CODE	1B6M (PDB)	Resolution	1.85
Name		Ring size	15
Formula	C33H49N4O6+	# Ligand atoms	43
Type	macrocycle	Scorpion Score	13.6

Mol. Weight (Da)	597.36	Saturated/ Unsaturated	U
cLogP	4.9968		
tPSA	142.6	Chiral centres.ring	2
#HBD's	5	Chiral centres.sub	3
#HBA's	5		
$N_{RB\ (RING)}$	10	$N_{RB\ (SUBSTITUENT)}$	10

Number of substituents	3	P/NP balance, substituents	5/21
Large (≥5HA)	1	P/NP balance, peripheral groups	2/0
Small (2-4HA)	2		
Proportion HA in substituents	60%	Degrees of unsaturation ring	15
Number of peripheral groups	2	N:O ratio	4:6
		Chiral centres	5

Polarity distribution ligand atoms

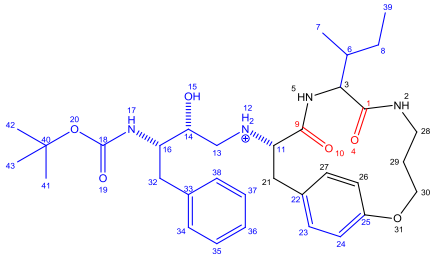
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	12	2	5
Substituent	5	21	3	6
Peripheral groups	2	-	2	0
Total	10	33	7	11

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'	21

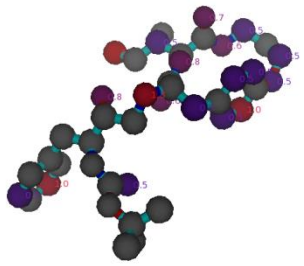
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	5	Hydrogen donor-π	2
Ionic interaction	2	π-π	-
Cation-dipole	-	VdW interaction	16
Cation-π	-	Unfavourable	-
Dipolar interaction	-	Poor-angle	2
Halogen bond	-	Unclassified	2
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



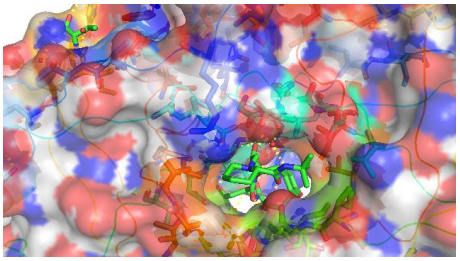
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



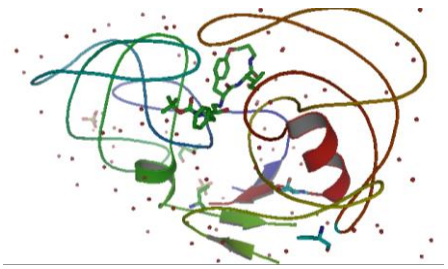
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis

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