

Product Name: VU 6019650

Catalog No.: 8055

Batch No.: 1

CAS Number: 2926782-31-0

IUPAC Name: (3*R*,4*S*)-*rel*-1-[(2,3-Dihydro-5-benzofuranyl)sulfonyl]-3-fluoro-4-[[[(1-methyl-1*H*-imidazol-2-yl)thio]methyl]piperidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₂FN₃O₃S₂.

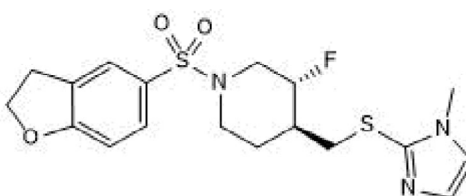
Batch Molecular Weight: 411.51

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



(and enantiomer)

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.54	5.39	10.21
Found	52.4	5.35	10.07

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

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Description:

VU 6019650 is a potent and selective M5 muscarinic acetylcholine receptor antagonist (human M5 IC₅₀ = 36 nM). Exhibits >100-fold selectivity against human and rat M1-4. In vivo, VU 6019650 inhibits the rewarding effects of oxycodone and reduces oxycodone self-administration in rats. VU 60196 is blood brain barrier penetrant.

Physical and Chemical Properties:

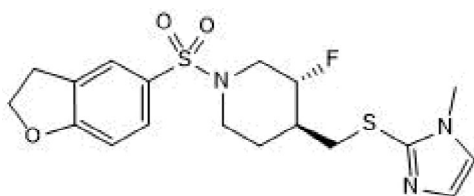
Batch Molecular Formula: C₁₈H₂₂FN₃O₃S₂.

Batch Molecular Weight: 411.51

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



(and enantiomer)

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Capstick *et al* (2022) Discovery of a potent M5 antagonist with improved clearance profile. Part 1: Piperidine amide-based antagonists. *Bioorg.Med.Chem.Lett.* **76** 128988. PMID: 36113671 .

Garrison *et al* (2022) Development of VU6019650: a potent, highly selective, and systemically active orthosteric antagonist of the M5 muscarinic acetylcholine receptor for the treatment of opioid use disorder. *J.Med.Chem.* **65** 6273. PMID: 35417155.

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