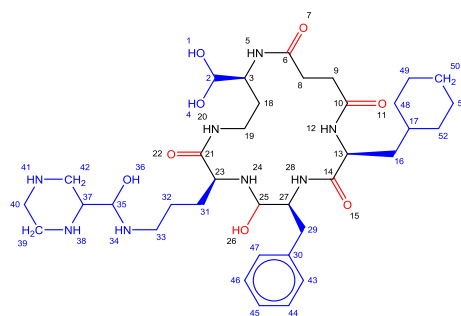
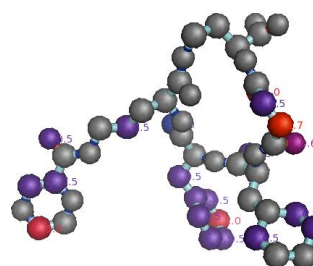


CODE	3U4W(PDB)		Resolution	1.9
Name	MC4b		Ring size	18
Formula	C36H60N8O8		# Ligand atoms	52
Type	Macrocycle		Scorpion Score	9.2
Mol. Weight (Da)	733	Saturated/Unsaturated	U	
cLogP	-1.85	Chiral centres.ring	5	
tPSA	245	Chiral centres.sub	2	
#HBD's	12			
#HBA's	16			
N _{RB} (RING)	14	N _{RB} (SUBSTITUENT)	11	
Number of substituents	4	P/NP balance, substituents	6/23	
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	5/0	
<i>Small (2-4HA)</i>	1	Degrees of unsaturation ring	11	
Proportion HA in substituents	55.8%	N:O ratio	8:8	
Number of peripheral groups	5	Chiral centres	7	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	5	13	-	2
Substituent	6	23	1	14
Peripheral groups	5	-	4	0
Total	11	23	5	16
Protein name	Src			
Organism	Gallus gallus			
Classification	Transferase/ transferase inhibitor			
Binding mode	Edge-on/ compact			
Receptor secondary structure topology				
Number of residue 'hotspots'	21			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	3	Hydrogen donor-π	2	
Ionic interaction		π-π		
Cation-dipole		VdW interaction	18	
Cation-π		Unfavourable	5	
Dipolar interaction	2	Poor-angle	5	
Halogen bond		Unclassified	3	
Water-mediated interaction	7			

2D-STRUCTURE LIGAND



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

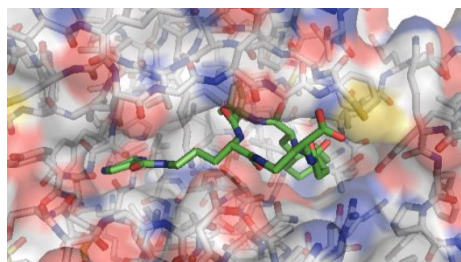


Physicochemical properties

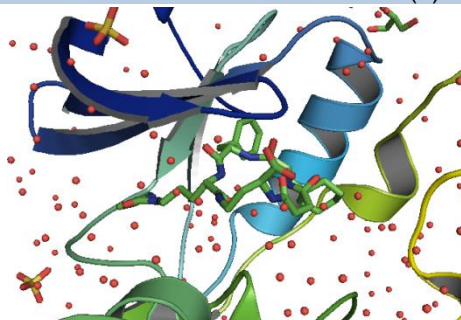
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Src IC50 (μM) ≤0.004

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis