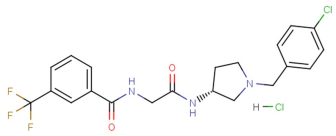
Data Sheet (Cat.No.T19230)

TargetMol
A DRUG SCREENING EXPERT

CCR2 antagonist 4 hydrochloride

Chemical Properties



CAS No.:	1313730-14-1
Formula:	C21H22Cl2F3N3O2
Molecular Weight:	476.32
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	CCR2 antagonist 4 hydrochloride is a specific CCR2 antagonist (IC50s: 180 nM for CCR2b). It potently inhibits MCP-1-induced chemotaxis (IC50: 24 nM).
Targets(IC_{50})	CCR2b: 180 nM
In vitro	Ile263 and Thr292 in CCR2 contribute significantly to the binding of CCR2 antagonist 4 in CCR2. His121 on TM3 and Ile263 on TM6 also strongly interact with CCR2 antagonist 4 hydrochloride. Residue Glu291 in TM7 contributes substantially to the binding of the protonated CCR2 antagonist 4 hydrochloride, and CCL2 [2].
In vivo	In ApoE-deficient mice, CCR2 antagonist 4 hydrochloride reduces the mouse monocyte/macrophage cell line (RAW 264.7) adhesion/ infiltration into the aorta [3].

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.099 mL	10.497 mL	20.994 mL
5 mM	0.42 mL	2.099 mL	4.199 mL
10 mM	0.21 mL	1.05 mL	2.099 mL
50 mM	0.042 mL	0.21 mL	0.42 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Moree WJ, et al. Potent antagonists of the CCR2b receptor. Part 3: SAR of the (R)-3-aminopyrrolidine series. Bioorg Med Chem Lett. 2008 Mar 15;18(6):1869-73.
2. Hall SE, et al. Elucidation of binding sites of dual antagonists in the human chemokine receptors CCR2 and CCR5. Mol Pharmacol. 2009 Jun;75(6):1325-36.
3. Calin M, et al. VCAM-1 directed target-sensitive liposomes carrying CCR2 antagonists bind to activated endothelium and reduce adhesion and transmigration of monocytes. Eur J Pharm Biopharm. 2015 Jan;89:18-29.

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