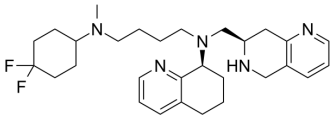
CXCR4 antagonist 4

Cat. No.:	HY-144285
CAS No.:	2761009-30-5
Molecular Formula:	$C_{29}H_{41}F_2N_5$
Molecular Weight:	497.67
Target:	CXCR; HIV
Pathway:	GPCR/G Protein; Immunology/Inflammation; Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

CXCR4 antagonist 4 is a potent, orally active CXCR4 antagonist (IC_{50}=24 nM) with diminished CYP 2D6 activity, improved PAMPA permeability, potent inhibition of human immunodeficiency virus entry (IC_{50}=7 nM)[1].

IC_{50} & Target

CXCR4	HIV
24 nM (IC_{50})	7 nM (IC_{50})

In Vitro

CXCR4 antagonist 4 (Compound 30, 0.1~10 μM, 48 hours) displays the inhibition potencies against the X4 virus in TZM-bl cells (IC_{50}=7 nM) [1].

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

Cell Cytotoxicity Assay[1]

Cell Line:	TZM-bl cells
Concentration:	0.1, 1, 10 μM
Incubation Time:	48 hours
Result:	Displayed inhibition potencies against the X4 virus (IC_{50}=7 nM)

In Vivo

CXCR4 antagonist 4 (3, 10, 30 mg/kg) demonstrates better oral Bioavailability in a dose dependent and reached 27% for the 30 mg/kg[1].Pharmacokinetic Parameters of CXCR4 antagonist 4 in mice[1].

Route	Dose(mg/kg)	$T_{1/2}$(h)	C_{max}(ng/mL)	C_{12h} (ng/mL)	AUC_{0-8h} (h*ng/mL)	% F_{PO} (0-8 h)	Cl (L/h/kg)	V_d (L/kg)
iv	3	5.89	116		265		11.3	96.3
po	3		12.8	1.50	34.3	12.9		
po	10		54.8	14.3	190	215		

po	30	169	34.8	717	27.1

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Animal Model:	mice[1]
Dosage:	3, 10, 30 mg/kg
Administration:	
Result:	Demonstrated better oral bioavailability in a dose dependent and reached 27% for the 30 mg/kg.

REFERENCES

[1]. Jecs E, et al. Synthesis and Evaluation of Novel Tetrahydronaphthyridine CXCR4 Antagonists with Improved Drug-like Profiles. J Med Chem. 2022, 65(5):4058-4084.

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

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA