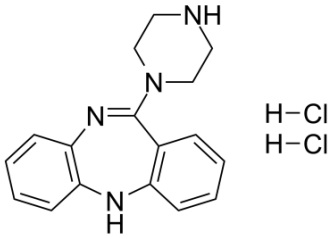
DREADD agonist 21 dihydrochloride

Cat. No.:	HY-100234A
Molecular Formula:	$C_{17}H_{20}Cl_2N_4$
Molecular Weight:	351.27
Target:	mAChR
Pathway:	GPCR/G Protein; Neuronal Signaling
Storage:	Please store the product under the recommended conditions in the COA.



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].
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].

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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