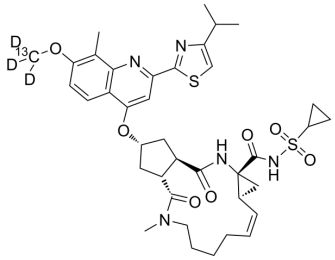
Simeprevir-$^{13}C,d_3$

Cat. No.:	HY-10241S
Molecular Formula:	$C_{37}{}^{13}CH_{44}D_3N_5O_7S_2$
Molecular Weight:	753.95
Target:	HCV Protease; SARS-CoV; HCV; DNA/RNA Synthesis; Isotope-Labeled Compounds
Pathway:	Anti-infection; Metabolic Enzyme/Protease; Cell Cycle/DNA Damage; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Simeprevir-$^{13}C,d_3$ is the ^{13}C- and deuterium labeled Simeprevir. Simeprevir is an oral, potent and highly specific hepatitis C virus (HCV) NS3/4A protease inhibitor with a Ki of 0.36 nM. Simeprevir inhibits HCV replication with an EC50 of 7.8 nM. Simeprevir also potently suppresses SARS-CoV-2 replication and synergizes with Remdesivir. Simeprevir inhibits the main protease (Mpro) and the RNA-dependent RNA polymerase (RdRp) of SARS-CoV-2, and also modulates host immune responses[1][2][5].
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Lo HS, et al. Simeprevir Potently Suppresses SARS-CoV-2 Replication and Synergizes with Remdesivir. ACS Cent Sci. 2021 May 26;7(5):792-802.

[2]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

[3]. Raboisson P, 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 Sep 1;18(17):4853-8.

[4]. Rajagopalan R, et al. Preclinical Characterization and Human Microdose Pharmacokinetics of ITMN-8187, a Nonmacrocyclic Inhibitor of the Hepatitis C Virus NS3 Protease. Antimicrob Agents Chemother. 2016 Dec 27;61(1). pii: e01569-16.

[5]. Lin TI, et al. In vitro activity and preclinical profile of TMC435350, a potent hepatitis C virus protease inhibitor.Antimicrob Agents Chemother. 2009 Apr;53(4):1377-85. Epub 2009 Jan 26.

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