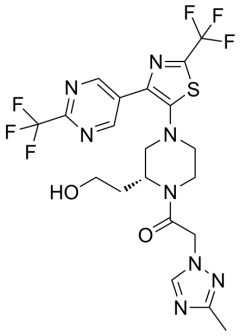
ACT-777991

Cat. No.:	HY-149055
CAS No.:	1967811-46-6
Molecular Formula:	$C_{20}H_{20}F_6N_8O_2S$
Molecular Weight:	550.48
Target:	CXCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	ACT-777991 is an orally active and selective CXCR3 antagonist. ACT-777991 has microsomes and hepatocytes stability across animal models. ACT-777991 inhibits the migration of activated T cells toward CXCL11[1].
IC_{50} & Target	CXCR3
In Vitro	ACT-777991 inhibits hEGR with an IC_{50} value of 26 μM in CHO cells[1]. ACT-777991 (1 μM; 45 min) is stable in microsomes and hepatocytes across humans, rats, and dogs[1]. ACT-777991 (0.01-1 μM;) inhibits the migration of both human and mouse-activated T cells toward CXCL11 with IC_{50}s range of 3.2-64 nM and 4.9-21 nM, respectively[1]. ACT-777991 (1 nM, 5 nM, 20 nM, and 50 nM) inhibits CXCR3-mediated chemotaxis of human and mouse T cells[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	ACT-777991 (0.5 mg/kg, 1 mg/kg; i.v.; single dose) has low in vivo plasma clearance in male Wistar rats (14/156) or Beagle dogs (5/15)[1]. ACT-777991 (0.006-2 mg/g food; po; started 3 days before and 72 h post LPS challenge) dose-dependently inhibits chemotaxis of $CXCR^{3+}$ T cells in vivo in mouse model[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	LPS challenge model in mice[1]
Dosage:	0.006, 0.02, 0.06, 0.2, 0.6, and 2 mg per g of food
Administration:	PO; started 3 days before LPS challenge and continued up to the end of the study (72 h post LPS challenge)
Result:	Reduced the number of BAL CD^{8+} T cells in a dose-dependent manner.

REFERENCES

[1]. Meyer EA, et al. Discovery of Clinical Candidate ACT-777991, a Potent CXCR3 Antagonist for Antigen-Driven and Inflammatory Pathologies. J Med Chem. 2023 Mar 23;66(6):4179-4196.

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

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