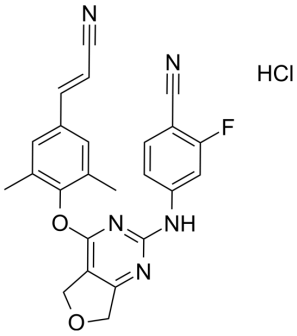
HIV-1 inhibitor-51

Cat. No.:	HY-152161
CAS No.:	2834087-82-8
Molecular Formula:	$C_{24}H_{19}ClFN_5O_2$
Molecular Weight:	463.89
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-51, a non-nucleoside reverse transcriptase inhibitor (NNRTI), exhibits outstanding antiviral activity against WT HIV-1 (IIIB) and a panel of mutant strains. HIV-1 inhibitor-51 has high binding affinity (K_D=2.50 μM) and inhibitory activity (IC_{50}=0.03 μM) to WT HIV-1 RT. HIV-1 inhibitor-51 has EC_{50}s of 2.22-53.3 nM for mutant strains (L100I, K103N, Y181C, Y188L, E138K, F227L + V106A, RES056)[1].

IC_{50} & Target

HIV-1 (WT) 0.03 μM (IC_{50})	HIV-1 (WT) 2.5 μM (Kd)	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)
HIV-1 (RES056) 53.3 nM (EC50)			

In Vivo

HIV-1 inhibitor-51 (compound 36a·HCl; 2 mg/kg; iv) has a $T_{1/2}$ of 1.43 hours, a CL of 103 L/h·kg, and C_{max} of 484 ng/mL[1].
HIV-1 inhibitor-51 (10 mg/kg; orally) has a $T_{1/2}$ of 5.12 hours, and C_{max} of 37.5 ng/mL[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	ICR mice[1]
Dosage:	2 mg/kg (Pharmacokinetic Analysis)
Administration:	IV
Result:	Had a $T_{1/2}$ of 5.12 hours, and C_{max} of 37.5 ng/mL.

REFERENCES

[1]. Yanying Sun, 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.

Caution: Product has not been fully validated for medical applications. For research use only.

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