

# **Certificate of Analysis**

Print Date: Jul 23rd 2019

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**Product Name:** PNU 282987 Catalog No.: 2303 Batch No.: 5

CAS Number: 711085-63-1

**IUPAC Name:** N-(3R)-1-Azabicyclo[2.2.2]oct-3-yl-4-chlorobenzamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

C<sub>14</sub>H<sub>17</sub>CIN<sub>2</sub>O **Batch Molecular Formula:** 

**Batch Molecular Weight:** 264.75 **Physical Appearance:** White solid

1eq. HCl to 100 mM Solubility:

DMSO to 100 mM

Storage: Store at RT

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

TLC:  $R_f = 0.3 (9:1 CHCl3:MeOH (NH4OH atmosphere))$ 

HPLC: Shows 99.4% purity

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

 $[\alpha]_D$  = +58.8 (Concentration = 24, Solvent = Chloroform) **Optical Rotation:** 

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 63.51 6.47 10.58 Found 63.28 6.52 10.59

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



## **Product Information**

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### **Description:**

Highly selective α7 nAChR agonist ( $K_i$  = 26 nM) displaying negligible blockade of  $\alpha_1\beta_1\gamma\delta$  and  $\alpha_3\beta_4$  nAChRs (IC<sub>50</sub> ≥ 60 μM). Found to be inactive against a panel of 32 receptors at 1 μM, except 5-HT<sub>3</sub> receptors ( $K_i$  = 930 nM).

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

Batch Molecular Formula: C<sub>14</sub>H<sub>17</sub>ClN<sub>2</sub>O Batch Molecular Weight: 264.75 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at RT

## Solubility & Usage Info:

1eq. HCl to 100 mM 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:

**Bodnar** et al (2005) Discovery and structure-activity relationship of quinuclidine benzamides as agonists of  $\alpha$ 7 nicotinic acetylcholine receptors. J.Med.Chem. **48** 905. PMID: 15715459.

**Hajós** *et al* (2005) The selective  $\alpha$ 7 nicotinic acetylcholine receptor agonist PNU-282987 [N-[(3R)-1-Azabicyclo[2.2.2]oct-3-yl]-4-chlorobenzamide hydrochloride] enhances GABAergic synaptic activity in brain slices and restores auditory gating deficits in anesthe J.Pharmacol.Exp.Ther. *312* 1213. PMID: 15523001.

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