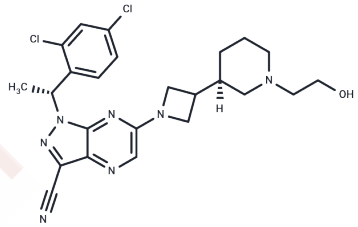
Data Sheet (Cat.No.T39661)

TargetMol

CCR4 antagonist 3

Chemical Properties



CAS No. : 2174938-70-4

Formula: C24H27Cl2N7O

Molecular Weight: 500.43

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	CCR4 antagonist 3 is an orally active, potent and selective CCR4 antagonist. CCR4 antagonist 3, featuring a novel piperidinyl-azetidine motif, has IC 50 s of 22 nM and 50 nM in the calcium flux and CTX assay. CCR4 antagonist 3 has antitumor activity.
Targets(IC50)	Others,CCR
In vitro	CCR4 antagonist 3 (compound 38) shows no activity in a CYP450 induction assay[1]. CCR4 antagonist 3 inhibits the migration of mouse iT reg cells with an IC 50 of 39 nM, while the IC 50 in human iT reg cells is 33 nM[1].
In vivo	CCR4 antagonist 3 demonstrated significant anti-tumor activity in a mouse model of Pan02-OVA tumors, administered as a 50 mg/kg oral dose daily for 40 days, resulting in a notable reduction in tumor growth. Pharmacokinetic profiles across species revealed that CCR4 antagonist 3, at a dosage of 0.5 mg/kg intravenously, exhibits low clearance (CL=10.2 mL/min/kg) and medium volume of distribution (Vss=5.2 L/kg) with a half-life (T 1/2) of 6.9 hours and 29% bioavailability in mice. In dogs, it showed a clearance of 7.3 mL/min/kg, a half-life of 12.7 hours, and 44% bioavailability. Cynomolgus monkeys demonstrated a clearance of 3.7 mL/min/kg, a long half-life of 10.7 hours, and 41% bioavailability. Additionally, when administered orally at 2 mg/kg in rats and 0.5 mg/kg intravenously or orally in mice, the compound achieved medium clearance (CL=47.6 mL/min/kg) with 49% bioavailability in rats and maintained its pharmacokinetic profile of low clearance, medium volume of distribution, a 6.9-hour half-life, and 29% bioavailability in mice.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9983 mL	9.9914 mL	19.9828 mL
5 mM	0.3997 mL	1.9983 mL	3.9966 mL
10 mM	0.1998 mL	0.9991 mL	1.9983 mL
50 mM	0.040 mL	0.1998 mL	0.3997 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Omar Robles, et al. Novel Piperidinyl-Azetidines as Potent and Selective CCR4 Antagonists Elicit Antitumor Response as Single Agent and in Combination with Checkpoint Inhibitors. J Med Chem. 2020 Jul 15.

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