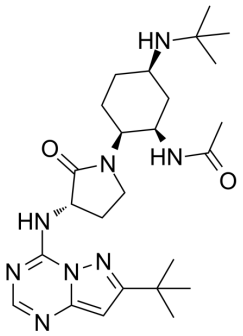
BMS-813160

Cat. No.:	HY-109593
CAS No.:	1286279-29-5
Molecular Formula:	$C_{25}H_{40}N_8O_2$
Molecular Weight:	484.64
Target:	CCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Storage:	4°C, protect from light * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (51.58 mM; Need ultrasonic and warming)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0634 mL	10.3169 mL	20.6339 mL
	5 mM	0.4127 mL	2.0634 mL	4.1268 mL
	10 mM	0.2063 mL	1.0317 mL	2.0634 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 (4.29 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.29 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.29 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BMS-813160 is a potent and selective CCR2/5 dual antagonist. BMS-813160 binds with CCR2 and CCR5 with IC_{50}s of 6.2 and 3.6 nM, respectively. BMS-813160 can be used for the research of inflammation[1][2].

IC_{50} & Target

CCR5	CCR2
3.6 nM (IC_{50})	6.2 nM (IC_{50})

In Vitro

BMS-813160 binds with CCR2, CCR5, CCR1, CCR4 and CXCR2 with IC_{50}s of 6.2 nM, 3.6 nM, ⊠25 μM, ⊠40 μM and ⊠40 μM, respectively[2].

BMS-813160 shows activities to CCR2 CTX, CCR2 CD11b, CCR5 CTX and CCR5 CD11b with IC_{50}s of 0.8, 4.8, 1.1 and 5.7 nM,

	respectively[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BMS-813160 (10-160 mg/kg; p.o. twice a day for two days) inhibits the migration of inflammatory monocytes and macrophages in mouse thioglycollate-induced peritonitis model, and shows excellent oral bioavailability[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Human-CCR2 knock-in C57BL/6 male mice with thioglycollate injection[2]
Dosage:	10, 50 and 160 mg/kg
Administration:	Oral gavage; 10-160 mg/kg twice a day; for two days
Result:	Dose-dependently reduced inflammatory monocyte and macrophage infiltration in the peritoneum.

CUSTOMER VALIDATION

- Research Square Preprint. 2020 Oct.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Cherney RJ, et al. BMS-813160: A Potent CCR2 and CCR5 Dual Antagonist Selected as a Clinical Candidate. ACS Med Chem Lett. 2021 Oct 15;12(11):1753-1758.

[2]. Norman P. et al. A dual CCR2/CCR5 chemokine antagonist, BMS-813160? Evaluation of WO2011046916. Expert Opin Ther Pat. 2011 Dec;21(12):1919-24.

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