Peniginsengins B–E, New Farnesylcyclohexenones from the Deep Sea-Derived Fungus *Penicillium* sp. YPGA11

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Abstract: Chemical examination of the EtOAc extract of the deep sea-derived fungus *Penicillium* sp. YPGA11 resulted in the isolation of four new farnesylcyclohexenones, peniginsengins B–E (**1–4**), and a known analog peniginsengin A (**5**). The structures of compounds **1–4** were determined on the basis of comprehensive analyses of the nuclear magnetic resonance (NMR) and mass spectroscopy (MS) data, and the absolute configurations of **1**, **2**, and **4** were determined by comparisons of experimental electronic circular dichroism (ECD) with calculated ECD spectra. Compounds **1–5**, characterized by a highly oxygenated 1-methylcyclohexene unit and a (4*E*,8*E*)-4,8-dimethyldeca-4,8-dienoic acid side chain, are rarely found in nature. Compounds **2–4** exhibited antibacterial activity against *Staphylococcus aureus*.

Keywords: *Penicillium* sp.; deep sea-derived fungus; farnesylcyclohexenones; antibacterial

Content

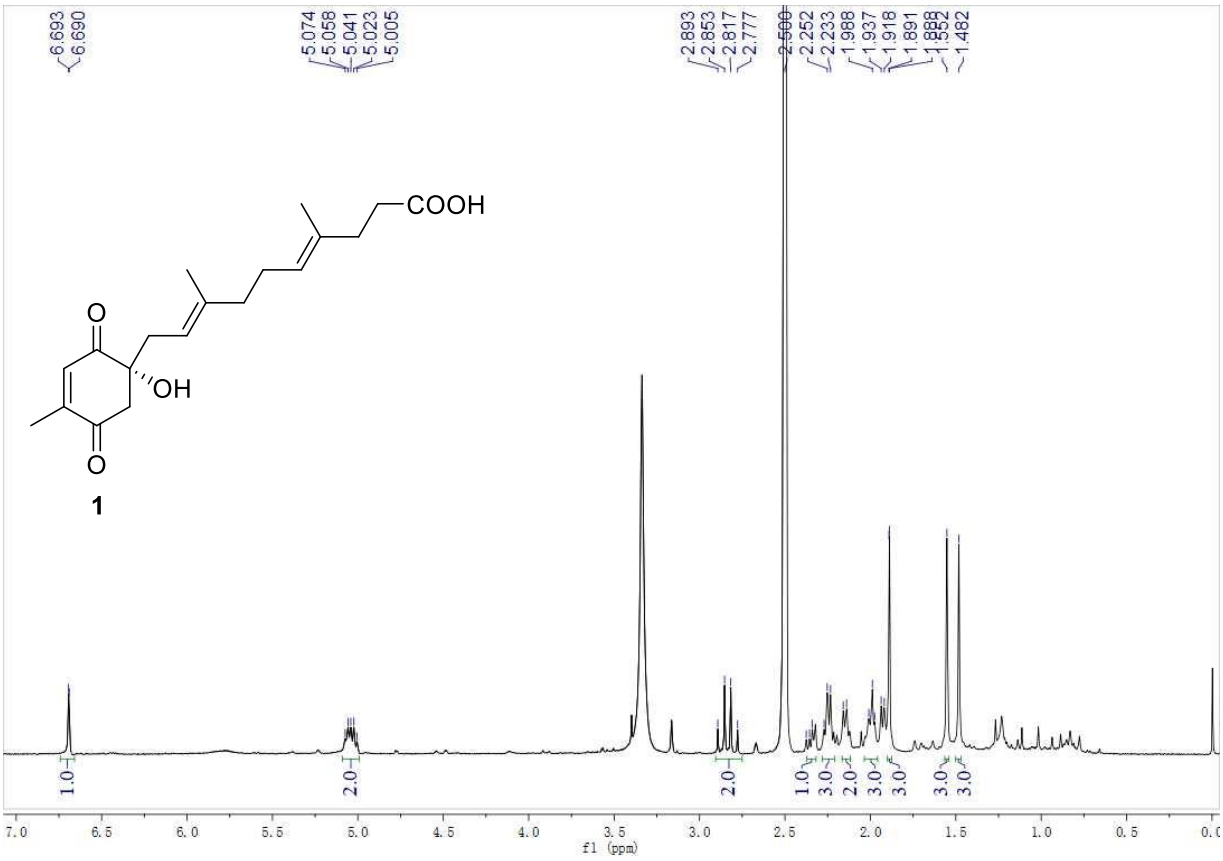

Figure S1. ^{1}H NMR Spectrum of **1** in DMSO-d_6 (400 MHz).

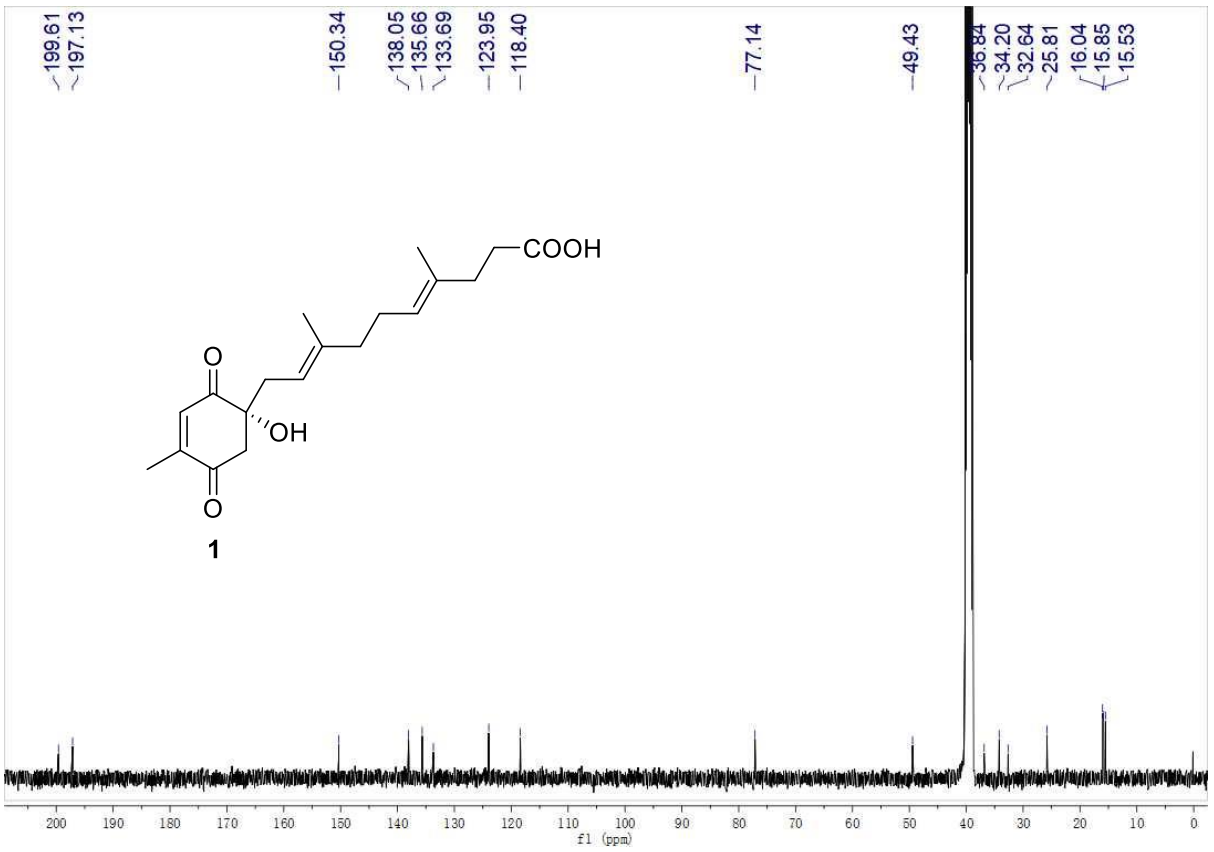

Figure S2. ^{13}C NMR Spectrum of **1** in DMSO-d_6 (100 MHz).

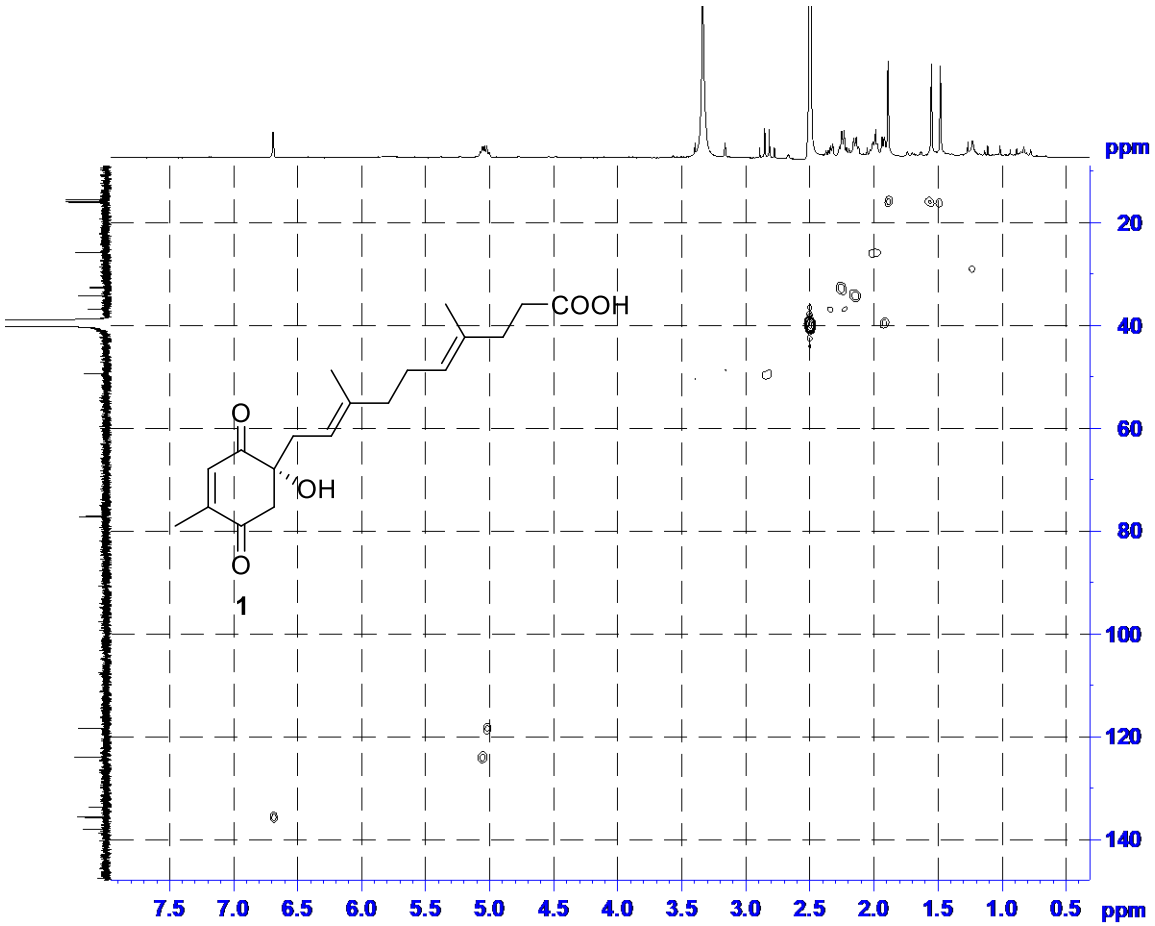

Figure S3. HSQC Spectrum of **1** in DMSO-d_6 (400 MHz)

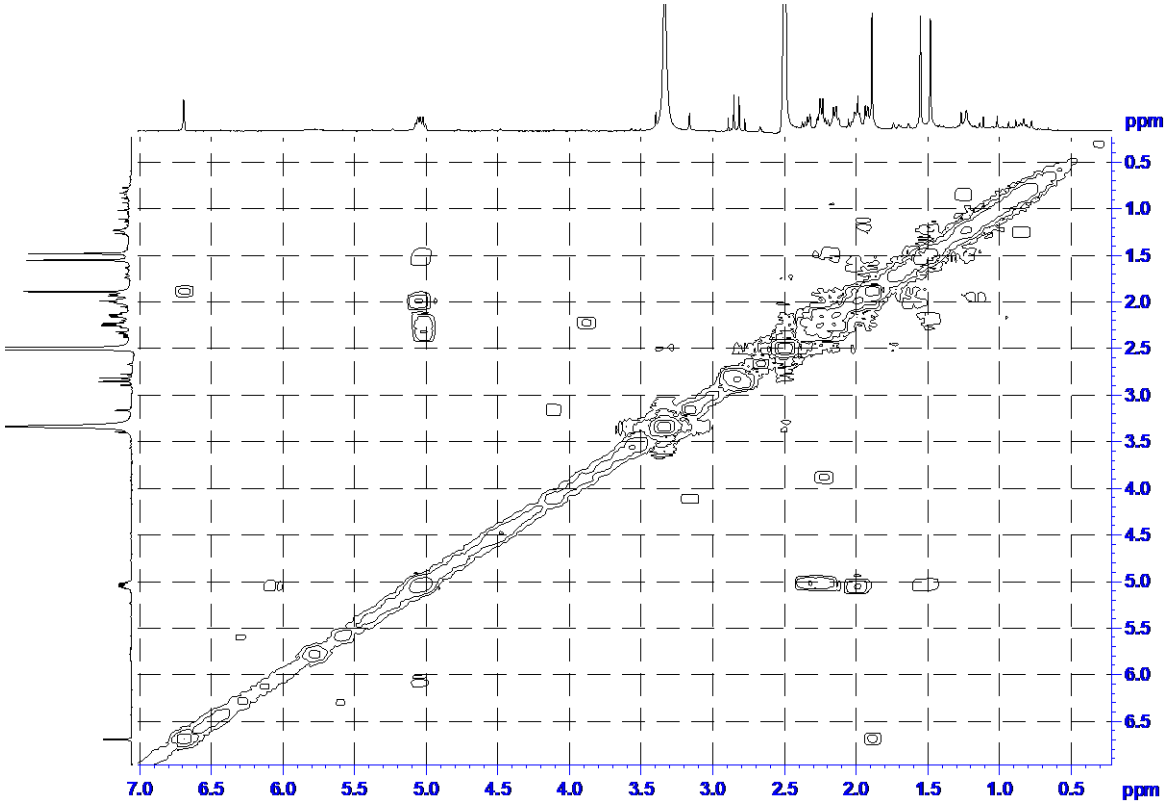

Figure S4. COSY Spectrum of **1** in DMSO-d_6 (400 MHz)

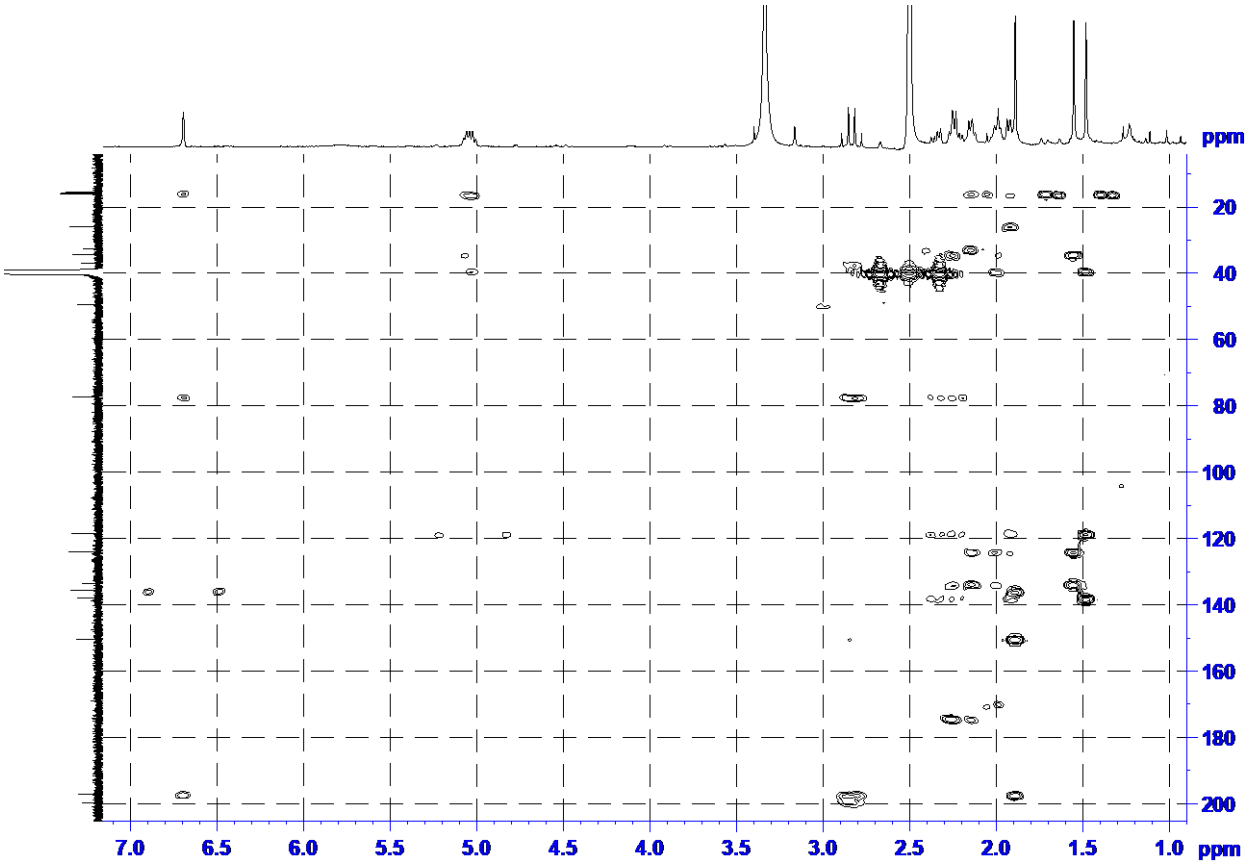

Figure S5. HMBC Spectrum of **1** in DMSO-d_6 (400 MHz)

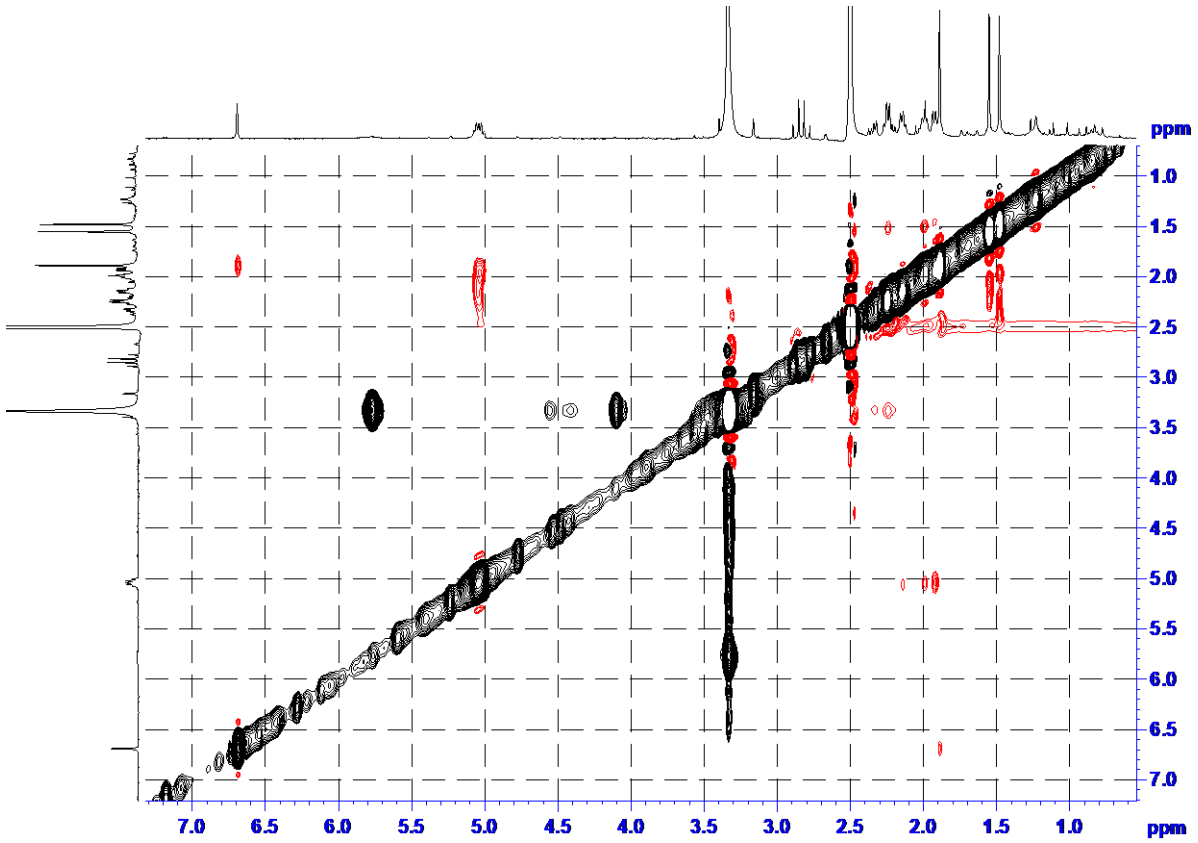

Figure S6. NOESY Spectrum of **1** in DMSO-d_6 (400 MHz)

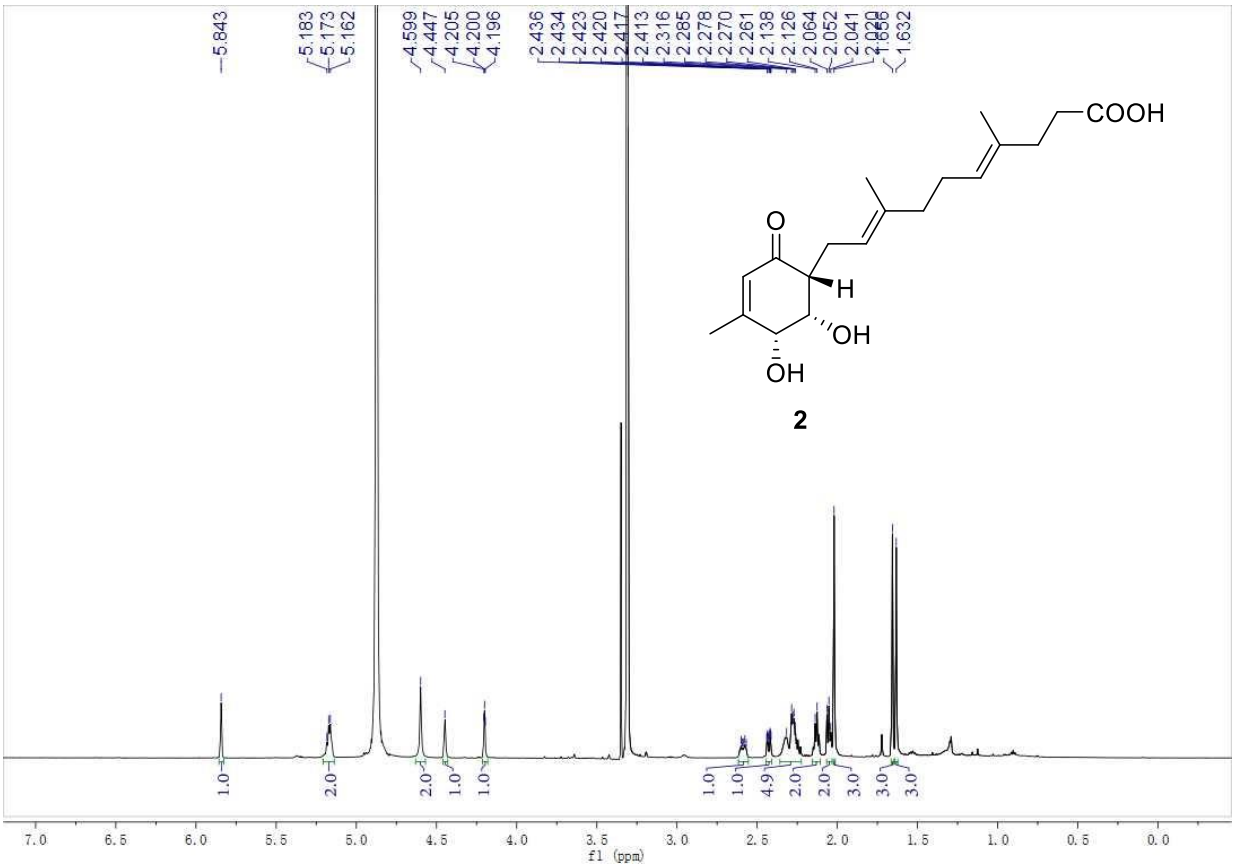

Figure S7. ^{1}H NMR Spectrum of **2** in Methanol-d_4 (600 MHz).

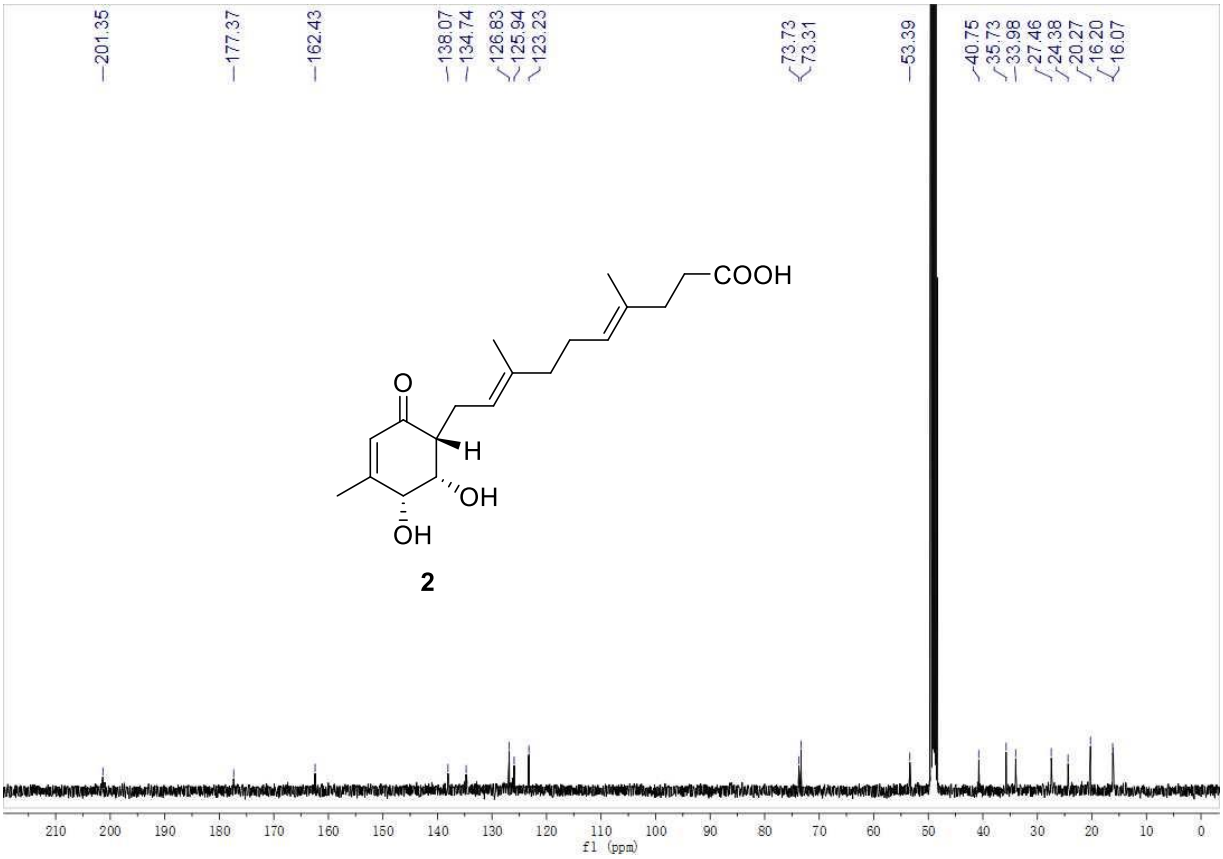

Figure S8. ^{13}C NMR Spectrum of **2** in Methanol-d_4 (150 MHz).

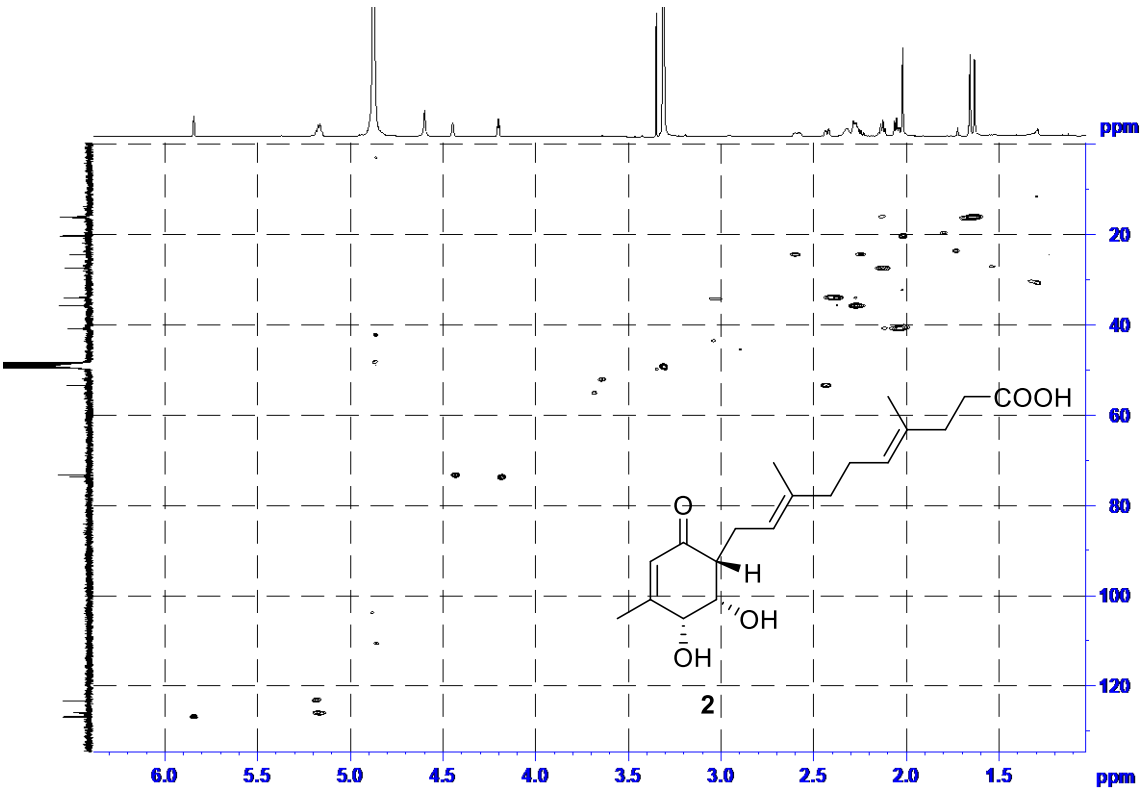

Figure S9. HSQC Spectrum of **2** in Methanol-d_4 (600 MHz).

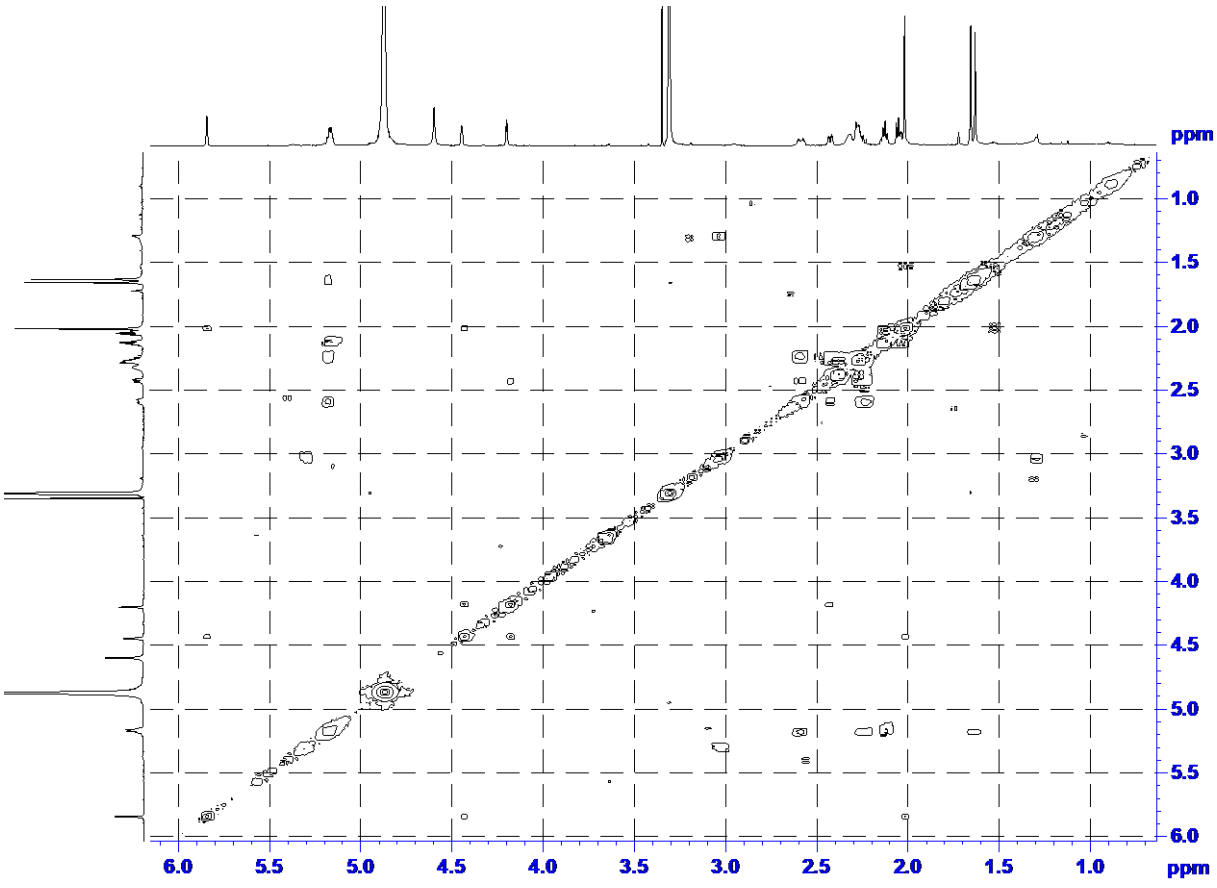

Figure S10. COSY Spectrum of **2** in Methanol-d_4 (600 MHz).

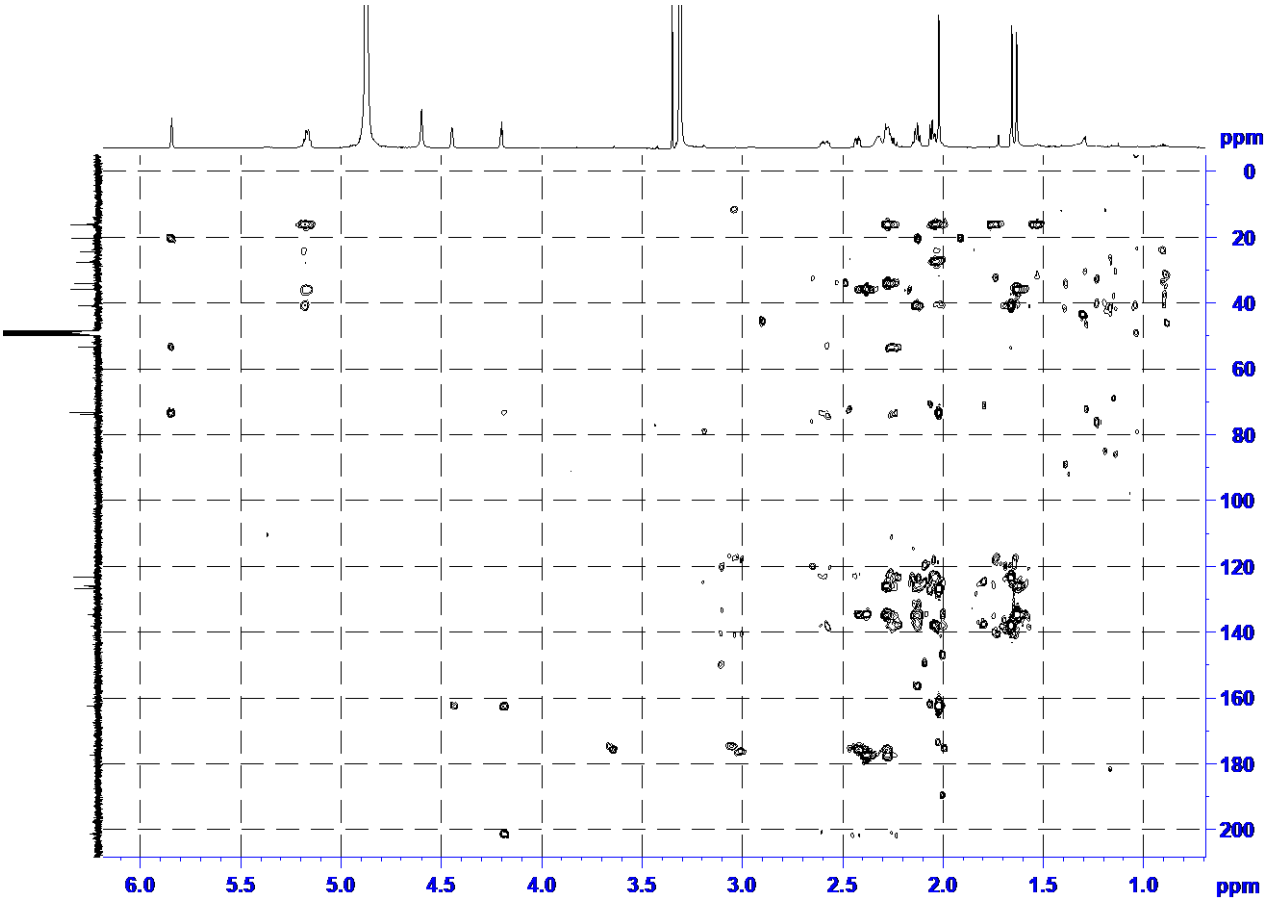

Figure S11. HMBC Spectrum of **2** in Methanol-d_4 (600 MHz).

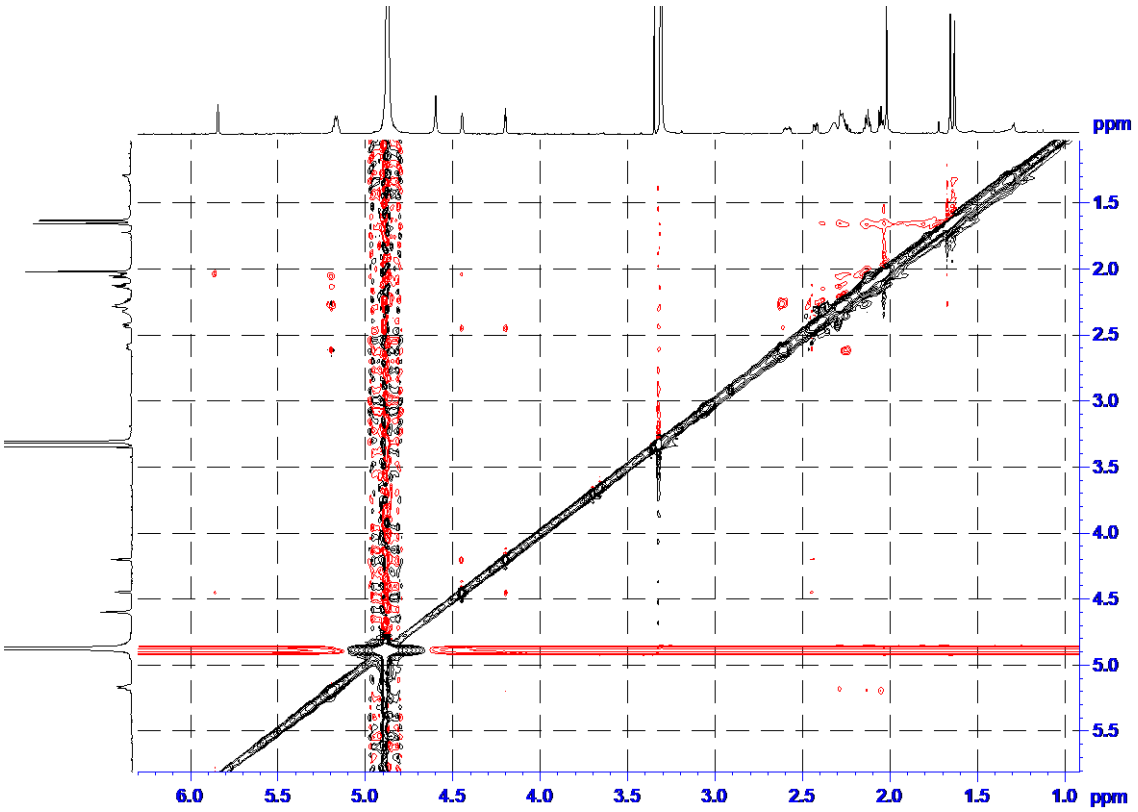

Figure S12. NOESY Spectrum of **2** in Methanol-d_4 (600 MHz).

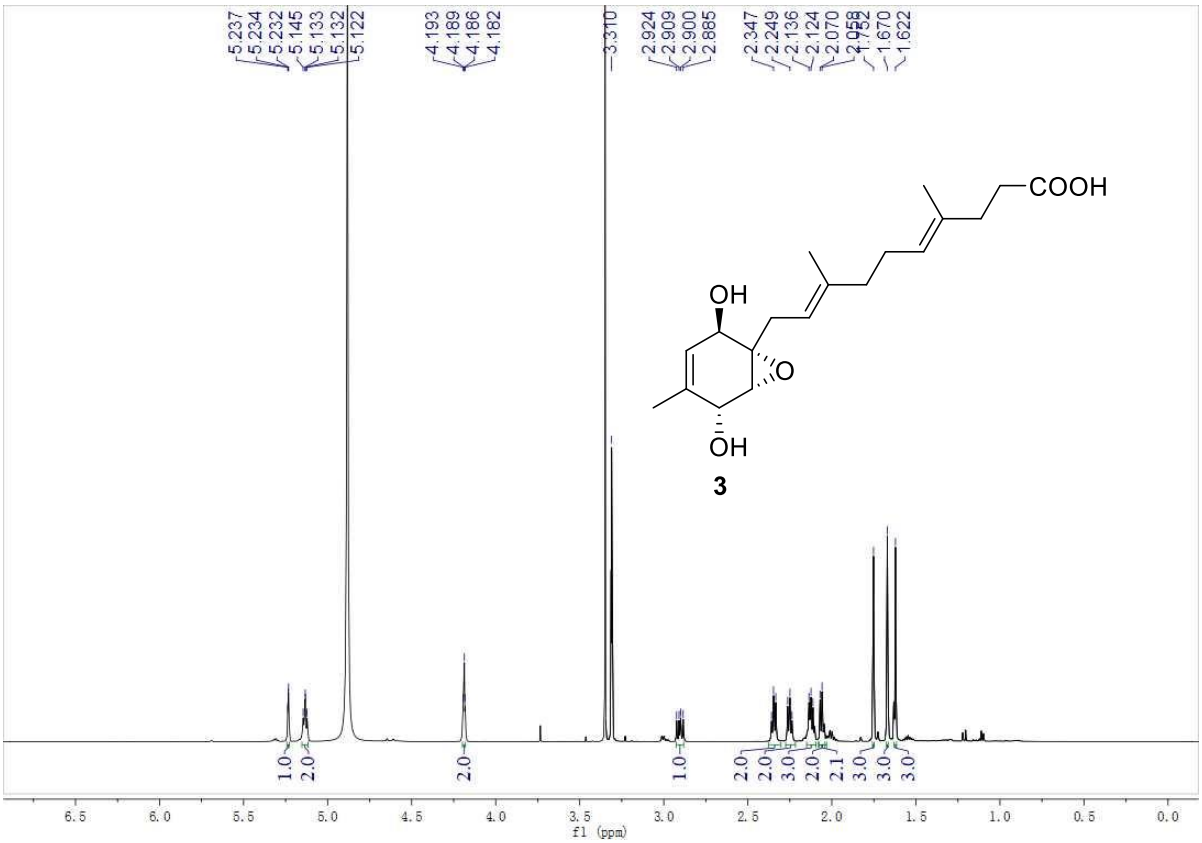

Figure S13. ^{1}H NMR Spectrum of **3** in Methanol-d_4 (600 MHz).

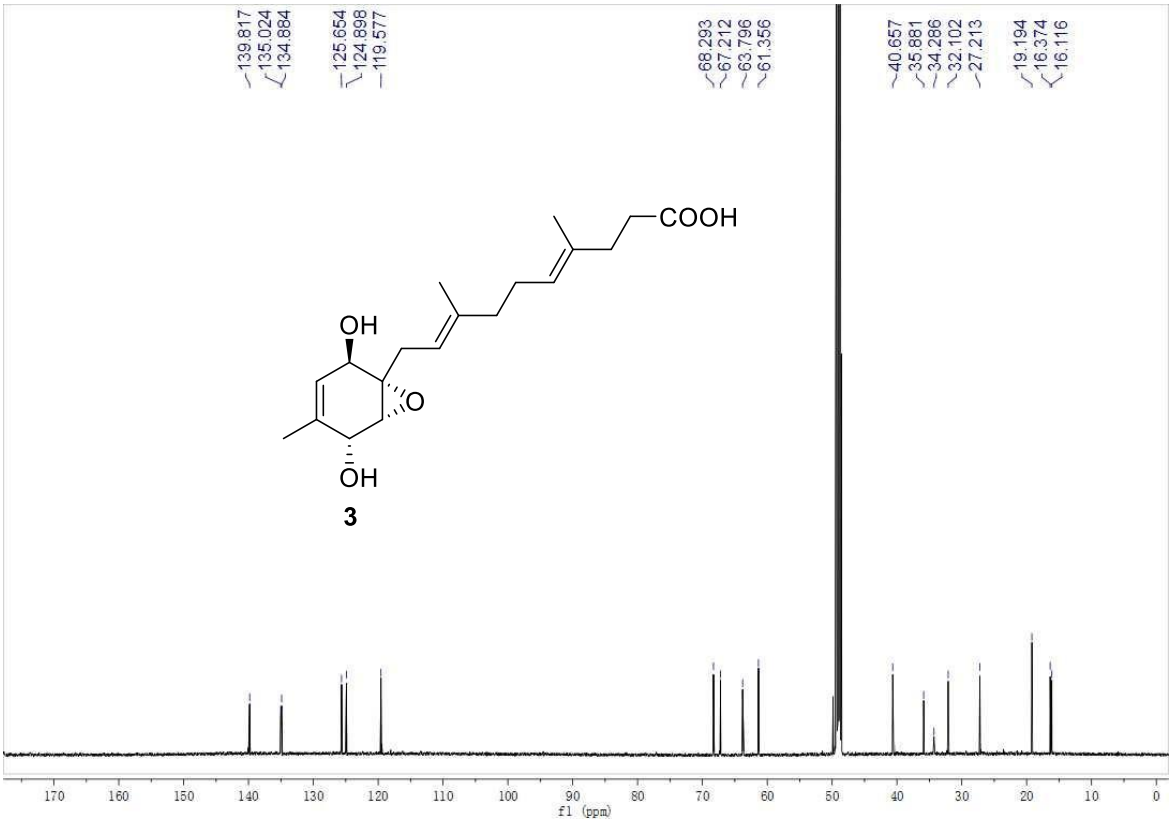

Figure S14. ^{13}C NMR Spectrum of **3** in Methanol-d_4 (150 MHz).

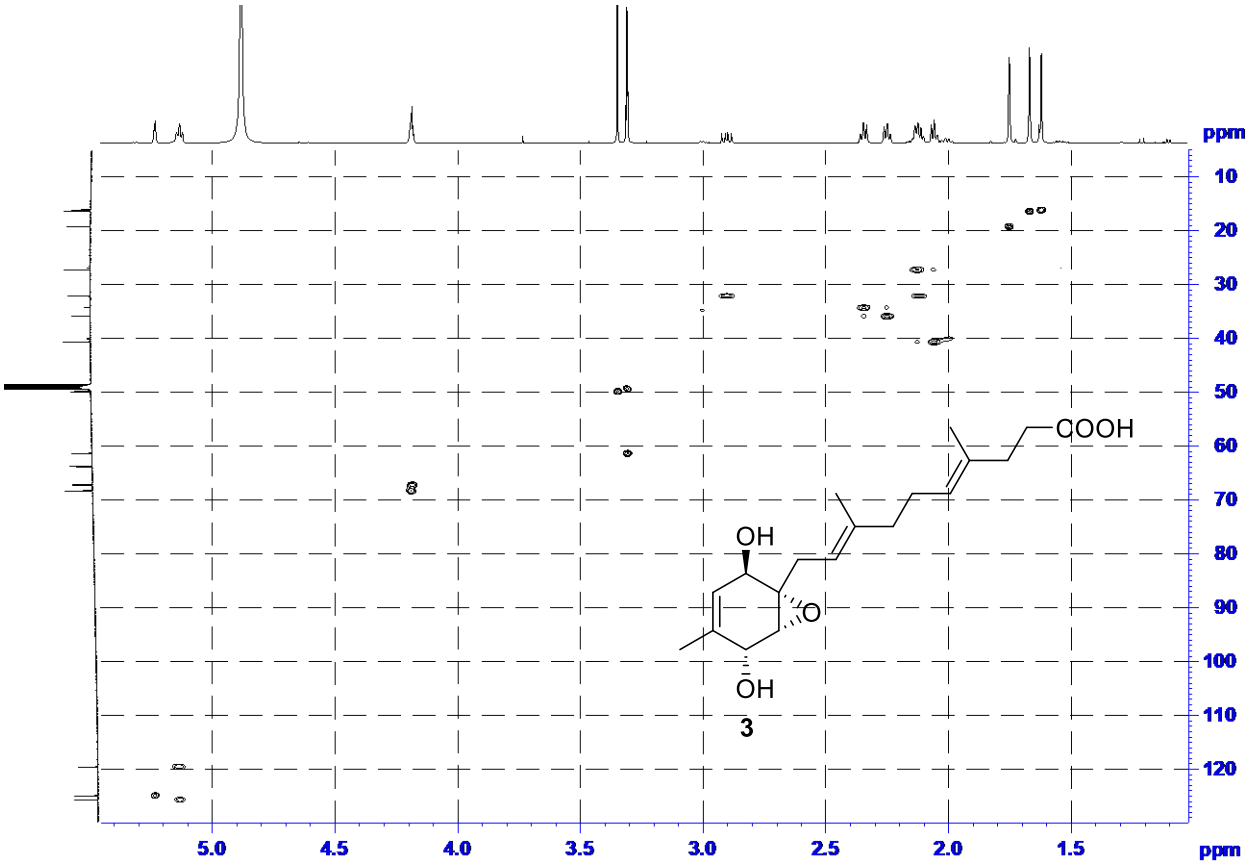

Figure S15. HSQC Spectrum of **3** in Methanol-d_4 (600 MHz).

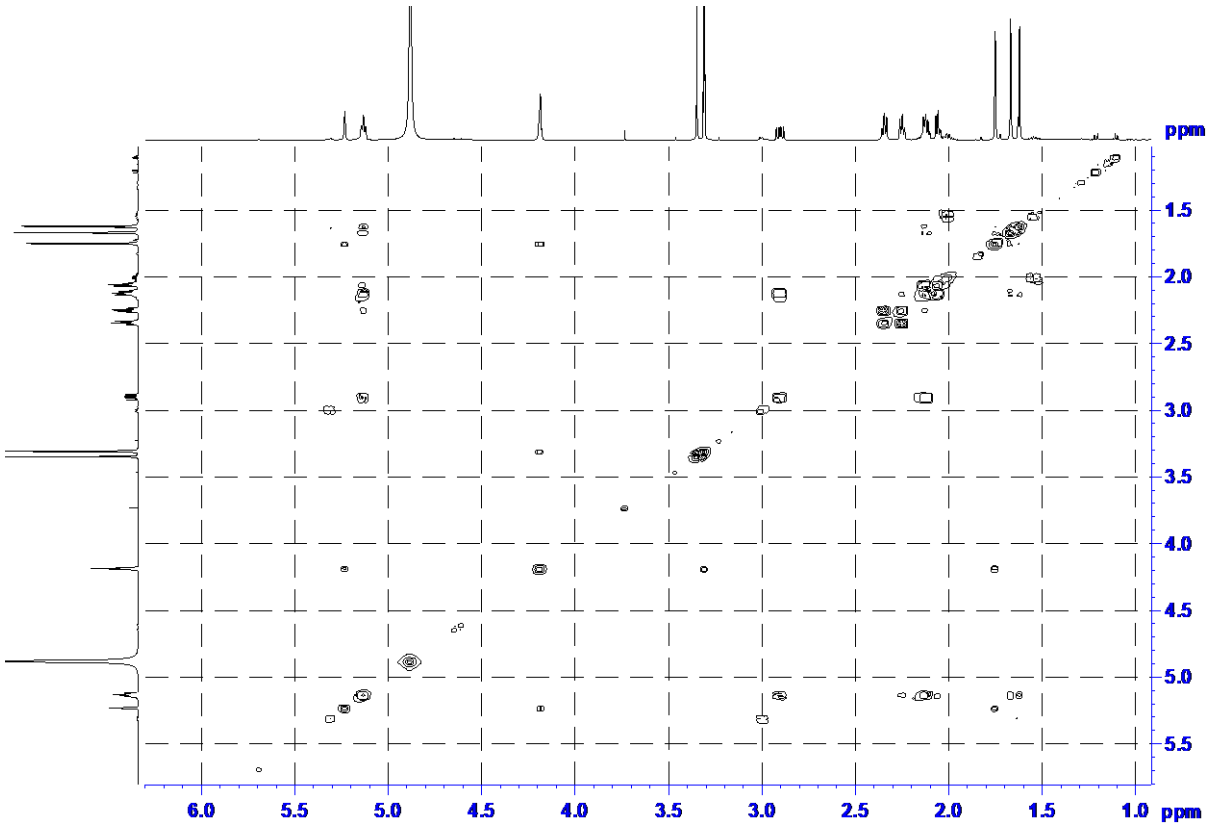

Figure S16. COSY Spectrum of **3** in Methanol-d_4 (600 MHz).

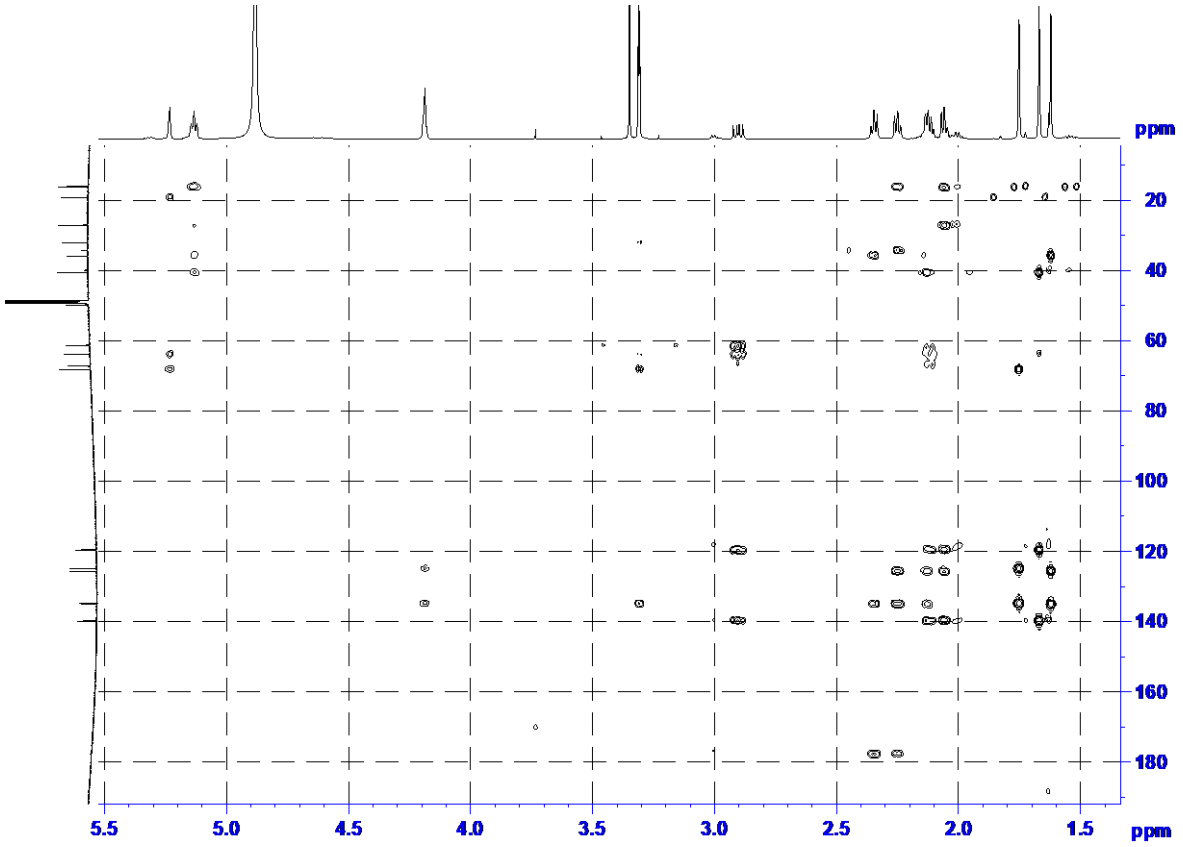

Figure S17. HMBC Spectrum of **3** in Methanol-d_4 (600 MHz).

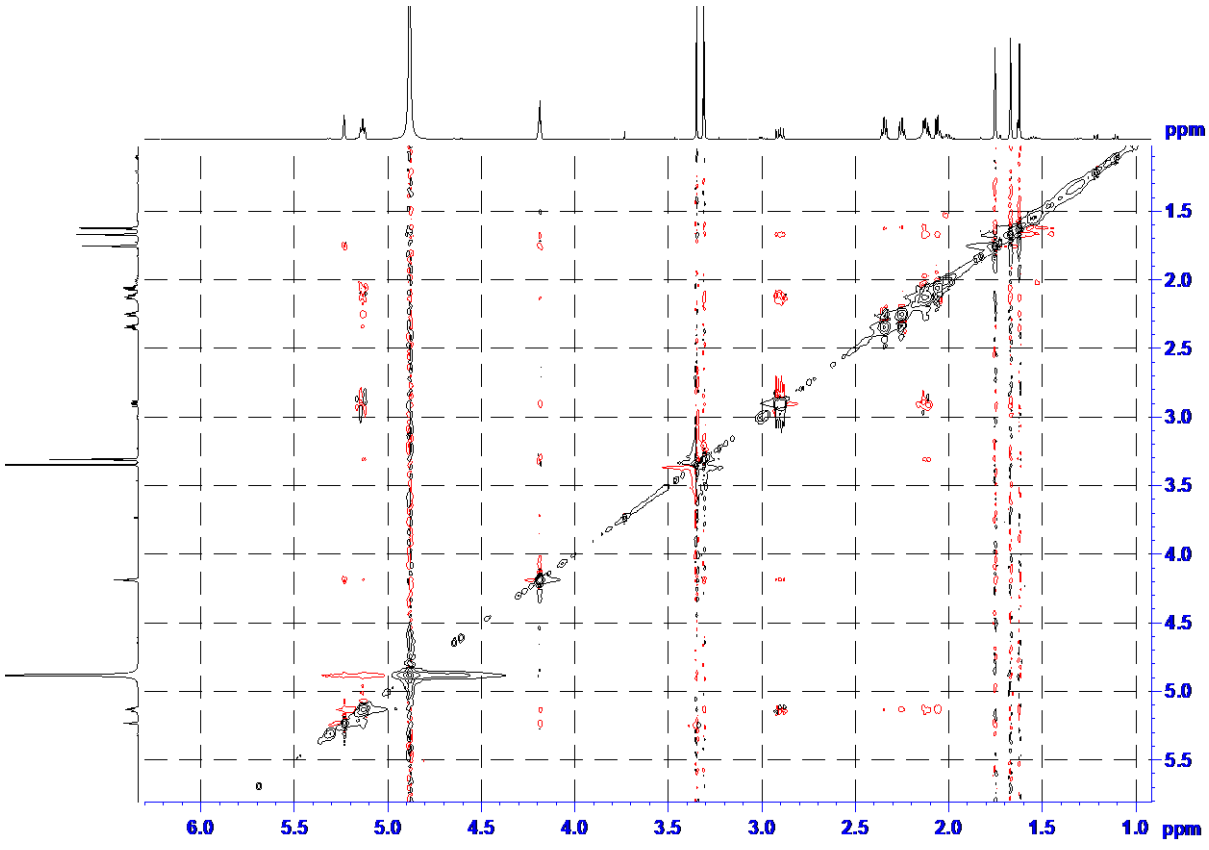

Figure S18. NOESY Spectrum of **3** in Methanol-d_4 (600 MHz).

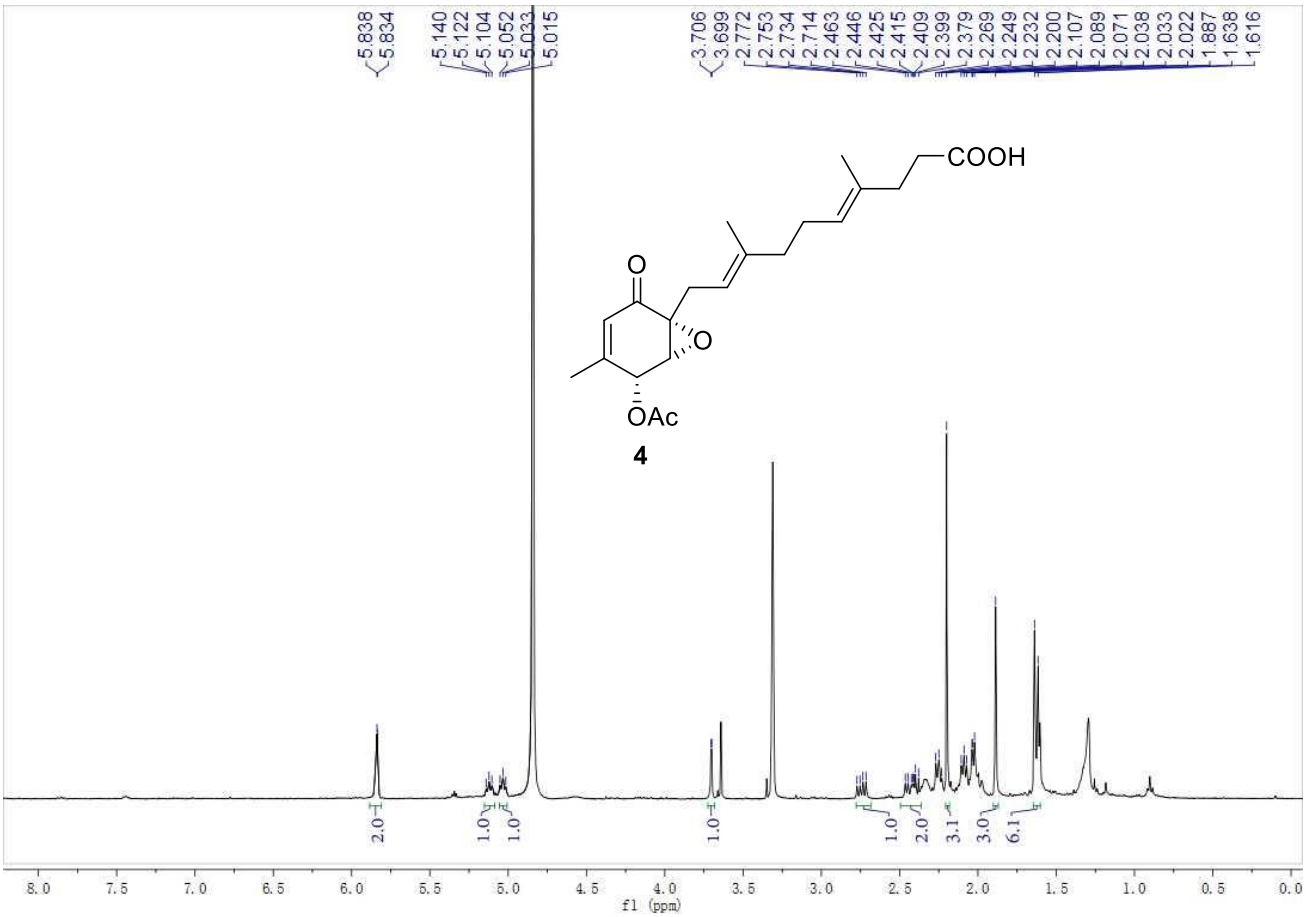

Figure S19. ^{1}H NMR Spectrum of **4** in Methanol-d_4 (600 MHz).

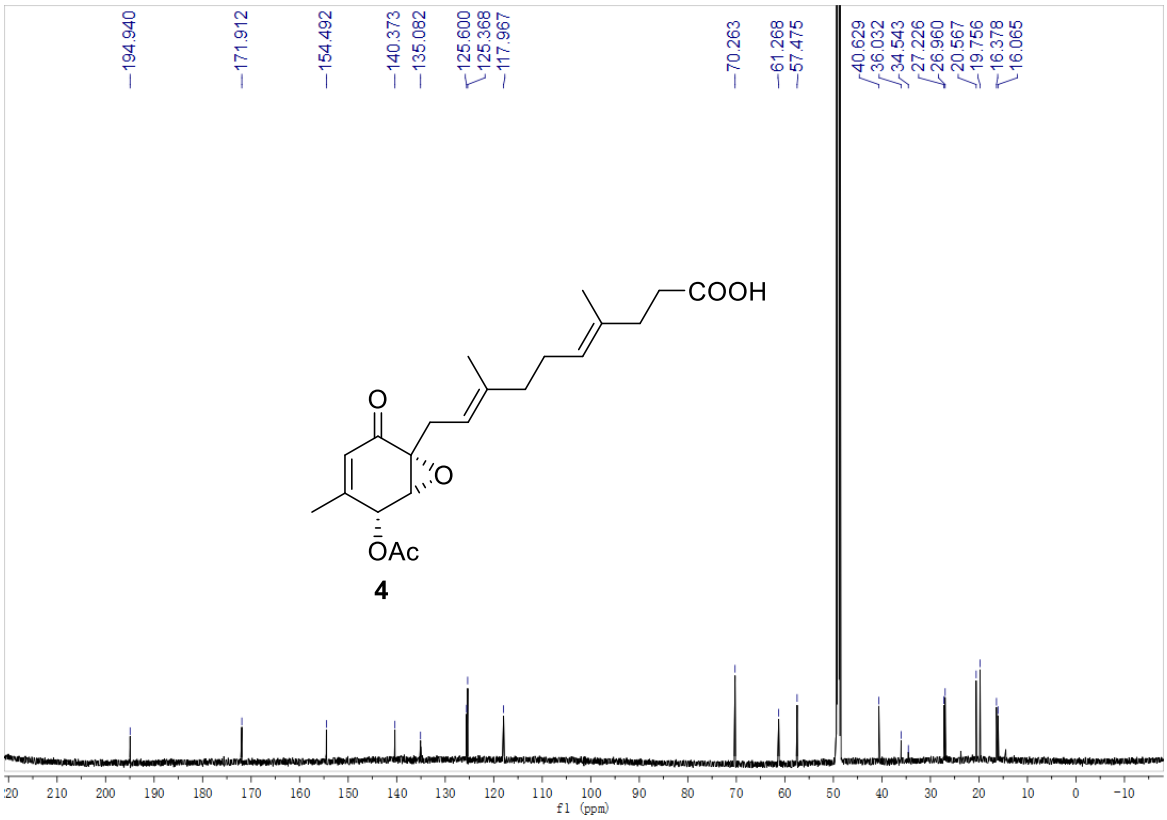

Figure S20. ^{13}C NMR Spectrum of **4** in Methanol-d_4 (150 MHz).

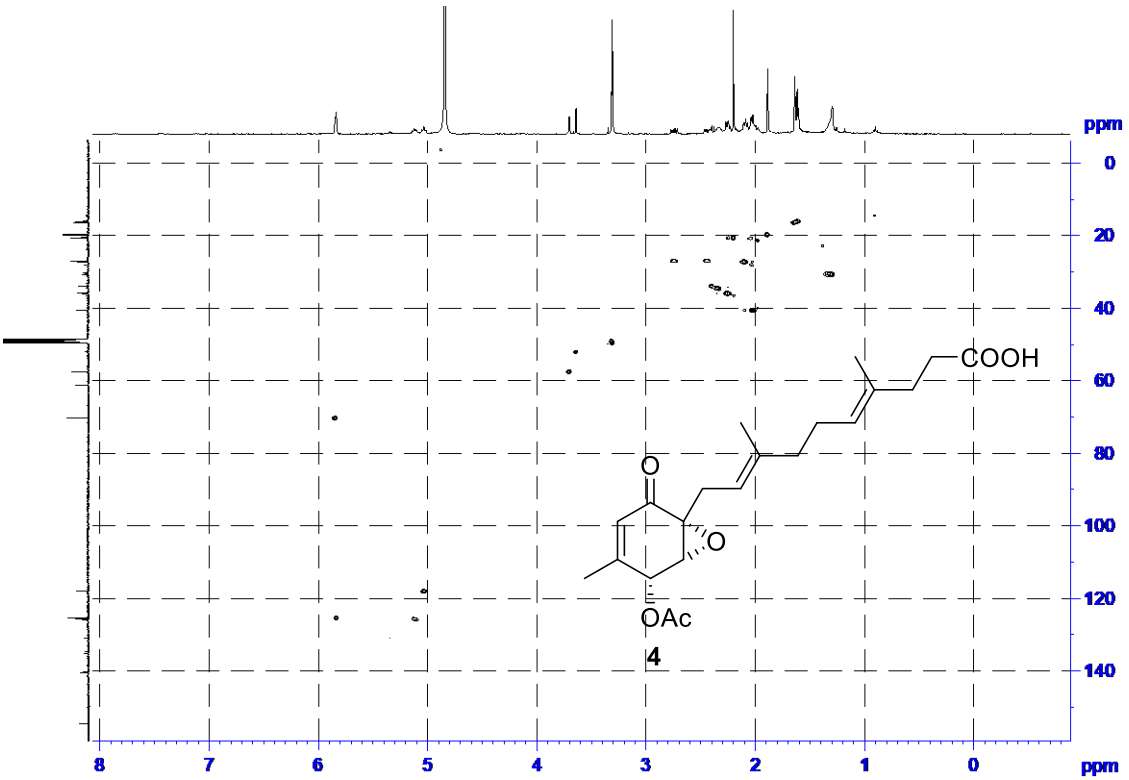

Figure S21. HSQC Spectrum of **4** in Methanol-d_4 (600 MHz).

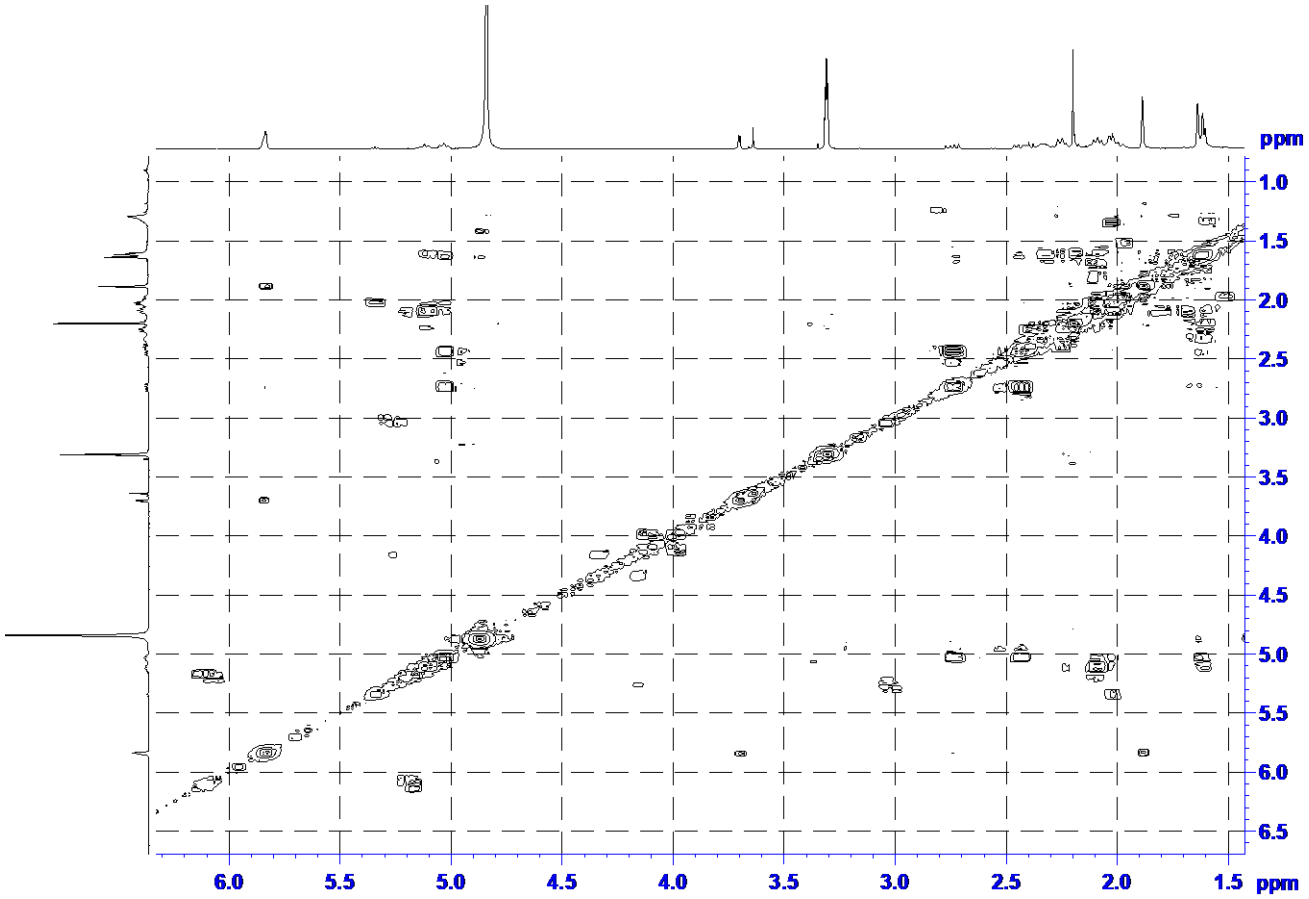

Figure S22. COSY Spectrum of **4** in Methanol-d_4 (600 MHz).

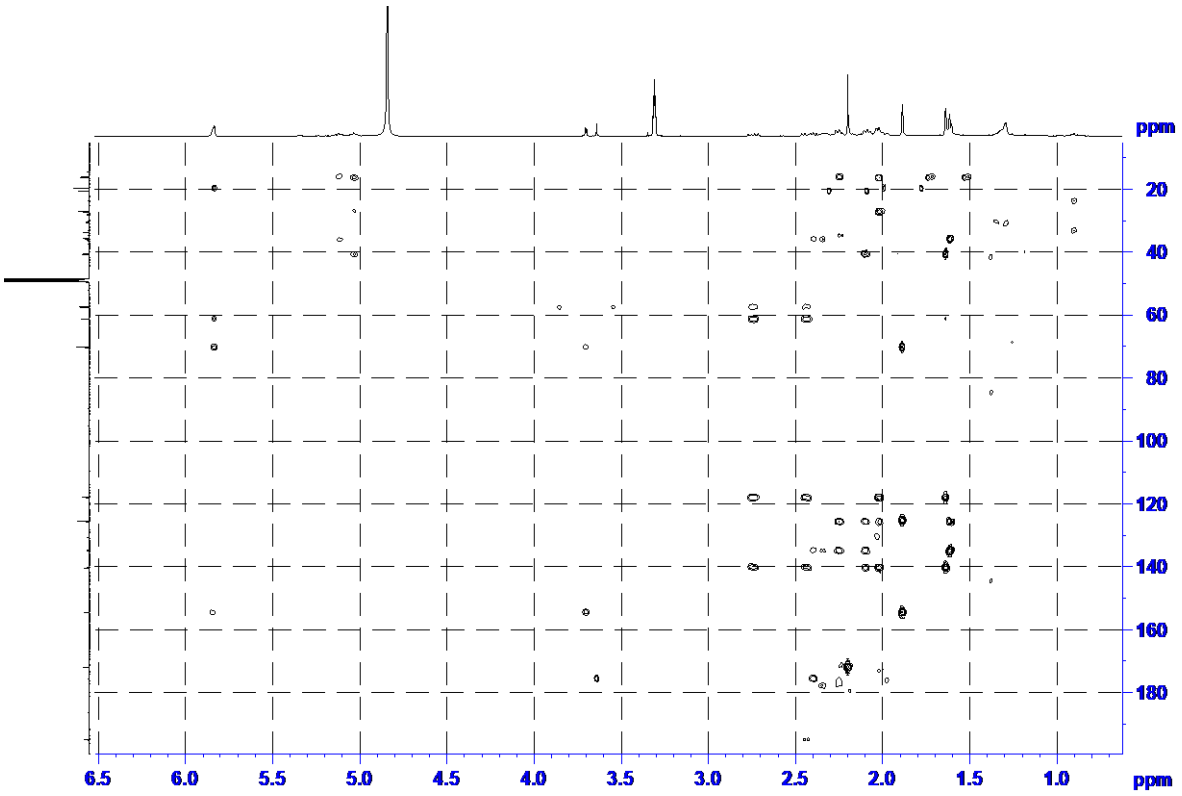

Figure S23. HMBC Spectrum of **4** in Methanol-d_4 (600 MHz).

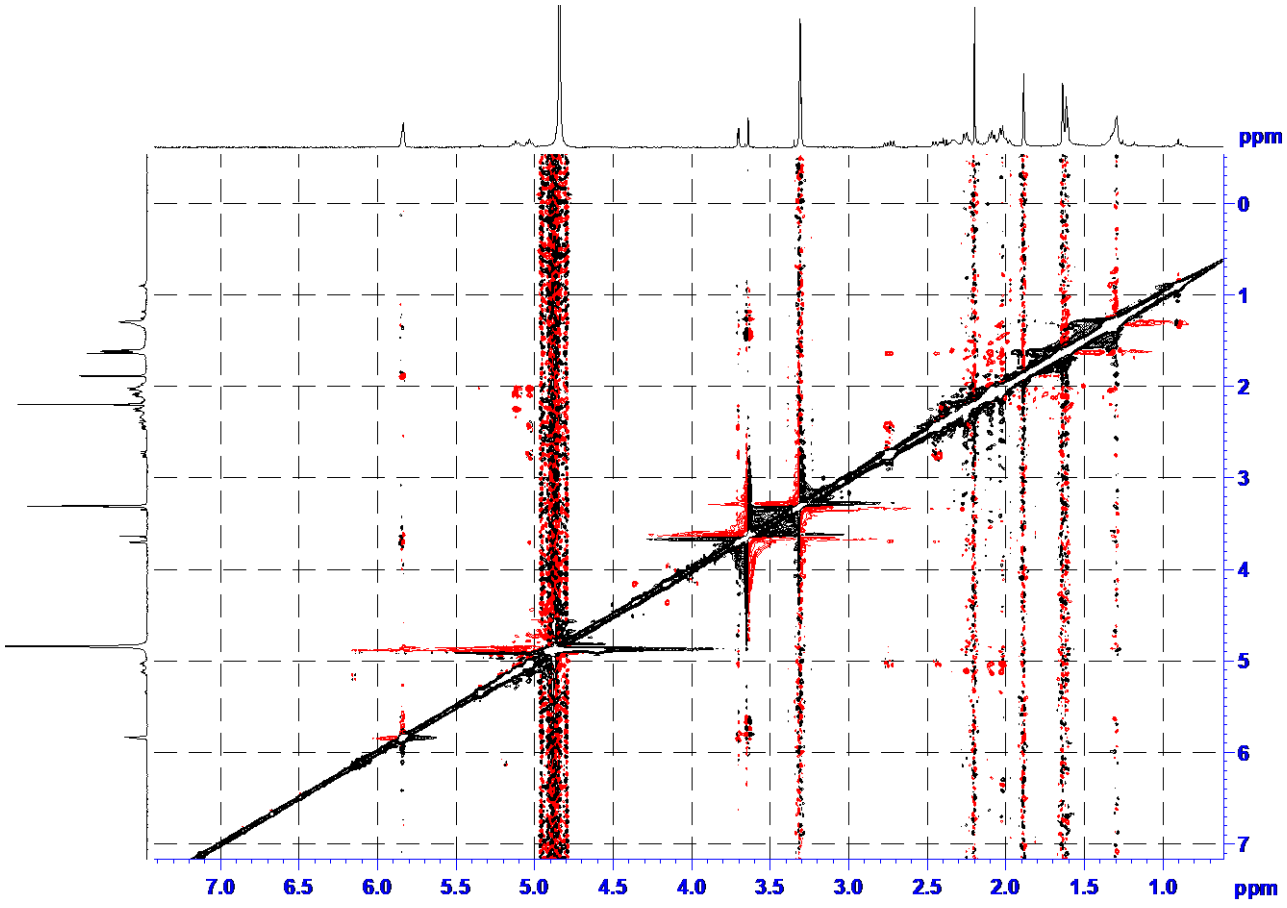

Figure S24. NOESY Spectrum of **4** in Methanol-d_4 (600 MHz).

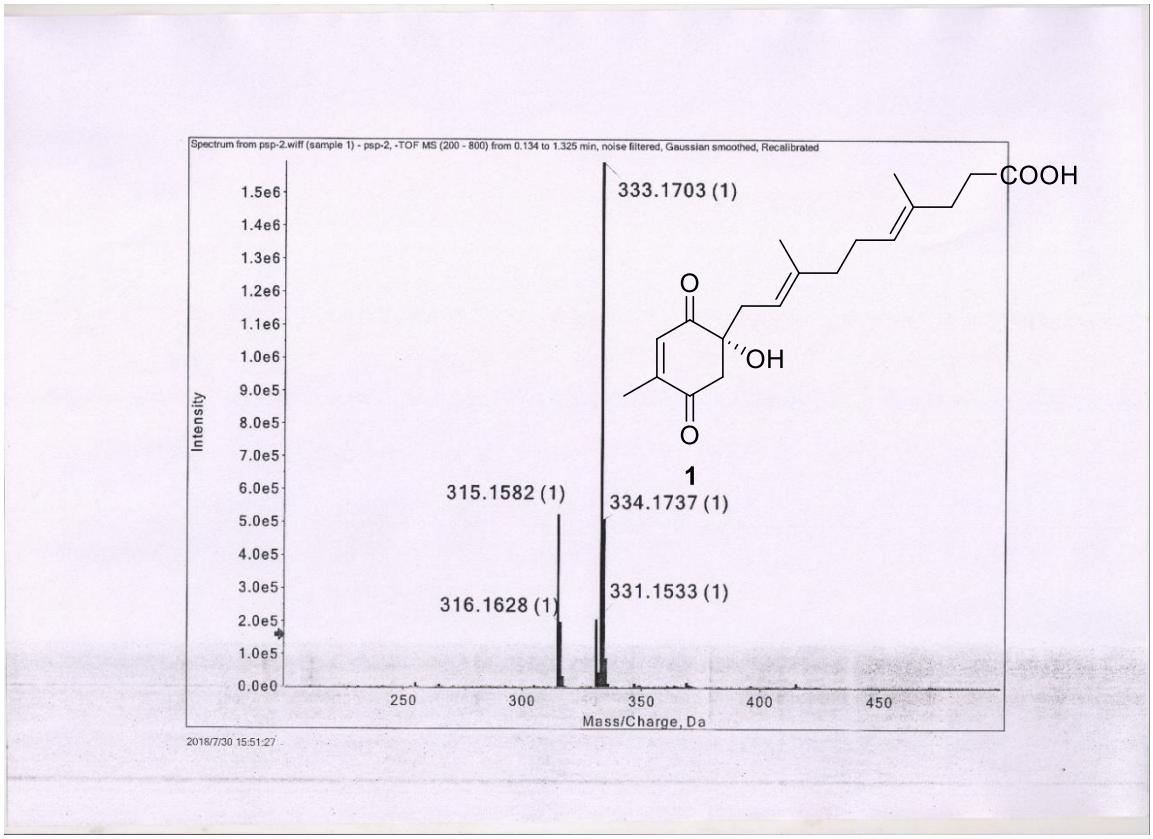

Figure S25. HRESIMS spectrum of **1**

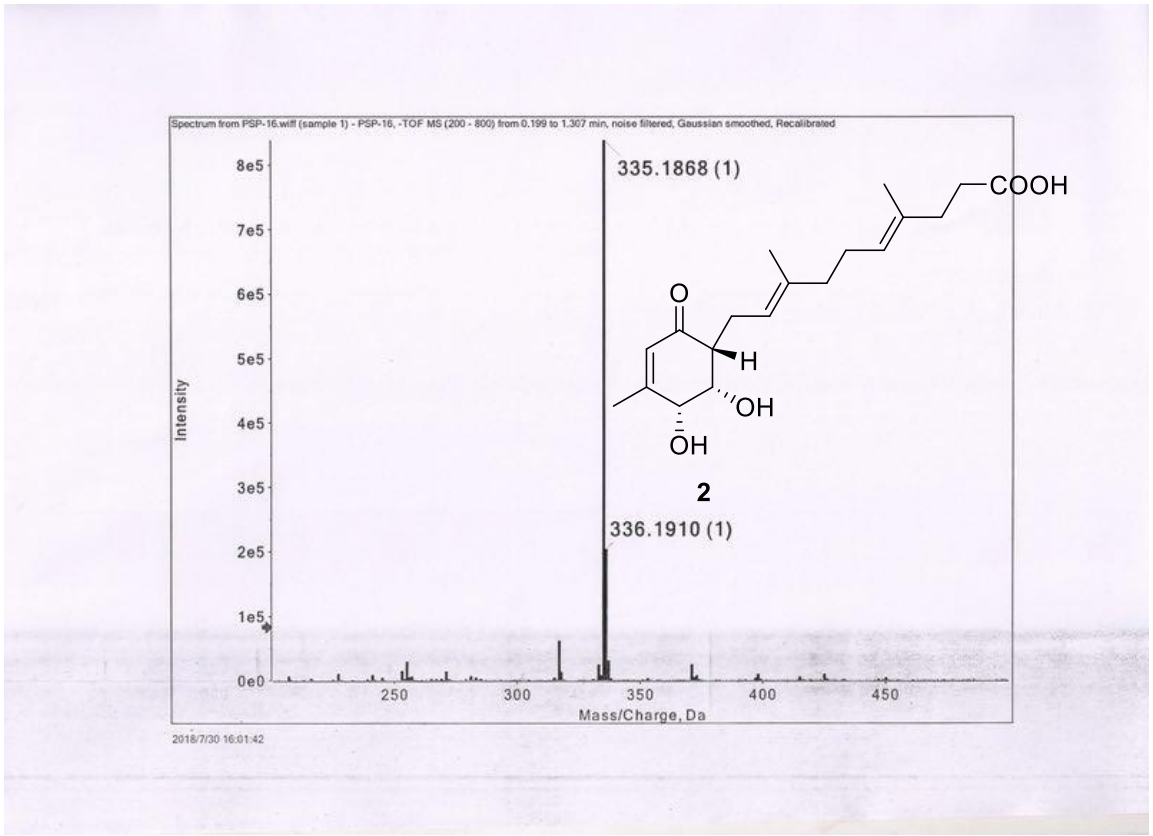

Figure S26. HRESIMS spectrum of **2**

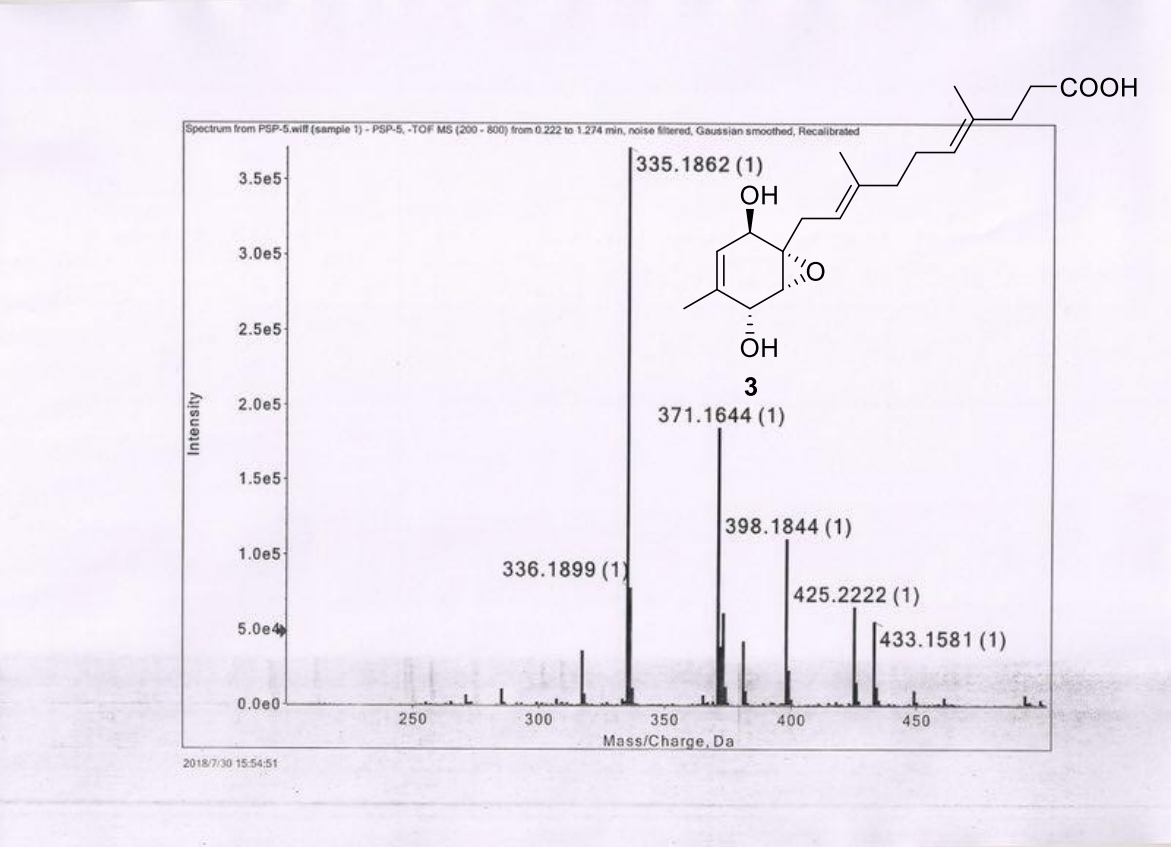

Figure S27. HRESIMS spectrum of **3**

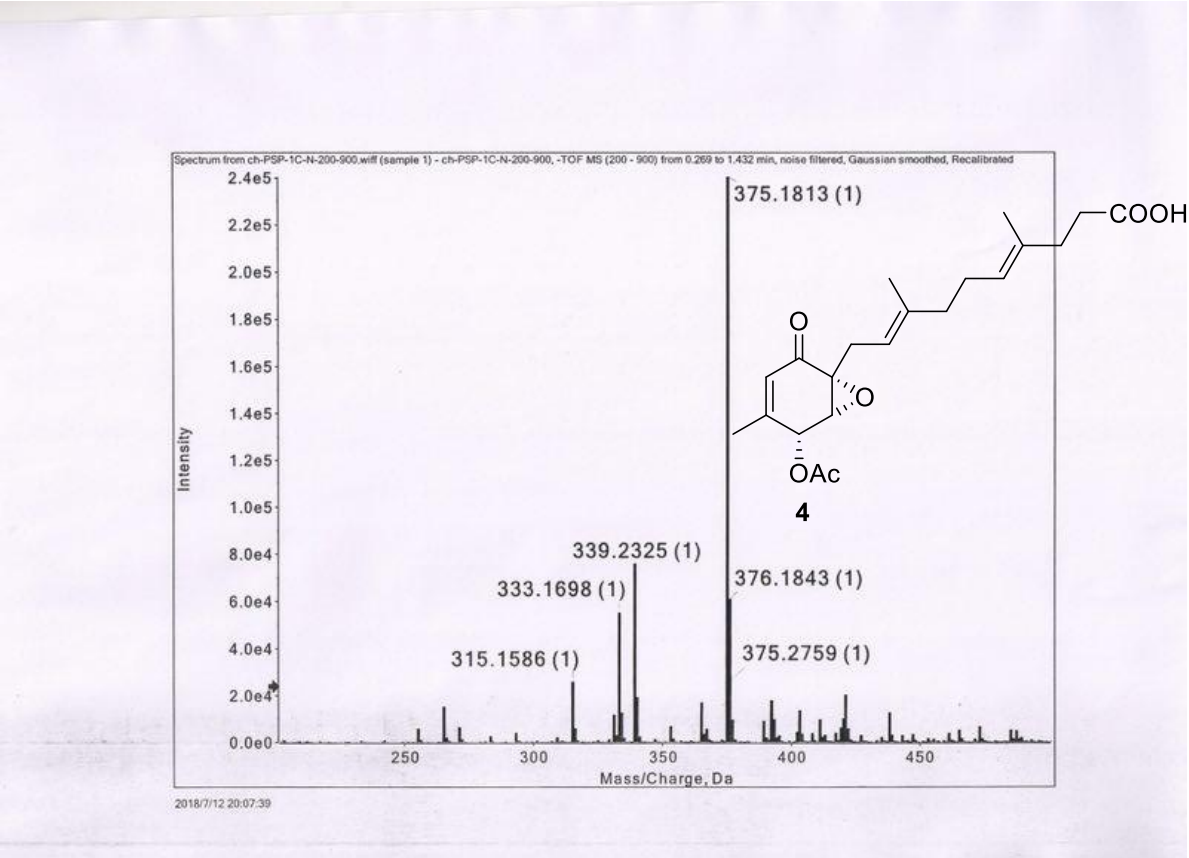

Figure S28. HRESIMS spectrum of **4**

Table S1. ^{1}H and ^{13}C NMR Data of Compounds **3** in DMSO-d_6

NO.	**3**	
	δ_H [a]	δ_C [b]
1	4.05, m	65.2, CH
2		62.0, C
3	3.13, d (2.3)	59.4, CH
4	4.07, d (2.3)	66.2, CH
5		132.8, C
6	5.07, m	123.9, CH
7	1.62, s	15.5, CH_3
1′	2.77, d (14.4, 8.7)	30.7, CH_2
	2.01, d (14.4, 8.7)	
2′	5.07, m	118.8, CH
3′		137.4, C
4′	1.97, m	39.2, CH_2
5′	2.04, m	25.9, CH_2
6′	5.07, m	124.0, CH
7′		133.7, C
8′	2.14, m	34.2, CH_2
9′	2.25, m	32.7, CH_2
10′		174.2, C
11′	1.55, s	15.9, CH_3
12′	1.60, s	16.1, CH_3

[a] Recorded at 400 MHz, [b] Recorded at 100 MHz, chemical shifts are in ppm, coupling constants *J* is in Hz.