

# **Certificate of Analysis**

Print Date: Jan 14th 2016

www.tocris.com

Product Name: SEN 12333 Catalog No.: 4441 Batch No.: 1

CAS Number: 874450-44-9

IUPAC Name: N-[4-(3-pyridinyl)phenyl]-4-morpholinepentanamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{20}H_{25}N_3O_2$ .  $^{1/2}H_2O$ 

Batch Molecular Weight: 348.44

**Physical Appearance:** White crystalline solid **Solubility:** DMSO to 100 mM

Storage: Store at RT

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.2$  (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.4% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.94 7.52 12.06 Found 69.01 7.55 12.25



## **Product Information**

Print Date: Jan 14th 2016

www.tocris.com

Product Name: SEN 12333 Catalog No.: 4441 Batch No.: 1

CAS Number: 874450-44-9

IUPAC Name: N-[4-(3-pyridinyl)phenyl]-4-morpholinepentanamide

#### **Description:**

 $\alpha7$  nicotinic acetylcholine receptor (nAChR) agonist (EC $_{50}$  = 1.6  $\mu M,~K_i$  = 260 nM at rat  $\alpha7$  nAChRs). Also displays functional antagonism at histamine  $H_3$  receptors (IC $_{50}$  = 103 nM) and weak agonist activity at human ganglionic  $\alpha3$  nAChRs (IC $_{50}$  = 8.5  $\mu M$ ). Neuroprotective in a rodent model of quisqualic acid-induced cholinergic degeneration. Brain penetrant and orally bioavailable.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>25</sub>N<sub>3</sub>O<sub>2</sub>. ½H<sub>2</sub>O

Batch Molecular Weight: 348.44

Physical Appearance: White crystalline solid

**Minimum Purity: >99%** 

#### **Batch Molecular Structure:**

Storage: Store at RT

#### Solubility & Usage Info:

DMSO 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:

Roncarati et al (2009) Procognitive and neuroprotective activity of a novel  $\alpha$ 7 nicotinic acetylcholine receptor agonist for treatment of neurodegenerative and cognitive disorders. J.Pharmacol.Exp.Ther. **329** 459. PMID: 19223665.

**Beinat** et al (2012) Consequences of linker length alteration of the  $\alpha$ 7 nicotinic acetylcholine receptor (nAChR) agonist, SEN12333. Bioorg.Med.Chem.Lett. **22** 2380. PMID: 22410083.