

## 15-4005: Simeprevir (sodium salt)

### Description

**Molecular Formula:** C<sub>38</sub>H<sub>47</sub>N<sub>5</sub>O<sub>7</sub>S<sub>2</sub> • XNa

**Molecular Weight:** 749.9

Simeprevir is an orally bioavailable and potent inhibitor of the hepatitis C virus (HCV) nonstructural protein 3/4A (NS3/4A) protease (K<sub>i</sub> = 0.36 nM), a serine protease essential for HCV replication. It inhibits HCV viral replication with an EC<sub>50</sub> value of 7.8 nM in Huh7 replicon cells using a luciferase-based assay. Simeprevir is effective against the HCV genotypes 1a and 1b in biochemical assays. In Huh7 replicon cells, it is synergistically effective when used in combination with IFN-α or NM-107 and has an additive effect when used with ribavirin (Item No. 16757). Formulations containing simeprevir have been used, alone or in combination with pegylated IFN-α and ribavirin, for the treatment of HCV.

### Product Info

**Amount :** 1 mg / 5 mg

**Purification :** ≥98%

**Content :** Simeprevir (sodium salt) is supplied as a crystalline solid.

**Storage condition :** Store at -20°C, product is stable for at least two years.

### Application Note

A stock solution may be made by dissolving the simeprevir (sodium salt) in the solvent of choice. Simeprevir (sodium salt) is soluble in organic solvents such as DMSO and dimethyl formamide, which should be purged with an inert gas. The solubility of simeprevir (sodium salt) in these solvents is approximately 30 mg/ml. Simeprevir (sodium salt) is also slightly soluble in ethanol.

Simeprevir (sodium salt) is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, simeprevir (sodium salt) should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Simeprevir (sodium salt) has a solubility of approximately 0.33 mg/ml in a 1:2 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

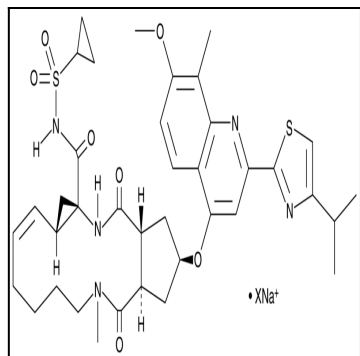


Figure-1: Structure of Simeprevir (sodium salt).