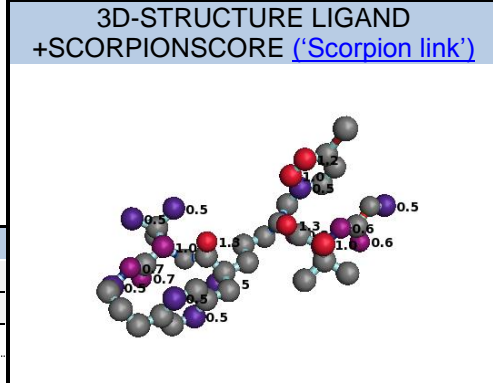
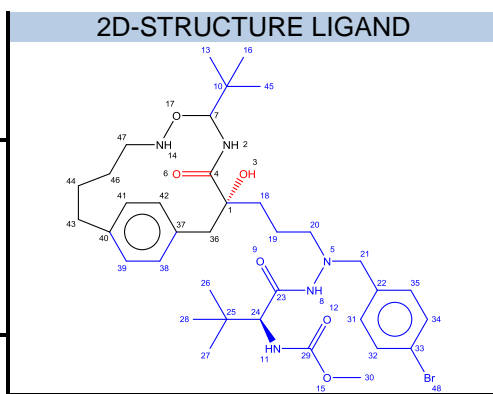


CODE	3ZPU(PDB)	Resolution	1.8	
Name	Compound 19b	Ring size	15	
Formula	C36H66BrN5O6	# Ligand atoms	49	
Type	macrocycle	Scorpion Score	14.1	
Mol. Weight (Da)	745	Saturated/Unsaturated	U	
cLogP	8.15	Chiral centres.ring	2	
tPSA	141	Chiral centres.sub	1	
#HBD's	4			
#HBA's	11			
N _{RB} (RING)	11	N _{RB} (SUBSTITUENT)	12	
Number of substituents	3	P/NP balance, substituents	7/24	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	2/0	
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	6	
Proportion HA in substituents	63.3%	N:O ratio	5:6	
Number of peripheral groups	2	Chiral centres	3	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	3	12	2	4
Substituent	7	24	4	7
Peripheral groups	2	-	2	-
Total	12	36	8	11

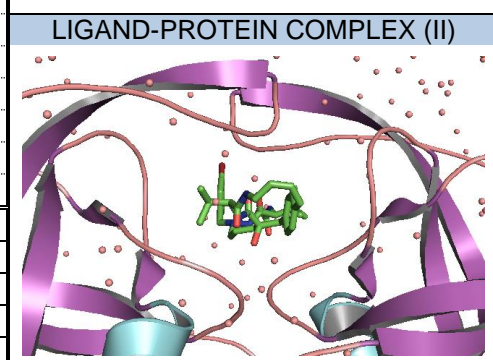
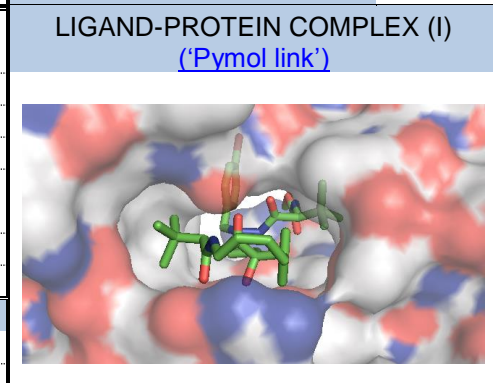
Protein name	HIV-1 Protease		
Organism	Human immunodeficiency virus 1		
Classification	Hydrolase		
Binding mode	Compact		
Receptor secondary structure topology			
Number of residue 'hotspots'	20		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	9	Hydrogen donor-π	
Ionic interaction		π-π	1
Cation-dipole		VdW interaction	14
Cation-π		Unfavourable	3
Dipolar interaction	1	Poor-angle	2
Halogen bond		Unclassified	
Water-mediated interaction	2		



Physicochemical properties

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Ki (nM)	4.2
EC50 (μM)	1.0
CC50 (μM)	30



*Based on Scorpion® analysis