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| Molecular Cluster  **Maping Molecular Cluster** **through Targets to ICD Categories** | Connected Targets | Connected ICD Categories |
| Molecular Cluster 1 | 4-Nitrophenol 2-monooxygenase inhibitor, Aspulvinone dimethylallyltransferase inhibitor, CYP2A11 substrate, CYP2A4 substrate, CYP2B5 substrate, CYP2C12 substrate, CYP2F1 substrate, Chlordecone reductase inhibitor, Lipid metabolism regulator, Lipid peroxidase inhibitor, Membrane integrity agonist, Spasmolytic, urinary | Digestive & Gastrointestinal System, Endocrine & Miscellaneous Metabolic Processes, Unclassified |
| Molecular Cluster 13 | Acylcarnitine hydrolase inhibitor, Alkenylglycerophosphocholine hydrolase inhibitor, Alkylacetylglycerophosphatase inhibitor, Antihypercholesterolemic, Caspase 3 stimulant, Chemopreventive, Cholesterol antagonist, DELTA14-sterol reductase inhibitor, Dextranase inhibitor, Hepatoprotectant, Hypolipemic, Linoleate diol synthase inhibitor, Proliferative diseases treatment, Prostaglandin-E2 9-reductase inhibitor, Respiratory analeptic, Testosterone 17beta-dehydrogenase (NADP+) inhibitor, UGT1A substrate, UGT1A4 substrate | Cardiovascular & Blood Circulatory System, Digestive & Gastrointestinal System, Endocrine & Miscellaneous Metabolic Processes, Nervous & Musculoskeletal System, Respiratory & Immune System, Skin, Soft Tissue, & Hepatic System, Unclassified, Urinary & Reproductive System |
| Molecular Cluster 30 | 2-Hydroxymuconate-semialdehyde hydrolase inhibitor, 3-Hydroxybenzoate 6-monooxygenase inhibitor, 5 Hydroxytryptamine release stimulant, 5-O-(4-coumaroyl)-D-quinate 3'-monooxygenase inhibitor, Aldehyde dehydrogenase 1 substrate, Aldehyde oxidase inhibitor, Alkane 1-monooxygenase inhibitor, Alkenylglycerophosphocholine hydrolase inhibitor, Arginine 2-monooxygenase inhibitor, Aryl-alcohol dehydrogenase inhibitor, Arylacetonitrilase inhibitor, Aspartate-phenylpyruvate transaminase inhibitor, Aspulvinone dimethylallyltransferase inhibitor, Bisphosphoglycerate phosphatase inhibitor, CDP-glycerol glycerophosphotransferase inhibitor, CYP2C12 substrate, CYP2J substrate, Cardiovascular analeptic, Chenodeoxycholoyltaurine hydrolase inhibitor, Chlordecone reductase inhibitor, Dehydro-L-gulonate decarboxylase inhibitor, Feruloyl esterase inhibitor, Glutamyl endopeptidase II inhibitor, Glutathione thiolesterase inhibitor, Membrane integrity agonist, Monodehydroascorbate reductase (NADH) inhibitor, Phobic disorders treatment, Phosphatidylcholine-retinol O-acyltransferase inhibitor, Prolyl aminopeptidase inhibitor, Pullulanase inhibitor, Ribulose-phosphate 3-epimerase inhibitor, Sugar-phosphatase inhibitor, Testosterone 17beta-dehydrogenase (NADP+) inhibitor, UDP-N-acetylglucosamine 4-epimerase inhibitor, Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor | Cardiovascular & Blood Circulatory System, Digestive & Gastrointestinal System, Endocrine & Miscellaneous Metabolic Processes, Nervous & Musculoskeletal System, Respiratory & Immune System, Skin, Soft Tissue, & Hepatic System, Unclassified |
| Molecular Cluster 40 | 2-Dehydropantoate 2-reductase inhibitor, Aldehyde oxidase inhibitor, Aryl-alcohol dehydrogenase (NADP+) inhibitor, CYP1A substrate, CYP1A1 inhibitor, CYP1A2 substrate, CYP1B substrate, CYP1B1 inhibitor, CYP2A6 substrate, Chlordecone reductase inhibitor, HIF1A expression inhibitor, Histidine kinase inhibitor, Kinase inhibitor, Membrane integrity agonist, Membrane permeability inhibitor, Monophenol monooxygenase inhibitor, P-benzoquinone reductase (NADPH) inhibitor, Peroxidase inhibitor, Quercetin 2,3-dioxygenase inhibitor, Ubiquinol-cytochrome-c reductase inhibitor | Endocrine & Miscellaneous Metabolic Processes, Respiratory & Immune System, Skin, Soft Tissue, & Hepatic System, Unclassified, Urinary & Reproductive System |
| Molecular Cluster 46 | Antiseborrheic, Arylsulfate sulfotransferase inhibitor, Aspulvinone dimethylallyltransferase inhibitor, CYP2H substrate, Calcium channel (voltage-sensitive) activator, Cardiovascular analeptic, Fibrinolytic, Fusarinine-C ornithinesterase inhibitor, Membrane integrity agonist, Mucomembranous protector, Phobic disorders treatment, Prolyl aminopeptidase inhibitor | Digestive & Gastrointestinal System, Endocrine & Miscellaneous Metabolic Processes, Nervous & Musculoskeletal System, Respiratory & Immune System, Skin, Soft Tissue, & Hepatic System, Unclassified |