CCR5 antagonist 2

Cat. No.: HY-152131

CAS No.: 1800570-93-7

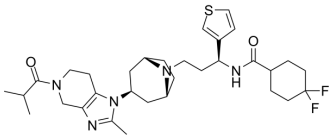
Molecular Formula: $C_{32}H_{45}F_2N_5O_2S$

Molecular Weight: 601.79

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 2 (Compound 25) is a CCR5 antagonist with an IC_{50} of 8.34 nM. CCR5 antagonist 2 shows broad-spectrum anti-HIV-1 activities[1].

IC_{50} & Target

CCR5	HIV-1
8.34 nM (IC_{50})	11 nM (EC50, TZM-bl cell)

In Vitro

CCR5 antagonist 2 (Compound 25) (48 h) shows excellent HIV-1 inhibitory activity with an EC_{50} of 0.011 ± 0.002 μM in TZM-bl cells[1].

CCR5 antagonist 2 (48 h) shows antiviral activities with an EC_{50} of 4.34 ± 1.61 nM against CCR5-tropic integrase inhibitor resistant strain HIV-$1_{YU\text{-}2(G140S/Q148H)}$ in TZM-bl cells[1].

CCR5 antagonist 2 shows HIV-1 inhibitory activity with EC_{50}s of 7.82, 8.73, 12.61, 15.99 and 16.93 nM against HIV-1 strains KIZ001, YU-2, KIZ006, SF162 and Ba-L, respectively[1].

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

In Vivo

PK Properties of CCR5 antagonist 2 (Compound 25) 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 2	p.o.	10	49.5 ± 18.6	2.0 ± 0.0	10.3 ± 2.5	229 ± 92	283 ± 105	13.2 ± 4.2	–	15.7
	i.v.	2	–	–	1.60 ± 0.03	291 ± 75	298 ± 76	1.81 ± 0.04	117 ± 29	

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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