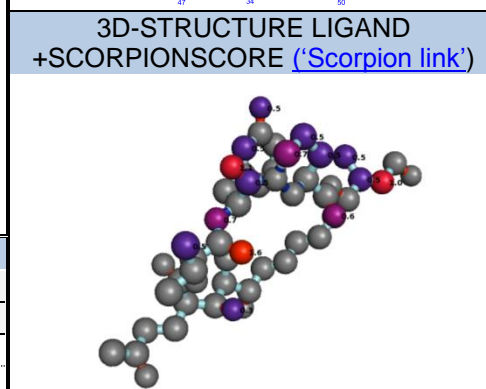
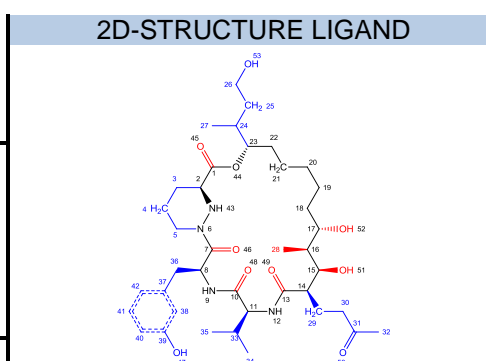
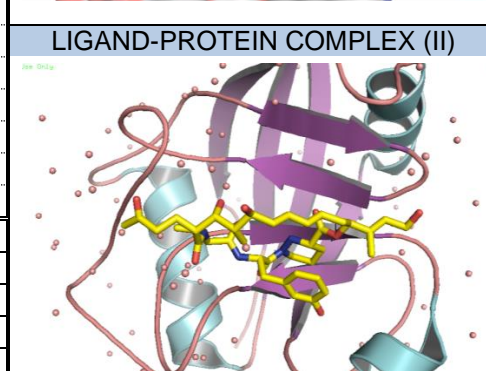
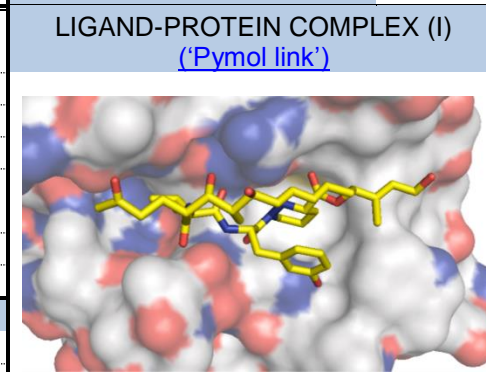


CODE	1NMK (PDB)	Resolution	2.1	
Name		Ring size	22	
Formula	C39H62N4O10	# Ligand atoms	53	
Type	macrocycle	Scorpion Score	9.4	
Mol. Weight (Da)	746,93	Saturated/ Unsaturated	S	
cLogP	3.72	Chiral centres.ring	8	
tPSA	215	Chiral centres.sub	2	
#HBD's	7			
#HBA's	14			
N _{RB} (RING)	16	N _{RB} (SUBSTITUENT)	9	
Number of substituents	5	P/NP balance, substituents	3/21	
<i>Large</i> (≥5HA)	3	P/NP balance, peripheral groups	6/1	
<i>Small</i> (2-4HA)	2	Degrees of unsaturation ring	11	
Proportion HA in substituents	45.3%	N:O ratio	4:10	
Number of peripheral groups	7	Chiral centres	10	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	5	17	1	1
Substituent	3	21	1	8
Peripheral groups	6	1	4	-
Total	14	39	6	9



Physicochemical properties
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Protein name	Cyclophilin		
Organism	Homo Sapiens		
Classification	Isomerase		
Binding mode			
Receptor secondary structure topology	Face-on		
Number of residue 'hotspots'	11		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	7	Hydrogen donor-π	1
Ionic interaction		π-π	
Cation-dipole	2	VdW interaction	10
Cation-π		Unfavourable	2
Dipolar interaction		Poor-angle	
Halogen bond		Unclassified	2
Water-mediated interaction	4		



*Based on Scorpion® analysis