

## *Supplementary Files:*

# **Experimental and Computational Study to Reveal the Potential of Non-Polar Constituents from *Hizikia fusiformis* as Dual Protein Tyrosine Phosphatase 1B and $\alpha$ -Glucosidase Inhibitors**

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Table S1. Molecular weight and molecular formula of isolated compounds.

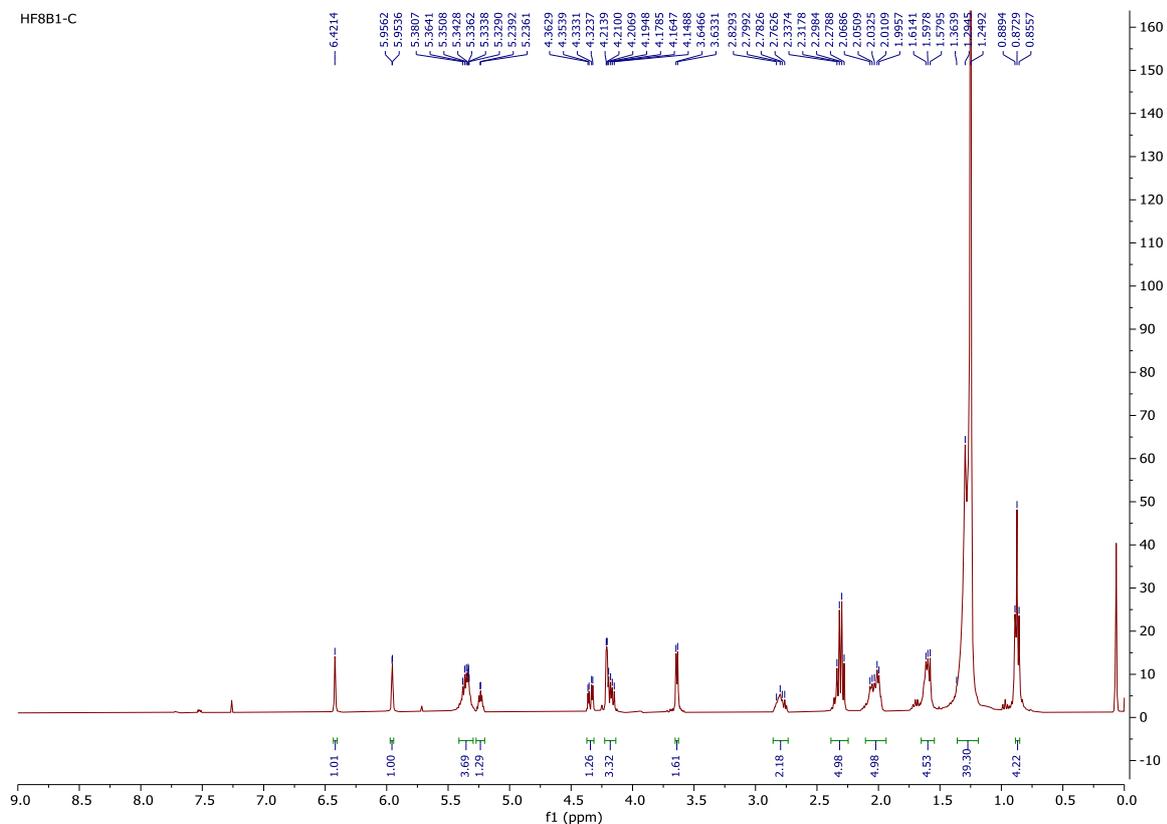
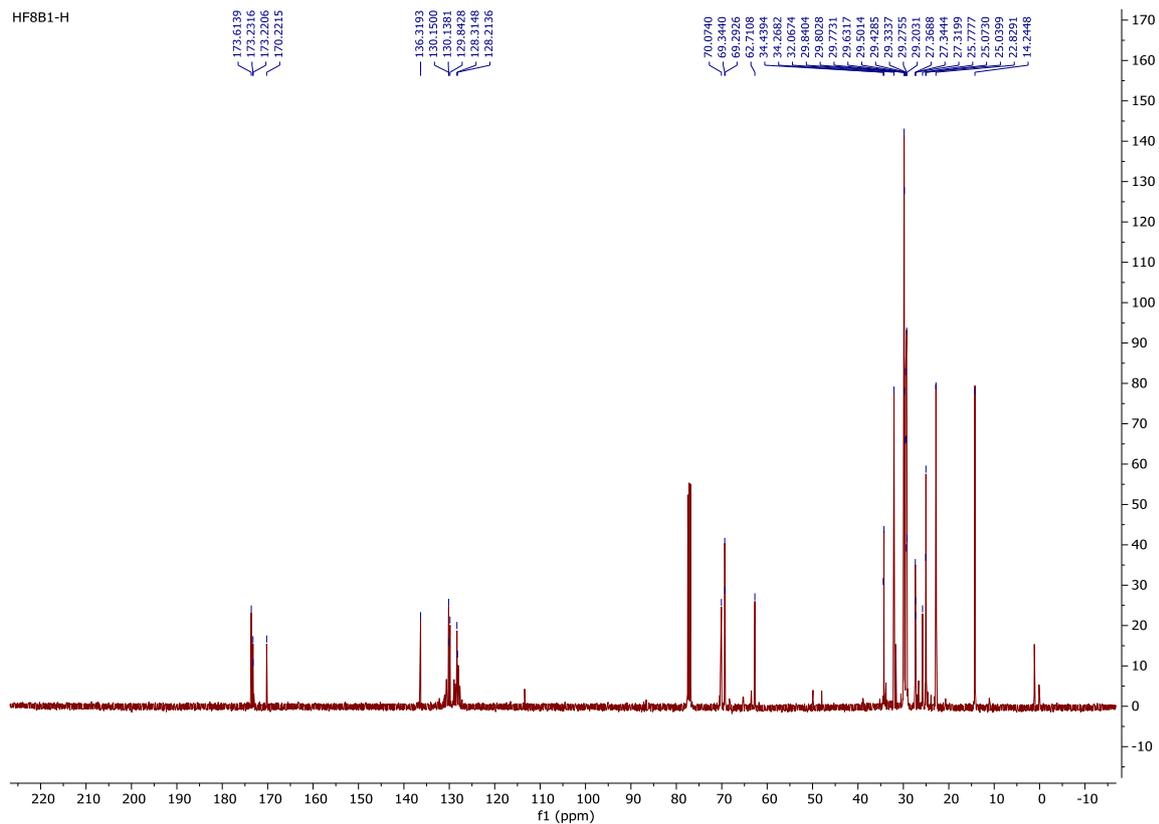


Figure S1.  $^{13}\text{C}$  (100 MHz in  $\text{CDCl}_3$ )- and  $^1\text{H}$  (400 MHz in  $\text{CDCl}_3$ )-NMR spectrum of compound 13.

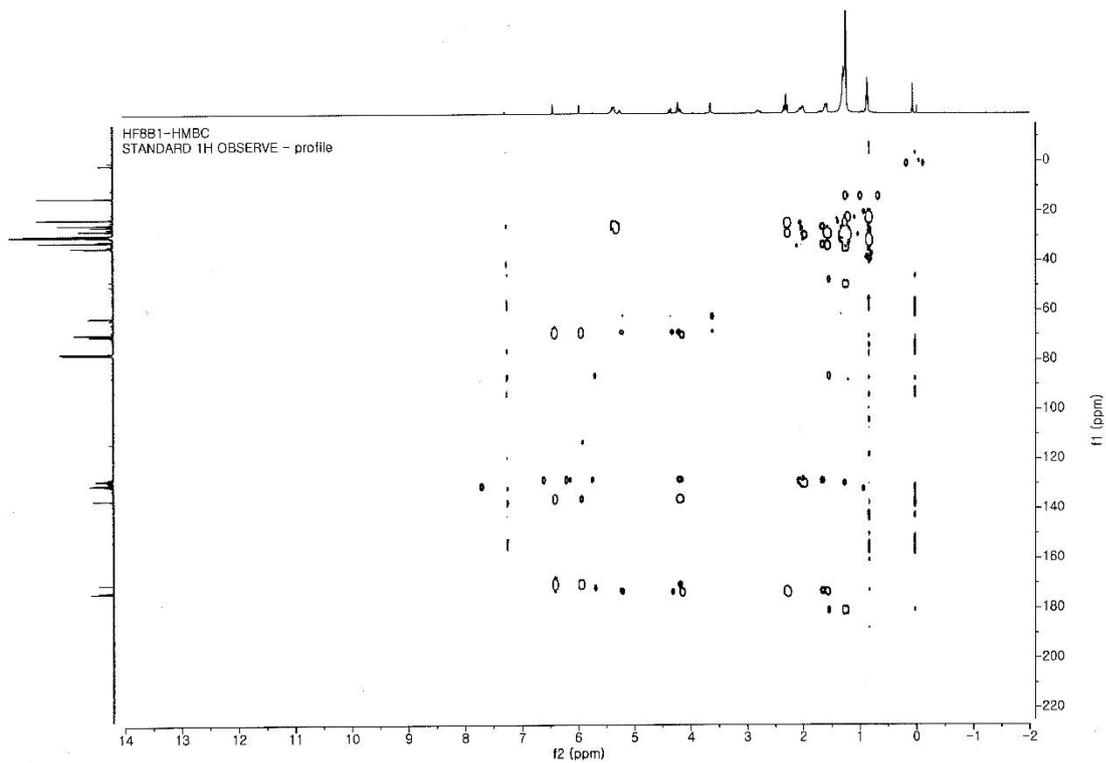


Figure S2. HMBC-NMR spectrum of compound 13.

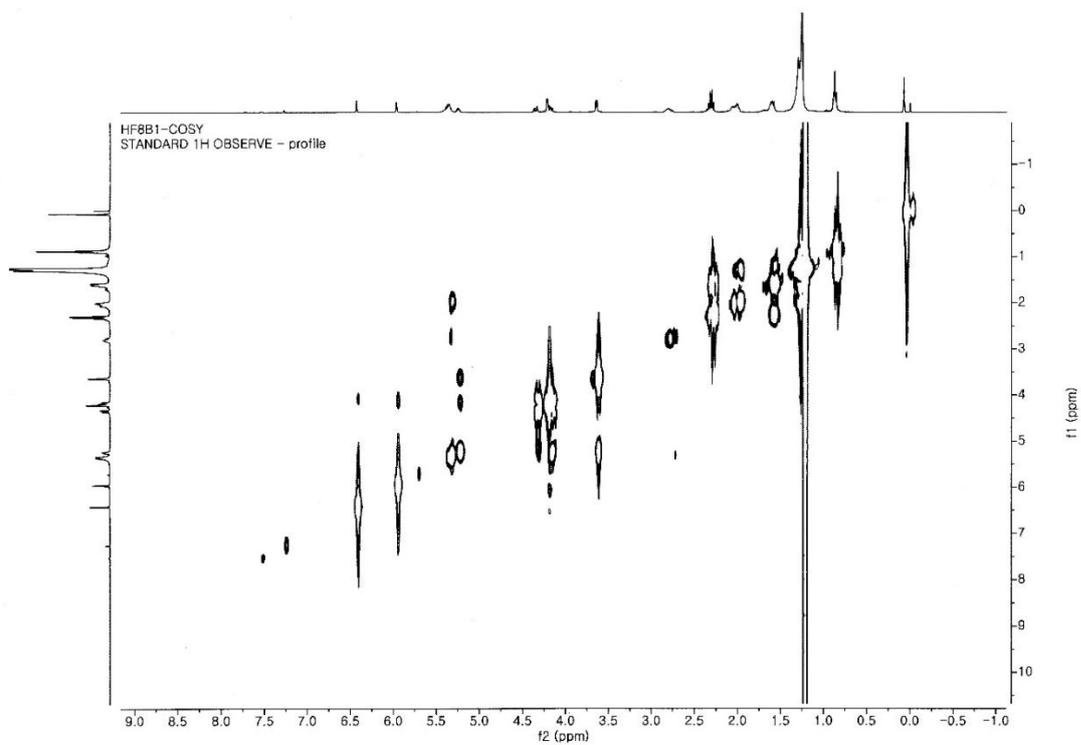


Figure S3. COSY-NMR spectrum of compound 13.

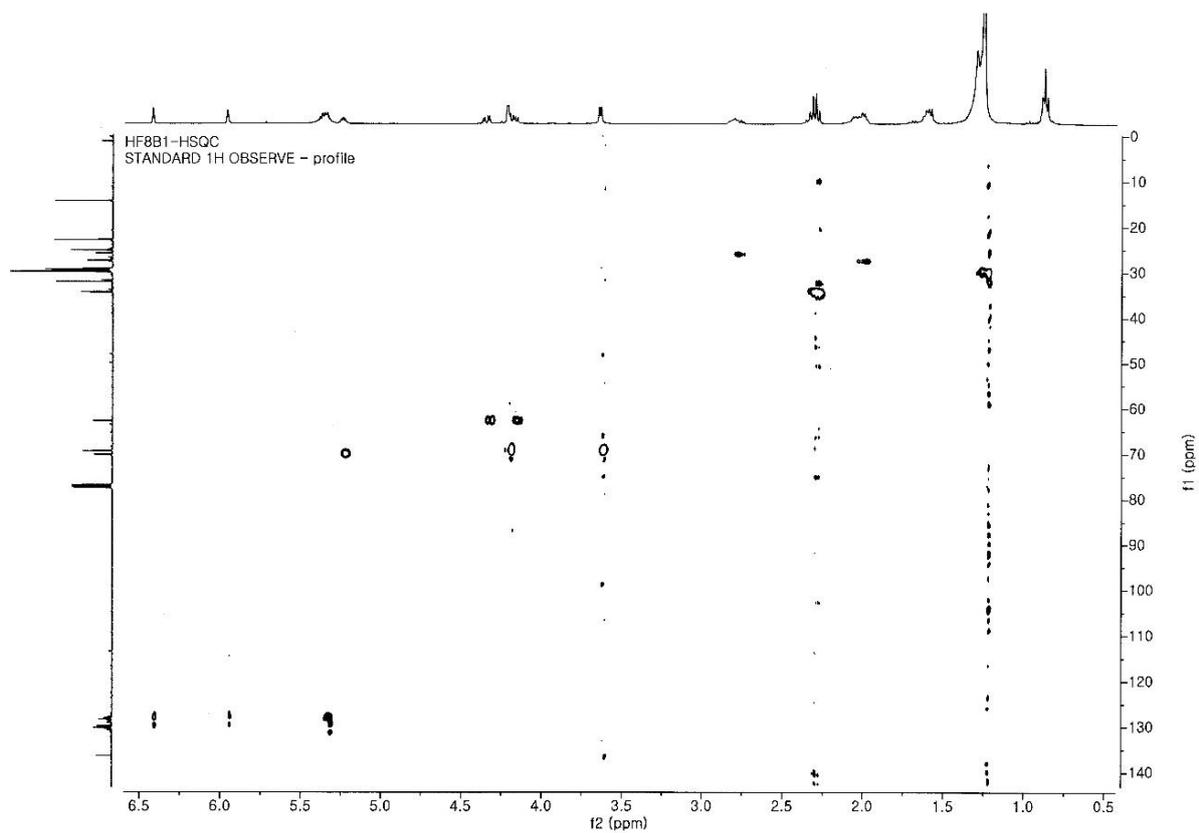


Figure S4. HSQC-NMR spectrum of compound 13.

# Display Report

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Operator BDAL@DE  
Instrument maxis HD 1820881.21289

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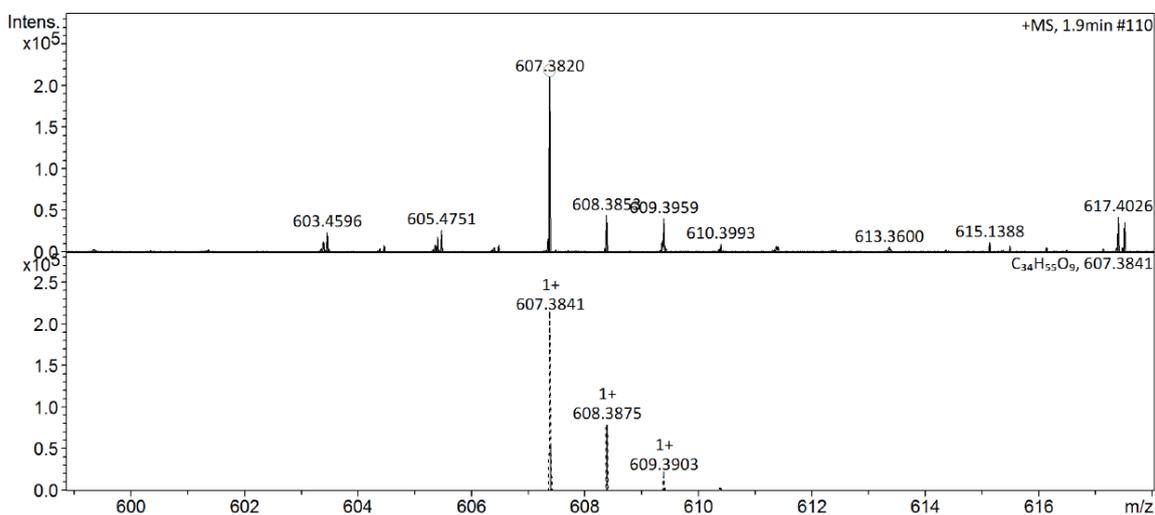
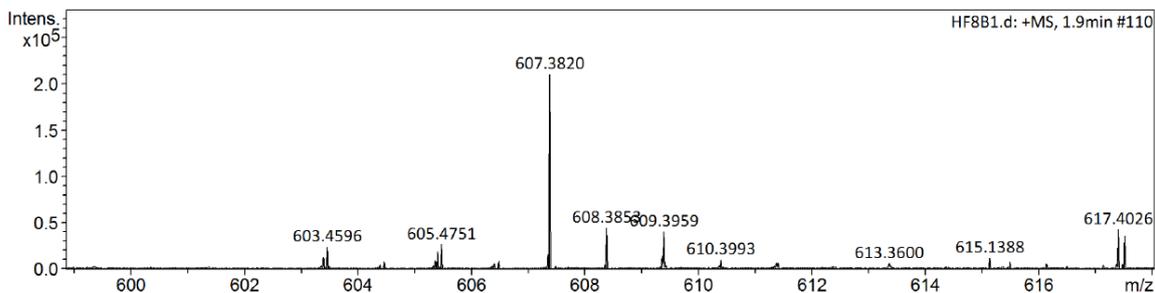
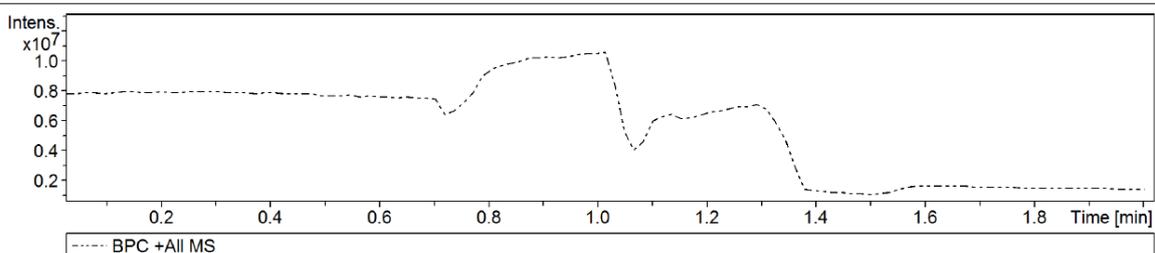


Figure S5. HR-ESI-MS data of compound 13.

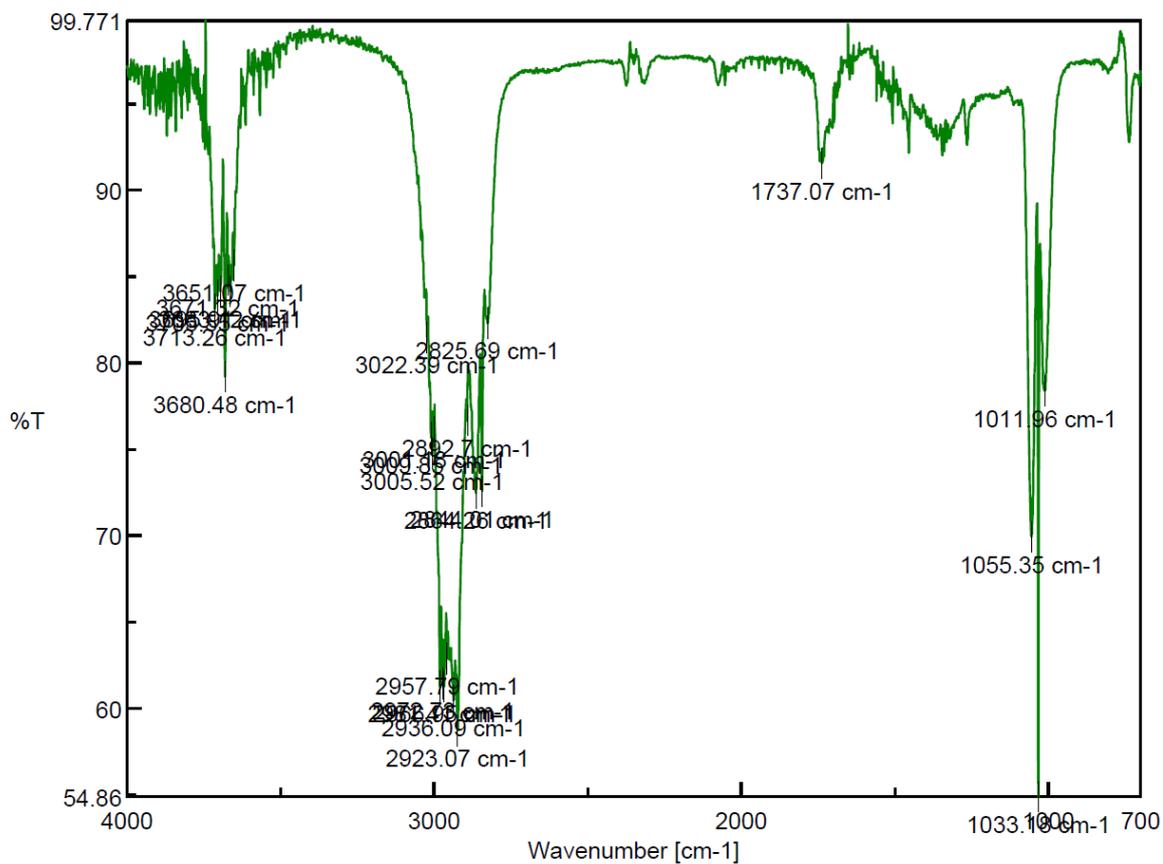


Figure S6. FT-IR spectrum of compound 13.

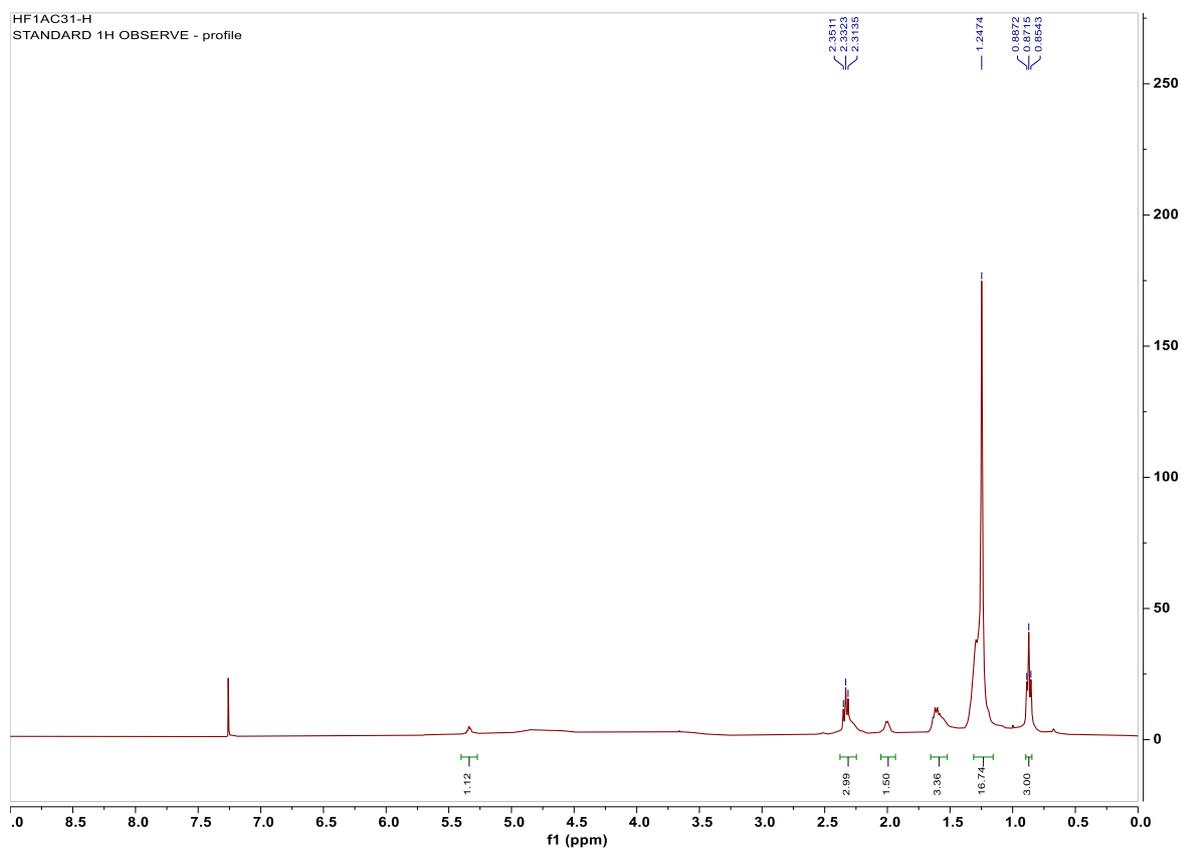
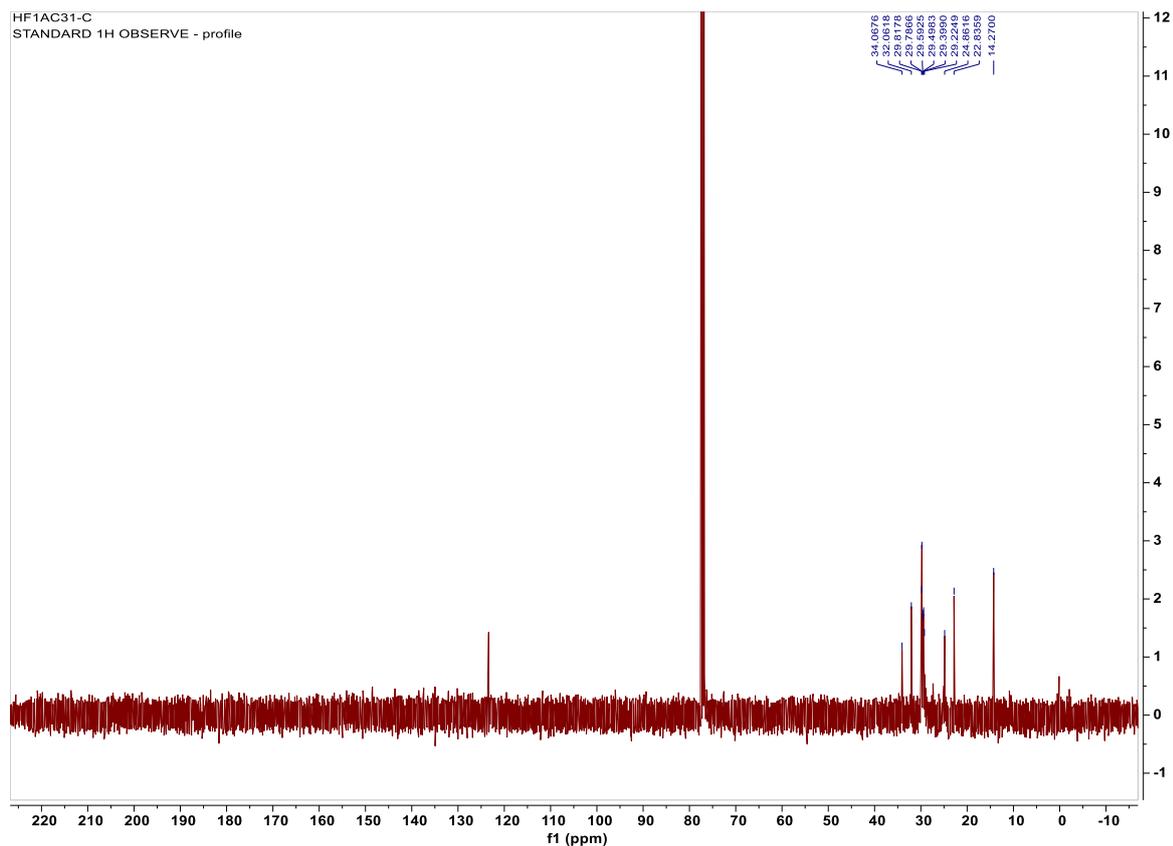


Figure S7.  $^{13}\text{C}$  (100 MHz in  $\text{CDCl}_3$ )- and  $^1\text{H}$  (400 MHz in  $\text{CDCl}_3$ )-NMR spectrum of compound **1**.

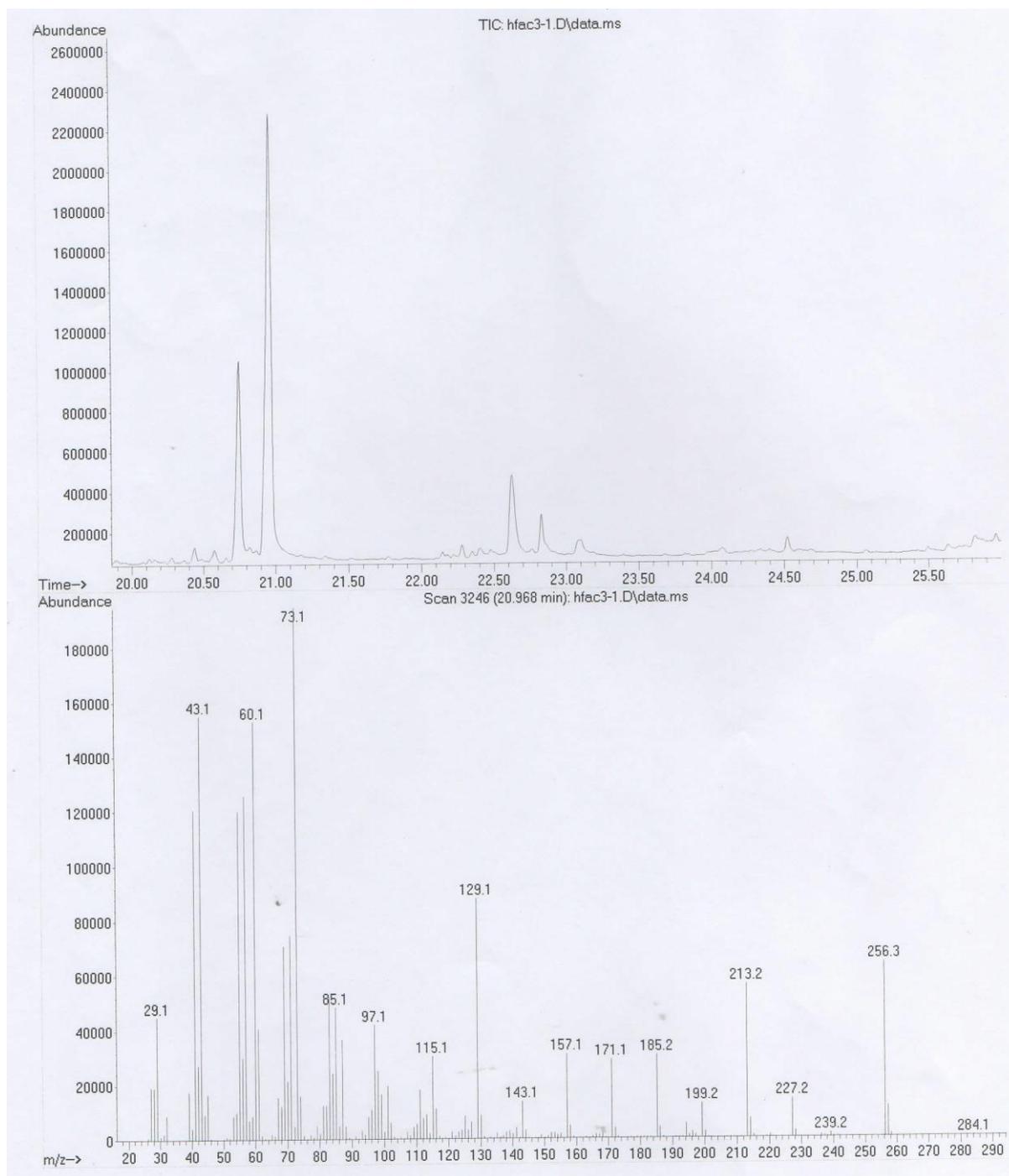
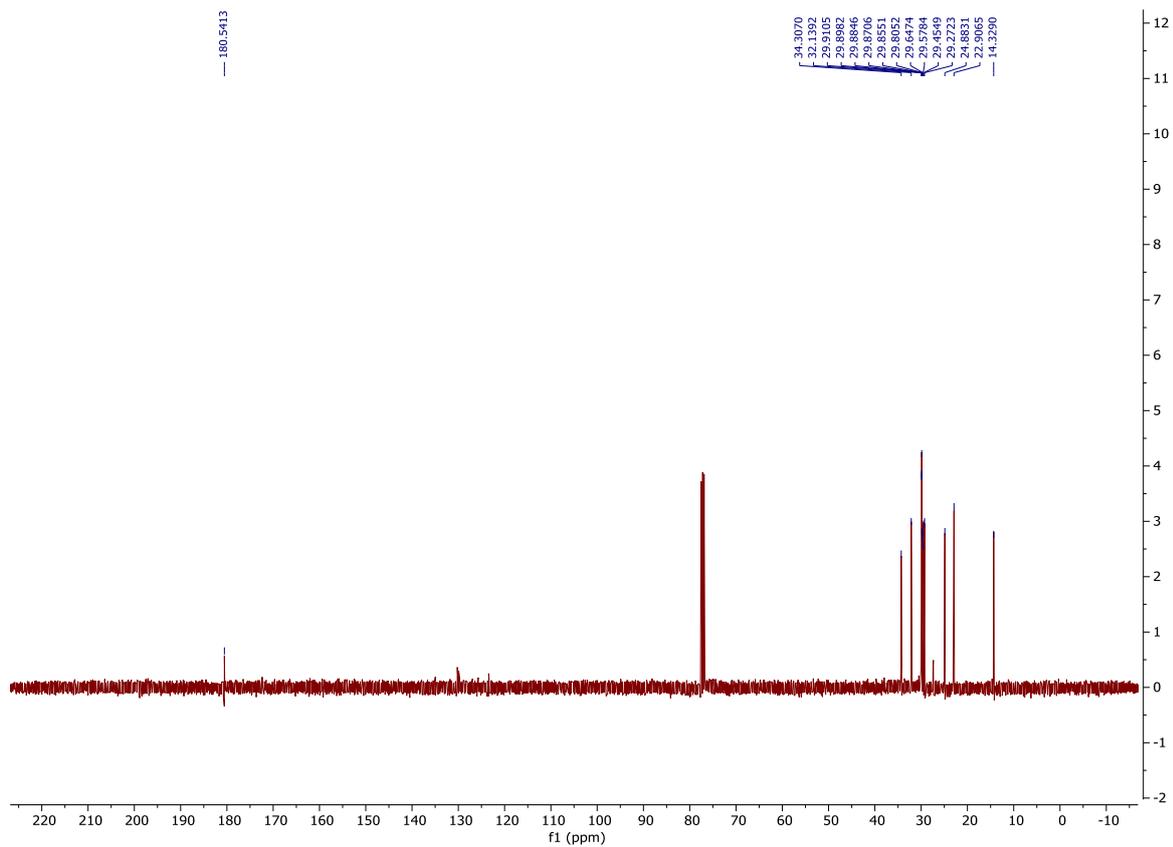


Figure S8. EI-MS spectrum of compound 1.



HF1C2-H  
STANDARD 1H OBSERVE - profile

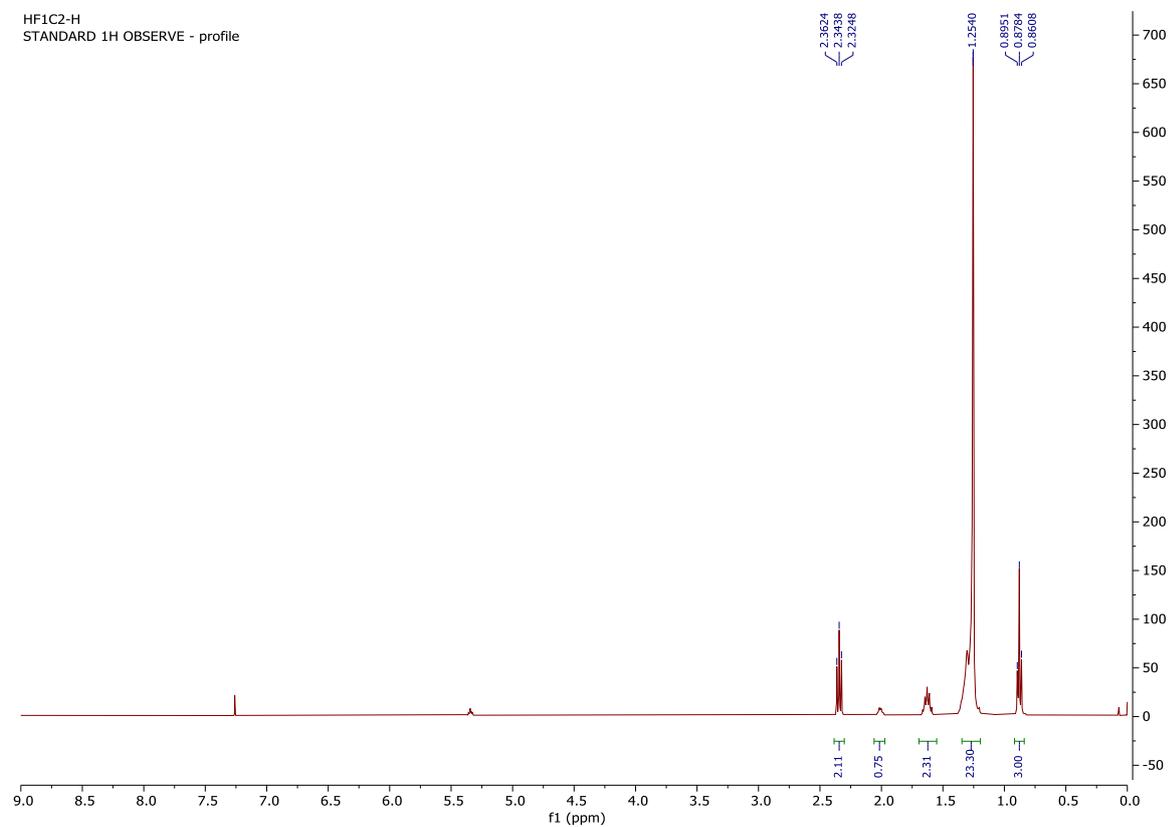


Figure S9.  $^{13}\text{C}$  (100MHz in  $\text{CDCl}_3$ )- and  $^1\text{H}$  (400MHz in  $\text{CDCl}_3$ )-NMR spectrum of compound 2.

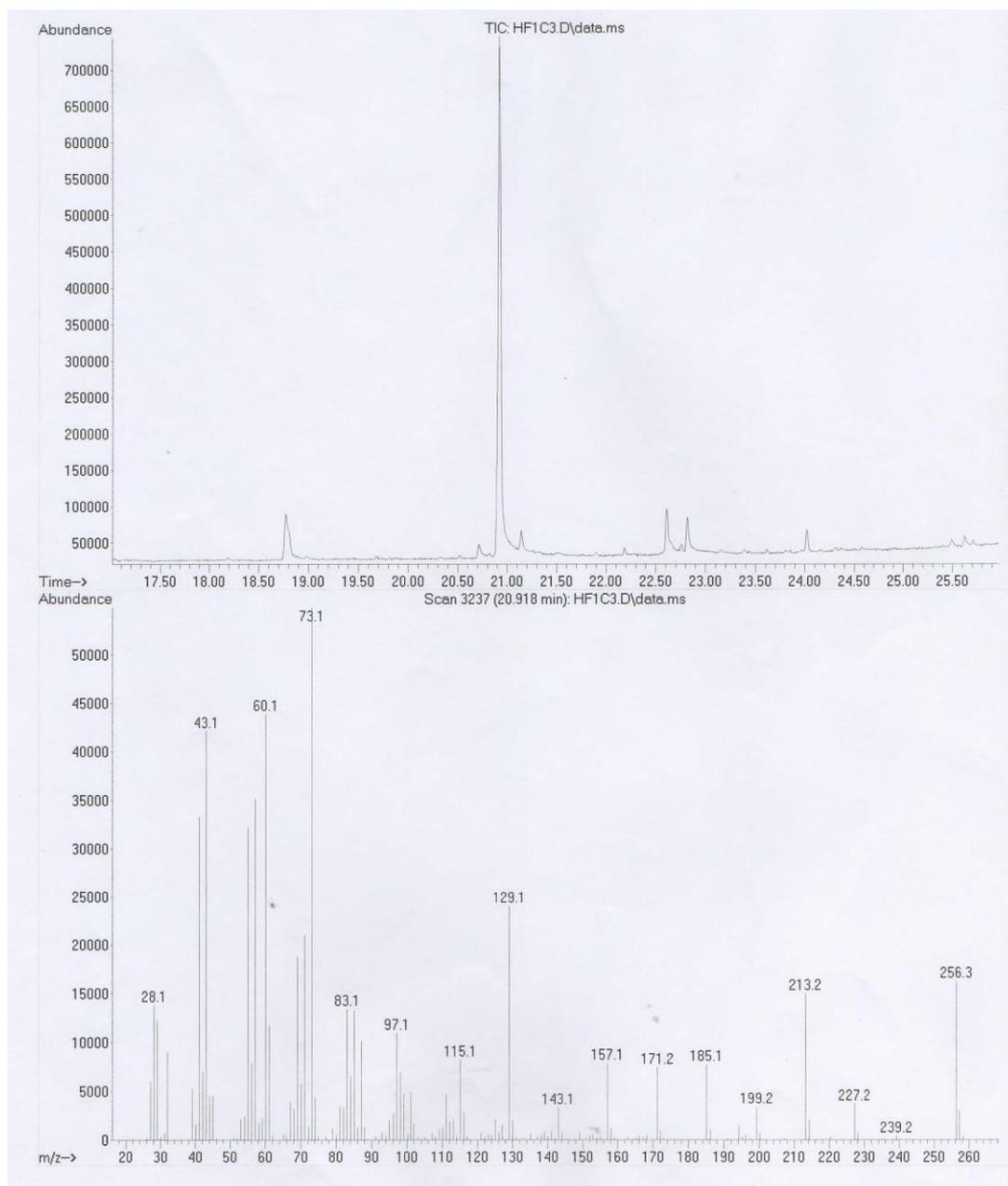
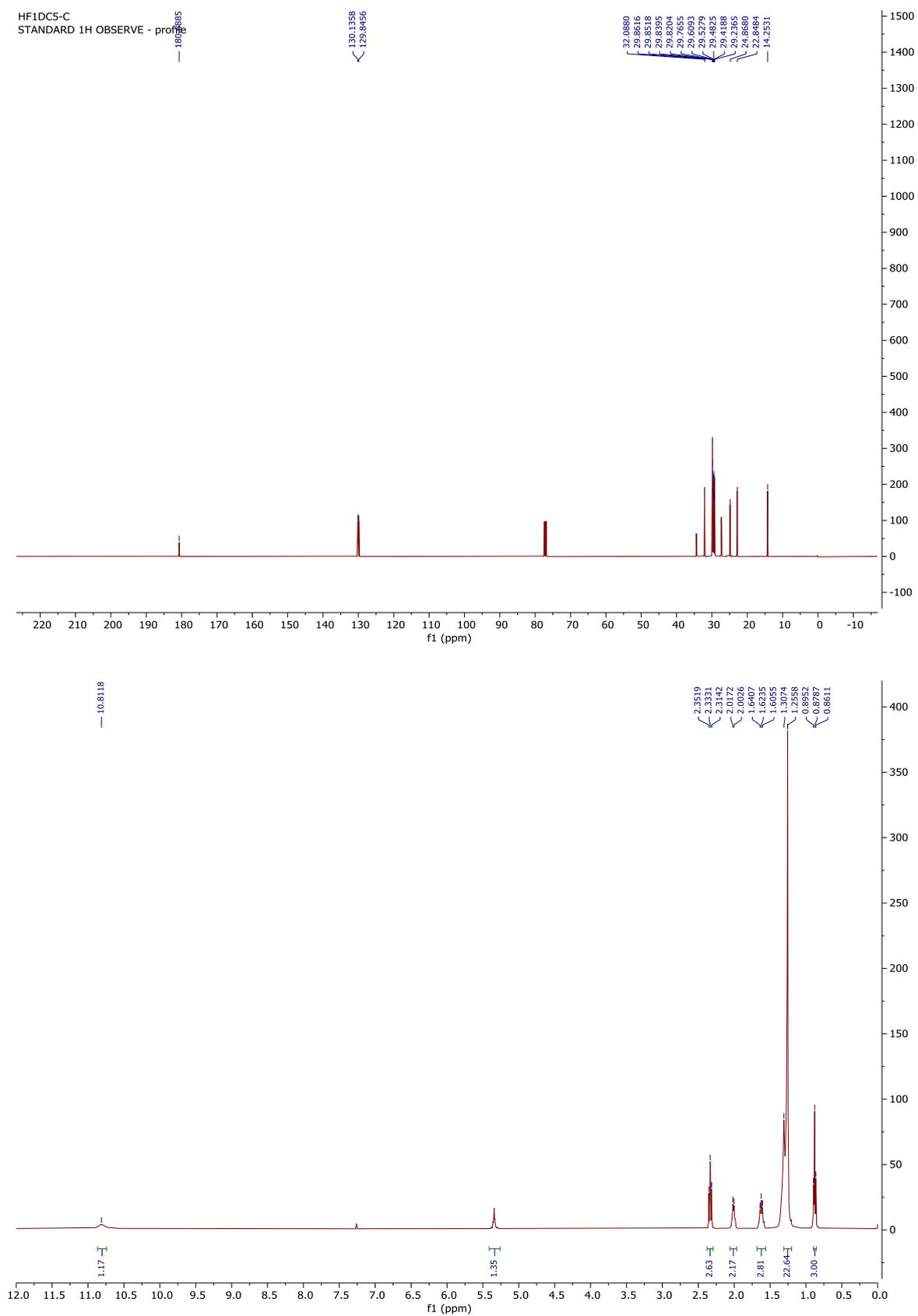


Figure S10. EI-MS spectrum of compound 2.



**Figure S11.** <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 3.

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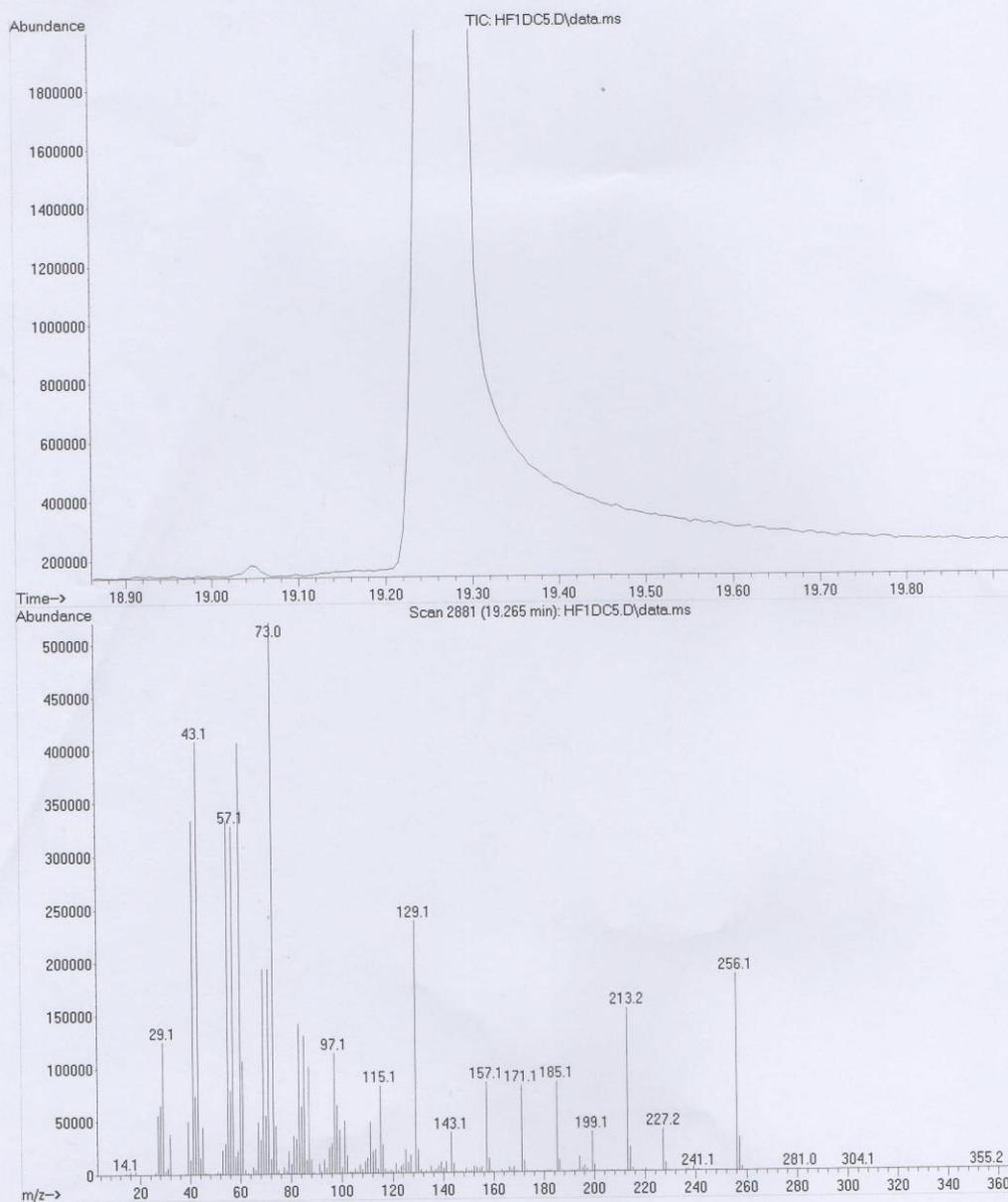


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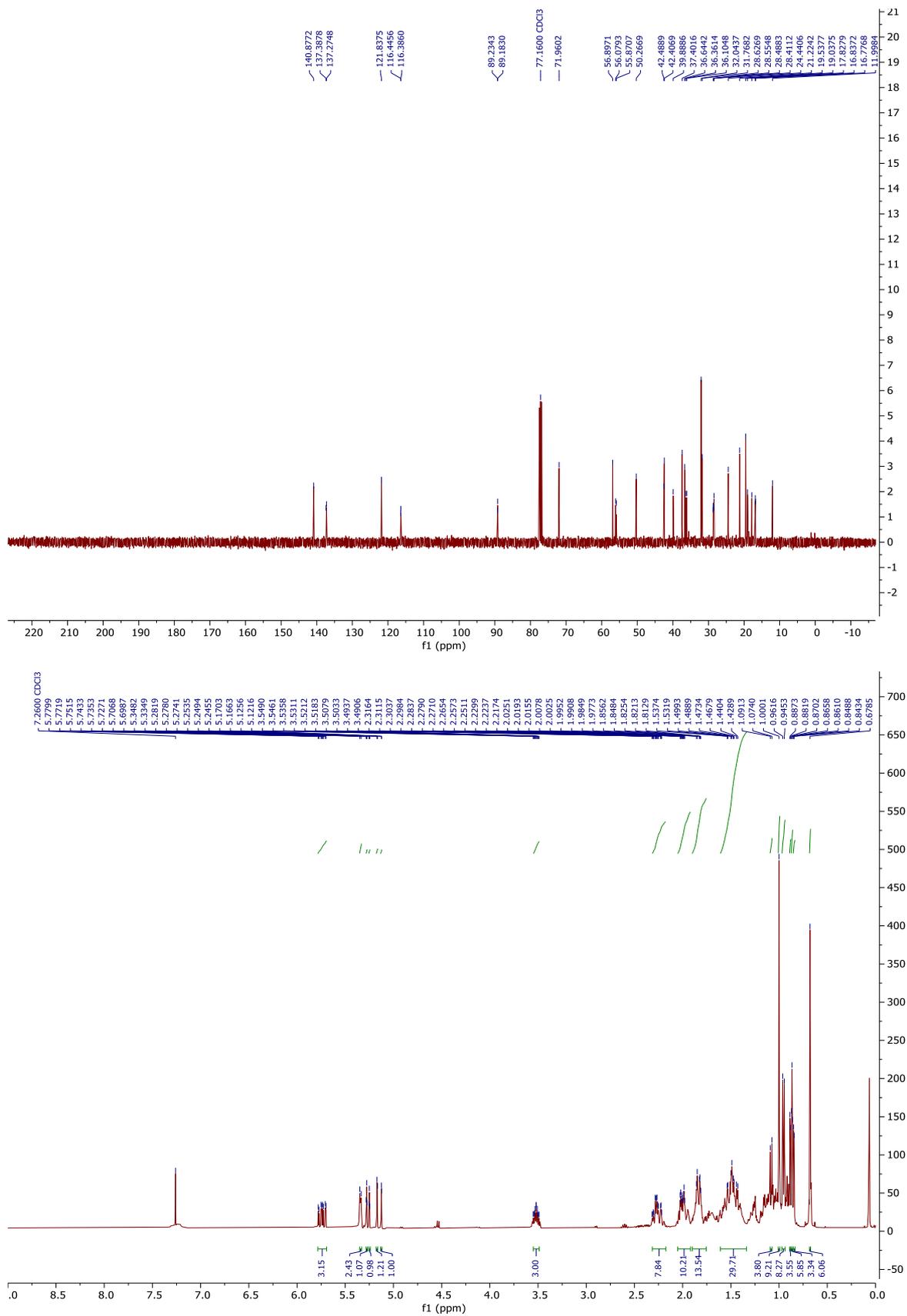
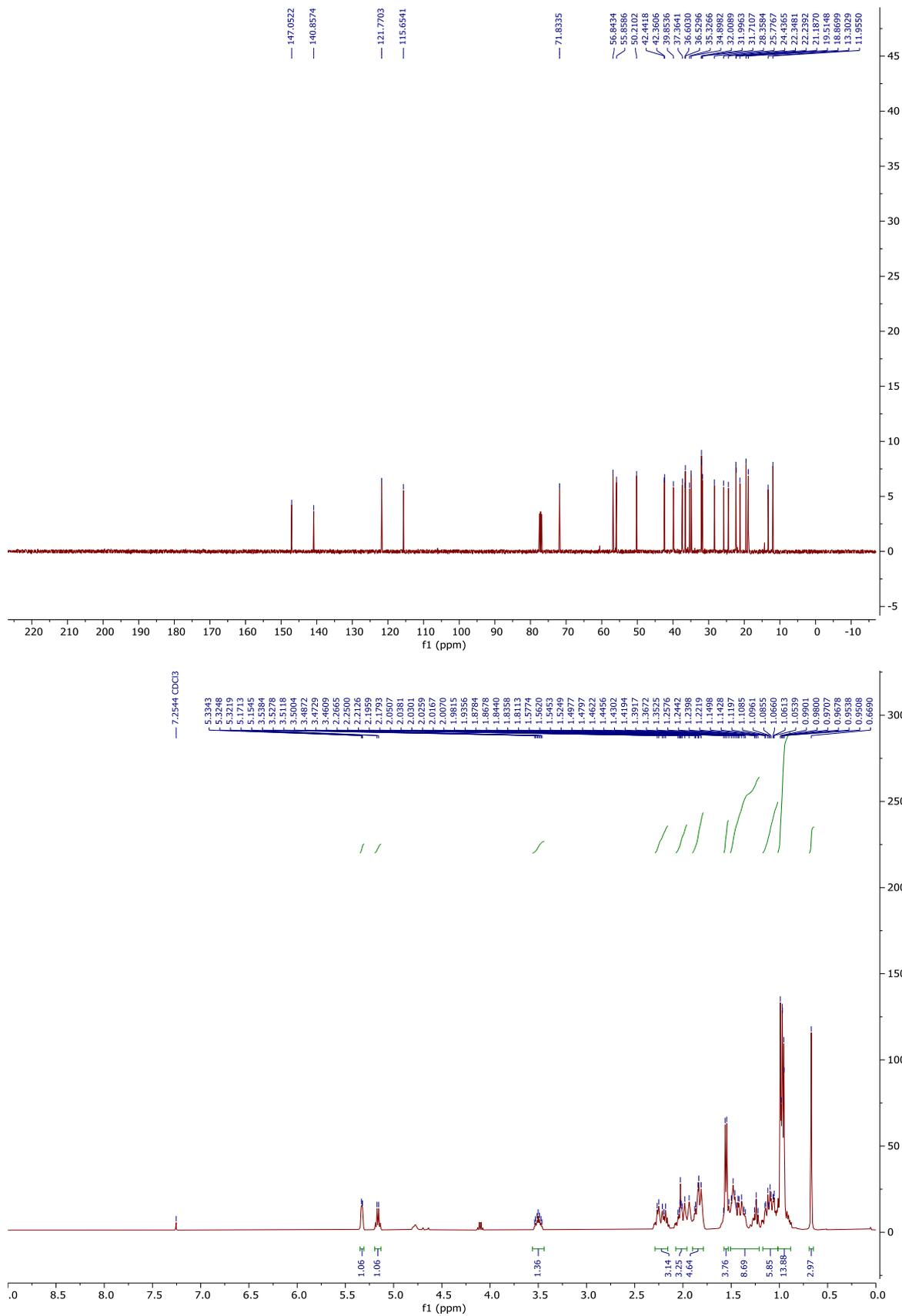


Figure S13. <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 4.



**Figure S14.** <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 5.

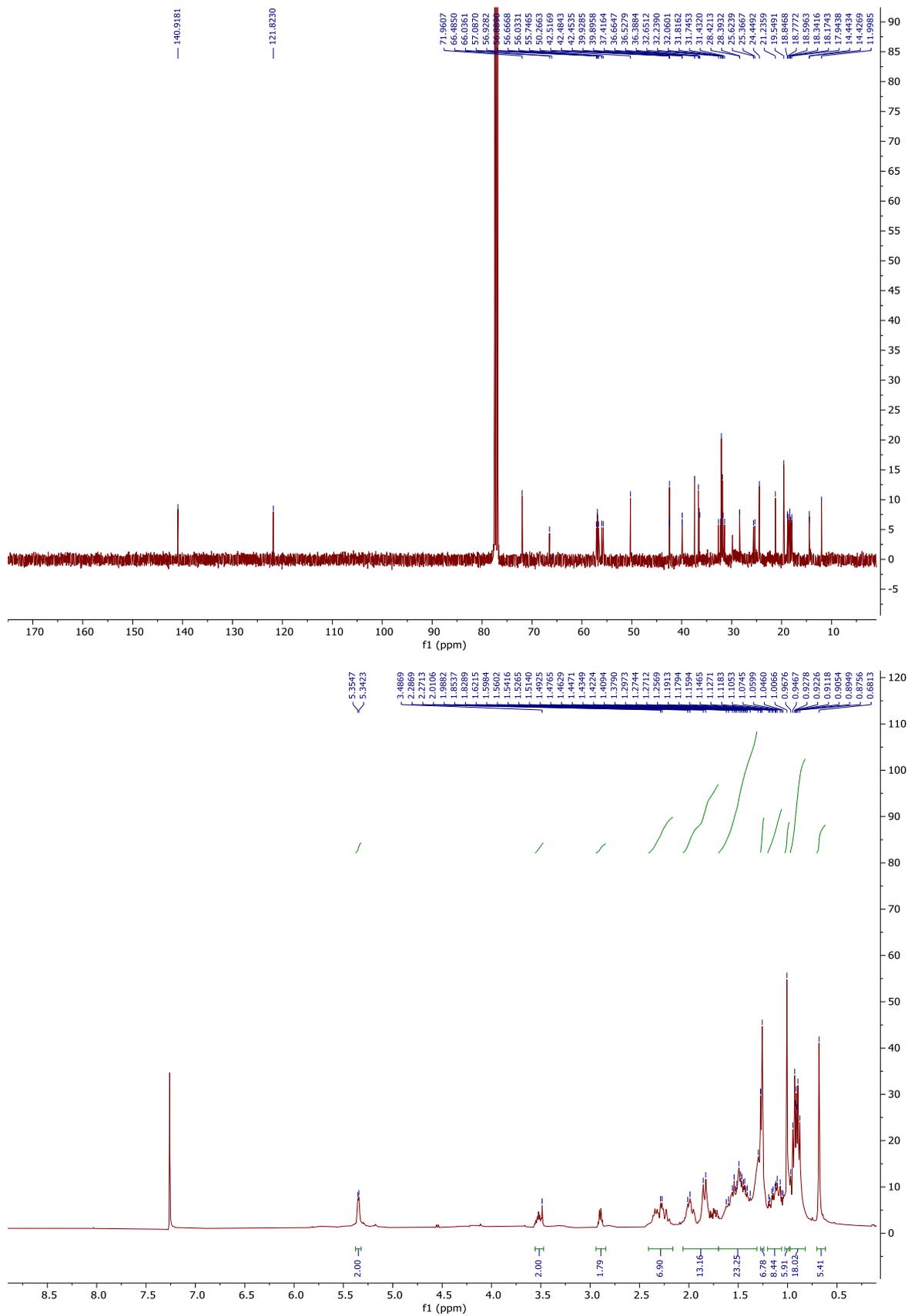


Figure S15. <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 6.

