CODE	1W25(PDB)	Resolution	2.7
Name		Ring size	12
Formula	$C_{20}H_{22}N_{10}O_{14}P_2^{2-}$	# Ligand atoms	46
Type	Macrocycle	Scorpion Score	3.8

Mol. Weight (Da)	688,08	Saturated/ Unsaturated	S
cLogP	-17.330		
tPSA	342.26	Chiral centres.ring	4
#HBD's	10	Chiral centres.sub	4
#HBA's	16		
$N_{RB\ (RING)}$	12	$N_{RB\ (SUBSTITUENT)}$	2

Number of substituents	2	P/NP balance, substituents	18/14
Large (≥5HA)	2	P/NP balance, peripheral groups	4/0
Small (2-4HA)	-		
Proportion HA in substituents	65.2%	Degrees of unsaturation ring	14
Number of peripheral groups	4	N:O ratio	10:14
		Chiral centres	8

Polarity distribution ligand atoms

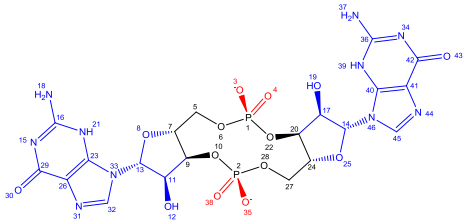
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	4	6		
Substituent	18	14		
Peripheral groups	4	-		
Total	26	20		

Protein name	STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN
Organism	Caulobater vibrioides
Classification	Signalling protein
Binding mode	Face - on
Receptor secondary structure topology	
Number of residue 'hotspots'	13

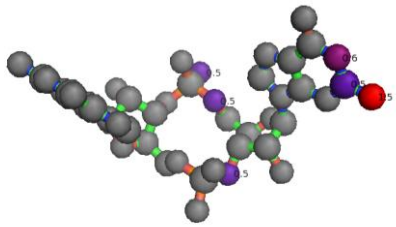
Number of protein-ligand interactions* ('Database link')

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

2D-STRUCTURE LIGAND



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

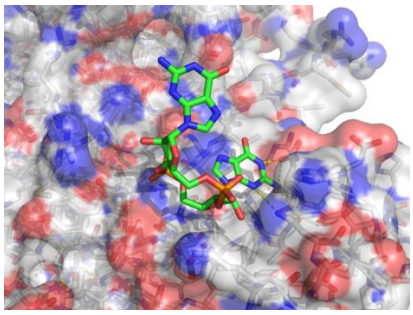


Physicochemical properties

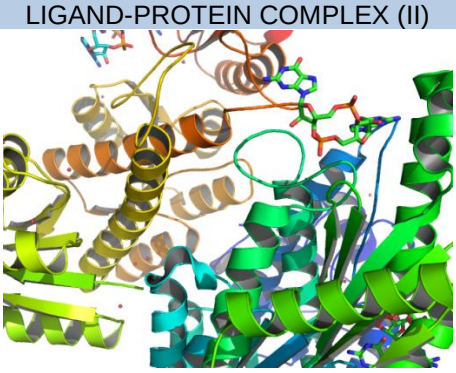
'click for publication'

K_i	0,5 µM

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis