CCR6 inhibitor 1

Cat. No.: HY-112701

CAS No.: 2437547-04-9

Molecular Formula: $C_{24}H_{23}F_3N_4O_3S$

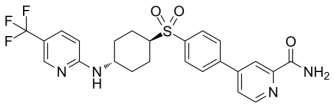
Molecular Weight: 504.52

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 : ≥ 125 mg/mL (247.76 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.9821 mL	9.9104 mL	19.8208 mL
5 mM	0.3964 mL	1.9821 mL	3.9642 mL
10 mM	0.1982 mL	0.9910 mL	1.9821 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 (4.12 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.12 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.12 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CCR6 inhibitor 1 is a potent and selective CCR6 inhibitor, with IC_{50}s of 0.45 and 6 nM for monkey and human CCR6, much more selective at CCR6 over human CCR1 (IC_{50}, > 30000 nM), and CCR7 (IC_{50}, 9400 nM). CCR6 inhibitor 1 markedly blocks ERK phosphorylation. CCR6 inhibitor 1 is used in the research of autoimmune diseases and cancer[1].

IC_{50} & Target			
	Moneky CCR6 0.45 nM (IC_{50})	Human CCR6 6 nM (IC_{50})	Human CCR7 9400 nM (IC_{50})

In Vitro	CCR6 inhibitor 1 (Compound 35) inhibits L20-induced human B cell migration[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Clin Transl Med. 2023 Feb;13(2):e1198.
- Stem Cell Res Ther. 2022 Jul 15;13(1):294.
- J Pathol. 2022 Apr;256(4):414-426.
- Dent J Iwate Med Univ. 46: 19-32, 2021.

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REFERENCES

[1]. Tawaraishi T, et al. Identification of a novel series of potent and selective CCR6 inhibitors as biological probes. Bioorg Med Chem Lett. 2018 Oct 1;28(18):3067-3072.

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