

Product Name	: Danoprevir
Synonyms	: ITMN-191;R-7227;RO-5190591;RG-7227
Cat No.	: M16181
CAS Number	: 850876-88-9
Molecular Formula	: C ₃₅ H ₄₆ FN ₅ O ₉ S
Formula Weight	: 731.83
Chemical Name	: 2H-Isoindole-2-carboxylic acid, 4-fluoro-1,3-dihydro-, (2R,6S,13aS,14aR,16aS)-14a-[[[(cyclopropylsulfonyl)amino]carbonyl]-6-[[[(1,1-dimethylethoxy)carbonyl]amino]-1,2,3,5,6,7,8,9,10,11,13a,14,14a,15,16,16a-hexadecahydro-5,16-dioxocyclopropa[e]pyrrolo[1,2-a]
Description	: A potent, highly selective, orally available, peptidomimetic HCV NS3/4A protease inhibitor with IC ₅₀ of 0.2-0.4 nM (GT1a, 1b, 4, 5 and 6), 1.6 nM (GT2b); shows favorable potency profile against multiple HCV genotypes 1-6 and key mutants (replicon GT1b, EC ₅₀ =1.6 nM). HCV Infection Approved
Pathway	: Microbiology/Virology
Target	: HCV
Receptor	: HCVNS3/4Aprotease
Solubility	: 10 mM in DMSO
SMILES	: <chem>O=C(N1CC2=C(C(F)=CC=C2)C1)O[C@@H](C3)C[C@](C(N[C@@](C4)(C(NS(=O)(C5CC5)=O)=O)[C@]4([H])C=C1CCCCC6NC(OC(C)(C)C)=O)=O)([H])N3C6=O</chem>
Storage	: (-20°C)
Stability	: ≥ 2 years
Reference	:

1. Bae A, et al. Antimicrob Agents Chemother. 2010 Dec;54(12):5288-97. | 2. Moucari R, et al. Gut. 2010 Dec;59(12):1694-8. | 3. Jiang Y, et al. J Med Chem. 2014 Mar 13;57(5):1753-69. | 4. Schaefer CJ, et al. Antimicrob Agents Chemother. 2011 Jul;55(7):3125-32.