CODE	2BCD(PDB)	Resolution	2.1
Name	Protein Phosphatase-1	Ring size	19
Formula	C40H65N5O10	# Ligand atoms	55
Type	Macrocycle	Scorpion Score	10.1

Mol. Weight (Da)	776	Saturated/ Unsaturated	S
cLogP	4.16		
tPSA	232	Chiral centres.ring	7
#HBD's	8	Chiral centres.sub	3
#HBA's	15		
$N_{RB\ (RING)}$	14	$N_{RB\ (SUBSTITUENT)}$	13
Number of substituents	5	P/NP balance, substituents	5/23
Large (≥5HA)	1	P/NP balance, peripheral groups	6/2
Small (2-4HA)	4		
Proportion HA in substituents	41.8%	Degrees of unsaturation ring	11
Number of peripheral groups	8	N:O ratio	5:10
		Chiral centres	10

Polarity distribution ligand atoms

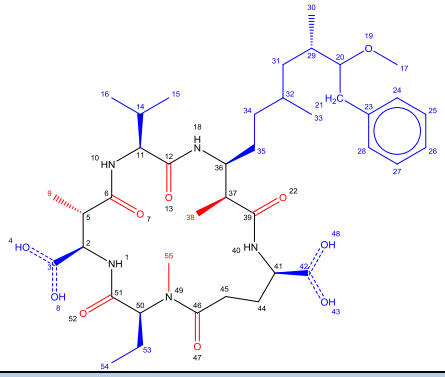
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	5	14	1	2
Substituent	5	23	3	5
Peripheral groups	6	2	3	1
Total	16	39	7	8

Protein name	Motuporin
Organism	Homo sapiens| Theonella sp.
Classification	Hydrolase/ hydrolase inhibitor
Binding mode	Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	11

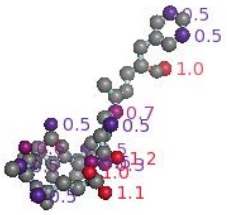
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	4	Hydrogen donor-π	2
Ionic interaction	2	π-π	
Cation-dipole	1	VdW interaction	9
Cation-π	2	Unfavourable	3
Dipolar interaction	-	Poor-angle	5
Halogen bond	-	Unclassified	-
Water-mediated interaction	5		

2D-STRUCTURE LIGAND



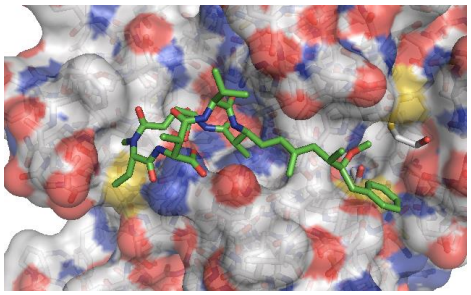
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



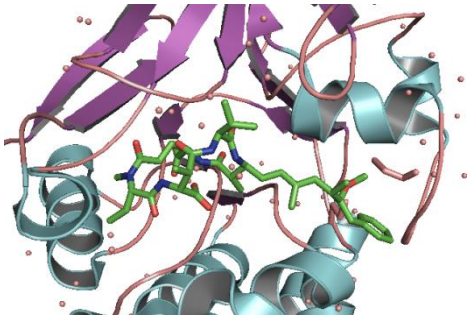
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis