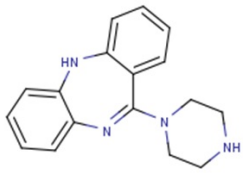
Data Sheet (Cat.No.T11095L)

TargetMol
A DRUG SCREENING EXPERT

DREADD agonist 21

Chemical Properties



CAS No.:	56296-18-5
Formula:	C17H18N4
Molecular Weight:	278.35
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	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 shows high binding affinities to 5HT2A and 5HT2C serotonin receptor, α1A adrenergic receptor, and H1 histamine receptor (Kis: 66, 170, 280, and 6 nM) [1]. DREADD agonist 21 potently activates hM1Dq, hM3Dq, and hM4Di. DREADD agonist 21 binds to hM1, hM4, hM1Dq, and hM4Di receptors (pKis: 5.97, 5.44, 7.20, and 6.75). DREADD agonist 21 potently activates hM3Dq in Chinese hamster ovary (CHO) cells transfected cells in vitro with a pEC50 of 8.48±0.05. 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].
Targets(IC_{50})	hM3Dq: (EC50) 1.7 nM hM1: (pki) 5.97 hM4: 5.44 (pki) hM1Dq: 7.2 (pki) hM4Di: 6.75 (pki) H1 histamine receptor: (ki) 6 nM 5HT2A serotonin receptor 5HT2A: 66 nM (ki) 5HT2C serotonin receptor: 170 nM (ki) α1A adrenergic receptor: 280 nM (ki)
In vitro	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 shows high binding affinities to 5HT2A and 5HT2C serotonin receptor, α1A adrenergic receptor, and H1 histamine receptor (Kis: 66, 170, 280, and 6 nM) [1]. DREADD agonist 21 potently activates hM1Dq, hM3Dq, and hM4Di. DREADD agonist 21 binds to hM1, hM4, hM1Dq, and hM4Di receptors (pKis: 5.97, 5.44, 7.20, and 6.75). DREADD agonist 21 potently activates hM3Dq in Chinese hamster ovary (CHO) cells transfected cells in vitro with a pEC50 of 8.48±0.05. 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].
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: 78 mg/mL (280.22 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.593 mL	17.963 mL	35.926 mL
5 mM	0.719 mL	3.593 mL	7.185 mL
10 mM	0.359 mL	1.796 mL	3.593 mL
50 mM	0.072 mL	0.359 mL	0.719 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. 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.

2. 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.

Inhibitors · Natural Compounds · Compound Libraries

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