Print Date: Oct 30th 2018

Certificate of Analysis

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Product Name: **JNJ 16259685** **Catalog No.: 2333** **Batch No.: 4**

CAS Number: 409345-29-5

IUPAC Name: (3,4-Dihydro-2*H*-pyrano[2,3-*b*]quinolin-7-yl)-(*cis*-4-methoxycyclohexyl)-methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{23}NO_3$

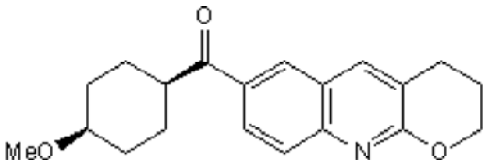
Batch Molecular Weight: 325.41

Physical Appearance: White solid

Solubility: ethanol to 100 mM
DMSO to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.14 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	73.82	7.12	4.3
Found	73.71	7.14	4.34

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Description:

Sub-nanomolar potent, non-competitive $mGlu_1$ antagonist (K_i = 0.34 nM). Inhibits glutamate-induced Ca^{2+} response at the human $mGlu_1$ receptor with an IC_{50} value of 0.55 nM. Selective over $mGlu_5$ (> 400-fold) and displays no activity at $mGlu_2$, $mGlu_3$, $mGlu_4$, $mGlu_6$, AMPA or NMDA receptors (IC_{50} > 10 µM). Centrally active following systemic administration.

Physical and Chemical Properties:

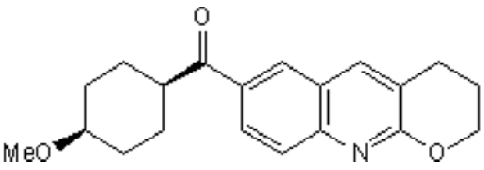
Batch Molecular Formula: $C_{20}H_{23}NO_3$

Batch Molecular Weight: 325.41

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

ethanol to 100 mM
DMSO to 25 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:

Xie *et al* (2010) Effects of mGluR1 antagonism in the dorsal hippocampus on drug context-induced reinstatement of cocaine-seeking behavior in rats. Psychopharmacology (Berl). ***208*** 1. PMID: 19847405.

Mabire *et al* (2005) Synthesis, structure-activity relationship, and receptor pharmacology of a new series of quinoline derivatives acting as selective, noncompetitive mGlu1 antagonists. J.Med.Chem. ***48*** 2134. PMID: 15771457.

Steckler *et al* (2005) Metabotropic glutamate receptor 1 blockade impairs acquisition and retention in a spatial water maze task. Behav.Brain Res. ***164*** 52. PMID: 16043241.

Lavreysen *et al* (2004) JNJ16259685, a highly potent, selective and systemically active mGlu1 receptor antagonist. Neuropharmacology ***47*** 961. PMID: 15555631.