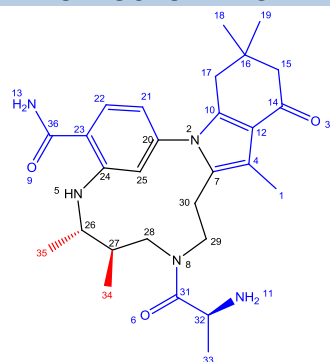
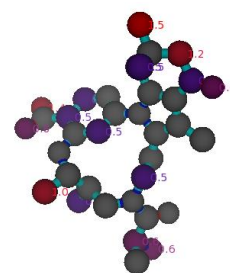


CODE	3RK2 (PDB)	Resolution	12	
Name		Ring size	12	
Formula	C28H39N5O3	# Ligand atoms	36	
Type	Macrocycle	Scorpion Score	12	
Mol. Weight (Da)	493.64	Saturated/Unsaturated	U	
cLogP	3.4348	Chiral centres.ring	2	
tPSA	121.76	Chiral centres.sub	1	
#HBD's	5			
#HBA's	8			
NRB (RING)	9	NRB (SUBSTITUENT)	2	
Number of substituents	3	P/NP balance, substituents	5/17	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	0/2	
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	12	
Proportion HA in substituents	61.1%	N:O ratio	5:3	
Number of peripheral groups	2	Chiral centres	3	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	3	9	0	2
Substituent	5	17	4	8
Peripheral groups	0	2	0	2
Total	8	28	4	12
Protein name	Hsp90			
Organism	Homo sapiens			
Classification	Chaperone/ Chaperone			
Binding mode				
Receptor secondary structure topology				
Number of residue 'hotspots'	11			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	3	Hydrogen donor-π		
Ionic interaction	1	π-π		
Cation-dipole		VdW interaction	13	
Cation-π		Unfavourable		
Dipolar interaction		Poor-angle	1	
Halogen bond		Unclassified	1	
Water-mediated interaction				

2D-STRUCTURE LIGAND

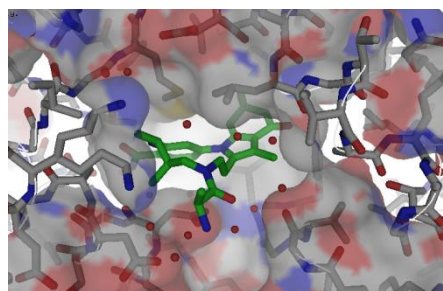


3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



Physicochemical properties

'click for publication'

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

LIGAND-PROTEIN COMPLEX (II)

