

## SUPPORTING INFORMATION (1)

# Klysimplexins I–T, Eunicellin-Based Diterpenoids from the Cultured Soft Coral *Klyxum simplex*

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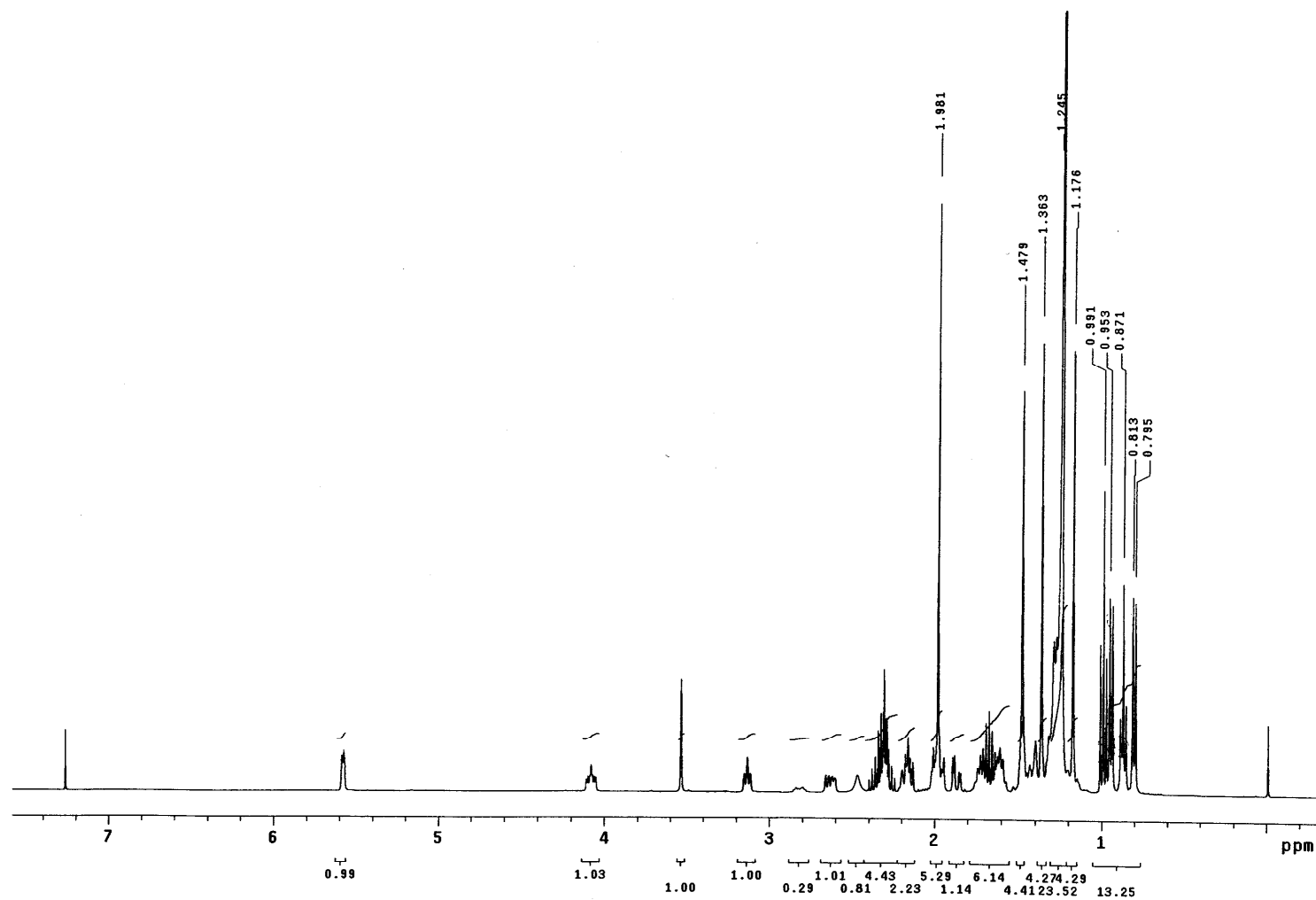
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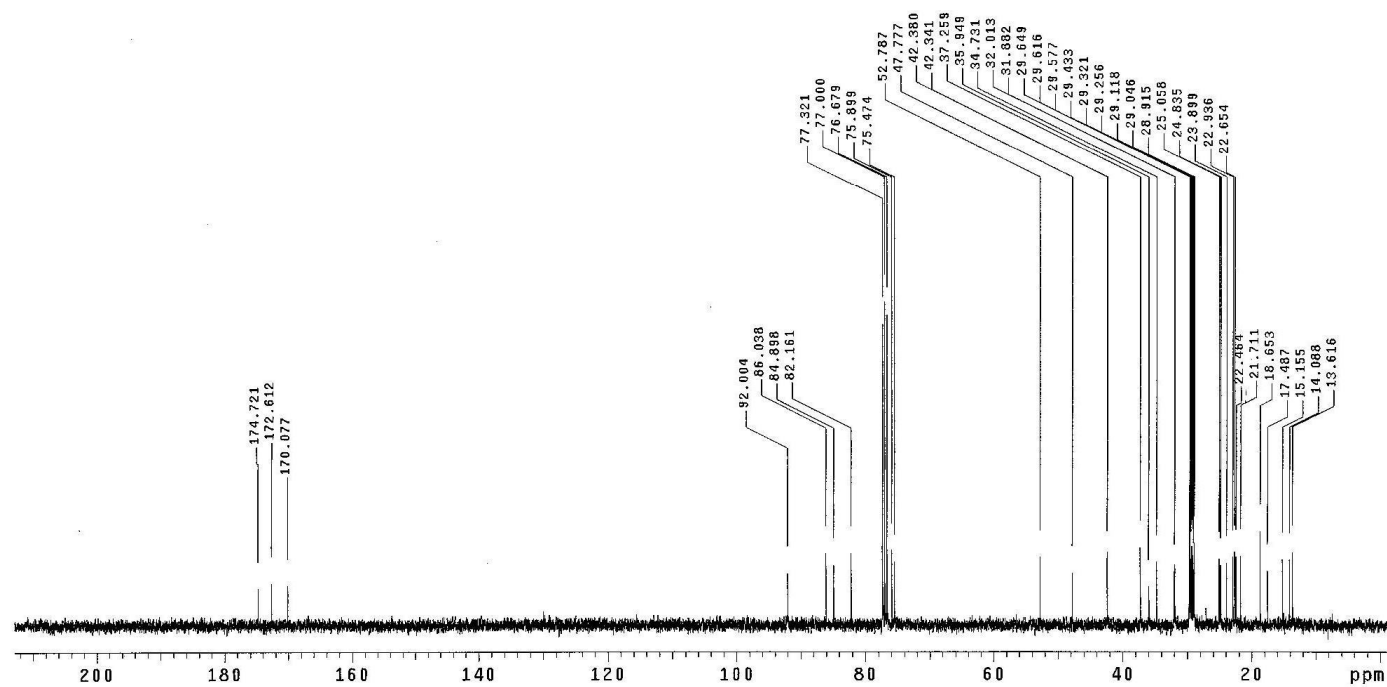
Corresponding author: [sheu@mail.nsysu.edu.tw](mailto:sheu@mail.nsysu.edu.tw)

## **List of Supporting Information:**

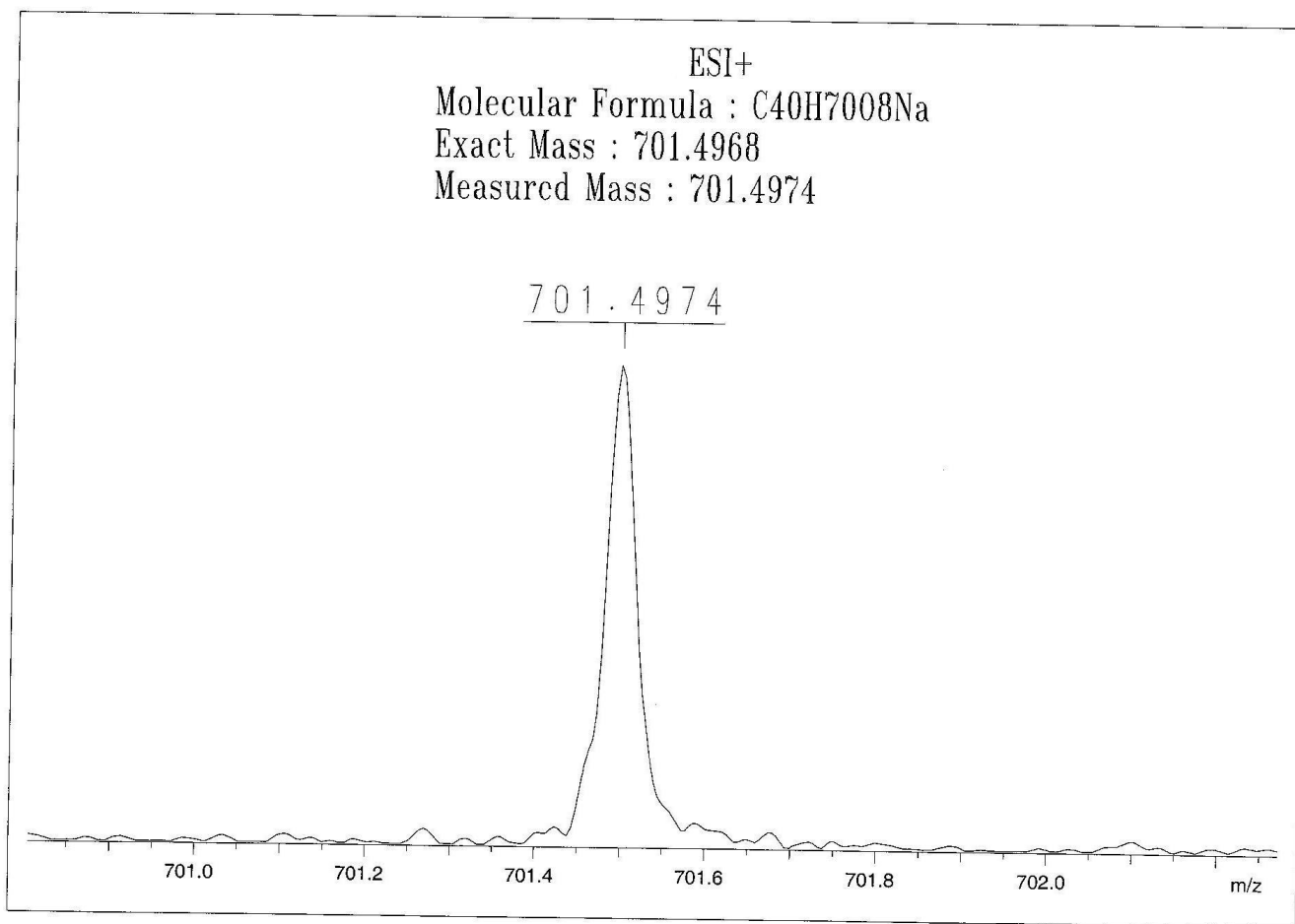
- S2.  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 400 MHz.
- S3.  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 100 MHz.
- S4. HRESIMS spectrum of **1**.
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- S6.  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CDCl}_3$  at 100 MHz.
- S7. HRESIMS spectrum of **2**.
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- S25.  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{CDCl}_3$  at 400 MHz.
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- S27. HRESIMS spectrum of **9**.
- S28.  $^{13}\text{C}$  NMR spectrum of **10** in  $\text{CDCl}_3$  at 500 MHz.
- S29.  $^{13}\text{C}$  NMR spectrum of **10** in  $\text{CDCl}_3$  at 125 MHz.
- S30. HRESIMS spectrum of **10**.
- S31.  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$  at 400 MHz.
- S32.  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$  at 100 MHz.
- S33. HRESIMS spectrum of **11**.
- S34.  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$  at 400 MHz.
- S35.  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$  at 100 MHz.
- S36. HRESIMS spectrum of **12**.



S2. <sup>1</sup>H NMR spectrum of **1** in CDCl<sub>3</sub> at 400 MHz.

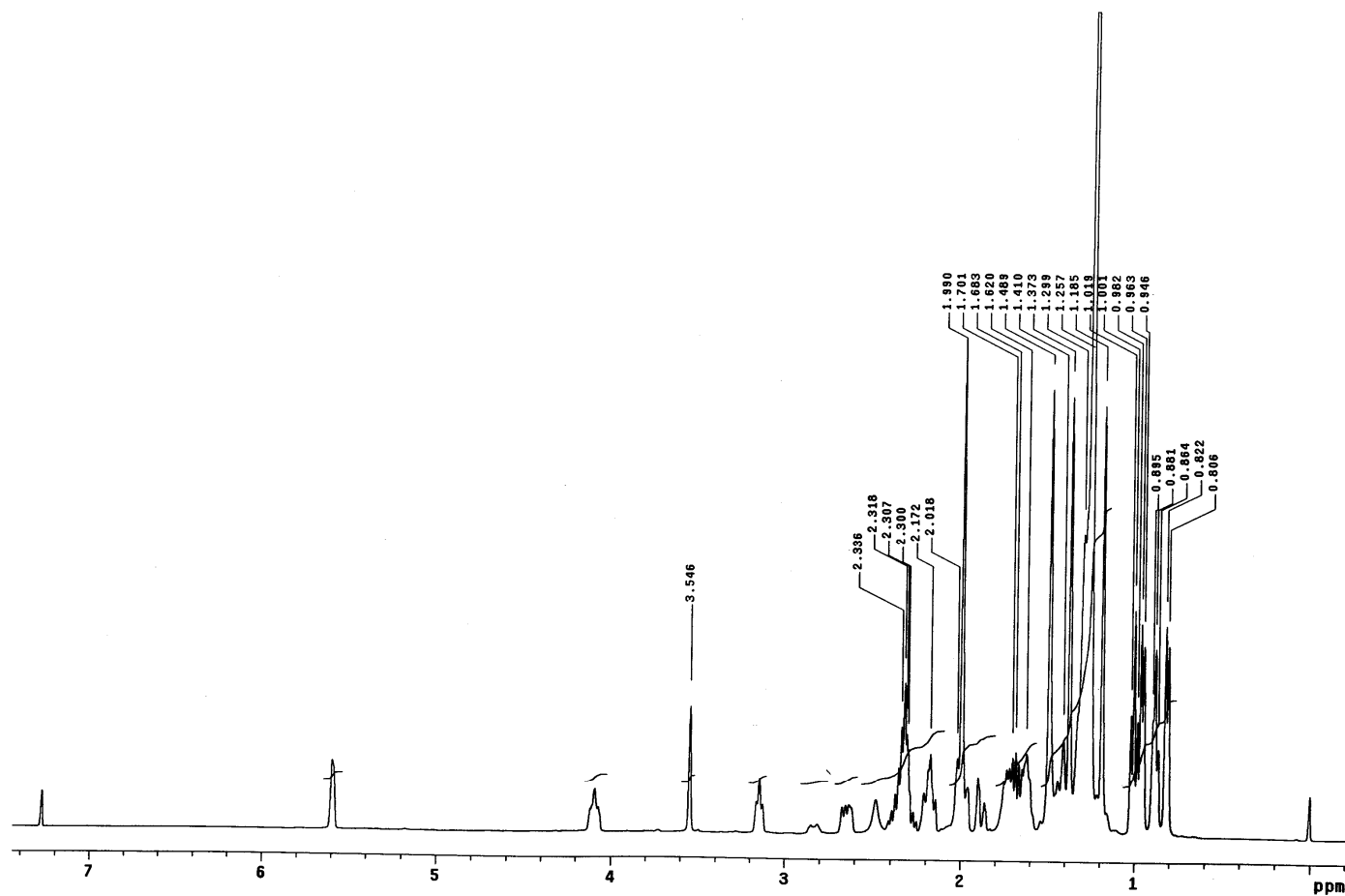


**S3** <sup>13</sup>C NMR spectrum of **1** in CDCl<sub>3</sub> at 100 MHz.

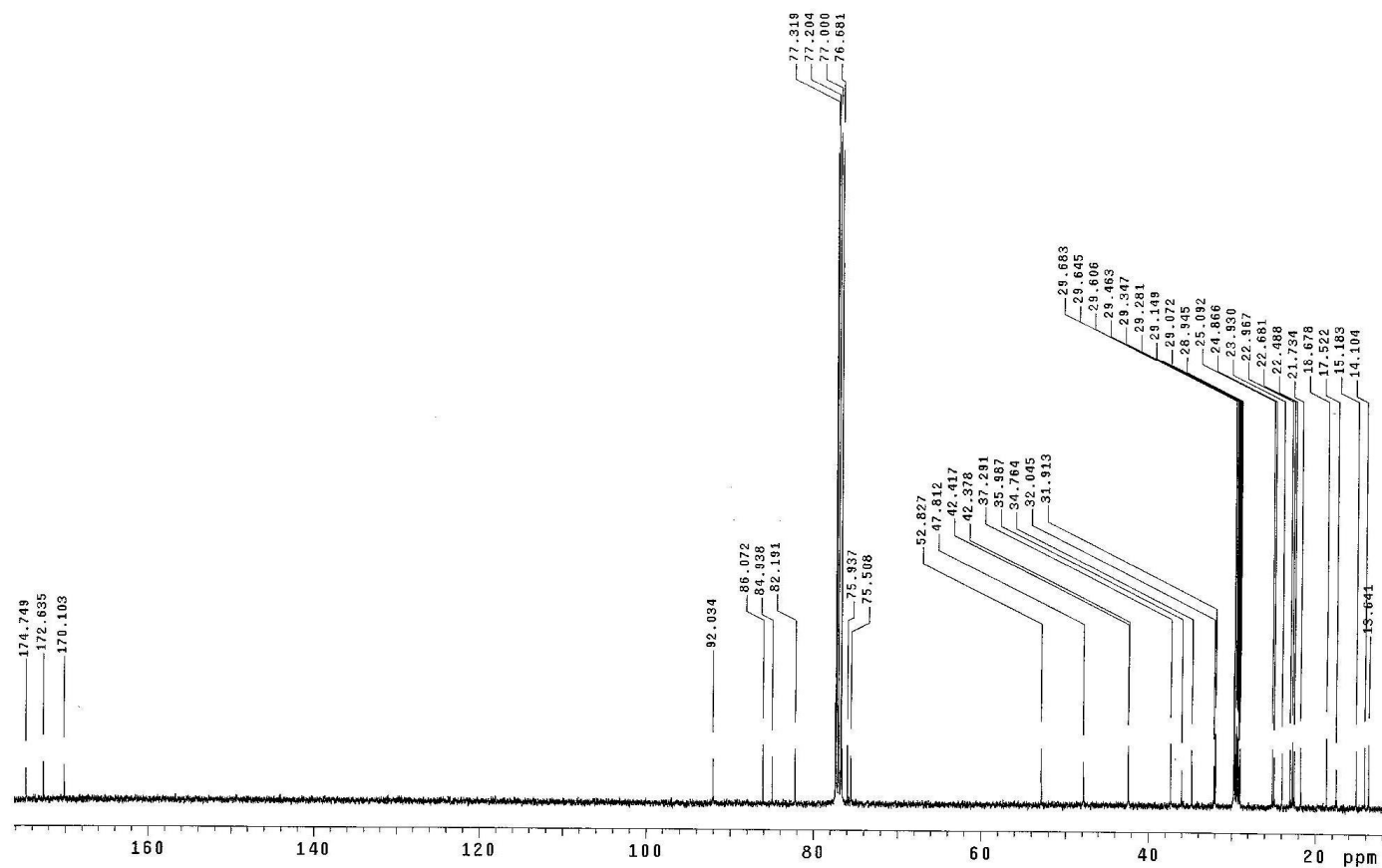


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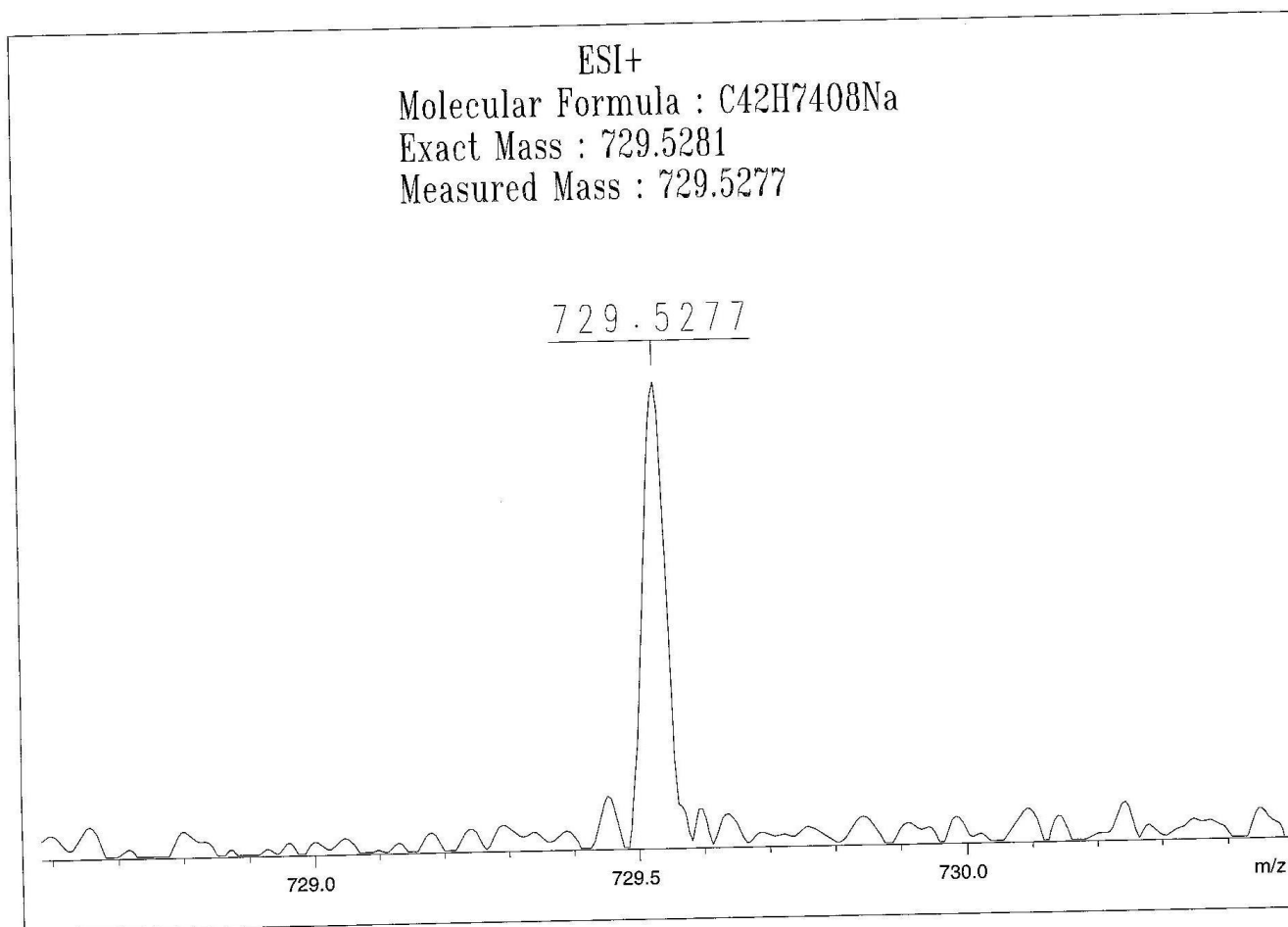
**S4 HRESIMS spectrum of 1.**



S5.  $^1\text{H}$  NMR spectrum of **2** in  $\text{CDCl}_3$  at 400 MHz.

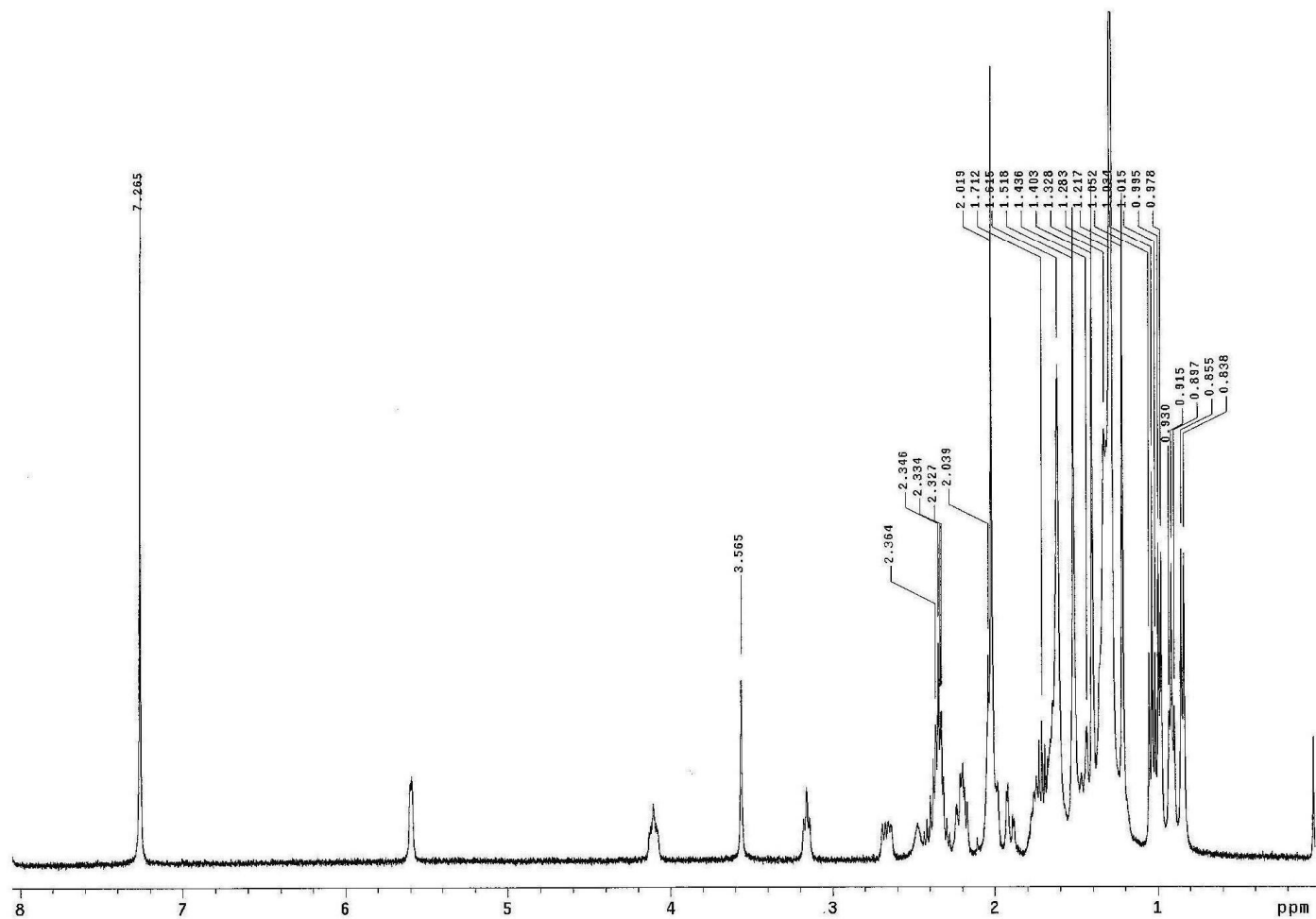


**S6.** <sup>13</sup>C NMR spectrum of **2** in CDCl<sub>3</sub> at 100 MHz.

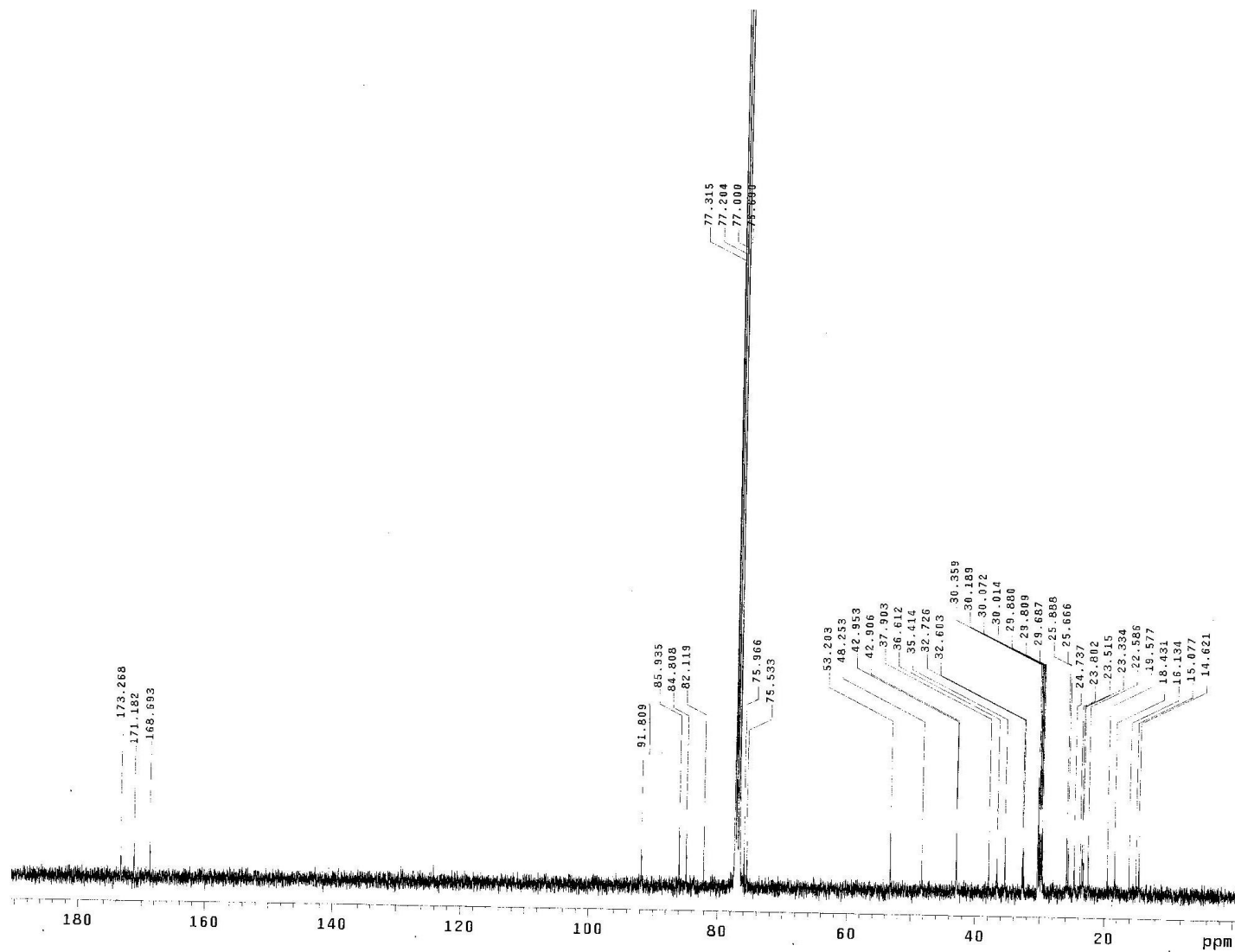


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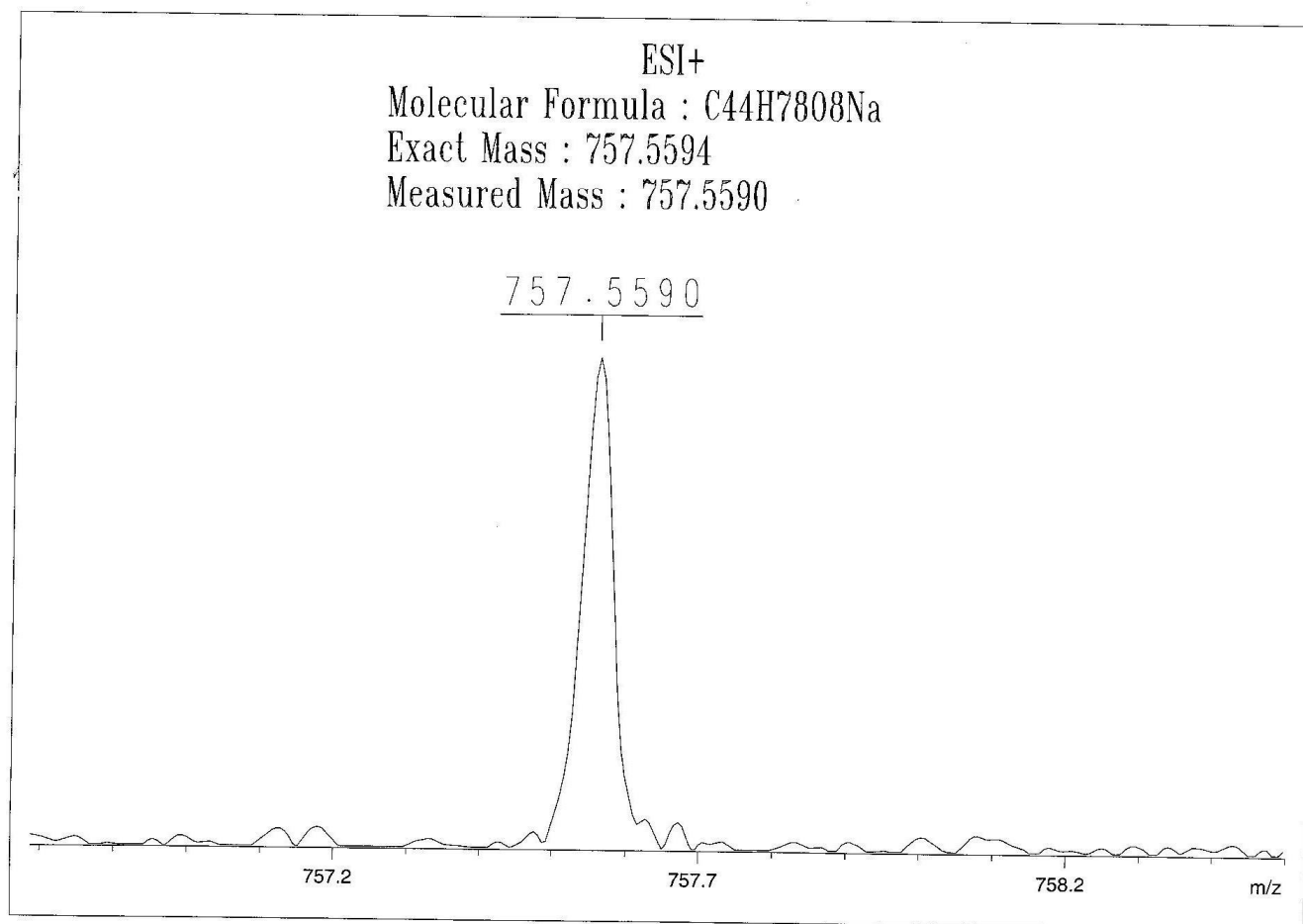
**S7** HRESIMS spectrum of **2**.



S8. <sup>1</sup>H NMR spectrum of **3** in CDCl<sub>3</sub> at 400 MHz.

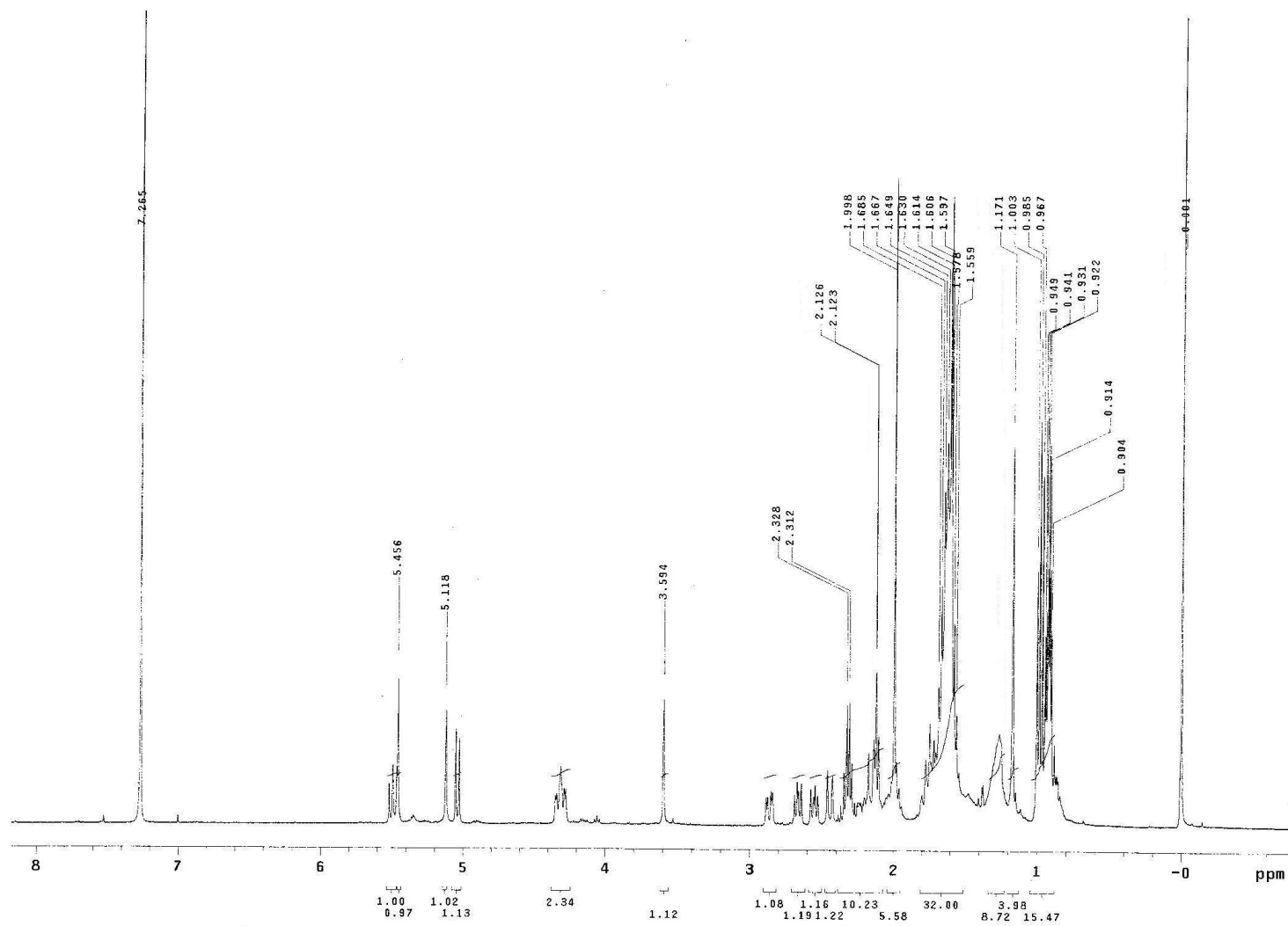


S9. <sup>13</sup>C NMR spectrum of **3** in CDCl<sub>3</sub> at 100 MHz.

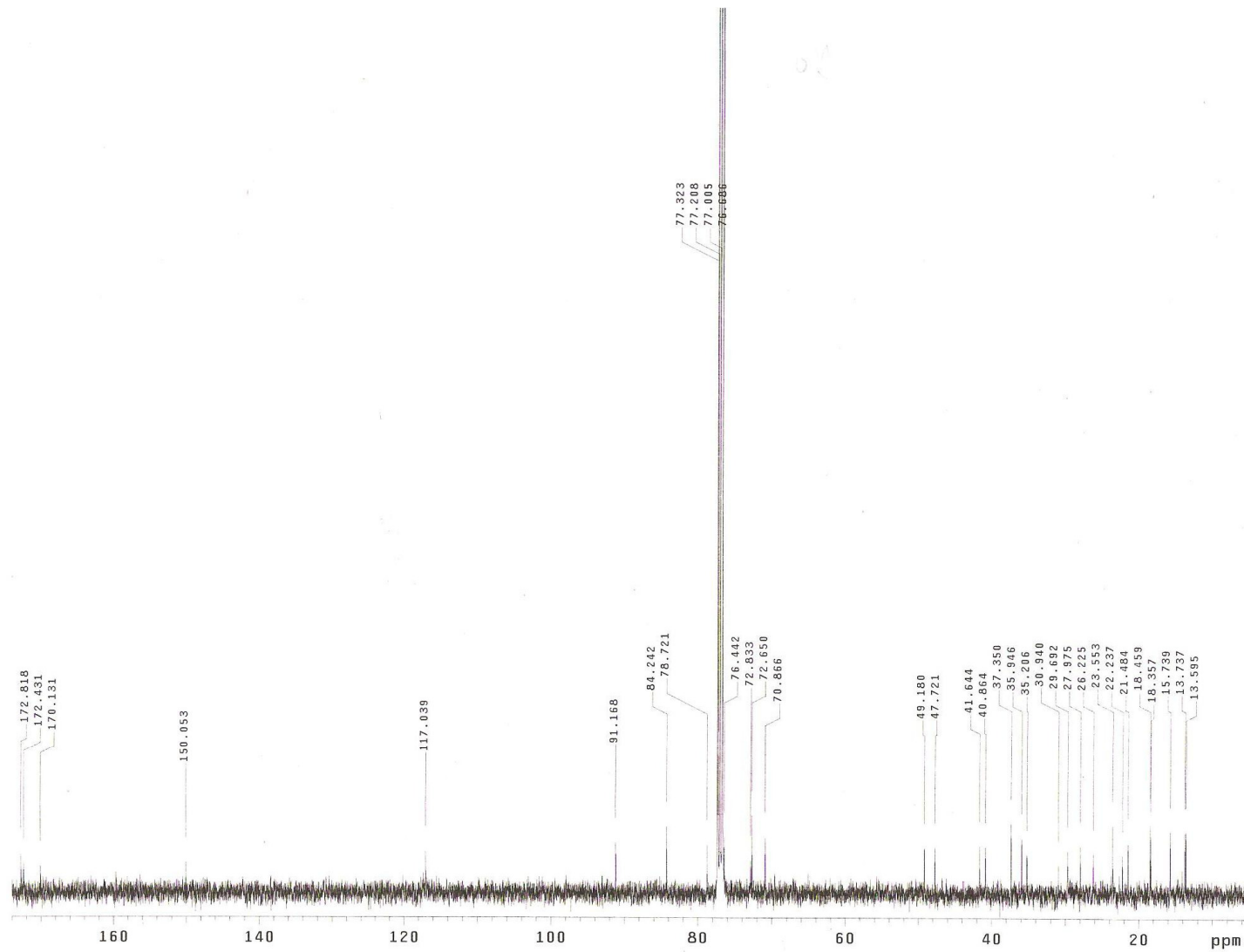


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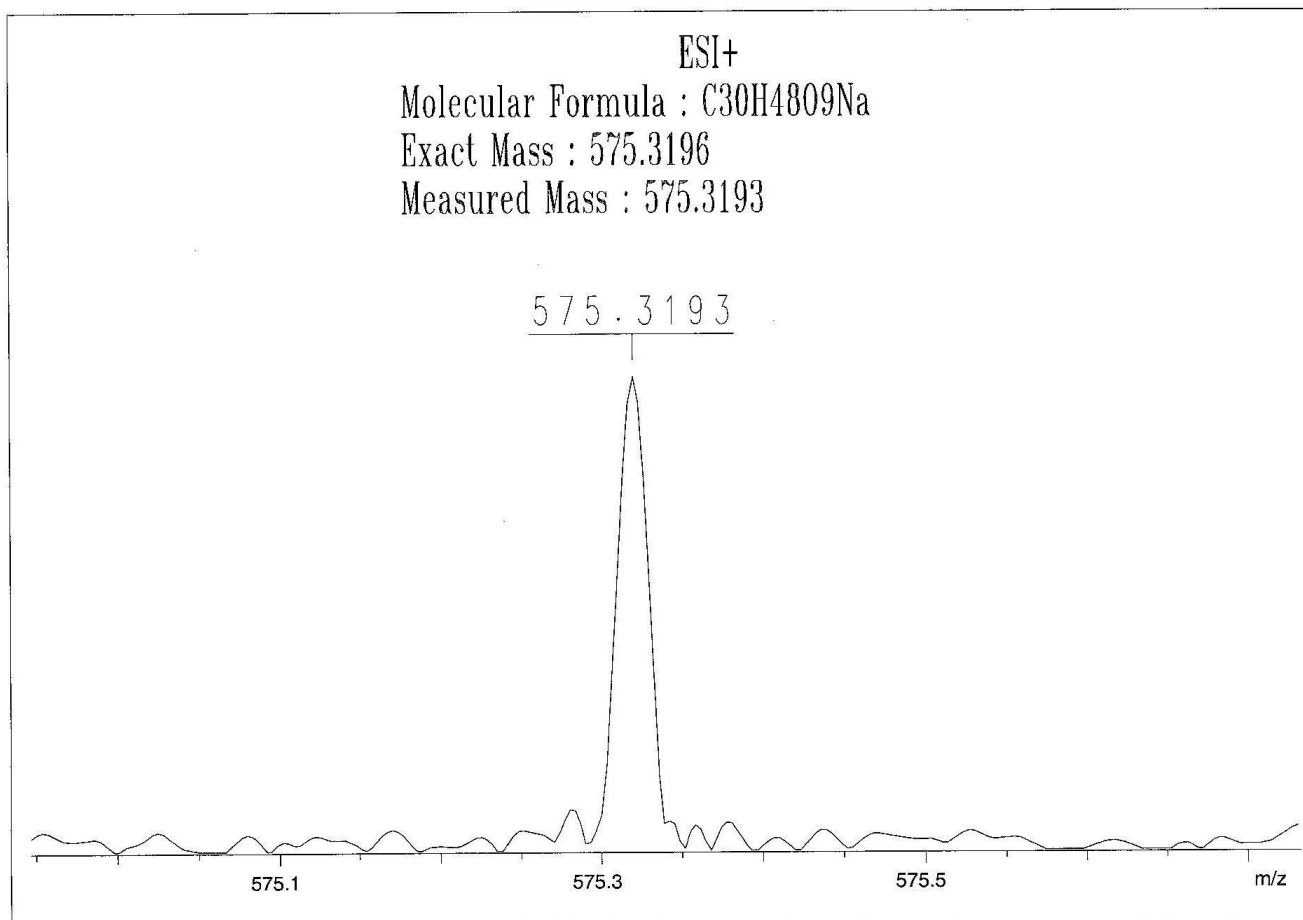
**S10.** HRESIMS spectrum of **3**.



**S11.** <sup>1</sup>H NMR spectrum of **4** in CDCl<sub>3</sub> at 400 MHz.

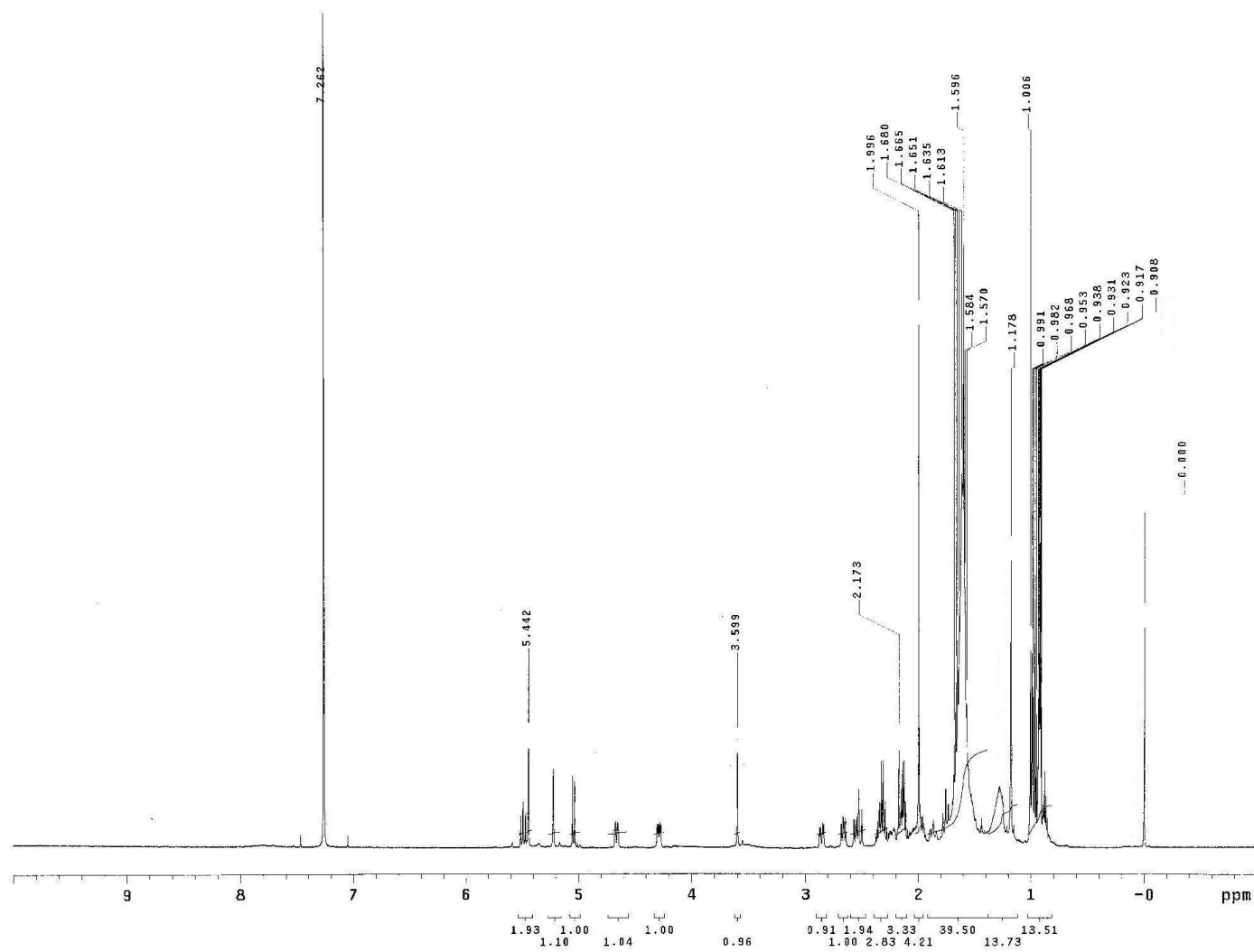


**S12.** <sup>13</sup>C NMR spectrum of **4** in CDCl<sub>3</sub> at 100 MHz.

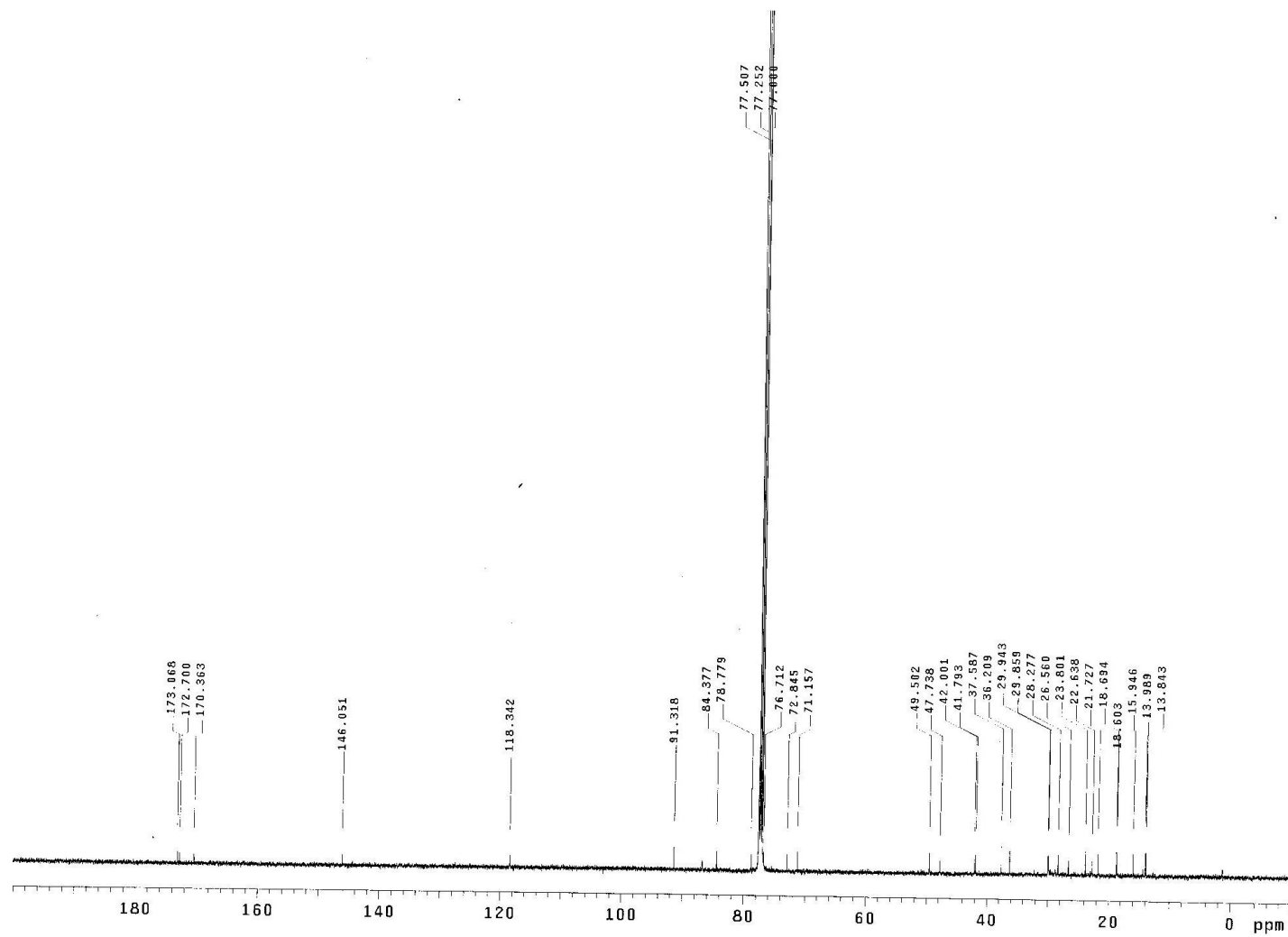


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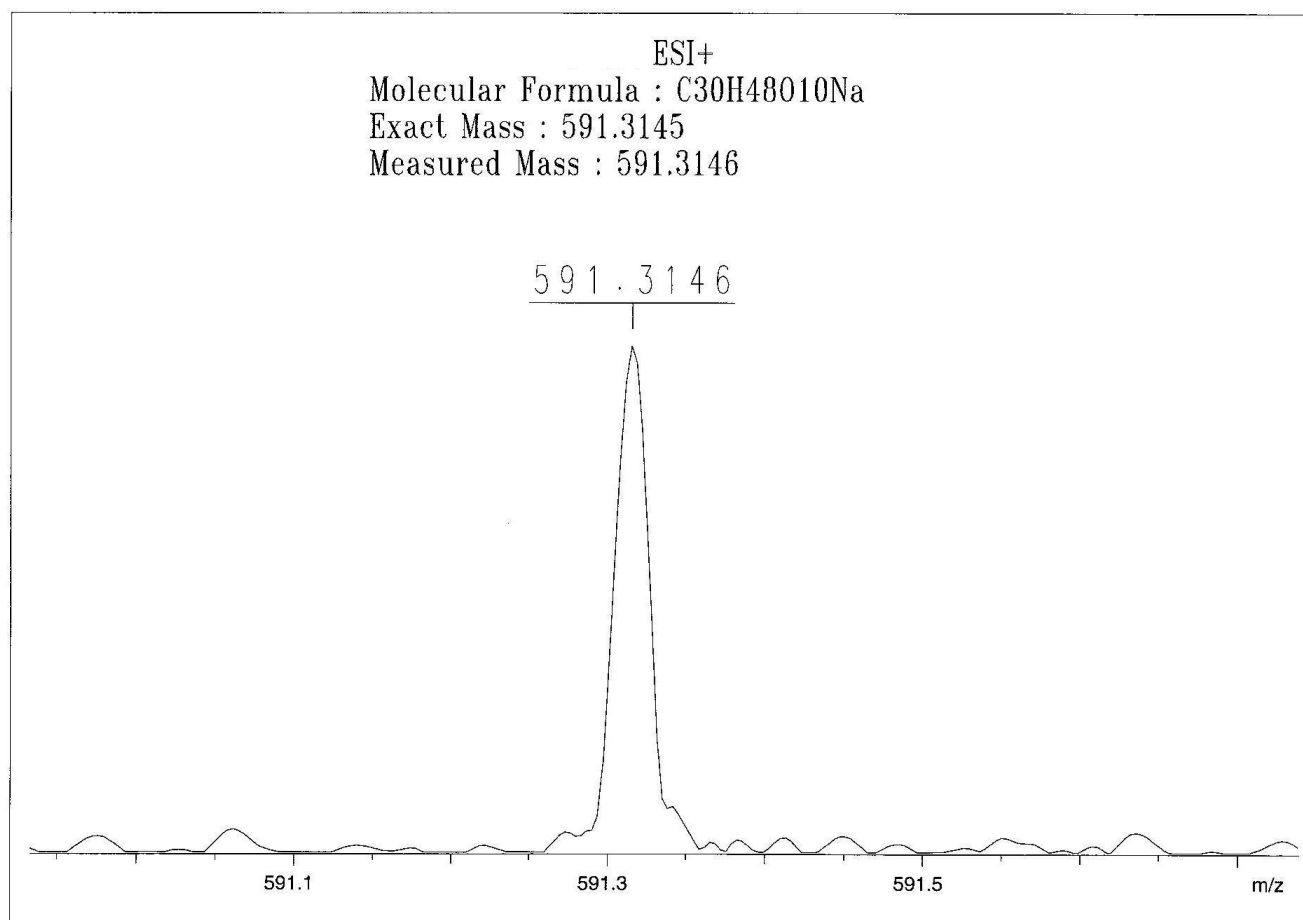
**S13** HRESIMS spectrum of **4**.



**S14.** <sup>1</sup>H NMR spectrum of **5** in CDCl<sub>3</sub> at 500 MHz.

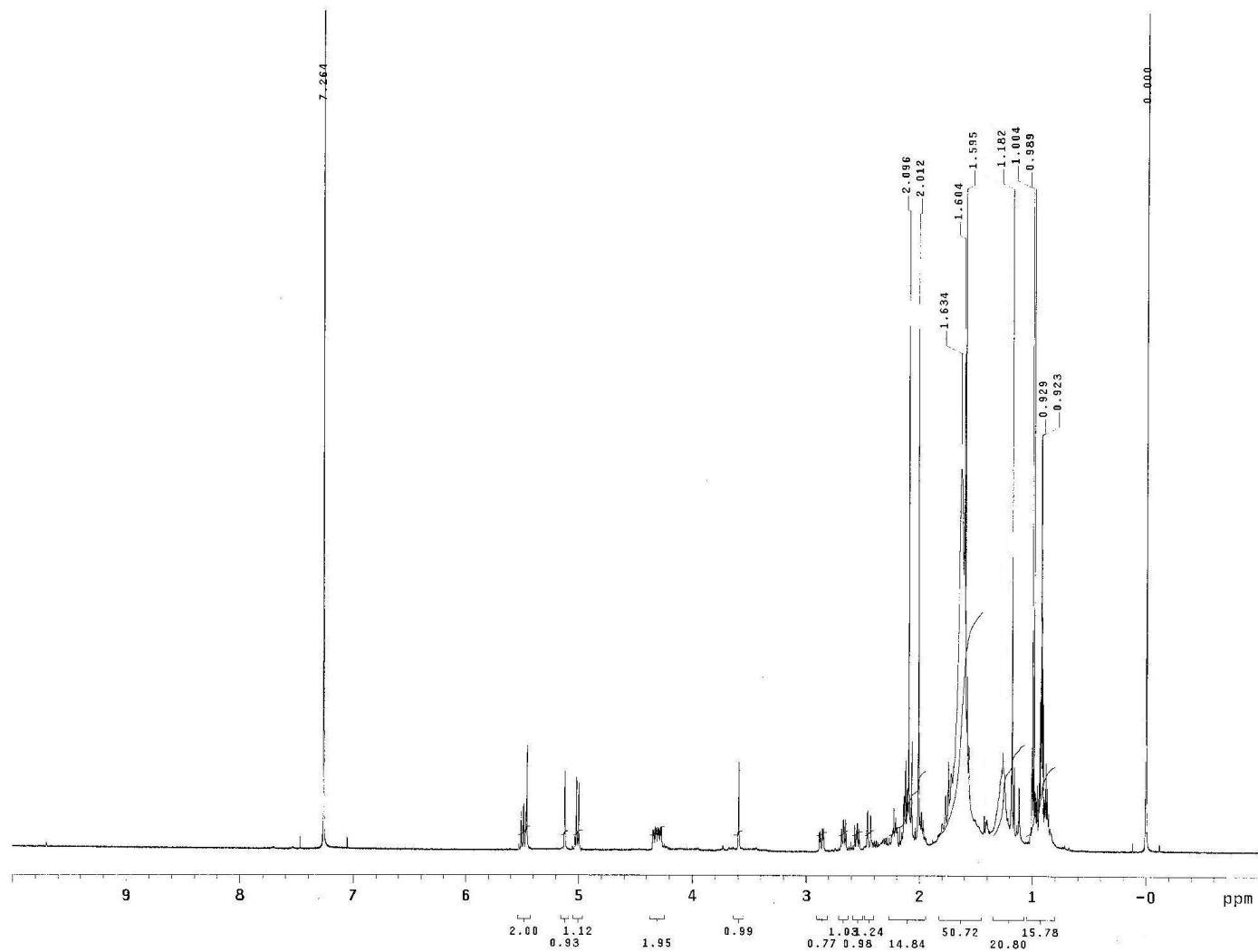


S15. <sup>13</sup>C NMR spectrum of **5** in CDCl<sub>3</sub> at 125 MHz.

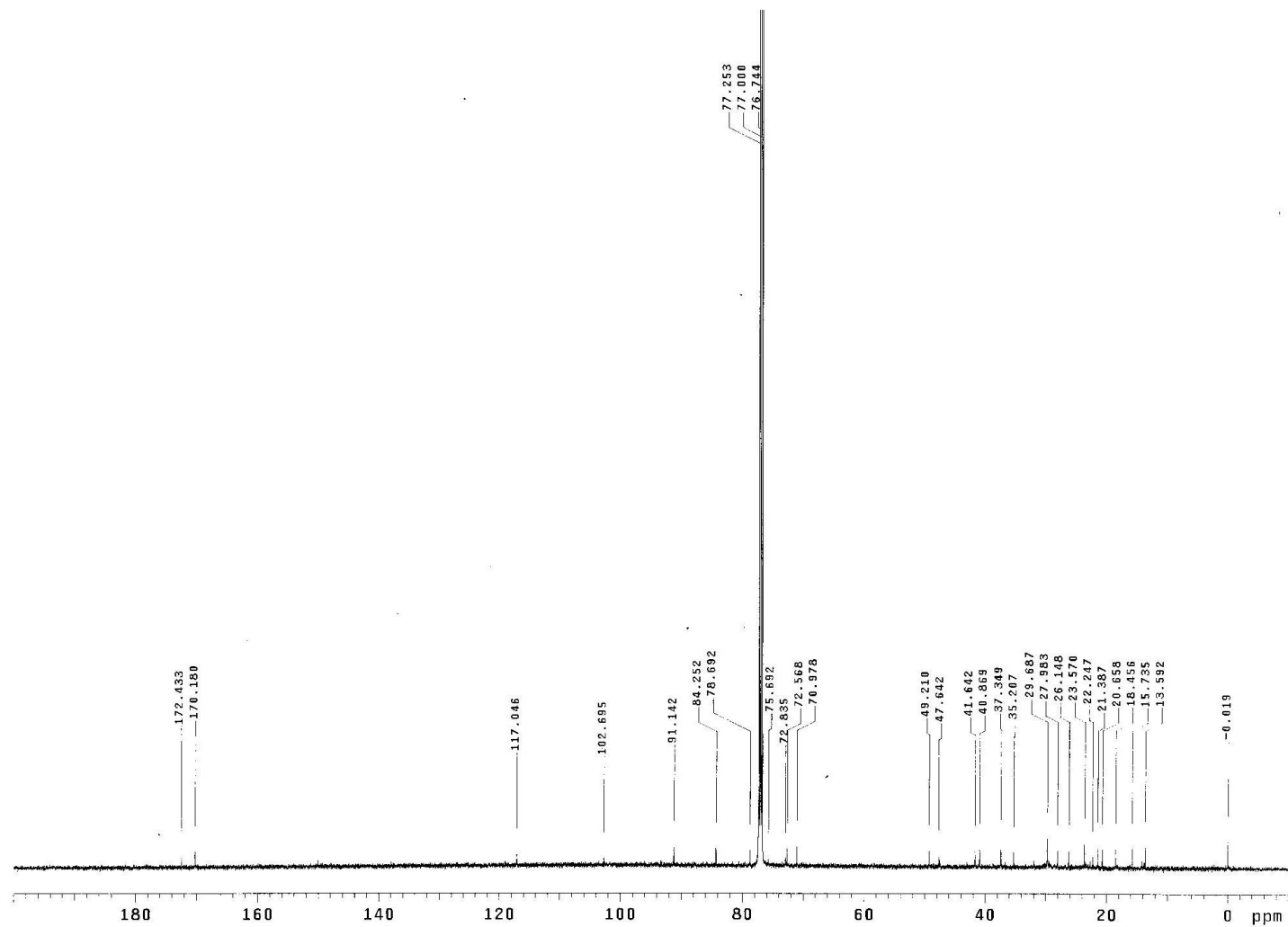


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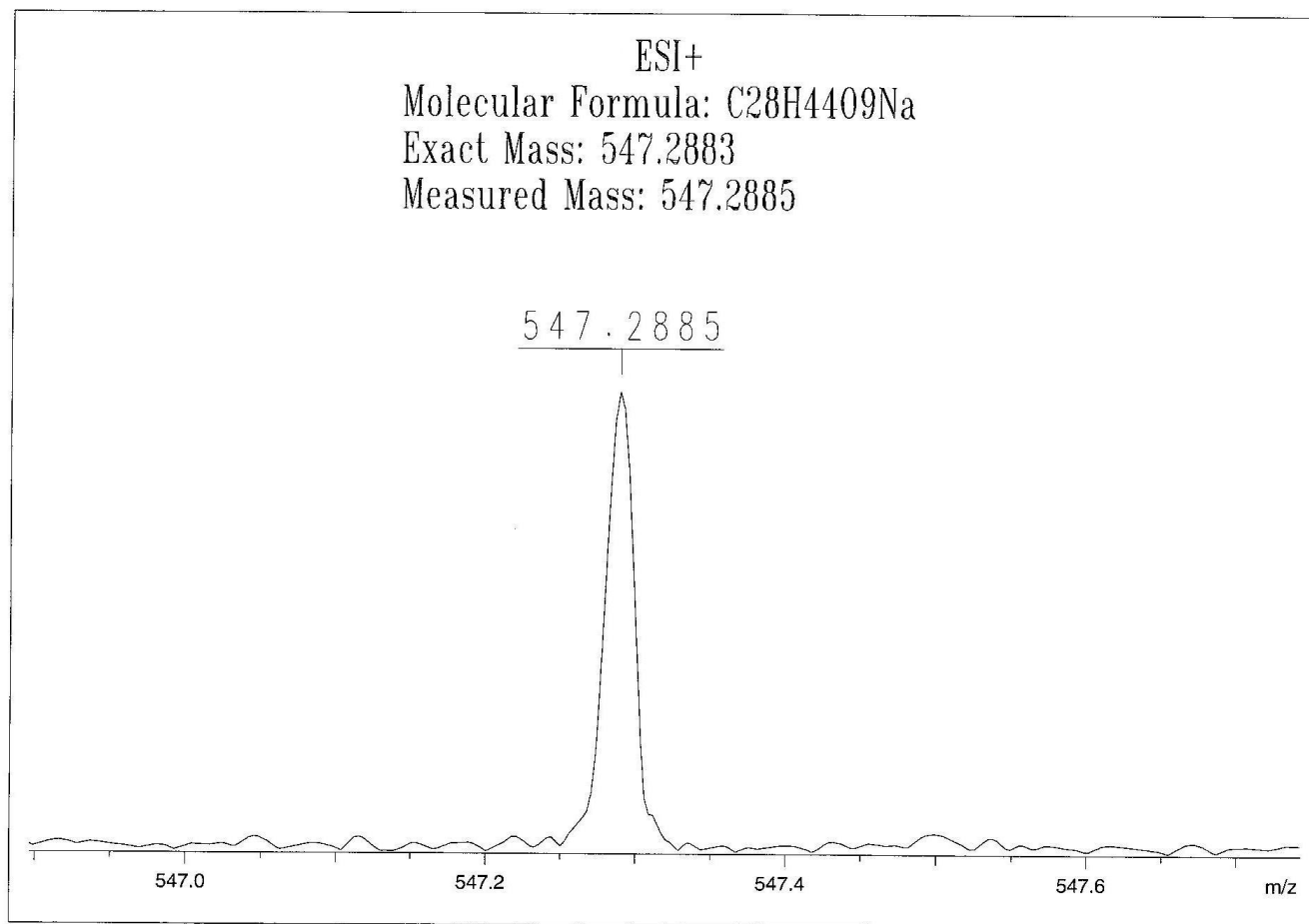
**S15** HRESIMS spectrum of **5**.



**S16.**  $^1\text{H}$  NMR spectrum of **6** in  $\text{CDCl}_3$  at 500 MHz.

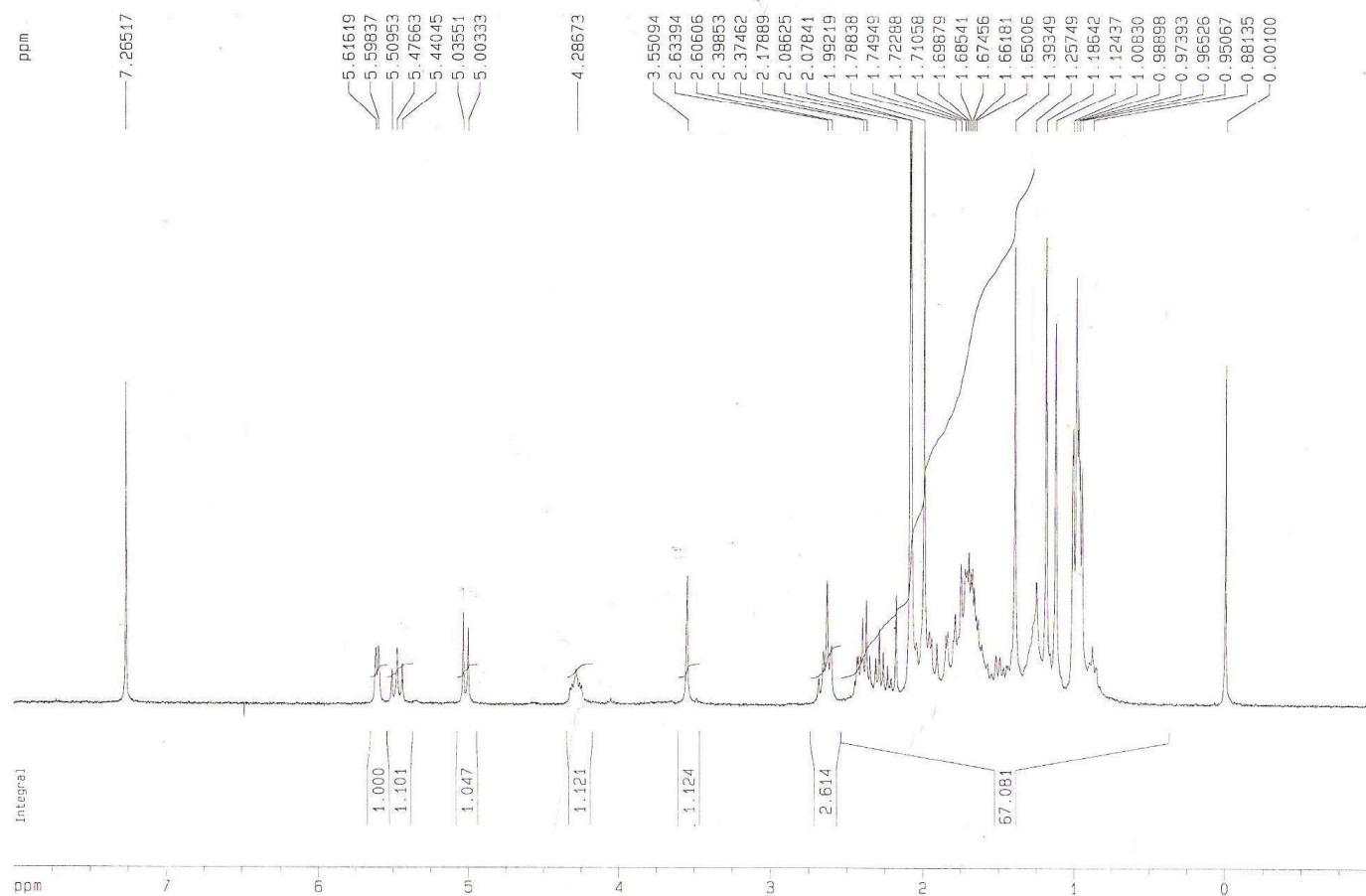


S17. <sup>13</sup>C NMR spectrum of **6** in CDCl<sub>3</sub> at 125 MHz.

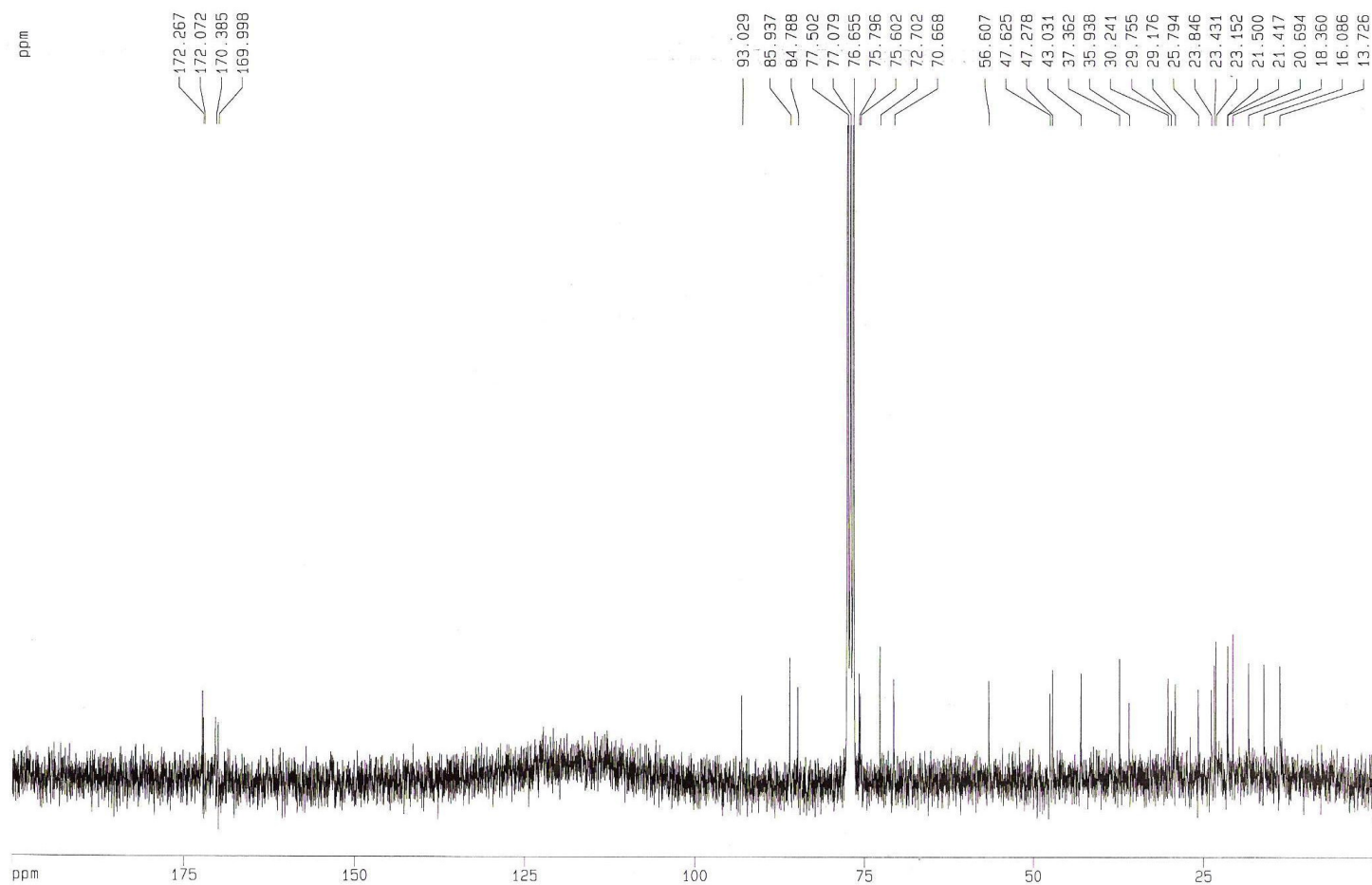


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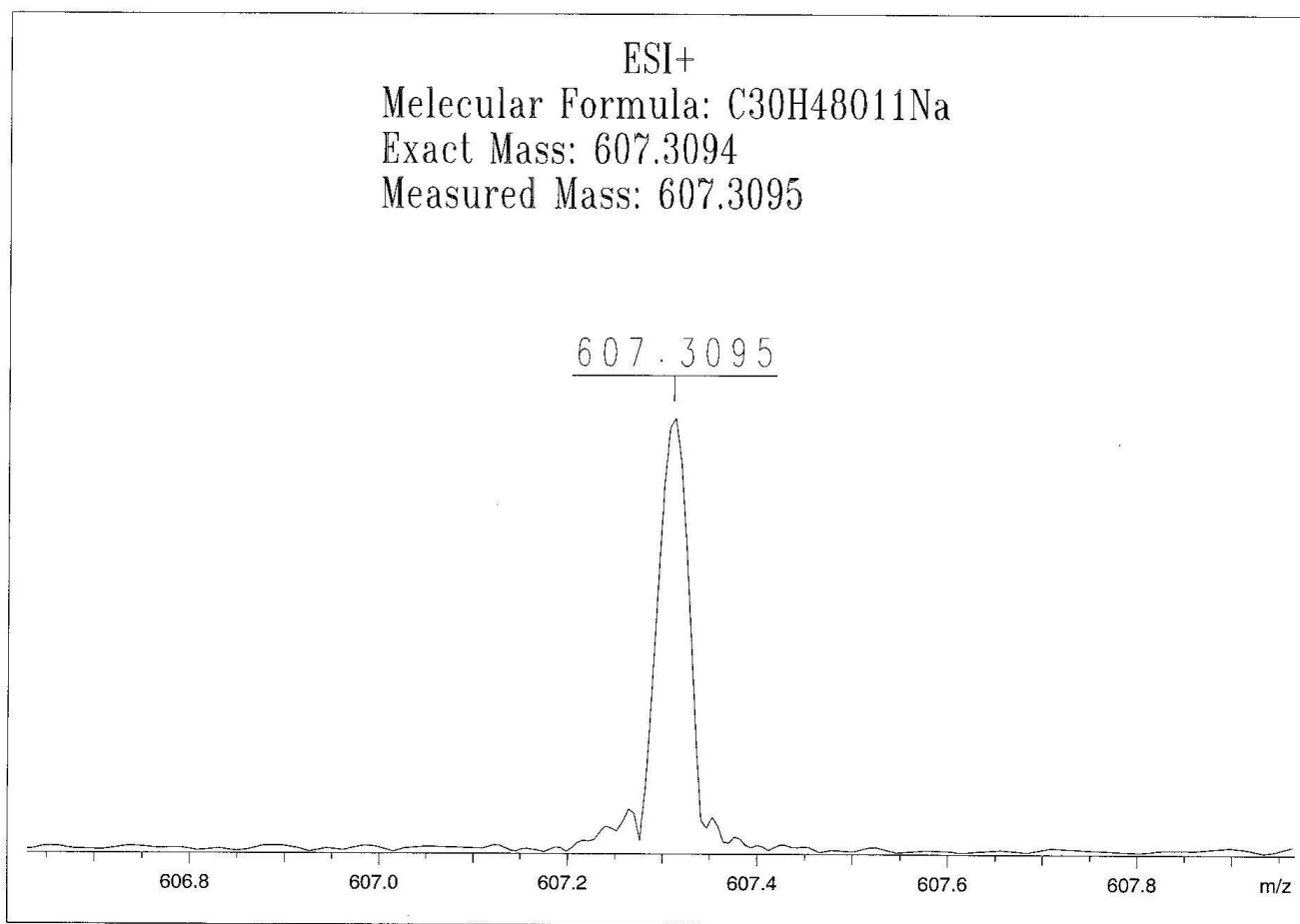
**S18 HRESIMS spectrum of 6.**



**S19.**  $^1\text{H}$  NMR spectrum of **7** in  $\text{CDCl}_3$  at 300 MHz.

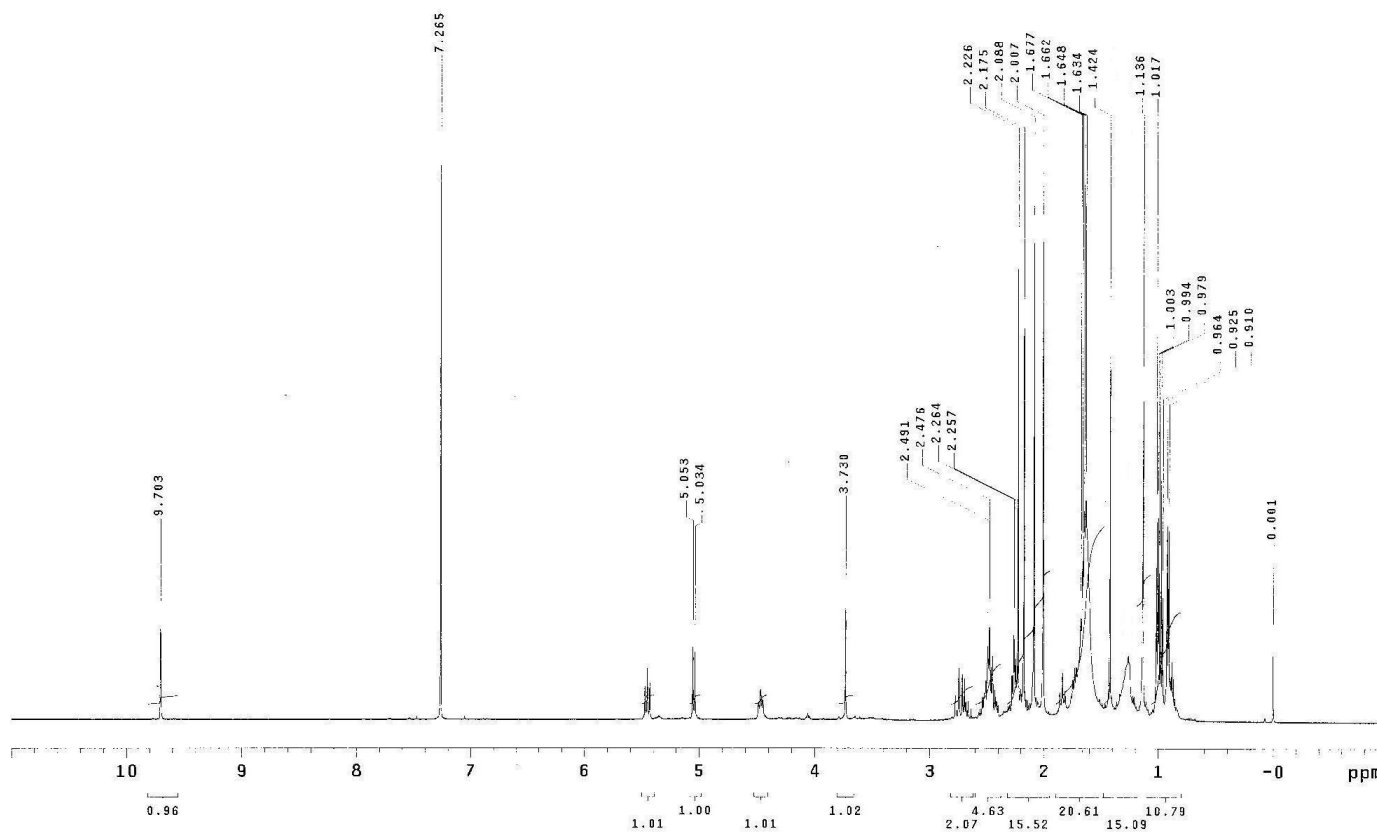


**S20.**  $^{13}\text{C}$  NMR spectrum of **7** in  $\text{CDCl}_3$  at 75 MHz.

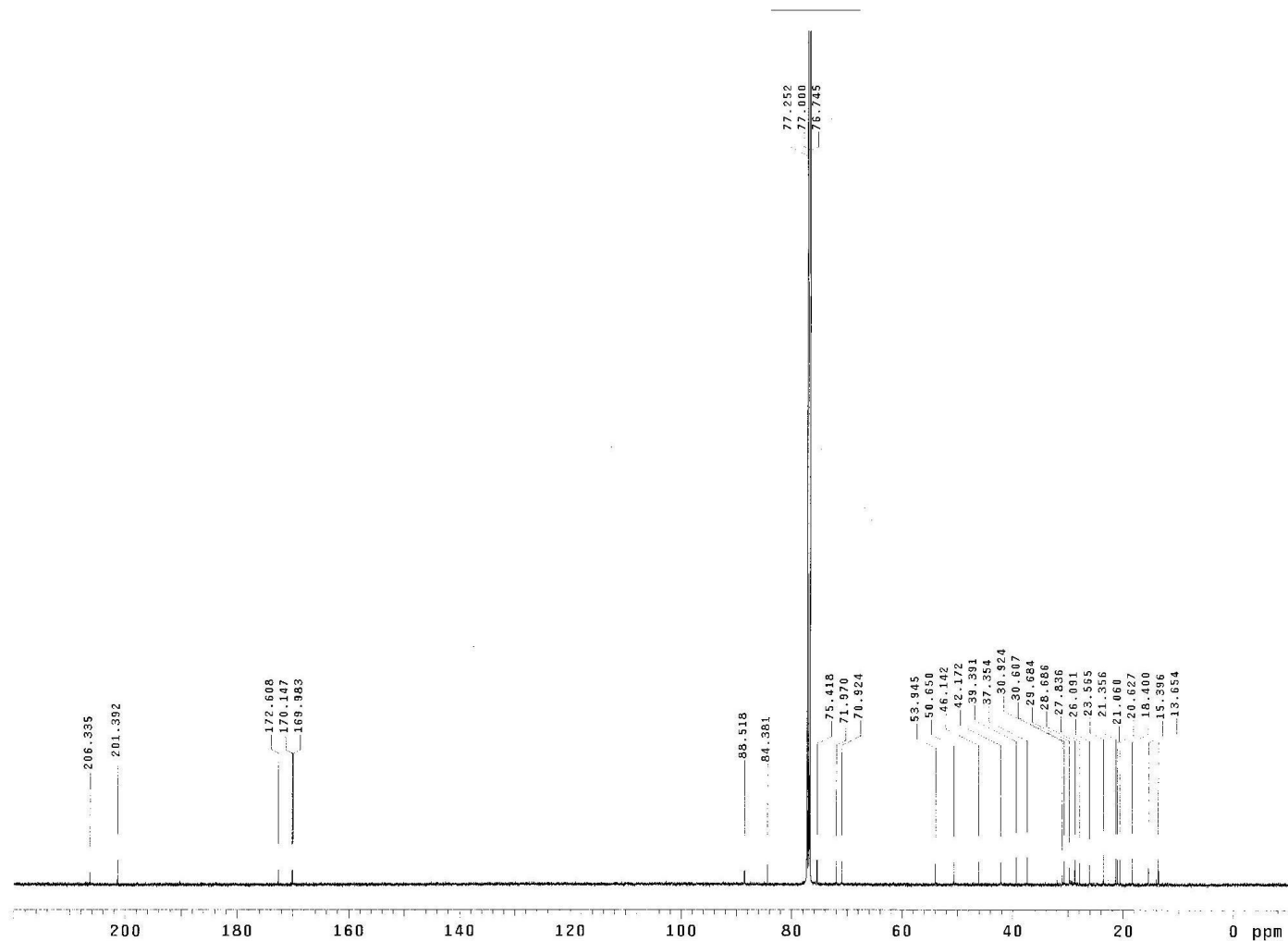


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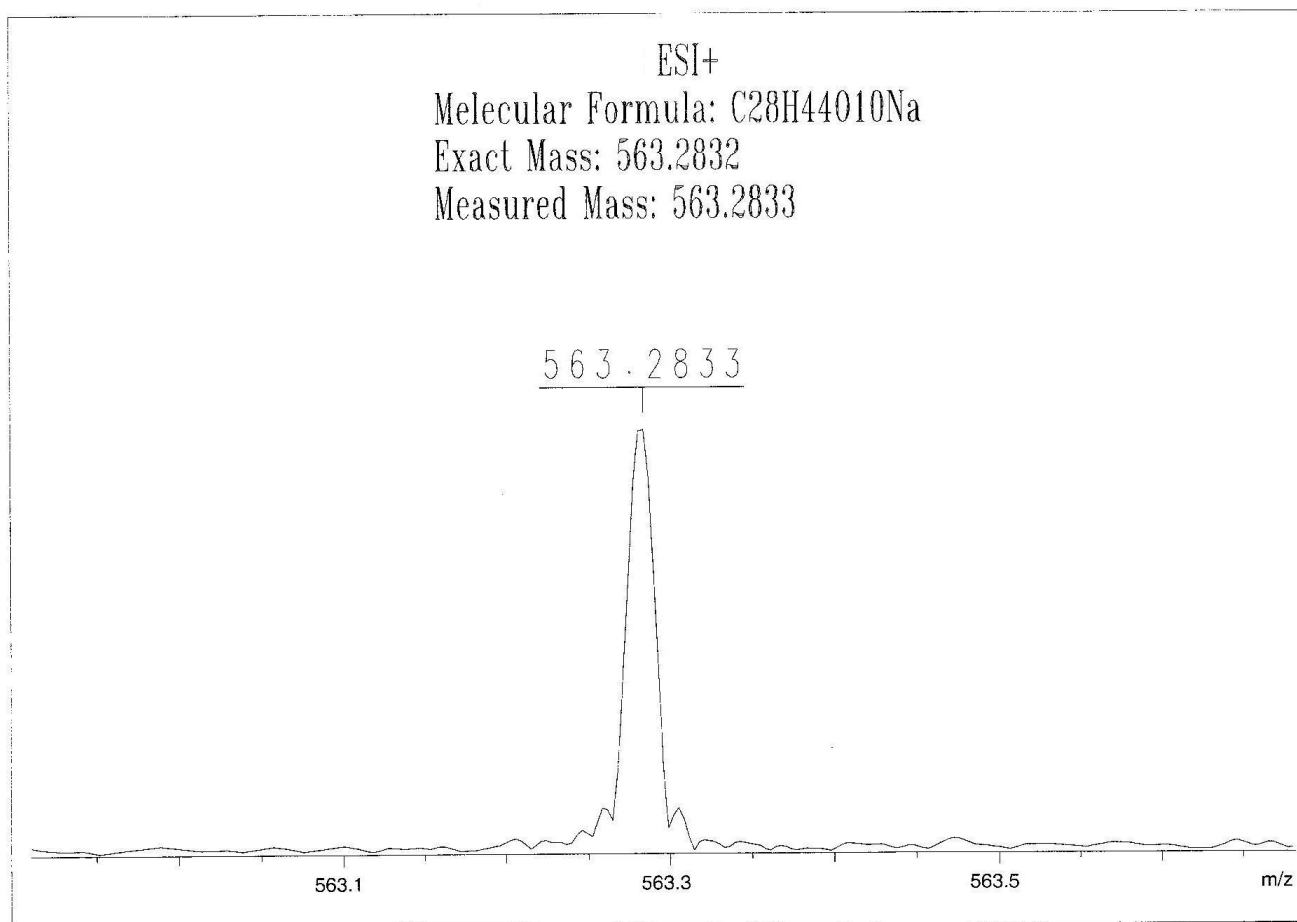
**S21** HRESIMS spectrum of **7**.



S22. <sup>13</sup>C NMR spectrum of **8** in CDCl<sub>3</sub> at 500 MHz.

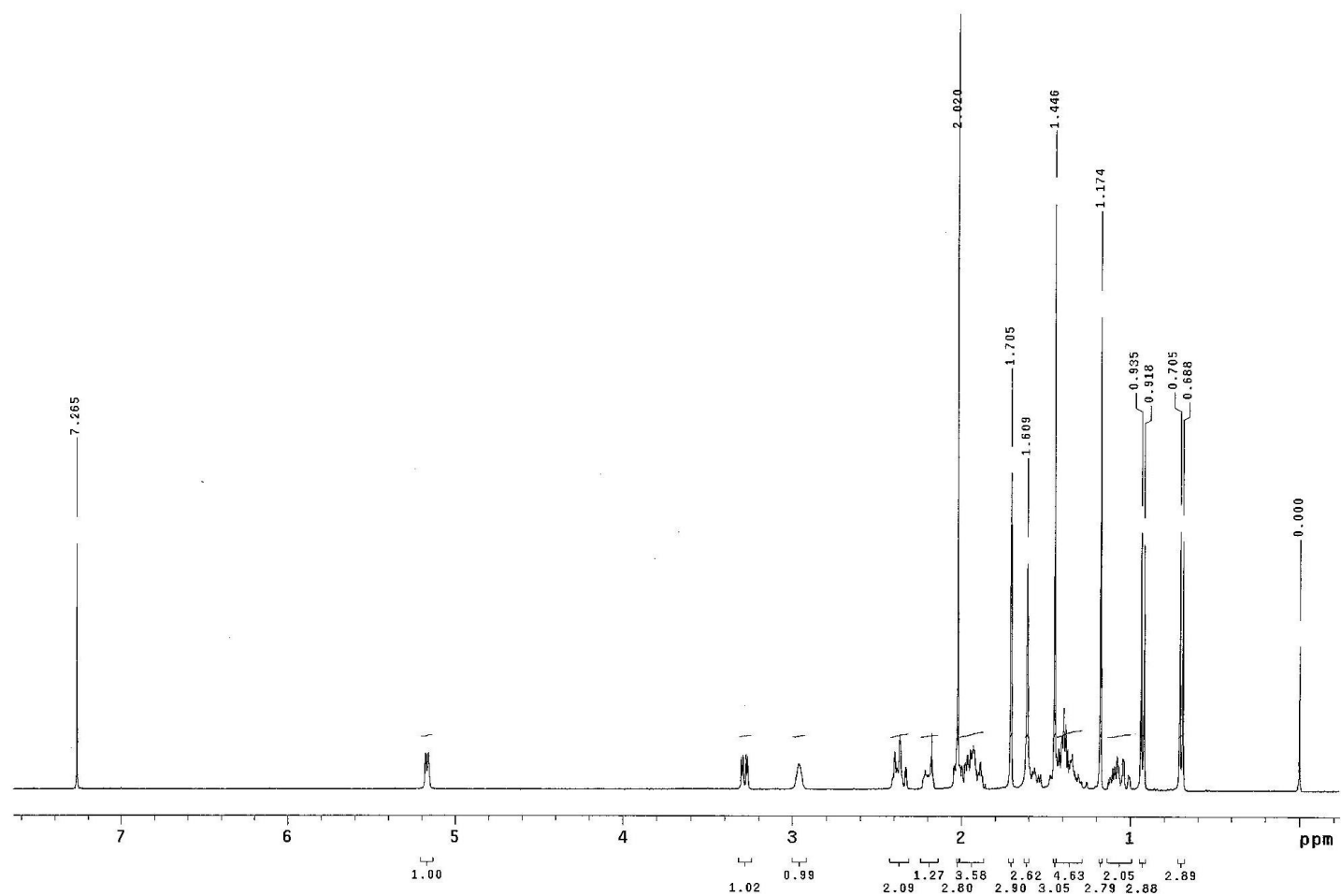


**S23.** <sup>13</sup>C NMR spectrum of **8** in CDCl<sub>3</sub> at 125 MHz.

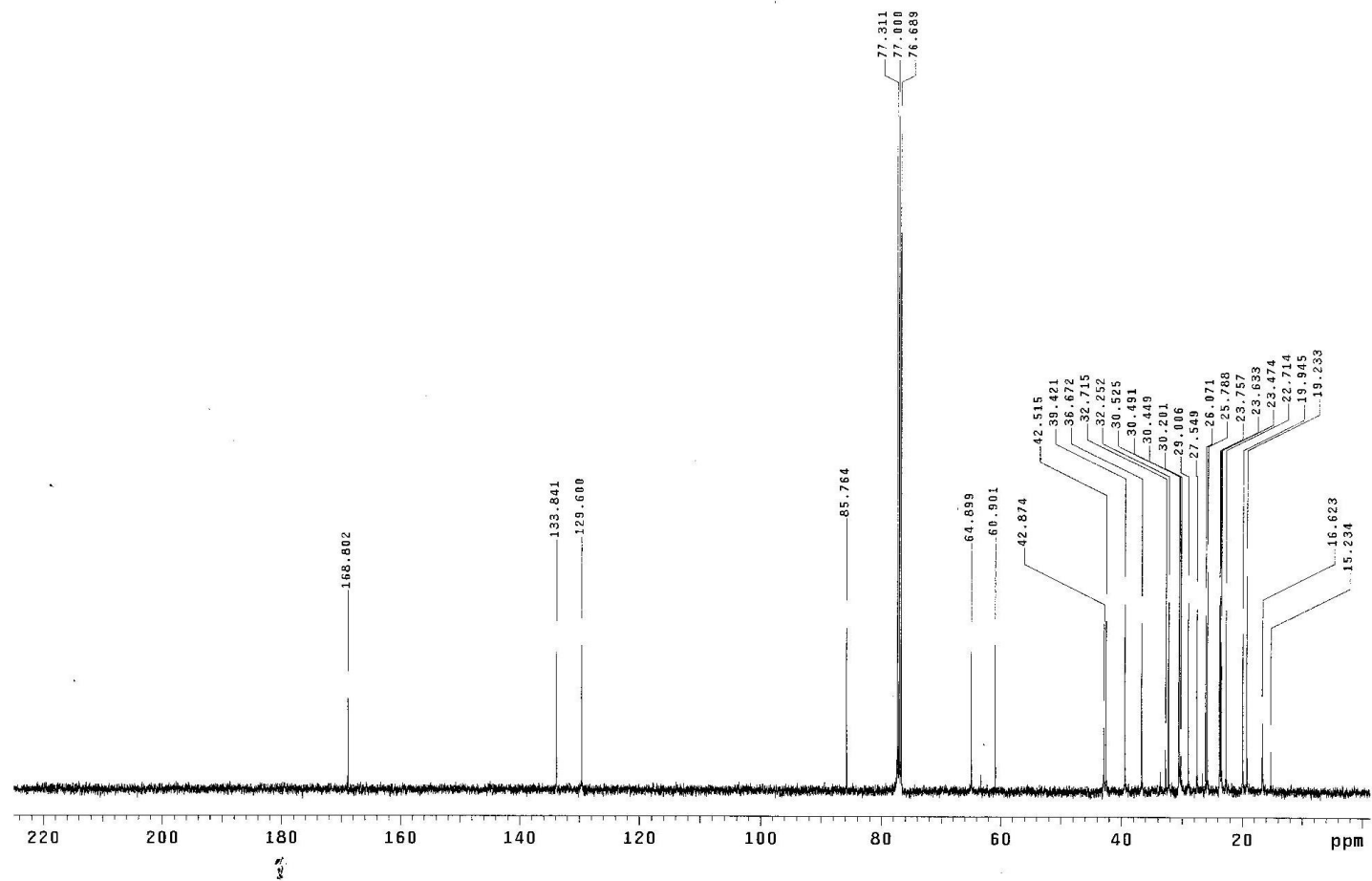


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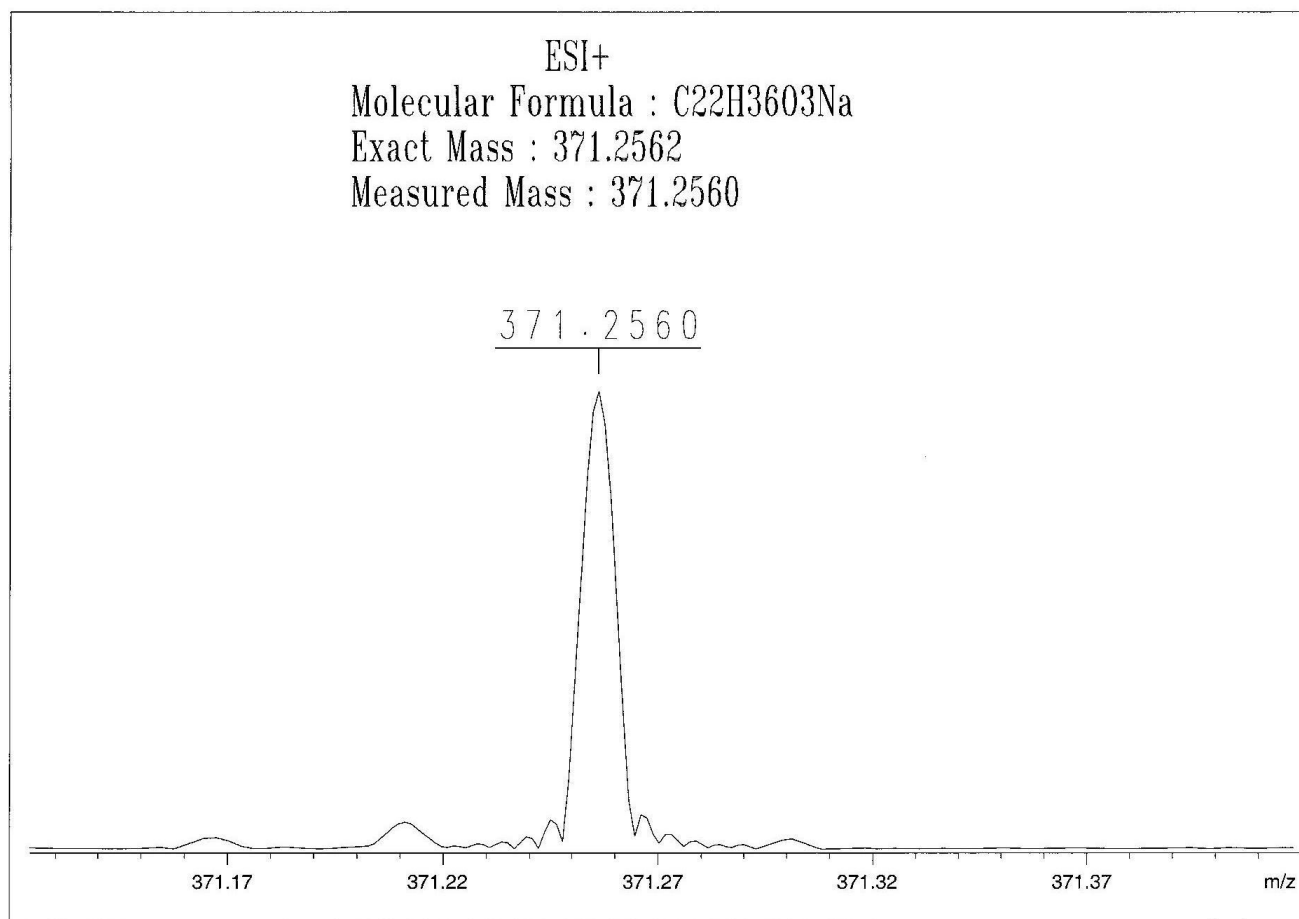
**S24** HRESIMS spectrum of **8**.



S25. <sup>13</sup>C NMR spectrum of **9** in CDCl<sub>3</sub> at 400 MHz.

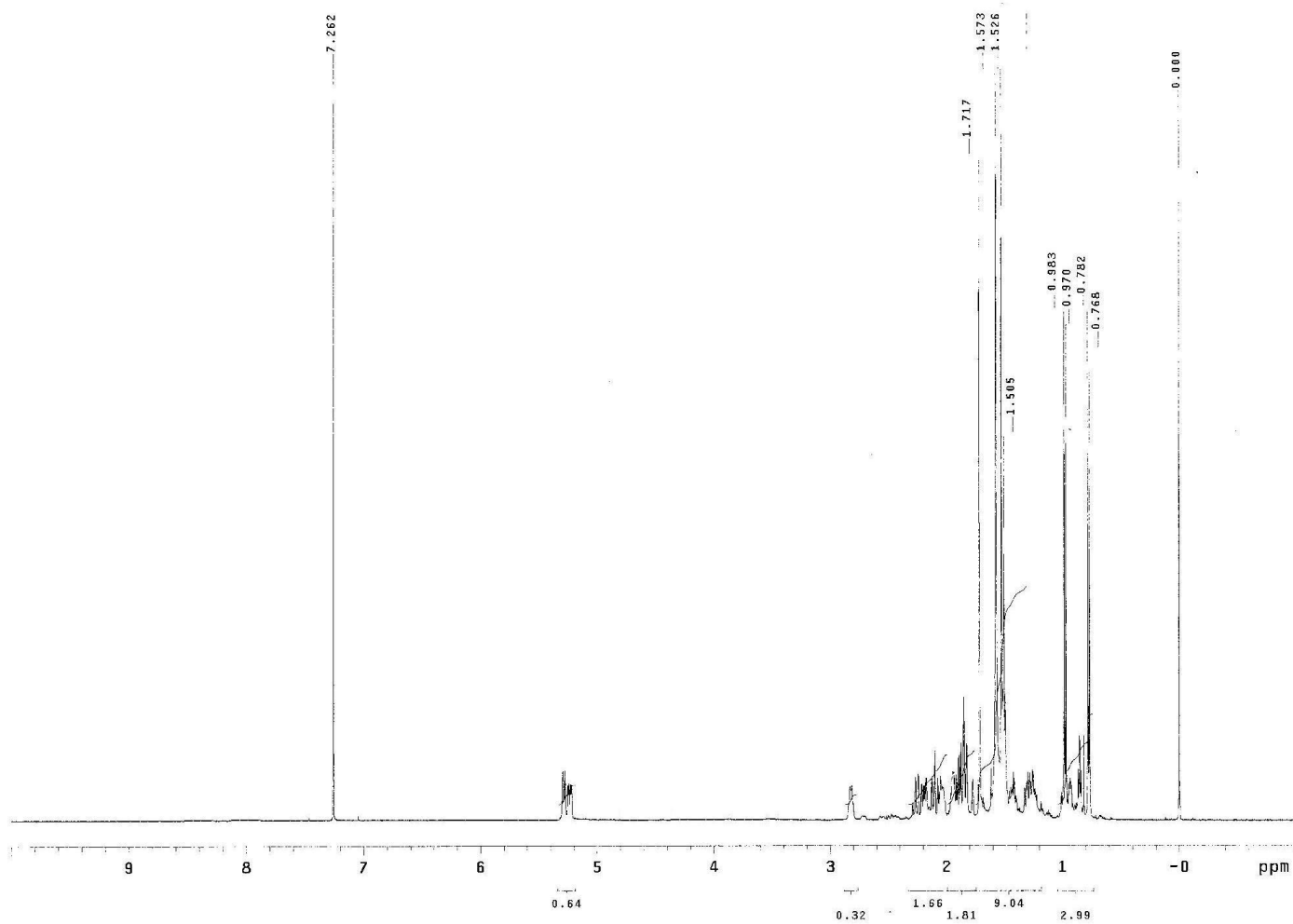


S26. <sup>13</sup>C NMR spectrum of **9** in CDCl<sub>3</sub> at 100 MHz.

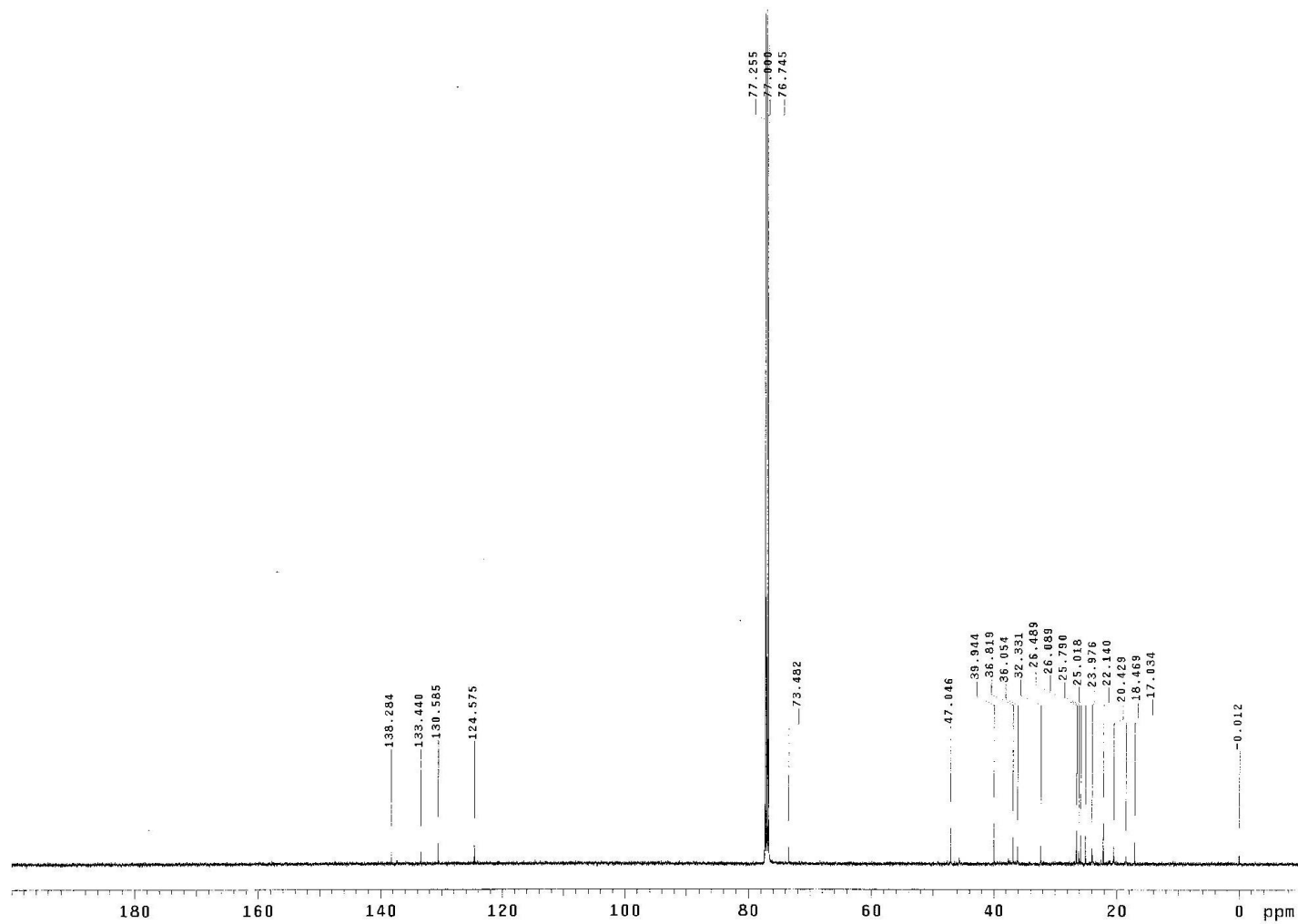


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**S27** HRESIMS spectrum of **9**.

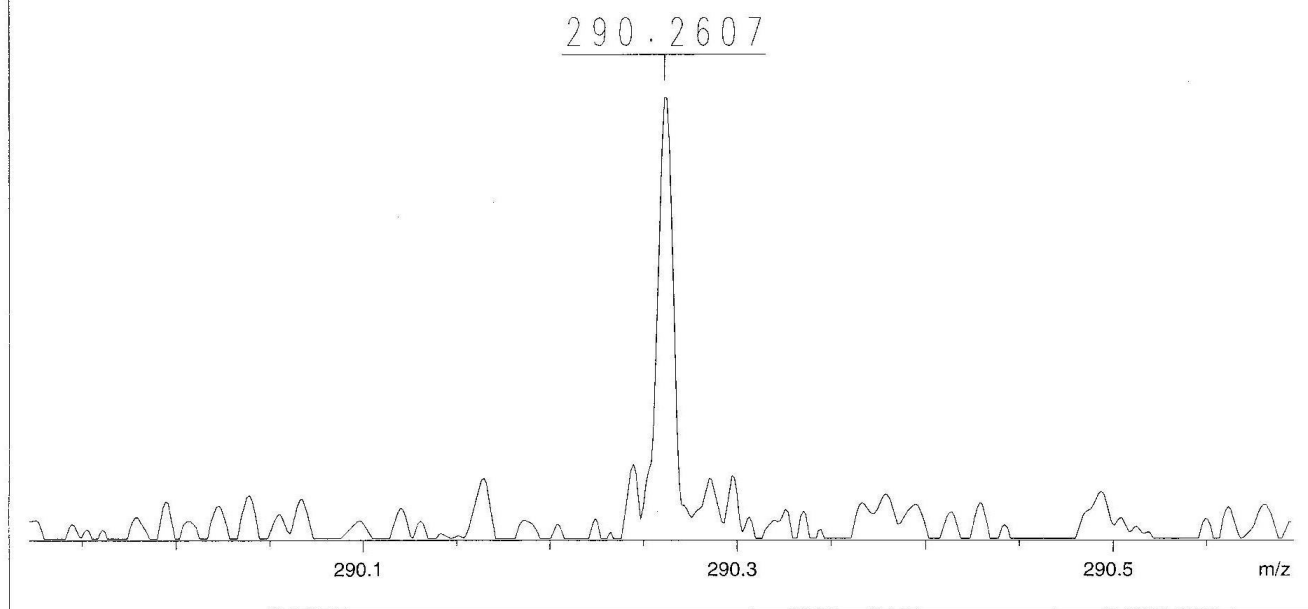


**S28.** <sup>13</sup>C NMR spectrum of **10** in CDCl<sub>3</sub> at 500 MHz.



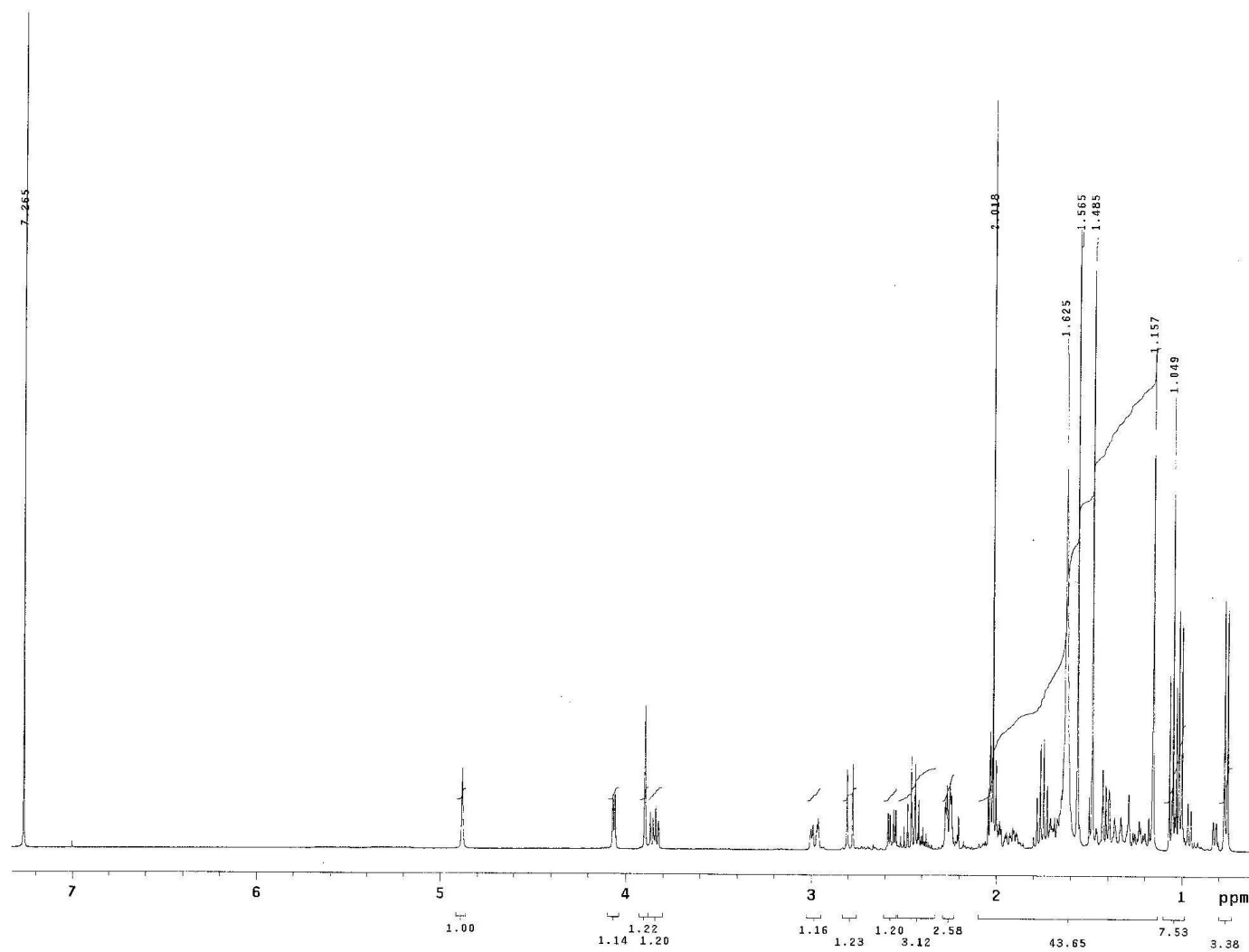
**S29.** <sup>13</sup>C NMR spectrum of **10** in CDCl<sub>3</sub> at 125 MHz.

El+  
Molecular Formula: C<sub>20</sub>H<sub>34</sub>O  
Exact Mass: 290.2610  
Measured Mass: 290.2607

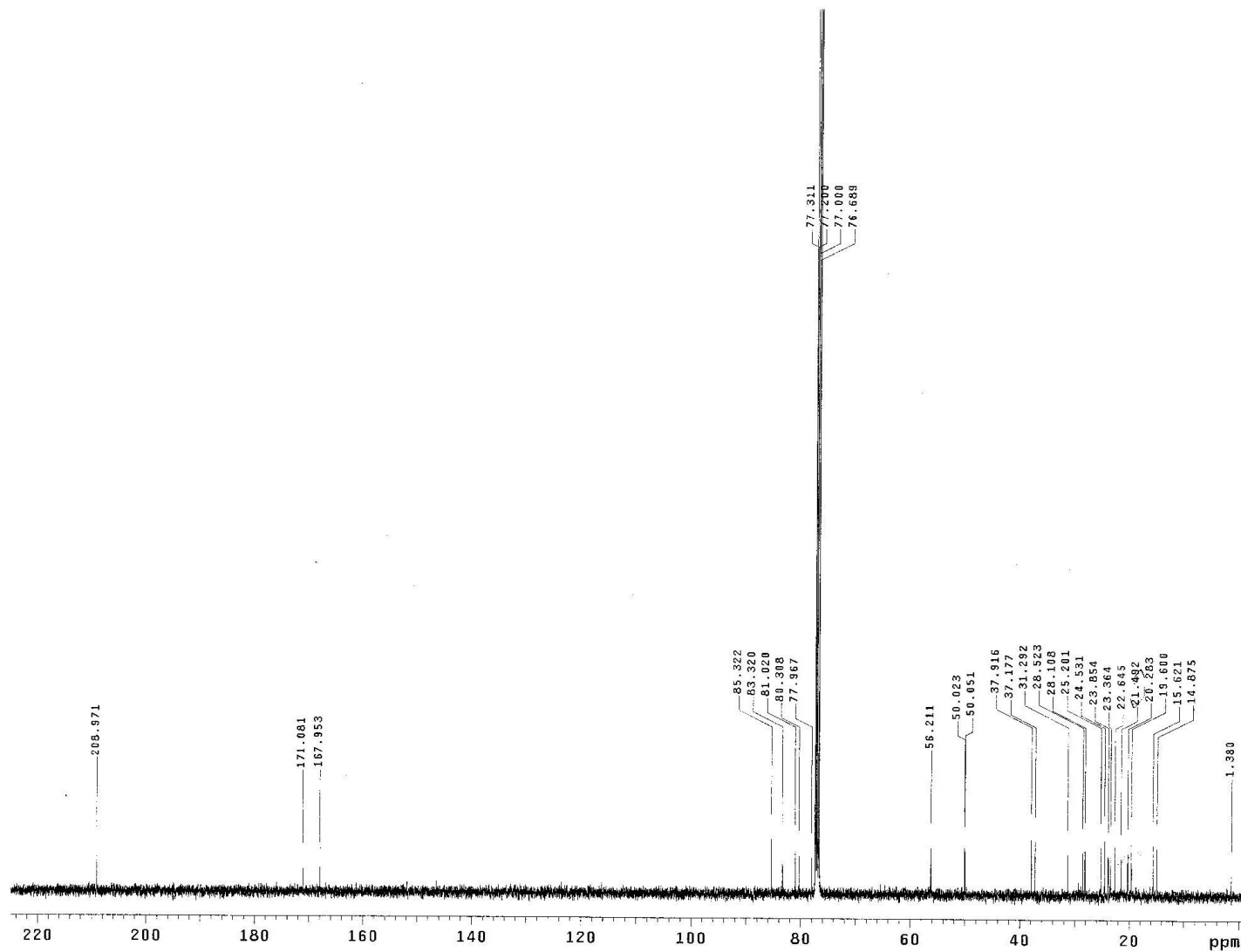


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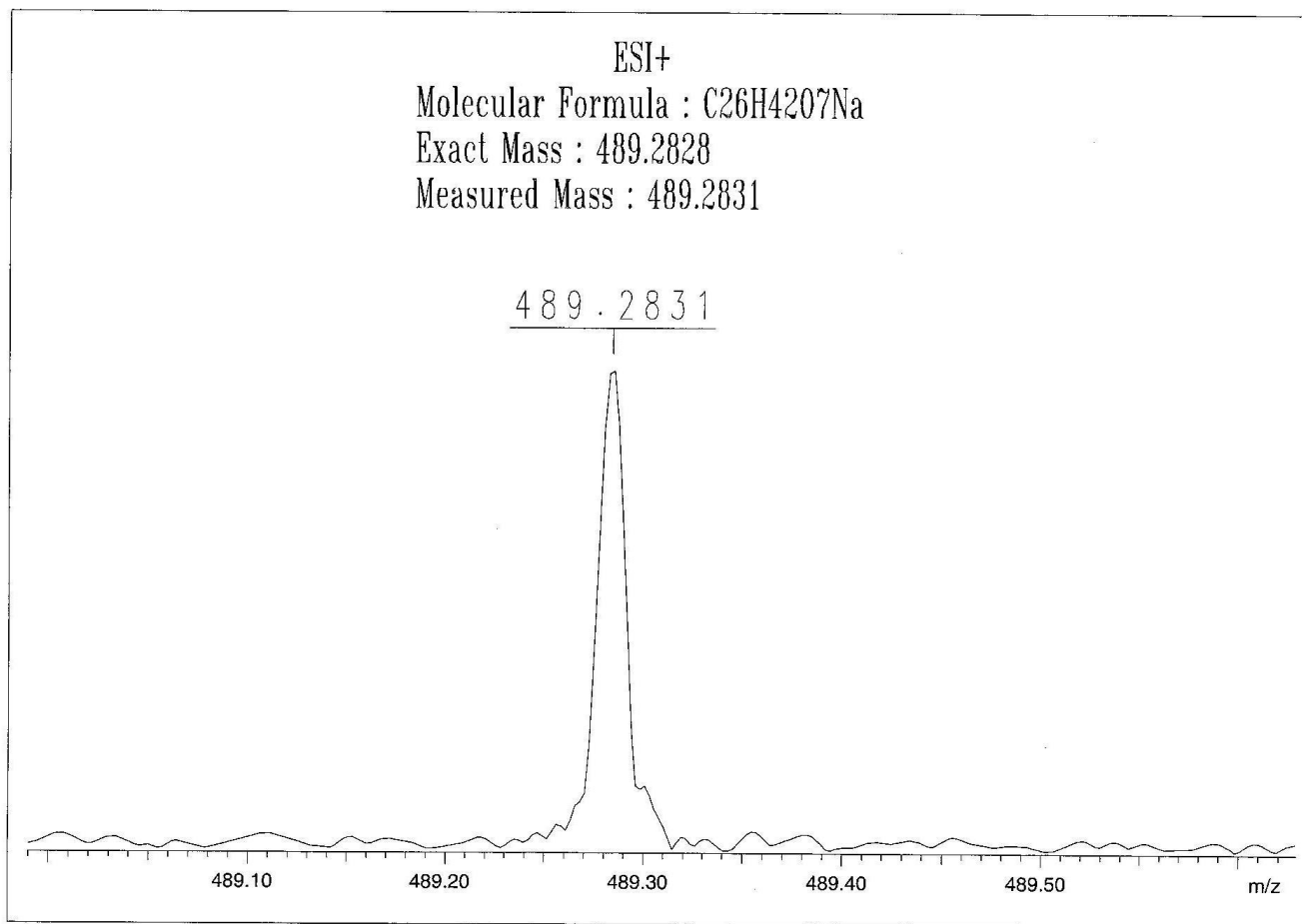
**S30 HRESIMS spectrum of 10.**



**S31.**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$  at 400 MHz.

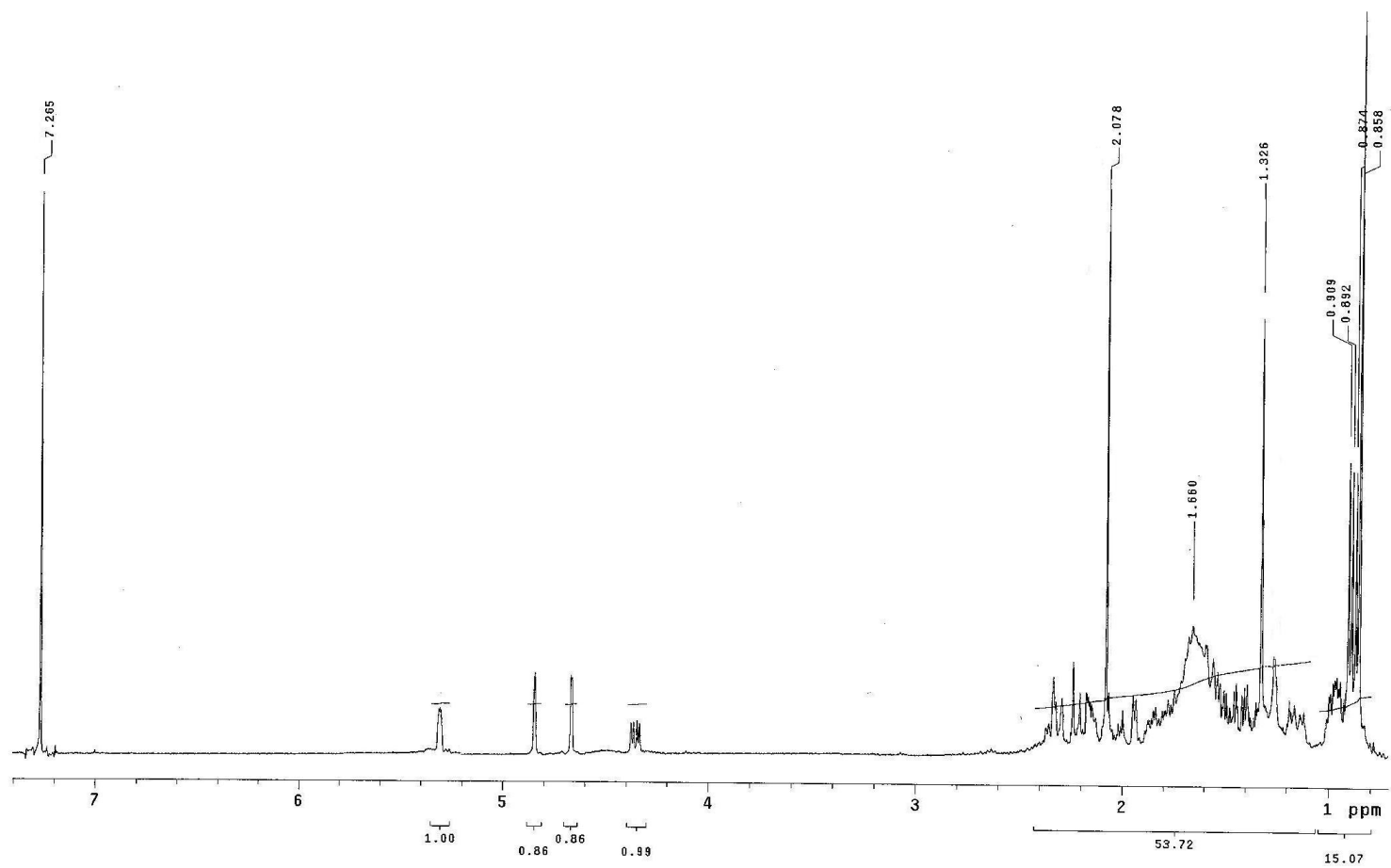


**S32.** <sup>13</sup>C NMR spectrum of **11** in CDCl<sub>3</sub> at 100 MHz.

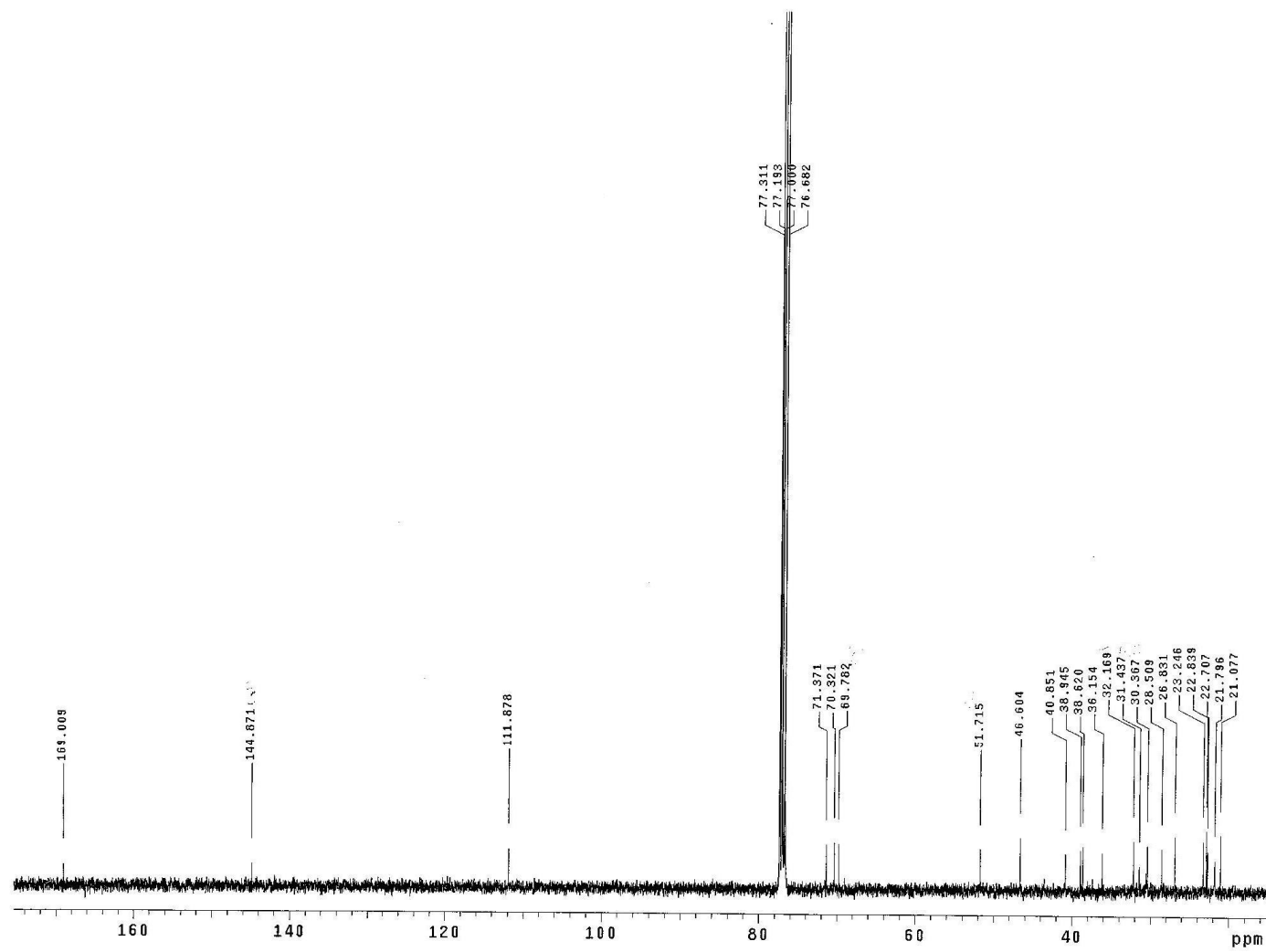


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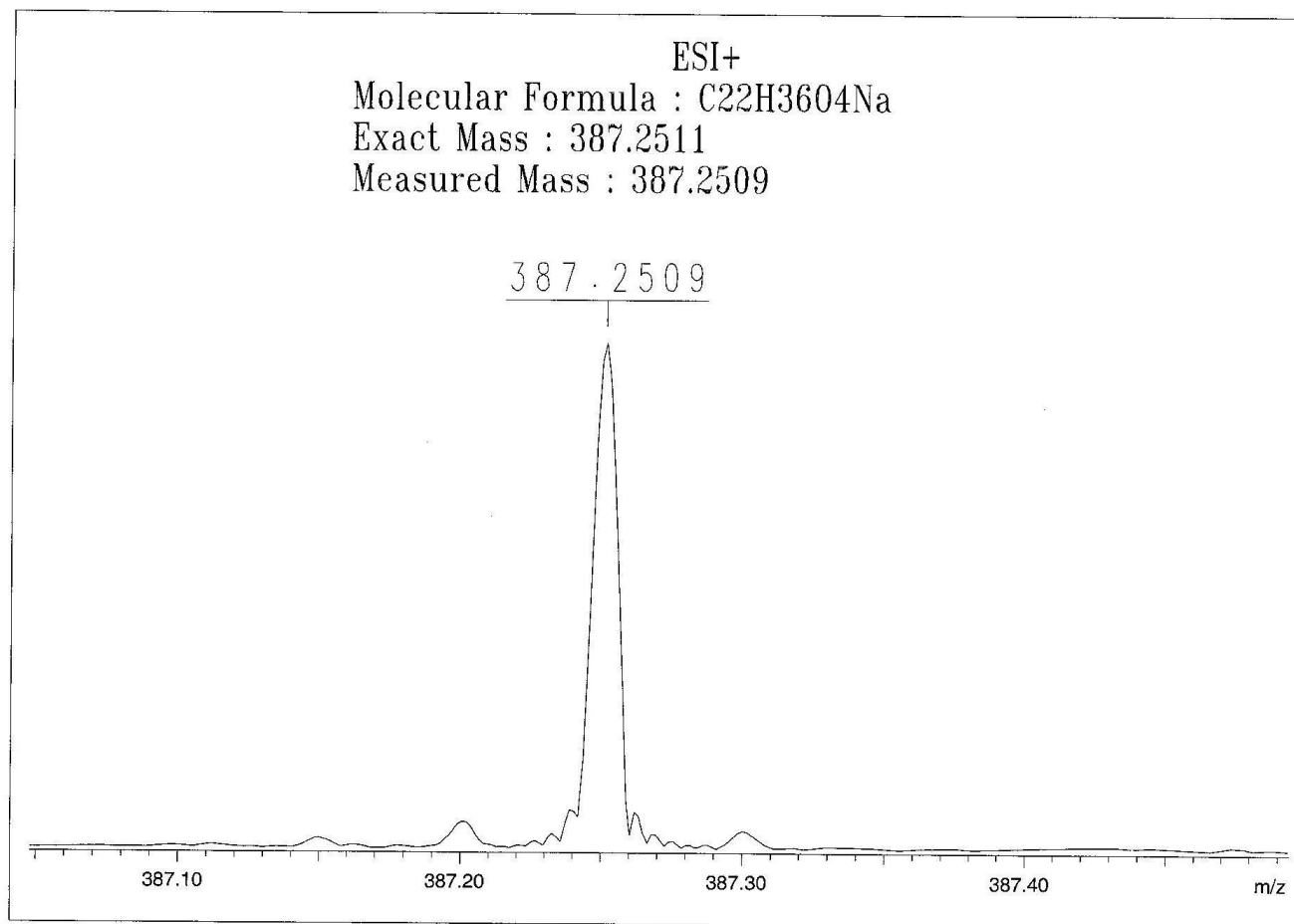
**S33** HRESIMS spectrum of **11**.



**S34.** <sup>13</sup>C NMR spectrum of **12** in CDCl<sub>3</sub> at 400 MHz.



S35. <sup>13</sup>C NMR spectrum of **12** in CDCl<sub>3</sub> at 100 MHz.



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**S36 HRESIMS spectrum of 12.**