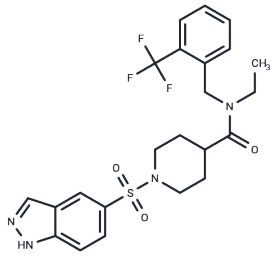
Data Sheet (Cat.No.T28069)

TargetMol

ML380

Chemical Properties



CAS No. : 1627138-52-6

Formula: C23H25F3N4O3S

Molecular Weight: 494.53

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	ML380 is a highly potent and the first CNS penetrant M5 positive allosteric modulator (PAM).
Targets(IC50)	AChR

Solubility Information

Solubility	DMSO: 90 mg/mL (181.99 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: 3.3 mg/mL (6.67 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	2.0221 mL	10.1106 mL	20.2212 mL
5 mM	0.4044 mL	2.0221 mL	4.0442 mL
10 mM	0.2022 mL	1.0111 mL	2.0221 mL
50 mM	0.0404 mL	0.2022 mL	0.4044 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

Berizzi AE, Gentry PR, Rueda P, Den Hoedt S, Sexton PM, Langmead CJ, Christopoulos A. Molecular Mechanisms of Action of M5 Muscarinic Acetylcholine Receptor Allosteric Modulators. Mol Pharmacol. 2016 Oct;90(4):427-36. doi: 10.1124/mol.116.104182.

Gentry PR, Kokubo M, Bridges TM, Daniels JS, Niswender CM, Smith E, Chase P, Hodder PS, Rosen H, Conn PJ, Engers J, Brewer KA, Lindsley CW, Wood MR. Development of the First CNS penetrant M5 Positive Allosteric Modulator (PAM) Based on a Novel, non-Isatin Core. 2013 Dec 15 [updated 2015 Feb 11]. Probe Reports from the NIH Molecular Libraries Program [Internet]. Bethesda (MD): National Center for Biotechnology Information (US); 2010-.

Gentry PR, Kokubo M, Bridges TM, Noetzel MJ, Cho HP, Lamsal A, Smith E, Chase P, Hodder PS, Niswender CM, Daniels JS, Conn PJ, Lindsley CW, Wood MR. Development of a highly potent, novel M5 positive allosteric modulator (PAM) demonstrating CNS exposure: 1-((1H-indazol-5-yl)sulfoneyl)-N-ethyl-N-(2-(trifluoromethyl)benzyl) piperidine-4- carboxamide (ML380). J Med Chem. 2014 Sep 25;57(18):7804-10. doi: 10.1021/jm500995y.