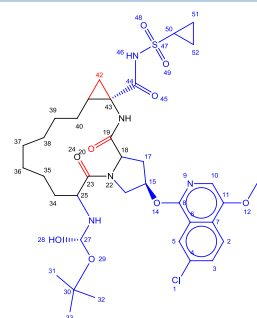
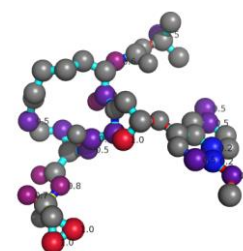


CODE	4WH8 (PDB)	Resolution	2.7	
Name	Asunaprevir	Ring size	15	
Formula	C36H46ClN5O9S	# Ligand atoms	98	
Type	macrocycle	Scorpion Score	13.6	
Mol. Weight (Da)	759.27	Saturated/Unsaturated	U	
cLogP	6.9047	Chiral centres.ring	3	
tPSA	181.8	Chiral centres.sub	2	
#HBD's	3			
#HBA's	12			
N _{RB} (RING)	11	N _{RB} (SUBSTITUENT)	9	
Number of substituents	3	P/NP balance, substituents	12/23	
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	2/0	
<i>Small (2-4HA)</i>	-	Degrees of unsaturation ring	15	
Proportion HA in substituents	36%	N:O ratio	5/9	
Number of peripheral groups	2	Chiral centres	5	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	2	13	1	5
Substituent	12	23	6	8
Peripheral groups	2	0	1	0
Total	16	36	8	13
Protein name	HCV NS3/ 4A protease			
Organism	Hepatitis C virus			
Classification	Hydrolase/ Hydrolase inhibitor			
Binding mode	Edge-on			
Receptor secondary structure topology				
Number of residue 'hotspots'	14			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	6	Hydrogen donor-π	2	
Ionic interaction	-	π-π	2	
Cation-dipole	-	VdW interaction	18	
Cation-π	-	Unfavourable	1	
Dipolar interaction	1	Poor-angle	2	
Halogen bond	-	Unclassified	2	
Water-mediated interaction	-			

2D-STRUCTURE LIGAND



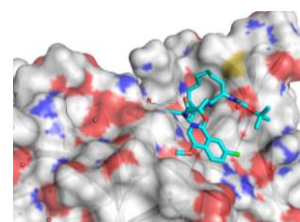
3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



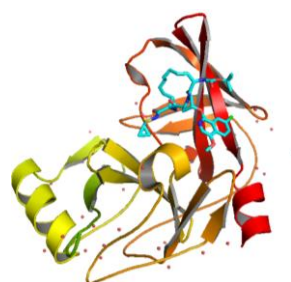
Physicochemical properties

['click for publication'](#)

LIGAND-PROTEIN COMPLEX (I) ('Pymol link')



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis