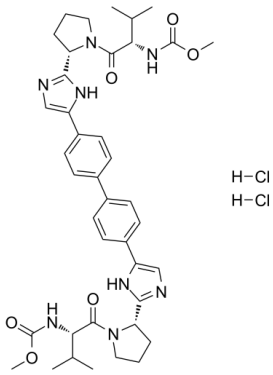
Data Sheet

Product Name:	Daclatasvir (dihydrochloride)
Cat. No.:	CS-0270
CAS No.:	1009119-65-6
Molecular Formula:	C40H52Cl2N8O6
Molecular Weight:	811.80
Target:	HCV
Pathway:	Anti-infection
Solubility:	DMSO : ≥ 56 mg/mL (68.98 mM); H2O : 50 mg/mL (61.59 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Daclatasvir dihydrochloride (BMS-790052 dihydrochloride) is a highly selective inhibitor of HCV NS5A with EC50 of 9-50 pM, for a broad range of HCV replicon genotypes and the JFH-1 genotype 2a infectious virus in cell culture. IC50 Value: 9-50 pM Target: HCV NS5A Daclatasvir has broad genotype coverage and exhibits picomolar in vitro potency against genotypes 1a (EC50 50pm) and 1b (EC50 9pm). Daclatasvir produces a robust decline in HCV RNA (-3.6 logs after 48 hours from a single 100 mg) dosefollowing a single dose in patients chronically infected with HCV genotype 1.

PROTOCOL (Extracted from published papers and Only for reference)

Cell assay [1] Replicon cells plated in 100- or 150-mm tissue culture dishes were maintained in medium supplemented with 0.5 mg/ml G418 and the desired concentration of BMS-790052 in DMSO. Control cells were maintained with an equivalent percent volume of DMSO (≤0.01%). Cells were split or fed with fresh medium containing inhibitor twice weekly to maintain a subconfluent monolayer. After approximately 4 to 5 weeks, pooled cells were expanded for phenotypic and genotypic analyses.

References:

[1]. Suzuki F, Sezaki H, Akuta N, Suzuki Y, Seko Y, Kawamura Y, Hosaka T, Kobayashi M, Saito S, Arase Y, Ikeda K, Kobayashi M, Mineta R, Watahiki S, Miyakawa Y, Kumada H.Prevalence of hepatitis C virus variants resistant to NS3 protease inhibitors or the NS5A inhibitor (BMS-790052) in hepatitis patients with genotype 1b.J Clin Virol. 2012 Aug;54(4):352-4. Epub 2012 Jun 1.

[2]. Jiang H, Zeng J, Kandoussi H, Liu Y, Wang X, Bifano M, Cojocaru L, Ryan J, Arnold ME.A sensitive and accurate liquid chromatography-tandem mass spectrometry method for quantitative determination of the novel hepatitis C NS5A inhibitor BMS-790052 (daclastasvir) in human plasma and urine.J Chromatogr A. 2012 Jul 6;1245:117-21. Epub 2012 May 14.

[3]. Sun JH, O'Boyle Ii DR, Zhang Y, Wang C, Nower P, Valera L, Roberts S, Nettles RE, Fridell RA, Gao M.Impact of a baseline polymorphism on the emergence of resistance to the hepatitis C virus nonstructural protein 5A replication complex inhibitor, BMS-790052.Hepatology. 2012 Jun;55(6):1692-9.

[4]. Wang C, Jia L, Huang H, Qiu D, Valera L, Huang X, Sun JH, Nower PT, O'Boyle DR 2nd, Gao M, Fridell RA.In vitro activity of BMS-790052 on hepatitis C virus genotype 4 NS5A.Antimicrob Agents Chemother. 2012 Mar;56(3):1588-90. Epub 2011 Dec 27.

[5]. Fridell RA et al. Resistance analysis of the hepatitis C virus NS5A inhibitor BMS-790052 in an in vitro replicon system. Antimicrob Agents Chemother. 2010 Sep;54(9):3641-50.

CAIndexNames:

Carbamic acid, N,N'-[[1,1'-biphenyl]-4,4'-diylbis[1H-imidazole-5,2-diyl-(2S)-2,1-pyrrolidinediyl[(1S)-1-(1-methylethyl)-2-oxo-2,1-ethanediyl]]]bis-, C,C'-dimethyl ester, hydrochloride (1:2)

SMILES:

O=C(N1CCC[C@H]1C2=NC=C(C3=CC=C(C4=CC=C(C=C4)C5=CN=C(N5)[C@@H]6CCCN6C([C@H](C(C)C)NC(OC)=O)=O)C=C3)N2)[C@H](C(C)C)NC(OC)=O.[H]Cl.[H]Cl

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

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