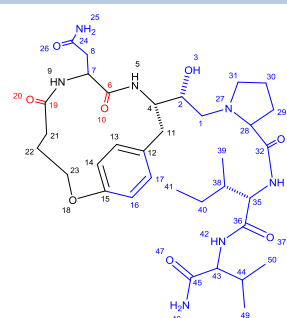
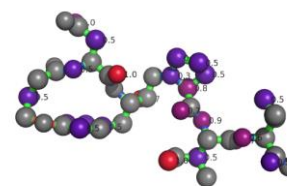


CODE	1B6J (PDB)	Resolution	1.85	
Name		Ring size	15	
Formula	C34H53N7O8	# Ligand atoms	49	
Type	macrocycle	Scorpion Score	14.5	
Mol. Weight (Da)	687.39	Saturated/Unsaturated	U	
cLogP		Chiral centers.ring	2	
tPSA		Chiral centers.sub	5	
#HBD's	9			
#HBA's	8			
N _{RB} (SUBSTITUENT)	13	N _{RB} (RING)	10	
Number of substituents	3	P/NP balance, substituents	10/19	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	2/0	
<i>Small (2-4HA)</i>	2			
Proportion HA in substituents	59%	Degrees of unsaturation ring	12	
Number of peripheral groups	2	N:O ratio	7:8	
		Chiral centres	7	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	3	12	1	4
Substituent	10	19	8	9
Peripheral groups	2	0	1	
Total	15	31	10	013
Protein name	HIV-1 protease			
Organism	Human immunodeficiency virus 1			
Classification	Hydrolase/ Hydrolase inhi			
Binding mode	Compact			
Receptor secondary structure topology				
Number of residue 'hotspots'	21			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	12	Hydrogen donor-π	1	
Ionic interaction	-	π-π	-	
Cation-dipole	-	VdW interaction	13	
Cation-π	-	Unfavourable	3	
Dipolar interaction	1	Poor-angle	5	
Halogen bond	-	Unclassified	-	
Water-mediated interaction	2			

2D-STRUCTURE LIGAND



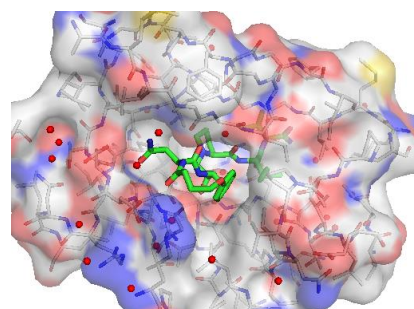
3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



Physicochemical properties

['click for publication'](#)

LIGAND-PROTEIN COMPLEX (I) ('Pymol link')



LIGAND-PROTEIN COMPLEX (II)

