

## Certificate of Analysis

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**Product Name:** MNI 137

**Catalog No.:** 4388

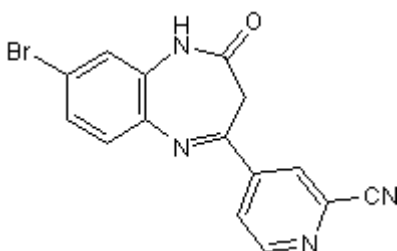
**Batch No.:** 1

CAS Number: 946619-21-2

IUPAC Name: 4-(8-Bromo-2,3-dihydro-2-oxo-1*H*-1,5-benzodiazepin-4-yl)-2-pyridinecarbonitrile

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>15</sub>H<sub>9</sub>BrN<sub>4</sub>O  
**Batch Molecular Weight:** 341.16  
**Physical Appearance:** Off-white solid  
**Solubility:** DMSO to 50 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.4 (Ethyl acetate:Petroleum ether [2:3])  
**HPLC:** Shows 98.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 52.81  | 2.66     | 16.42    |
| Found       | 52.92  | 2.82     | 16.3     |

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

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**Description:**

Selective negative allosteric modulator of group II mGlu receptors (IC<sub>50</sub> values are 8.3 and 12.6 nM for human and rat mGlu<sub>2</sub> inhibition of glutamate-induced calcium mobilization). Displays no activity at mGlu<sub>1</sub>, mGlu<sub>4</sub>, mGlu<sub>5</sub> or mGlu<sub>6</sub> receptors in a calcium mobilization assay.

**Physical and Chemical Properties:**

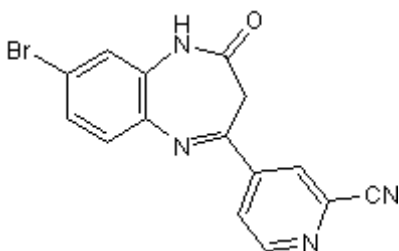
Batch Molecular Formula: C<sub>15</sub>H<sub>9</sub>BrN<sub>4</sub>O

Batch Molecular Weight: 341.16

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Hemstapat et al (2007)** A novel family of potent negative allosteric modulators of group II metabotropic glutamate receptors. *J.Pharmacol.Exp.Ther.* **322** 254. PMID: 17416742.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 50 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.

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