

Certificate of Analysis

Print Date: Aug 23rd 2017

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Product Name: Clozapine N-oxide Catalog No.: 4936 Batch No.: 11

CAS Number: 34233-69-7

IUPAC Name: 8-Chloro-11-(4-methyl-4-oxido-1-piperazinyl)-5*H*-dibenzo[*b*,*e*][1,4]diazepine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{19}CIN_4O.1\frac{1}{2}H_2O$

Batch Molecular Weight:369.84Physical Appearance:Yellow solidSolubility:DMSO to 20 mM

ethanol to 10 mM with gentle warming

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogon Nitrogo

Carbon Hydrogen Nitrogen

Theoretical 58.46 6 15.15 Found 58.11 6.13 15.07



Product Information

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Description:

Metabolite of clozapine (Cat. No. 0444). Activates human muscarinic designer receptors (DREADDs) in vitro. Silences hippocampal neurons expressing hM $_4$ DREADDs in vitro. Activates G $_8$ -linked DREADDS- AgRP in mice via intracerebroventricular (i.c.v) injection. Recently shown to be a P-glycoprotein (P-gp) efflux pump substrate. Other potent and selective hM $_3$ Dq DREADD agonists available: DREADD agonist 21 (Cat. No. 5548) and Perlapine (Cat. No. 5549)

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₉ClN₄O.1½H₂O

Batch Molecular Weight: 369.84 Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 20 mM

ethanol to 10 mM with gentle warming

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:

Gomez et al (2017) Chemogenetics revealed: DREADD occupancy and activation via converted clozapine. Science 357 503. PMID: 28774929

Nakajima *et al* (2016) G_s-coupled GPCR signalling in AgRP neurons triggers sustained increase in food intake. Nat. Commun. *8* 10268. PMID: 26743492.

Roth et al (2016) DREADDs for Neuroscientists Neuron 89 683. PMID: 26889809.

Zaman *et al* (2014) LMO4 is essential for paraventricular hypothalamic neuronal activity and calcium channel expression to prevent hyperphagia. J.Neurosci. **34** 140. PMID: 24381275.

Armbruster *et al* (2007) Evolving the lock to fit the key to create a family of G protein-coupled receptors potently activated by an inert ligand. Proc.Natl.Acad.Sci.U.S.A. *104* 5163. PMID: 17360345.

Eiermann et al (1997) The involvement of CYP1A2 and CYP3A4 in the metabolism of clozapine. Br.J.Clin.Pharmacol. **44** 439. PMID: 9384460.

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