

Product Name: BMS CCR2 22

Catalog No.: 3129

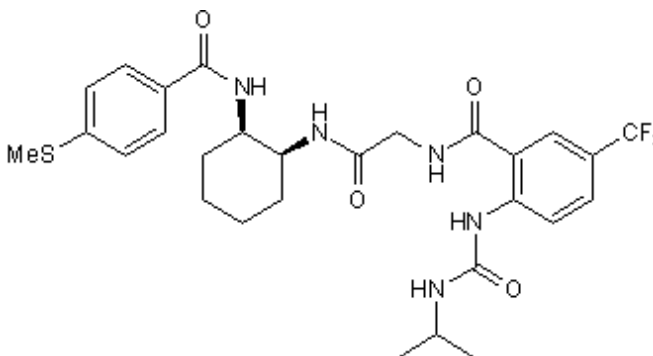
Batch No.: 4

CAS Number: 445479-97-0

IUPAC Name: 2-[(Isopropylaminocarbonyl)amino]-N-[2-[[*cis*-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₈ H ₃₄ F ₃ N ₅ O ₄ S
Batch Molecular Weight:	593.66
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 10 mM
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.85 (Ethyl acetate)
HPLC:	Shows 99% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	56.65	5.77	11.8
Found	56.49	5.5	11.67

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

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Description:

High affinity CCR2 chemokine receptor antagonist ($IC_{50} = 5.1$ nM). Displays potent functional antagonism, IC_{50} values are 1 and 18 nM for chemotaxis and antagonism of calcium flux respectively. Selective over CCR3.

Physical and Chemical Properties:

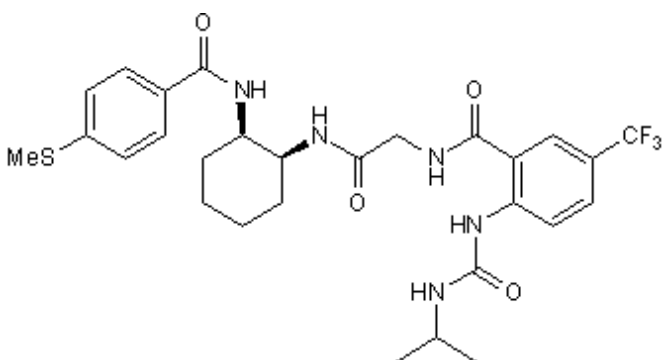
Batch Molecular Formula: $C_{28}H_{34}F_3N_5O_4S$

Batch Molecular Weight: 593.66

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 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:

Cherney et al (2008) Discovery of disubstituted cyclohexanes as a new class of CC chemokine receptor 2 antagonists. *J.Med.Chem.* **51** 721. PMID: 18232650.

You et al (2010) CCR2 receptor ligands inhibit $Ca_v3.2$ T-type calcium channels. *Mol.Pharmacol.* **77** 211. PMID: 19864434.

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