

## Certificate of Analysis

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**Product Name:** 3-Bromocytisine

**Catalog No.:** 3549

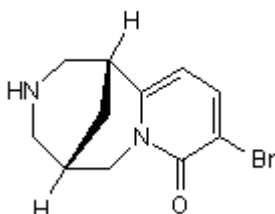
**Batch No.:** 1

CAS Number: 207390-14-5

IUPAC Name: (1*R*,5*S*)-9-Bromo-1,2,3,4,5,6-hexahydro-1,5-methano-8*H*-pyrido[1,2-*a*][1,5]diazocin-8-one

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>11</sub>H<sub>13</sub>BrN<sub>2</sub>O  
**Batch Molecular Weight:** 269.14  
**Physical Appearance:** White solid  
**Solubility:** water to 100 mM  
DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.25 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 99.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 49.09  | 4.87     | 10.41    |
| Found       | 48.94  | 4.85     | 10.41    |

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

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**Description:**

Potent agonist of  $\alpha 4\beta 4$ ,  $\alpha 4\beta 2$  and  $\alpha 7$  nACh receptors ( $IC_{50}$  values are 0.28, 0.30 and 31.6 nM respectively). Displays different effects on high (HS) and low (LS) ACh sensitivity  $\alpha 4\beta 2$  nAChRs ( $EC_{50}$  values are 0.008 and 0.05  $\mu$ M respectively).

**Physical and Chemical Properties:**

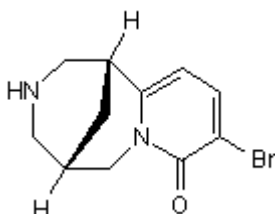
Batch Molecular Formula:  $C_{11}H_{13}BrN_2O$

Batch Molecular Weight: 269.14

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

water 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:**

**Houlihan et al** (2001) Activity of cytosine and its brominated isoteres on recombinant human  $\alpha 7$ ,  $\alpha 4\beta 2$  and  $\alpha 4\beta 4$  nicotinic acetylcholine receptors. *J.Neurochem.* **78** 1029. PMID: 11553677.

**Moroni et al** (2006)  $\alpha 4\beta 2$  nicotinic receptors with high and low acetylcholine sensitivity: pharmacology, stoichiometry, and sensitivity to long-term exposure to nicotine. *Mol.Pharmacol.* **70** 755. PMID: 16720757.

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