Daclatasvir dihydrochloride

Cat. No.: HY-10465

CAS No.: 1009119-65-6

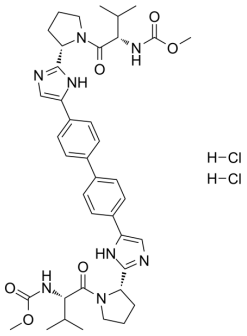
Molecular Formula: $C_{40}H_{52}Cl_2N_8O_6$

Molecular Weight: 811.8

Target: HCV

Pathway: Anti-infection

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 56 mg/mL (68.98 mM)
H_2O : 50 mg/mL (61.59 mM; Need ultrasonic)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.2318 mL	6.1592 mL	12.3183 mL
	5 mM	0.2464 mL	1.2318 mL	2.4637 mL
	10 mM	0.1232 mL	0.6159 mL	1.2318 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1 mg/mL (1.23 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1 mg/mL (1.23 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1 mg/mL (1.23 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Daclatasvir dihydrochloride (BMS-790052 dihydrochloride) is a potent and orally active HCV NS5A protein inhibitor with EC_{50} s range of 9-146 pM for multiple HCV replicon genotypes. Daclatasvir dihydrochloride is also an organic anion transporting polypeptide 1B (OATP1B) and OATP1B3 inhibitor with IC_{50}s of 1.5 μM and 3.27 μM, respectively[1][2][3].

IC_{50} & Target

EC50: 50 pM (HCV replicon genotype 1a), 9 pM (HCV replicon genotype 1b), 71 pM (HCV replicon genotype 2a), 146 pM (HCV replicon genotype 3a), 12 pM (HCV replicon genotype 4a) and 33 pM (HCV replicon genotype 5a)[1]
Kd: 8 nM (NS5A33-202) and 210 nM (NS5A26-202)[2]

	IC50: 1.5 μM (OATP1B) and 3.27 μM (OATP1B3)[3]
In Vitro	Daclatasvir (BMS-790052) demonstrates potent inhibitory activity towards all genotypes tested, with EC_{50} values ranging from 9 pM to 146 pM. Daclatasvir inhibits HCV replicon genotype 1a, 1b, 2a, 3a, 4a and 5a with EC_{50} values of 50 pM, 9 pM, 71 pM, 146 pM, 12 pM and 33 pM, respectively. Daclatasvir is a potent inhibitor of the JFH-1 genotype 2a infectious virus that replicates in cell culture (EC_{50}=28 pM)[1].Daclatasvir (BMS-790052) binds tightly to NS5A33-202 and NS5A26-202 with K_ds of 8 nM and 210 nM, respectively[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Daclatasvir (BMS-790052; 30 mg/kg; oral administration; daily; for 27 days) treatment reduces serum HCV RNA titers very rapidly by ~1.5 log_{10} at day 3[4]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	NOD/SCID male mice (5 weeks of age, 18-20 g) bearing HCV RNA-transfected cells[4]
Dosage:	30 mg/kg
Administration:	Oral administration; daily; for 27 days
Result:	Reduced serum HCV RNA titers very rapidly by ~1.5 log_{10} at day 3.

CUSTOMER VALIDATION

- Hepatology. 2019 May;69(5):1861-1872.
- Int J Antimicrob Agents. 2015 Oct;46(4):381-8.
- Cell Rep. 2021 Nov 23;37(8):110049.
- EMBO Rep. 2016 Jul;17(7):1013-28.
- PLoS Pathog. 2018 Sep 18;14(9):e1007284.

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REFERENCES

[1]. Min Gao, et al. Chemical genetics strategy identifies an HCV NS5A inhibitor with a potent clinical effect. Nature. 2010 May 6;465(7294):96-100.

[2]. David B Ascher, et al. Potent hepatitis C inhibitors bind directly to NS5A and reduce its affinity for RNA. Sci Rep. 2014 Apr 23;4:4765.

[3]. Tomomi Furihata, et al. Different interaction profiles of direct-acting anti-hepatitis C virus agents with human organic anion transporting polypeptides. Antimicrob Agents Chemother. 2014 Aug;58(8):4555-64.

[4]. Seung-Hoon Lee, et al. HA1077 displays synergistic activity with daclatasvir against hepatitis C virus and suppresses the emergence of NS5A resistance-associated substitutions in mice. Sci Rep. 2018 Aug 20;8(1):12469.

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