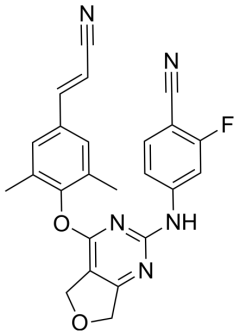
HIV-1 inhibitor-50

Cat. No.:	HY-152160
CAS No.:	2834087-69-1
Molecular Formula:	$C_{24}H_{18}FN_5O_2$
Molecular Weight:	427.43
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 invistor-50 is a non-nucleoside reverse transcriptase inhibitor (NNRTI) that targets HIV-1 reverse transcriptase (RT) (IC_{50}=50 nM). HIV-1 inhibitor-50 shows significant antiviral activity, with EC_{50}s of 2.22-53.3nM against HIV-1 IIIB and its mutant strains[1].

IC_{50} & Target

HIV-1 (WT) 3.04 nM (EC50)	HIV-1 (L100I) 3.04 nM (EC50)	HIV-1 (K103N) 2.87 nM (EC50)	HIV-1 (Y181C) 10.2 nM (EC50)
HIV-1 (Y188L) 13.2 nM (EC50)	HIV-1 (E138K) 9.77 nM (EC50)	HIV-1 (F227L+V106A) 19.8 nM (EC50)	

In Vitro

HIV-1 inhibitor-50 (compound 36a) protects MT-4 cells from HIV-1 IIIB and RES056 with EC_{50}s of 2.22 nM and 53.3 nM, respectively[1].

HIV-1 inhibitor-50 inhibits MT-4 cells viability with an CC_{50} value of 45.6 μM[1].

HIV-1 inhibitor-50 (hydrochloride;) shows a lower intrinsic clearance rates in microsomes (CL=87.6 μL/min/mg) and liver (CL=16.6 μL/min/mg), and leads to a higher metabolic stability ($T_{1/2}$=11.3 min)[1].

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

Cell Viability Assay[1]

Cell Line:	MT-4 cells
Concentration:	
Incubation Time:	
Result:	Inhibited HIV-1 infection in MT-4 cells with EC_{50} values of 3.04 nM (L100I), 2.87 nM (K103N), 10.2 nM (Y181C), 13.2 nM (Y188L), 9.77 nM (E138K), 19.8 nM (F227L+V106A), respectively.

In Vivo

HIV-1 inhibitor-50 (compound 36a) (hydrochloride; 2 mg/kg; i.v.; single dose) has a high clearance (CL=103 L/h/kg) and a modest half-life ($T_{1/2}$=1.43 h)[1].

HIV-1 inhibitor-50 (hydrochloride; 2000 mg/kg; p.o.; single dose) doesn't result any abnormal behaviors or significant changes in body weight compared with the control in 7 days, indicating no acute toxicity[1].

Pharmacokinetic Analysis[1]

Route	Dose (mg/kg)	$T_{1/2}$ (h)	T_{max} (h)	C_{max} (ng/mL)	AUC_{0-t} (h·ng/mL)	$AUC_{0-\infty}$ (h·ng/mL)	CL (L/h/kg)	F (%)
i.v.	2	1.43	0	484	250	255	103	/
p.o.	10	5.12	0.25	37.5	107	154	/	12.1

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

REFERENCES

[1]. Sun Y, et al. Lead Optimization and Avoidance of Metabolic-perturbing Motif Developing Novel Diarylpyrimidines as Potent HIV-1 NNRTIs. J Med Chem. 2022 Dec 8;65(23):15608-15626.

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