TOCRIS
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Print Date: Jul 28th 2018

Certificate of Analysis

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Product Name: **DREADD agonist 21 dihydrochloride** **Catalog No.: 6422** **Batch No.: 1**

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{18}N_4.2HCl.1¼H_2O$

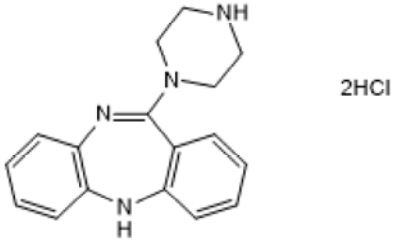
Batch Molecular Weight: 373.79

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.13 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.63	6.07	14.99
Found	54.45	6.02	14.88

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

Description:

Water soluble version of DREADD agonist 21 (Cat. No. 5548). Potent hM_3D_q DREADD agonist.

Physical and Chemical Properties:

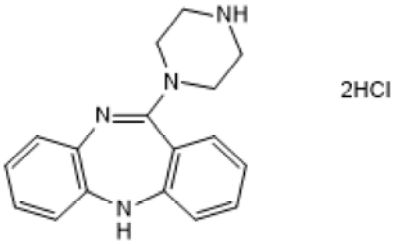
Batch Molecular Formula: $C_{17}H_{18}N_4.2HCl.1¼H_2O$

Batch Molecular Weight: 373.79

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO 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:

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.