

Supplementary Information

Lophiostomins A-D, new 3,4-dihydroisocoumarin derivatives from the endophytic fungus *Lophiostoma* sp. Sigrf10

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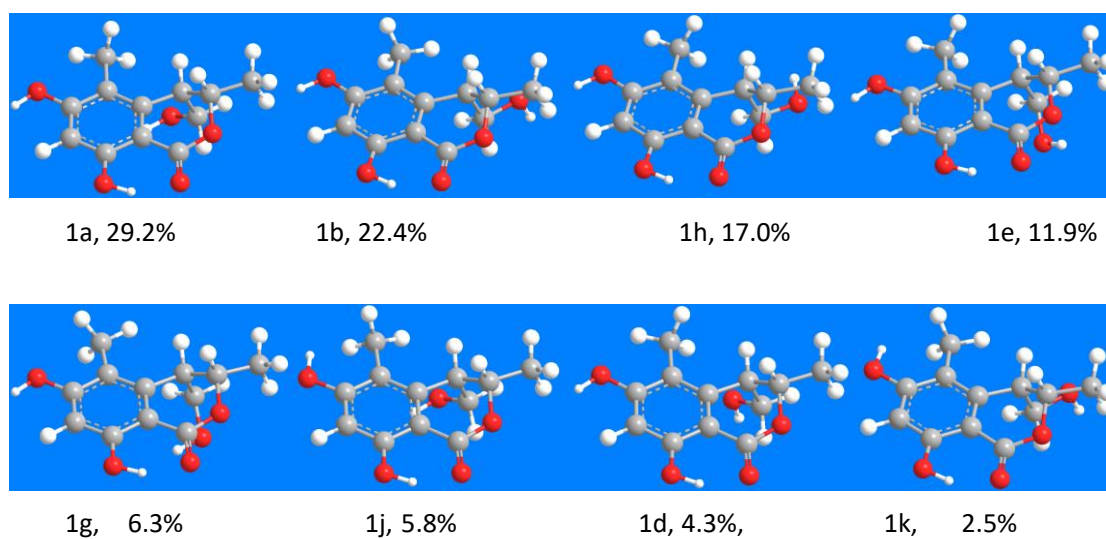


Figure S1. The optimized, predominant conformers of **1** calculated at the B3lyp/6-31 g(d) level in the gas phase ($\geq 1\%$ population)

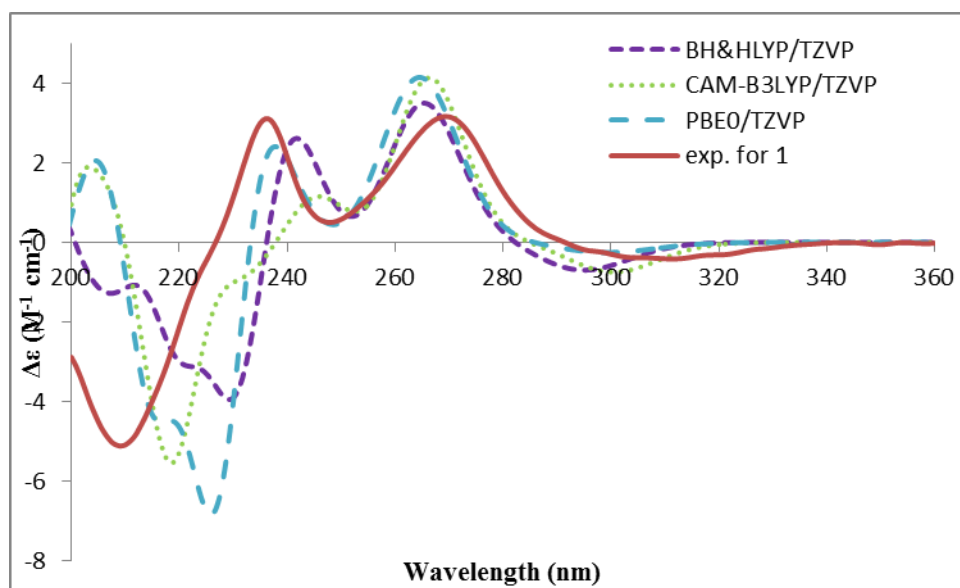


Figure S2. Calculated CD spectra for **1** at three different levels and the experimental spectrum of **1**

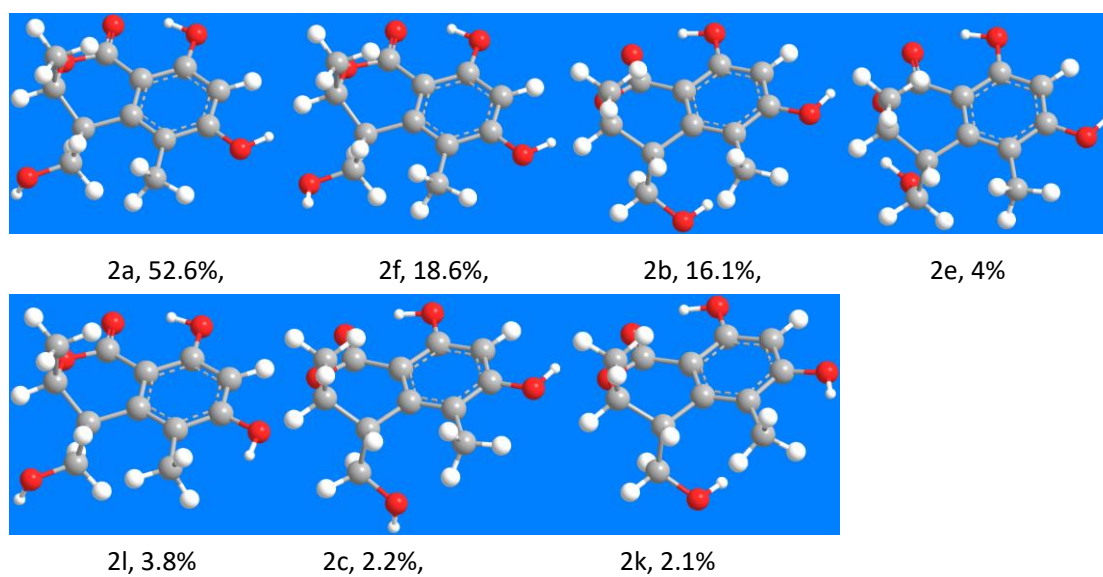
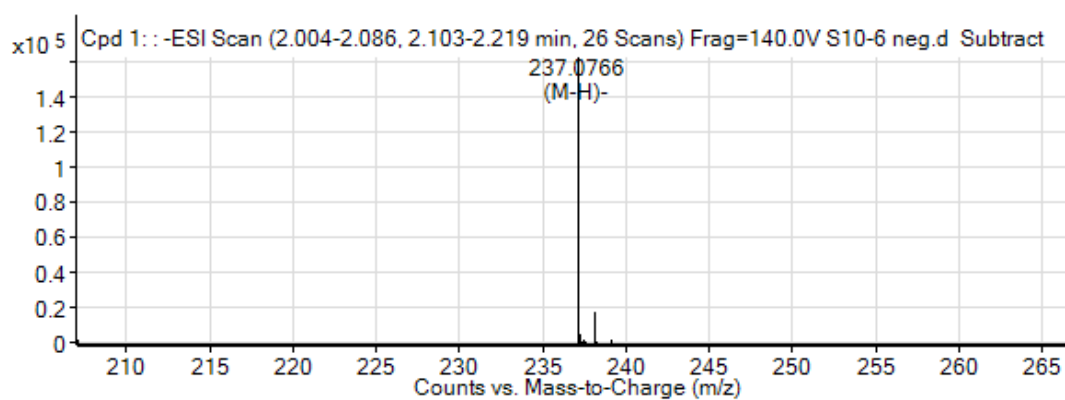


Figure S3. The optimized, predominant conformers of (3*R*, 4*R*)-**2** calculated at the B3lyp/6-31 g(d) level in the gas phase ($\geq 1\%$ population)



<i>m/z</i>	<i>Calc m/z</i>	Diff (ppm)	Z	Abund	Formula	Ion
237.0766	237.0768	-1.06	-1	162370	C ₁₂ H ₁₃ O ₅	(M-H) ⁻

Figure S4. HRESIMS spectrum of **1**

S10-6

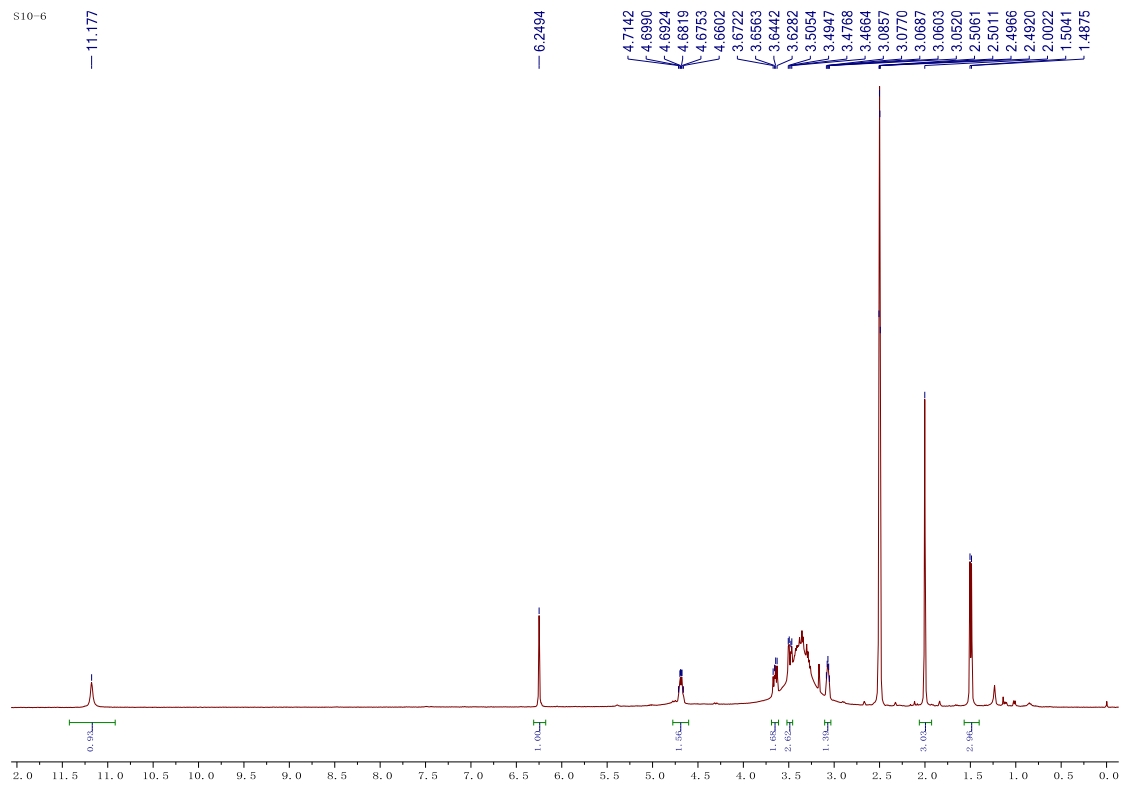


Figure S5. ^1H NMR spectrum of **1** ($\text{DMSO-}d_6$, 400 MHz)

S10-6_13C

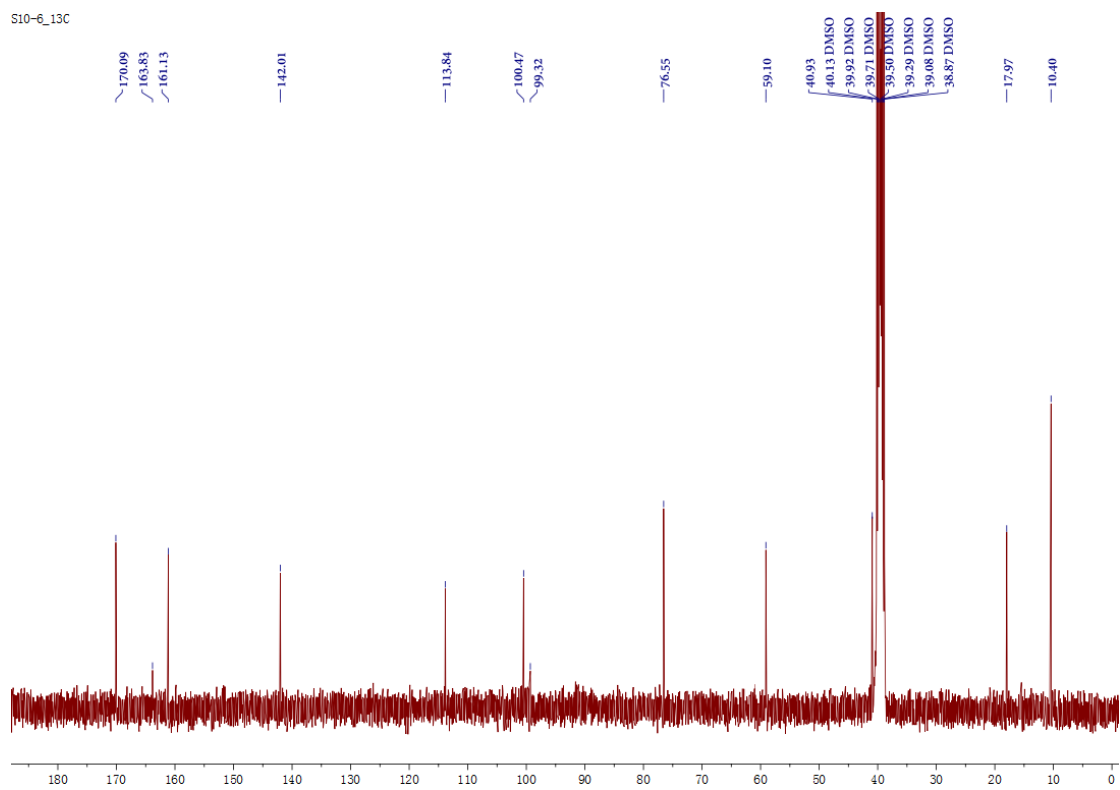


Figure S6. ^{13}C NMR spectrum of **1** ($\text{DMSO-}d_6$, 100 MHz)

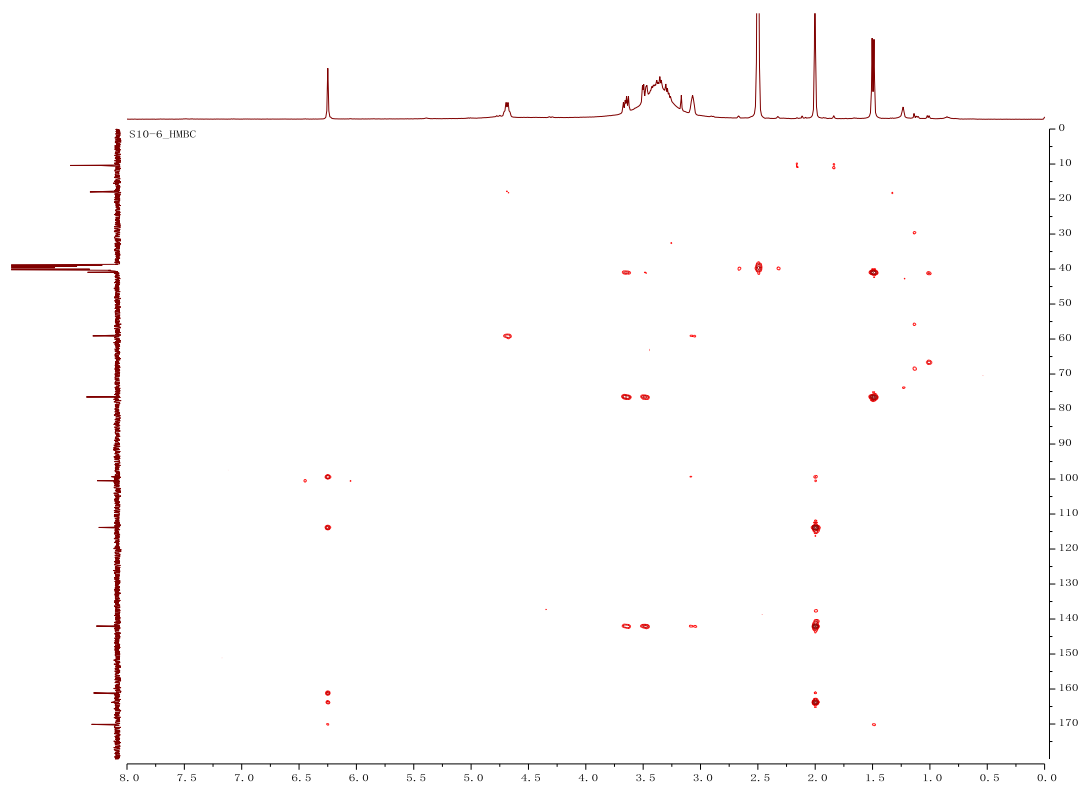


Figure S7. HMBC spectrum of **1**

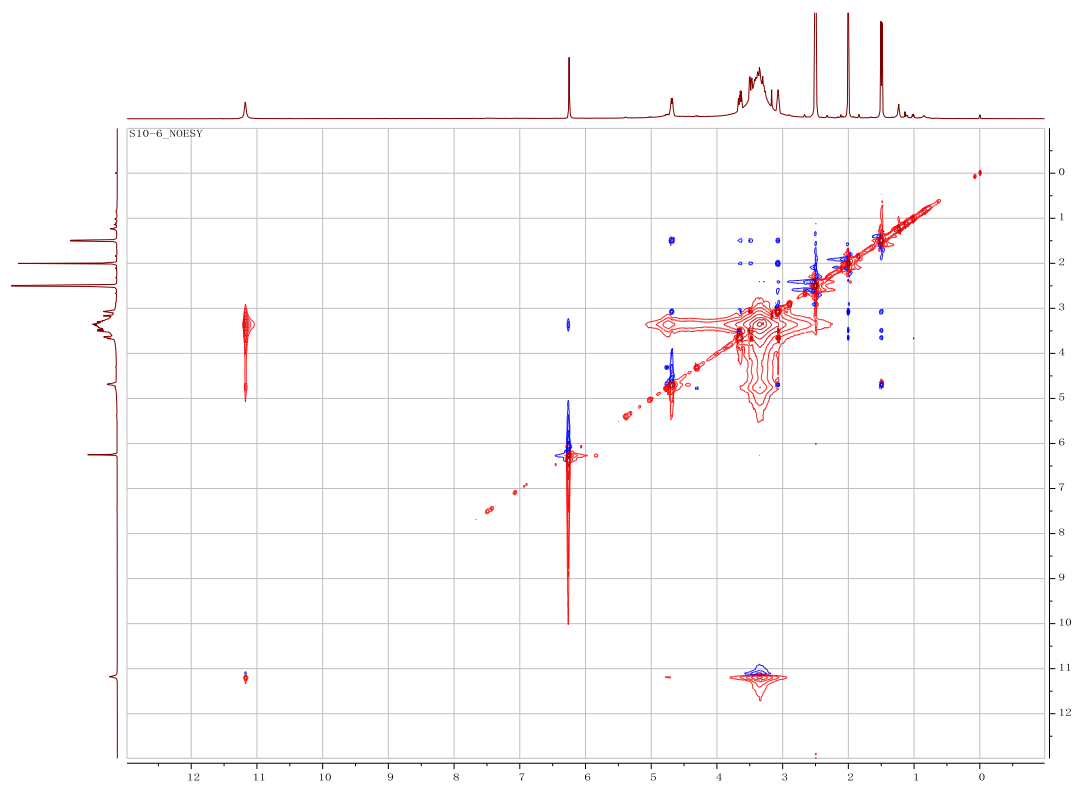
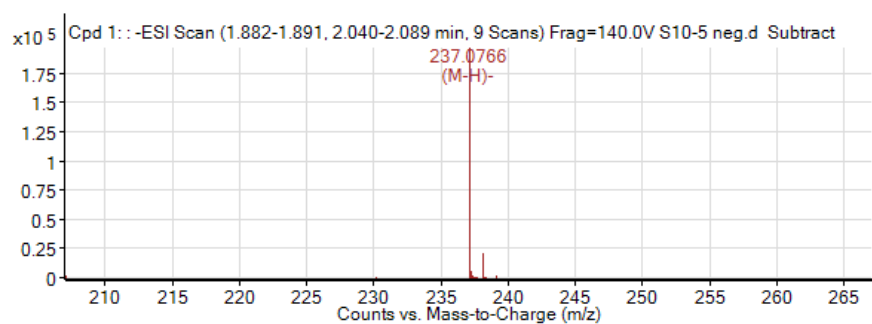


Figure S8. NOESY spectrum of **1**



<i>m/z</i>	<i>Calc m/z</i>	Diff (ppm)	Z	Abund	Formula	Ion
237.0766	237.0768	-0.95	-1	197103.5	C ₁₂ H ₁₃ O ₅	(M-H) ⁻

Figure S9. HRESIMS spectrum of **2**.

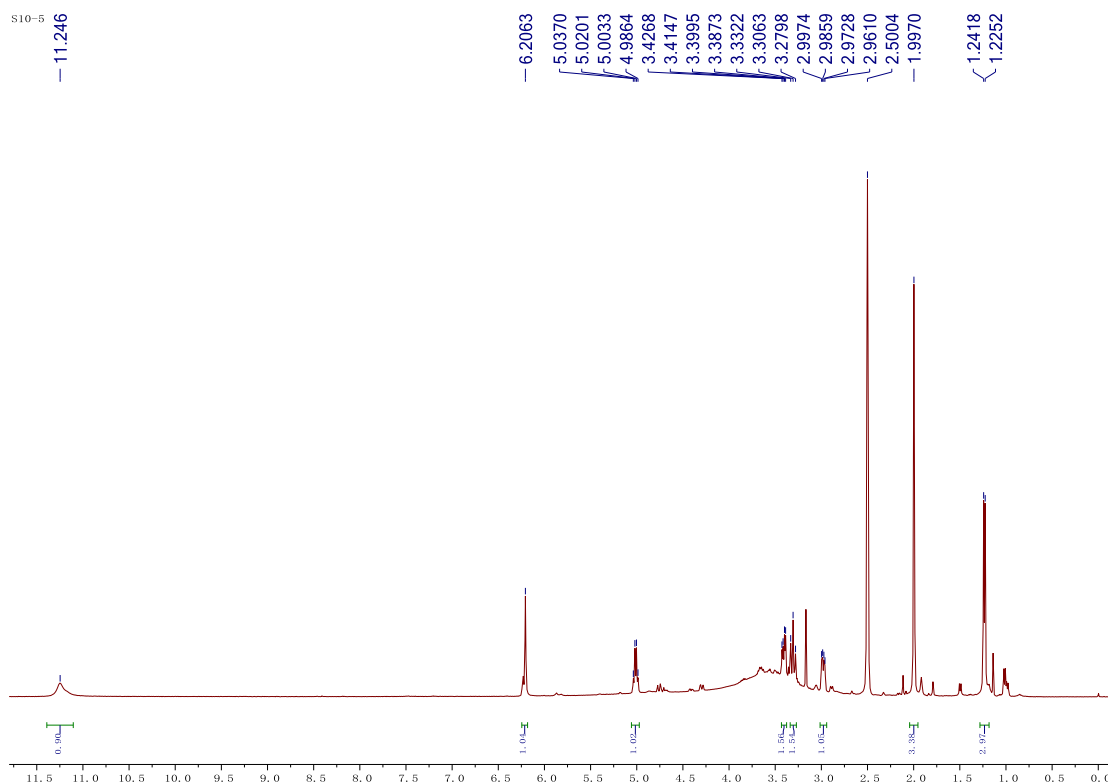


Figure S10. ¹H NMR spectrum of **2** (DMSO-*d*₆, 400 MHz)

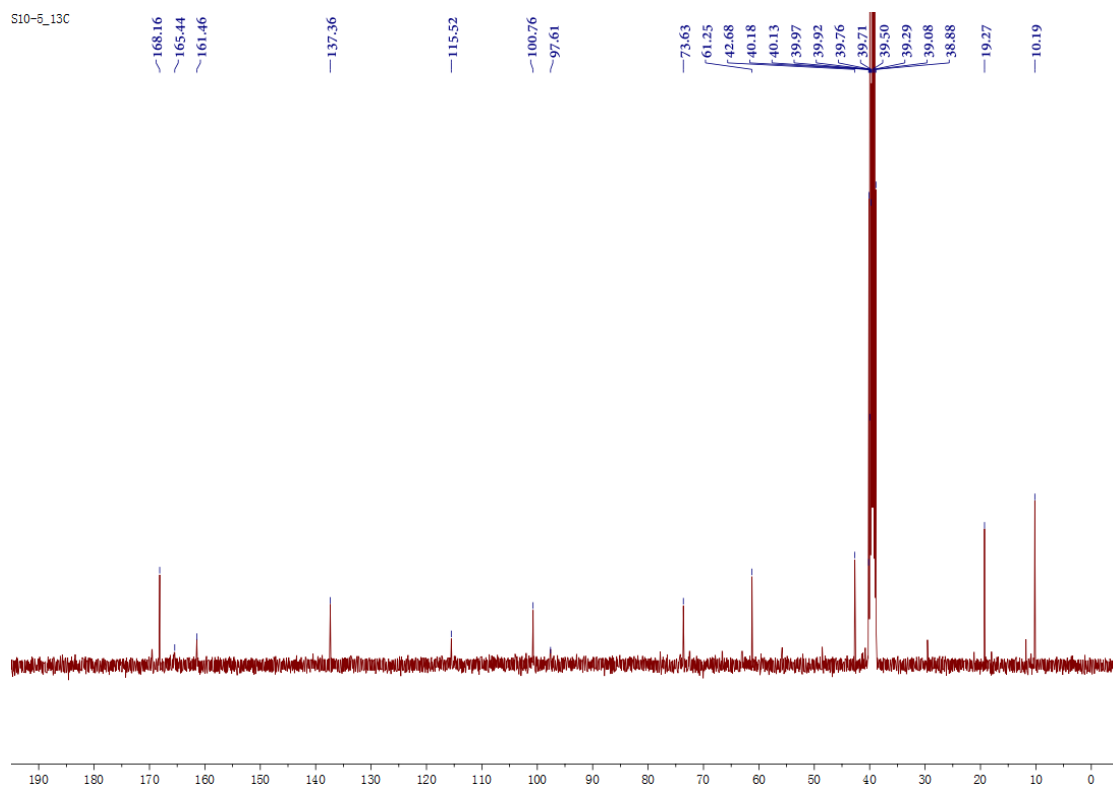


Figure S11. ^{13}C NMR spectrum of **2** (DMSO- d_6 , 100 MHz)

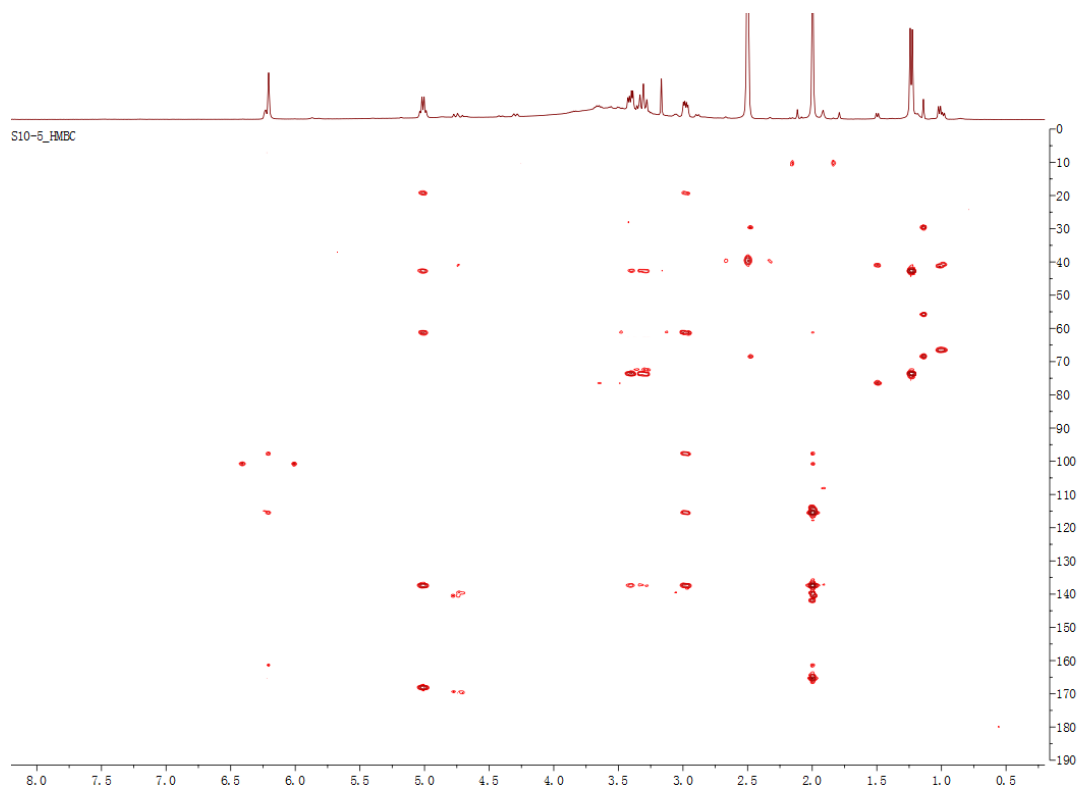


Figure S12. HMBC spectrum of **2**

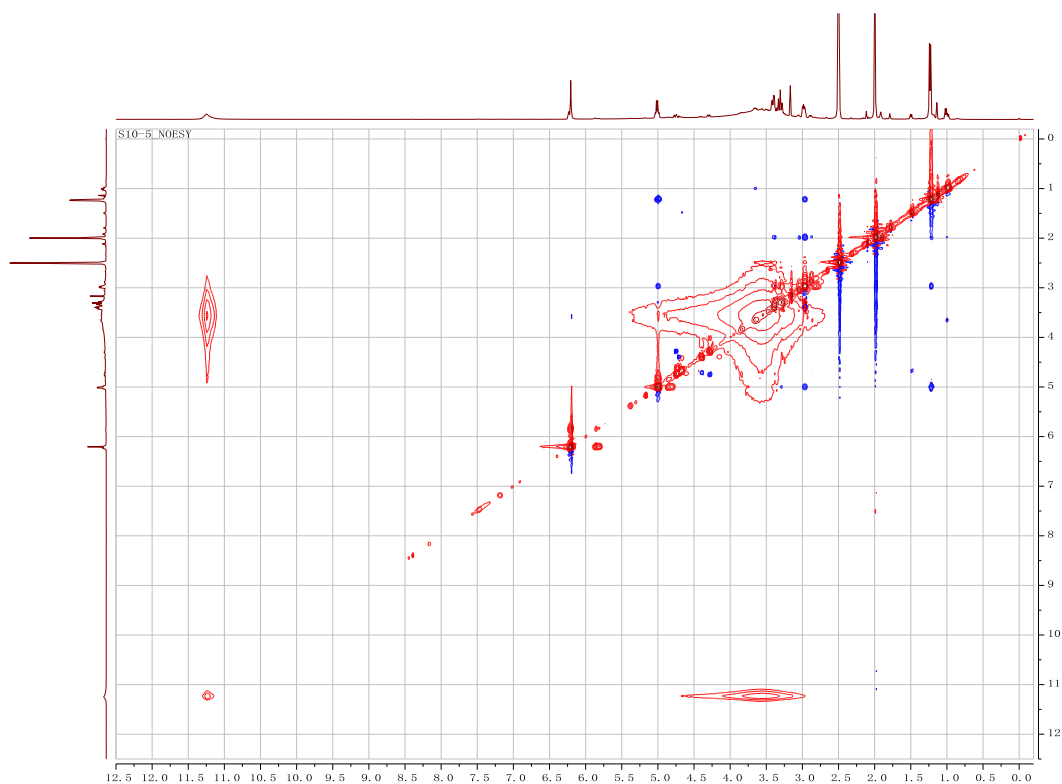
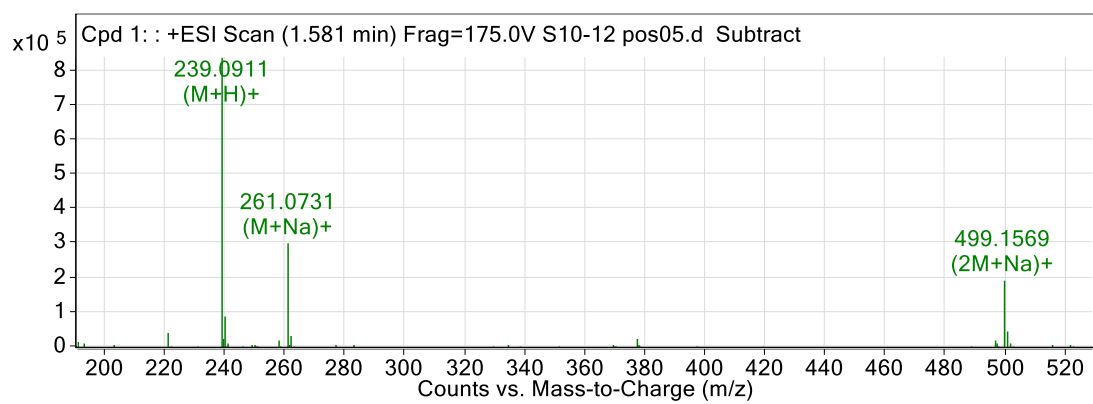


Figure S13. NOESY spectrum of **2**



<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
239.0911	239.0914	-1.19	1	837256.6	C ₁₂ H ₁₅ O ₅	(M+H) ⁺
261.0731	261.0733	-0.77	1	302155.1	C ₁₂ H ₁₄ NaO ₅	(M+Na) ⁺
499.1569	499.1575	-1.06	1	195147.1	C ₂₄ H ₂₈ NaO ₁₀	(2M+Na) ⁺

Figure S14. HRESIMS spectrum of **3**

S10-12

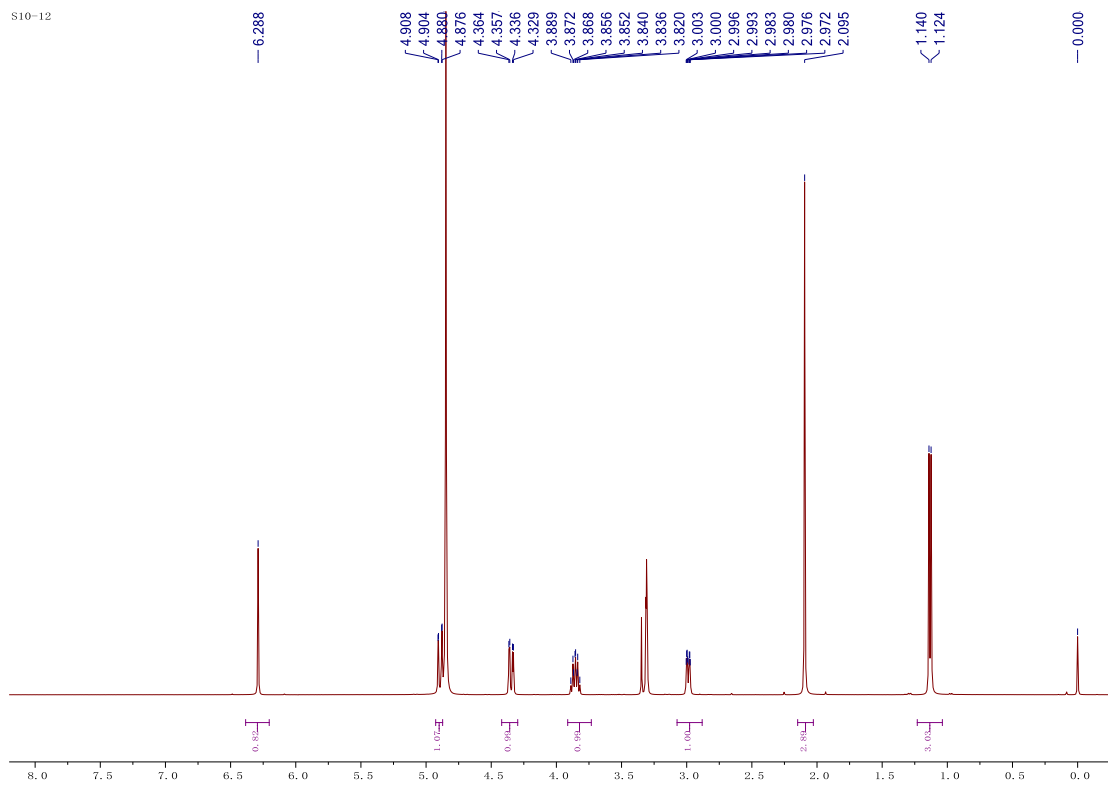


Figure S15. ^1H NMR spectrum of **3** (CD_3OD , 400 MHz)

S10-12_13C

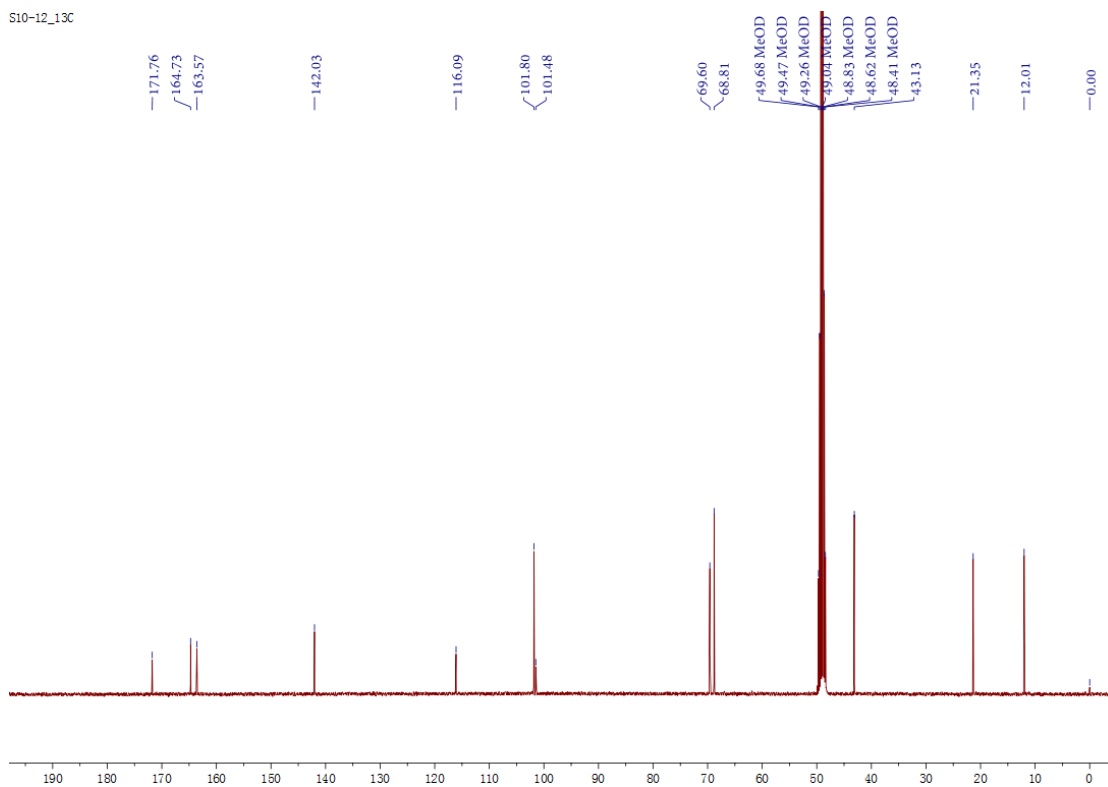


Figure S16. ^{13}C NMR spectrum of **3** (CD_3OD , 100 MHz)

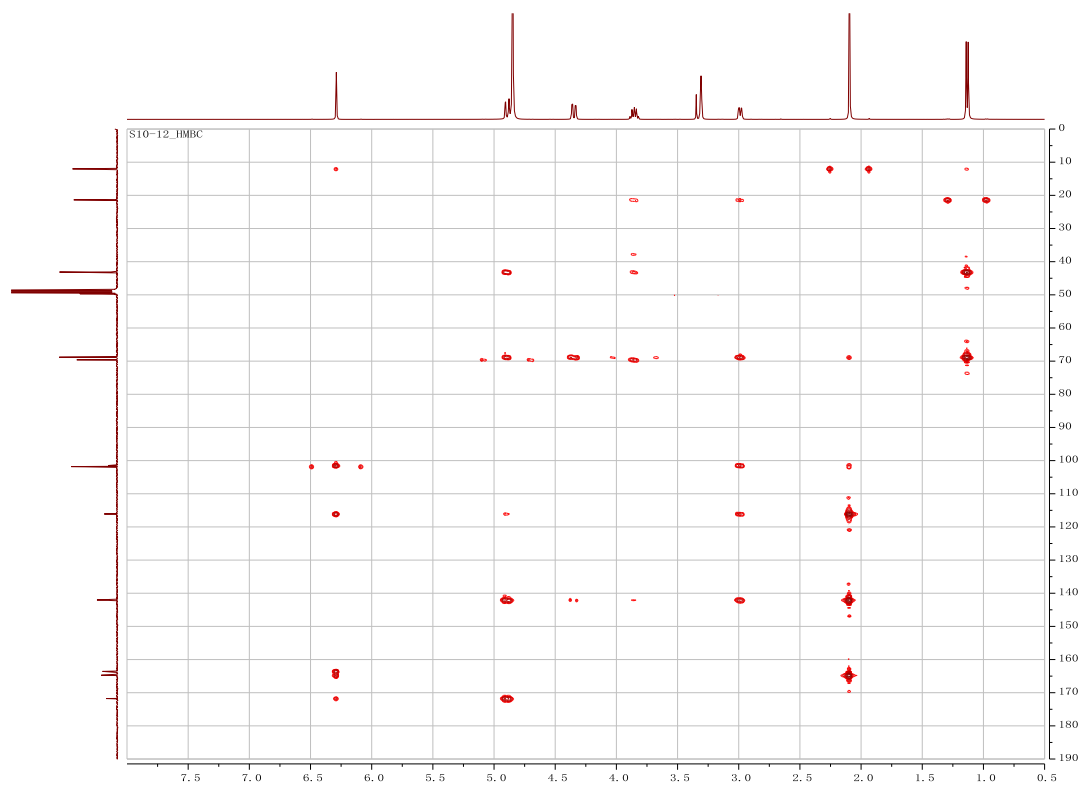


Figure S17. HMBC spectrum of **3**

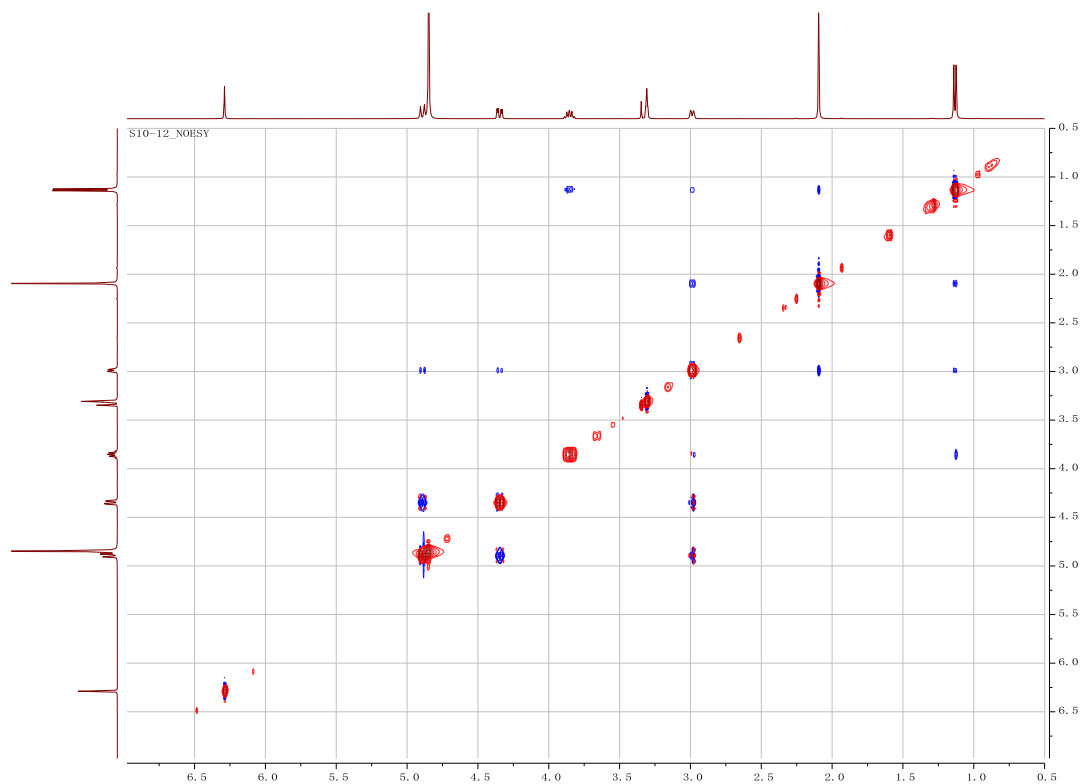
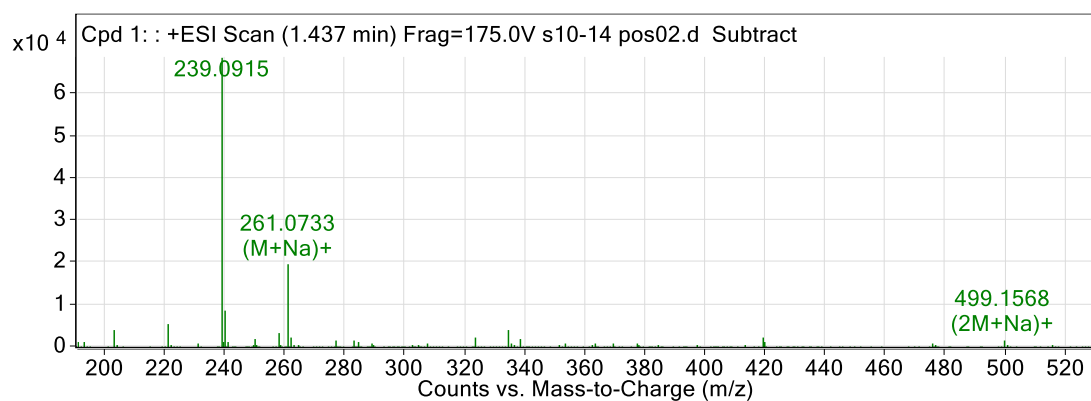


Figure S18. NOESY spectrum of **3**



m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
239.0915	239.0914	0.3	1	68578	C ₁₂ H ₁₅ O ₅	(M+H) ⁺
261.0733	261.0733	-0.03	1	19660	C ₁₂ H ₁₄ NaO ₅	(M+Na) ⁺
499.1568	499.1575	-1.26	1	1805.9	C ₂₄ H ₂₈ NaO ₁₀	(2M+Na) ⁺

Figure S19. HRESIMS spectrum of **4**

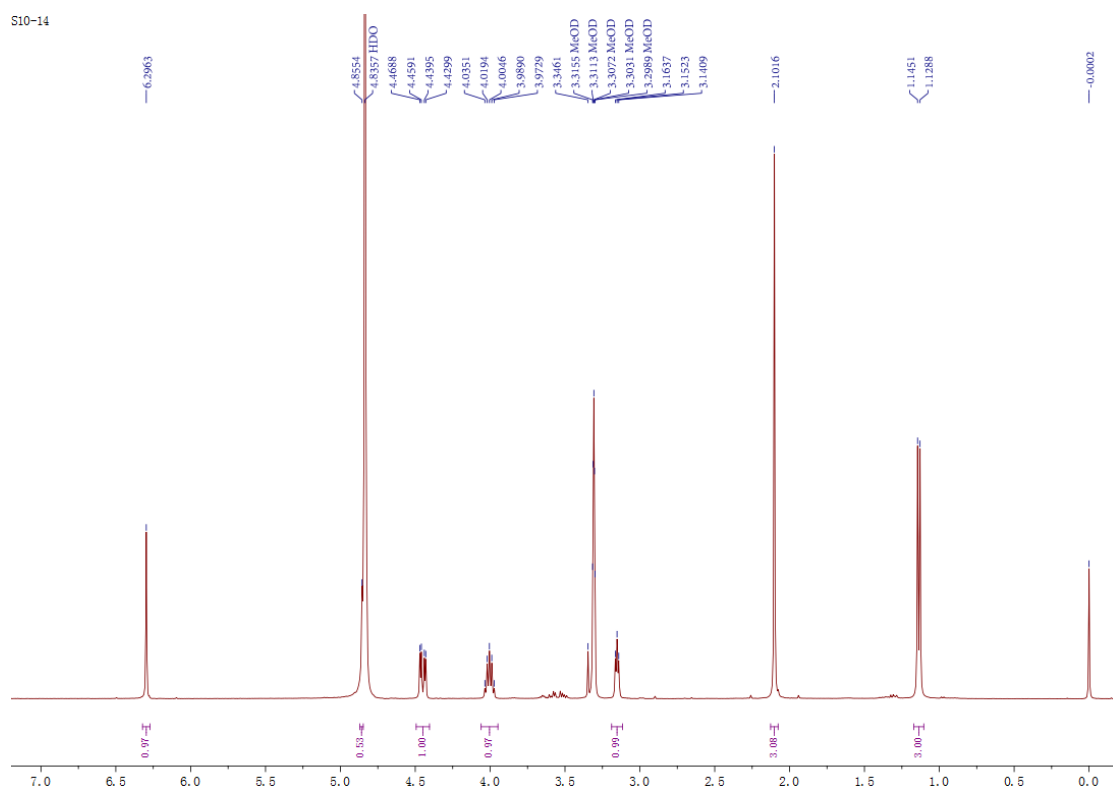


Figure S20. ¹H NMR spectrum of **4** (CD₃OD, 400 MHz)

S10-14_13C

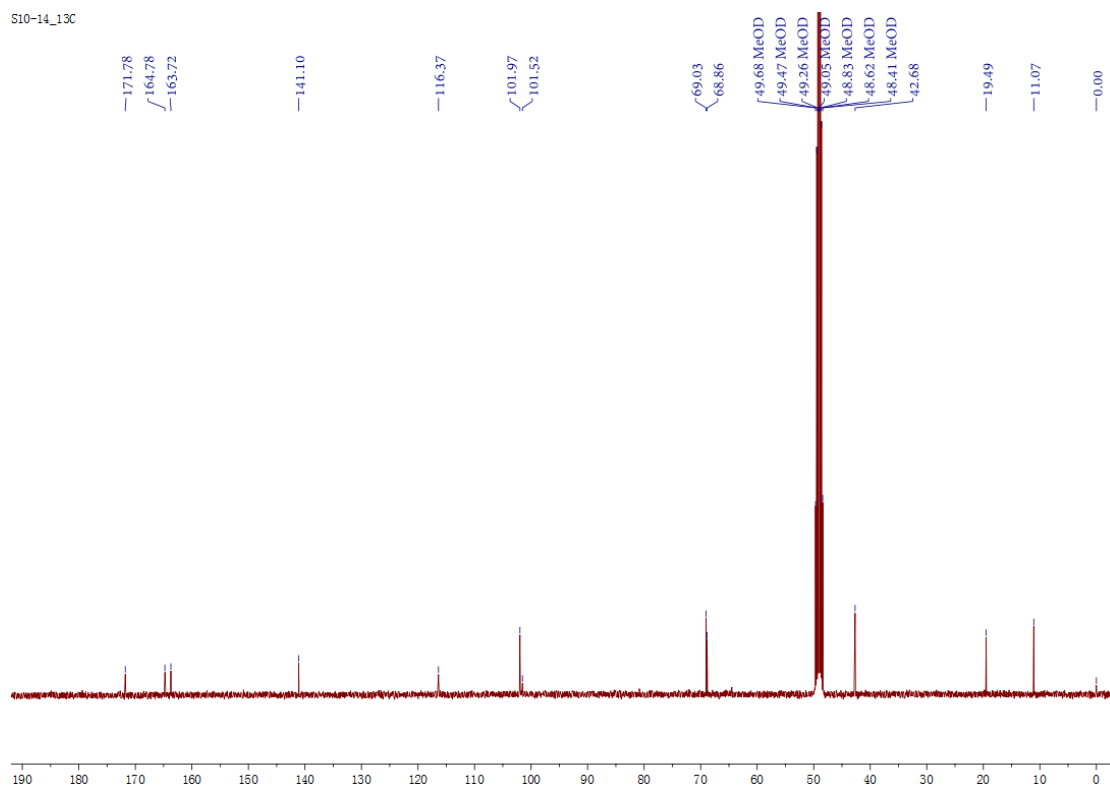


Figure S21. ^{13}C NMR spectrum of **4** (CD_3OD , 100 MHz)

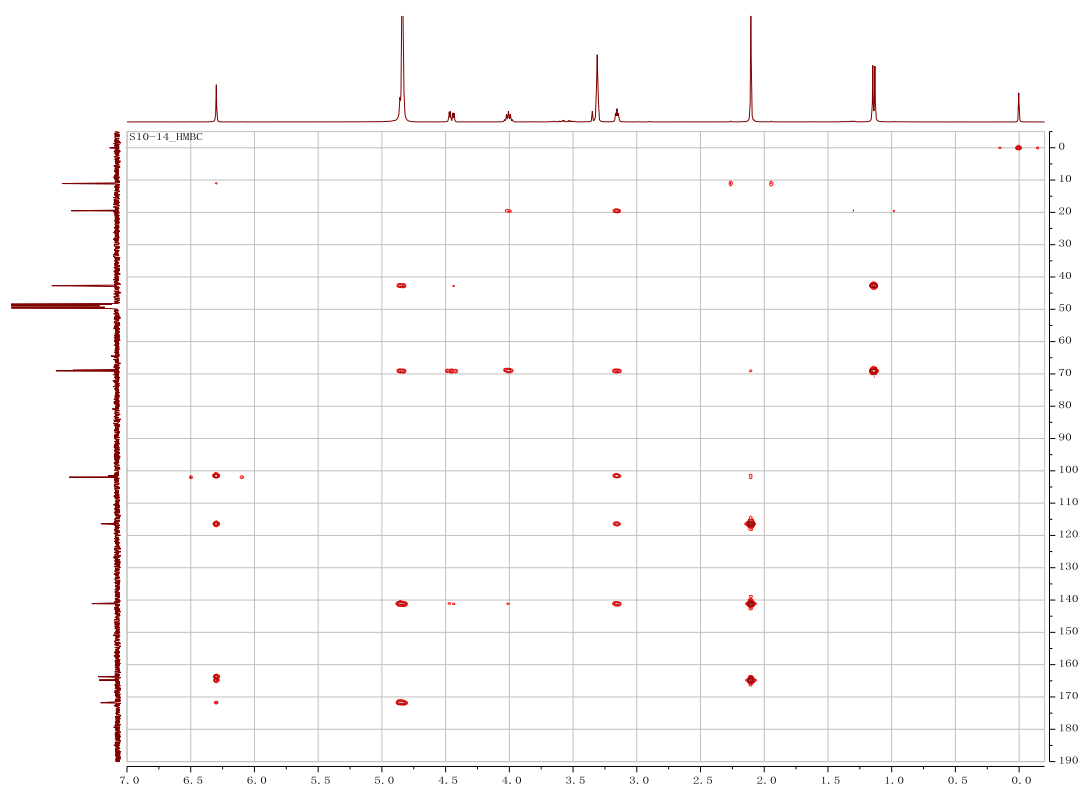


Figure S22. HMBC spectrum of **4**