

# Two Gracilioethers Containing a [2(5H)-Furanylidene]ethanoate Moiety and 9,10-Dihydroplakortone G: New Polyketides from the Caribbean Marine Sponge *Plakortis halichondrioides*

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## Supplementary Material

**Table S1.** NMR spectral data for plakortone G (**9**) in CDCl<sub>3</sub>.

atom	$\delta_C^a$ , Type	$\delta_H^b$ , mult ( <i>J</i> in Hz)	<sup>1</sup> H- <sup>1</sup> H COSY	<sup>1</sup> H- <sup>13</sup> C HMBC
1	173.5, C			
2	135.8, C			
3	150.1, CH	6.82, br s		1, 2, 4, 13
4	89.3, C			
5	37.2, CH <sub>2</sub>	1.60, m		3, 4, 15, 16
		1.60, m		3, 4, 15, 16
6	21.2, CH <sub>2</sub>	1.10-1.38, br m		
7	35.1, CH <sub>2</sub>	1.10-1.38, br m		8
		1.10-1.38, br m		8
8	44.3, CH	1.73, m	9	
9	132.9, CH	5.01, dd (8.9, 15.2)	8, 10	8
10	132.4, CH	5.34, m	9, 11	8
11	25.6, CH <sub>2</sub>	1.97, m	10, 12	9, 10, 12
12	14.2, CH <sub>3</sub>	0.94, t (7.5)	11	10, 11
13	18.5, CH <sub>2</sub>	2.28, m	14	1, 2, 3, 14
14	12.0, CH <sub>3</sub>	1.15, t (7.5)	13	2, 13
15	29.9, CH <sub>2</sub>	1.70, m	16	3, 4, 5, 16
15	29.9, CH <sub>2</sub>	1.70, m	16	3, 4, 5, 16
16	7.7, CH <sub>3</sub>	0.80, m	15 $\alpha$ , 15 $\beta$	4, 5, 15
17	28.2, CH <sub>2</sub>	1.10-1.38, br m		8
		1.10-1.38, br m		8
18	11.6, CH <sub>3</sub>	0.80, m		8

\* All Assignments are based on COSY, HSQC, and HMBC experiments. <sup>a</sup> Recorded at 125 MHz. Multiplicities were obtained from the Attached Proton Test (APT) experiments. <sup>b</sup> Recorded at 500 MHz.



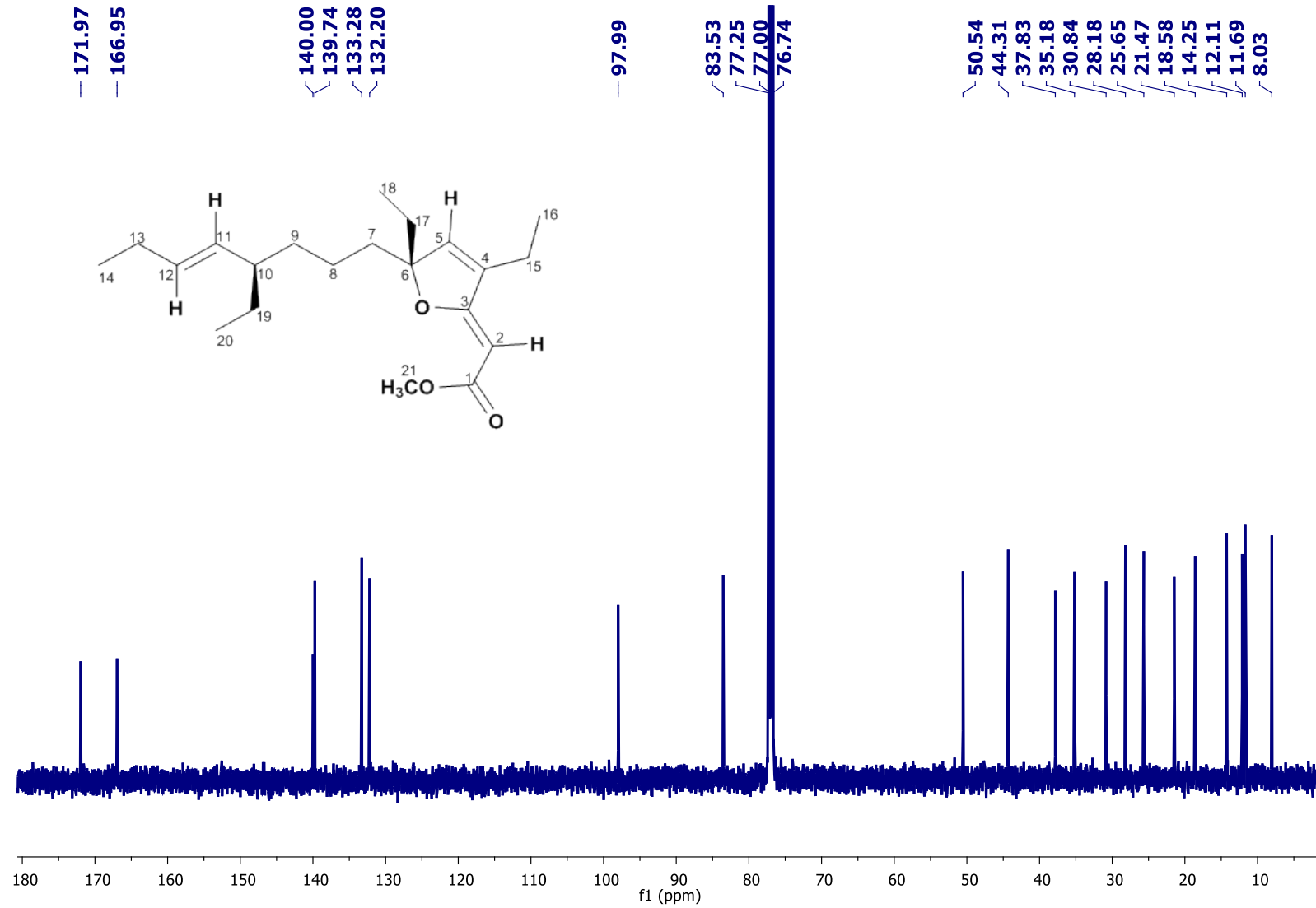


Figure S2. <sup>13</sup>C-NMR spectrum (CDCl<sub>3</sub>, 125 MHz) of gracilioether M (**6**).

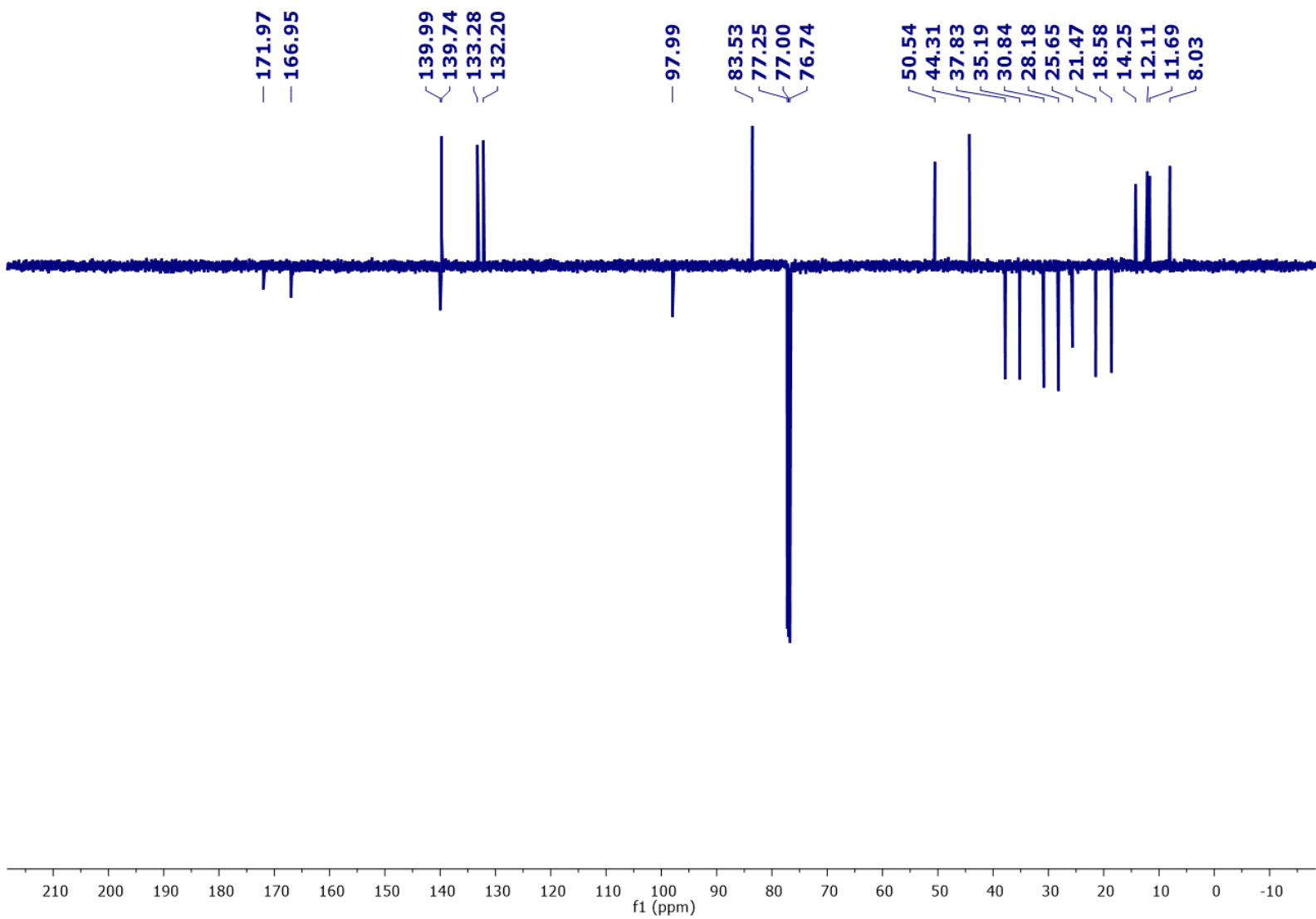


Figure S3. APT spectrum (CDCl<sub>3</sub>, 125 MHz) of gracilioether M (**6**).

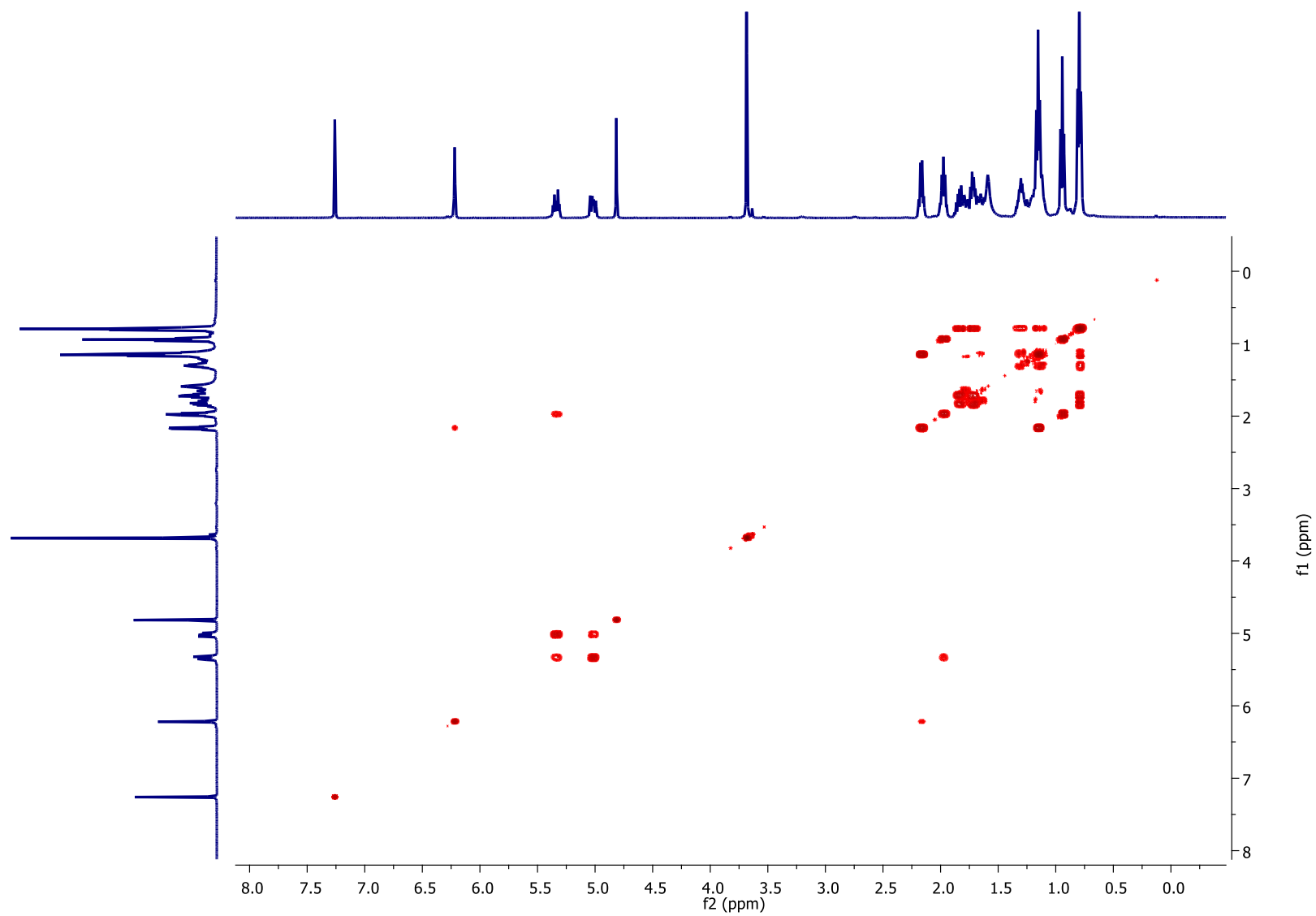


Figure S4.  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum ( $\text{CDCl}_3$ ) of gracilioether M (**6**).

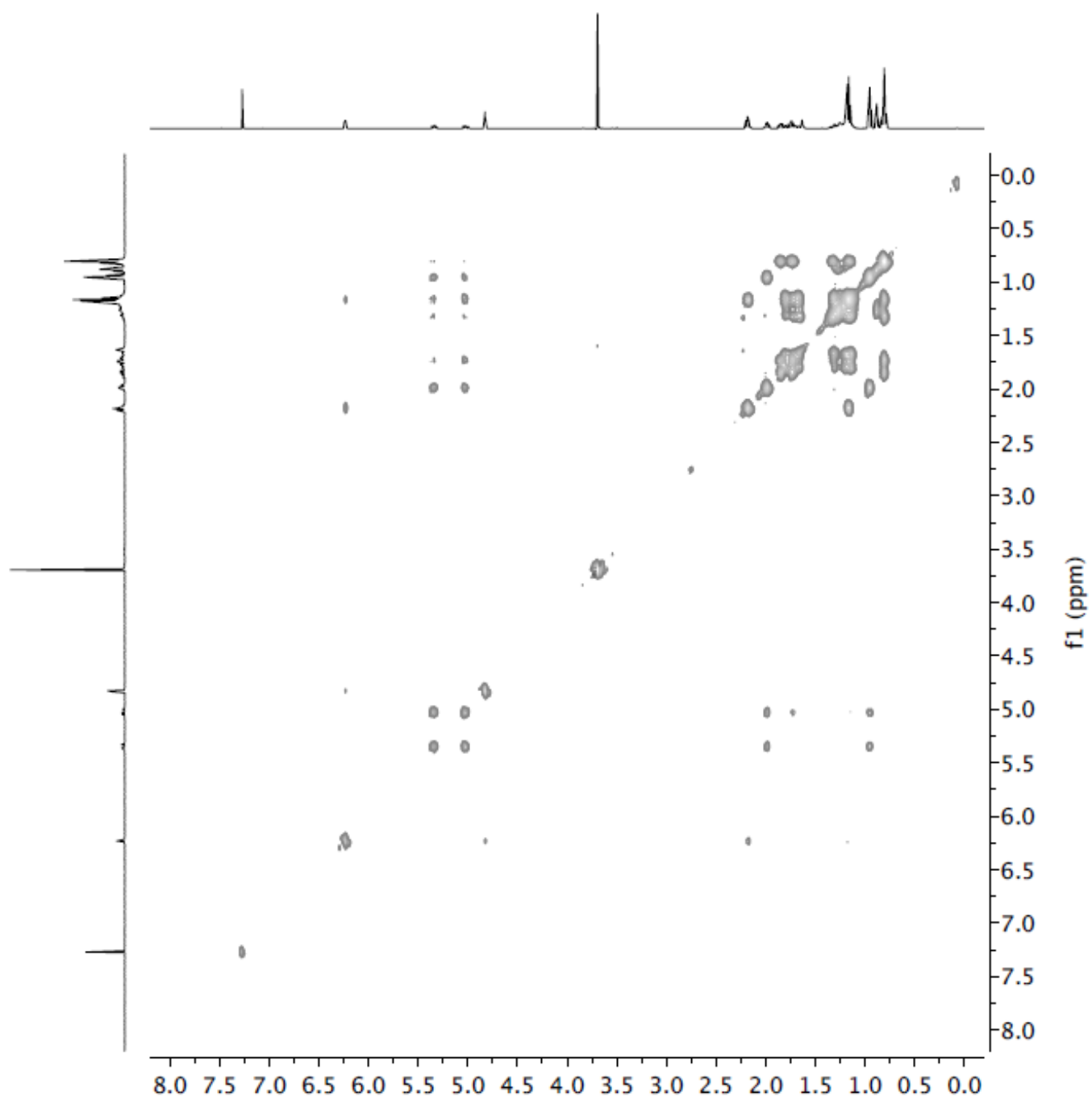


Figure S5.  $^1\text{H}$ - $^1\text{H}$ -TOCSY spectrum ( $\text{CDCl}_3$ ) of gracilioether M (**6**)

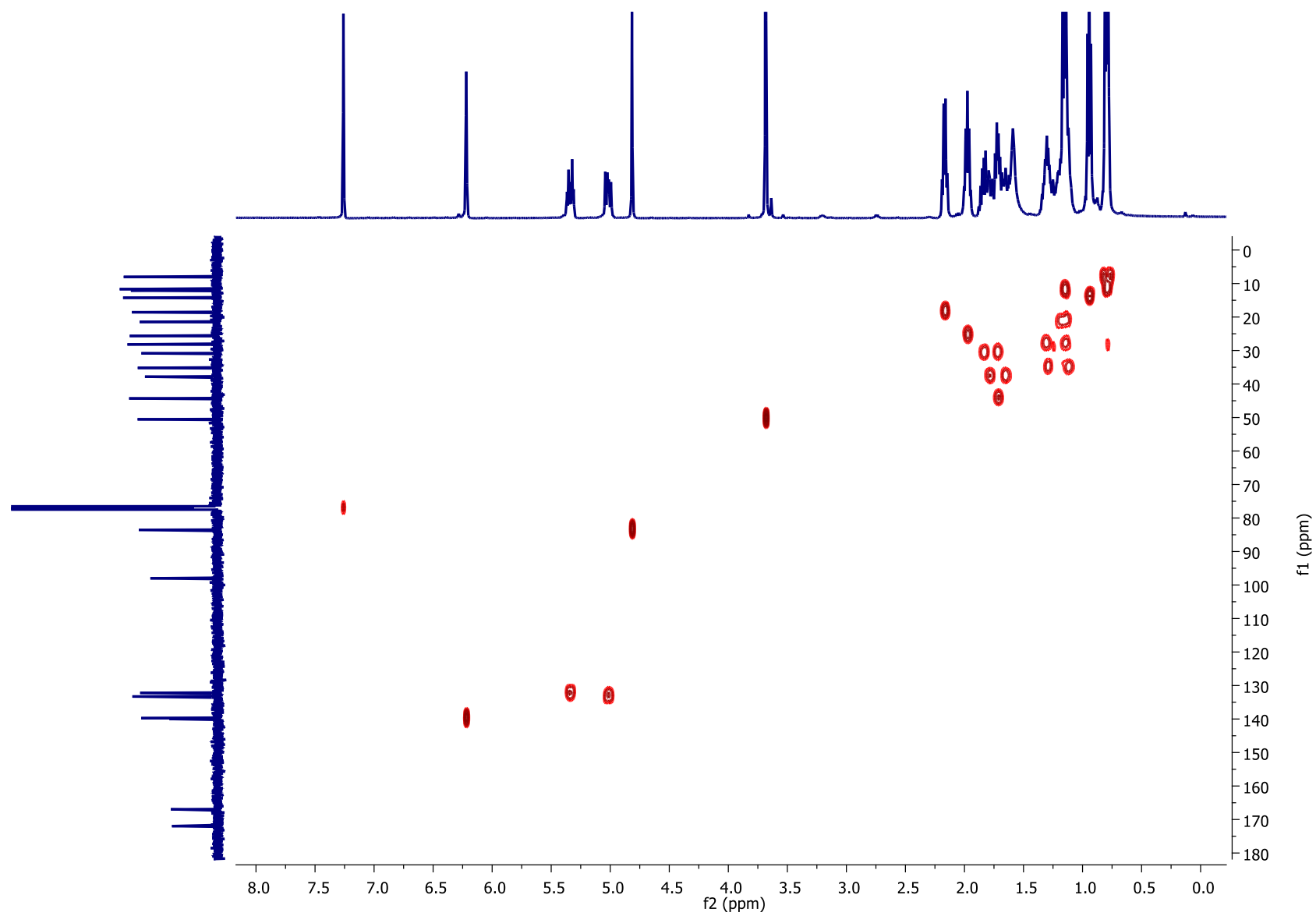


Figure S6.  $^1\text{H}$ - $^{13}\text{C}$ -HSQC spectrum ( $\text{CDCl}_3$ ) of gracilioether M (6).

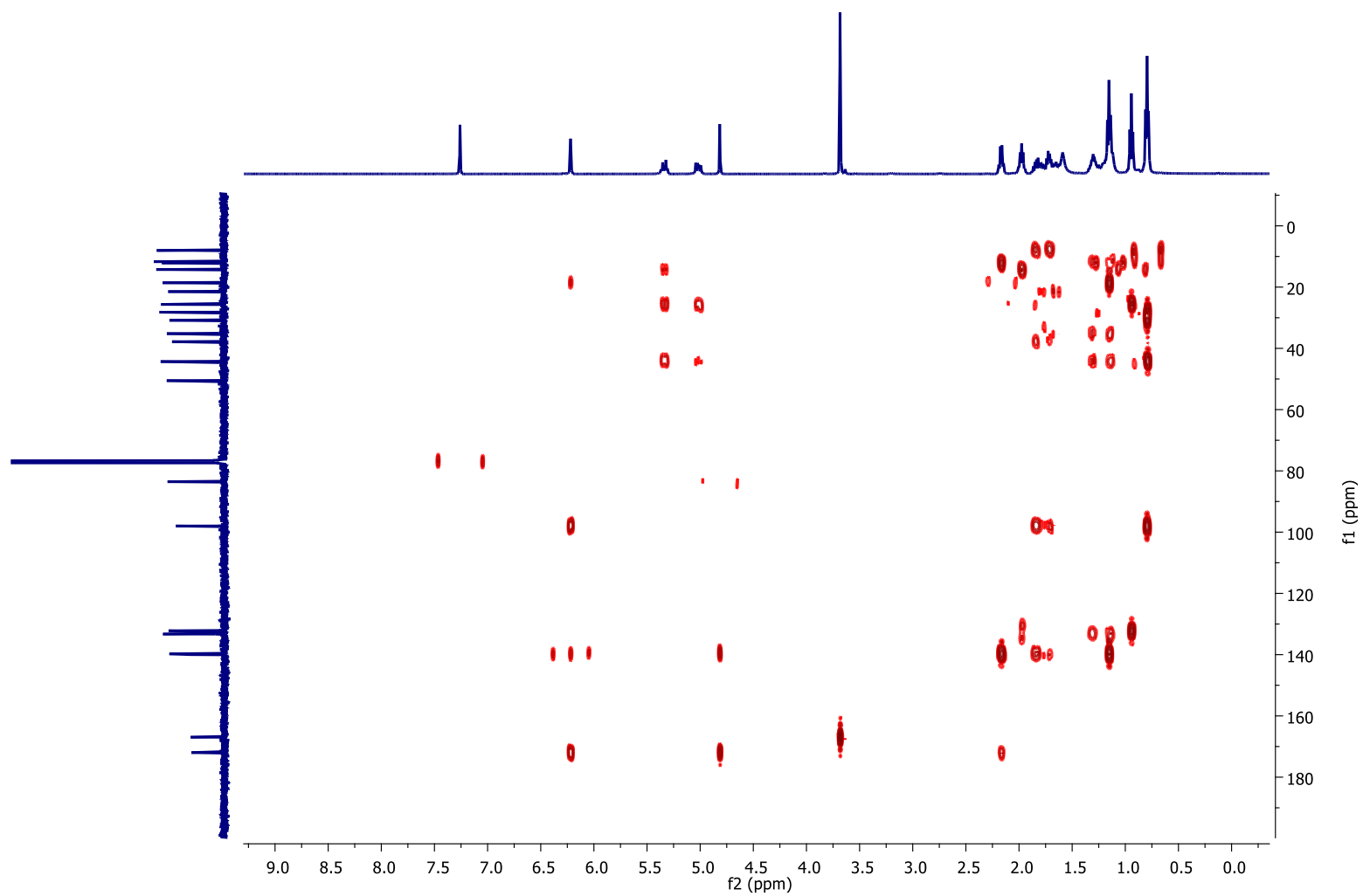


Figure S7.  $^1\text{H}$ - $^{13}\text{C}$ -HMBC spectrum ( $\text{CDCl}_3$ ) of gracilioether M (6).



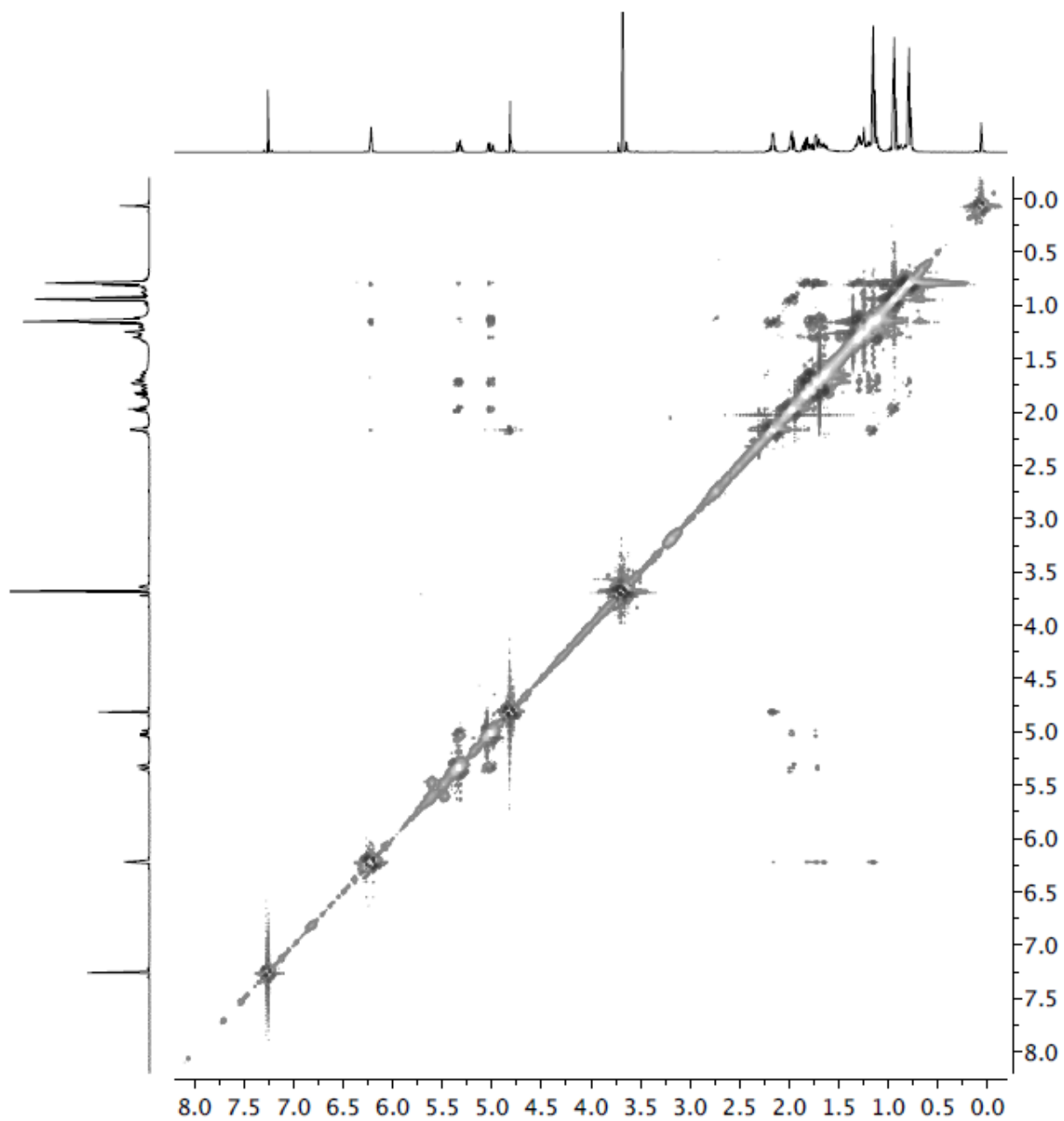


Figure S8.  $^1\text{H}$ - $^1\text{H}$ -NOESY spectrum ( $\text{CDCl}_3$ ) of gracilioether M (**6**).

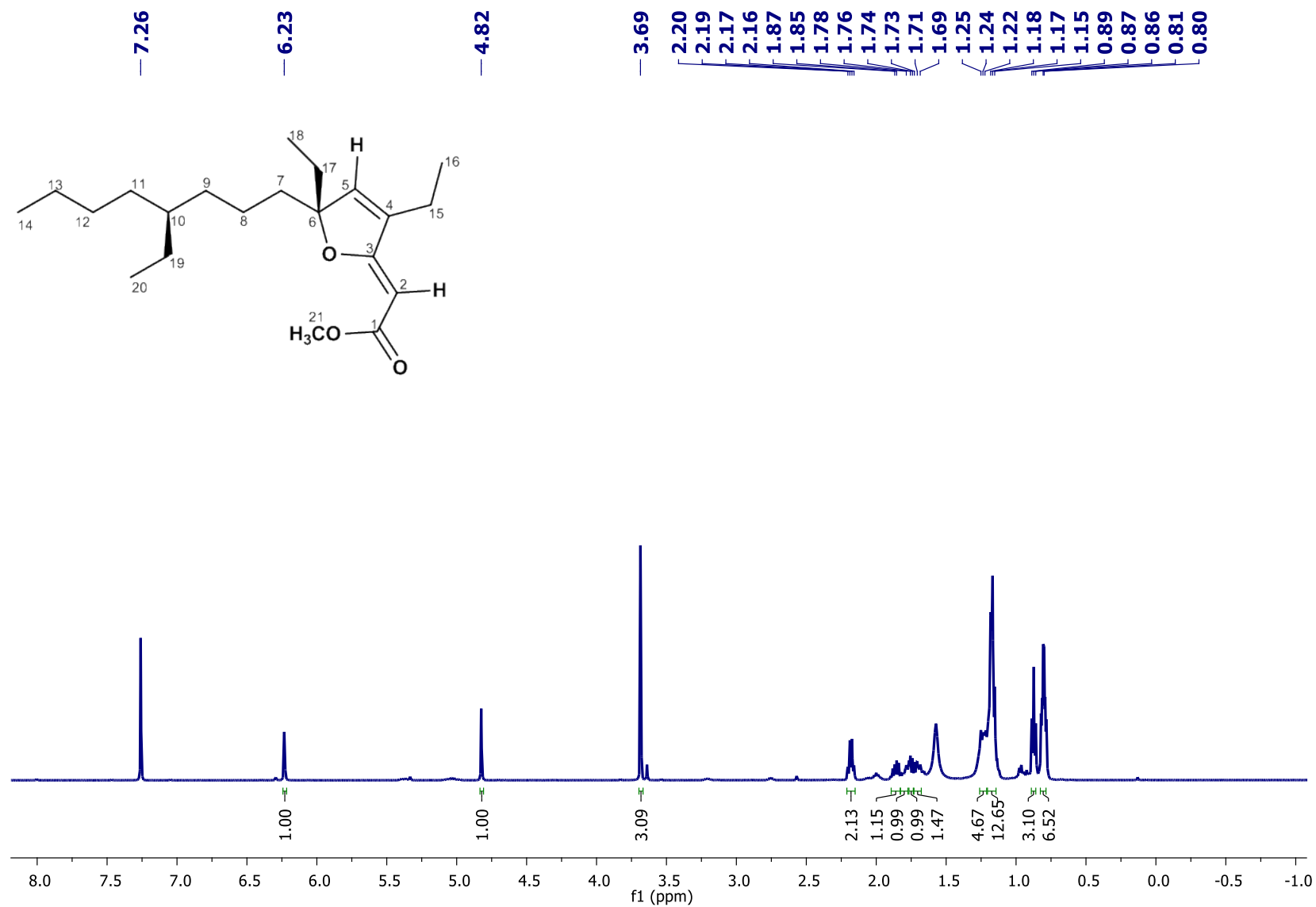


Figure S9.  $^1\text{H}$ -NMR spectrum ( $\text{CDCl}_3$ , 500 MHz) of 11,12-dihydrogracilioether M (7).

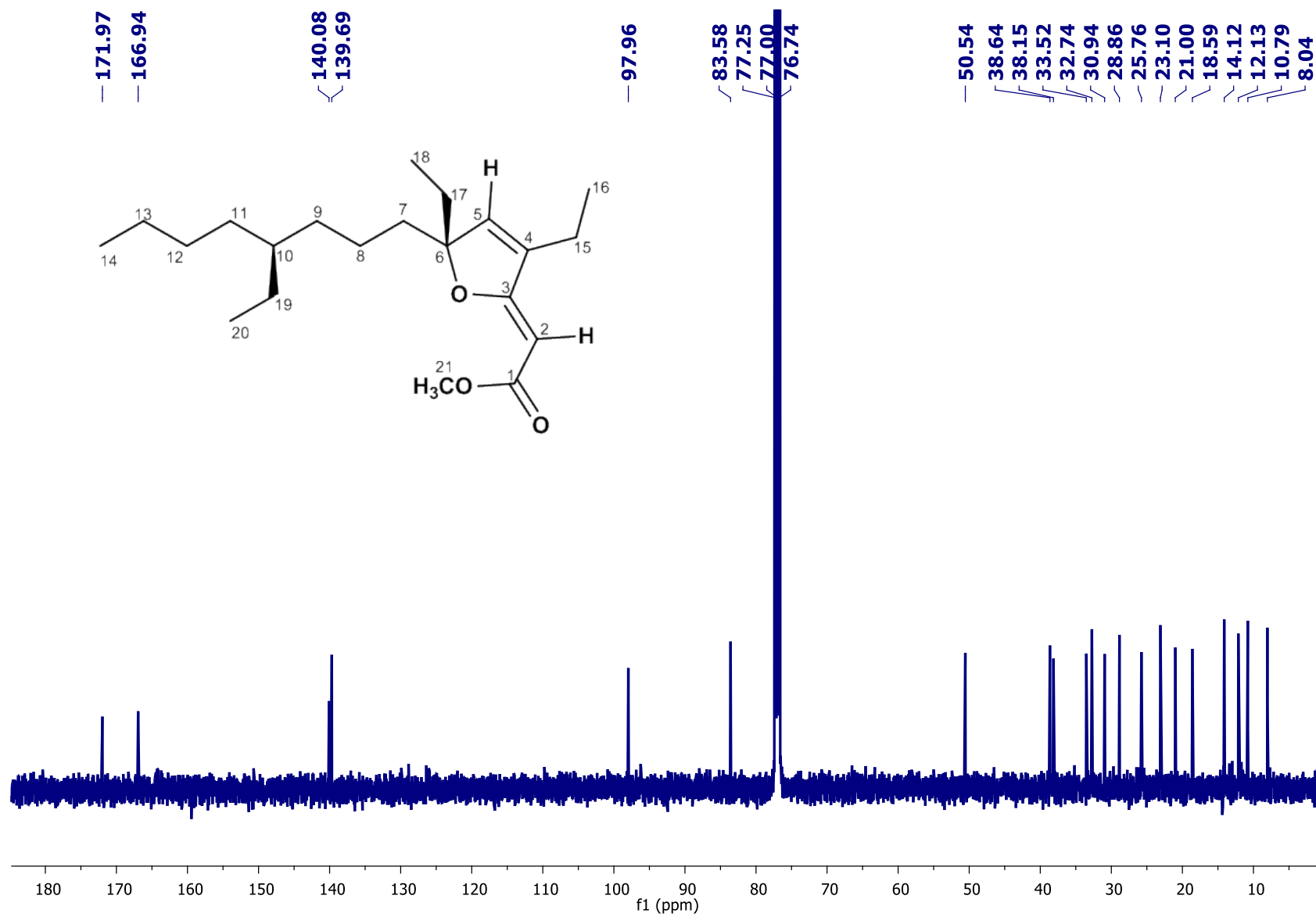


Figure S10. <sup>13</sup>C-NMR spectrum (CDCl<sub>3</sub>, 125 MHz) of 11,12-dihydrogracilioether M (7).

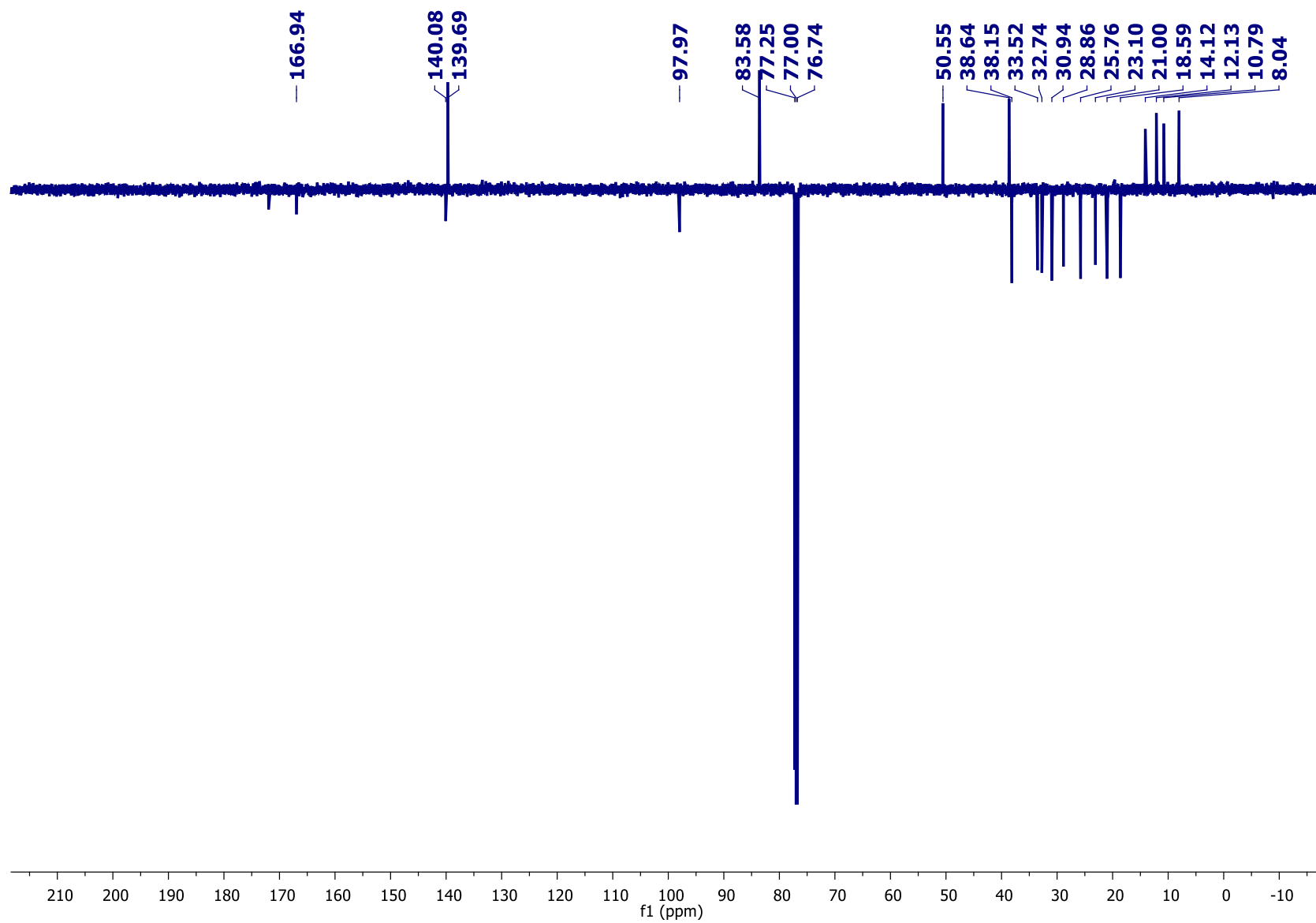


Figure S11. APT spectrum (CDCl<sub>3</sub>, 125 MHz) of 11,12-dihydrogracilioether M (7).

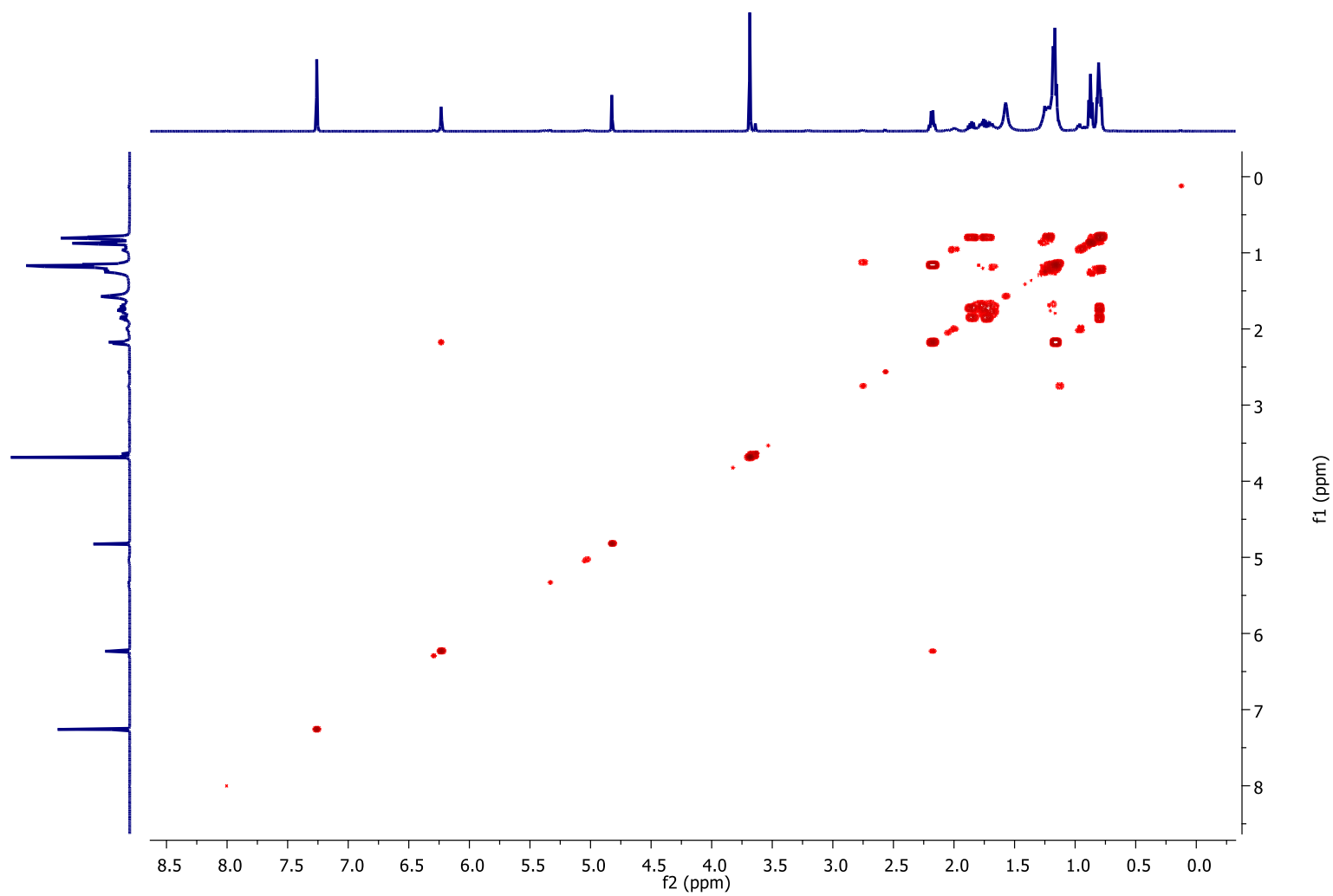


Figure S12.  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum ( $\text{CDCl}_3$ ) of 11,12-dihydrogracilioether M (7).

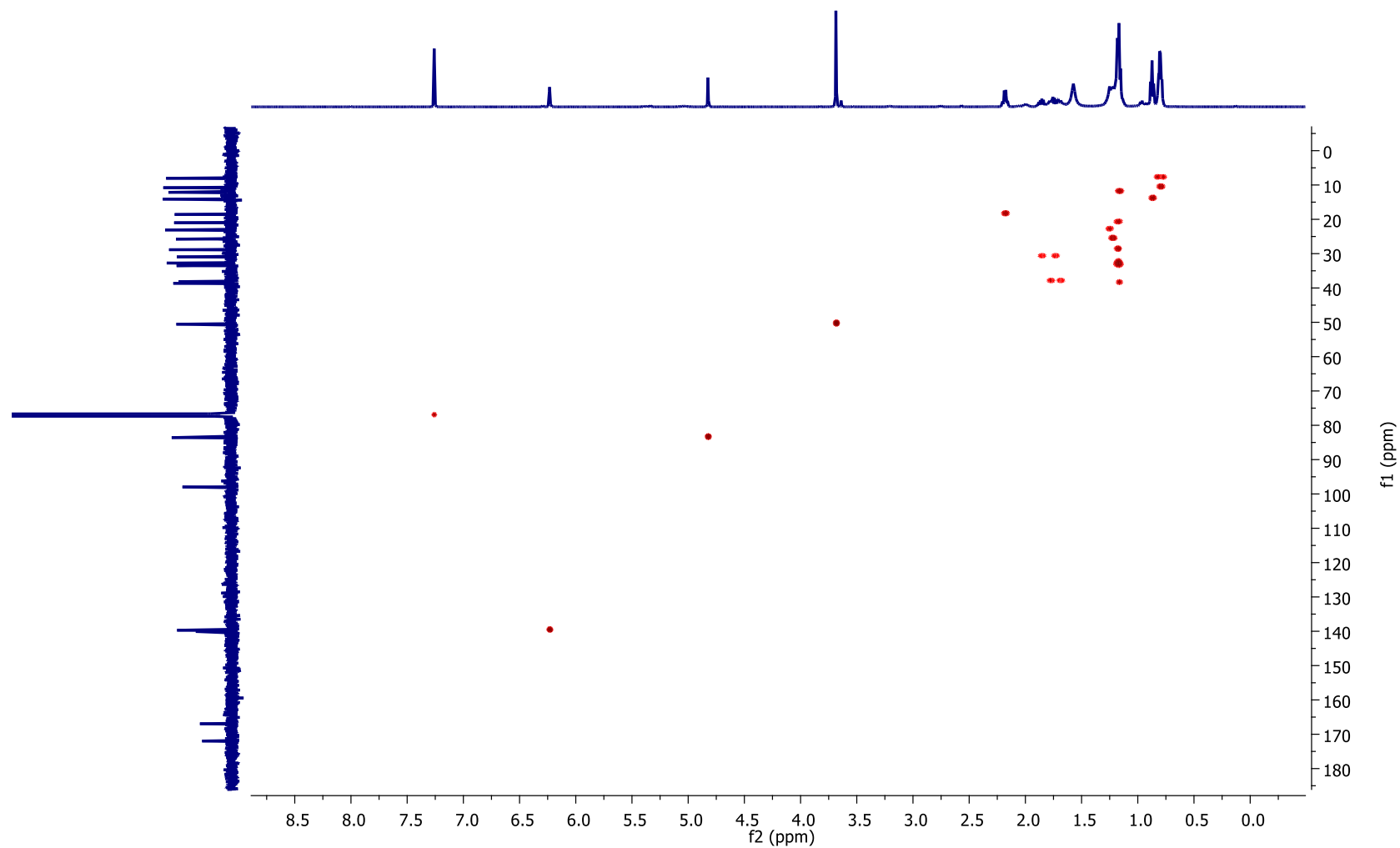


Figure S13.  $^1\text{H}$ - $^{13}\text{C}$ -HSQC spectrum ( $\text{CDCl}_3$ ) of 11,12-dihydrogracilioether M (7).

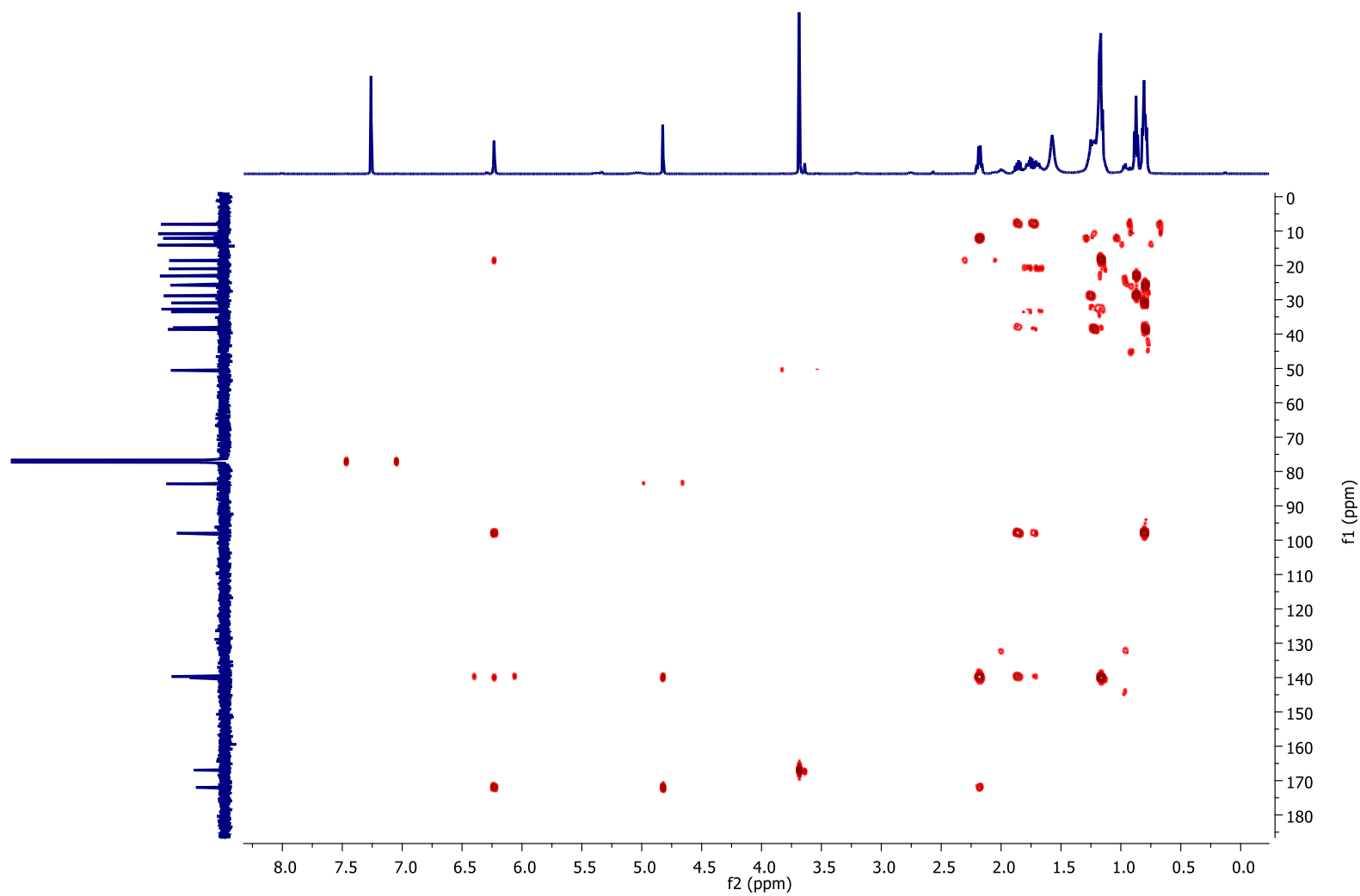


Figure S14.  $^1\text{H}$ - $^{13}\text{C}$ -HMBC spectrum ( $\text{CDCl}_3$ ) of 11,12-dihydrogracilioether M (7).

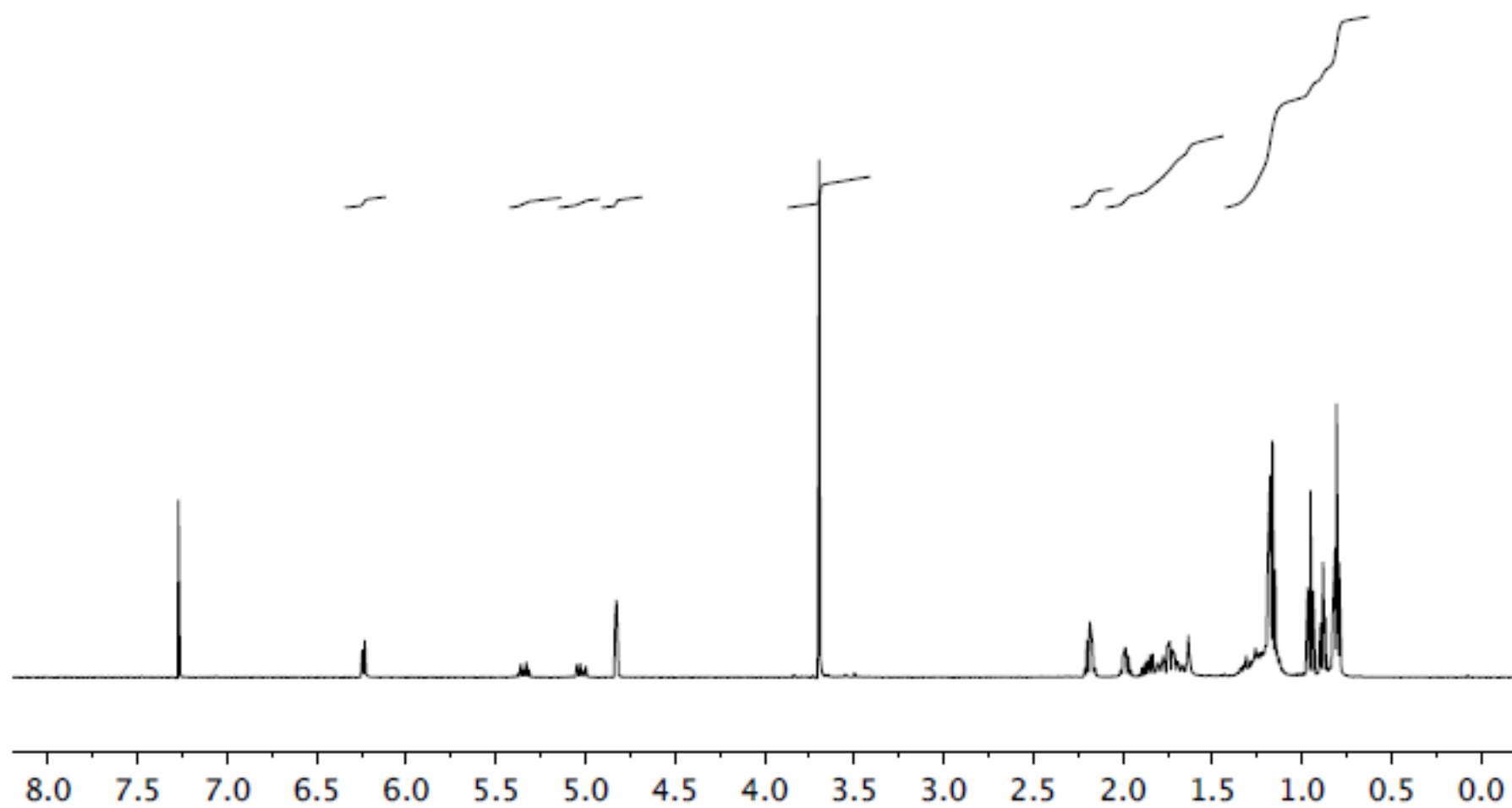


Figure S15.  $^1\text{H}$ -NMR spectrum ( $\text{CDCl}_3$ , 500 MHz) of a mixture of compounds **8–9**.



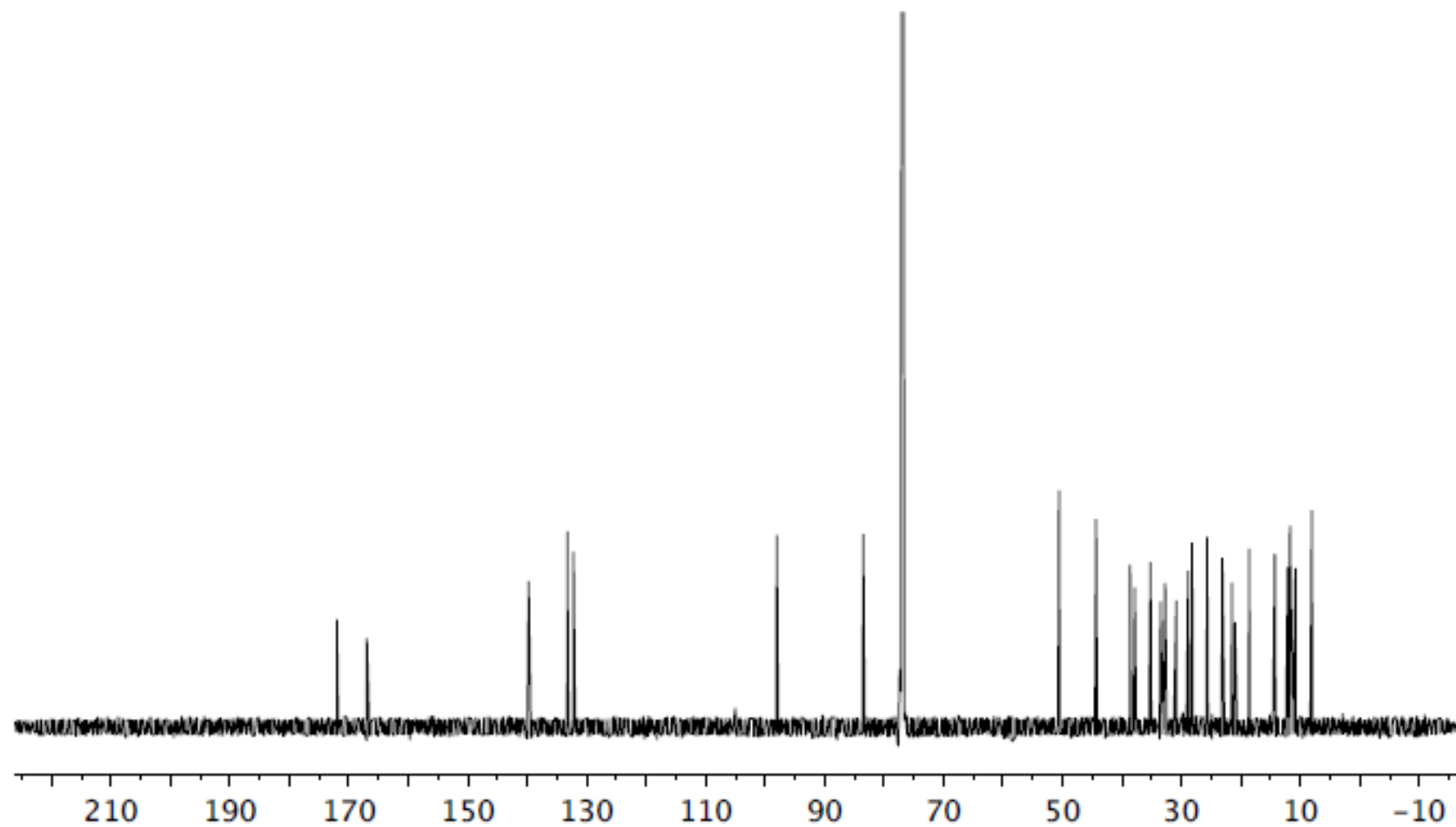


Figure S16.  $^{13}\text{C}$ -NMR spectrum ( $\text{CDCl}_3$ , 125 MHz) of a mixture of compounds **8–9**.

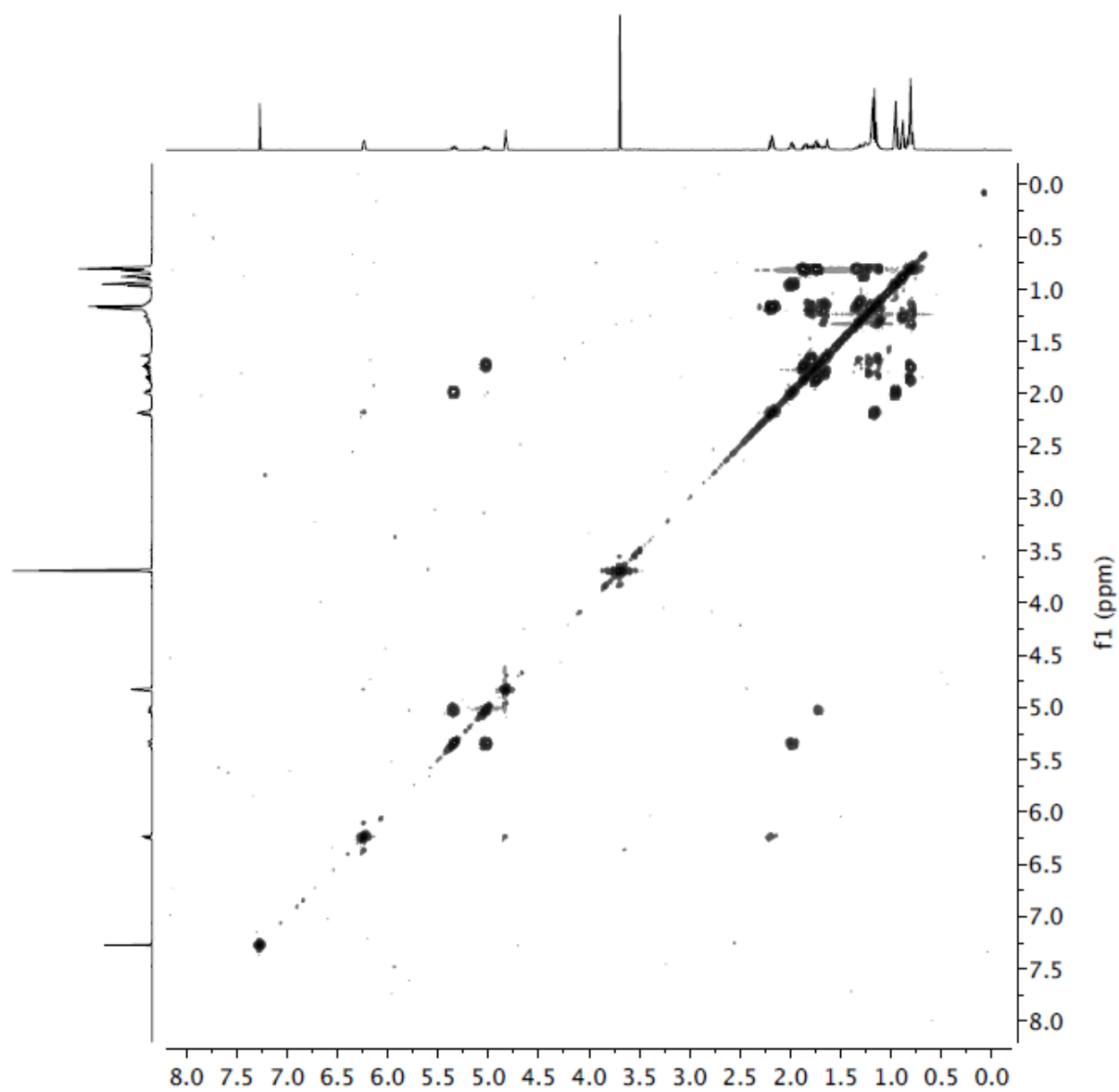


Figure S17.  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum ( $\text{CDCl}_3$ ) of a mixture of compounds **8–9**.

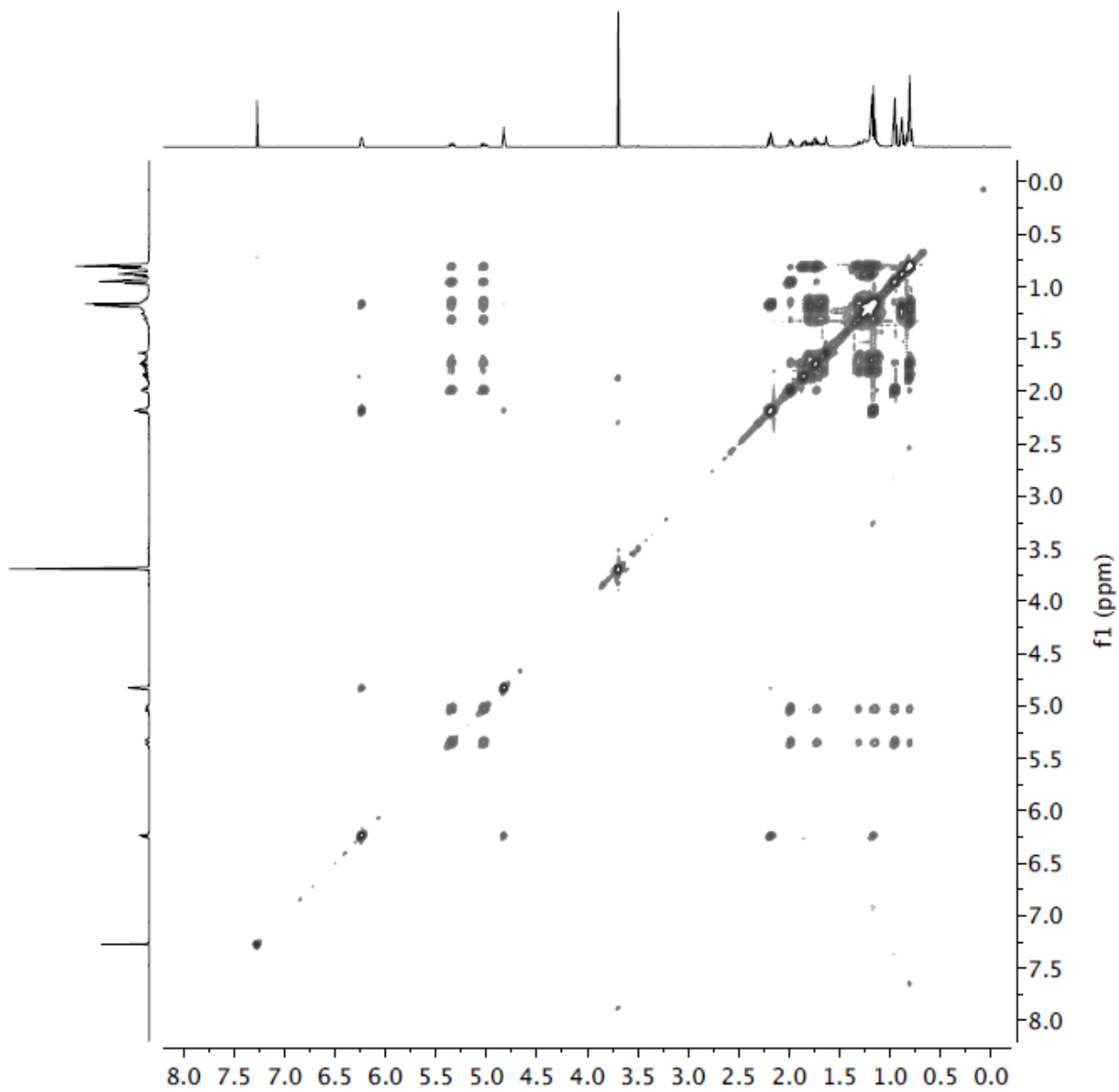


Figure S18.  $^1\text{H}$ - $^1\text{H}$ -TOCSY spectrum ( $\text{CDCl}_3$ ) of a mixture of compounds **8–9**.

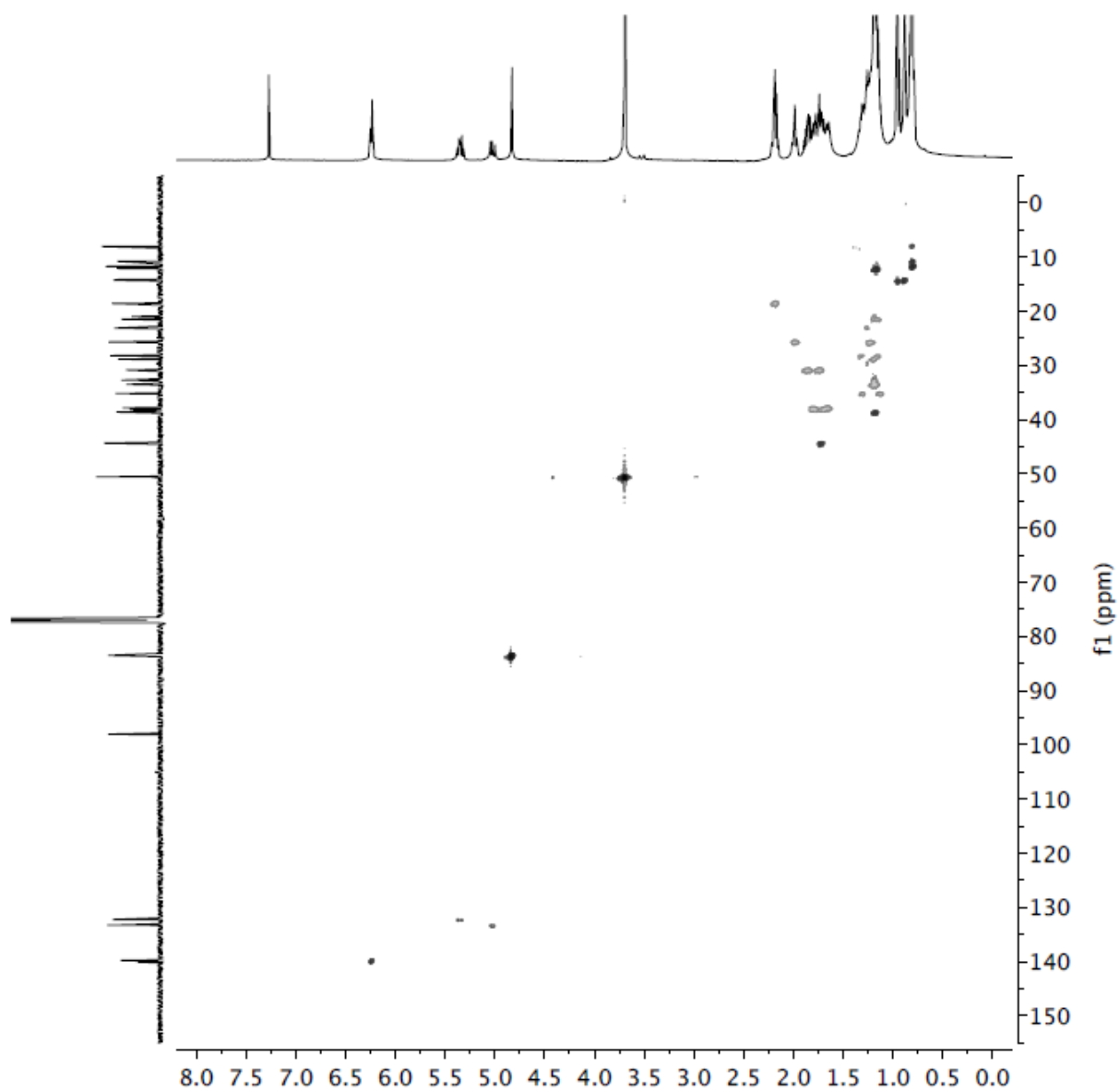


Figure S19.  $^1\text{H}$ - $^{13}\text{C}$ -HSQC spectrum ( $\text{CDCl}_3$ ) of a mixture of compounds **8–9**.

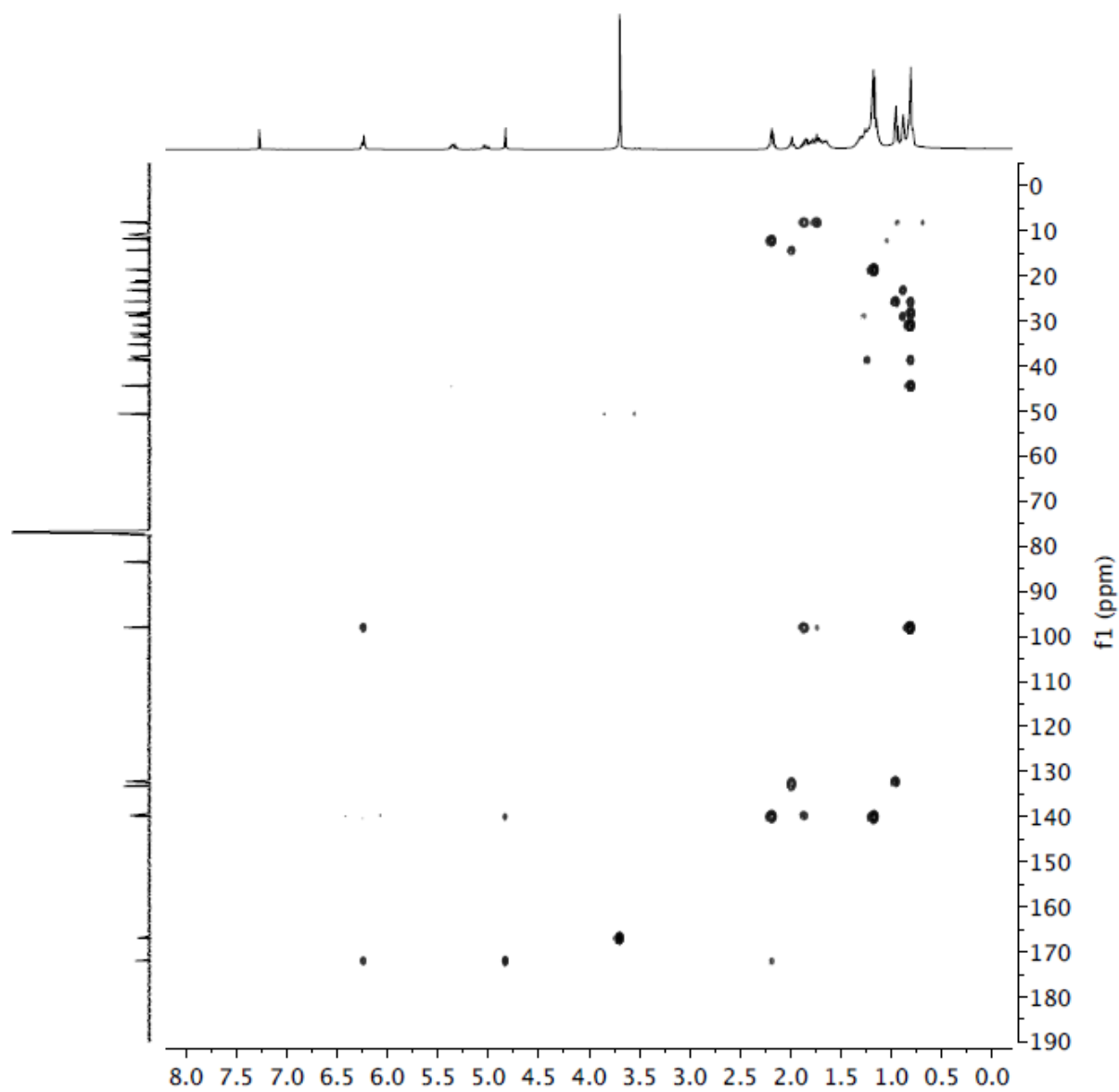


Figure S20.  $^1\text{H}$ - $^{13}\text{C}$ -HMBC spectrum ( $\text{CDCl}_3$ ) of a mixture of compounds **8-9**.

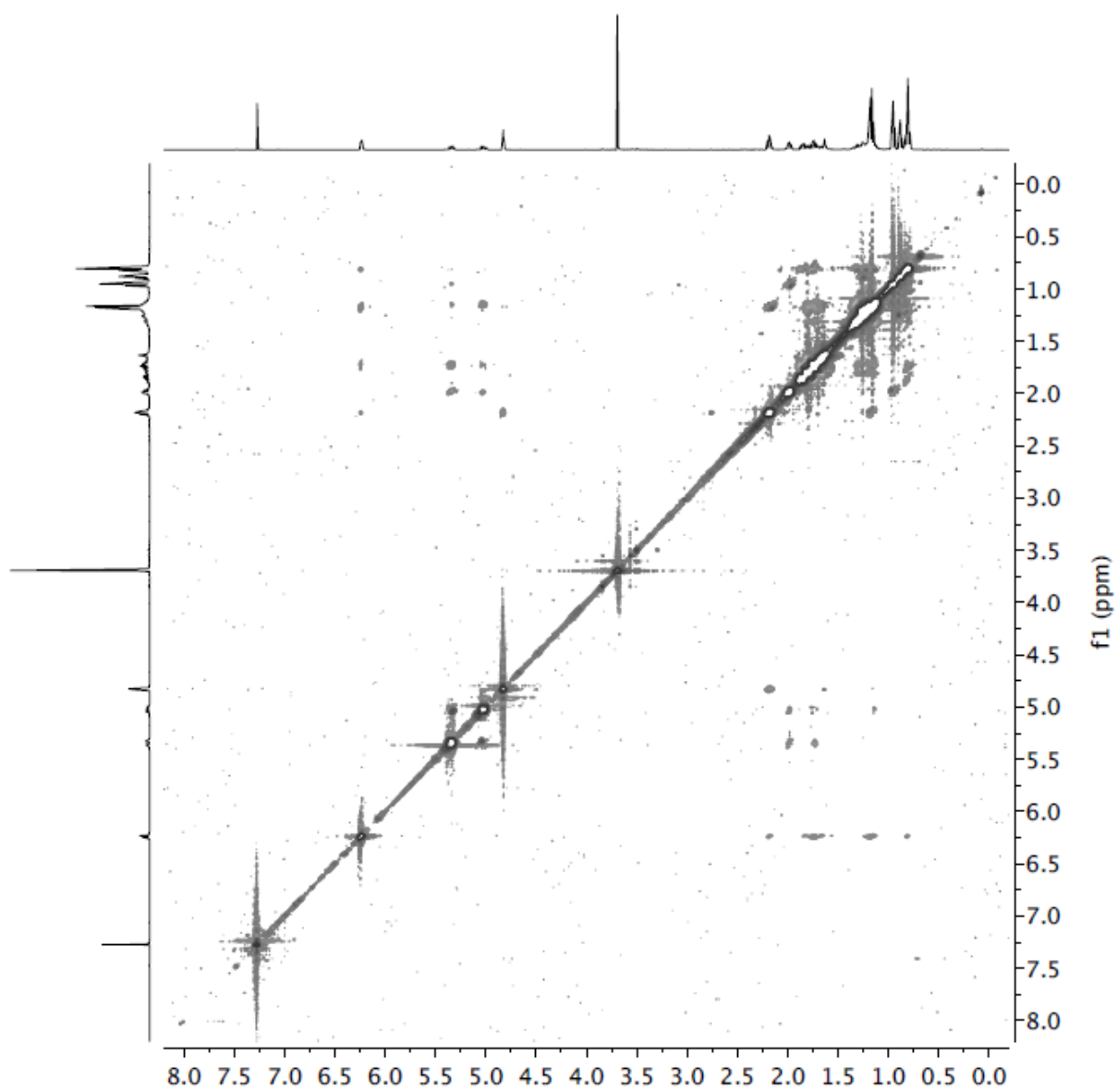


Figure S21.  $^1\text{H}$ - $^1\text{H}$ -NOESY spectrum ( $\text{CDCl}_3$ ) of a mixture of compounds **8–9**.

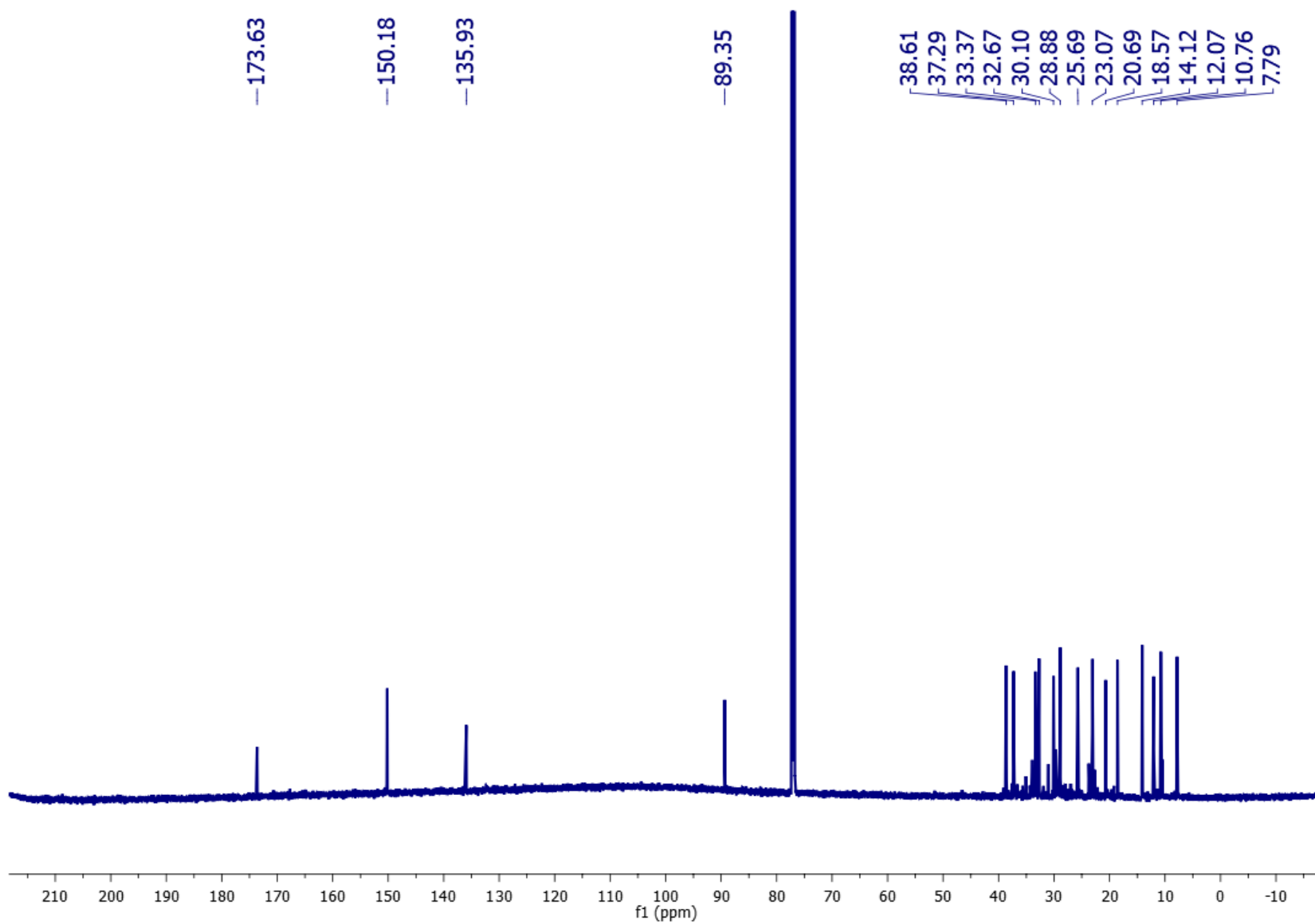


Figure S22.  $^{13}\text{C}$ -NMR spectrum ( $\text{CDCl}_3$ , 125 MHz) for semi-synthetic 9,10-dihydroplakortone G (**8**) (~90% pure).

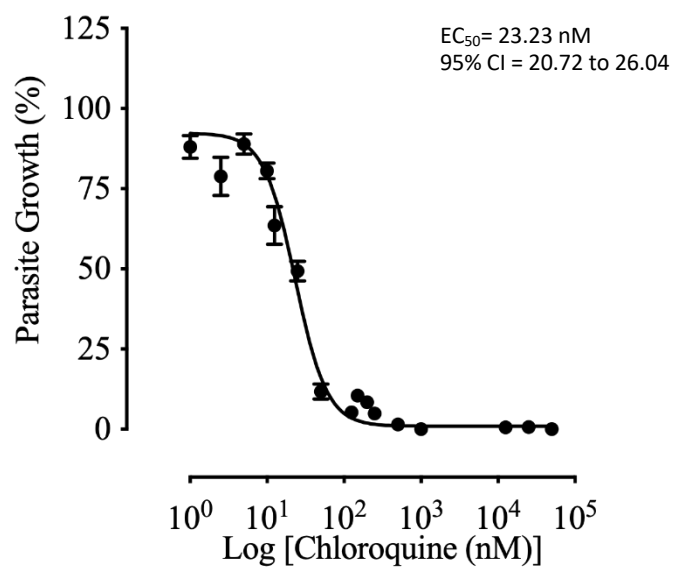


Figure S23. Dose-response curve of the parasite *Plasmodium berghei* for chloroquine (positive control).

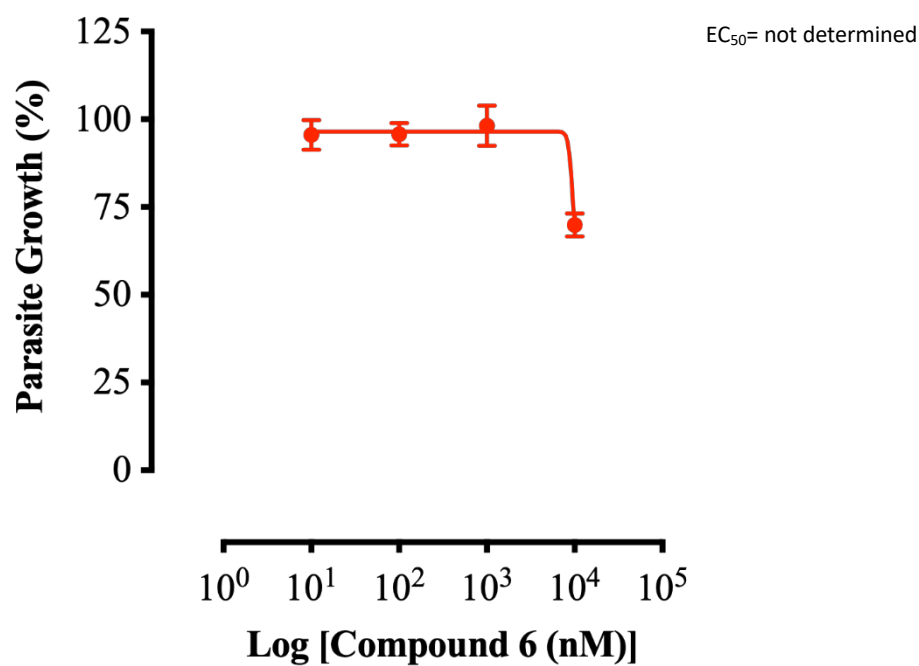


Figure S24. Dose-response curve of the parasite *Plasmodium berghei* for gracilioether M (**6**)



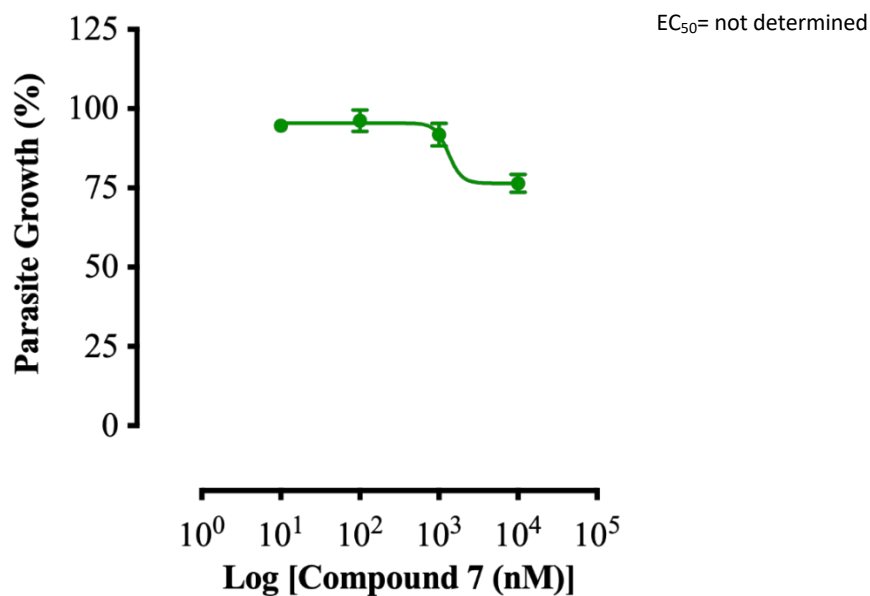


Figure S25. Dose-response curve of the parasite *Plasmodium berghei* for 11,12-dihydrogracilioether M (7).

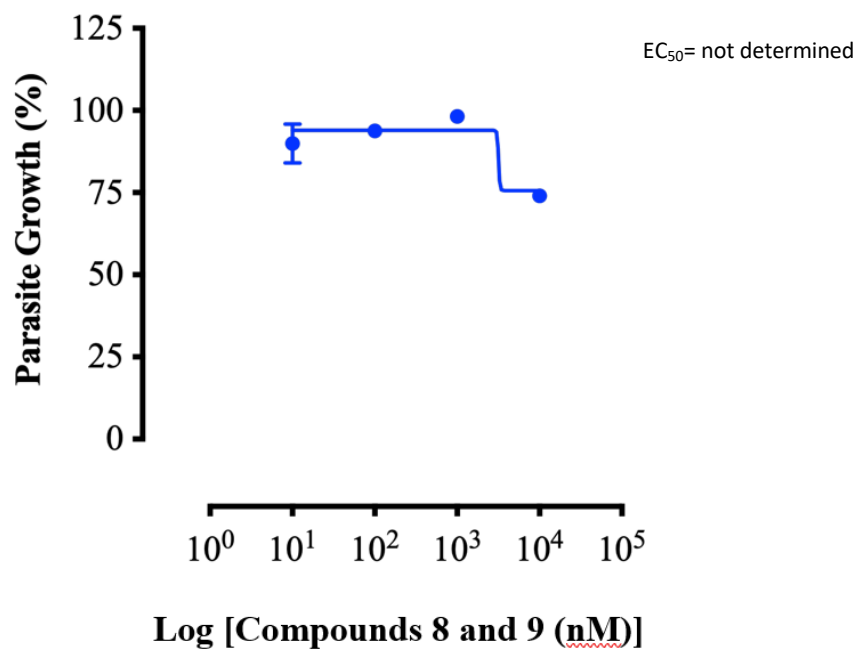


Figure S26. Dose-response curve of the parasite *Plasmodium berghei* for a mixture of compounds **8–9**