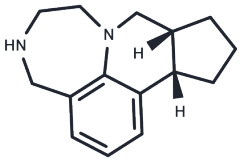
Data Sheet (Cat.No.T13275)

TargetMol

Vabicaserin hydrochloride

Chemical Properties



CAS No. : 887258-94-8

Formula: C15H21ClN2

Molecular Weight: 264.79

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	Vabicaserin hydrochloride (SCA 136) is a selective agonist of 5-hydroxytryptamine 2C (5-HT2C) receptor (EC50: 8 nM).
Targets(IC50)	5-HT Receptor
In vitro	In Chinese hamster ovary cell membranes, Vabicaserin displaces 125I-(2,5-dimethoxy) phenylisopropylamine binding from human 5-HT2C receptor sites (Ki: 3 nM) and is >50-fold selective over a number of serotonergic, noradrenergic, and dopaminergic receptors. The binding affinity determined for the human 5-HT2B receptor subtype using [3H]5HT is 14 nM. Vabicaserin is a potent and full agonist (EC50, 8 nM; Emax, 100%) in stimulating 5-HT2C receptor-coupled calcium mobilization and exhibits 5-HT2A receptor antagonism and 5-HT2B antagonist or partial agonist activity in transfected cells, depending on the level of receptor expression. Vabicaserin showed a lower affinity at the binding site (22 nM) of 5-HT2C antagonist labeled with [3H]methsulamide. Other binding studies have shown that Vabicaserin has an affinity for 5-HT2B and 5-HT1A receptors with Ki values of 14 and 112 nM, respectively [1].
In vivo	After administering a single oral dose of [14C]Vabicaserin (50 mg/kg in mice, 5 mg/kg in rats, and 15 mg/kg in dogs), the unchanged drug accounted for less than 19%, 20%, and 35% of the total plasma radioactivity in mice, rats, and dogs, respectively, at all examined time points. The carbamoyl glucuronide (CG) comprised approximately 7-36% of plasma radioactivity in mice, 2-28% in dogs, and was absent in rat plasma following the single [14C]Vabicaserin dose, yet observed in rat plasma after multiple-dose administration of Vabicaserin at higher doses, being roughly 20 times lower than Vabicaserin based on AUC0-24 values at steady state. The plasma AUC0-24 ratios of CG to Vabicaserin were 1.5 in mice and 1.7 in dogs post-single dose. At doses used for safety assessment, these ratios at steady state were lower for mice (0.2-0.6) but slightly higher for dogs (1.8-4.0). CG was detected in dog urine at amounts comparable to the parent drug but was not found in mouse or rat urine post-single dose. Following a 5 mg/kg [14C]Vabicaserin dose in rats, 19-24% of the administered dose was recovered in bile over 24 hours, with CG representing up to 30% of biliary radioactivity. In monkeys, after a single oral 25-mg/kg dose of Vabicaserin, CG plasma concentrations surpassed those of Vabicaserin at all examined postdose intervals (2-24 h), though the CG-to-Vabicaserin ratio declined by 24 h postdose, from 17.5 at 2 h to 1.7 at 24 h, indicating that CG is a major metabolite with a 12:1 AUC0-24 ratio to Vabicaserin.

Solubility Information

Solubility	DMSO: 55 mg/mL (207.71 mM),Sonication is recommended. H2O: 4 mg/mL (15.11 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.7766 mL	18.8829 mL	37.7658 mL
5 mM	0.7553 mL	3.7766 mL	7.5532 mL
10 mM	0.3777 mL	1.8883 mL	3.7766 mL
50 mM	0.0755 mL	0.3777 mL	0.7553 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

Dunlop J, et al. Characterization of Vabicaserin (SCA-136), a selective 5-hydroxytryptamine 2C receptor agonist. J Pharmacol Exp Ther. 2011 Jun;337(3):673-80.

Tong Z, et al. Species differences in the formation of Vabicaserin carbamoyl glucuronide. Drug Metab Dispos. 2010 Apr;38(4):581-90.