CODE	3R92 (PDB)	Resolution	1.58
Name		Ring size	12
Formula	C26H34N4O2	# Ligand atoms	32
Type	Macrocycle	Scorpion Score	11.3

Mol. Weight (Da)	434.58	Saturated/ Unsaturated	U
cLogP	4.27		
tPSA	80	Chiral centres.ring	1
#HBD's	3	Chiral centres.sub	0
#HBA's	6		
$N_{RB\ (RING)}$	8	$N_{RB\ (SUBSTITUENT)}$	1
Number of substituents	3	P/NP balance, substituents	3/17
Large (≥5HA)	2	P/NP balance, peripheral groups	-
Small (2-4HA)	1		
Proportion HA in substituents	62.5%	Degrees of unsaturation ring	12
Number of peripheral groups	-	N:O ratio	2:1
		Chiral centres	1

Polarity distribution ligand atoms

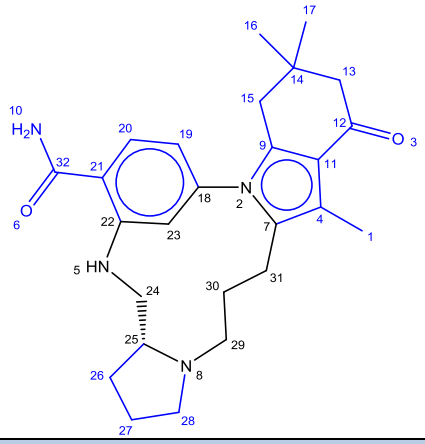
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	9	1	3
Substituent	3	17	3	7
Peripheral groups	-	-	-	-
Total	6	26	4	10

Protein name	Hsp90
Organism	Homo sapiens
Classification	Chaperone/ Chaperone inhibitor
Binding mode	Compact
Receptor secondary structure topology	
Number of residue 'hotspots'	8

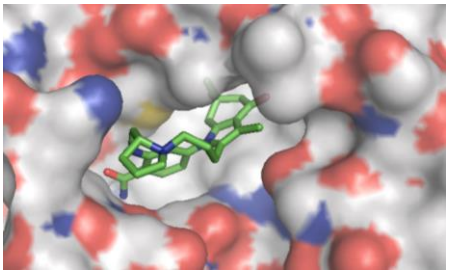
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	3	Hydrogen donor-π	
Ionic interaction		π-π	
Cation-dipole		VdW interaction	13
Cation-π		Unfavourable	
Dipolar interaction		Poor-angle	2
Halogen bond		Unclassified	1
Water-mediated interaction			

2D-STRUCTURE LIGAND

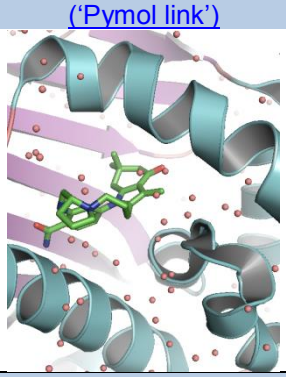


3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



Physicochemical properties
'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)

*Based on Scorpion® analysis