CODE	1AY6 (PDB)	Resolution	1.8
Name	Comp 3i	Ring size	19
Formula	C30H45N7O5	# Ligand atoms	42
Type	Macrocycle	Scorpion Score	4.5

Mol. Weight (Da)	583,72	Saturated/ Unsaturated	U
cLogP	3.3804		
tPSA	186.58	Chiral centers(ring)	3
#HBD's	7	Chiral centers(sub)	0
#HBA's	6		
$N_{RB\ (SUBSTITUENT)}$	7	$N_{RB\ (RING)}$	15

Number of substituents	3	P/NP balance, substituents	3/15
Large (≥5HA)	2	P/NP balance, peripheral groups	5/0
Small (2-4HA)	1		
Proportion HA in substituents	43%	Degrees of unsaturation ring	12
Number of peripheral groups	5	N:O ratio	7/5
		Chiral centres	3

Polarity distribution ligand atoms

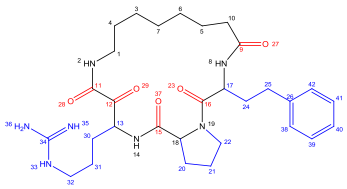
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	4	15	1	2
Substituent	3	15	2	7
Peripheral groups	5	0	1	0
Total	12	30	4	9

Protein name	Thrombin
Organism	Homo sapiens
Classification	Hydrolase/ Hydrolase inhibitor
Binding mode	Edge on
Receptor secondary structure topology	
Number of residue 'hotspots'	15

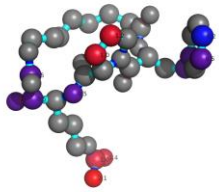
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	5	Hydrogen donor-π	-
Ionic interaction	2	π-π	1
Cation-dipole	-	VdW interaction	12
Cation-π	1	Unfavourable	6
Dipolar interaction	-	Poor-angle	3
Halogen bond	-	Unclassified	1
Water-mediated interaction	3		

2D-STRUCTURE LIGAND



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

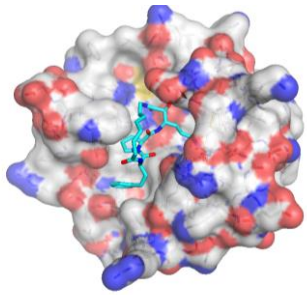


Physicochemical properties

'click for publication'

Ki thrombin [b]	20 + 2.8
Ki trypsin [b]	14 + 2.4

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



LIGAND-PROTEIN COMPLEX (II)

*Based on Scorpion® analysis

*Based on Scorpion® analysis