

Product Name: VU 6028418 hydrochloride

Catalog No.: 7658

Batch No.: 1

IUPAC Name: (3a*R*,5*s*,6a*S*)-2-((Tetrahydro-2*H*-pyran-4-yl)methyl)-*N*-(6-(2,3,5-trifluorophenyl)pyridazin-3-yl)octahydrocyclopenta[*c*]pyrrol-5-amine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₇F₃N₄O.HCl.2¼H₂O

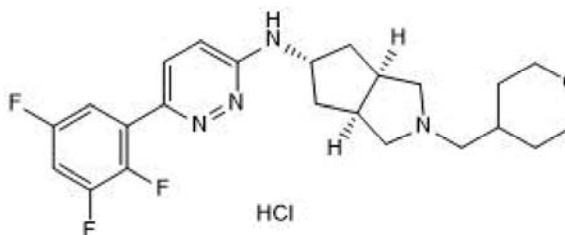
Batch Molecular Weight: 509.48

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.22	6.43	11
Found	54.22	6.03	11.03

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

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Description:

VU 6028418 hydrochloride is a potent and selective M₄ mAChR antagonist (IC₅₀ = 4.1 nM and 57 nM for human and rat M₄ respectively). VU 6028418 hydrochloride dose-dependently reduces the latency to withdraw and reverses cataleptic behavior in haloperidol-treated animals. Orally bioavailable.

Physical and Chemical Properties:

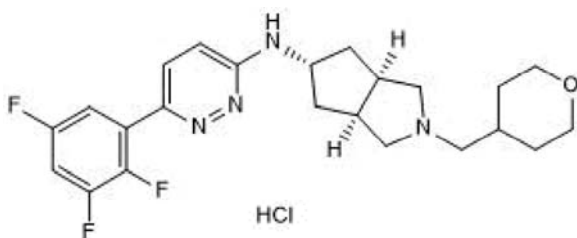
Batch Molecular Formula: C₂₃H₂₇F₃N₄O.HCl.2¼H₂O

Batch Molecular Weight: 509.48

Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°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.

Licensing Information:

Sold under license from Vanderbilt University

References:

Spock et al (2021) Discovery of VU6028418: a highly selective and orally bioavailable M₄ muscarinic acetylcholine receptor antagonist. ACS Med.Chem.Lett. **12** 1342. PMID: 34413964.

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