CODE	1T7D(PDB)	Resolution	2.5
Name		Ring size	14
Formula	C32H39N6O11-	# Ligand atoms	49
Type	macrocycle	Scorpion Score	6.2

Mol. Weight (Da)	684	Saturated/ Unsaturated	U
cLogP	-3.45		
tPSA	258	Chiral centres.ring	3
#HBD's	7	Chiral centres.sub	2
#HBA's	16		
$N_{RB\ (RING)}$	8	$N_{RB\ (SUBSTITUENT)}$	9
Number of substituents	4	P/NP balance, substituents	2/12
Large (≥5HA)	1	P/NP balance, peripheral groups	2/1
Small (2-4HA)	3		
Proportion HA in substituents	65.3%	Degrees of unsaturation ring	16.5
Number of peripheral groups	3	N:O ratio	6/11
		Chiral centres	5

Polarity distribution ligand atoms

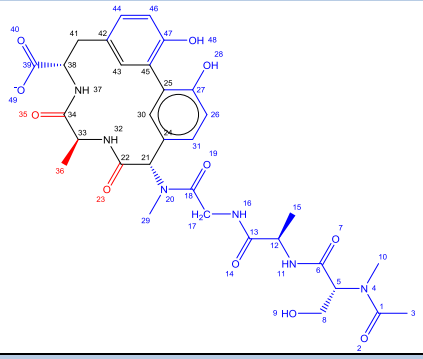
	All		Contact	
	Polar	*Nonpolar*	*Polar*	*Nonpolar*
Ring	2	12	1	4
Substituent	13	19	3	1
Peripheral groups	2	1	1	-
Total	17	32	5	5

Protein name	Signal peptidase type 1
Organism	Escherichia coli| Streptomyces sp.
Classification	Hydrolase/ antibiotic
Binding mode	Edge-on
Receptor secondary structure topology	
Number of residue 'hotspots'	9

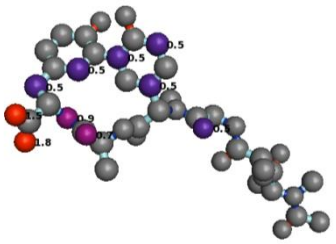
Number of protein-ligand interactions* ('Database link')

Hydrogen bond	6	Hydrogen donor-π	1
Ionic interaction	1	π-π	-
Cation-dipole	-	VdW interaction	5
Cation-π	-	Unfavourable	2
Dipolar interaction	-	Poor-angle	5
Halogen bond	-	Unclassified	1
Water-mediated interaction	3		

2D-STRUCTURE LIGAND

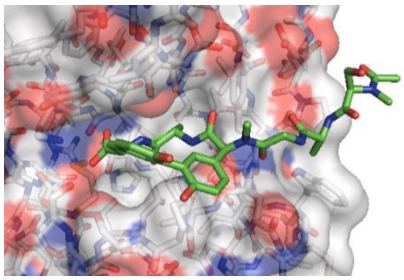


3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

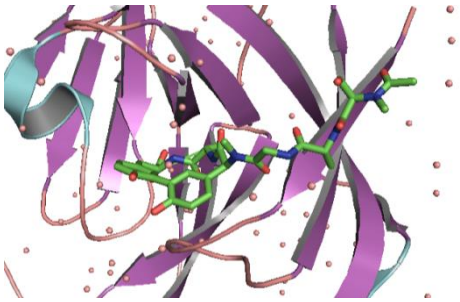


Physicochemical properties
'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis