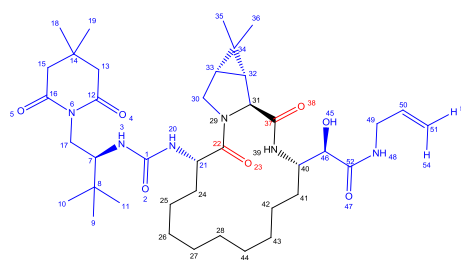
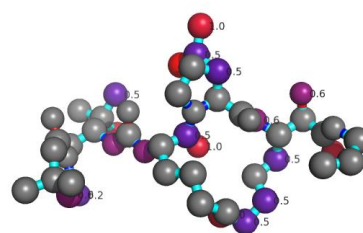


CODE	3KNX (PDB)	Resolution		
Name	Comp 52	Ring size	16	
Formula	C39H64N6O7	# Ligand atoms	54	
Type	Macrocycle	Scorpion Score	12.7	
Mol. Weight (Da)	728,96	Saturated/ Unsaturated	U	
cLogP		Chiral centres.ring	3	
tPSA		Chiral centres.sub	4	
#HBD's	5			
#HBA's	8			
N _{RB} (RING)	13	N _{RB} (SUBSTITUENT)	9	
Number of substituents	3	P/NP balance, substituents	9/25	
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	2/0	
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	11	
Proportion HA in substituents	63%	N:O ratio	6:7	
Number of peripheral groups	2	Chiral centres	7	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	2	14	1	5
Substituent	9	25	5	7
Peripheral groups	2	-	1	-
Total	13	39	7	12
Protein name	HCV NS3 protease			
Organism	Hepatitis C virus			
Classification	Viral protein			
Binding mode	Face on			
Receptor secondary structure topology				
Number of residue 'hotspots'	16			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	10	Hydrogen donor-π	-	
Ionic interaction	-	π-π	-	
Cation-dipole	-	VdW interaction	16	
Cation-π	-	Unfavourable	2	
Dipolar interaction	-	Poor-angle	1	
Halogen bond	-	Unclassified	-	
Water-mediated interaction	1			

2D-STRUCTURE LIGAND



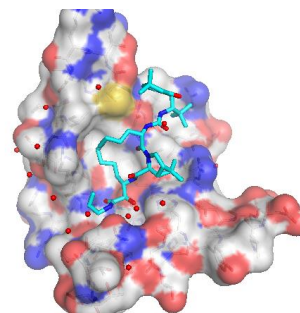
3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



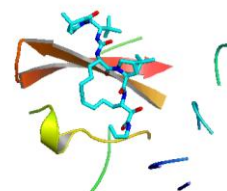
Physicochemical properties 'click for publication'

EC90 (μM) 0.020
K(μM) 0.002

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis