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Lieferung & Zahlungsart

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Zuschläge

- Mindermengenzuschlag
- Trockeneiszuschlag
- Gefahrgutzuschlag
- Expressversand

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CXCR4-IN-3

Cat. No.: HY-161735

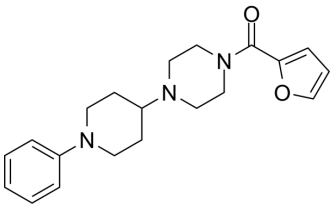
Molecular Formula: $C_{20}H_{25}N_3O_2$

Molecular Weight: 339.43

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

CXCR4-IN-3 (compound XVI) is an orally active and potent inhibitor targeting the inflammation-related receptor CXCR4, with an IC_{50} of 3.2 nM. CXCR4-IN-3 exhibits potent antichemotactic activity, at 79.19±2.33% inhibition. CXCR4-IN-3 shows anti-inflammatory activity. CXCR4-IN-3 can be used for IBD (inflammatory bowel disease) research[1].

IC_{50} & Target

CXCR4
3.2 nM (IC_{50})

In Vivo

CXCR4-IN-3 (compound XVI) (25 mg/kg, IG, twice a day for 14 consecutive days) alleviates DSS (dextran sulfate sodium)-induced IBD (inflammatory bowel disease) and is associated with reduced numbers of inflammatory cells and reduced secretion of inflammatory factors[1].

CXCR4-IN-3 (iv (2 mg/kg) ig (20 mg/kg); once) shows reasonable pharmacokinetic properties[1].

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

Animal Model:	Male C57BL/6 mice (8 weeks, n=8 per group, DSS-Induced Colitis Model)[1]
Dosage:	25 mg/kg
Administration:	Intragastrically, 100 μL/10 g, twice a day for 14 consecutive days
Result:	Markedly relieved the condition of IBD; Significantly decreased the myeloperoxidase (MPO) levels; Blocked chronic inflammation of the intestinal tract.

Animal Model:	Male Sprague-Dawley rats[1]
Dosage:	iv (2 mg/kg) ig (20 mg/kg)
Administration:	IV or IG, once (Pharmacokinetic Analysis)
Result:	Pharmacokinetic Parameters of CXCR4-IN-3 in male Sprague-Dawley rats[1].

	IV (2 mg/kg)	IG (20 mg/kg)

T_{max} (h)	0.08	0.25
$t_{1/2}$ (h)	0.81±0.10	1.71±0.08
C_{max} (ng/mL)	351.42±18.92	1436.41±805.36
AUC_{0-t} (ng/mL*h)	330.37±22.00	3010.81±283.96
$AUC_{0-\infty}$ (ng/mL*h)	340.29±26.61	3070.77±325.73
CL (mL/h/kg)	5901.52±463.48	6565.45±741.43
V (mL/kg)	6037.79±278.59	16161.66±1798.44
F (%)		91.14

REFERENCES

[1]. Jiang X, et al. Synthetically Feasible De Novo Molecular Design of Leads Based on a Reinforcement Learning Model: AI-Assisted Discovery of an Anti-IBD Lead Targeting CXCR4. J Med Chem. 2024 Jun 27;67(12):10057-10075.

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