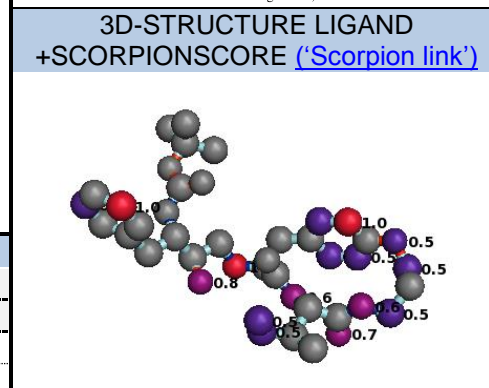
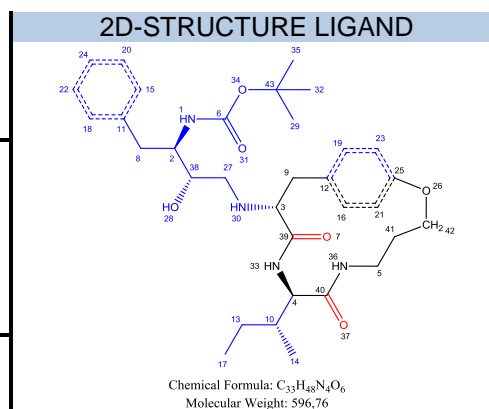


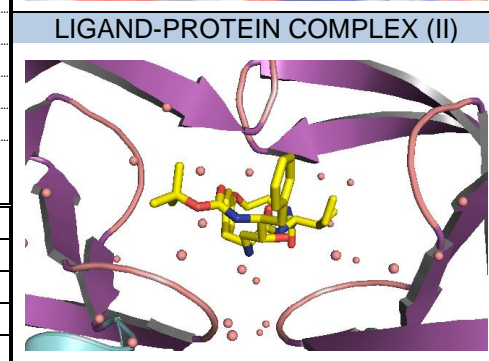
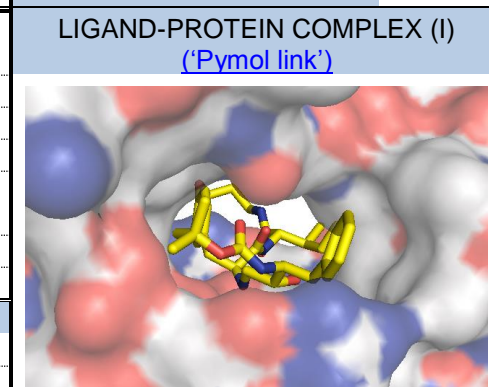
CODE	1MTR (PDB)	Resolution	1.8	
Name		Ring size	15	
Formula	C ₃₃ H ₄₈ N ₄ O ₆	# Ligand atoms	43	
Type	Macrocycle	Scorpion Score	10.8	
Mol. Weight (Da)	596,76	Saturated/ Unsaturated	U	
cLogP	4.72	Chiral centres.ring	2	
tPSA	138	Chiral centres.sub	3	
#HBD's	5			
#HBA's	10			
N _{RB} (RING)	10	N _{RB} (SUBSTITUENT)	11	
Number of substituents	3	P/NP balance, substituents	5/21	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	2/0	
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	12	
Proportion HA in substituents	60.5%	N:O ratio	4:6	
Number of peripheral groups	2	Chiral centres	5	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	3	12	3	4
Substituent	5	21	2	6
Peripheral groups	2	-	1	-
Total	10	33	6	10



Physicochemical properties

'click for publication' (not available)

Protein name	HIV-1 protease		
Organism	Human immunodeficiency virus 1		
Classification	Hydrolase/ hydrolase inhibitor		
Binding mode			
Receptor secondary structure topology			
Number of residue 'hotspots'			
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	6	Hydrogen donor-π	2
Ionic interaction	2	π-π	
Cation-dipole		VdW interaction	13
Cation-π		Unfavourable	2
Dipolar interaction		Poor-angle	3
Halogen bond		Unclassified	1
Water-mediated interaction	1	Intermolecular h-bond (H ₂ O mediated)	1



*Based on Scorpion® analysis