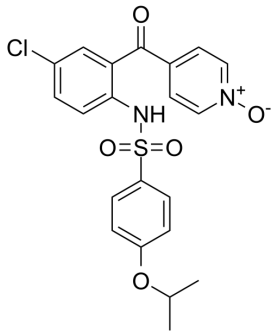
MLN3126

Cat. No.:	HY-123763
CAS No.:	628300-71-0
Molecular Formula:	$C_{21}H_{19}ClN_2O_5S$
Molecular Weight:	446.9
Target:	CCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (55.94 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2376 mL	11.1882 mL	22.3764 mL
	5 mM	0.4475 mL	2.2376 mL	4.4753 mL
	10 mM	0.2238 mL	1.1188 mL	2.2376 mL

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

BIOLOGICAL ACTIVITY

Description

MLN3126 is an orally active and potent CCR9 antagonist. MLN3126 inhibits CCL25-induced calcium mobilization and chemotaxis of mouse primary thymocytes, wiht an IC_{50} value of 6.3 nM for calcium influx[1].

In Vitro

MLN3126 inhibits CCL25-induced calcium mobilization with an IC_{50} value of 6.3 nM in CCR9 expressing cells[1].
MLN3126 inhibits the binding of biotinylated CCL25 to CCR9 with an IC_{50} of 14.2 nM[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Invasion Assay[1]

Cell Line:	Mouse thymocytes
Concentration:	0.01, 0.03, 0.1, 0.3, 1, 3 μM
Incubation Time:	90 min
Result:	Inhibited CCL25-induced chemotaxis of mouse thymocytes.

In Vivo

MLN3126 (2.5% w/w; p.o.) decreases colonic level of IFN-γ, largely produced by T cells[1].
MLN3126 (0.05, 0.25 and 1% (w/w); p.o.) has the potential activity for alleviating inflammatory bowel disease (IBD)[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Activated T cell transferred colitis mouse model[1]
Dosage:	0.05, 0.25 and 1% (w/w) (around 4 g/day)
Administration:	Oral gavage; 21 days
Result:	Blocked CCR9/CCL25 interaction by inhibiting migration of T cells to the colon and resulted in the amelioration of colitis.

REFERENCES

[1]. Igaki K, et al. MLN3126, an antagonist of the chemokine receptor CCR9, ameliorates inflammation in a T cell mediated mouse colitis model. Int Immunopharmacol. 2018 Jul;60:160-169.

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