

CODE	2AOA(PDB)	Resolution	2.0
Name	F222	Ring size	15
Formula	C41H53N4O10	# Ligand atoms	55
Type	Cyclic peptide	Scorpion Score	16.9

Mol. Weight (Da)	762	Saturated/Unsaturated	S
cLogP	3.90	Chiral centres.ring	5
tPSA	262	Chiral centres.sub	-
#HBD's	12	NRB (SUBSTITUENT)	
#HBA's	14	NRB (PERIPHERAL)	

Number of substituents	5	P/NP balance, substituents	2/9
Large ($\geq 5HA$)	3	P/NP balance, peripheral groups	3/0
Small (2-4HA)	2	Degrees of unsaturation ring	17.5
Proportion HA in substituents	60.0%	N:O ratio	2:5
Number of peripheral groups	3	Chiral centres	5

Polarity distribution ligand atoms

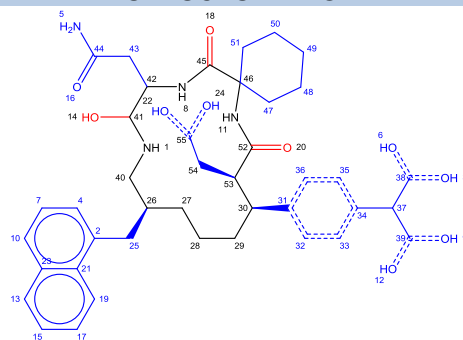
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	3	12	-	2
Substituent	6	27	8	10
Peripheral groups	3	-	-	-
Total	9	39	8	12

Protein name	Grb2 SH2 domain		
Organism	Homo sapiens		
Classification	Transferase		
Binding mode	Face-om		
Receptor secondary structure topology			
Number of residue 'hotspots'	11		

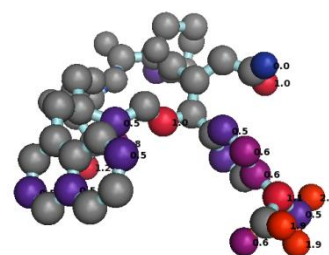
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	14	Hydrogen donor- π	1
Ionic interaction	6	π - π	1
Cation-dipole	-	VdW interaction	10
Cation- π	2	Unfavourable	2
Dipolar interaction	-	Poor-angle	3
Halogen bond	-	Unclassified	-
Water-mediated interaction	-		

2D-STRUCTURE LIGAND



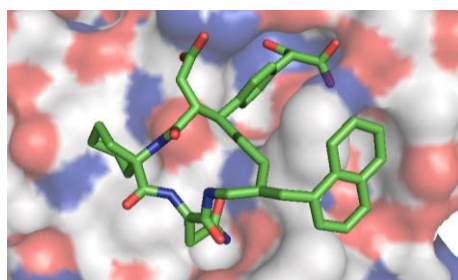
3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



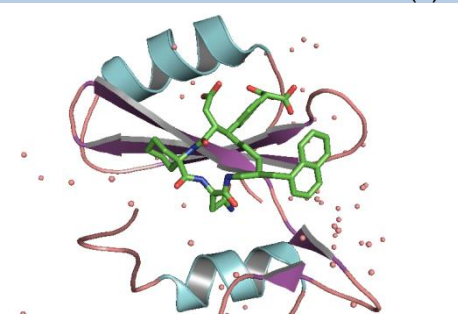
Physicochemical properties

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis