CODE	2AOB(PDB)	Resolution	1.8
Name		Ring size	15
Formula	C41H51N4O10	# Ligand atoms	55
Type	macrocycle	Scorpion Score	20.3

Mol. Weight (Da)	760	Saturated/ Unsaturated	S
cLogP	4.21		
tPSA	259	Chiral centres.ring	4
#HBD's	10	Chiral centres.sub	-
#HBA's	13		
$N_{RB\ (RING)}$	12	$N_{RB\ (SUBSTITUENT)}$	10
Number of substituents	5	P/NP balance, substituents	1/4
Large (≥5HA)	3	P/NP balance, peripheral groups	3/0
Small (2-4HA)	2		
Proportion HA in substituents	27.3%	Degrees of unsaturation ring	18.5
Number of peripheral groups	3	N:O ratio	2:5
		Chiral centres	4

Polarity distribution ligand atoms

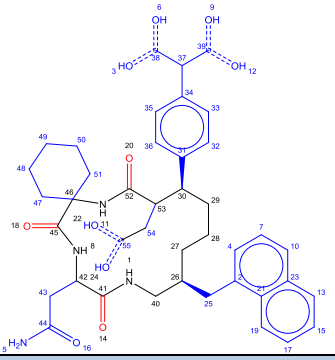
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	12	1	2
Substituent	6	27	8	11
Peripheral groups	3	-	-	-
Total	9	39	9	13

Protein name	Grb2 SH2 domain
Organism	Homo sapiens
Classification	Transferase
Binding mode	Face-on
Receptor secondary structure topology	
Number of residue 'hotspots'	12

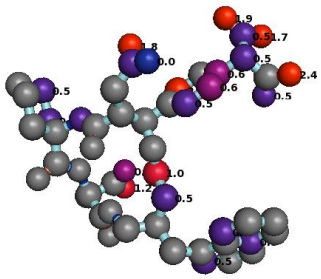
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	15	Hydrogen donor-π	2
Ionic interaction	6	π-π	1
Cation-dipole	-	VdW interaction	15
Cation-π	-	Unfavourable	1
Dipolar interaction	-	Poor-angle	-
Halogen bond	-	Unclassified	-
Water-mediated interaction	2		

2D-STRUCTURE LIGAND



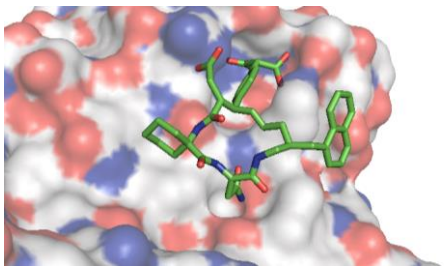
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



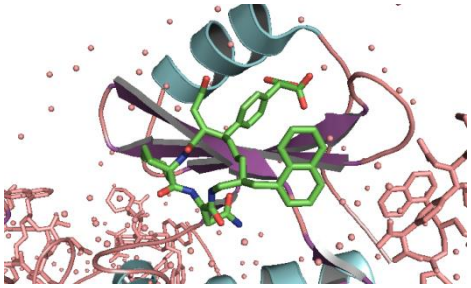
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis