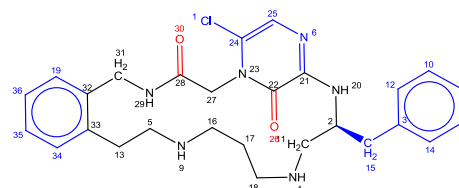
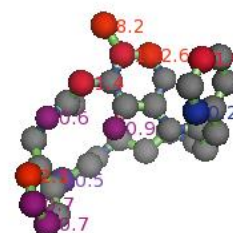


CODE	1NM6(PDB)	Resolution	1.8	
Name		Ring size	19	
Formula	C27H33ClN6O2	# Ligand atoms	36	
Type	Macrocycle	Scorpion Score	19.5	
Mol. Weight (Da)	509,04	Saturated/ Unsaturated	U	
cLogP	3.26	Chiral centres.ring	1	
tPSA	100	Chiral centres.sub	-	
#HBD's	4			
#HBA's	8			
N <sub>RB</sub> (RING)	15	N <sub>RB</sub> (SUBSTITUENT)	2	
Number of substituents	3	P/NP balance, substituents	5/14	
Large (≥5HA)	2	P/NP balance, peripheral groups	2/0	
Small (2-4HA)	1	Degrees of unsaturation ring	14	
Proportion HA in substituents	41.7%	N:O ratio	3:1	
Number of peripheral groups	2	Chiral centres	1	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	5	14	1	2
Substituent	1	14	-	8
Peripheral groups	2	-	1	-
Total	8	28	2	10
Protein name	Thrombin			
Organism	Homo Sapiens  Hirudo medicinalis			
Classification	Blood clotting/ hydrolase inhibitor			
Binding mode	Edge-on			
Receptor secondary structure topology				
Number of residue 'hotspots'	14			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	4	Hydrogen donor-π	2	
Ionic interaction	-	π-π	5	
Cation-dipole	-	VdW interaction	18	
Cation-π	-	Unfavourable	4	
Dipolar interaction	-	Poor-angle	3	
Halogen bond	-	Unclassified	1	
Water-mediated interaction	2			

## 2D-STRUCTURE LIGAND



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

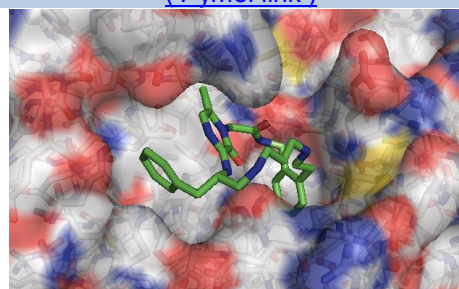


## Physicochemical properties

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Thrombin Ki (nM)	0.09
2x APTT (μM)	0.47
Trypsin Ki (μM)	2.1

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



## LIGAND-PROTEIN COMPLEX (II)

