

Supplementary material

Structure elucidation and functional studies of a novel β -hairpin antimicrobial peptide from the marine polychaeta *Capitella teleta*

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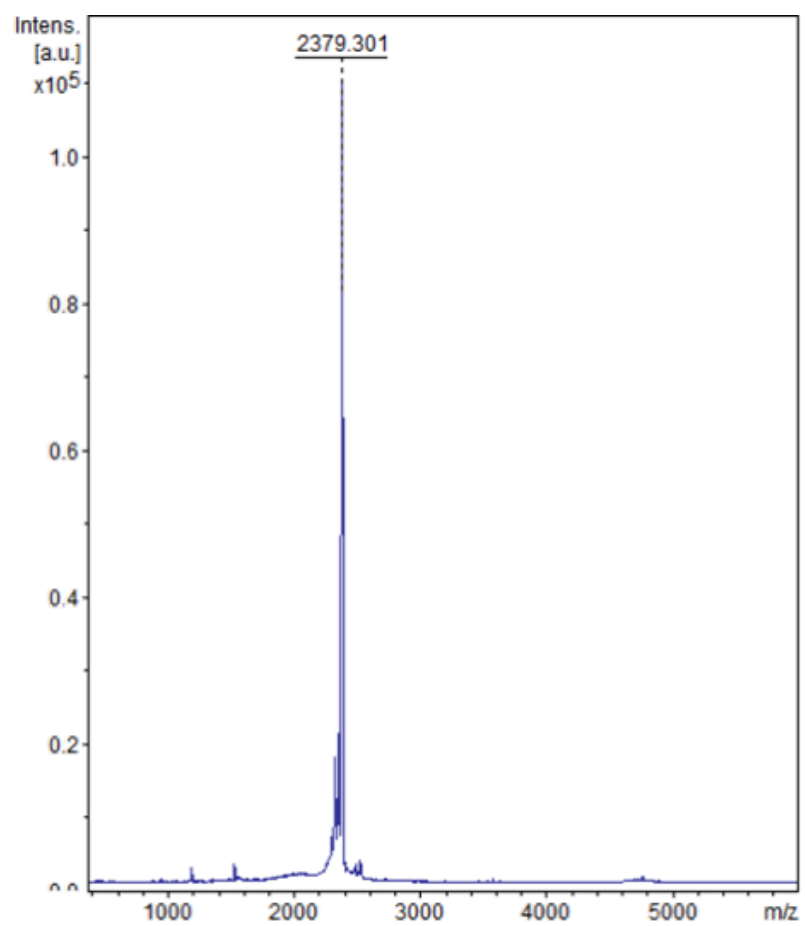


Figure S1. MALDI-MS analysis of the recombinant capitellacin. The experimental $[M+H]^+$ monoisotopic mass is indicated in the picture.

Table S1. Statistics for the best CYANA structures of capitellacin.

Distance and angle restraints	
Total NOE contacts	157
intraresidual	70
sequential ($ i-j =1$)	53
medium-range ($1< i-j <4$)	6
long-range ($ i-j >4$)	28
Hydrogen bonds restraints (6 bonds, upper/lower)	12/12
S-S bond restraints (2 bonds, upper/lower)	6/6
Torsion angle restraints	25
Angle φ	16
Angle χ_1	9
Total restraints/per residue:	218/11
Statistics for calculated structures	
Structures calculated/selected	200/20
CYANA target function (\AA^2)	0.22 \pm 0.3
Violations of restraints	
Distance ($>0.2 \text{\AA}$)	2
Distance ($>0.4 \text{\AA}$)	0
Dihedral angles ($>1^\circ$)	0
RMSD (\AA) overall (Ser1-Gly20)	
Backbone	0.42 \pm 0.15
Heavy atoms	1.13 \pm 0.13
Ramachandran analysis (backbone)	
Residues in favored regions (%)	75%
Residues in allowed regions (%)	25%
Residues in disallowed regions (%)	0%