Simeprevir

Catalog No.C10634 Batch:C1063403

Product Datasheet

Technical Data

Formula	$C_{38}H_{47}N_5O_7S_2$					
Molecular Weight	749.94	**CAS No.**	923604-59-5			
Solubility (25°C)*	In vitro	DMSO	100 mg/mL (133.34 mM)			
		Ethanol	5 mg/mL (6.66 mM)			
		Water	Insoluble			
	In vivo (Add solvents to the product individually and in order)	Oral Administration	Homogeneous suspension	CMC-NA	≥5mg/ml	Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml.
		Injection	Clear solution	5%DMSO [1]→ 40%PEG300 [2]→ 5%Tween80 [3]→ 50%ddH2O Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	0.830mg/ml (1.11mM)	Taking the 1 mL working solution as an example, add 50 μL of 16.6 mg/ml clarified DMSO stock solution to 400 μL of PEG300, mix evenly to clarify it; add 50 μL of Tween80 to the above system, mix evenly to clarify; then continue to add 500 μL of ddH2O to adjust the volume to 1 mL. The mixed solution should be used immediately for optimal results.
			Clear solution	5% DMSO [1]→ 95% Corn oil Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	0.830mg/ml (1.11mM)	Taking the 1 mL working solution as an example, add 50 μL of 16.6 mg/ml clear DMSO stock solution to 950 μL of corn oil and mix evenly. The mixed solution should be used immediately for optimal results.

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

Preparing Stock Solutions

Biological Activity

Description	Simeprevir is a competitive, reversible, macrocyclic, noncovalent **hepatitis C virus (HCV) NS3/4A protease** inhibitor that acts directly against the hepatitis C virus. It has a medium inhibitory concentration (IC50) <13 nM for all HCV NS3/4A enzymes(genotypes 1a, 1b, 2, 4, 5, and 6), but has an IC50 value of 37 nM for genotype 3.
Targets	HCV NS3/4A protease [1]
In vitro	Simeprevir exhibits potent inhibition on NS3/4A protease of genotypes 1a, 1b, 2, 4, 5, and 6, with a medium inhibitory concentration (IC50) <13 nM for all HCV NS3/4A enzymes tested. However, the IC50 for genotype 3 is 37 nM. In vitro, this compound is also an inhibitor of bilirubin transporters OATP1B1 and MRP2. It is a more potent inhibitor of OATP1B1 (IC50=720 nM), which is primarily responsible for transporting unconjugated bilirubin, than MRP2 (IC50 around 10,000 nM), primarily a conjugated bilirubin transporter[1].
In vivo	In vivo, simeprevir has a relatively long absorption phase, reaching maximum concentration (Cmax) after 4-6 hours. It is extensively (99.9%) bound to plasma proteins, mainly to albumin. The absolute bioavailability is 44% after a single oral administration. In rats, the liver to blood ratio is 29:1, which means good distribution to the liver. For humans, in preclinical studies, the liver to plasma concentration ratio is really high (ratio of 39). The highest tissue/plasma AUC ratios are observed in the small intestine (ratio of 128). While tissue concentrations of this compound reach peak values within 4 hours postdosing, its concentrations in liver remain above the EC99 for up to 31 hours postdosing, and plasma concentrations are higher than the EC99 at 8 hours and around the EC50 at 24 hours postdosing. The AUC24h of this chemical is increased by 61%-69% when administered with food. It should therefore be taken with food. This compound is also a substrate and inhibitor of P-glycoprotein. It is metabolized by CYP3A4 and eliminated by biliary excretion. It is also an inhibitor of gut cytochrome 3A4 but not hepatic CYP3A4[1].

References

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4157399/#b20-p…

RETURN POLICY

Capsid Bio's Unconditional Return Policy ensures a smooth online shopping experience for our customers. If you are in any way unsatisfied with your purchase, you may return any item(s) within 7 days of receiving it. In the event of product quality issues, either protocol related or product related problems, you may return any item(s) within 365 days from the original purchase date. Please follow the instructions below when returning products.

SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

EU Headquarters
Gajeva ulica 28, HR-10000 Zagreb, Croatia

US Headquarters
12222 Merit Dr STE 130 Dallas, Texas, 75251

UK Headquarters
121 ABILITY HOUSE, BROOKER ROAD, EN9 1JH, ESSEX

Orders: Sales@capsidbio.com
Enquiries: info@capsidbio.com
www.capsidbio.com