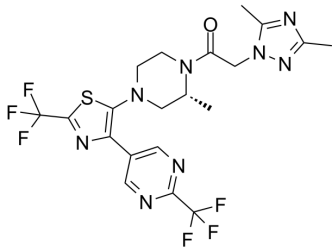
ACT-660602

Cat. No.:	HY-151096
CAS No.:	1646267-59-5
Molecular Formula:	$C_{20}H_{20}F_6N_8OS$
Molecular Weight:	534.48
Target:	CXCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 110 mg/mL (205.81 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8710 mL	9.3549 mL	18.7098 mL
	5 mM	0.3742 mL	1.8710 mL	3.7420 mL
	10 mM	0.1871 mL	0.9355 mL	1.8710 mL

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

BIOLOGICAL ACTIVITY

Description

ACT-660602 is an orally active antagonist of chemokine receptor (CXCR3) with an IC_{50} value of 204 nM. ACT-660602 inhibits T-cell migration and shows efficacy in acute lung ingury model. ACT-660602 can be used for autoimmune diseases research[1] [2].

IC_{50} & Target

CXCR3
204 nM (IC_{50})

In Vitro

ACT-660602 shows selectivity to CXCR3 over hERG, with IC_{50}s of 18 μM (hERG)[1].
ACT-660602 (112 nM; 6 h) inhibits cell migration and improves the metabolic stability[1].
ACT-660602 (5, 20, 100 or 500 nM) displays an non-competitive binding mode to CXCL10 and CXCL11 in different concentration, with more stable IC_{50}s[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Migration Assay [1]

Cell Line:	CD3/CD28-activated primary human T cells

Concentration:	112 nM
Incubation Time:	45 min
Result:	Inhibited cell migration.

In Vivo

ACT-660602 (1 μM; 6 h) intrinsic metabolic clearance (CLint) in human, rat, mouse liver microsomes (HLM, RLM, MLM)[1].
ACT-660602 (30 mg/kg; p.o.; once daily) displays anti-inflammatory activity and exerts efficacy in the mouse model of acute lung ingury[1].
Range for Pharmacokinetics of ACT-660602[1]

Animal	Route	Dose (range) (mg/kg)	C_{max} (range) (ng/mL)	T_{max} (range) (h)	AUC (range) (ng•h/mL)	F (%)	CL (range) (mL/min/kg)	V_{ss} (range) (L/kg)	$T_{1/2}$ (range) (h)
Dog	p.o.	2	1380	1	20000	8	1.3	1.7	14.5
	i.v.	0.5	1300-1450	0.5-2.0	10400-32000	/	0.6-3.0	1.6-1.7	6.3-
Rat	p.o.	2	1520	0.5	14000	80	1.9	1.1	7.1
	i.v.	0.5	1250-1860	0.5-1.0	11600-15641	/	1.9-1.9	0.9-1.3	5.7-8.8

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	LPS-induced lung inflammation model (72 h post LPS challenge)[1]
Dosage:	30 mg/kg
Administration:	Oral gavage; once daily
Result:	Significantly reduced recruitment of the CXCR3+ CD8+ T cell in the bronchoalveolar lavage compartment.

REFERENCES

[1]. Meyer EA, et al. Discovery and In Vivo Evaluation of ACT-660602: A Potent and Selective Antagonist of the Chemokine Receptor CXCR3 for Autoimmune Diseases. J Med Chem. 2022 Aug 10.

[2]. Caroff Eva, et al. Preparation of piperazinyltriazolylethanone derivatives for use as CXCR3 receptor modulators: World Intellectual Property Organization, WO2015011099. 2015-01-29.

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