

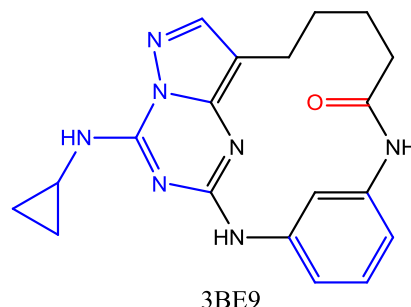
CODE	3BE9(PDB)	Resolution	2
Name		Ring size	14
Formula	C19H22N7O	# Ligand atoms	27
Type	Macrocycle	Scorpion Score	15.7
Mol. Weight (Da)	364	Saturated/ Unsaturated	U
cLogP	-	Chiral centres.ring	0
tPSA	100	Chiral centres.sub	0
#HBD's	4		
#HBA's	8		
N _{RB} (RING)	8	N _{RB} (SUBSTITUENT)	2
Number of substituents	2	P/NP balance, substituents	4/8
Large (≥5HA)	1	P/NP balance, peripheral groups	1/0
Small (2-4HA)	1	Degrees of unsaturation ring	12.5
Proportion HA in substituents	44.4%	N:O ratio	7:1
Number of peripheral groups	1	Chiral centres	0

Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	3	11	-	8
Substituent	4	8	2	7
Peripheral groups	1	-	1	-
Total	8	19	3	15

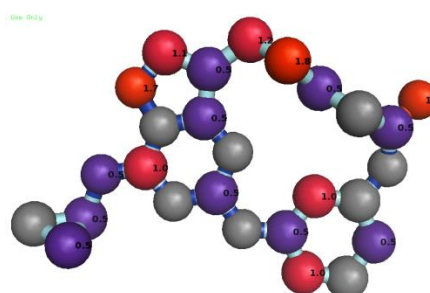
Protein name	Protein kinase CK2		
Organism	Zea mays		
Classification	Transferase		
Binding mode	Edge-on		
Receptor secondary structure topology			
Number of residue 'hotspots'	14		

Number of protein-ligand interactions* ('Database link')			
Hydrogen bond	4	Hydrogen donor-π	1
Ionic interaction		π-π	
Cation-dipole	1	VdW interaction	23
Cation-π		Unfavourable	
Dipolar interaction		Poor-angle	4
Halogen bond		Unclassified	1
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



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

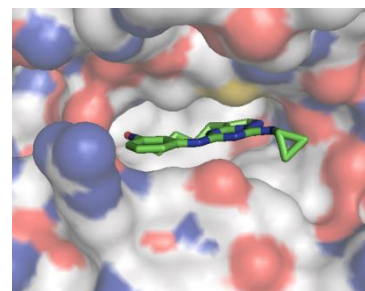


Physicochemical properties

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IC ₅₀ (μM)HCT 116	0.29
IC ₅₀ (μM) PC3	0.88
Ki CK2 (nM)	24

LIGAND-PROTEIN COMPLEX (I) (Pymol link)



LIGAND-PROTEIN COMPLEX (II)

