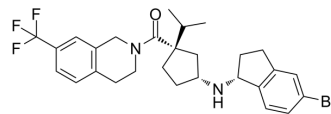


## CCR2 antagonist 1

Cat. No.:	HY-112792		
CAS No.:	1683534-96-4		
Molecular Formula:	C <sub>28</sub> H <sub>32</sub> BrF <sub>3</sub> N <sub>2</sub> O		
Molecular Weight:	549.47		
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 (227.49 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	Preparing Stock Solutions	1 mM	1.8199 mL	9.0997 mL	18.1994 mL
		5 mM	0.3640 mL	1.8199 mL	3.6399 mL
10 mM		0.1820 mL	0.9100 mL	1.8199 mL	
Please refer to the solubility information to select the appropriate solvent.					
In Vivo	1. Add each solvent one by one: 5 % DMSO >> 45 % PEG300 >> 50% sterile water Solubility: 11 mg/mL (20.02 mM); Suspended solution; Need ultrasonic				
	2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (3.79 mM); Clear solution				

### BIOLOGICAL ACTIVITY

Description	CCR2 antagonist 1 is a high-affinity and long-residence-time CCR2 antagonist, with a K <sub>i</sub> of 2.4 nM.
IC <sub>50</sub> & Target	CCR2 2.4 nM (K <sub>i</sub> )
In Vitro	The combination of SAR and SKR in the hit-to-lead process results in the discovery of a new high-affinity and long-residence-time CCR2 antagonist (CCR2 antagonist 1 (compound 15a), K <sub>i</sub> =2.4 nM; RT=714 min) <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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## CUSTOMER VALIDATION

- Sci Adv. 2023 Aug 2;9(31):eadg6856.

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## REFERENCES

[1]. Vilums M, et al. When structure-affinity relationships meet structure-kinetics relationships: 3-((Inden-1-yl)amino)-1-isopropyl-cyclopentane-1-carboxamides as CCR2 antagonists. Eur J Med Chem. 2015 Mar 26;93:121-34.

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**Caution: Product has not been fully validated for medical applications. For research use only.**

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