CODE	2J9M(PDB)	Resolution	2.5
Name		Ring size	13
Formula	C13H14BrN5O2S	# Ligand atoms	22
Type	Macrocycle	Scorpion Score	5.6

Mol. Weight (Da)	384	Saturated/ Unsaturated	U
cLogP	3.07		
tPSA	384	Chiral centres.ring	0
#HBD's	3	Chiral centres.sub	0
#HBA's	7		
$N_{RB\ (RING)}$	9	$N_{RB\ (SUBSTITUENT)}$	0
Number of substituents	2	P/NP balance, substituents	1/6
Large (≥5HA)	-	P/NP balance, peripheral groups	2/0
Small (2-4HA)	2		
Proportion HA in substituents	31.8%	Degrees of unsaturation ring	9
Number of peripheral groups	2	N:O ratio	5:2
		Chiral centres	0

Polarity distribution ligand atoms

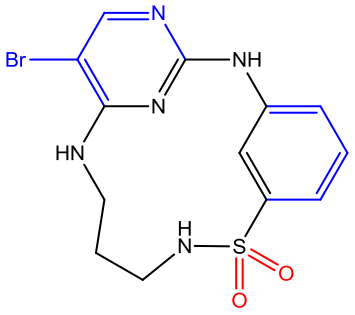
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	4	9	2	2
Substituent	1	6	1	4
Peripheral groups	2	-	1	-
Total	7	15	4	6

Protein name	CDK2
Organism	Homo sapiens
Classification	Transferase
Binding mode	Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	10

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

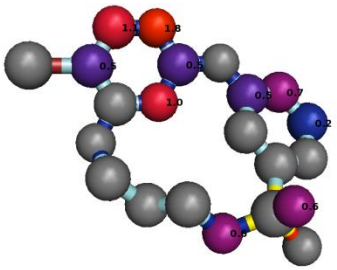
Hydrogen bond	4	Hydrogen donor-π	1
Ionic interaction	-	π-π	2
Cation-dipole	-	VdW interaction	8
Cation-π	1	Unfavourable	4
Dipolar interaction	-	Poor-angle	2
Halogen bond	-	Unclassified	1
Water-mediated interaction	-		

2D-STRUCTURE LIGAND



2J9M

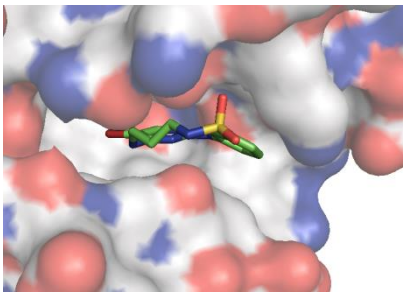
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



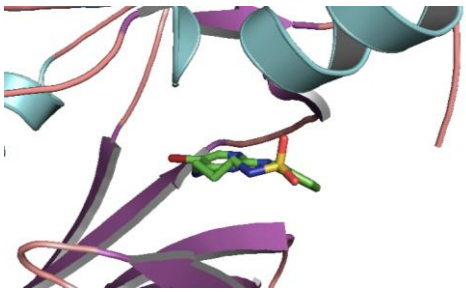
Physicochemical properties
'click for publication'

IC 50 CDK1 (nM)	*20*
IC 50 CDK2 (nM)	*140*
IC50 VEGF-R2 (nM)	*40*
IC50 MCF7 (nM)	*200*

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis