

Product Name: Teijin compound 1

Catalog No.: 3664

Batch No.: 2

CAS Number: 1313730-14-1

IUPAC Name: *N*-[2-[[*(3R)*-1-[(4-chlorophenyl)methyl]-3-pyrrolidinyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₁ClF₃N₃O₂.HCl

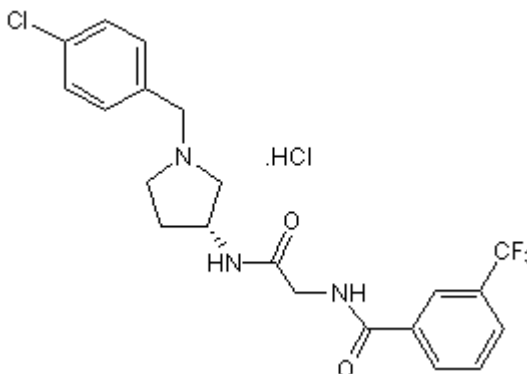
Batch Molecular Weight: 476.32

Physical Appearance: White solid

Solubility: water to 10 mM
DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.37 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +31.2 (Concentration = 1, Solvent = Ethanol)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 52.95 4.66 8.82

Found 52.97 4.61 8.8

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

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Description:

Potent chemokine CCR2b receptor antagonist (IC_{50} = 180 nM). Potently inhibits cell chemotaxis induced by MCP-1 (EC_{50} = 24 nM).

Physical and Chemical Properties:

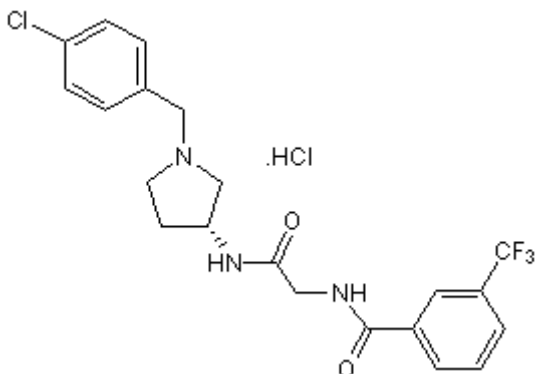
Batch Molecular Formula: $C_{21}H_{21}ClF_3N_3O_2 \cdot HCl$

Batch Molecular Weight: 476.32

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Moree et al (2004) Small molecule antagonists of the CCR2b receptor. Part 2: discovery process and initial structure-activity relationships of diamine derivatives. *Bioorg.Med.Chem.Letts.* **14** 5413.

Moree et al (2008) Potent antagonists of the CCR2b receptor. Part 3: SAR of the (*R*)-3-aminopyrrolidine series. *Bioorg.Med.Chem.Letts.* **18** 1869.

Hall et al (2009) Elucidation of binding sites of dual antagonists in the human chemokine receptors CCR2 and CCR5. *Mol.Pharmacol.* **75** 1325. PMID: 19297521.

Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 10 mM
DMSO 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.

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