

## Certificate of Analysis

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**Product Name:** A 867744

**Catalog No.:** 4571

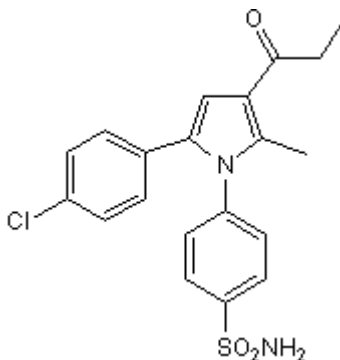
**Batch No.:** 1

CAS Number: 1000279-69-5

IUPAC Name: 4-[5-(4-Chlorophenyl)-2-methyl-3-(1-oxopropyl)-1H-pyrrol-1-yl]benzenesulfonamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>20</sub> H <sub>19</sub> ClN <sub>2</sub> O <sub>3</sub> S.¼H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	407.39
<b>Physical Appearance:</b>	Off-white solid
<b>Solubility:</b>	DMSO to 100 mM ethanol to 10 mM with gentle warming
<b>Storage:</b>	Store at +4°C
<b>Batch Molecular Structure:</b>	



### 2. ANALYTICAL DATA

<b>Melting Point:</b>	At 245°C
<b>HPLC:</b>	Shows 97.2% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	
	Carbon Hydrogen Nitrogen
	Theoretical 58.97 4.82 6.88
	Found 59.12 4.86 6.8

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

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**Description:**

Positive allosteric modulator of  $\alpha 7$  nAChRs ( $IC_{50}$  values are 0.98 and 1.12  $\mu$ M for human and rat  $\alpha 7$  receptor ACh-evoked currents respectively, in *X. laevis* oocytes). Displays no activity at 5-HT<sub>3A</sub>,  $\alpha 3\beta 4$  or  $\alpha 4\beta 2$  nAChRs. Brain penetrant.

**Physical and Chemical Properties:**

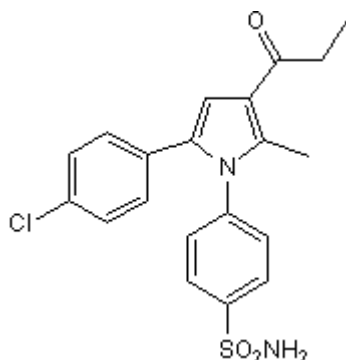
Batch Molecular Formula: C<sub>20</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>3</sub>S·¼H<sub>2</sub>O

Batch Molecular Weight: 407.39

Physical Appearance: Off-white solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 10 mM with gentle warming

**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:**

**Malysz et al** (2009) In vitro pharmacological characterization of a novel allosteric modulator of  $\alpha 7$  neuronal acetylcholine receptor, 4-(5-(4-chlorophenyl)-2-methyl-3-propionyl-1H-pyrrol-1-yl)benzenesulfonamide (A-867744), exhibiting unique pharmacological profile. *J.Pharmacol.Exp.Ther.* **330** 257. PMID: 19389923.

**Faghiih et al** (2009) Discovery of 4-(5-(4-chlorophenyl)-2-methyl-3-propionyl-1H-pyrrol-1-yl)benzenesulfonamide (A-867744) as a novel positive allosteric modulator of the  $\alpha 7$  nicotinic acetylcholine receptor. *J.Med.Chem.* **28** 3377. PMID: 19419141.

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