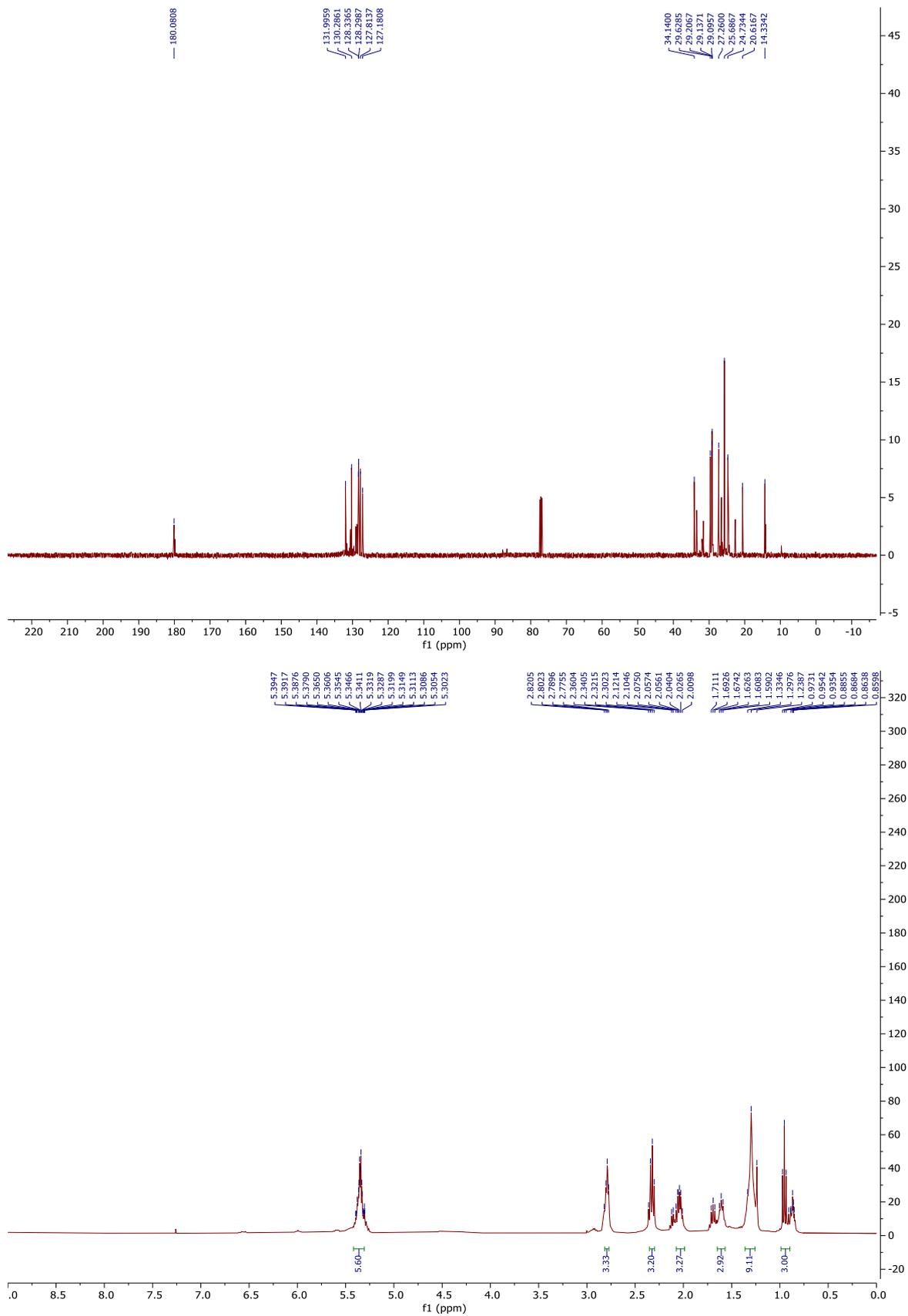


Figure S16. <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 7.

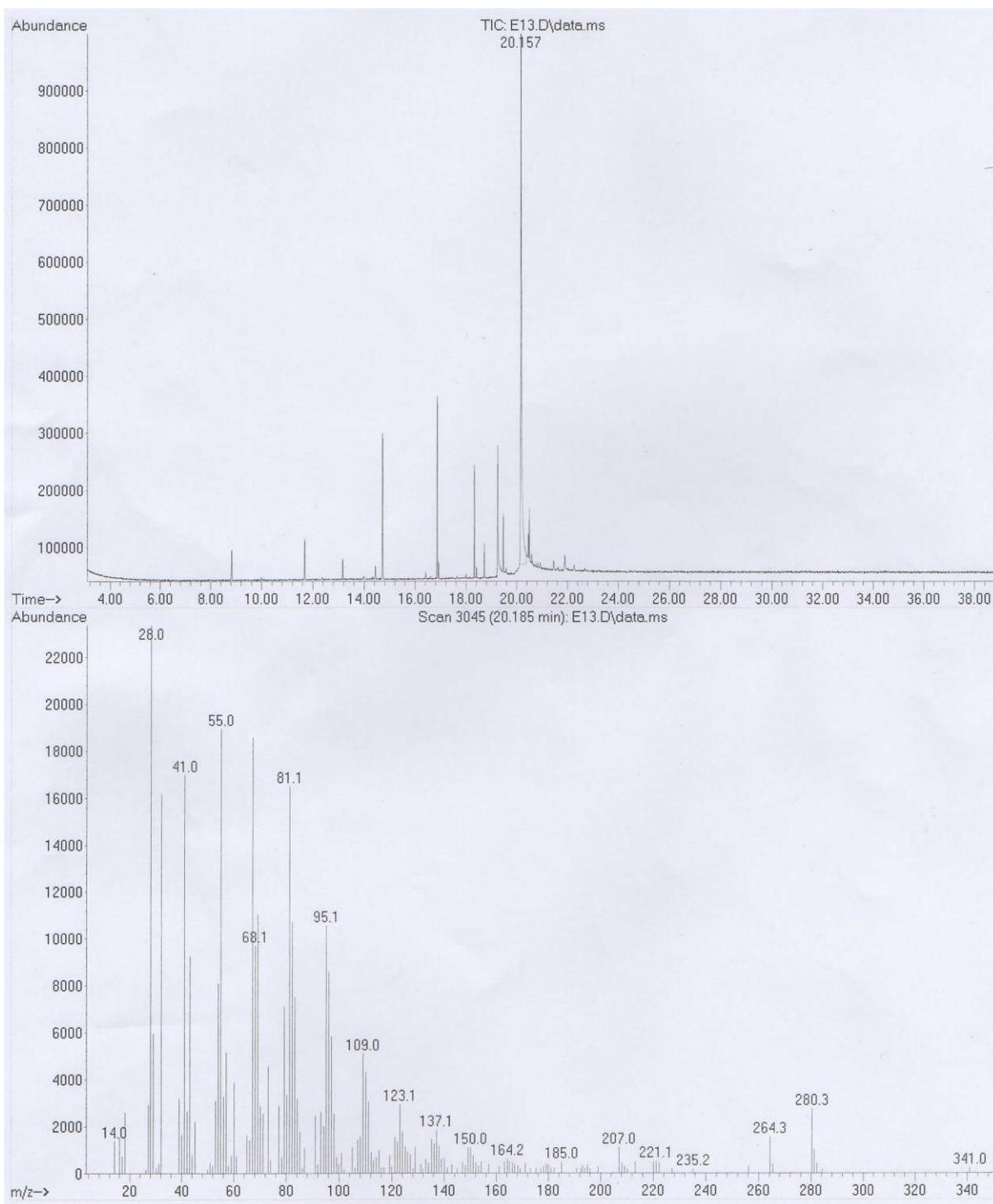
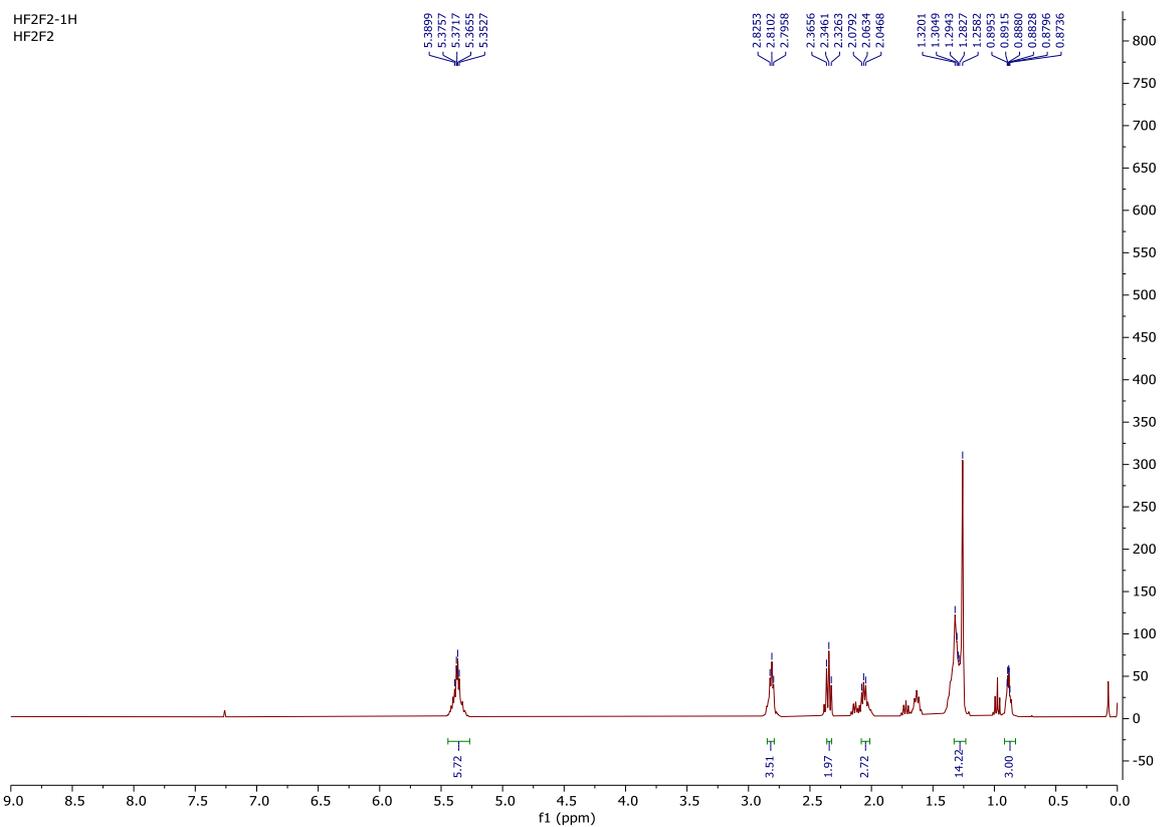
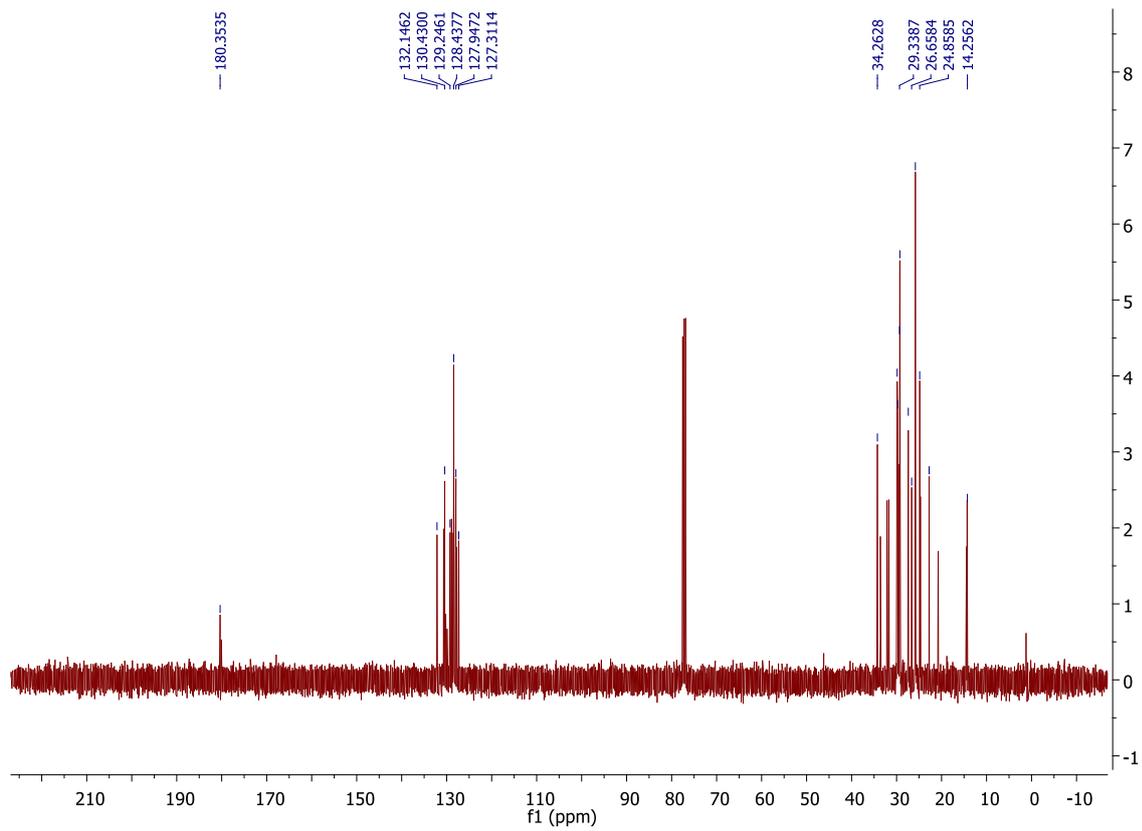


Figure S17. EI-MS spectrum of compound 7.



**Figure S18.**  $^{13}\text{C}$  (100MHz in  $\text{CDCl}_3$ )- and  $^1\text{H}$  (400MHz in  $\text{CDCl}_3$ )-NMR spectrum of compound 8.

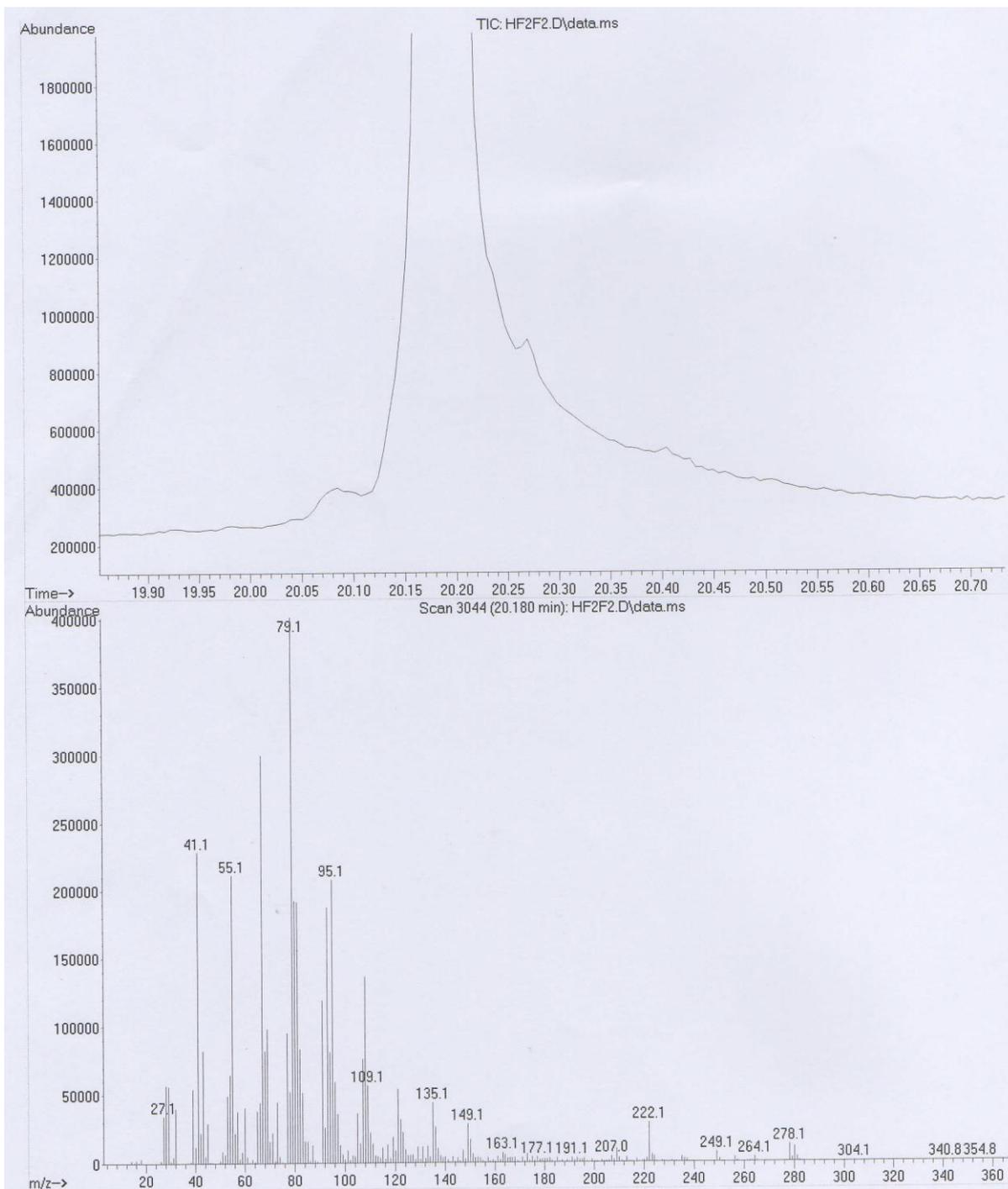
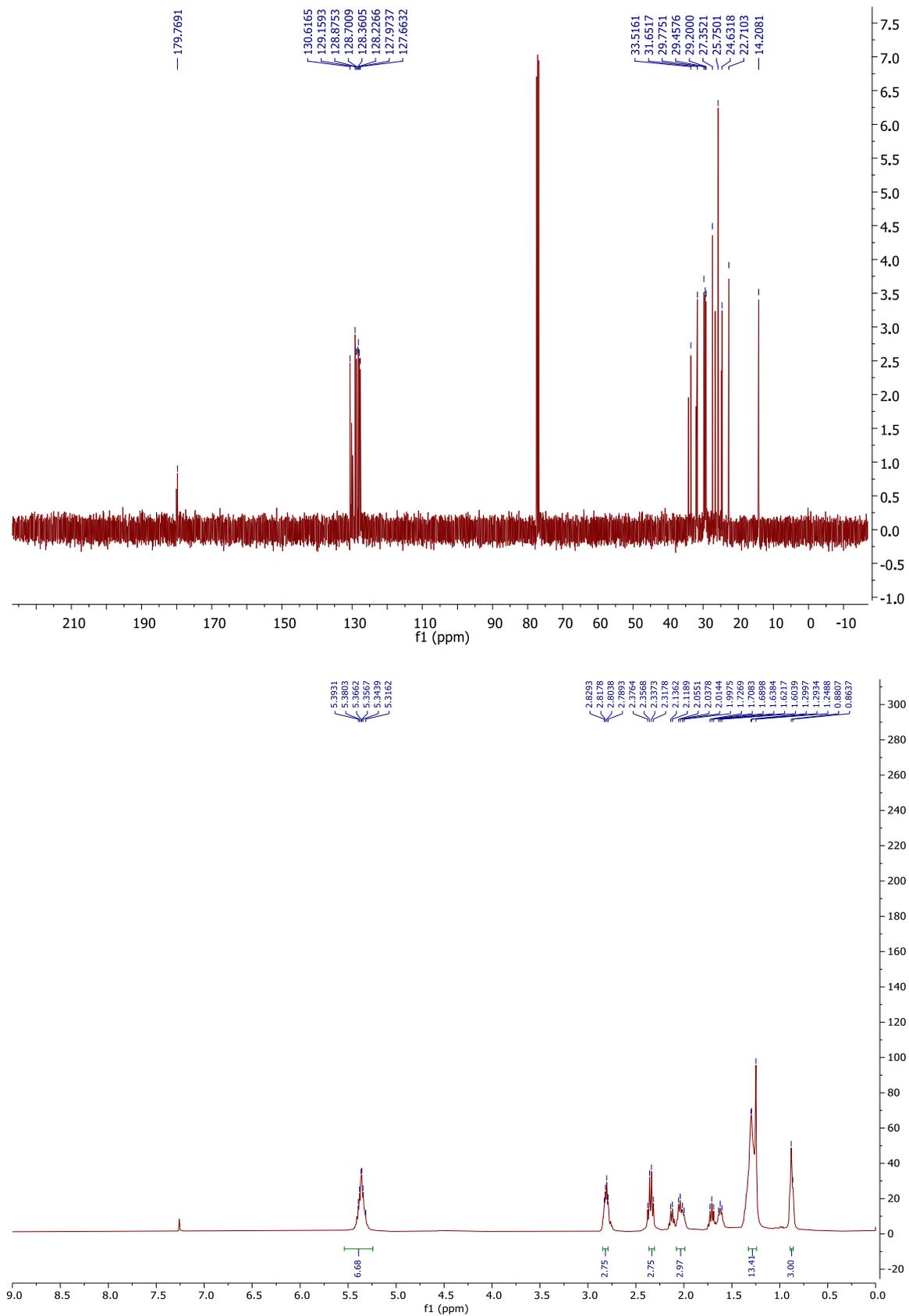


Figure S19. EI-MS spectrum of compound 8.



**Figure S20.** <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 9.

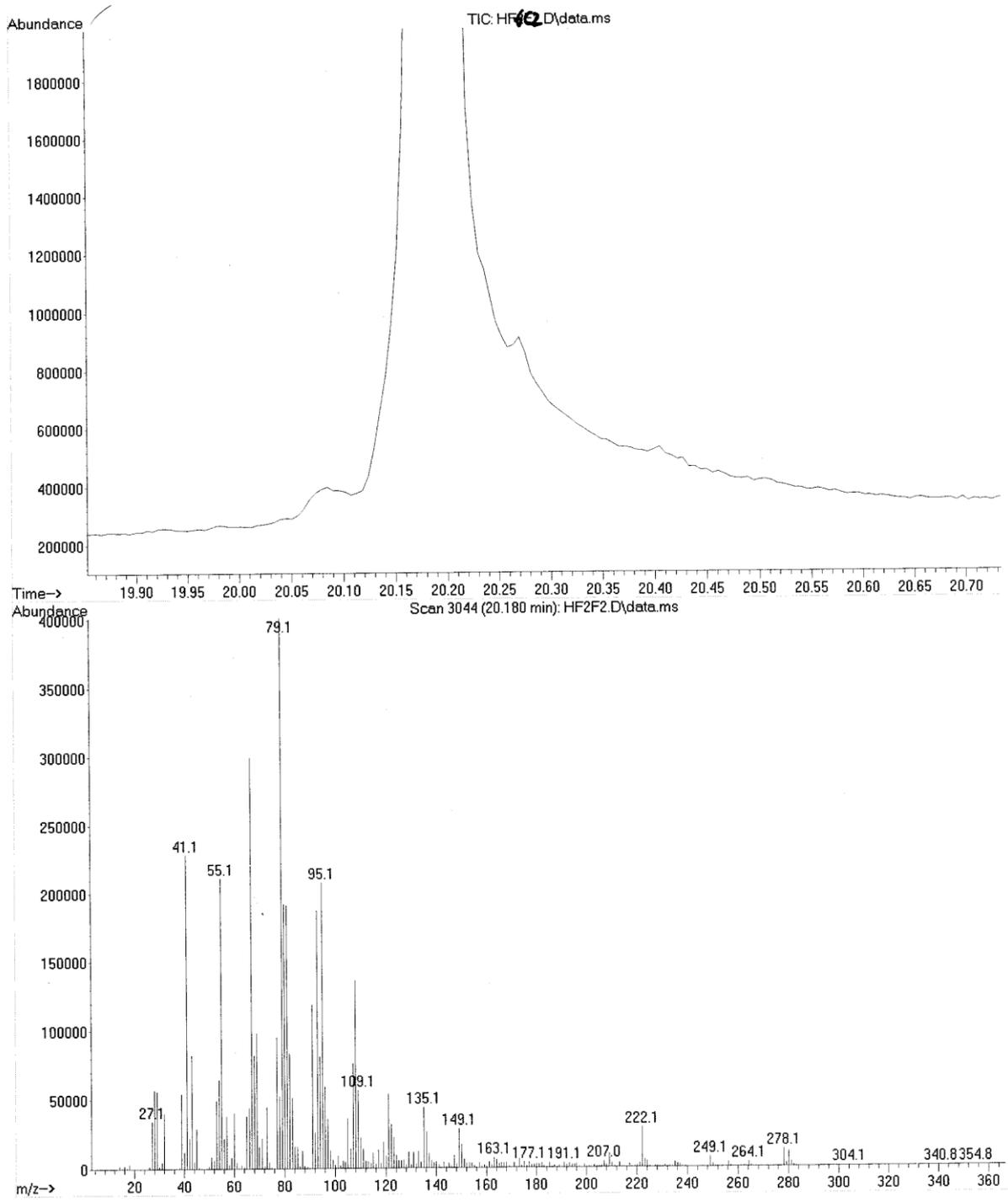


Figure S21. EI-MS spectrum of compound 9.

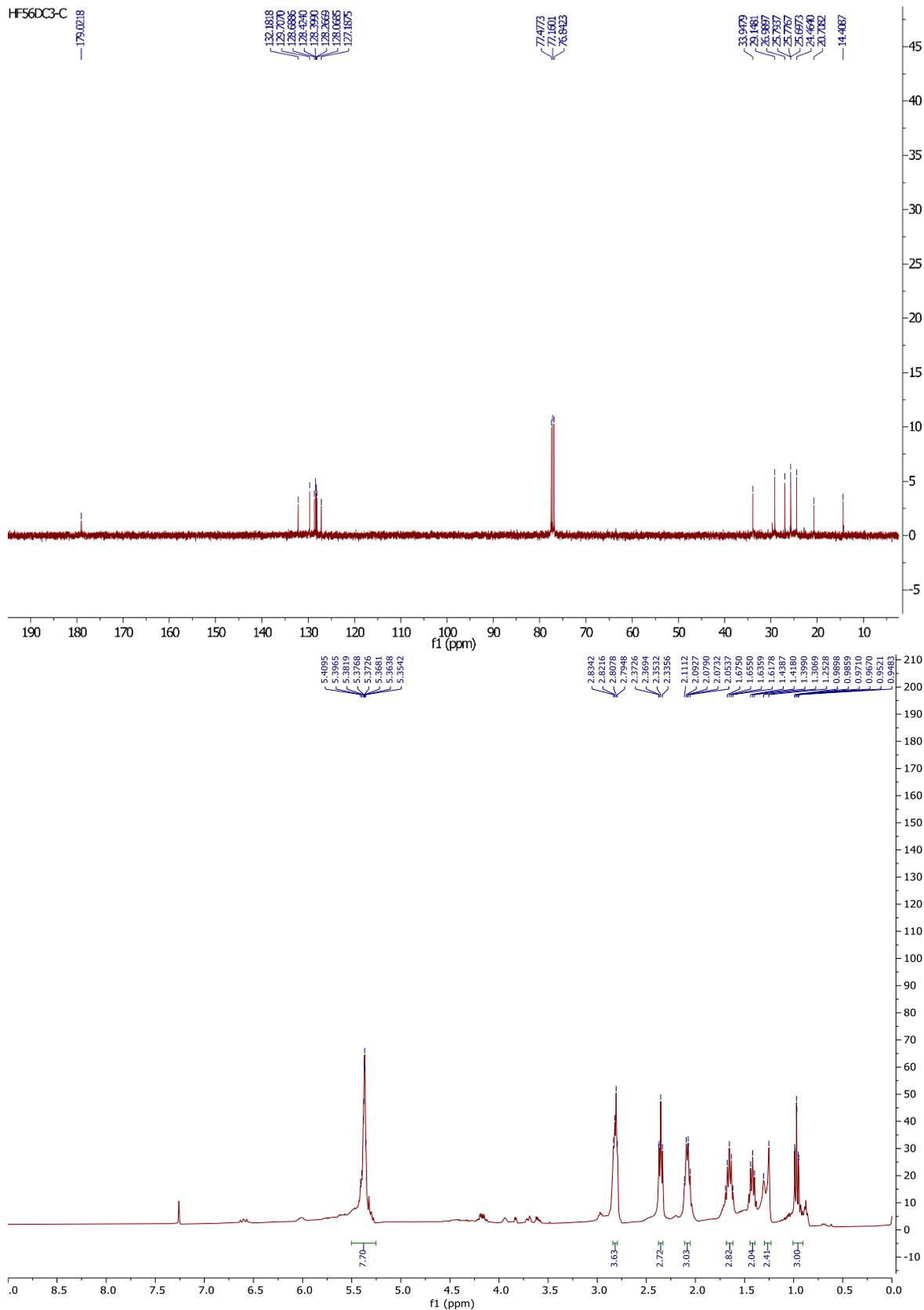


Figure S22.  $^{13}\text{C}$  (100MHz in  $\text{CDCl}_3$ )- and  $^1\text{H}$  (400MHz in  $\text{CDCl}_3$ )-NMR spectrum of compound 10.

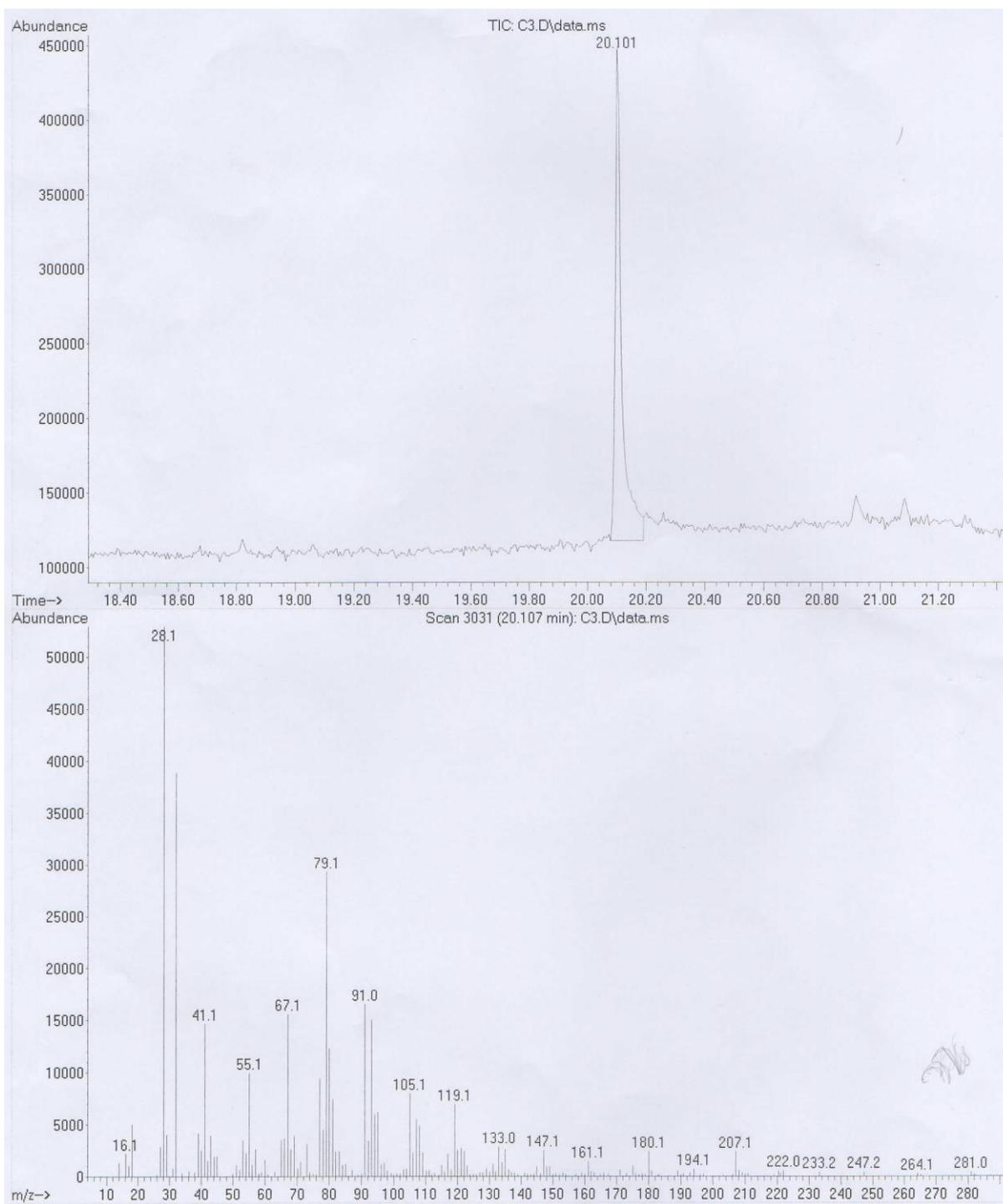


Figure S23. EI-MS spectrum of compound 10.

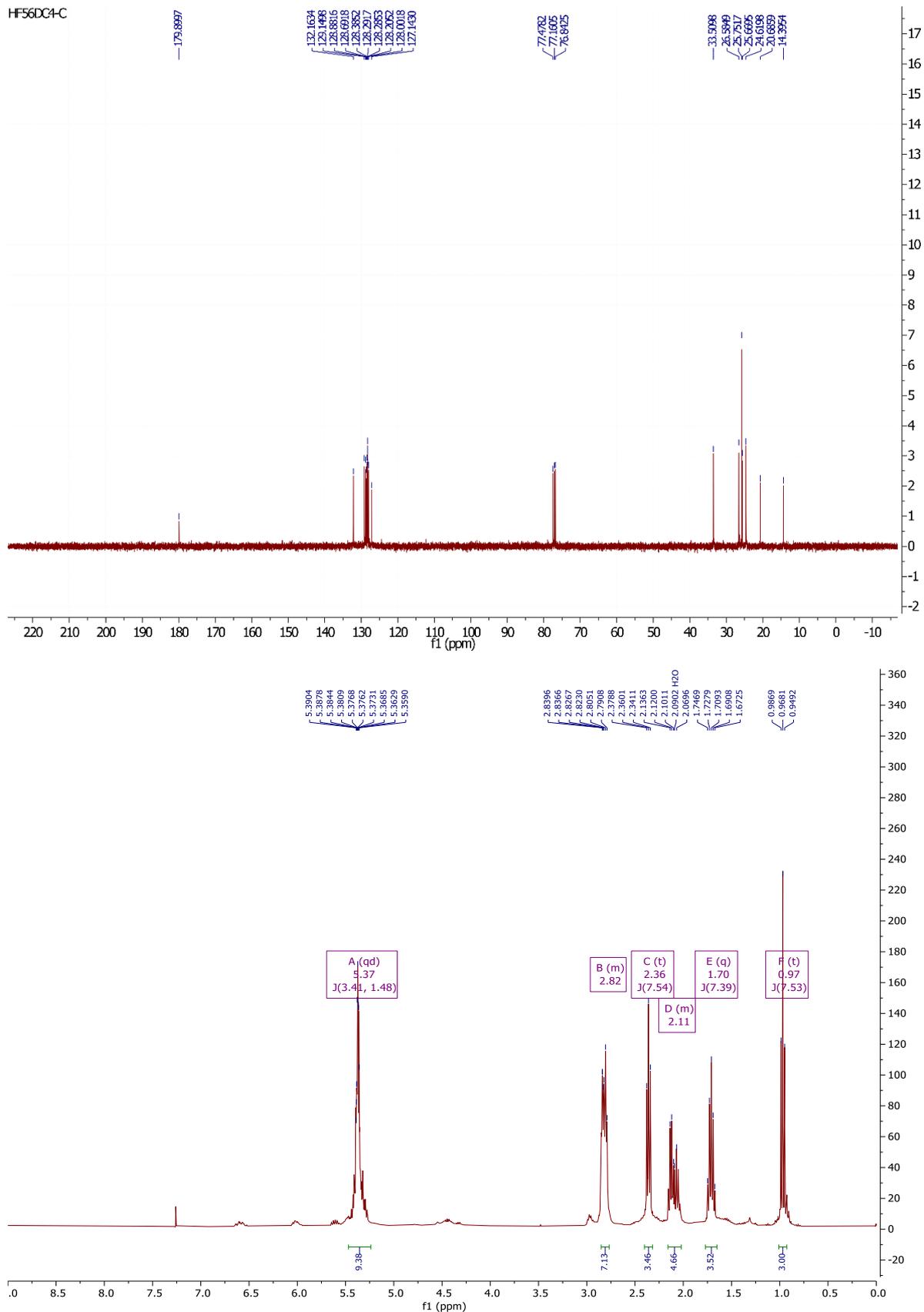


Figure S24. <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 11.

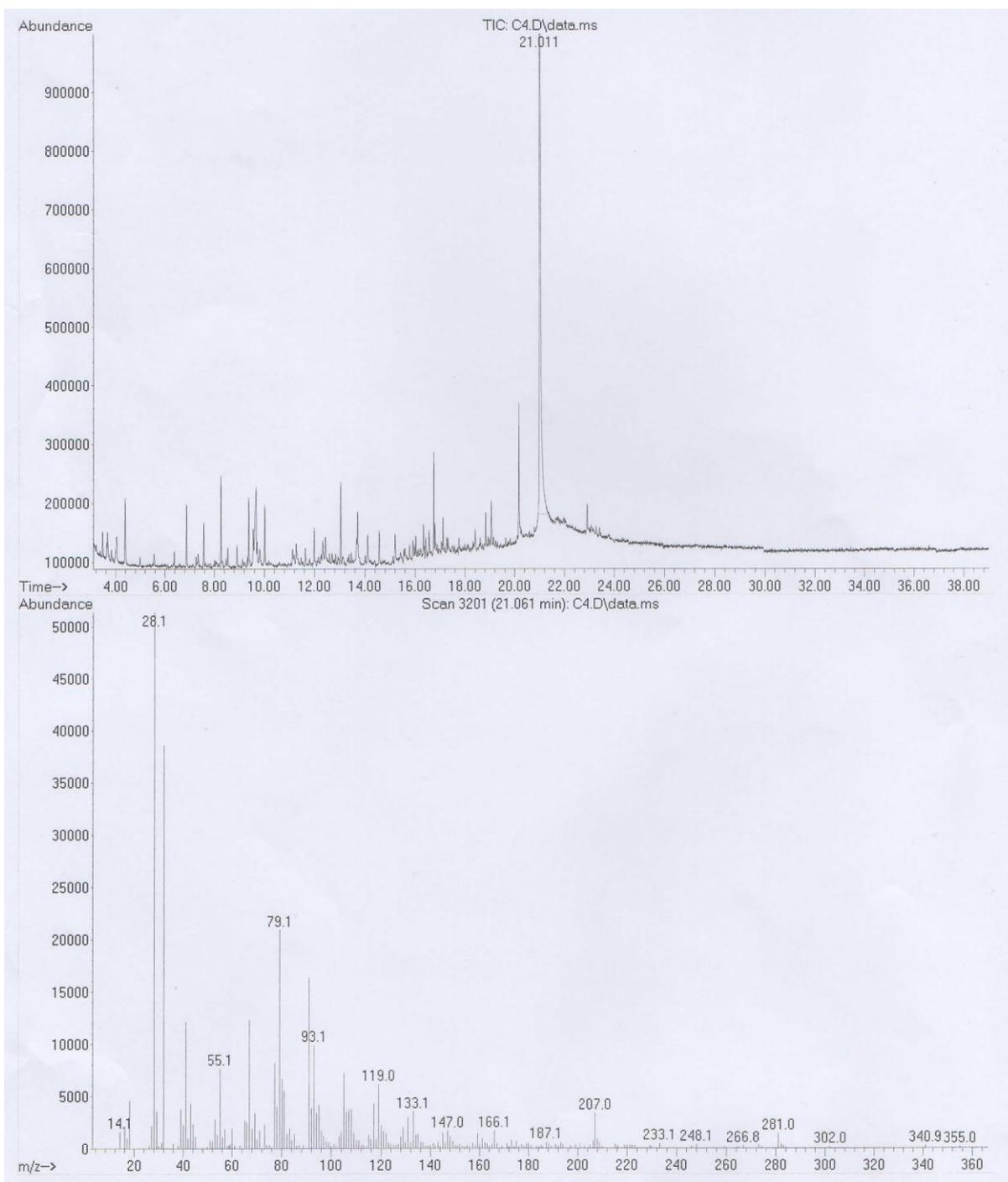


Figure S25. EI-MS spectrum of compound **11**.

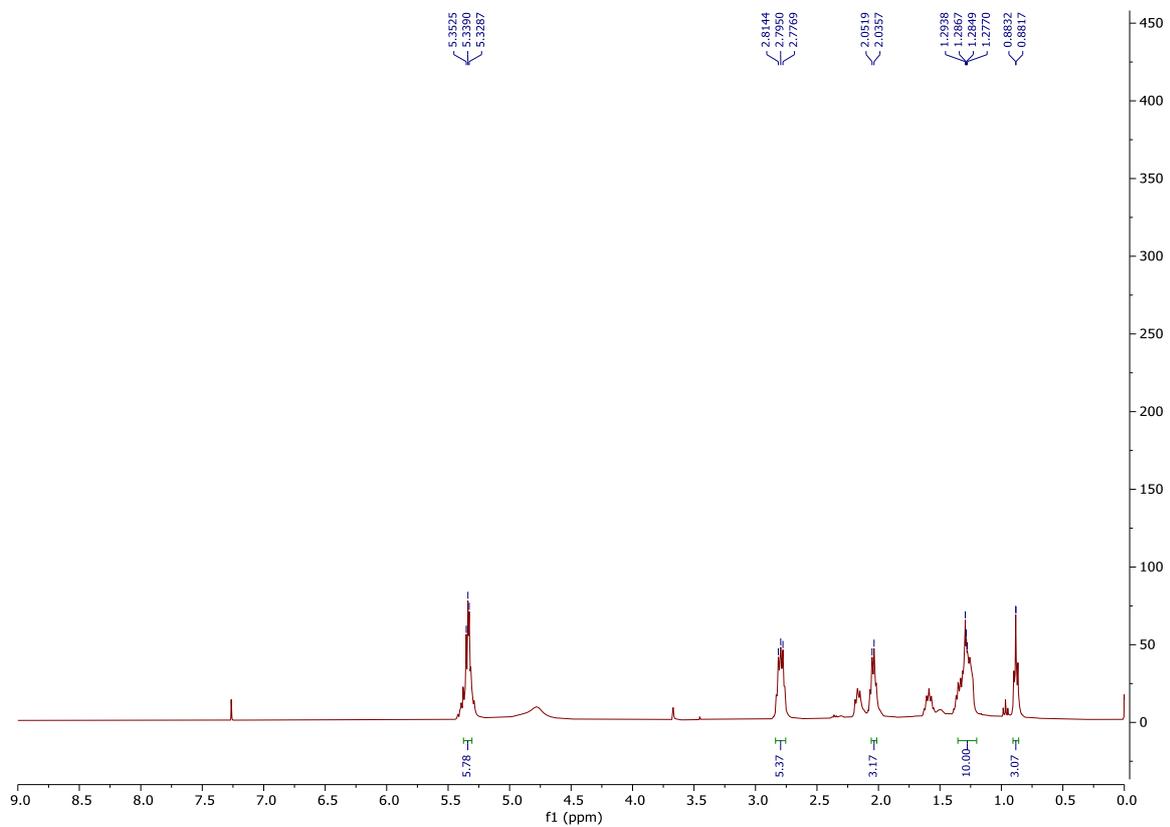
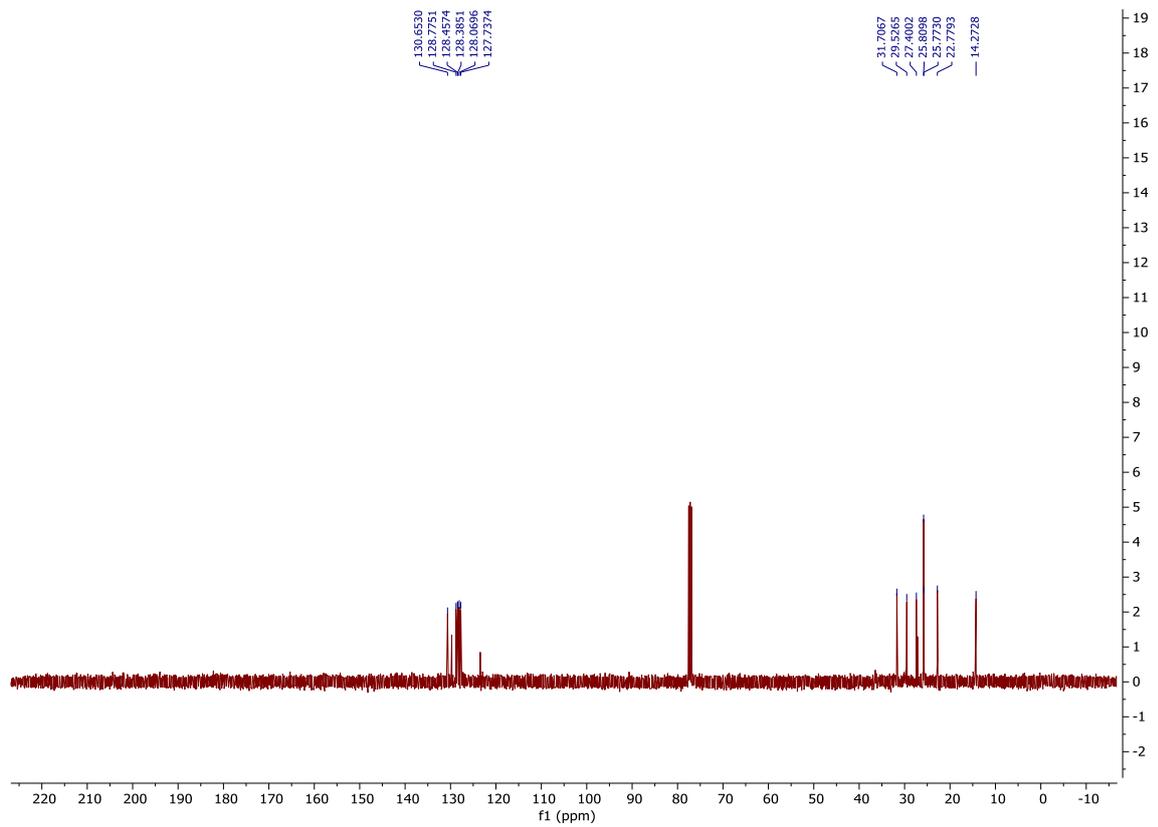


Figure S26. <sup>13</sup>C (100MHz in CDCl<sub>3</sub>)- and <sup>1</sup>H (400MHz in CDCl<sub>3</sub>)-NMR spectrum of compound 12.

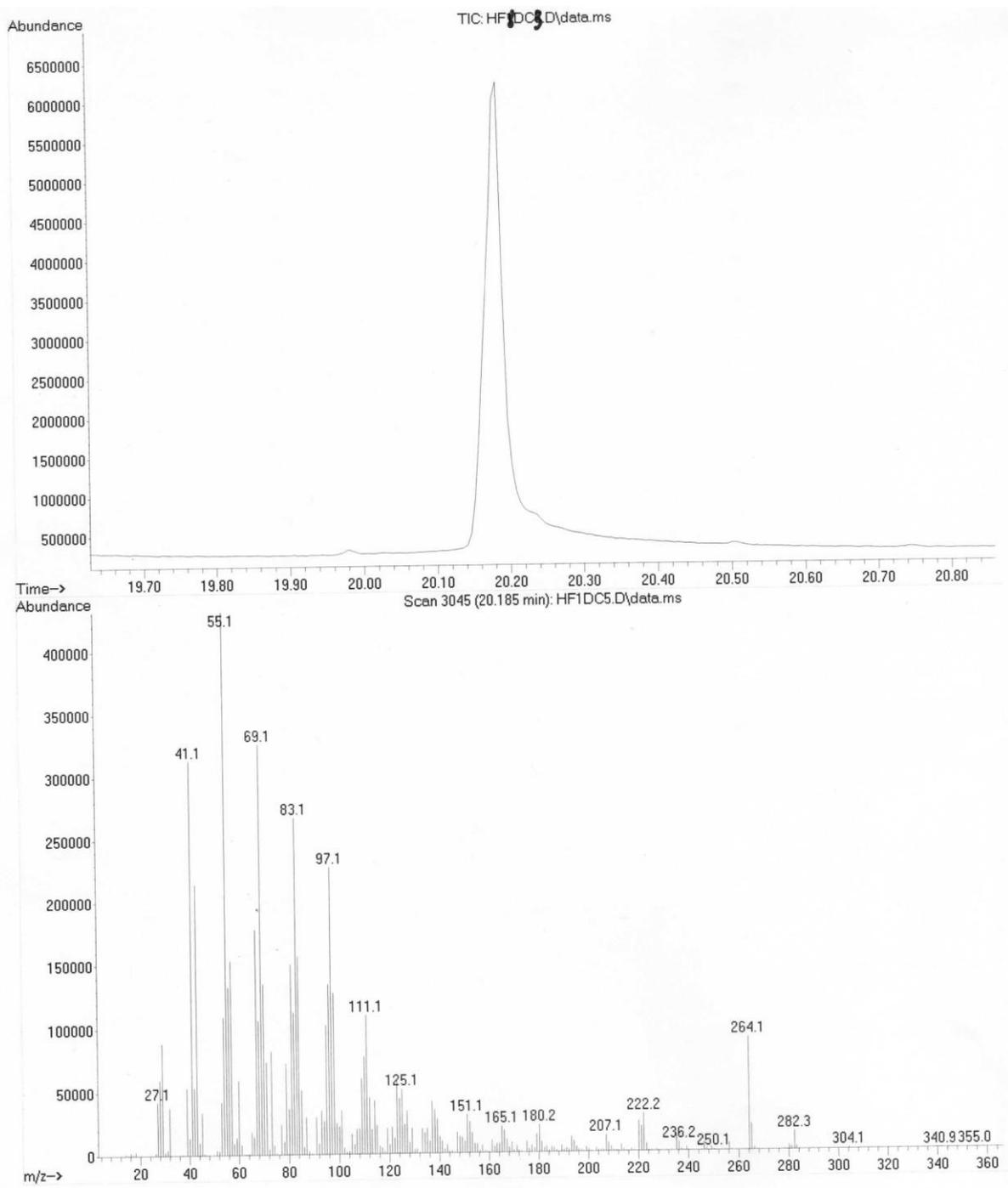


Figure S27. EI-MS spectrum of compound 12.

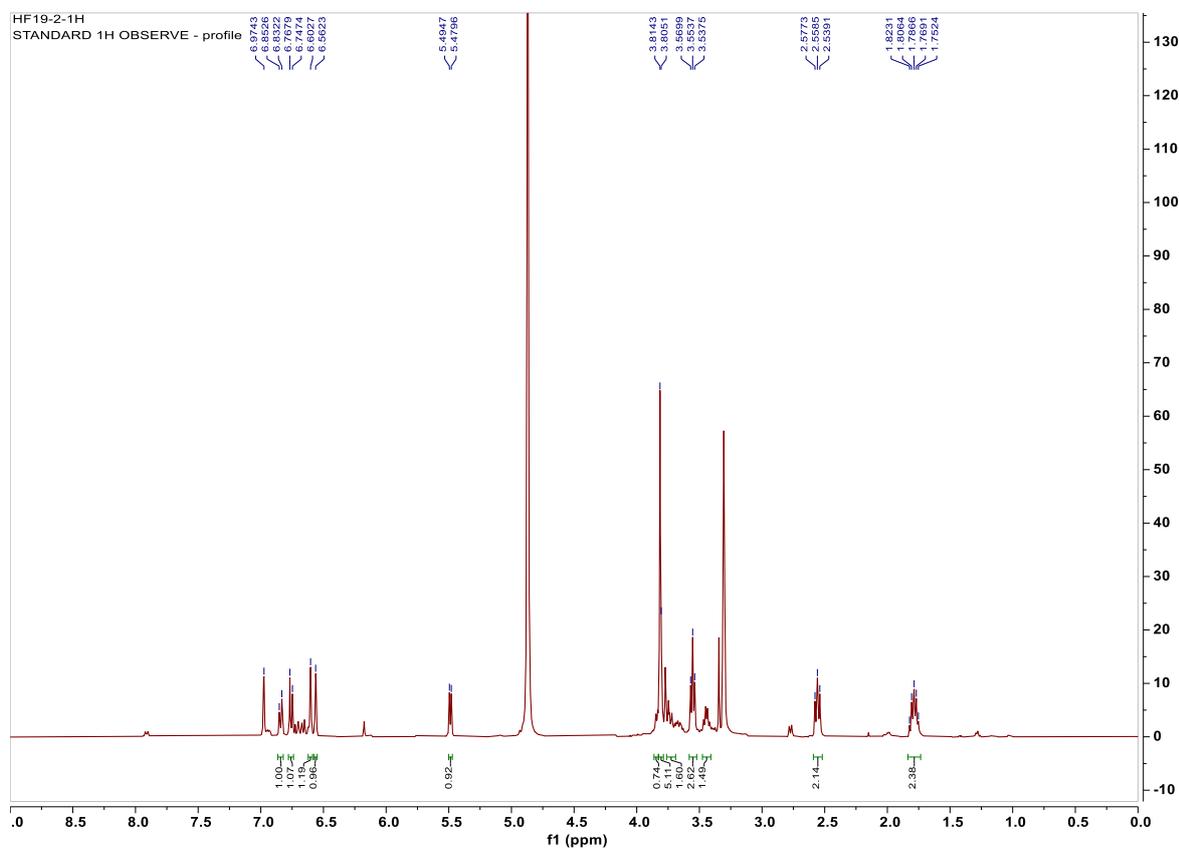
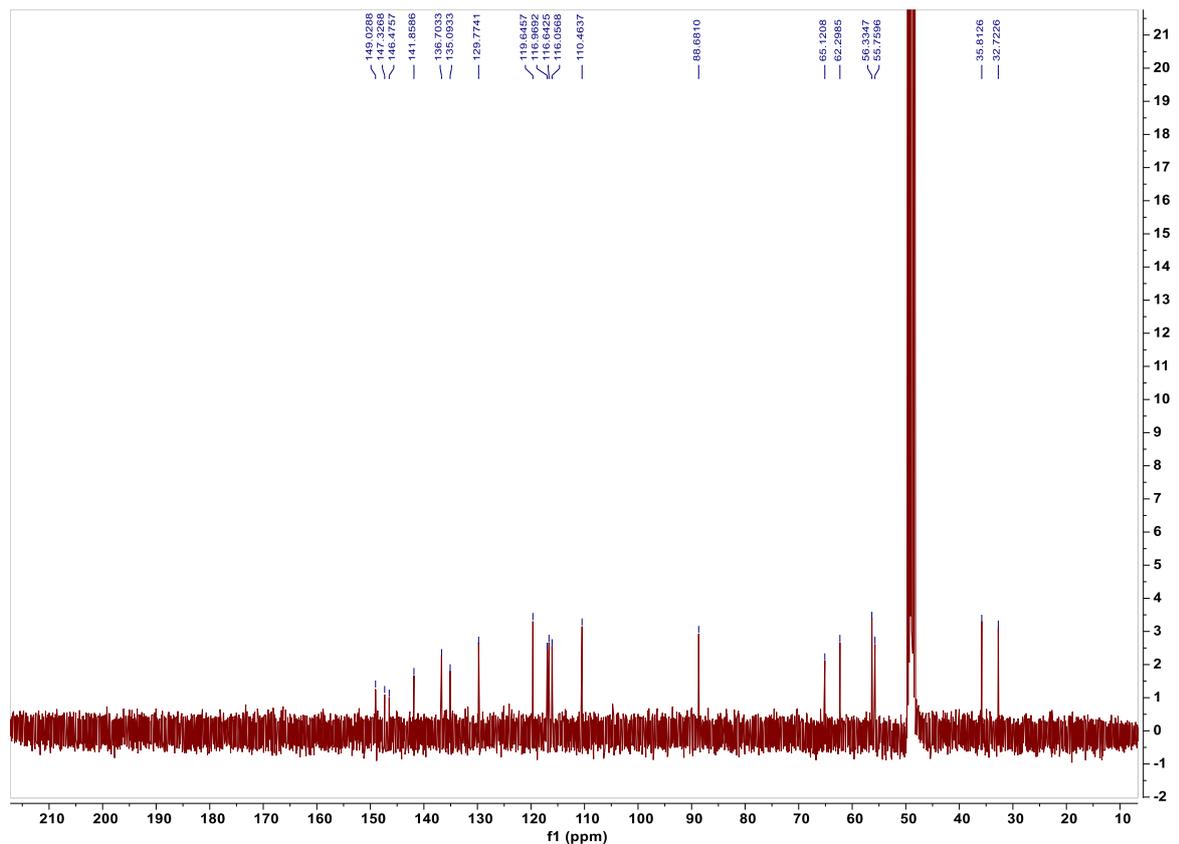


Figure S28.  $^{13}\text{C}$  (100MHz in  $\text{CD}_3\text{OD}$ )- and  $^1\text{H}$  (400MHz in  $\text{CD}_3\text{OD}$ )-NMR spectrum of compound 14.

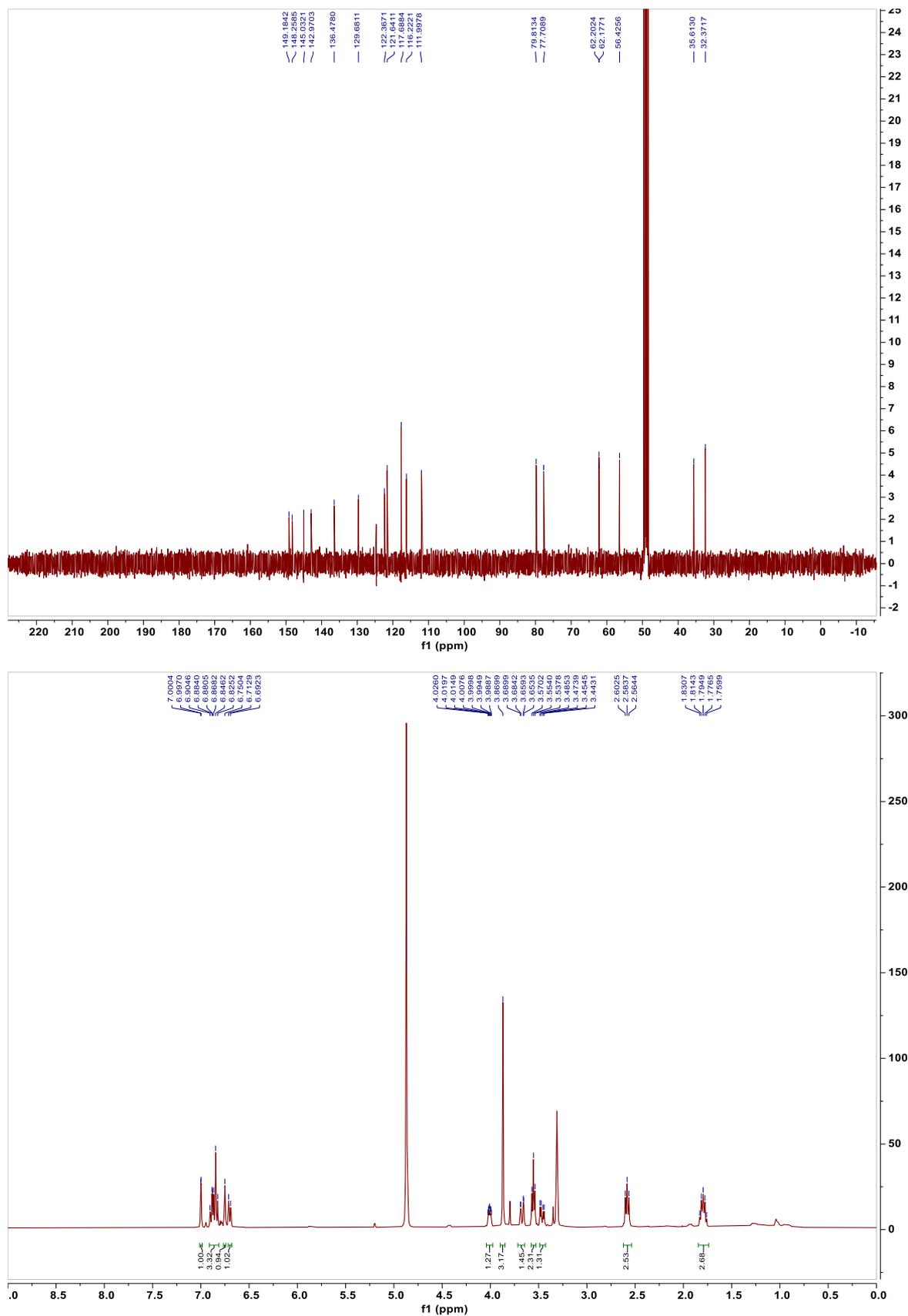


Figure S29. <sup>13</sup>C (100MHz in CD<sub>3</sub>OD)- and <sup>1</sup>H (400MHz in CD<sub>3</sub>OD)-NMR spectrum of compound 15.

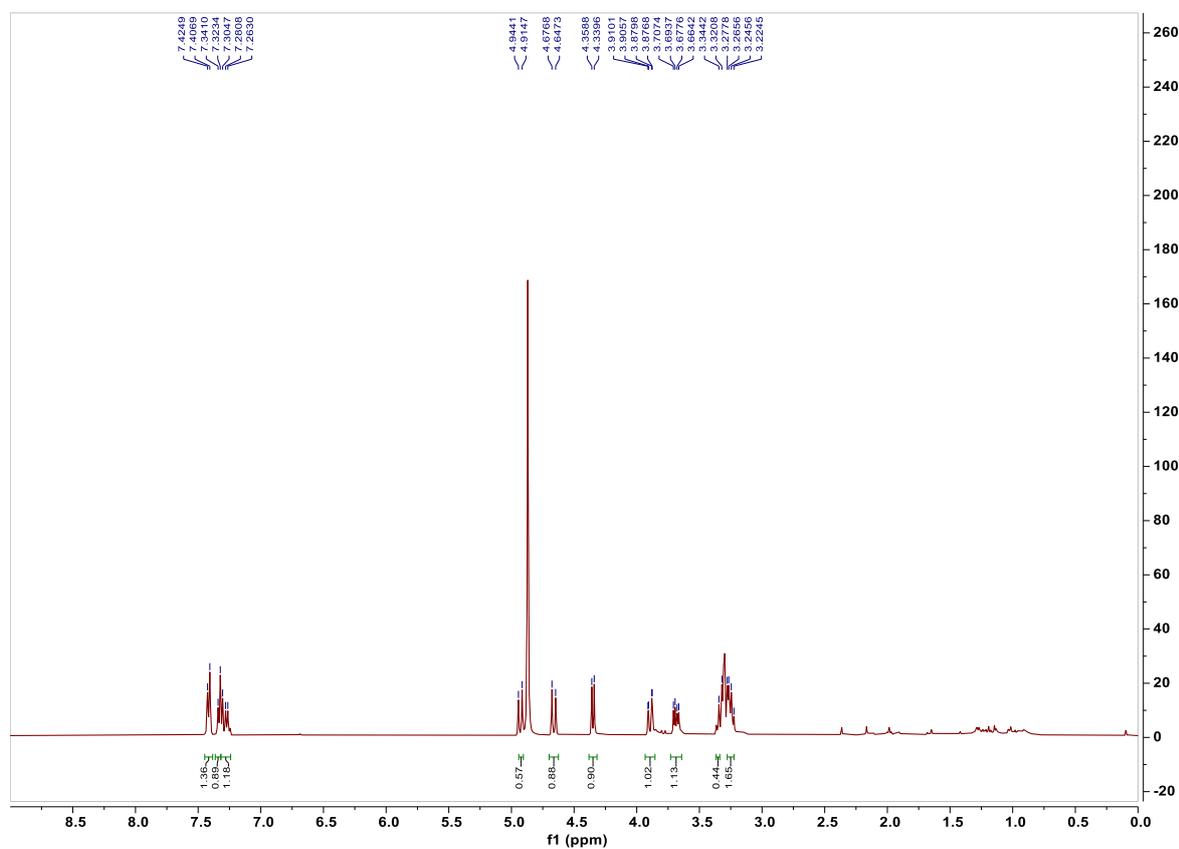
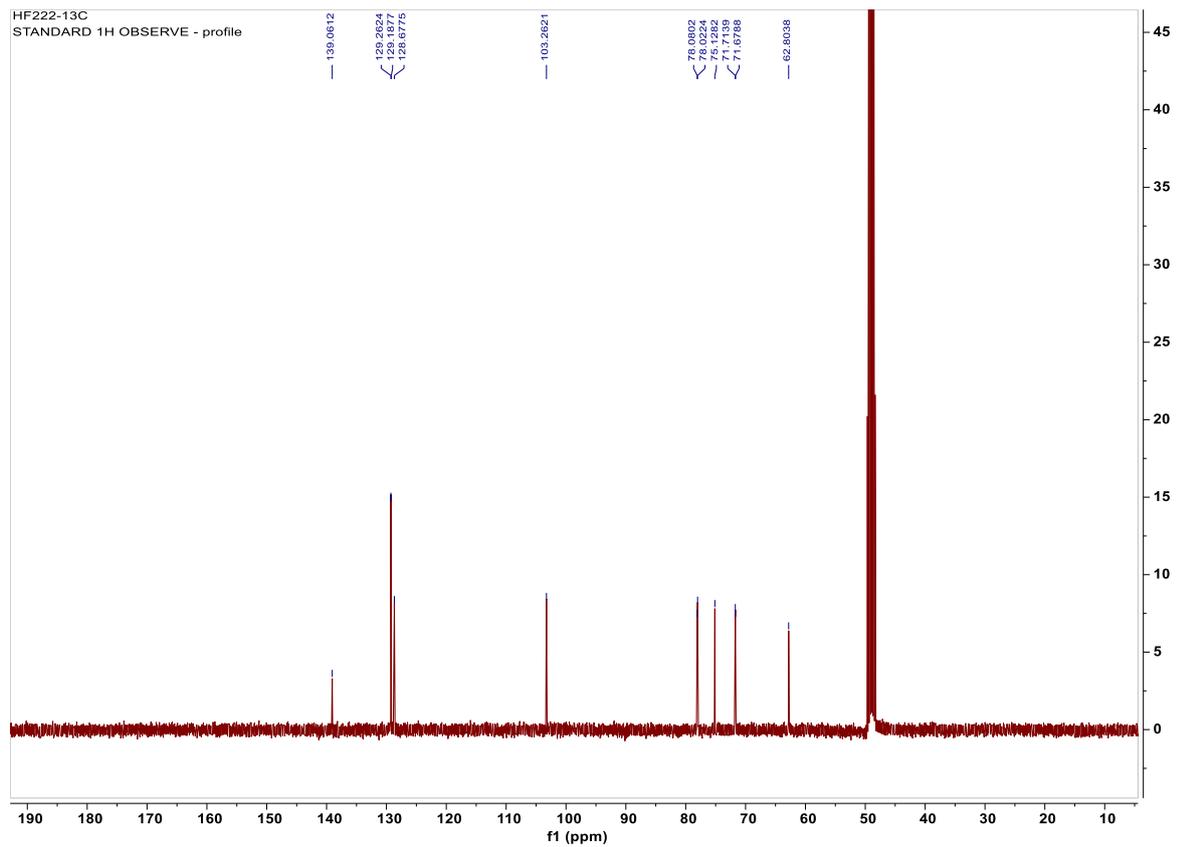


Figure S30.  $^{13}\text{C}$  (100MHz in  $\text{CD}_3\text{OD}$ )- and  $^1\text{H}$  (400MHz in  $\text{CD}_3\text{OD}$ )-NMR spectrum of compound 16.

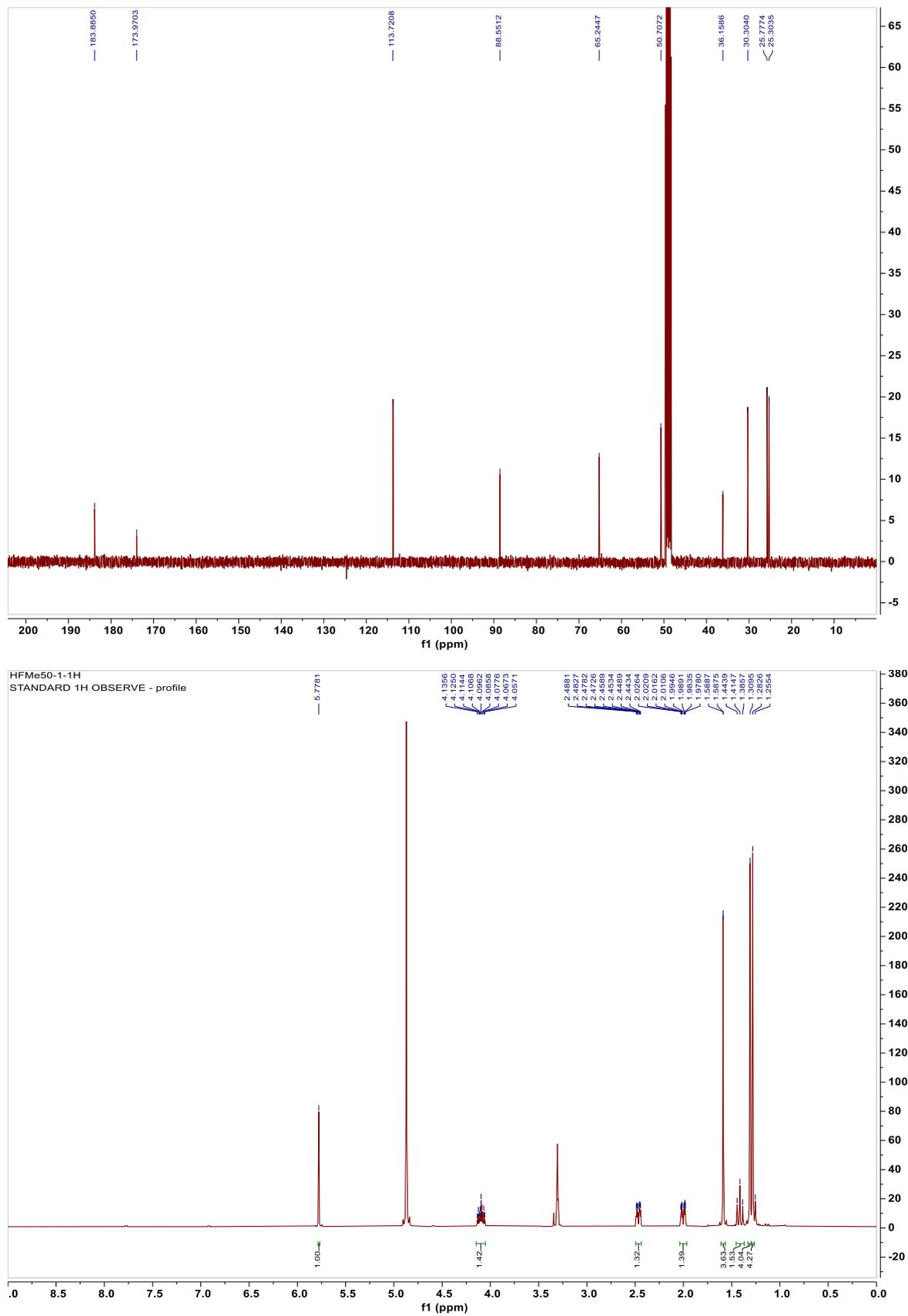


Figure S31. <sup>13</sup>C (100MHz in CD<sub>3</sub>OD)- and <sup>1</sup>H (400MHz in CD<sub>3</sub>OD)-NMR spectrum of compound 17.

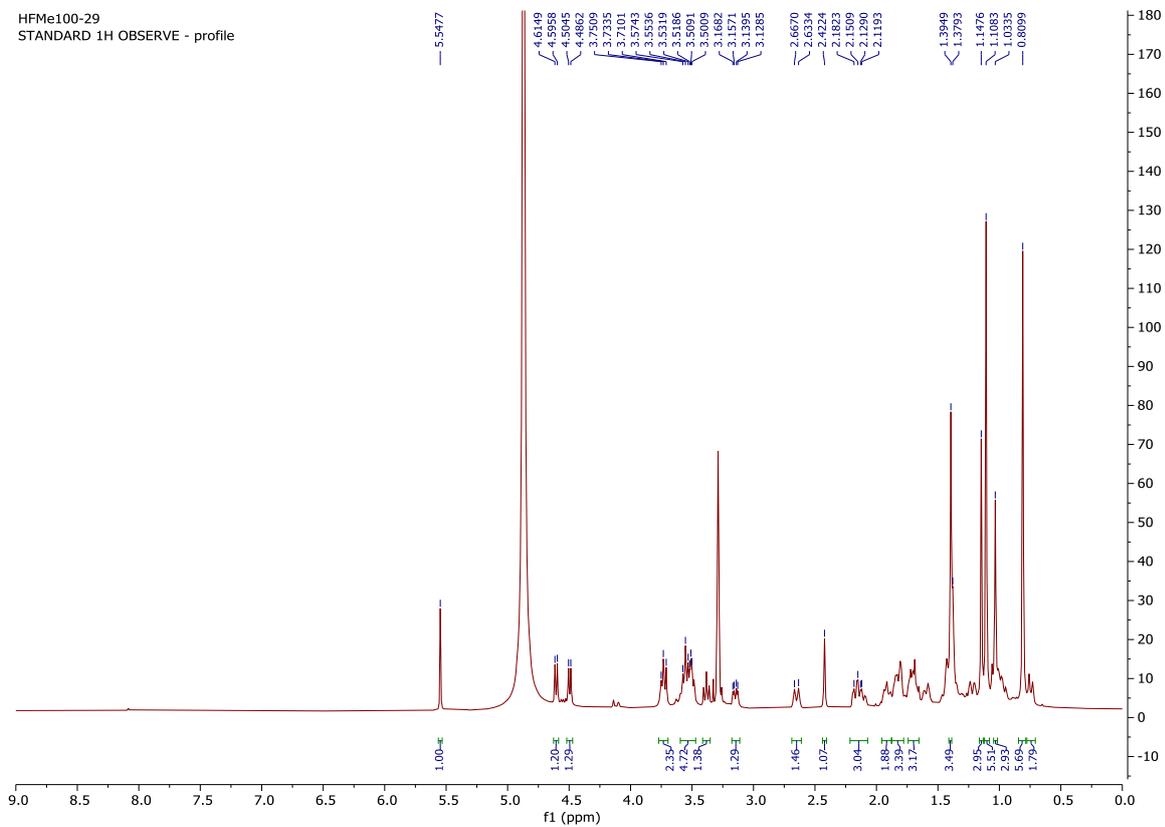
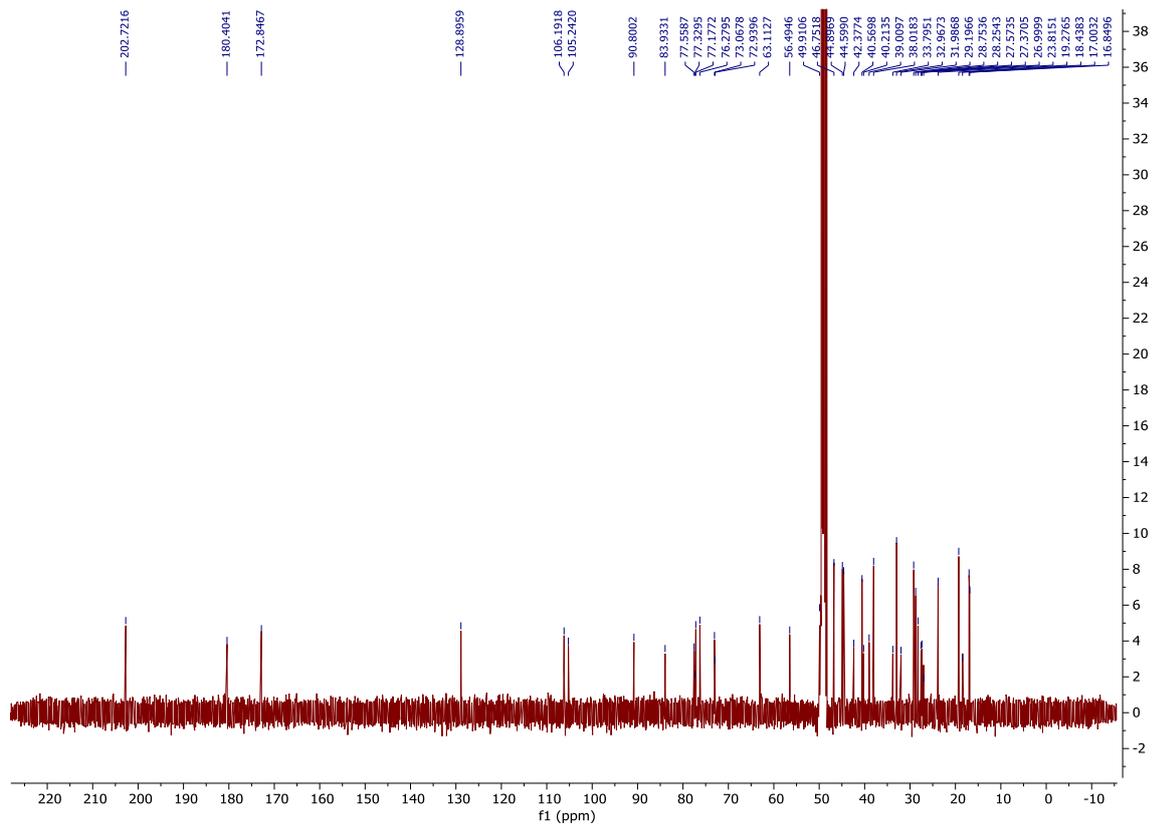


Figure S32.  $^{13}\text{C}$  (100MHz in  $\text{CD}_3\text{OD}$ )- and  $^1\text{H}$  (400MHz in  $\text{CD}_3\text{OD}$ )-NMR spectrum of compound 18.

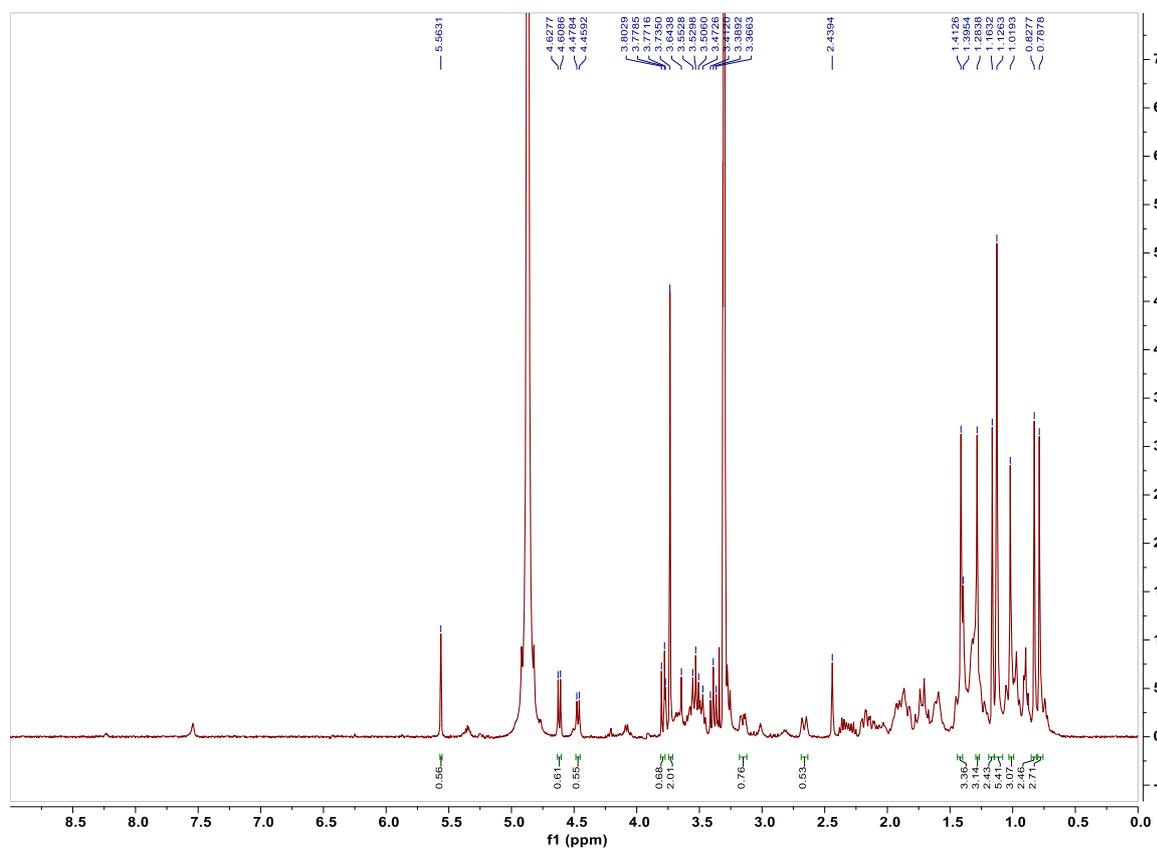
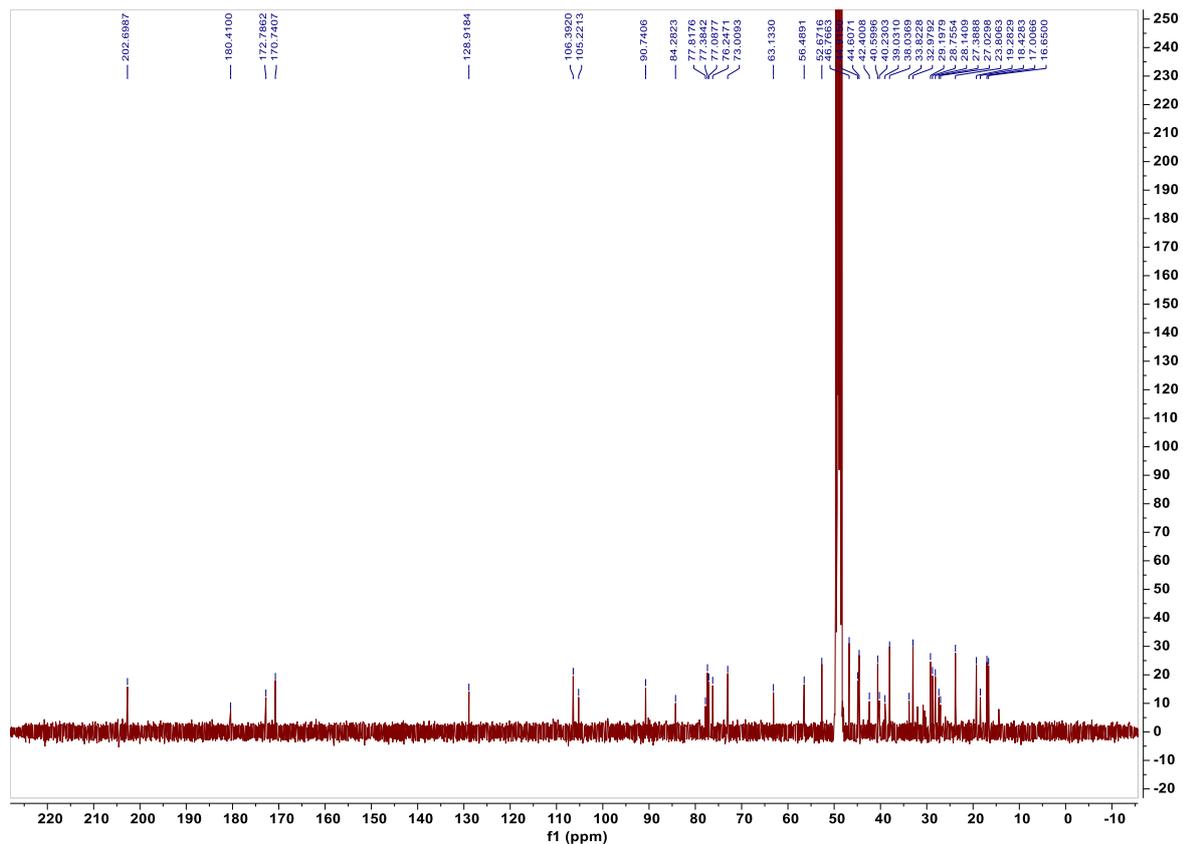


Figure S33. <sup>13</sup>C (100MHz in CD<sub>3</sub>OD)- and <sup>1</sup>H (400MHz in CD<sub>3</sub>OD)-NMR spectrum of compound 19.

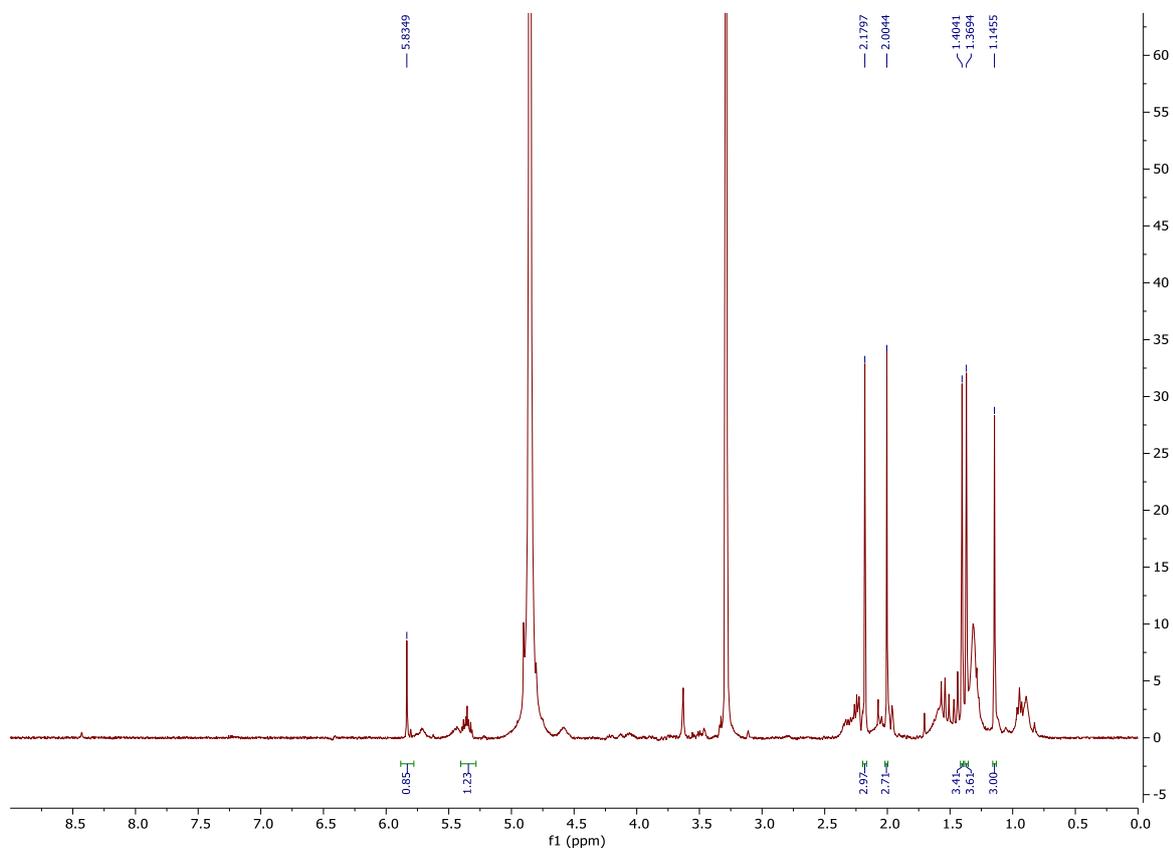
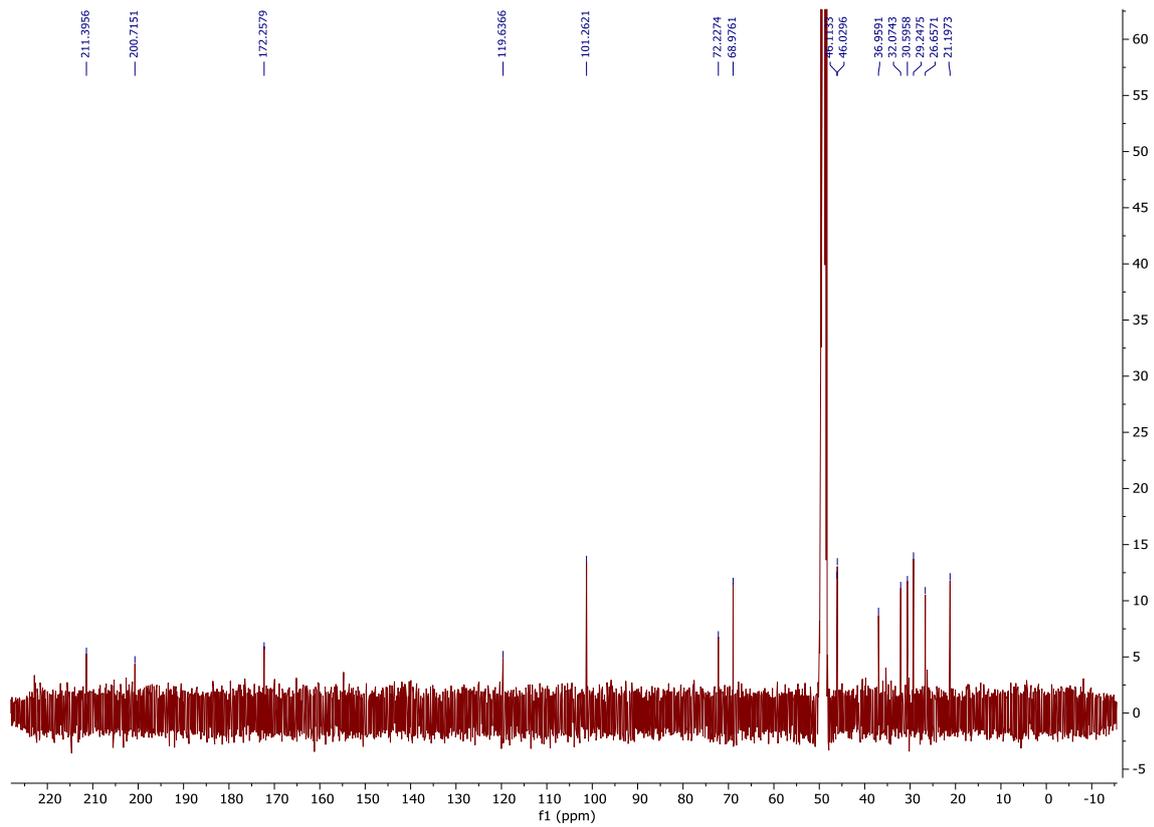


Figure S34. <sup>13</sup>C (100MHz in CD<sub>3</sub>OD)- and <sup>1</sup>H (400MHz in CD<sub>3</sub>OD)-NMR spectrum of compound 20.

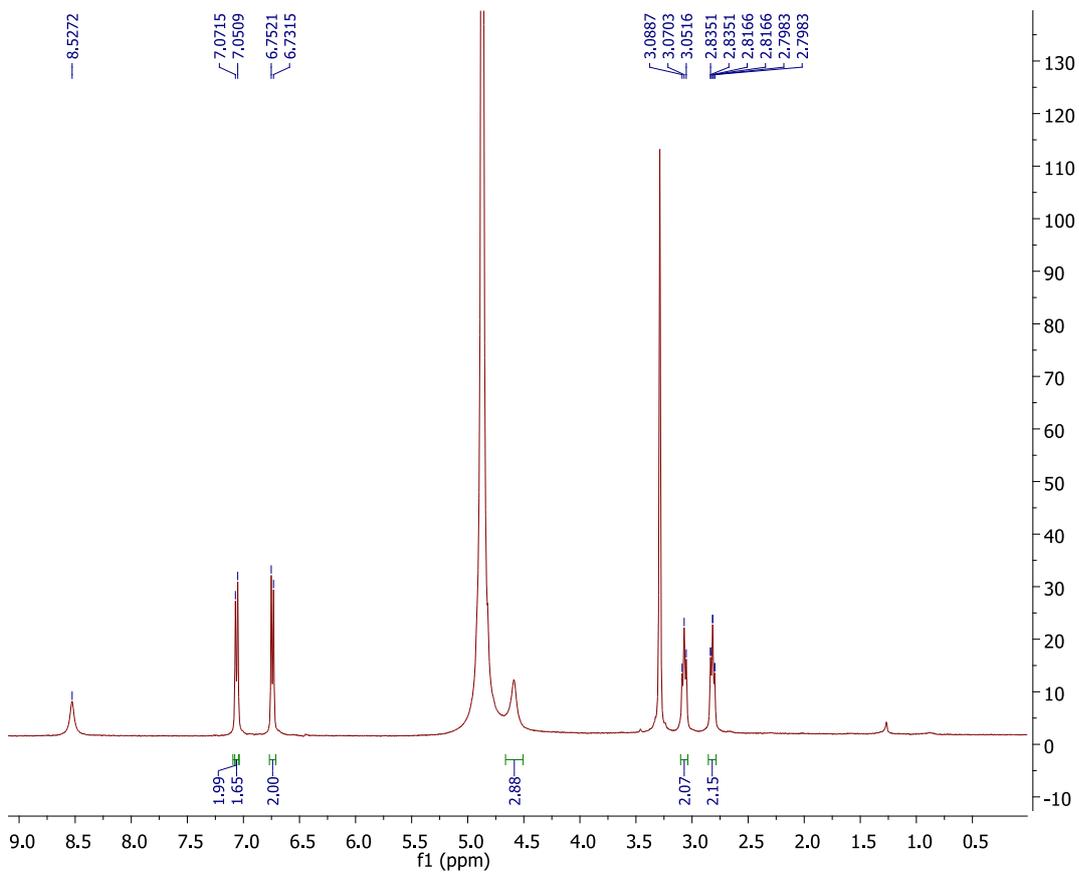
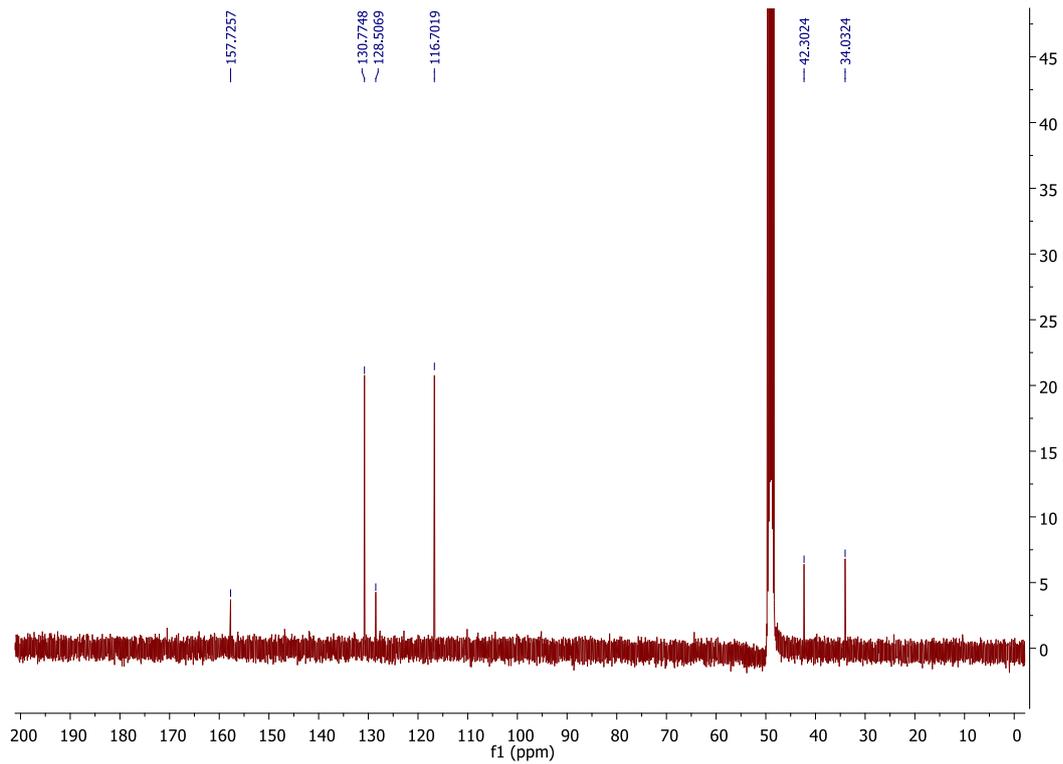


Figure S35.  $^{13}\text{C}$  (100MHz in  $\text{CD}_3\text{OD}$ )- and  $^1\text{H}$  (400MHz in  $\text{CD}_3\text{OD}$ )-NMR spectrum of compound 21.

Table S1. Molecular weight and molecular formula of 21 isolated compounds.

Compounds	Molecular formula	Observed molecular weight	Exact molecular weight
1	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	254 <sup>a</sup>	254.2245
2	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256 <sup>a</sup>	256.2402
3	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282 <sup>a</sup>	282.2558
4	C <sub>29</sub> H <sub>48</sub> O <sub>2</sub>	428 <sup>a</sup>	428.3654
5	C <sub>29</sub> H <sub>48</sub> O	412 <sup>a</sup>	412.3705
6	C <sub>29</sub> H <sub>48</sub> O <sub>2</sub>	428 <sup>a</sup>	428.3654
7	C <sub>17</sub> H <sub>28</sub> O <sub>2</sub>	264 <sup>a</sup>	264.2089
8	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	278 <sup>a</sup>	278.2245
9	C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>	304 <sup>a</sup>	304.2402
10	C <sub>18</sub> H <sub>28</sub> O <sub>2</sub>	276 <sup>a</sup>	276.2089
11	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>	302 <sup>a</sup>	302.2245
12	C <sub>17</sub> H <sub>28</sub> O <sub>2</sub>	264 <sup>a</sup>	264.2089
13	C <sub>34</sub> H <sub>54</sub> O <sub>9</sub>	607.3820 [M + H] <sup>+ b</sup>	607.3846 (C <sub>34</sub> H <sub>55</sub> O <sub>9</sub> )
14	C <sub>19</sub> H <sub>22</sub> O <sub>6</sub>	— <sup>c</sup>	346.1416
15	C <sub>19</sub> H <sub>24</sub> O <sub>7</sub>	— <sup>c</sup>	364.1522
16	C <sub>13</sub> H <sub>18</sub> O <sub>6</sub>	— <sup>c</sup>	270.1103
17	C <sub>11</sub> H <sub>16</sub> O <sub>3</sub>	219.0992 [M + Na] <sup>+ b</sup>	219.0997 (C <sub>11</sub> H <sub>16</sub> NaO <sub>3</sub> )
18	C <sub>42</sub> H <sub>62</sub> O <sub>16</sub>	— <sup>c</sup>	822.4037
19	C <sub>43</sub> H <sub>64</sub> O <sub>16</sub>	— <sup>c</sup>	836.4194
20	C <sub>15</sub> H <sub>22</sub> O <sub>4</sub>	— <sup>c</sup>	266.1518
21	C <sub>8</sub> H <sub>11</sub> NO	— <sup>c</sup>	137.0840

<sup>a</sup> Observed from EI-MS.

<sup>b</sup> Observed from ESI-MS.

<sup>a</sup> Structures were elucidated based on the NMR data.