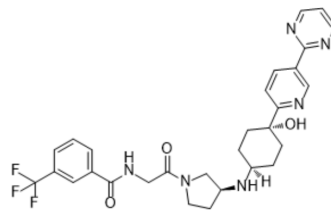


PF-4136309

Cat. No.:	HY-13245		
CAS No.:	1341224-83-6		
Molecular Formula:	C ₂₉ H ₃₁ F ₃ N ₆ O ₃		
Molecular Weight:	568.59		
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

Ethanol : 133.33 mg/mL (234.49 mM; Need ultrasonic)
 DMSO : ≥ 34 mg/mL (59.80 mM)
 H₂O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)
 * "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	1 mM	1.7587 mL	8.7937 mL	17.5874 mL
	5 mM	0.3517 mL	1.7587 mL	3.5175 mL
	10 mM	0.1759 mL	0.8794 mL	1.7587 mL

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

In Vivo

- Add each solvent one by one: 0.5% Methylcellulose/saline water
Solubility: 10 mg/mL (17.59 mM); Suspended solution; Need ultrasonic
- Add each solvent one by one: 10% EtOH >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 5 mg/mL (8.79 mM); Clear solution
- Add each solvent one by one: 10% EtOH >> 90% (20% SBE-β-CD in saline)
Solubility: ≥ 5 mg/mL (8.79 mM); Clear solution
- Add each solvent one by one: 10% EtOH >> 90% corn oil
Solubility: ≥ 5 mg/mL (8.79 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 2.08 mg/mL (3.66 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 2.08 mg/mL (3.66 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.08 mg/mL (3.66 mM); Clear solution

8. Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.08 mg/mL (3.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	PF-4136309 is a potent, selective, and orally bioavailable CCR2 antagonist, with IC ₅₀ s of 5.2 nM, 17 nM and 13 nM for human, mouse and rat CCR2.		
IC₅₀ & Target	Human CCR2 5.2 nM (IC ₅₀)	Mouse CCR2 13 nM (IC ₅₀)	Rat CCR2 17 nM (IC ₅₀)
In Vitro	PF-4136309 is potent in human chemotaxis activity (IC ₅₀ =3.9 nM) and in the whole blood assay (IC ₅₀ =19 nM), with IC ₅₀ of 16 and 2.8 nM in mouse and rat chemotaxis assays. PF-4136309 is potent in inhibiting CCR2 mediated signaling events such as intracellular calcium mobilization and ERK (extracellular signal-regulated kinase) phosphorylation with IC ₅₀ values of 3.3 and 0.5 nM, respectively. In hERG patch clamp assay, PF-4136309 inhibits hERG potassium current with an IC ₅₀ of 20 μ M. PF-4136309 is not a cytochrome P450 (CYP) inhibitor, with IC ₅₀ values of >30 μ M against five major CYP isozymes CYP1A2, CYP2C9, CYP2C19, CYP2D6, and CYP3A4. Moreover, PF-4136309 is not a CYP inducer at concentrations up to 30 μ M ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		
In Vivo	PF-4136309 (2 mg/kg) exhibits a moderate half-life in both species after iv administration (2.5 and 2.4 h). When administered orally, PF-4136309 (10 mg/kg) is absorbed rapidly, with peak concentration time (T _{max}) at 1.2 h for rats and 0.25 h for dogs. A similar half-life is observed in both species between iv dosing and po dosing. PF-4136309 is well absorbed, with an oral bioavailability of 78% in both species ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		

CUSTOMER VALIDATION

- Materials Today. 2022.
- Int J Mol Sci. 2023, 24(1), 123.

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REFERENCES

[1]. Wang W, Chen XK, Zhou L, et al. Chemokine CCL2 promotes cardiac regeneration and repair in myocardial infarction mice via activation of the JNK/STAT3 axis. Acta Pharmacol Sin. Published online December 12, 2023.

[2]. Xue CB, et al. Discovery of INCB8761/PF-4136309, a Potent, Selective, and Orally Bioavailable CCR2 Antagonist. ACS Med. Chem. Lett., 2011, 2 (12), pp 913-918.

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

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