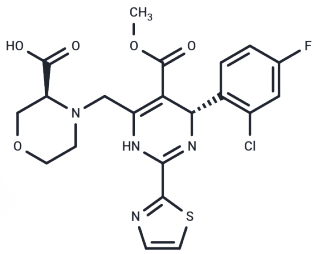
Data Sheet (Cat.No.T9054)

RO6889678

Chemical Properties



CAS No. : 1578153-27-1

Formula: C21H20ClFN4O5S

Molecular Weight: 494.92

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	RO6889678 is HBV inhibitor with a complex ADME profile.
Targets(IC50)	Cytochromes P450,HBV
In vitro	RO6889678, a novel inhibitor of HBV with a complex absorption, distribution, metabolism, and excretion (ADME) profile.?RO6889678 showed an intracellular enrichment of 78-fold in hepatocytes, with an apparent intrinsic clearance of 5.2 l/min per mg protein and uptake and biliary clearances of 2.6 and 1.6 l/min per mg protein, respectively.?When apparent intrinsic clearance was incorporated into a PBPK model, the simulated oral human profiles were in good agreement with observed data at low doses but were underestimated at high doses due to unexpected overproportional increases in exposure with dose.?In addition, the induction potential of RO6889678 on cytochrome P450 (P450) enzymes and transporters at steady state was assessed and cotreatment with ritonavir revealed a complex drug-drug interaction with concurrent P450 inhibition and moderate UDP-glucuronosyltransferase induction.

Solubility Information

Solubility	DMSO: 55 mg/mL (111.13 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.0205 mL	10.1026 mL	20.2053 mL
5 mM	0.4041 mL	2.0205 mL	4.0411 mL
10 mM	0.2021 mL	1.0103 mL	2.0205 mL
50 mM	0.0404 mL	0.2021 mL	0.4041 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Kratochwil N A , Triyatni M , Mueller M B , et al. Simultaneous Assessment of Clearance, Metabolism, Induction and Drug-Drug Interaction Potential using a Long-Term In Vitro Liver Model for a Novel Hepatitis B Virus Inhibitor[J]. Journal of Pharmacology & Experimental Therapeutics, 2018:jpet.117.245712.