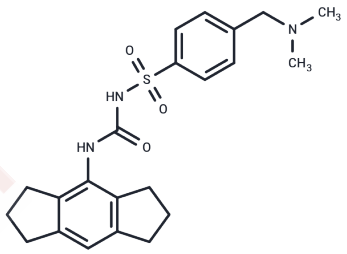
Data Sheet (Cat.No.T79733)

TargetMol

NLRP3-IN-20

Chemical Properties



CAS No. : 2428478-22-0

Formula: C22H27N3O3S

Molecular Weight: 413.53

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	NLRP3-IN-20 is an effective oral inhibitor of NLRP3 inflammatory corpuscles, and the IC_{50} secreted by IL-1β is 25nM. NLRP3-IN-20 showed good pharmacokinetic characteristics, and showed significant pharmacological activities in animal models such as nonalcoholic steatohepatitis, septic shock and colitis.
Targets(IC50)	NOD-like Receptor (NLR)
In vivo	Pharmacokinetic analysis in mice [1] showed that an intravenous (i.v.) administration of the compound at a dose of 5 mg/kg resulted in a half-life (T 1/2) of 4.01 hours, time to peak concentration (T max) of 0.083 hours, peak concentration (C max) of 22567 ng/mL, area under the curve from time zero to infinity (AUC 0-inf) of 130240 ng·h/mL, mean residence time from time zero to infinity (MRT 0-inf) of 5.30 hours, volume of distribution (V z) of 226 mL/kg, clearance (Cl) of 38.8 mL/h/kg, and absolute bioavailability (F) of -%. In contrast, oral administration (p.o.) of a 10 mg/kg dose showed a T 1/2 of 3.50 hours, T max of 0.667 hours, C max of 33867 ng/mL, AUC 0-inf of 221955 ng·h/mL, MRT 0-inf of 4.79 hours, and an F of 85.21%.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4182 mL	12.091 mL	24.182 mL
5 mM	0.4836 mL	2.4182 mL	4.8364 mL
10 mM	0.2418 mL	1.2091 mL	2.4182 mL
50 mM	0.0484 mL	0.2418 mL	0.4836 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

Li Z, et al. Novel Sulfonylurea-Based NLRP3 Inflammasome Inhibitor for Efficient Treatment of Nonalcoholic Steatohepatitis, Endotoxic Shock, and Colitis. J Med Chem. 2023 Sep 28;66(18):12966-12989.

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