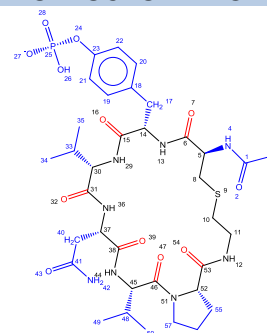
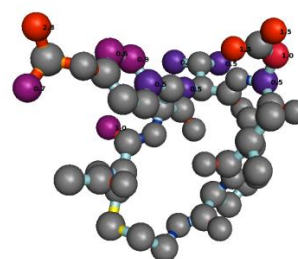


CODE	2BM2(PDB)	Resolution	2.1	
Name		Ring size	22	
Formula	C35H58N8O12PS-	# Ligand atoms	57	
Type	Cyclic peptide	Scorpion Score	14	
Mol. Weight (Da)	846	Saturated/ Unsaturated	S	
cLogP	0.62	Chiral centres.ring	6	
tPSA	308	Chiral centres.sub	-	
#HBD's	9	NRB (SUBSTITUENT)		
#HBA's	29	NRB (PERIPHERAL)		
NRB (RING)				
Number of substituents	6	P/NP balance, substituents	9/20	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	6/0	
<i>Small (2-4HA)</i>	5	Degrees of unsaturation ring	11	
Proportion HA in substituents	50.9%	N:O ratio	2:3	
Number of peripheral groups	6	Chiral centres	6	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	6	16	1	1
Substituent	9	20	5	6
Peripheral groups	6	-	1	-
Total	21	36	7	7
Protein name	GRB2-SH2 domain			
Organism	Homo Sapiens			
Classification	Hormone/ Growth factor			
Binding mode	Edge-on			
Receptor secondary structure topology				
Number of residue 'hotspots'	12			
Number of protein-ligand interactions* (Database link)				
Hydrogen bond	15	Hydrogen donor-π	-	
Ionic interaction	2	π-π	1	
Cation-dipole		VdW interaction	7	
Cation-π	1	Unfavourable	-	
Dipolar interaction	-	Poor-angle	2	
Halogen bond	-	Unclassified	2	
Water-mediated interaction	1			

2D-STRUCTURE LIGAND



3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))

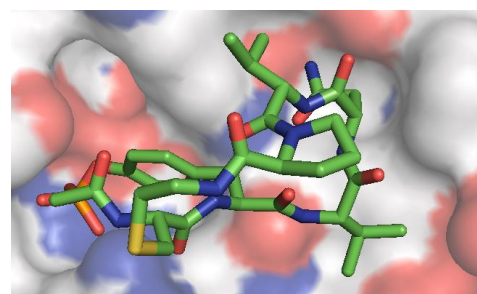


Physicochemical properties

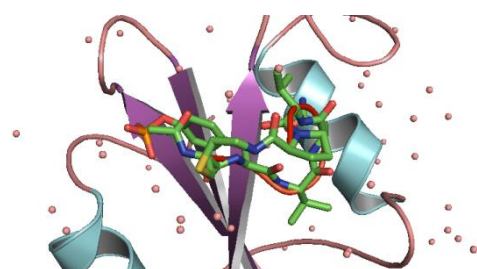
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IC50 (μM) Grb2-SH2b	0.11 ± 0.03
IC50 (μM) Src-SH2c	88

LIGAND-PROTEIN COMPLEX (I) ([Pymol link](#))



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis