

Certificate of Analysis

Print Date: Oct 20th 2022

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

680590-49-2 CAS Number:

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

1. PHYSICAL AND CHEMICAL PROPERTIES

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

Batch Molecular Weight: 454.54

Off White solid **Physical Appearance:**

DMSO to 100 mM Solubility: ethanol to 50 mM

Store at -20°C

Storage:

Batch Molecular Structure:

2. ANALYTICAL DATA

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

HPLC: Shows 99.1% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.77 5.77 12.33 60.43 Found 5.86 12.14

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Product Information

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

Description:

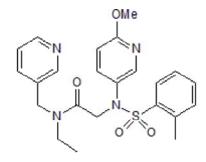
EMPA is a highly potent, selective OX_2 receptor antagonist (IC_{50} values are 2.3 nM and 1900 nM for OX_2 and OX_1 respectively). Displays negligible or no inhibition of a panel of 80 receptors. Blocks orexin-B- and orexin-A-invoked calcium mobilization in hOX_2 -expressing CHO cells (IC_{50} values 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 OX1 antagonist SB-674042 and the selective OX2 antagonist N-ethyl-2-[(6-methoxy-pyridin-3-yl)-(toluene-Mol.Pharmacol. **78** 81. PMID: 20404073.

Malherbe et al (2009) Biochemical and behavioural characterization of EMPA, a novel high-affinity, selective antagonist for the OX₂ receptor. Br.J.Pharmacol. **156** 1326. PMID: 19751316.

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