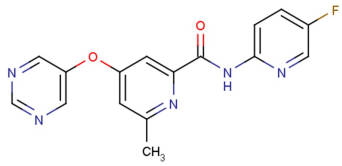
Data Sheet (Cat.No.T17241)

TargetMol
A DRUG SCREENING EXPERT

Auglurant

Chemical Properties



CAS No.:	1396337-04-4
Formula:	C16H12FN5O2
Molecular Weight:	325.3
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Auglurant is a novel and selective mGlu5 antagonist (IC50: 11 nM (rat) and an IC50: 14 nM (human)). Auglurant has an acceptable CNS penetration.
Targets(IC_{50})	Others: None
In vitro	Auglurant has an IC50 value of 14 nM in HEK293A cells. It also binding a known allosteric site (Ki: 4.4 nM in HEK293A cells).
In vivo	Auglurant had a clearance of 19.3 mL/min/kg in rats and demonstrates 50% mGlu5 PET ligand occupancy at an oral dose of 0.8 mg/kg in rats. Auglurant also had a clearance of 15.5 mL/min/kg in cynomolgus monkeys and demonstrates 50% mGlu5 PET ligand occupancy at an oral dose of 0.06 mg/kg in baboons [1].

Solubility Information

Solubility	DMSO: 22.73 mg/mL (69.87 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.074 mL	15.37 mL	30.741 mL
5 mM	0.615 mL	3.074 mL	6.148 mL
10 mM	0.307 mL	1.537 mL	3.074 mL
50 mM	0.061 mL	0.307 mL	0.615 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Felts AS, et al. Discovery of N-(5-Fluoropyridin-2-yl)-6-methyl-4-(pyrimidin-5-yloxy)picolinamide (VU0424238): A Novel Negative Allosteric Modulator of Metabotropic Glutamate Receptor Subtype 5 Selected for Clinical Evaluation. J Med Chem. 2017 Jun 22;60(12):5072-5085.

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