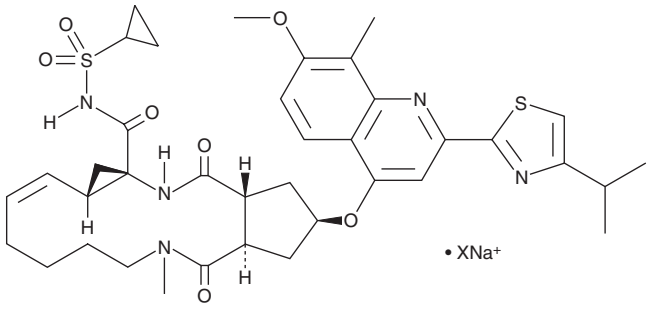
PRODUCT INFORMATION

Simeprevir (sodium salt)

Item No. 22144

CAS Registry No.: 1241946-89-3
Formal Name: (2R,3aR,10Z,11aS,12aR,14aR)-N-(cyclopropylsulfonyl)-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetradecahydro-2-[[7-methoxy-8-methyl-2-[4-(1-methylethy)-2-thiazolyl]-4-quinolinyl]oxy]-5-methyl-4,14-dioxo-cyclopenta[c]cyclopropa[g][1,6]diazacyclotetradecine-12a(1H)-carboxamide, sodium salt
MF: $C_{38}H_{47}N_5O_7S_2$ • XNa
FW: 749.9
Purity: ≥98%
UV/Vis.: λ_{max}: 221, 289, 332 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

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

Description

Simeprevir is an orally bioavailable and potent inhibitor of the hepatitis C virus (HCV) nonstructural protein 3/4A (NS3/4A) protease (K_i = 0.36 nM), a serine protease essential for HCV replication.[1] It inhibits HCV viral replication with an EC_{50} 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.[2] 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.

References

1. Raboisson, P., de Kock, H., Rosenquist, A., *et al.* Structure-activity relationship study on a novel series of cyclopentane-containing macrocyclic inhibitors of the hepatitis C virus NS3/4A protease leading to the discovery of TMC435350. *Bioorg. Med. Chem. Lett.* **18(17)**, 4853-4858 (2008).
2. Lin, T.-I., Lenz, O., Fanning, G., *et al.* In vitro activity and preclinical profile of TMC435350, a potent hepatitis C virus protease inhibitor. *Antimicrob. Agents Chemother.* **53(4)**, 1377-1385 (2009).

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