Product Data Sheet

ML604086

Cat. No.:HY-124416CAS No.:850330-18-6Molecular Formula: $C_{27}H_{32}N_4O_4S$ Molecular Weight:508.63

Target: CCR

Pathway: GPCR/G Protein; Immunology/Inflammation

Storage: Powder -20°C 3 years

4°C 2 years In solvent -80°C 2 years

-20°C 1 year

SOLVENT & SOLUBILITY

In Vitro

DMSO: 120 mg/mL (235.93 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	1.9661 mL	9.8303 mL	19.6607 mL
	5 mM	0.3932 mL	1.9661 mL	3.9321 mL
	10 mM	0.1966 mL	0.9830 mL	1.9661 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: \geq 6.25 mg/mL (12.29 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 6.25 mg/mL (12.29 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	ML604086 is a selective CCR8 inhibitor, inhibiting CCL1 binding to CCR8 on circulating T-cells. ML604086 inhibits CCL1 mediated chemotaxis and increases in intracellular Ca^{2+} concentrations ^{[1][2]} .
IC ₅₀ & Target	$CCR8^{[1][2]}$.
In Vitro	ML604086 (0-100 μ M) inhibits CCL1 mediated chemotaxis and increases in intracellular Ca ²⁺ concentrations of cell lines stably expressing cyno CCR8 with IC ₅₀ s of 1.3 μ M and 1.0 μ M, respectively ^[2] . ML604086 (10, 30 μ M; 64 h) inhibits CCL1 binding to CCR8 on CD4 T-cells, and inhibits the serotonin receptor 5HT1a with the inhibition rate of 30%, 70% at 10, 30 μ M respectively ^[2] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo	ML604086 (1.038 mg/kg; intravenous infusion) shows no effect on airway eosinophilia, pro-inflammatory cytokine production or airway resistance and compliance in Macaca fascicularis ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
	Animal Model:	3.0-5.0 kg male and female adult Macaca fascicularis (primate modelof asthma) ^[2]	
	Dosage:	1.038 mg/kg	
	Administration:	Intravenous infusion	
	Result:	Did not effected the Changes in airway resistance and compliance induced by allergen provocation and increasing concentrations of methacholine.	

REFERENCES

- [1]. James E. Pease, et al. Chemokine Receptors in Allergy, Inflammation, and Infectious Disease. Top Med Chem (2015) 14: 1-40.
- [2]. Lin Wang, et al. Antagonism of chemokine receptor CCR8 is ineffective in a primate model of asthma. Thorax 2013;68:506–512.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA