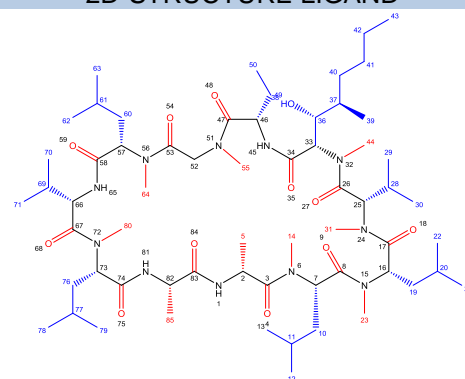
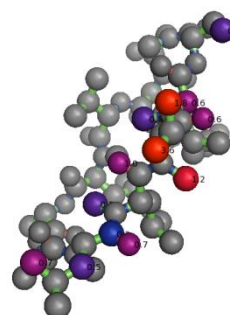


CODE	1C5F(PDB)	Resolution	2.7	
Name	Cyclosporin A	Ring size	33	
Formula	C62H113N11O12	# Ligand atoms	85	
Type	Cyclic peptide	Scorpion Score	12.4	
Mol. Weight (Da)	1205	Saturated/ Unsaturated	S	
cLogP	14.8	Chiral centres.ring	8	
tPSA	279	Chiral centres.sub	2	
#HBD's	5	NRB (SUBSTITUENT)		
#HBA's	22	NRB (PERIPHERAL)		
NRB (RING)				
Number of substituents	8	P/NP balance, substituents	1/31	
Large ($\geq 5HA$)	1	P/NP balance, peripheral groups	11/9	
Small (2-4HA)	7	Degrees of unsaturation ring	12	
Proportion HA in substituents	37.6%	N:O ratio	11:12	
Number of peripheral groups	20	Chiral centres	10	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	11	22	-	-
Substituent	1	31	-	5
Peripheral groups	11	9	3	4
Total	23	62	3	9
Protein name	Cyclophilin –like domain			
Organism	Brugia malayi Toxoplasma gondii			
Classification	Isomerase/ Immunosuppressant			
Binding mode	Edge-on			
Receptor secondary structure topology				
Number of residue 'hotspots'	13			
Number of protein-ligand interactions* (Database link)				
Hydrogen bond	5	Hydrogen donor- π	2	
Ionic interaction		π - π	2	
Cation-dipole		VdW interaction	14	
Cation- π		Unfavourable	3	
Dipolar interaction	1	Poor-angle	1	
Halogen bond		Unclassified	1	
Water-mediated interaction	-			

2D-STRUCTURE LIGAND



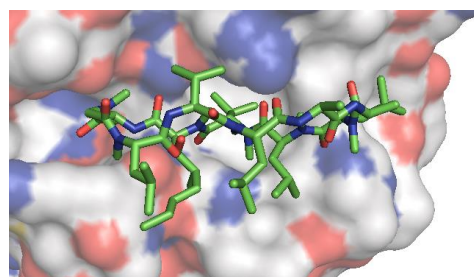
3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))



Physicochemical properties

[click for publication](#)

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



LIGAND-PROTEIN COMPLEX (II)

