranase inhibitor
Alpha-amylase inhibitor
Phosphodiesterase 1B inhibitor
Oxygen scavenger
Arachidonic acid antagonist
Growth factor agonist
Squalene epoxidase inhibitor
Antineoplastic (bone cancer)
Squalene-hopene cyclase inhibitor
Contraceptive
Antiviral (Herpes)
Glutaminase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Gluconate 5-dehydrogenase inhibitor
Nicotinic alpha2beta2 receptor antagonist
Serine protease unspecified inhibitor
Caspase 2 inhibitor
CYP1B1 inhibitor
Exoribonuclease II inhibitor
Ribulose-phosphate 3-epimerase inhibitor
Hydroxylamine oxidase inhibitor
Glyceryl-ether monooxygenase inhibitor
UGT1A substrate
Retinopathy treatment
Gametolysin inhibitor
Pappalysin-1 inhibitor
Cathepsin T inhibitor
Sigma 1 receptor agonist
HERG 1 channel blocker
Nav1.3 sodium channel blocker
Fructose 5-dehydrogenase inhibitor
Antiprotozoal (Trichomonas)
Enteropeptidase inhibitor
Pancreatic endopeptidase E inhibitor

Urolithiasis treatment
MMP9 expression inhibitor
Steroid N-acetylglucosaminyltransferase inhibitor
Acetylcholine neuromuscular blocking agent
D-lactaldehyde dehydrogenase inhibitor
Antineoplastic (lymphoma)
Antihematotoxic
Acetylcholine nicotinic antagonist
CYP2C9 inducer
Aldehyde dehydrogenase 2 substrate
Choline sulfotransferase inhibitor
JAK2 expression inhibitor
Phosphodiesterase I inhibitor
Phosphoinositide 5-phosphatase inhibitor
Glycerol-3-phosphate oxidase inhibitor
Sulfite dehydrogenase inhibitor
Antineoplastic (ovarian cancer)
Thioredoxin reductase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Antineoplastic (lymphocytic leukemia)
Cytokine modulator
Tropinesterase inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Phosphatidylglycerophosphatase inhibitor
Sigma receptor agonist
Carnitine dehydratase inhibitor
Phospholipase D1 inhibitor
Opioid kappa 3 receptor antagonist
Aldehyde dehydrogenase substrate
Octopamine antagonist
Eye irritation, inactive
Putrescine oxidase inhibitor
ICAM1 expression inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
5 Hydroxytryptamine 2B agonist
Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Diacylglycerol cholinephosphotransferase inhibitor
D-benzoylarginine-4-nitroanilide amidase inhibitor
Antiperistaltic
Poly(beta-D-mannuronate) lyase inhibitor
Peptidylamidoglycolate lyase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Glucose oxidase inhibitor
Epoxide hydrolase substrate
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Phospholipase D inhibitor
Histamine H1 receptor antagonist
UGT1A10 substrate

Thromboxane B2 antagonist
Sulfite oxidase inhibitor
Phosphatidate phosphatase inhibitor
UGT1A8 substrate
Nav1.4 sodium channel blocker
Fumarate reductase (NADH) inhibitor
Aldehyde dehydrogenase 1 substrate
Phosphopantothenoylcysteine decarboxylase inhibitor
Nav1.2 sodium channel blocker
Calcium antagonist
Protein-tyrosine sulfotransferase inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Leishmanolysin inhibitor
Chemoprotective
2-Enoate reductase inhibitor
Antifibrinolytic
Cyclic AMP agonist
Linoleoyl-CoA desaturase inhibitor
Myt1 kinase inhibitor
Wee-1 tyrosine kinase inhibitor
Envelysin inhibitor
Granzyme A inhibitor
Choline kinase inhibitor
Cycloartenol synthase inhibitor
Trypanothione-disulfide reductase inhibitor
2,3-Oxidosqualene-lanosterol cyclase inhibitor
Antiviral (Adenovirus)
(S)-carnitine 3-dehydrogenase inhibitor
Mucositis treatment
X-methyl-His dipeptidase inhibitor
Antineurotic
Thiamine pyridinylase inhibitor
Histamine release stimulant
Lysine 2,3-aminomutase inhibitor
Candidapepsin inhibitor
Sodium/calcium exchanger inhibitor
Telomerase inhibitor
Carnosine synthase inhibitor
Anabolic
Fructan beta-fructosidase inhibitor
Mannitol-1-phosphatase inhibitor
Polygalacturonase inhibitor
Actin depolymerization stimulant
Glycerophosphocholine phosphodiesterase inhibitor
Methylamine-glutamate N-methyltransferase inhibitor
Gamma-glutamyltransferase inhibitor
Gamma-butyrobetaine dioxygenase inhibitor
N-acylmannosamine kinase inhibitor
Signal peptidase I inhibitor
Sorbose dehydrogenase inhibitor

Arylamine N-acetyltransferase inhibitor
Acylcarnitine hydrolase inhibitor
Glycerophosphocholine cholinephosphodiesterase inhibitor
Nicotine dehydrogenase inhibitor
Aspartate-phenylpyruvate transaminase inhibitor
Galactolipase inhibitor
Amidase inhibitor
MAO A substrate
Cholesterol synthesis inhibitor
GABA B receptor agonist
Polyamine-transporting ATPase inhibitor
(R)-limonene 6-monooxygenase inhibitor
IgA-specific serine endopeptidase inhibitor
Carnitine 3-dehydrogenase inhibitor
(R)-aminopropanol dehydrogenase inhibitor
H⁺-exporting ATPase inhibitor
Cyanoalanine nitrilase inhibitor
Loop diuretic
Sodium/calcium exchanger 1 inhibitor
Kexin inhibitor
Psychosexual dysfunction treatment
Chloride channel blocker
Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
Penicillin amidase inhibitor
Dichloromethane dehalogenase inhibitor
Nav1.8 sodium channel blocker
Thermitase inhibitor
Cyclomaltodextrinase inhibitor
Mucinaminyserine mucinaminidase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
DNA intercalator
Venombin A inhibitor
Prolactin inhibitor
Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Isopenicillin-N synthase inhibitor
Aminoacylase inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Cutinase inhibitor
Hypoxia inducible factor 1 alpha inhibitor
Glyoxylate reductase inhibitor
Anaphylatoxin receptor antagonist
GABA uptake inhibitor
Pin1 inhibitor
Alkanal monooxygenase (FMN-linked) inhibitor
Photosensitizer
Plastoquinol-plastocyanin reductase inhibitor
CYP3A4 inhibitor
Tripeptide aminopeptidase inhibitor
Thyroid hormone antagonist
Gluconate 2-dehydrogenase (acceptor) inhibitor

Para amino benzoic acid antagonist
Thymidylate 5'-phosphatase inhibitor
Agmatinase inhibitor
Triose-phosphate isomerase inhibitor
Gamma-glutamyl hydrolase inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Sodium channel blocker class Ib
CYP2J2 substrate
Antihelminthic
Gastrointestinal motility stimulant
Thimet oligopeptidase inhibitor
MAO B substrate
Clavamate synthase inhibitor
Phosphoserine phosphatase inhibitor
3-Phytase inhibitor
Ethanolamine ammonia-lyase inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Diphosphomevalonate decarboxylase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Aminobutyraldehyde dehydrogenase inhibitor
Neuronal nicotinic receptor antagonist
Dopamine D1A antagonist
GABA transporter 2 inhibitor
Shab potassium channel blocker
Antitoxic
Spermidine dehydrogenase inhibitor
Carnitine O-octanoyltransferase inhibitor
Transketolase inhibitor
Polyneuridine-aldehyde esterase inhibitor
Glycine amidinotransferase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
UDP-glucuronosyltransferase substrate
Feruloyl esterase inhibitor
Acetylspermidine deacetylase inhibitor
Anthranilate synthase inhibitor
Endothelial growth factor antagonist
Lassitude treatment
Alkylacetylgllycerophosphatase inhibitor
Antihistaminic
Nav1.5 sodium channel blocker
Histamine N-methyltransferase inhibitor
Lysostaphin inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
6,7-Dihydropteridine reductase inhibitor
1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
Prion diseases treatment
Inositol 1,4,5-trisphosphate 3-kinase inhibitor
DNA synthesis inhibitor
Phthalate 4,5-dioxygenase inhibitor
Ubiquitin thiolesterase inhibitor

Atherosclerosis treatment
CYP2E1 inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Brachyurin inhibitor
Limulus clotting factor B inhibitor
Carnitine palmitoyltransferase inhibitor
Atrolysin A inhibitor
Isopentenyl-diphosphate DELTA-isomerase inhibitor
Histamine antagonist
Fragilysin inhibitor
Heat shock protein agonist
Ecdysone 20-monooxygenase inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor

Vorinostat

Molecular Mechanism (initial) :

histone deacetylase 6, 2, 1, 3 inhibitor

Molecular Mechanism (repurposed) :

histone deacetylase 6, 2, 1, 3 inhibitor

initial indication(s):

cutaneous T-cell lymphoma

Repurposed indication(s):

multiple myeloma

Predicted Activities

Histone deacetylase 3 inhibitor

Linoleate diol synthase inhibitor
Histone deacetylase class IIb inhibitor
Antiarthritic

Histone deacetylase 6 inhibitor

Histone deacetylase class II inhibitor
Fragilysin inhibitor
Fibrolase inhibitor
Urease inhibitor

Histone deacetylase inhibitor

Acrocyllindropepsin inhibitor
Chymosin inhibitor
Saccharopepsin inhibitor
Peroxidase inhibitor

Histone deacetylase class I inhibitor

Antineoplastic (sarcoma)
Histone deacetylase 1 inhibitor
Catechol oxidase inhibitor
AR expression inhibitor
Phobic disorders treatment
Ubiquinol-cytochrome-c reductase inhibitor
Acetylspermidine deacetylase inhibitor
Botulin neurotoxin A light chain inhibitor
Tumour necrosis factor alpha release inhibitor
Histone deacetylase 2 inhibitor

Pitrilysin inhibitor
Pseudolysin inhibitor
IgA-specific serine endopeptidase inhibitor
Antiviral (Picornavirus)
Polyporopepsin inhibitor
Chemosensitizer
Coccolysin inhibitor
L-glutamate oxidase inhibitor
Macrophage colony stimulating factor agonist
CYP2J substrate
Testosterone 17beta-dehydrogenase (NADP+) inhibitor
Glutamine-tRNA ligase inhibitor
CYP2J2 substrate
Histone deacetylase class IIa inhibitor
Histone deacetylase 4 inhibitor
Fusarinine-C ornithinesterase inhibitor
Radiosensitizer
CYP3A1 substrate
Glutamine-phenylpyruvate transaminase inhibitor
Histone deacetylase 8 inhibitor
Hydrogen dehydrogenase inhibitor
Sugar-phosphatase inhibitor
Metalloproteinase-2 inhibitor
Cyclic AMP agonist
Pro-opiomelanocortin converting enzyme inhibitor
Fibroblast growth factor agonist
Calcium channel (voltage-sensitive) activator
Mucositis treatment
CYP3A2 substrate
CYP2F1 substrate
Manganese peroxidase inhibitor
Endopeptidase So inhibitor
Gastrin inhibitor
Flavin-containing monooxygenase substrate
Antineoplastic
Thioredoxin inhibitor
Cl--transporting ATPase inhibitor
Taurine-2-oxoglutarate transaminase inhibitor
Taurine dehydrogenase inhibitor
Polyamine-transporting ATPase inhibitor
Aspulvinone dimethylallyltransferase inhibitor
Sulfur reductase inhibitor
Limulus clotting factor B inhibitor
Electron-transferring-flavoprotein dehydrogenase inhibitor
Chloride peroxidase inhibitor
Glucan endo-1,3-beta-D-glucosidase inhibitor
Glucan 1,4-alpha-maltotriohydrolase inhibitor
Gluconate 5-dehydrogenase inhibitor
CYP2C18 substrate
Vanilloid 1 agonist

S-formylglutathione hydrolase inhibitor
RNA-directed RNA polymerase inhibitor
Carboxypeptidase Taq inhibitor
GST A substrate
Erythropoiesis stimulant
PfA-M1 aminopeptidase inhibitor
Glyoxylate reductase inhibitor
Matrix metalloproteinase inhibitor
Aminopeptidase B inhibitor
Alkylacetyl glycerophosphatase inhibitor
Yeast ribonuclease inhibitor
Atrolysin A inhibitor
Leukopoiesis stimulant
Excitatory amino acid transporter EAAC1 inhibitor
Protein-disulfide reductase (glutathione) inhibitor
Phospholipid-translocating ATPase inhibitor
Ribonucleoside triphosphate reductase inhibitor
Astacin inhibitor
CYP2A3 substrate
Glutamyl endopeptidase II inhibitor
Metalloproteinase-9 inhibitor
TP53 expression enhancer
Antineoplastic (melanoma)
Sickle-cell anemia treatment
Aminobutyraldehyde dehydrogenase inhibitor
Gelatinase inhibitor
TNF expression inhibitor
Growth factor agonist
Laccase inhibitor
Dimethylargininase inhibitor
Wound healing agent
Ribulose-phosphate 3-epimerase inhibitor
Spermidine dehydrogenase inhibitor
Anthrax lethal factor inhibitor
Glycerol-3-phosphate dehydrogenase inhibitor
Fucosterol-epoxide lyase inhibitor
Acylcarnitine hydrolase inhibitor
Adenylate cyclase V inhibitor
Alanine-tRNA ligase inhibitor
Omptin inhibitor
Platelet aggregation stimulant
HIV-2 reverse transcriptase inhibitor
Pterin deaminase inhibitor
Mannan endo-1,4-beta-mannosidase inhibitor
Atrolysin C inhibitor
Lysine 2,3-aminomutase inhibitor
3-Hydroxybenzoate 6-monooxygenase inhibitor
Simian immunodeficiency virus proteinase inhibitor
Dactylisin inhibitor
Methylamine-glutamate N-methyltransferase inhibitor

Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor
Mycothiol-S-conjugate amidase inhibitor
Neutrophil collagenase inhibitor
Interleukin 6 antagonist
NADPH peroxidase inhibitor
Biotinidase inhibitor
Arginine 2-monooxygenase inhibitor
Immunosuppressant
Antileprosy
Kidney function stimulant
Antidote
Aspergillopepsin I inhibitor
Exoribonuclease II inhibitor
FMO3 substrate
Aspartate-phenylpyruvate transaminase inhibitor
Apoptosis agonist
CYP2C12 substrate
Alopecia treatment
Muramoyltetrapeptide carboxypeptidase inhibitor
Matrix metalloproteinase 1 inhibitor
5-O-(4-coumaroyl)-D-quinat 3'-monooxygenase inhibitor
Formaldehyde transketolase inhibitor
Methylumbelliferyl-acetate deacetylase inhibitor
Prostaglandin-A1 DELTA-isomerase inhibitor
Nicotinic alpha6beta3beta4alpha5 receptor antagonist
Cutinase inhibitor
CYP4A2 substrate
Phosphatidylcholine-retinol O-acyltransferase inhibitor
Venombin AB inhibitor
Acetylcholinesterase inhibitor
CYP2C29 substrate
Glycosylphosphatidylinositol phospholipase D inhibitor
Antipyretic
5 Hydroxytryptamine uptake stimulant
S-alkylcysteine lyase inhibitor
Plastoquinol-plastocyanin reductase inhibitor
Asparaginase inhibitor
Lipoprotein lipase inhibitor
Membrane integrity agonist
2-Haloacid dehalogenase inhibitor
Meprin A inhibitor
Thymidylate 5'-phosphatase inhibitor
Tumour necrosis factor antagonist
2-Dehydropantoate 2-reductase inhibitor
Phosphopantothenoylcysteine decarboxylase inhibitor
Antineoplastic (small cell lung cancer)
Septic shock treatment
Phthalate 4,5-dioxygenase inhibitor
Thiamine pyridinylase inhibitor
Xylose isomerase inhibitor

Leukotriene-C4 synthase inhibitor
Intermittent claudication treatment
NADPH-cytochrome-c2 reductase inhibitor
Antiinflammatory, intestinal
Sweetener
UDP-N-acetylglucosamine 4-epimerase inhibitor
Blasticidin-S deaminase inhibitor
4-Hydroxymandelate oxidase inhibitor
Antiviral (Influenza A)
X-His dipeptidase inhibitor
All-trans-retinyl-palmitate hydrolase inhibitor
Mannose isomerase inhibitor
Growth hormone agonist
N-acylmannosamine kinase inhibitor
Oxygen scavenger
Phosphatidylserine decarboxylase inhibitor
N-formylmethionyl-peptidase inhibitor
Amine dehydrogenase inhibitor
Protein-S-isoprenylcysteine O-methyltransferase inhibitor
Chitosanase inhibitor
Complement factor D inhibitor
5 Hydroxytryptamine release inhibitor
Antineoplastic (non-small cell lung cancer)
Antineoplastic (multiple myeloma)
Arylamine N-acetyltransferase inhibitor
Carnitinamidase inhibitor
Aromatic-hydroxylamine O-acetyltransferase inhibitor
Adenylyl-sulfate reductase inhibitor
Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor
2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor
Oryzin inhibitor
Agaritine gamma-glutamyltransferase inhibitor
Pancreatic elastase inhibitor
Nicotinic alpha2beta2 receptor antagonist
Poly(beta-D-mannuronate) lyase inhibitor
Dihydroorotase inhibitor
Antineoplastic (bladder cancer)
Phenol O-methyltransferase inhibitor
Chitinase inhibitor
Glucose oxidase inhibitor
Hyaluronic acid agonist
Mucinaminylserine mucinaminidase inhibitor
(R)-6-hydroxynicotine oxidase inhibitor
Fatty-acyl-CoA synthase inhibitor
Thiosulfate dehydrogenase inhibitor
3-Chloro-D-alanine dehydrochlorinase inhibitor
Huntington's disease treatment
N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor
Antitoxic
Aspergillus nuclease S1 inhibitor

Matrix metalloproteinase 3 (membrane-type) inhibitor
Glucan 1,4-alpha-maltotetraohydrolase inhibitor
Renal tissue kallikrein inhibitor
Stromelysin 2 inhibitor
Platelet adhesion inhibitor
N-methylhydantoinase (ATP-hydrolysing) inhibitor
Endothelin-converting enzyme inhibitor
Glutamate decarboxylase inhibitor
Sodium channel blocker class Ib
Corneal wound healing stimulator
Aspergillopepsin II inhibitor
Collagenase 3 inhibitor
Procollagen N-endopeptidase inhibitor
Gamma-glutamyltransferase inhibitor
CYP2A5 substrate
1,4-Lactonase inhibitor
Coenzyme-B sulfoethylthiotransferase inhibitor
Cyclomaltodextrinase inhibitor
Malate oxidase inhibitor
Interleukin 2 agonist
Phosphoinositide 5-phosphatase inhibitor
Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor
Diabetic neuropathy treatment
CYP2C8 inhibitor
Anticataract
Nitric oxide antagonist
Leishmanolysin inhibitor
Cytosol alanyl aminopeptidase inhibitor
Cyclic AMP modulator
Myosin ATPase inhibitor
Gaucher disease treatment
Antiviral (Influenza)
Dipeptidase E inhibitor
Rhizopuspepsin inhibitor
Caspase 3 stimulant
Retinoic acid metabolism inhibitor
Rhodotorulapepsin inhibitor
Lipoxygenase substrate
Reductant
CYP4A substrate
N-acetyllactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor
Nicotinate dehydrogenase inhibitor
Gingipain K inhibitor
Antineoplastic (colorectal cancer)
Alpha-N-acetylglucosaminidase inhibitor
Enteropeptidase inhibitor
Matrix metalloproteinase (membrane-type) inhibitor
Limulus clotting factor C inhibitor
Alkylglycerone-phosphate synthase inhibitor
Pullulanase inhibitor

Preneoplastic conditions treatment
Periodontitis treatment
GABA aminotransferase inhibitor
Linoleate isomerase inhibitor
4-Hydroxyglutamate transaminase inhibitor
Hydroxylamine oxidase inhibitor
Bcr-Abl kinase inhibitor
Prion diseases treatment
Aspartate-ammonia ligase inhibitor
DNA-3-methyladenine glycosylase I inhibitor
Antineoplastic (colon cancer)
ATP phosphoribosyltransferase inhibitor
Chenodeoxycholytaurine hydrolase inhibitor
5 Hydroxytryptamine 7 agonist
Trimethylamine-oxide aldolase inhibitor
Fructose 5-dehydrogenase inhibitor
CYP2G1 substrate
(R)-Pantolactone dehydrogenase (flavin) inhibitor
Alkenylglycerophosphocholine hydrolase inhibitor
Vanilloid agonist
Antinephritic
Hydroxylamine reductase (NADH) inhibitor
Alcohol dehydrogenase (acceptor) inhibitor
Phosphatidylcholine-sterol O-acyltransferase inhibitor
(S)-6-hydroxynicotine oxidase inhibitor
Indoleacetaldoxime dehydratase inhibitor
NAT1 substrate
Xylan endo-1,3-beta-xylosidase inhibitor
Na⁺-transporting two-sector ATPase inhibitor
Aminopeptidase microsomal inhibitor
CYP2D16 substrate
Levanase inhibitor
Glycolate dehydrogenase inhibitor
Nuclease inhibitor
CYP2E1 inducer
Aspartate transaminase inhibitor
CYP2B10 substrate
Tpr proteinase (*Porphyromonas gingivalis*) inhibitor
Leucine transaminase inhibitor
Glutarate-semialdehyde dehydrogenase inhibitor
Sphinganine kinase inhibitor
N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
Histone deacetylase 1A inhibitor
Urethanase inhibitor
Multiple sclerosis treatment
Diamine N-acetyltransferase inhibitor
Hematopoietic
Membrane integrity antagonist
Opine dehydrogenase inhibitor
D-alanine 2-hydroxymethyltransferase inhibitor

N-(long-chain-acyl)ethanolamine deacylase inhibitor
Glucuronate isomerase inhibitor
Formyltetrahydrofolate dehydrogenase inhibitor
Macrophage elastase inhibitor
Muscular dystrophy treatment
Omega-amidase inhibitor
Antiinflammatory, ophthalmic
Alpha-glucuronidase inhibitor
Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
Matrix metalloproteinase 2 (membrane-type) inhibitor
Analgesic stimulant
Thiol oxidase inhibitor
Cathepsin T inhibitor
Glucan endo-1,6-beta-glucosidase inhibitor
Tumour necrosis factor alpha antagonist
Leukopoiesis inhibitor
Cholestanetriol 26-monooxygenase inhibitor
Immunoglobulin Fc receptor antagonist
3-Methylbutanal reductase inhibitor
Age-related macular degeneration treatment
Methylenetetrahydrofolate reductase (NADPH) inhibitor
Nicotine dehydrogenase inhibitor
CYP2C3 substrate
Poly(alpha-L-guluronate) lyase inhibitor
Arylmalonate decarboxylase inhibitor
EIF4E expression inhibitor
Methionine decarboxylase inhibitor
Antiviral (Poxvirus)
Dimethylmaleate hydratase inhibitor
Antimyopathies
Histidine N-acetyltransferase inhibitor
Antiprotozoal (Plasmodium)
Prostate cancer treatment
Glutathione thiolesterase inhibitor
Acute neurologic disorders treatment
Leukotriene-B4 20-monooxygenase inhibitor
Adenylate cyclase inhibitor
Choline-phosphate cytidyltransferase inhibitor
Iron-cytochrome-c reductase inhibitor
Anthranilate-CoA ligase inhibitor
Bacterial leucyl aminopeptidase inhibitor
3-Phytase inhibitor
Sclerosant
Membrane dipeptidase inhibitor
Aspartoacylase inhibitor
3-Cyanoalanine hydratase inhibitor
3-Hydroxybenzoate 4-monooxygenase inhibitor
D-Alanine-poly(phosphoribitol) ligase inhibitor
Aminopeptidase N inhibitor
1,4-Alpha-glucan branching enzyme inhibitor

Diamine oxidase inhibitor
Bontoxilysin inhibitor
Glutamate-tRNA ligase inhibitor
Endopeptidase La inhibitor
Alpha-N-acetylgalactosaminidase inhibitor
Glycine amidinotransferase inhibitor
Aggrecanase inhibitor
K(Ca) 3.1 channel activator
Potassium channel intermediate-conductance Ca-activated activator
O-aminophenol oxidase inhibitor
2-Hydroxyquinoline 8-monooxygenase inhibitor
Tyrosine 3 hydroxylase inhibitor
Cellulose 1,4-beta-cellobiosidase inhibitor
Gamma-guanidinobutyraldehyde dehydrogenase inhibitor
Neuropeptide Y2 antagonist
Glycerol-3-phosphate oxidase inhibitor
Trimethylamine dehydrogenase inhibitor
Falcipain 3 inhibitor
Beta-alanine-pyruvate transaminase inhibitor
Galactose 1-dehydrogenase (NADP+) inhibitor
Histidine ammonia-lyase inhibitor
Linoleoyl-CoA desaturase inhibitor
Superoxide dismutase inhibitor
Gallate decarboxylase inhibitor
Beta-carotene 15,15'-monooxygenase inhibitor
Lipotropic
5-Formyltetrahydrofolate cyclo-ligase inhibitor
Hyponitrite reductase inhibitor
Diabetic retinopathy treatment
Guanidinoacetate N-methyltransferase inhibitor
Sorbitol-6-phosphate 2-dehydrogenase inhibitor
Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
Alkenylglycerophosphoethanolamine hydrolase inhibitor
Thiopurine S-methyltransferase inhibitor
5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor
Mandelate 4-monooxygenase inhibitor
Quisqualate antagonist
NAT2 substrate
Octopamine antagonist
Picornain 3C inhibitor
Cyclohexyl-isocyanide hydratase inhibitor
GABA C receptor agonist
Stem cell growth factor agonist
Phenylalanine(histidine) transaminase inhibitor
Venombin A inhibitor
Antineoplastic (breast cancer)
Antiviral (CMV)
Matrix metalloproteinase 1 (membrane-type) inhibitor
CYP2A8 substrate
Ethanolamine-phosphate cytidyltransferase inhibitor

DNA polymerase I inhibitor
N-benzyloxycarbonylglycine hydrolase inhibitor
Dehydro-L-gulonate decarboxylase inhibitor
Peptide agonist
Glutathione peroxidase inhibitor
Phosphodiesterase 1B inhibitor
Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor
2-Hydroxy-3-oxoadipate synthase inhibitor
Phosphoenolpyruvate carboxykinase (ATP) inhibitor
Pappalysin-1 inhibitor
Arylamine N-Acetyltransferase substrate
Peptidyl-dipeptidase Dcp inhibitor
Glyoxylate oxidase inhibitor
D-lactaldehyde dehydrogenase inhibitor
Beta-adrenergic receptor kinase inhibitor
G-protein-coupled receptor kinase inhibitor
2-Aminoethylphosphonate-pyruvate transaminase inhibitor
Antiemphysemic
Iron antagonist
Tryptophan 2,3-dioxygenase inhibitor
Galactolipase inhibitor
Acyl-CoA oxidase inhibitor
Glutaminy-peptide cyclotransferase inhibitor
Ferredoxin-NAD⁺ reductase inhibitor
Naphthalene 1,2-dioxygenase inhibitor
Antibacterial, ophthalmic
Glucuronolactone reductase inhibitor
Sulfite oxidase inhibitor
Anti-Helicobacter pylori
Ornithine cyclodeaminase inhibitor
Macrophage scavenger receptor antagonist
4-Hydroxyproline epimerase inhibitor
Opheline kinase inhibitor
Taurocyamine kinase inhibitor
4-Chlorobenzoyl-CoA dehalogenase inhibitor
Cyclooxygenase substrate
Signal peptidase I inhibitor
Radioprotector
2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor
Cyanoalanine nitrilase inhibitor
Aggrecanase 2 inhibitor
Sphingosine 1-phosphate receptor 5 agonist
Nitrite reductase (NO-forming) inhibitor
Nitrile hydratase inhibitor
Quinoprotein glucose dehydrogenase inhibitor
Collagenase inhibitor
Aldehyde dehydrogenase 2 substrate
N-acetyl-gamma-glutamyl-phosphate reductase inhibitor
Pin1 inhibitor
D-proline reductase (dithiol) inhibitor

Pseudouridylate synthase inhibitor
Undecaprenyl-diphosphatase inhibitor
2-Dehydropantoate aldolase inhibitor
2,4-Diaminopentanoate dehydrogenase inhibitor
3-Hydroxybutyryl-CoA dehydrogenase inhibitor
Lysine 6-dehydrogenase inhibitor
Bisphosphoglycerate phosphatase inhibitor
Glutamine-pyruvate transaminase inhibitor
Caspase 2 inhibitor
8-Amino-7-oxononanoate synthase inhibitor
Arylsulfate sulfotransferase inhibitor
Arginase inhibitor
NADH kinase inhibitor
Peptide alpha-N-acetyltransferase inhibitor
Shikimate O-hydroxycinnamoyltransferase inhibitor
Arginine decarboxylase inhibitor
Dynein ATPase inhibitor
Isopenicillin-N epimerase inhibitor
Albendazole monooxygenase inhibitor
Benzaldehyde dehydrogenase (NADP+) inhibitor
Isopenicillin-N synthase inhibitor
Lactose synthase inhibitor
3-Oxadipate enol-lactonase inhibitor
Calcium-sensing receptor agonist
Prolyl aminopeptidase inhibitor
Bile-salt sulfotransferase inhibitor
Tauropine dehydrogenase inhibitor
Liver fibrosis treatment
Camphor 1,2-monooxygenase inhibitor
Prunasin beta-glucosidase inhibitor
[acyl-carrier-protein] S-acetyltransferase inhibitor
Tentoxilysin inhibitor
UGT1A9 substrate
Monodehydroascorbate reductase (NADH) inhibitor
Peptide deformylase inhibitor
Phosphoenolpyruvate mutase inhibitor
Thermitase inhibitor
Glycine C-acetyltransferase inhibitor
Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
JAK2 expression inhibitor
N-methyl-2-oxoglutaramate hydrolase inhibitor
Aerobactin synthase inhibitor
Dihydroxyacetanilide dehydrogenase inhibitor
Dihydroxyacetanilide epoxidase inhibitor
Guanidinoacetate kinase inhibitor
Antidiabetic (type 1)
CYP1A2 inducer
Serine-tRNA ligase inhibitor
Lactaldehyde reductase (NADPH) inhibitor
Clavamate synthase inhibitor

Saccharolysin inhibitor
Melanin inhibitor
Allophanate hydrolase inhibitor
Subtilisin inhibitor
Acetylserotonin O-methyltransferase inhibitor
Long-chain-aldehyde dehydrogenase inhibitor
Narcolepsy treatment
Uroporphyrinogen-III synthase inhibitor
Antidyskinetic
(S)-3-amino-2-methylpropionate transaminase inhibitor
Heat shock protein agonist
N-hydroxy-2-acetamidofluorene reductase inhibitor
Bisphosphoglycerate mutase inhibitor
CYP1A3 substrate
15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor
Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor
Crotonoyl-[acyl-carrier-protein] hydratase inhibitor
Nitrate reductase (cytochrome) inhibitor
Hematopoietic inhibitor
ErbB antagonist
Polyamine oxidase inhibitor
Tropinesterase inhibitor
Antiprotozoal (Babesia)
Mitochondrial processing peptidase inhibitor
27-Hydroxycholesterol 7alpha-monooxygenase inhibitor
ErbB-2 antagonist
NMDA receptor agonist
Cellulase inhibitor
Neuropeptide Y4 antagonist
Cysteine-S-conjugate beta-lyase inhibitor
Sedoheptulose-bisphosphatase inhibitor
CYP26A substrate
Granzyme A inhibitor
Loop diuretic
UGT1A3 substrate
Endonuclease (influenza) inhibitor
Deoxyribose-phosphate aldolase inhibitor
Cytochrome-b5 reductase substrate
Penicillopepsin inhibitor
2,6-Dihydroxypyridine 3-monooxygenase inhibitor
Alanine transaminase inhibitor
Autophagy inducer
Antihelminthic (Nematodes)
Lysozyme inhibitor
Thimet oligopeptidase inhibitor
Procollagen C-endopeptidase inhibitor
Acrosin inhibitor
CYP2C6 substrate
Neurotransmitter antagonist
Allantoin racemase inhibitor

Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor
Carboxypeptidase D inhibitor
Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor
Bothrolysin inhibitor
Cytochrome P450 stimulant
Creatininase inhibitor
TNF convertase inhibitor
Dihydrouracil dehydrogenase (NAD⁺) inhibitor
Guanidinoacetase inhibitor
Phosphatidylinositol diacylglycerol-lyase inhibitor
Asparagine-tRNA ligase inhibitor
Arylesterase inhibitor
Imidazoline receptor agonist
Plasmanylethanolamine desaturase inhibitor
N-Acyl-D-aspartate deacylase inhibitor
Cyclooxygenase 1 substrate
Tryptophan alpha,beta-oxidase inhibitor
Gluconolactonase inhibitor
NMDA receptor glycine site agonist
UGT2B10 substrate
Lysine 2-monooxygenase inhibitor
N-Carbamoyl-D-amino acid hydrolase inhibitor
Histone deacetylase SIRT1 inhibitor
Serine-pyruvate transaminase inhibitor
CYP2C10 substrate
Brachyurin inhibitor
Pyruvate carboxylase inhibitor
Styrene-oxide isomerase inhibitor
UGT2B28 substrate
Hydroxymethylbilane synthase inhibitor
Homospermidine synthase inhibitor
Iduronate-2-sulfatase inhibitor
Aggrecanase 1 inhibitor
Thermolysin inhibitor
4-Nitrophenol 2-monooxygenase inhibitor
Myeloblastin inhibitor
Glutamate (mGluR4) antagonist
Dihydroorotate oxidase inhibitor
CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
N-hydroxyarylamine O-acetyltransferase inhibitor
Phenylacetate-CoA ligase inhibitor
D-amino-acid dehydrogenase inhibitor
Phosphodiesterase I inhibitor
Aldehyde ferredoxin oxidoreductase inhibitor
Furin inhibitor
Ribonucleoside diphosphate reductase inhibitor
Heat shock protein 70 agonist
Peptidyl-glycinamidase inhibitor
Glutamin-(asparagin-)ase inhibitor
Arylalkyl acylamidase inhibitor

Mitochondrial intermediate peptidase inhibitor
Peptidoglycan glycosyltransferase inhibitor
Fructan beta-fructosidase inhibitor
Arginine deiminase inhibitor
Acaricide
Endo-1,3(4)-beta-glucanase inhibitor
Tripeptidyl-peptidase I inhibitor
Protein-glutamate methylesterase inhibitor
BRAF expression inhibitor
Raynaud's phenomenon treatment
Vibriolysin inhibitor
CYP2A4 substrate
tRNA-pseudouridine synthase I inhibitor
Lysase inhibitor
Saccharopine dehydrogenase (NADP+, L-lysine-forming) inhibitor
Aspartate-ammonia ligase (ADP-forming) inhibitor
Diguanidinobutanase inhibitor
Glycine dehydrogenase (decarboxylating) inhibitor
Phenylalanine racemase (ATP-hydrolysing) inhibitor
Cyclin-dependent kinase 7 inhibitor
D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor
NMDA receptor polyamine site antagonist
Metalloproteinase inhibitor
2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
Para amino benzoic acid antagonist
ADP-thymidine kinase inhibitor
Glutamate-1-semialdehyde 2,1-aminomutase inhibitor
Apyrase inhibitor
Meprin B inhibitor
GST T substrate
GST T1-1 substrate
Oxidizing agent
Antimutagenic
Pantoate 4-dehydrogenase inhibitor
Acetylenecarboxylate hydratase inhibitor
Histamine release stimulant
Ferrochelataase inhibitor
Nucleoside oxidase (H₂O₂-forming) inhibitor
Cyclamate sulfohydrolase inhibitor
CYP2C9 inducer
CDP-4-dehydro-6-deoxyglucose reductase inhibitor
CYP4A11 substrate
Immunostimulant
Indolepyruvate C-methyltransferase inhibitor
Aldehyde dehydrogenase [NAD(P)+] inhibitor
Corticosteroid side-chain-isomerase inhibitor
Glyoxylate reductase (NADP+) inhibitor
Cytochrome-b5 reductase inhibitor
Carbon-monoxide dehydrogenase inhibitor
Butyrylcholinesterase stimulant

UGT1A6 substrate
Antineoplastic antimetabolite
Methane monooxygenase inhibitor
Diaminopropionate ammonia-lyase inhibitor
Chlordecone reductase inhibitor
GST M substrate
Phosphodiesterase 4C inhibitor
Inulinase inhibitor
Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor
2-Nitrophenol 2-monooxygenase inhibitor
Choline-sulfatase inhibitor
Metalloproteinase-3 inhibitor
12-Lipoxygenase inhibitor
Ganglioside galactosyltransferase inhibitor
Methanol dehydrogenase inhibitor
2-Aminohexano-6-lactam racemase inhibitor
Oligopeptidase B inhibitor
Cerebroside-sulfatase inhibitor
Beta-N-acetylgalactosaminidase inhibitor
Transketolase inhibitor
Antituberculosic
Diaminopimelate dehydrogenase inhibitor
Adenylate kinase inhibitor
Opioid dependency treatment
Acylaminoacyl-peptidase inhibitor
Phosphodiesterase 5A inhibitor
Glutamate N-acetyltransferase inhibitor
Urticaria treatment
Flavin-containing monooxygenase inhibitor
Antipsoriatic
N-acetyllactosamine synthase inhibitor
D-alanine transaminase inhibitor
Transcription factor NF kappa A inhibitor
Lombricine kinase inhibitor
Ornithine-oxo-acid transaminase inhibitor
Trimethyllysine dioxygenase inhibitor
Sphinganine-1-phosphate aldolase inhibitor
Glutamate 5-kinase inhibitor
Alpha-Methylacyl-CoA racemase inhibitor
Arginine kinase inhibitor
Maltose-transporting ATPase inhibitor
Phosphatidylglycerophosphatase inhibitor
Monophenol monooxygenase inhibitor
CYP4F2 substrate
Aryl hydrocarbon receptor agonist
Phosphoinositide phospholipase C inhibitor
Deacetoxycephalosporin-C synthase inhibitor
Anthranilate 3-monooxygenase (deaminating) inhibitor
Acyl-lysine deacylase inhibitor
Nardilysin inhibitor

Phosphodiesterase 4D inhibitor
3-Isopropylmalate dehydratase inhibitor
K(Ca) 3.1 channel blocker
Succinate-CoA ligase (ADP-forming) inhibitor
CF transmembrane conductance regulator agonist
Cysteine synthase inhibitor
Chaperonin ATPase inhibitor
D-glutamate oxidase inhibitor
Arylacetonitrilase inhibitor
2-Aminoadipate transaminase inhibitor
Lipoxygenase inhibitor
Transactivator transcription protein inhibitor
Phosphonoacetate hydrolase inhibitor
Cystathionine beta-lyase inhibitor
Urate-ribonucleotide phosphorylase inhibitor
Di-trans,poly-cis-decaprenylcistransferase inhibitor
Sphingosine 1-phosphate receptor 4 agonist
Heparan-alpha-glucosaminide N-acetyltransferase inhibitor
Envelysin inhibitor
Acetylornithine deacetylase inhibitor
Carboxymethylenebutenolidase inhibitor
Histidinol-phosphatase inhibitor
Pancreatic endopeptidase E inhibitor
Choline acetyltransferase stimulant
Microbial collagenase inhibitor
Diaminopimelate epimerase inhibitor
Metallo-carboxypeptidase D inhibitor
Histone deacetylase 1B inhibitor
Antiviral (Adenovirus)
L-lysine oxidase inhibitor
Tryptophan transaminase inhibitor
N-acetylneuraminase 4-O-acetyltransferase inhibitor
Malonate-semialdehyde dehydrogenase inhibitor
Adenylate cyclase I inhibitor
Carbonic anhydrase inhibitor
Adenylate cyclase stimulant
Leucine dehydrogenase inhibitor
Phosphodiesterase 4B inhibitor
Maleylacetoacetate isomerase inhibitor
3-Hydroxyphenylacetate 6-hydroxylase inhibitor
CTGF expression inhibitor
Horrisysin inhibitor
GABA B receptor agonist
Venom exonuclease inhibitor
Vascular adhesion protein 1 inhibitor
CYP7 inhibitor
Glycerol dehydrogenase (NADP+) inhibitor
Excitatory amino acid transporter 1 inhibitor
N-acetylneuraminase synthase inhibitor
1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor

D-cysteine desulfhydrase inhibitor
Caspase 8 stimulant
Sulfite dehydrogenase inhibitor
Carnitine dehydratase inhibitor
Interleukin 10 agonist
Feruloyl esterase inhibitor
Glutamate synthase (ferredoxin) inhibitor
Lysostaphin inhibitor
Rubredoxin-NAD⁺ reductase inhibitor
P-benzoquinone reductase (NADPH) inhibitor
Antihematotoxic
Pantothenase inhibitor
Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor
Trypanothione-disulfide reductase inhibitor
Membrane permeability inhibitor
Lysyl oxidase inhibitor
Carbamoyl-serine ammonia-lyase inhibitor
Serine-glyoxylate transaminase inhibitor
Farnesyltranstransferase inhibitor
Benzoate-CoA ligase inhibitor
Pyruvate dehydrogenase (cytochrome) inhibitor
Trans-2-enoyl-CoA reductase (NAD⁺) inhibitor
Centromere associated protein inhibitor
Adrenaline release stimulant
Gingipain R inhibitor
Antispirochetal
Saccharopine dehydrogenase (NAD⁺, L-glutamate-forming) inhibitor
Polyneuridine-aldehyde esterase inhibitor
Carbonic anhydrase II inhibitor
Telomerase inhibitor
D-stereospecific aminopeptidase inhibitor
Selenocysteine lyase inhibitor
Protein synthesis stimulant
Rhamnulose-1-phosphate aldolase inhibitor
Fumarate reductase (NADH) inhibitor
Pyruvate decarboxylase inhibitor
ADAM10 endopeptidase inhibitor
Glutamate (mGluR group III) antagonist
Licheninase inhibitor
ADP-ribosylarginine hydrolase inhibitor
Glutathione reductase (NADPH) stimulant
Glutathione reductase stimulant
Amino-acid N-acetyltransferase inhibitor
Cytochrome-c3 hydrogenase inhibitor
(S)-carnitine 3-dehydrogenase inhibitor
Allantoicase inhibitor
2-Hydroxy-3-oxopropionate reductase inhibitor
Thiamine-triphosphatase inhibitor
Glutathione dehydrogenase (ascorbate) inhibitor
Dihydrolipoamide S-acetyltransferase inhibitor

Dipeptidyl peptidase II inhibitor
Antineoplastic (ovarian cancer)
Pyridoxine 4-oxidase inhibitor
Cysteine desulfurase inhibitor
Antiperistaltic
Peptidoglycan beta-N-acetylmuramidase inhibitor
Trehalose-phosphatase inhibitor
Benzoylformate decarboxylase inhibitor
Ketol-acid reductoisomerase inhibitor
Carbonic anhydrase I inhibitor
3-Hydroxyacyl-CoA dehydrogenase inhibitor
tRNA nucleotidyltransferase inhibitor
2-Hydroxymuconate-semialdehyde hydrolase inhibitor
Arginyltransferase inhibitor
Deoxycytidylate 5-hydroxymethyltransferase inhibitor
Trans-pentaprenyltranstransferase inhibitor
Isomaltulose synthase inhibitor
DNA-(apurinic or apyrimidinic site) lyase inhibitor
Formimidoylglutamase inhibitor
Glycerol 2-dehydrogenase (NADP+) inhibitor
Aromatic-amino-acid transaminase inhibitor
Aminopeptidase A inhibitor
Glucosamine-1-phosphate N-acetyltransferase inhibitor
Tryptophan-tRNA ligase inhibitor
Sphingomyelinase inhibitor
Bone morphogenic protein inhibitor
Galactose oxidase inhibitor
Aspartate 1-decarboxylase inhibitor
Alkane 1-monooxygenase inhibitor
Secretase alpha stimulant
Secretase stimulant
Liver X receptor antagonist
NAD⁺ synthase (glutamine-hydrolysing) inhibitor
Arginine-tRNA ligase inhibitor
Paget's disease treatment
Hydroxylamine reductase inhibitor
Glucarate dehydratase inhibitor
Glycine N-methyltransferase inhibitor
Peptidyltransferase inhibitor
Glutathione synthase inhibitor
CYP26 substrate
Carnitine 3-dehydrogenase inhibitor
Nitrite reductase [NAD(P)H] inhibitor
Tryptophan 2-monooxygenase inhibitor
Angiogenesis inhibitor
Beta-mannosidase inhibitor
Sarcosine oxidase inhibitor
Endoglycosylceramidase inhibitor
CYP2A13 substrate
Inorganic diphosphatase inhibitor

Amidase inhibitor
Aspartate racemase inhibitor
Antineoplastic (cervical cancer)
Leukotriene C antagonist
Decylcitrate synthase inhibitor
Urocanate hydratase inhibitor
Antirickettsial
Serratia marcescens nuclease inhibitor
Beta-ureidopropionase inhibitor
Salicylate 1-monooxygenase inhibitor
Glucosyl transferase inhibitor
Antipruritic, non-allergic
Homoserine dehydrogenase inhibitor
5-Lipoxygenase inhibitor
Ethanolamine oxidase inhibitor
CYP2B5 substrate
Cyclopentanone monooxygenase inhibitor
Carbonic anhydrase V inhibitor
Kynureninase inhibitor
Carbonic anhydrase VII inhibitor
Cytosole dipeptidase inhibitor
Alpha-amylase inhibitor
Farnesoid X receptor antagonist
Polar-amino-acid-transporting ATPase inhibitor
Potassium channel small-conductance Ca-activated 3 activator
Acetate kinase inhibitor
Antifibrinolytic
Chelator
Acetyl-CoA C-acyltransferase inhibitor
Ovulation inhibitor
Phosphoenolpyruvate-protein phosphotransferase inhibitor
Lysine decarboxylase inhibitor
Adenylosuccinate synthase inhibitor
Retinoic acid beta receptor agonist
Dextranase inhibitor
Cyclohexanone monooxygenase inhibitor
4-Hydroxybenzoate nonaprenyltransferase inhibitor
Cyclin-dependent kinase 9 inhibitor
IgA-specific metalloendopeptidase inhibitor
Malate-CoA ligase inhibitor
Galacturan 1,4-alpha-galacturonidase inhibitor
Haloacetate dehalogenase inhibitor
Prepilin peptidase inhibitor
Methionyl aminopeptidase 1 inhibitor
N-Acyl-D-amino-acid deacylase inhibitor
5-Oxoprolinase (ATP-hydrolysing) inhibitor
pFOX inhibitor
Coagulant
Glycine hydroxymethyltransferase inhibitor
Gamma-glutamyl hydrolase inhibitor

2-Haloacid dehalogenase (configuration-inverting) inhibitor
Malate dehydrogenase (acceptor) inhibitor
Ferredoxin hydrogenase inhibitor
Bone morphogenic protein 1 inhibitor
(R,R)-butanediol dehydrogenase inhibitor
FMO1 substrate
Carbonic anhydrase XIV inhibitor
Peptidyl-dipeptidase B inhibitor
Aconitate decarboxylase inhibitor
5 Hydroxytryptamine 1E antagonist
ADAM inhibitor
Homogentisate 1,2-dioxygenase inhibitor
X-methyl-His dipeptidase inhibitor
Dichloromuconate cycloisomerase inhibitor
Cholate-CoA ligase inhibitor
D-Ornithine 4,5-aminomutase inhibitor
Cancer procoagulant inhibitor
Cyanate hydratase inhibitor
L-threonine 3-dehydrogenase inhibitor
Beta-cyclopiazonate dehydrogenase inhibitor
NAD(P)⁺-arginine ADP-ribosyltransferase inhibitor
Neuropsin inhibitor
Tyrosine kinase stimulant
Valine decarboxylase inhibitor
2-Oxoglutarate decarboxylase inhibitor
Allantoate deiminase inhibitor
2-Acylglycerol O-acyltransferase inhibitor
3C-like protease (Human coronavirus) inhibitor
Cysteine transaminase inhibitor
Carbonic anhydrase IV inhibitor
Deoxyhypusine synthase inhibitor
Matrilysin inhibitor
Saccharopine dehydrogenase (NADP⁺, L-glutamate-forming) inhibitor
UGT2B4 substrate
Lactate 2-monooxygenase inhibitor
CYP2B18 substrate
Endocannabinoid uptake inhibitor
Antihelminthic (Fasciola)
Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
Putrescine oxidase inhibitor
L-lysine 6-transaminase inhibitor
TRPA1 agonist
Antidote, heavy metal
Calpain inhibitor
Antiprotozoal (Trypanosoma)
Hydroxymethylglutaryl-CoA lyase inhibitor
MAP-kinase-activated kinase 1 inhibitor
3-Aminobutyryl-CoA ammonia-lyase inhibitor
3-Oxoacid CoA-transferase inhibitor
UGT1A substrate

Carboxypeptidase E inhibitor
Alpha-N-arabinofuranosidase inhibitor
Allantoinase inhibitor
Asparagine-oxo-acid transaminase inhibitor
CYP2B11 substrate
2-Oxoisovalerate dehydrogenase (acylating) inhibitor
Phosphogluconate 2-dehydrogenase inhibitor
Arabinose-5-phosphate isomerase inhibitor
Tyrosine 2,3-aminomutase inhibitor
Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor
Formaldehyde dehydrogenase (glutathione) inhibitor
Photosensitizer
NADPH-ferrihemoprotein reductase inhibitor
Glutamate formimidoyltransferase inhibitor
Protein kinase stimulant
2-Methylcitrate dehydratase inhibitor
Polygalacturonase inhibitor
Methionyl aminopeptidase inhibitor
Histone acetyltransferase inhibitor
Glycine N-acyltransferase inhibitor
Glycine transaminase inhibitor
Carnosine synthase inhibitor
Opioid kappa 3 receptor antagonist
Acylglycerone-phosphate reductase inhibitor
Protein-tyrosine sulfotransferase inhibitor
(S)-3-hydroxyacid ester dehydrogenase inhibitor
Orotate reductase (NADH) inhibitor
CYP4A1 substrate
Dihydroorotate dehydrogenase inhibitor
Excitatory amino acid transporter 2 inhibitor
Lysophosphatidic acid receptor antagonist
Glutaminase inhibitor
Galactosylgalactosylglucosylceramidase inhibitor
Guanidinodeoxy-scylo-inositol-4-phosphatase inhibitor
Aryl-alcohol dehydrogenase (NADP+) inhibitor
Dopamine release stimulant
Insulysin inhibitor
Neurolysin inhibitor
Thiosulfate sulfurtransferase inhibitor
Heparanase inhibitor
Mucorpepsin inhibitor
Antiviral (Parainfluenza)
Polynucleotide 5'-hydroxy-kinase inhibitor
NAD(P)+ transhydrogenase (AB-specific) inhibitor
Ubiquitin thiolesterase inhibitor
3-Carboxyethylcatechol 2,3-dioxygenase inhibitor
Tryptophanyl aminopeptidase inhibitor
1-Aminocyclopropane-1-carboxylate deaminase inhibitor
Serine 3-dehydrogenase inhibitor
Mandelate racemase inhibitor

Glycerol-1-phosphatase inhibitor
Glutamate dehydrogenase [NAD(P)+] inhibitor
Dihydrouracil oxidase inhibitor
X-Pro dipeptidase inhibitor
Tyrosine-ester sulfotransferase inhibitor
Aminomuconate-semialdehyde dehydrogenase inhibitor
Homocysteine desulfhydrase inhibitor
3-Ketovalidoxylamine C-N-lyase inhibitor
Creatinase inhibitor
Sterol 3-beta-glucosyltransferase inhibitor
Free radical scavenger
Antidote, organophosphates
Threonine aldolase inhibitor
Adenosine deaminase inhibitor
6-Carboxyhexanoate-CoA ligase inhibitor
Biotin-CoA ligase inhibitor
Homoaconitate hydratase inhibitor
Triacetate-lactonase inhibitor
Orotate reductase (NADPH) inhibitor
4-Phytase inhibitor
Cell wall biosynthesis inhibitor
2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor
Guanidinobutyrase inhibitor
UDP-3-O-acyl-N-acetylglucosamine deacetylase inhibitor
Oxytocic
Aspartate carbamoyltransferase inhibitor
Deoxyribonuclease I inhibitor
Sphingosine 1-phosphate receptor 3 agonist
Phosphatidylinositol 3-kinase stimulant
Acidifying agent gastric
RNA-directed RNA polymerase (Influenza A) inhibitor
Tryptophan synthase inhibitor
Retinal dehydrogenase inhibitor
Formaldehyde dehydrogenase inhibitor
(S)-2-Methylmalate dehydratase inhibitor
Mannan endo-1,6-alpha-mannosidase inhibitor
Glutamate (mGluR6) antagonist
Melatonin agonist
Candidapepsin inhibitor
Histone acetylation inducer
Ribonucleotide reductase inhibitor
Acetoacetate decarboxylase inhibitor
Phenol 2-monooxygenase inhibitor
CDC25C inhibitor
Kexin inhibitor
Methylaspartate ammonia-lyase inhibitor
CYP3A3 substrate
Leukotriene C4 antagonist
Heparin epidermal growth factor antagonist

CC chemokine receptor agonist
Chemokine receptor agonist
Chitin synthase inhibitor
2,4-Dichlorophenol 6-monooxygenase inhibitor
2-Nitropropane dioxygenase inhibitor
Beta lactamase TEM-1 inhibitor
Mannitol-1-phosphatase inhibitor
Chloramphenicol O-acetyltransferase inhibitor
Oxalate oxidase inhibitor
Cytoprotectant
Delayed rectifier potassium channel activator
Potassium channel (Voltage-sensitive) activator
Potassium channel KCNQ activator
Nitrilase inhibitor
3-Dehydroquate dehydratase inhibitor
L-ascorbate peroxidase inhibitor
tRNA (cytosine-5-)-methyltransferase inhibitor
Amino-acid racemase inhibitor
Peptide-tryptophan 2,3-dioxygenase inhibitor
Hepatocyte nuclear factor 4 alpha antagonist
Hepatocyte nuclear factor antagonist
Galactoside O-acetyltransferase inhibitor
Endopeptidase inhibitor
2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
Pectin lyase inhibitor
UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor
Scyllo-inosamine-4-phosphate amidinotransferase inhibitor
Dihydrofolate synthase inhibitor
HDL-cholesterol increasing
Sphingosine 1-phosphate receptor 4 antagonist
L-aminoadipate-semialdehyde dehydrogenase inhibitor
PRL phosphatase inhibitor
Skin whitener
Biotin carboxylase inhibitor
Antihyperlipoproteinemic
Endo-beta-N-acetylglucosaminidase inhibitor
Hydroxyacylglutathione hydrolase inhibitor
DNA-3-methyladenine glycosylase II inhibitor
tRNA (guanine-N2-)-methyltransferase inhibitor
Thermomycin inhibitor
HMOX1 expression enhancer
Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
Purine biosynthesis inhibitor
Creatinine deaminase inhibitor
Neuropeptide FF agonist
Neuropeptide FF2 agonist
D-threo-aldose 1-dehydrogenase inhibitor
Toll-Like receptor antagonist
ATP deaminase inhibitor
Picornain 2A inhibitor

Acetylcholinesterase stimulant
Tryptophan dimethylallyltransferase inhibitor
Glucan 1,4-beta-glucosidase inhibitor
Dihydroxy-acid dehydratase inhibitor
Ribulose-bisphosphate carboxylase inhibitor
Sphingosine kinase inhibitor
6-Pyruvoyltetrahydropterin synthase inhibitor
Biliary tract disorders treatment
Glutamate (mGluR8) agonist
Malyl-CoA lyase inhibitor
Potassium channel KCNQ2 activator
Synaptic vesicle protein SV2, levetiracetam binding site antagonist
Aminopeptidase Y inhibitor
4a-Hydroxytetrahydrobiopterin dehydratase inhibitor
Cerevisin inhibitor
Aryldialkylphosphatase inhibitor
Leucolysin inhibitor
Endothelial growth factor antagonist
2-Methyleneglutarate mutase inhibitor
3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor
UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor
Glutamate carboxypeptidase inhibitor
Cyclooxygenase 3 inhibitor
Snapalysin inhibitor
N6-methyl-lysine oxidase inhibitor
CYP4B1 substrate
Sulfite reductase inhibitor
CYP4B substrate
Glycine N-choloyltransferase inhibitor
Glyceryl-ether monooxygenase inhibitor
Mucomembranous protector
Renilla-luciferin 2-monooxygenase inhibitor
Histone deacetylase SIRT2 inhibitor
Tryptophanamidase inhibitor
Proline racemase inhibitor
D-lactate dehydrogenase inhibitor
Proline dehydrogenase inhibitor
Pyruvate dehydrogenase kinase inhibitor
Homoserine O-succinyltransferase inhibitor
Retinol O-fatty-acyltransferase inhibitor
CXC chemokine 1 receptor antagonist
Cell wall synthesis inhibitor
Carboxylate reductase inhibitor
Leukotriene A4 hydrolase inhibitor
Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor
Azobenzene reductase inhibitor
3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor
NMDA receptor polyamine site agonist
Mycolysin inhibitor
CMP-N-acylneuraminate phosphodiesterase inhibitor

Homocitrate synthase inhibitor
Dipeptidyl peptidase inhibitor
4-Chlorophenylacetate 3,4-dioxygenase inhibitor
Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
Alternansucrase inhibitor
ATM kinase inhibitor
D-xylulose reductase inhibitor
Fatty-acyl-ethyl-ester synthase inhibitor
O-acetylhomoserine aminocarboxypropyltransferase inhibitor
N-Acetylated alpha-linked acidic dipeptidase inhibitor
Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
Neutral endopeptidase inhibitor
Deoxycytidine deaminase inhibitor
Bis(5'-adenosyl)-triphosphatase inhibitor
Agmatinase inhibitor

