
Product Data Sheet

Product Name: Simeprevir-13C,d3

Cat. No.: GC64038

Chemical Properties

Cas. No. 923604-59-5

Formula C3713CH44D3N5O7S2

M.Wt 753.95

Solubility DMSO : 14.29 mg/mL (19.05 mM; Need ultrasonic) Storage Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure

Background

Simeprevir-13C,d3 (TMC435-13C,d3) is the 13C- and deuterium labeled Simeprevir. Simeprevir (TMC435) is an oral and potent HCV NS3/4A protease inhibitor with a K_i of 0.36 nM. Simeprevir inhibits HCV replication with an EC_{50} of 7.8 nM[1]. Simeprevir inhibits SARS-CoV-2 3CLpro activity[4].

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].

- [1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother.* 2019;53(2):211-216. [2]. 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. [3]. 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. [4]. Rajagopalan R, et al. Preclinical Characterization and Human Microdose

Caution: Product has not been fully validated for medical applications. For research use only.

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Pharmacokinetics of ITMN-8187, a Nonmacrocytic Inhibitor of the Hepatitis C Virus NS3 Protease. *Antimicrob Agents Chemother.* 2016 Dec 27;61(1). pii: e01569-16.

[5]. Qi Sun, et al. Bardoxolone and bardoxolone methyl, two Nrf2 activators in clinical trials, inhibit SARS-CoV-2 replication and its 3C-like protease. *Signal Transduct Target Ther.* 2021 May 29;6(1):212.

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