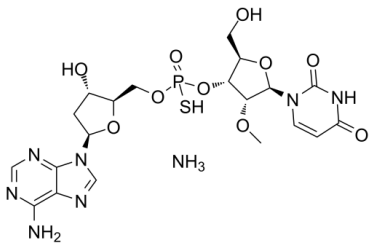
Data Sheet

Product Name:	Inarigivir (ammonium)
Cat. No.:	CS-0203894
CAS No.:	2172788-92-8
Molecular Formula:	$C_{20}H_{29}N_8O_{10}PS$
Molecular Weight:	604.53
Target:	HBV
Pathway:	Anti-infection
Solubility:	H2O : 100 mg/mL (165.42 mM; Need ultrasonic); DMSO : 100 mg/mL (165.42 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Inarigivir (ORI-9020) ammonium is a dinucleotide antiviral drug that can significantly reduce liver **HBV** DNA in transgenic mice expressing hepatitis B virus. Inarigivir (ORI-9020) ammonium acts as a **RIG-I (Retinoic acid-inducible gene-I)** agonist to activate cellular innate immune responses[1][2]. IC50 & Target: Target: HBV[1]. **In Vitro:** Inarigivir (SB 9200) is active against HBV variants carrying resistance markers against all the nucleos(t)ide analogues approved for treating chronic hepatitis B[2]. **In Vivo:** Inarigivir (100 mg/kg/day, ip) significantly reduces viral DNA in the liver and shows anti-HBV activity. Serum HBV DNA is not reduced in response to treatment. Inarigivir does not affect levels of HBV RNA in liver, levels of HBeAg in serum, or mean titers of HBsAg. The minimal effective dose is identified to be between 1.6 and 0.5 mg/kg/day using liver HBV DNA values[1].

References:

[1]. Iyer RP, et al. Anti-hepatitis B virus activity of ORI-9020, a novel phosphorothioate dinucleotide, in a transgenic mouse model. Antimicrob Agents Chemother. 2004 Jun;48(6):2318-20.

[2]. Danni Colledge, et al. The Novel Antiviral Agent Inarigivir Inhibits Both Nucleos(t)ide Analogue and Capsid Assembly Inhibitor Resistant HBV in vitro.

CAIndexNames:

O-(((2R,3S,5R)-5-(6-Amino-9H-purin-9-yl)-3-hydroxytetrahydrofuran-2-yl)methyl) O-((2R,3R,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-2-(hydroxy methyl)-4-methoxytetrahydrofuran-3-yl) S-hydrogen phosphorothioate, ammonia salt

SMILES:

NC1=C(N=CN2[C@@H]3O[C@H](COP(O[C@H]4[C@@H](OC)[C@H](N5C=CC(NC5=O)=O)O[C@@H]4CO)(S)=O)[C@@H](O)C3)C2=NC=N1.N

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