CODE	3SO4(PDB)	Resolution	2.44
Name	Arylomycin	Ring size	14
Formula	C38H48N6O16-	# Ligand atoms	60
Type	Macrocycle	Scorpion Score	9.8

Mol. Weight (Da)	845	Saturated/ Unsaturated	U
cLogP			
tPSA	334	Chiral centres.ring	3
#HBD's	9	Chiral centres.sub	10
#HBA's	22		
$N_{RB\ (RING)}$	8	$N_{RB\ (SUBSTITUENT)}$	11
Number of substituents	4	P/NP balance, substituents	28/25
Large (≥5HA)	2	P/NP balance, peripheral groups	2/1
Small (2-4HA)	2		
Proportion HA in substituents	70.0%	Degrees of unsaturation ring	18
Number of peripheral groups	3	N:O ratio	3:8
		Chiral centres	13

Polarity distribution ligand atoms

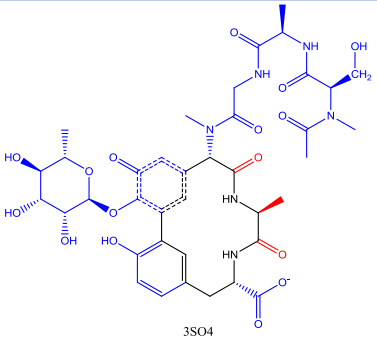
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	12	2	3
Substituent	28	25	5	3
Peripheral groups	2	3	-	1
Total			7	7

Protein name	Type 1 Signal peptidase
Organism	Escherichia coli | Streptomyces sp.
Classification	Transferase
Binding mode	Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	13

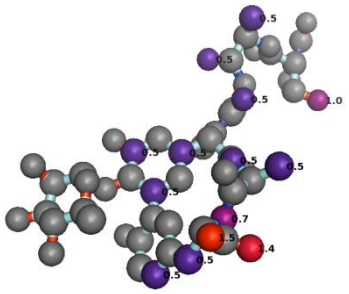
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	11	Hydrogen donor-π	1
Ionic interaction	1	π-π	
Cation-dipole		VdW interaction	7
Cation-π		Unfavourable	
Dipolar interaction		Poor-angle	4
Halogen bond		Unclassified	2
Water-mediated interaction	0		

2D-STRUCTURE LIGAND

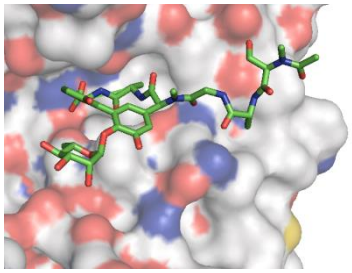


3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

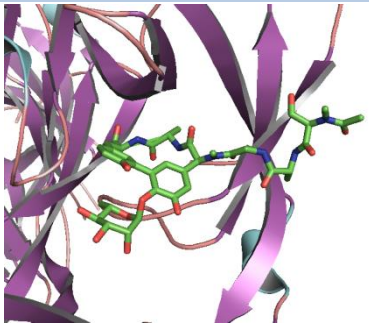


Physicochemical properties 'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis