CODE	1YND(PDB)	Resolution	1.6
Name		Ring size	22
Formula	C60H99N5O13	# Ligand atoms	78
Type	macrocycle	Scorpion Score	8

Mol. Weight (Da)	1098	Saturated/ Unsaturated	S
cLogP	7.96		
tPSA	273	Chiral centres.ring	8
#HBD's	11	Chiral centres.sub	11
#HBA's	19		
$N_{RB\ (RING)}$	19	$N_{RB\ (SUB)}$	17
Number of substituents	5	P/NP balance, substituents	7/42
Large (≥5HA)	3	P/NP balance, peripheral groups	6/1
Small (2-4HA)	2		
Proportion HA in substituents	62.8%	Degrees of unsaturation ring	14
Number of peripheral groups	7	N:O ratio	5:13
		Chiral centres	19

Polarity distribution ligand atoms

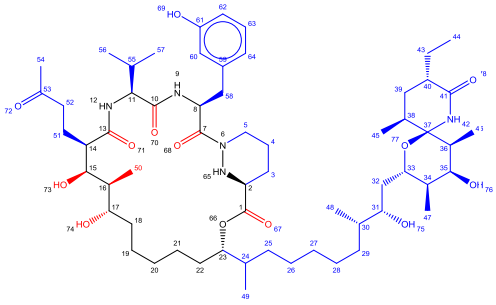
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	5	17	1	-
Substituent	7	42	1	8
Peripheral groups	6	1	4	-
Total	18	60	6	8

Protein name	Cyclophilin A
Organism	Homo Sapiens
Classification	Isomerase
Binding mode	Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	8

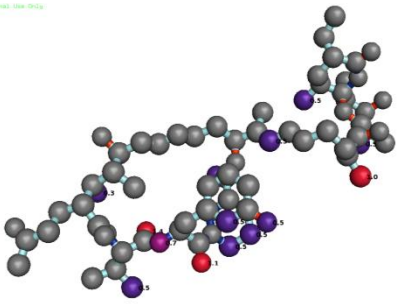
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	6	Hydrogen donor-π	2
Ionic interaction	-	π-π	-
Cation-dipole	2	VdW interaction	9
Cation-π	-	Unfavourable	2
Dipolar interaction	-	Poor-angle	1
Halogen bond	-	Unclassified	-
Water-mediated interaction	4		

2D-STRUCTURE LIGAND



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



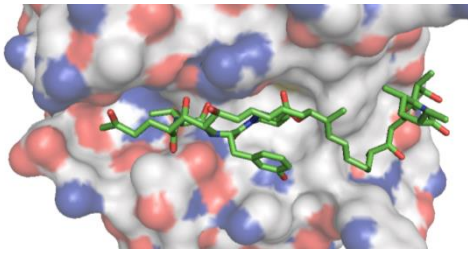
Physicochemical properties

'click for publication'

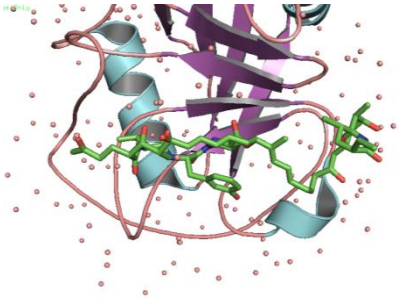
CypA binding (nM)	3.6 ÷1.2
MLR (nM)	170 ÷ 30

LIGAND-PROTEIN COMPLEX (I)

('Pymol link')



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis