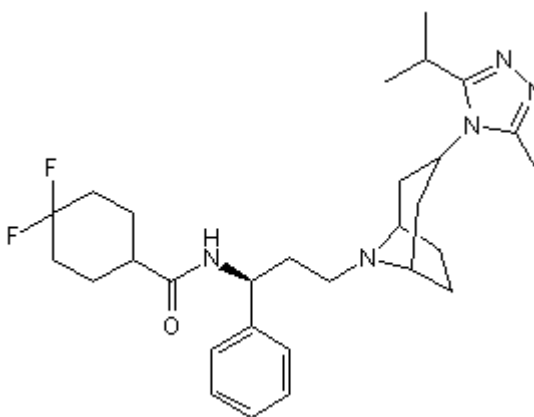


Product Name: Maraviroc **Catalog No.:** 3756 **Batch No.:** 1
CAS Number: 376348-65-1
IUPAC Name: 4,4-Difluoro-N-((1S)-3-[3-(3-isopropyl-5-methyl-4H-1,2,4-triazol-4-yl)-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl)cyclohexanecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₄₁F₂N₅O
Batch Molecular Weight: 513.67
Physical Appearance: White solid
Solubility: DMSO to 75 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -26.6 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.81	8.05	13.63
Found	67.91	8.03	13.75

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

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Description:

Selective CCR5 antagonist; displays potent anti-HIV-1 activity. Prevents the interaction of HIV-1 gp120 and CCR5 (IC₅₀ = 6.4 nM), inhibiting HIV-1 entry. Exhibits antinociceptive effects in a rat model of neuropathic pain. Also inhibits CCL3 (MIP-1α) binding to CCR5. Orally bioavailable.

Physical and Chemical Properties:

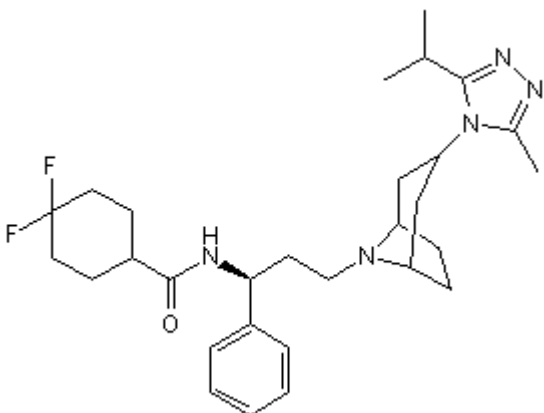
Batch Molecular Formula: C₂₉H₄₁F₂N₅O

Batch Molecular Weight: 513.67

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 75 mM
ethanol to 100 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:

Piotrowska et al (2016) Maraviroc reduces neuropathic pain through polarization of microglia and astroglia - Evidence from *in vivo* and *in vitro* studies. *Neuropharmacology* **S0028-3908** 30164. PMID: 27117708.

Garcia-Perez et al (2011) New insights into the mechanisms whereby low molecular weight CCR5 ligands inhibit HIV-1 infection. *J.Biol.Chem.* **286** 4978. PMID: 21118814.

Kuritzkes et al (2008) Fresh from the pipeline - maraviroc. *Nat.Rev.Drug Discov.* **7** 15.

Dorr et al (2005) Maraviroc (UK-427,857), a potent, orally bioavailable, and selective small-molecule inhibitor of chemokine receptor CCR5 with broad-spectrum anti-human immunodeficiency virus type 1 activity. *Antimicrob.Agents Chemother.* **49** 4721. PMID: 16251317.

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