

Certificate of Analysis

Print Date: Feb 3rd 2016

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Product Name: VU 0357017 hydrochloride Catalog No.: 4295 Batch No.: 3

CAS Number: 1135242-13-5

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

Store at +4°C

1. PHYSICAL AND CHEMICAL PROPERTIES

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

Batch Molecular Weight: 369.89

Physical Appearance: White solid

Solubility: water to 25 mM DMSO to 5 mM

Batch Molecular Structure:

2. ANALYTICAL DATA

Storage:

TLC: $R_f = 0.6$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.45 7.63 11.35 Found 58.5 7.87 11.37



Product Information

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

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 μ M. 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 & Usage 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 M₁ receptor function in the central nervous system. ACS Chem.Neurosci. *1* 104.