CODE	3VHD (PDB)	Resolution	12.2
Name		Ring size	16
Formula	C19H23N5O2S	# Ligand atoms	27
Type	Macrocycle	Scorpion Score	12.2

Mol. Weight (Da)	385	Saturated/ Unsaturated	U
cLogP	1.4		
tPSA	110	Chiral centres.ring	0
#HBD's	4	Chiral centres.sub	0
#HBA's	7		
$N_{RB\ (RING)}$	10	$N_{RB\ (SUBSTITUENT)}$	0

Number of substituents	2	P/NP balance, substituents	3/6
Large (≥5HA)	1	P/NP balance, peripheral groups	2/0
Small (2-4HA)	1		
Proportion HA in substituents	33.3%	Degrees of unsaturation ring	11
Number of peripheral groups	2	N:O ratio	5:2
		Chiral centres	0

Polarity distribution ligand atoms

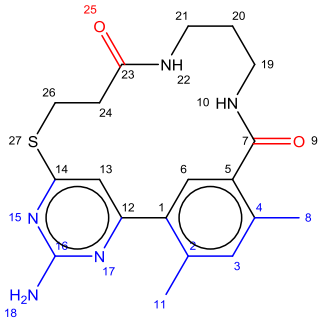
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	14	-	4
Substituent	3	6	3	3
Peripheral groups	2	-	1	-
Total	7	20	4	7

Protein name	Hsp90
Organism	Homo sapiens
Classification	Chaperone/ Chaperone inhibitor
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	9

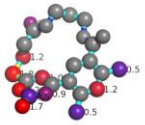
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	1	Hydrogen donor-π	
Ionic interaction		π-π	
Cation-dipole		VdW interaction	14
Cation-π	1	Unfavourable	
Dipolar interaction		Poor-angle	
Halogen bond		Unclassified	1
Water-mediated interaction	6		

2D-STRUCTURE LIGAND



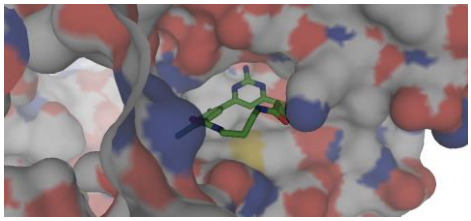
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



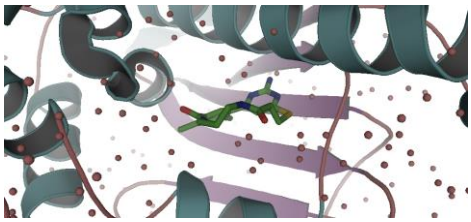
Physicochemical properties

'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis