HIV-1 inhibitor-8

Cat. No.: HY-132291

CAS No.: 2826996-78-3

Molecular Formula: $C_{25}H_{21}N_5OS$

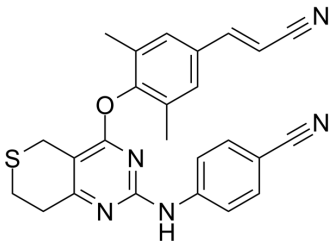
Molecular Weight: 439.53

Target: HIV

Pathway: Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (113.76 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2752 mL	11.3758 mL	22.7516 mL
	5 mM	0.4550 mL	2.2752 mL	4.5503 mL
	10 mM	0.2275 mL	1.1376 mL	2.2752 mL

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

BIOLOGICAL ACTIVITY

Description

HIV-1 inhibitor-8 is an orally active, low-toxicity and potent HIV-1 non-nucleoside reverse transcriptase inhibitor (NNRTI). HIV-1 inhibitor-8 yields exceptionally potent antiviral activities (EC_{50}=4.44~54.5 nM) against various HIV-1 strains. The IC_{50} of HIV-1 inhibitor-8 against WT HIV-1 reverse transcriptase is 0.081 μM[1].

IC_{50} & Target

HIV-1 (WT)
0.081 μM (IC_{50})

In Vitro

HIV-1 inhibitor-8 yields exceptionally potent antiviral activities (EC_{50}=4.44~54.5 nM) against various HIV-1 strains and improves resistance profiles (RF = 0.5~5.6). HIV-1 inhibitor-8 exhibits reduces cytotoxicity (CC_{50}=284 μM) and higher SI values (SI = 5210~63992). HIV-1 inhibitor-8 displays better solubility (sol. =12.8 μg/mL) and no significant inhibition of the main CYP enzymes. HIV-1 inhibitor-8 displays an extremely low hERG inhibition with an IC_{50} value of 19.84 μM in CHO-hERG cells.
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

HIV-1 inhibitor-8 (2 mg/kg; i.v.) shows a favorable mean CL, volume of distribution and a long terminal half-life[1].
HIV-1 inhibitor-8 (20 mg/kg; p.o.) absorption reaches maximum at 0.25 hours with a plasma concentration value of 16.6

ng/mL and the mean residence time is 2.90 hours[1].

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

Animal Model:	Sprague-Dawley (SD) rat[1]
Dosage:	2 mg/kg
Administration:	I.v.
Result:	Showed a favorable mean CL, volume of distribution and a long terminal half-life.

Animal Model:	Sprague-Dawley (SD) rat[1]
Dosage:	20 mg/kg
Administration:	P.o.
Result:	Absorption reached maximum at 0.25 hours with a plasma concentration value of 16.6 ng/mL and the mean residence time was 2.90 hours.

REFERENCES

[1]. Wang Z, et al. Discovery of Novel Dihydrothiopyrano[4,3-d]pyrimidine Derivatives as Potent HIV-1 NNRTIs with Significantly Reduced hERG Inhibitory Activity and Improved Resistance Profiles [published online ahead of print, 2021 Aug 25]. J Med Chem. 2021;10.1021/acs.jmedchem.1c01015.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA