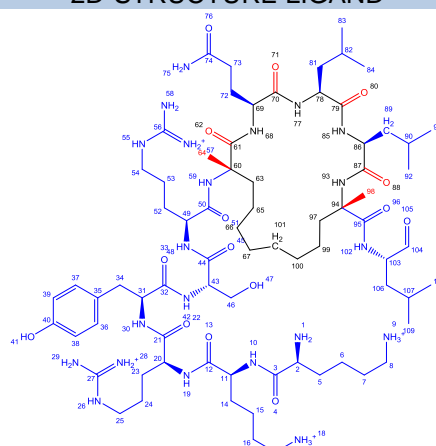
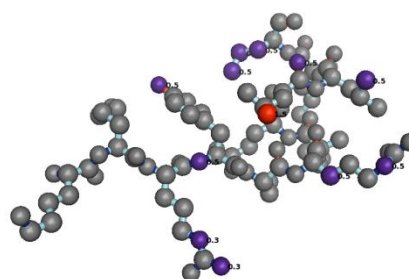


CODE	4BEA(PDB)	Resolution	2.57
Name		Ring size	21
Formula	C73H133N21O15	# Ligand atoms	109
Type	Stapled peptide	Scorpion Score	7.2
Mol. Weight (Da)	1545	Saturated/ Unsaturated	S
cLogP	0.13		
tPSA	629		
#HBD's	51		
#HBA's	77	NRB (SUBSTITUENT)	
NRB (RING)		NRB (PERIPHERAL)	
Number of substituents	5	P/NP balance, substituents	28/54
Large ($\geq 5HA$)	5	P/NP balance, peripheral groups	4/2
Small (2-4HA)	-	Degrees of unsaturation ring	18
Proportion HA in substituents	75.2%	N:O ratio	21:15
Number of peripheral groups	6	Chiral centres	
Polarity distribution ligand atoms			
	All		Contact
	Polar	Nonpolar	Polar Nonpolar
Ring	4	17	
Substituent	28	54	
Peripheral groups	4	2	
Total	36	73	
Protein name	eIF4E		
Organism	Homo sapiens synthetic construct		
Classification	Translation		
Binding mode			
Receptor secondary structure topology			
Number of residue 'hotspots'	12		
Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	4	Hydrogen donor- π	
Ionic interaction	1	π - π	
Cation-dipole	1	VdW interaction	9
Cation- π		Unfavourable	2
Dipolar interaction		Poor-angle	4
Halogen bond		Unclassified	
Water-mediated interaction	4		

2D-STRUCTURE LIGAND



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

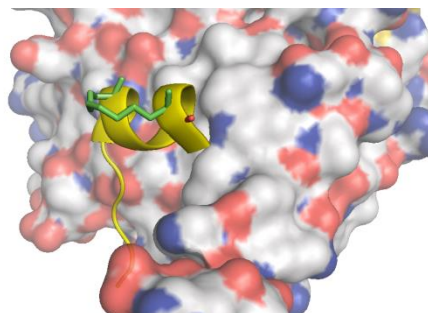


Physicochemical properties

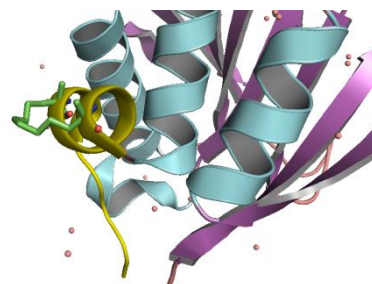
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Kd SPR (nM)	5.0 ± 0.7
Kd FP (nM)	11.5 ± 3.6

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis

