

DREADD agonist 21 dihydrochloride

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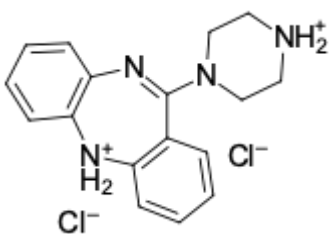
DREADD agonist 21 (Compound 21, C21) is a synthetic compound for selective activation of hM3Dq (excitatory) and hM4Di (inhibitory) DREADDs (*D*esigner *R*eceptor *E*xclusively *A*ctivated by *D*esigner *D*rugs) derived from the human muscarinic acetylcholine M3 (hM3) receptor. It does not agonize the hM3 receptor and displays weaker binding affinities for histamine H1, serotonin 5-HT_{2A}, 5-HT_{2C}, and α 1A-adrenergic receptors (K_i = 6, 66, 170, and 280 nM, respectively) [1].

DREADD agonist 21 is routinely used as a chemogenetic tool for remotely controlling neuronal activity. It displays excellent brain permeability and capability to activate neurons expressing hM3Dq DREADDs and inhibit activity in neurons expressing hM4Di DREADDs *in vivo* [2].

This product is dihydrochloride salt, a water-soluble version of DREADD agonist 21.

[1] Chen X. et al. The first structure-activity relationship studies for designer receptors exclusively activated by designer drugs. *ACS Chem. Neurosci.* 2015. 6(3). 476-484.

[2] Thompson K.J. et al. DREADD agonist 21 is an effective agonist for muscarinic-based DREADDs *in vitro* and *in vivo*. *ACS Pharmacol. Transl. Sci.* 2018. 1(1). 61-72.



Structure of DREADD agonist 21 dihydrochloride

General properties

Appearance: yellow-brown powder

Molecular weight: 351.28

CAS number: 2250025-92-2

Molecular formula: C₁₇H₁₈N₄

IUPAC name: 11-(1-piperazinyl)-5H-dibenzo[b,e][1,4]diazepine dihydrochloride

Solubility: in water, DMSO

Quality control: NMR ¹H and HPLC-MS (95+%)

Storage conditions: 24 months after receipt at -20°C in the dark. Transportation: at room temperature for up to 3 weeks. Desiccate.

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