# Simeprevir

**Cat. No.:** HY-10241  
**CAS No.:** 923604-59-5  
**Molecular Formula:** C₃₈H₄₇N₅O₇S₂  
**Molecular Weight:** 749.94  
**Target:** HCV; HCV Protease  
**Pathway:** Anti-infection; Metabolic Enzyme/Protease  
**Storage:**  
- **Powder:** -20°C 3 years  
- **4°C:** 2 years  
- **In solvent:**  
  - **-80°C:** 6 months  
  - **-20°C:** 1 month

## SOLVENT & SOLUBILITY

### In Vitro

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMSO</td>
<td>1 mM</td>
<td>1.3334 mL</td>
<td>6.6672 mL</td>
<td>13.3344 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.2667 mL</td>
<td>1.3334 mL</td>
<td>2.6669 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.1333 mL</td>
<td>0.6667 mL</td>
<td>1.3334 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: ≥ 1.43 mg/mL (1.91 mM); Clear solution
2. Add each solvent one by one:  
   - **10% DMSO** >> **90% corn oil**  
   Solubility: ≥ 1.43 mg/mL (1.91 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**  
Simeprevir (TMC435) is an oral and potent HCV NS3/4A protease inhibitor with a $K_i$ of 0.36 nM, and inhibits HCV replication with an $EC_{50}$ of 7.8 nM[1].

**IC₅₀ & Target**  
- $K_i$: 0.36 nM (HCV NS3/4A protease)[1]  
- $EC_{50}$: 7.8 nM (HCV replication)[1]

**In Vitro**  
In Huh7-Luc cells, antiviral activity of simeprevir (TMC435) is dose dependent, and the $EC_{50}$ and $EC_{90}$ values determined for simeprevir (TMC435) are 8 nM and 24 nM, respectively[2]. Simeprevir (TMC435) inhibits NS3/4A proteases from HCV genotypes 1 to 6 with $IC_{50}$s of 1/0.9/7/30/1.5/2.2/1.6 nM.
Simeprevir (TMC435) has moderate terminal elimination half-life ($t_{1/2} = 1.5$ h and 4.1 h for rat (3 mg/kg, p.o.), monkey (3 mg/kg, p.o.))\(^3\).

**In Vivo**

<table>
<thead>
<tr>
<th>Animal Model:</th>
<th>Sprague-Dawley (SD) rats and cynomolgus monkeys(^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dosage:</td>
<td>3 mg/kg</td>
</tr>
<tr>
<td>Administration:</td>
<td>Oral administration</td>
</tr>
<tr>
<td>Result:</td>
<td>Time at which peak concentration ($T_{\text{max}}$) of 1 hour and 2 hour for rat and monkey, respectively. Concentration at 24 h after dosing ($C_{24,\text{h}}$) of 0.9 and 2.3 ng/mL for rat and monkey, respectively. AUC$_{0-24,\text{h}}$=1173 and 1409 ng • h/mL for rat and monkey, respectively.</td>
</tr>
</tbody>
</table>

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### REFERENCES


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

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