Print Date: Jun 14th 2017

Certificate of Analysis

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Product Name: **EMPA** **Catalog No.: 4558** **Batch No.: 2**

CAS Number: 680590-49-2

IUPAC Name: *N*-Ethyl-2-[(6-methoxy-3-pyridinyl)[(2-methylphenyl)sulfonyl]amino]-*N*-(3-pyridinylmethyl)-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{26}N_4O_4S$

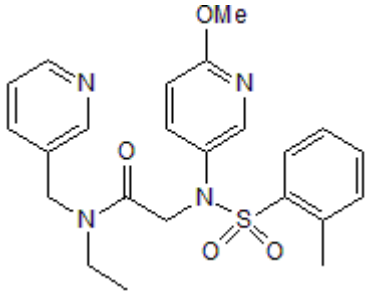
Batch Molecular Weight: 454.54

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

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

HPLC: Shows >99.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.77	5.77	12.33
Found	60.43	5.86	12.14

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Product Information

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Description:

Highly potent, selective OX_2 receptor antagonist (IC_{50} values are 2.3 nM and 1900 nM for OX_2 and OX_1 respectively). Displays negligible or no inhibition of a panel of 80 receptors. Blocks orexin-B- and orexin-A-invoked calcium mobilization in hOX_2-expressing CHO cells (IC_{50} values are 7.9 nM and 8.8 nM respectively); reverses orexin-B-induced hyperlocomotion in mice. Brain penetrant.

Physical and Chemical Properties:

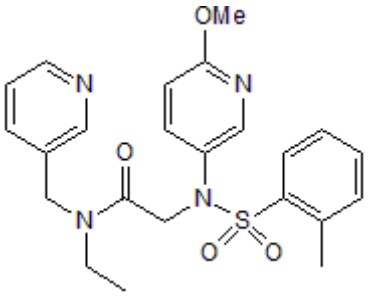
Batch Molecular Formula: $C_{23}H_{26}N_4O_4S$

Batch Molecular Weight: 454.54

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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:

Mochizuki *et al* (2011) Orexin receptor 2 expression in the posterior hypothalamus rescues sleepiness in narcoleptic mice. Proc.Natl.Acad.Sci.U.S.A ***108*** 4471. PMID: 21368172.

Malherbe *et al* (2010) Mapping the binding pocket of dual antagonist almorexant to human orexin 1 and orexin 2 receptors: comparison with the selective OX_1 antagonist SB-674042 and the selective OX_2 antagonist N-ethyl-2-[(6-methoxy-pyridin-3-yl)-(toluene-2-sulfonyl)-amino]-N-pyridin-3-ylmethyl-acetamide (EMPA). Mol.Pharmacol. ***78*** 81. PMID: 20404073.

Malherbe *et al* (2009) Biochemical and behavioural characterization of EMPA, a novel high-affinity, selective antagonist for the OX_2 receptor. Br.J.Pharmacol. ***156*** 1326. PMID: 19751316.

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