

# Supporting Information

## Discovering a New Okadaic Acid Derivative as Potent HIV Latency-Reversing Agent from *Prorocentrum lima* PL11: Isolation, Structural Modification, and Mechanistic Study

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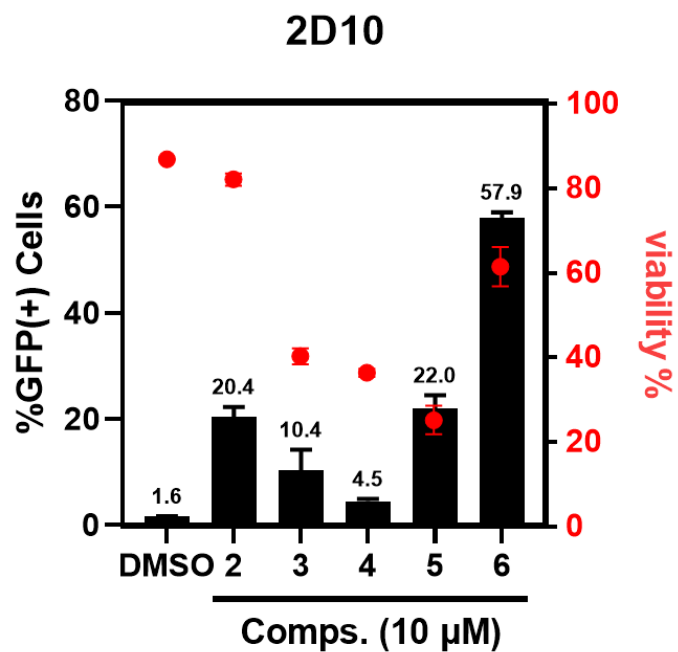
**Figure S36.** HSQC spectrum of **7** in  $\text{CDCl}_3$ .

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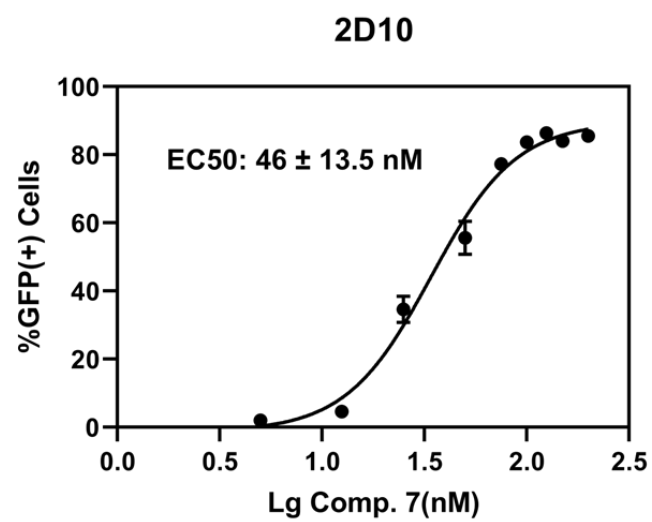
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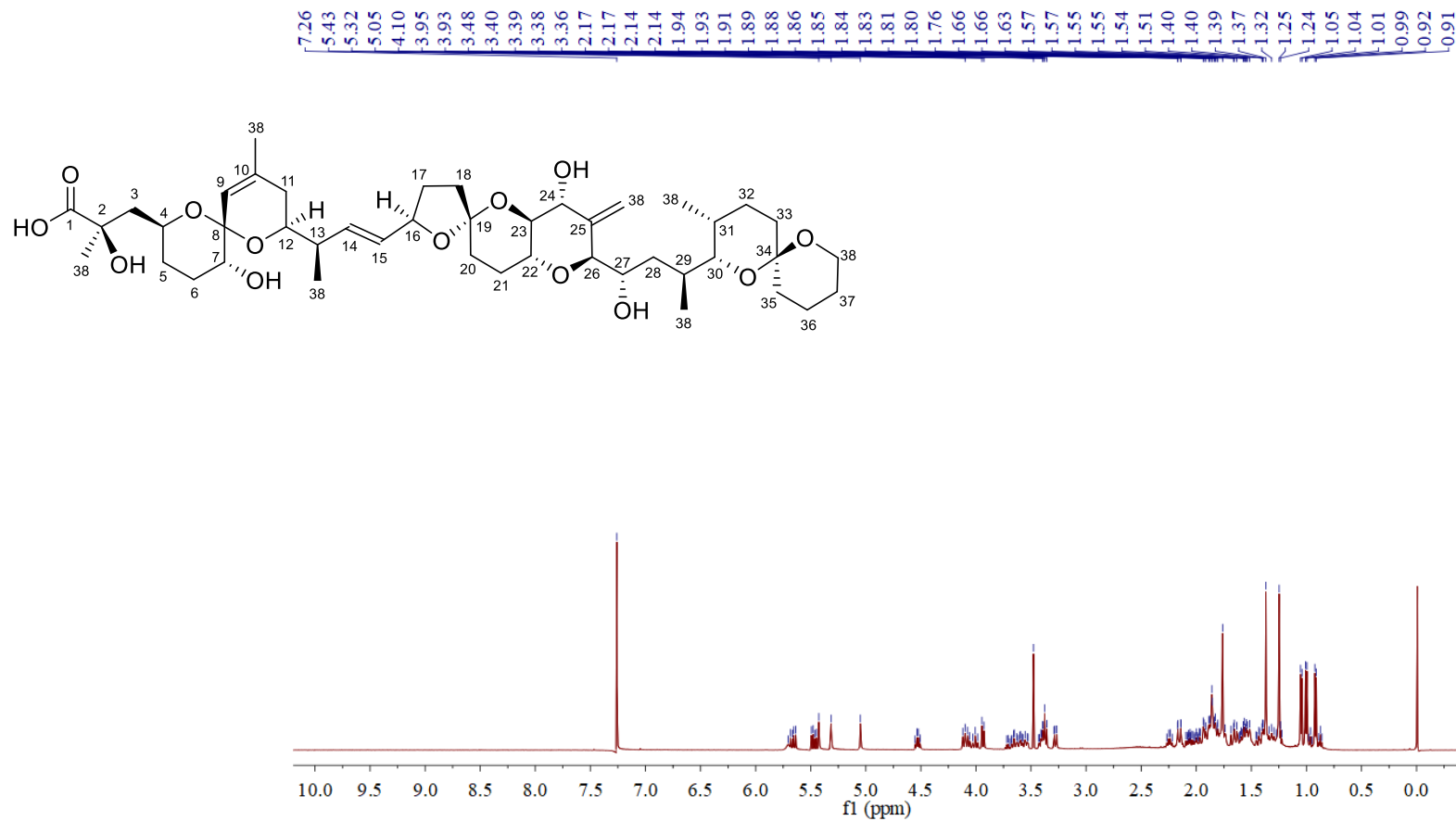
**Figure S1.** The HIV-latency-reversing activity of OA derivatives 2–6 at 10  $\mu$ M measured in 2D10 cell. Cell viability was labeled as red dots. Black bars represented GFP expression.



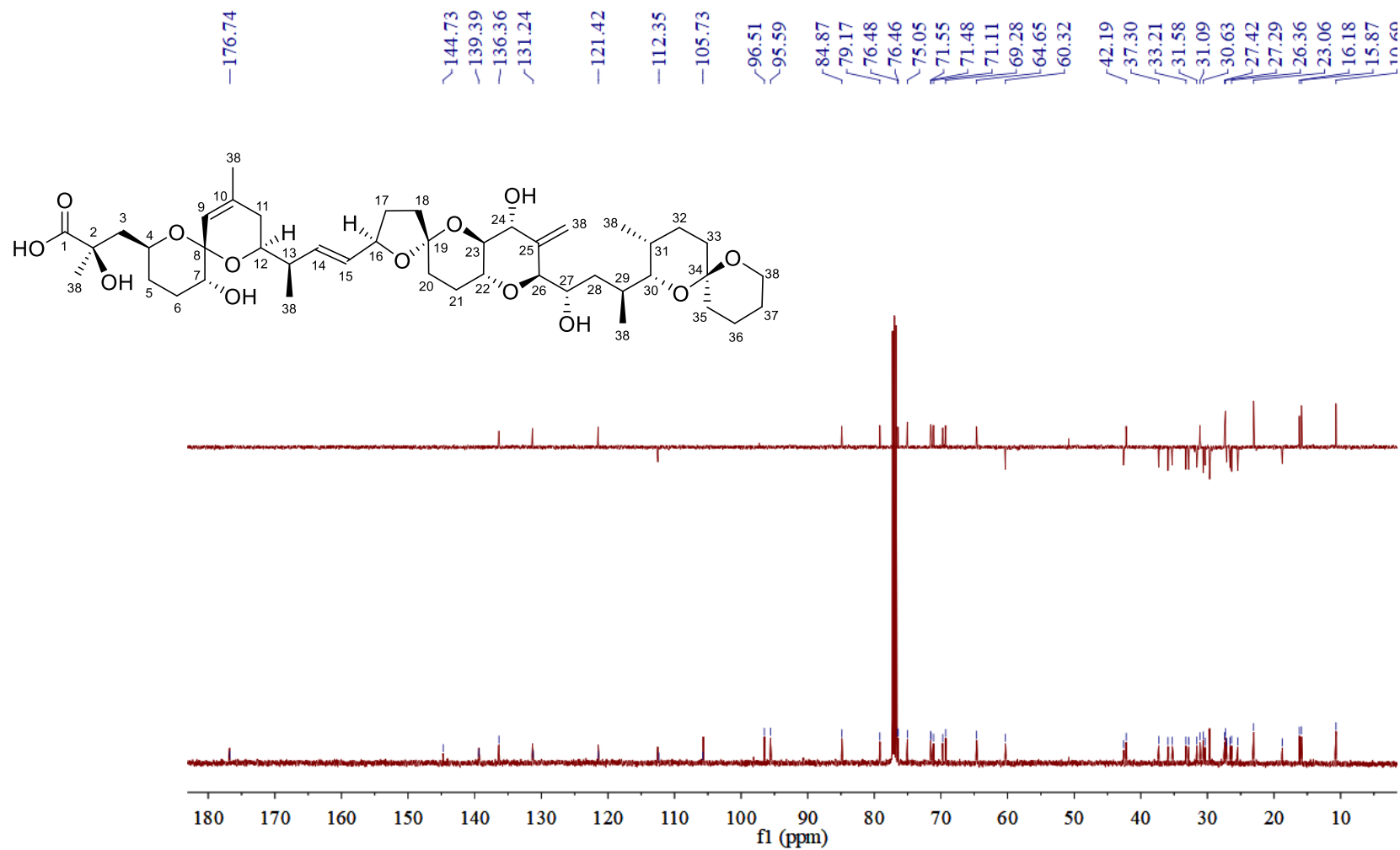
**Figure S2.** The HIV-latency-reversing activity of compound **7** (EC<sub>50</sub>) measured in 2D10 cell.

## 2. NMR, HRESIMS, and IR spectra of 1–7.

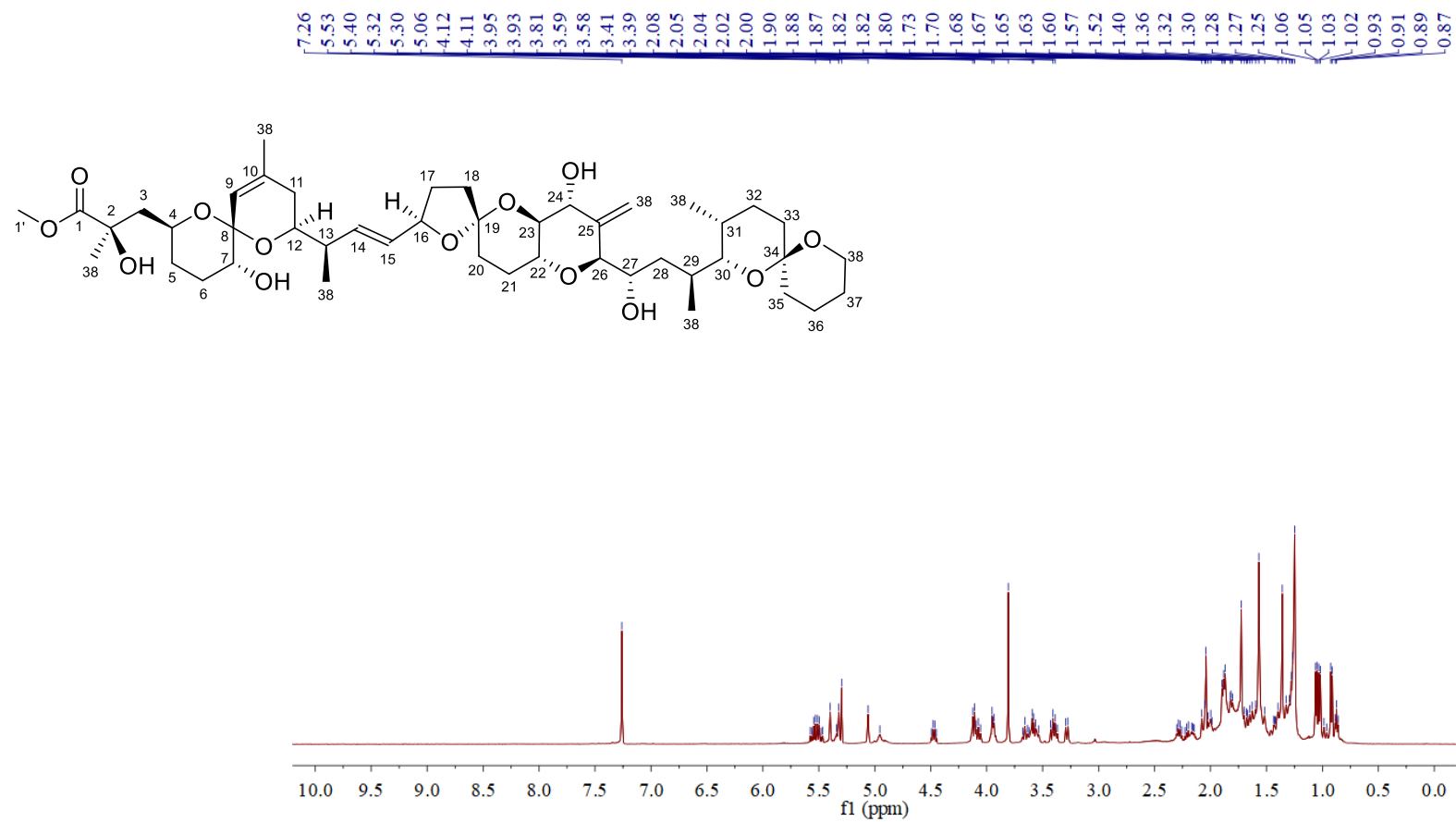
**Figure S3.**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$ .



**Figure S4.**  $^{13}\text{C}$  NMR and DEPT 135 spectra of **1** in  $\text{CDCl}_3$ .



**Figure S5.**  $^1\text{H}$  NMR spectrum of **2** in  $\text{CDCl}_3$ .



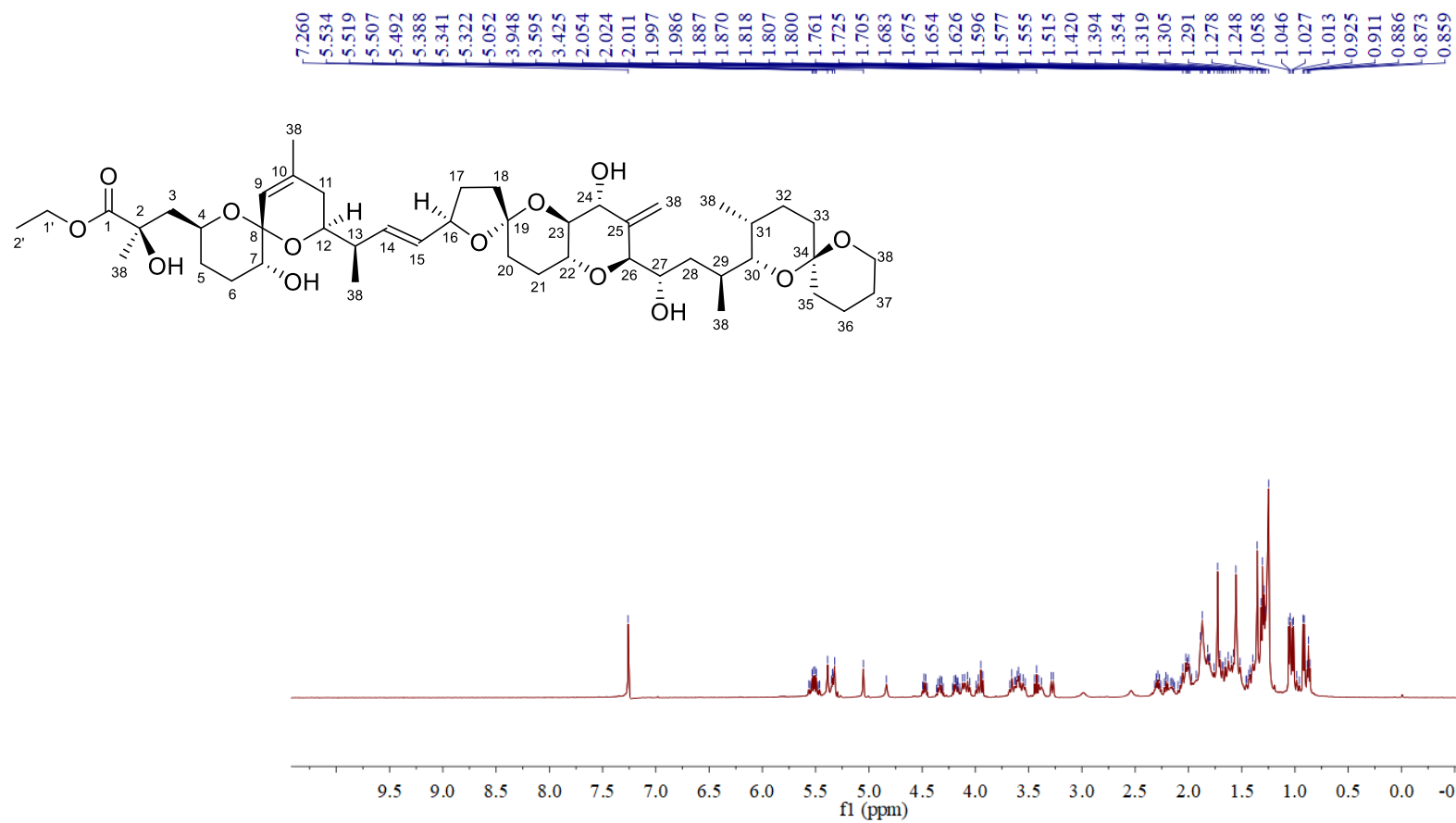


Chemical structure of compound 1 is shown above the  $^{13}\text{C}$  NMR spectrum. The spectrum displays peaks corresponding to the carbon atoms in the molecule, with chemical shifts (ppm) labeled on the right side of the plot.

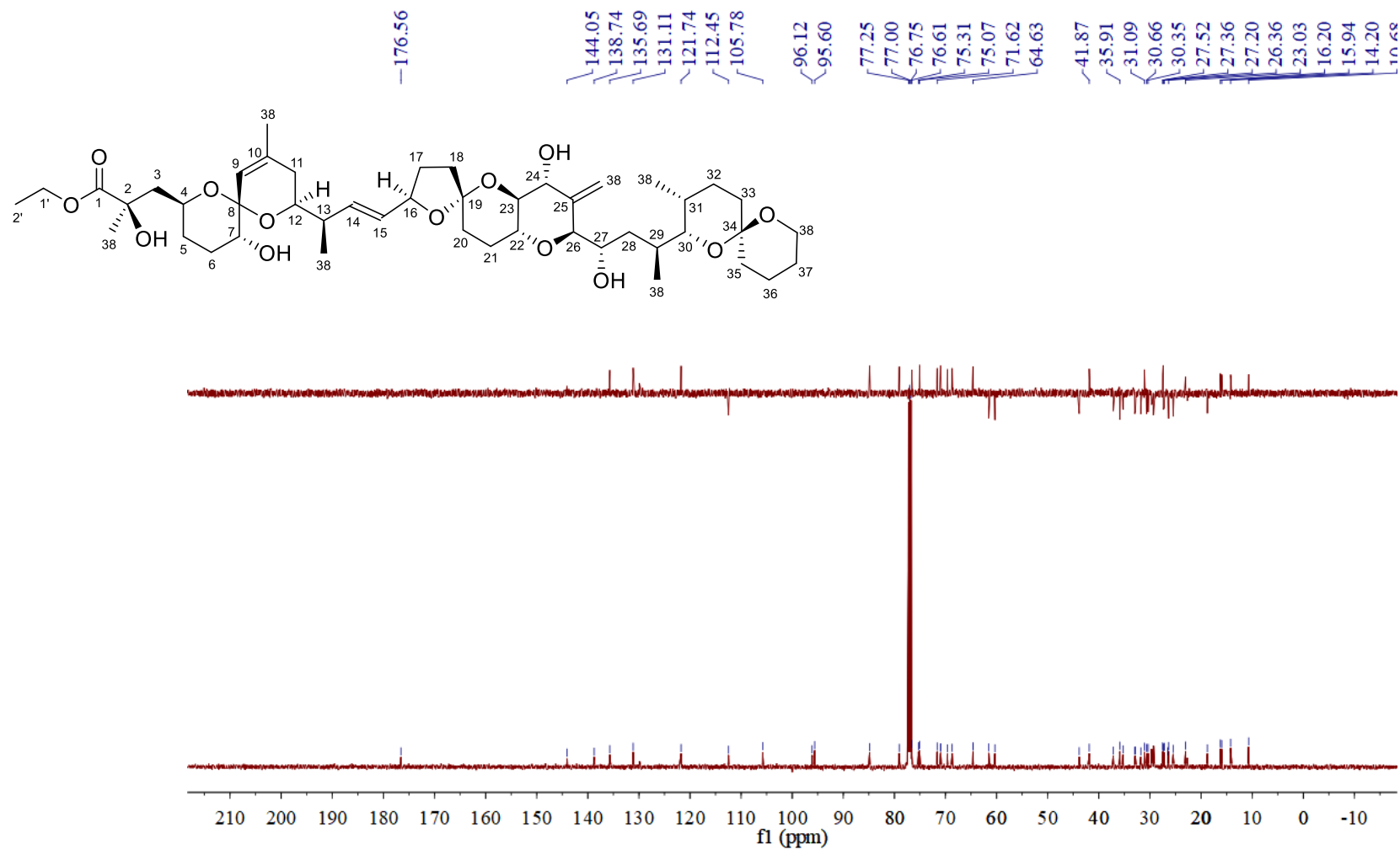
Chemical shifts (ppm) labeled on the right side of the spectrum:

- 176.92
- 144.01
- 138.78
- 135.69
- 130.90
- 121.65
- 112.47
- 105.80
- 105.77
- 96.06
- 95.61
- 84.86
- 79.01
- 76.65
- 75.57
- 75.07
- 71.61
- 70.96
- 70.90
- 69.60
- 52.78
- 41.90
- 37.17
- 35.90
- 35.25
- 31.08
- 27.70
- 27.41
- 25.45
- 23.03
- 18.76
- 16.20
- 15.90
- 10.68

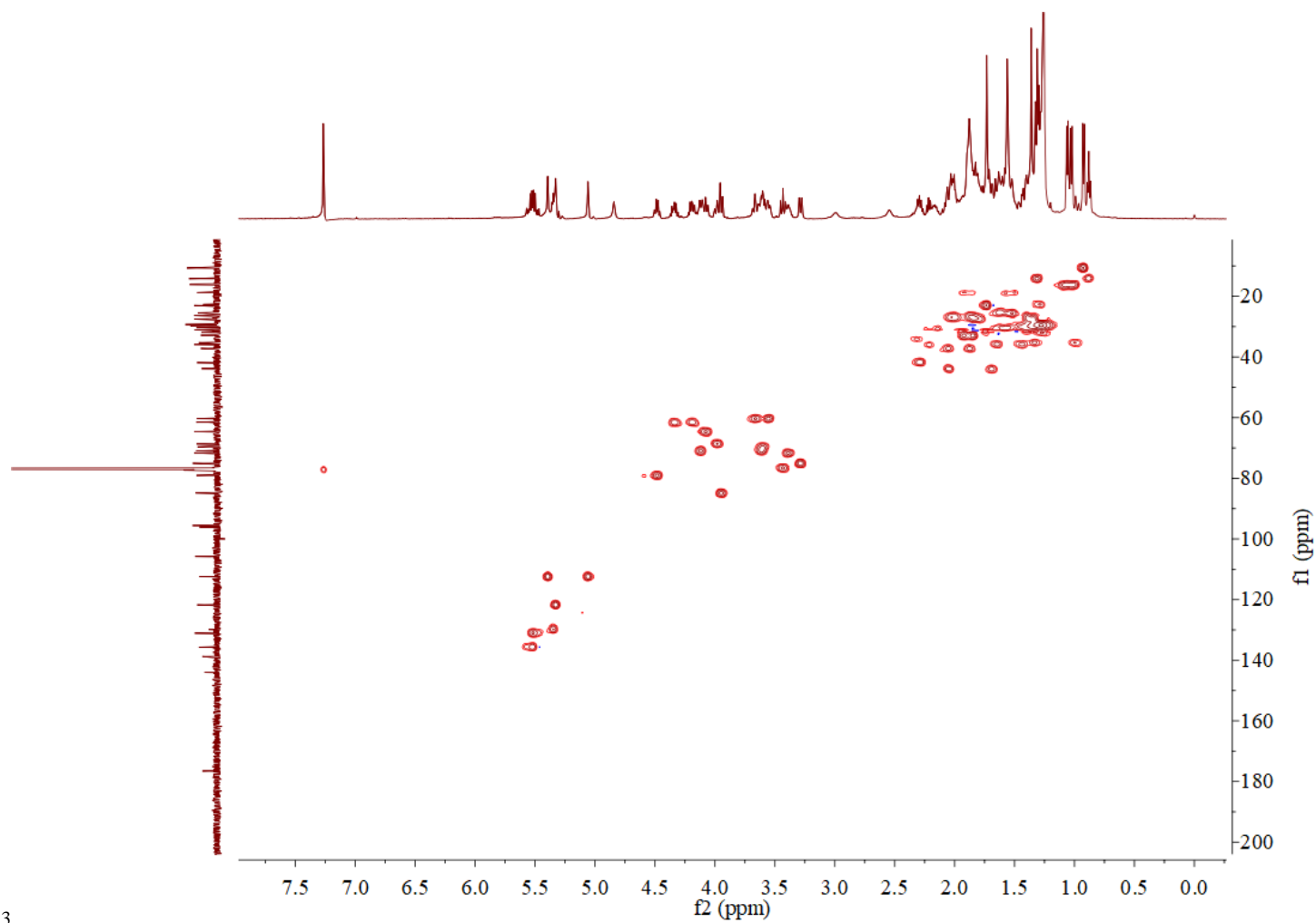
**Figure S7.**  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$ .



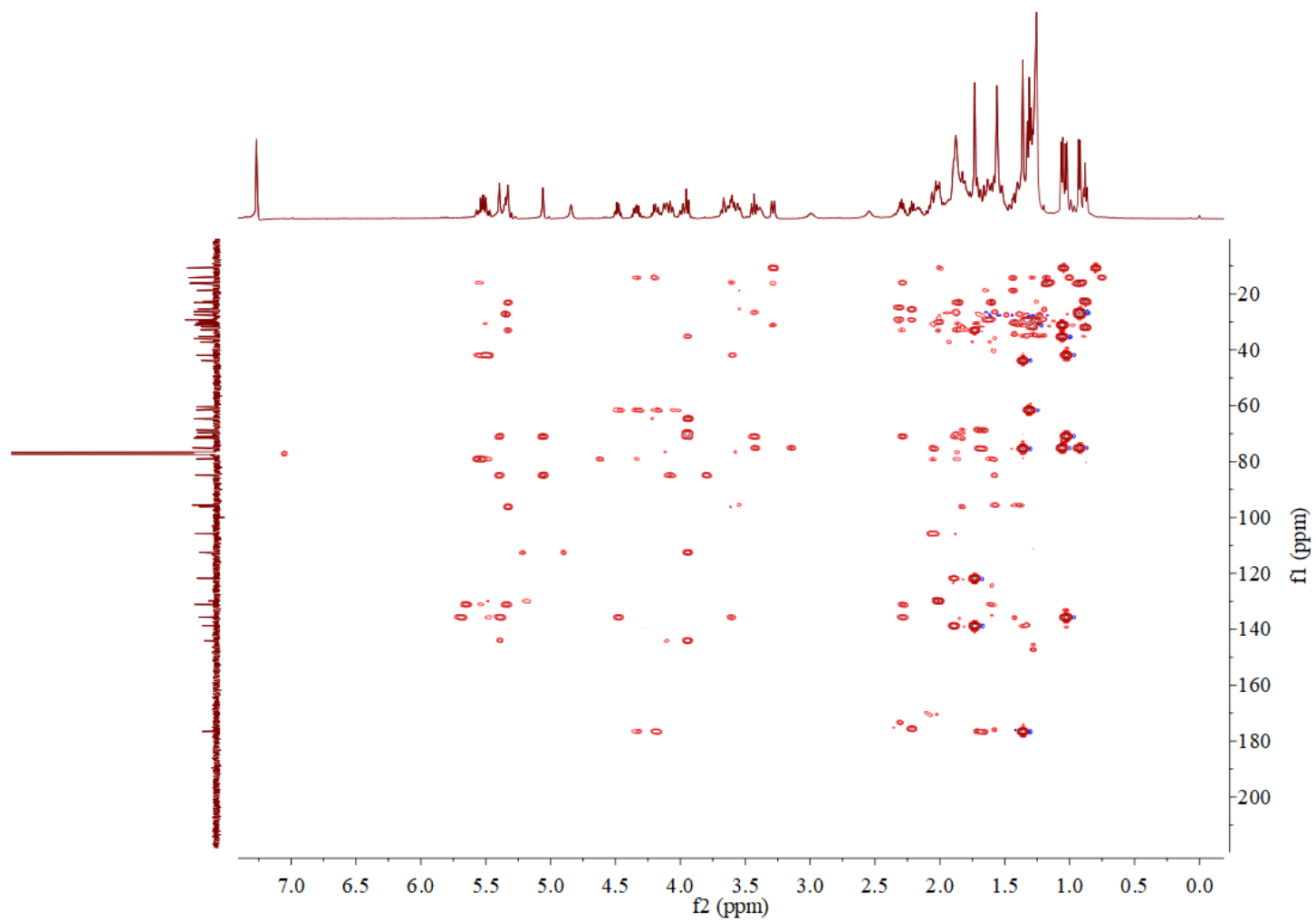
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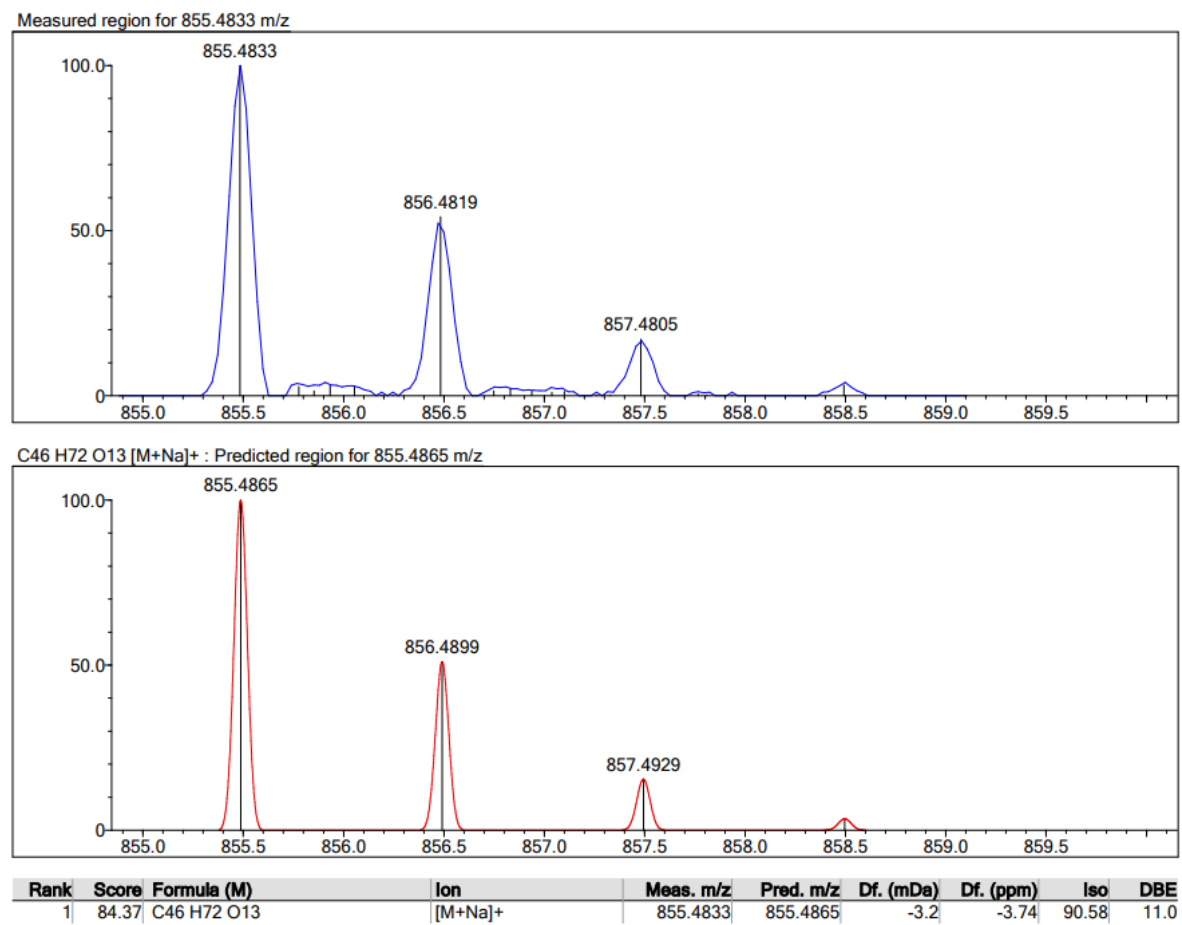
**Figure S9.** HSQC spectrum of **3** in CDCl<sub>3</sub>.



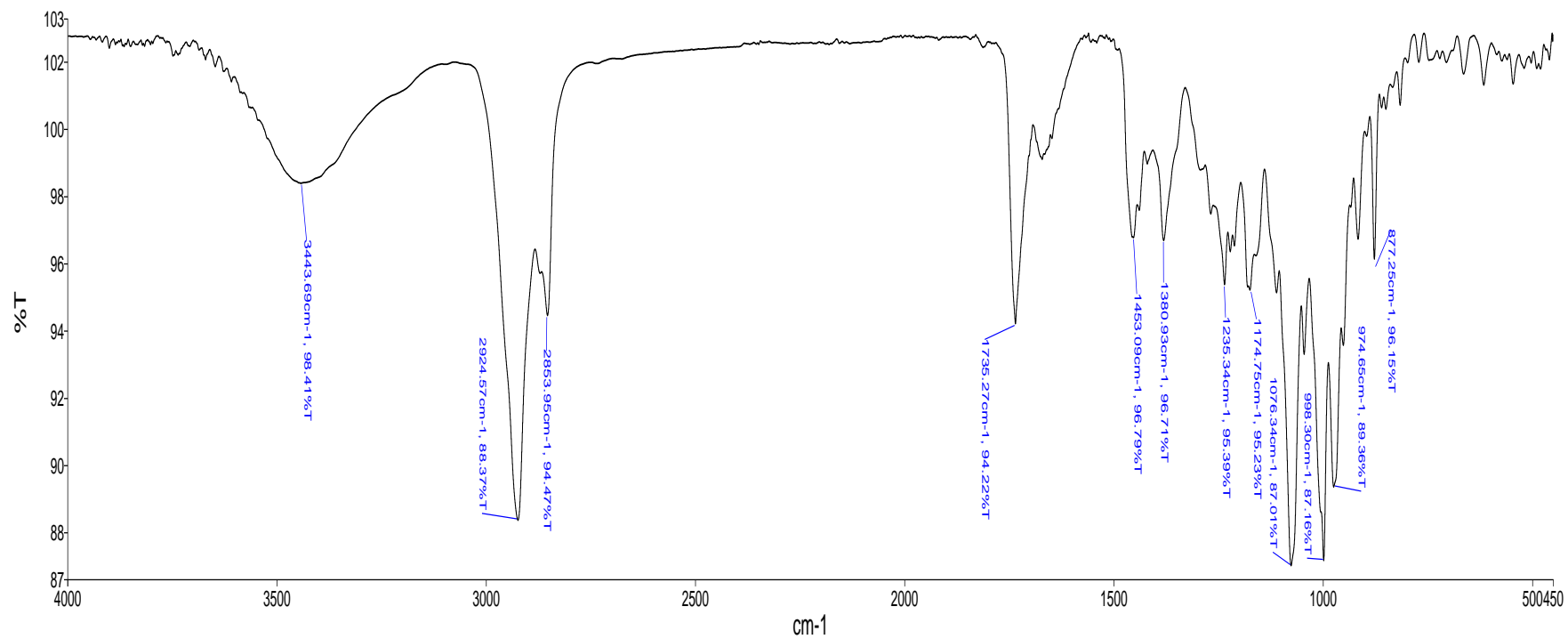
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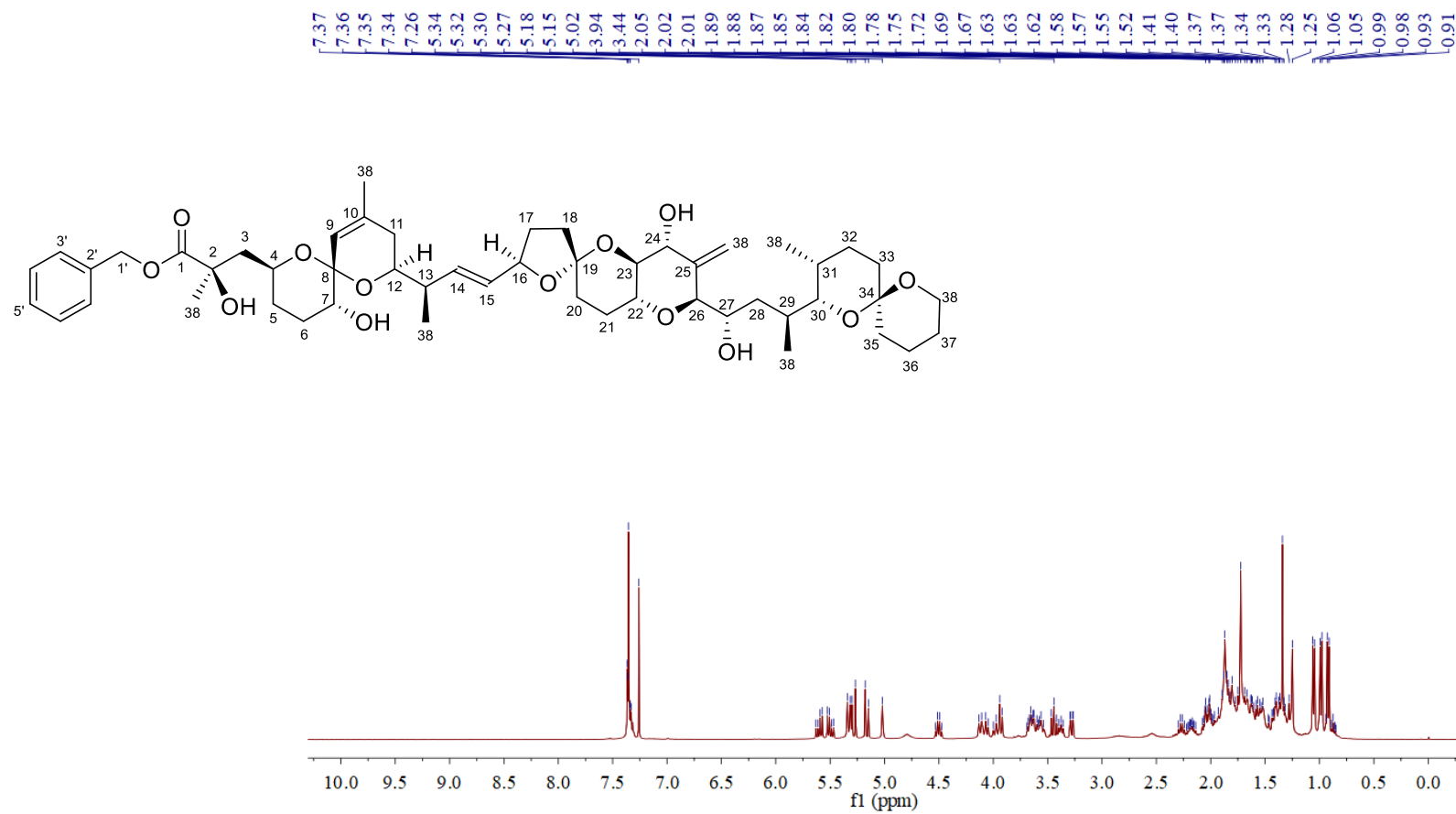
**Figure S11.** HRESIMS spectrum of **3**.



**Figure S12.** IR (KBr disc) spectrum of **3**.

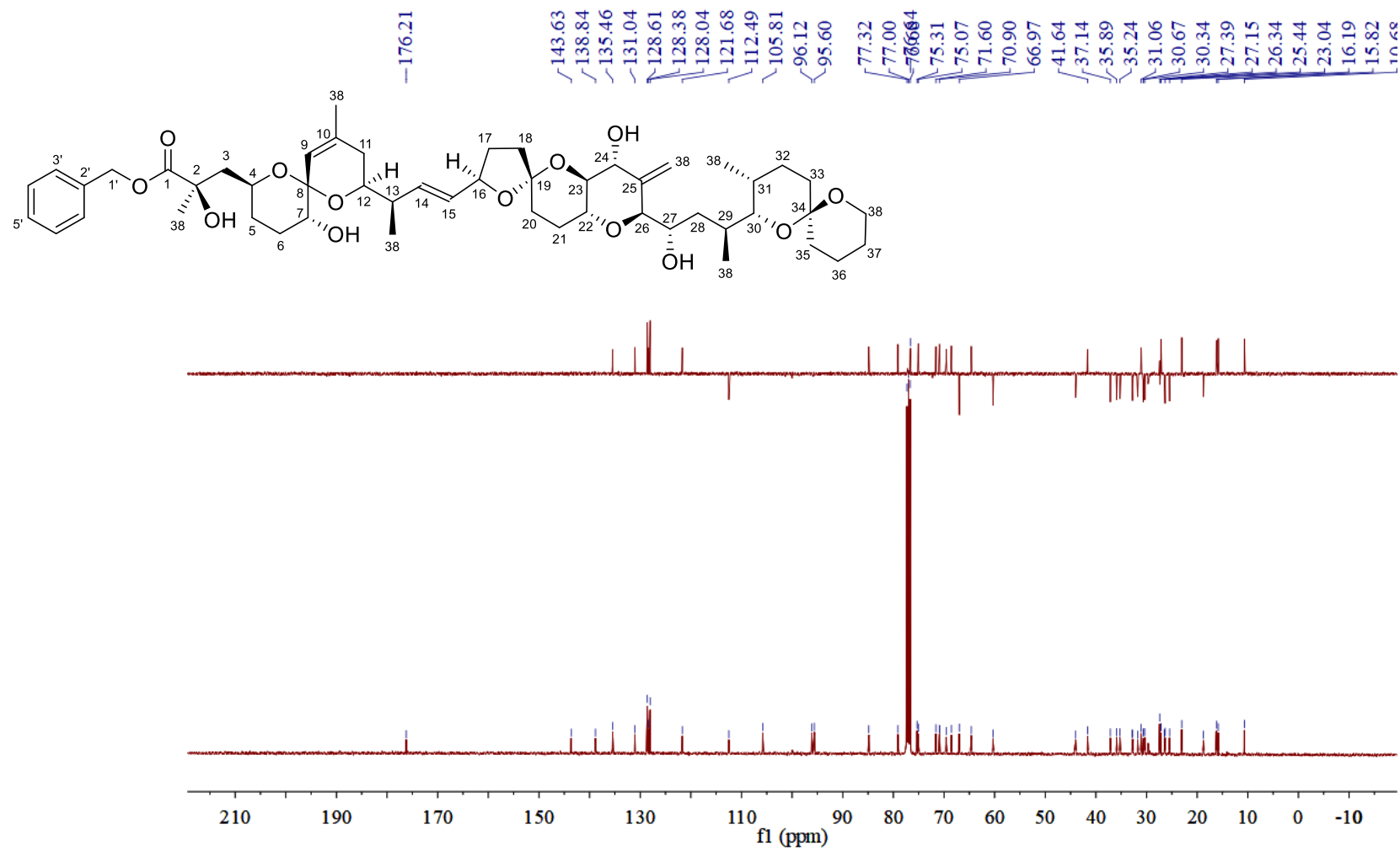


**Figure S13.**  $^1\text{H}$  NMR spectrum of **4** in  $\text{CDCl}_3$ .

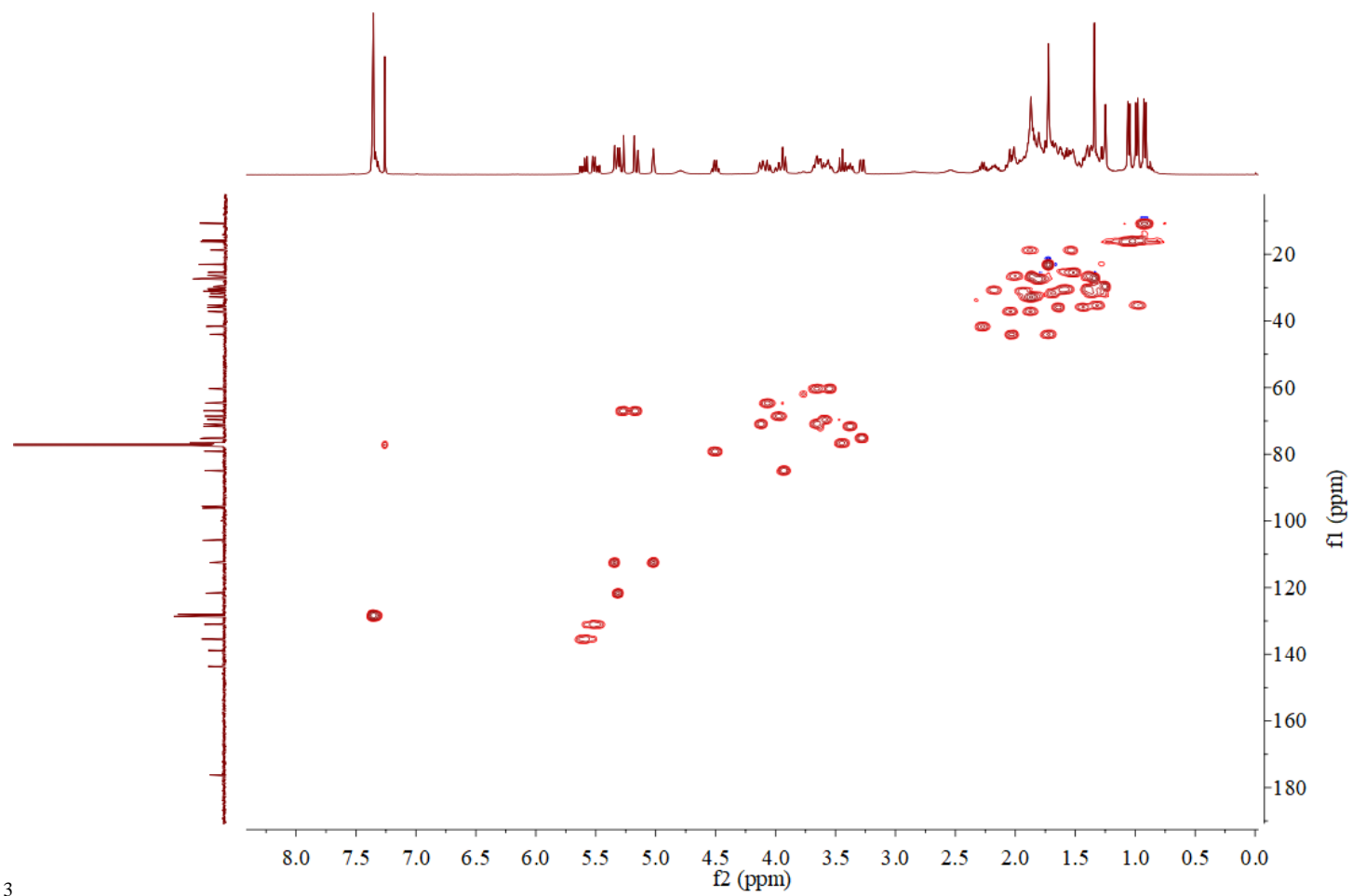




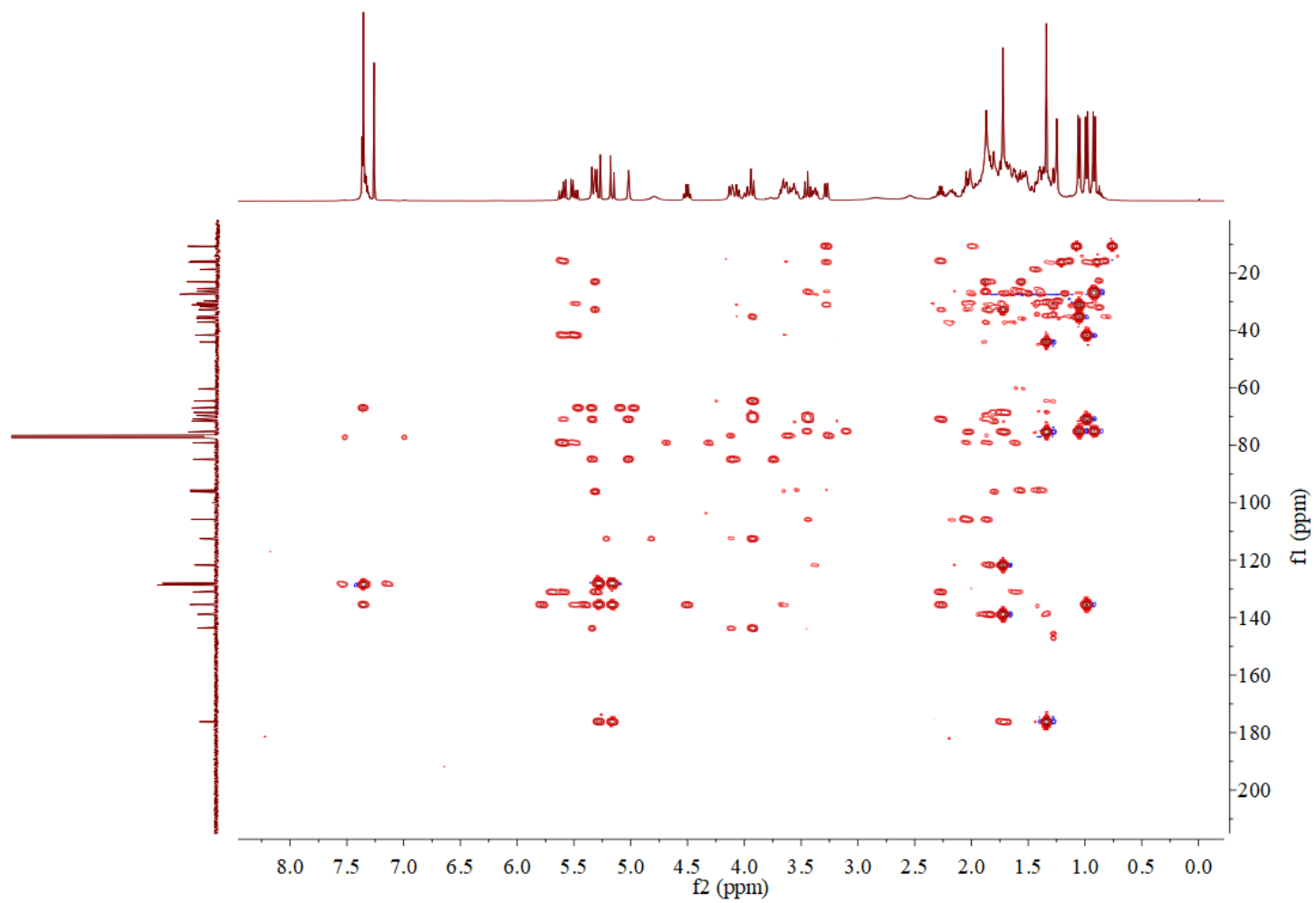
**Figure S14.**  $^{13}\text{C}$  NMR and DEPT 135 spectra of **4** in  $\text{CDCl}_3$ .



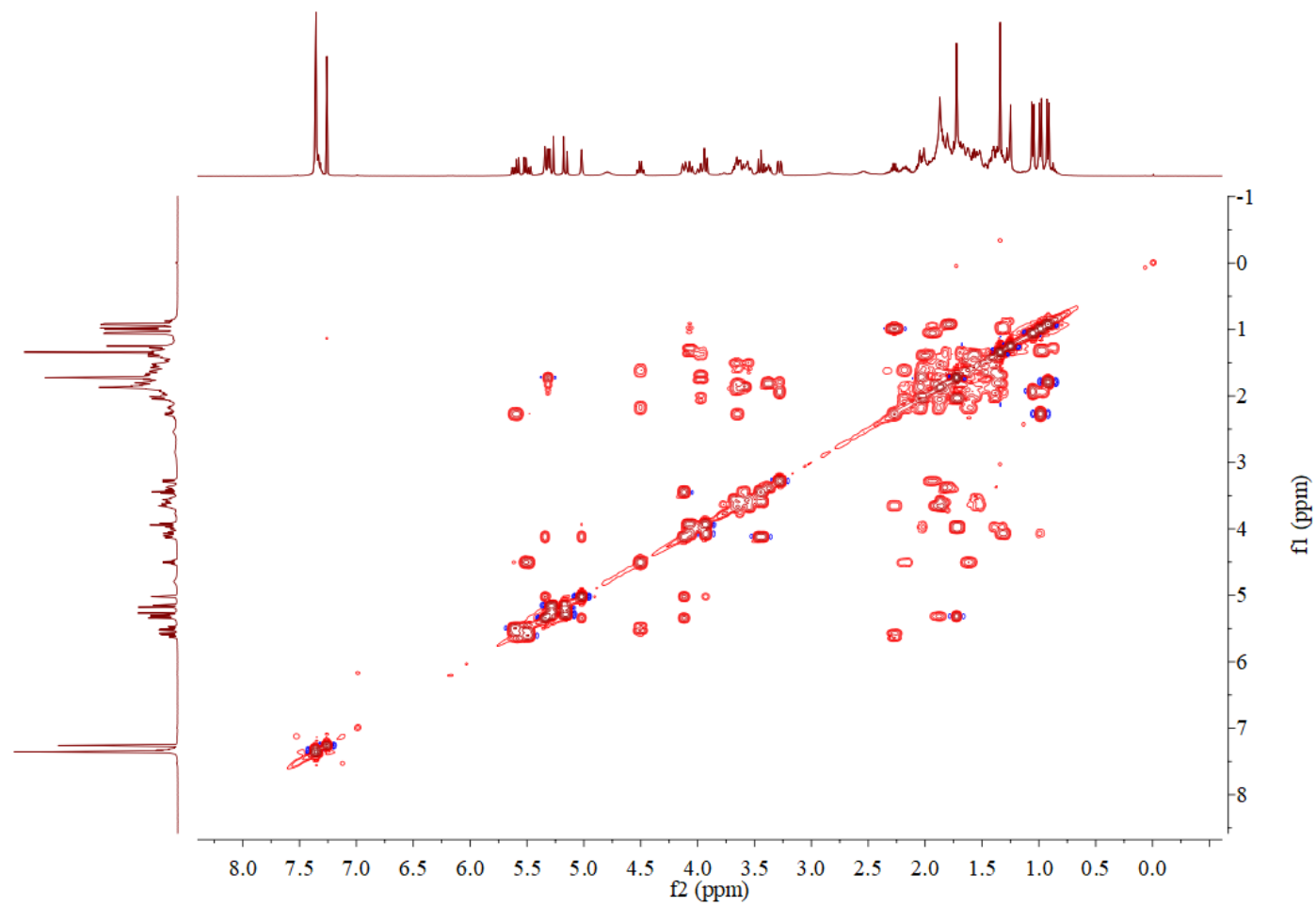
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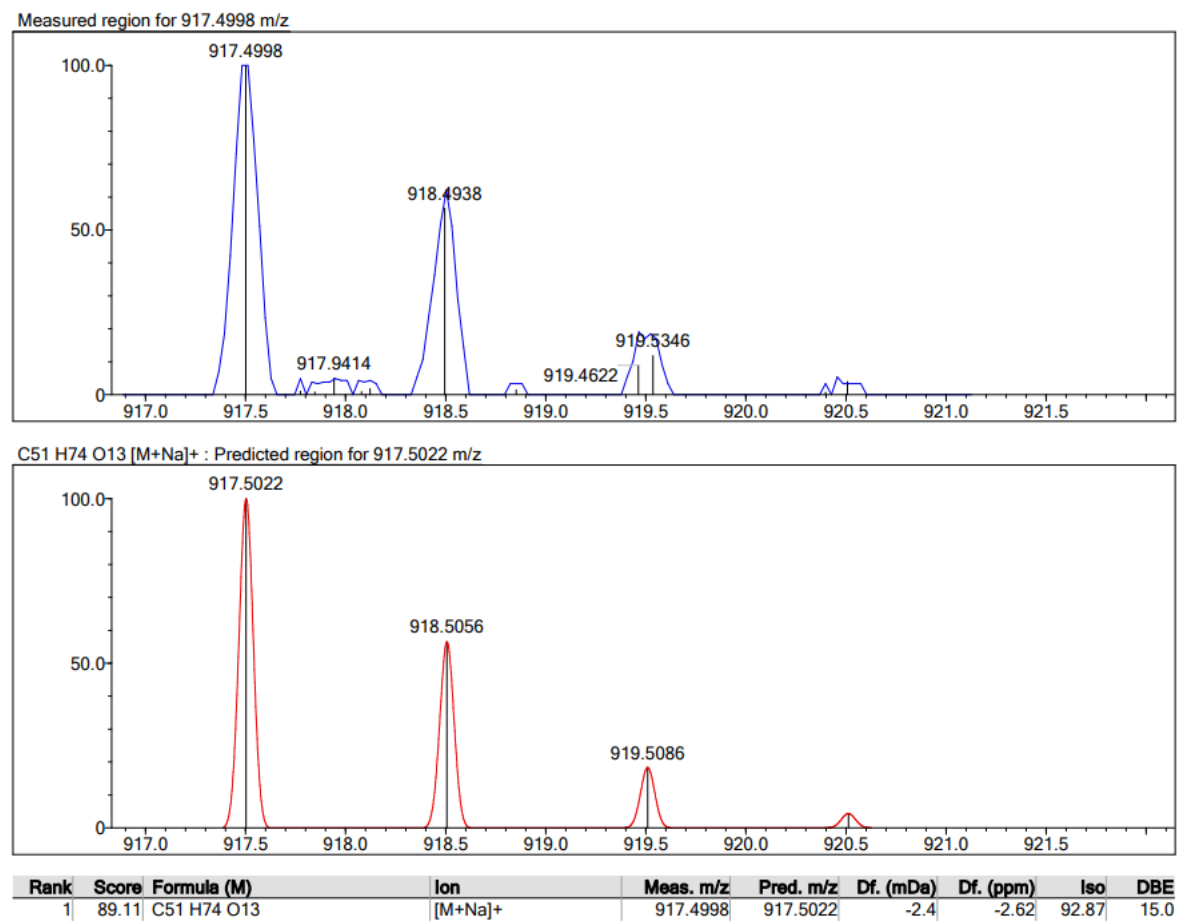
**Figure S16.** HMBC spectrum of **4** in CDCl<sub>3</sub>.



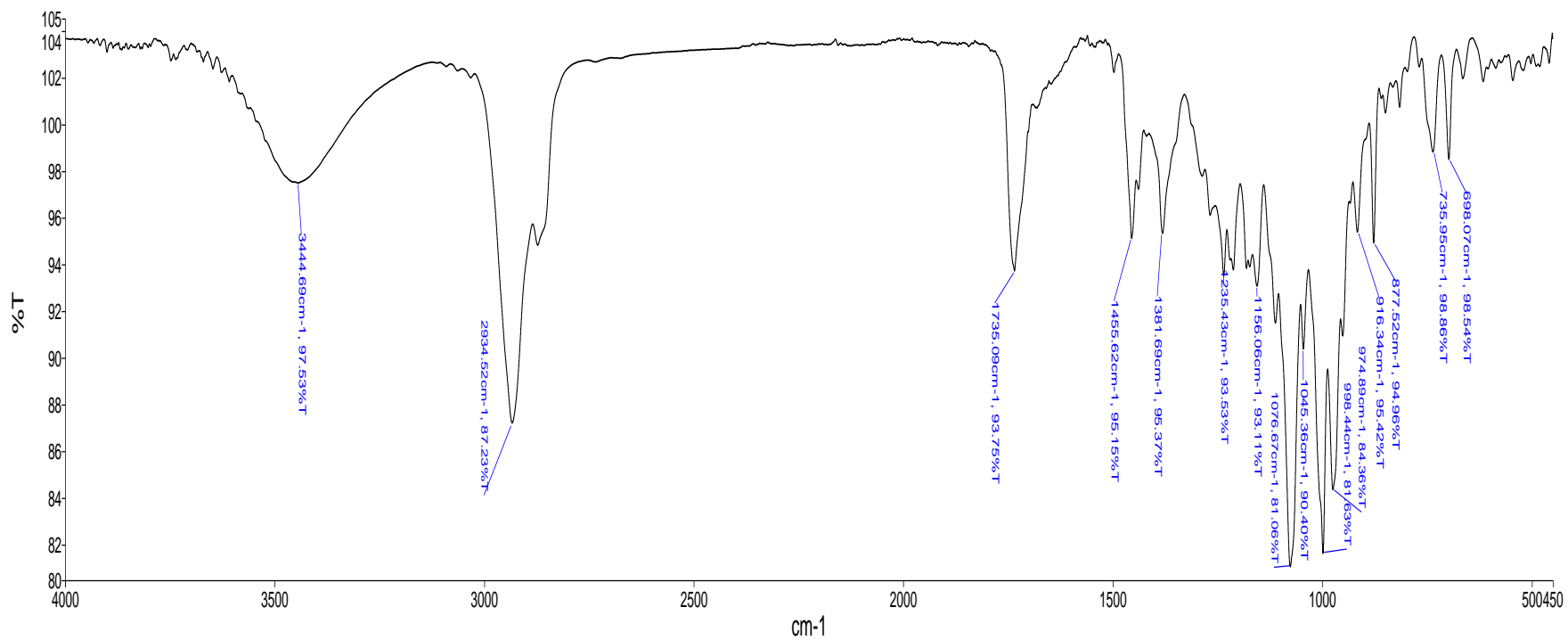
**Figure S17.**  $^1\text{H}$ – $^1\text{H}$  COSY spectrum of **4** in  $\text{CDCl}_3$ .



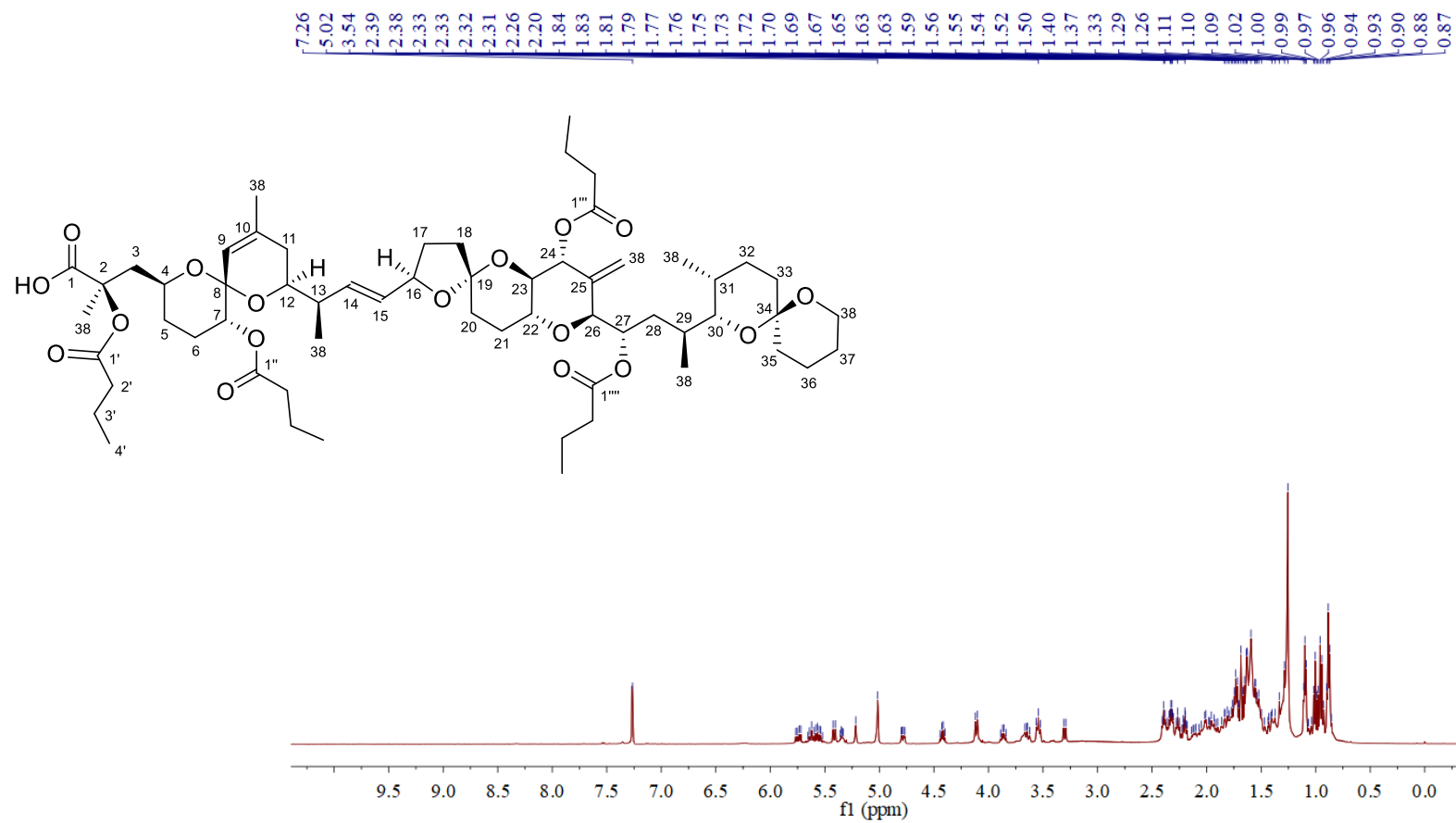
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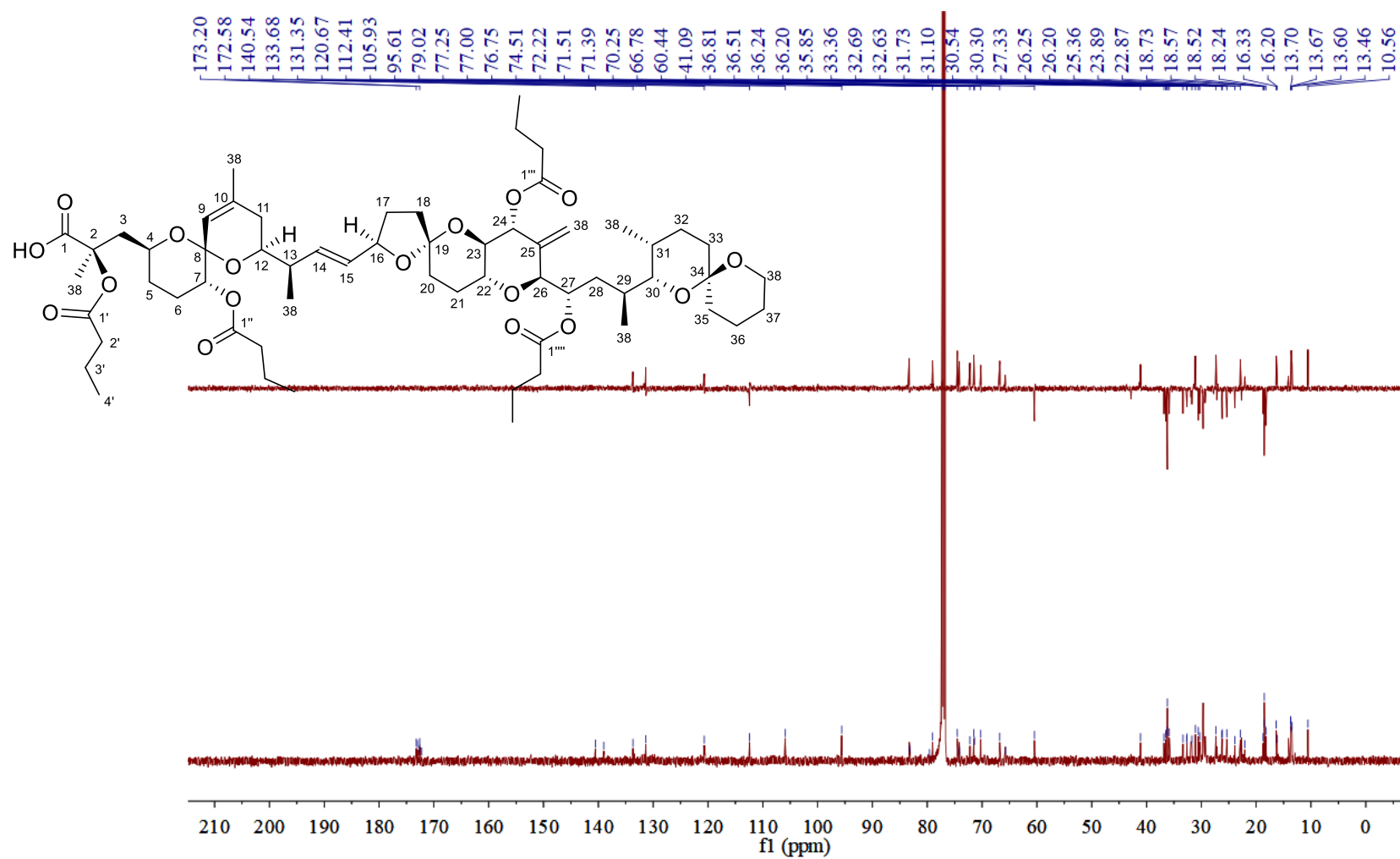
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**Figure S20.**  $^1\text{H}$  NMR spectrum of **5** in  $\text{CDCl}_3$ .

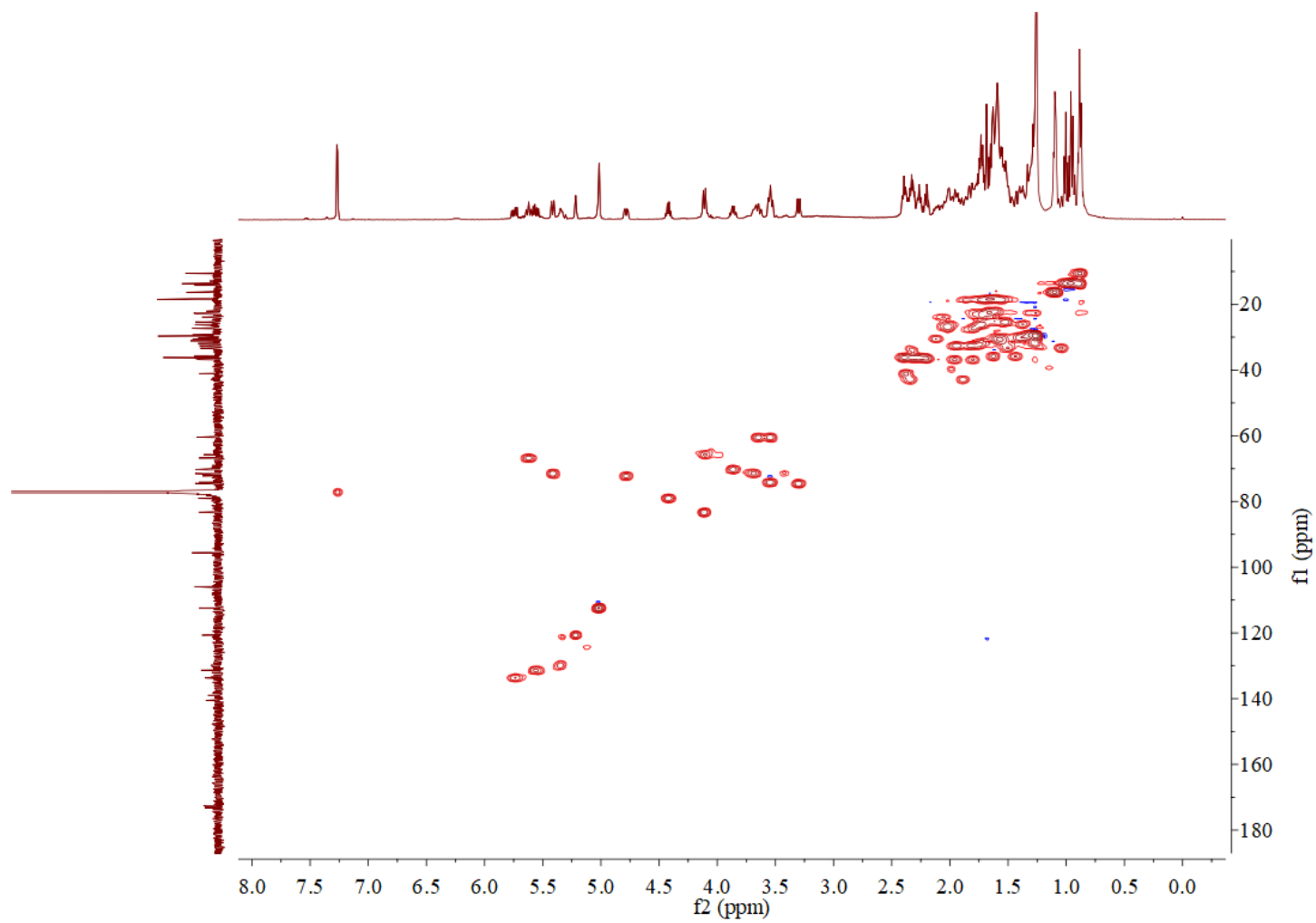


**Figure S21.**  $^{13}\text{C}$  NMR and DEPT 135 spectra of **5** in  $\text{CDCl}_3$ .

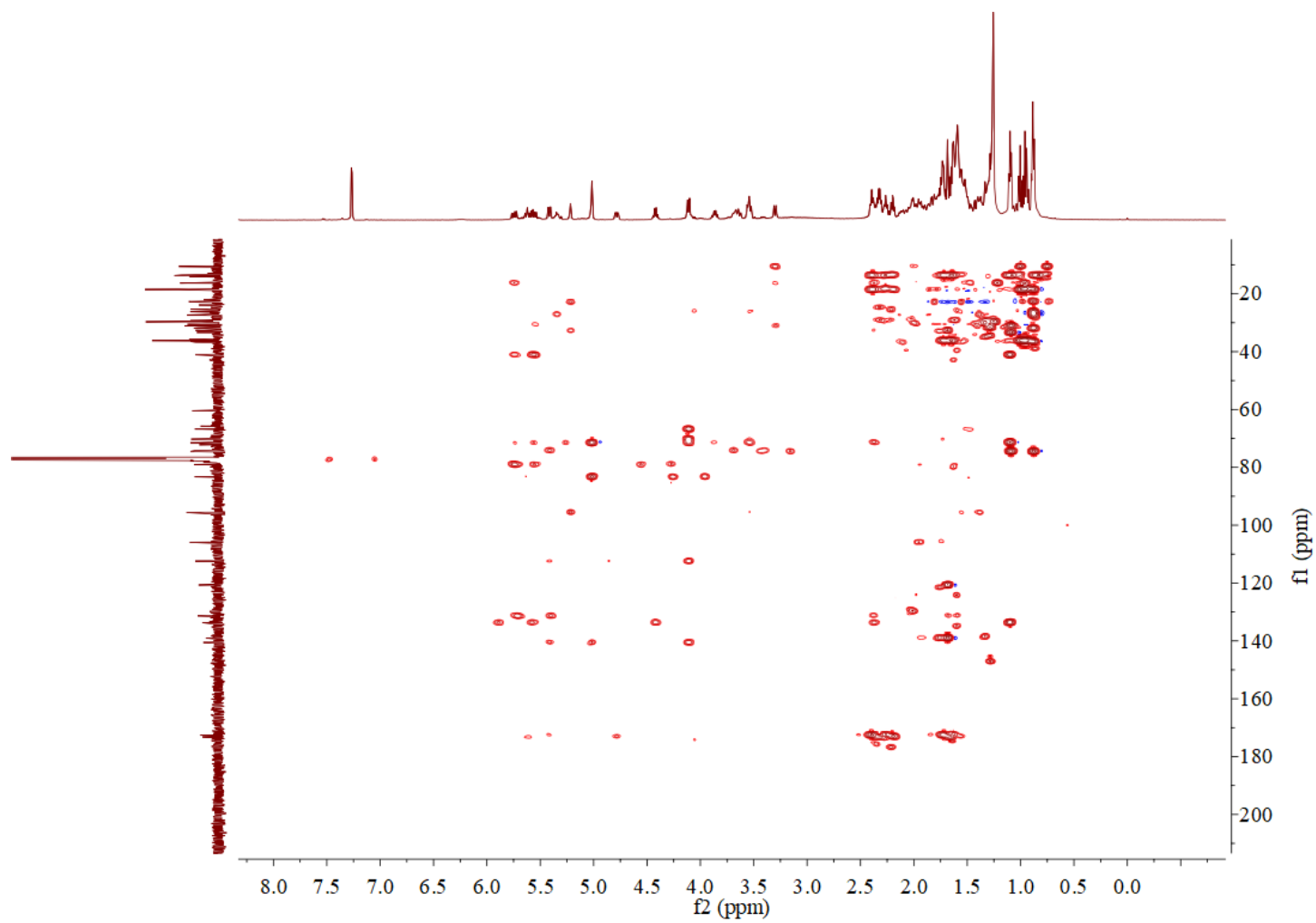




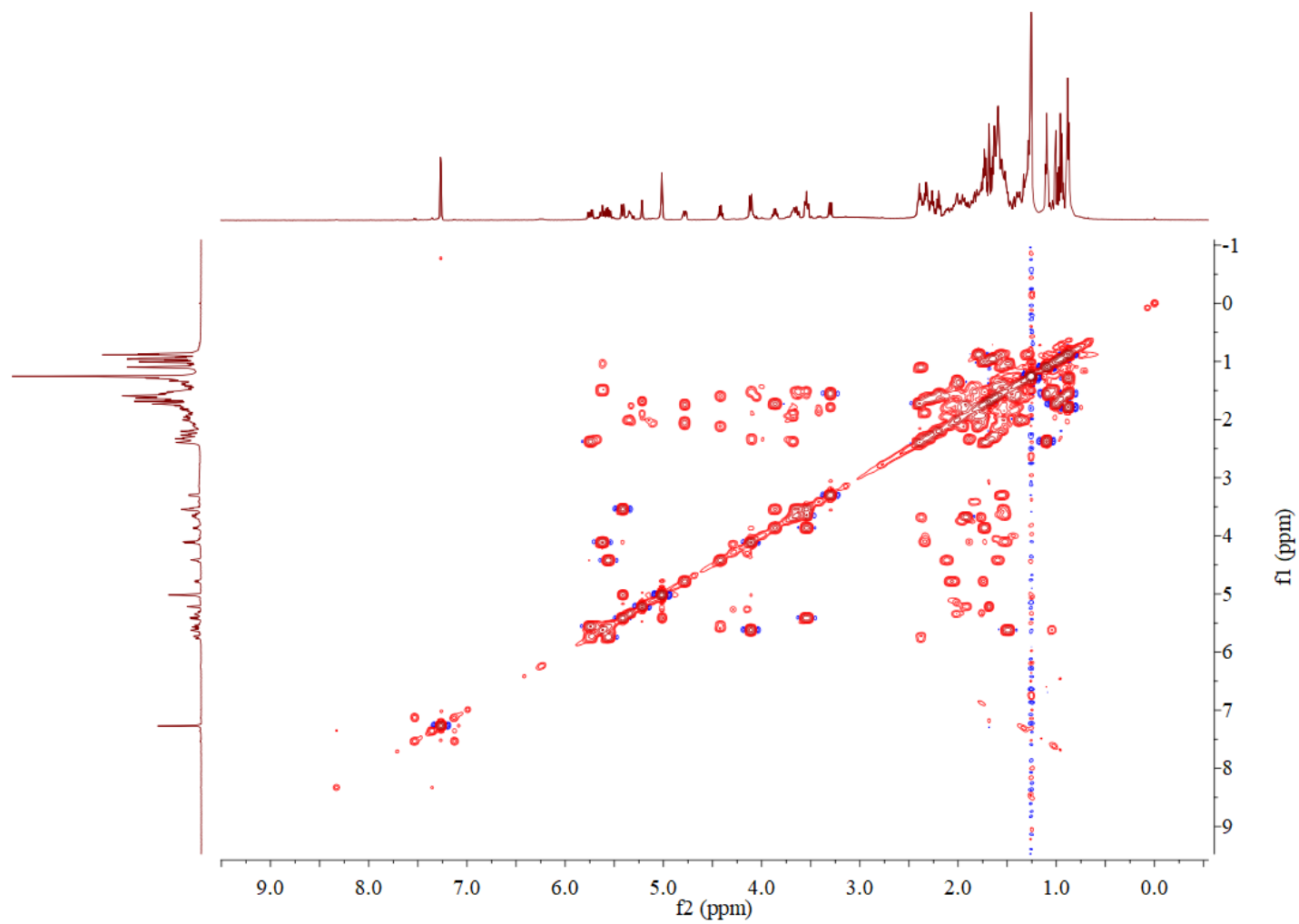
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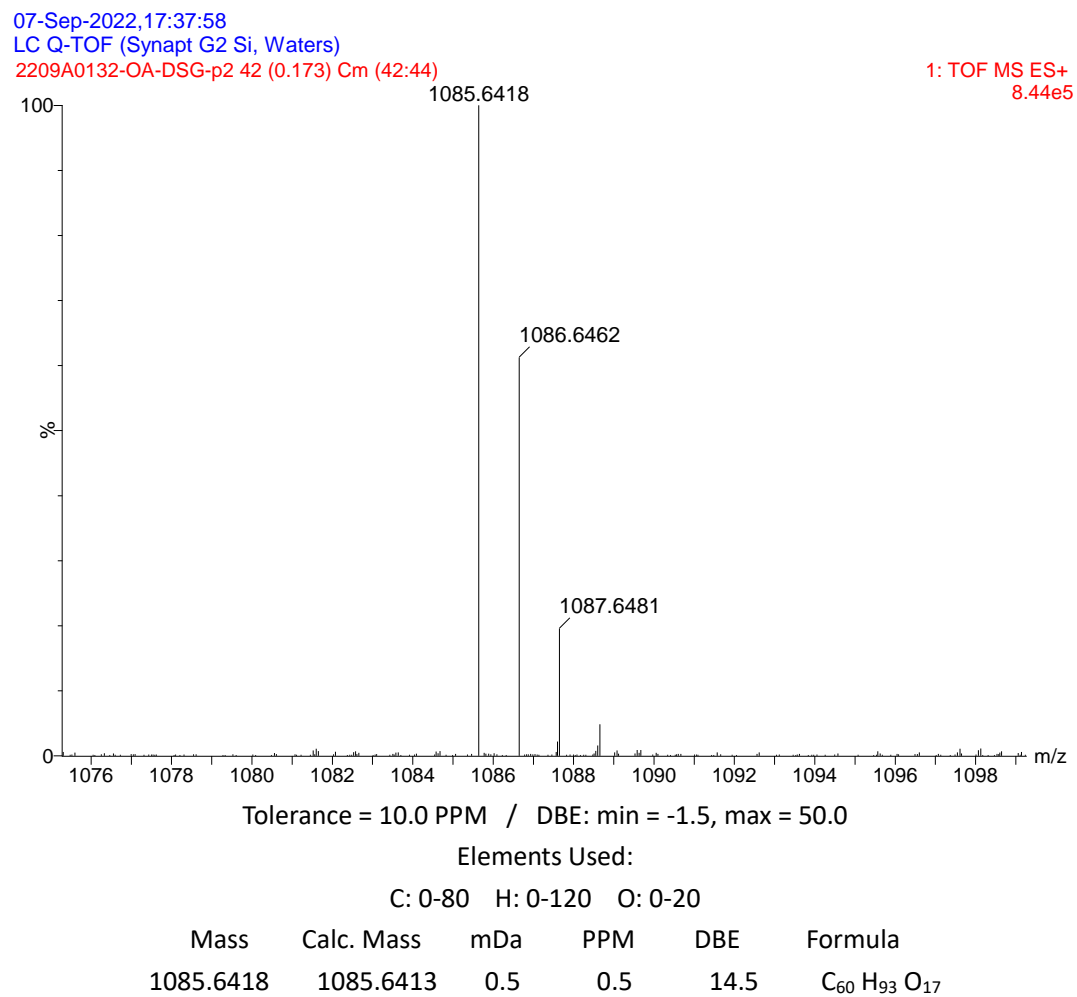
**Figure S23.** HMBC spectrum of **5** in CDCl<sub>3</sub>.



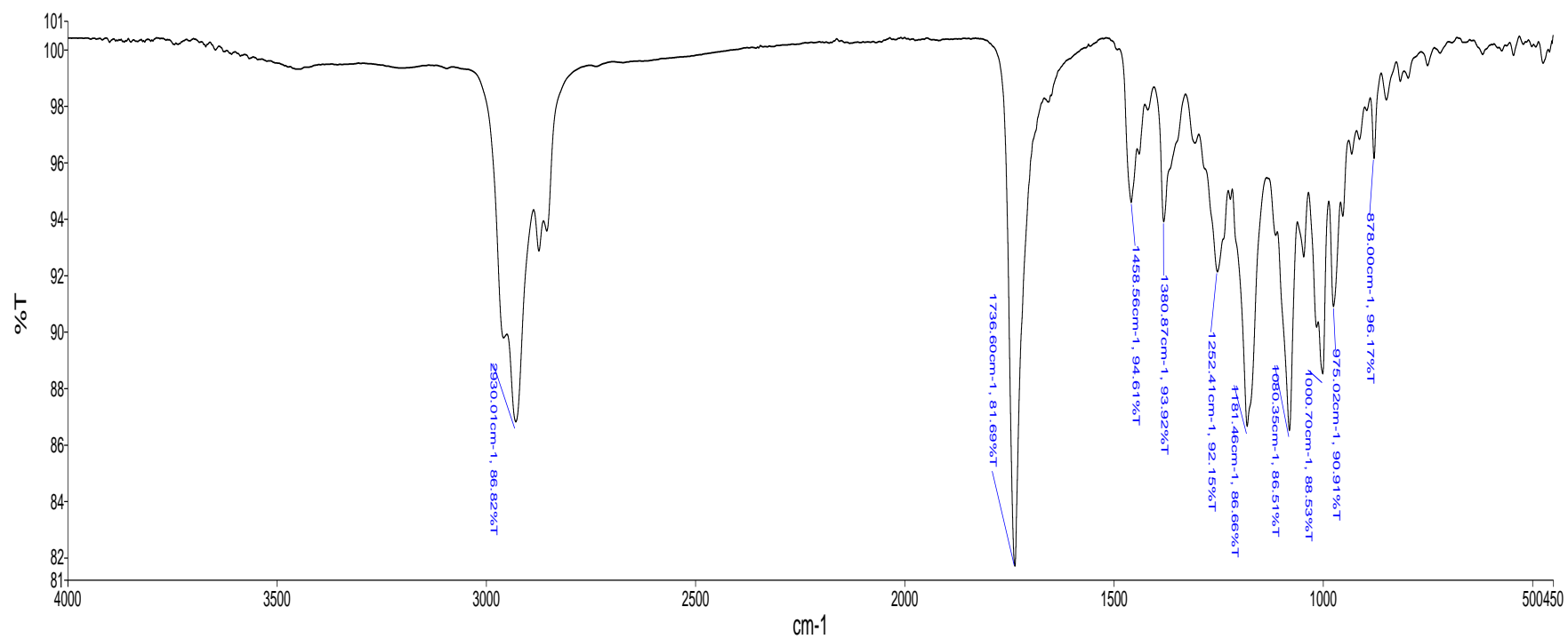
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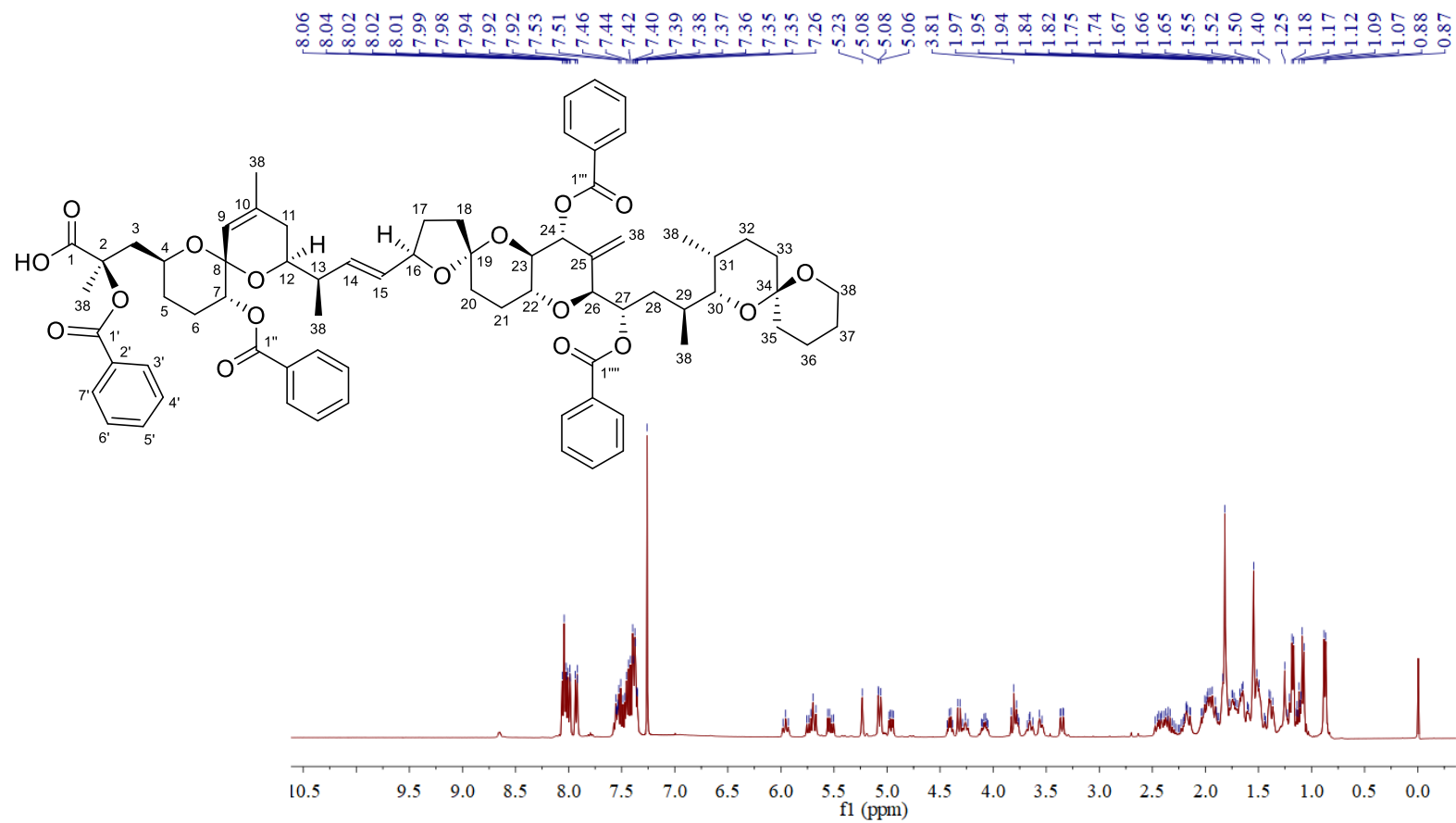
**Figure S25.** HRESIMS spectrum of **5**.



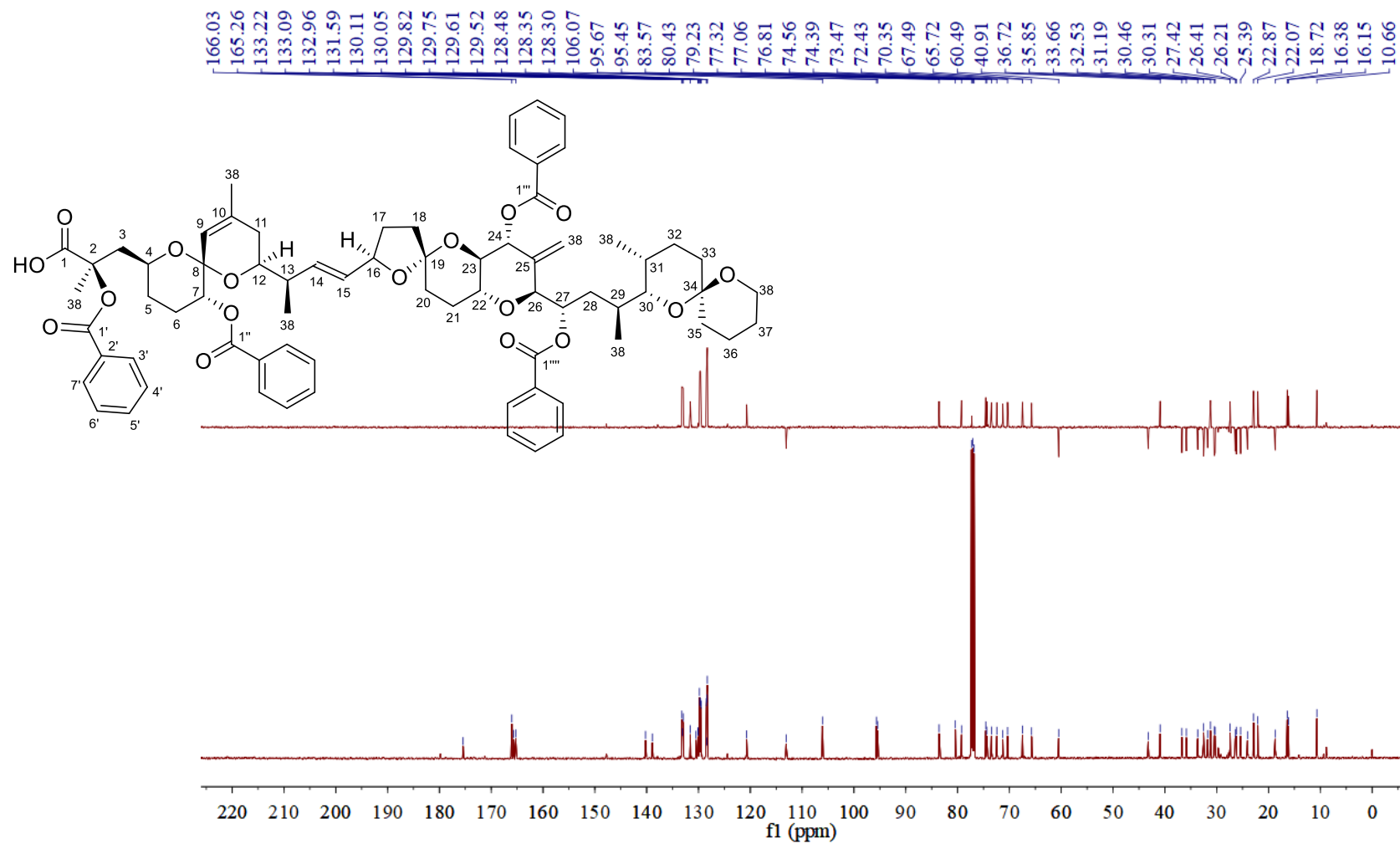
**Figure S26.** IR (KBr disc) spectrum of **5**.



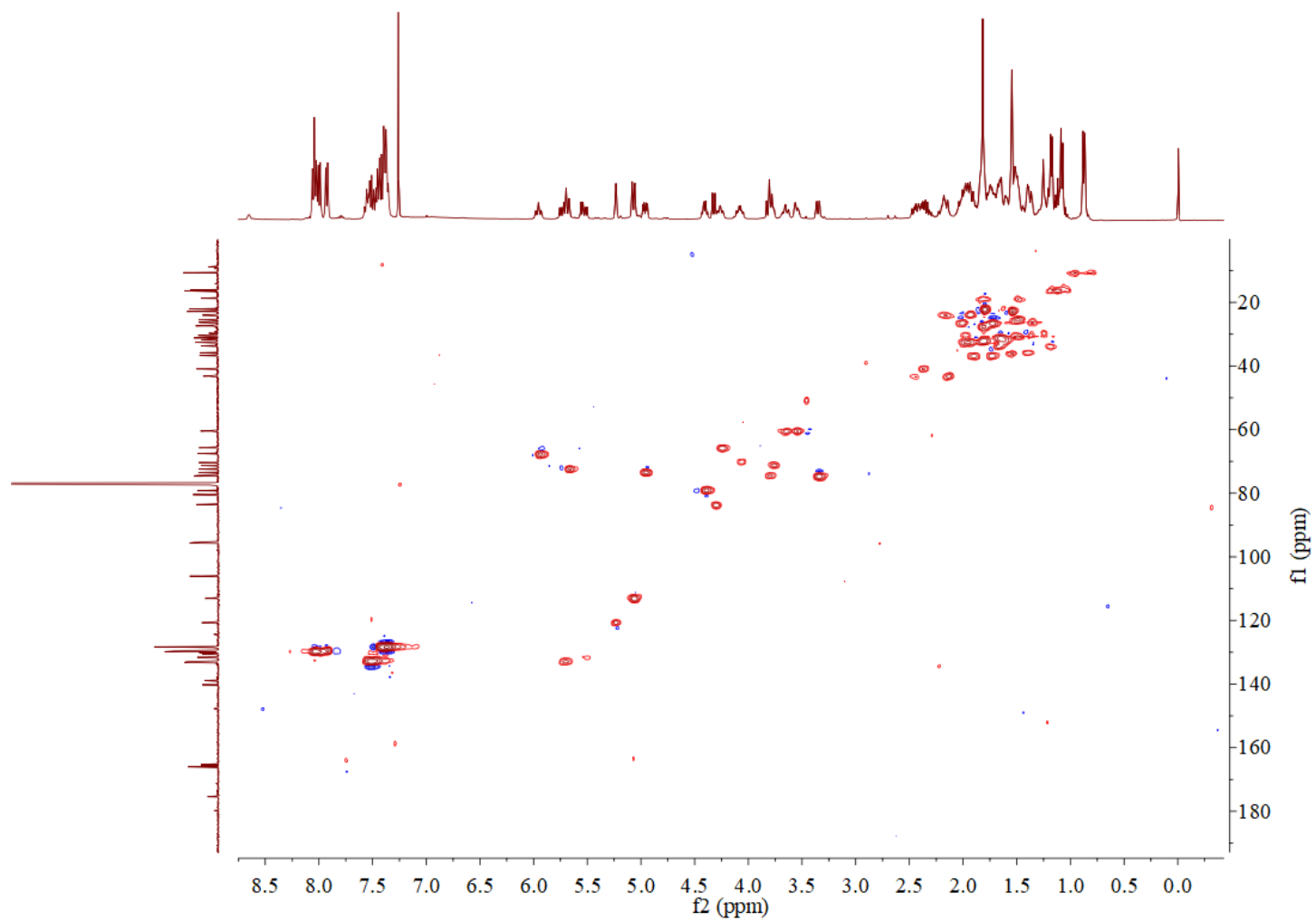
**Figure S27.**  $^1\text{H}$  NMR spectrum of **6** in  $\text{CDCl}_3$ .



**Figure S28.**  $^{13}\text{C}$  NMR and DEPT 135 spectra of **6** in  $\text{CDCl}_3$ .

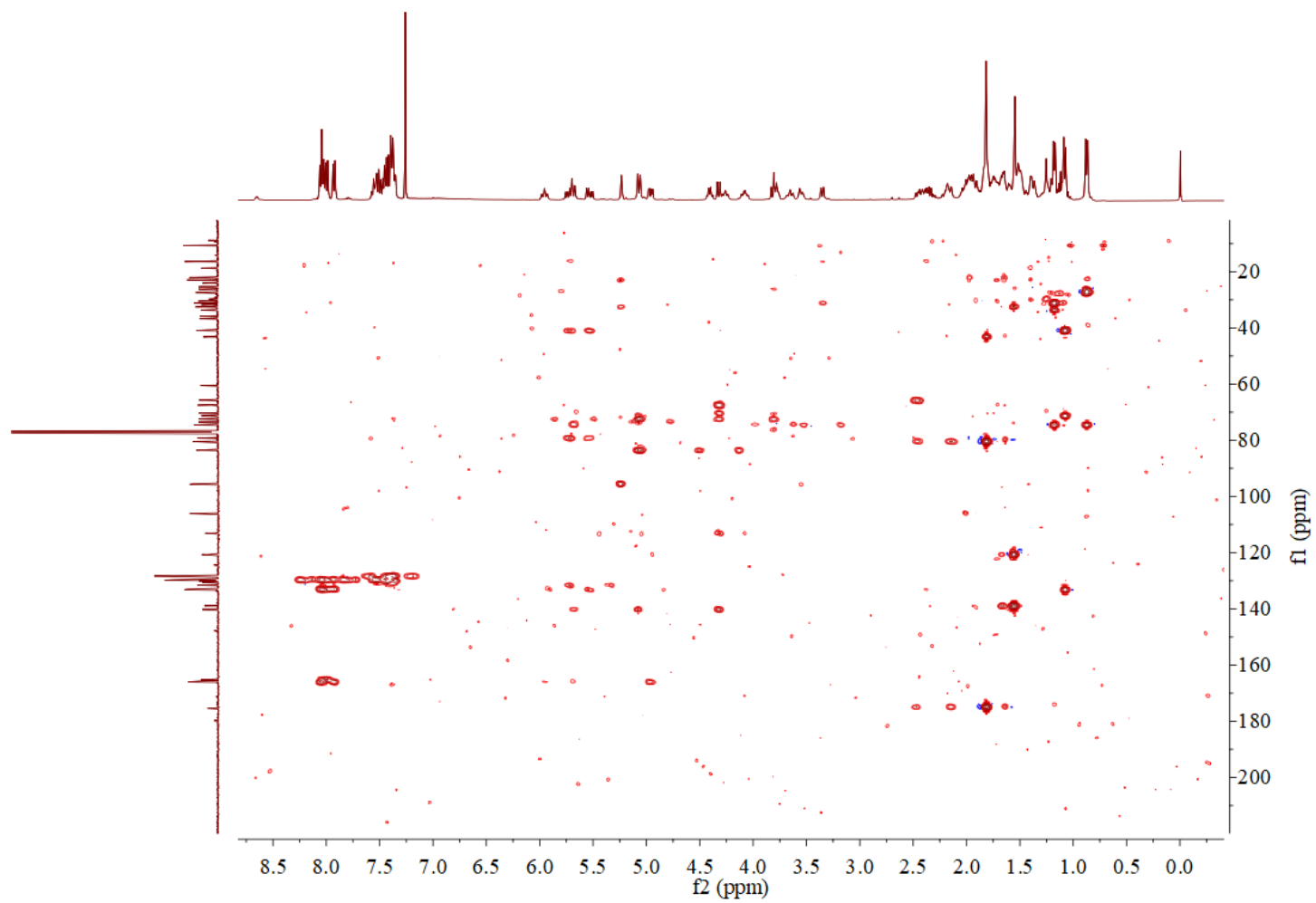


**Figure S29.** HSQC spectrum of **6** in CDCl<sub>3</sub>.

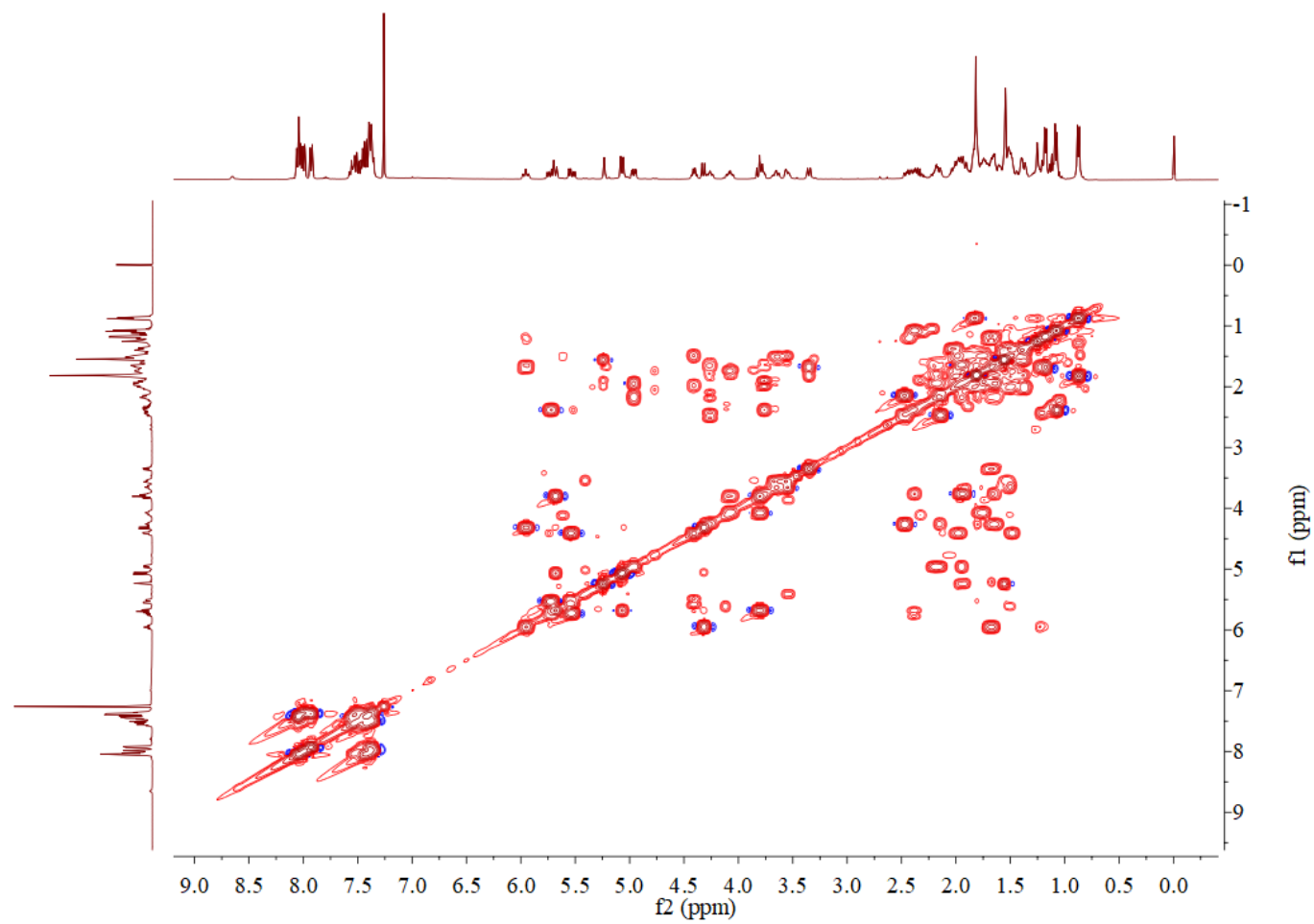




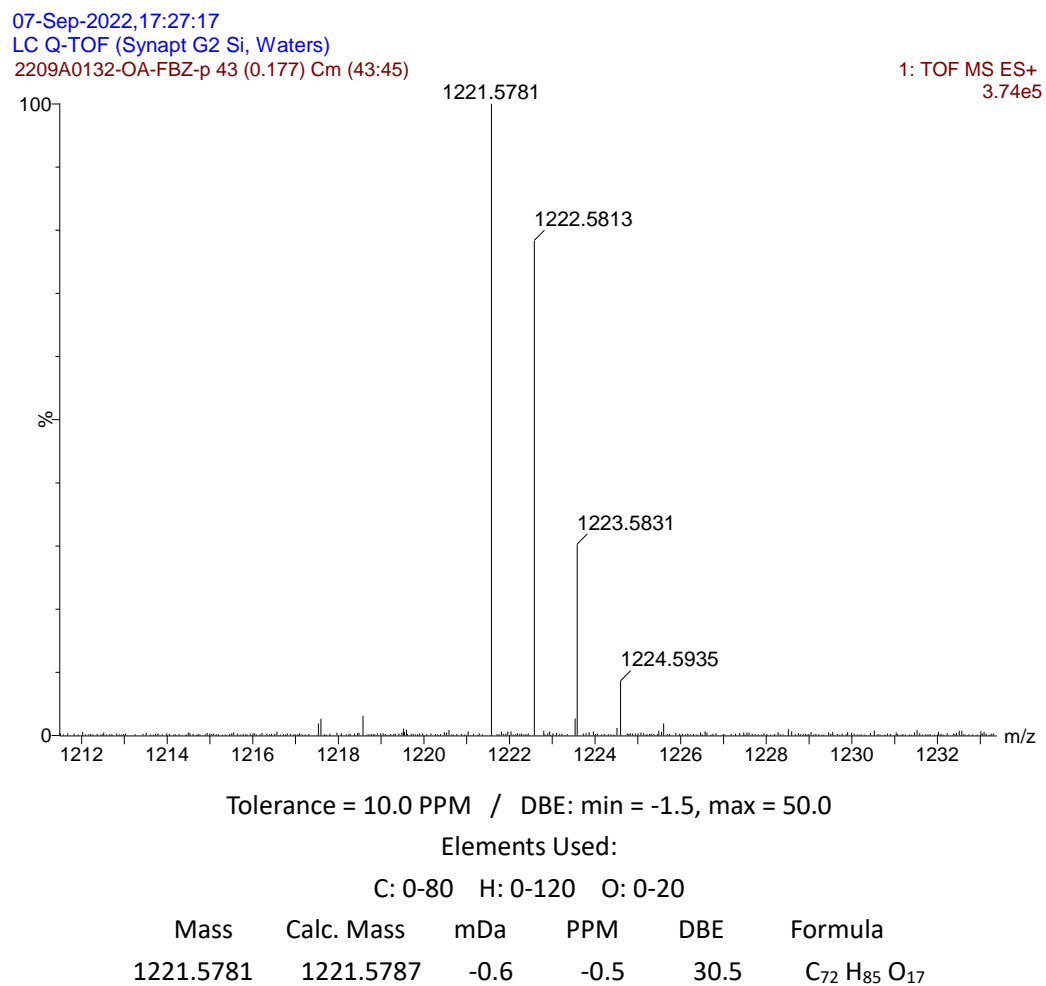
**Figure S30.** HMBC spectrum of **6** in CDCl<sub>3</sub>.



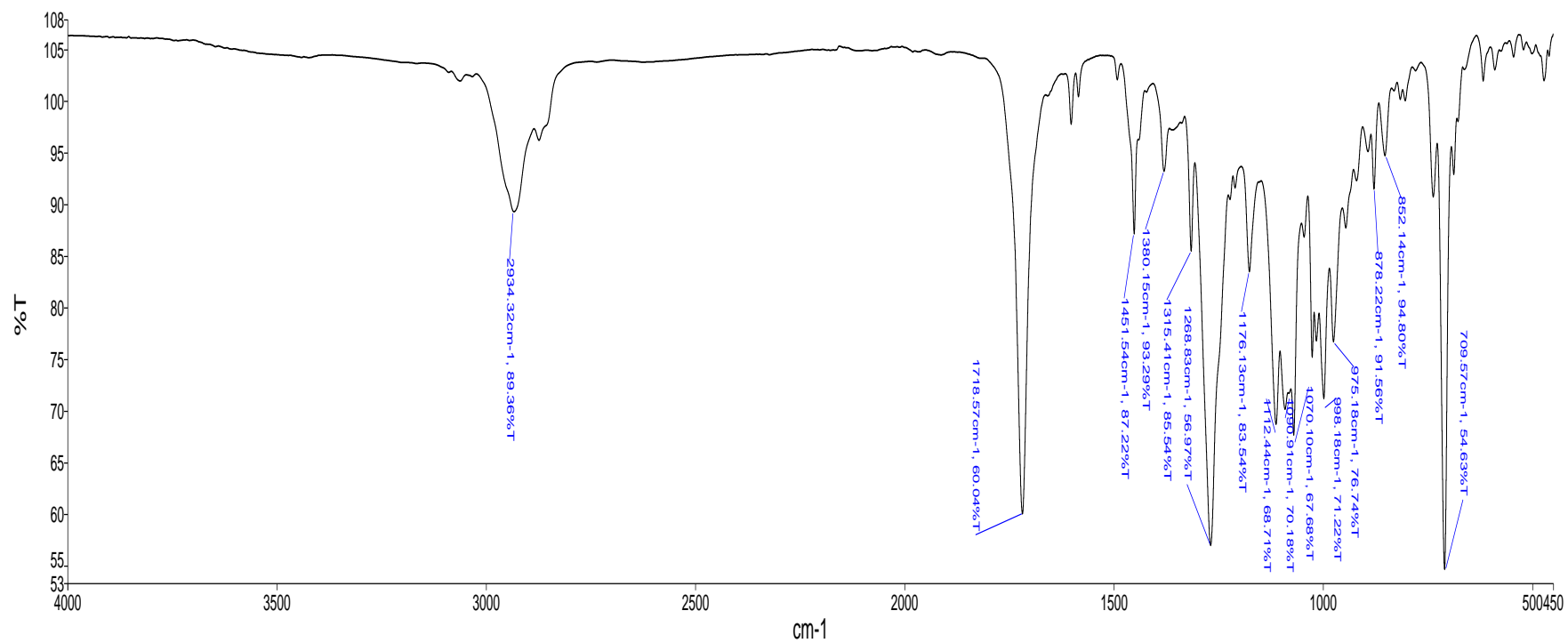
**Figure S31.**  $^1\text{H}$ – $^1\text{H}$  COSY spectrum of **6** in  $\text{CDCl}_3$ .



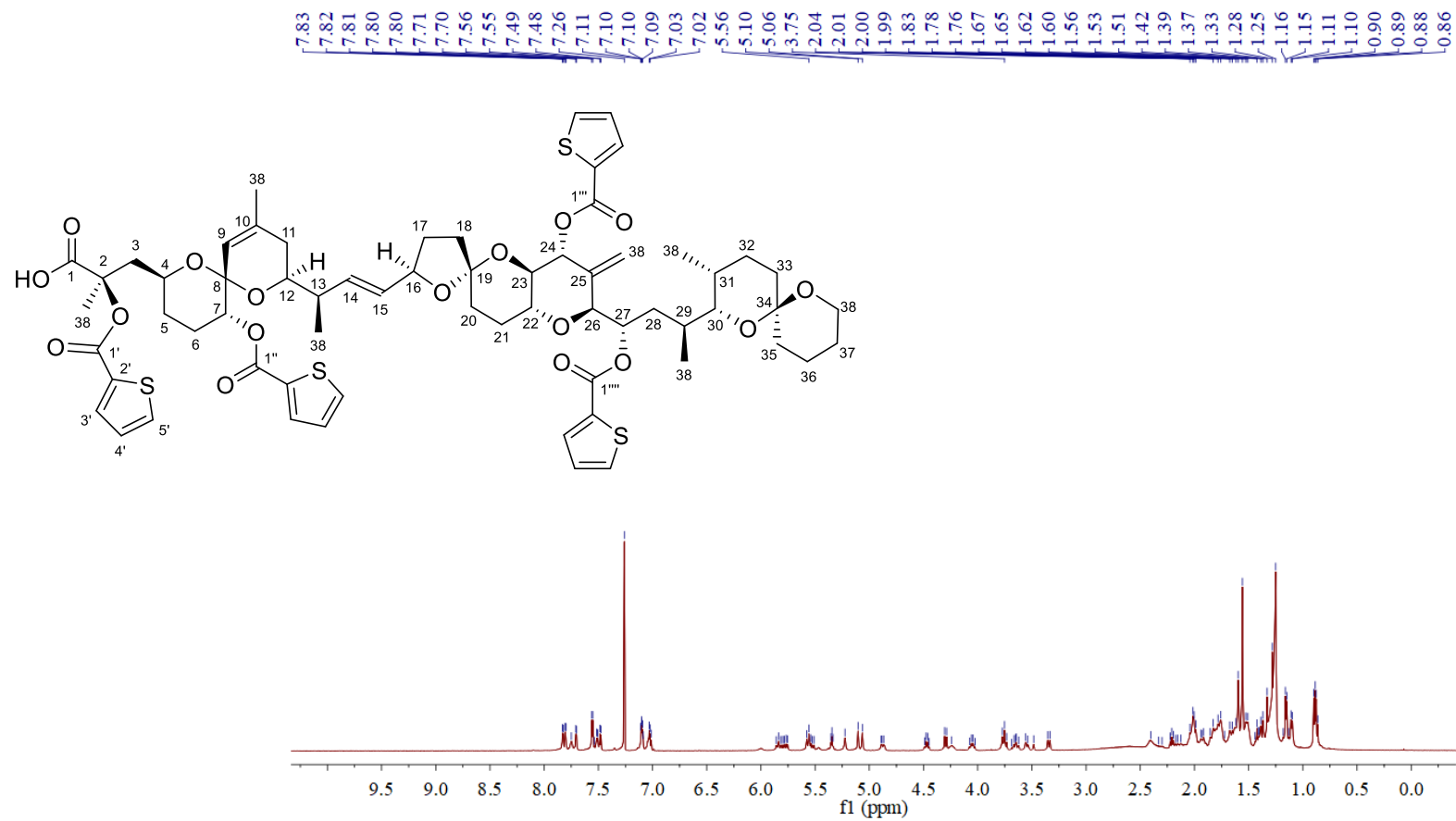
**Figure S32.** HRESIMS spectrum of **6**.



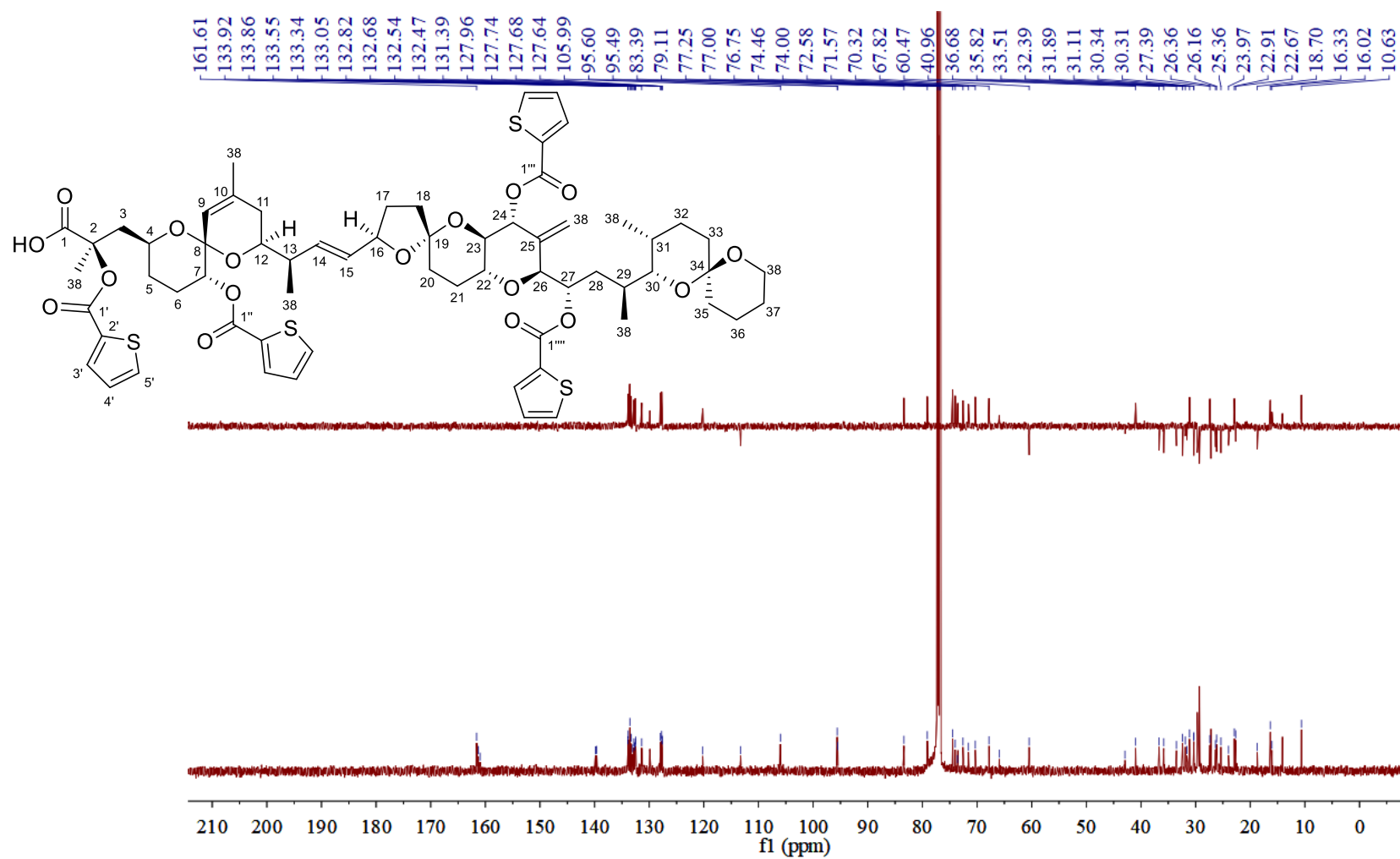
**Figure S33.** IR (KBr disc) spectrum of **6**.



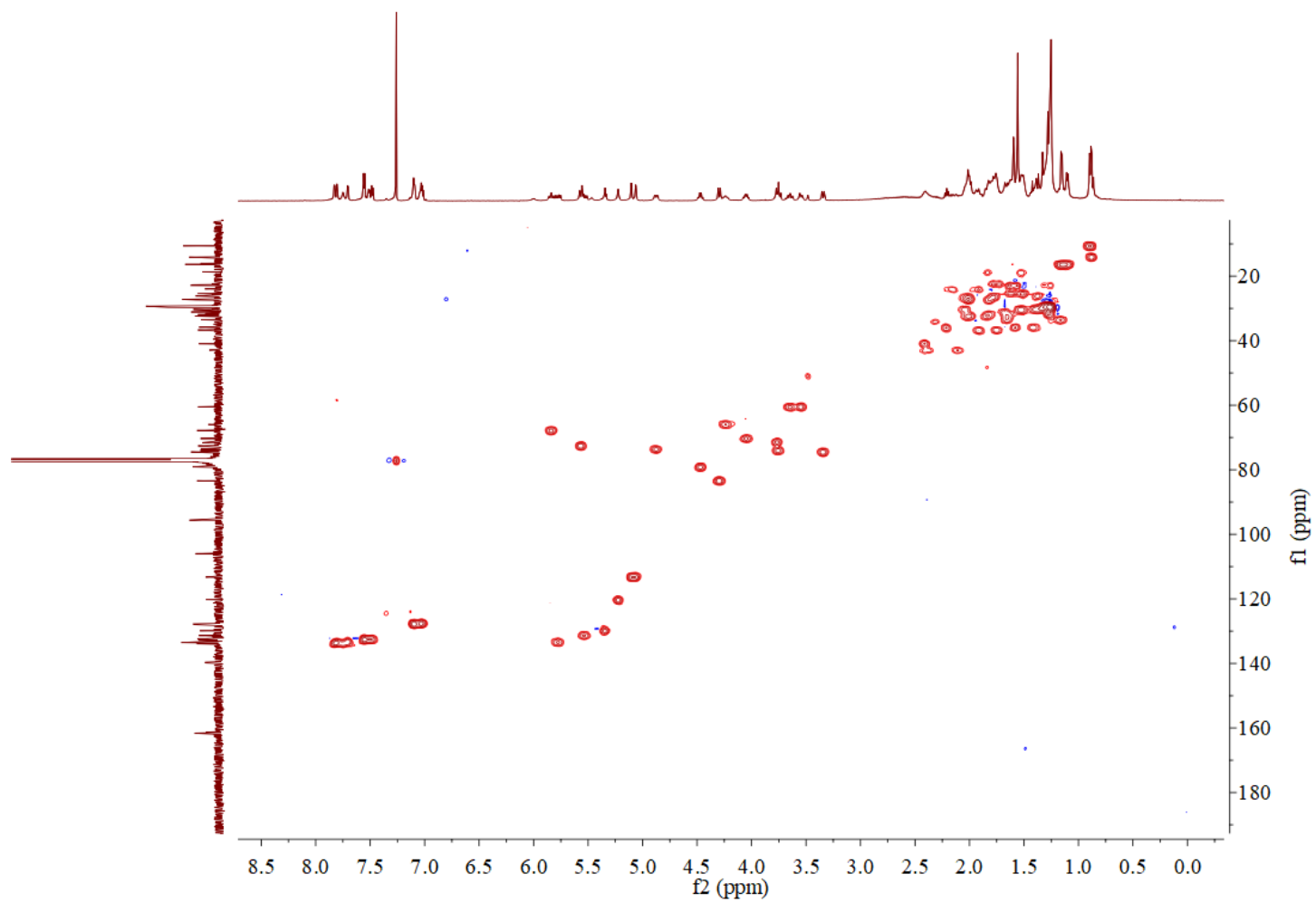
**Figure S34.**  $^1\text{H}$  NMR spectrum of **7** in  $\text{CDCl}_3$ .



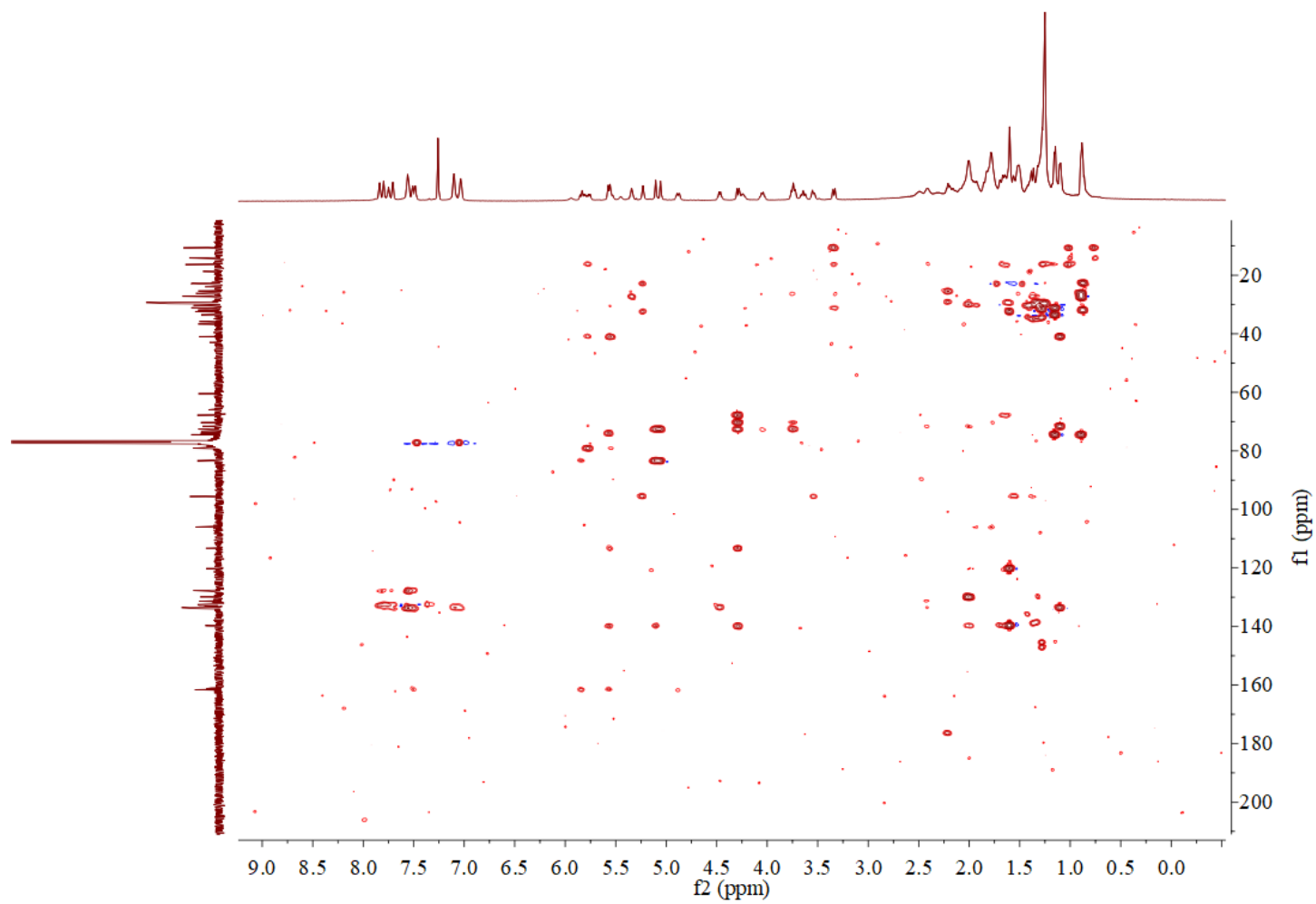
**Figure S35.**  $^{13}\text{C}$  NMR and DEPT 135 spectra of **7** in  $\text{CDCl}_3$ .



**Figure S36.** HMBC spectrum of **7** in CDCl<sub>3</sub>.

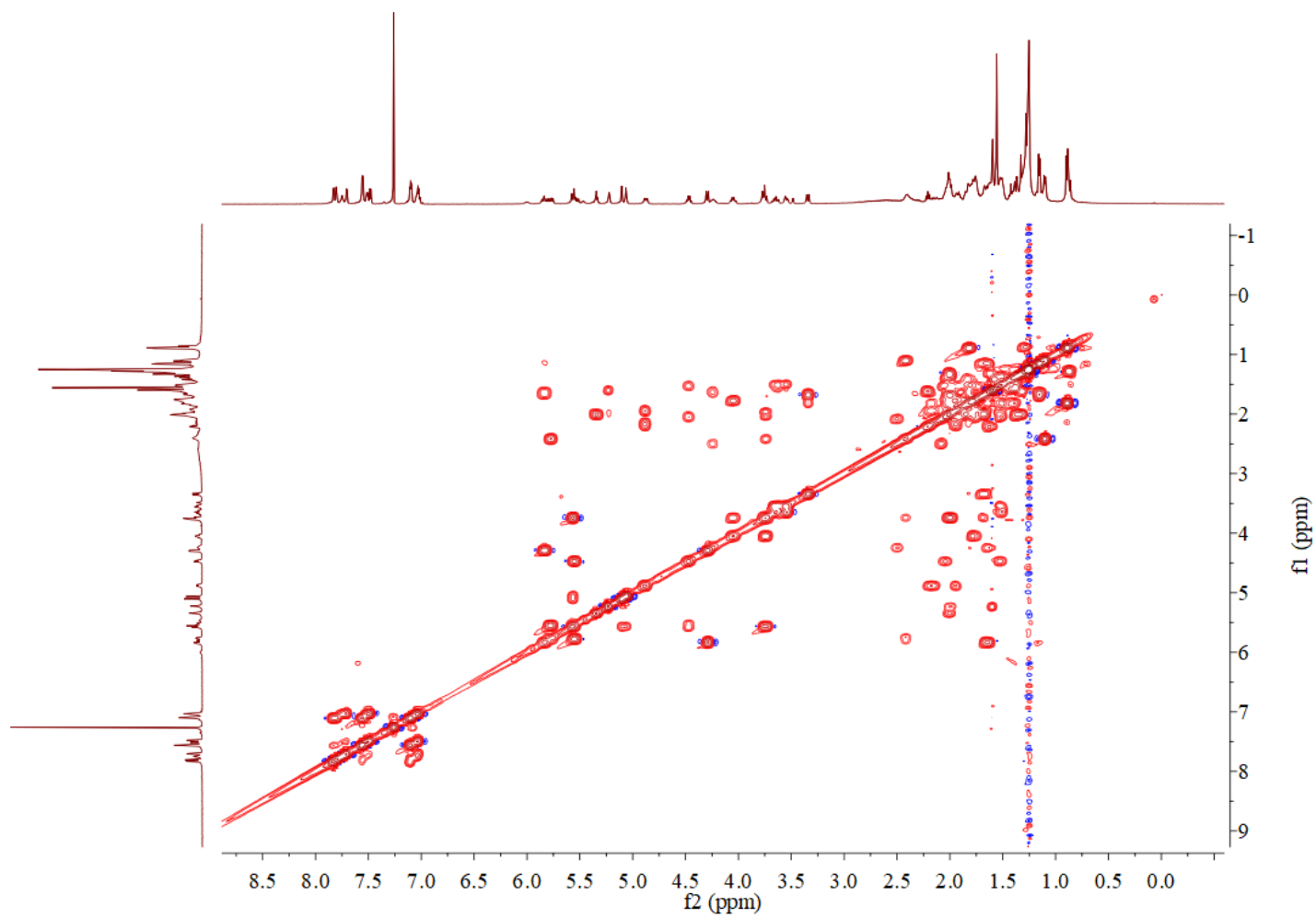


**Figure S37.** HMBC spectrum of **7** in CDCl<sub>3</sub>.

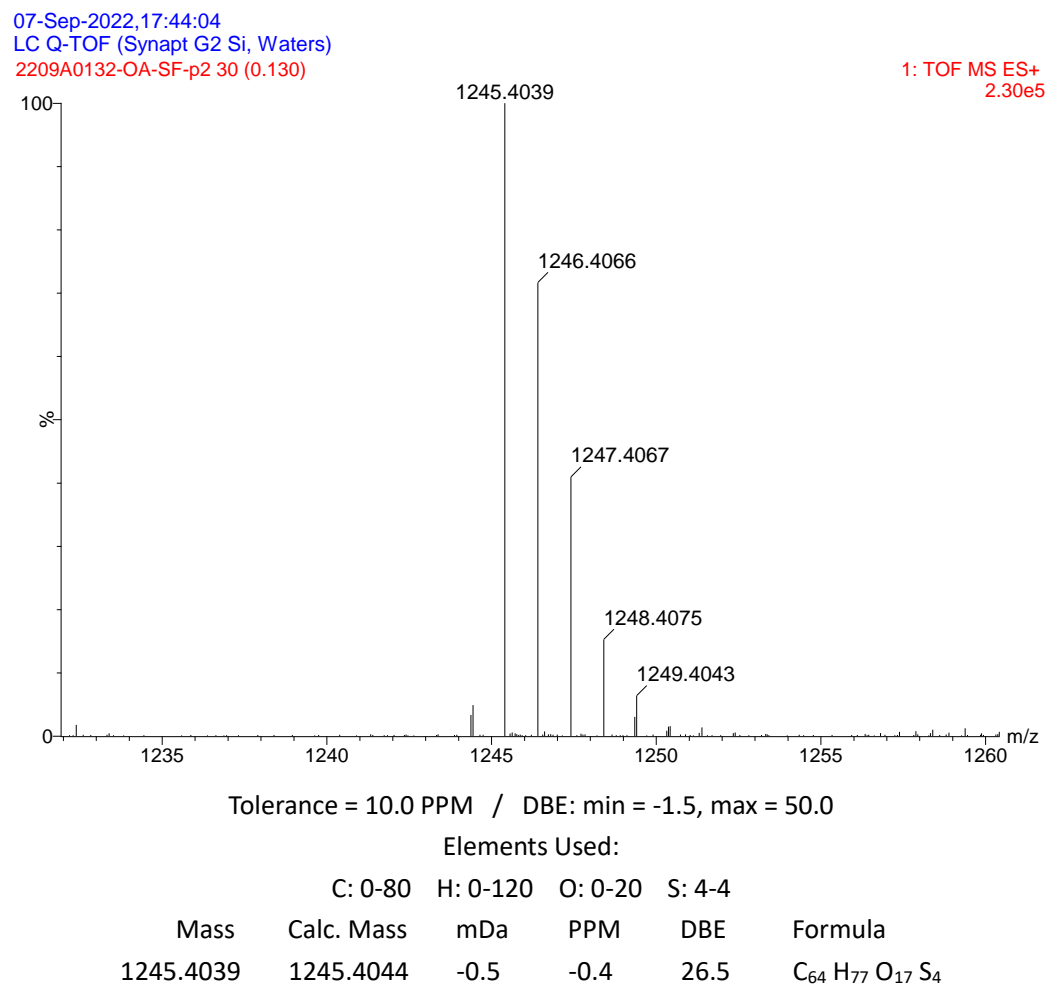




**Figure S38.**  $^1\text{H}$ – $^1\text{H}$  COSY spectrum of **7** in  $\text{CDCl}_3$ .



**Figure S39.** HRESIMS spectrum of **7**.



**Figure S40.** IR (KBr disc) spectrum of **7**.

