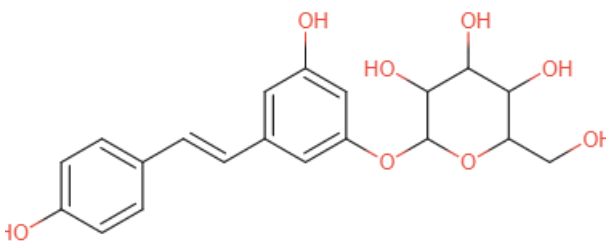
Pharmacokinetic Properties

Molecule Depiction



SMILES

Molecule properties:

Descriptor	Value
Molecular Weight	390.388
LogP	0.4469
#Rotatable Bonds	5
#Acceptors	8
#Donors	6
Surface Area	160.705

Property	Model Name	Predicted Value	Unit

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	**-2.575**	Numeric (log mol/L)
Absorption	Caco2 permeability	**-0.077**	Numeric (log Papp in 10^{-6} cm/s)
Absorption	Intestinal absorption (human)	**51.086**	Numeric (% Absorbed)
Absorption	Skin Permeability	**-2.735**	Numeric (log Kp)
Absorption	P-glycoprotein substrate	**Yes**	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	**Yes**	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	**No**	Categorical (Yes/No)
Distribution	VDss (human)	**0.125**	Numeric (log L/kg)
Distribution	Fraction unbound (human)	**0.274**	Numeric (Fu)
Distribution	BBB permeability	**-1.029**	Numeric (log BB)
Distribution	CNS permeability	**-3.61**	Numeric (log PS)
Metabolism	CYP2D6 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	**No**	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitior	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitior	**No**	Categorical (Yes/No)
Excretion	Total Clearance	**0.057**	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)	**0.569**	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	**No**	Categorical (Yes/No)
Toxicity	hERG II inhibitor	**No**	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	**2.516**	Numeric (mol/kg)

Property	Model Name	Predicted Value	Unit
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	**4.473**	Numeric (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	**No**	Categorical (Yes/No)
Toxicity	Skin Sensitisation	**No**	Categorical (Yes/No)
Toxicity	*T.Pyriformis* toxicity	**0.285**	Numeric (log ug/L)
Toxicity	Minnow toxicity	**4.39**	Numeric (log mM)

Run another prediction

Back

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