CODE	**2A4Q** (PDB)	Resolution	2.45
Name	Comp. 18	Ring size	17
Formula	C41H58N5O8	# Ligand atoms	54
Type	Macrocycle	Scorpion Score	15

Mol. Weight (Da)	749	Saturated/ Unsaturated	U
cLogP	6.44		
tPSA	209	Chiral centres.ring	2
#HBD's	8	Chiral centres.sub	3
#HBA's	13		
$N_{RB(RING)}$	13	$N_{RB(SUB)}$	12

Number of substituents	3	P/NP balance, substituents	9/29
Large (≥5HA)	2	P/NP balance, peripheral groups	2/0
Small (2-4HA)	1		
Proportion HA in substituents	70.4%	Degrees of unsaturation ring	15.5
Number of peripheral groups	2	N:O ratio	5:8
		Chiral centres	5

Polarity distribution ligand atoms

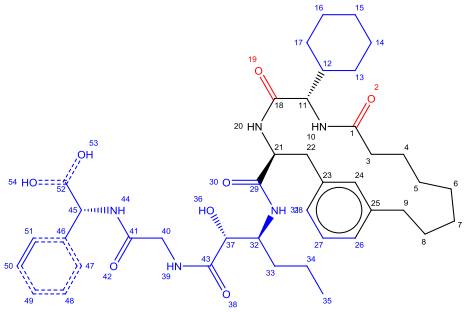
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	15	-	7
Substituent	9	27	5	9
Peripheral groups	2	0	1	0
Total	13	42	6	16

Protein name	HCV NS3 protease
Organism	Hepatitis C virus
Classification	Viral protein
Binding mode	Face-on
Receptor secondary structure topology	
Number of residue 'hotspots'	13

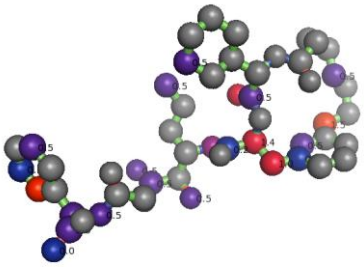
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	7	Hydrogen donor-π	3
Ionic interaction		π-π	3
Cation-dipole		VdW interaction	17
Cation-π		Unfavourable	2
Dipolar interaction		Poor-angle	4
Halogen bond		Unclassified	1
Water-mediated interaction			

2D-STRUCTURE LIGAND



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

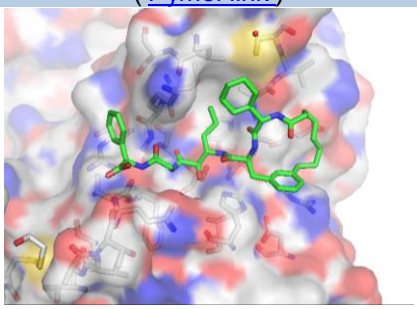


Physicochemical properties

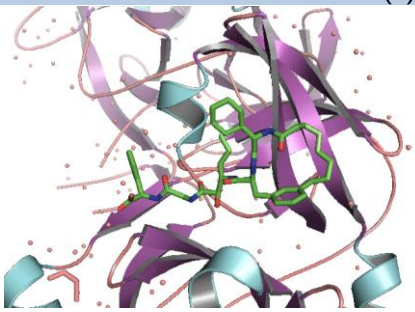
'click for publication'

KI (µM)	0.066

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis