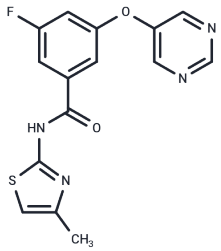
Data Sheet (Cat.No.T29132)

TargetMol

VU0409106

Chemical Properties



CAS No. : 1276617-62-9

Formula: C15H11FN4O2S

Molecular Weight: 330.34

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	VU0409106 is a potent and highly selective mGlu5 negative allosteric modulator with an IC_{50} of 24 nM. It exhibits concentration-dependent anxiolytic effects in mouse models and can penetrate the blood-brain barrier.
Targets(IC50)	GluR
In vivo	Methods: Mice received a single intraperitoneal injection of 10 mg/kg VU0409106, and its blood-brain barrier penetration ability and brain/plasma distribution ratio were determined. Results: VU0409106 penetrated the blood-brain barrier (BBB) with a brain/plasma ratio close to 1, demonstrating favorable brain distribution properties [1].

Solubility Information

Solubility	DMSO: 1.6 mg/mL (4.84 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.0272 mL	15.1359 mL	30.2718 mL
5 mM	0.6054 mL	3.0272 mL	6.0544 mL
10 mM	0.3027 mL	1.5136 mL	3.0272 mL
50 mM	0.0605 mL	0.3027 mL	0.6054 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

Felts AS, et al. Discovery of VU0409106: A negative allosteric modulator of mGlu5 with activity in a mouse model of anxiety. Bioorg Med Chem Lett. 2013 Nov 1;23(21):5779-85.

Morrison RD, et al. The role of aldehyde oxidase and xanthine oxidase in the biotransformation of a novel negative allosteric modulator of metabotropic glutamate receptor subtype 5. Drug Metab Dispos. 2012 Sep;40(9):1834-45.

Felts AS, Rodriguez AL, Morrison RD, Venable DF, Manka JT, Bates BS, Blobaum AL, Byers FW, Daniels JS, Niswender CM, Jones CK, Conn PJ, Lindsley CW, Emmitte KA. Discovery of VU0409106: A negative allosteric modulator of mGlu5 with activity in a mouse model of anxiety. Bioorg Med Chem Lett. 2013 Nov 1;23(21):5779-85. doi: 10.1016/j.bmcl.2013.09.001. Epub 2013 Sep 10. PubMed PMID: 24074843; PubMed Central PMCID: PMC3846293.

Morrison RD, Blobaum AL, Byers FW, Santomango TS, Bridges TM, Stec D, Brewer KA, Sanchez-Ponce R, Corlew MM, Rush R, Felts AS, Manka J, Bates BS, Venable DF, Rodriguez AL, Jones CK, Niswender CM, Conn PJ, Lindsley CW, Emmitte KA, Daniels JS. The role of aldehyde oxidase and xanthine oxidase in the biotransformation of a novel negative allosteric modulator of metabotropic glutamate receptor subtype 5. Drug Metab Dispos. 2012 Sep;40(9):1834-45. doi: 10.1124/dmd.112.046136. Epub 2012 Jun 18. PubMed PMID: 22711749; PubMed Central PMCID: PMC3422546.