

Certificate of Analysis

Product Name: IPSU

Catalog No.: 5645

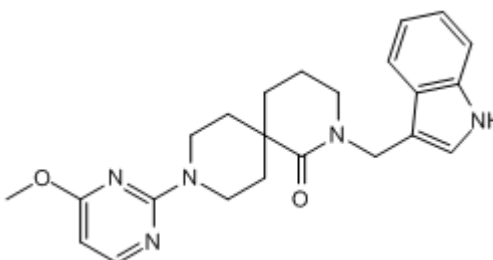
Batch No.: 1

CAS Number: 1373765-19-5

IUPAC Name: 2-(1*H*-Indol-3-ylmethyl)-9-(4-methoxy-2-pyrimidinyl)-2,9-diazaspiro[5.5]undecan-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₇N₅O₂
Batch Molecular Weight: 405.49
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 1eq. HCl to 100 mM
 ethanol to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate:Petroleum ether [1:3])
HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.13	6.71	17.27
Found	67.96	6.76	16.93

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

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Description:

OX₂ receptor antagonist. Exhibits approximately six-fold selectivity for OX₂ versus OX₁ receptors. Decreases activity and increases sleep time in mice during the active phase, without affecting REM/NREM balance. Orally bioavailable. Brain penetrant.

Physical and Chemical Properties:

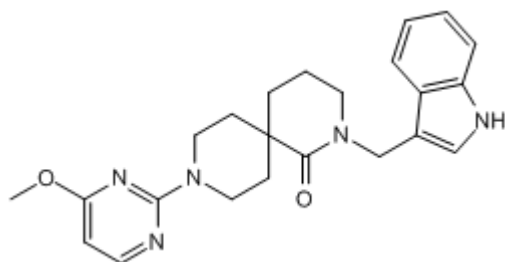
Batch Molecular Formula: C₂₃H₂₇N₅O₂

Batch Molecular Weight: 405.49

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Hoyer *et al* (2013) Distinct effects of IPSU and suvorexant on mouse sleep architecture. *Front.Neurosci.* **7** 230. PMID: 24376396.

Betschart *et al* (2013) Identification of a novel series of orexin receptor antagonists with a distinct effect on sleep architecture for the treatment of insomnia. *J.Med.Chem.* **56** 7590. PMID: 23964859.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl 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.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956