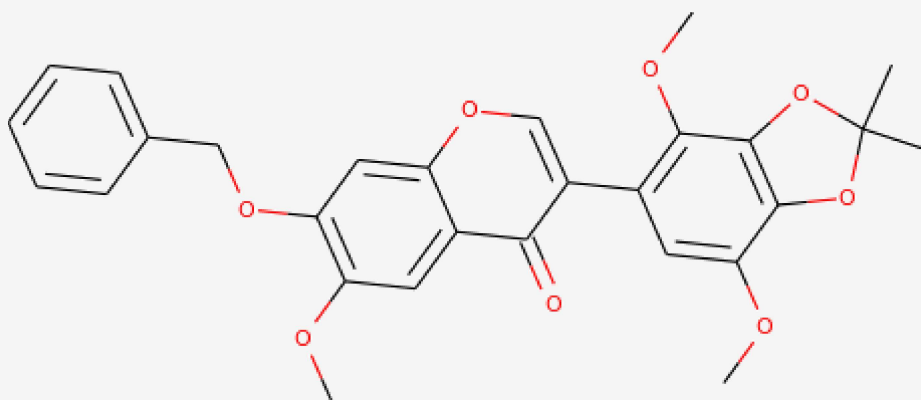


Pharmacokinetic Properties

Molecule Depiction

[SMILES](#)

Molecule properties:

| Descriptor | Value |
|------------------|---------|
| Molecular Weight | 490.508 |
| LogP | 5.5721 |
| #Rotatable Bonds | 7 |
| #Acceptors | 8 |
| #Donors | 0 |
| Surface Area | 207.424 |

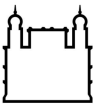
| Property | Model Name | Predicted Value | Unit |
|-------------------|--------------------|-----------------|---|
| Absorption | Water solubility | -3.93 | Numeric (log mol/L) |
| Absorption | Caco2 permeability | 1.404 | Numeric (log Papp in 10 ⁻⁶ cm/s) |

| Property | Model Name | Predicted Value | Unit |
|--------------|-----------------------------------|-----------------|----------------------------|
| Absorption | Intestinal absorption (human) | 99.409 | 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) | -0.451 | Numeric (log L/kg) |
| Distribution | Fraction unbound (human) | 0.205 | Numeric (Fu) |
| Distribution | BBB permeability | -1.195 | Numeric (log BB) |
| Distribution | CNS permeability | -3.082 | 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 | 0.523 | 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) | 0.7 | 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) | 2.775 | Numeric (mol/kg) |
| Toxicity | Oral Rat Chronic Toxicity (LOAEL) | 1.057 | 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 | -1.427 | Numeric (log mM) |

Run another prediction

Back



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