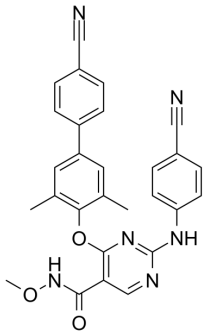
NNRT-IN-1

Cat. No.:	HY-149928
CAS No.:	2925364-09-4
Molecular Formula:	$C_{28}H_{22}N_6O_3$
Molecular Weight:	490.51
Target:	HIV
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	NNRTIs-IN-1 is a potent non-nucleoside reverse transcriptase inhibitor featuring significantly anti-resistance efficacy. NNRTIs-IN-1 inhibits the wild-type HIV-1 and five mutant strains with EC_{50}s in the nanomolar range. NNRTIs-IN-1 displays favorable pharmacokinetic properties[1].
In Vitro	NNRTIs-IN-1 (compound 8r) inhibits the wild-type HIV-1 (EC_{50}=2.3 nM) and five mutant strains, K103N (EC_{50}=8 nM), E138K (EC_{50}=6 nM), double-digit potency against L100I (EC_{50}=13 nM), Y181C (EC_{50}=29 nM), and Y188L (EC_{50}=52 nM)[1]. NNRTIs-IN-1 shows no apparent inhibitory effect on CYP1A2, CYP2D6, CYP3A4-T, and CYP3A4-M with IC_{50} values over 50 μM, and exhibits extremely weak activity toward RPV-sensitive CYP2C9 and CYP2C19 subtypes (IC_{50}=18.5 and 23.6 μM)[1]. NNRTIs-IN-1 displays very weak inhibition of hERG (IC_{50}>40 μM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	NNRTIs-IN-1 (1 mg/kg; i.v.) exhibits a favorable half-life of 3.66 h and a mean residence time (MRT) of 3.75 h, and the maximal concentration (C_{max}) is up to 431 ng/mL[1]. NNRTIs-IN-1 (5 mg/kg; p.o.) exhibits a half-life of 5.18 h, a MRT of 5.21 h, a C_{max} value of 616 ng/mL, and the oral bioavailability (F) of 31.19%[1]. NNRTIs-IN-1 (p.o.) is well tolerated at a dose of 2 g/kg[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Sang YL, et, al. Fragment Hopping-Based Design of Novel Biphenyl-DAPY Derivatives as Potent Non-Nucleoside Reverse Transcriptase Inhibitors Featuring Significantly Improved Anti-Resistance Efficacy. J Med Chem. 2023 Apr 13;66(7):4755-4767.

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