

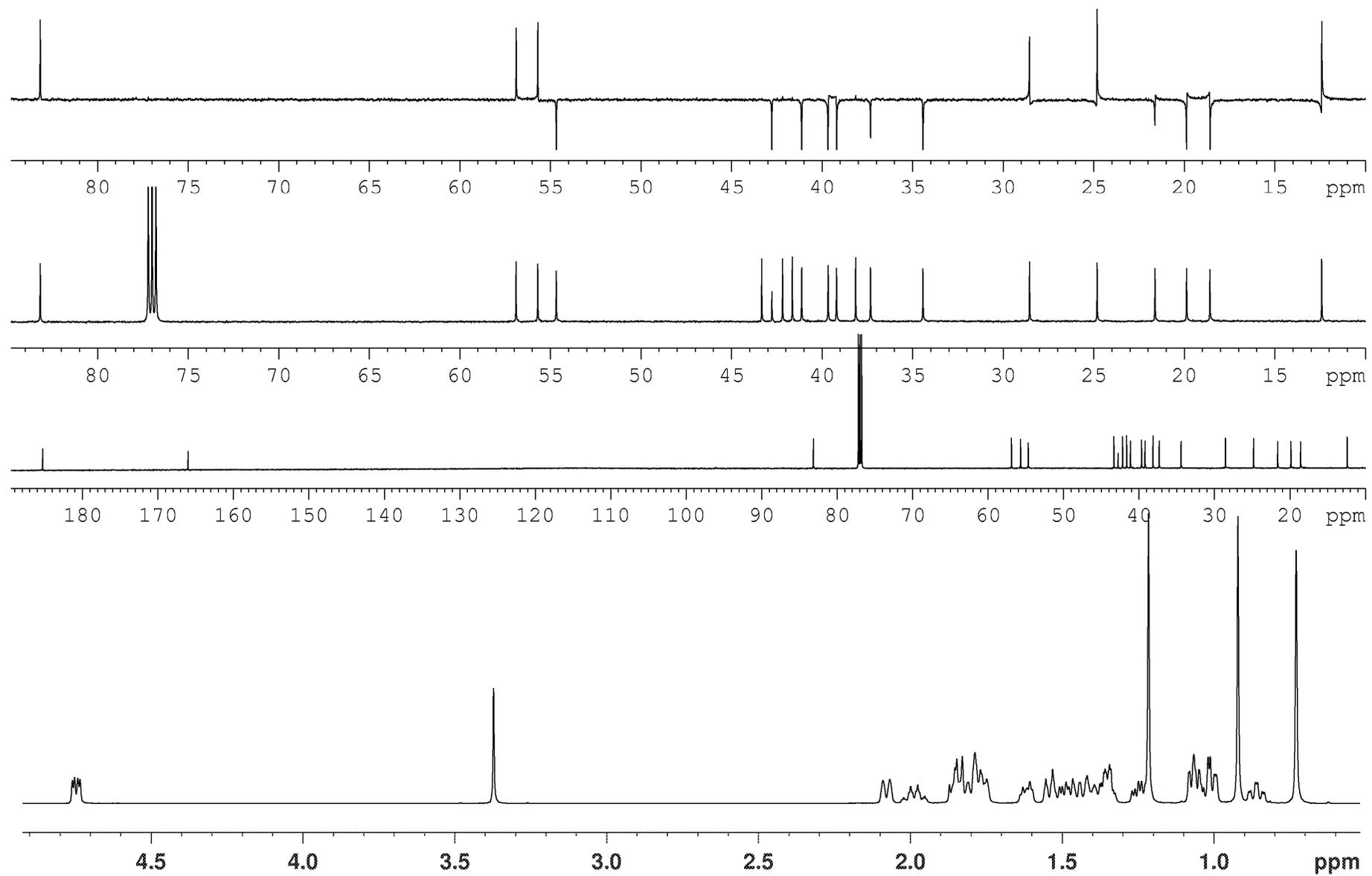
**New malonate macrocycle bearing two isosteviol moieties and its adduct with fullerene C<sub>60</sub>**

**Ravil N. Khaybullin, Irina Yu. Strobyskina, Valentina P. Gubskaya, Guzel M. Fazleeva, Shamil K. Latypov and Vladimir E. Kataev\***

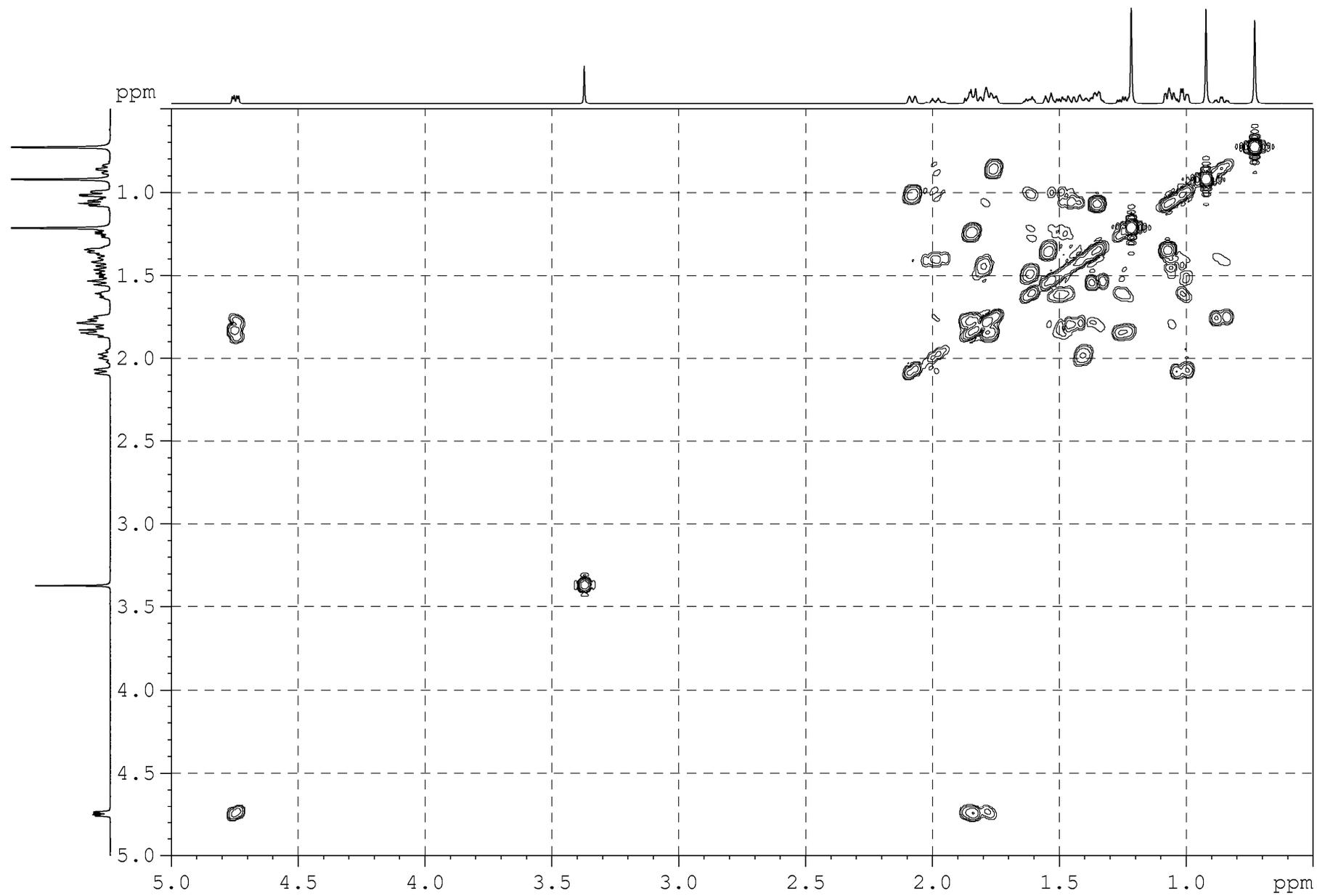
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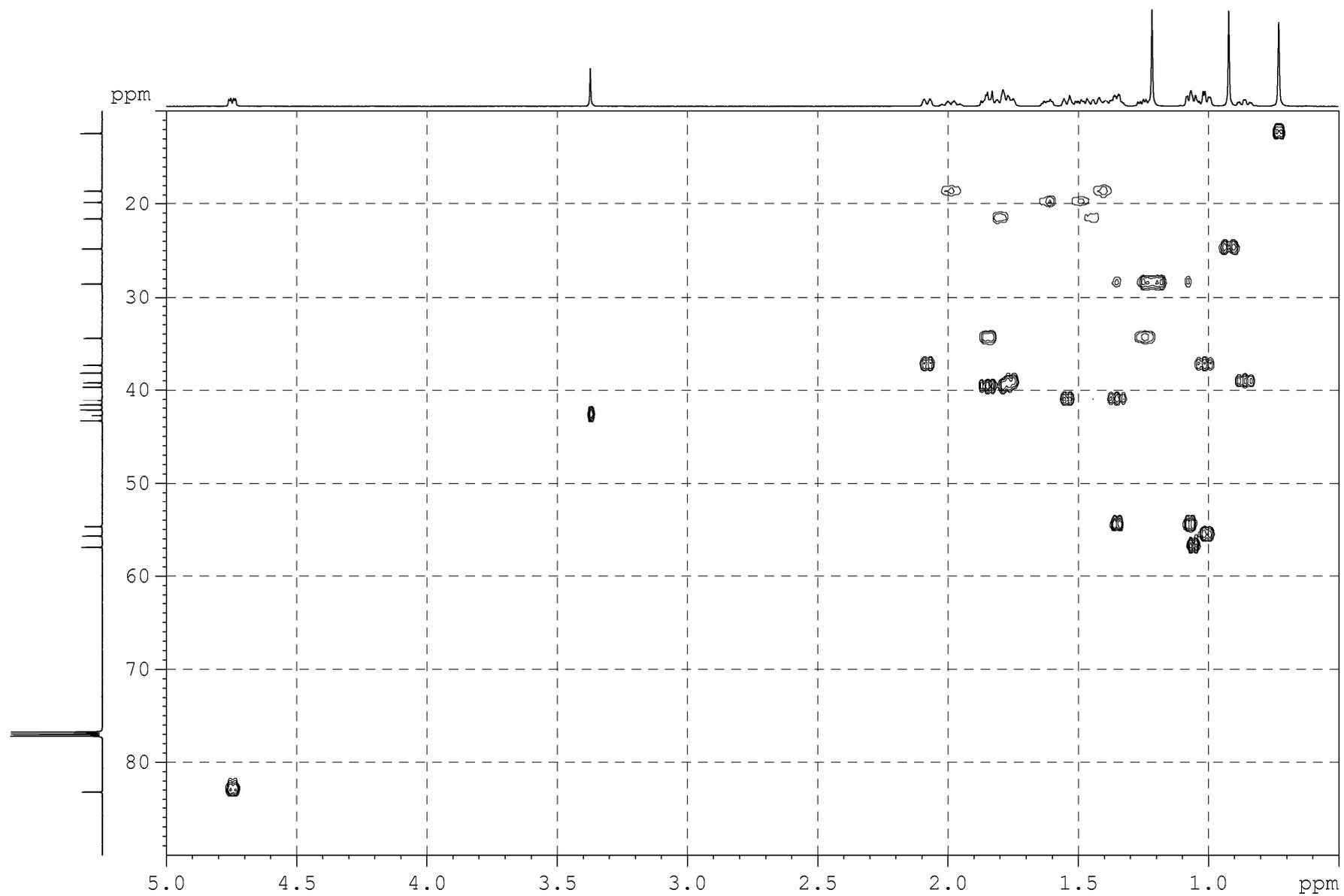
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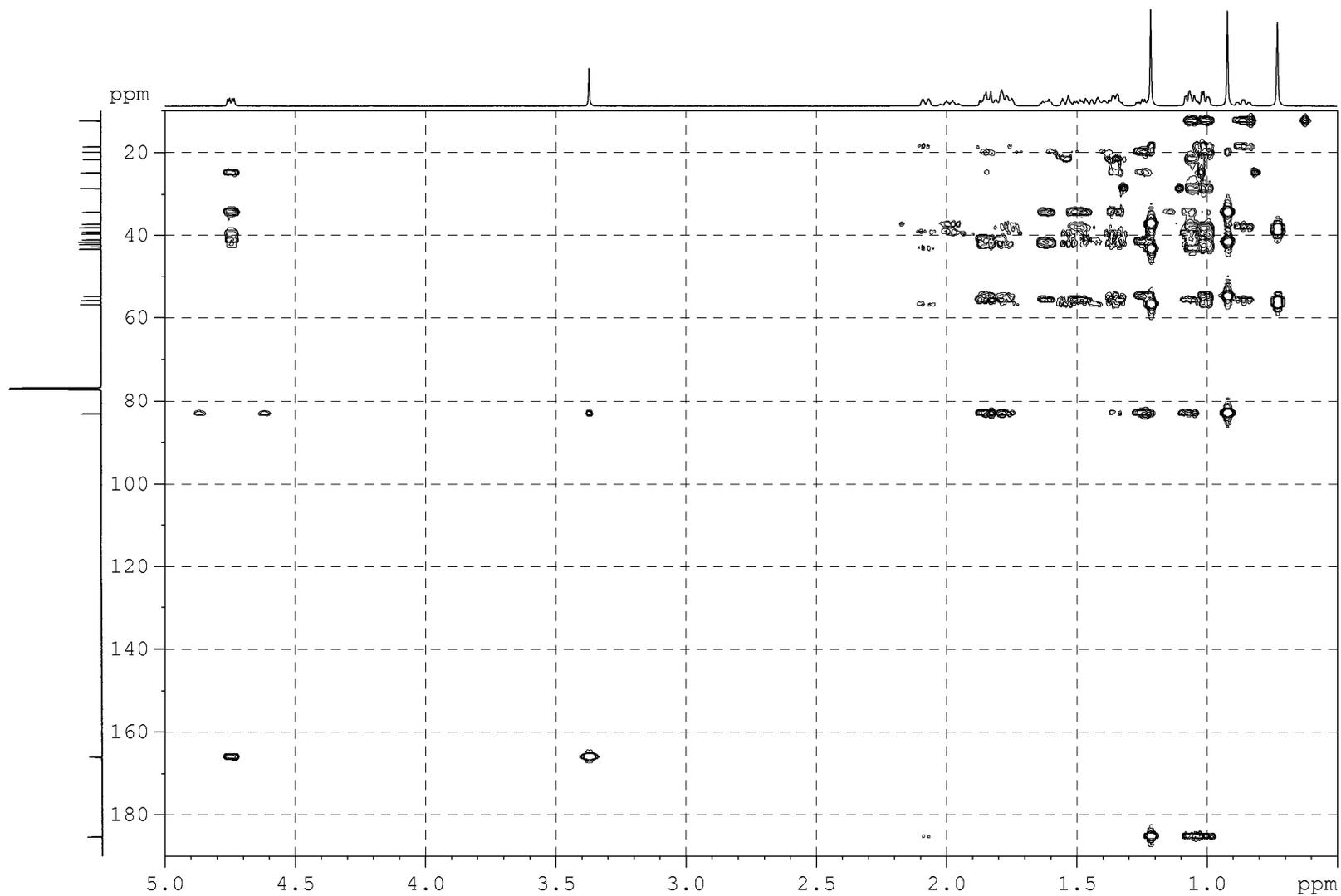
**Figure S1.** 1D <sup>1</sup>H, <sup>13</sup>C and DEPT spectra in CDCl<sub>3</sub> of 7 (T=303K).



**Figure S2.** 2D  $^1\text{H}$ - $^1\text{H}$  COSY spectra in  $\text{CDCl}_3$  of **7** ( $T=303\text{K}$ ).

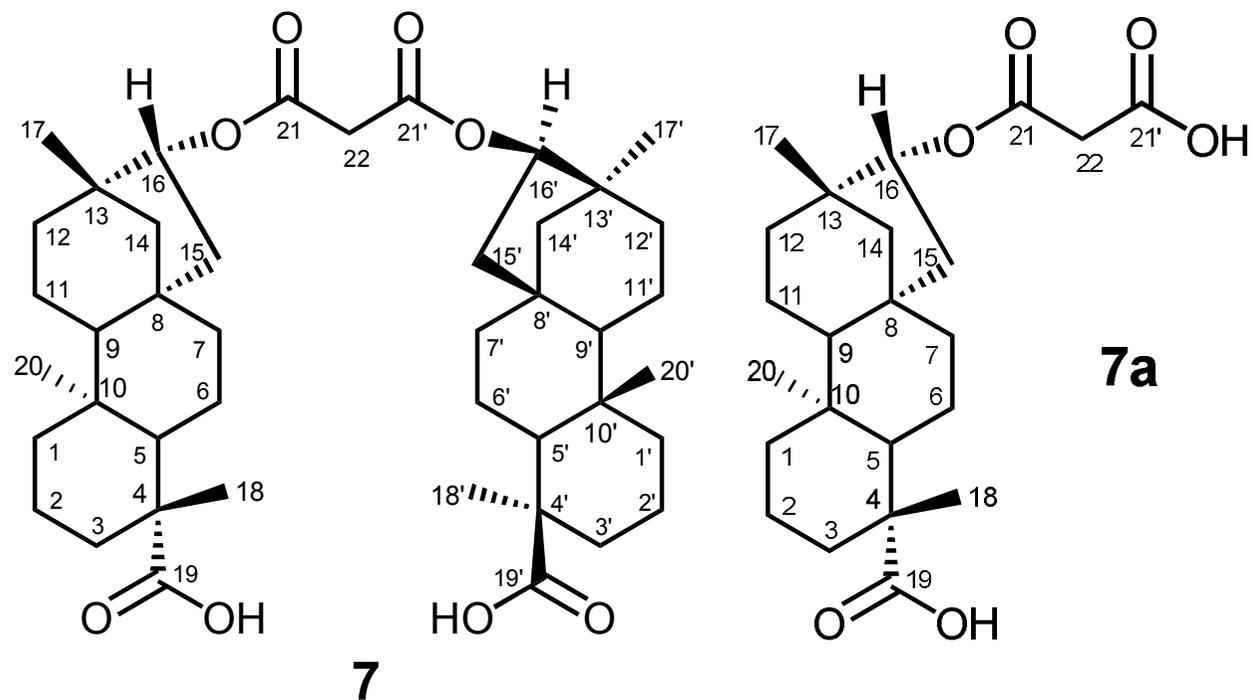


**Figure S3.** 2D  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectra in  $\text{CDCl}_3$  of **7** ( $T=303\text{K}$ ).

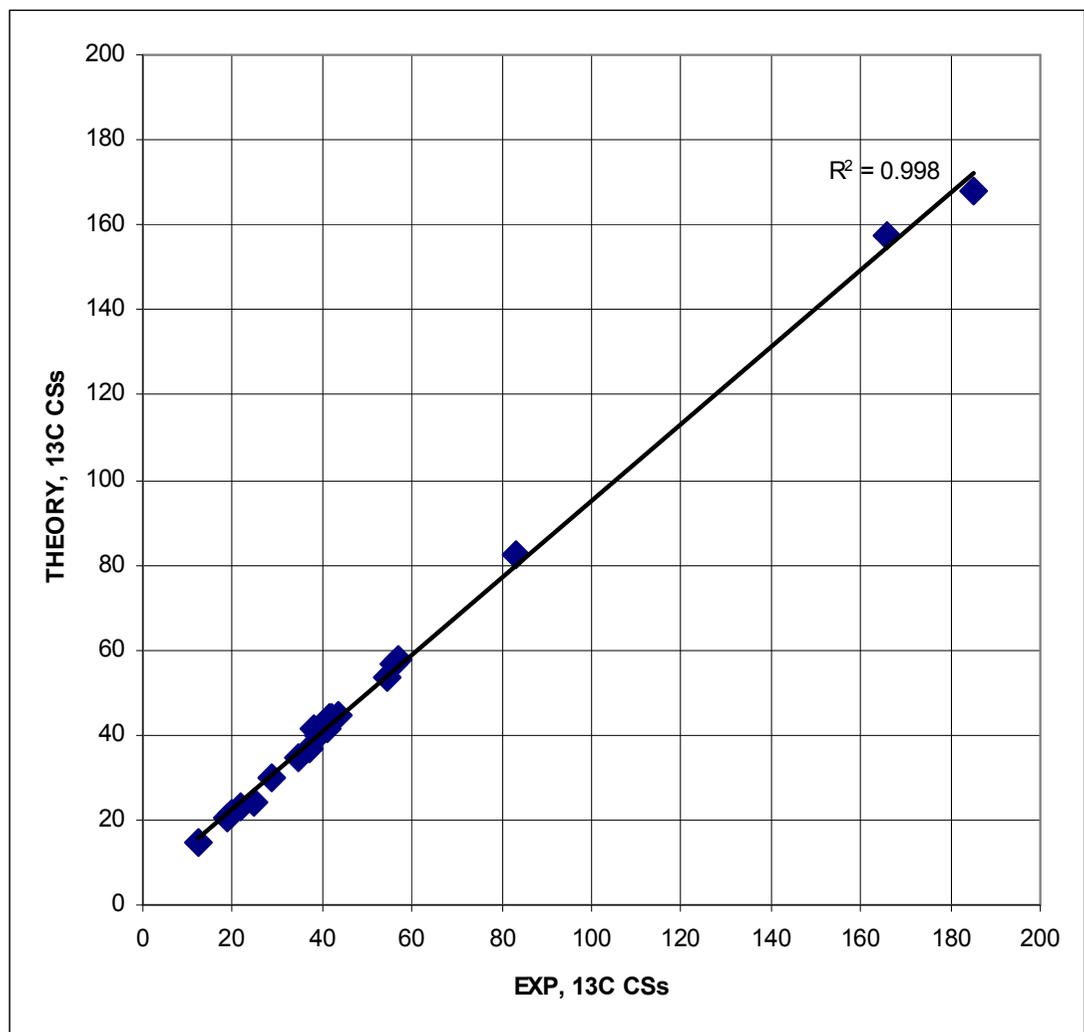


**Figure S4.** 2D  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectra in  $\text{CDCl}_3$  of **7** ( $T=303\text{K}$ ).

**Table S1.** NMR  $^{13}\text{C}$  chemical shifts (CS) for compound **7** and calculated for model **7a**.



C, n	Experiment for 7	Theory for 7a
1	39,21	39,6651
2	18,58	20,4285
3	37,33	36,9512
4	42,19	44,0037
5	56,9	57,7273
6	21,62	22,889
7	41,13	41,3343
8	43,34	44,366
9	55,7	56,7743
10	38,15	41,2827
11	19,87	21,4745
12	34,43	34,5394
13	41,65	43,9565
14	54,68	53,6094
15	39,67	40,7807
16	83,16	82,3213
17	24,82	24,3074
18	28,55	30,1667
19	185,25	168,0134
20	12,42	14,5887
21	166,03	157,4432



**Figure S5.** The correlation of <sup>13</sup>C NMR chemical shift calculated (GIAO B3LYP/6-31G(d)//HF/6-31G)<sup>22</sup> for simple model **7a** versus experimental values observed for compound **7**.

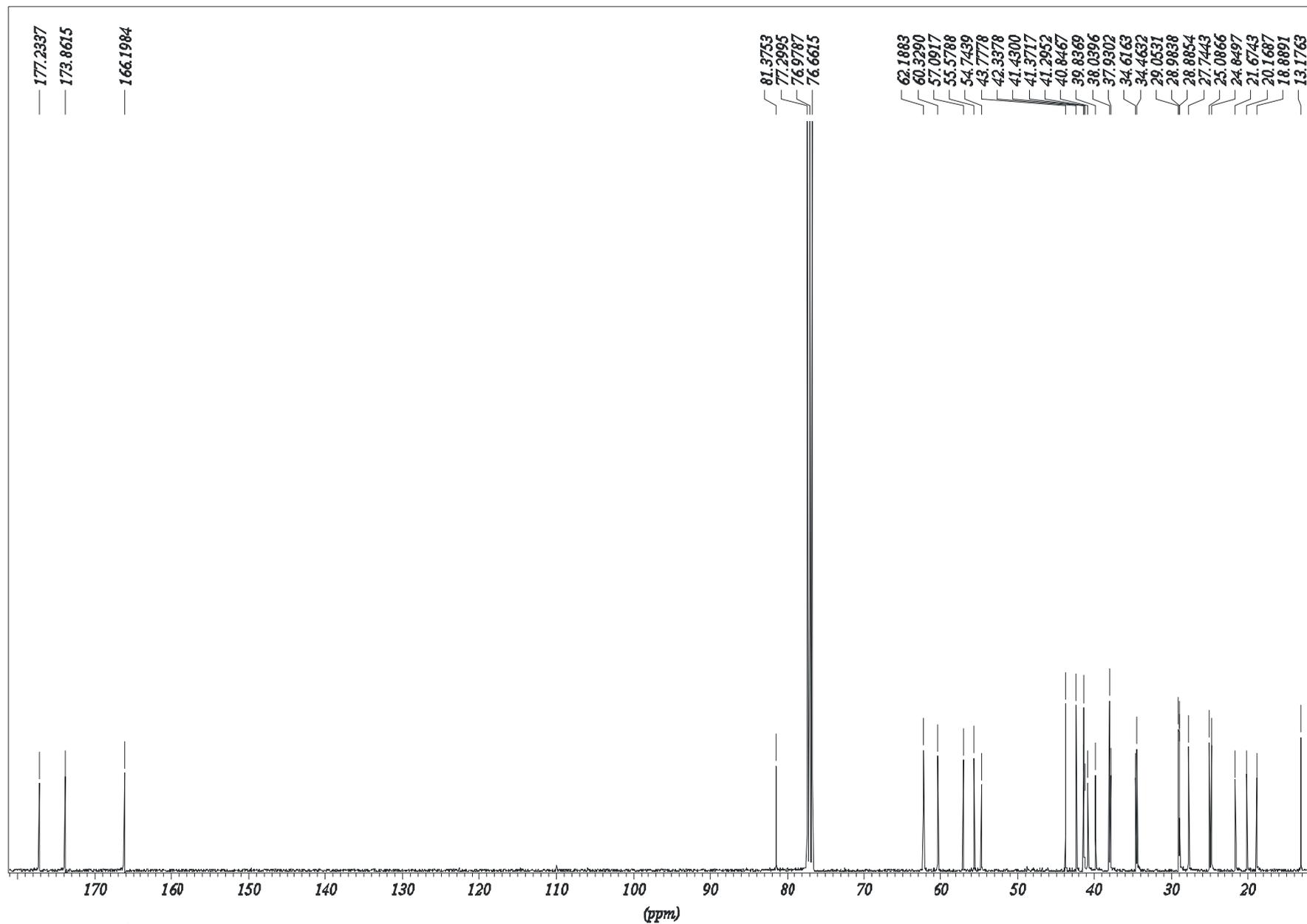


Figure S6.  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ,  $T=303\text{K}$ ) of malonate macrocycle 7.

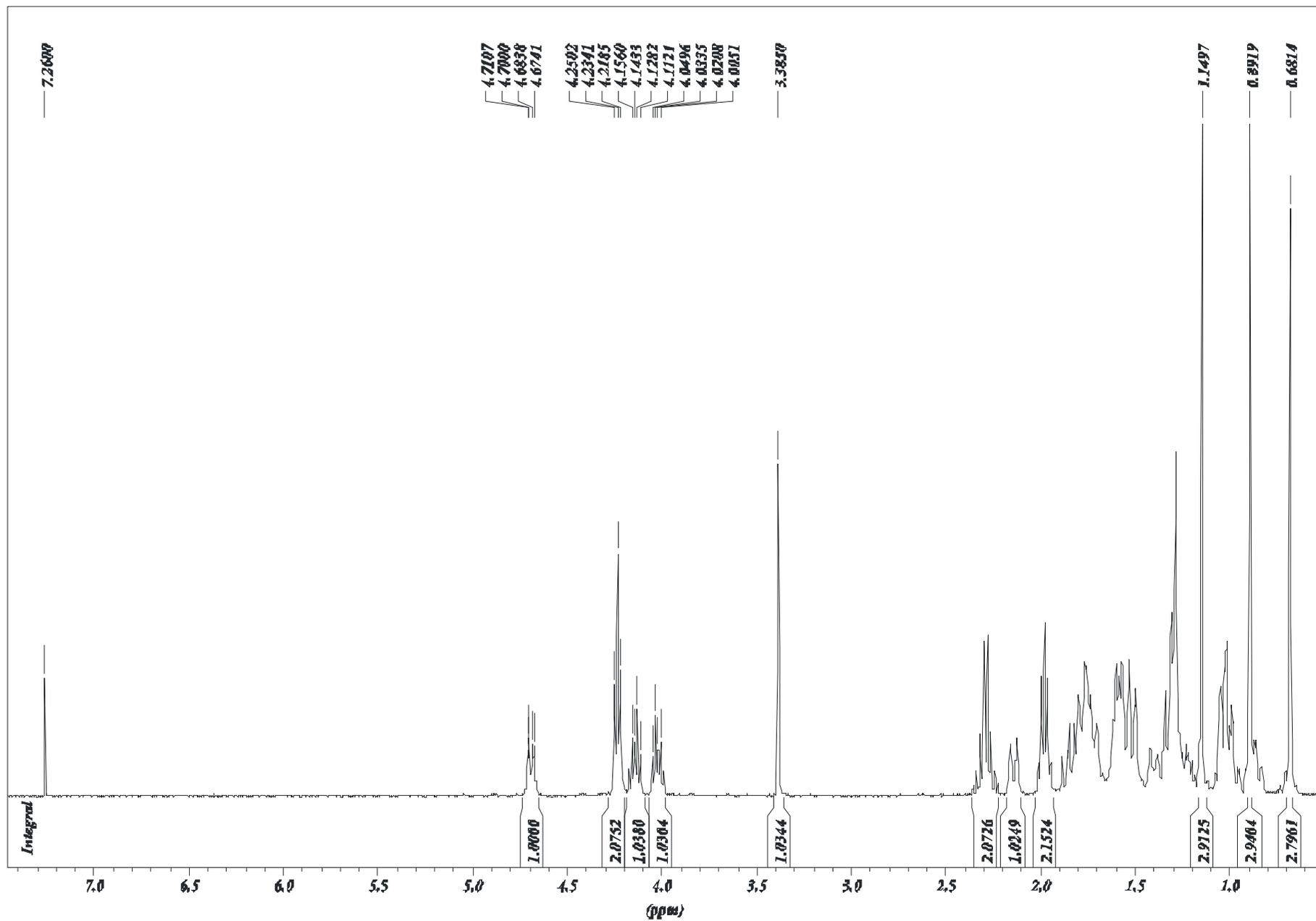


Figure S7.  $^1\text{H}$  NMR spectrum (600 MHz,  $\text{CDCl}_3$ ,  $T=303\text{K}$ ) of malonate macrocycle 7.

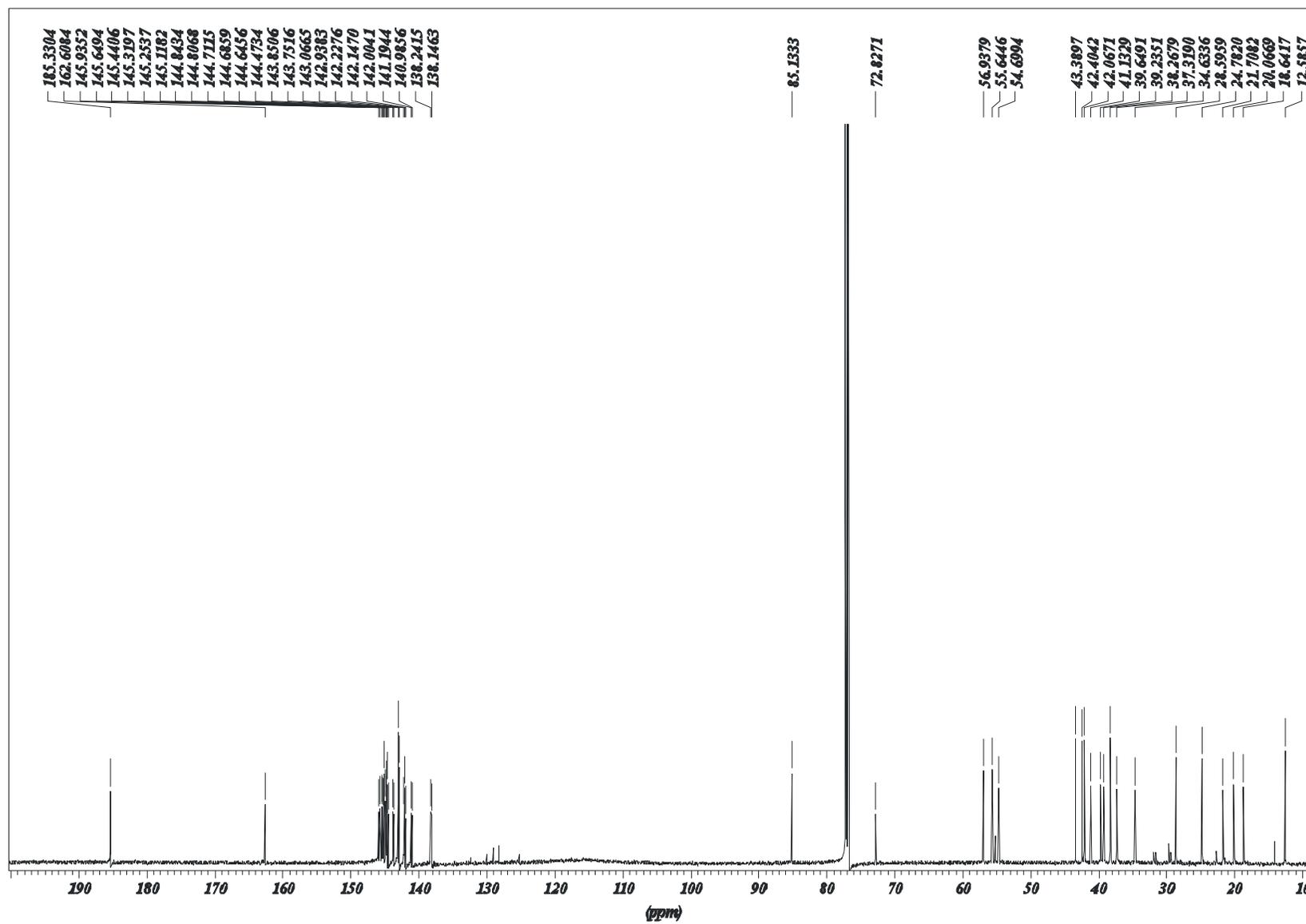
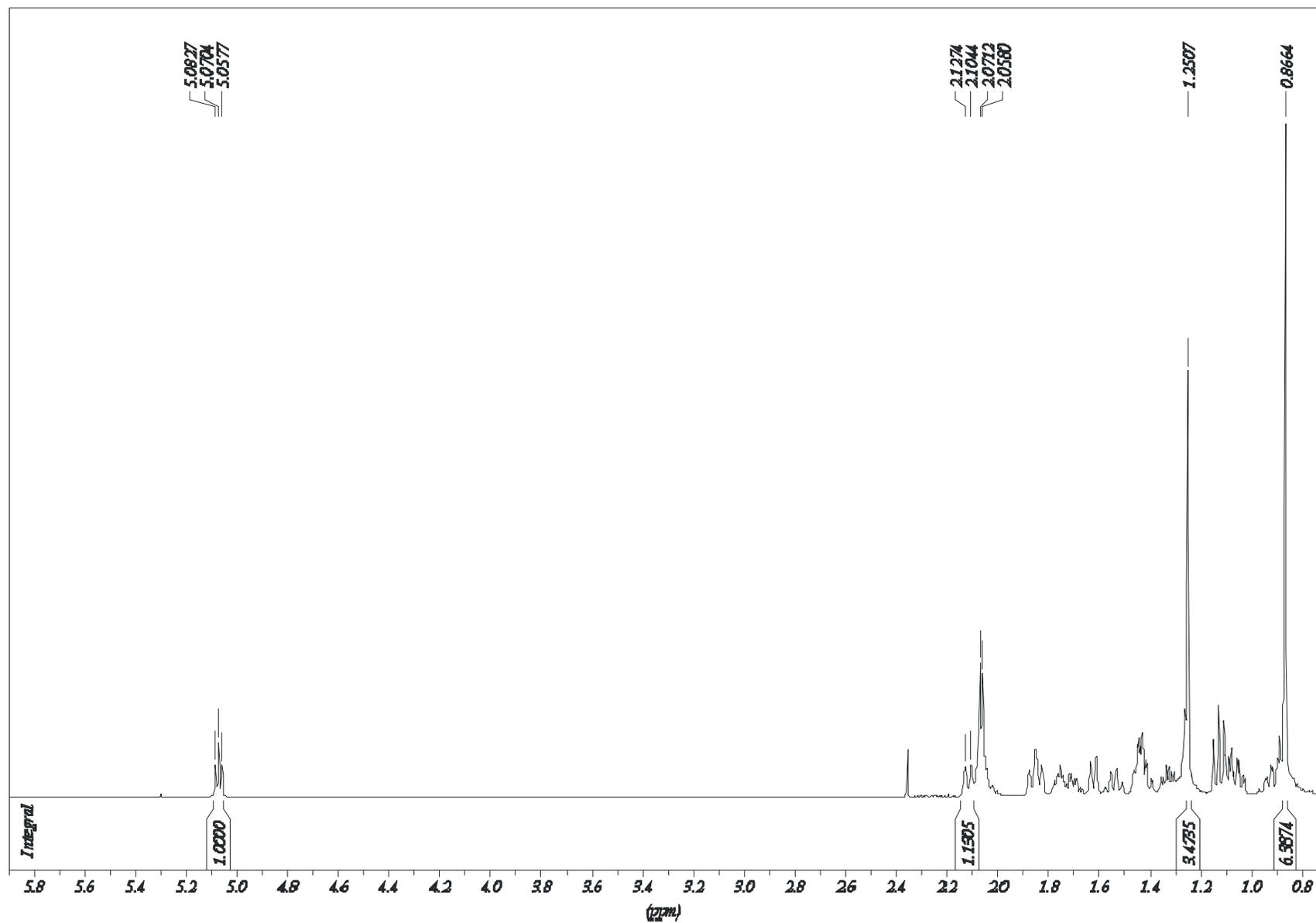
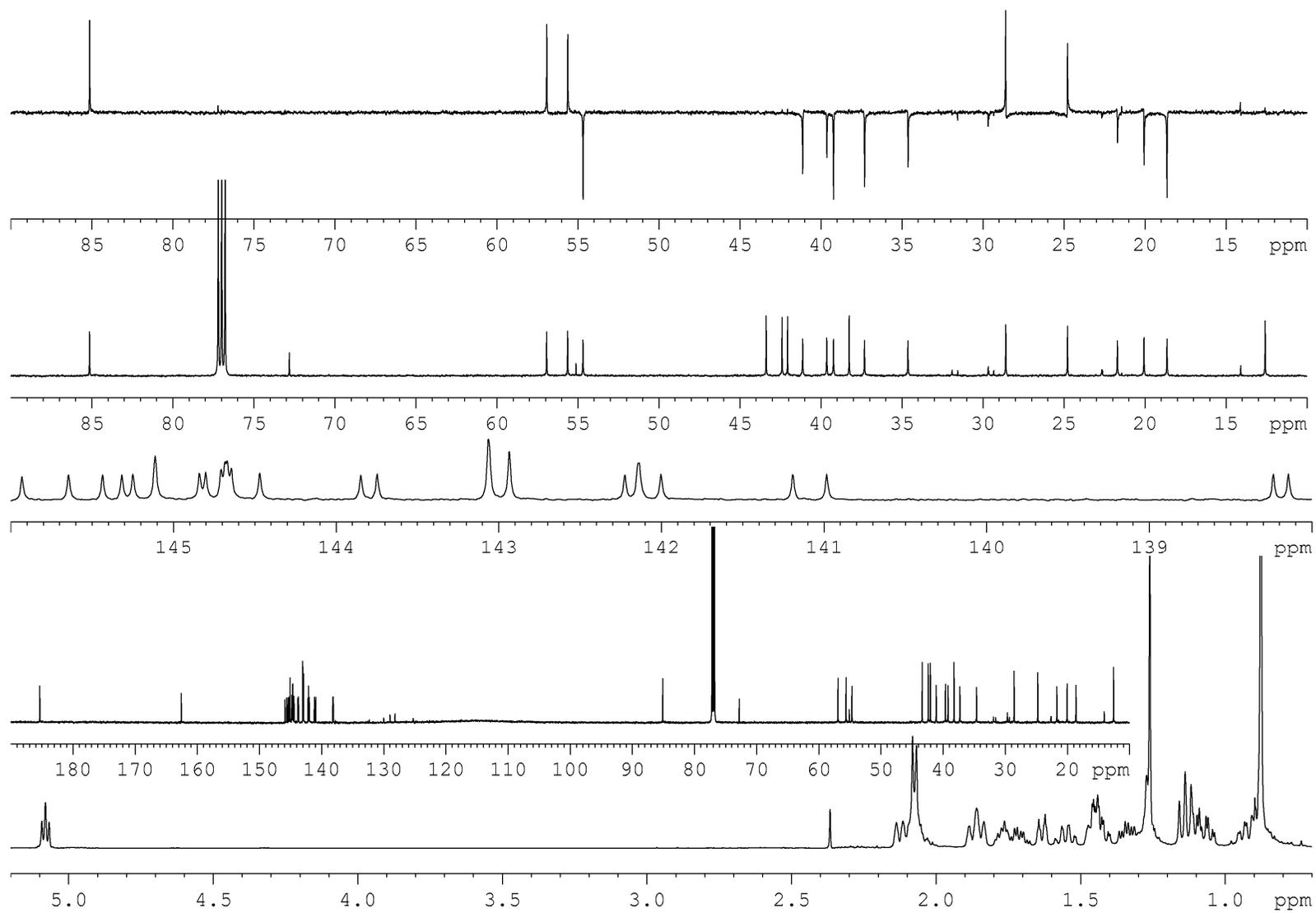


Figure S8.  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ,  $\text{CDCl}_3$ ,  $T=303\text{K}$ ) of methanofullerene **8**.

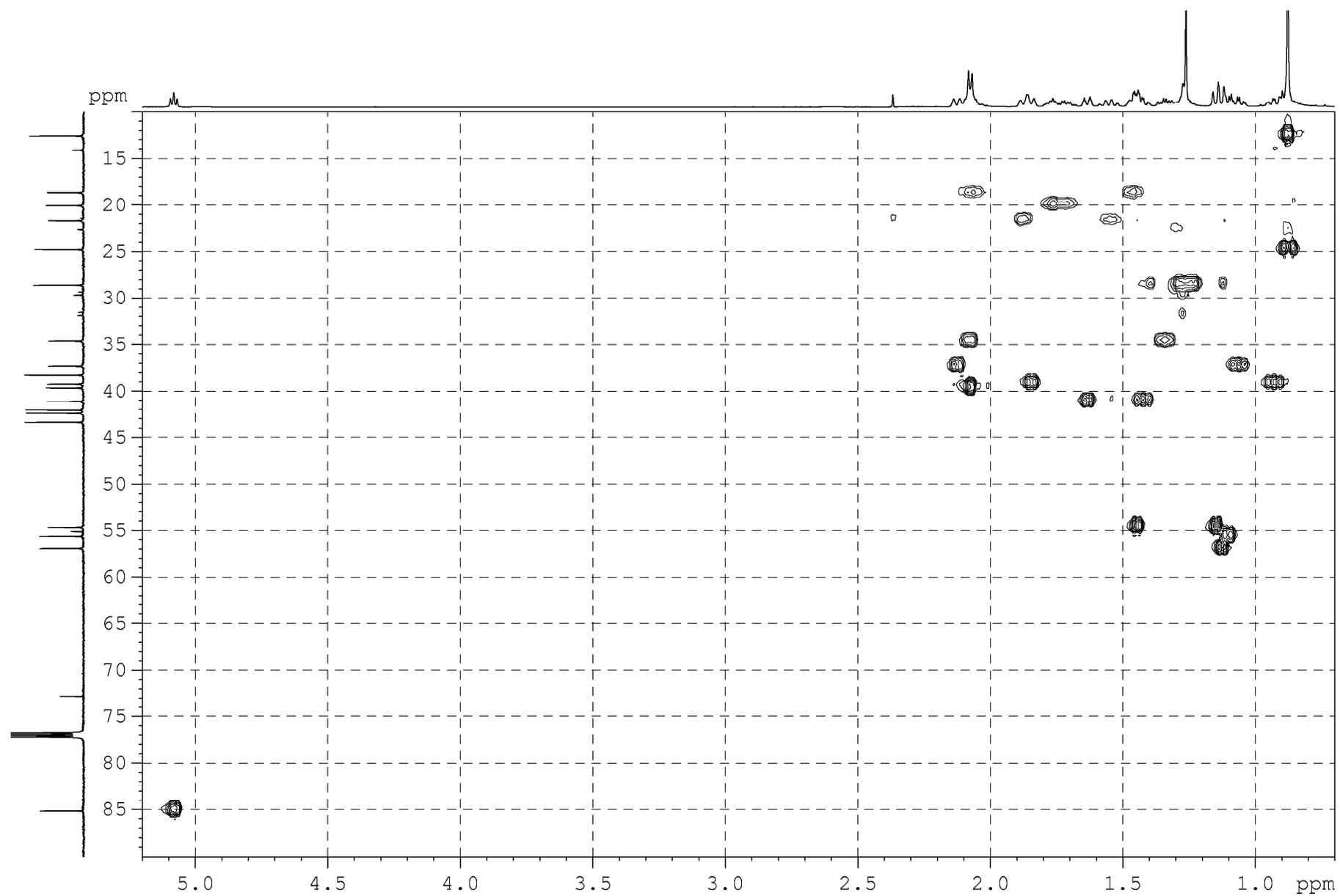


**Figure S9.** <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>, T=303K) of methanofullerene **8**.

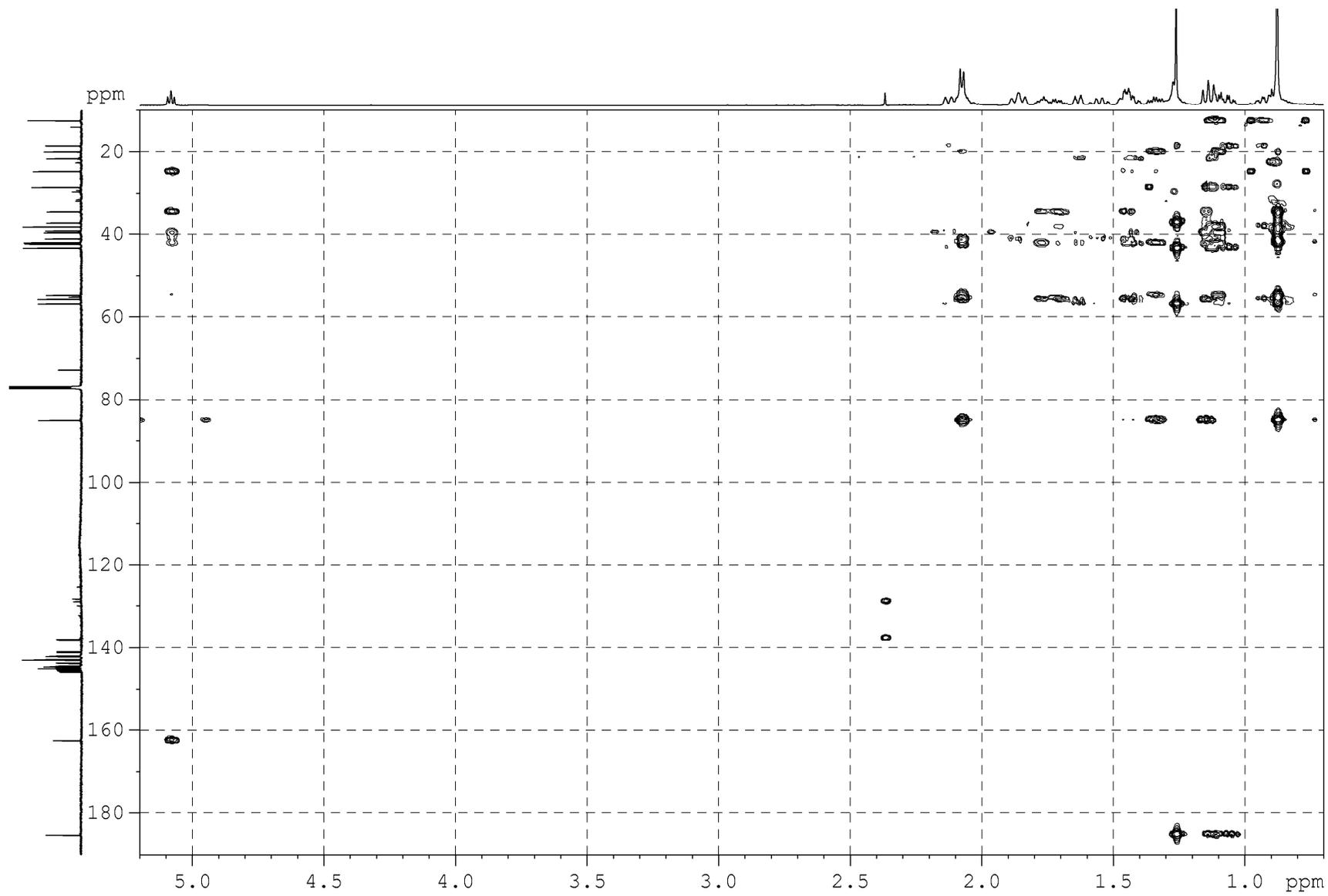


**Figure S10.** 1D <sup>1</sup>H, <sup>13</sup>C and DEPT spectra in CDCl<sub>3</sub> of **8** (T=303K).





**Figure S12.** 2D  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectra in  $\text{CDCl}_3$  of **8** ( $T=303\text{K}$ ).



**Figure S13.** 2D  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectra in  $\text{CDCl}_3$  of **8** ( $T=303\text{K}$ ).

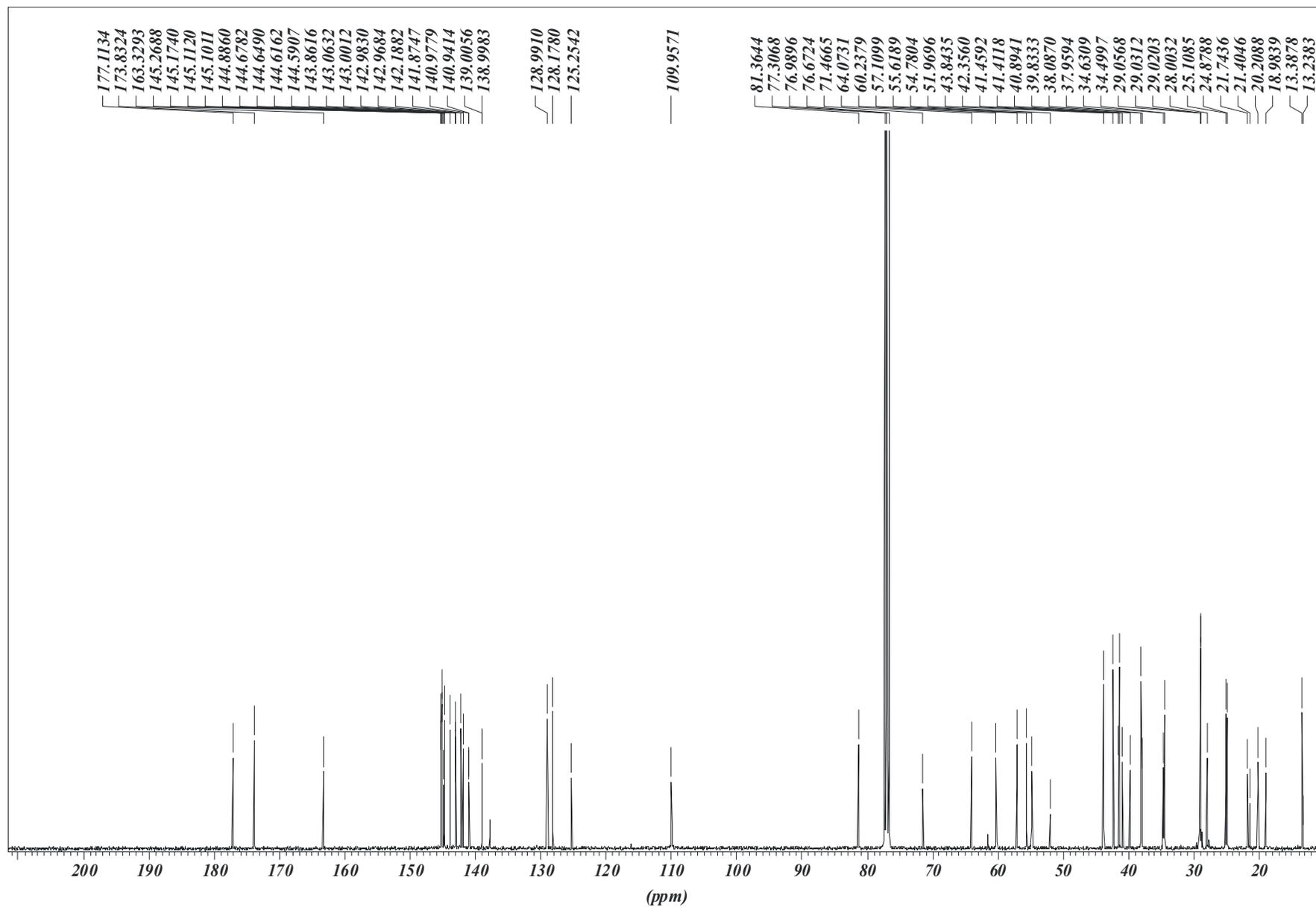
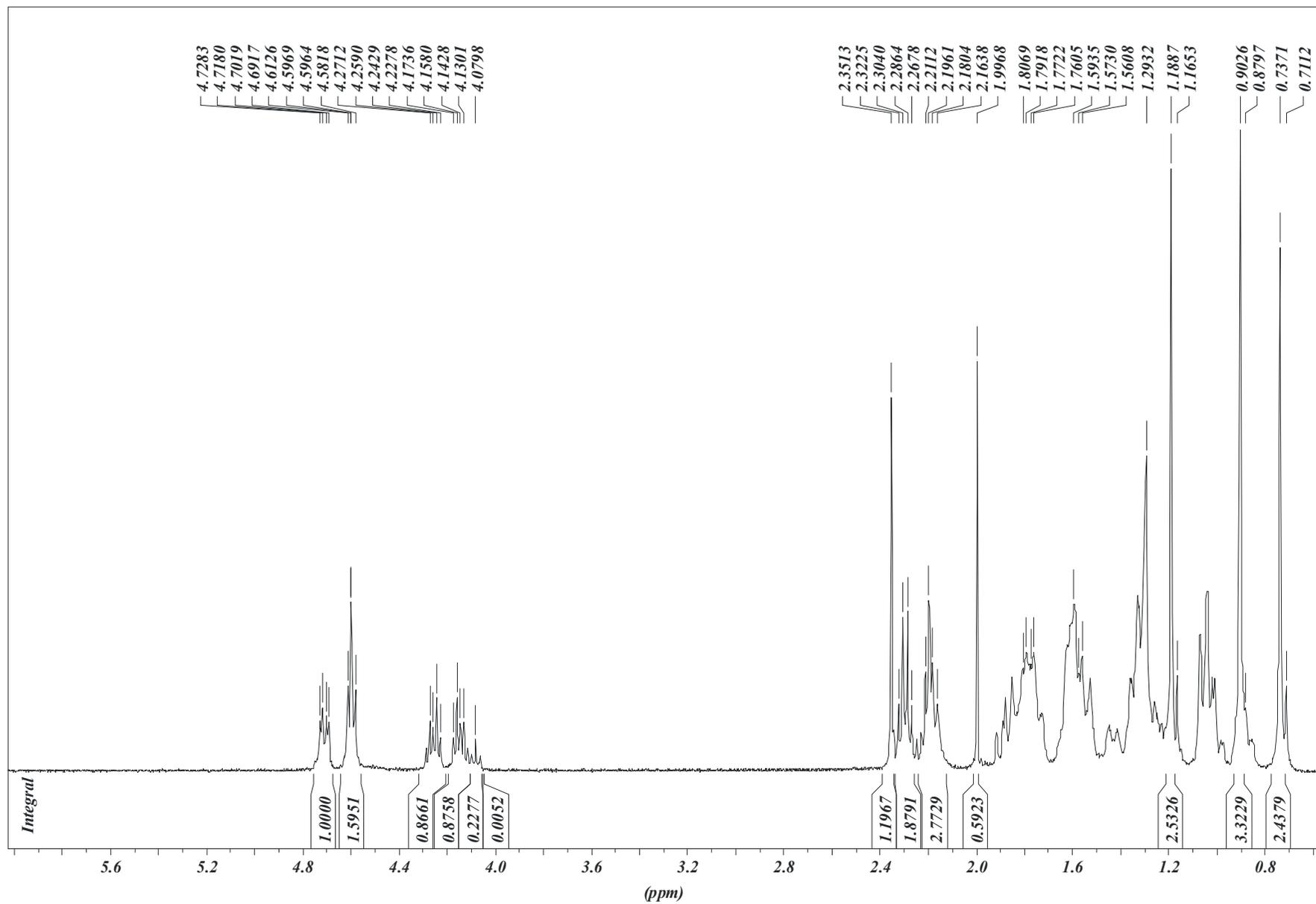
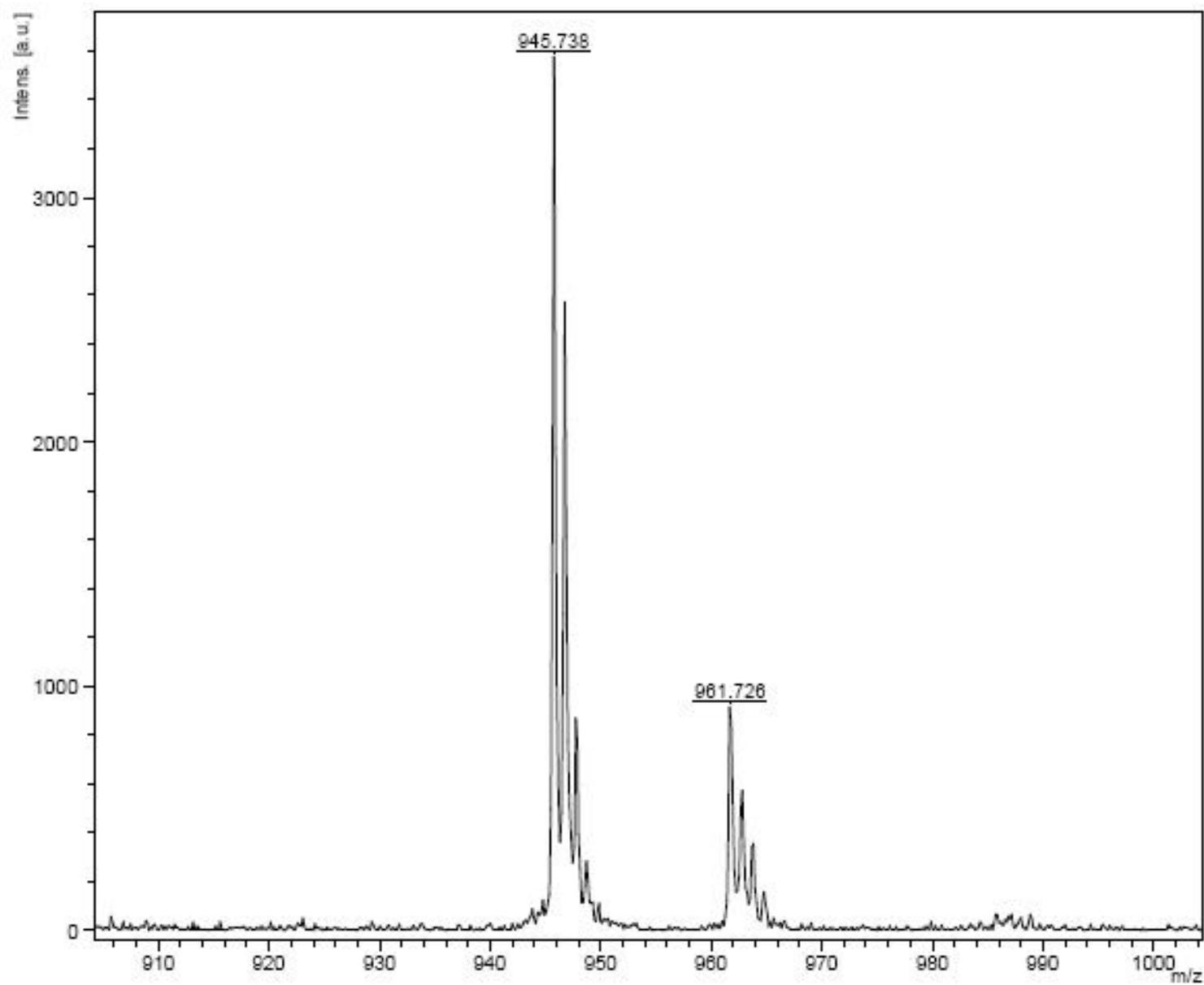
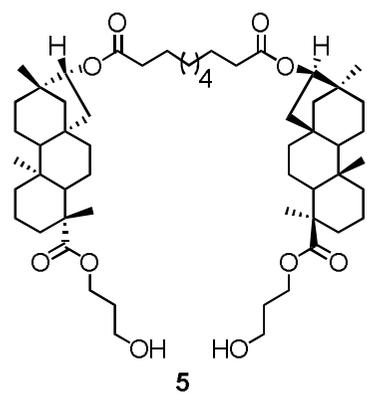


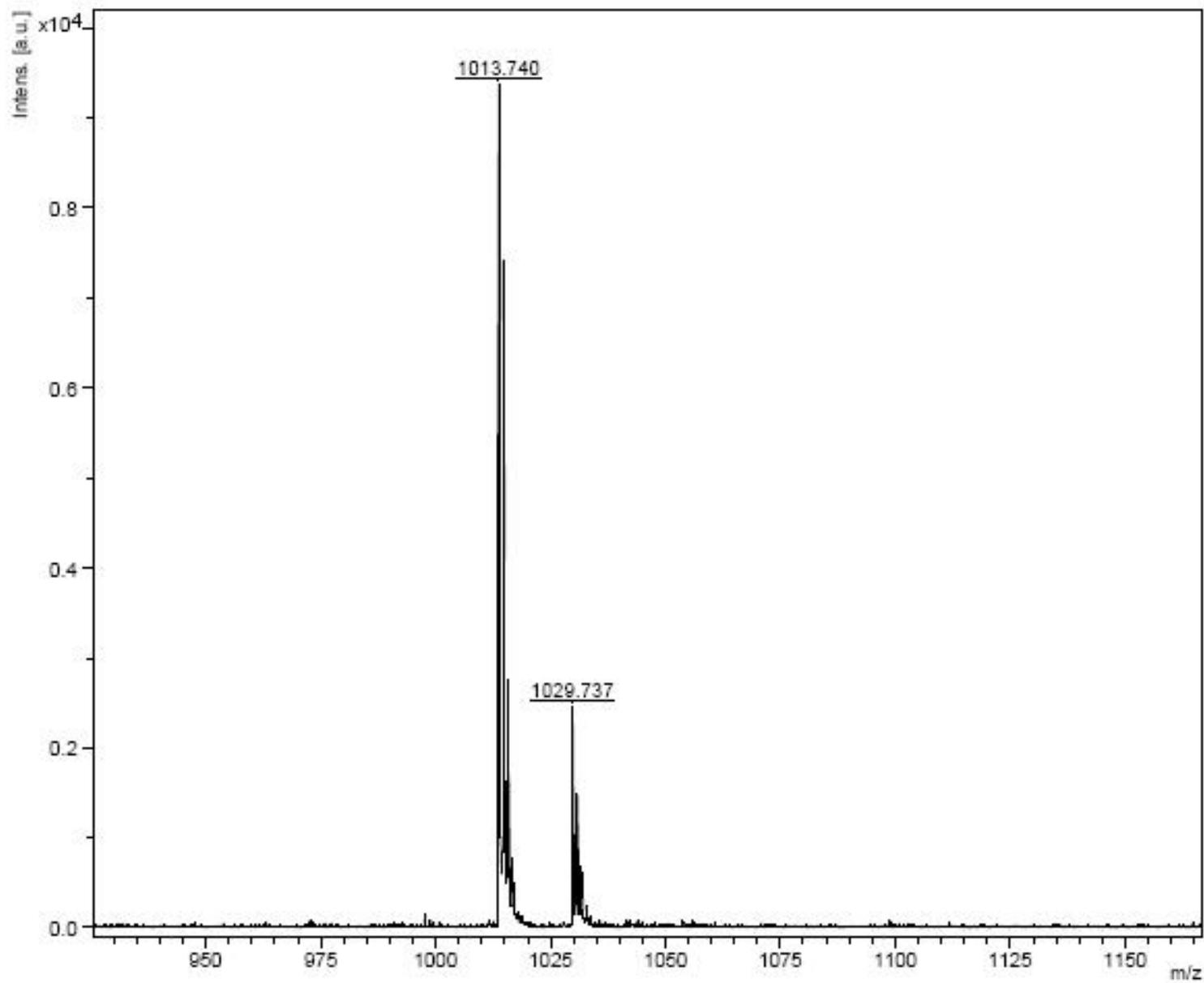
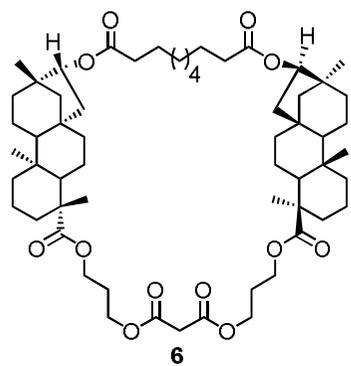
Figure S14.  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ,  $T=303\text{K}$ ) of methanofullerene **9**.



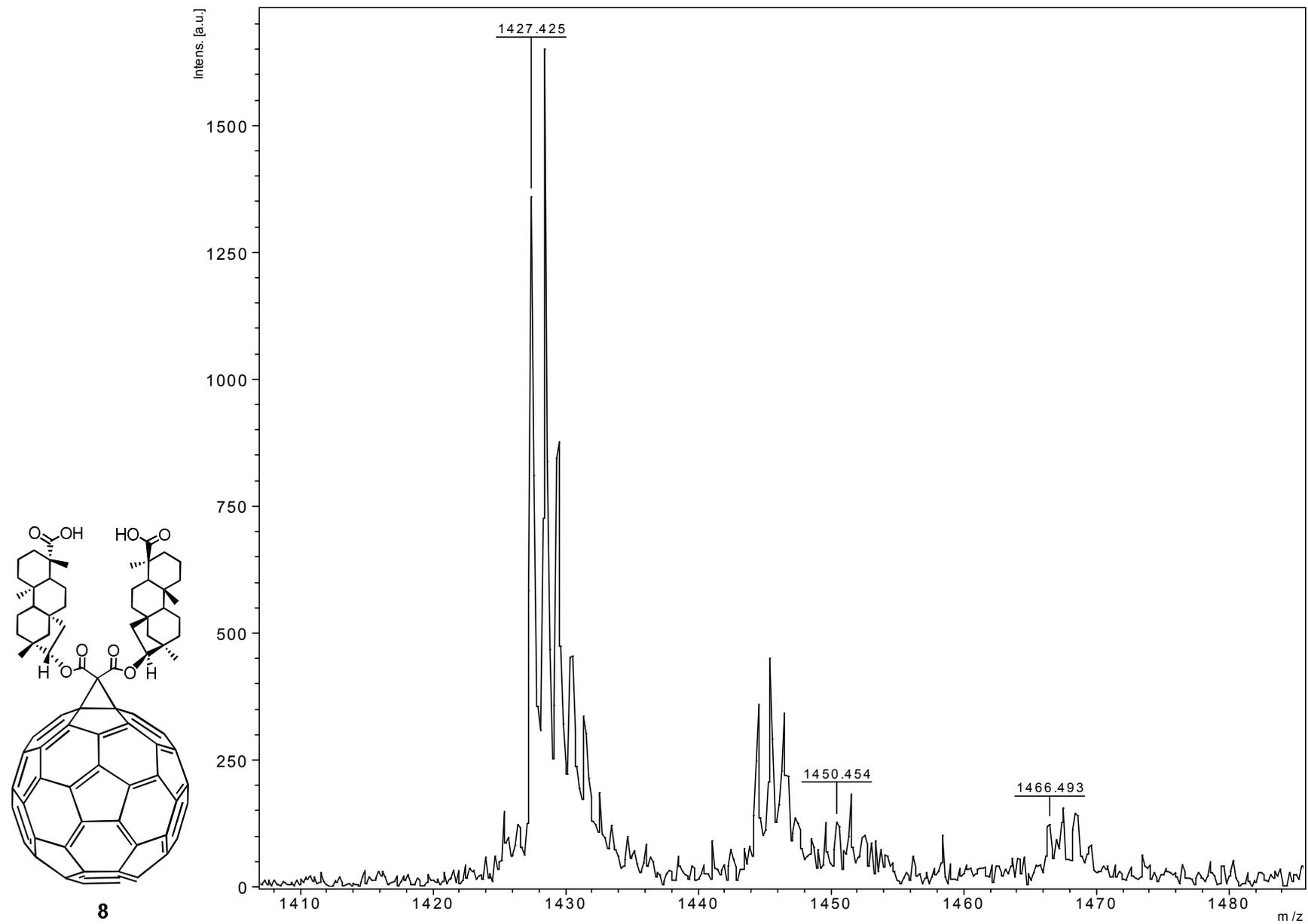
**Figure S15.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ,  $T=303\text{K}$ ) of methanofullerene **9**.



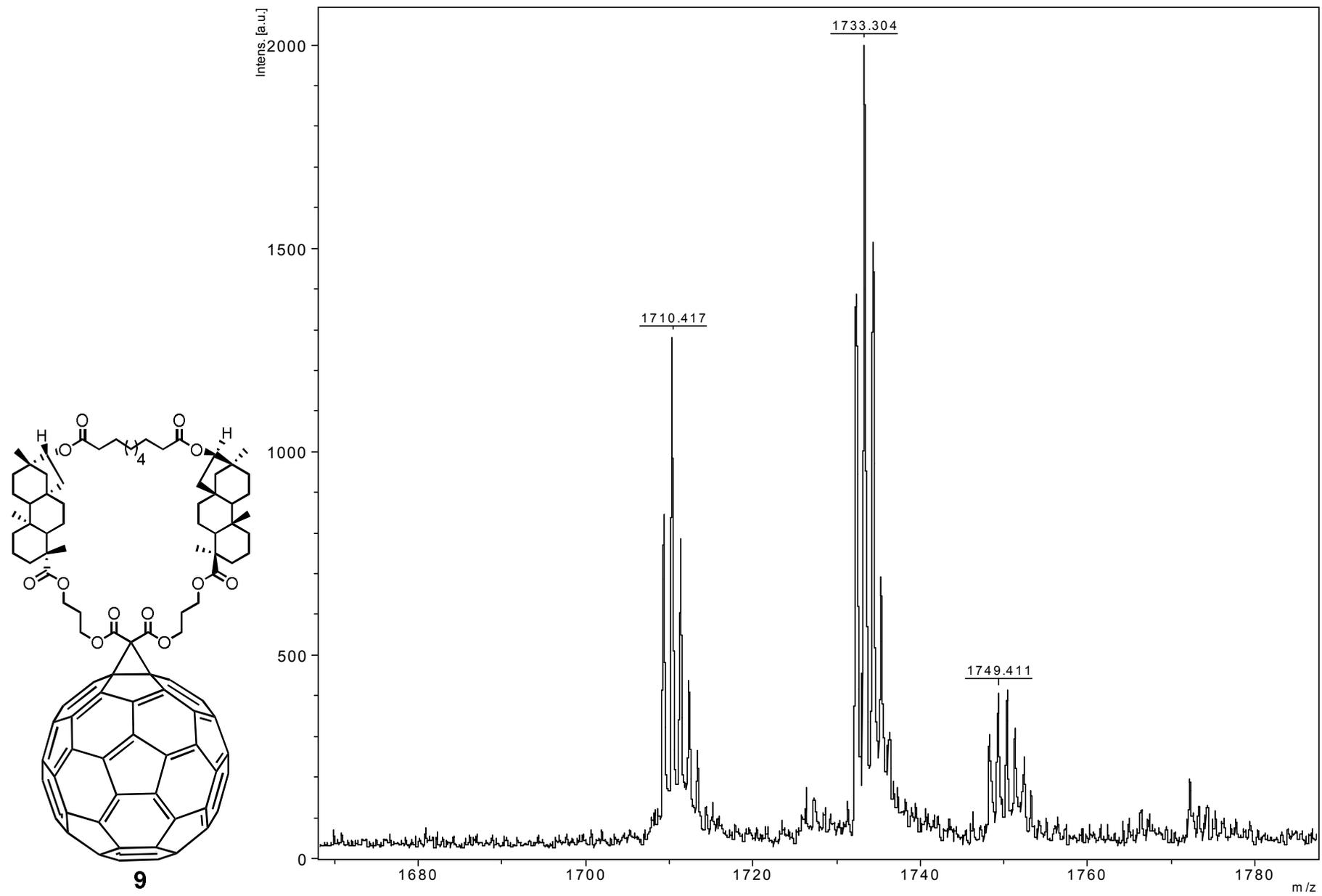
**Figure S16.** MALDI TOF mass spectrum of diol 5.



**Figure S17.** MALDI TOF mass spectrum of macrocycle **6**.



**Figure S18.** MALDI TOF mass spectrum of methanofullerene **8**.



**Figure S19.** MALDI TOF mass spectrum of methanofullerene **9**.