

**Product Name:** Maraviroc

**Catalog No.:** 3756

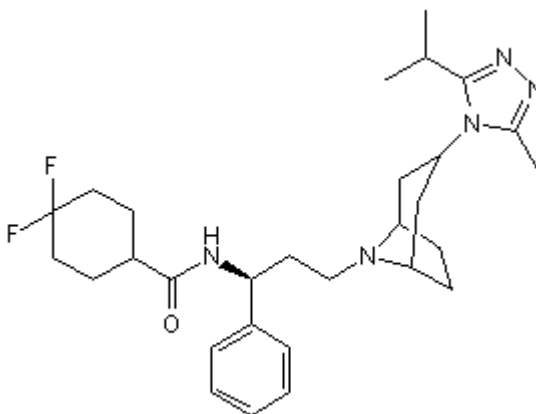
**Batch No.:** 1

**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:** C<sub>29</sub>H<sub>41</sub>F<sub>2</sub>N<sub>5</sub>O  
**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  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -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 (IC<sub>50</sub> = 6.4 nM), inhibiting HIV-1 entry. Also inhibits CCL3 (MIP-1α) binding to CCR5.

**Physical and Chemical Properties:**

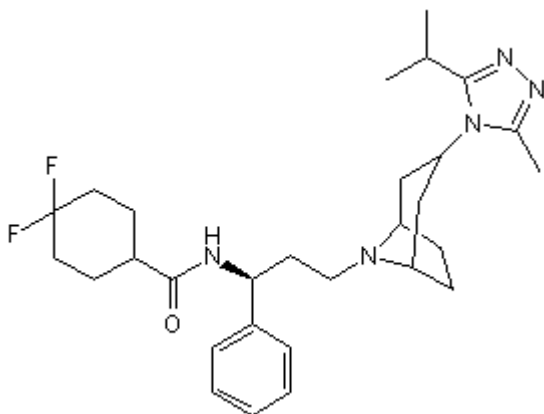
Batch Molecular Formula: C<sub>29</sub>H<sub>41</sub>F<sub>2</sub>N<sub>5</sub>O

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:**

**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.

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

**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.

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