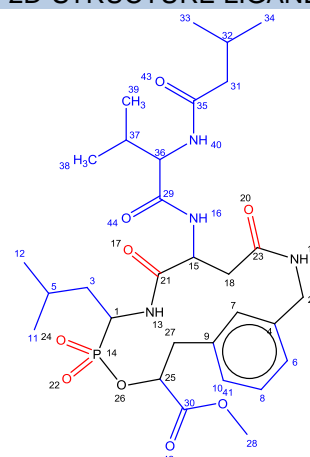
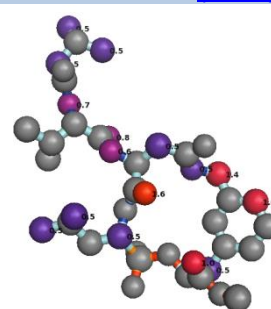


CODE	1BXO ( <a href="#">PDB</a> )	Resolution	0.95	
Name		Ring size	15	
Formula	C30H46N4O9P	# Ligand atoms	44	
Type	Macrocycle	Scorpion Score	10.2	
Mol. Weight (Da)	637,68	Saturated/ Unsaturated	U	
cLogP	3.0	Chiral centres.ring	3	
tPSA	186	Chiral centres.sub	1	
#HBD's	4			
#HBA's	13			
NRB (RING)	11	NRB (SUBSTITUENT)	10	
Number of substituents	4	P/NP balance, substituents	6/19	
Large ( $\geq 5HA$ )	1	P/NP balance, peripheral groups	4/0	
Small (2-4HA)	3	Degrees of unsaturation ring	10	
Proportion HA in substituents	56.8%	N:O ratio	4:9	
Number of peripheral groups	4	Chiral centres	4	
Polarity distribution ligand atoms				
	All		Contact	
	Polar	Nonpolar	Polar	Nonpolar
Ring	3	12	1	4
Substituent	6	19	4	6
Peripheral groups	4	-	1	-
Total	13	31	6	10
Protein name	Acid proteinase (penicillopepsin)			
Organism	Penicillium janthinellum			
Classification	Hydrolase			
Binding mode	Face-on/compact			
Receptor secondary structure topology				
Number of residue 'hotspots'	20			
Number of protein-ligand interactions* ( <a href="#">Database link</a> )				
Hydrogen bond	8	Hydrogen donor- $\pi$	2	
Ionic interaction		$\pi$ - $\pi$	1	
Cation-dipole		VdW interaction	12	
Cation- $\pi$		Unfavourable	7	
Dipolar interaction	2	Poor-angle	2	
Halogen bond		Unclassified		
Water-mediated interaction	2			

### 2D-STRUCTURE LIGAND



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



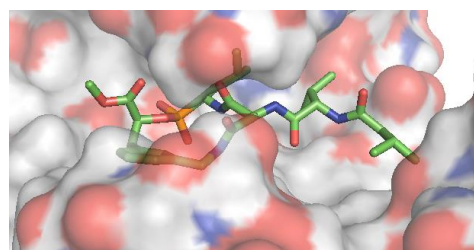
### Physicochemical properties

[click for publication](#)

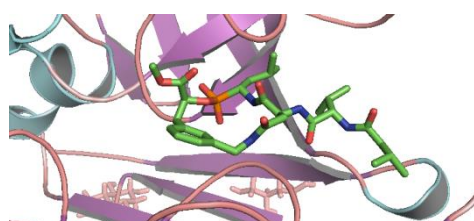
Ki (nM) 0.10

### LIGAND-PROTEIN COMPLEX (I)

([Pymol link](#))



### LIGAND-PROTEIN COMPLEX (II)



\*Based on Scorpion® analysis