

Certificate of Analysis

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Product Name: VU 0255035

Catalog No.: 3727

Batch No.: 2

CAS Number: 1135243-19-4

IUPAC Name: *N*-[3-Oxo-3-[4-(4-pyridinyl)-1-piperazinyl]propyl]-2,1,3-benzothiadiazole-4-sulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

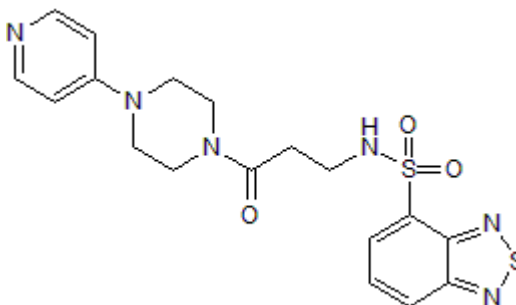
Batch Molecular Formula: C₁₈H₂₀N₆O₃S₂·³/₄H₂O

Batch Molecular Weight: 446.03

Physical Appearance: Yellow solid

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.68 (Dichloromethane-2M:NH₃:Methanol [10:1])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	48.47	4.86	18.84
Found	48.47	4.93	18.86

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Description:

Highly selective muscarinic M₁ antagonist (K_i = 14.87 nM). Targets the M₁ orthosteric site with greater than 75-fold selectivity over the other receptor subtypes. Reduces pilocarpine-induced seizures in mice. Brain penetrant.

Physical and Chemical Properties:

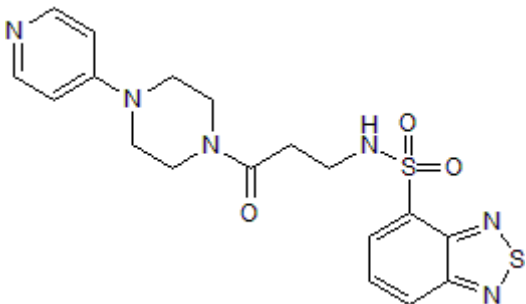
Batch Molecular Formula: C₁₈H₂₀N₆O₃S₂·¾H₂O

Batch Molecular Weight: 446.03

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Sheffler et al (2009) A novel selective muscarinic acetylcholine receptor subtype 1 antagonist reduces seizures without impairing hippocampus-dependent learning. *Mol.Pharmacol.* **76** 356. PMID: 19407080.

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