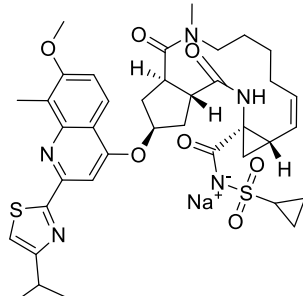


Product data sheet



MedKoo Cat#: 314237 Name: Simeprevir sodium CAS#: 1241946-89-3 (sodium) Chemical Formula: C ₃₈ H ₄₆ N ₅ NaO ₇ S ₂ Molecular Weight: 771.9238		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	
Shipping conditions	Ambient temperature	
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

1. Product description:

Simeprevir, also known as TMC43, is a drug for the treatment and cure of hepatitis C. In the United States, simeprevir is approved by the Food and Drug Administration for use in combination with peginterferon-alfa and ribavirin for hepatitis C and hepatitis B. Simeprevir has been approved in Japan for the treatment of chronic hepatitis C infection, genotype 1.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	30.0	38.86
DMSO:PBS (pH 7.2) (1:2)	0.33	0.43
DMF	30.0	38.86

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.30 mL	6.48 mL	12.95 mL
5 mM	0.26 mL	1.30 mL	2.59 mL
10 mM	0.13 mL	0.65 mL	1.30 mL
50 mM	0.03 mL	0.13 mL	0.26 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

- Librelotto CS, Souza AP, Álvares-DA-Silva MR, Simon D, Dihl RR. Evaluation of the genetic toxicity of sofosbuvir and simeprevir with and without ribavirin in a human-derived liver cell line. *An Acad Bras Cienc.* 2021 Sep 24;93(4):e20200632. doi: 10.1590/0001-3765202120200632. PMID: 34586319.
- Murai K, Shimakami T, Welsch C, Shirasaki T, Liu F, Kitabayashi J, Tanaka S, Funaki M, Omura H, Nishikawa T, Sumiyadorj A, Honda M, Kaneko S. Unexpected Replication Boost by Simeprevir for Simeprevir-Resistant Variants in Genotype 1a Hepatitis C Virus. *Antimicrob Agents Chemother.* 2018 Jun 26;62(7):e02601-17. doi: 10.1128/AAC.02601-17. PMID: 29661883; PMCID: PMC6021633.

In vivo study

- Li Y, She P, Xu L, Liu Y, Liu S, Li Z, Yang Y, Li L, Hussain Z, Wu Y. Anti-hepatitis C virus drug simeprevir: a promising antimicrobial agent against MRSA. *Appl Microbiol Biotechnol.* 2022 Apr;106(7):2689-2702. doi: 10.1007/s00253-022-11878-2. Epub 2022 Mar 26. PMID: 35338386.
- Muturi E, Hong W, Li J, Yang W, He J, Wei H, Yang H. Effects of simeprevir on the replication of SARS-CoV-2 in vitro and in transgenic hACE2 mice. *Int J Antimicrob Agents.* 2022 Jan;59(1):106499. doi: 10.1016/j.ijantimicag.2021.106499. Epub 2021 Dec 17. PMID: 34929295; PMCID: PMC8679493.

Product data sheet



7. Bioactivity

Biological target:

Simeprevir is a potent NS3/4A protease inhibitor.

In vitro activity

Simeprevir demonstrated genotoxic effects in HepG2 cells; the highest concentration of simeprevir exhibited cytotoxicity. Simeprevir increased micronuclei frequency at higher concentrations. Combinations with ribavirin showed significant results for both simeprevir and sofosbuvir. Interestingly, the combination index indicated antagonism, suggesting a reduction in the genotoxic effects of ribavirin when combined with sofosbuvir or simeprevir.

Reference: An Acad Bras Cienc. 2021 Sep 24;93(4):e20200632. <https://pubmed.ncbi.nlm.nih.gov/34586319/>

In vivo activity

The results of this study imply that simeprevir does not inhibit SARS-CoV-2 in vivo. In a transgenic hACE2 mouse model of SARS-CoV-2 infection, intraperitoneal administration of simeprevir for 3 consecutive days failed to suppress viral replication.

Reference: Int J Antimicrob Agents. 2022 Jan;59(1):106499. <https://pubmed.ncbi.nlm.nih.gov/34929295/>

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.