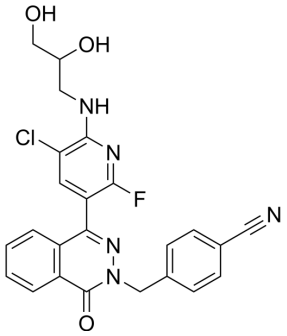
HBV-IN-4

Cat. No.:	HY-131343
CAS No.:	2305897-84-9
Molecular Formula:	$C_{24}H_{19}ClFN_5O_3$
Molecular Weight:	479.89
Target:	HBV; DNA/RNA Synthesis
Pathway:	Anti-infection; Cell Cycle/DNA Damage
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 : 100 mg/mL (208.38 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0838 mL	10.4191 mL	20.8381 mL
	5 mM	0.4168 mL	2.0838 mL	4.1676 mL
	10 mM	0.2084 mL	1.0419 mL	2.0838 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: ≥ 2.5 mg/mL (5.21 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.21 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.21 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

HBV-IN-4, a phthalazinone derivative, is a potent and orally active HBV DNA replication inhibitor with an IC_{50} of 14 nM. HBV-IN-4 induces the formation of genome-free capsids and has potent anti-HBV potencies[1].

IC_{50} & Target

IC50: 14 nM (HBV DNA replication)[1]

In Vitro

HBV-IN-4 (compound 19f; 0-1 μM; 8 days) treatment inhibits the various forms (relaxed circular [rc] and single-stranded [ss] HBV DNA) in a dose-dependent manner in HepG2.2.15 cells. HBV-IN-4 treatment could also reduce capsidassociated DNAs

	dose-dependently. HBV-IN-4 could induce the formation of genome-free capsids, including a phenotype of faster-migrating ones[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	HBV-IN-4 (Compound 19f; 50-150 mg/kg; oral administration; twice a day; for 4 weeks; Balb/c male mice) treatment achieves 2.67 log viral load reduction in AAV-HBV/mouse model[1]. HBV-IN-4 (compound 19f) exhibits favorable drug characteristics with low plasma clearance (CL=4.1 mL/min/kg), excellent drug exposure (AUC_{0-t}=49 744 h•ng/L), $T_{1/2}$ (2.15 hours) and oral bioavailability (F=60.4%) using 20 mg/kg oral administration in mice. HBV-IN-4 also shows good distribution in liver exposure[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Balb/c male mice (8-week-old) injected with a recombinant adenoassociated virus (AAV[1]
Dosage:	50 mg/kg, 150 mg/kg
Administration:	Oral administration; twice a day; for 4 weeks
Result:	Resulted in a 2.67 log reduction of the HBV DNA viral load during a 4-week treatment.

REFERENCES

[1]. Wuhong Chen, et al. Discovery of Phthalazinone Derivatives as Novel Hepatitis B Virus Capsid Inhibitors. J Med Chem. 2020 Jul 21.

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