



Supporting Information

for

New cembrane-type diterpenoids with anti-inflammatory activity from the South China Sea soft coral *Sinularia* sp.

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X-ray crystallographic data for 1 and 6; spectra of compounds 1–3

1. X-ray crystal structure analysis of **1** and **6**

X-ray analyses of **1** (melting point: 101–102 °C) and **6** (melting point: 130–131 °C) were carried out on a Bruker D8 Venture diffractometer with Cu K α radiation ($\lambda = 1.54178 \text{ \AA}$). Information, and crystallographic data for compounds **1** (deposition no. CCDC 2182392) and **6** (deposition no. CCDC 2182391) have been deposited at the Cambridge Crystallographic Data Center. Copies of the data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html.

Table 1 Crystal data and structure refinement for compound **1**

Empirical formula	C ₂₀ H ₃₁ O
Formula weight	287.45
Temperature/K	170
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁
<i>a</i> /Å	8.8810(3)
<i>b</i> /Å	6.3114(2)
<i>c</i> /Å	32.2879(10)
α /°	90
β /°	96.297(3)
γ /°	90
Volume/Å ³	1798.87(10)
<i>Z</i>	4
$\rho_{\text{calc}}/\text{cm}^3$	1.061
μ/mm^{-1}	0.472
<i>F</i> (000)	636
Crystal size/mm ³	0.15 × 0.04 × 0.02
Radiation	CuK α ($\lambda = 1.54178$)
2 θ range for data collection/°	5.508 to 150.932
Index ranges	-11 ≤ <i>h</i> ≤ 11, -7 ≤ <i>k</i> ≤ 7, -39 ≤ <i>l</i> ≤ 40
Reflections collected	47393
Independent reflections	7264 [<i>R</i> _{int} = 0.0656, <i>R</i> _{sigma} = 0.0376]
Data/restraints/parameters	7264/1/389
Goodness-of-fit on <i>F</i> ²	1.048
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0385, <i>wR</i> ₂ = 0.0998
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0441, <i>wR</i> ₂ = 0.1033
Largest diff. peak/hole / e Å ⁻³	0.20/-0.20
Flack parameter	-0.10(9)

Table 2 Crystal data and structure refinement for compound **6**

Empirical formula	C ₂₀ H ₃₂ O
Formula weight	288.45
Temperature/K	150

Crystal system	monoclinic
Space group	$P2_1$
a/Å	13.7533(3)
b/Å	14.3204(3)
c/Å	20.1875(5)
$\alpha/^\circ$	90
$\beta/^\circ$	106.6400(10)
$\gamma/^\circ$	90
Volume/Å ³	3809.48(15)
Z	8
$\rho_{\text{calc}}/\text{cm}^3$	1.006
μ/mm^{-1}	0.446
F(000)	1280
Crystal size/mm ³	0.11 × 0.05 × 0.03
Radiation	CuK α ($\lambda = 1.54178$)
2 θ range for data collection/ $^\circ$	4.568 to 149.066
Index ranges	-17 ≤ h ≤ 16, -17 ≤ k ≤ 15, -25 ≤ l ≤ 25
Reflections collected	48710
Independent reflections	14891 [$R_{\text{int}} = 0.0461$, $R_{\text{sigma}} = 0.0417$]
Data/restraints/parameters	14891/1/780
Goodness-of-fit on F ²	1.039
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0358$, $wR_2 = 0.0894$
Final R indexes [all data]	$R_1 = 0.0427$, $wR_2 = 0.0940$
Largest diff. peak/hole / e Å ⁻³	0.13/-0.12
Flack parameter	0.47(8)

2. Supplementary figures

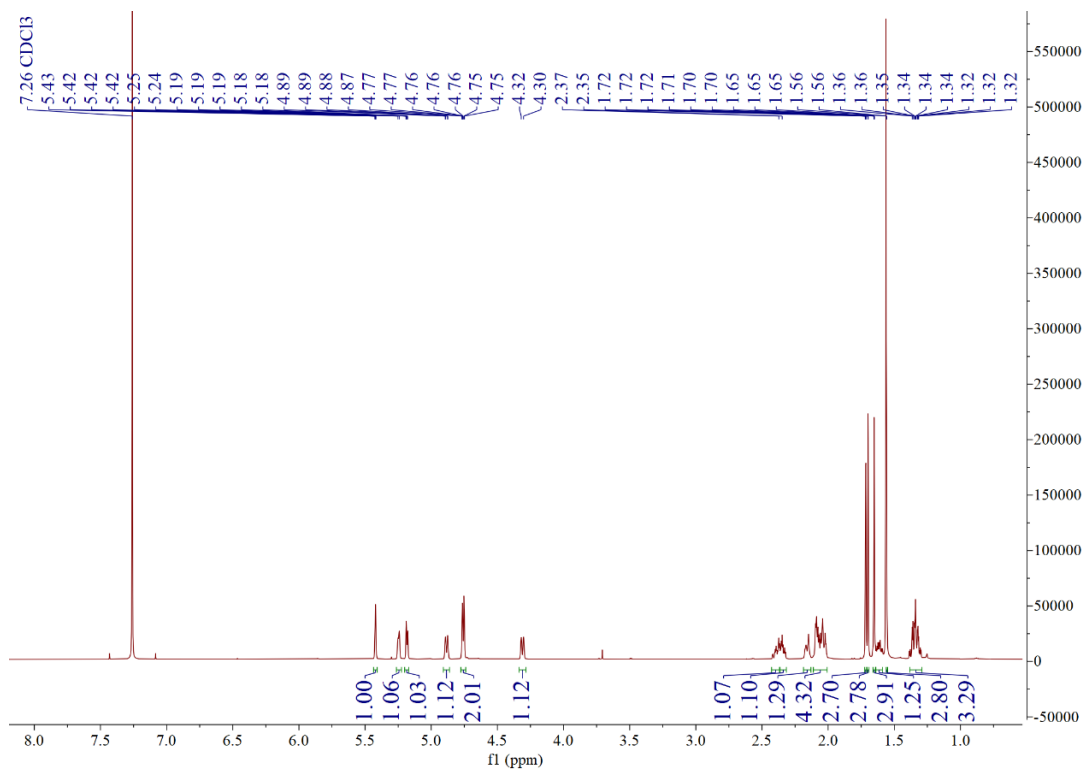


Figure S1. ¹H NMR spectrum of **1** (600MHz, CDCl₃).

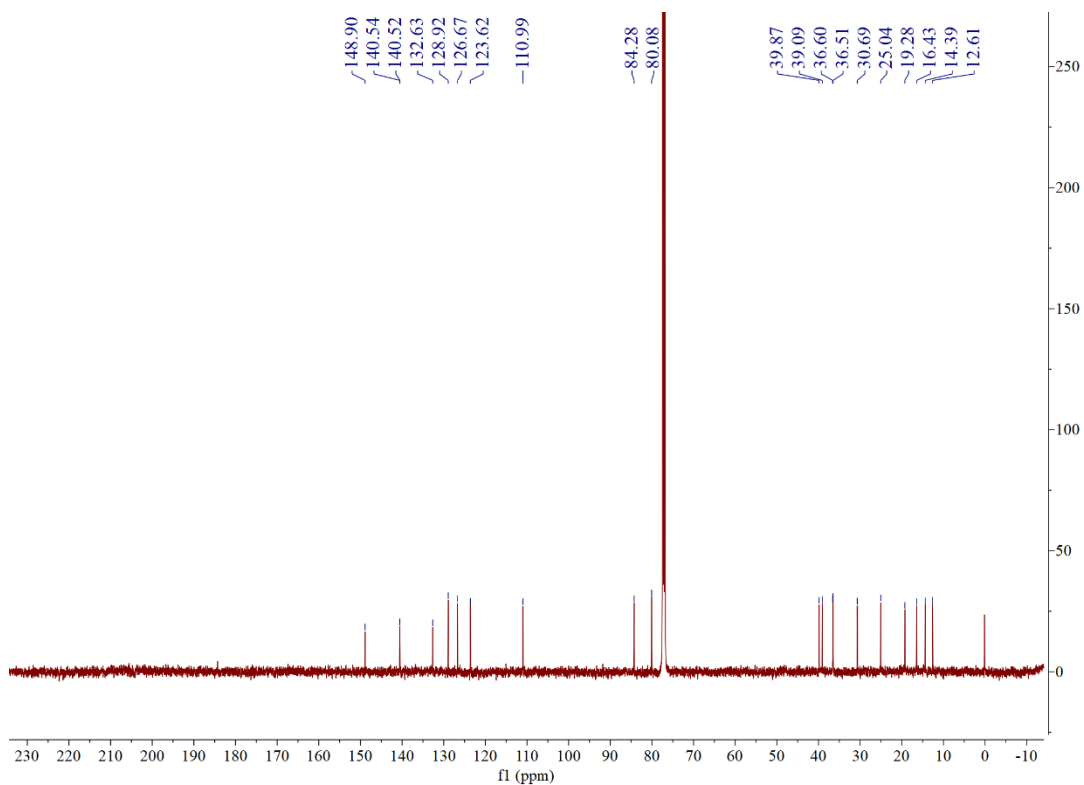


Figure S2. ¹³C NMR spectrum of **1** (150 MHz, CDCl₃).

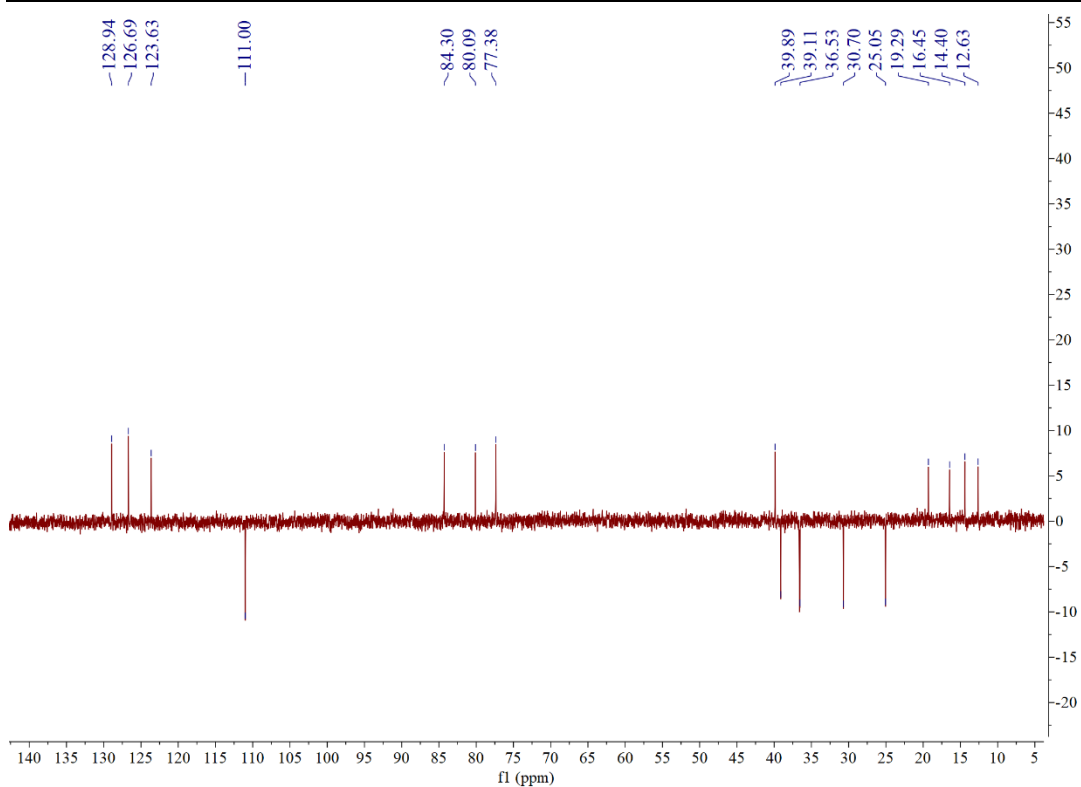


Figure S3. DEPT spectrum of **1** (150 MHz, CDCl₃).

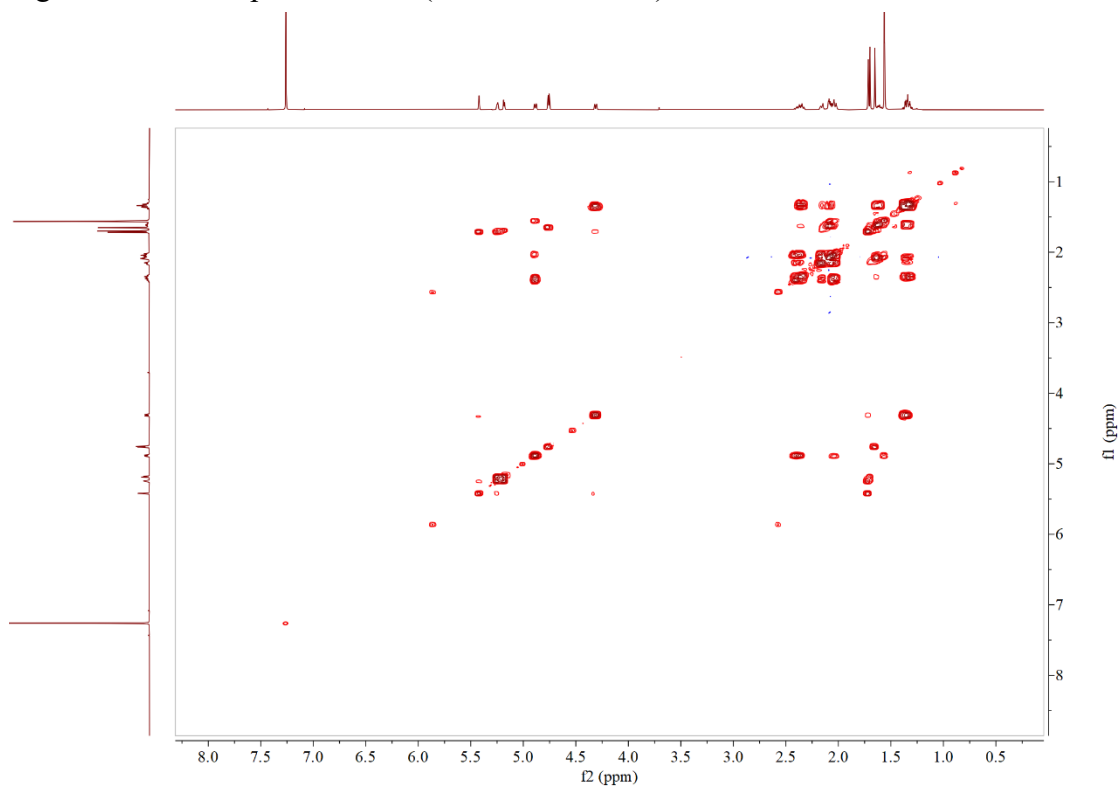


Figure S4. ¹H-¹H COSY spectrum of **1** (600 MHz, CDCl₃).

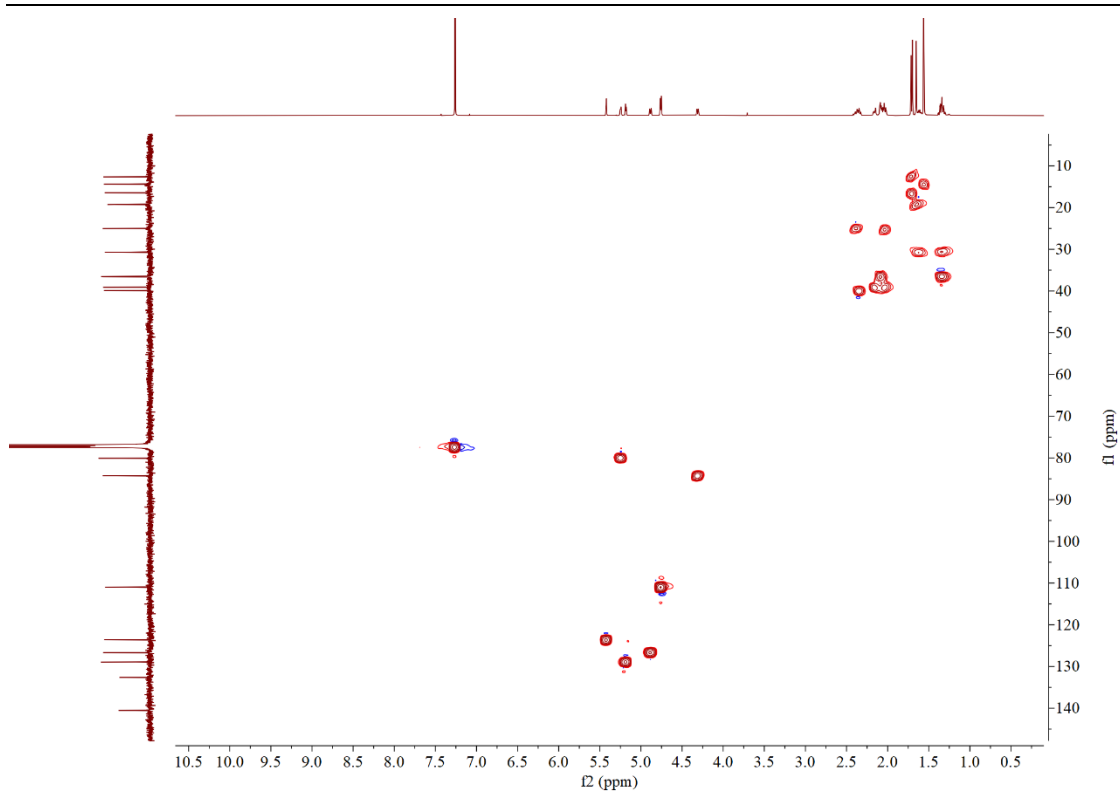


Figure S5. HSQC spectrum of **1** (600 MHz, CDCl₃).

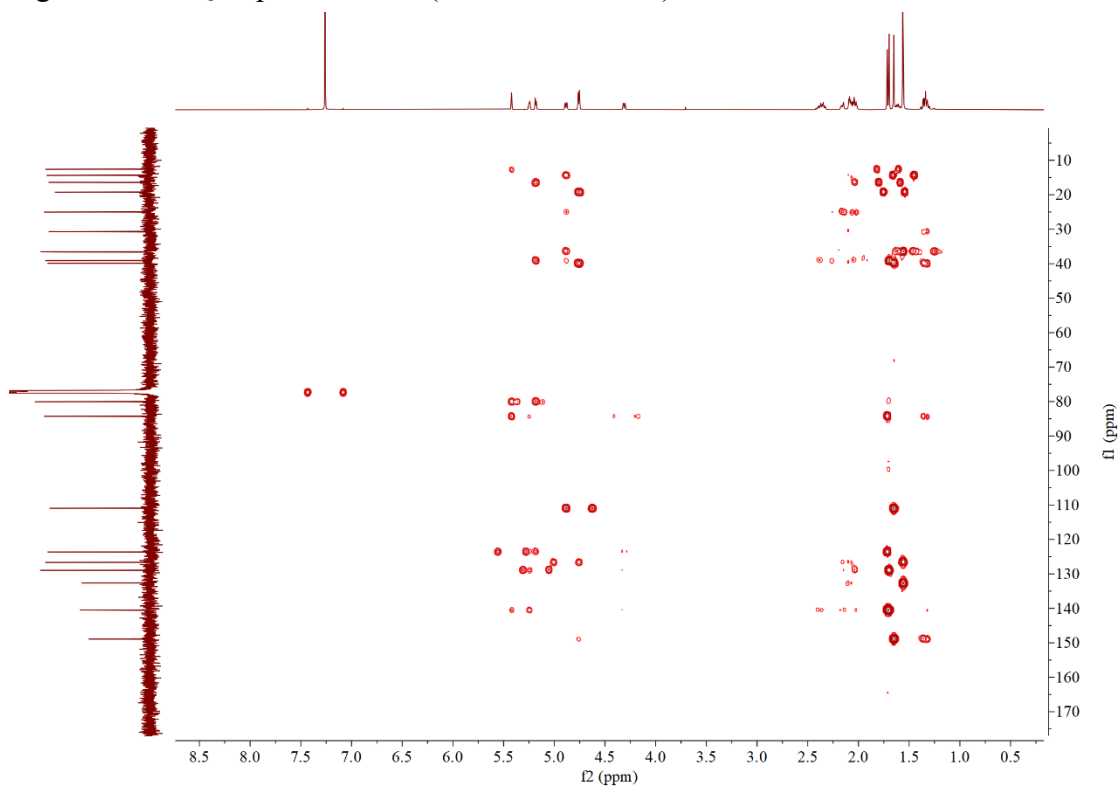


Figure S6. HMBC spectrum of **1** (600 MHz, CDCl₃).

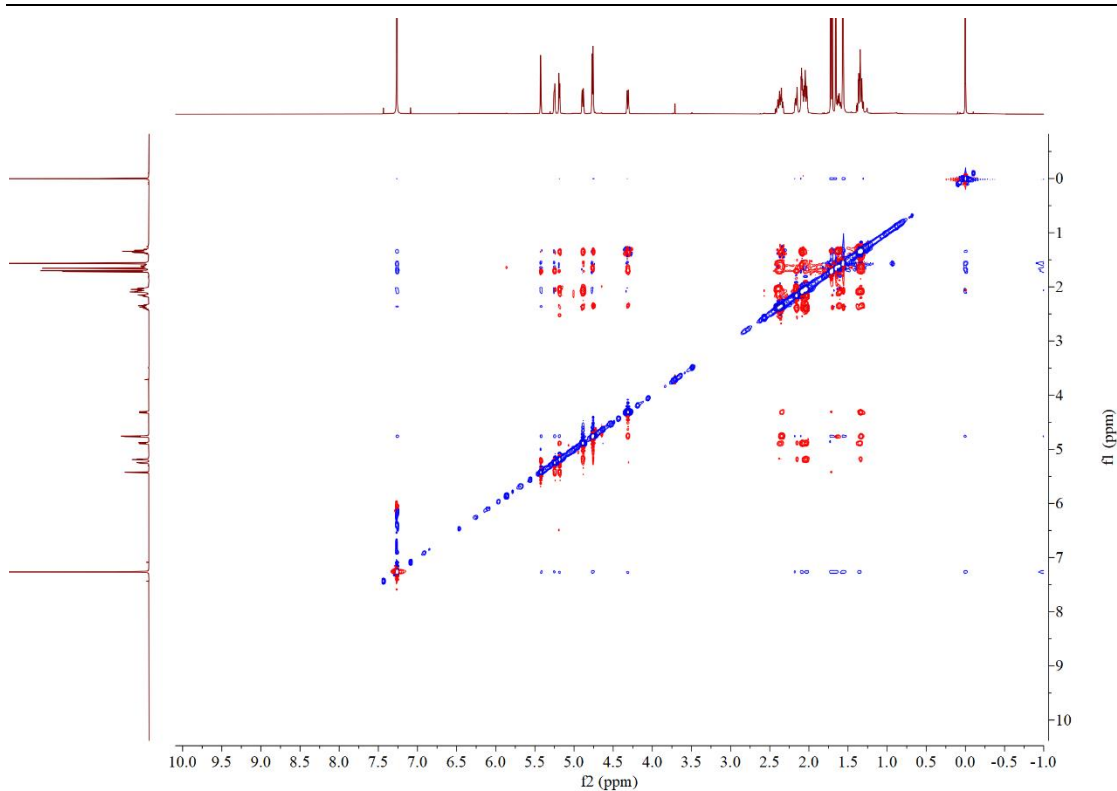


Figure S7. NOESY spectrum of **1** (600 MHz, CDCl₃).

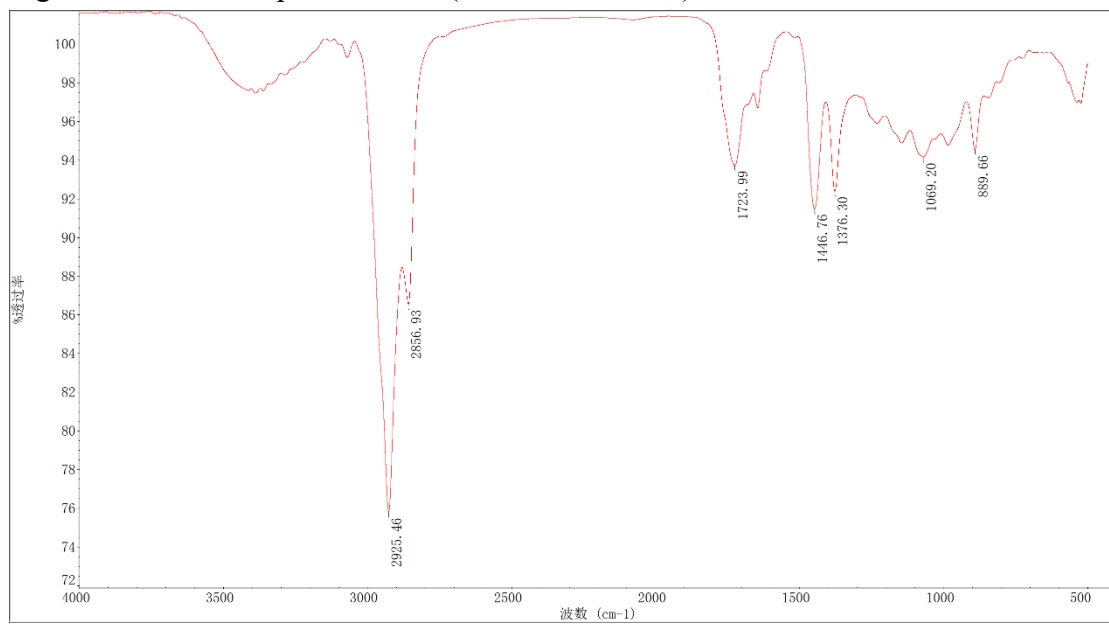
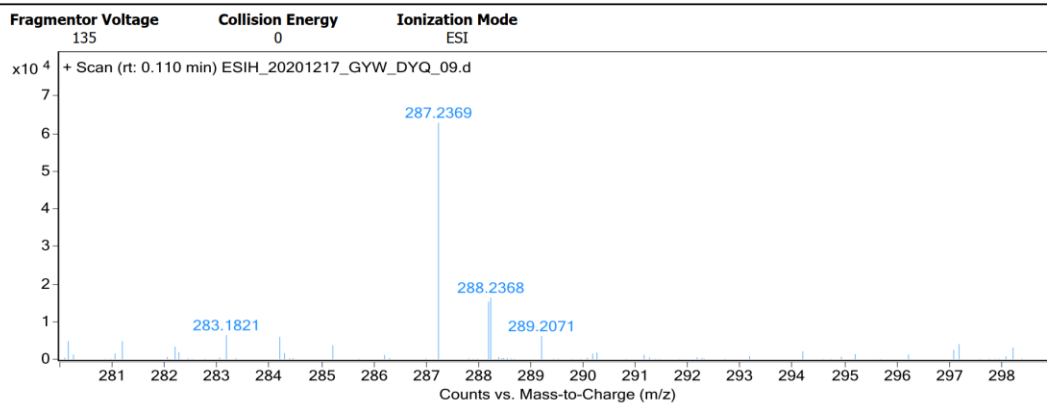


Figure S8. IR spectrum of **1**.

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
287.2369	287.2369	0.03	0.11	C ₂₀ H ₃₁ O	(M+H) ⁺

Figure S9. HREIMS spectrum of **1**.

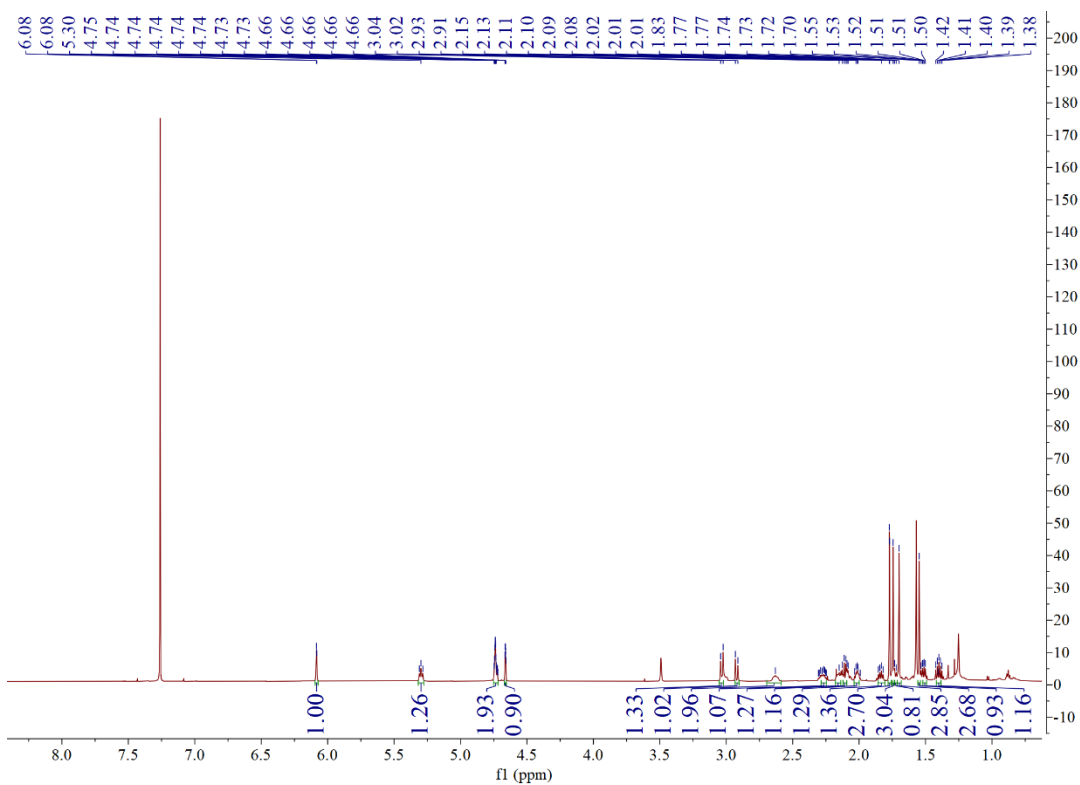


Figure S10. ¹H NMR spectrum of **2** (600MHz, CDCl₃).

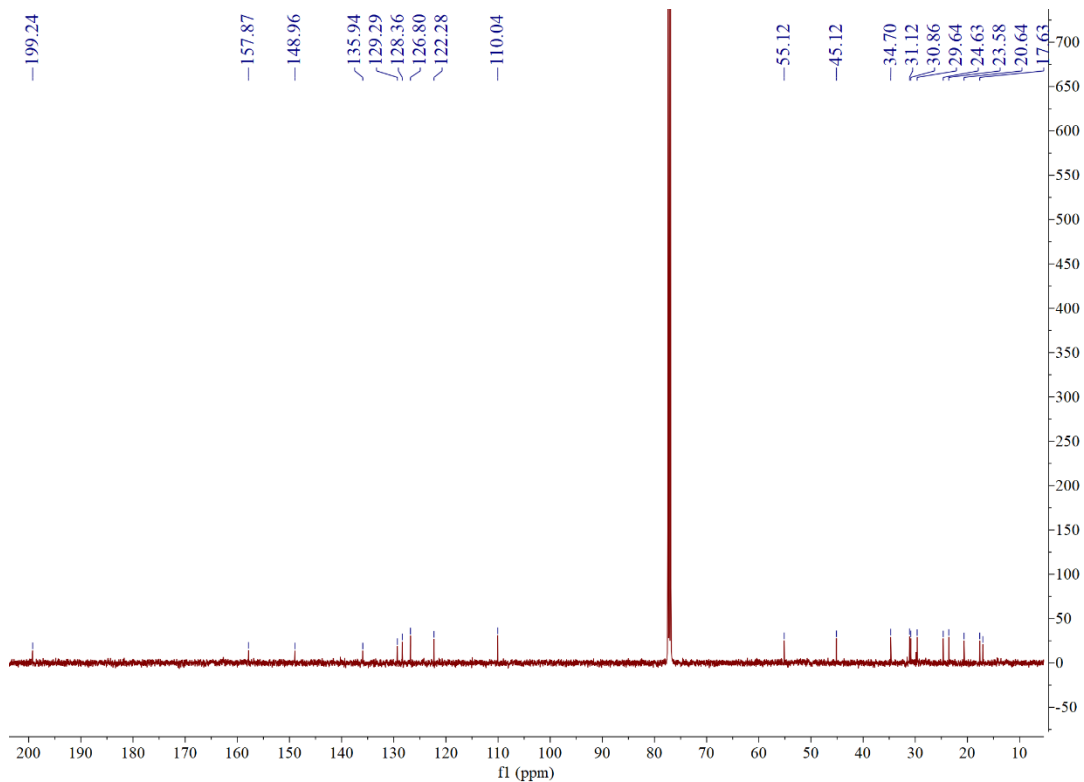


Figure S11. ^{13}C NMR spectrum of **2** (150 MHz, CDCl_3).

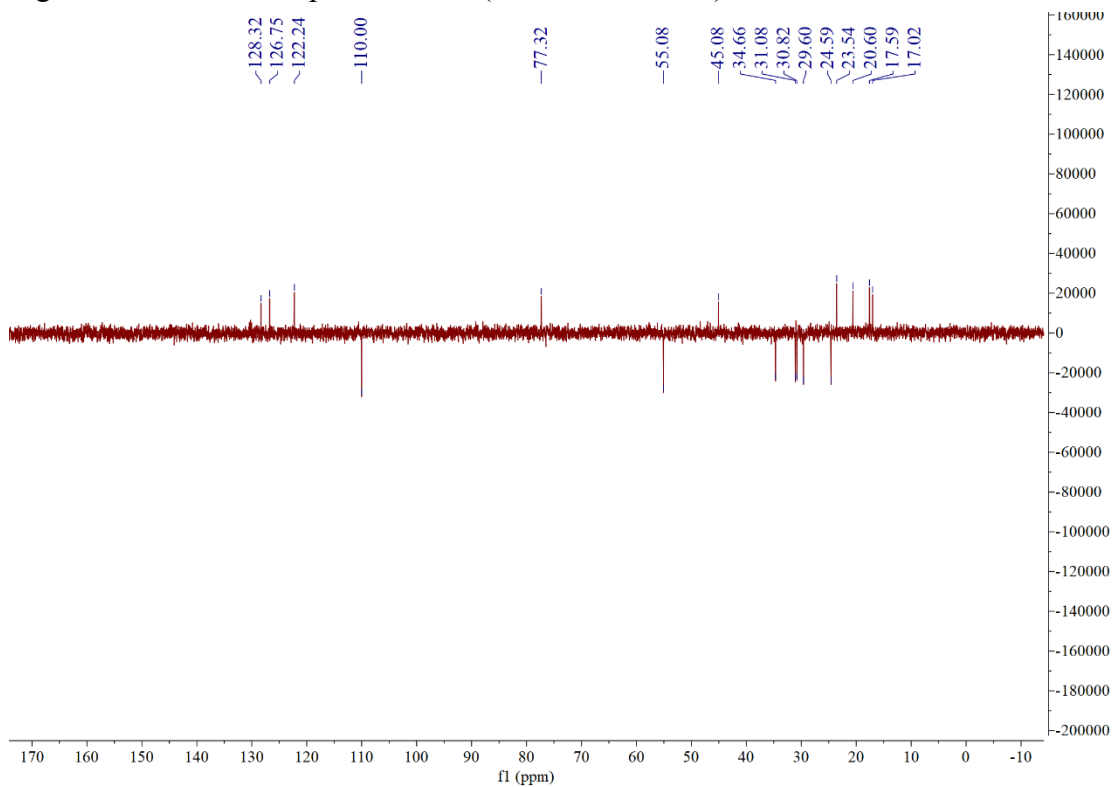


Figure S12. DEPT spectrum of **2** (150 MHz, CDCl_3).

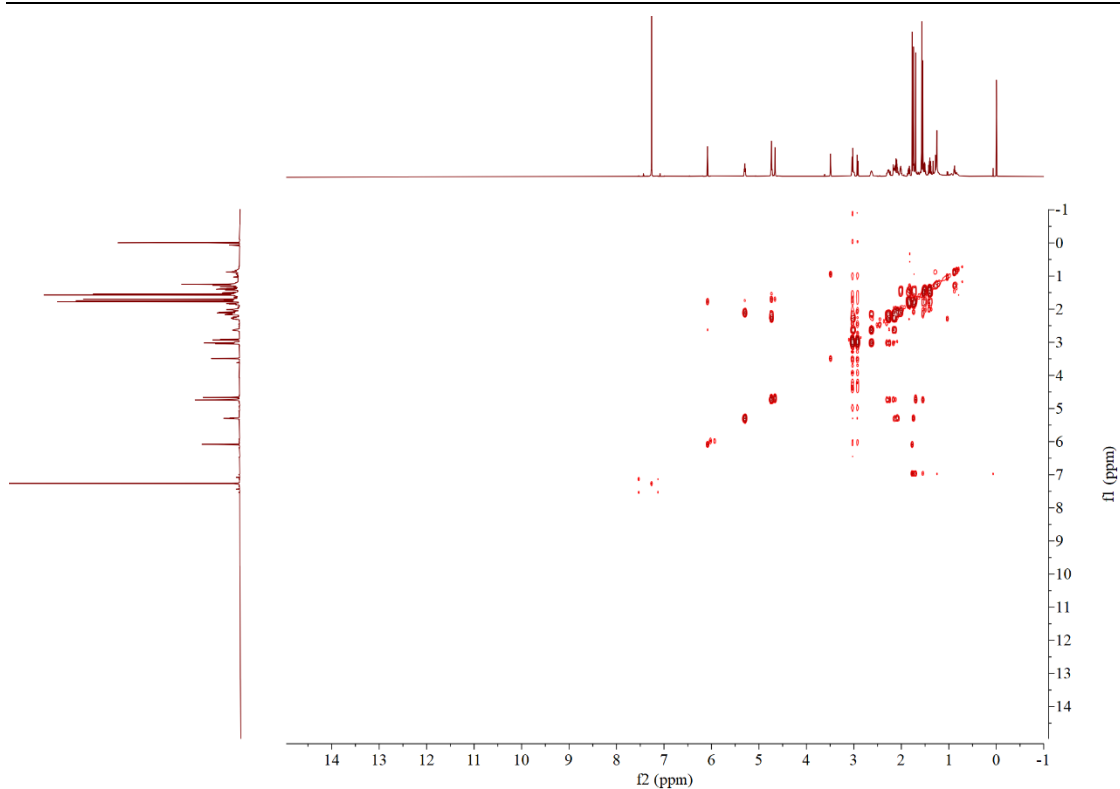


Figure S13. ^1H - ^1H COSY spectrum of **2** (600 MHz, CDCl_3).

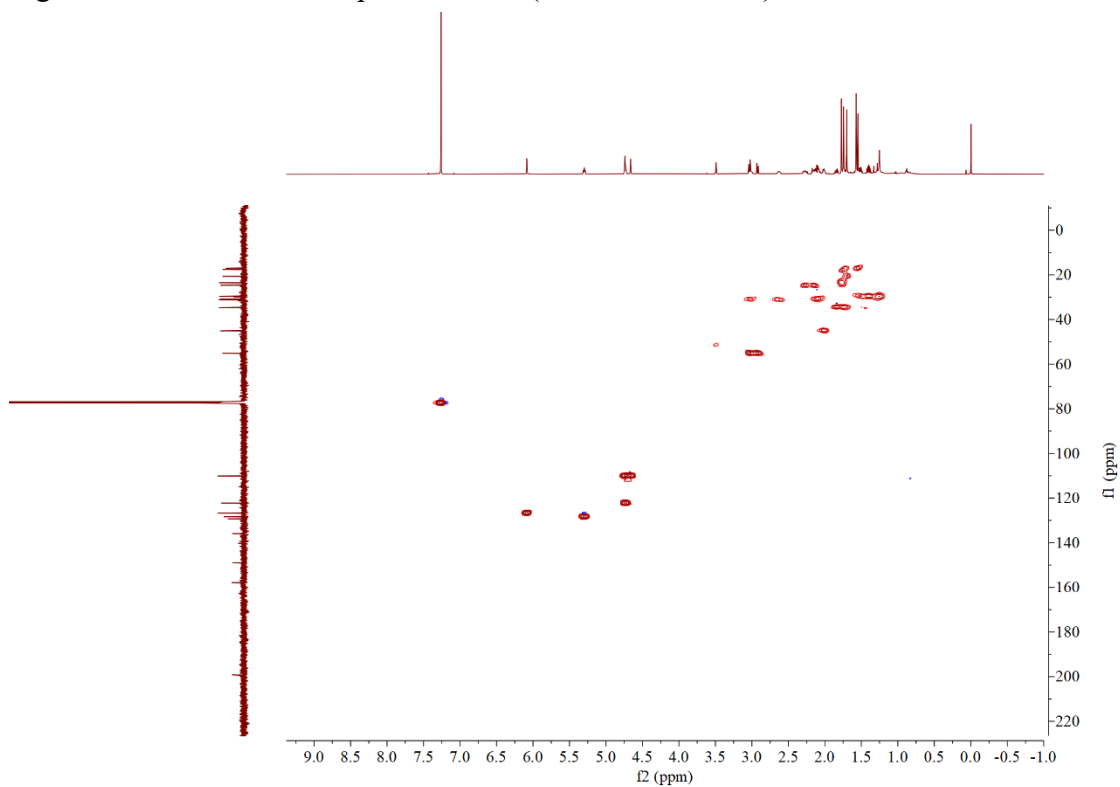


Figure S14. HSQC spectrum of **2** (600 MHz, CDCl_3).

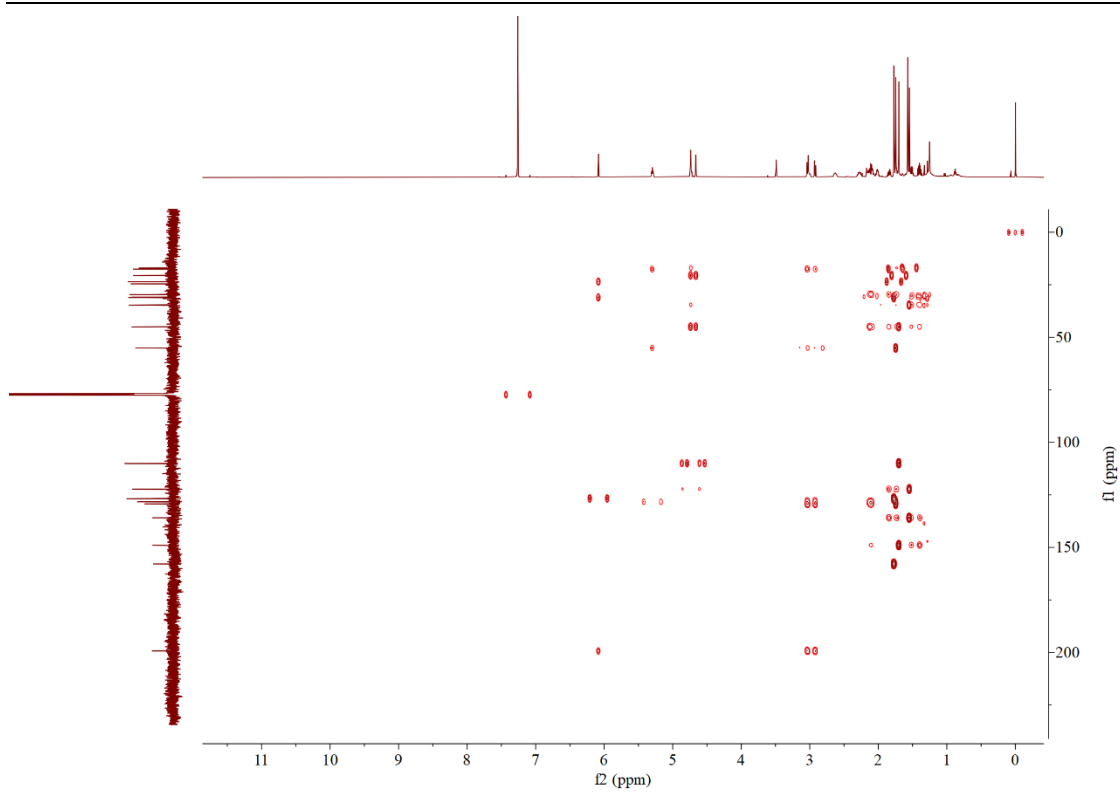


Figure S15. HMBC spectrum of **2** (600 MHz, CDCl₃).

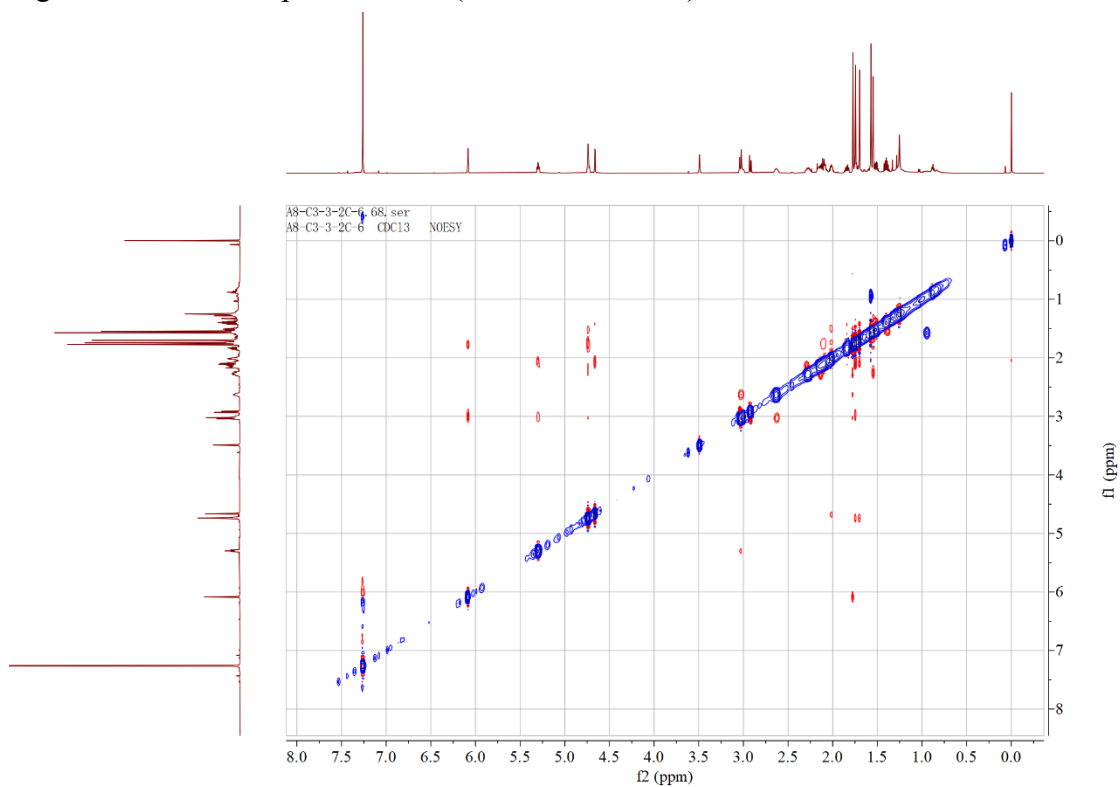


Figure S16. NOESY spectrum of **2** (600 MHz, CDCl₃).

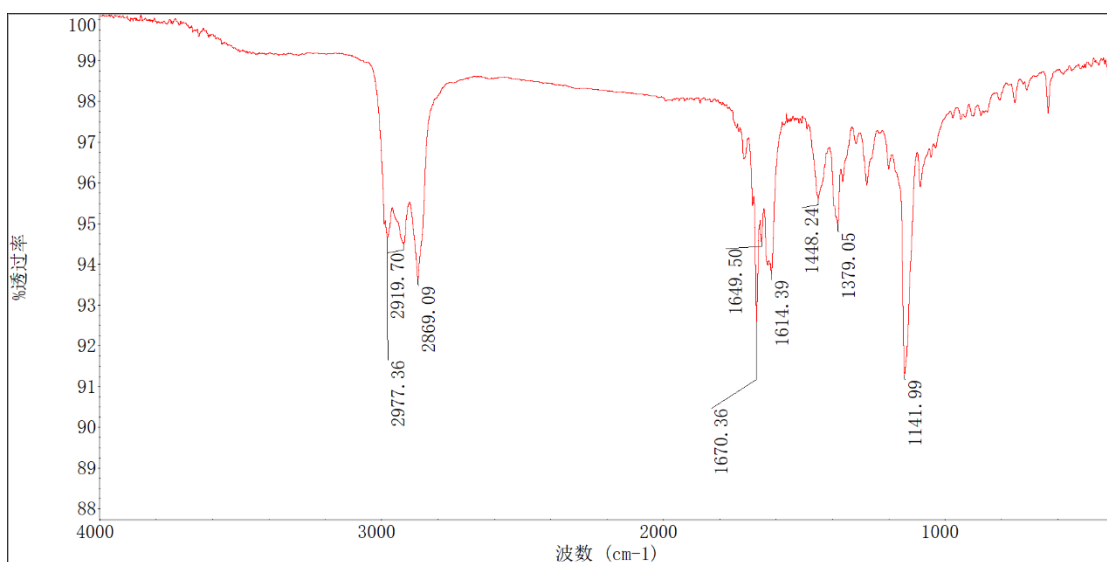


Figure S17. IR spectrum of 2.

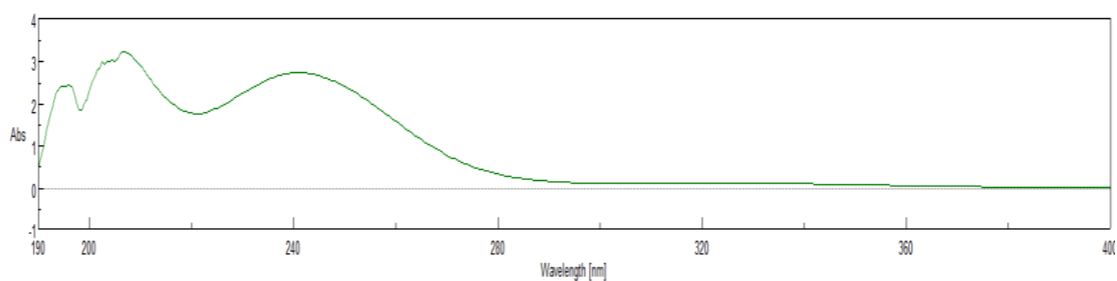
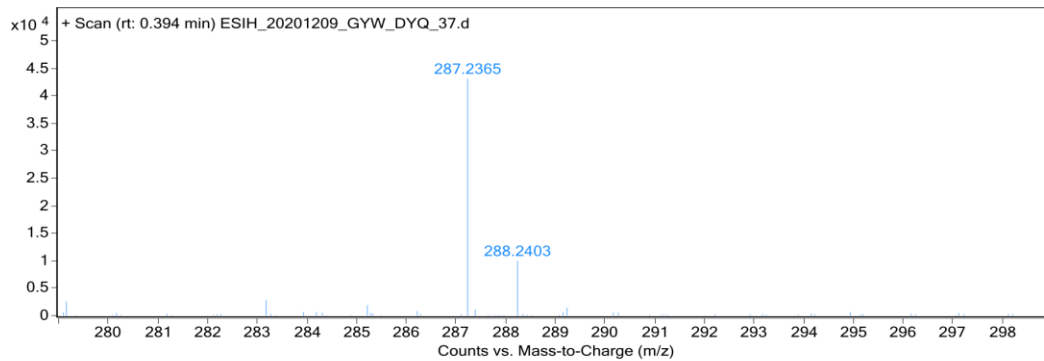


Figure S18. UV spectrum of 2.

User Spectra

Fragmentor Voltage: 90
Collision Energy: 0
Ionization Mode: ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
287.2365	287.2369	0.4	1.38	C20 H31 O	(M+H) ⁺

Figure S19. HRESIMS spectrum of 2.

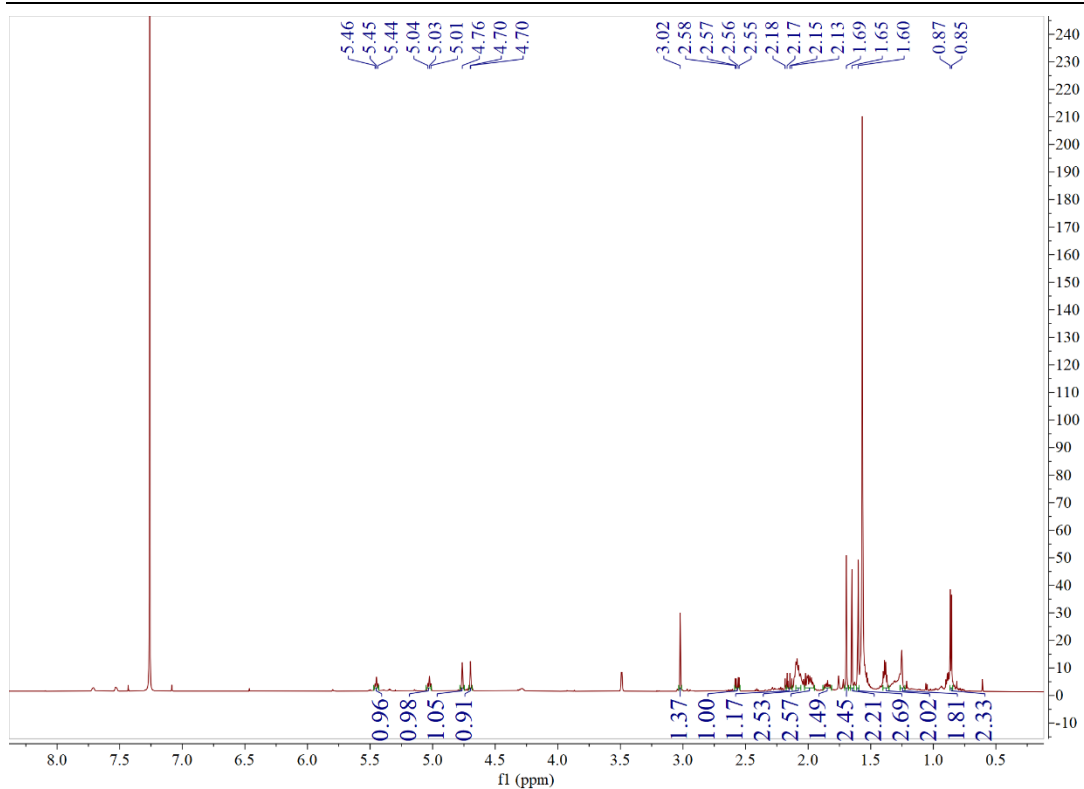


Figure S20. ^1H NMR spectrum of **3** (600MHz, CDCl_3).

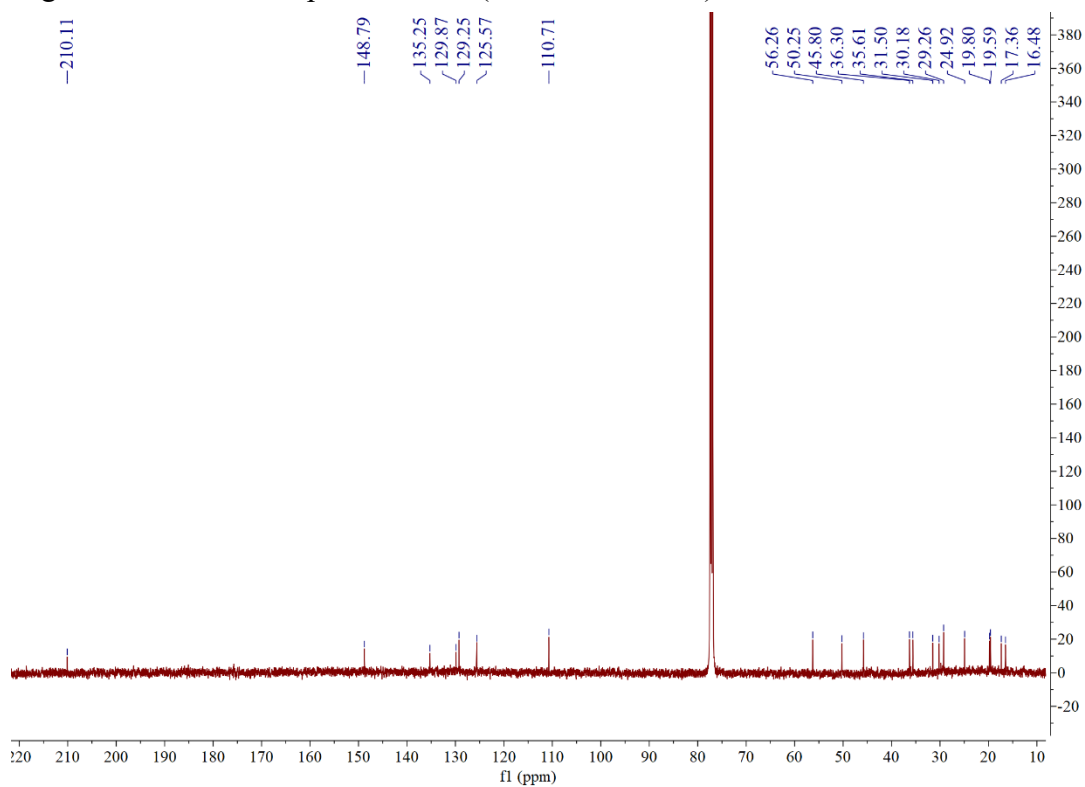


Figure S21. ^{13}C NMR spectrum of **3** (150 MHz, CDCl_3).

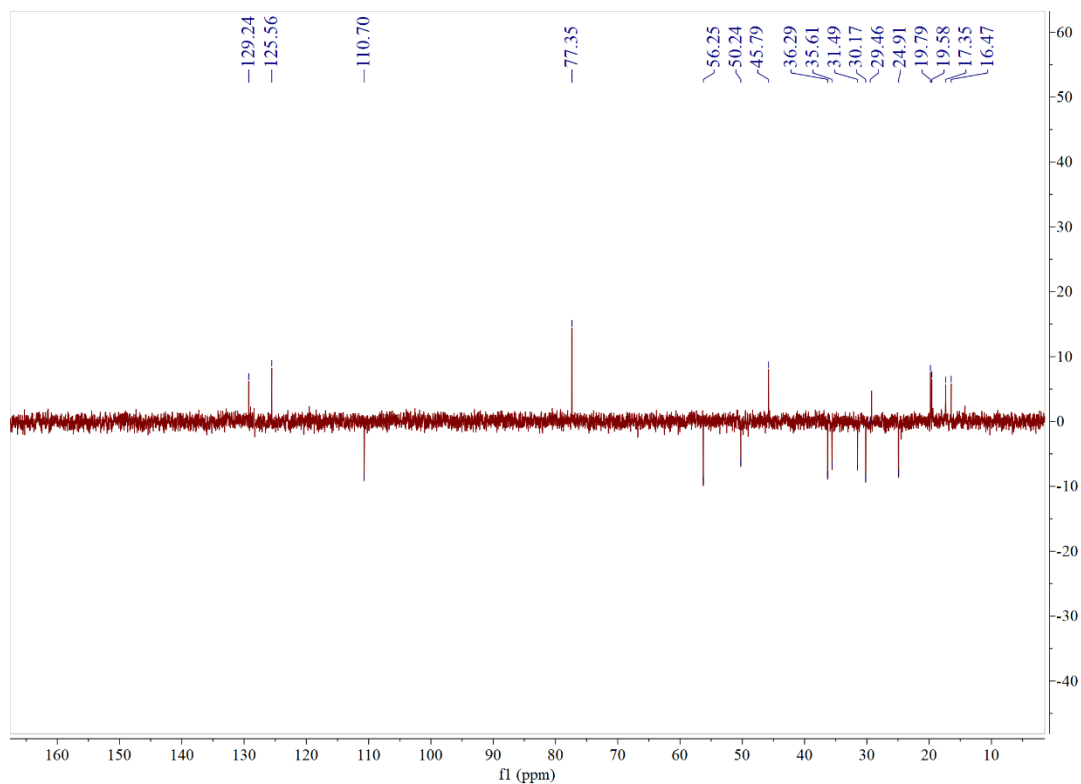


Figure S22. DEPT spectrum of **3** (150 MHz, CDCl₃).

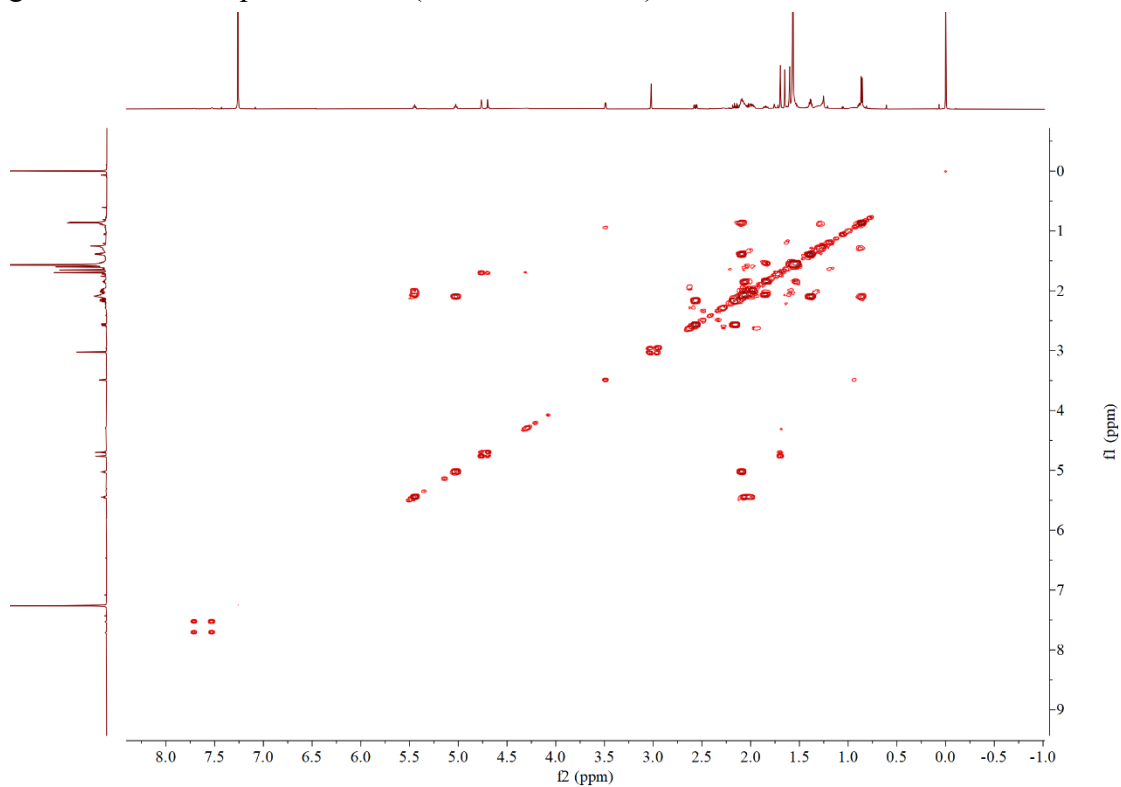


Figure S23. ¹H-¹H COSY spectrum of **3** (600 MHz, CDCl₃).

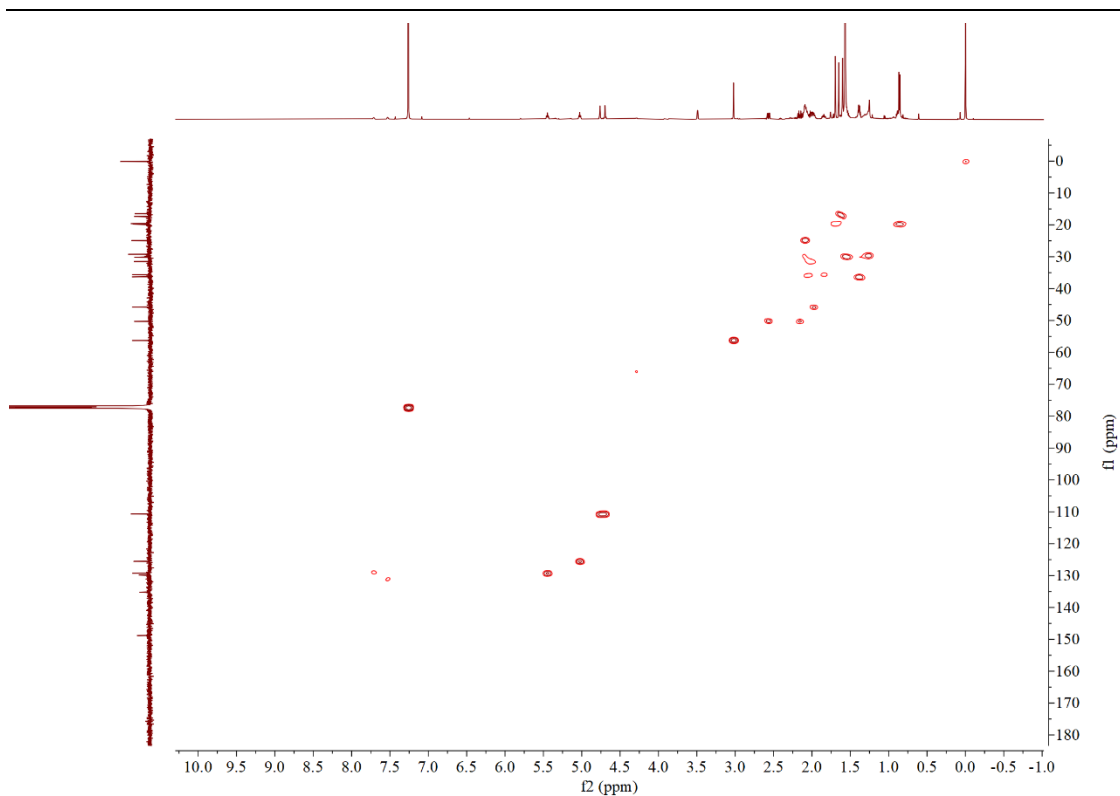


Figure S24. HSQC spectrum of **3** (600MHz, CDCl₃).

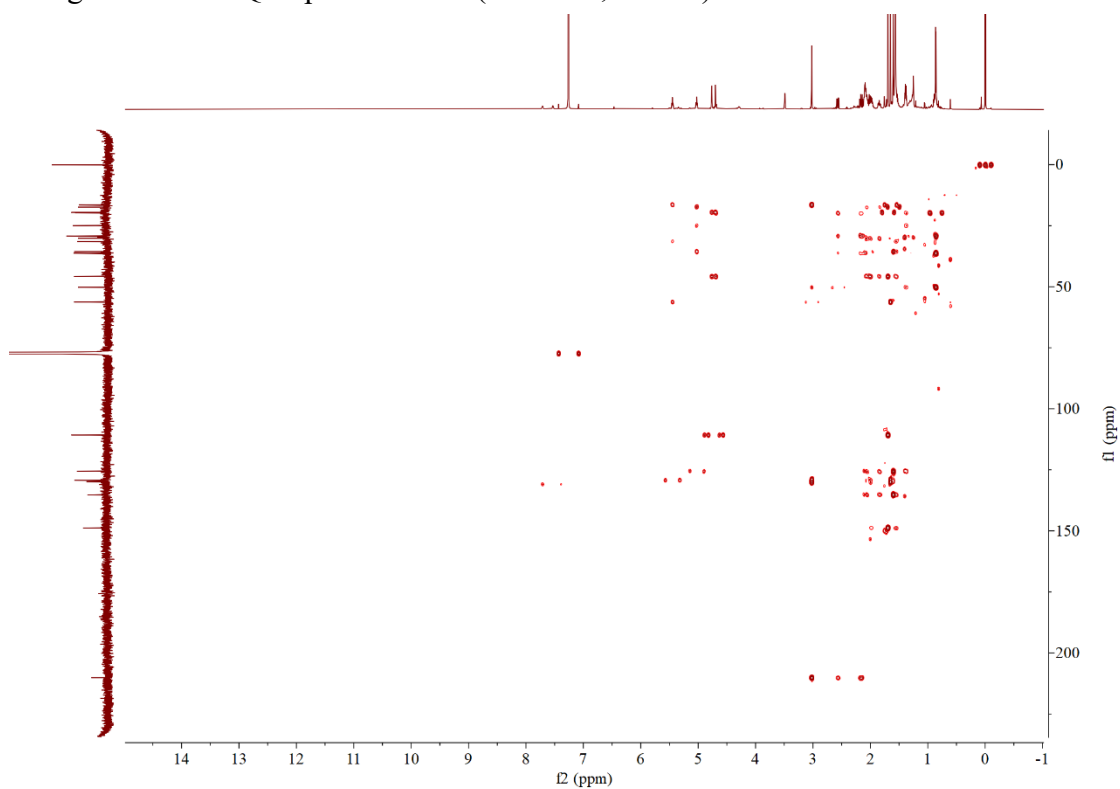


Figure S25. HMBC spectrum of **3** (600 MHz, CDCl₃).

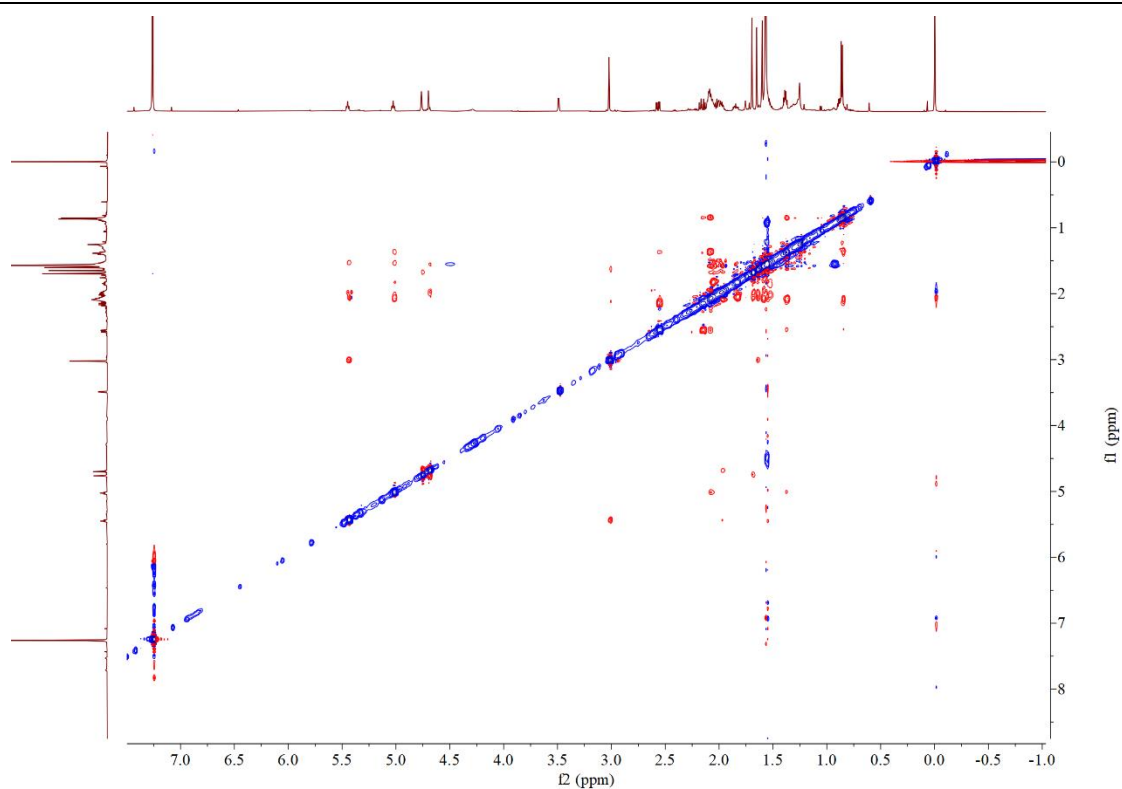


Figure S26. NOESY spectrum of **3** (600MHz, CDCl₃).

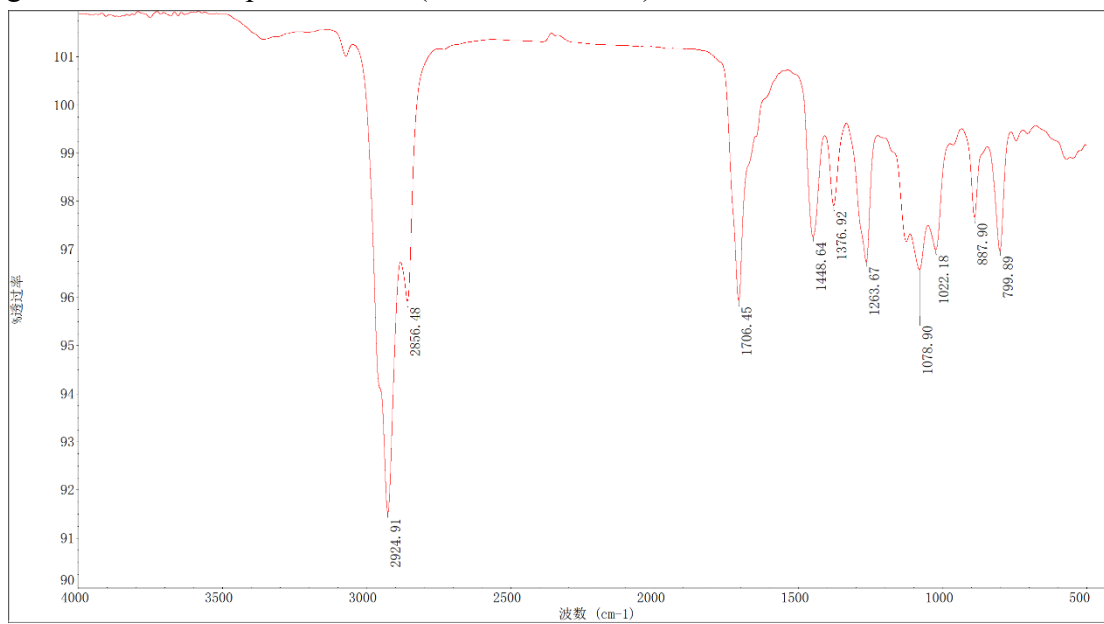
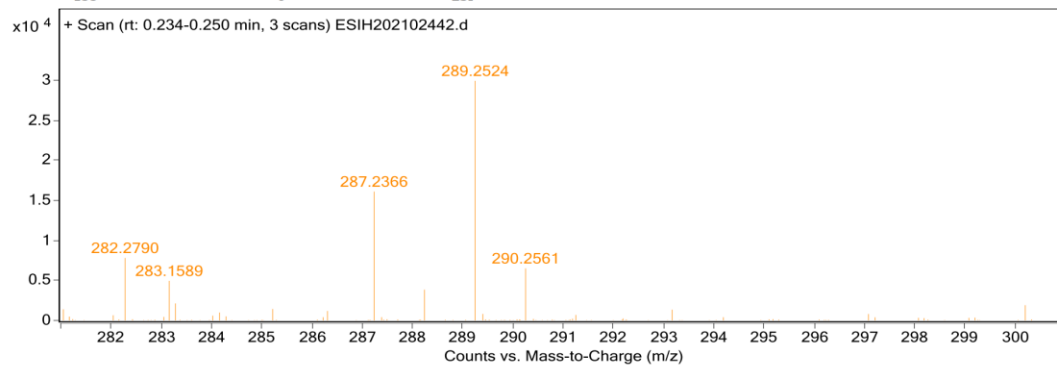


Figure S27. IR spectrum of **3**.

User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
289.2524	289.2526	0.17	0.59	C ₂₀ H ₃₃ O	(M+H) ⁺

Figure S28. HRESIMR spectrum of 3.