

Product Name : Simeprevir

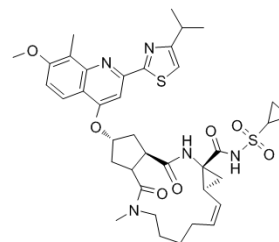
Synonyms : TMC-435; TMC435; TMC435350; TMC-435350

Cat No. : M16618

CAS Number : 923604-59-5

Molecular Formula : C₃₈H₄₇N₅O₇S₂

Formula Weight : 749.94



Chemical Name : Cyclopenta[c]cyclopropa[g][1,6]diazacyclotetradecine-12a(1H)-carboxamide, N-(cyclopropylsulfonyl)-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetradecahydro-2-[[7-methoxy-8-methyl-2-[4-(1-methylethyl)-2-thiazolyl]-4-quinolinyl]oxy]-5-methyl-4,14-dioxo-, (2R,3aR,1

Description : A potent, orally available inhibitor of HCV NS3/4A protease with K_i of 0.36 nM, replicon EC₅₀ of 7.8 nM; inhibits NS3/4A proteases of genotypes 1a and 1b with K_i of 0.5 and 0.4 nM, shows synergistic effect with α-Interferon and an NS5B inhibitor in the replicon model and additive with ribavirin; exerts favorable pharmacokinetic profile and antiviral activity in vivo. HCV Infection Approved

Pathway : Microbiology/Virology

Target : HCV

Receptor : HCV

Solubility : 10 mM in DMSO

SMILES : CC1=C(C=CC2=C1N=C(C=C2OC3CC4C(C3)C(=O)N(CCCCC=CC5CC5(NC4=O)C(=O)NS(=O)(=O)C6CC6)C)C7=NC(=CS7)C(C)C)OC

Storage : (-20°C)

Stability : ≥ 2 years

Reference :

1. Raboisson P, et al. Bioorg Med Chem Lett. 2008 Sep 1;18(17):4853-8. | 2. Lin TI, et al. Antimicrob Agents Chemother. 2009 Apr;53(4):1377-85. | 3. Lenz O, et al. Antimicrob Agents Chemother. 2010 May;54(5):1878-87.