Print Date: Dec 14th 2011

# Certificate of Analysis

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**Product Name:** **VU 0357017 hydrochloride** **Catalog No.: 4295** **Batch No.: 2**

CAS Number: 1135242-13-5

IUPAC Name: 4-[[2-[(2-Methylbenzoyl)amino]ethyl]amino]-1-piperidinecarboxylic acid ethyl ester hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{18}H_{27}N_3O_3.HCl$

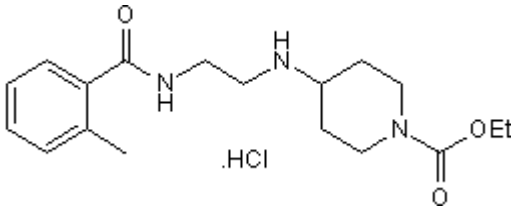
**Batch Molecular Weight:** 369.89

**Physical Appearance:** White solid

**Solubility:** water to 25 mM
DMSO to 5 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.35 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

**HPLC:** Shows 99.1% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 58.45 | 7.63 | 11.36 |
| Found | 58.38 | 7.7 | 11.28 |

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**Description:**

Positive allosteric modulator of muscarinic $M_1$ receptors ($EC_{50}$ = 198 nM). Displays no activity at $M_2$-$M_5$ at concentrations up to 30 µM. Potentiates NMDA receptor currents in hippocampal neurons; activity reverses cognitive decifits in a rodent model of hippocampal-dependent memory. CNS penetrant.

**Physical and Chemical Properties:**

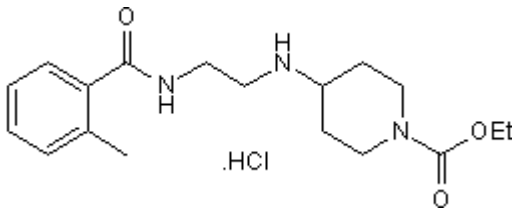
Batch Molecular Formula: $C_{18}H_{27}N_3O_3$.HCl

Batch Molecular Weight: 369.89

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at +4°C

**Solubility & Useage Info:**

water to 25 mM
DMSO to 5 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:**

**Bridges** *et al* (2010) Chemical lead optimization of a pan $G_q$ mAChR $M_1$, $M_3$, $M_5$ positive allosteric modulator (PAM) Lead. Part II. Development of potent and highly selective $M_1$ PAM. Bioorg.Med.Chem.Lett. ***20*** 1972. PMID: 20156687.

**Lebois** *et al* (2010) Discovery and characterization of novel subtype-selective allosteric agonists for the investigation of $M_1$ receptor function in the central nervous system. ACS Chem.Neurosci. ***1*** 104.