Scientific names of Indian medicinal plants

Manual curation of the list identify synonyms for removal of redundant information

Indexing a unique scientific name to each curatede Indian medicinal plant and its synonyms

Curated list of Indian medicinal plants

Literature

Databases

Natural Language Processing (NLP)

PubMed.gov

List of plant-phytochemical associations

Manual search for phytochemical ontologies (Phytochemical name, synonyms and Standard chemical identifiers)

Indexing a unique standard chemical identifier to each phytochemical in a chosen ontological order

Pubchem
ChEBI
CAS
CHEMSPIDER

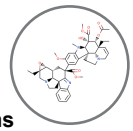
Plant classification

Tropicos
PlantList

Kingdom
Family

Indian Medicinal Plant

Phytochemical



Unique list of Plant-Phytochemical associations

Phytochemical classification

ClassyFire

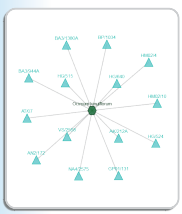
Kingdom
Superclass
Class
Subclass

Traditional Indian medicine Formulations

TKDL

Plant-Formulation associations

INDIAN MEDICINAL PLANT	FORMULATION IDENTIFIER
Ocimum tenuiflorum	AK/212A
Ocimum tenuiflorum	AT/87
Ocimum tenuiflorum	BP/1034
Ocimum tenuiflorum	HG/515
Ocimum tenuiflorum	HG/524
Ocimum tenuiflorum	HG/640
Ocimum tenuiflorum	VS/2558



Literature

List of Plant-Therapeutic use associations

Manual search for therapeutic ontologies (Therapeutics name, synonyms and standard identifiers)

Indexing a unique therapeutic use and its synonyms

Unique list of Plant-Therapeutic use associations

Cheminformatics

STITCH

Human target proteins

Predicted human target proteins

Protein identifier	HGNC symbol	Combined score from STITCH database
ENSP00000461516	TRPV1	770
ENSP00000350841	HSPA4	600
ENSP00000367959	NTRK1	600
ENSP00000340019	HSPD1	600
ENSP00000311032	CASP3	700
ENSP00000320239	TRPM7	862
ENSP00000262209	TRPA1	770
ENSP00000341045	UGT2B15	700

Cytoscape network of predicted human targets of CAPNORDL

admetSAR

ADMET properties

ADMET Properties

Property	Value	Probability
Human Intestinal Absorption	+	0.996
Blood Brain Barrier	+	0.938
Caco-2 permeable	+	0.915
P-glycoprotein substrate	Non-substrate	0.722
P-glycoprotein inhibitor I	Non-inhibitor	0.934
P-glycoprotein inhibitor II	Non-inhibitor	0.988

FAF-*Drugs*4
RDKit
Open Babel

Physicochemical and drug-likeness properties

Physicochemical Properties

Property	Value
Molecular weight	150.22 g/mol
LogP	2.82
LogD	3.43
LogSw	-3.08
Number of stereocenters	0
Stereochemical complexity	0.000
Fsp3	0.400
Topological polar surface area	20.23 Å²

Drug-likeness Properties

Property	Value
Lipinski's rule of 5 violations	0
Veber rule	Good
Egan rule	Good
Oral PhysChem score (Traffic Lights)	1
GSK's 4/400 score	Good

Balloon
Open Babel

3D Structure