A

Boletus edulis

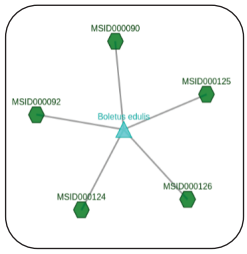
Family: Boletaceae

System of Traditional medicine: Traditional Chinese Medicine

Reference: PMID:30668382, ISBN:1-57067-143-5

Genome sequence

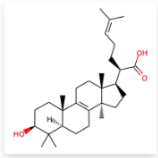
Medicinal fungi	Secondary metabolite identifier	Secondary metabolite name	Reference
Boletus edulis	MSID000090	(1S)-(3-ethenylphenyl)-1,2-ethanediol	PMID:17440922
Boletus edulis	MSID000092	(1S)-(4-acetylphenyl)-1,2-ethanediol	PMID:17440922
Boletus edulis	MSID000124	1-(3-Ethylphenyl)-1,2-ethanediol	PMID:17440922
Boletus edulis	MSID000125	1-(3-Formylphenyl)-ethanone	PMID:17440922
Boletus edulis	MSID000126	1-(4-Ethylphenyl)-1,2-ethanediol	PMID:17440922



B

Secondary metabolite: Trametenolic acid B

Summary | Physicochemical properties | Drug-likeness properties | ADMET properties | Descriptors | Predicted human target proteins



Summary

Molecular formula: C30H48O3

SMILES: CC(=CCC[C@H](C[C@H]1CC[C@@]2([C@]1(C)CCC1=C2CC[C@@H]2[C@]1(C)CC[C@@H](C2(C)C)O)C)C(=O)O)C

InChI: InChI=1S/C30H48O3/c1-19(2)9-8-10-20(26(32)33)21-13-17-30(7)23-11-12-24-27(3,4)25(31)15-16-28(24,5)22(23)14-18-29(21,30)6/h9,20-21,24-25,31H,8,10-18H2,1-7H3,(H,32,33)/t20-,21-,24+,25+,28-,29-,30+/m1/s1

InChIKey: NBSBUIQBEPROBM-GIICLEHTSA-N

Chemical classification

Kingdom: Organic compounds

Super class: Lipids and lipid-like molecules

Class: Prenol lipids

Sub class: Triterpenoids

Synonymous chemical names:

(+)-trametenolic acid b, 3b-hydroxy-5 a -lanosta-8,24-dien-21-oic acid, 3β-hydroxy-5α-lanosta-8,24-diene-21-oic acid, trametenolic acid b

External chemical identifiers:

CID_12309443; CAS_24160-36-9; NPATLAS_NPA011620; CHEMSPIDER_10193870

Chemical structure download

2D: 2D MOL | 2D MOL2 | 2D SDF

3D: 3D MOL | 3D MOL2 | 3D SDF | 3D PDB | 3D PDBQT

Physicochemical properties

Property name	Tool	Property value
Molecular weight (g/mol)	RDKit	456.71
Log P	RDKit	7.54
Topological polar surface area (Å^2)	RDKit	57.53
Number of hydrogen bond acceptors	RDKit	2
Number of hydrogen bond donors	RDKit	2

Drug-likeness properties

Property name	Tool	Property value
Number of Lipinski's rule of 5 violations	RDKit	1
Lipinski's rule of 5 filter	RDKit	Passed
Number of Ghose filter violations	RDKit	3
Ghose filter	RDKit	Failed
Veber filter	RDKit	Good
Egan filter	RDKit	Bad
Pfizer's 3/75 filter	RDKit	Bad
GSK 4/400 filter	RDKit	Bad
Number of Leadlikeness violations	SwissADME	2
Weighted quantitative estimate of drug-likeness (QEDw) score	RDKit	0.42

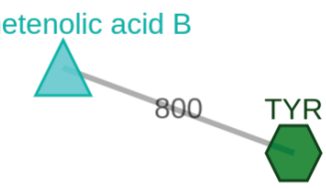
ADMET properties

Property name	Tool	Property value
Bioavailability score	SwissADME	0.85
Solubility class [ESOL]	SwissADME	Poorly soluble
Solubility class [Silicos-IT]	SwissADME	Poorly soluble
Blood Brain Barrier permeation	SwissADME	No
Gastrointestinal absorption	SwissADME	Low
Log K_p (Skin permeation, cm/s)	SwissADME	-3.78
Number of PAINS structural alerts	SwissADME	0
Number of Brenk structural alerts	SwissADME	1

Descriptors

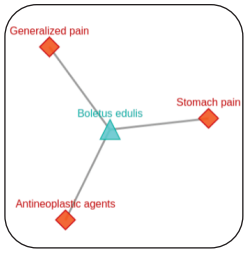
Tool	Type	Descriptor	Description	Descriptor class	Result
PaDEL	2D	nAcid	Number of acidic groups. The list of acidic groups is defined by these SMARTS "${[O;H1]-[C,S,P]=O)", "${[*;-!S(*~[*;+])])", "${[NH](S(=O)=O)C(F)(F)F)", and "${n1nnnc1)" originally presented in JOELib	Acidic Group Count descriptor	1
PaDEL	2D	ALogP	Ghose-Crippen LogKow	ALOGP descriptor	3.3496
PaDEL	2D	ALogp2	Square of ALogP	ALOGP descriptor	11.2198
PaDEL	2D	AMR	Molar refractivity	ALOGP descriptor	135.1754

Predicted human target proteins



C

Medicinal fungi	Therapeutic use	Therapeutic use identifier	Reference
Boletus edulis	Antineoplastic agents	MESH:D000970, MESH:D009369; ICD-9:199.1, ICD-9:239.9, ICD-9:E933.1; DOID:162	PMID:30668382
Boletus edulis	Generalized pain	ICD-9:780.96	PMID:30668382
Boletus edulis	Stomach pain		PMID:30668382



D

Physicochemical filter | Drug-like filter | Chemical similarity filter

Molecular Weight — Choose here

LogP — Choose here

Topological Polar Surface Area (TPSA) — Choose here

Hydrogen Bond Acceptors (HBA) — Choose here

Hydrogen Bond Donors (HBD) — Choose here

Heavy Atoms — Choose here

Heteroatoms — Choose here

Number of Rings — Choose here

Rotatable Bonds — Choose here

Stereochemical Complexity — Choose here

Shape Complexity — Choose here

Search

Physicochemical filter | Drug-like filter | Chemical similarity filter

Lipinski RO5 Violation — Choose here

Ghose Rule Violation — Choose here

GSK 4/400 — Choose here

Pfizer 3/75 — Choose here

Veber Rule — Choose here

Egan Rule — Choose here

QEDw — Choose here

Search

Physicochemical filter | Drug-like filter | Chemical similarity filter

Enter SMILES

Choose Fingerprint — Choose here

Search