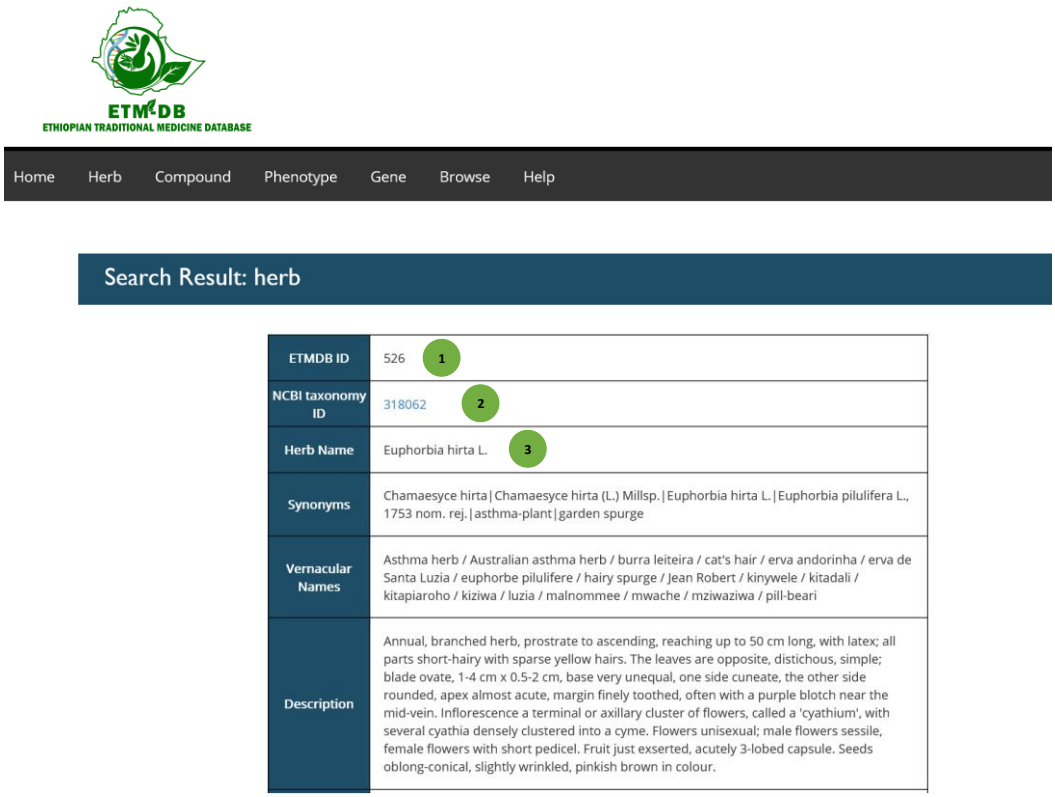
Contents

1. Help general description

The ETM-DB website interface allows users to search for entities and relationships using (a) names, ETM-DB identifiers, NCBI taxonomy identifiers for herbs, (b) names, ETM-DB identifiers, InChI, InChIkey, smiles, formula for compounds, (c) names, ETM-DB identifiers, UMLS names, UMLS IDs for phenotypes, or (d) gene names, ETM-DB identifiers, Entrez ID, gene symbol. Search results for entities and relationships including references to the sources are displayed in the web interface. The herbs search result page shows the herb attributes and related compounds, phenotypes and prescriptions. Search results for compounds display compound attributes and related herbs, phenotypes and genes. It includes detailed information on 2D and 3D chemical structure, predicted physicochemical and ADMET properties for the selected phytochemical. Users can also download 2D and 3D structure of the phytochemical in the form of a structure-data file (SDF). For phenotype search results, associated herbs, compounds, genes and prescriptions are included. Similarly, gene query results show gene attributes, related compounds, and phenotypes. For each query result, users can click each entity identifier to view a different page including detailed data about the entities. Users can also click the button "Browse" on the the homepage to browse compounds and herbs in the database.

2. Herb search

You can search the herb of interest using names, ETM-DB identifiers, and NCBI taxonomy identifiers. Users can also browse herbs alphabetically in the browse menu.



- ✧ Each herb has a unique ID. The ID (1) can be used in the search field to access the herb directly. If you know the NCBI taxonomy ID (2) or name (3) of the herb, you can insert in the herb search box to directly access the herb.
- ✧ The herb search result is displayed as shown above.

3. Compound search

The search options for compounds include name, ETM-DB ID, SMILES, InChI, InChIkey, Formula and Structure.

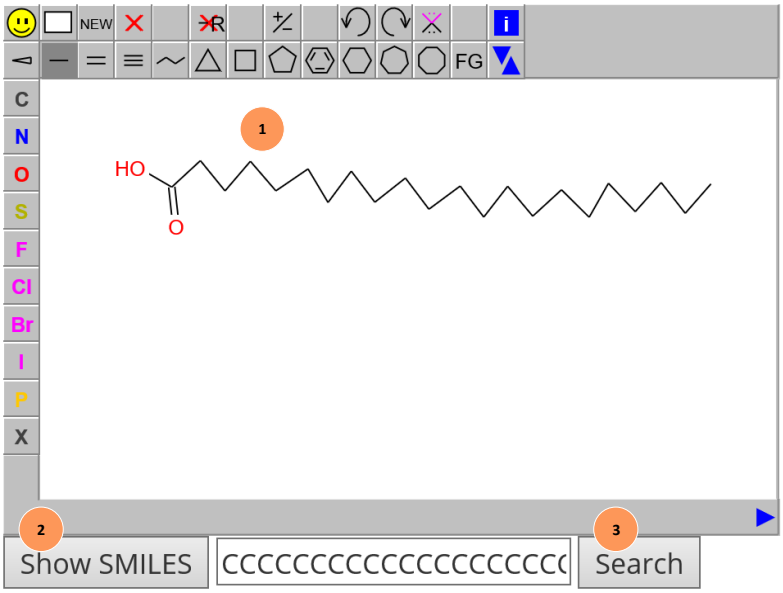
Users can also browse compounds alphabetically in the browse menu.

3.1.1. Direct keyword search

A. If you know the name (1) of the compound of interest just type in compound search menu.

B. Each compound has the SMILES (2). Similarly, users can also enter compound ETMDB ID, InChi Key, InChi or Formula in the compound search to access the compound information directly.

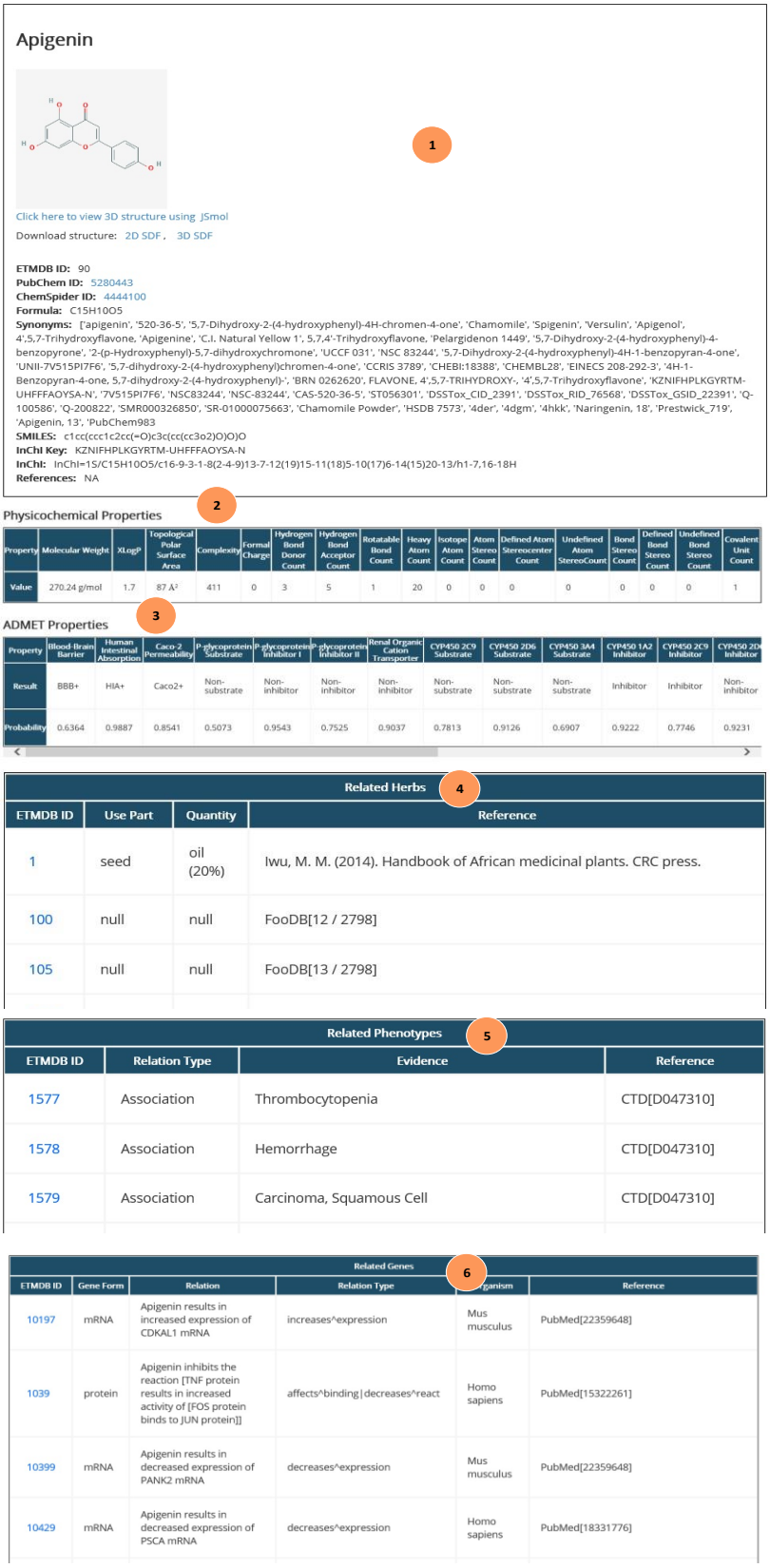
3.1.2. Structure search



A. Users can draw a structure of the compound to search for similar compound. For example, the structure drawn on the Field (1) window is behenic acid. It can be drawn by selecting single bond from the top panel and attaching hydroxyl group by selecting O from the left panel. Then selecting double bond from the top panel followed by selecting O from the left panel to draw the oxygen on the double bond. The other carbon chain is drawn by concatenating single bond.

B. Once the structure is drawn, users have to click show SMILES (2) button to generate the SMILES from the structure, followed by hitting the Search (3) button to submit the query and the results page will be displayed.

3.1.3. Compound search result (Example: Apigenin)



Apigenin

1

Click here to view 3D structure using JSmol

Download structure: 2D SDF , 3D SDF

ETMDB ID: 90
PubChem ID: 5280443
ChemSpider ID: 4444100
Formula: C15H10O5
Synonyms: ['apigenin', '520-36-5', '5,7-Dihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one', 'Chamomile', 'Spigenin', 'Versulin', 'Apigenol', 4',5,7-Trihydroxyflavone, 'Apigenine', 'C.I. Natural Yellow 1', 5,7,4'-Trihydroxyflavone, 'Pelargidenon 1449', '5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-benzopyrone', '2-(p-Hydroxyphenyl)-5,7-dihydroxychromone', 'UCCF 031', 'NSC 83244', '5,7-Dihydroxy-2-(4-hydroxyphenyl)-4H-1-benzopyran-4-one', 'UNII-7V515PI7F6', '5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one', 'CCRIS 3789', 'CHEBI:18388', 'CHEMBL28', 'EINECS 208-292-3', '4H-1-Benzopyran-4-one, 5,7-dihydroxy-2-(4-hydroxyphenyl)-', 'BRN 0262620', FLAVONE, 4',5,7-TRIHYDROXY-, '4',5,7-Trihydroxyflavone', 'KZNIFHPLKGYRTM-UHFFFAOYSA-N', '7V515PI7F6', 'NSC83244', 'NSC-83244', 'CAS-520-36-5', 'ST056301', 'DSSTox_CID_2391', 'DSSTox_RID_76568', 'DSSTox_GSID_22391', 'Q-100586', 'Q-200822', 'SMR000326850', 'SR-01000075663', 'Chamomile Powder', 'HSDB 7573', '4der', '4dgm', '4hkk', 'Naringenin, 18', 'Prestwick_719', 'Apigenin, 13', 'PubChem983
SMILES: c1cc(ccc1c2cc(=O)c3c(cc(cc3o2)O)O)O
InChI Key: KZNIFHPLKGYRTM-UHFFFAOYSA-N
InChI: InChI=1S/C15H10O5/c16-9-3-1-8(2-4-9)13-7-12(19)15-11(18)5-10(17)6-14(15)20-13/h1-7,16-18H
References: NA

Physicochemical Properties

2

Property	Molecular Weight	XLogP	Topological Polar Surface Area	Complexity	Formal Charge	Hydrogen Bond Donor Count	Hydrogen Bond Acceptor Count	Rotatable Bond Count	Heavy Atom Count	Isotope Atom Count	Atom Stereo Count	Defined Atom Stereocenter Count	Undefined Atom StereoCount	Bond Stereo Count	Defined Bond Stereo Count	Undefined Bond Stereo Count	Covalent Unit Count
Value	270.24 g/mol	1.7	87 Å²	411	0	3	5	1	20	0	0	0	0	0	0	0	1

ADMET Properties

3

Property	Blood-Brain Barrier	Human Intestinal Absorption	Caco-2 Permeability	P-glycoprotein Substrate	P-glycoprotein Inhibitor I	P-glycoprotein Inhibitor II	Renal Organic Cation Transporter	CYP450 2C9 Substrate	CYP450 2D6 Substrate	CYP450 3A4 Substrate	CYP450 1A2 Inhibitor	CYP450 2C9 Inhibitor	CYP450 2D6 Inhibitor
Result	BBB+	HIA+	Caco2+	Non-substrate	Non-inhibitor	Non-inhibitor	Non-inhibitor	Non-substrate	Non-substrate	Non-substrate	Inhibitor	Inhibitor	Non-inhibitor
Probability	0.6364	0.9887	0.8541	0.5073	0.9543	0.7525	0.9037	0.7813	0.9126	0.6907	0.9222	0.7746	0.9231

Related Herbs

4

ETMDB ID	Use Part	Quantity	Reference
1	seed	oil (20%)	Iwu, M. M. (2014). Handbook of African medicinal plants. CRC press.
100	null	null	FooDB[12 / 2798]
105	null	null	FooDB[13 / 2798]

Related Phenotypes

5

ETMDB ID	Relation Type	Evidence	Reference
1577	Association	Thrombocytopenia	CTD[D047310]
1578	Association	Hemorrhage	CTD[D047310]
1579	Association	Carcinoma, Squamous Cell	CTD[D047310]

Related Genes

6

ETMDB ID	Gene Form	Relation	Relation Type	Organism	Reference
10197	mRNA	Apigenin results in increased expression of CDKAL1 mRNA	increases^expression	Mus musculus	PubMed[22359648]
1039	protein	Apigenin inhibits the reaction [TNF protein results in increased activity of [FOS protein binds to JUN protein]]	affects^binding|decreases^react	Homo sapiens	PubMed[15322261]
10399	mRNA	Apigenin results in decreased expression of PANK2 mRNA	decreases^expression	Mus musculus	PubMed[22359648]
10429	mRNA	Apigenin results in decreased expression of PSCA mRNA	decreases^expression	Homo sapiens	PubMed[18331776]

A. The general properties (chemical structures, PubChem ID, ChemSpider ID, formula, synonym, smiles, InChIKey, and InChI) of the corresponding compound is shown at the top of the compound search result as shown in Field (1). PubChem and ChemSpider IDs are linked, if available, and users can click the link to be redirected to the PubChem and ChemSpider page, where additional information about this compound can be accessed.

B. This is followed by predicted physicochemical properties (2) and ADMET properties (3) of the compounds.

C. Field (4) shows the information about the related phenotypes to the respective comound. This relation contains informations about relation type, evidence, and reference. Similarly field (5) is information about related target gene/protein with attributes shown