CODE	1TMB(PDB)	Resolution	2.3
Name	Cyclotheonamide A	Ring size	19
Formula	C36H53N9O8	# Ligand atoms	53
Type	Cyclic peptide	Scorpion Score	14.1

Mol. Weight (Da)	740	Saturated/ Unsaturated	U
cLogP			
tPSA	269	Chiral centres.ring	6
#HBD's	11	Chiral centres.sub	1
#HBA's	17		
$N_{RB\ (RING)}$	13	$N_{RB\ (SUBSTITUENT)}$	10
Number of substituents	5	P/NP balance, substituents	6/22
Large (≥5HA)	3	P/NP balance, peripheral groups	6/0
Small (2-4HA)	2		
Proportion HA in substituents	52.8%	Degrees of unsaturation ring	15
Number of peripheral groups	6	N:O ratio	9:8
		Chiral centres	7

Polarity distribution ligand atoms

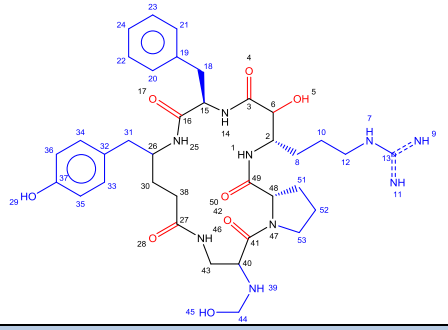
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	5	14	1	2
Substituent	6	22	4	7
Peripheral groups	6	-	3	-
Total	17	36	8	9

Protein name	Human alpha-thrombin
Organism	Homo sapiens| Hirudo medicinalis| Theonella sp.
Classification	Hydrolase/ hydrolase inhibitor
Binding mode	Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	16

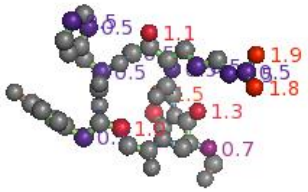
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	10	Hydrogen donor-π	3
Ionic interaction	2	π-π	-
Cation-dipole	-	VdW interaction	16
Cation-π	1	Unfavourable	4
Dipolar interaction	-	Poor-angle	4
Halogen bond	-	Unclassified	2
Water-mediated interaction	-	Intermol. hbond	1

2D-STRUCTURE LIGAND



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

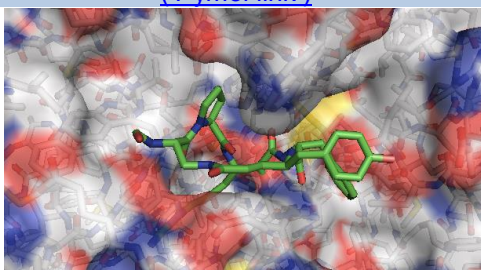


Physicochemical properties

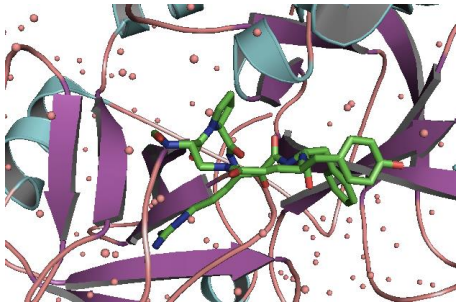
'click for publication'

Thrombin Ki (µM)	0.18 ±0.04
Plasmin Ki (µM)	0.37±0.08
Kalikrein Ki (µM)	0.51±0.21
See publ. table 2 for more	

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis