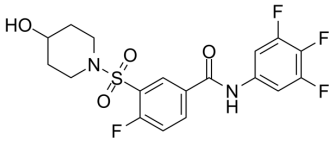
NVR 3-778

Cat. No.:	HY-124600
CAS No.:	1445790-55-5
Molecular Formula:	$C_{18}H_{16}F_4N_2O_4S$
Molecular Weight:	432.39
Target:	HBV
Pathway:	Anti-infection
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (578.18 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3127 mL	11.5636 mL	23.1273 mL
	5 mM	0.4625 mL	2.3127 mL	4.6255 mL
	10 mM	0.2313 mL	1.1564 mL	2.3127 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: ≥ 2.08 mg/mL (4.81 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.81 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.81 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NVR 3-778 is a first-in-Class and oral bioavailable HBV CAM (capsid assembly modulator) belonging to the SBA (sulfamoylbenzamide) class, with anti-HBV activity[1].

IC_{50} & Target

HBV[1]

In Vitro

NVR 3-778 targets HBV core protein and inhibits viral replication[1].
NVR 3-778 inhibits the generation of infectious HBV DNA-containing virus particles with a mean antiviral with an EC_{50} of 0.40 μM in HepG2.2.15 cells[1].

NVR 3-778 exhibits pan-genotypic antiviral activity and a lack of cross-resistance with nucleos(t)ide inhibitors of HBV replication[1].
NVR 3-778 inhibits pregenomic RNA encapsidation, viral replication, and the production of HBV DNA- and HBV RNA-containing particles[1].
NVR 3-778 also inhibits de novo infection and viral replication in primary human hepatocytes with EC_{50}s of 0.81 μM against HBV DNA and between 3.7μM and 4.8 μM against the production of HBV antigens and intracellular HBV RNA[1].
The EC_{50} values of NVR 3-778 are increased by 4.5-, 9.3-, and 15.8-fold in the presence of 10%, 20%, and 40% human serum, respectively[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

NVR 3-778 (1.5 mg/kg; i.g.) displays the mean C_{max} and AUC_{0-inf} values of 0.56 μg/ml and 3.50 μg·h/ml, respectively, in dogs following oral administration. And the mean oral bioavailability is determined to be 84.6%[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Dogs[1]
Dosage:	1.5 mg/kg (Pharmacokinetic Analysis)
Administration:	Oral gavage
Result:	The mean C_{max} and AUC_{0-inf} values are 0.56 μg/ml and 3.50 μg·h/ml and the oral bioavailability is 84.6%.

CUSTOMER VALIDATION

- Anal Methods. 2021 Dec 17.

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REFERENCES

[1]. Lam AM, et al. Preclinical Characterization of NVR 3-778, a First-in-Class Capsid Assembly Modulator against Hepatitis B Virus. Antimicrob Agents Chemother. 2018 Dec 21;63(1).

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

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