

Halogenated C₁₅ Acetogenin Analogues of Obtusallene III from a *Laurenciella* sp. Collected in Corsican

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- **Figure S1.** ^1H NMR spectrum of compound **1** at 20°C (CDCl_3 , 400 MHz).
- **Figure S2.** ^1H NMR spectrum of compound **1** at -40°C (CDCl_3 , 400 MHz).
- **Figure S3.** ^{13}C NMR spectrum of compound **1** at 20°C (CDCl_3 , 125.5 MHz).
- **Figure S4.** ^{13}C NMR spectrum of compound **1** at -40°C (CDCl_3 , 125.5 MHz).
- **Figure S5.** HMQC spectrum of compound **1** at -40°C (CDCl_3 , 400 MHz).
- **Figure S6.** HMBC spectrum of compound **1** at -40°C (CDCl_3 , 400 MHz).
- **Figure S7.** COSY spectrum of compound **1** at $+20^\circ\text{C}$ (CDCl_3 , 400 MHz).
- **Figure S8.** COSY spectrum of compound **1** at -40°C (CDCl_3 , 400 MHz).
- **Figure S9.** NOESY spectrum of compound **1** at $+20^\circ\text{C}$ (CDCl_3 , 400 MHz).
- **Figure S10.** HRMS spectrum of compound **1** in negative ionization.
- **Figure S11.** HRMS spectrum of compound **1** (Zoom) in negative ionization.
- **Figure S12.** UV spectra of compound **1**.
- **Figure S13.** Experimental ECD spectra of **1**.
- **Figure S14.** ^1H NMR spectrum of compound **2** at 20°C (CDCl_3 , 400 MHz).
- **Figure S15.** ^1H NMR spectrum of compound **2** at -40°C (CDCl_3 , 400 MHz).
- **Figure S16.** ^{13}C NMR spectrum of compound **2** at 20°C (CDCl_3 , 125.5 MHz).
- **Figure S17.** ^{13}C NMR spectrum of compound **2** at -40°C (CDCl_3 , 125.5 MHz).
- **Figure S18.** HMQC spectrum of compound **2** at -40°C (CDCl_3 , 400 MHz).
- **Figure S19.** HMBC spectrum of compound **2** at -40°C (CDCl_3 , 400 MHz).
- **Figure S20.** COSY spectrum of compound **2** at $+20^\circ\text{C}$ (CDCl_3 , 400 MHz).
- **Figure S21.** COSY spectrum of compound **2** at -40°C (CDCl_3 , 400 MHz).
- **Figure S22.** NOESY spectrum of compound **2** at $+20^\circ\text{C}$ (CDCl_3 , 400 MHz).
- **Figure S23.** HRMS spectrum of compound **2** in negative ionization.
- **Figure S24.** HRMS spectrum of compound **2** (Zoom) in negative ionization.
- **Figure S25.** UV spectra of compound **2**.
- **Figure S26.** ^1H NMR spectrum of compound **3** at 20°C (CDCl_3 , 400 MHz).
- **Figure S27.** ^1H NMR spectrum of compound **3** at -40°C (CDCl_3 , 400 MHz).
- **Figure S28.** ^{13}C NMR spectrum of compound **3** at 20°C (CDCl_3 , 125.5 MHz).
- **Figure S29.** ^{13}C NMR spectrum of compound **3** at -40°C (CDCl_3 , 125.5 MHz).
- **Figure S30.** HMQC spectrum of compound **3** at -40°C (CDCl_3 , 400 MHz).
- **Figure S31.** HMBC spectrum of compound **3** at -40°C (CDCl_3 , 400 MHz).

- **Figure S32.** COSY spectrum of compound **3** at +20°C (CDCl₃, 400 MHz).
- **Figure S33.** COSY spectrum of compound **3** at -40°C (CDCl₃, 400 MHz).
- **Figure S34.** NOESY spectrum of compound **3** at +20°C (CDCl₃, 400 MHz).
- **Figure S35.** HRMS spectrum of compound **3** in negative ionization.
- **Figure S36.** UV spectra of compound **3**.
- **Figure S37.** ¹H NMR spectrum of compound **4** at 20°C (CDCl₃, 400 MHz).
- **Figure S38.** ¹H NMR spectrum of compound **4** at -40°C (CDCl₃, 400 MHz).
- **Figure S39.** ¹³C NMR spectrum of compound **4** at 20°C (CDCl₃, 125.5 MHz).
- **Figure S40.** HMQC spectrum of compound **4** at -40°C (CDCl₃, 400 MHz).
- **Figure S41.** HMBC spectrum of compound **4** at -40°C (CDCl₃, 400 MHz).
- **Figure S42.** COSY spectrum of compound **4** at +20°C (CDCl₃, 400 MHz).
- **Figure S43.** COSY spectrum of compound **4** at -40°C (CDCl₃, 400 MHz).
- **Figure S44.** NOESY spectrum of compound **4** at +20°C (CDCl₃, 400 MHz).
- **Figure S45.** UV spectra of compound **4**.
- **Figure S46.** HRMS spectrum of compound **4** (Zoom) negative ionization.
- **Figure S47.** HRMS spectrum of compound **4** (Zoom) positive ionization.
- **Figure S48.** ¹H NMR spectrum of compound **5** (CDCl₃, 400 MHz).
- **Figure S49.** ¹³C NMR spectrum of compound **5** (CDCl₃, 125.5 MHz).
- **Figure S50.** HSQC spectrum of compound **5** (CDCl₃, 400 MHz).
- **Figure S51.** HMBC spectrum of compound **5** (CDCl₃, 400 MHz).
- **Figure S52.** COSY spectrum of compound **5** (CDCl₃, 400 MHz).
- **Figure S53.** NOESY spectrum of compound **5** (CDCl₃, 400 MHz).
- **Figure S54.** UV spectra of compound **5**.
- **Figure S55.** HRMS spectrum of compound **5** in positive ionization.
- **Figure S56.** ¹H NMR spectrum of compound **6** (CDCl₃, 400 MHz).
- **Figure S57.** Experimental CD spectra of **6** in MeOH
- **Figure S58.** Picture of a specimen of *Laurenciella* sp. collected in Ajaccio bay, Corsica, France.
- **Figure S59.** Known C₁₅ acetogenins and sesquiterpens identified from *Laurenciella* sp. extract.
- **Table S60.** Crystallographic and structure refinement parameters for **1**.

Figure S1. ^1H NMR spectrum of compound **1** at 20°C (CDCl_3 , 400 MHz).

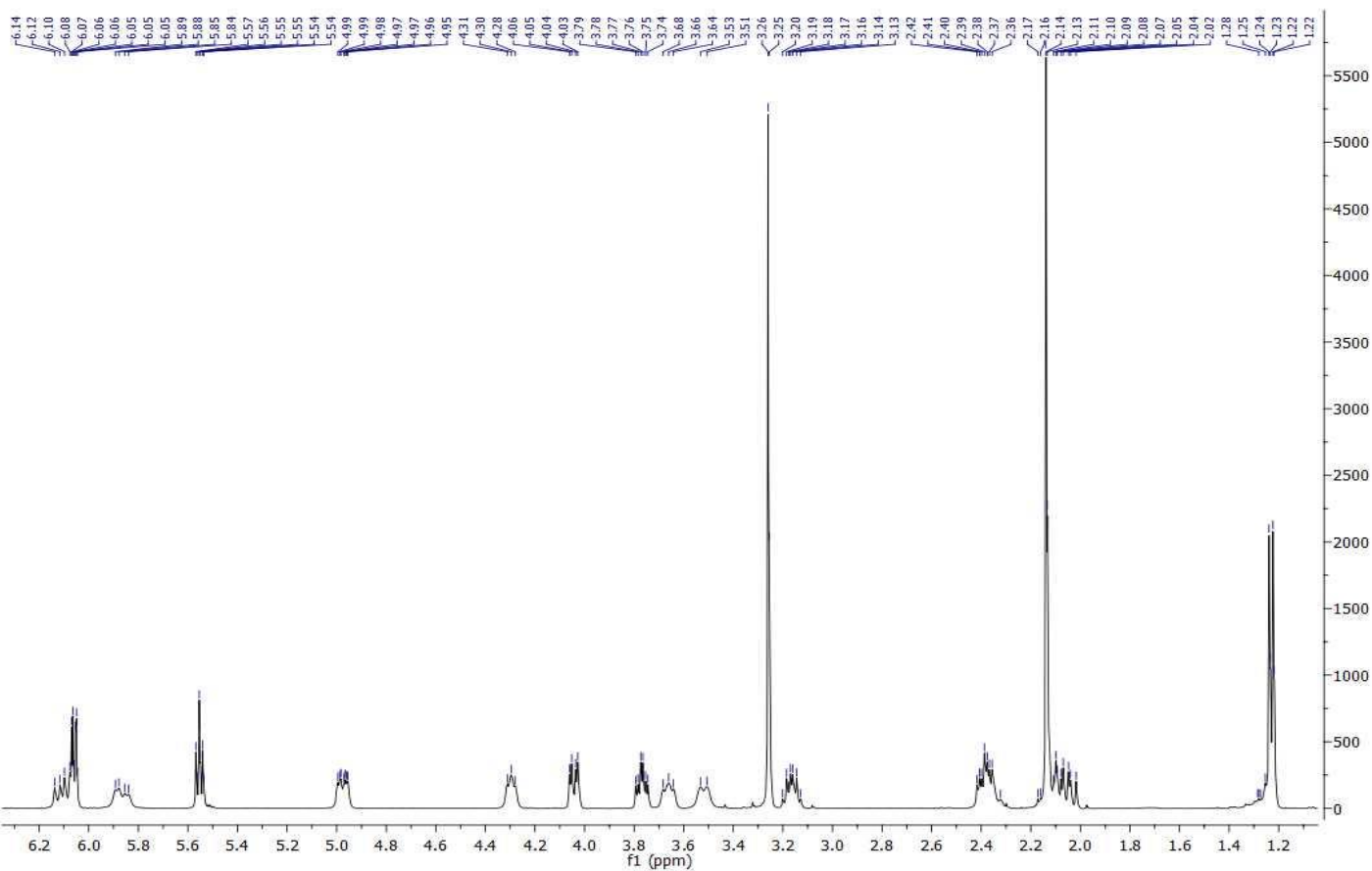


Figure S2. ^1H NMR spectrum of compound **1** at -40°C (CDCl_3 , 400 MHz).

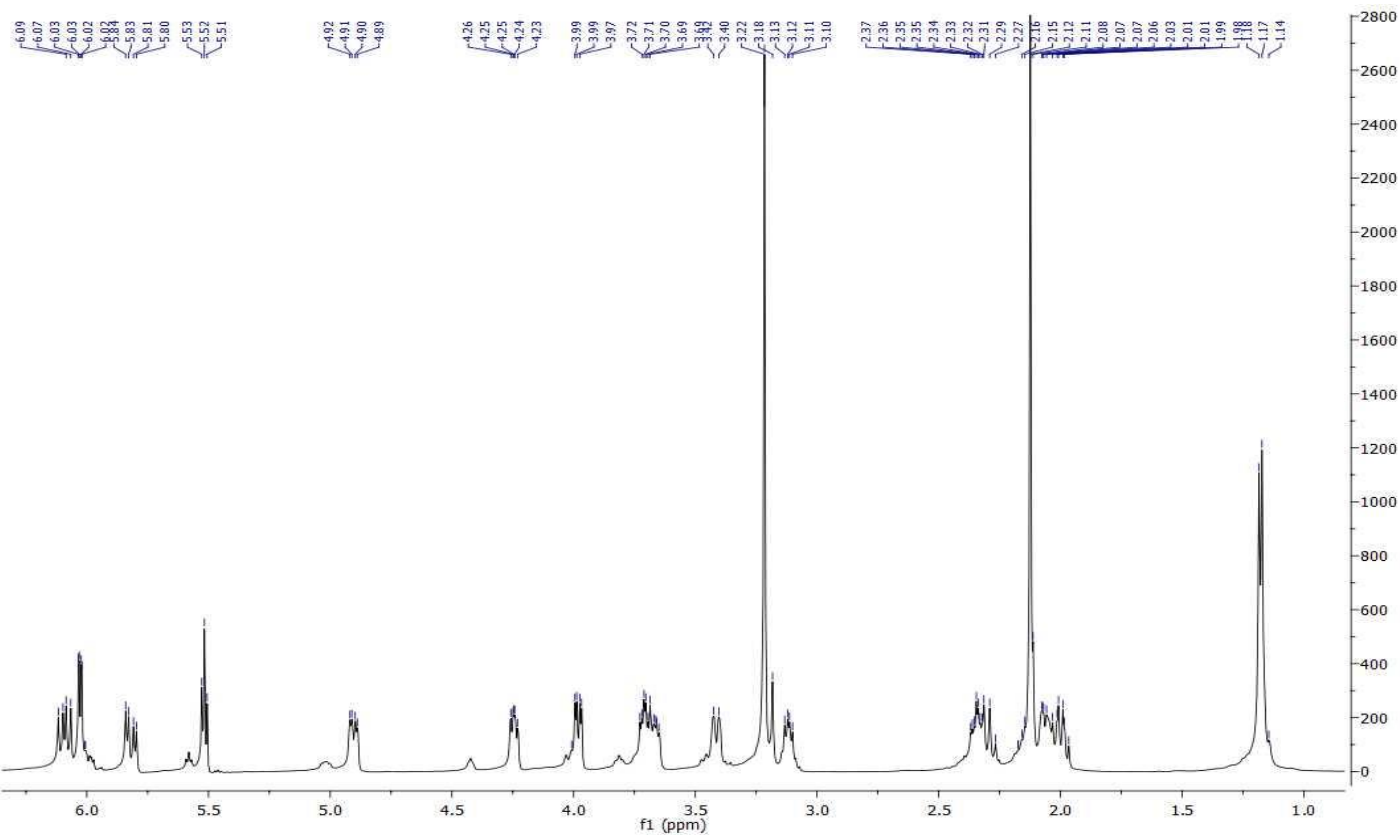


Figure S3. ^{13}C NMR spectrum of compound **1** at 20°C (CDCl_3 , 125.5 MHz).

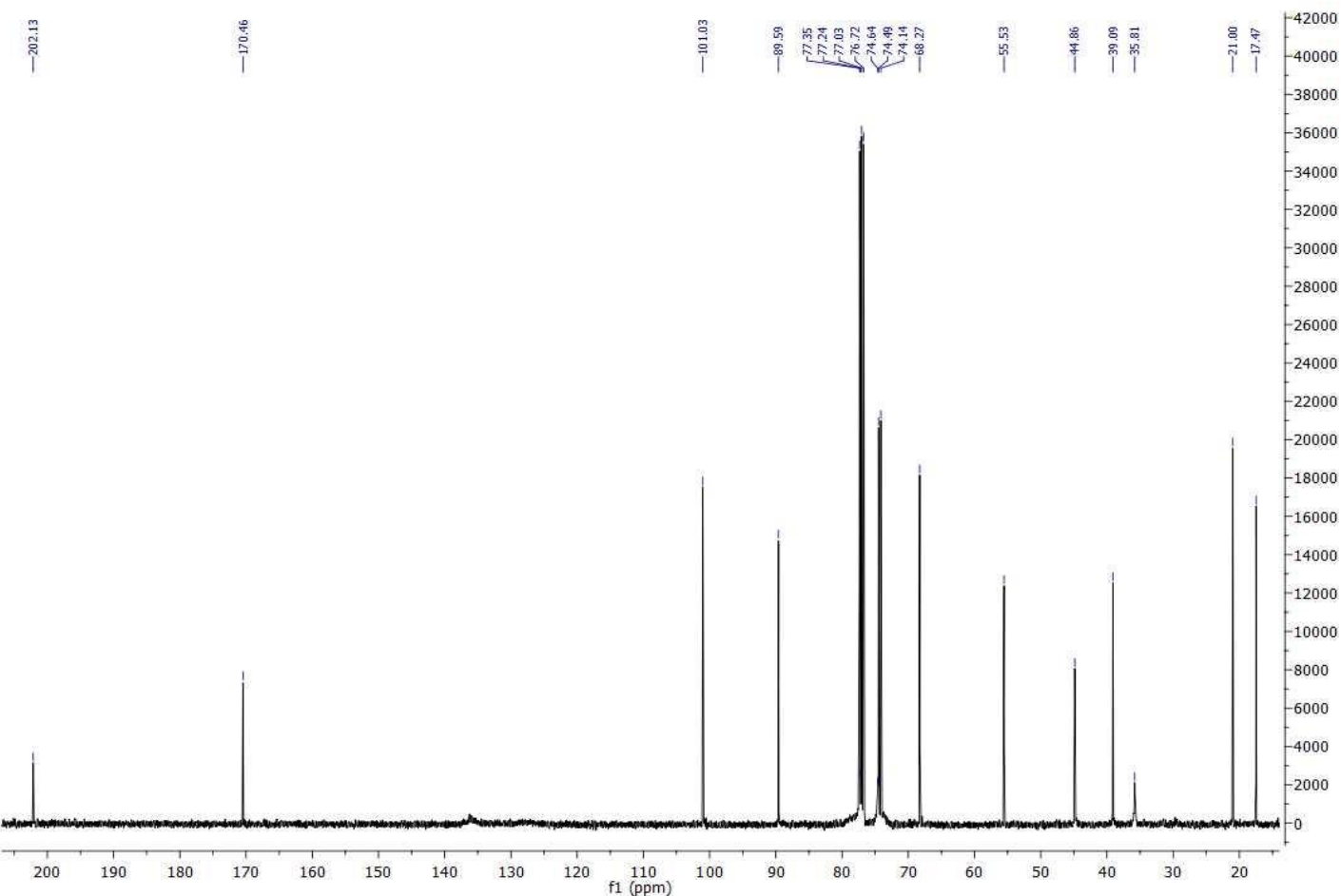


Figure S4. ^{13}C NMR spectrum of compound **1** at -40°C (CDCl_3 , 125.5 MHz).

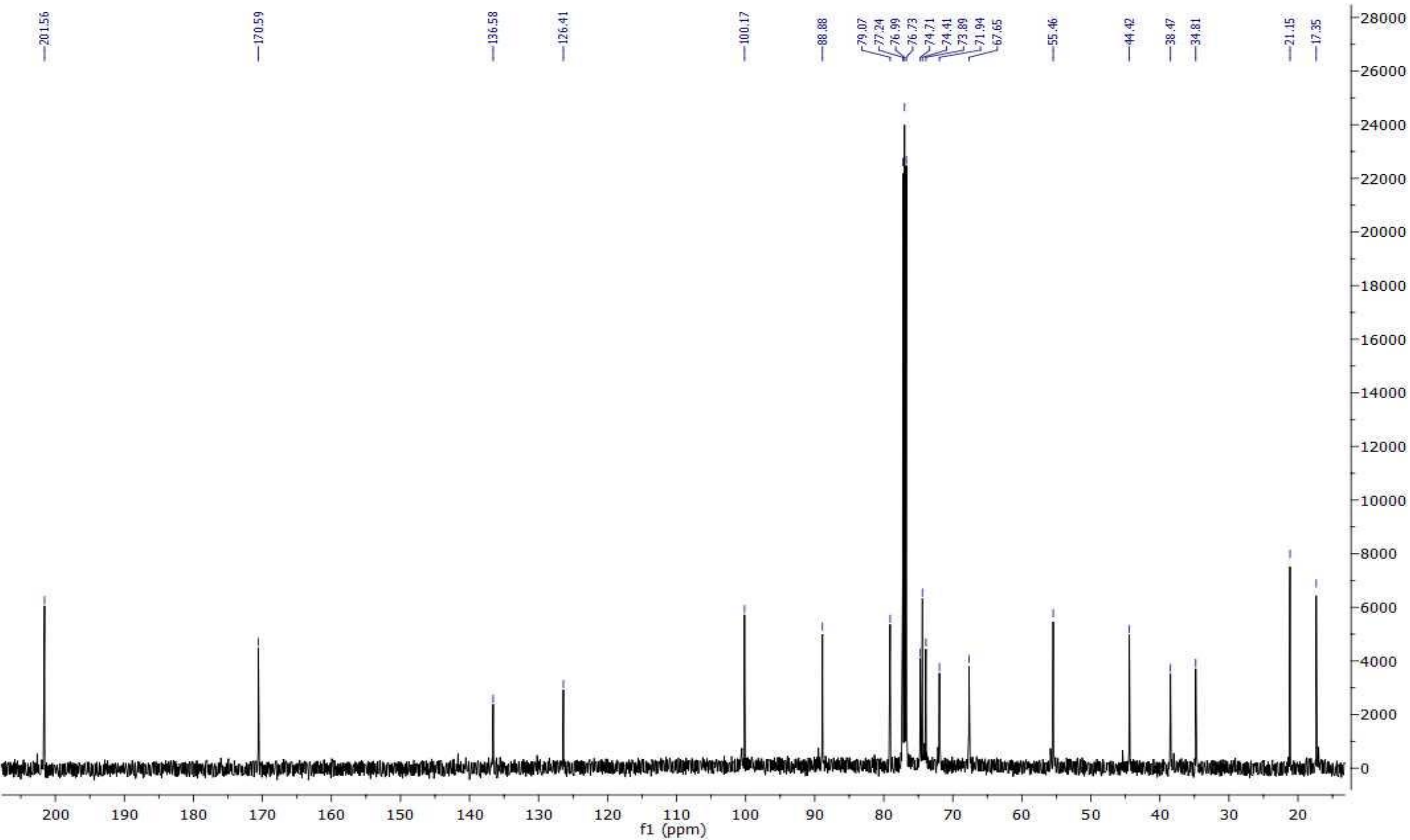


Figure S5. HMQC spectrum of compound **1** at - 40°C (CDCl₃, 400.0 MHz).

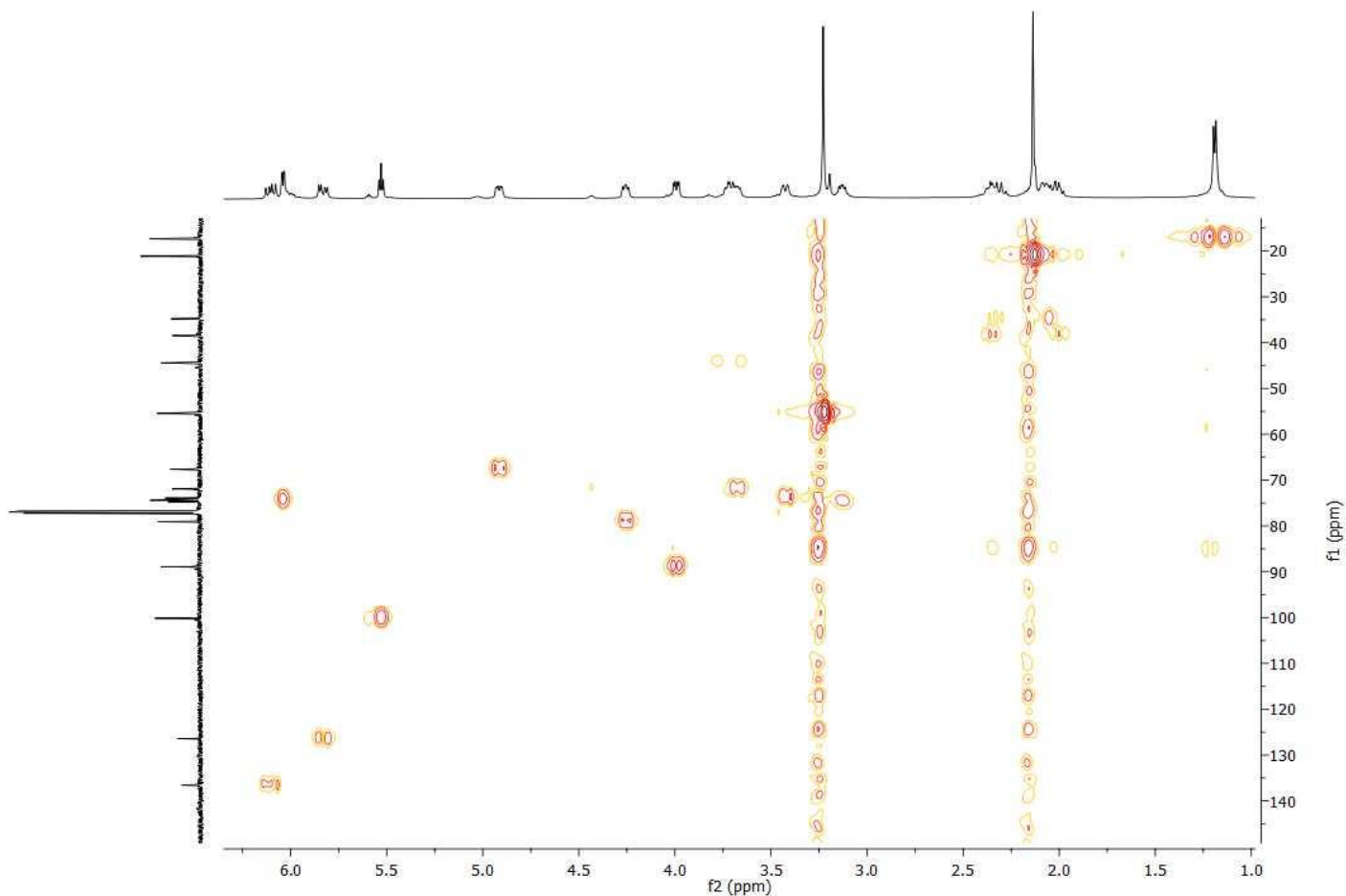


Figure S6. HMBC spectrum of compound **1** at - 40°C (CDCl₃, 400.0 MHz).

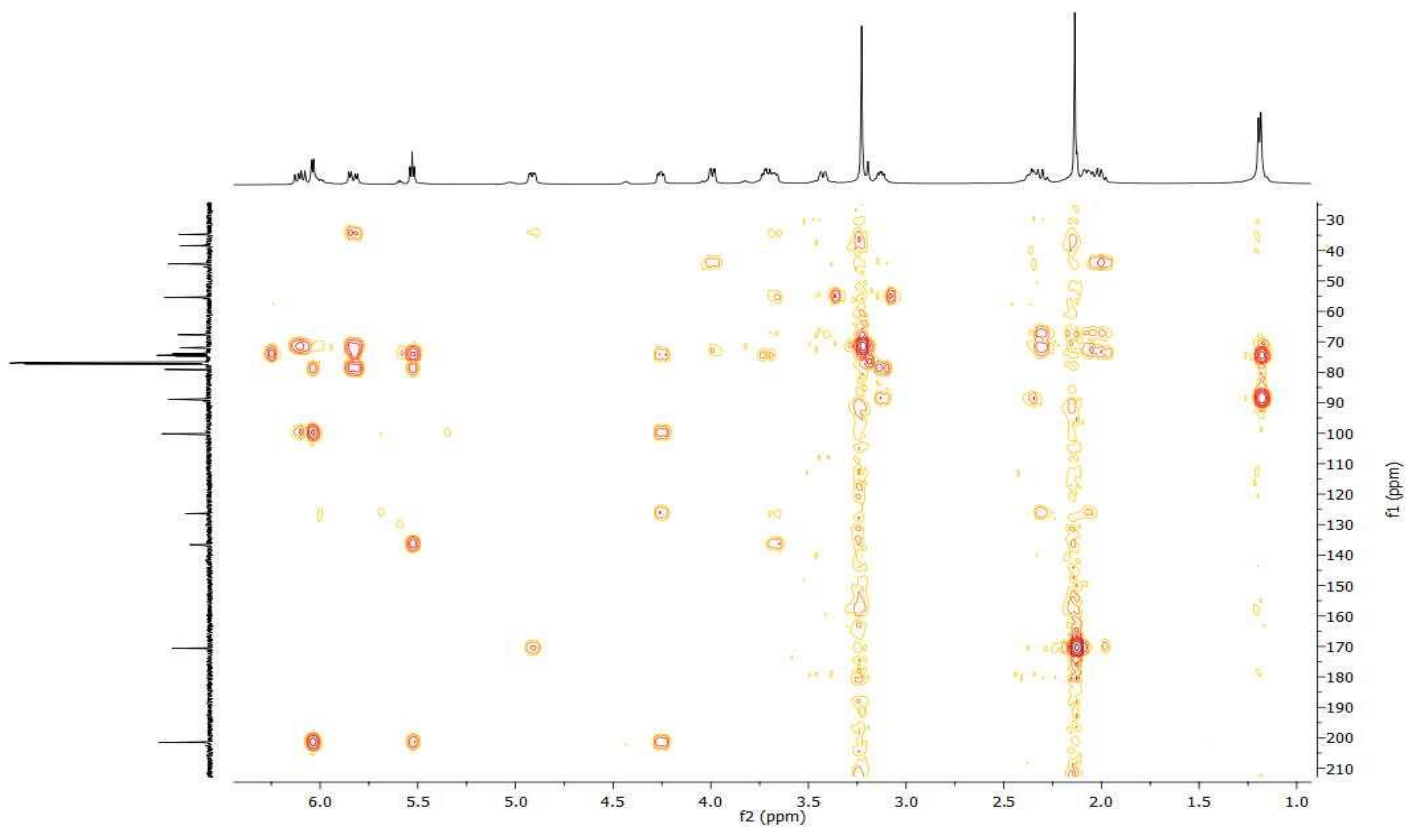


Figure S7. COSY spectrum of compound **1** at 20°C (CDCl₃, 400.0 MHz).

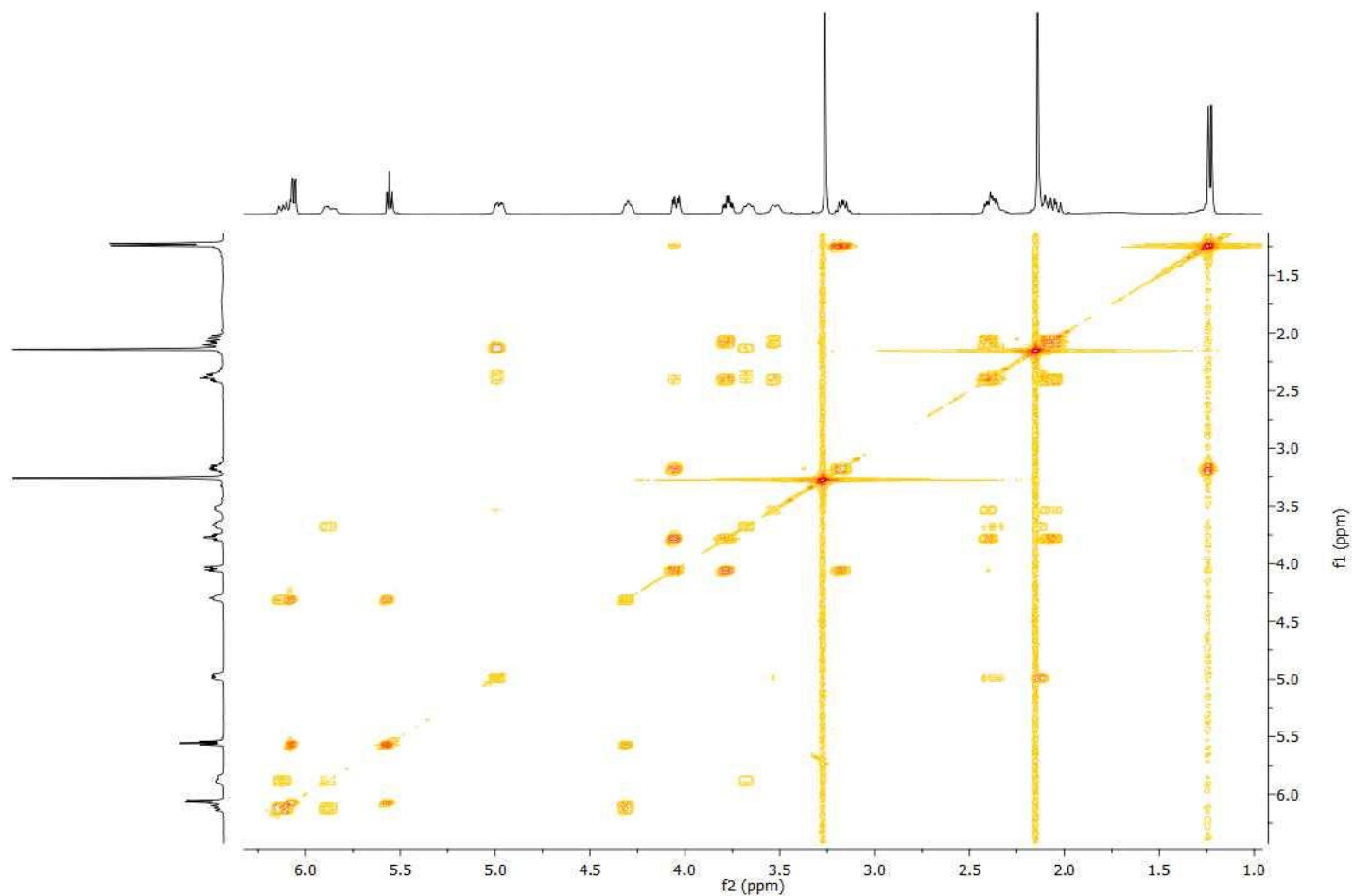


Figure S8. COSY spectrum of compound **1** at -40°C (CDCl₃, 400.0 MHz).

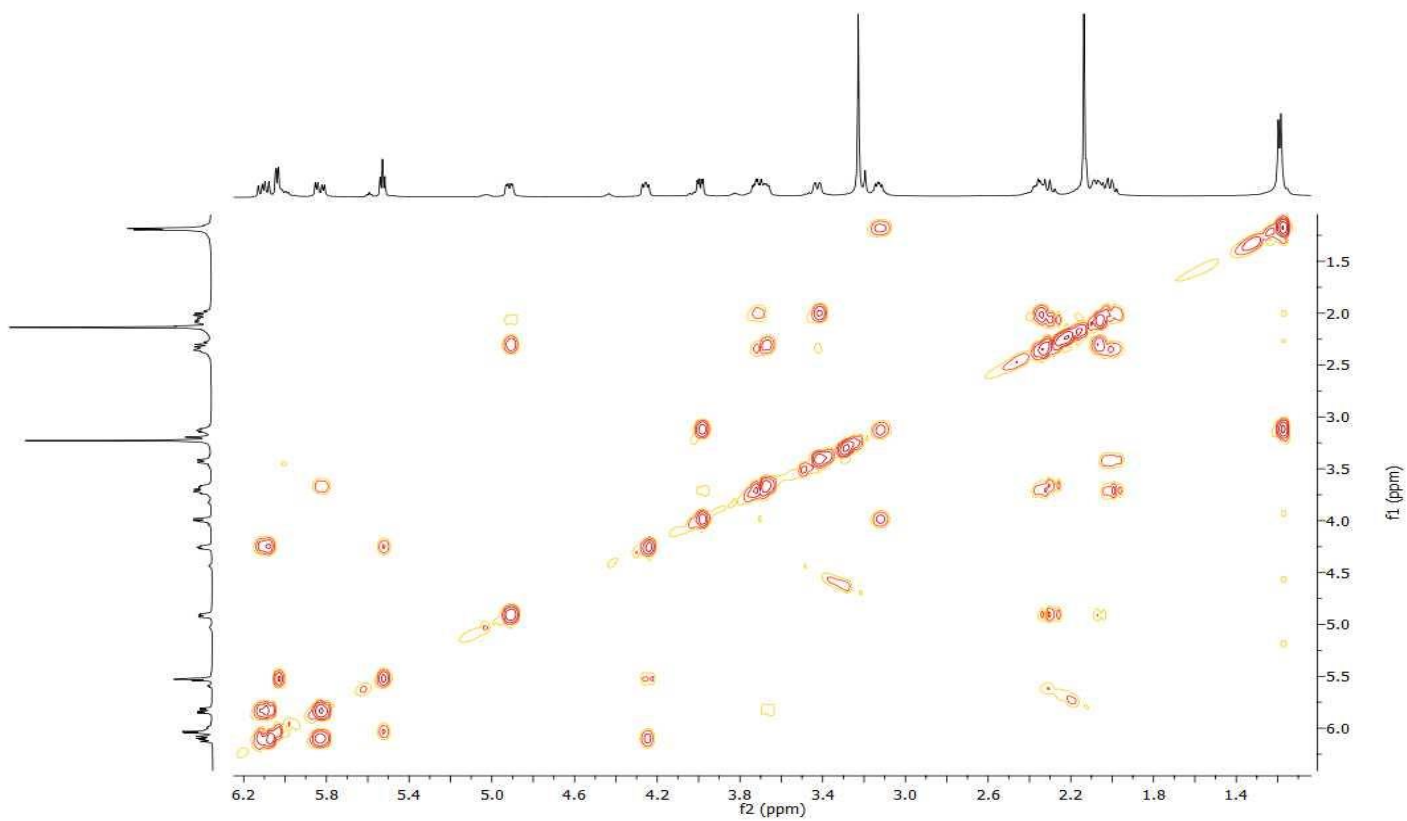


Figure S9. NOESY spectrum of compound **1** at 20°C (CDCl₃, 125.5 MHz).

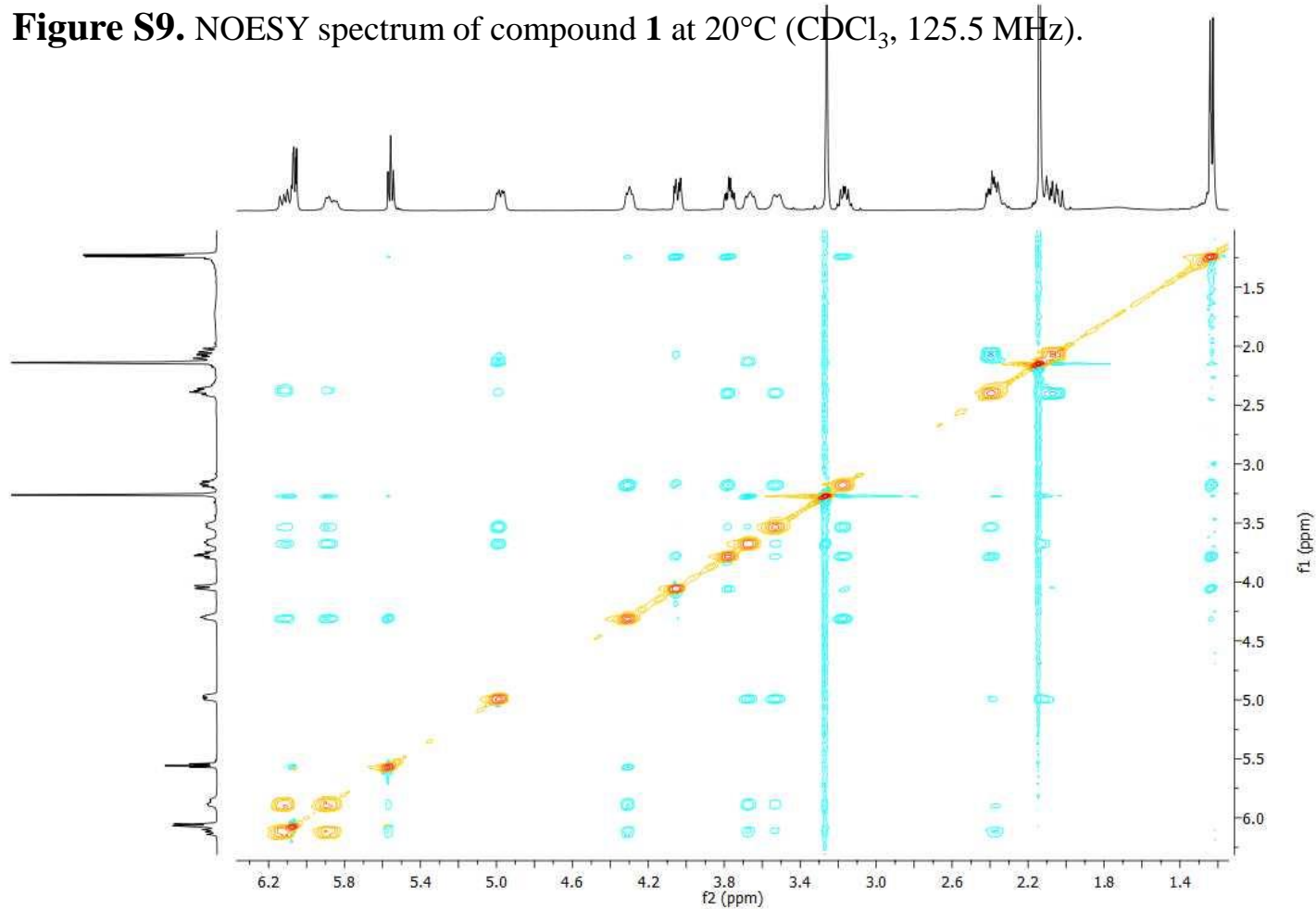


Figure S10. HRMS spectrum of compound **1** in negative ionization.

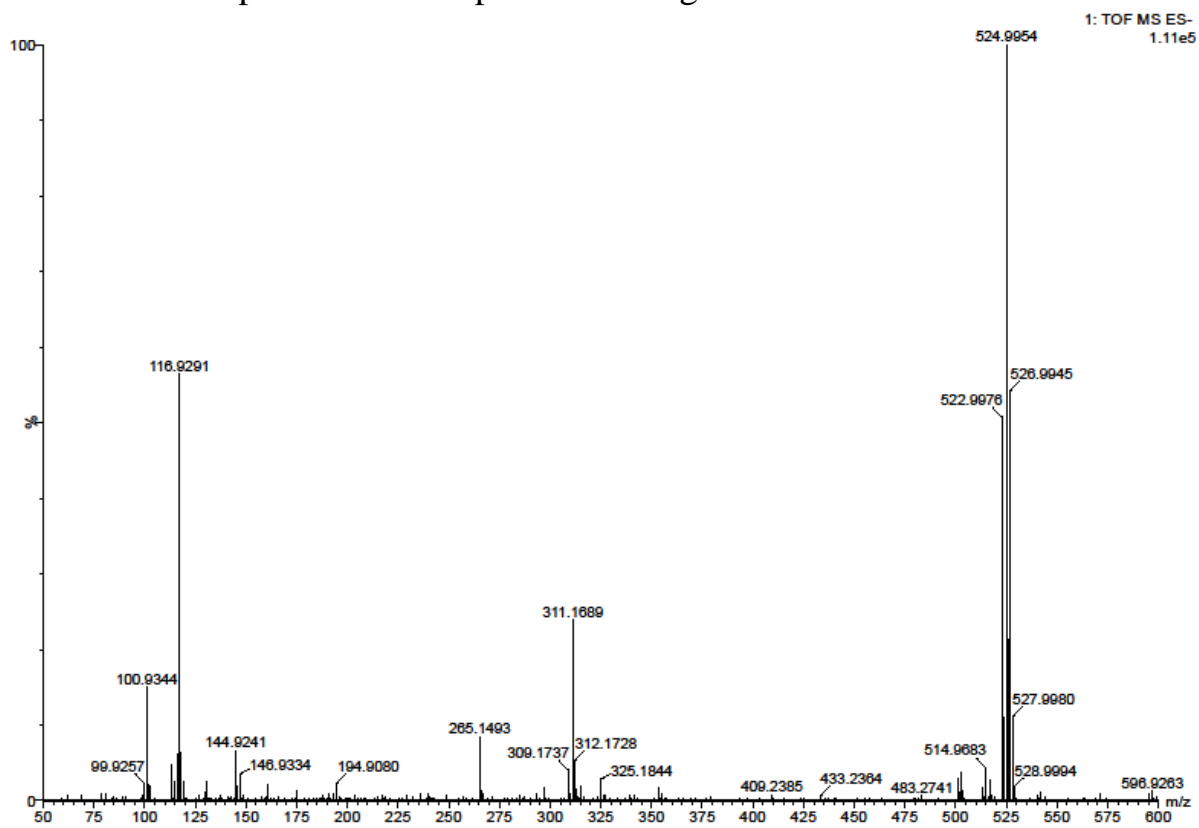


Figure S11. HRMS spectrum of compound **1** (Zoom) in negative ionization.

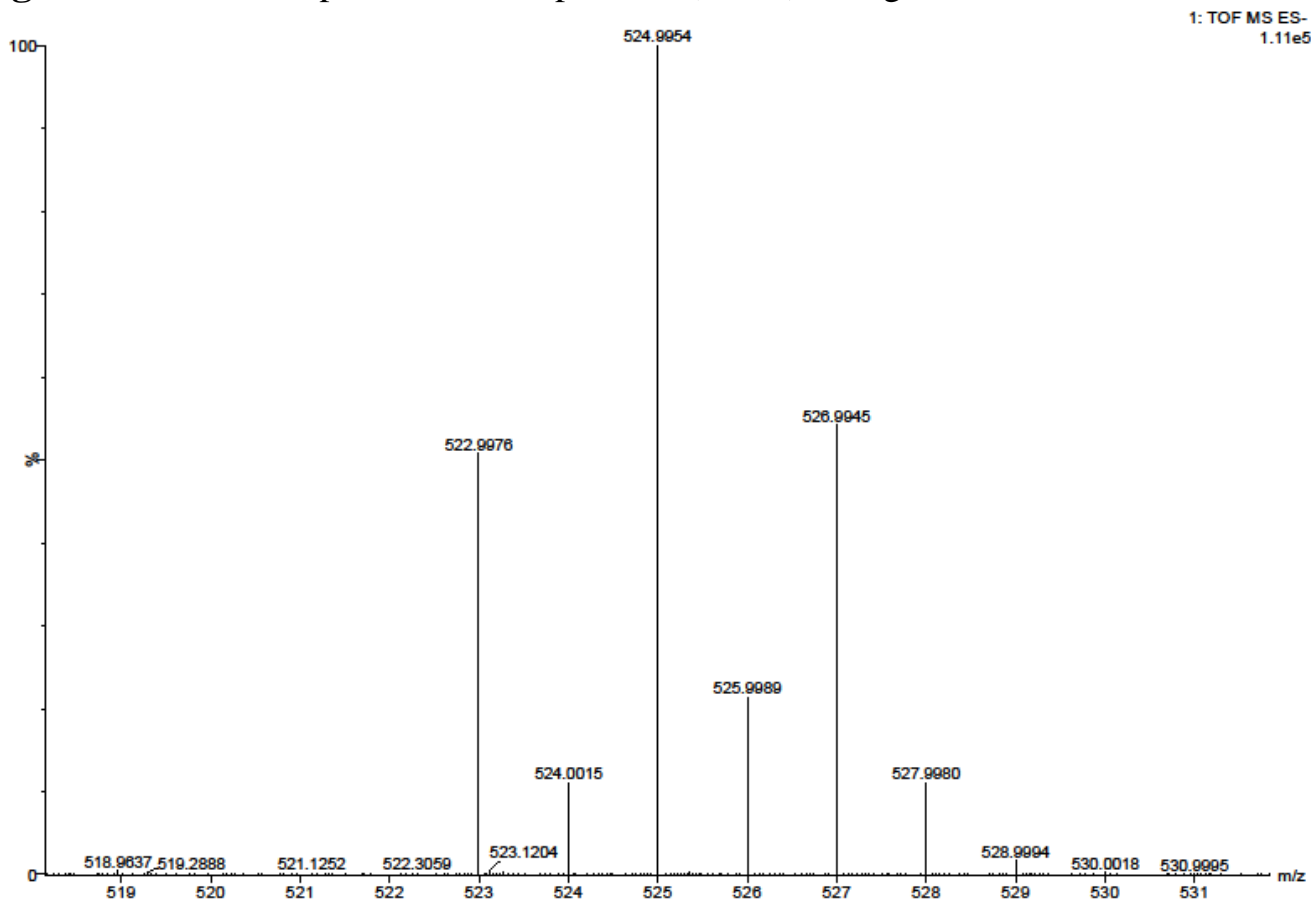


Figure S12. UV spectrum of compound **1**.

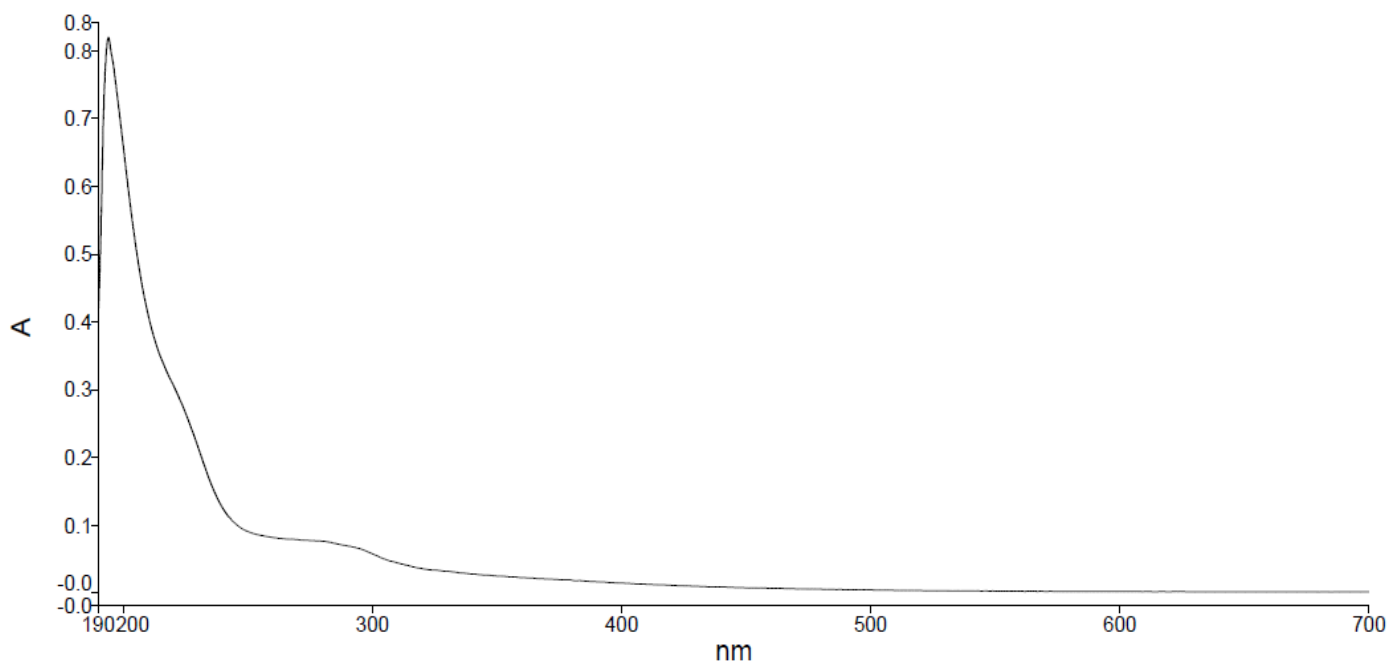


Figure S13. Experimental ECD spectra of **1**.

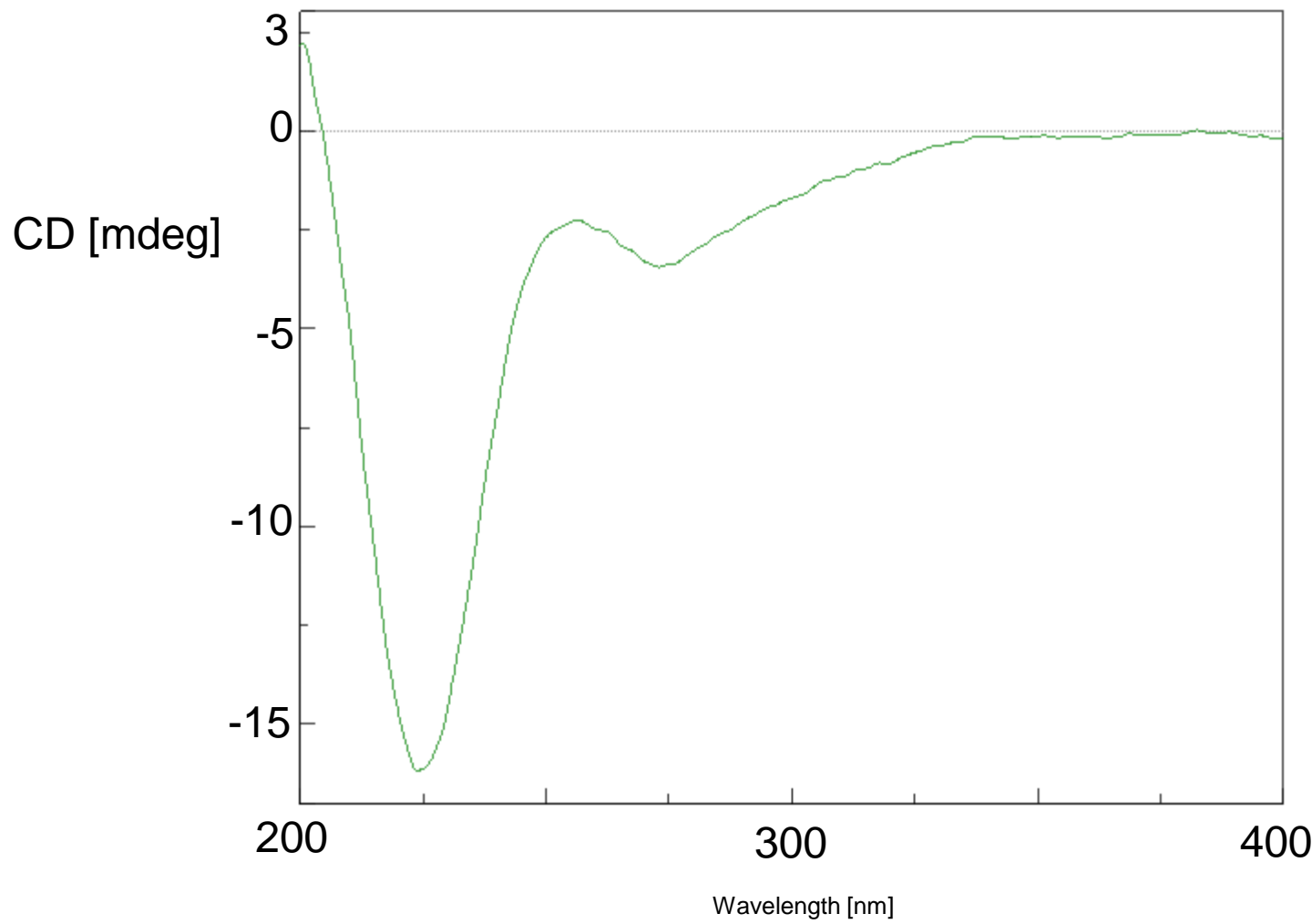


Figure S14. ^1H NMR spectrum of compound **2** at 20°C (CDCl_3 , 400 MHz).

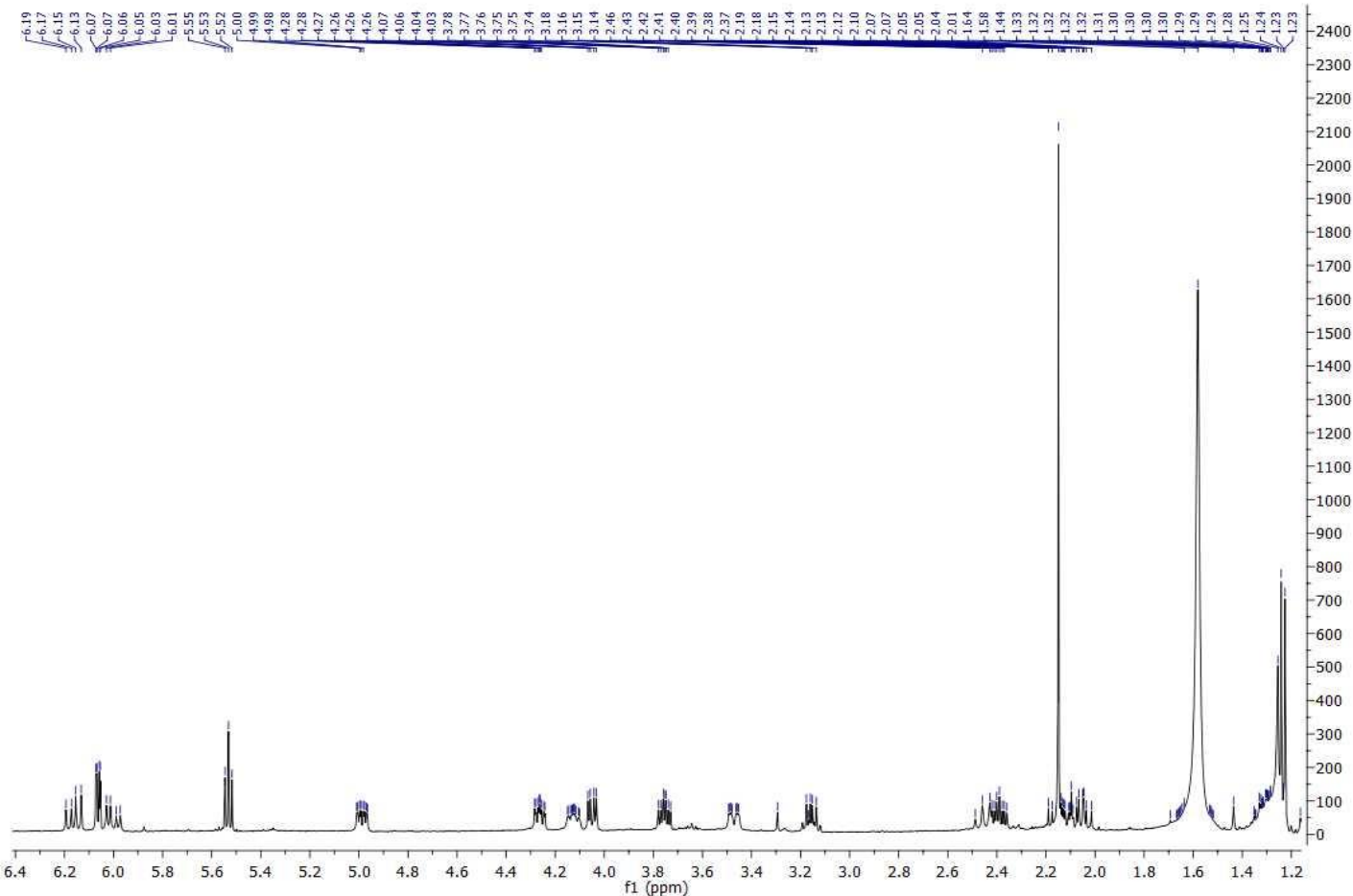


Figure S15. ^1H NMR spectrum of compound **2** at -40°C (CDCl_3 , 400 MHz).

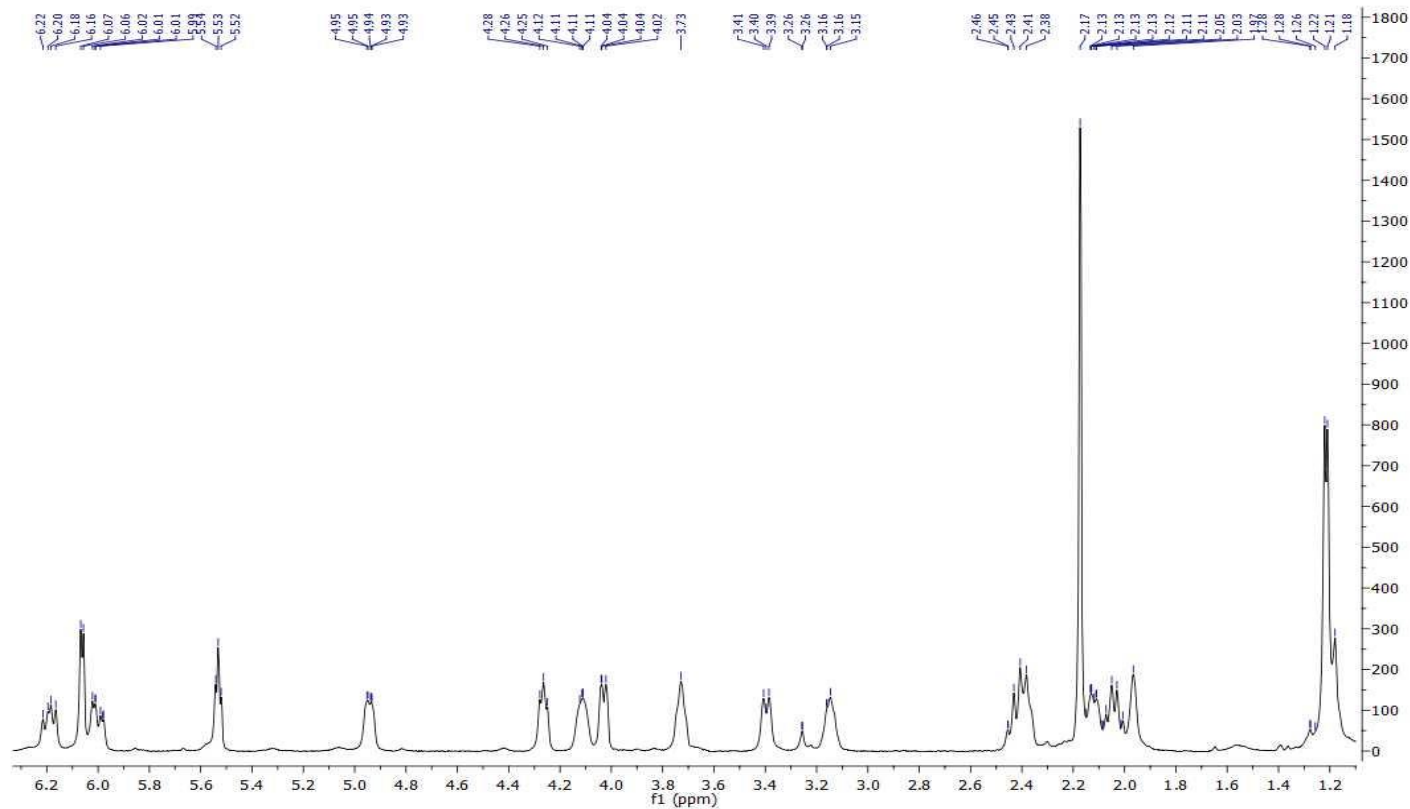


Figure S16. ^{13}C NMR spectrum of compound **2** at 20°C (CDCl_3 , 125.5 MHz).

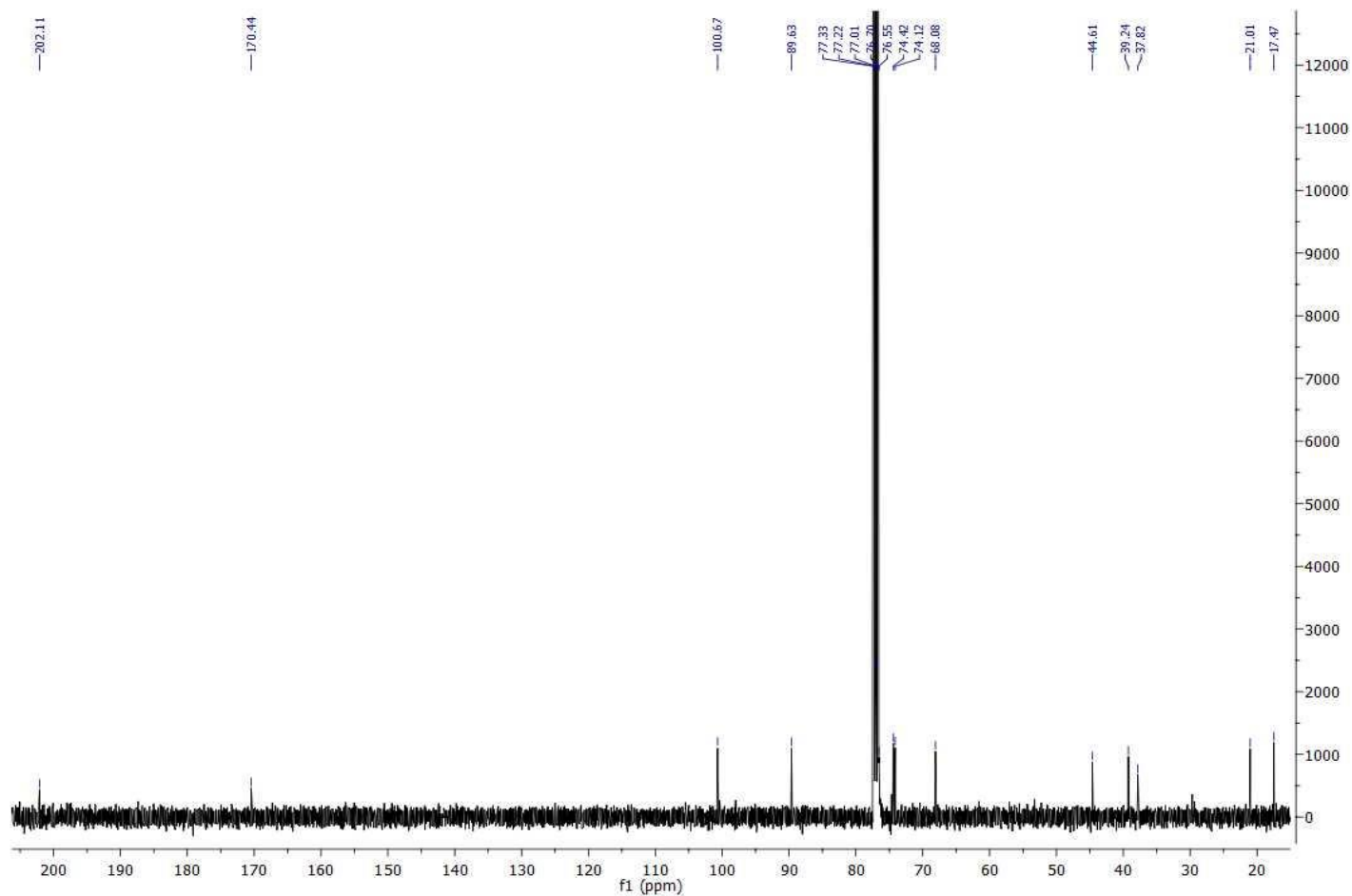


Figure S17. ^{13}C NMR spectrum of compound **2** at -40°C (CDCl_3 , 125.5 MHz).

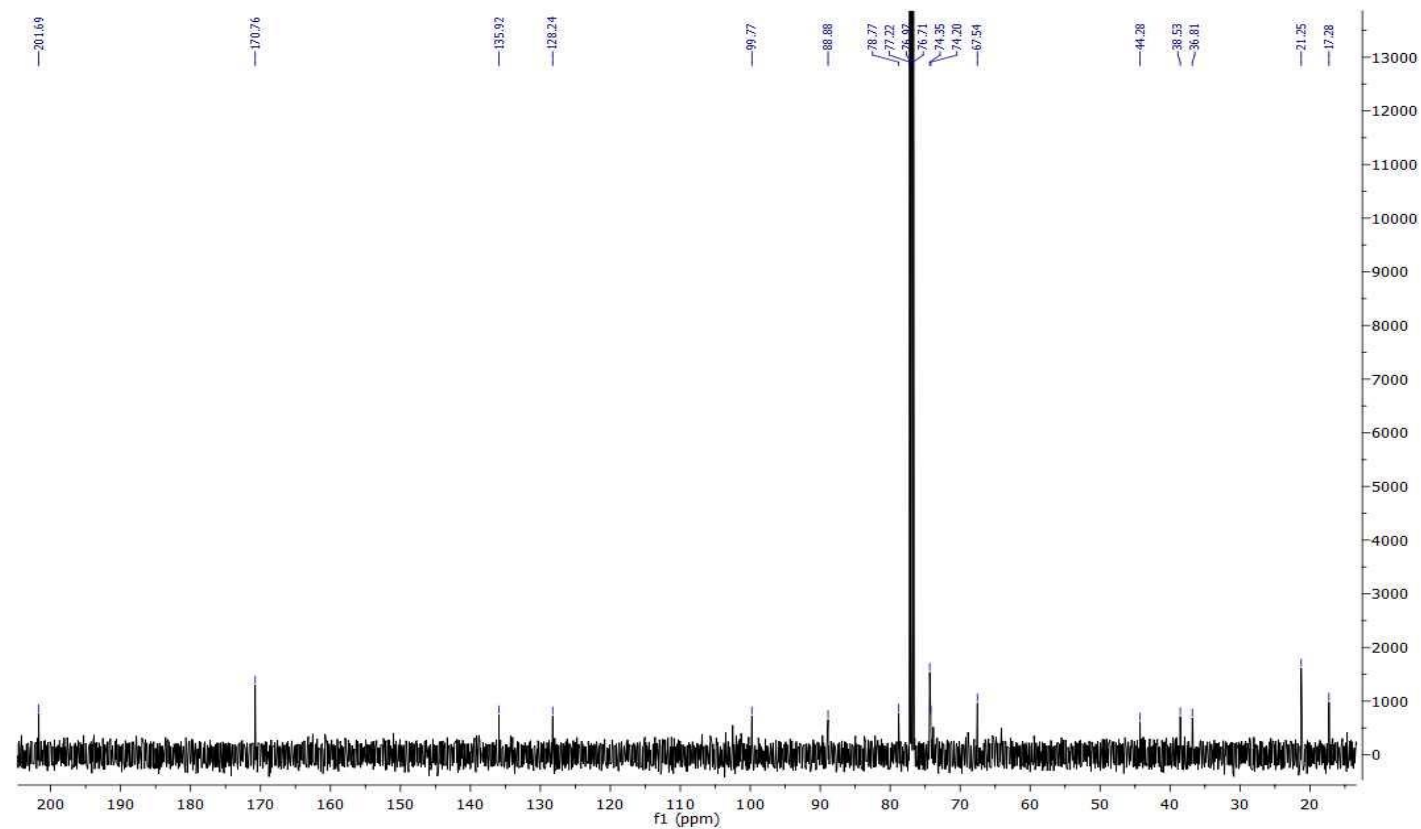


Figure S18. HMQC spectrum of compound **2** at - 40°C (CDCl₃, 400.0 MHz).

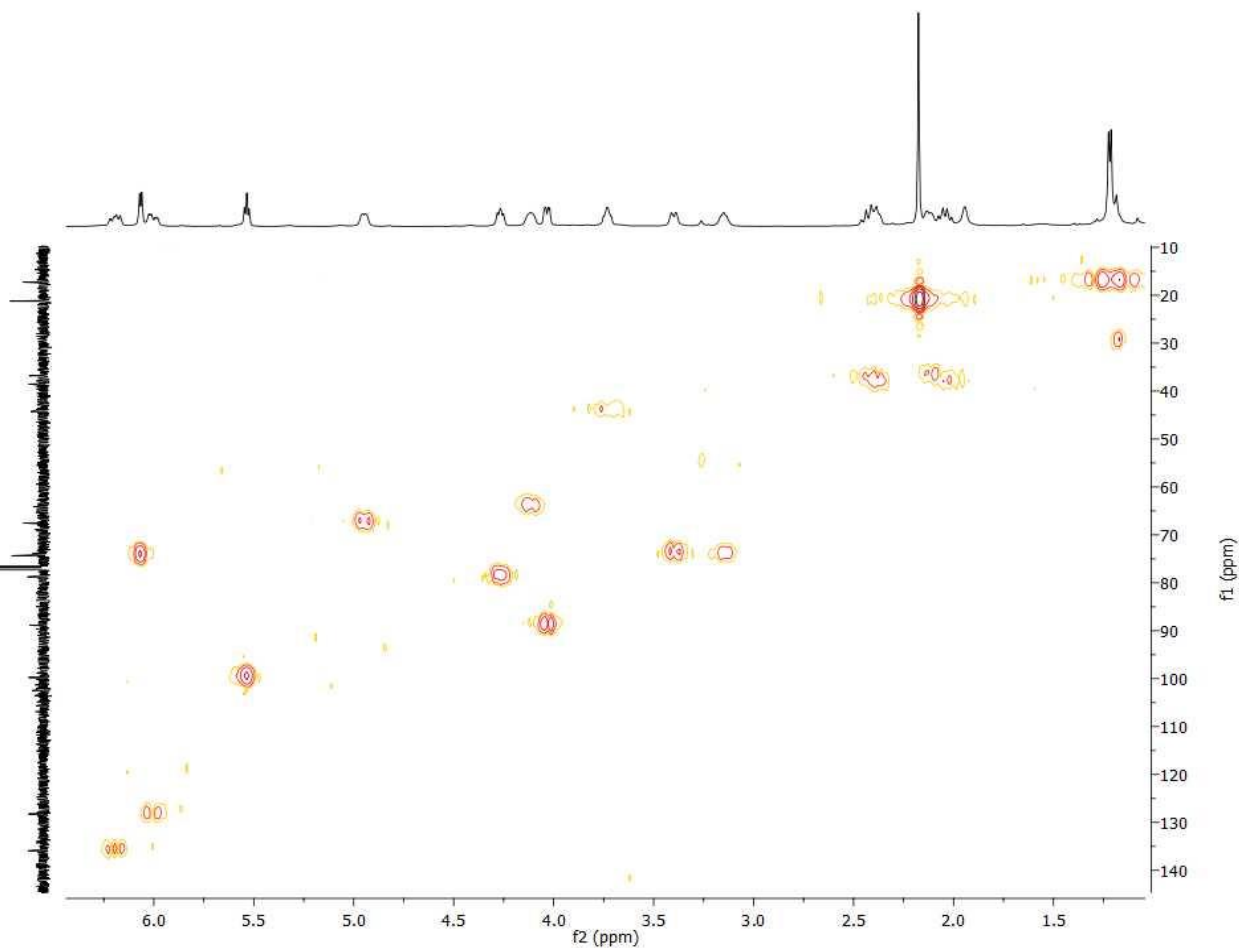


Figure S19. HMBC spectrum of compound **2** at - 40°C (CDCl₃, 400.0 MHz).

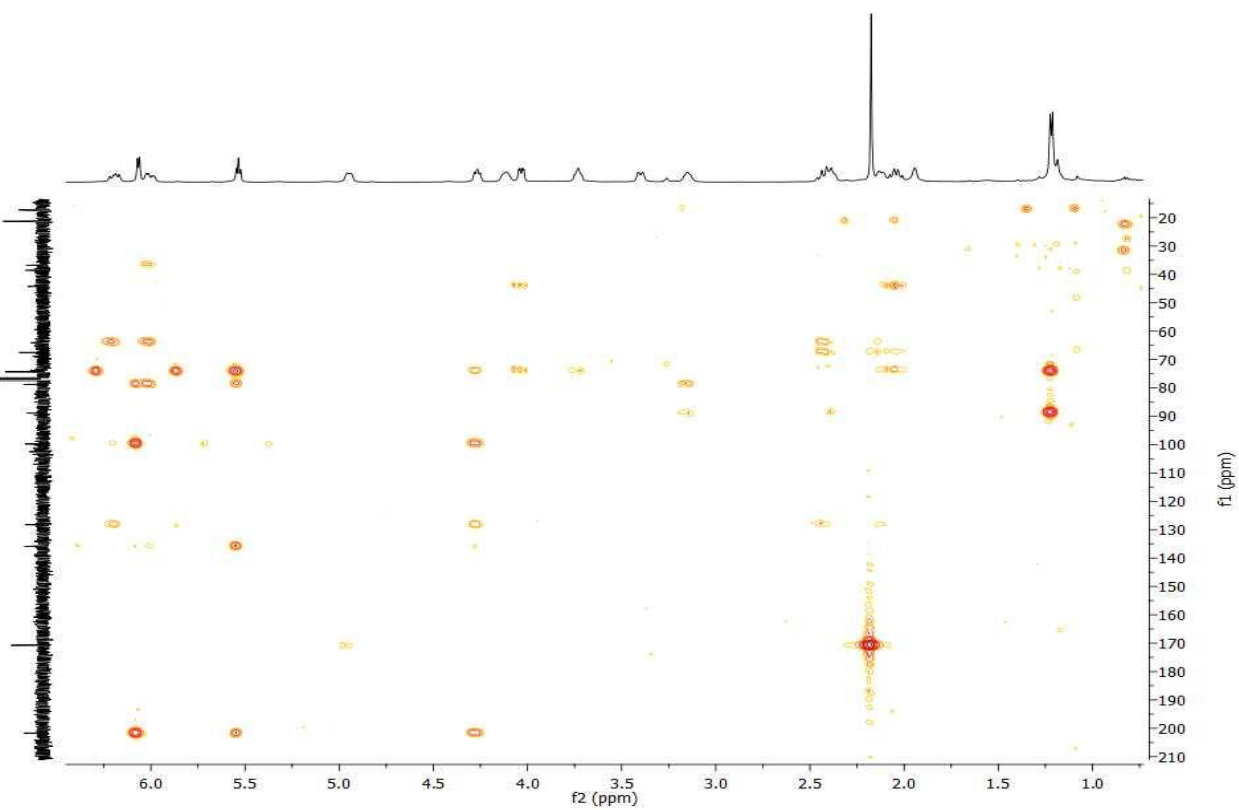


Figure S22. NOESY spectrum of compound **2** at 20°C (CDCl₃, 125.5 MHz).

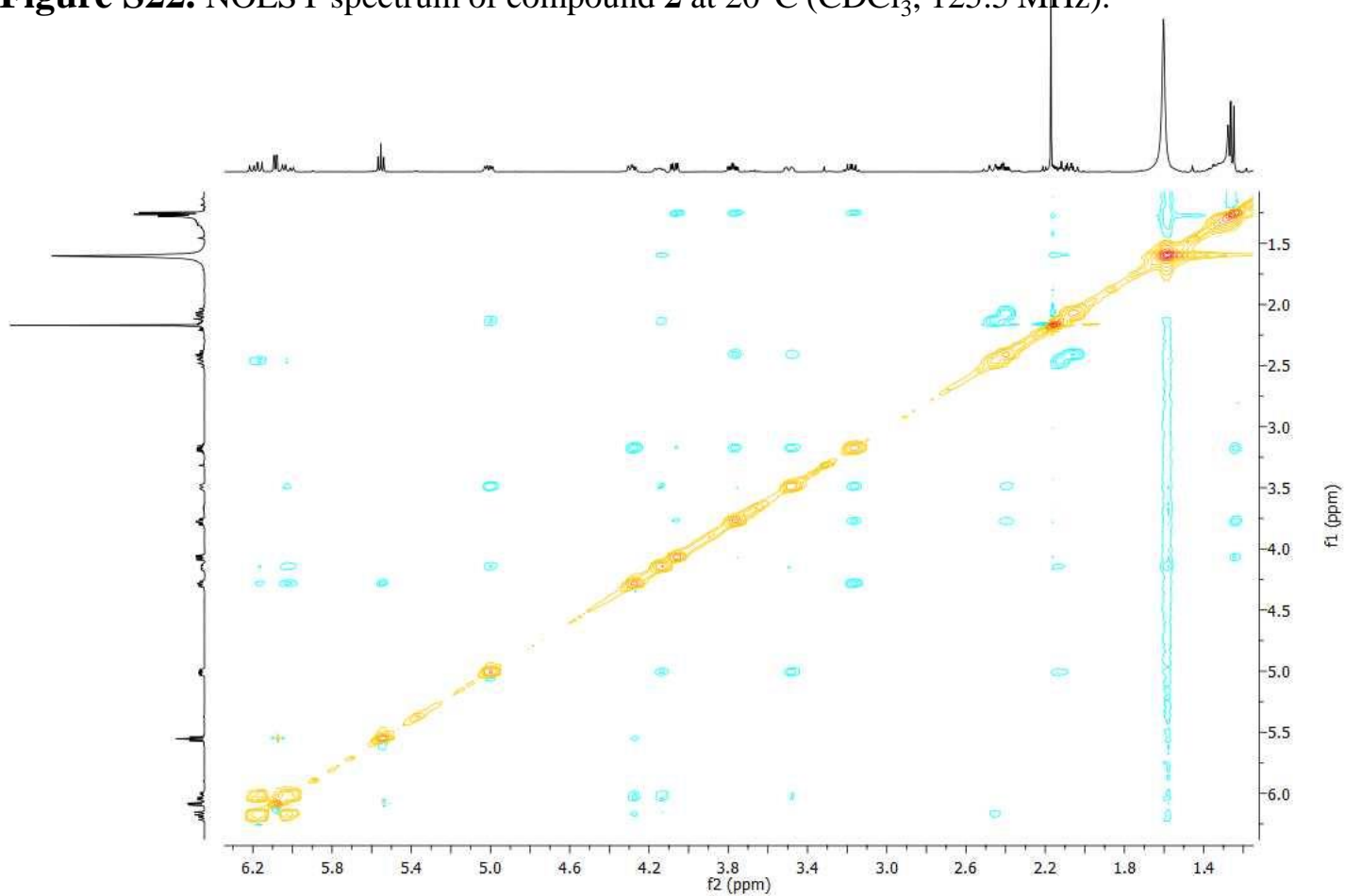


Figure S23. HRMS spectrum of compound **2**.

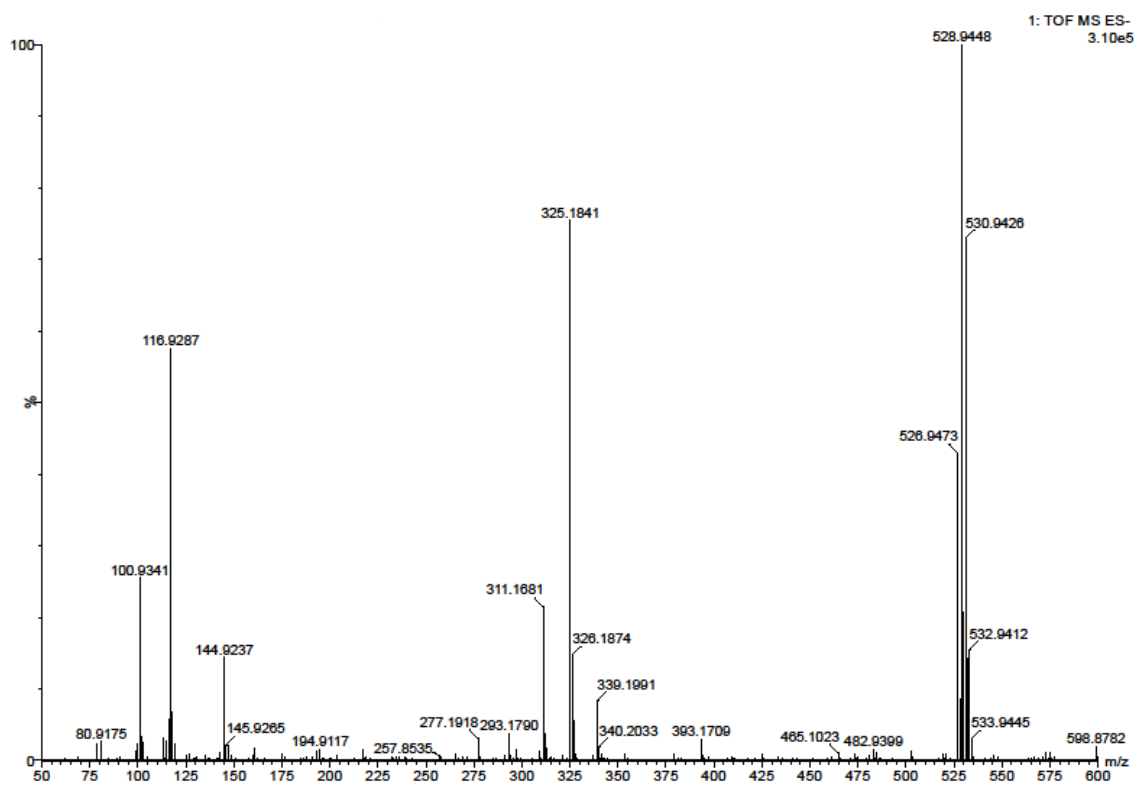


Figure S24. HRMS spectrum of compound **2** (Zoom).

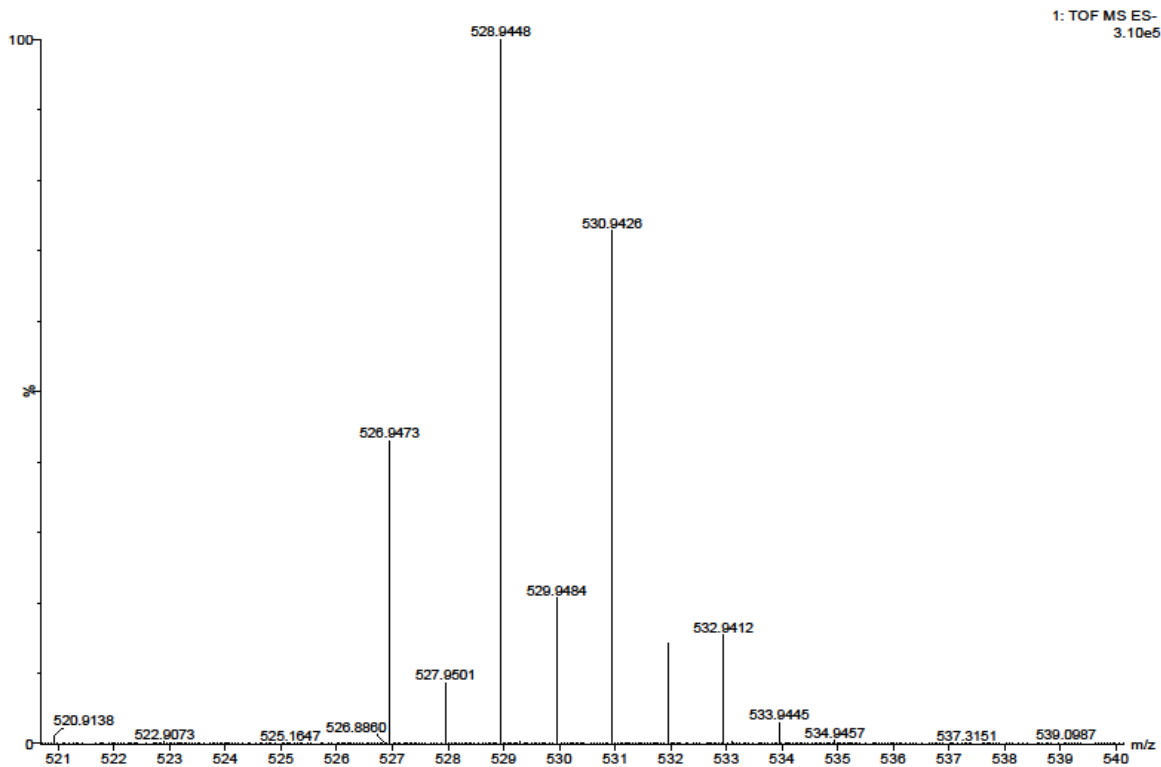


Figure S25. UV spectrum of compound **2**.

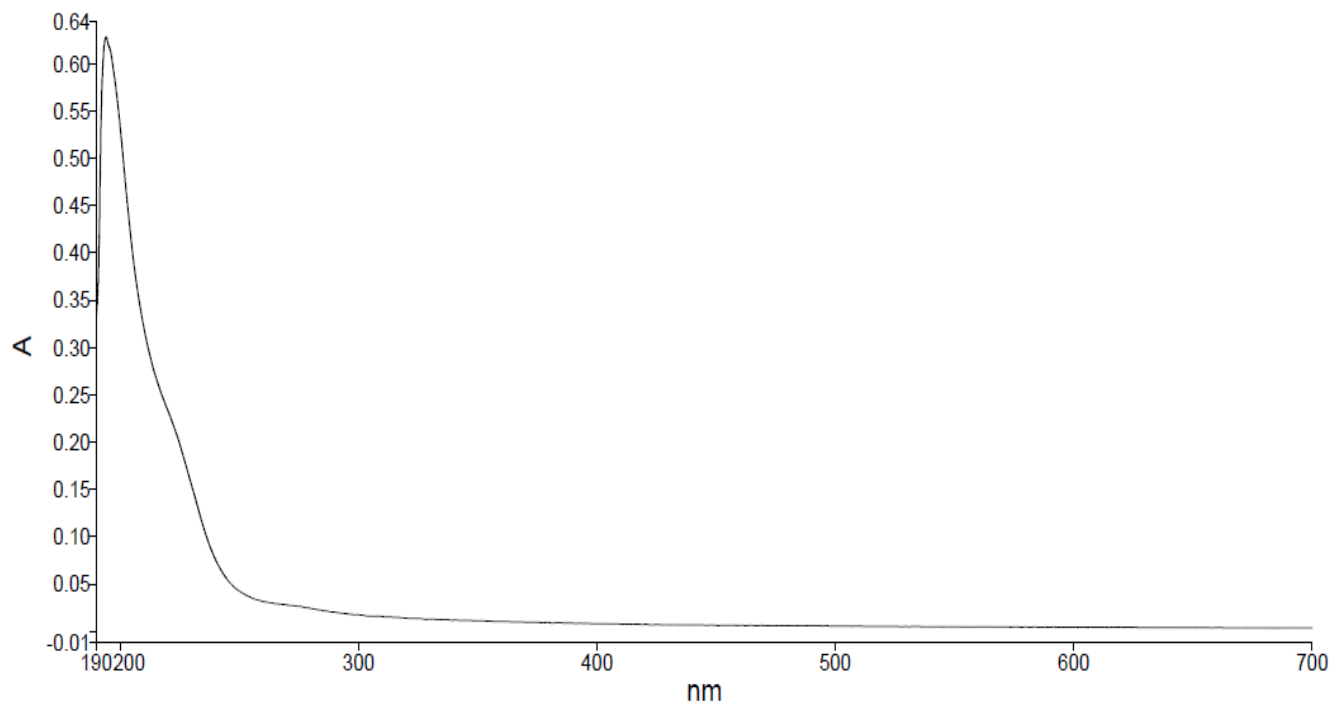


Figure S26. ^1H NMR spectrum of compound **3** at 20°C (CDCl_3 , 400 MHz).

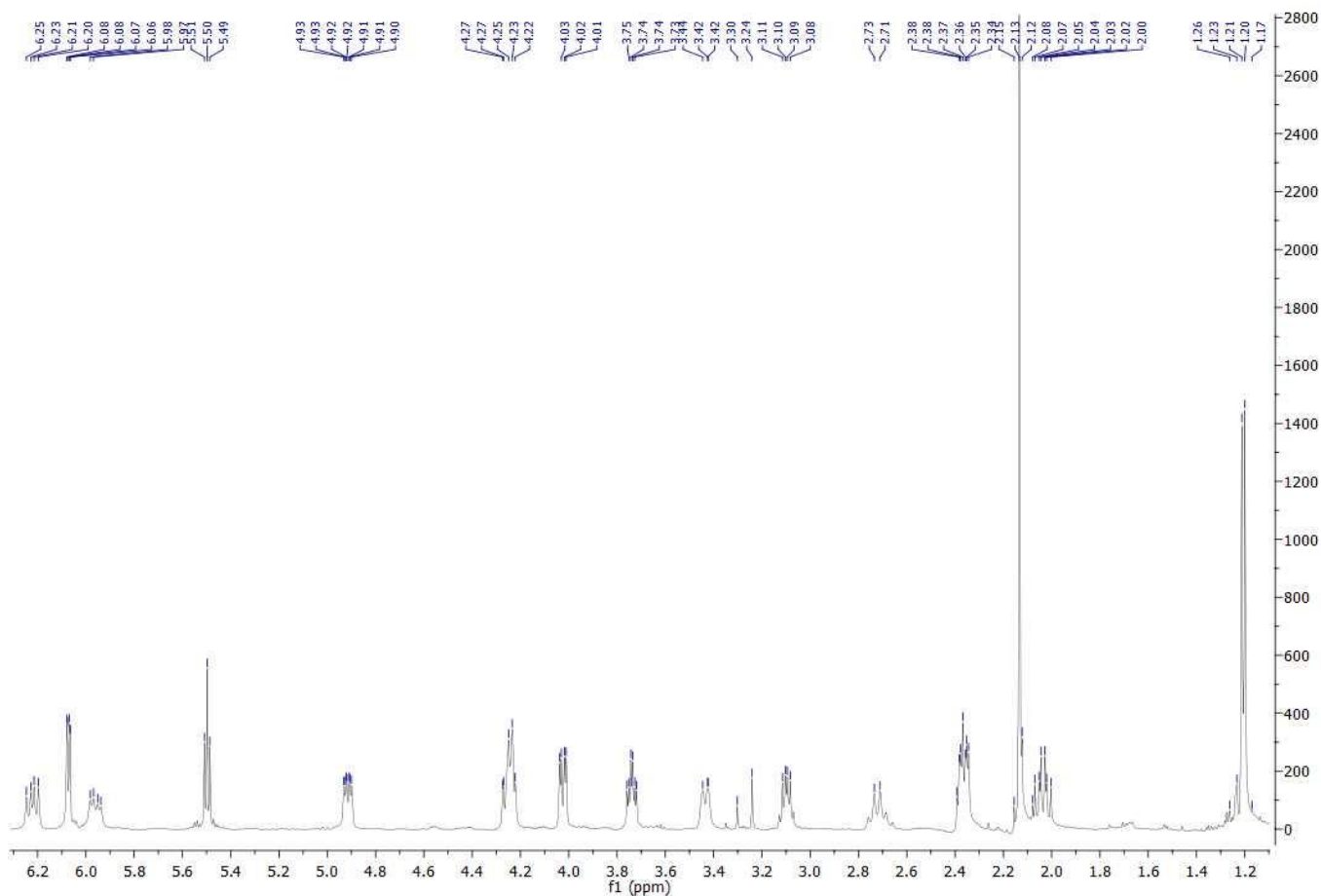


Figure S27. ^1H NMR spectrum of compound **3** at -40°C (CDCl_3 , 400 MHz).

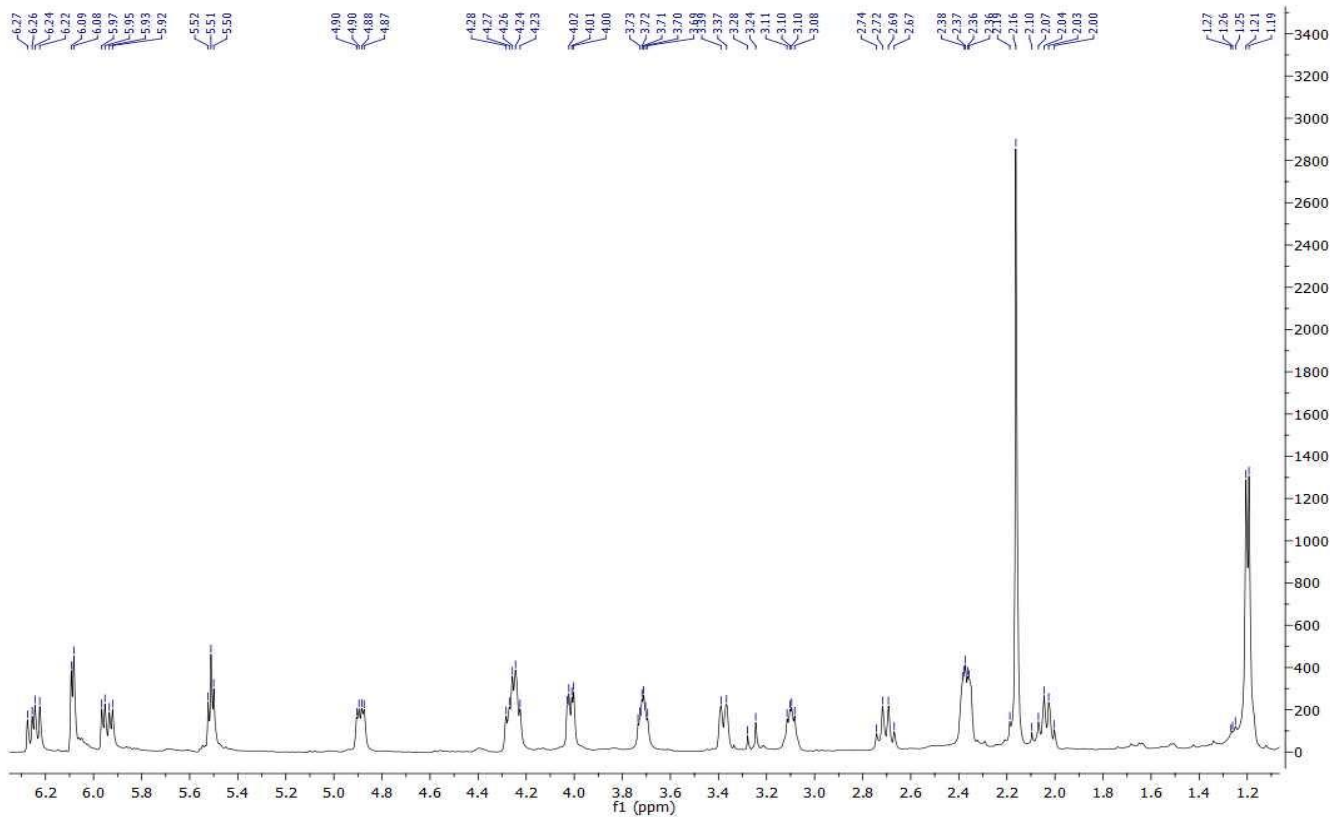


Figure S28. ^{13}C NMR spectrum of compound **3** at 20°C (CDCl_3 , 125.5 MHz).

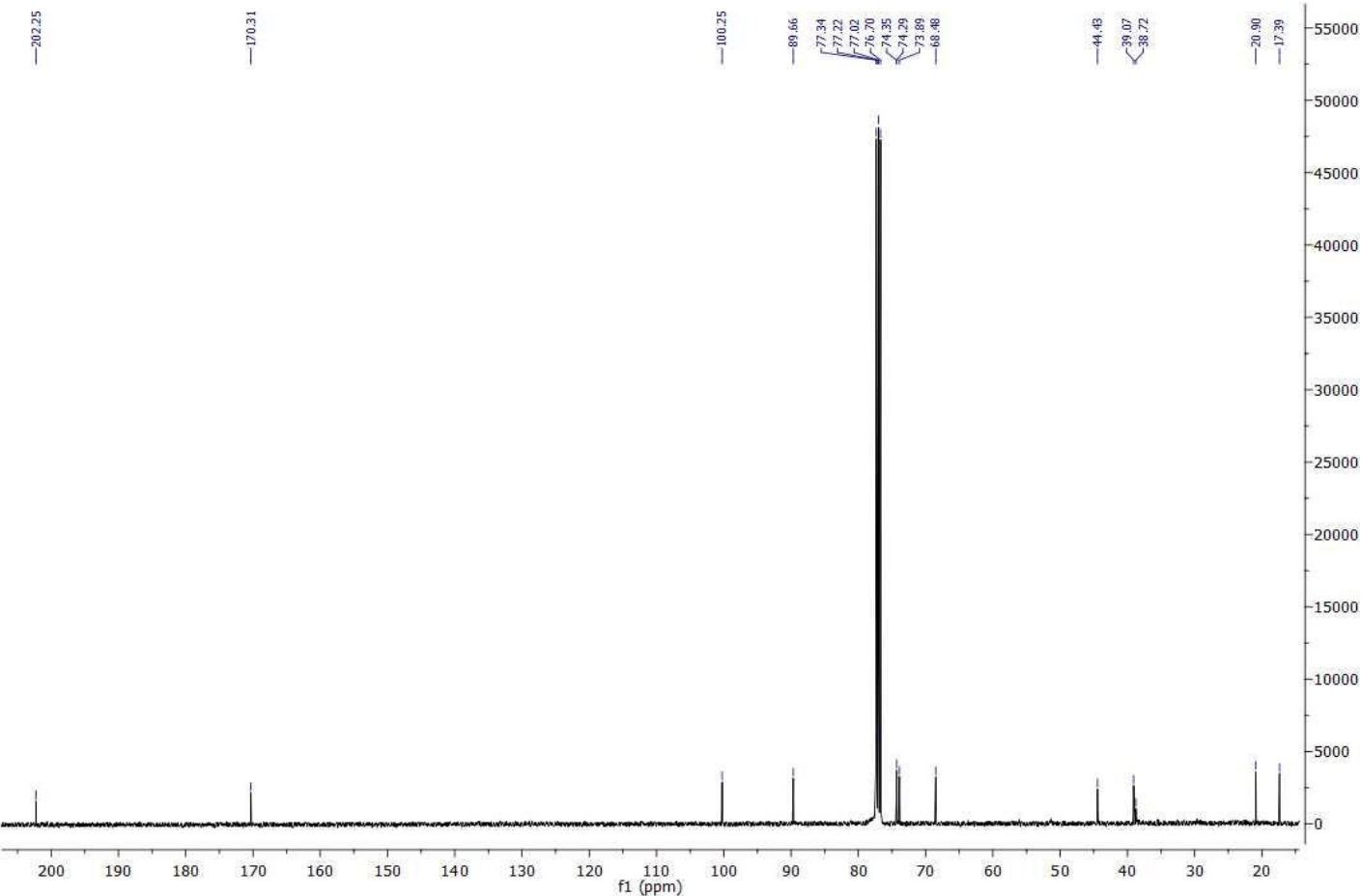


Figure S29. ^{13}C NMR spectrum of compound **3** at -40°C (CDCl_3 , 125.5 MHz).

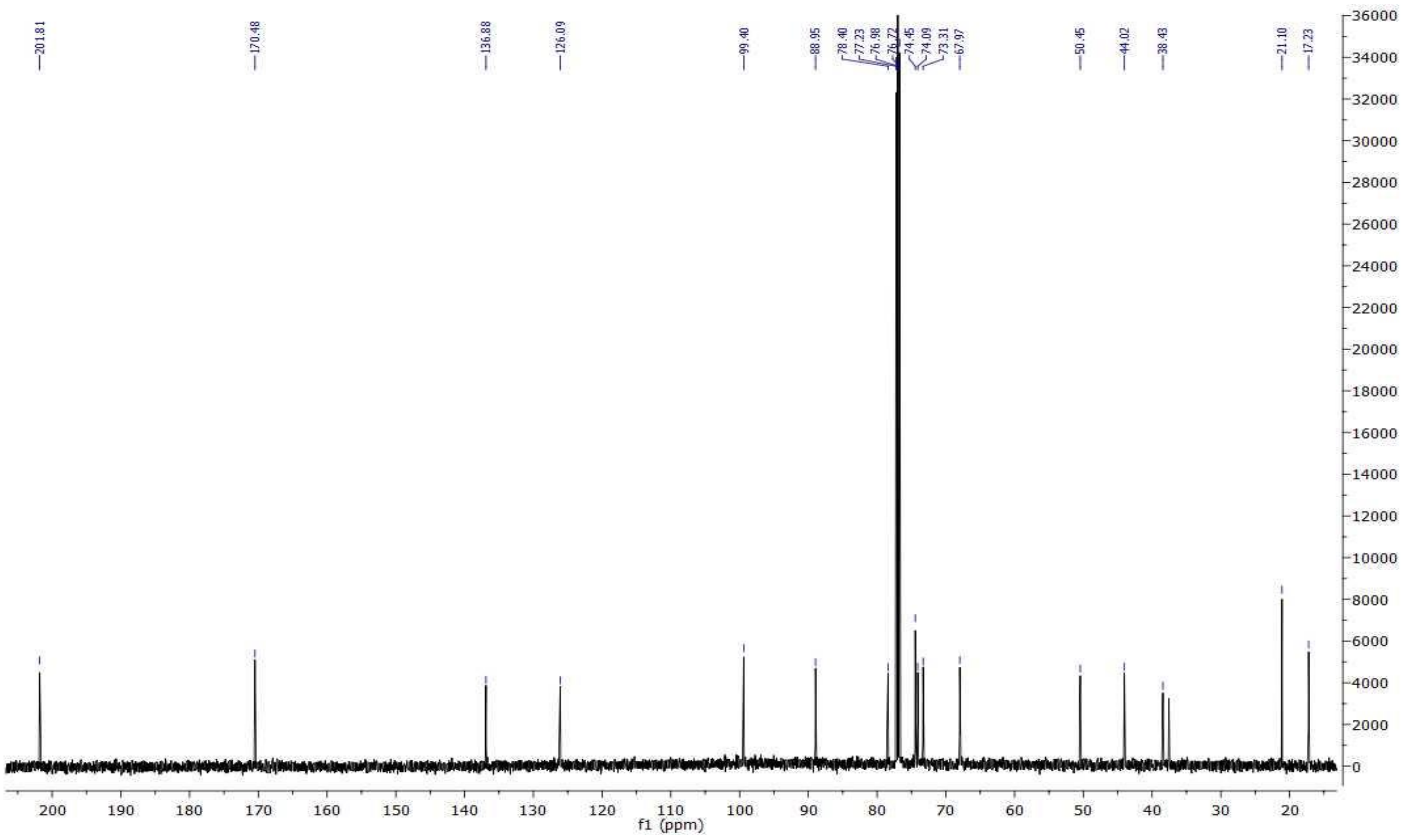


Figure S30. HMQC spectrum of compound **3** at - 40°C (CDCl₃, 400.0 MHz).

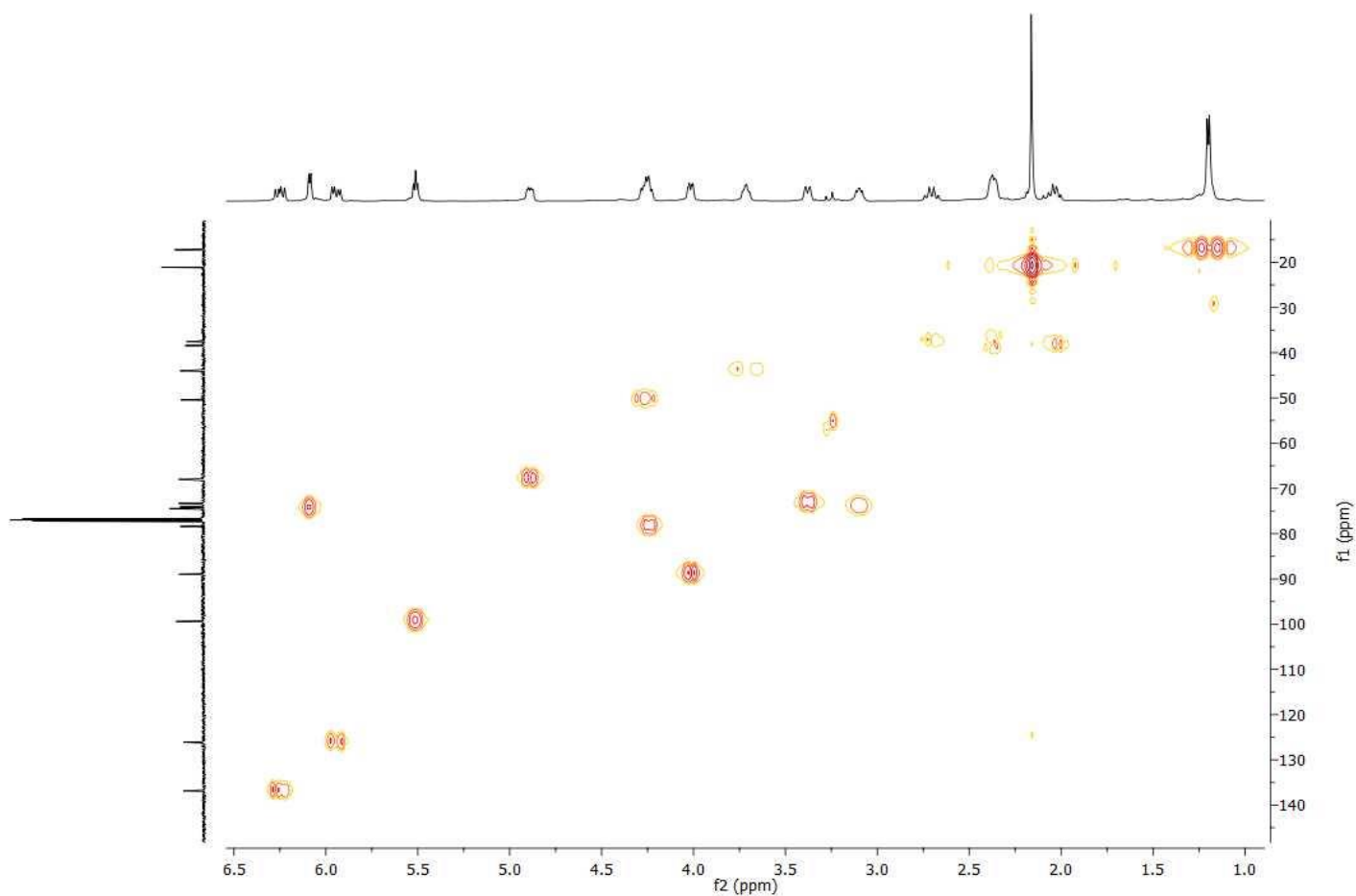


Figure S31. HMBC spectrum of compound **3** at - 40°C (CDCl₃, 400.0 MHz).

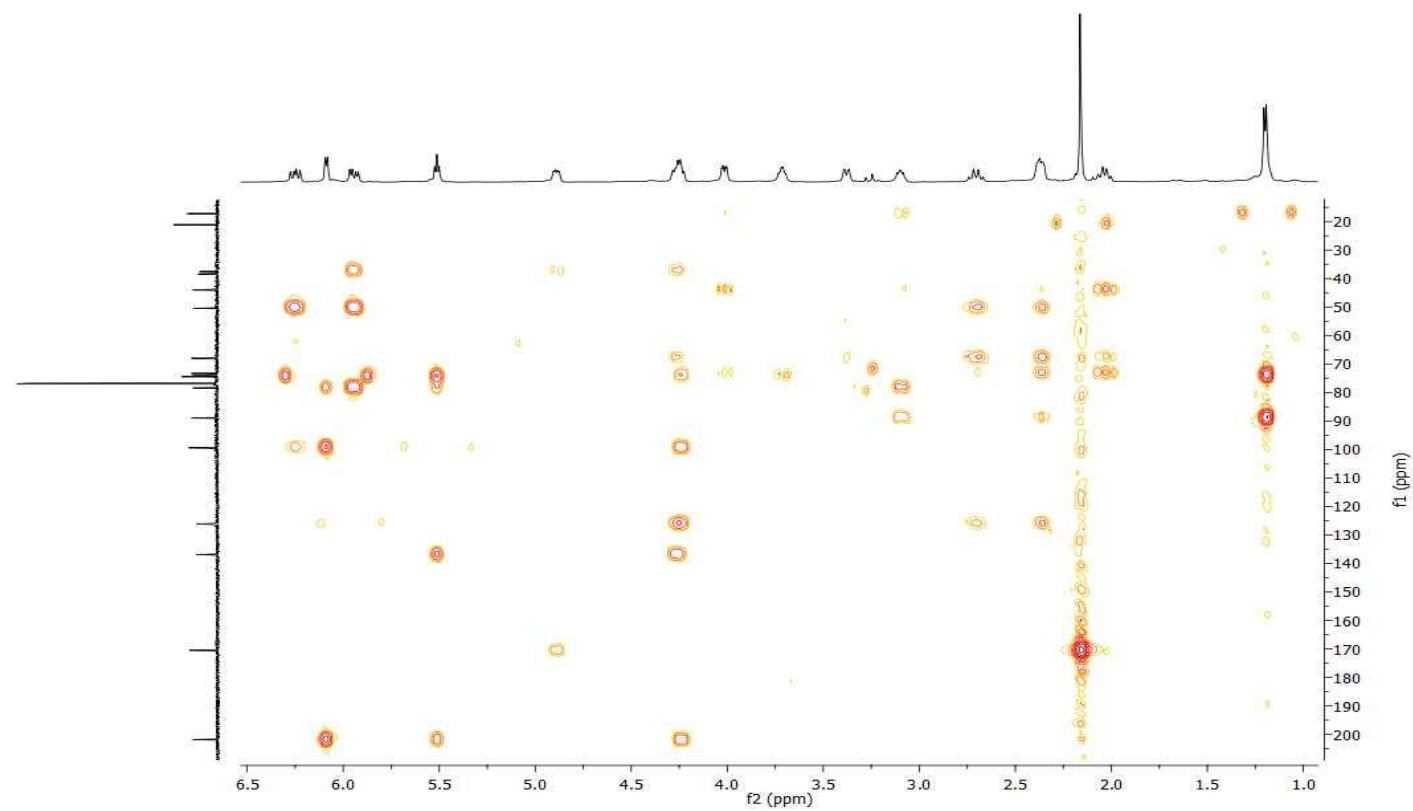


Figure S34. NOESY spectrum of compound **3** at 20°C (CDCl₃, 125.5 MHz).

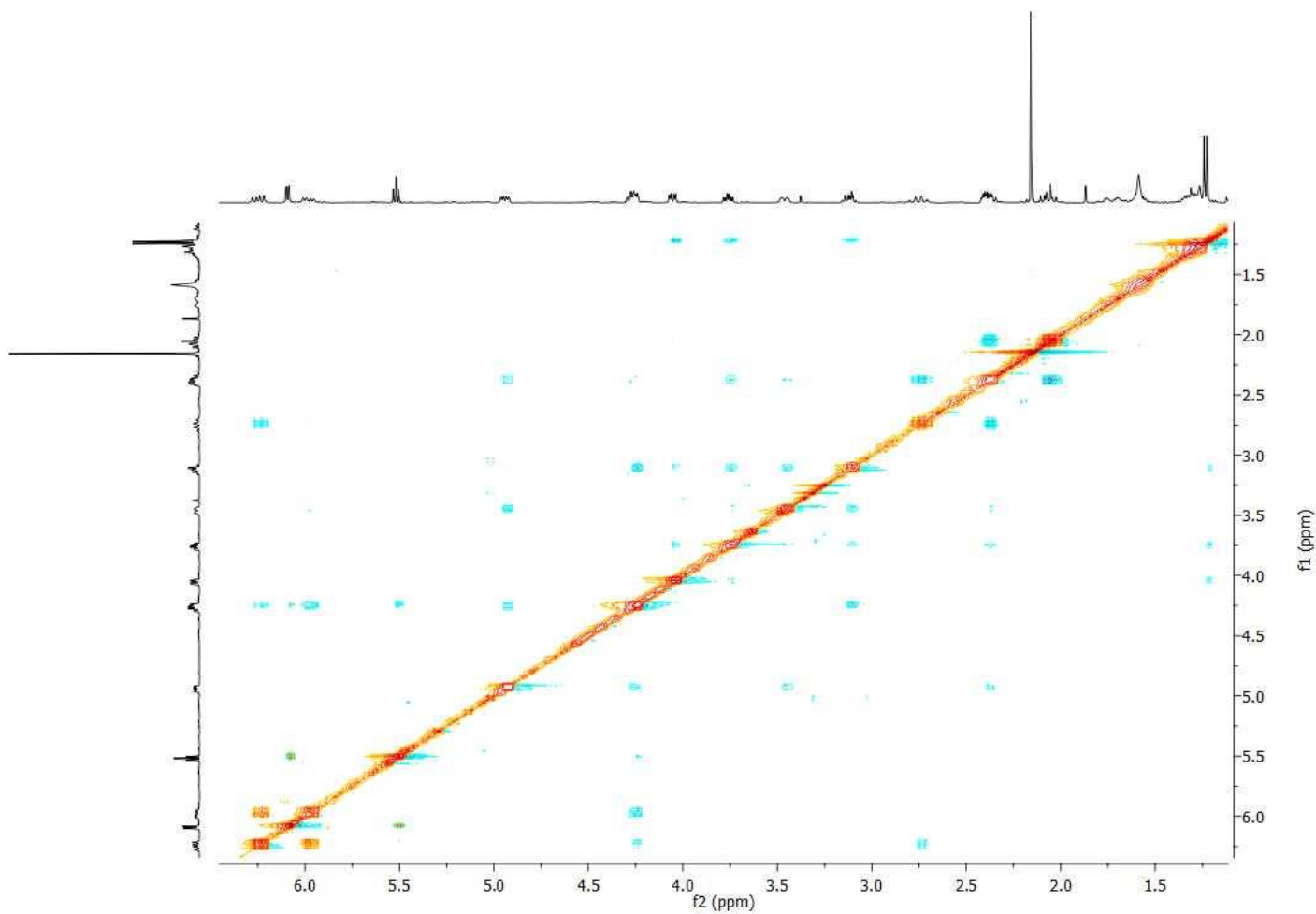


Figure S35. HRMS spectrum of compound **3** (Zoom), in negative ionization.

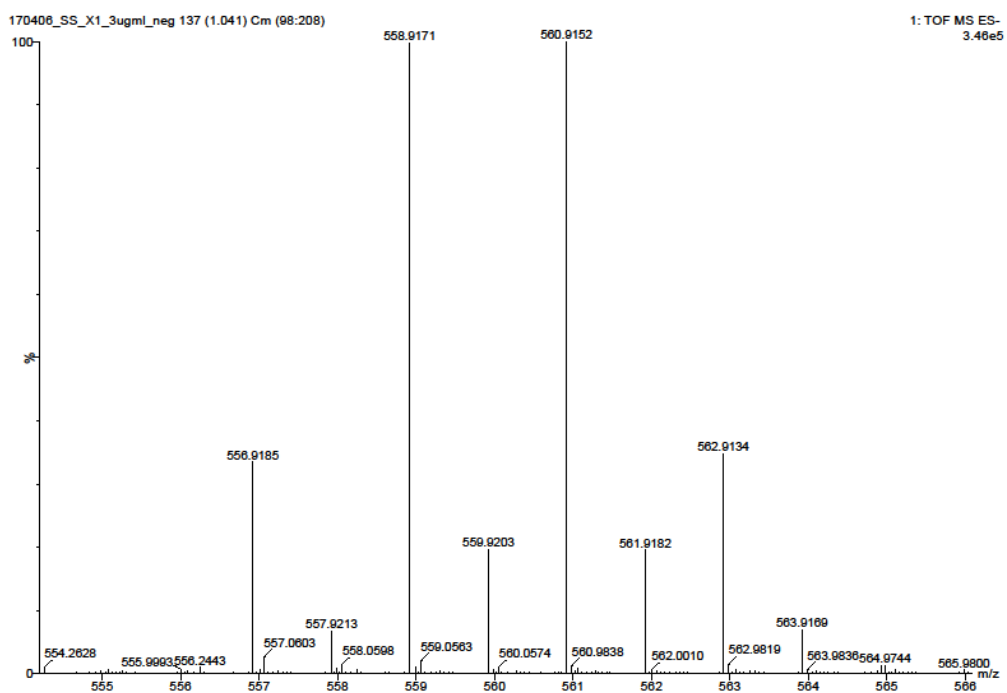


Figure S36. UV spectrum of compound **3**.

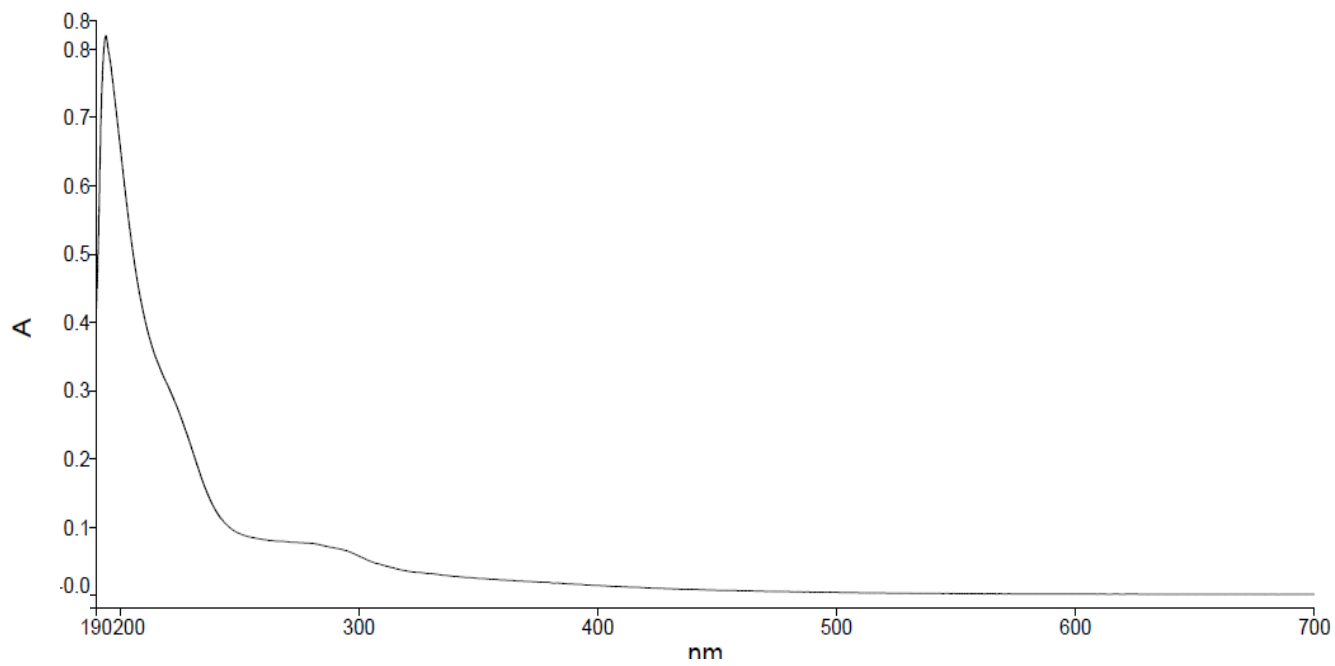


Figure S39. ^{13}C NMR spectrum of compound **4** at 20°C (CDCl_3 , 125.5 MHz).

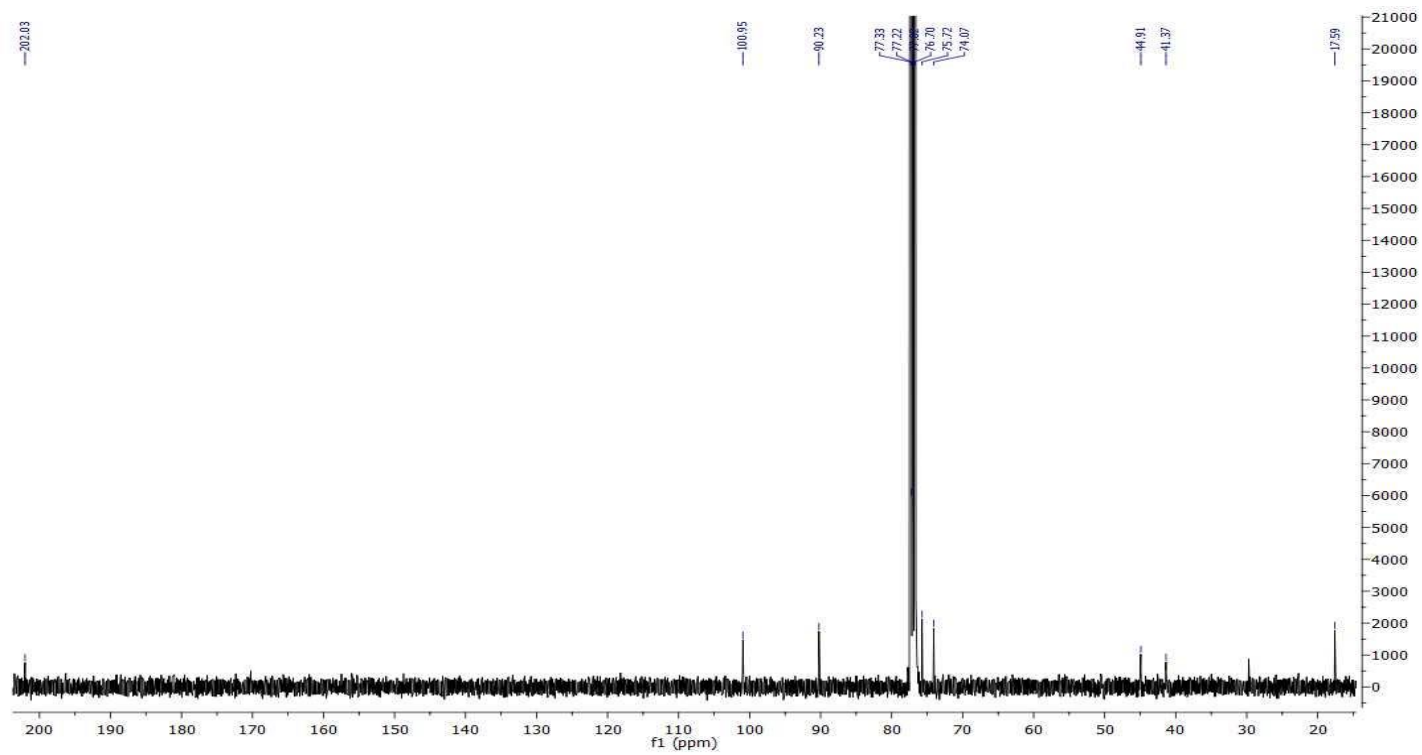


Figure S40. HMQC spectrum of compound **4** at - 40°C (CDCl₃, 400.0 MHz).

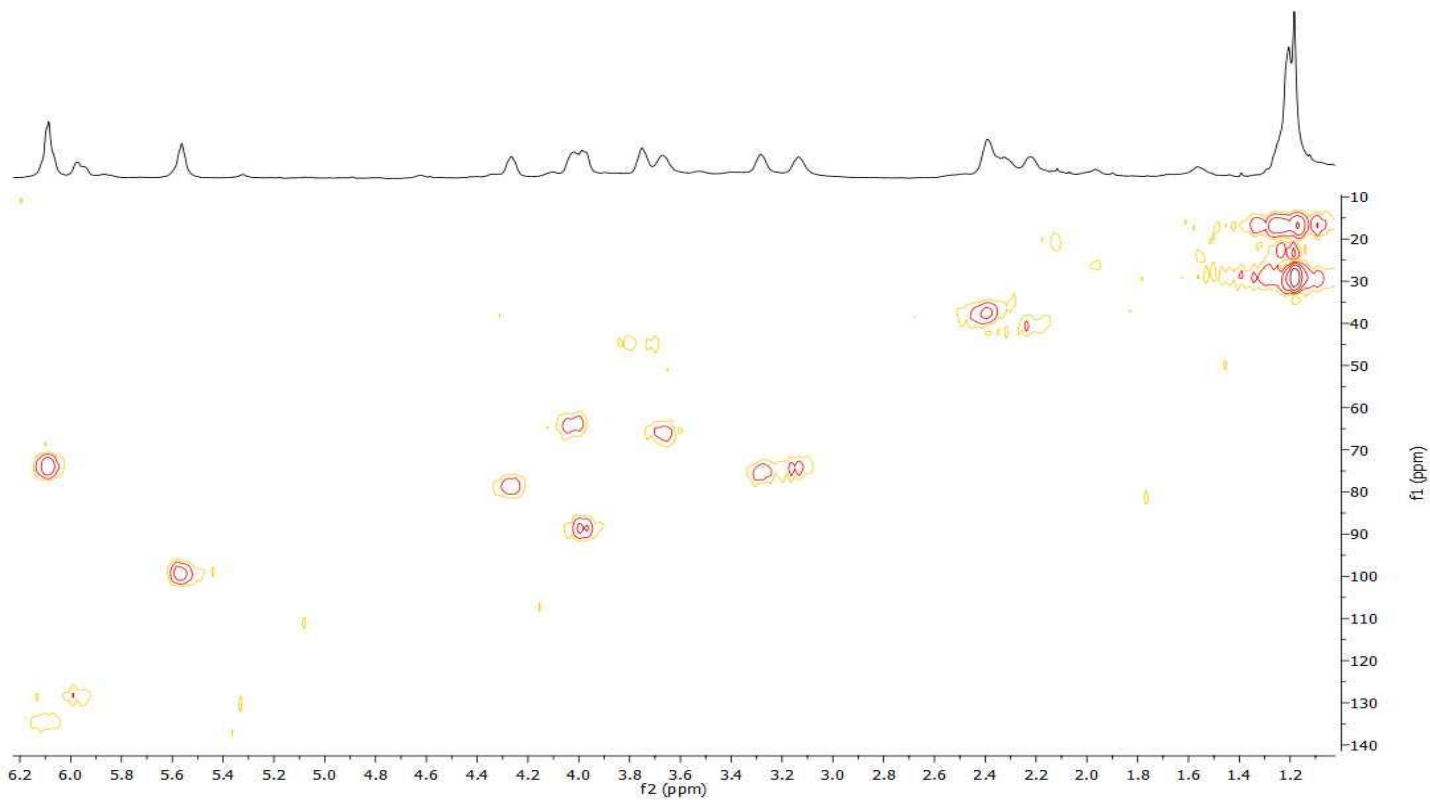


Figure S41. HMBC spectrum of compound **4** at - 40°C (CDCl₃, 400.0 MHz).

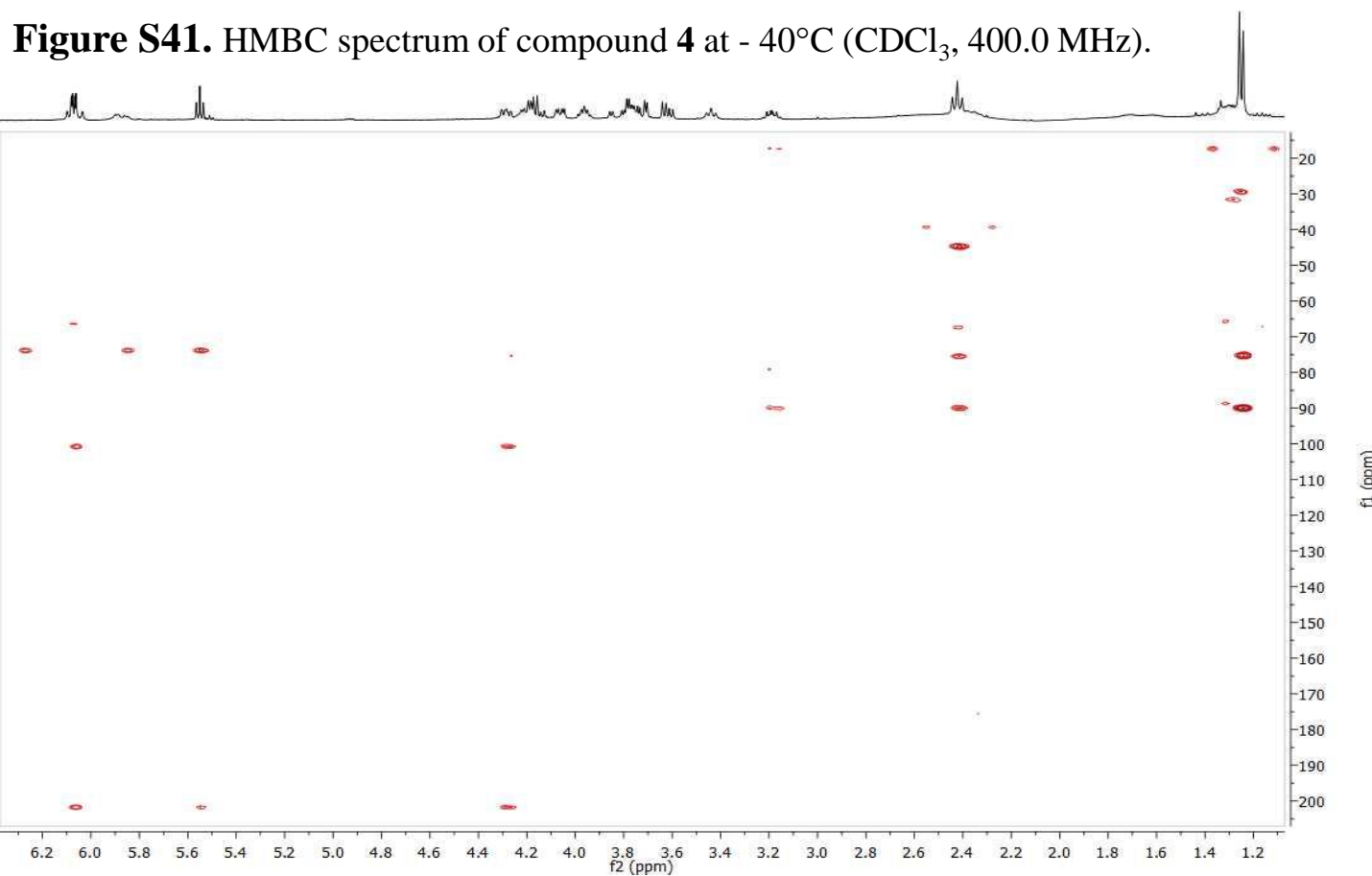


Figure S42. COSY spectrum of compound **4** at 20°C (CDCl₃, 400.0 MHz).

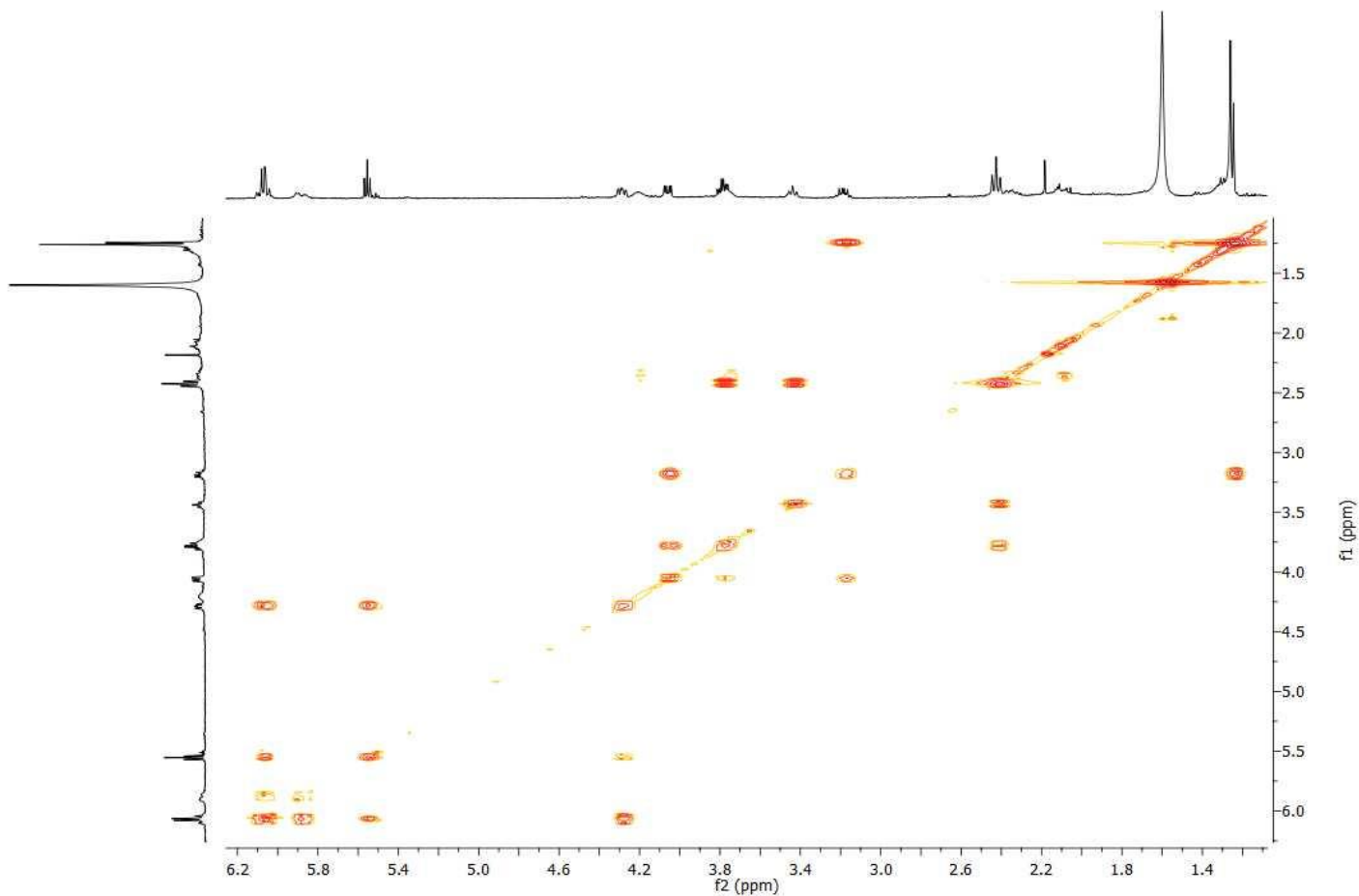


Figure S43. COSY spectrum of compound **4** at -40°C (CDCl₃, 400.0 MHz).

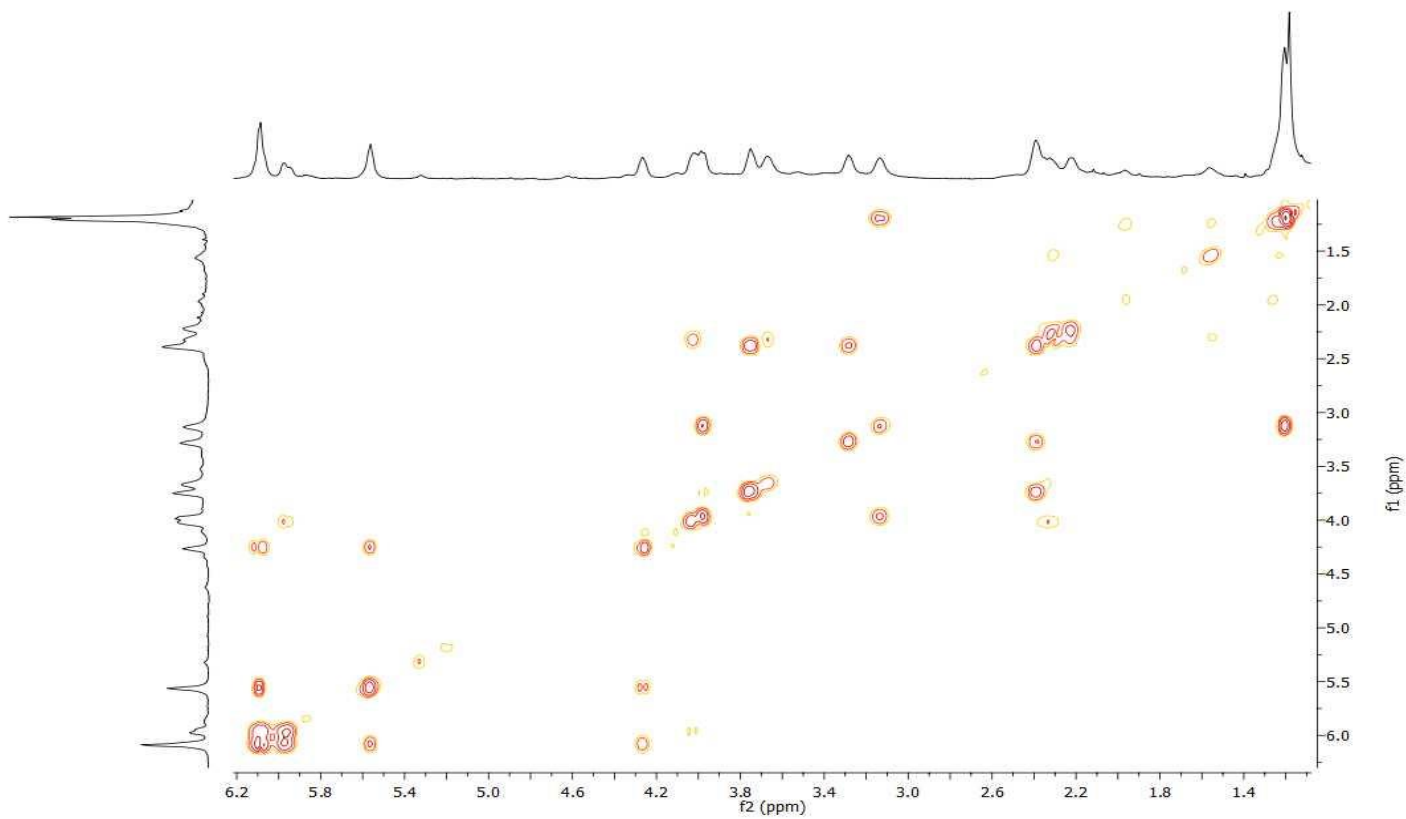


Figure S44. NOESY spectrum of compound **4** at 20°C (CDCl₃, 125.5 MHz).

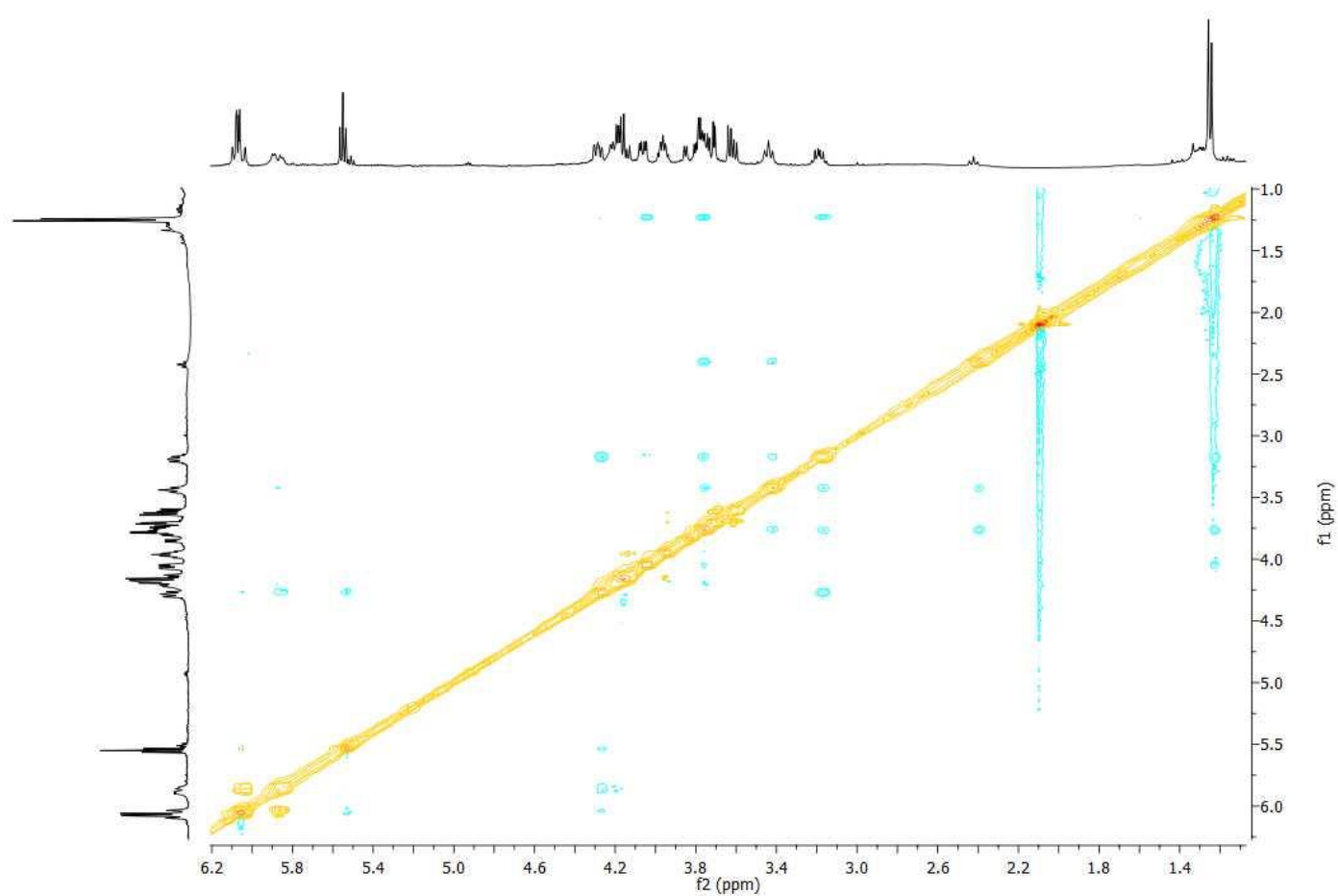


Figure S45. UV spectrum of compound **4**.

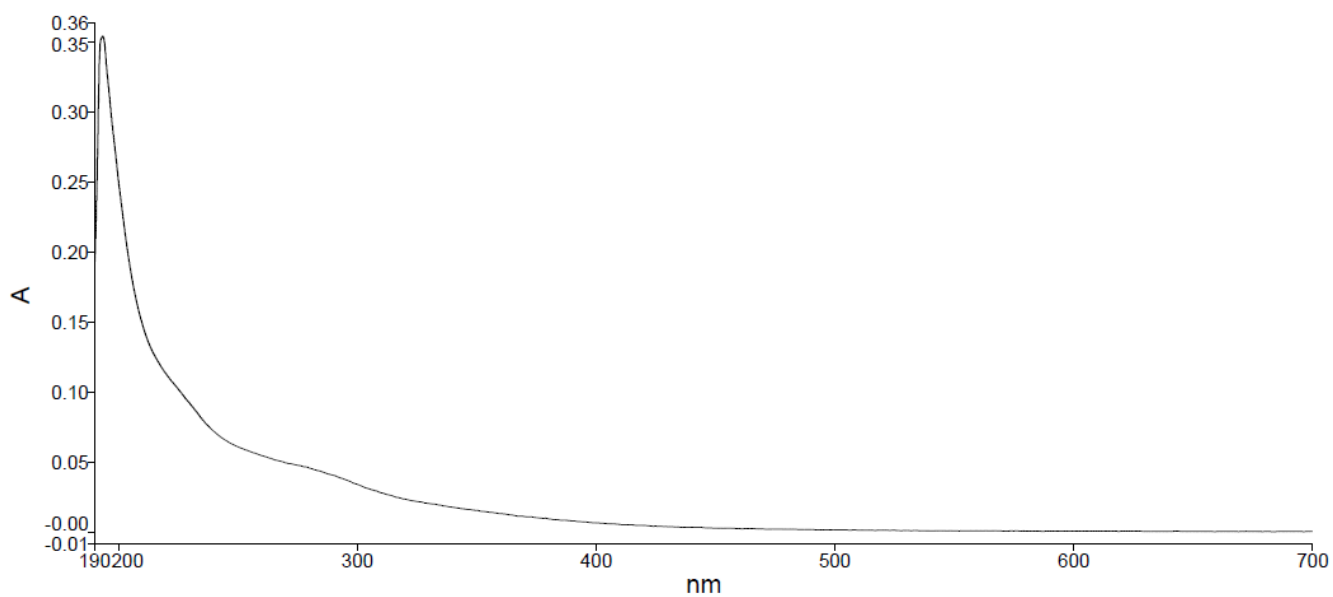


Figure S46. HRMS spectrum of compound **4** (Zoom) in negative ionization.

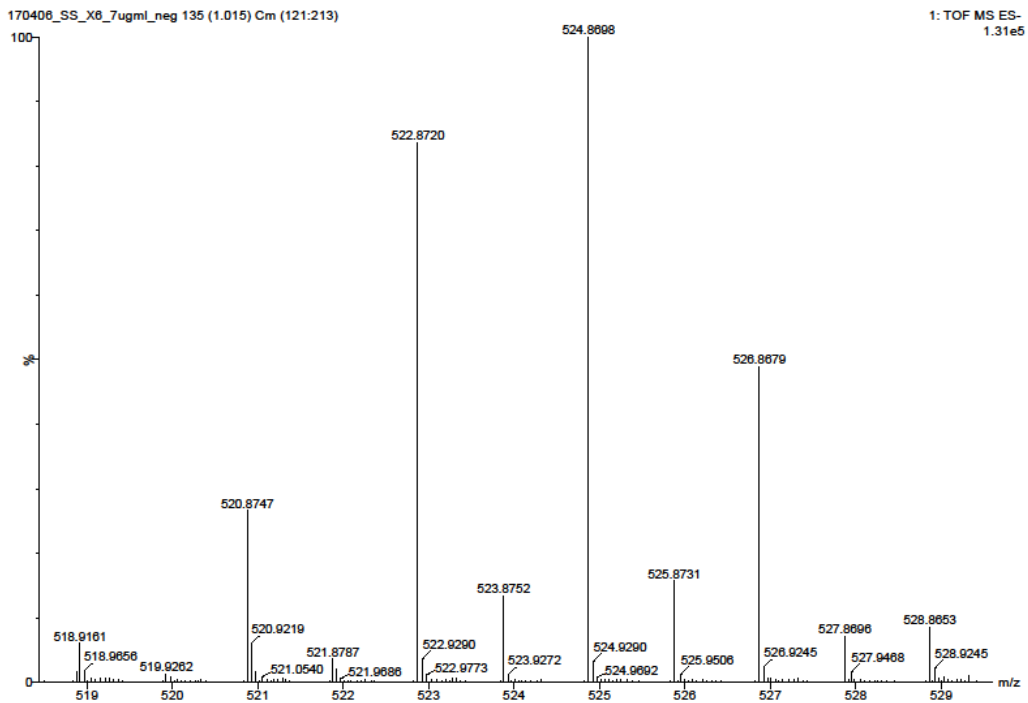


Figure S47. HRMS spectrum of compound **4** (Zoom) in positive ionization.

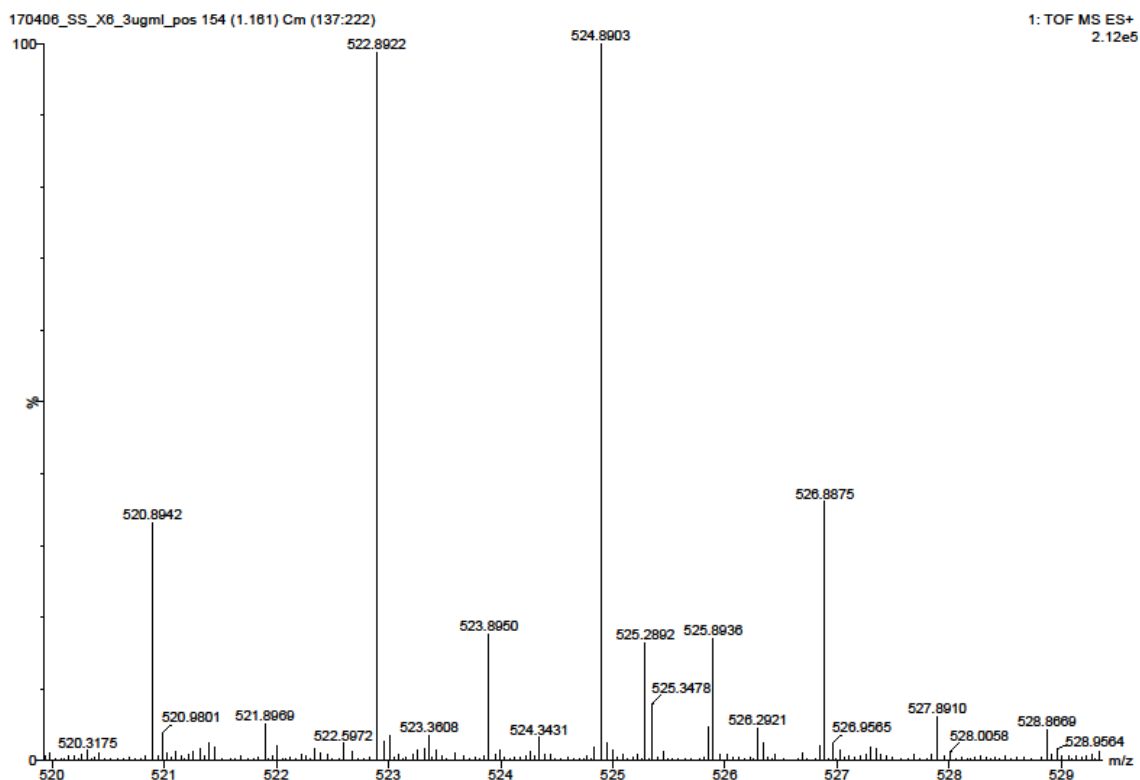


Figure S48. ^1H NMR spectrum of compound **5** (CDCl_3 , 400 MHz).

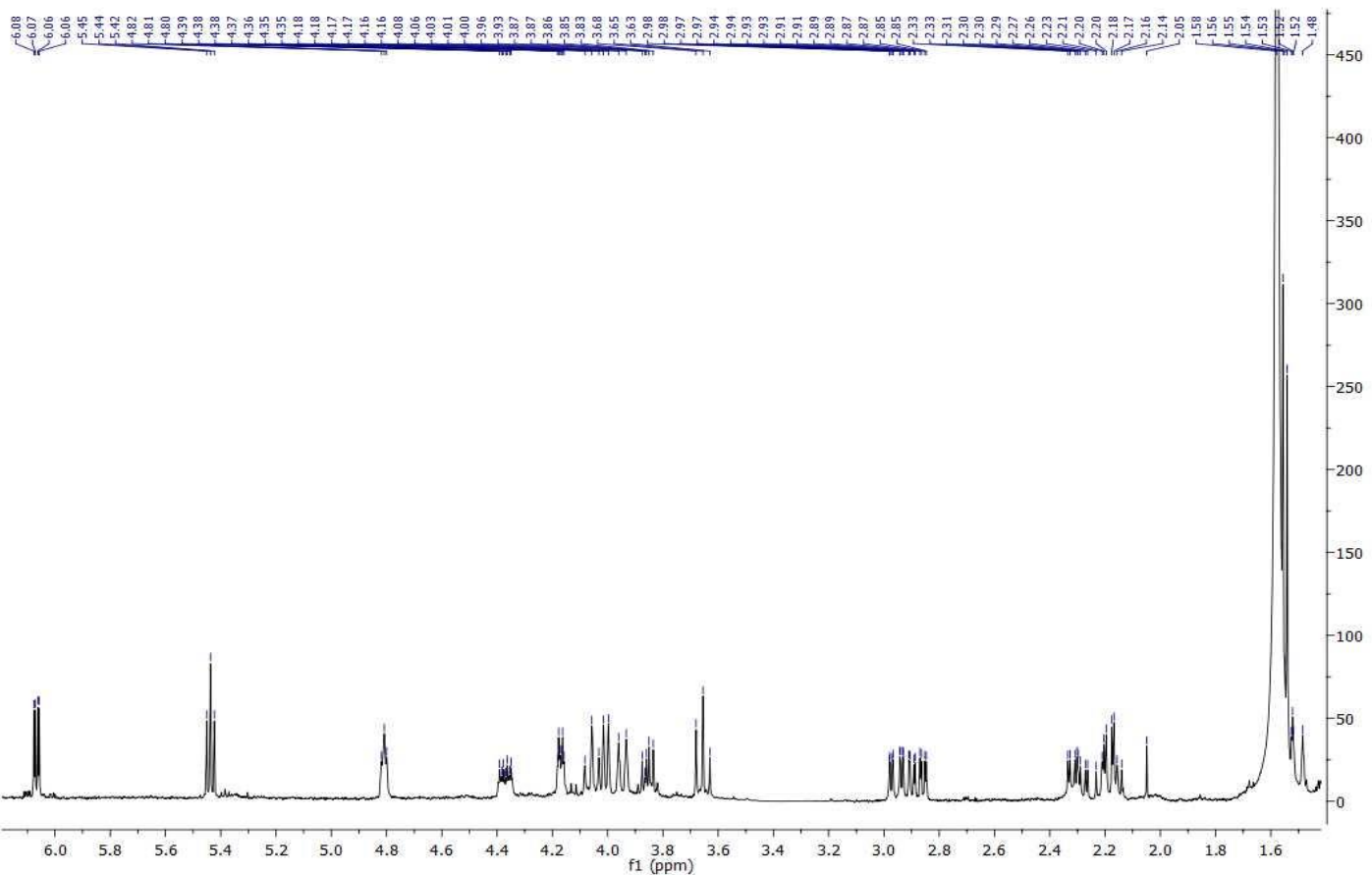


Figure S49. ^{13}C NMR spectrum of compound **5** (CDCl_3 , 125.5 MHz).

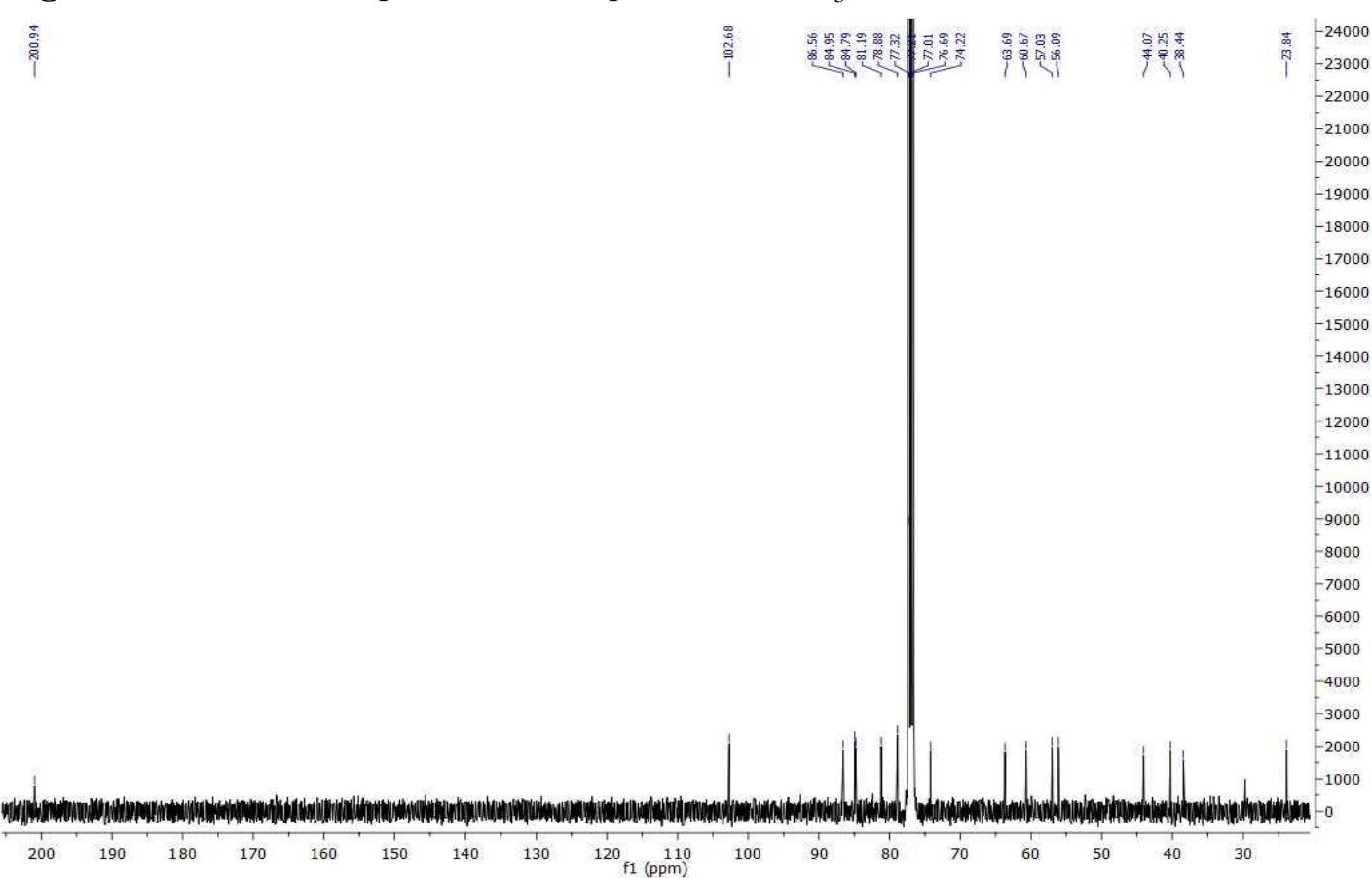


Figure S50. HSQC spectrum of compound **5** (CDCl₃, 400.0 MHz).

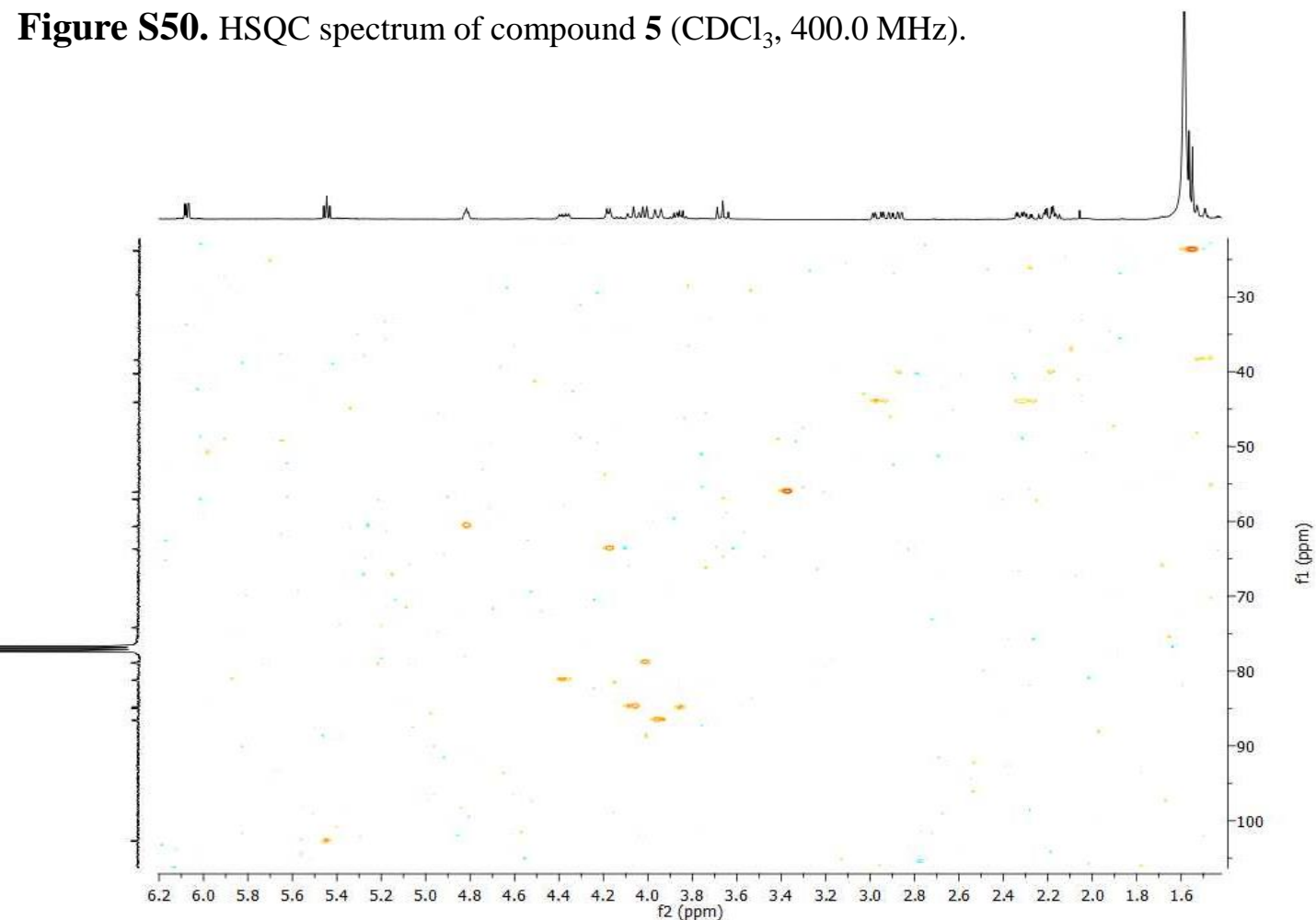


Figure S51. HMBC spectrum of compound **5** (CDCl₃, 400.0 MHz).

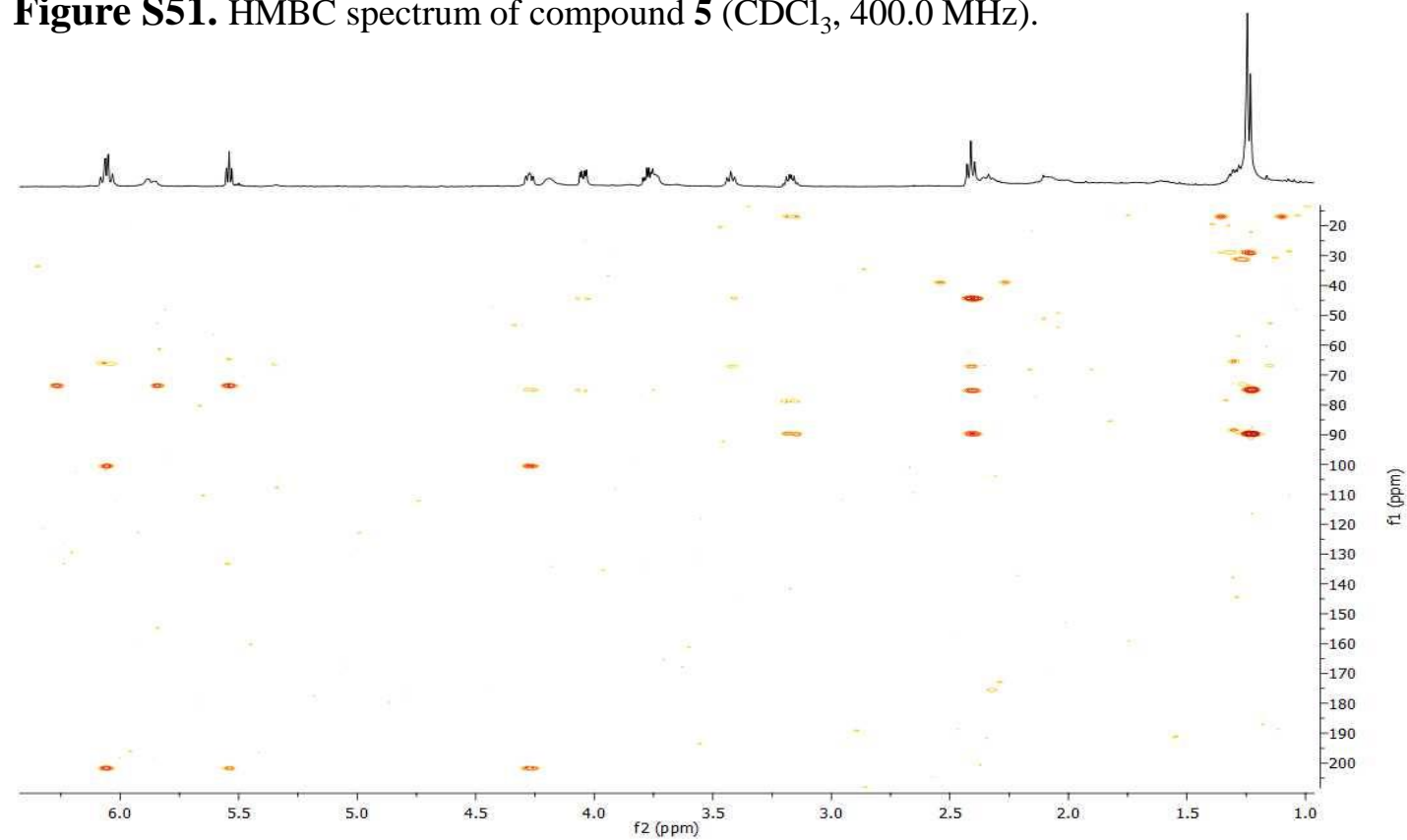


Figure S52. COSY spectrum of compound **5** at 20°C (CDCl₃, 400.0 MHz).

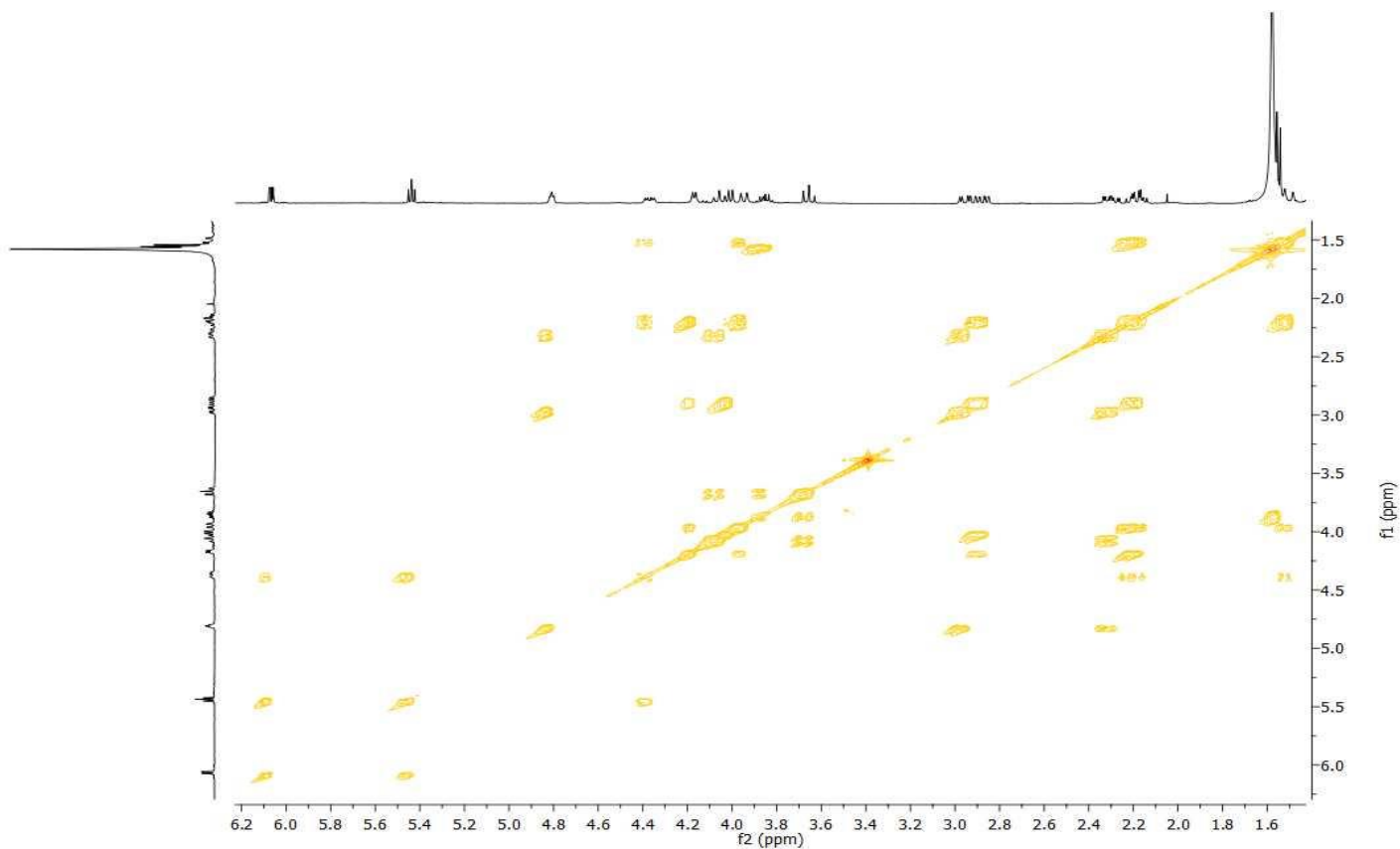


Figure S53. NOESY spectrum of compound **5** at 20°C (CDCl₃, 125.5 MHz).

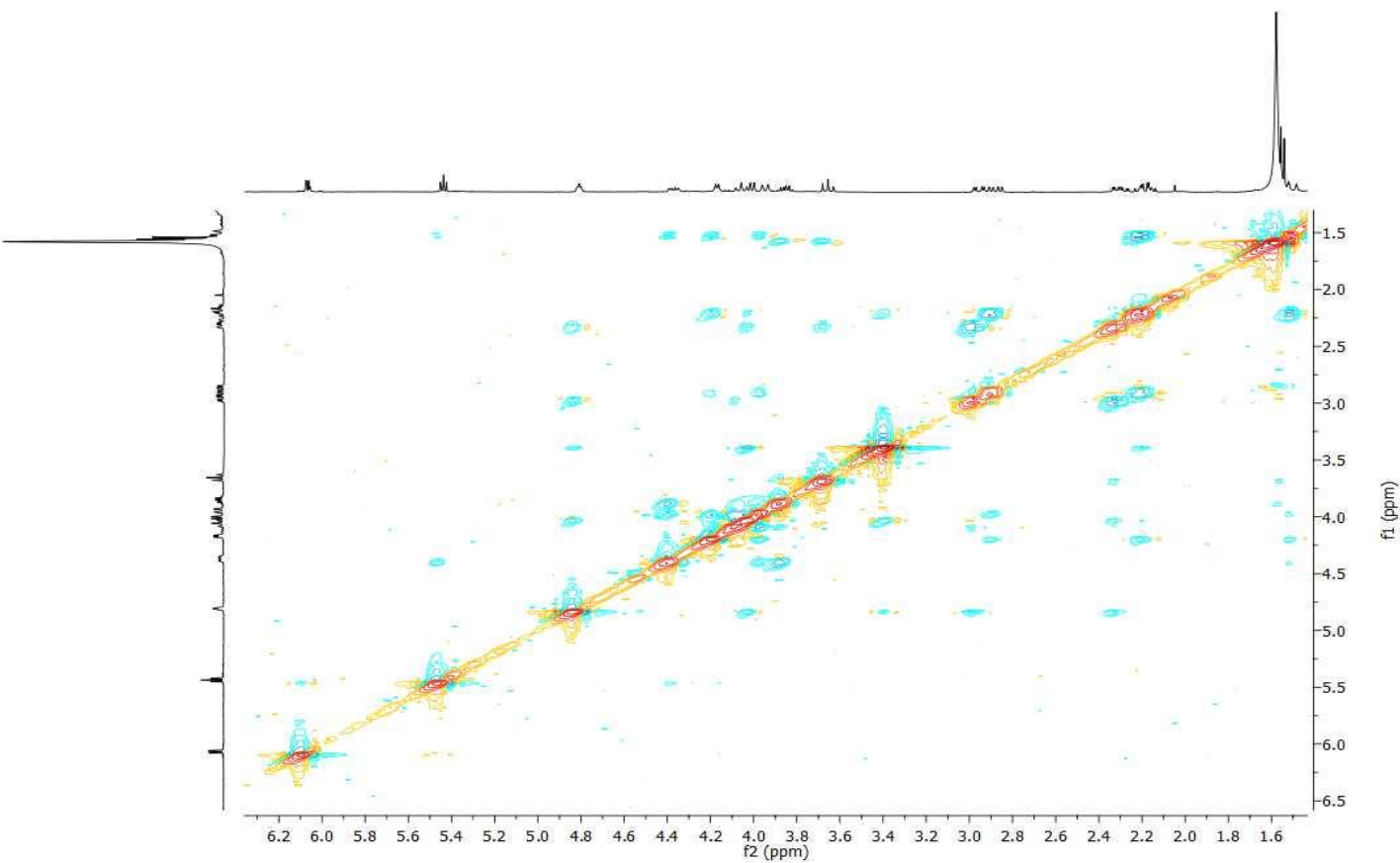


Figure S54. UV spectrum of compound **5**.

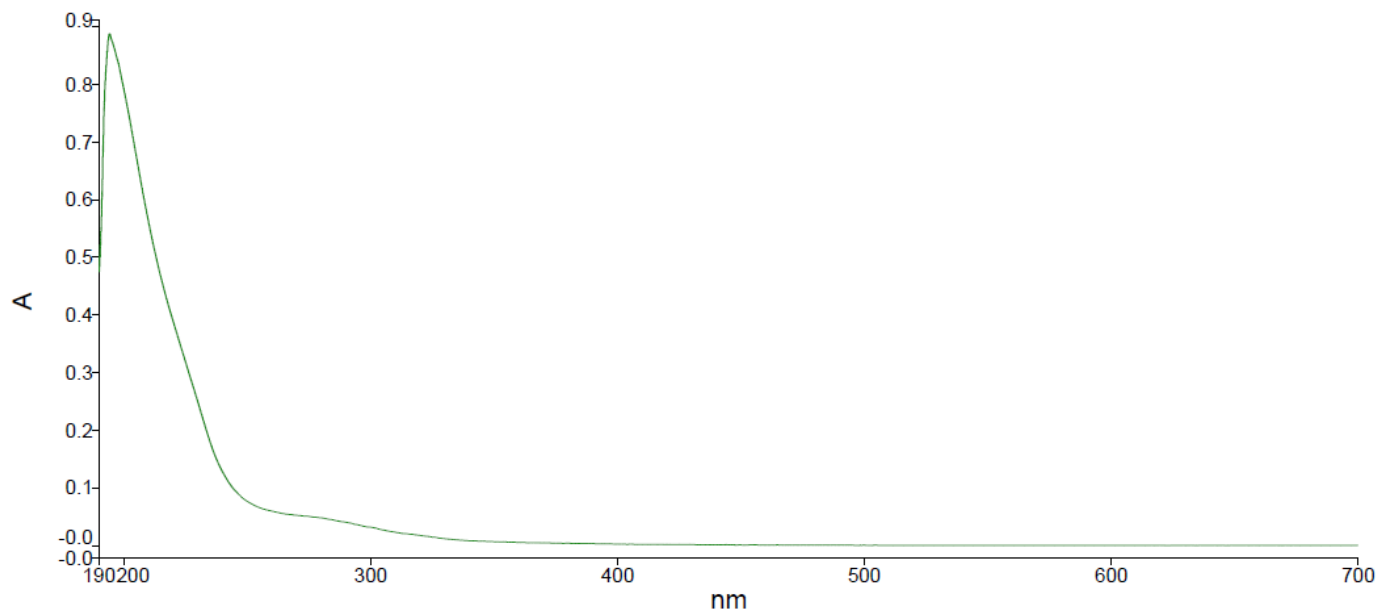
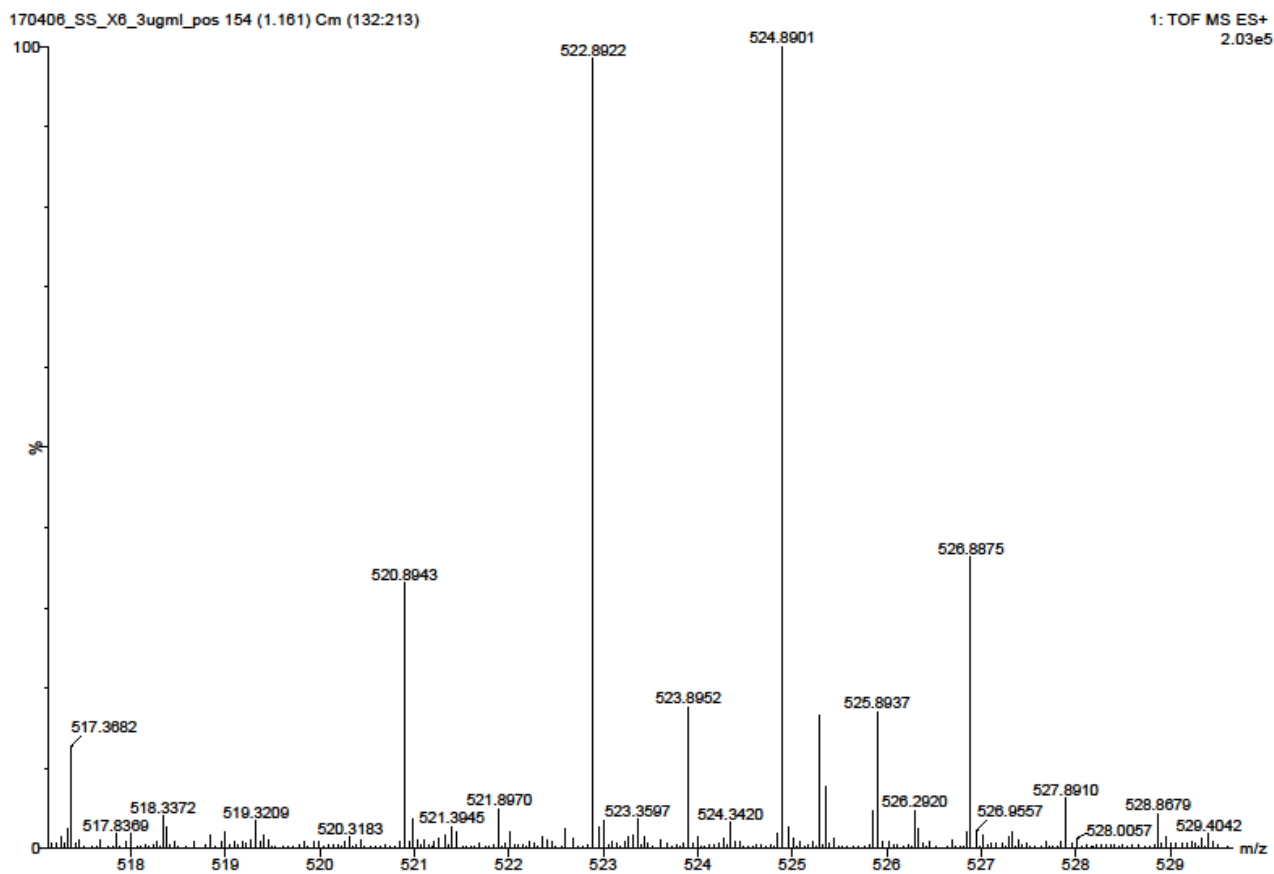
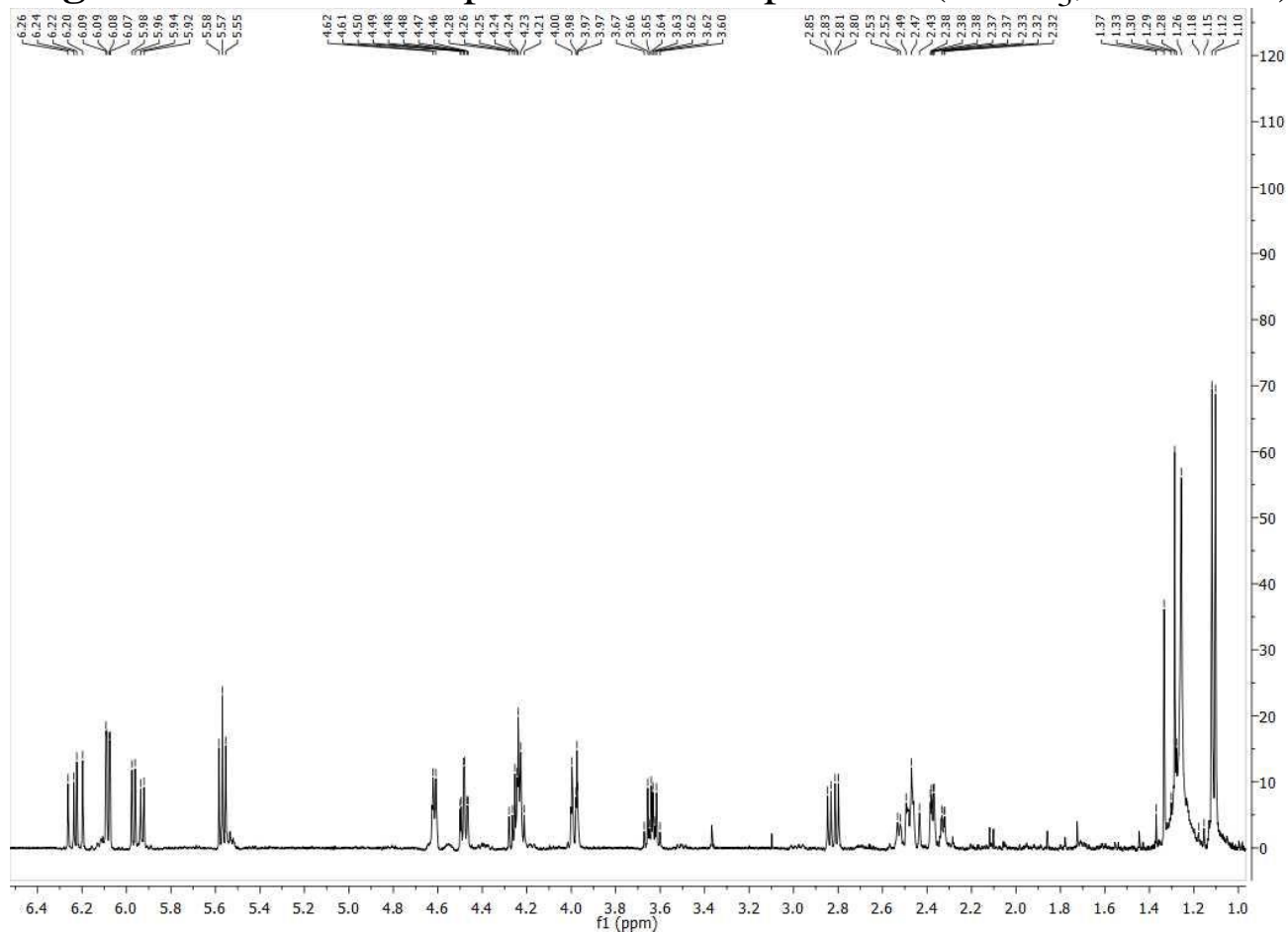


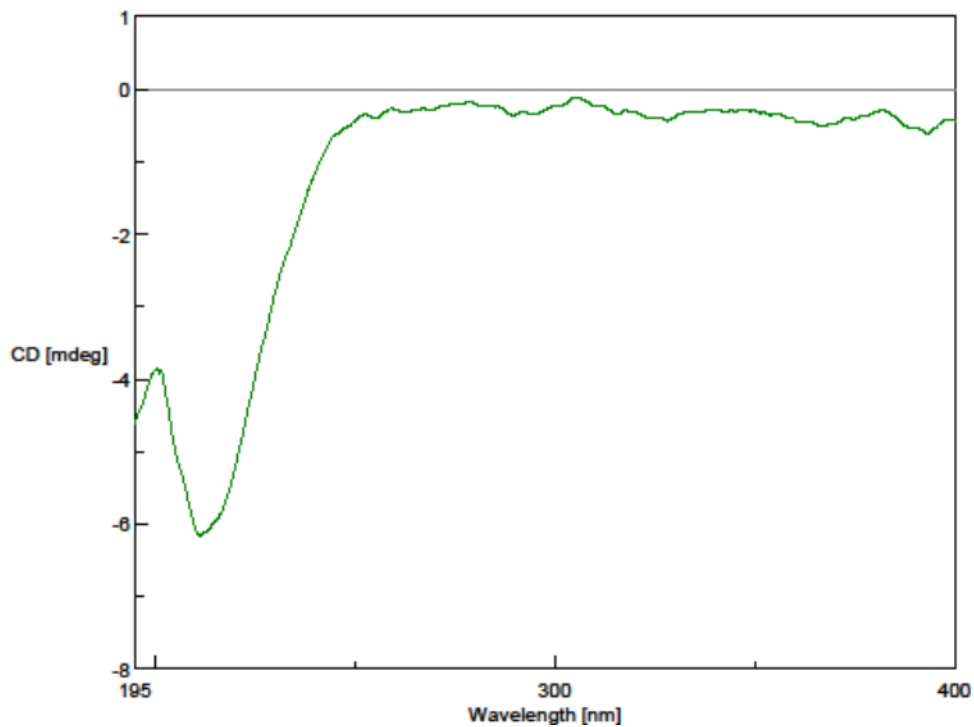
Figure S55. HRMS spectrum of compound **5** (Zoom) in positive ionization.



- **Figure S56.** ^1H NMR spectrum of compound **6** (CDCl_3 , 400 MHz).



- **Figure S57.** Experimental CD spectra of **6** in MeOH



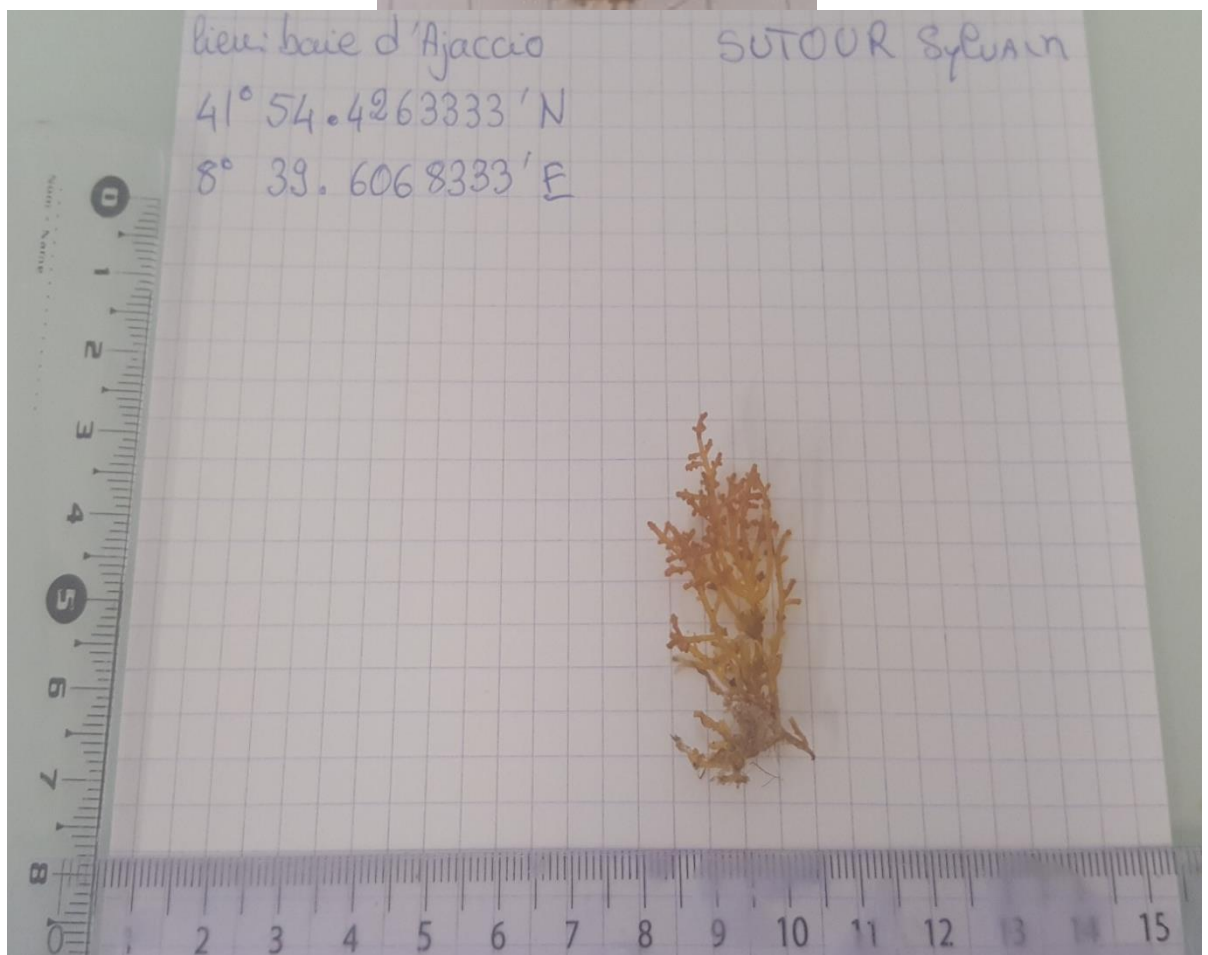
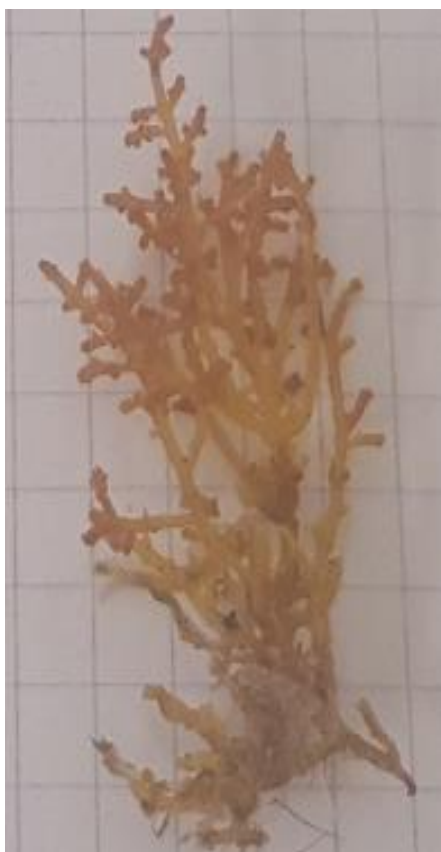
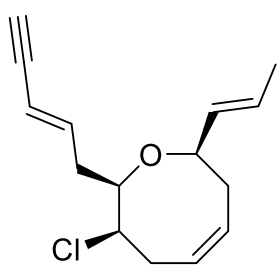
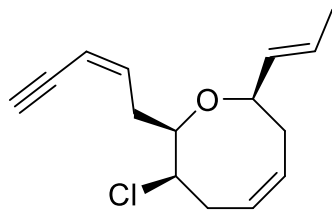


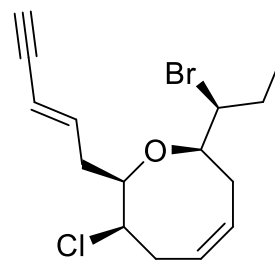
Figure S58. Picture of a specimen of *Laurenciella* sp. collected in Ajaccio bay, Corsica, France.



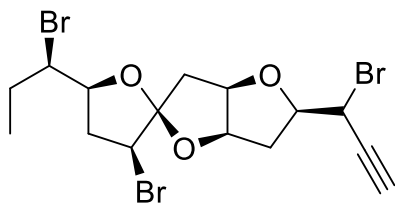
3-(*E*)-laurenyne



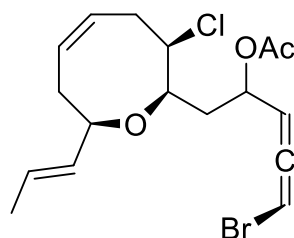
3-(*Z*)-laurenyne



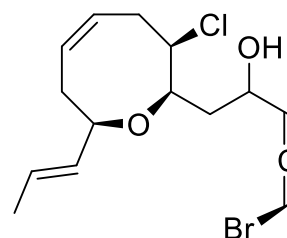
(*E*)-pinnatifidenyne



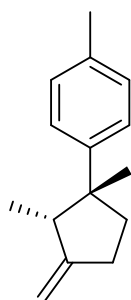
obtusin



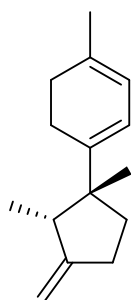
4-acetoxymarilzallene



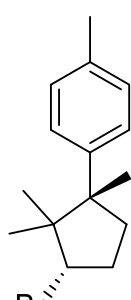
marilzallene B



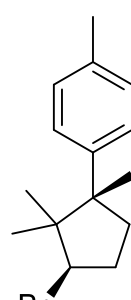
laurene



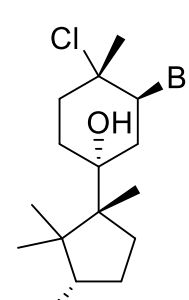
dihydro-laurene



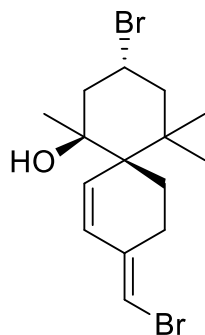
α -bromocuparene



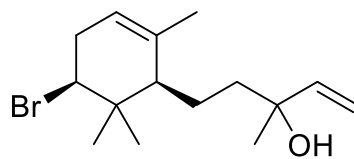
α -
cuparene



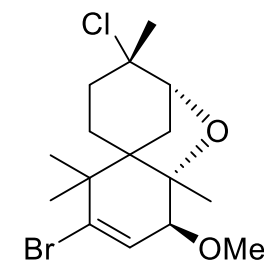
1-deacetoxy-8-
deoxyalgaove



9,15-dibromo-
1,3(15)-
chamigradien-11-ol



α -snyderol



cycloelatenene A

Figure S59. Known C_{15} acetogenins and sesquiterpens identified from *Laurenciella* sp. extract.

	1
Chemical formula	C ₁₈ H ₂₄ Br ₂ O ₅
Formula weight	480.19
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ (no. 4)
Crystal colour and shape	Colorless plate
Crystal size	0.43 x 0.18 x 0.16
<i>a</i> (Å)	4.7521(3)
<i>b</i> (Å)	25.2432(16)
<i>c</i> (Å)	17.1496(11)
<i>B</i> (°)	90.701(5)
<i>V</i> (Å ³)	2057.1(2)
<i>Z</i>	4
<i>T</i> (K)	293(2)
<i>D_c</i> (g·cm ⁻³)	1.550
<i>μ</i> (mm ⁻¹)	3.964
Scan range (°)	1.613 < <i>θ</i> < 29.364
Unique reflections	11216
Observed refls [<i>I</i> > 2σ(<i>I</i>)]	5616
<i>R_{int}</i>	0.0693
Flack parameter	-0.014(7)
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]*	0.0656, <i>wR</i> ₂ 0.1390
<i>R</i> indices (all data)	0.1318, <i>wR</i> ₂ 0.1563
Goodness-of-fit	1.022
Max, Min Δρ/e (Å ⁻³)	0.992, -0.628

* Structures were refined on *F*₀²: $wR_2 = [\sum[w(F_0^2 - F_c^2)^2] / \sum w(F_0^2)^2]^{1/2}$, where $w^{-1} = [\Sigma(F_0^2) + (aP)^2 + bP]$ and $P = [\max(F_0^2, 0) + 2F_c^2]/3$

Table S60. Crystallographic and structure refinement parameters for **1**.