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Print Date: Jun 14th 2021

Certificate of Analysis

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Product Name: **DREADD agonist 21 dihydrochloride** **Catalog No.: 6422** **Batch No.: 2**

CAS Number: 2250025-92-2

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{18}N_4.2HCl.2½H_2O$

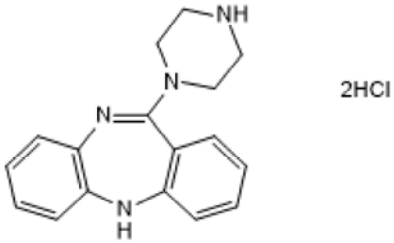
Batch Molecular Weight: 396.31

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	51.52	6.36	14.14	17.89
Found	51.95	6.23	14.01	17.6

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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

Description:

DREADD agonist 21 dihydrochloride is a water soluble version of DREADD agonist 21 (Cat. No. 5548). Potent muscarinic DREADD agonist.

Physical and Chemical Properties:

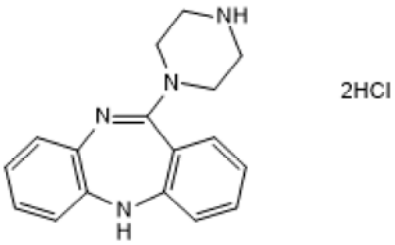
Batch Molecular Formula: $C_{17}H_{18}N_4.2HCl.2½H_2O$

Batch Molecular Weight: 396.31

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.