

## Supplementary Information

### **Application of an Ionic Liquid in the Microwave Assisted Extraction of Cytotoxic Metabolites from Fruits of *Schinus terebinthifolius* Raddi (Anacardiaceae)**

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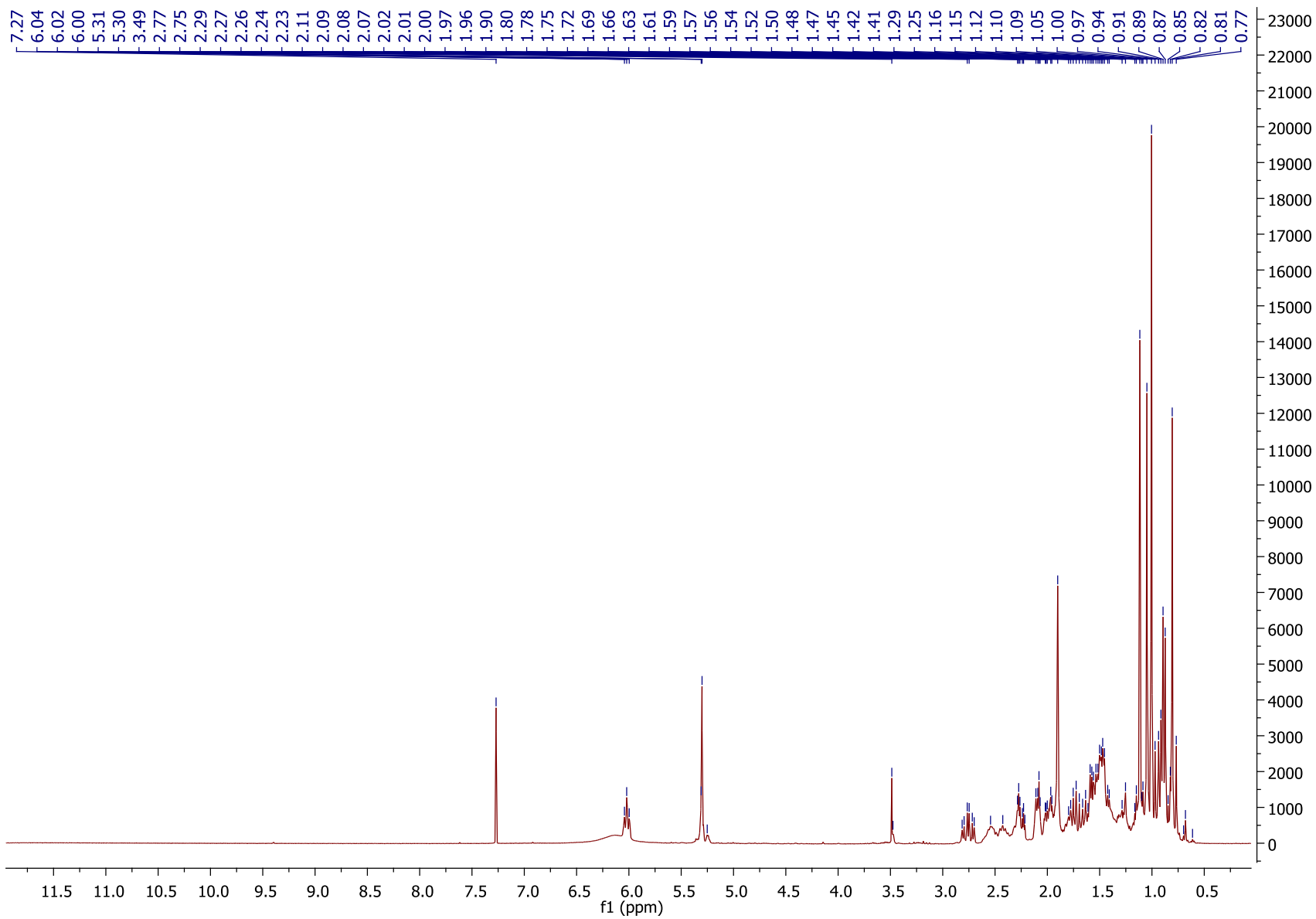
**Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of compounds **1**, **2** and **3** ( $\delta$  in ppm, 300 and 75 MHz,  $\text{CDCl}_3$ )

Position	<b>1</b>		<b>2</b>		<b>3</b>	
	$\delta_{\text{H}}$ (multiplicity, <i>J</i> , Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (multiplicity, <i>J</i> , Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (multiplicity, <i>J</i> , Hz)	$\delta_{\text{C}}$
1	1.41 (m)	38.5	1.46 (m)	36.1	1.48 (m)	36.0
2	2.23 (m) 2.77 (td, 15.1 and 6.0)	35.0	2.04 (m)	36.4	1.59 (m)	24.2
3	–	217.1	3.46 (dd, 10.2 and 5.4)	76.4	4.54 (dd, 10.5 and 4.5)	81.1
4	–	47.9	–	37.4	–	37.8
5	2.27 (m)	48.6	1.91 (m)	44.5	1.90 (m)	50.7
6	2.09 (m)	24.5	1.91 (m)	24.3	1.98 (m)	23.7
7	5.30 (t, 3.0)	117.8	5.28 (m)	117.8	5.26 (br s)	117.7
8	–	146.1	–	147.0	–	145.7
9	1.90 (m)	38.5	2.50 (m)	48.6	2.31 (m)	50.7
10	–	35.7	–	35.6	–	34.8
11	0.89 (m)	18.2	1.56 (m)	18.5	1.54 (m)	18.2
12	1.50 (m)	34.1	1.59 (m)	34.7	1.54 (m)	33.9
13	–	43.5	–	43.9	–	43.5
14	–	51.2	–	51.6	–	51.2
15	1.52 (m)	35.7	1.43 (m)	34.0	1.53 (m)	34.6
16	1.97 (m)	28.2	1.97 (m)	28.2	1.70 (m)	28.2
17	1.47 (m)	52.9	1.42 (m)	53.3	1.44 (m)	52.8
18	0.87 (s)	18.3	0.83 (s)	21.37	0.93 (s)	21.8
19	0.77 (s)	13.0	0.77 (s)	13.0	0.77 (s)	13.1
20	1.54 (m)	36.1	1.39 (m)	36.1	1.42 (m)	36.8
21	0.88 (d, 6.0)	18.0	0.89 (d, 6.0)	18.7	0.86 (m)	18.2
22	1.57 (m)	33.8	1.37 (m)	36.1	1.42 (m)	36.0
23	2.56 (m)	26.9	2.46 (m)	26.9	1.87 (m)	27.0
24	6.02 (t, 6.0)	146.1	6.07 (t, 6.3)	146.1	6.90 (m)	146.0
25	–	126.5	–	125.7	–	126.6
26	1.90 (s)	20.6	2.05 (s)	20.6	1.84 (s)	171.0
27	–	173.4	–	172.4	–	11.9
28	1.12 (s)	27.4	0.93 (s)	28.2	0.85 (s)	27.2
29	1.00 (s)	27.3	0.90 (s)	22.5	0.93 (s)	21.4
30	1.05 (s)	25.4	1.95 (s)	27.4	0.97 (s)	21.8
C=O	–	–	–	–	–	171.0
CH <sub>3</sub>	–	–	–	–	2.07 (s)	21.0

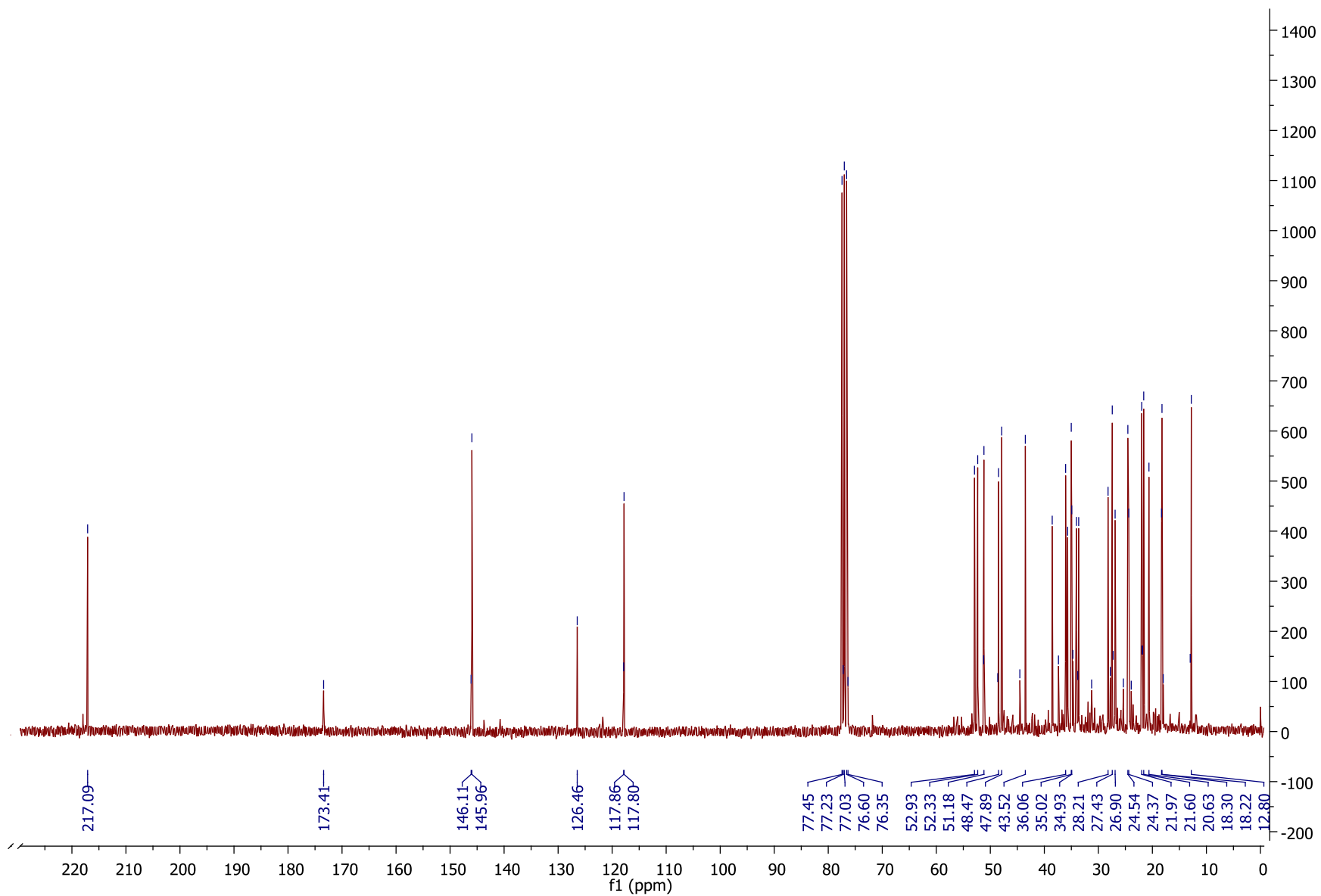
**Table S2.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR data of compounds **4** and **5** ( $\delta$  in ppm, 300 and 75 MHz,  $\text{CD}_3\text{OD}$ )

Position	<b>4</b>		<b>5</b>	
	$\delta_{\text{H}}$ (multiplicity)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (multiplicity, <i>J</i> , Hz)	$\delta_{\text{C}}^{\text{a}}$
1	–	120.9	–	122.0
2	6.92 (s)	109.5	7.02 (s)	109.0
3	–	145.8	–	144.7
4	–	138.4	–	137.3
5	–	145.8	–	144.7
6	6.92 (s)	109.5	7.02 (s)	109.0
7	–	167.9	–	166.3
OH	9.36 (s)	–	–	–
OCH <sub>2</sub>	–	–	3.60 (q, 7.2)	60.0
CH <sub>3</sub>	–	–	1.24 (q, 7.2)	14.1

<sup>a</sup>in  $\text{CDCl}_3 + \text{CD}_3\text{OD}$ .



**Figure S1.**  $^1\text{H}$  NMR spectrum ( $\delta$  in ppm, 300 MHz,  $\text{CDCl}_3$ ) of compound 1.



**Figure S2.** <sup>13</sup>C NMR spectrum (δ in ppm, 75 MHz, CDCl<sub>3</sub>) of compound **1**.

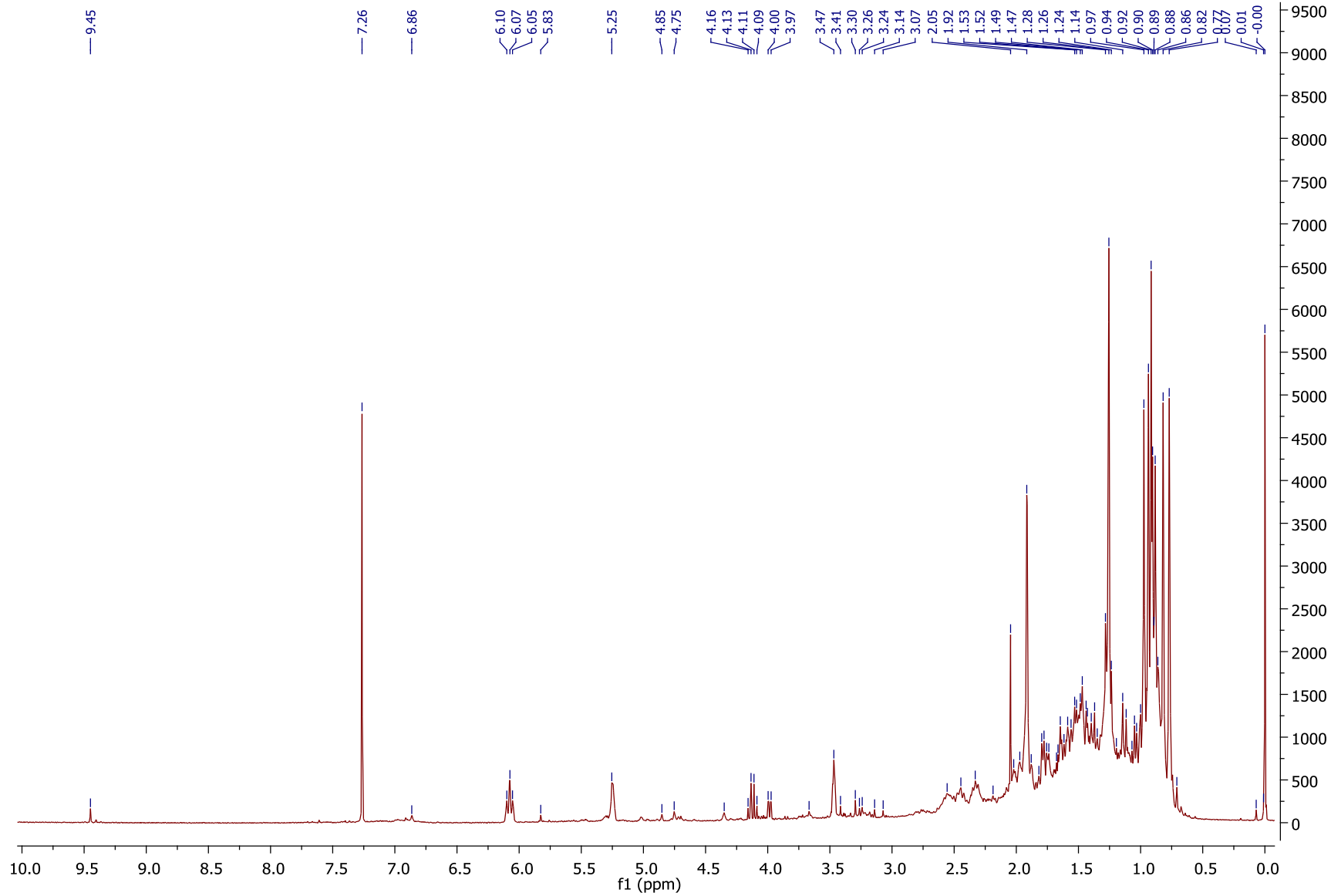
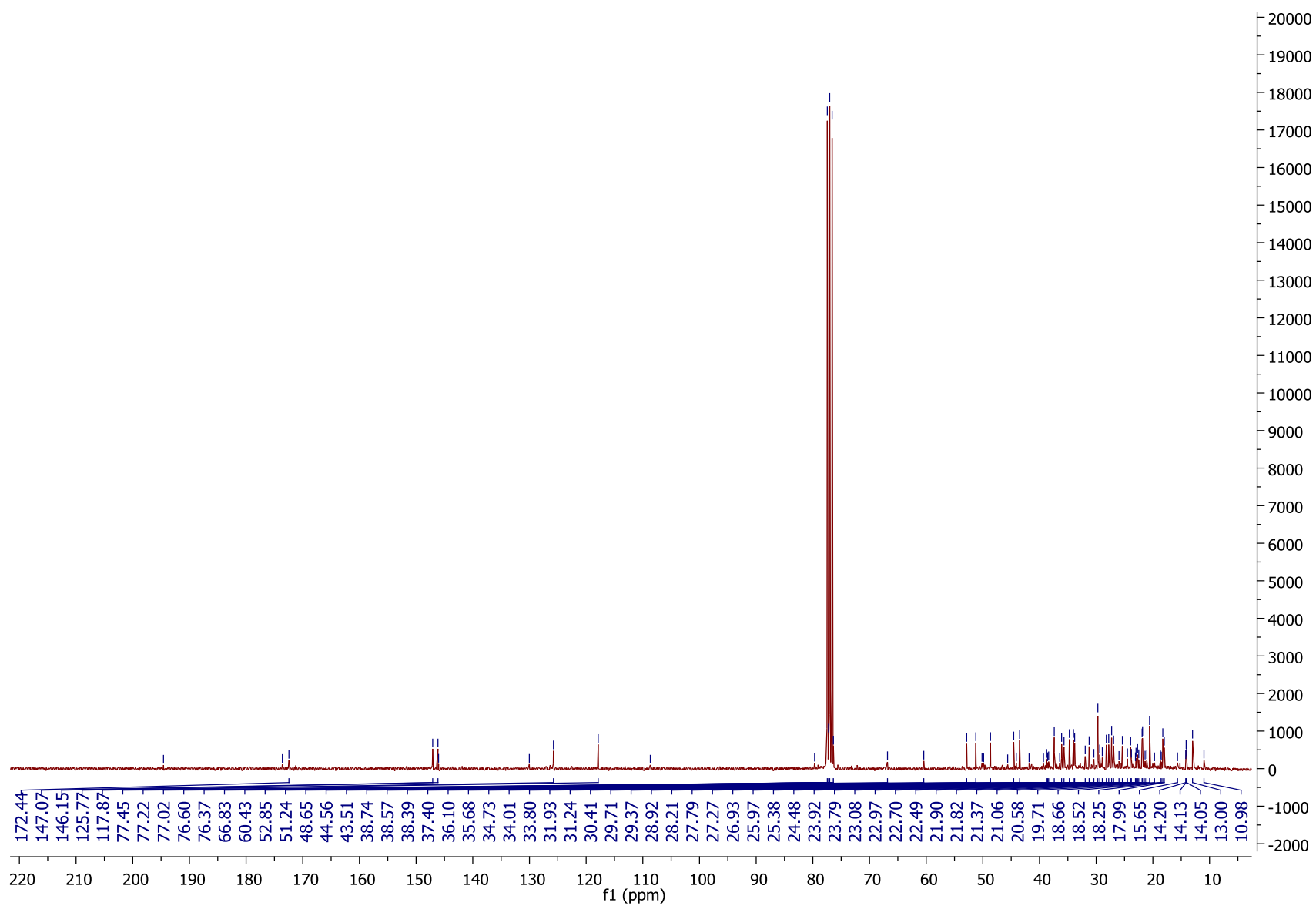


Figure S3. <sup>1</sup>H NMR spectrum ( $\delta$  in ppm, 300 MHz, CDCl<sub>3</sub>) of compound **2**.



**Figure S4.**  $^{13}\text{C}$  NMR spectrum ( $\delta$  in ppm, 75 MHz,  $\text{CDCl}_3$ ) of compound 2.

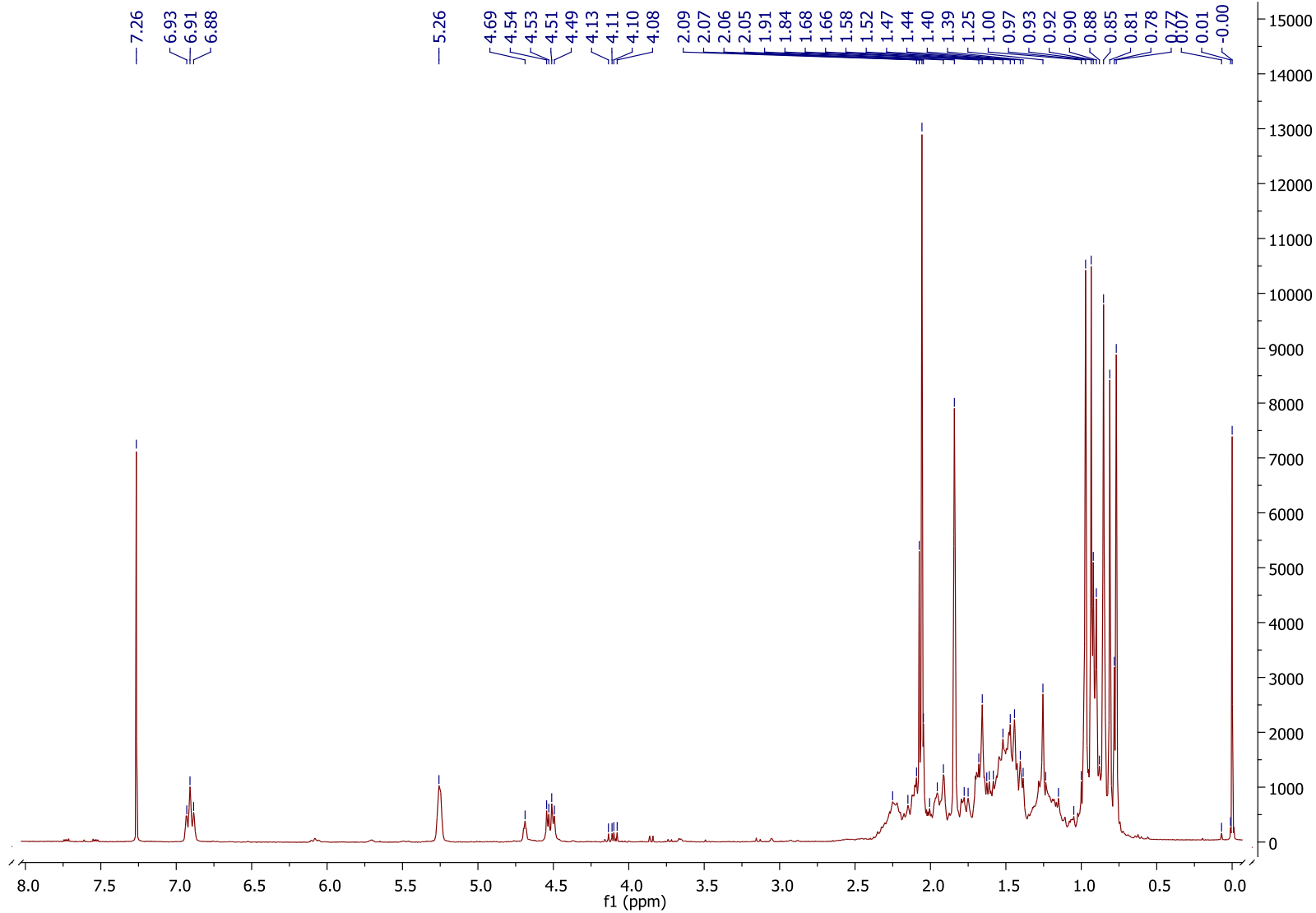
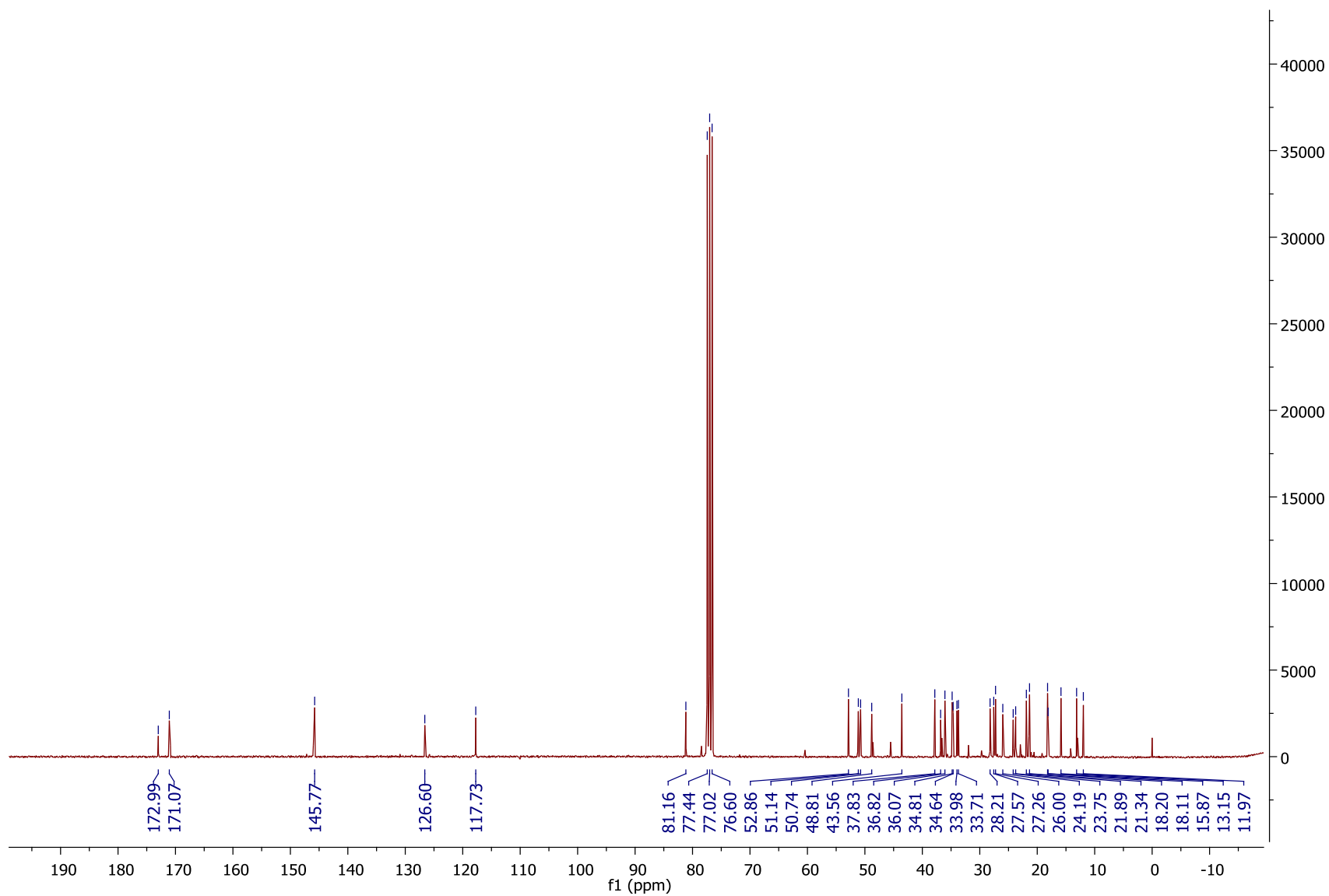
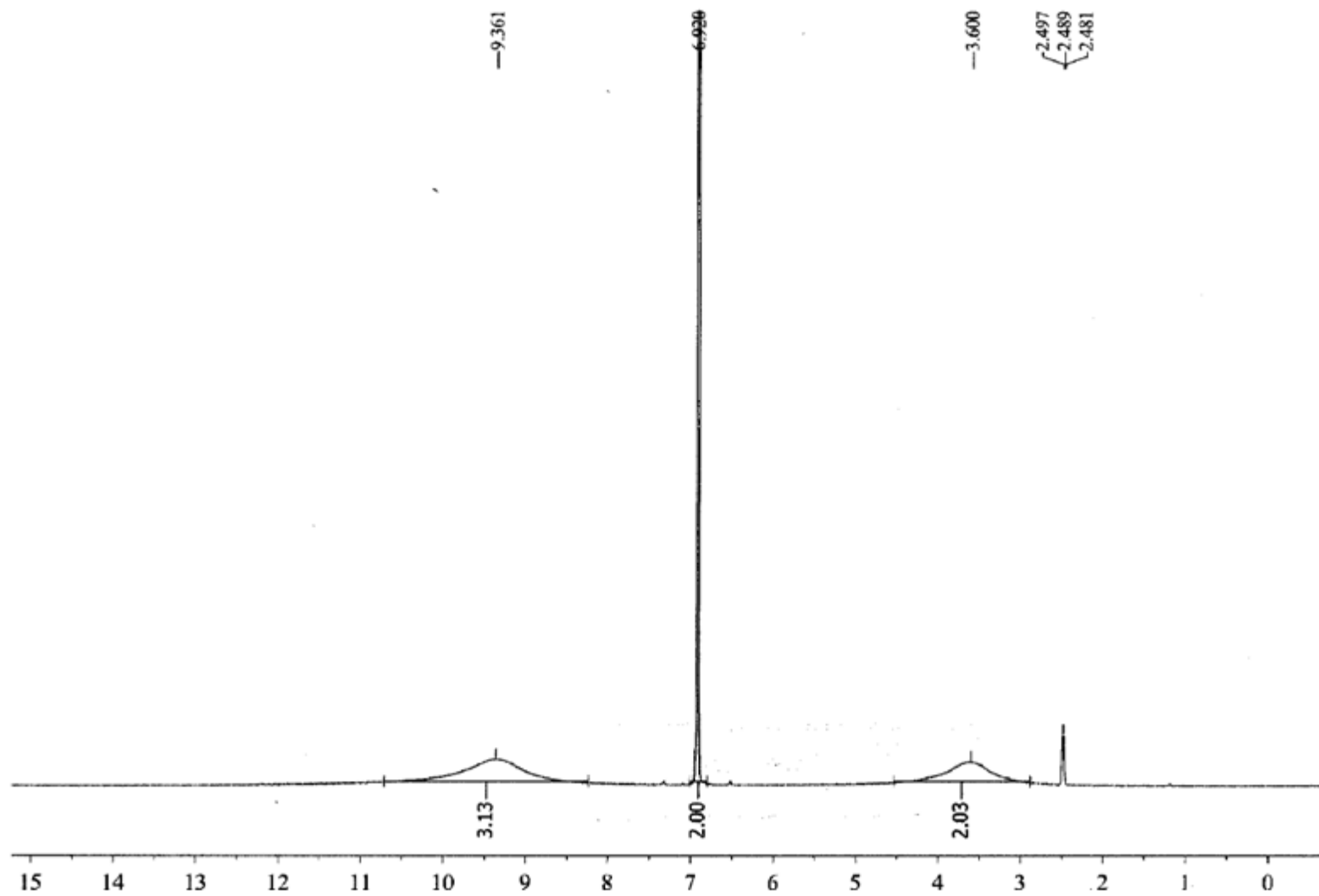


Figure S5. <sup>1</sup>H NMR spectrum (δ in ppm, 300 MHz, CDCl<sub>3</sub>) of compound 3.





**Figure S6.** <sup>13</sup>C NMR spectrum (δ in ppm, 75 MHz, CDCl<sub>3</sub>) of compound **3**.



**Figure S7.**  $^1\text{H}$  NMR spectrum ( $\delta$  in ppm, 300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **4**.

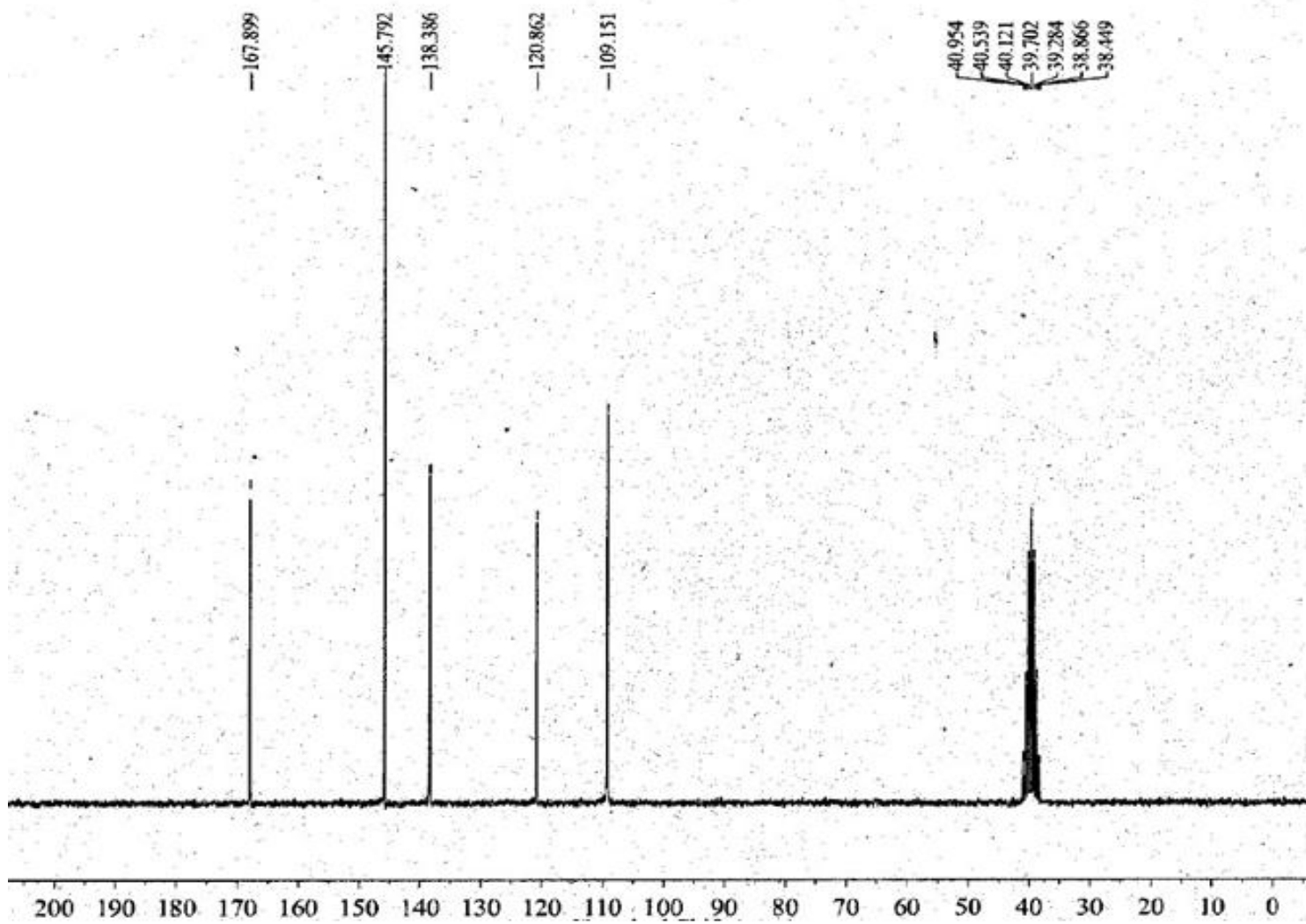


Figure S8.  $^{13}\text{C}$  NMR spectrum ( $\delta$  in ppm, 75 MHz,  $\text{CD}_3\text{OD}$ ) of compound 4.

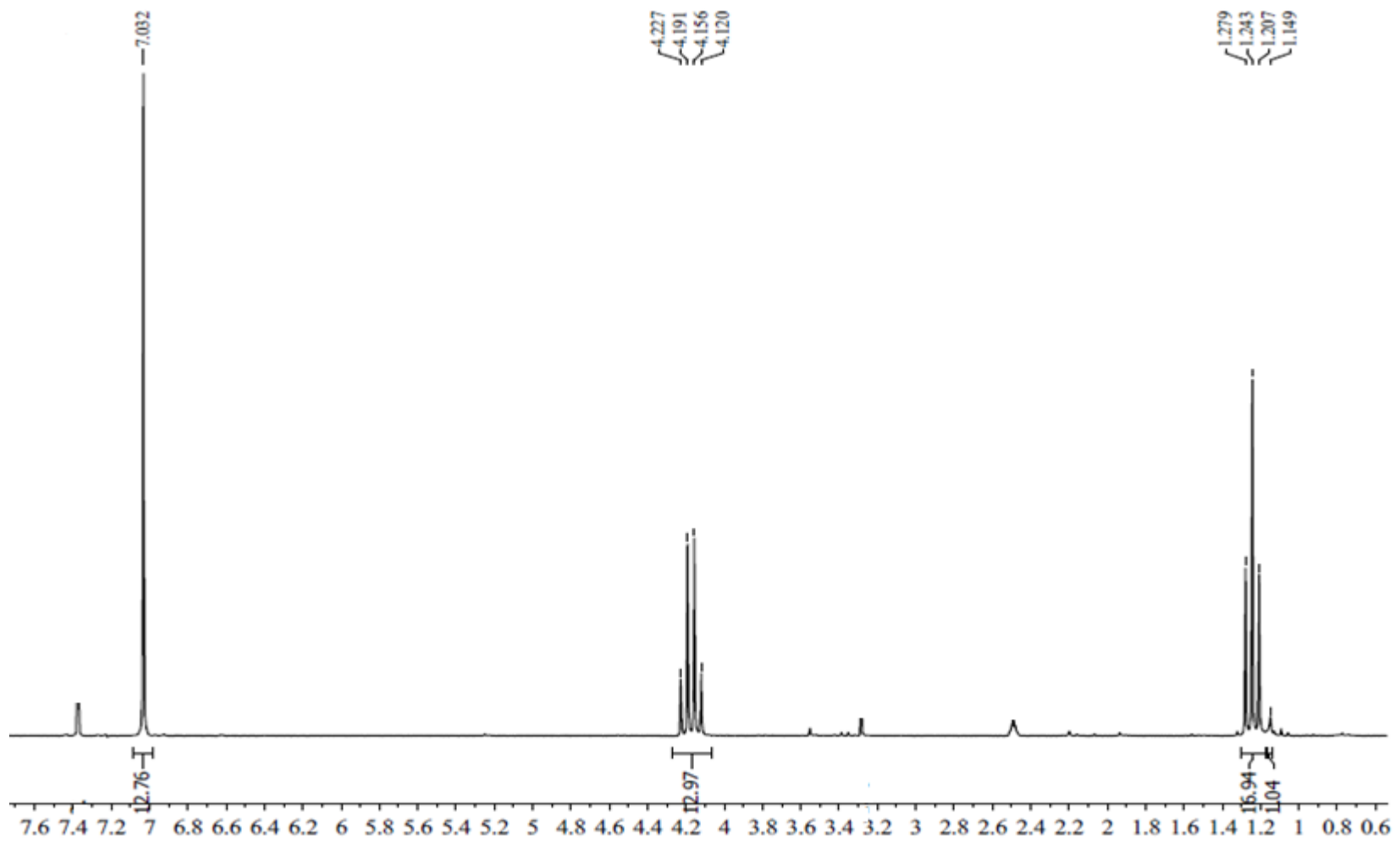
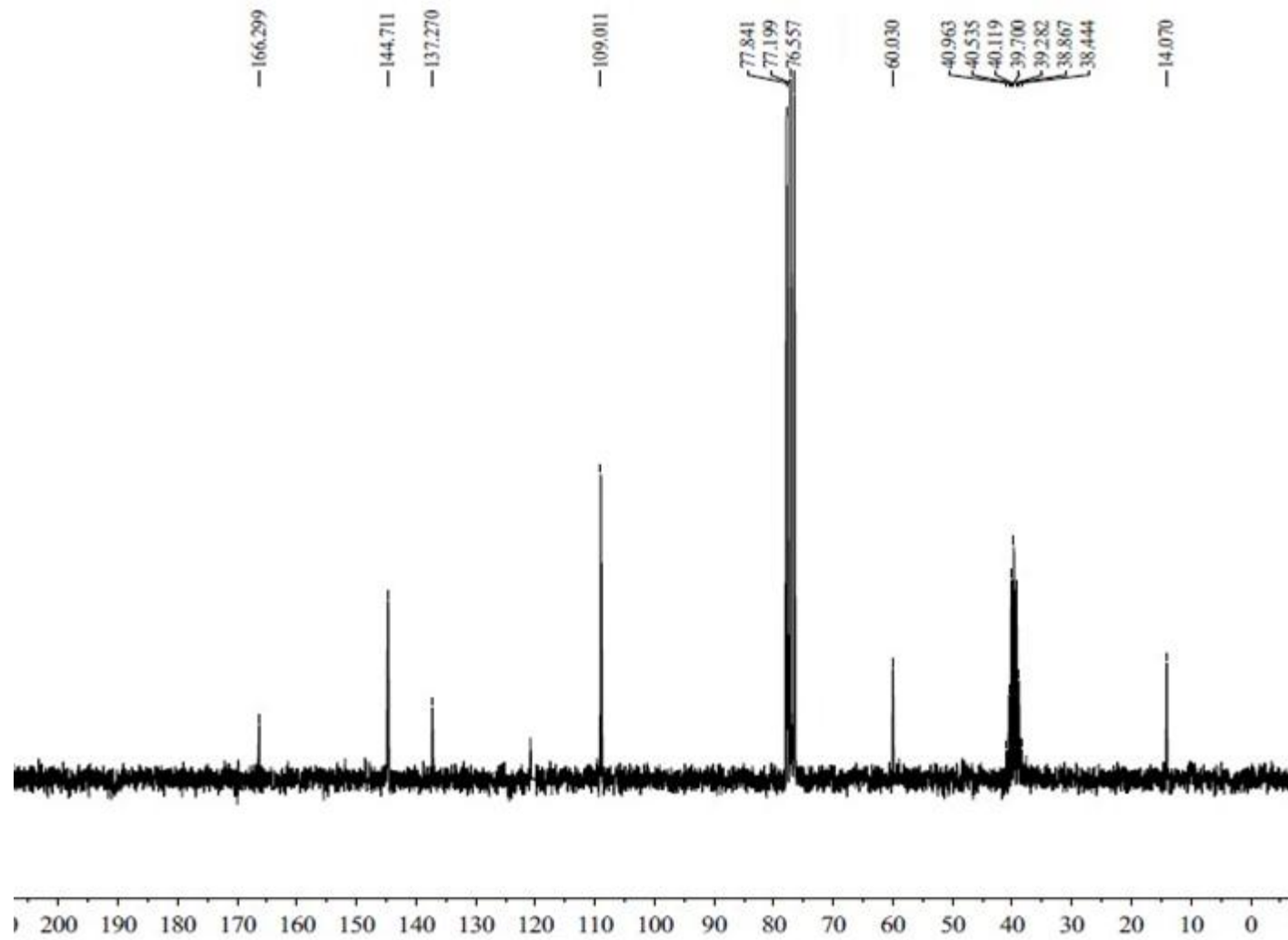


Figure S9.  $^1\text{H}$  NMR spectrum ( $\delta$  in ppm, 300 MHz,  $\text{CD}_3\text{OD}$ ) of compound 5.



**Figure S10.**  $^{13}\text{C}$  NMR spectrum ( $\delta$  in ppm, 75 MHz,  $\text{CDCl}_3 + \text{CD}_3\text{OD}$ ) of compound **5**.