

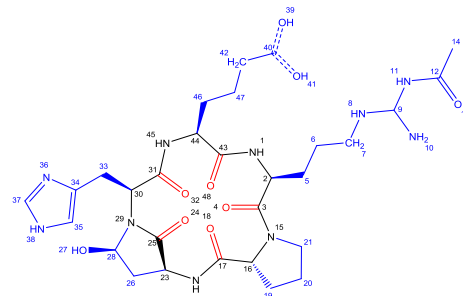
CODE	1W9U (PDB)	Resolution	1.85
Name		Ring size	15
Formula	C29H45N10O9	# Ligand atoms	48
Type	macrocycle	Scorpion Score	19.6
Mol. Weight (Da)	678	Saturated/ Unsaturated	S
cLogP	-3.3	Chiral centres.ring	5
tPSA	282	Chiral centres.sub	3
#HBD's	11		
#HBA's	18		
NRB (RING)	9	NRB (SUBSTITUENT)	12
Number of substituents	5	P/NP balance, substituents	9/19
<i>Large (≥5HA)</i>	3	P/NP balance, peripheral groups	5/0
<i>Small (2-4HA)</i>	2	Degrees of unsaturation ring	12.5
Proportion HA in substituents	79.2%	N:O ratio	10:9
Number of peripheral groups	5	Chiral centres	8

Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	5	10	1	3
Substituent	9	19	4	15
Peripheral groups	5	-	3	-
Total	19	29	8	18

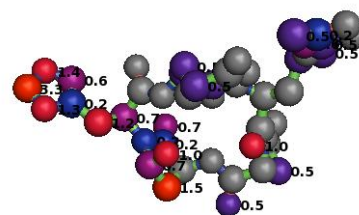
Protein name	Chitinase		
Organism	Aspergillus fumigatus Clonostachys		
Classification	Hydrolase/ Hydrolase inhibitors		
Binding mode	Edge-on		
Receptor secondary structure topology			
Number of residue 'hotspots'	13		

Number of protein-ligand interactions* (Database link)			
Hydrogen bond	8	Hydrogen donor-π	
Ionic interaction		π-π	8
Cation-dipole		VdW interaction	17
Cation-π	1	Unfavourable	2
Dipolar interaction		Poor-angle	1
Halogen bond		Unclassified	
Water-mediated interaction	1		

2D-STRUCTURE LIGAND



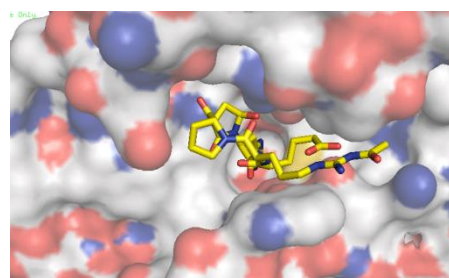
3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))



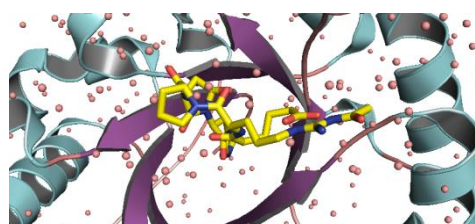
Physicochemical properties

[click for publication](#)

LIGAND-PROTEIN COMPLEX (I) ([Pymol link](#))



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis