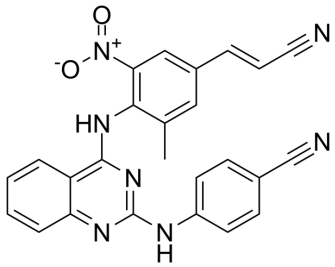
Reverse transcriptase-IN-1

Cat. No.:	HY-130241
CAS No.:	2380001-43-2
Molecular Formula:	$C_{25}H_{17}N_7O_2$
Molecular Weight:	447.45
Target:	HIV
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 12.5 mg/mL (27.94 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2349 mL	11.1744 mL	22.3489 mL
	5 mM	0.4470 mL	2.2349 mL	4.4698 mL
	10 mM	0.2235 mL	1.1174 mL	2.2349 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.25 mg/mL (2.79 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 1.25 mg/mL (2.79 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Reverse transcriptase-IN-1 (Compound 12z), a diarylbenzopyrimidine (DABP) analogue, is a potent, orally active HIV-1 nonnucleoside reverse transcriptase inhibitor. Reverse transcriptase-IN-1 has antiviral activity with EC_{50} values of 3.4 nM, 4.3 nM and 3.6 nM for HIV-1 III_B, E138K and K103N mutants, respectively. Reverse transcriptase-IN-1 also has an $IC_{50}$of 13.7 nM against HIV-1 reverse transcriptase enzyme[1].

IC_{50} & Target

HIV-1

In Vivo

The oral bioavailability of Reverse transcriptase-IN-1 (Compound 12z) is significantly improved to 16.5% at a dose of 5 mg/kg in rats. The intrinsic rat microsome clearance of Reverse transcriptase-IN-1 is 33.2 μL/min/mg proteins. The PK study and safety assessment of Reverse transcriptase-IN-1 shows that it is absorbed with mean residence times (MRTs) of 11.8 hours (5 mg/kg, p.o.) and 11.4 hours (1 mg/kg, i.v.) at these two doses. The C_{max} of Reverse transcriptase-IN-1 is 39.9 ng/mL at a dose

of 5 mg/kg. A single-dose toxicity test of Reverse transcriptase-IN-1 in rats shows no mortality, and there is no abnormal body weight decrease in the animals in the week following an intragastrical dose at 293 mg/kg body weigh. The above results indicate that Reverse transcriptase-IN-1 could be an orally bioavailable candidate for human HIV-1 infection research [1].

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

REFERENCES

[1]. Han S, et al. Molecular Hybridization-Inspired Optimization of Diarylbenzopyrimidines as HIV-1 Nonnucleoside Reverse Transcriptase Inhibitors with Improved Activity against K103N and E138K Mutants and Pharmacokinetic Profiles. ACS Infect Dis. 2019 Oct 24.

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