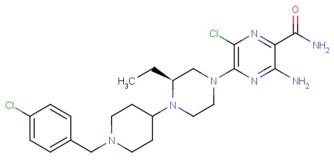
Data Sheet (Cat.No.T16863)

TargetMol
A DRUG SCREENING EXPERT

SCH 546738

Chemical Properties



CAS No.:	906805-42-3
Formula:	C23H31Cl2N7O
Molecular Weight:	492.44
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	SCH 546738 is an effective and non-competitive CXCR3 antagonist. SCH 546738 bindings to the human CXCR3 receptor is determined (Ki: 0.4 nM) in multiple experiments.
Targets(IC_{50})	Human CXCR3: 0.4 nM (ki)
In vitro	SCH 546738 effectively and specifically inhibits CXCR3-mediated chemotaxis in human activated T cells (IC90: 10 nM). SCH 546738 displaces radiolabeled CXCL10 and CXCL11 from human CXCR3 (IC50: ranging from 0.8 to 2.2 nM) in a non-competitive manner. Competition of human CXCL10 and CXCL11 binding to human CXCR3 by SCH 546738 is determined at various concentrations of [125I]hCXCL10 and [125I]hCXCL11 around the Kd (50-100 pM) for the receptor [1].
In vivo	SCH 546738 is a selective and effective CXCR3 antagonist with a good PK for in vivo studies. SCH 546738 has a favorable pharmacokinetic profile in rodents, the plasma concentrations of SCH 546738 in Lewis rat, and C57BL/6 mouse over 24 hr post-dose. SCH 546738 has strong cross-species activities with IC50 of 1.3 nM, 6.4 nM, 5.9 nM, and 4.2 nM in inhibiting the binding of [125I]hCXCL10 to CXCR3 of monkey, dog, mouse and rat origin, respectively [1].

Solubility Information

Solubility	DMSO: 4.5 mg/mL (9.14 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.031 mL	10.154 mL	20.307 mL
5 mM	0.406 mL	2.031 mL	4.061 mL
10 mM	0.203 mL	1.015 mL	2.031 mL
50 mM	0.041 mL	0.203 mL	0.406 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. Jenh CH, et al. A selective and potent CXCR3 antagonist SCH 546738 attenuates the development of autoimmune diseases and delays graft rejection. BMC Immunol. 2012 Jan 10;13:2.
2. Zhang X, et al. CXC chemokine receptor 3 promotes steatohepatitis in mice through mediating inflammatory cytokines, macrophages and autophagy. J Hepatol. 2016 Jan;64(1):160-70.
3. Yue C, et al. STAT3 in CD8

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