

CODE	1W96 (PDB)	Resolution	1.8
Name	Soraphen A	Ring size	16
Formula	C29H46O8	# Ligand atoms	37
Type	Natural product macrocycle	Scorpion Score	12.5

Mol. Weight (Da)	522.67	Saturated/Unsaturated	U
cLogP	3.3826	Chiral centres.ring	7
tPSA	103.68	Chiral centres.sub	3
#HBD's	2		
#HBA's	6		
NRB (RING)	16	NRB (SUBSTITUENT)	4

Number of substituents	4	P/NP balance, substituents	4/13
Large ($\geq 5HA$)	2	P/NP balance, peripheral groups	2/2
Small (2-4HA)	2	Degrees of unsaturation ring	7
Proportion HA in substituents	46%	N:O ratio	0/8
Number of peripheral groups	4	Chiral centres	10

Polarity distribution ligand atoms

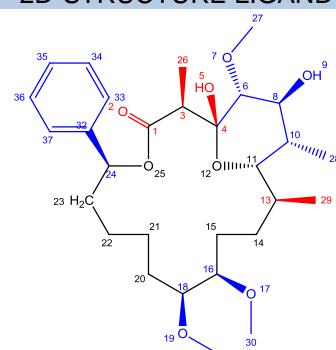
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	2	14	-	5
Substituent	4	13	2	6
Peripheral groups	2	2	1	3
Total	8	29	3	14

Protein name	Eukaryotic Acetyl-Coenzyme A Carboxylase		
Organism	Saccharomyces cerevisiae		
Classification	Ligase		
Binding mode	Face on		
Receptor secondary structure topology			
Number of residue 'hotspots'	11		

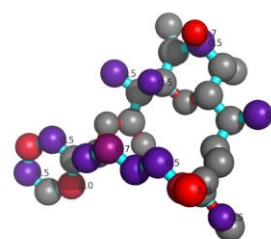
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	5	Hydrogen donor- π	-
Ionic interaction	-	π - π	-
Cation-dipole	-	VdW interaction	18
Cation- π	-	Unfavourable	1
Dipolar interaction	-	Poor-angle	2
Halogen bond	-	Unclassified	-
Water-mediated interaction	-		

2D-STRUCTURE LIGAND



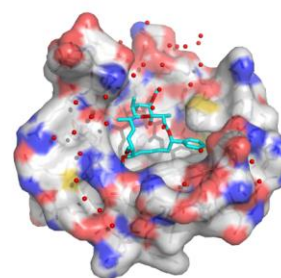
3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



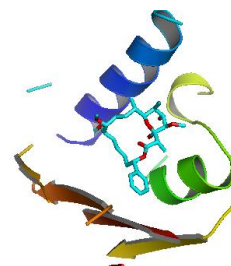
Physicochemical properties

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis