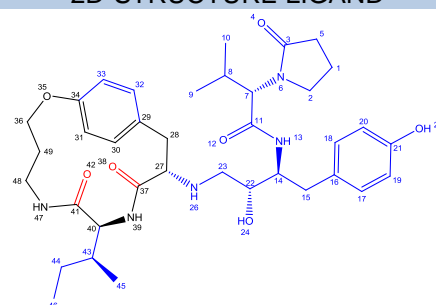


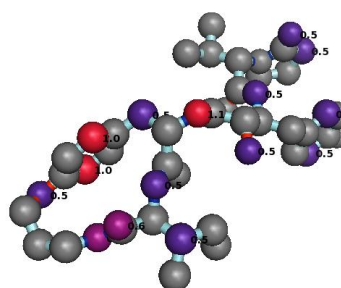
CODE	1B6K(PDB)	Resolution	1.85	
Name	HIVKI-5	Ring size	15	
Formula	C37H50N5O7	# Ligand atoms	49	
Type	macrocycle	Scorpion Score	9.4	
Mol. Weight (Da)	679,84	Saturated/ Unsaturated	U	
cLogP	3.54	Chiral centre.ring	2	
tPSA	171	Chiral centre.sub	4	
#HBD's	6			
#HBA's	12			
N _{RB} (RING)	12	N _{RB} (SUBSTITUENT)	12	
Number of substituents	3	P/NP balance, substituents	7/25	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	2/0	
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	15.5	
Proportion HA in substituents	65%	N:O ratio	5:7	
Number of peripheral groups	2	Chiral centres	6	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	3	12	3	2
Substituent	7	25	4	5
Peripheral groups	2	-	1	-
Total	12	37	8	7
Protein name	HIV-1 Protease			
Organism	Human immunodeficiency virus 1			
Classification	Hydrolase/Hydrolase inhibitor			
Binding mode	Compact			
Receptor secondary structure topology				
Number of residue 'hotspots'	17			
Number of protein-ligand interactions* (Database link)				
Hydrogen bond	8	Hydrogen donor-π	1	
Ionic interaction	2	π-π		
Cation-dipole		VdW interaction	10	
Cation-π		Unfavourable		
Dipolar interaction		Poor-angle	3	
Halogen bond		Unclassified	2	
Water-mediated interaction	5	Intramolecular hydrogen bond water mediated	1	

2D-STRUCTURE LIGAND



Chemical Formula: C₃₇H₄₃N₅O₇
Molecular Weight: 679.8460

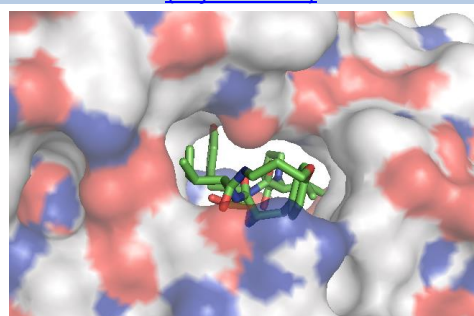
3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))



Physicochemical properties

[click for publication](#)

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



LIGAND-PROTEIN COMPLEX (II)

