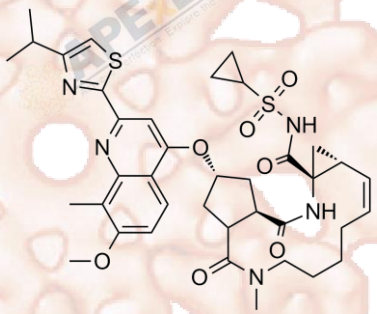
Product Data Sheet

Simeprevir



Cat. No.:	A3820
CAS No.:	923604-59-5
Formula:	C38H47N5O7S2
M.Wt:	749.96
Synonyms:	TMC435,TMC435350,TMC-435350,Simeprevir
Target:	Proteases
Pathway:	HCV Protease
Storage:	Store at -20°C

Solvent & Solubility

In Vitro

insoluble in H2O; insoluble in EtOH; ≥18.75 mg/mL in DMSO

Preparing Stock Solutions

Mass / Solvent / Concentration	1mg	5mg	10mg
1 mM	1.3334 mL	6.6670 mL	13.3340 mL
5 mM	0.2667 mL	1.3334 mL	2.6668 mL
10 mM	0.1333 mL	0.6667 mL	1.3334 mL

Please refer to the solubility information to select the appropriate solvent.

Biological Activity

Shortsummary	Inhibitor of HCV NS3/4A protease
IC_{50} & Target	

In Vitro

Cell Viability Assay

Cell Line:	Huh7-Luc HCV genotype 1b replicon cell line
Preparation method:	The solubility of this compound in DMSO is > 18.8 mg/mL. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below - 20 °C for several months.

	Reacting conditions:	0.1 ~ 1000 nM; 72 hrs
	Applications:	In Huh7-Luc HCV genotype 1b replicon cell line, Simeprevir exhibited dose-dependent inhibitory effects, with the EC50 and EC90 values of 8 nM and 24 nM, respectively. Meanwhile, Simeprevir did not show significant effect on the cellular ribosomal protein RPL13A transcript level. According to the immunoblot analysis of replicon cell lysates collected after 72 hrs, NS5B expression was dose-dependently reduced, but α-tubulin expression was not suppressed.
In Vivo	**Animal experiment**	
	Animal models:	Male SD rats
	Dosage form:	2 mg/kg, i.v. or 20 mg/kg, p.o.
	Applications:	In male SD rats, Simeprevir was well distributed in the liver, with a high liver/plasma ratio after oral administration reaching 32. The T1/2 value for oral administration of Simeprevir was 2.8 hrs. When Simeprevir was given intravenously, Simeprevir showed a low clearance (Cl = 0.505 L/h/kg) associated with a low Vdss (0.490 L/kg).
	Other notes:	Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

Product Citations

1. Lee SH, Moon JS, et al. "HA1077displays synergistic activity with daclatasvir against hepatitis C virus and suppresses the emergence of NS5A resistance-associated substitutions in mice." Sci Rep. 2018 Aug 20;8(1):12469.PMID:30127498

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References

[1]. Lin TI, Lenz O, Fanning G, et al. In vitro activity and preclinical profile of TMC435350, a potent hepatitis C virus protease inhibitor. Antimicrob Agents Chemother, 2009, 53(4): 1377-1385.

[2]. Raboisson P, de Kock H, Rosenquist A, et al. Structure-activity relationship study on a novel series of cyclopentane-containing macrocyclic inhibitors of the hepatitis C virus NS3/4A protease leading to the discovery of TMC435350. Bioorg Med Chem Lett, 2008, 18(17): 4853-4858.

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most APExBIO products are stable

under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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