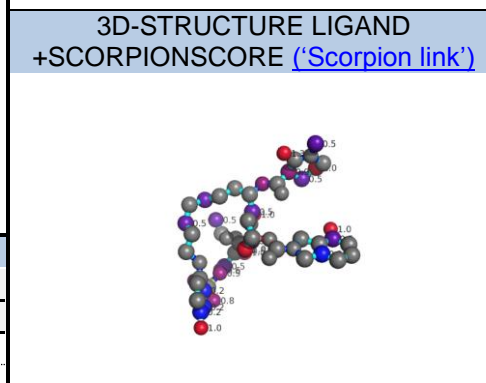
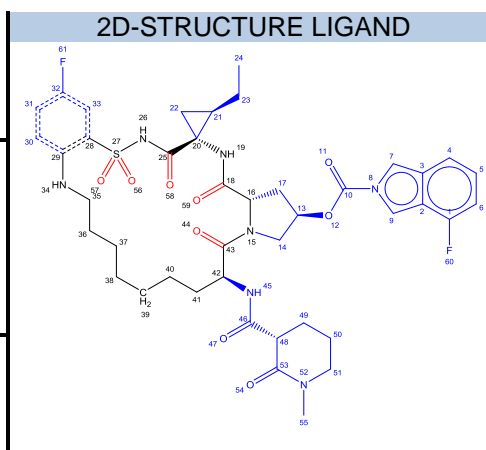
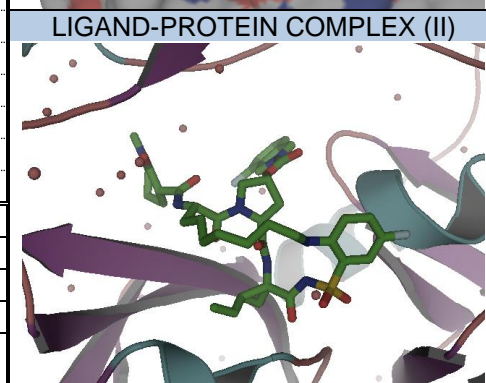
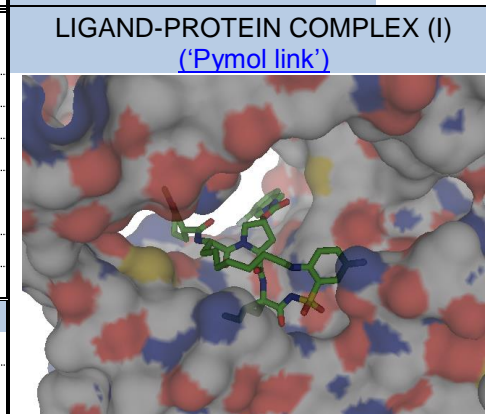


CODE	4A92 ( <a href="#">PDB</a> )	Resolution	2.7	
Name		Ring size	20	
Formula	C42H51F2N7O9S	# Ligand atoms	61	
Type	Macrocycle	Scorpion Score	17.8	
Mol. Weight (Da)	868	Saturated/ Unsaturated	U	
cLogP	6.3	Chiral centres.ring	3	
tPSA	205	Chiral centres.sub	3	
#HBD's	4			
#HBA's	18			
NRB (RING)	15	NRB (SUBSTITUENT)	5	
Number of substituents	4	P/NP balance, substituents	9/27	
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	5/0	
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	20	
Proportion HA in substituents	59.0%	N:O ratio	7:9	
Number of peripheral groups	5	Chiral centres	6	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	4	16	2	6
Substituent	9	27	4	11
Peripheral groups	5	-	4	-
Total	18	43	10	17

Protein name	NS3/4A protease-helicase		
Organism	Hepatitis C virus		
Classification	Hydrolase		
Binding mode	Face-on/ Compact		
Receptor secondary structure topology			
Number of residue 'hotspots'	21		
Number of protein-ligand interactions* ( <a href="#">Database link</a> )			
Hydrogen bond	11	Hydrogen donor-π	2
Ionic interaction		π-π	4
Cation-dipole		VdW interaction	19
Cation-π		Unfavourable	4
Dipolar interaction		Poor-angle	6
Halogen bond		Unclassified	1
Water-mediated interaction	0		



Physicochemical properties  
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\*Based on Scorpion® analysis