Boceprevir

Cat. No.: HY-10237
CAS No.: 394730-60-0
Molecular Formula: C\textsubscript{27}H\textsubscript{45}N\textsubscript{5}O\textsubscript{5}
Molecular Weight: 519.68
Target: HCV Protease; HCV
Pathway: Metabolic Enzyme/Protease; Anti-infection
Storage:
- Powder: -20°C 3 years
- 4°C  2 years
- In solvent: -80°C 6 months
- -20°C 1 month

**SOLVENT & SOLUBILITY**

In Vitro

DMSO: ≥ 10 mg/mL (19.24 mM)
H\textsubscript{2}O: < 0.1 mg/mL (insoluble)

* "≥" means soluble, but saturation unknown.

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td></td>
<td>1.9243 mL</td>
<td>9.6213 mL</td>
<td>19.2426 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td></td>
<td>0.3849 mL</td>
<td>1.9243 mL</td>
<td>3.8485 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td></td>
<td>0.1924 mL</td>
<td>0.9621 mL</td>
<td>1.9243 mL</td>
</tr>
</tbody>
</table>

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 is a novel, potent, highly selective, orally bioavailable HCV NS3 protease inhibitor with Ki of 14 nM in both enzyme assay and EC\textsubscript{90} of 350 nM in cell-based replicon assay.

IC\textsubscript{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$^{[1]}$.

**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$^{[2]}$.

**PROTOCOL**

**Animal Administration $^{[2]}$**

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**


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**REFERENCES**


