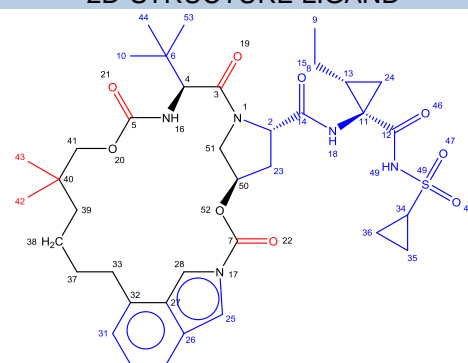


CODE	3SU3 (PDB)	Resolution	1.3	
Name		Ring size	20	
Formula	C38H55N5O9S	# Ligand atoms	53	
Type	Macrocycle	Scorpion Score	16.6	
Mol. Weight (Da)	758	Saturated/ Unsaturated	U	
cLogP	7.44	Chiral centres.ring	2	
tPSA	182	Chiral centres.sub	3	
#HBD's	3			
#HBA's	14			
N _{RB} (RING)	12	N _{RB} (SUBSTITUENT)	6	
Number of substituents	3	P/NP balance, substituents	6/22	
<i>Large (≥5HA)</i>	2	P/NP balance, peripheral groups	3/2	
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	14	
Proportion HA in substituents	86.8%	N:O ratio	5:9	
Number of peripheral groups	5	Chiral centres	5	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	5	15	1	3
Substituent	6	22	5	13
Peripheral groups	3	2	1	1
Total	14	39	7	17
Protein name	NS3/4A protease			
Organism	Hepatitis C virus			
Classification	Hydrolase/Inhibitor			
Binding mode	Face-on			
Receptor secondary structure topology				
Number of residue 'hotspots'	17			
Number of protein-ligand interactions* (Database link)				
Hydrogen bond	8	Hydrogen donor-π		
Ionic interaction		π-π	1	
Cation-dipole		VdW interaction	17	
Cation-π	2	Unfavourable	1	
Dipolar interaction		Poor-angle	6	
Halogen bond		Unclassified		
Water-mediated interaction	4			

2D-STRUCTURE LIGAND

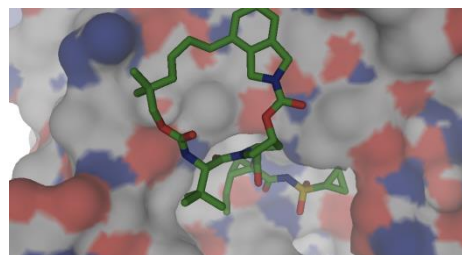


3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))

Physicochemical properties

[click for publication](#)

LIGAND-PROTEIN COMPLEX (I) ([Pymol link](#))



LIGAND-PROTEIN COMPLEX (II)

