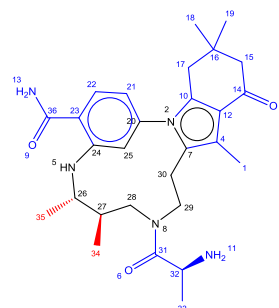


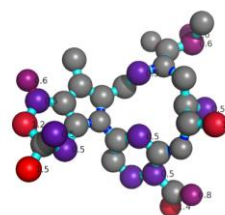
CODE	3RKZ (PDB)	Resolution	1.57	
Name		Ring size	12	
Formula	C28H39N5O3	# Ligand atoms	36	
Type	Macrocycle	Scorpion Score	12	
Mol. Weight (Da)	494	Saturated/ Unsaturated	U	
cLogP	3.4	Chiral centres.ring	2	
tPSA	123	Chiral centres.sub	1	
#HBD's	4			
#HBA's	8			
NRB (RING)	9	NRB (SUBSTITUENT)	2	
Number of substituents	3	P/NP balance, substituents	5/17	
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	0/2	
<i>Small (2-4HA)</i>	-	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	-	2
Substituent	5	17	4	8
Peripheral groups	-	2	-	2
Total	8	28	4	12

Protein name	Hsp90		
Organism	Homo sapiens		
Classification	Chaperone/ chaperone inhibitor		
Binding mode	Compact		
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	6		

2D-STRUCTURE LIGAND



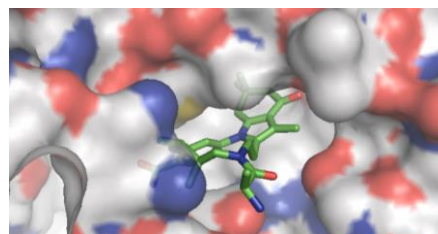
3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))



Physicochemical properties

[click for publication](#)

LIGAND-PROTEIN COMPLEX (I) ([Pymol link](#))



LIGAND-PROTEIN COMPLEX (II)

