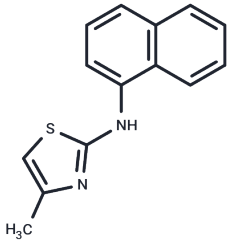
Data Sheet (Cat.No.T60336)

TargetMol

CCR4 antagonist 3-1

Chemical Properties



CAS No. : 1957-01-3

Formula: C14H12N2S

Molecular Weight: 240.32

Storage: Store at low temperature
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 3-1 is a less active chemokine receptor 4 (CCR4) antagonist that inhibits [125I]TARC (thymus and activation-regulated chemokine) with an IC50 value of 1.7 μM. CCR4 antagonist 3-1 inhibits the binding of radiolabeled [125I]TARC and macrophage-derived chemokine (MDC) to CEM cell surface and inhibits TARC-mediated CEM cell migration in vitro with an IC50 value of 6.4 μM. CCR4 antagonist 3 inhibited the binding of radiolabeled [125I]TARC and macrophage-derived chemokine (MDC) to the CCR4 receptor on the surface of CEM cells and inhibited TARC-mediated migration of CEM cells in vitro with an IC50 value of 6.4 μM.
Targets(IC50)	CCR
In vivo	CCR4 antagonist 3-1 (compound 1) (0.5 mg/kg, i.v.; 2 mg/kg, p.o.; single dosage) exhibited a high clearance of 4.2 L/h/kg a short half-life of 0.4 h, and the oral bioavailability of 2%.[1]

Solubility Information

Solubility	DMSO: 45 mg/mL (187.25 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	4.1611 mL	20.8056 mL	41.6112 mL
5 mM	0.8322 mL	4.1611 mL	8.3222 mL
10 mM	0.4161 mL	2.0806 mL	4.1611 mL
50 mM	0.0832 mL	0.4161 mL	0.8322 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

Wang X, et al. Optimization of 2-aminothiazole derivatives as CCR4 antagonists. Bioorg Med Chem Lett. 2006 May 15;16(10):2800-3.