

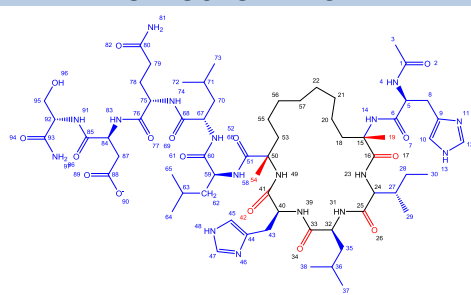
CODE	2YJD(PDB)	Resolution	1.93
Name		Ring size	21
Formula	C64H104N17O16	# Ligand atoms	97
Type	Staple peptide	Scorpion Score	6.4
Mol. Weight (Da)	1368	Saturated/Unsaturated	S
cLogP	-1.35	Chiral centres.ring	5
tPSA	515	Chiral centres.sub	7
#HBD's	22	N _{RB} (SUBSTITUENT)	
#HBA's	53	N _{RB} (PERIPHERAL)	
N _{RB} (RING)			
Number of substituents	5	P/NP balance, substituents	25/45
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	4/2
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	21.5
Proportion HA in substituents	72.2%	N:O ratio	17:16
Number of peripheral groups	6	Chiral centres	12

Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	4	17	-	3
Substituent	25	45	2	5
Peripheral groups	4	2	-	-
Total	33	64	2	8

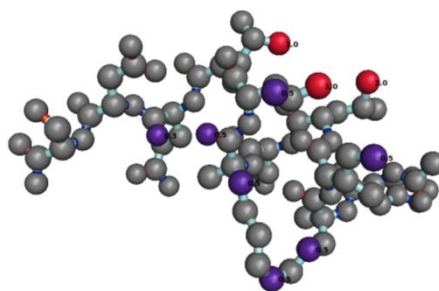
Protein name	Estrogen receptor beta		
Organism	Homo Sapiens		
Classification	Hormone receptor/ Peptide		
Binding mode			
Receptor secondary structure topology			
Number of residue 'hotspots'	7		

Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	1	Hydrogen donor-π	
Ionic interaction	1	π-π	
Cation-dipole	1	VdW interaction	11
Cation-π		Unfavourable	1
Dipolar interaction		Poor-angle	
Halogen bond		Unclassified	
Water-mediated interaction			

2D-STRUCTURE LIGAND



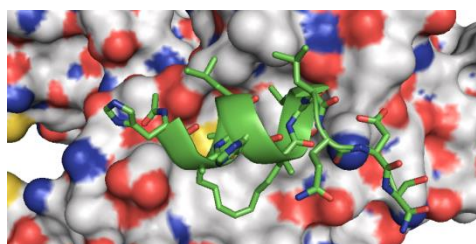
3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



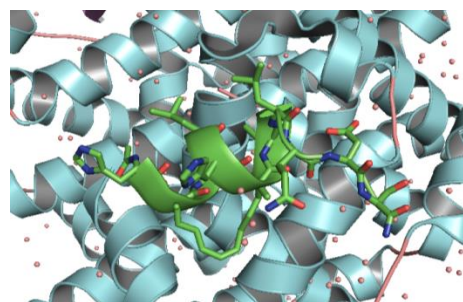
Physicochemical properties

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis