Screening Libraries

CCR1 antagonist 9

Cat. No.: HY-124759

CAS No.: 1220026-26-5 Molecular Formula: $C_{20}H_{16}FN_{5}O_{3}S$

Molecular Weight: 425.44 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

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 83.33 mg/mL (195.87 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.3505 mL	11.7525 mL	23.5051 mL
	5 mM	0.4701 mL	2.3505 mL	4.7010 mL
	10 mM	0.2351 mL	1.1753 mL	2.3505 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: ≥ 2.08 mg/mL (4.89 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (4.89 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	CCR1 antagonist 9 is a potent and selective CCR1 antagonist with an IC ₅₀ of 6.8 nM in calcium flux assay ^[1] .
IC ₅₀ & Target	CCR1 6.8 nM (IC ₅₀ , in calcium flux assay)
In Vitro	CCR1 antagonist 9 (Compound 19e) blocks the CCR1 chemotaxis of THP-1 cells with an IC $_{50}$ of 28 nM. CCR1 antagonist 9 also blocks hERG with an IC $_{50}$ of 30 μ M $^{[1]}$. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES				
[1]. Harcken C, et al. Identification of novel azaindazole CCR1 antagonist clinical candidates. Bioorg Med Chem Lett. 2019 Feb 1;29(3):441-448.				
Cautian Dual				
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