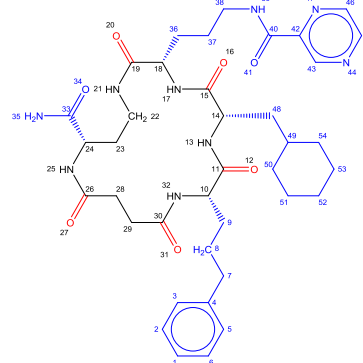
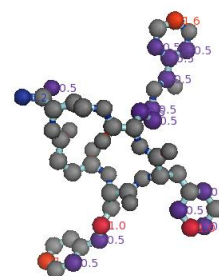


CODE	3U51(PDB)	Resolution	2.2	
Name		Ring size	18	
Formula	C38H53N9O7	# Ligand atoms	54	
Type	MACROCYCLE	Scorpion Score	11.1	
Mol. Weight (Da)	748	Saturated/Unsaturated	U	
cLogP	2.12	Chiral centres.ring	4	
tPSA	243	Chiral centres.sub	0	
#HBD's	8			
#HBA's	16			
N _{RB} (RING)	13	N _{RB} (SUBSTITUENT)	12	
Number of substituents	4	P/NP balance, substituents	6/25	
Large (≥5HA)	3	P/NP balance, peripheral groups	5/0	
Small (2-4HA)	1	Degrees of unsaturation ring	17	
Proportion HA in substituents	57.4%	N:O ratio	9:7	
Number of peripheral groups	5	Chiral centres	4	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	5	13	-	-
Substituent	6	25	3	15
Peripheral groups	5	-	-	-
Total	16	38	3	15
Protein name	Src			
Organism	Gallus gallus			
Classification	Transferase/ transferase inhibitor			
Binding mode	Edge-on			
Receptor secondary structure topology				
Number of residue 'hotspots'	24			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	2	Hydrogen donor-π		
Ionic interaction		π-π	1	
Cation-dipole		VdW interaction	21	
Cation-π		Unfavourable	7	
Dipolar interaction	1	Poor-angle	6	
Halogen bond		Unclassified		
Water-mediated interaction	0			

2D-STRUCTURE LIGAND



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

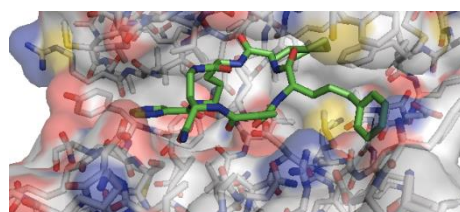


Physicochemical properties

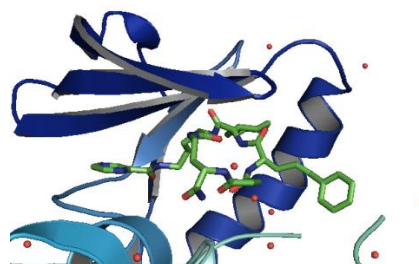
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Src IC50 (μM) 25±3.0

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis