CCR5 antagonist 3

Cat. No.: HY-152132

CAS No.: 1800570-92-6

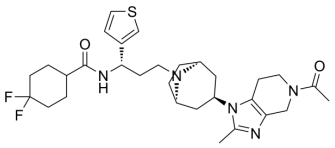
Molecular Formula: $C_{30}H_{41}F_2N_5O_2S$

Molecular Weight: 573.74

Target: CCR; 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

CCR5 antagonist 3 (Compound 26) is a CCR5 antagonist with an IC_{50} of 15.90 nM. CCR5 antagonist 3 shows broad-spectrum anti-HIV-1 activities[1].

IC_{50} & Target

CCR5	HIV-1
15.90 nM (IC_{50})	0.010 μM (EC50, In TZM-bl cells)

In Vitro

CCR5 antagonist 3 (Compound 26) (48 h) shows excellent HIV-1 inhibitory activity with an EC_{50} of 0.010 ± 0.004 μM in TZM-bl cells[1].

CCR5 antagonist 3 (48 h) shows antiviral activities with an EC_{50} of 2.71 ± 0.34 nM against CCR5-tropic integrase inhibitor resistant strain HIV-$1_{YU\text{-}2(G140S/Q148H)}$ in TZM-bl cells[1].

CCR5 antagonist 3 shows HIV-1 inhibitory activity with EC_{50}s of 2.89, 5.26, 7.64, 9.96 and 19.01 nM against HIV-1 strains YU-2, KIZ001, SF162, Ba-L and KIZ006 respectively[1].

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

In Vivo

PK Properties of CCR5 antagonist 3 (Compound 26) in SD Rats[1]

compd	admin	dose (mg/kg)	C_{max} (ng/mL)	T_{max} (h)	$T_{1/2}$ (h)	AUC_{0-last} (ng·h/mL)	$AUC_{0-\infty}$ (ng·h/mL)	MRT (h)	CL (mL/min/kg)	F (%)
CCR5 antagonist 3	p.o.	10	66.4 ± 64.0	2.67 ± 1.15	6.44 ± 2.10	249 ± 149	270 ± 145	9.16 ± 4.17	–	11.9
	i.v.	2	–	–	3.34 ± 1.55	420 ± 36	426 ± 34	2.43 ± 0.74	78.7 ± 6.6	

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

Animal Model:	SD rats[1]
Dosage:	2 mg/kg and 10 mg/kg
Administration:	Intravenous and oral administration (Pharmacokinetic Analysis)

Result:	Displayed good PK profiles.

REFERENCES

[1]. Xie X, et al. Structure-Based Design of Tropane Derivatives as a Novel Series of CCR5 Antagonists with Broad-Spectrum Anti-HIV-1 Activities and Improved Oral Bioavailability. J Med Chem. 2022 Dec 22;65(24):16526-16540.

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