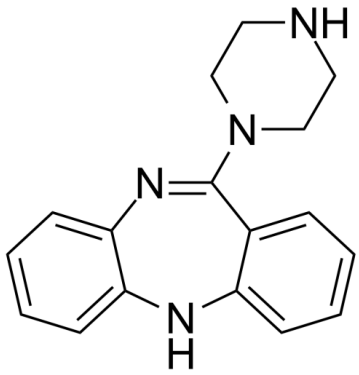
Data Sheet

Product Name:	DREADD agonist 21
Cat. No.:	CS-6102
CAS No.:	56296-18-5
Molecular Formula:	C17H18N4
Molecular Weight:	278.35
Target:	mAChR
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : ≥ 78 mg/mL (280.22 mM)



BIOLOGICAL ACTIVITY:

DREADD agonist 21 is a potent human muscarinic acetylcholine M3 receptors (**hM3Dq**) agonist(**EC_{50}**=1.7 nM). IC50 & Target: EC50: 1.7 nM (hM3Dq)[1]

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].

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.

CAIndexNames:

5H-Dibenzo[b,e][1,4]diazepine, 11-(1-piperazinyl)-

SMILES:

C12=CC=CC=C1NC3=CC=CC=C3C(N4CCNCC4)=N2

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