

Supplementary file

Killing effect of *Bacillus velezensis* FZB42 on a *Xanthomonas campestris* pv. *campestris* (Xcc) strain newly isolated from cabbage *Brassica oleracea* convar. *capitata* (L.): a metabolomic study

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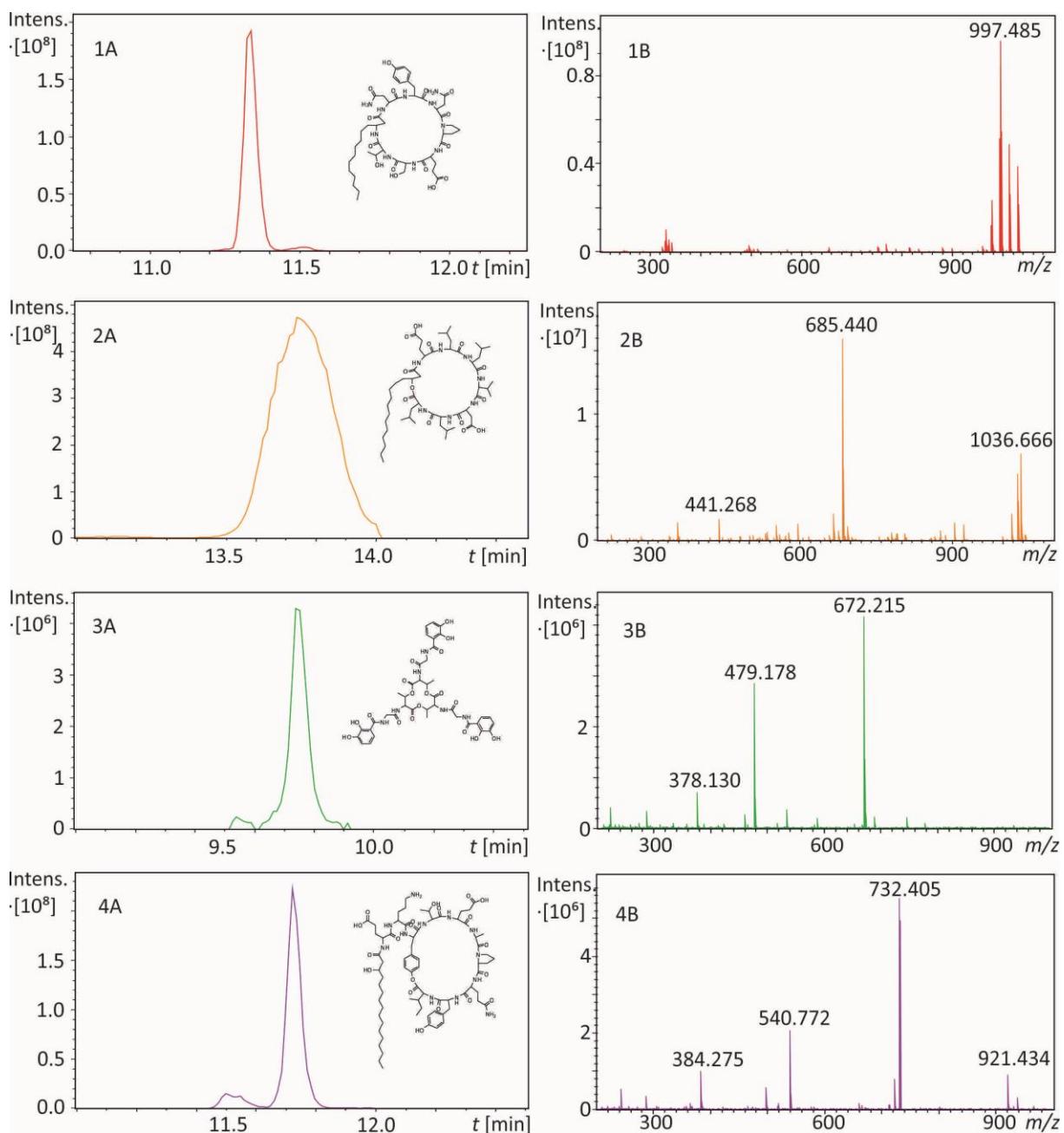
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Table S1: Metabolites detected in dual culture of *B. velezensis* FZB42 and Xcc-SU

metabolite	ion type	measured m/z	Molecular formula	Calculated m/z	LC-MS spectra
Bacillomycin D (C12)	[M+H] ⁺	1003.506	C ₄₆ H ₇₀ N ₁₀ O ₁₅	1003.509	
Bacillomycin D (C13)	[M+H] ⁺	1017.514	C ₄₇ H ₇₂ N ₁₀ O ₁₅	1017.525	
Bacillomycin D (C14)	[M+H] ⁺	1031.548	C ₄₈ H ₇₄ N ₁₀ O ₁₅	1031.541	Fig.S1A,B
	[M+Na] ⁺	1053.523	C ₄₈ H ₇₄ N ₁₀ O ₁₅	1053.523	
Bacillomycin D (C15)	[M+H] ⁺	1045.551	C ₄₉ H ₇₆ N ₁₀ O ₁₅	1045.556	
	[M+Na] ⁺	1067.546	C ₄₉ H ₇₆ N ₁₀ O ₁₅	1067.538	
Bacillomycin D (C16)	[M+H] ⁺	1059.564	C ₅₀ H ₇₈ N ₁₀ O ₁₅	1059.572	
	[M+Na] ⁺	1081.547	C ₅₀ H ₇₈ N ₁₀ O ₁₅	1081.554	
Bacillomycin D (C17)	[M+H] ⁺	1073.584	C ₅₁ H ₈₀ N ₁₀ O ₁₅	1073.588	
Surfactin (C50)	[M+H] ⁺	994.639	C ₅₀ H ₈₇ N ₇ O ₁₃	994.643	
	[M+Na] ⁺	1016.623	C ₅₀ H ₈₇ N ₇ O ₁₃	1016.625	
Surfactin (C51)	[M+H] ⁺	1008.654	C ₅₁ H ₈₉ N ₇ O ₁₃	1008.659	
	[M+Na] ⁺	1030.637	C ₅₁ H ₈₉ N ₇ O ₁₃	1030.641	
Surfactin (C52)	[M+H] ⁺	1022.669	C ₅₂ H ₉₁ N ₇ O ₁₃	1022.675	
	[M+Na] ⁺	1044.648	C ₅₂ H ₉₁ N ₇ O ₁₃	1044.657	
Surfactin (C53)	[M+H] ⁺	1036.697	C ₅₃ H ₉₃ N ₇ O ₁₃	1036.690	Fig.S2A,B
	[M+Na] ⁺	1058.669	C ₅₃ H ₉₃ N ₇ O ₁₃	1058.672	
Bacillibactin	[M+H] ⁺	883.263	C ₃₉ H ₄₂ N ₆ O ₁₈	883.263	Fig.S3A,B
	[M+Na] ⁺	905.244	C ₃₉ H ₄₂ N ₆ O ₁₈	905.245	
Fengycin A (C15-un-saturated)	[M+2H] ²⁺	724.411	C ₇₁ H ₁₀₆ N ₁₂ O ₂₀	724.390	
Fengycin A (C15)	[M+2H] ²⁺	725.398	C ₇₁ H ₁₀₈ N ₁₂ O ₂₀	725.397	
Fengycin A (C16-un-saturated)	[M+2H] ²⁺	731.403	C ₇₂ H ₁₀₈ N ₁₂ O ₂₀	731.397	
Fengycin A (C16)	[M+2H] ²⁺	732.406	C ₇₂ H ₁₁₀ N ₁₂ O ₂₀	732.405	Fig.S4A,B
Fengycin A (C17-un-saturated)	[M+2H] ²⁺	738.428	C ₇₃ H ₁₁₀ N ₁₂ O ₂₀	738.405	
Fengycin A (C17)	[M+2H] ²⁺	739.412	C ₇₃ H ₁₁₂ N ₁₂ O ₂₀	739.413	
Fengycin A (C18)	[M+2H] ²⁺	746.428	C ₇₄ H ₁₁₄ N ₁₂ O ₂₀	746.421	
Fengycin A (C19)	[M+2H] ²⁺	753.429	C ₇₅ H ₁₁₆ N ₁₂ O ₂₀	753.429	
Fengycin A (C20)	[M+2H] ²⁺	760.427	C ₇₆ H ₁₁₈ N ₁₂ O ₂₀	760.437	
Fengycin A (C21)	[M+2H] ²⁺	767.433	C ₇₇ H ₁₂₀ N ₁₂ O ₂₀	767.444	
Fengycin A (C22)	[M+2H] ²⁺	774.435	C ₇₈ H ₁₂₂ N ₁₂ O ₂₀	774.452	
Fengycin A (C23)	[M+2H] ²⁺	781.444	C ₇₉ H ₁₂₄ N ₁₂ O ₂₀	781.460	
Fengycin A (C24)	[M+2H] ²⁺	788.447	C ₈₀ H ₁₂₆ N ₁₂ O ₂₀	788.468	

Figure S1: Extracted ion chromatograms of bacillomycin D ($[M+H]^+=1031.541\text{ }m/z$, 1A), surfactin ($[M+H]^+=1036.690\text{ }m/z$, 2A), bacilibactin ($[M+H]^+=883.263\text{ }m/z$, 3A), and fengycin A ($[M+2H]^{2+}=732.405\text{ }m/z$, 4A) at particular retention times. Corresponding fragmentation spectra of selected parent ions of bacillomycin D (1B), surfactin (2B), bacilibactin (3B), and fengycin A (4B) are in agreement with the literature [41,49].



Abbreviations: BH, Bushnel-Haas medium; CBS, concentric backscatter detector; CFU, colony forming unit; ESI, electrospray ionization; ETD, Everhart-Thornley Detector; HPLC, high-performance liquid chromatography; LB, Luria-Bertani broth; LC-MS, liquid chromatography-mass spectrometry; LOD, limit of detection; LOQ, limit of quantitation; M9, mineral medium; M9TE, M9 mineral medium supplemented with trace elements; MS, mass spectrometry; PCR, polymerase chain reaction; SEM, scanning electron microscopy; TLD, through-the-lens detector; Xcc, *Xanthomonas campestris* pv. *campestris*

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