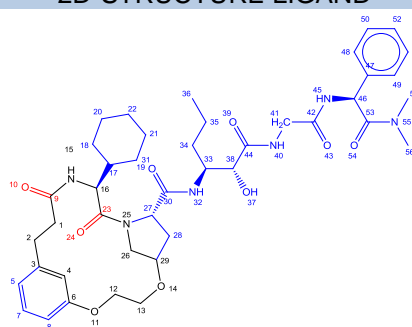


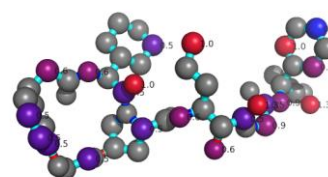
CODE	2GVF (PDB)	Resolution	
Name	Comp 38	Ring size	16
Formula	C42H58N6O9	# Ligand atoms	57
Type	Macrocycle	Scorpion Score	15.6
Mol. Weight (Da)	790,94	Saturated/ Unsaturated	U
cLogP		Chiral centres.ring	3
tPSA		Chiral centres.sub	4
#HBD's	5		
#HBA's	10		
N _{RB} (RING)	10	N _{RB} (SUBSTITUENT)	12
Number of substituents	3	P/NP balance, substituents	9/30
<i>Large (≥5HA)</i>	2	P/NP balance, peripheral groups	2/0
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	17
Proportion HA in substituents	68%	N:O ratio	6:9
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	3	13	
Substituent	9	30	
Peripheral groups	2	0	
Total	14	43	

Protein name	HCV NS3-4A protease		
Organism	Hepatitis C virus		
Classification	Hydrolase		
Binding mode	Face on		
Receptor secondary structure topology			
Number of residue 'hotspots'	14		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	12	Hydrogen donor-π	1
Ionic interaction	-	π-π	1
Cation-dipole	-	VdW interaction	14
Cation-π	-	Unfavourable	1
Dipolar interaction	-	Poor-angle	3
Halogen bond	-	Unclassified	1
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



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

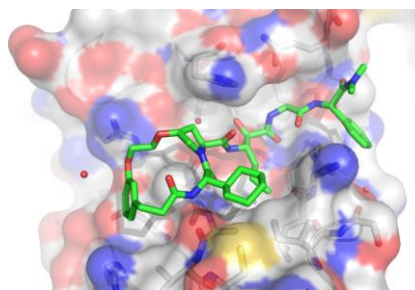


Physicochemical properties

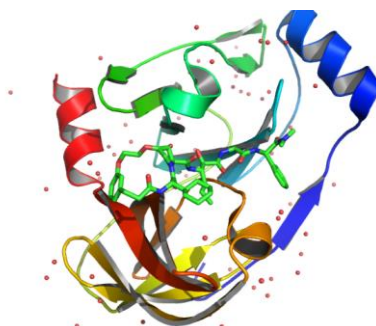
'click for publication'

K_i= 25nM

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis