

Table S6. NMR analysis of xantholysin A. ^1H and ^{13}C NMR assignment of xantholysin A in DMF-d7 solution, 55°C.

		^1H δ [ppm]	^{13}C δ [ppm]			^1H δ [ppm]	^{13}C δ [ppm]		
<u>HDA</u>	CO		173.28	<u>Gln3</u>					
	CH ₂ α	2.43	44.11		$^3J_{\text{HNH}\alpha}$ [Hz]	6.14	NH	8.34	
	CH β	4.02	68.71				CH α	4.26	55.64
	CH ₂ γ	1.48	37.91				CO		n.a.
	CH ₂ δ 1	1.36	25.76				CH ₂ β	2.13	27.17
	CH ₂ δ 2	1.48	25.76				CH ₂ γ	2.38	32.38
	CH ₂ ϵ	1.31	29.97				CO δ		n.a.
	CH ₂ ζ	1.28	29.60				NH ₂	6.71/7.40	
	CH ₂ η	1.28	32.07						
	CH ₂ θ	1.28	22.72						
CH ₃ ι	0.88	13.91							
	OH	n.a.							
<u>Leu1</u>				<u>Val4</u>					
	$^3J_{\text{HNH}\alpha}$ [Hz]	6.50			$^3J_{\text{HNH}\alpha}$ [Hz]	6.93	NH	7.70	
	NH	8.30					CH α	4.02	61.85
	CH α	4.30	52.87				CO		n.a.
	CO		n.a.				CH β	2.26	29.93
	CH ₂ β 1	1.67	40.96				CH ₃ γ	0.96	19.22
	CH ₂ β 2	1.74	40.96				CH ₃ γ	1.01	19.46
	CH γ	1.74	24.85						
	CH ₃ δ	0.91	21.80						
	CH ₃ δ	0.95	23.13						
<u>Glu2</u>				<u>Leu5</u>					
	$^3J_{\text{HNH}\alpha}$ [Hz]	ca 4.5			$^3J_{\text{HNH}\alpha}$ [Hz]	n.d.	NH	7.95	
	NH	8.72					CH α	4.18	54.65
	CH α	4.27	55.78				CO		n.a.
	CO		174.31				CH ₂ β	1.71	40.39
	CH ₂ β 1	2.04	27.02				CH γ	1.74	24.97
	CH ₂ β 2	2.15	27.02				CH ₃ δ	0.89	21.26
	CH ₂ γ	2.45	31.38				CH ₃ δ	0.94	22.63
	CO δ		n.a.						
	OH	n.a.							
<u>Gln6</u>				<u>Gln6</u>					
					$^3J_{\text{HNH}\alpha}$ [Hz]	6.58	NH	8.24	
							CH α	4.09	53.91
							CO		172.54
							CH ₂ β	2.05	27.08
							CH ₂ γ	2.28	32.18
							CO δ		n.a.
							NH ₂	6.55/7.19	

n.d. = not determined

n.a. = not assigned

Table S6. NMR analysis of xantholysin A. ^1H and ^{13}C NMR assignment of xantholysin A in DMF-d7 solution, 55°C (continued).

^1H δ [ppm] ^{13}C δ [ppm]				^1H δ [ppm] ^{13}C δ [ppm]			
Ser7				Leu11			
$^3J_{\text{HNH}\alpha}$ [Hz]	5.32	NH	7.89	$^3J_{\text{HNH}\alpha}$ [Hz]	n.d.	NH	7.95
		CH α	4.58			CH α	4.32
		CO				CO	53.62
		CH ₂ β 1	64.01			CH ₂ β 1	173.51
		CH ₂ β 2	4.38			CH ₂ β 2	41.18
			4.50			CH γ	41.18
						CH ₃ δ	24.94
						CH ₃ δ	21.92
						CH ₃ δ	22.91
Val8				Leu12			
$^3J_{\text{HNH}\alpha}$ [Hz]	6.79	NH	8.20	$^3J_{\text{HNH}\alpha}$ [Hz]	7.12	NH	7.79
		CH α	4.09			CH α	4.34
		CO				CO	53.23
		CH β	173.90			CH ₂ β	173.76
		CH ₃ γ	2.40			CH ₂ β	1.71
		CH ₃ γ	0.98			CH γ	1.76
			1.08			CH ₃ δ	25.02
						CH ₃ δ	21.61
						CH ₃ δ	23.33
Leu9				Gln13			
$^3J_{\text{HNH}\alpha}$ [Hz]	n.d.	NH	8.03	$^3J_{\text{HNH}\alpha}$ [Hz]	6.70	NH	7.25
		CH α	4.20			CH α	4.25
		CO				CO	54.27
		CH ₂ β 1	174.04			CH ₂ β 1	172.30
		CH ₂ β 2	1.59			CH ₂ β 2	27.32
		CH γ	1.84			CH ₂ β 2	2.32
		CH ₃ δ	1.83			CH ₂ γ	2.22
		CH ₃ δ	0.87			CO δ	n.a.
		CH ₃ δ	0.92			NH ₂	6.63/7.19
			23.05				
Gln10				Ile14			
$^3J_{\text{HNH}\alpha}$ [Hz]	6.84	NH	7.74	$^3J_{\text{HNH}\alpha}$ [Hz]	8.51	NH	7.48
		CH α	4.33			CH α	4.37
		CO				CO	n.a.
		CH ₂ β 1	172.98			CH β	1.89
		CH ₂ β 2	2.04			CH ₃ γ	37.06
		CH ₂ γ	2.18			CH ₂ γ 1	15.82
		CO δ	2.38			CH ₂ γ 2	25.30
		NH ₂	n.a.			CH ₃ δ	25.30
			6.55/7.19				11.00

n.d. = not determined

n.a. = not assigned