4,5-Dimethoxycanthin-6-one

Cat. No.: HY-N1882

CAS No.: 18110-87-7

Molecular Formula: $C_{16}H_{12}N_2O_3$

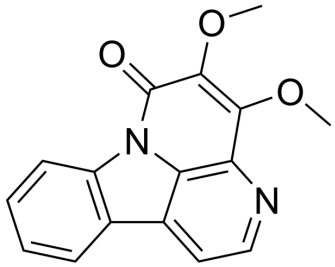
Molecular Weight: 280.28

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 10 mg/mL (35.68 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.5679 mL	17.8393 mL	35.6786 mL
	5 mM	0.7136 mL	3.5679 mL	7.1357 mL
	10 mM	0.3568 mL	1.7839 mL	3.5679 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1 mg/mL (3.57 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1 mg/mL (3.57 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1 mg/mL (3.57 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

4,5-Dimethoxycanthin-6-one is a potent and uncompetitive inhibitor of CYP1A2-mediated phenacetin O-deethylation with an IC_{50} value of 1.7μM and a K_i value of 2.6 μM. 4,5-Dimethoxycanthin-6-one, as an alkaloid, is isolated from the wood of Picrasma quassioides BENNET (Simaroubaceae)[1][2].

IC_{50} & Target

CYP1A2 1.7 μM (IC_{50})	CYP1A2 2.6 μM (Ki)

In Vitro

4,5-Dimethoxycanthin-6-one is a potent and uncompetitive inhibitor of CYP1A2-mediated phenacetin O-deethylation with an IC_{50} value of 1.7μM and a K_i value of 2.6 μM[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Taichi O, et al. Studies on the Constituents of Picrasma quassioides BENNET. III. The Alkaloidal Constituents

[2]. Miao X,et al. In vitro metabolism of 4, 5-dimethoxycanthin-6-one by human liver microsomes and its inhibition on human CYP1A2. Life Sci. 2017;190:46-51.

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