Data Sheet (Cat.No.T2395L)

TargetMol

Vortioxetine hydrobromide

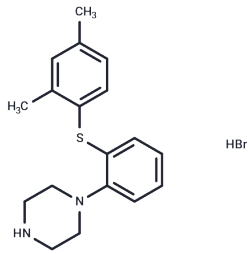
Chemical Properties

CAS No. : 960203-27-4

Formula: C18H22N2S·HBr

Molecular Weight: 379.36

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.



Biological Description

Description	Vortioxetine hydrobromide (Lu AA21004 hydrobromide) is a serotonin (5-HT) modulator and stimulator (SMS), inhibits 5-HT1A/1B/3A/7 receptor and SERT (IC50: 15/33/3.7/19/1.6 nM).
Targets(IC50)	5-HT Receptor,Serotonin Transporter
In vitro	Subcutaneous injection of Lu AA21004 (2.5-10.0 mg/kg) into the medial prefrontal cortex and ventral hippocampal area of rats was found to elevate extracellular levels of 5-HT, DA, and NA. A specific dose of Lu AA21004 (5 mg/kg) targeting the rats' ventral hippocampal region resulted in a 200% increase in extracellular 5-HT levels. Additionally, administration of Lu AA21004 (at doses of 5 and 10 mg/kg) showed a significant elevation in ACh levels to 224% and 204% respectively, 20 minutes post-injection. This compound, when administered to the ventral hippocampal area of awake rats at doses of 5 and 10 mg/kg, enhanced extracellular 5-HT levels, and a 3-day treatment of the medial prefrontal cortex with Lu-AA21004 (at 5 and 10 mg/kg) substantially raised the basal levels of 5-HT. Furthermore, Lu AA21004 (10 mg/kg) notably decreased pain perception in rats. In terms of pharmacokinetics within rats, Lu-AA21004 exhibited a liver clearance rate of 7.1 (L/h)/kg and an oral bioavailability of 16%. Lastly, Lu AA21004 dose-dependently affected the rats' Bezold-Jarisch reflex by inhibiting transient bradycardia (ED50: 0.11 mg/kg).
In vivo	Lu AA21004 acts as an agonist for the h5-HT1B receptor, with an EC50 value of 460 nM and demonstrating 22% intrinsic activity in whole-cell assays. It inhibits recombinant human cytochrome P450 enzymes CYP1A2, CYP2C9, CYP2D6, and CYP3A4 with IC50 values of 40 μM, 39 μM, 9.8 μM, and 10 μM, respectively. Furthermore, Lu AA21004 binds to the r5-HT7 receptor with a Ki value of 200 nM in vitro whole-cell cAMP assays and functions as a competitive antagonist with an IC50 of 2 μM.
Kinase Assay	Assay of MEK Kinase Activity: Anti-MEK1 antibody is used to immunoprecipitate MEK1 molecules. MEK kinase activity is measured as the ability of immuno-isolated MEK1 to activate recombinant ERK1 in a coupled assay using MBP as the end point of the assay. Phosphorylated MBP is resolved on a 14% SDS-PAGE gel and vacuum-dried before exposure to X-ray film.

Solubility Information

Solubility	Ethanol: 14 mg/mL (36.9 mM),Sonication is recommended. DMSO: 45 mg/mL (118.62 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.27 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.636 mL	13.1801 mL	26.3602 mL
5 mM	0.5272 mL	2.636 mL	5.272 mL
10 mM	0.2636 mL	1.318 mL	2.636 mL
50 mM	0.0527 mL	0.2636 mL	0.5272 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.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Bang-Andersen B, et al. J Med Chem, 2011, 54(9), 3206-3221.
Mørk A, et al. J Pharmacol Exp Ther, 2012, 340(3), 666-675.
Mørk A, et al. Pharmacol Biochem Behav, 2013, 105C, 41-50.