

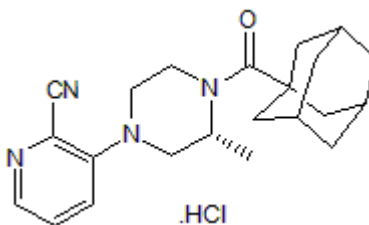
## Certificate of Analysis

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**Product Name:** VU 0469650 hydrochloride **Catalog No.:** 5379 **Batch No.:** 1  
**CAS Number:** 1443748-47-7  
**IUPAC Name:** 3-[(3R)-3-Methyl-4-(tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-ylcarbonyl)-1-piperazinyl]-2-pyridinecarbonitrile hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>22</sub>H<sub>28</sub>N<sub>4</sub>O.HCl  
**Batch Molecular Weight:** 400.94  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 50 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.32 (Ethyl acetate:Petroleum ether [5:5])  
**HPLC:** Shows 99.8% purity  
**Chiral HPLC:** Shows 100% purity  
<sup>1</sup>H NMR: Consistent with structure  
 Mass Spectrum: Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -50 (Concentration = 4, Solvent = Methanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	65.9	7.29	13.97
Found	66.15	7.28	14.03

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**Description:**

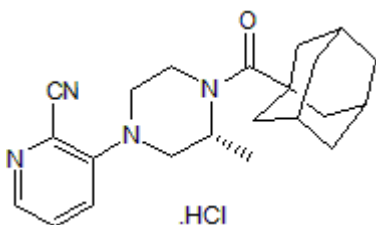
Potent and selective negative allosteric modulator of mGlu<sub>1</sub> (IC<sub>50</sub> = 99 nM). Exhibits >100-fold selectivity for mGlu<sub>1</sub> over mGlu<sub>2-8</sub> and 68 other GPCRs, ion channels, kinases and transporters. Brain penetrant.

**Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>22</sub>H<sub>28</sub>N<sub>4</sub>O.HCl  
 Batch Molecular Weight: 400.94  
 Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
 ethanol 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.

**References:**

**Lovell et al (2013)** *N*-Acyl-*N'*-aryl piperazines as negative allosteric modulators of mGlu<sub>1</sub>: Identification of VU0469650, a potent and selective tool compound with CNS exposure in rats. *Bioorg.Med.Chem.Lett.* **23** 3713. PMID: 23727046 .

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