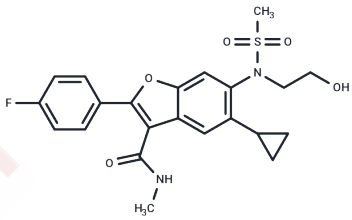
Data Sheet (Cat.No.TQ0090)

TargetMol

Nesbuvir

Chemical Properties



CAS No. : 691852-58-1

Formula: C22H23FN2O5S

Molecular Weight: 446.49

Storage: Keep away from direct sunlight
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Nesbuvir is a selective hepatitis C virus (HCV) nonstructural protein 5B (NS5B) RNA-dependent polymerase inhibitor.Nesbuvir has an IC50 of 9 nM against hepatocellular carcinoma cells containing 1b HCV replicons.
Targets(IC50)	HCV Protease
In vitro	Nesbuvir (40 or 80 nM) (approximately 10 and 20 times the EC50 in a 3-day replicon inhibition assay, respectively). The EC50 for Nesbuvir in the transient expression assay is 14 nM, whereas it is 5 nM for the stable replicon.[1] Nesbuvir (0.1 and 1 μM; Huh-7 cells; for 16 days) reduced about 3.6 log10 and 4.2 log10 HCV RNA levels, respectively.[3]
In vivo	Nesbuvir is demonstrated to yield significant antiviral effects in mice with chimeric human livers and in patients infected with HCV.[2] Nesbuvir (chimeric mouse model) treatment resulted in a 2.02 +/- 0.55 log reduction in HCV titer, whereas in combination with interferon using a suboptimal dose of 30 mg/kg three times per day showed a 2.44 log reduction and were better than interferon treatment only.[5]
Cell Research	Huh7-BB7 cells are seeded at a density of 20,000 cells per 100 mm dish in DMEM supplemented with 2% FBS, 1 mg/mL G418, and various concentrations of Nesbuvir and/or Boceprevir with DMSO at a final concentration of 0.5% (vol/vol). The medium is removed and is replaced with a fresh medium with the appropriate compound concentrations every 3 or 4 days. After 7 days, the cells are split 1 to 10, placed into fresh 100 mm dishes, and incubated with medium with the appropriate compound concentrations. After 20 days, the medium is removed and the cells are fixed with 7% (wt/vol) formaldehyde and stained with 1% (wt/vol) crystal violet in 50% (vol/vol) ethanol [1].

Solubility Information

Solubility	DMSO: 45 mg/mL (100.79 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.48 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2397 mL	11.1985 mL	22.3969 mL
5 mM	0.4479 mL	2.2397 mL	4.4794 mL
10 mM	0.224 mL	1.1198 mL	2.2397 mL
50 mM	0.0448 mL	0.224 mL	0.4479 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Flint M, et al. Selection and characterization of hepatitis C virus replicons dually resistant to the polymerase and protease inhibitors HCV-796 and boceprevir (SCH 503034). Antimicrob Agents Chemother. 2009;53(2):401-411.
Reich S, et al. Mechanisms of activity and inhibition of the hepatitis C virus RNA-dependent RNA polymerase. J Biol Chem. 2010;285(18):13685-13693.
Howe AY, et al. Molecular mechanism of hepatitis C virus replicon variants with reduced susceptibility to a benzofuran inhibitor, HCV-796. Antimicrob Agents Chemother. 2008;52(9):3327-3338.
Meshram RJ, et al. Effective epitope identification employing phylogenetic, mutational variability, sequence entropy, and correlated mutation analysis targeting NS5B protein of hepatitis C virus: from bioinformatics to therapeutics. J Mol Recognit. 2015;28(8):492-505.
Kneteman NM, et al. HCV796: A selective nonstructural protein 5B polymerase inhibitor with potent anti-hepatitis C virus activity in vitro, in mice with chimeric human livers, and in humans infected with hepatitis C virus. Hepatology. 2009;49(3):745-752.