CODE	1B6L (PDB)	Resolution	1.75
Name		Ring size	15
Formula	C28H44N5O6+	# Ligand atoms	46
Type	macrocycle	Scorpion Score	11

Mol. Weight (Da)	545,67	Saturated/ Unsaturated	U
cLogP	1.18		
tPSA	164.29	Chiral centre.ring	2
#HBD's	7	Chiral centre.sub	2
#HBA's	5		
$N_{RB\ (RING)}$	10	$N_{RB\ (SUBSTITUENT)}$	7

Number of substituents	3	P/NP balance, substituents	6/16
Large (≥5HA)	1	P/NP balance, peripheral groups	2/0
Small (2-4HA)	2		
Proportion HA in substituents	48%	Degrees of unsaturation ring	9.5
Number of peripheral groups	2	N:O ratio	5/6
		Chiral centres	4

Polarity distribution ligand atoms

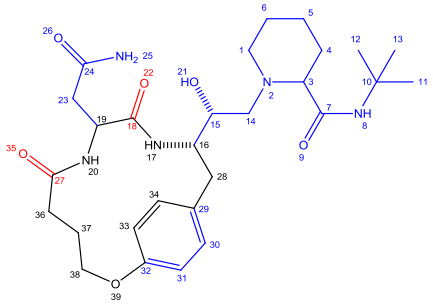
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	12	2	2
Substituent	6	16	4	6
Peripheral groups	2	-	1	0
Total	11	28	7	8

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'	14

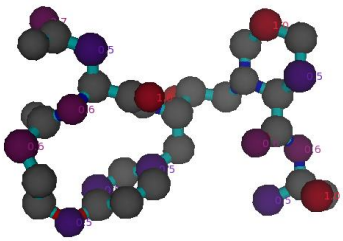
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	7	Hydrogen donor-π	-
Ionic interaction	-	π-π	1
Cation-dipole	-	VdW interaction	10
Cation-π	-	Unfavourable	4
Dipolar interaction	1	Poor-angle	5
Halogen bond	-	Unclassified	1
Water-mediated interaction	2		

2D-STRUCTURE LIGAND



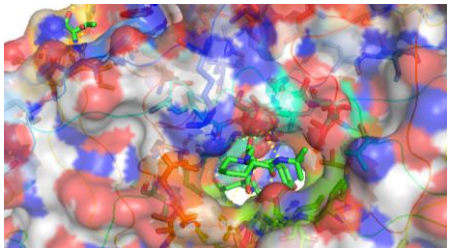
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



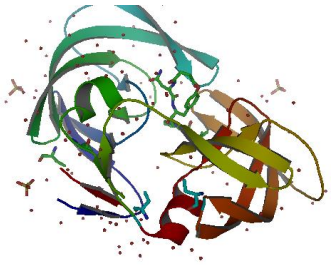
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis

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