

# **Certificate of Analysis**

Print Date: Nov 24th 2017

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**Product Name:** IC 87201 Catalog No.: 6226 Batch No.: 2

CAS Number: 866927-10-8

**IUPAC Name:** 2-[(1H-Benzotriazol-6-ylamino)methyl]-4,6-dichlorophenol

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>13</sub>H<sub>10</sub>Cl<sub>2</sub>N<sub>4</sub>O.H<sub>2</sub>O

**Batch Molecular Weight:** 327.17

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

ethanol to 100 mM

Storage: Store at +4°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

Microanalysis:

TLC: R<sub>f</sub> = 0.57 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99.5% purity

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

Carbon Hydrogen Nitrogen

Theoretical 47.73 3.7 17.12 47.87 Found 3.6 17.38

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



# **Product Information**

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IUPAC Name: 2-[(1H-Benzotriazol-6-ylamino)methyl]-4,6-dichlorophenol

#### **Description:**

Inhibits binding of the NMDA receptor postsynaptic density protein 95 kDa (PSD95) to nNOS (EC $_{50}$  = 23.94  $\mu$ M), while not affecting the PSD95-ErbB4 interaction. Inhibits glutamate-induced cell death in cultured cortical neurons. Exhibits antinociceptive effects in inflammatory pain models in vivo. Also exhibits antidepressant-like activity in animal models.

# **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>13</sub>H<sub>10</sub>Cl<sub>2</sub>N<sub>4</sub>O.H<sub>2</sub>O

Batch Molecular Weight: 327.17 Physical Appearance: Off 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:

Lee et al (2015) Small molecule inhibitors of PSD95-nNOS protein-protein interactions as novel analgesics. Neuropharmacology. 97 464. PMID: 26071110.

**Doucet** *et al* (2013) Small-molecule inhibitors at the PSD-95/nNOS interface have antidepressant-like properties in mice. Neuropsychopharmacology. **38** 1575. PMID: 23446451.

**Florio** *et al* (2009) Disruption of nNOS-PSD95 protein-protein interaction inhibits acute thermal hyperalgesia and chronic mechanical allodynia in rodents. Br.J.Pharmacol. *158* 494. PMID: 19732061.