bio-techne
TOCRIS

Print Date: Aug 10th 2023

Certificate of Analysis

www.tocris.com

Product Name: **DREADD agonist 21** **Catalog No.: 5548** **Batch No.: 4**

CAS Number: 56296-18-5

IUPAC Name: 11-(1-Piperazinyl)-5*H*-dibenzo[*b*,*e*][1,4]diazepine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{18}N_4.H_2O$

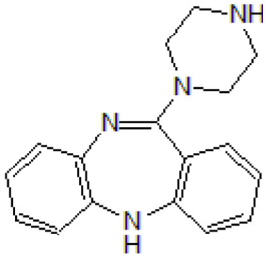
Batch Molecular Weight: 296.37

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6 % purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.9	6.8	18.9
Found	68.81	6.97	18.74

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Description:

DREADD agonist 21 is a potent muscarinic DREADD agonist (pEC_{50} values are 8.91, 8.48 and 7.77 for hM_1D_q, hM_3D_q and hM_4D_i in vitro, respectively). Exhibits > 10-fold higher affinity for hM_1D_q and hM_4D_i compared to wild type receptors. Also displays little to no activity at wild type M_3 receptors. Activates neurons expressing hM_3D_q DREADDS and inhibits activity in neurons expressing hM_4D_i in vivo. Displays excellent brain permeability. Water soluble salt also available, DREADD agonist 21 hydrochloride (Cat. No. 6422). Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

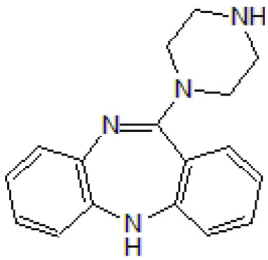
Batch Molecular Formula: $C_{17}H_{18}N_4.H_2O$

Batch Molecular Weight: 296.37

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Thompson *et al* (2018) DREADD agonist 21 (C21) is an effective agonist for muscarinic-based DREADDs *in vitro* and *in vivo*. ACS Pharmacol.Transl.Sci. ***1*** 61. PMID: 30868140 .

Chen *et al* (2015) The first structure-activity relationship studies for designer receptors exclusively activated by designer drugs. ACS Chem.Neurosci. ***18*** 476. PMID: 25587888.