

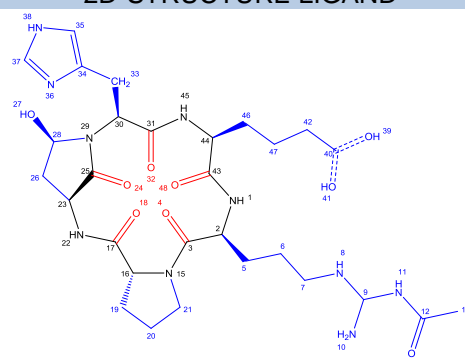
CODE	1WAW (PDB)	Resolution	1.75
Name		Ring size	15
Formula	C2945N10O9	# Ligand atoms	48
Type	macrocycle	Scorpion Score	23.8
Mol. Weight (Da)	678	Saturated/ Unsaturated	S
cLogP	-3.3	Chiral centres.ring	5
tPSA	282	Chiral centres.sub	3
#HBD's	11		
#HBA's	18		
N _{RB} (RING)	9	N _{RB} (SUB)	12
Number of 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	58.3%	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	4
Substituent	9	19	4	15
Peripheral groups	5	-	2	-
Total	19	29	7	19

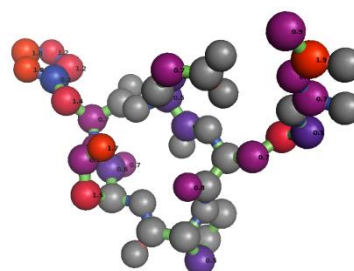
Protein name	Human chitinase		
Organism	Homo sapiens Clonostachys		
Classification	Hydrolase/ Hydrolase inhibitor		
Binding mode	Edge-on		
Receptor secondary structure topology			
Number of residue 'hotspots'	14		

Number of protein-ligand interactions* (Database link)			
Hydrogen bond	6	Hydrogen donor-π	1
Ionic interaction		π-π	9
Cation-dipole	1	VdW interaction	20
Cation-π	1	Unfavourable	1
Dipolar interaction		Poor-angle	1
Halogen bond		Unclassified	
Water-mediated interaction	5		

2D-STRUCTURE LIGAND



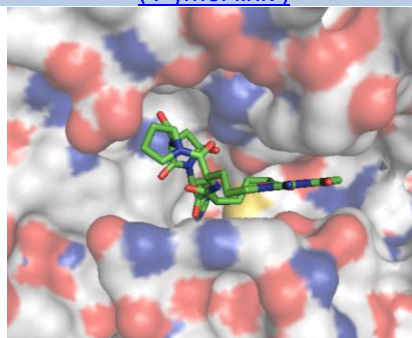
3D-STRUCTURE LIGAND +SCORPIONSORE ([Scorpion link](#))



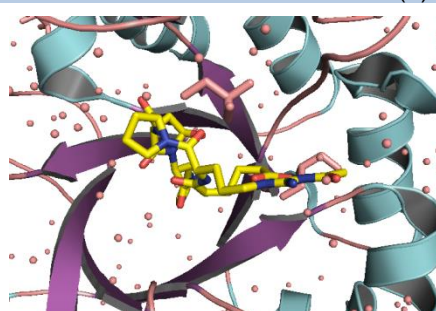
Physicochemical properties

[click for publication](#)

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis