Print Date: Nov 12th 2020

Certificate of Analysis

www.tocris.com

Product Name: **JHU 37152** **Catalog No.: 7197** **Batch No.: 1**

CAS Number: 2369979-67-7

IUPAC Name: 8-Chloro-11-(4-ethylpiperazin-1-yl)-1-fluoro-5*H*-dibenzo[*b*,*e*][1,4]diazepine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{20}ClFN_4.½H_2O$

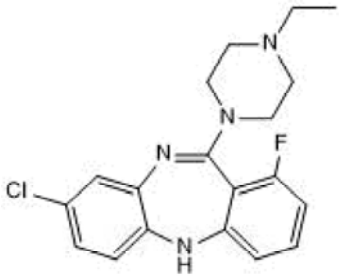
Batch Molecular Weight: 367.86

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 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.04	5.75	15.23
Found	62.28	5.74	15.14

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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Description:

High affinity and highly potent activator of hM_3D_q and hM_4D_i DREADDs (K_i values are 1.8 nM and 8.7 nM for hM_3D_q and hM_4D_i in vitro, respectively; EC_{50} values are 5 nM and 0.5 nM for hM_3D_q and hM_4D_i in vitro, respectively). Selectively displaces [^{3}H]clozapine from DREADDs in vivo, but not from other clozapine binding sites. Inhibits locomotor activity in mice expressing hM_3D_q and hM_4D_i in D_1-expressing neurons. Brain penetrant in mice, rats and non-human primates. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

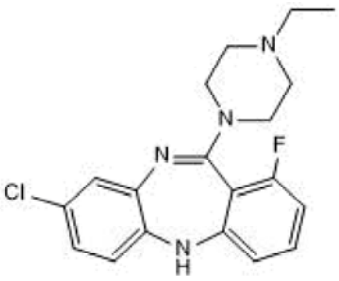
Batch Molecular Formula: $C_{19}H_{20}ClFN_4.½H_2O$

Batch Molecular Weight: 367.86

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:

Bonaventura *et al* (2019) High-potency ligands for DREADD imaging and activation in rodents and monkeys. Nat.Commun. ***10*** 4627. PMID: 31604917.