

CODE	2XNI (PDB)	Resolution	3.3
Name		Ring size	20
Formula	C32H47BN4O9	# Ligand atoms	46
Type	Macrocycle	Scorpion Score	6
Mol. Weight (Da)	643	Saturated/ Unsaturated	U
cLogP	4.6	Chiral centres.ring	2
tPSA	180	Chiral centres.sub	2
#HBD's	5		
#HBA's	12		
NRB (RING)	12	NRB (SUBSTITUENT)	6

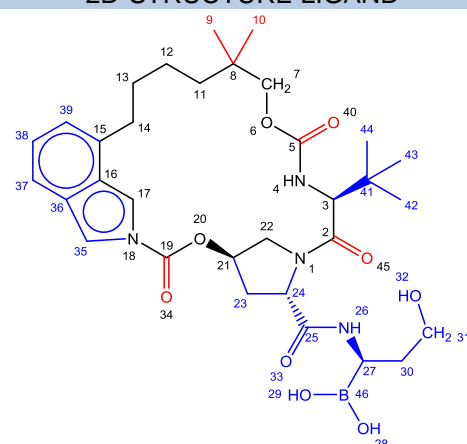
Number of substituents	3	P/NP balance, substituents	5/16
Large ($\geq 5HA$)	2	P/NP balance, peripheral groups	3/2
Small (2-4HA)	1	Degrees of unsaturation ring	11.5
Proportion HA in substituents	45.7%	N:O ratio	4:9
Number of peripheral groups	5	Chiral centres	4

	Polarity distribution ligand atoms			
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	5	15	-	1
Substituent	5	16	2	5
Peripheral groups	3	2	1	1
Total	13	33	3	7

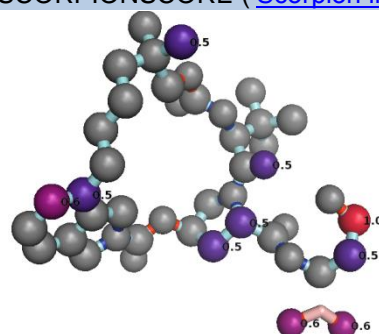
Protein name	HCV NS3 protease
Organism	Hepatitis C virus
Classification	Hydrolase/ Hydrolase regulator
Binding mode	Face-on
Receptor secondary structure topology	
Number of residue 'hotspots'	10

Number of protein-ligand interactions* (Database link)			
Hydrogen bond	3	Hydrogen donor- π	-
Ionic interaction	-	π - π	-
Cation-dipole	-	VdW interaction	7
Cation- π	1	Unfavourable	2
Dipolar interaction	-	Poor-angle	2
Halogen bond	-	Unclassified	-
Water-mediated interaction	-		

2D-STRUCTURE LIGAND



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

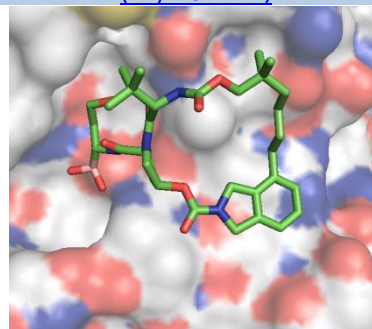


Physicochemical properties

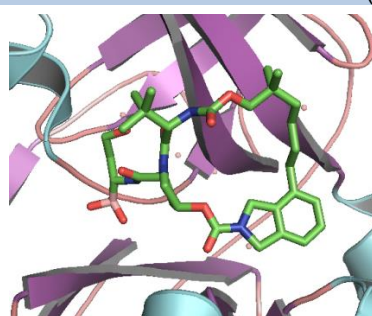
[click for publication](#)

NS3/4A IC50 (μM)	0.43
HCV replicon EC50 (μM)	0.78/ 0.52

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis