DREADD agonist 21

Cat. No.: HY-100234

CAS No.: 56296-18-5

Molecular Formula: $C_{17}H_{18}N_4$

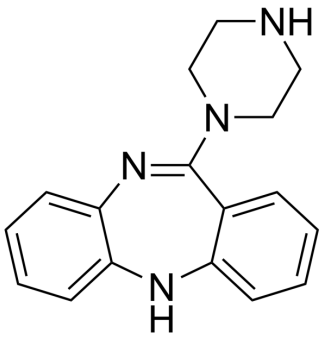
Molecular Weight: 278.35

Target: mAChR

Pathway: GPCR/G Protein; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 78 mg/mL (280.22 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.5926 mL	17.9630 mL	35.9260 mL
	5 mM	0.7185 mL	3.5926 mL	7.1852 mL
	10 mM	0.3593 mL	1.7963 mL	3.5926 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (8.98 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (8.98 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

DREADD agonist 21 is a potent human muscarinic acetylcholine M3 receptors (hM3Dq) agonist (EC_{50}=1.7 nM)[1].

IC_{50} & Target

mAChR3

In Vitro

DREADD agonist 21 is a potent human muscarinic acetylcholine M3 receptors (hM3Dq) agonist (EC_{50}=1.7 nM) and does not activate human M3 receptor (hM3). In addition to being inactive at hM3, DREADD agonist 21, a potent full agonist of hM3Dq (EC_{50}=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 with K_i values of 66, 170, 280, and 6 nM, respectively[1].

	?DREADD agonist 21 potently activates hM1Dq, hM3Dq, and hM4Di. DREADD agonist 21 binds to hM1, hM4, hM1Dq and hM4Di receptors with pK_is of 5.97, 5.44, 7.20, and 6.75, respectively. DREADD agonist 21 potently activates hM3Dq in Chinese hamster ovary (CHO) cells transfected cells in vitro with a pEC_{50} of 8.48±0.05. DREADD agonist 21 is a highly selective and potent agonist for muscarinic DREADDs (pEC_{50} for hM1Dq=6.54 and that for hM4Di=7.77 in pERK assays)[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	DREADD agonist 21 (0.3, 1.0, and 3.0 mg/kg; i.p.) activates neuronal hM3Dq in mice[2]. ?DREADD agonist 21 has excellent bioavailability, pharmacokinetic properties, and brain penetrability. DREADD agonist 21 (0.1, 1, and 10 mg/kg; i.p.) displays 95.1% plasma protein binding and 95% brain protein bounding in mice[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Brain Res Bull. 2021 May 15;S0361-9230(21)00143-X.

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REFERENCES

[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.

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