DREADD agonist 21 dihydrochloride

Cat. No.: HY-100234A

CAS No.: 2250025-92-2

Molecular Formula: $C_{17}H_{20}Cl_2N_4$

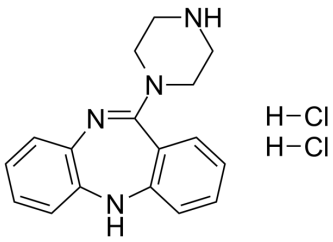
Molecular Weight: 351.27

Target: mAChR

Pathway: GPCR/G Protein; Neuronal Signaling

Storage: 4°C, stored under nitrogen

* In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 200 mg/mL (569.36 mM; ultrasonic and warming and heat to 60°C)

H_2O : 100 mg/mL (284.68 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.8468 mL	14.2341 mL	28.4681 mL
5 mM	0.5694 mL	2.8468 mL	5.6936 mL
10 mM	0.2847 mL	1.4234 mL	2.8468 mL

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

BIOLOGICAL ACTIVITY

Description

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

IC_{50} & Target

EC50: 1.7 nM (hM3Dq)[1]

pKi: 5.97 (hM1), 5.44 (hM4), 7.20 (hM1Dq), and 6.75 (hM4Di)[2]

Ki: 6 nM (H1 histamine receptor), 66 nM (5HT2A serotonin receptor 5HT2A), 170 nM (5HT2C serotonin receptor), 280 nM (α1A adrenergic receptor)[1]

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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