Boceprevir

Cat. No.: HY-10237

CAS No.: 394730-60-0

Molecular Formula: $C_{27}H_{45}N_5O_5$

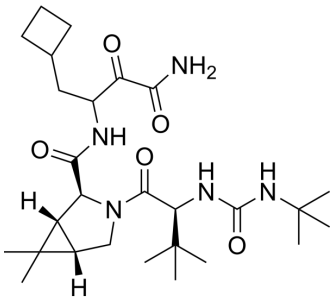
Molecular Weight: 520

Target: HCV Protease; HCV; SARS-CoV

Pathway: Anti-infection; Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 180 mg/mL (346.15 mM; Need ultrasonic)

H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9231 mL	9.6154 mL	19.2308 mL
	5 mM	0.3846 mL	1.9231 mL	3.8462 mL
	10 mM	0.1923 mL	0.9615 mL	1.9231 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: ≥ 1.67 mg/mL (3.21 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 1.67 mg/mL (3.21 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.67 mg/mL (3.21 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Boceprevir (EBP 520) is a potent, highly selective, orally bioavailable HCV NS3 protease inhibitor with a K_i of 14 nM in both enzyme assay and an EC_{90} of 350 nM in cell-based replicon assay[1][2][3][4][5]. Boceprevir inhibits SARS-CoV-2 $3CL^{pro}$ activity [6].

IC_{50} & Target

Ki: 14 nM (HCV NS3 protease)[1]

In Vitro

In the HCV NS3 protease continuous assay, Boceprevir (SCH 503034) has a potency of 14 nM (K_i) average over a large number

	of runs. In the 72-h bicistronic subgenomic cell-based replicon assay in HuH-7 cells, the EC_{50} and EC_{90} values are determined to be 0.20 μM and 0.35 μM, respectively. Boceprevir is also found to be a very weak inhibitor of HNE (K_i=26 μM) representing a selectivity of 2200[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Boceprevir, an HCV Protease Inhibitor for the Treatment of Hepatitis C Virus Infection. The pharmacokinetic profile of Boceprevir is evaluated in several animal species. Following oral administration, Boceprevir is moderately absorbed in rats (10 mg/kg), dogs (3 mg/kg), and monkeys (3 mg/kg). Absorption is relatively rapid in dogs but slower in mice (10 mg/kg), rats, and monkeys, as evidenced by mean absorption times (MAT) ranging from 0.5 to 1.4 h. The AUC is good in dogs and rats, moderate in mouse, and low in monkeys. The absolute oral bioavailability is modest in mouse, rats, and dogs (26-34%) but low in monkeys (4%)[1]. Boceprevir (100 mg/kg, orally) inhibit HCV NS3/4A protease activity in triple-transgenic mice[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Animal Administration [2]	Mice[2] Boceprevir is purchased from MedChem Express. To evaluate the effect of Boceprevir, triple-transgenic mice are induced with Doxycycline (Dox) for 10 days (n=5 per group). On the third day after Dox induction, when plasma Gluc activity reaches its peak, the mice are administered either Boceprevir (100 mg/kg) or DMSO via oral gavage twice daily for 7 days. During this period, blood is collected from the caudal vein daily to detect plasma Gluc activity. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cancer Cell. 2022 Aug 26;S1535-6108(22)00372-5.
- Nat Methods. 2018 Jul;15(7):519-522.
- Signal Transduct Target Ther. 2021 May 29;6(1):212.
- ACS Cent Sci. February 2, 2022.
- Nat Commun. 2020 Sep 4;11(1):4417.

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REFERENCES

[1]. Njoroge FG, et al. Challenges in modern drug discovery: a case study of boceprevir, an HCV protease inhibitor for the treatment of hepatitis C virus infection. Acc Chem Res. 2008 Jan;41(1):50-9.

[2]. Yao M, et al. Conditional Inducible Triple-Transgenic Mouse Model for Rapid Real-Time Detection of HCV NS3/4A ProteaseActivity. PLoS One. 2016 Mar 4;11(3):e0150894.

[3]. Coilly A, et al. Practical management of boceprevir and immunosuppressive therapy in liver transplant recipients with hepatitis C virus recurrence. Antimicrob Agents Chemother. 2012 Nov;56(11):5728-34.

[4]. Berenguer M, et al. New developments in the management of hepatitis C virus infection: focus on boceprevir. Biologics. 2012;6:249-56.

[5]. Burton MJ, et al. Telaprevir and boceprevir in african americans with genotype 1 chronic hepatitis C: implications for patients and providers. South Med J. 2012 Aug;105(8):431-6.

[6]. Qi Sun, et al. Bardoxolone and bardoxolone methyl, two Nrf2 activators in clinical trials, inhibit SARS-CoV-2 replication and its 3C-like protease. Signal Transduct Target Ther. 2021 May 29;6(1):212.

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

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