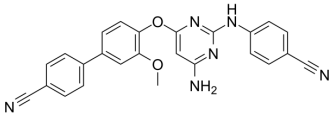
HIV-1 inhibitor-40

Cat. No.:	HY-147807
CAS No.:	2789676-44-2
Molecular Formula:	$C_{25}H_{18}N_6O_2$
Molecular Weight:	434.45
Target:	HIV; Cytochrome P450
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	HIV-1 inhibitor-40 (Compound 4ab) is a non-nucleoside reverse transcriptase inhibitor (NNRTI) of HIV-1 with an EC_{50} of 1.9 nM. HIV-1 inhibitor-40 displays weak CYP sensitivity with IC_{50} values of 5.16 μM and 4.51 μM against CYP2C9 and CYP2C19, respectively. HIV-1 inhibitor-40 has no apparent in vivo acute toxicity[1].			
IC_{50} & Target	HIV-1 (WT) 1.9 nM (EC50)	HIV-1 (K103N) 0.004 μM (EC50)	HIV-1 (E138K) 0.009 μM (EC50)	HIV-1 (L100I) 0.019 μM (EC50)
	HIV-1 (Y181C) 0.029 μM (EC50)	HIV-1 (Y188L) 0.570 μM (EC50)	CYP2C19 4.51 μM (IC_{50})	CYP2C9 5.16 μM (IC_{50})
In Vitro	HIV-1 inhibitor-40 (Compound 4ab) displays inhibitory activity with EC_{50} values of 0.019 ± 0.005, 0.004 ± 0.001, 0.029 ± 0.007, 0.570 ± 0.099 and 0.009 ± 0.006 μM against L100I, K103N, Y181C, Y188L and E138K HIV-1 mutant strains, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.			

REFERENCES

[1]. Jin X, et al. Structure-Based Discovery of Novel NH2-Biphenyl-Diarylpyrimidines as Potent Non-Nucleoside Reverse Transcriptase Inhibitors with Significantly Improved Safety: From NH2-Naphthyl-Diarylpyrimidine to NH2-Biphenyl-Diarylpyrimidine. J Med Chem. 2022 Jun 23;65(12):8478-8492.

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