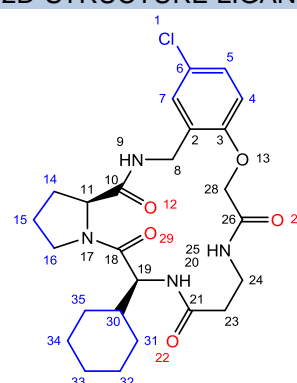


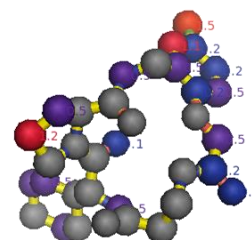
CODE	1NT1(PDB)	Resolution	2.0	
Name	Comp. 8	Ring size	17	
Formula	C23H33ClN4O5	# Ligand atoms	35	
Type	MACROCYCLE	Scorpion Score	9.3	
Mol. Weight (Da)	505	Saturated/Unsaturated	U	
cLogP	3.30	Chiral centres.ring	2	
tPSA	117	Chiral centres.sub	-	
#HBD's	3			
#HBA's	10			
N _{RB} (ring)	11	N _{RB} (SUBSTITUENT)	1	
Number of substituents	3	P/NP balance, substituents	0/14	
<i>Large (≥5HA)</i>	2	P/NP balance, peripheral groups	4/0	
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	11	
Proportion HA in substituents	40%	N:O ratio	4:5	
Number of peripheral groups	4	Chiral centres	2	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	5	12	2	4
Substituent	0	17	-	10
Peripheral groups	4	-	2	-
Total	5	29	4	14

Protein name	Thrombin		
Organism	Homo sapiens Hirudo medicinalis		
Classification	Blood clotting/ Hydrolase inhibitor		
Binding mode	Compact		
Receptor secondary structure topology			
Number of residue 'hotspots'	13		
Number of protein-ligand interactions* (Database link)			
Hydrogen bond	3	Hydrogen donor-π	2
Ionic interaction		π-π	6
Cation-dipole		VdW interaction	13
Cation-π		Unfavourable	1
Dipolar interaction	1	Poor-angle	
Halogen bond		Unclassified	2
Water-mediated interaction	-		

2D-STRUCTURE LIGAND



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

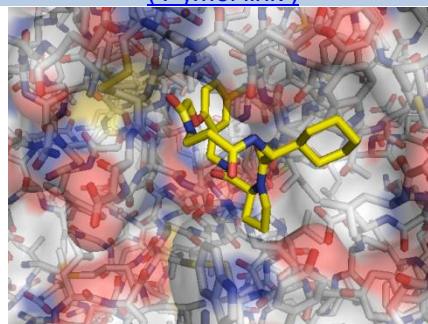


Physicochemical properties

[click for publication](#)

Thrombin Ki(nM)	1.3
2xAPTT (μM)	0.36
Trypsin Ki (μM)	21.5
tPA Ki (μM)	5.6

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



LIGAND-PROTEIN COMPLEX (II)

