CODE	4X9R (PDB)	Resolution	
Name		Ring size	20
Formula	C46H76N8O12P-	# Ligand atoms	138
Type	macrocycle	Scorpion Score	14.4

Mol. Weight (Da)	963,53	Saturated/ Unsaturated	U
cLogP			
tPSA		Chiral centres.ring	5
#HBD's	8	Chiral centres.sub	4
#HBA's	10		
$N_{RB\ (RING)}$	14	$N_{RB\ (SUBSTITUENT)}$	21

Number of substituents	4	P/NP balance, substituents	15/29
Large (≥5HA)	2	P/NP balance, peripheral groups	2/0
Small (2-4HA)	2		
Proportion HA in substituents	32%	Degrees of unsaturation ring	12.5
Number of peripheral groups	2	N:O ratio	8:12
		Chiral centres	8

Polarity distribution ligand atoms

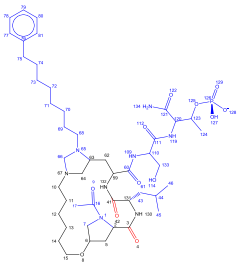
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	4	16	-	3
Substituent	15	29	7	11
Peripheral groups	2	-	2	-
Total	21	45	9	14

Protein name	PLK-1 polo-box domain
Organism	Homo sapiens
Classification	Transferase/ Transferase inhibitor
Binding mode	Face on
Receptor secondary structure topology	
Number of residue 'hotspots'	14

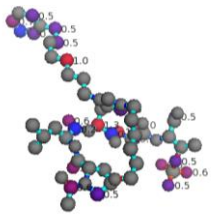
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	10	Hydrogen donor-π	-
Ionic interaction	1	π-π	5
Cation-dipole	-	VdW interaction	12
Cation-π	1	Unfavourable	1
Dipolar interaction	-	Poor-angle	1
Halogen bond	-	Unclassified	-
Water-mediated interaction	3		

2D-STRUCTURE LIGAND



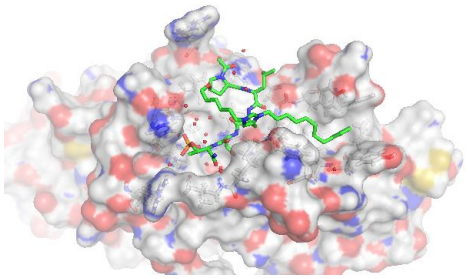
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



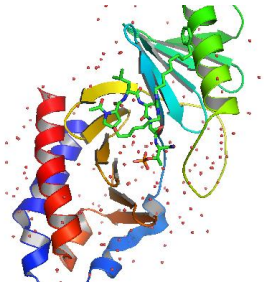
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis