

Product Name: DREADD agonist 21

Catalog No.: 5548

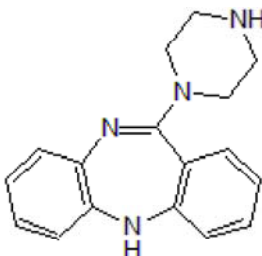
Batch No.: 3

CAS Number: 56296-18-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₈N₄·¼H₂O
Batch Molecular Weight: 282.85
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.13 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.19	6.59	19.81
Found	72.15	6.68	19.44

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent muscarinic DREADD agonist (pEC₅₀ values are 8.91, 8.48 and 7.77 for hM₁D_q, hM₃D_q and hM₄D_i in vitro, respectively). Exhibits > 10-fold higher affinity for hM₁D_q and hM₄D_i compared to wild type receptors. Also displays little to no activity at wild type M₃ receptors. Activates neurons expressing hM₃D_q DREADDs and inhibits activity in neurons expressing hM₄D_i in vivo. Displays excellent brain permeability. Water soluble salt also available, DREADD agonist 21 hydrochloride (Cat. No. 6422). Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

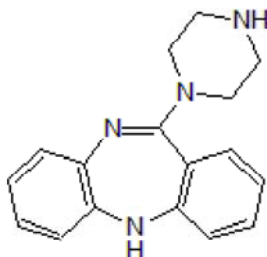
Batch Molecular Formula: C₁₇H₁₈N₄·¼H₂O

Batch Molecular Weight: 282.85

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. Our standard recommendations are:

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.

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