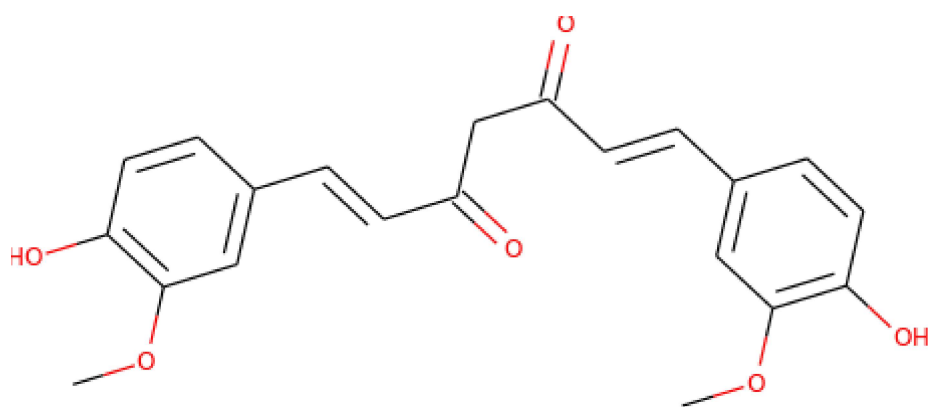


Pharmacokinetic Properties

Molecule Depiction



SMILES

Molecule properties:

Descriptor	Value
Molecular Weight	368.385
LogP	3.3699
#Rotatable Bonds	8
#Acceptors	6
#Donors	2
Surface Area	156.532

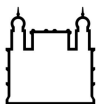
Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	-4.01	Numeric (log mol/L)
Absorption	Caco2 permeability	-0.093	Numeric (log Papp in 10 ⁻⁶ cm/s)

Property	Model Name	Predicted Value	Unit
Absorption	Intestinal absorption (human)	82.19	Numeric (% Absorbed)
Absorption	Skin Permeability	-2.764	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	Yes	Categorical (Yes/No)
Distribution	VDss (human)	-0.215	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0	Numeric (Fu)
Distribution	BBB permeability	-0.562	Numeric (log BB)
Distribution	CNS permeability	-2.99	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	Yes	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	Yes	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	-0.002	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)	0.081	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)	1.833	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity (LOAEL)	2.228	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	0.494	Numeric (log ug/L)
Toxicity	Minnow toxicity	-0.081	Numeric (log mM)

Run another prediction

Back



Instituto
René Rachou
FIOCRUZ MINAS



THE UNIVERSITY OF
MELBOURNE



UNIVERSITY OF
CAMBRIDGE

OPEN KNOWLEDGE

Best viewed using [Chrome](#) on 1280x1024 resolution and above