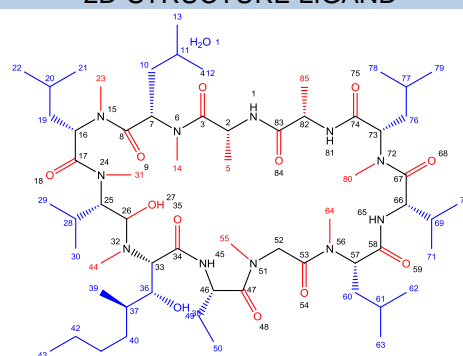
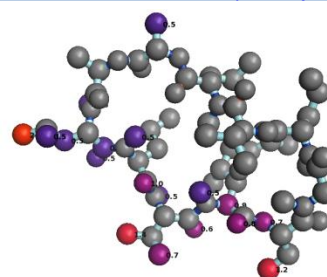


CODE	2X2C (PDB)	Resolution	2.41	
Name	Cyclosporine	Ring size	33	
Formula	C62H117N11O13	# Ligand atoms	85	
Type	Cyclic peptide	Scorpion Score	14.6	
Mol. Weight (Da)	1225	Saturated/ Unsaturated	S	
cLogP	14.19	Chiral centres.ring	10	
tPSA	313	Chiral centres.sub	2	
#HBD's	6	NRB (SUBSTITUENT)		
#HBA's	29	NRB (PERIPHERAL)		
NRB (RING)				
Number of substituents	8	P/NP balance, substituents	11/22	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	11/9	
<i>Small (2-4HA)</i>	7	Degrees of unsaturation ring	10	
Proportion HA in substituents	38.8%	N:O ratio	11:13	
Number of peripheral groups	20	Chiral centres	12	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	11	22	1	2
Substituent	2	31	-	6
Peripheral groups	11	9	4	5
Total	24	62	5	13
Protein name	Acetyl-Cyclophilin A (CYPA)			
Organism	Tolypocladium inflatum Homo sapiens			
Classification	Isomerase/ immunosuppressant			
Binding mode				
Receptor secondary structure topology	Edge-on			
Number of residue 'hotspots'	13			
Number of protein-ligand interactions* (Database link)				
Hydrogen bond	7	Hydrogen donor-π	-	
Ionic interaction	-	π-π	-	
Cation-dipole	-	VdW interaction	17	
Cation-π	-	Unfavourable	1	
Dipolar interaction	1	Poor-angle	2	
Halogen bond	-	Unclassified	1	
Water-mediated interaction	-			

2D-STRUCTURE LIGAND



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

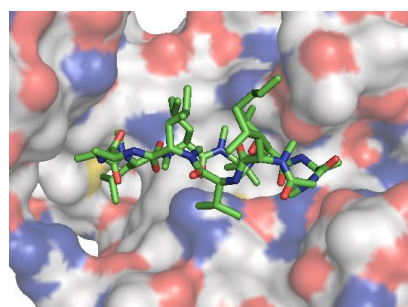


Physicochemical properties

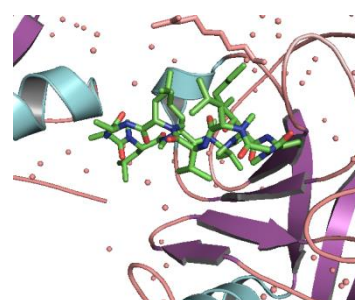
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Ki	27 ± 5.6 nM
Kd	1 ± 1.2 nM

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis

