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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **JNJ 10397049** **Catalog No.: 4317** **Batch No.: 1**

CAS Number: 708275-58-5

IUPAC Name: *N*-(2,4-Dibromophenyl)-*N*'-[(4*S*,5*S*)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]-urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{20}Br_2N_2O_3$

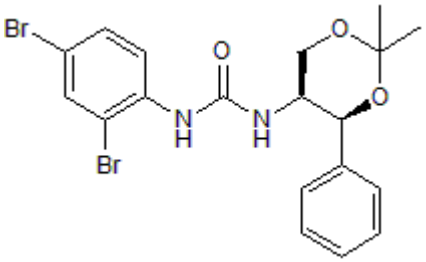
Batch Molecular Weight: 484.18

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.13	4.16	5.79
Found	47.51	4.25	5.86

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Description:

Selective OX_2 receptor antagonist (pIC_{50} = 7.4 for chimeric OX_2 receptors; pK_B values are 5.9 and 8.5 for OX_1 and OX_2 receptors respectively). Shows no significant activity in a panel of over 50 other neurotransmitters and neuropeptide receptors. Achieves high level of OX_2 receptor occupancy in the rat brain; exhibits sleep-promoting effects in rats.

Physical and Chemical Properties:

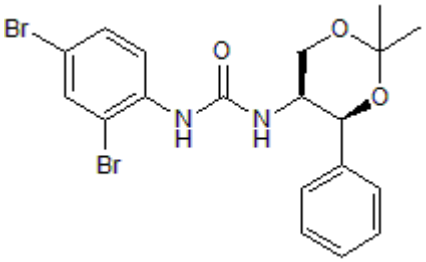
Batch Molecular Formula: $C_{19}H_{20}Br_2N_2O_3$

Batch Molecular Weight: 484.18

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

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:

Dugovic *et al* (2009) Blockade of orexin-1 receptors attenuates orexin-2 receptor antagonism-induced sleep promotion in the rat. J.Pharmacol.Exp.Ther. ***330*** 142. PMID: 19363060.

Tran *et al* (2011) Chimeric, mutant orexin receptors show key interactions between orexin receptors, peptides and antagonists. Eur.J.Pharmacol. ***667*** 120. PMID: 21679703.

Gozzi *et al* (2011) Functional magnetic resonance imaging reveals different neural substrates for the effects of orexin-1 and orexin-2 receptor antagonists. PLoS ONE ***6*** e16406. PMID: 21307957.