

## Certificate of Analysis

**Product Name:** ACT 462206

**Catalog No.:** 5319

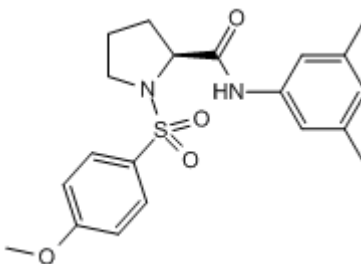
**Batch No.:** 1

CAS Number: 1361321-96-1

IUPAC Name: (2S)-N-(3,5-Dimethylphenyl)-1-[(4-methoxyphenyl)sulfonyl]-2-pyrrolidinecarboxamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>S  
**Batch Molecular Weight:** 388.48  
**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<sub>f</sub> = 0.62 (Ethyl acetate:Petroleum ether [1:1])  
**HPLC:** Shows 99.9% purity  
**Chiral HPLC:** Shows >99.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.83	6.23	7.21
Found	61.94	6.17	7.14

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

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**Description:**

Potent, dual orexin receptor antagonist (IC<sub>50</sub> values are 11 and 60 nM for OX<sub>2</sub> and OX<sub>1</sub> receptors respectively). Exhibits anxiolytic-like properties in vivo. Brain penetrant.

**Physical and Chemical Properties:**

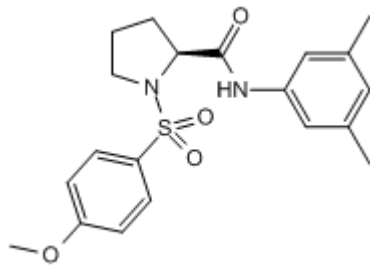
Batch Molecular Formula: C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>S

Batch Molecular Weight: 388.48

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:**

**Boss et al** (2014) Structure-activity relationship, biological, and pharmacological characterization of the proline sulfonamide ACT-462206: a potent, brain-penetrant dual orexin 1/orexin 2 receptor antagonist. *ChemMedChem*. **9** 2486. PMID: 25147058.

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