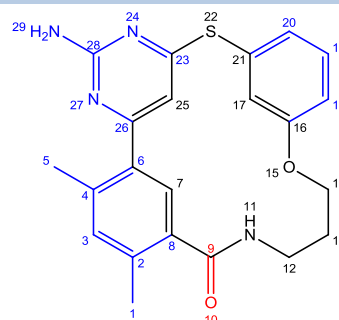
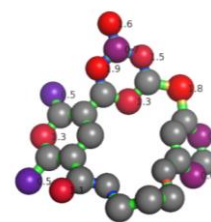


CODE	3VHC (PDB)	Resolution	1.4	
Name		Ring size	16	
Formula	C22H22N4O2S	# Ligand atoms	29	
Type	MACROCYCLE	Scorpion Score	13.5	
Mol. Weight (Da)	406.50	Saturated/Unsaturated	U	
cLogP	4.3756	Chiral centres.ring	0	
tPSA	89.07	Chiral centres.sub	0	
#HBD's	3			
#HBA's	5			
N _{RB} (RING)	9	N _{RB} (SUBSTITUENT)	0	
Number of substituents	3	P/NP balance, substituents	3/9	
<i>Large (≥5HA)</i>	1	P/NP balance, peripheral groups	1/0	
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	13	
Proportion HA in substituents	33.3%	N:O ratio	4:2	
Number of peripheral groups	1	Chiral centres	0	
Polarity distribution ligand atoms				
	All		Contact	
	<i>Polar</i>	<i>Nonpolar</i>	<i>Polar</i>	<i>Nonpolar</i>
Ring	3	13	1	1
Substituent	3	9	3	6
Peripheral groups	1	0	1	-
Total	7	22	5	7
Protein name	HSP90			
Organism	Homo sapiens			
Classification	Chaperone/ inhibitor			
Binding mode	compact			
Receptor secondary structure topology				
Number of residue 'hotspots'	12			
Number of protein-ligand interactions* ('Database link')				
Hydrogen bond	2	Hydrogen donor-π	-	
Ionic interaction	-	π-π	-	
Cation-dipole	-	VdW interaction	13	
Cation-π	1	Unfavourable	-	
Dipolar interaction	-	Poor-angle	2	
Halogen bond	-	Unclassified	-	
Water-mediated interaction	0			

2D-STRUCTURE LIGAND



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

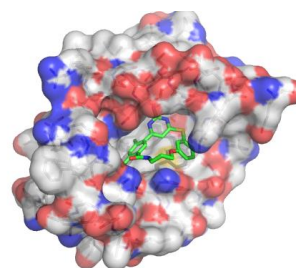


Physicochemical properties

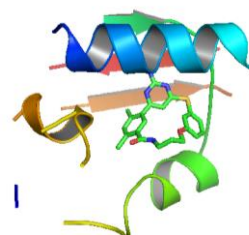
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K _d	1,3 nM
IC ₅₀ HCT116	0,78 μM
IC ₅₀ NCI-N87	0,94 μM

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis