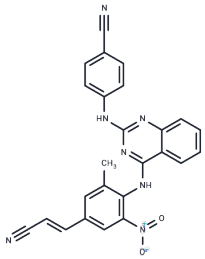
Data Sheet (Cat.No.T12715)

TargetMol

Reverse transcriptase-IN-1

Chemical Properties



CAS No. : 2380001-43-2

Formula: C25H17N7O2

Molecular Weight: 447.45

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Reverse transcriptase-IN-1 is a diarylbenzopyrimidine (DABP) analogue and a potent inhibitor of HIV-1 nonnucleoside reverse transcriptase with an IC50of 13.7 nM.
Targets(IC50)	HIV Protease
In vitro	Reverse transcriptase-IN-1 has antiviral activity with EC50 values of 3.4 nM, 4.3 nM and 3.6 nM for HIV-1 IIIB, E138K and K103N mutants, respectively[1].
In vivo	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 Cmax of Reverse transcriptase-IN-1 is 39.9 ng/mL at a dose of 5 mg/kg. The oral bioavailability of Reverse transcriptase-IN-1 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[1].

Solubility Information

Solubility	DMSO: 12 mg/mL (26.82 mM),Sonication and heating to 60°C are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (2.23 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2349 mL	11.1744 mL	22.3489 mL
5 mM	0.447 mL	2.2349 mL	4.4698 mL
10 mM	0.2235 mL	1.1174 mL	2.2349 mL
50 mM	0.0447 mL	0.2235 mL	0.447 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.