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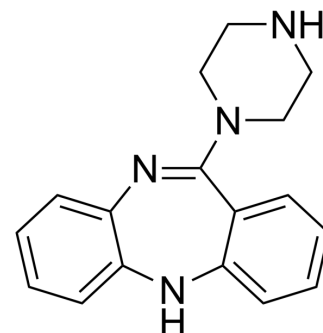
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DREADD agonist 21

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.

	Solvent Concentration	Mass	1 mg	5 mg	10 mg
Preparing Stock Solutions	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

- 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
- 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_s 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 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]. 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.

Caution: Product has not been fully validated for medical applications. For research use only.

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