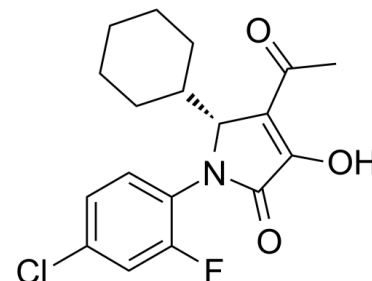


Data Sheet

Product Name:	CCR2-RA-[R]
Cat. No.:	CS-0002114
CAS No.:	512177-83-2
Molecular Formula:	C ₁₈ H ₁₉ ClFNO ₃
Molecular Weight:	351.80
Target:	CCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Solubility:	DMSO : ≥ 125 mg/mL (355.32 mM); H ₂ O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

CCR2-RA-[R] is an allosteric antagonist of the **C-C chemokine receptor type 2 (CCR2)** with an **IC₅₀** of 103 nM. IC₅₀ & Target: IC₅₀: 103 nM (CCR2)^[1] **In Vitro:** The chemokine receptor CCR2 is a G protein-coupled receptor that is involved in many diseases characterized by chronic inflammation, and therefore a large variety of CCR2 small molecule antagonists has been developed. CCR2-RA-[R] displaces [¹²⁵I]CCL2 from CCR2 with an pIC₅₀ value of 6.1. The pK_D of CCR2-RA-[R] for CCR2 and CCR5 is 8.8±0.1 and 7.0±0.1, respectively^[2]. CCR2-RA-[R] inhibits CCR2 non-competitively by blocking activation-associated conformational changes and formation of the G protein-binding interface. The binding pocket of CCR2-RA-[R] is highly enclosed and possesses a balanced combination of hydrophobic and polar features, all of which favors pocket "druggability"^[3].

References:

- [1]. Zweemer AJ, et al. Multiple binding sites for small-molecule antagonists at the CC chemokine receptor 2. *Mol Pharmacol*. 2013 Oct;84(4):551-61.
- [2]. Zweemer AJ, et al. Discovery and mapping of an intracellular antagonist binding site at the chemokine receptor CCR2. *Mol Pharmacol*. 2014 Oct;86(4):358-68.
- [3]. Zheng Y, et al. Structure of CC chemokine receptor 2 with orthosteric and allosteric antagonists. *Nature*. 2016 Dec 15;540(7633):458-461.

CAIndexNames:

2H-Pyrrol-2-one, 4-acetyl-1-(4-chloro-2-fluorophenyl)-5-cyclohexyl-1,5-dihydro-3-hydroxy-, (5R)-

SMILES:

O=C1C(O)=C(C(C)=O)[C@@H](C2CCCC2)N1C(C(F)=C3)=CC=C3Cl

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

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