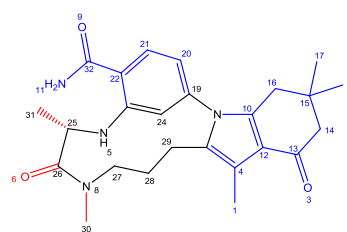
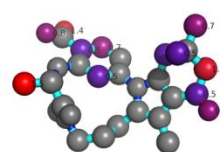


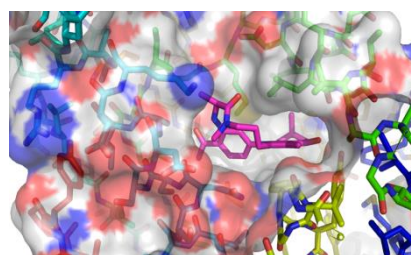
CODE	3R91(PDB)	Resolution		
Name		Ring size	12	
Formula	C25H32N4O3	# Ligand atoms	32	
Type	Macrocycle	Scorpion Score	9.5	
Mol. Weight (Da)	436,25	Saturated/ Unsaturated	U	
cLogP	3.9	Chiral centres.ring	1	
tPSA	95.74	Chiral centres.sub	0	
#HBD's	3			
#HBA's	6			
NRB (RING)	8	NRB (SUBSTITUENT)	1	
Number of substituents	2	P/NP balance, substituents	3/14	
Large ($\geq 5HA$)	2	P/NP balance, peripheral groups	1/3	
Small (2-4HA)	-	Degrees of unsaturation ring	12	
Proportion HA in substituents	53.1%	N:O ratio	4:3	
Number of peripheral groups	3	Chiral centres	1	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	3	9	-	1
Substituent	3	14	3	7
Peripheral groups	1	2	-	1
Total	7	25	3	9
Protein name	Hsp90			
Organism	Homo sapiens			
Classification	Chaperone/ Chaperone inhibitor			
Binding mode	Edge - on			
Receptor secondary structure topology				
Number of residue 'hotspots'	9			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	3	Hydrogen donor- π		
Ionic interaction		π - π		
Cation-dipole		VdW interaction	11	
Cation- π		Unfavourable		
Dipolar interaction		Poor-angle	2	
Halogen bond		Unclassified	1	
Water-mediated interaction				

2D-STRUCTURE LIGAND

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

Physicochemical properties

['click for publication'](#)

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

LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis