

Product Name : Nalraprevir

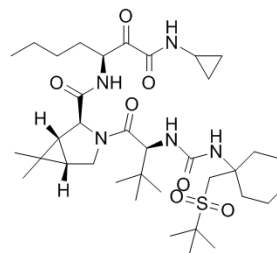
Synonyms : SCH 900518;SCH900518;SCH-900518

Cat No. : M16286

CAS Number : 865466-24-6

Molecular Formula : C₃₆H₆₁N₅O₇S

Formula Weight : 707.96



Chemical Name : 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-1-[2-(cyclopropylamino)-2-oxoacetyl]pentyl]-3-[(2S)-2-[[[1-[(1,1-dimethylethyl)sulfonyl]methyl]cyclohexyl]amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)-

Description : A potent, second generation HCV NS3 serine protease inhibitor with K_i of 6 nM; displays no significant issues in the in vitro CYP or hERG assay; shows replicon EC₉₀ of 40 nM; exhibits improved potency (~10-fold over Boceprevir), pharmacokinetic profile and physicochemical characteristics.

Pathway : Microbiology/Virology

Target : HCV

Receptor : HCV

Solubility : 10 mM in DMSO

SMILES : O=C([C@@H]1[C@@]2([H])C(C)(C)[C@@]2([H])CN1C([C@H](C(C)(C)NC(NC3CS(=O)(C(C)(C)C)=O)CCCCC3)=O)=O)N[C@H](C(C(=O)NC4CC4)=O)=O)CCCC

Storage : (-20°C)

Stability : ≥ 2 years

Reference :

1. Arasappan A, et al. ACS Med Chem Lett. 2010 Feb 15;1(2):64-9. 2. Tong X, et al. Antimicrob Agents Chemother. 2010 Jun;54(6):2365-70. 3. de Bruijne J, et al. Hepatology. 2010 Nov;52(5):1590-9.