

Supporting Information

Secondary Metabolites with Agricultural Antagonistic Potentials from *Beauveria felina*, a Marine-derived Entomopathogenic Fungus

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Figure S1. HR-ESI-MS spectrum of compound **1**.

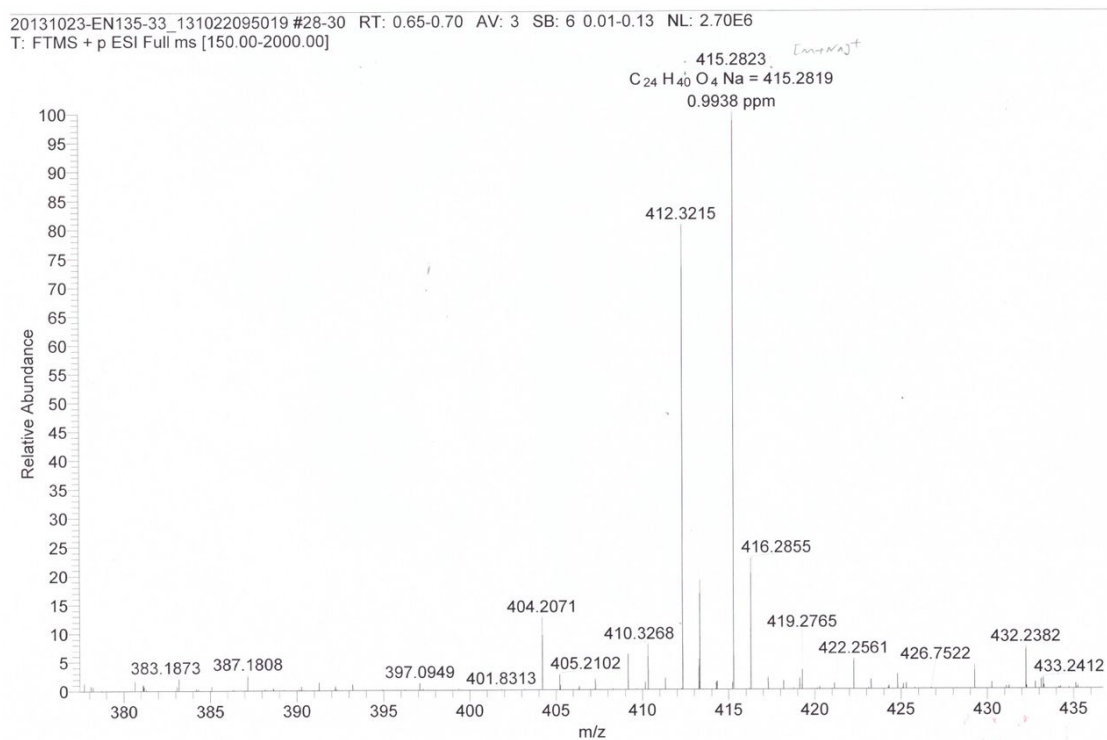


Figure S2. 1H NMR (500 MHz, $DMSO-d_6$) spectrum of compound **1**.

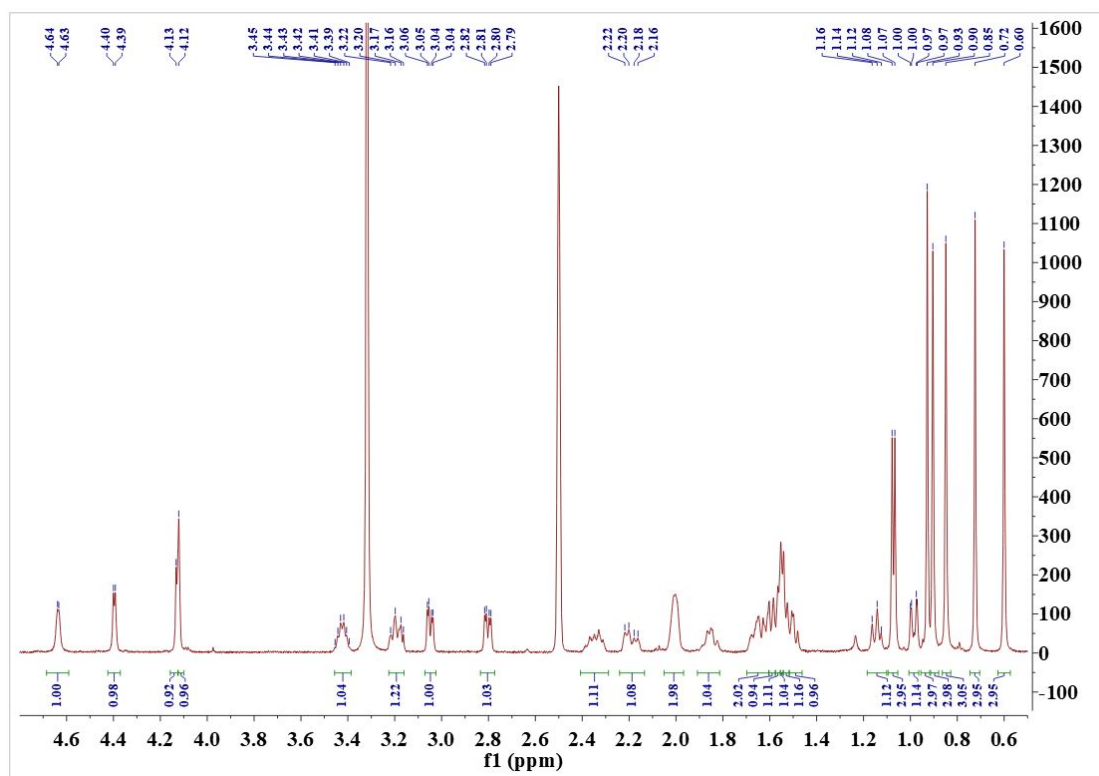


Figure S3. ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) and DEPT spectra of compound **1**.

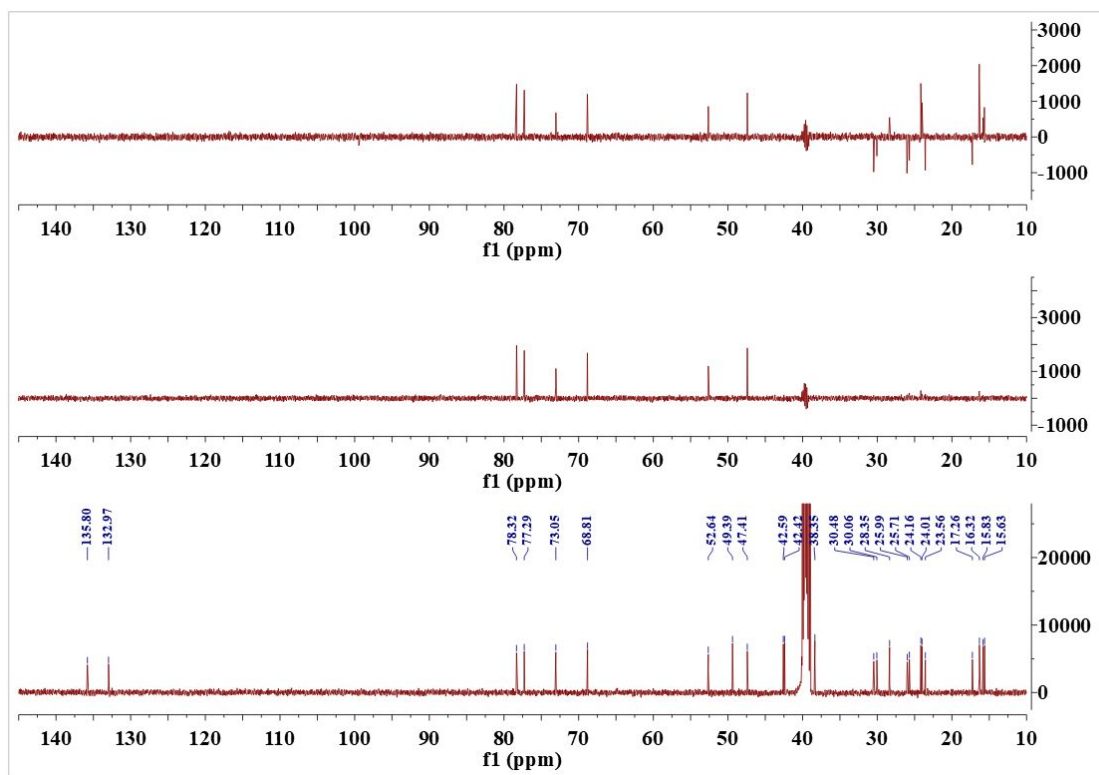


Figure S4. ^1H - ^1H COSY spectrum of compound **1**.

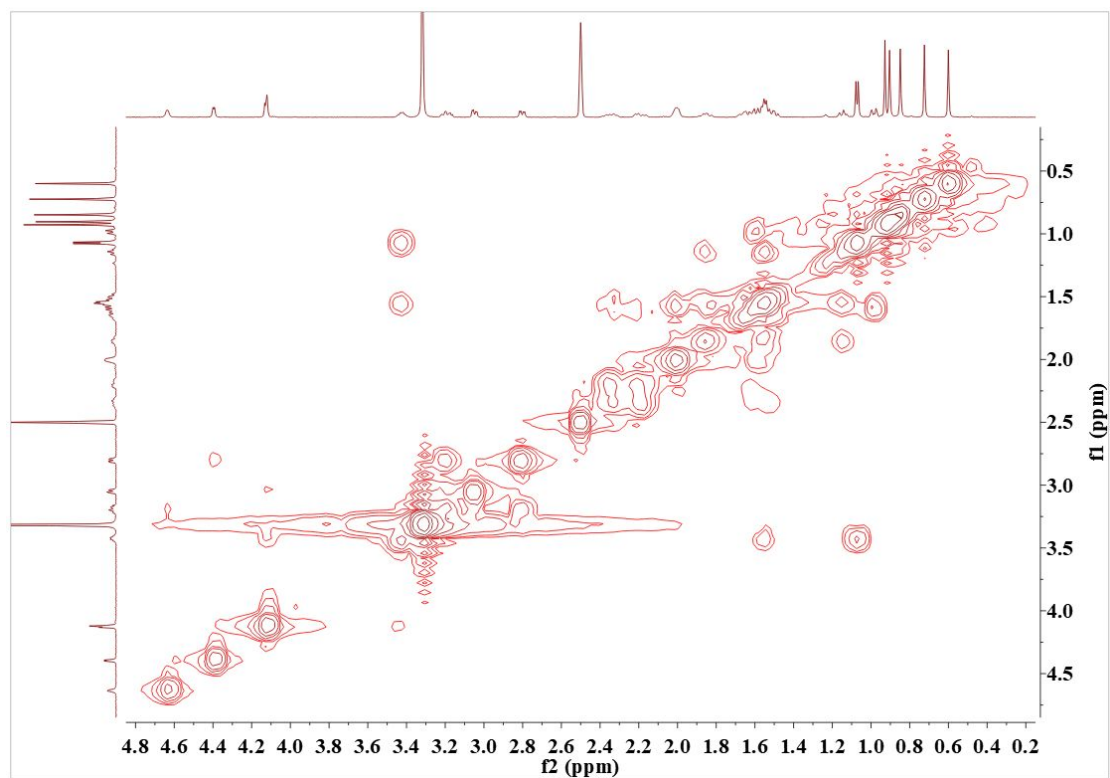


Figure S5. HSQC spectrum of compound **1**.

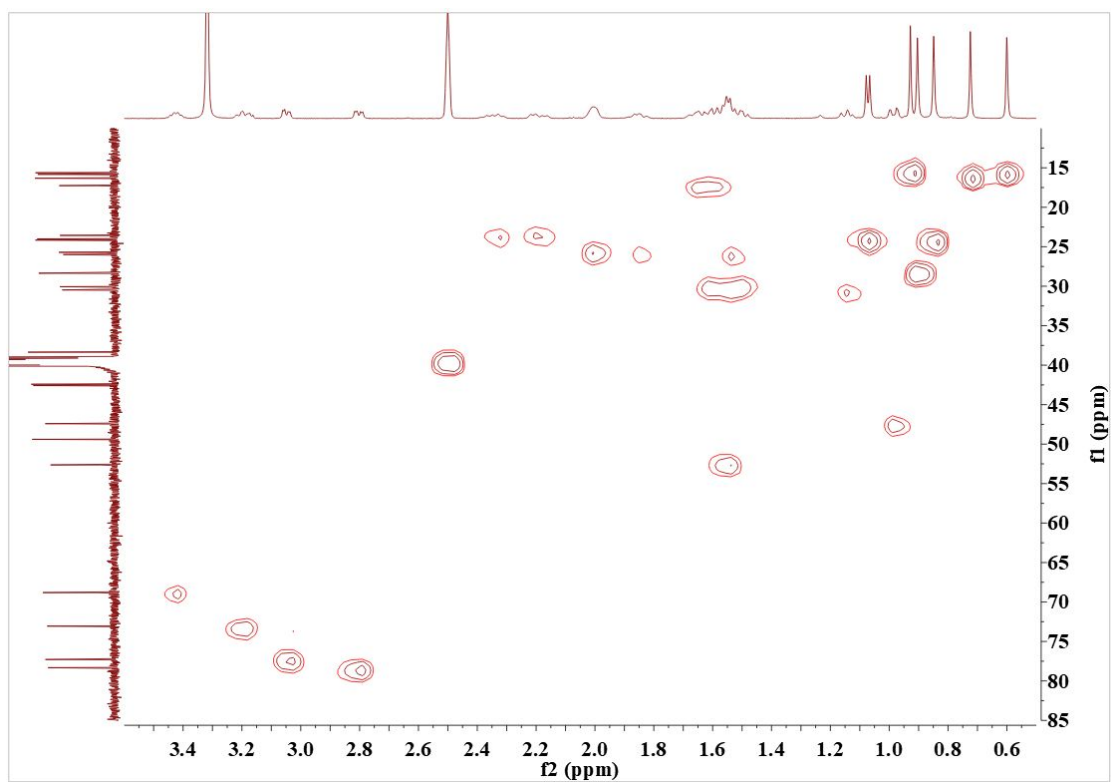


Figure S6. HMBC spectrum of compound **1**.

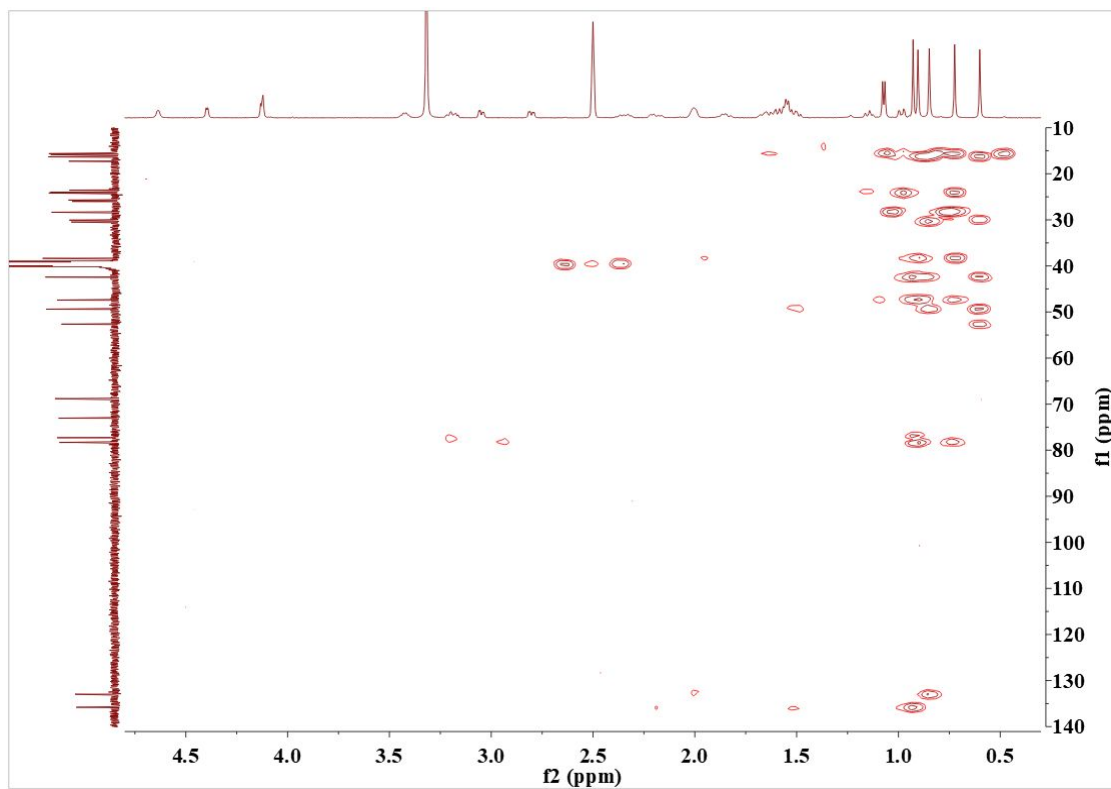


Figure S7. NOESY spectrum of compound 1.

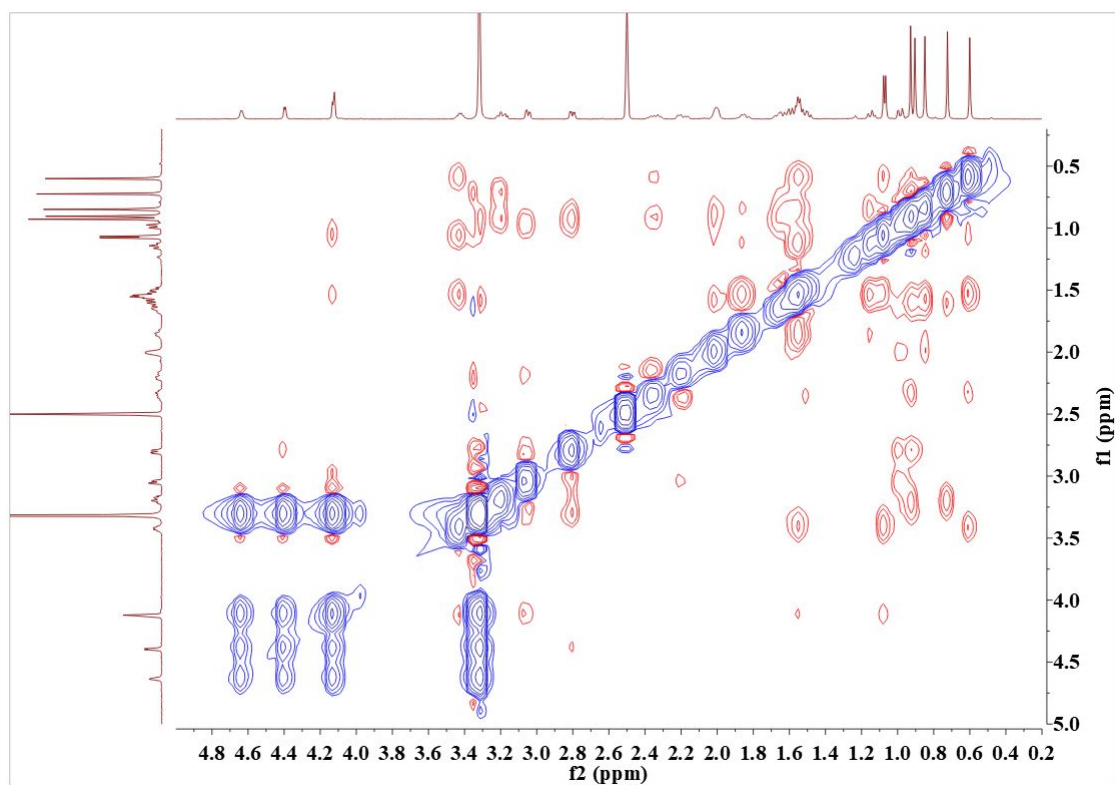


Figure S8. HR-ESI-MS spectrum of compound 2.

20130608-EN135-62_130606155538 #93-104 RT: 0.75-0.84 AV: 12 NL: 1.21E6
T: FTMS + p ESI Full ms [130.00-1500.00]

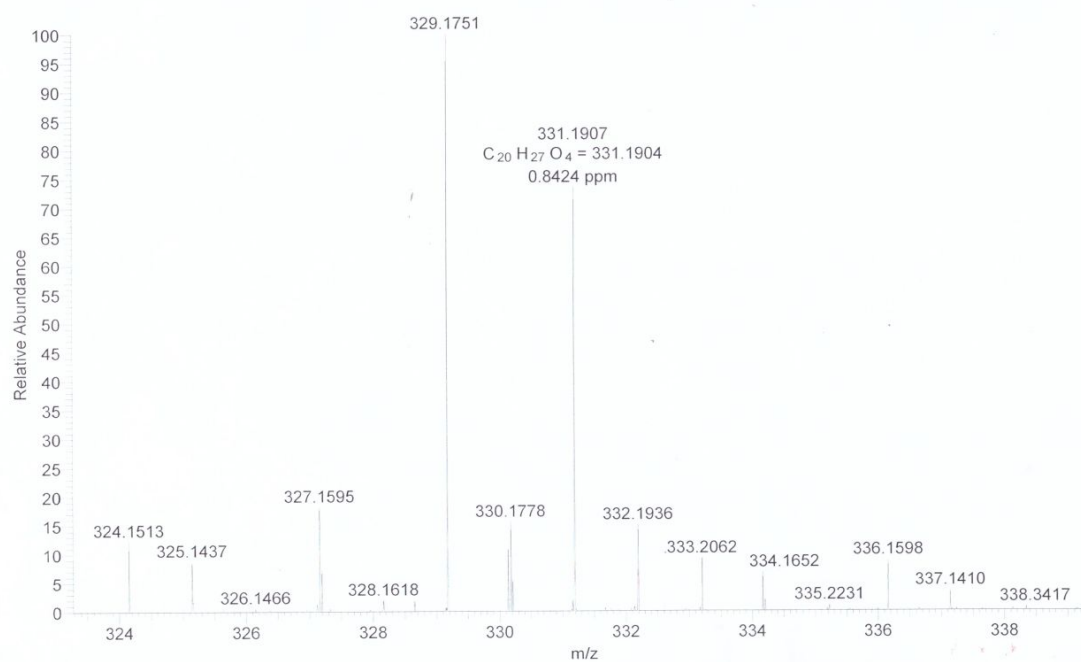


Figure S9. ^1H NMR (500 MHz, acetone- d_6) spectrum of compound **2**.

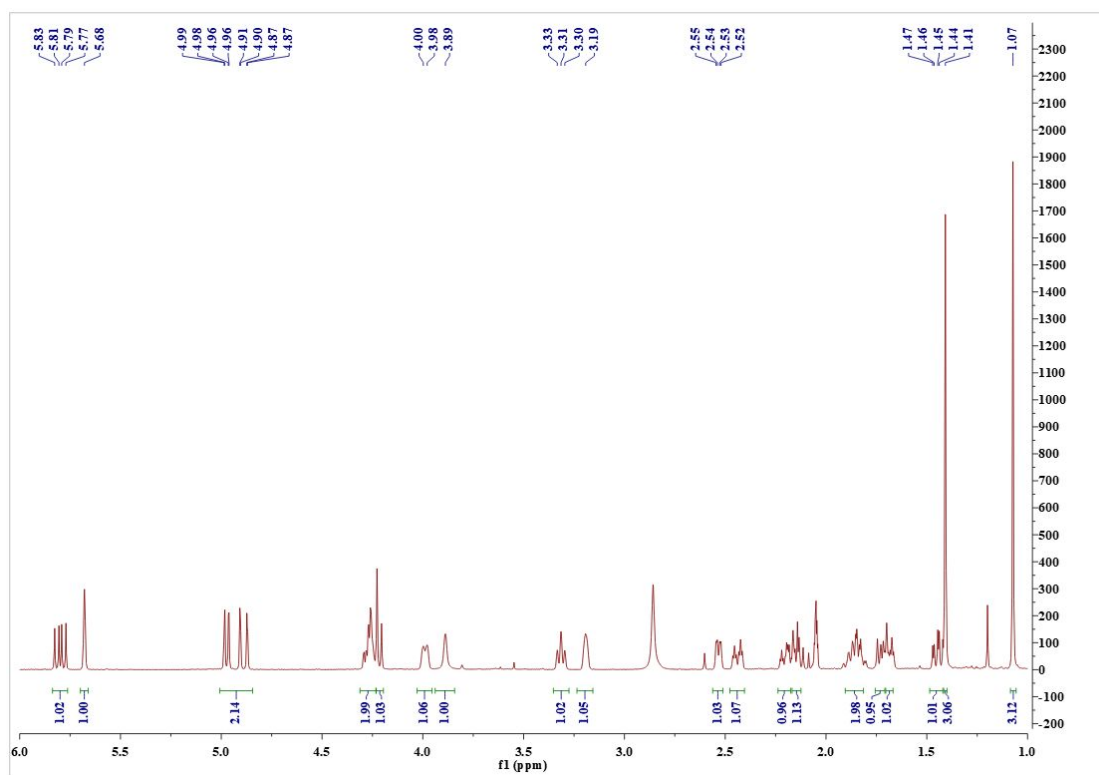


Figure S10. ^{13}C NMR (125 MHz, acetone- d_6) and DEPT spectra of compound **2**.

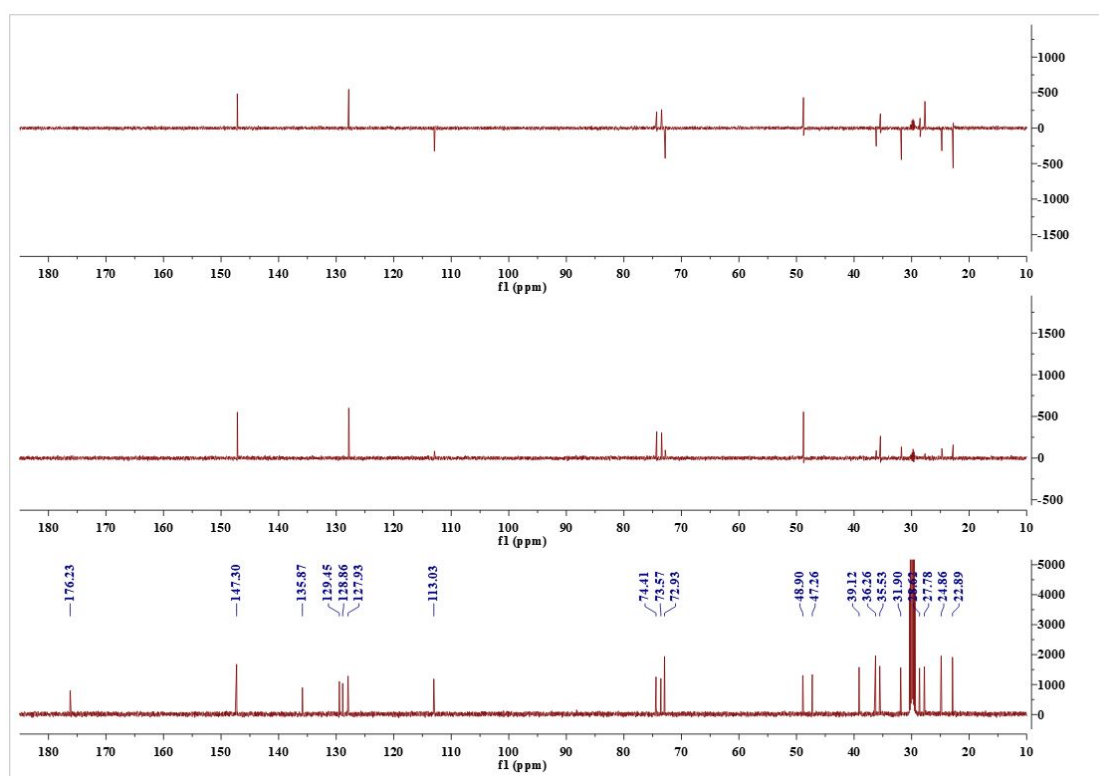


Figure S13. HMBC spectrum of compound **2**.

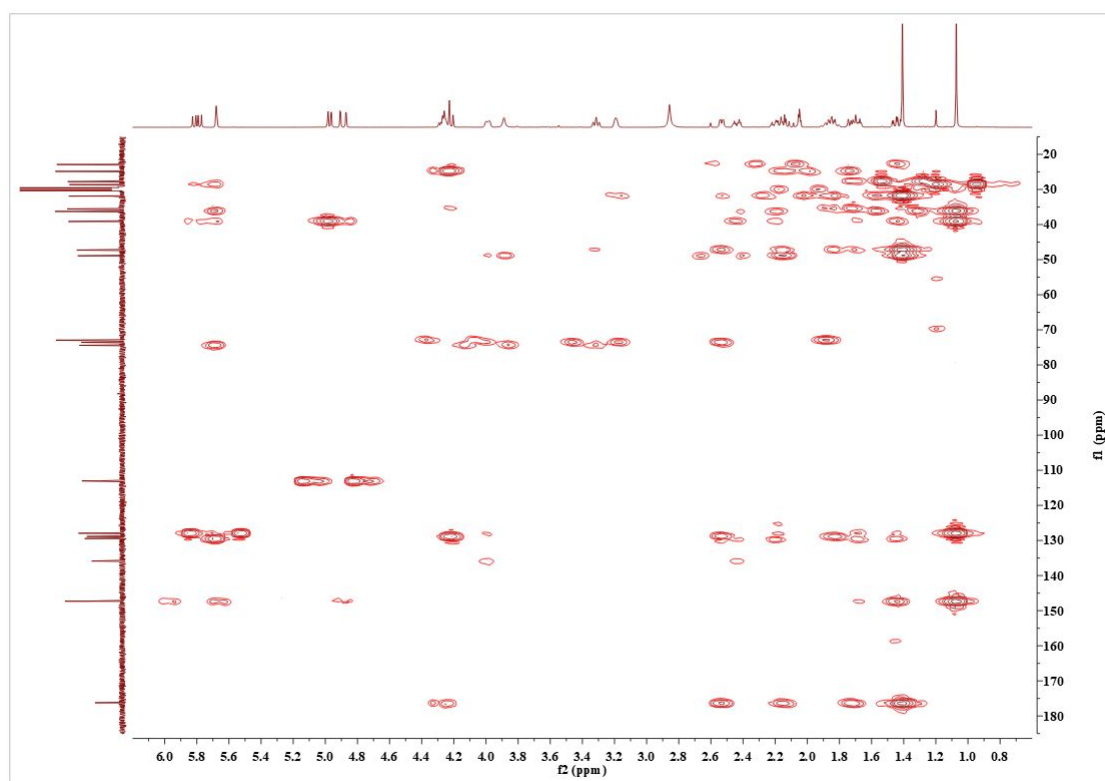


Figure S14. NOESY spectrum of compound **2**.

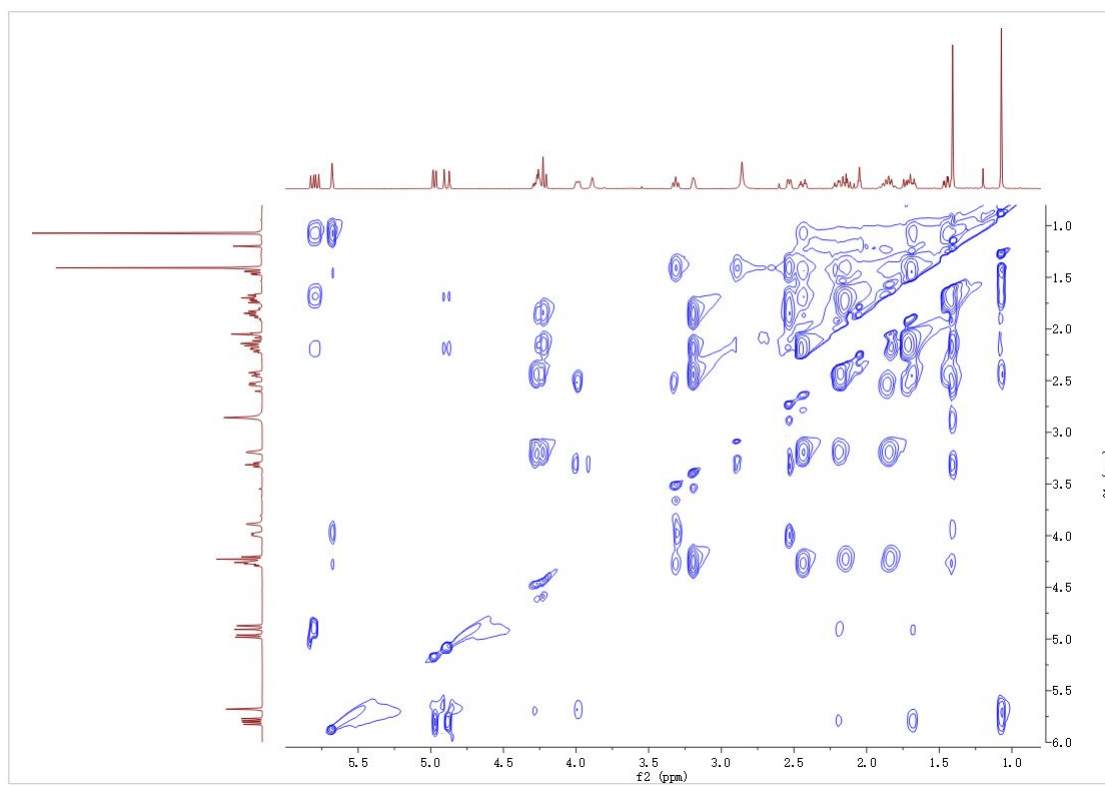


Figure S15. HR-ESI-MS spectrum of compound **3**.

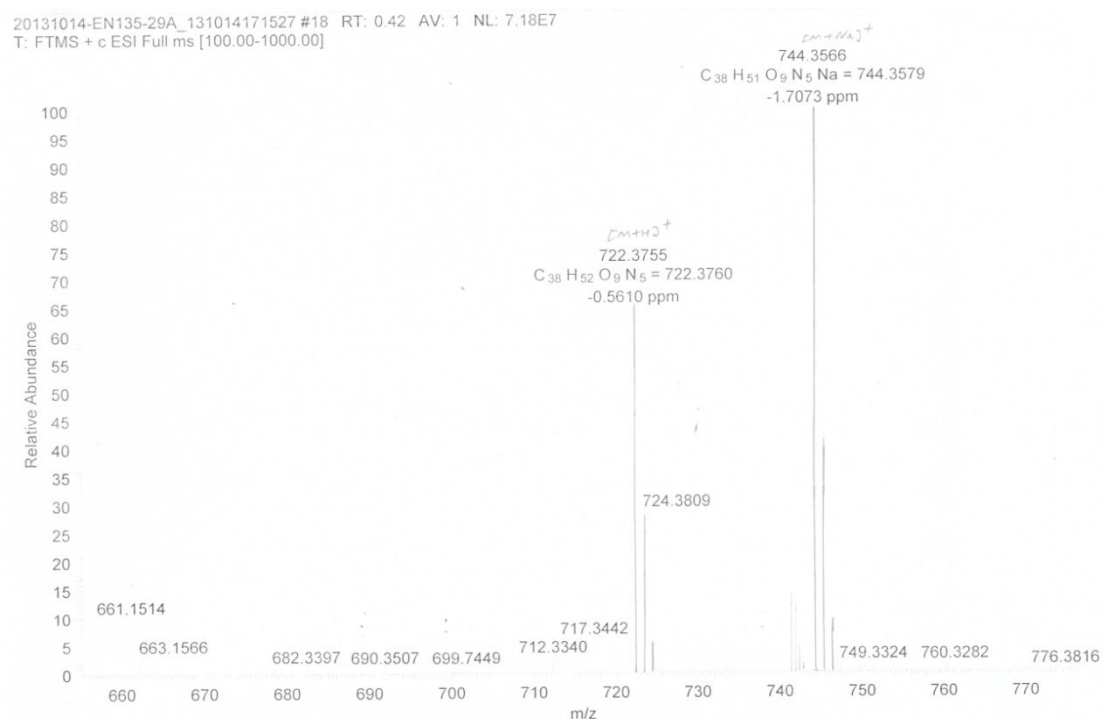


Figure S16. ^{13}C NMR (125 MHz, acetone- d_6) of compound **3**.

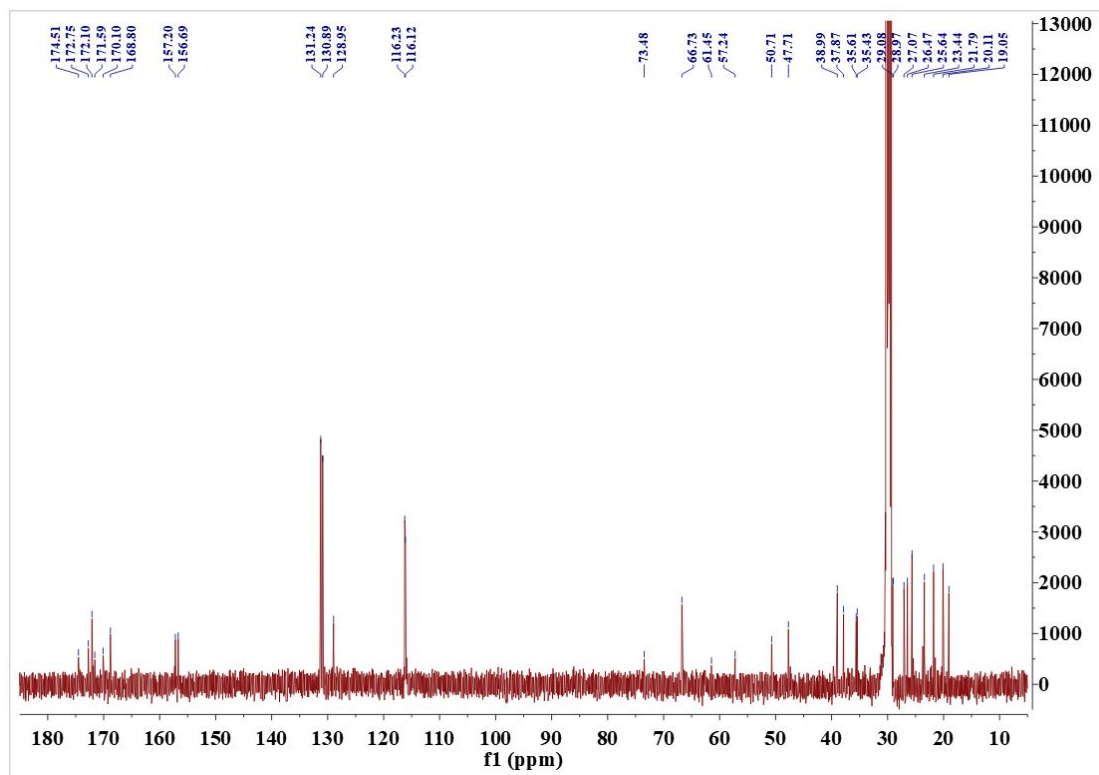


Figure S17. DEPT spectra of compound **3**.

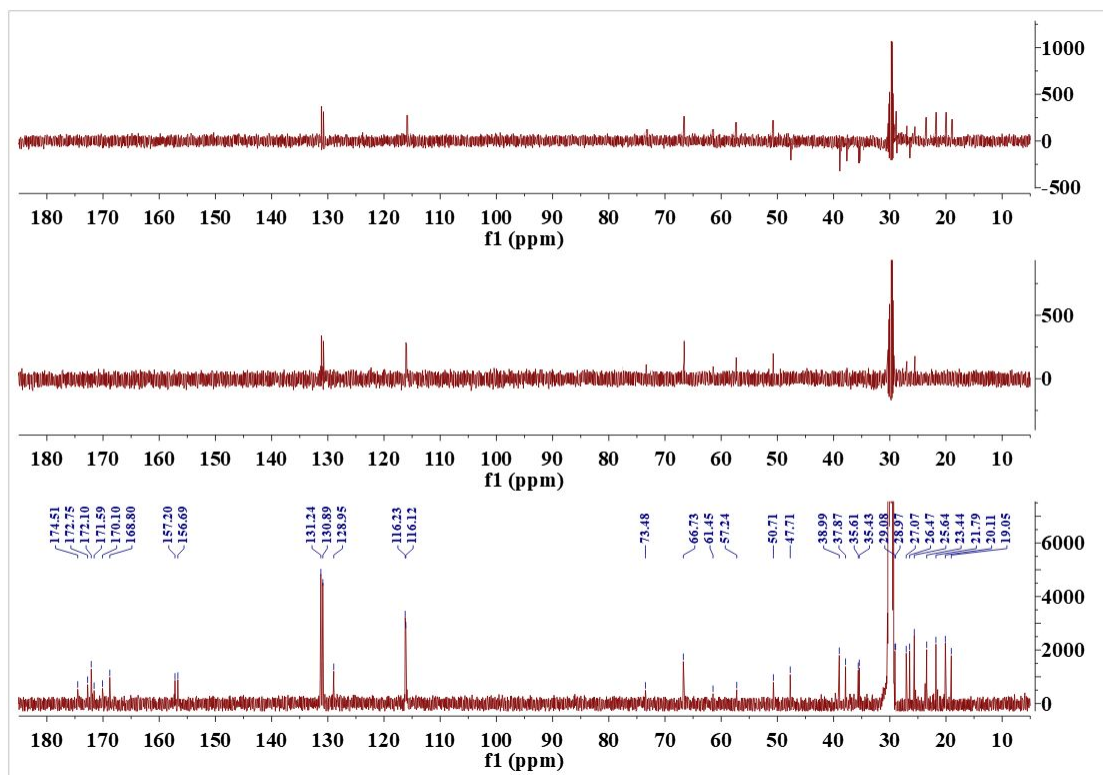


Figure S18. ^1H NMR (500 MHz, acetone- d_6) spectrum of compound **3**.

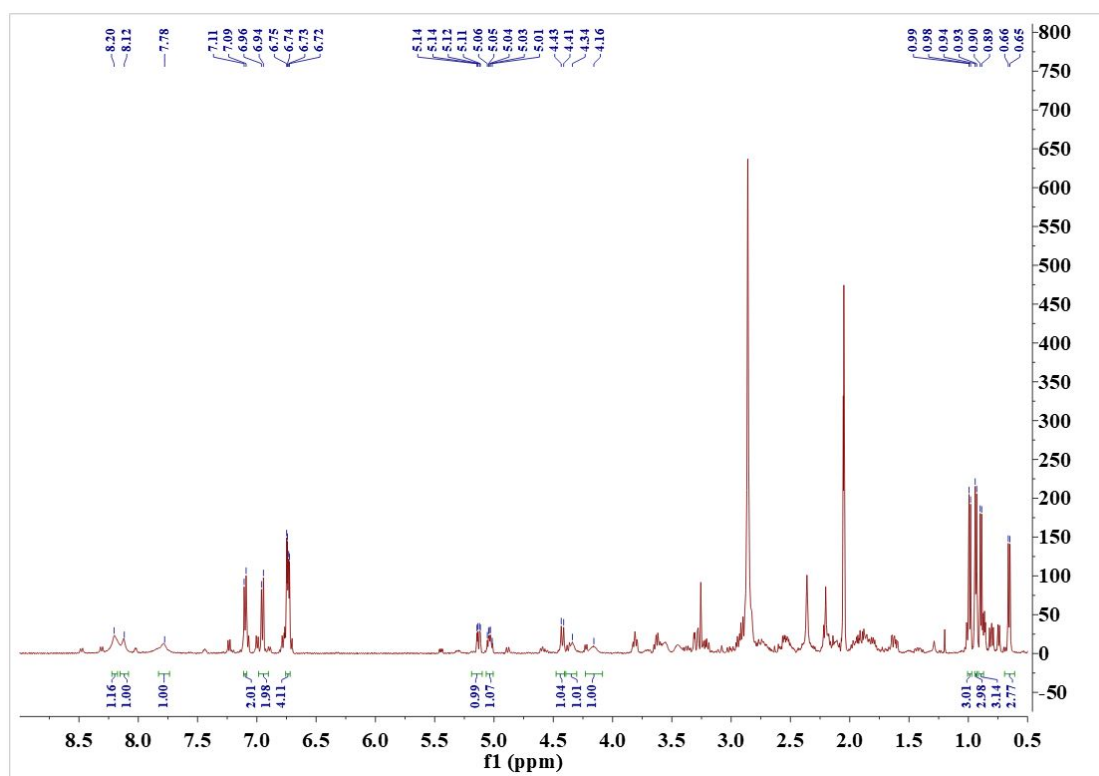


Figure S19. Inhibitory activity of the positive control of 2,4-dichlorophenoxyacetic acid against the radicle growth of *A. retroflexus* seedlings.



Figure S20. The structures of compound **3** and desmethyisaridin G.

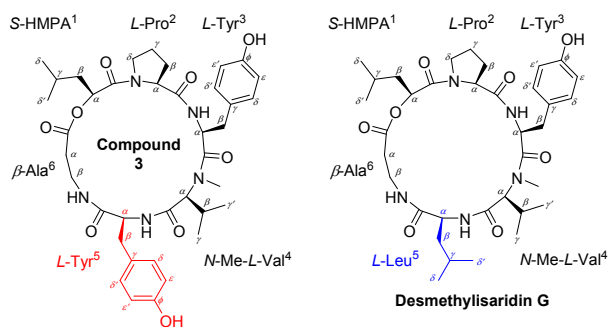


Table S1. Comparison of ^{13}C NMR data of compound **3** and desmethyisaridin G (Acetone- d_6 , δ : ppm).

Compound 3 ^a		Desmethyisaridin G ^a		Compound 3		Desmethyisaridin G	
HMPA		HMPA		N-Me-Val		N-Me-Val	
CO	170.1, C	CO	169.1, C	CO	168.8, C	CO	167.9, C
α	73.5, CH	α	73.7, CH	α	66.7, CH	α	66.0, CH
β	39.0, CH ₂	β	38.1, CH ₂	β	27.1, CH	β	26.2, CH
γ	25.6, CH	γ	24.7, CH	γ	20.1, CH ₃	γ	19.1, CH ₃
δ	23.4, CH ₃	δ	22.9, CH ₃	γ'	19.1, CH ₃	γ'	18.1, CH ₃
δ'	21.8, CH ₃	δ'	20.9, CH ₃	N-Me	29.1, CH ₃	N-Me	28.4, CH ₃
Pro ²		Pro ²		Tyr ⁵		Leu ⁵	
CO	174.5, C	CO	173.7, C	CO	172.1, C	CO	171.1, C
α	61.5, CH	α	61.6, CH	α	57.2, CH	α	52.1, CH
β	29.0, CH ₂	β	28.2, CH ₂	β	39.0, CH ₂	β	39.5, CH ₂
γ	26.5, CH ₂	γ	25.6, CH ₂	γ	129.0, C	γ	24.5, CH
δ	47.7, CH ₂	δ	46.9, CH ₂	δ/δ'	130.9, CH	δ	22.5, CH ₃
Tyr ³		Tyr ³		ϵ/ϵ'	116.1, CH	δ'	20.6, CH ₃
CO	172.8, C	CO	172.2, C	θ	156.7, C		
α	50.7, CH	α	49.9, CH	β-Ala ⁶		β-Ala ⁶	
β	37.9, CH ₂	β	37.0, CH ₂	CO	171.6, C	CO	171.3, C
γ	129.0, C	γ	128.0, C	α	35.4, CH ₂	α	34.4, CH ₂
δ/δ'	131.2, CH	δ/δ'	130.3, CH	β	35.6, CH ₂	β	34.5, CH ₂
ϵ/ϵ'	116.2, CH	ϵ/ϵ'	115.2, CH				
θ	157.2, C	θ	156.3, C				

^a Both determined in acetone- d_6 .

Table S2. Back bone torsion angels (ω) in the crystal structure of **3**.

Amide bonds	Torsion angel (°)
HMPA ¹ -Pro ²	-7.6
Pro ² -Tyr ³	173.0
Tyr ³ -NMeVal ⁴	-3.7
NMeVal ⁴ -Tyr ⁵	179.7
Tyr ⁵ - β -Ala ⁶	-178.7
β -Ala ⁶ -HMPA ¹	166.0