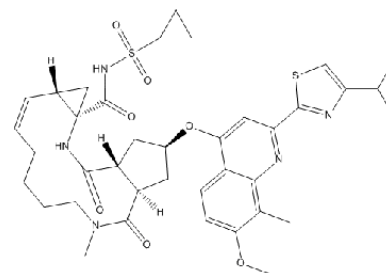


Simeprevir

Catalog Number: BC-0813

CAS Number: 923604-59-5

Price: [Online Inquiry](#)



Catalog Number	Price
BC-0813	Online Inquiry

Product Information	
Molecular Formula	C ₃₈ H ₄₇ N ₅ O ₇ S ₂
Molecular Weight	749.96
Purity	≥98% by HPLC
SMILES	<chem>CC1=C(C=CC2=C1N=C(C=C2OC3CC4C(C3)C(=O)N(CCCCC=CC5CC5(NC4=O)C(=O)NS(=O)(=O)C6CC6)C)C7=NC(=CS7)C(C)C)OC</chem>
InChi	InChI=1S/C38H47N5O7S2/c1-21(2)30-20-51-35(40-30)29-18-32(26-13-14-31(49-5)22(3)33(26)39-29)50-24-16-27-28(17-24)36(45)43(4)15-9-7-6-8-10-23-19-38(23,41-34(27)44)37(46)42-52(47,48)25-11-12-25/h8,10,13-14,18,20-21,23-25,27-28H,6-7,9,11-12,15-17,19H2,1-5H3,(H,41,44)(H,42,46)/b10-8-/t23-,24-,27-,28-,38-/m1/s1
InChi Key	JTZZSQYMACOLNN-VDWJNHBNSA-N
Alternate Name	(2R,3aR,10Z,11aS,12aR,14aR)-N-(Cyclopropylsulfonyl)-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetrahydro-2-[[7-methoxy-8-methyl-2-[4-(1-methylethyl)-2-thiazolyl]-4-quinolinyl]oxy]-5-methyl-4,14-dioxo-cyclopenta[c]cyclopropa[g][1,6]diazacyclotetradecine-12a(1H)-carboxamide; TMC 435; TMC 435350
Appearance	Off-white solid

Properties	
Storage Conditions	-20°C
Shipping Conditions	Gel Pack
Solubility	DMSO