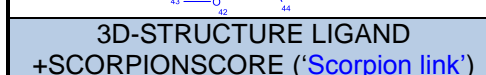
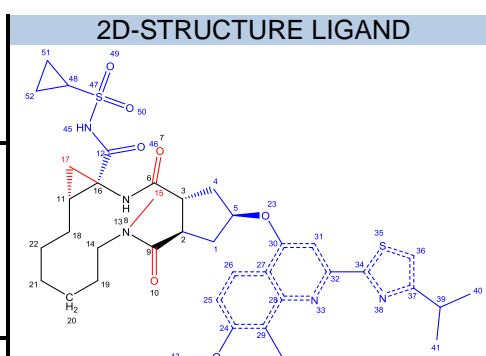


CODE	3KEE (PDB)	Resolution	2.4
Name	(TMC435)	Ring size	12
Formula	C38H49N5O7S2	# Ligand atoms	52
Type	Macrocyclic	Scorpion Score	21
Mol. Weight (Da)	751.96	Saturated/ Unsaturated	S
cLogP	5.78	Chiral centres.ring	4
tPSA	157	Chiral centres.sub	1
#HBD's	2		
#HBA's	12		
N _{RB} (RING)	10	N _{RB} (SUBSTITUENT)	8
Number of substituents	2	P/NP balance, substituents	8/26
<i>Large (≥5HA)</i>	2	P/NP balance, peripheral groups	2/2
<i>Small (2-4HA)</i>	-	Degrees of unsaturation ring	17
Proportion HA in substituents	78.8%	N:O ratio	5:7
Number of peripheral groups	4	Chiral centres	5

Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	2	12	1	4
Substituent	8	26	7	14
Peripheral groups	2	2	1	1
Total	12	40	9	19

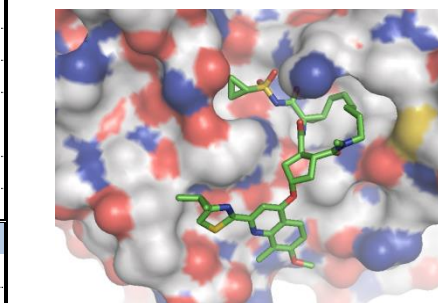
Protein name	HCV NS3/NS4A		
Organism	Hepatitis C virus		
Classification	Hydrolase		
Binding mode	Edge-on		
Receptor secondary structure topology			
Number of residue 'hotspots'	18		

Number of protein-ligand interactions* (Database link)			
Hydrogen bond	6	Hydrogen donor-π	
Ionic interaction		π-π	
Cation-dipole		VdW interaction	26
Cation-π	1	Unfavourable	1
Dipolar interaction		Poor-angle	1
Halogen bond		Unclassified	2
Water-mediated interaction			

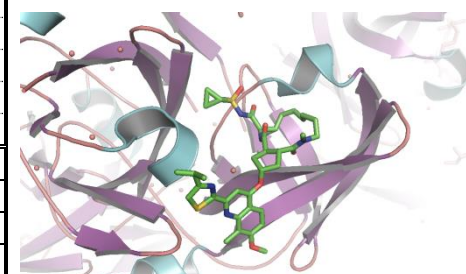


Physicochemical properties
[click for publication](#)

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis