CODE	3QTF(PDB)	Resolution	
Name		Ring size	12
Formula	C24H32N4O2	# Ligand atoms	30
Type	Macrocycle	Scorpion Score	8.9

Mol. Weight (Da)	408,25	Saturated/ Unsaturated	U
cLogP	4.073		
tPSA	87.46	Chiral centres.ring	1
#HBD's	4	Chiral centres.sub	0
#HBA's	3		
$N_{RB\ (RING)}$	9	$N_{RB\ (SUBSTITUENT)}$	1

Number of substituents	2	P/NP balance, substituents	3/14
Large (≥5HA)	2	P/NP balance, peripheral groups	0/1
Small (2-4HA)	-		
Proportion HA in substituents	56.7%	Degrees of unsaturation ring	11
Number of peripheral groups	1	N:O ratio	3:2
		Chiral centres	1

Polarity distribution ligand atoms

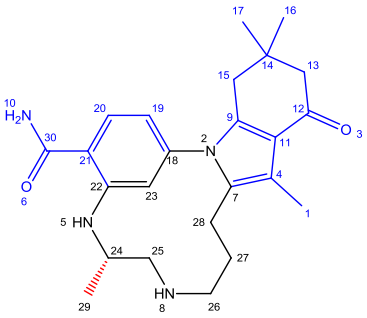
	All		Contact**	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	3	9	1	1
Substituent	3	14	3	7
Peripheral groups	-	1	-	1
Total	6	24	4	9

Protein name	Hsp90
Organism	Homo sapiens
Classification	Chaperone/ Chaperone inhibitor
Binding mode	Compact/ Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	10

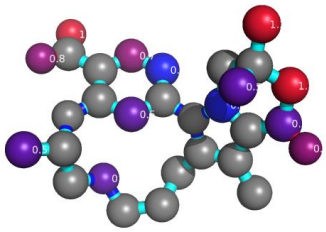
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	3	Hydrogen donor-π	
Ionic interaction	-	π-π	2
Cation-dipole	-	VdW interaction	8
Cation-π	-	Unfavourable	-
Dipolar interaction	-	Poor-angle	2
Halogen bond	-	Unclassified	1
Water-mediated interaction	8		

2D-STRUCTURE LIGAND



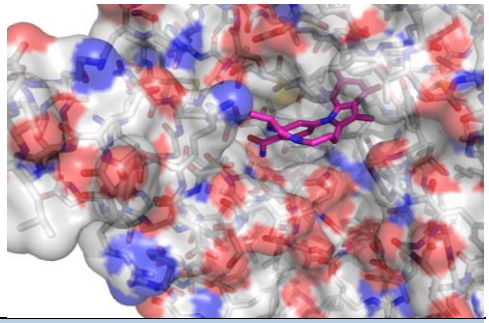
3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')



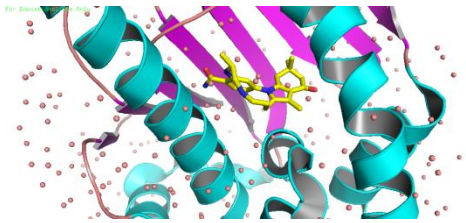
Physicochemical properties
'click for publication'

Hsp90 IC50 (µM)	0.11
HCT1 16 EC50 (µM)	0.09
Solubility (µg/mL)	>100
T1/2 in rat microsomes (min)	>30

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis
** Based on Scorpion score