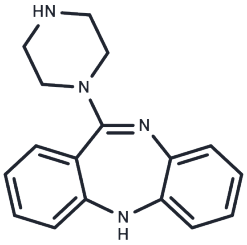
Data Sheet (Cat.No.T11095L)

TargetMol

DREADD agonist 21

Chemical Properties



CAS No. : 56296-18-5

Formula: C17H18N4

Molecular Weight: 278.35

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	DREADD agonist 21 is a potent agonist of human muscarinic acetylcholine M3 receptors (EC50=1.7 nM).
Targets(IC50)	5-HT Receptor,Adrenergic Receptor,AChR,Histamine Receptor
In vitro	DREADD agonist 21 is a highly selective and potent agonist for muscarinic DREADDs (pEC50 for hM1Dq=6.54 and that for hM4Di=7.77 in pERK assays)[2]. DREADD agonist 21 potently activates hM3Dq in Chinese hamster ovary (CHO) cells transfected cells in vitro (pEC50: 8.48±0.05) and it also potently activates hM1Dq, hM3Dq, and hM4Di. DREADD agonist 21 does not activate human M3 receptor (hM3). DREADD agonist 21 displays high binding affinities to 5HT2A and 5HT2C serotonin receptor, α1A adrenergic receptor, and H1 histamine receptor with Ki values of 66, 170, 280, and 6 nM, respectively[1]. In addition to being inactive at hM3, DREADD agonist 21, a potent full agonist of hM3Dq (EC50=1.7 nM), is only 3.5-fold selective for hM3Dq over H1, 40-fold selective over 5HT2A, 100-fold selective over 5HT2C, and 165-fold selective over α1A. DREADD agonist 21 binds to hM1, hM4, hM1Dq and hM4Di receptors (pKis of 5.97, 5.44, 7.20, and 6.75, respectively).
In vivo	DREADD agonist 21 has excellent pharmacokinetic properties, bioavailability and brain penetrability. DREADD agonist 21 (0.3, 1.0, and 3.0 mg/kg; i.p.) activates neuronal hM3Dq in mice. DREADD agonist 21 (0.1, 1, and 10 mg/kg; i.p.) shows 95.1% plasma protein binding and 95% brain protein bounding in mice[2].

Solubility Information

Solubility	DMSO: 75 mg/mL (269.44 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 (7.19 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	3.5926 mL	17.963 mL	35.926 mL
5 mM	0.7185 mL	3.5926 mL	7.1852 mL
10 mM	0.3593 mL	1.7963 mL	3.5926 mL
50 mM	0.0719 mL	0.3593 mL	0.7185 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

Chen X, et al. The first structure-activity relationship studies for designer receptors exclusively activated by designer drugs. ACS Chem Neurosci. 2015 Mar 18;6(3):476-84.
Thompson KJ, et al. DREADD Agonist 21 Is an Effective Agonist for Muscarinic-Based DREADDs in Vitro and in Vivo. ACS Pharmacol Transl Sci. 2018 Sep 14;1(1):61-72.