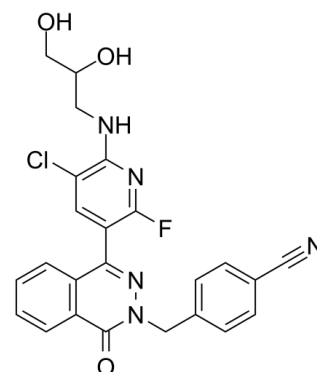


Data Sheet

Product Name:	HBV-IN-4
Cat. No.:	CS-0133443
CAS No.:	2305897-84-9
Molecular Formula:	C ₂₄ H ₁₉ ClFN ₅ O ₃
Molecular Weight:	479.89
Target:	DNA/RNA Synthesis; HBV
Pathway:	Anti-infection; Cell Cycle/DNA Damage
Solubility:	DMSO : 100 mg/mL (208.38 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

HBV-IN-4, a phthalazinone derivative, is a potent and orally active **HBV DNA replication** inhibitor with an **IC₅₀** of 14 nM. HBV-IN-4 induces the formation of genome-free capsids and has potent anti-**HBV** potencies^[1]. IC₅₀ & 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 capsid-associated DNAs dose-dependently. HBV-IN-4 could induce the formation of genome-free capsids, including a phenotype of faster-migrating ones^[1]. **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].

References:

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

CAIndexNames:

Benzonitrile, 4-[[4-[5-chloro-6-[(2,3-dihydroxypropyl)amino]-2-fluoro-3-pyridinyl]-1-oxo-2(1H)-phthalazinyl]methyl]-

SMILES:

N#CC1=CC=C(CN(N=C(C2=CC(Cl)=C(NCC(O)CO)N=C2F)C3=C4C=CC=C3)C4=O)C=C1

Caution: Product has not been fully validated for medical applications. For research use only.

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