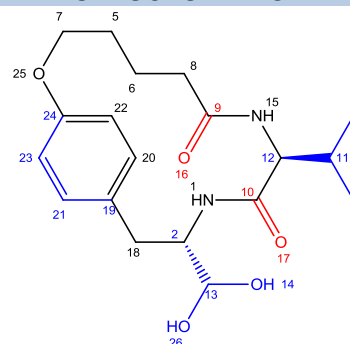
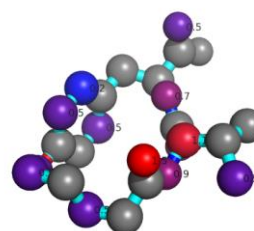


CODE	3BXS (PDB)	Resolution		
Name		Ring size	16	
Formula	C19H28N2O5	# Ligand atoms	26	
Type	Macrocycle	Scorpion Score	8.9	
Mol. Weight (Da)	364.44	Saturated/Unsaturated	U	
cLogP	1.445	Chiral centres.ring	2	
tPSA	107.89	Chiral centres.sub	0	
#HBD's	4			
#HBA's	3			
NRB (RING)	11	NRB (SUBSTITUENT)	2	
Number of substituents	3	P/NP balance, substituents	2/6	
Large ($\geq 5HA$)	-	P/NP balance, peripheral groups	2/0	
Small (2-4HA)	3	Degrees of unsaturation ring	7	
Proportion HA in substituents	31%	N:O ratio	2:5	
Number of peripheral groups	2	Chiral centres	2	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	3	13	3	5
Substituent	2	6	1	2
Peripheral groups	2	-	2	-
Total	7	19	5	7
Protein name	HIV-1 protease			
Organism	Human immunodeficiency virus 1			
Classification	Hydrolase			
Binding mode	Compact mode			
Receptor secondary structure topology				
Number of residue 'hotspots'	11			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	6	Hydrogen donor- π	1	
Ionic interaction	-	π - π	1	
Cation-dipole	-	VdW interaction	5	
Cation- π	-	Unfavourable	1	
Dipolar interaction	-	Poor-angle	1	
Halogen bond	-	Unclassified	-	
Water-mediated interaction	2			

2D-STRUCTURE LIGAND

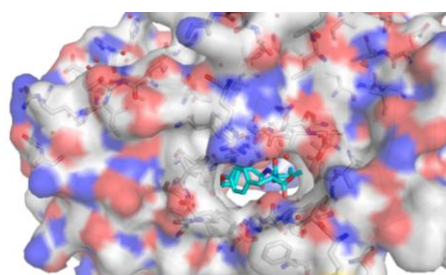


3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



Physicochemical properties

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

LIGAND-PROTEIN COMPLEX (II)

