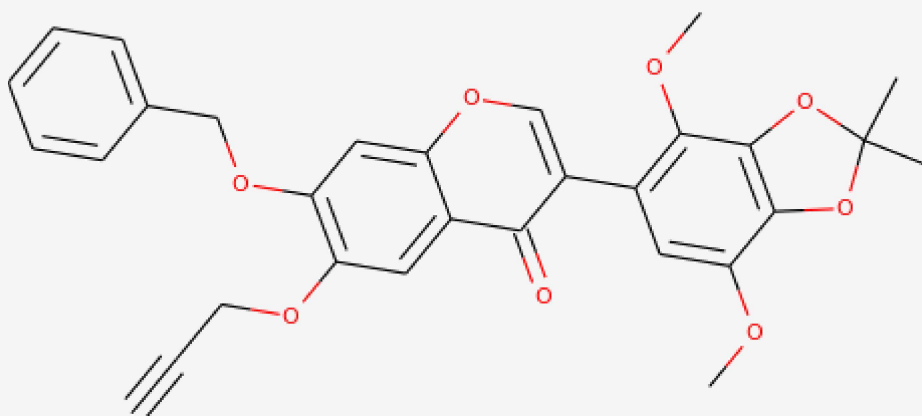


Pharmacokinetic Properties

Molecule Depiction

[SMILES](#)

Molecule properties:

Descriptor	Value
Molecular Weight	514.53
LogP	5.5755
#Rotatable Bonds	8
#Acceptors	8
#Donors	0
Surface Area	219.153

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	-4.6	Numeric (log mol/L)
Absorption	Caco2 permeability	1.358	Numeric (log Papp in 10 ⁻⁶ cm/s)

Property	Model Name	Predicted Value	Unit
Absorption	Intestinal absorption (human)	98.797	Numeric (% Absorbed)
Absorption	Skin Permeability	-2.735	Numeric (log Kp)
Absorption	P-glycoprotein substrate	No	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	Yes	Categorical (Yes/No)
Distribution	VDss (human)	-0.464	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.195	Numeric (Fu)
Distribution	BBB permeability	-1.173	Numeric (log BB)
Distribution	CNS permeability	-2.952	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	Yes	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	Yes	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	Yes	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	Yes	Categorical (Yes/No)
Excretion	Total Clearance	0.563	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	No	Categorical (Yes/No)
Toxicity	AMES toxicity	No	Categorical (Yes/No)
Toxicity	Max. tolerated dose (human)	0.726	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	No	Categorical (Yes/No)
Toxicity	hERG II inhibitor	Yes	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	2.853	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	1.066	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	No	Categorical (Yes/No)
Toxicity	Skin Sensitisation	No	Categorical (Yes/No)

Property	Model Name	Predicted Value	Unit
Toxicity	<i>T.Pyriformis</i> toxicity	0.285	Numeric (log ug/L)
Toxicity	Minnow toxicity	-1.269	Numeric (log mM)

Run another prediction

Back

