CODE	3MK8 (PDB)	Resolution	2.32
Name		Ring size	21
Formula	C91H158N31O26	# Ligand atoms	148
Type	Stapled peptide	Scorpion Score	22.8

Mol. Weight (Da)	2102	Saturated/ Unsaturated	S
cLogP	-		
tPSA	946	Chiral centres.ring	5
#HBD's	56	Chiral centres.sub	14
#HBA's	105	$N_{RB\ (SUBSTITUENT)}$	
$N_{RB\ (RING)}$		$N_{RB\ (PERIPHERAL)}$	
Number of substituents	5	P/NP balance, substituents	49/72
Large (≥5HA)	4	P/NP balance, peripheral groups	4/2
Small (2-4HA)	1		
Proportion HA in substituents	81.6%	Degrees of unsaturation ring	28.5
Number of peripheral groups	6	N:O ratio	31:26
		Chiral centres	19

Polarity distribution ligand atoms

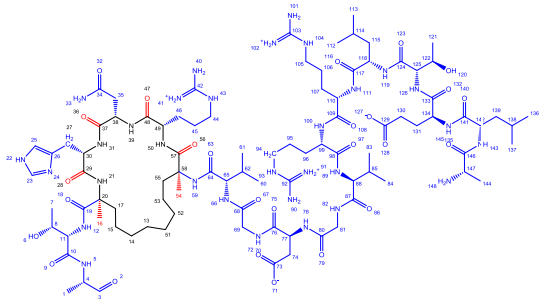
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	4	17	-	1
Substituent	49	72	8	17
Peripheral groups	4	2	1	1
Total	57	91	9	19

Protein name	MCL-1 BH3
Organism	Homo Sapiens
Classification	Apoptosis/Apoptosis regulator
Binding mode	Face-on
Receptor secondary structure topology	
Number of residue 'hotspots'	14

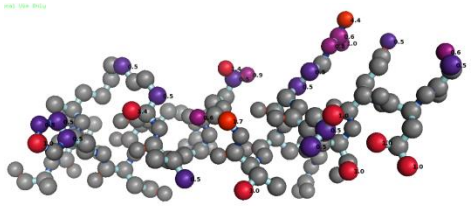
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	9	Hydrogen donor-π	1
Ionic interaction	7	π-π	
Cation-dipole	1	VdW interaction	29
Cation-π	3	Unfavourable	2
Dipolar interaction		Poor-angle	
Halogen bond		Unclassified	
Water-mediated interaction	1		

2D-STRUCTURE LIGAND

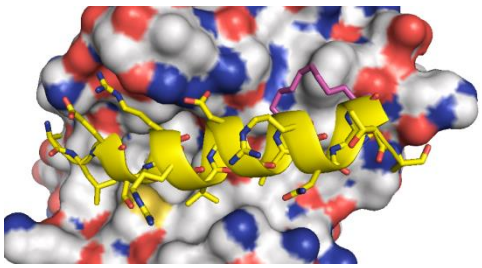


3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

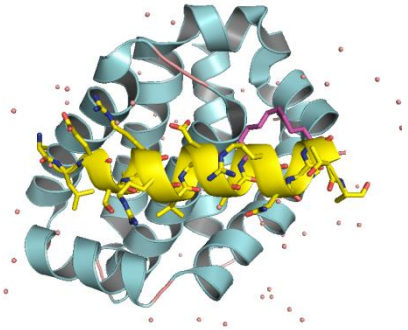


Physicochemical properties 'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis