HIV-1 inhibitor-49

Cat. No.: HY-151933

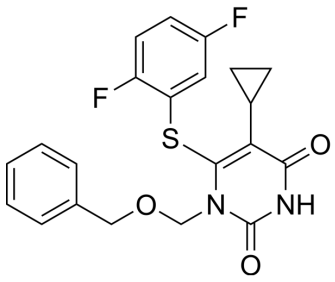
Molecular Formula: $C_{21}H_{18}F_2N_2O_3S$

Molecular Weight: 416.44

Target: HIV; Reverse Transcriptase

Pathway: Anti-infection

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

HIV-1 inhibitor-49 is an orally active HIV-1 inhibitor, is a HEPT analog. HIV-1 inhibitor-49 possesses great pharmacokinetics profiles and potent non-nucleoside reverse transcriptase inhibitory activity (IC_{50}=30 nM). HIV-1 inhibitor-49 exerts potential safety without acute toxicity in mouse model[1].

IC_{50} & Target

HIV-1 (WT)	HIV-1 (L100I)	HIV-1 (K103N)	HIV-1 (Y181C)
17 nM (EC50)	0.38 μM (EC50)	2.64 μM (EC50)	1.85 μM (EC50)

HIV-1 (E138K)
0.09 μM (EC50)

In Vitro

HIV-1 inhibitor-49 (compound 9h) (EC_{50}=17 nM-39.21 μM) inhibits WT HIV-1 with much higher selectivity index over other HIV-1 mutant (L100I, K103N, Y181C, and E138K)[1].

HIV-1 inhibitor-49 (0-50 μM) shows little CYP enzyme, hERG inhibition in CHO-hERG cells, with IC_{50}s of 27.6 μM (CYP2C9), 30.3 μM (CYP2C19), and >50 μM (others)[1].

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

In Vivo

HIV-1 inhibitor-49 (compound 9h) (1000 mg/kg; i.g.; single dose) does not induce mice death and obvious pathological damage in healthy mouse model[1].

HIV-1 inhibitor-49 (10 mg/kg; p.o.; single dose) shows excellent oral bioavailability in rats[1].

Rat PK profile[1]

Route	Dose (mg/kg)	AUC_{0-t} (ng·h/mL)	$AUC_{0-\infty}$ (ng·h/mL)	$T_{1/2}$ (h)	T_{max} (h)	V_z (mL/kg)	Cl (mL/h/kg)	C_{max} (ng/mL)	F (%)
i.v.	1.0	1102	1100	0.514	0.083	698	936	2033	
p.o.	10	9557	8663	2.51	0.583			3523	86.72%

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

REFERENCES

[1]. Zhou RL, et al. Structure-guided design of novel HEPT analogs with enhanced potency and safety: From Isopropyl-HEPTs to Cyclopropyl-HEPTs. Eur J Med Chem. 2022 Nov 24;246:114939.

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