

## SUPPORTING INFORMATION (1)

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

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## **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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**S8.**  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at 400 MHz.

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**S12.**  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{CDCl}_3$  at 100 MHz.

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

**S13.**  $^1\text{H}$  NMR spectrum of **5** in  $\text{CDCl}_3$  at 500 MHz.

**S14.**  $^{13}\text{C}$  NMR spectrum of **5** in  $\text{CDCl}_3$  at 125 MHz.

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

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

**S17.**  $^{13}\text{C}$  NMR spectrum of **6** in  $\text{CDCl}_3$  at 125 MHz.

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**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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**S22.**  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{CDCl}_3$  at 500 MHz.

**S23.**  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{CDCl}_3$  at 125 MHz.

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

**S25.**  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{CDCl}_3$  at 400 MHz.

**S26.**  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{CDCl}_3$  at 100 MHz.

**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.

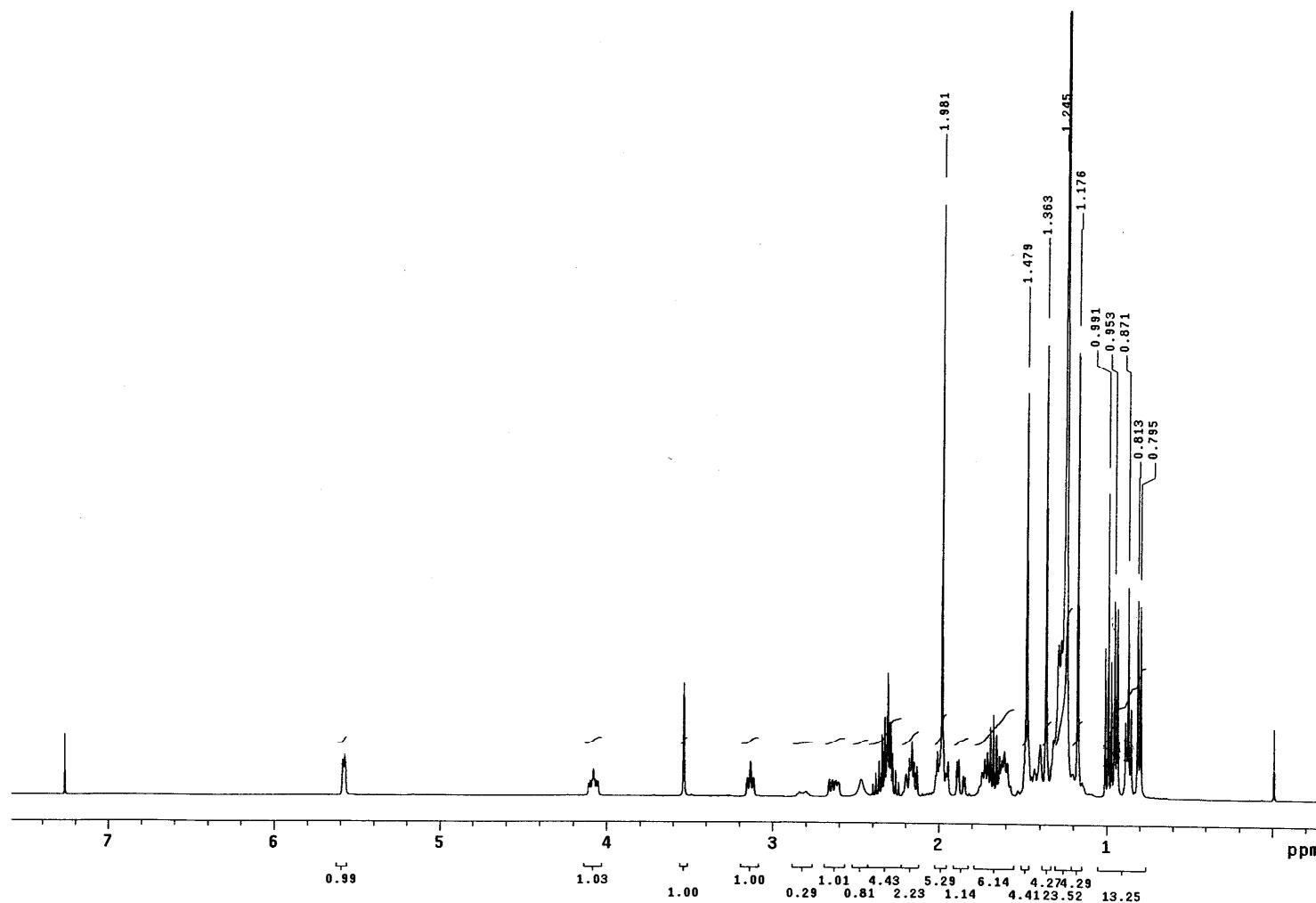
**S32.**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$  at 100 MHz.

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

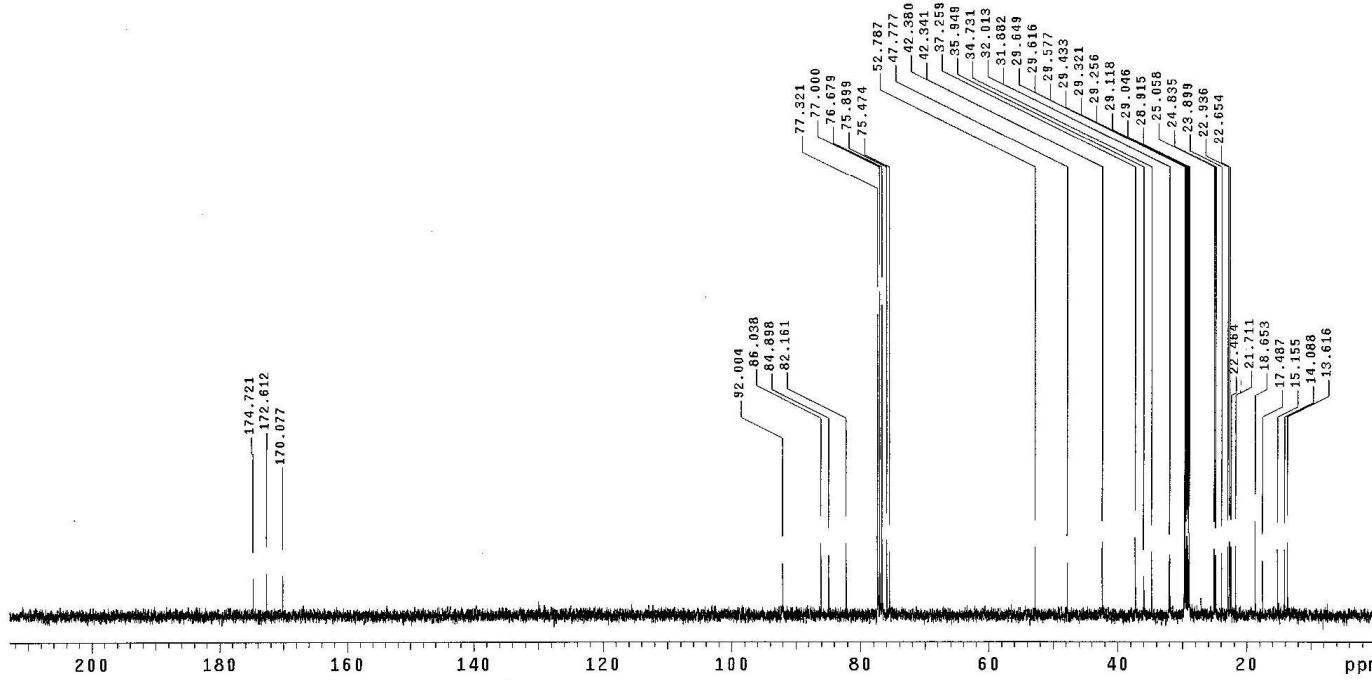
**S34.**  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$  at 400 MHz.

**S35.**  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$  at 100 MHz.

**S36.** HRESIMS spectrum of **12**.

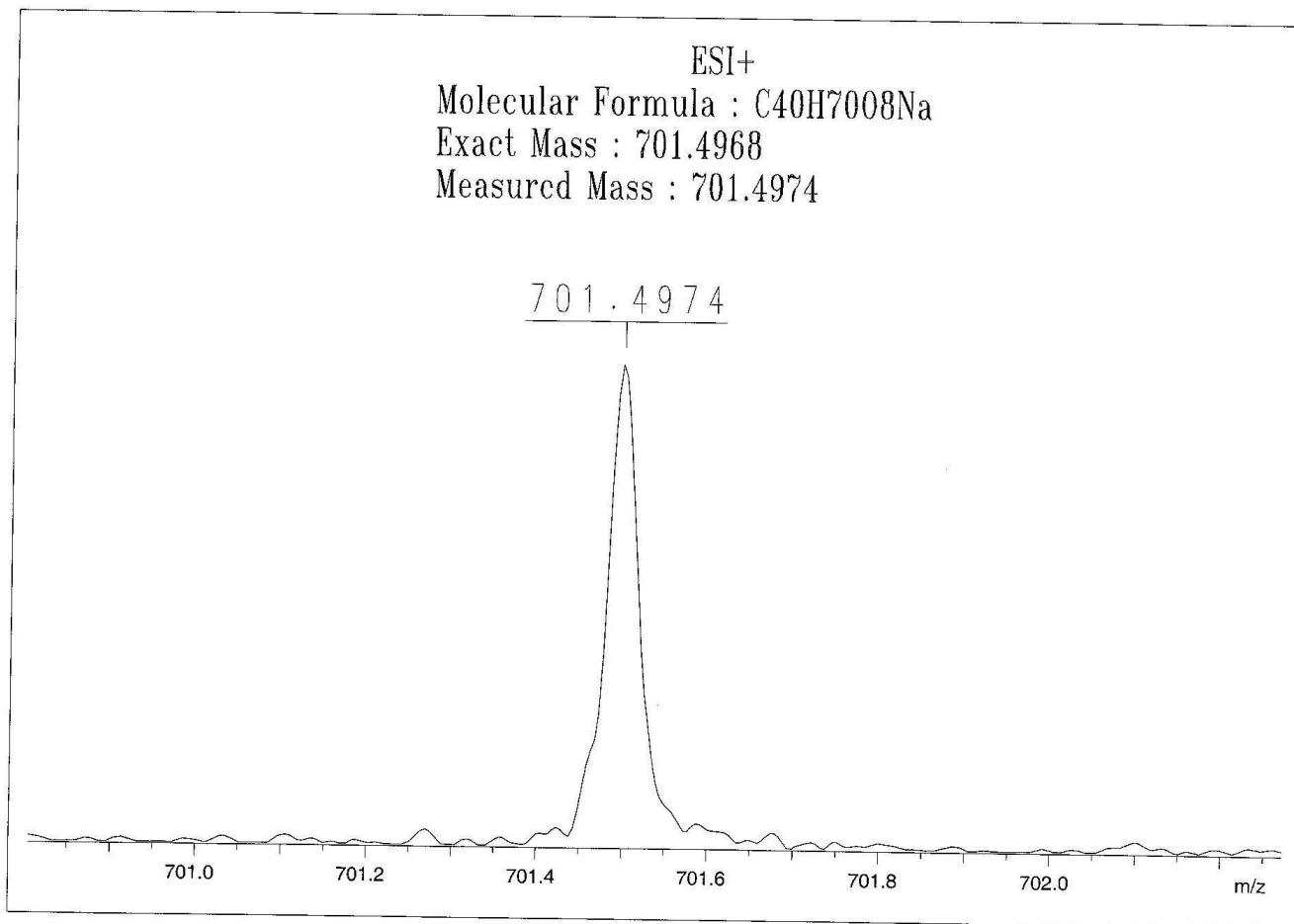


**S2.** <sup>1</sup>H NMR spectrum of **1** in  $\text{CDCl}_3$  at 400 MHz.



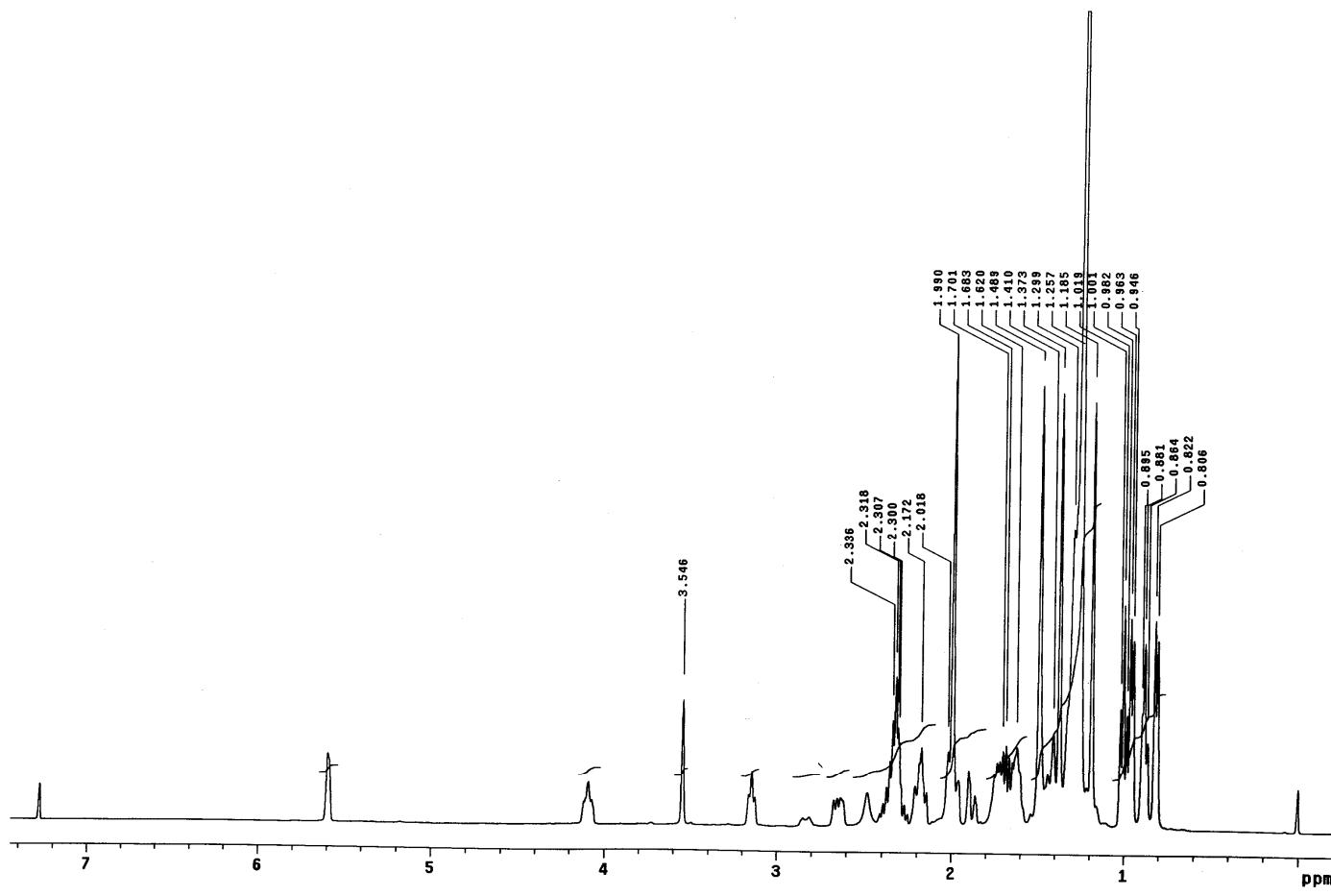
**S3**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 100 MHz.

ESI+  
Molecular Formula : C<sub>40</sub>H<sub>70</sub>O<sub>8</sub>Na  
Exact Mass : 701.4968  
Measured Mass : 701.4974

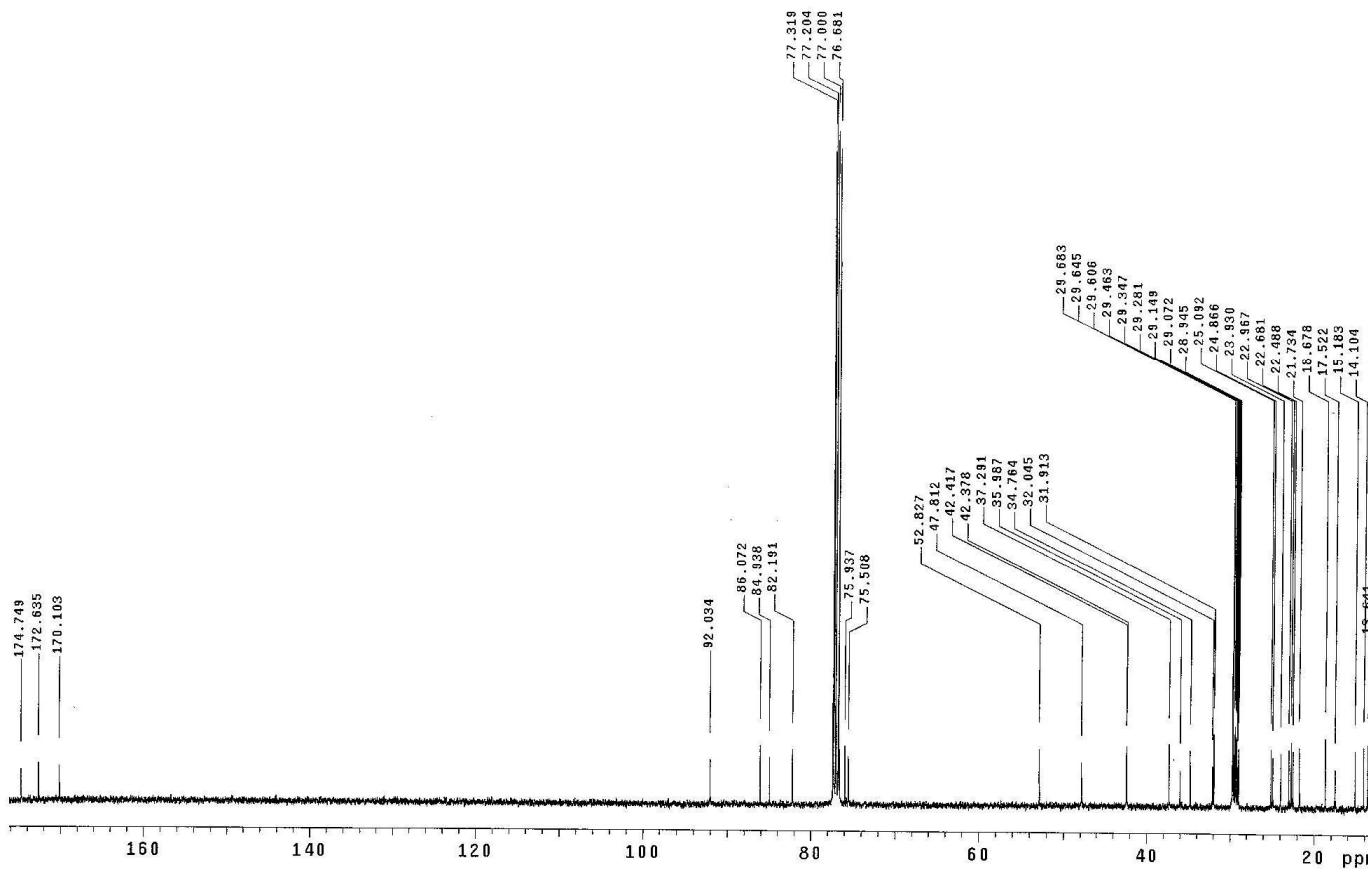


/d=/Data/yu/FSC42145MIN/1/pdata/1 Administrator Mon May 26 15:30:16 2008

**S4** HRESIMS spectrum of **1**.

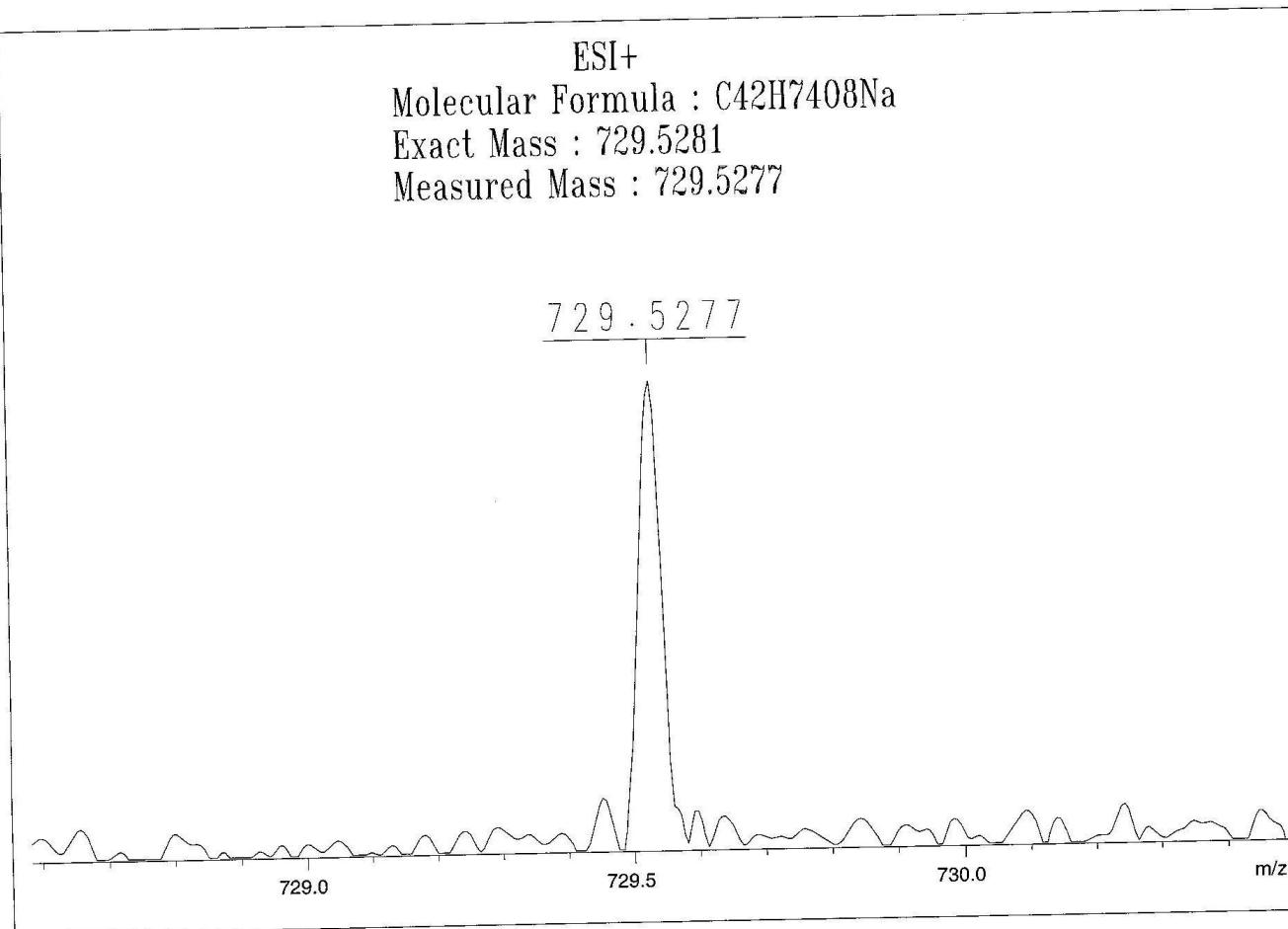


**S5.**  $^1\text{H}$  NMR spectrum of **2** in  $\text{CDCl}_3$  at 400 MHz.



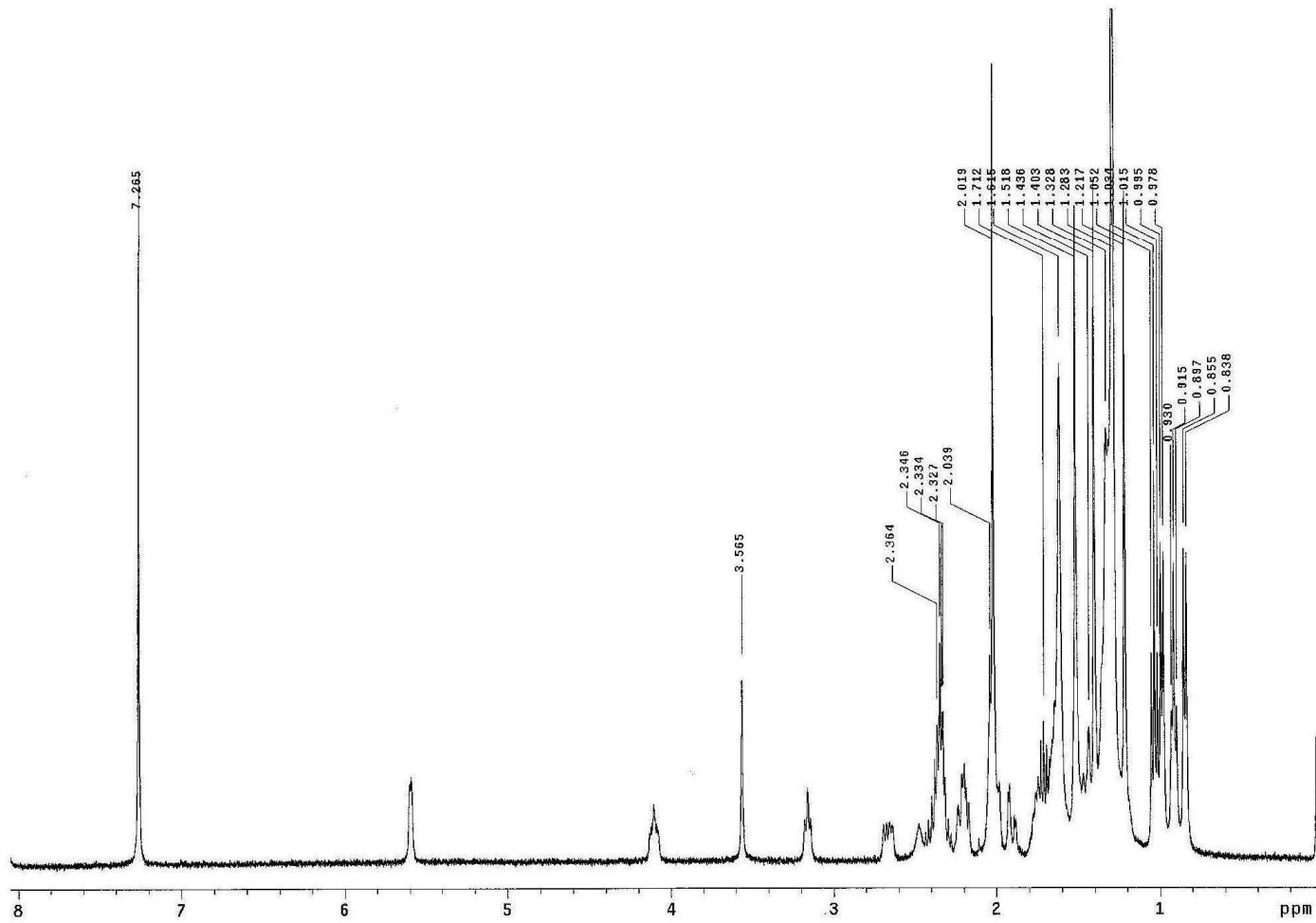
**S6.**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CDCl}_3$  at 100 MHz.

ESI+  
Molecular Formula : C42H74O8Na  
Exact Mass : 729.5281  
Measured Mass : 729.5277

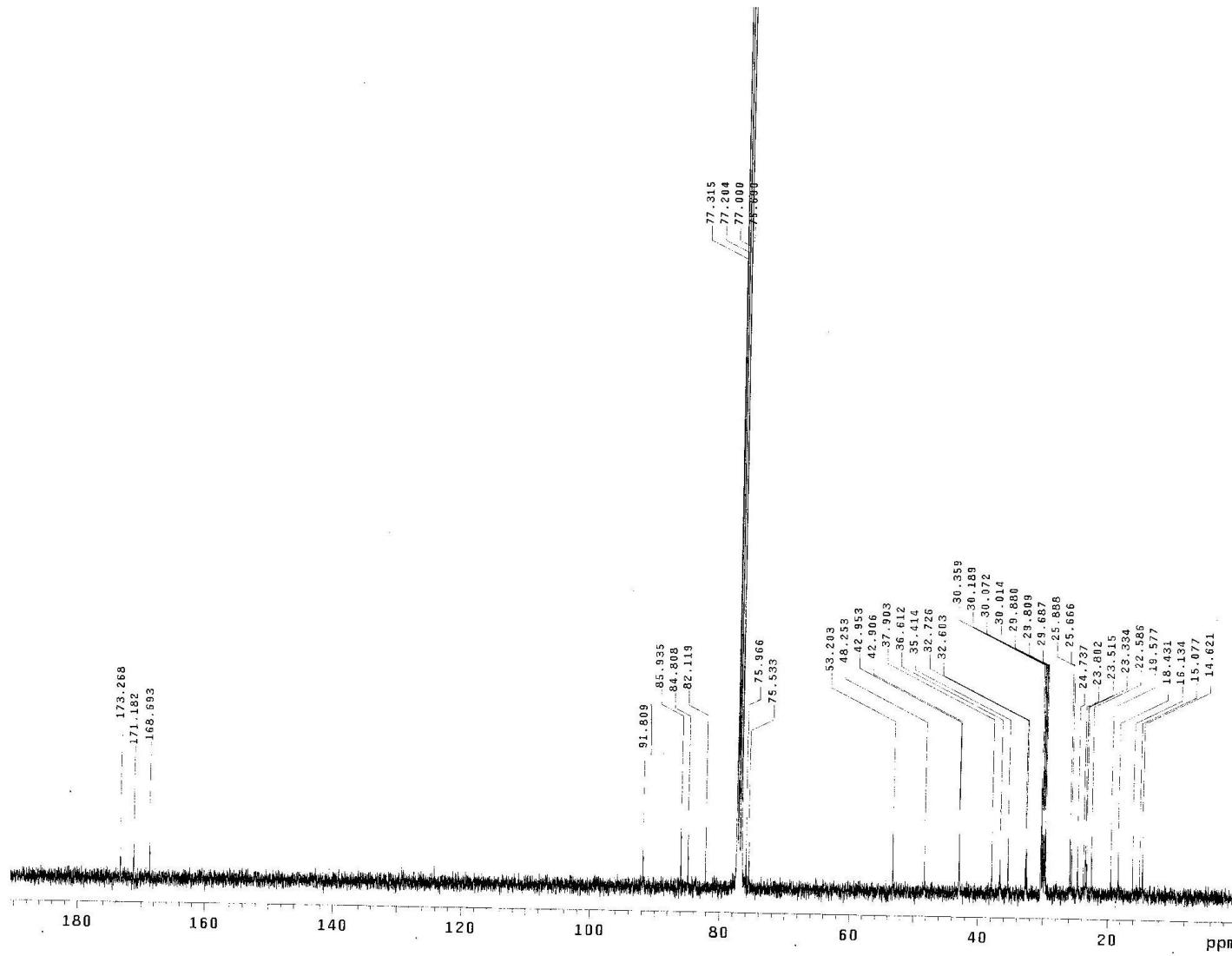


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**S7** HRESIMS spectrum of **2**.



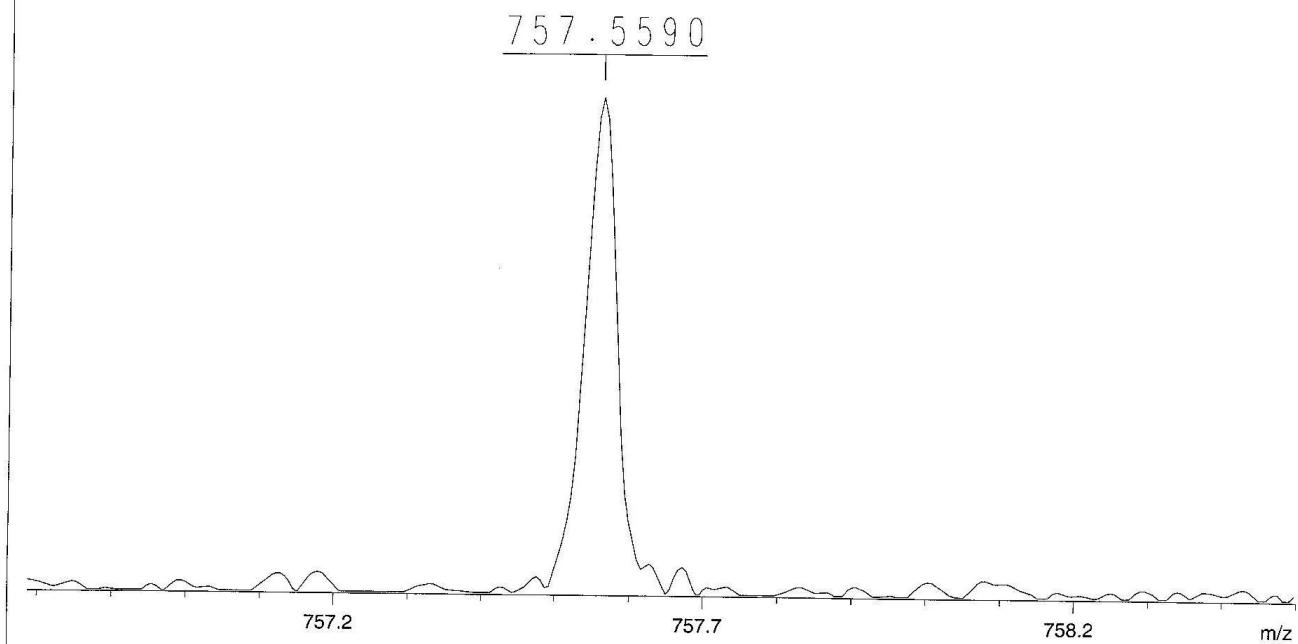
**S8.**  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at 400 MHz.



**S9.**  $^{13}\text{C}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at 100 MHz.

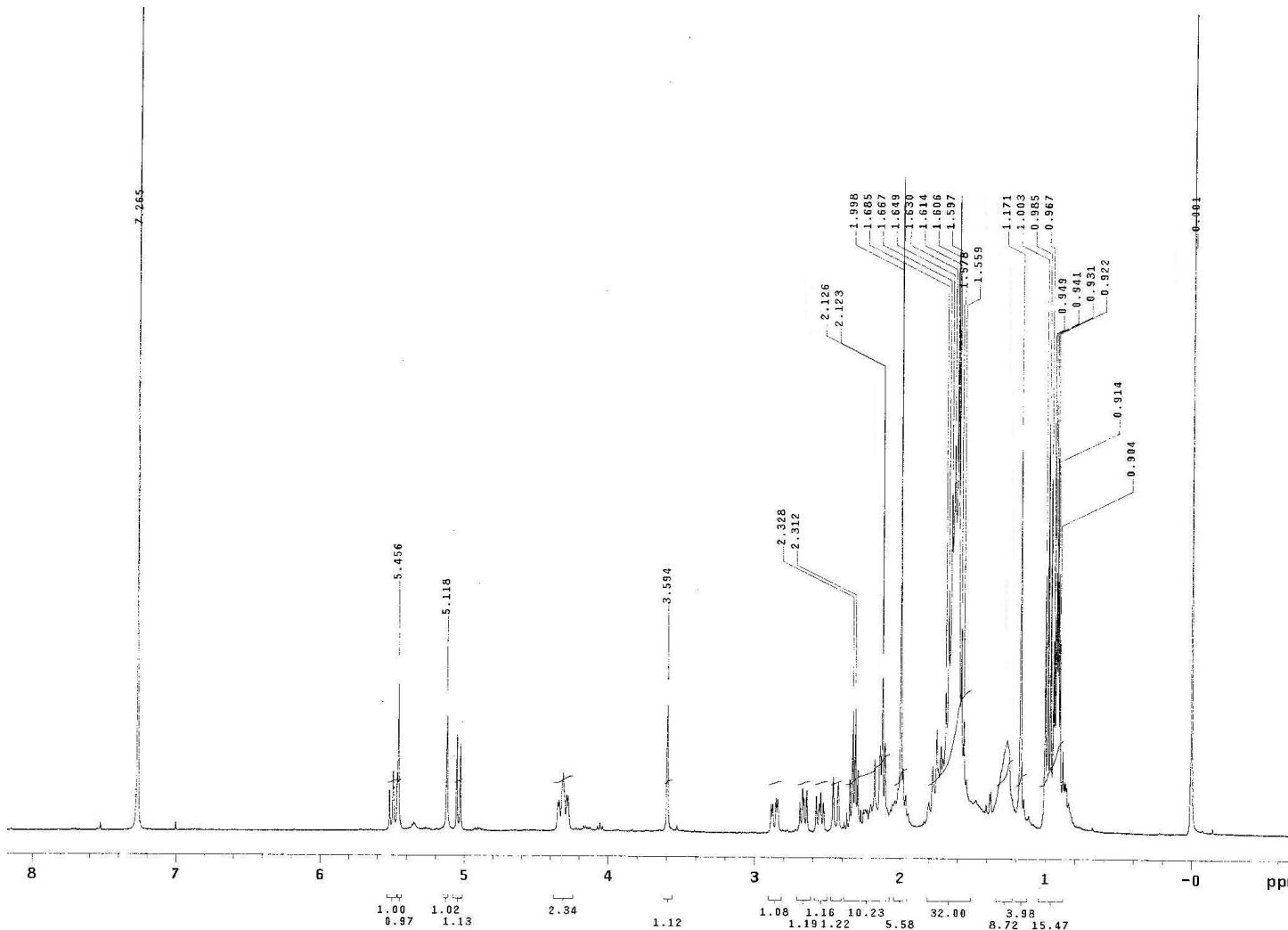
ESI+

Molecular Formula : C<sub>44</sub>H<sub>78</sub>O<sub>8</sub>Na  
Exact Mass : 757.5594  
Measured Mass : 757.5590

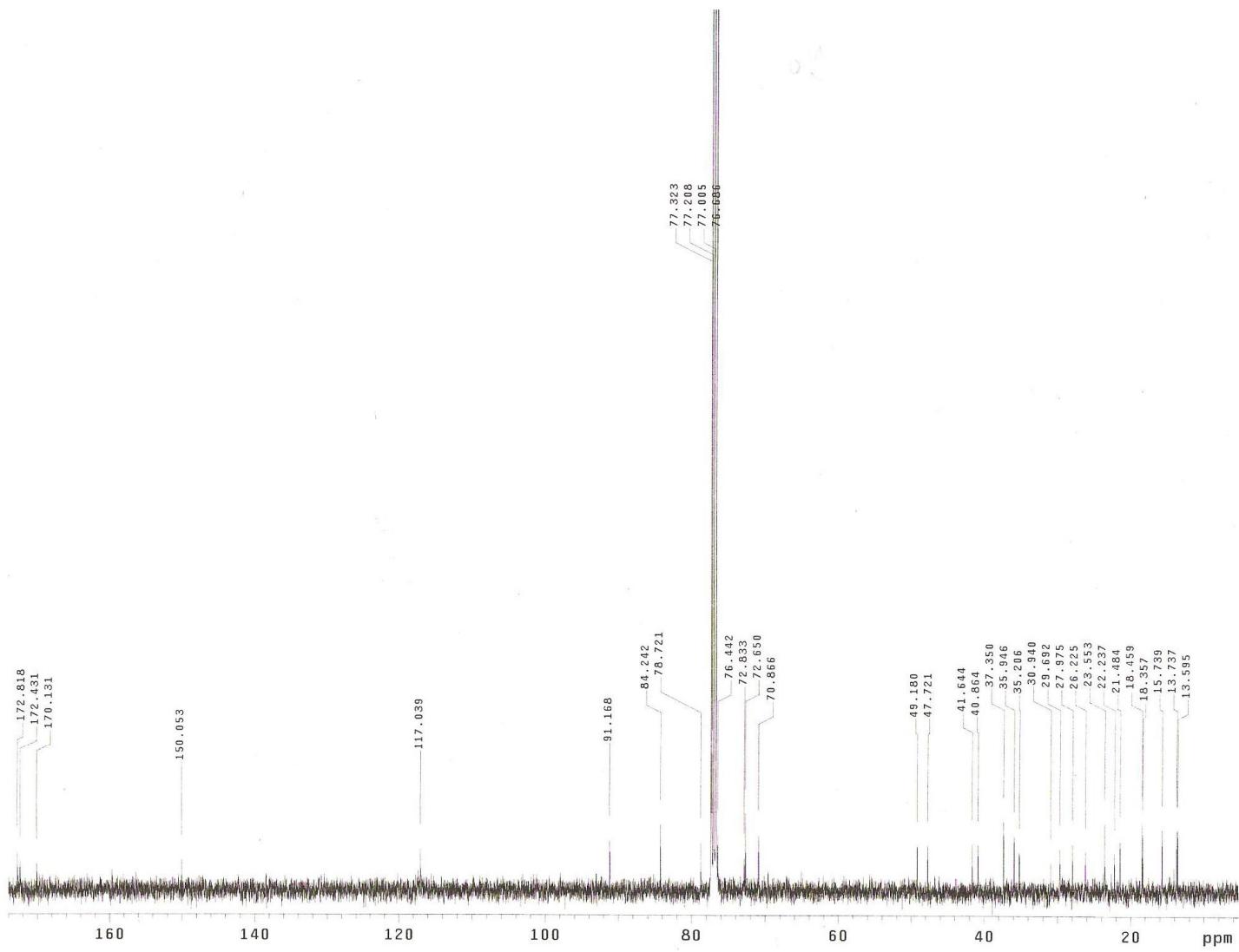


/d=/Data/yu/FSC42140MIN/2/pdata/1 Administrator Mon May 26 15:48:14 2008

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



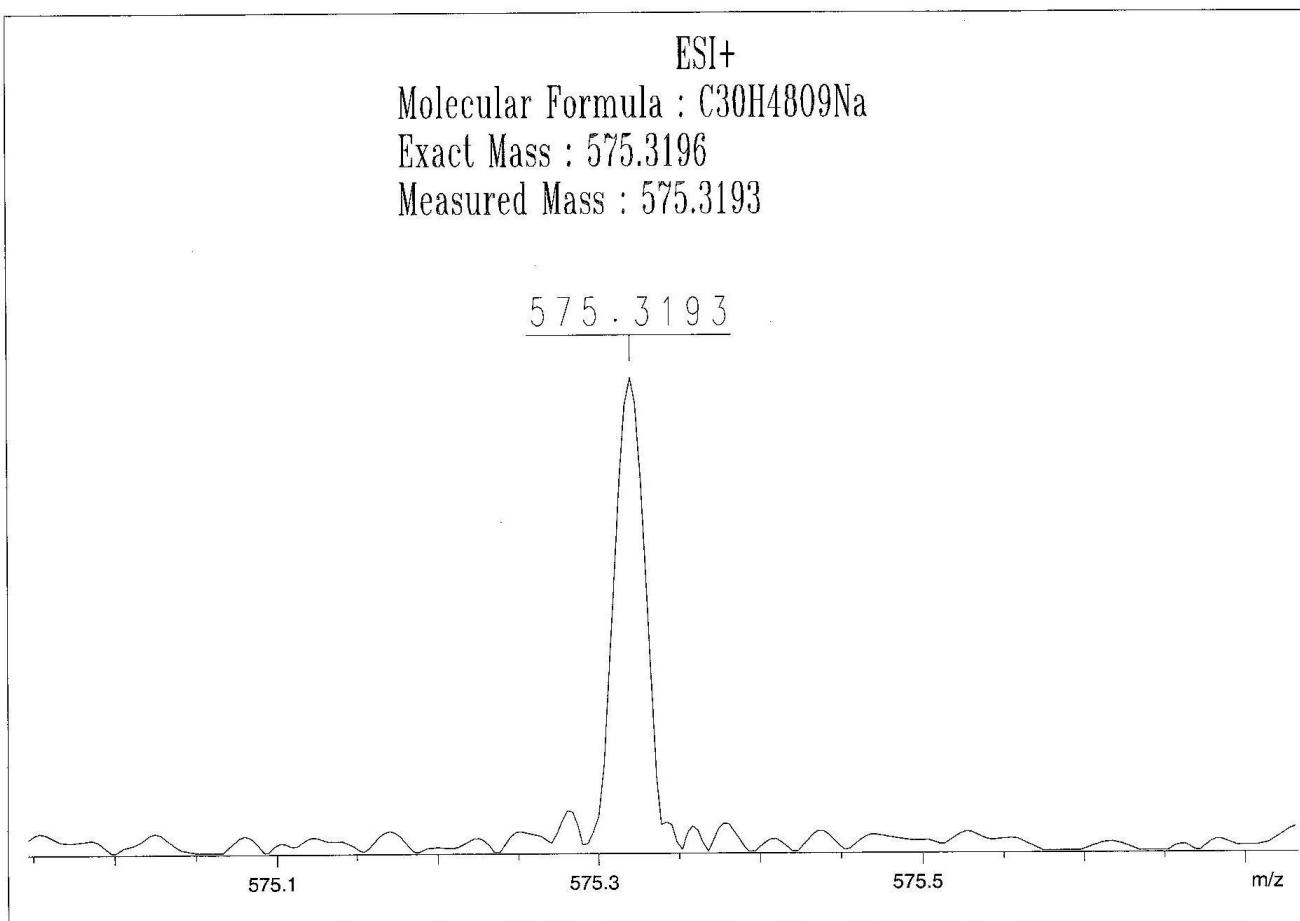
**S11.** <sup>1</sup>H NMR spectrum of **4** in  $\text{CDCl}_3$  at 400 MHz.



**S12.**  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{CDCl}_3$  at 100 MHz.

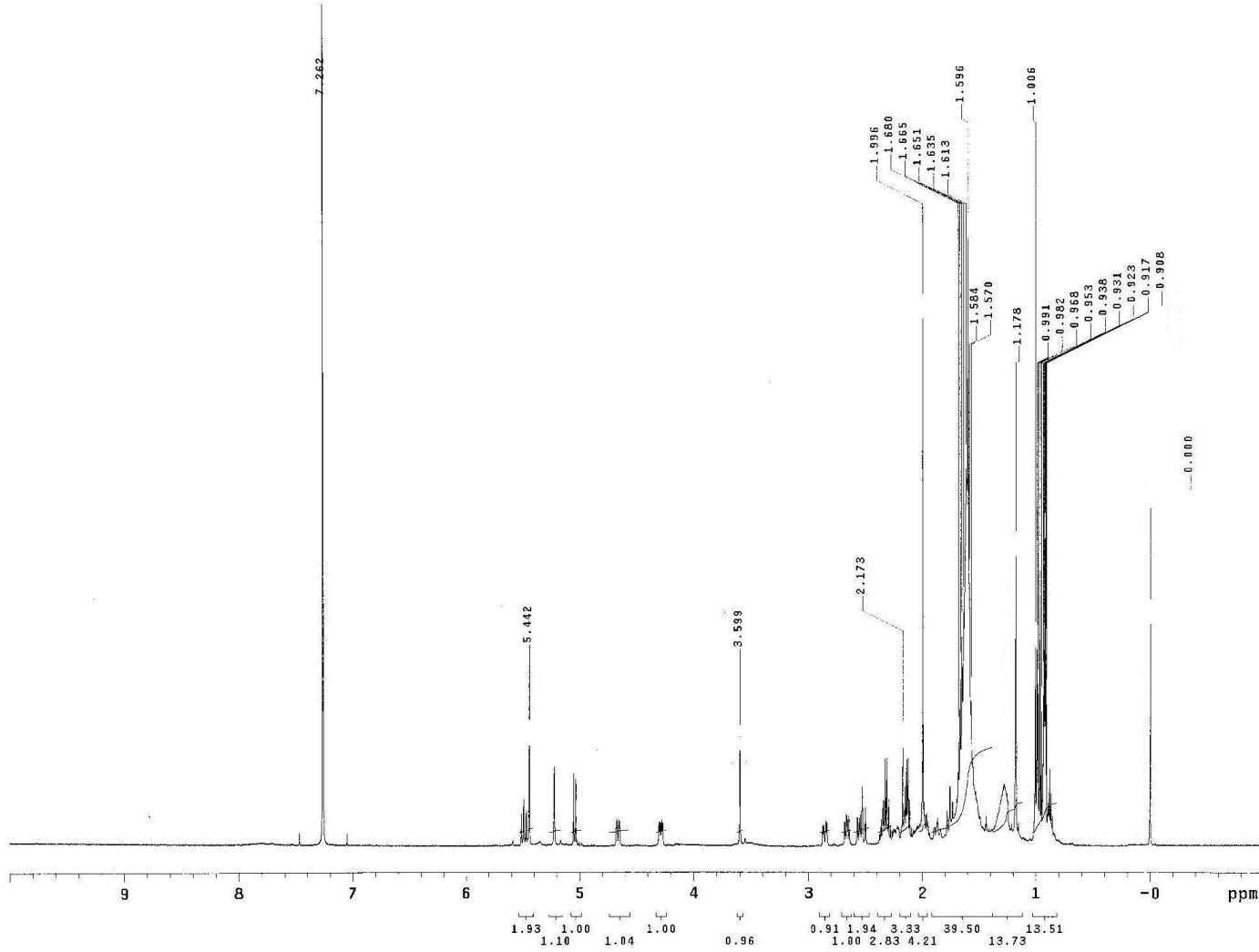
ESI+

Molecular Formula : C<sub>30</sub>H<sub>48</sub>O<sub>9</sub>Na  
Exact Mass : 575.3196  
Measured Mass : 575.3193

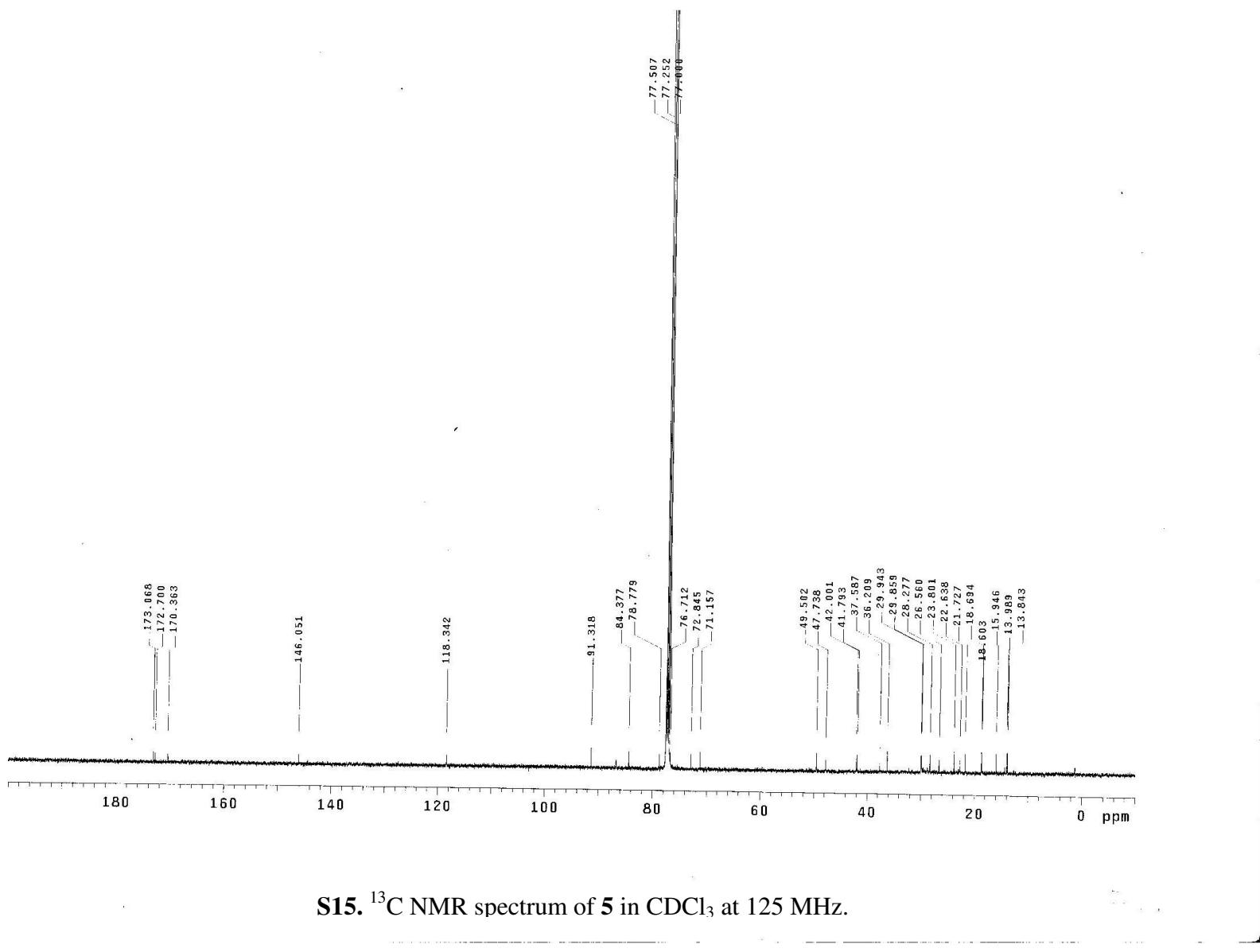


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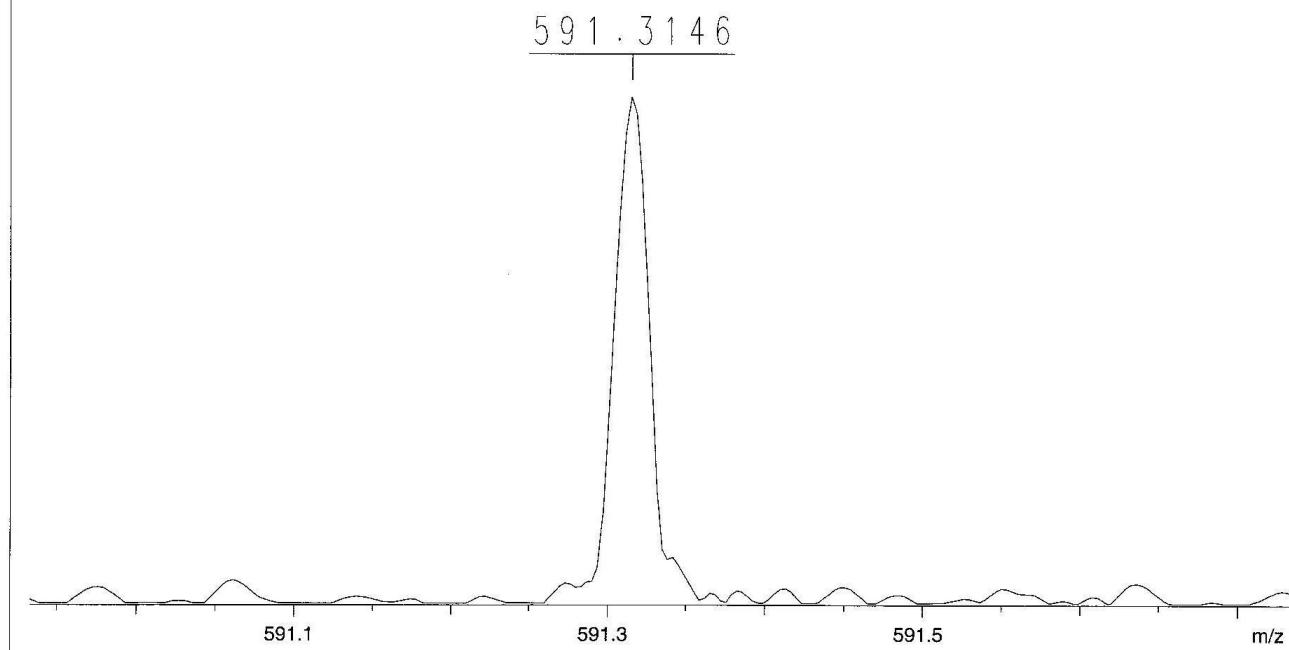
S13 HRESIMS spectrum of 4.



**S14.**  $^1\text{H}$  NMR spectrum of **5** in  $\text{CDCl}_3$  at 500 MHz.

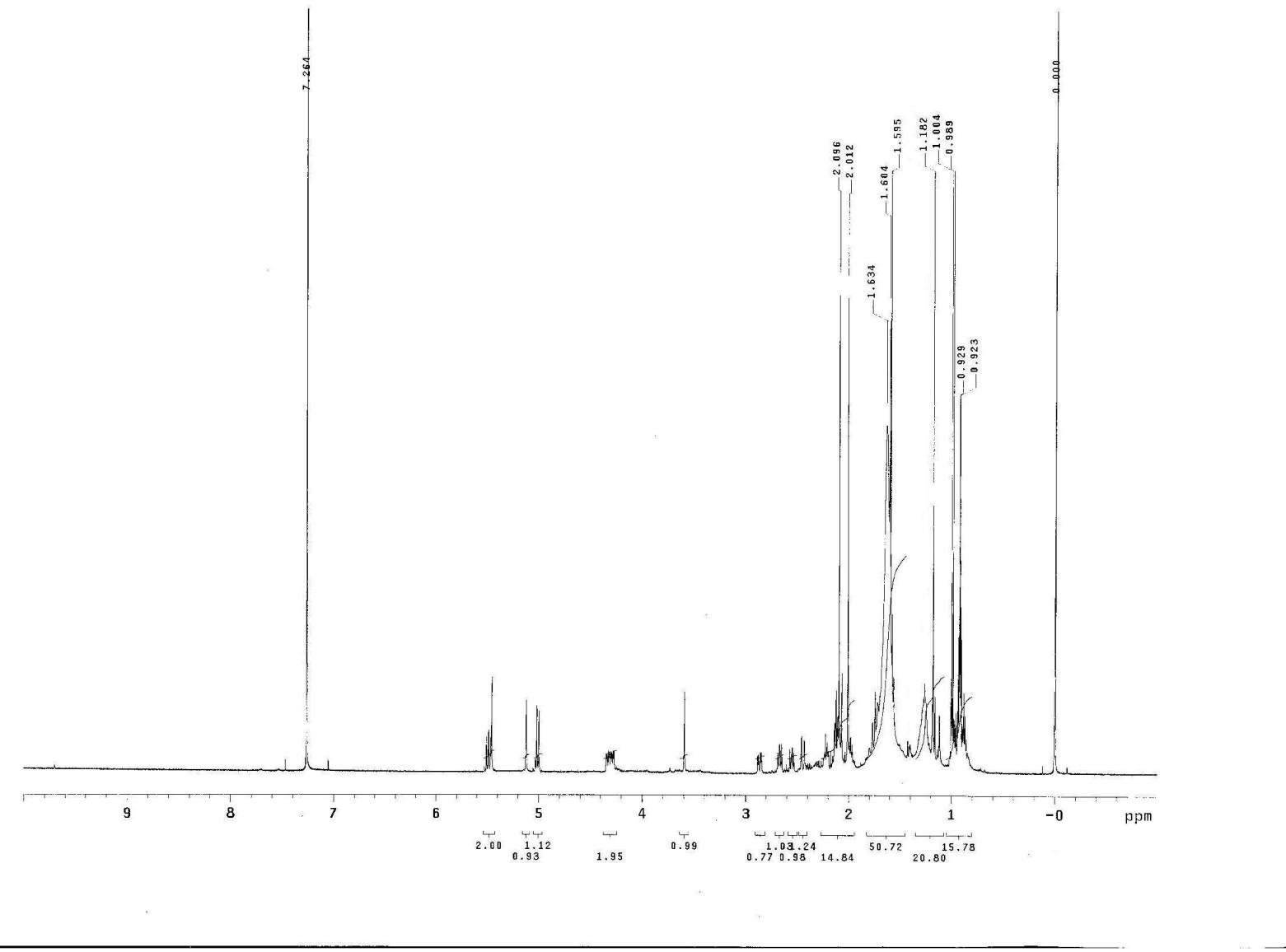


ESI+  
Molecular Formula : C<sub>30</sub>H<sub>48</sub>O<sub>10</sub>Na  
Exact Mass : 591.3145  
Measured Mass : 591.3146

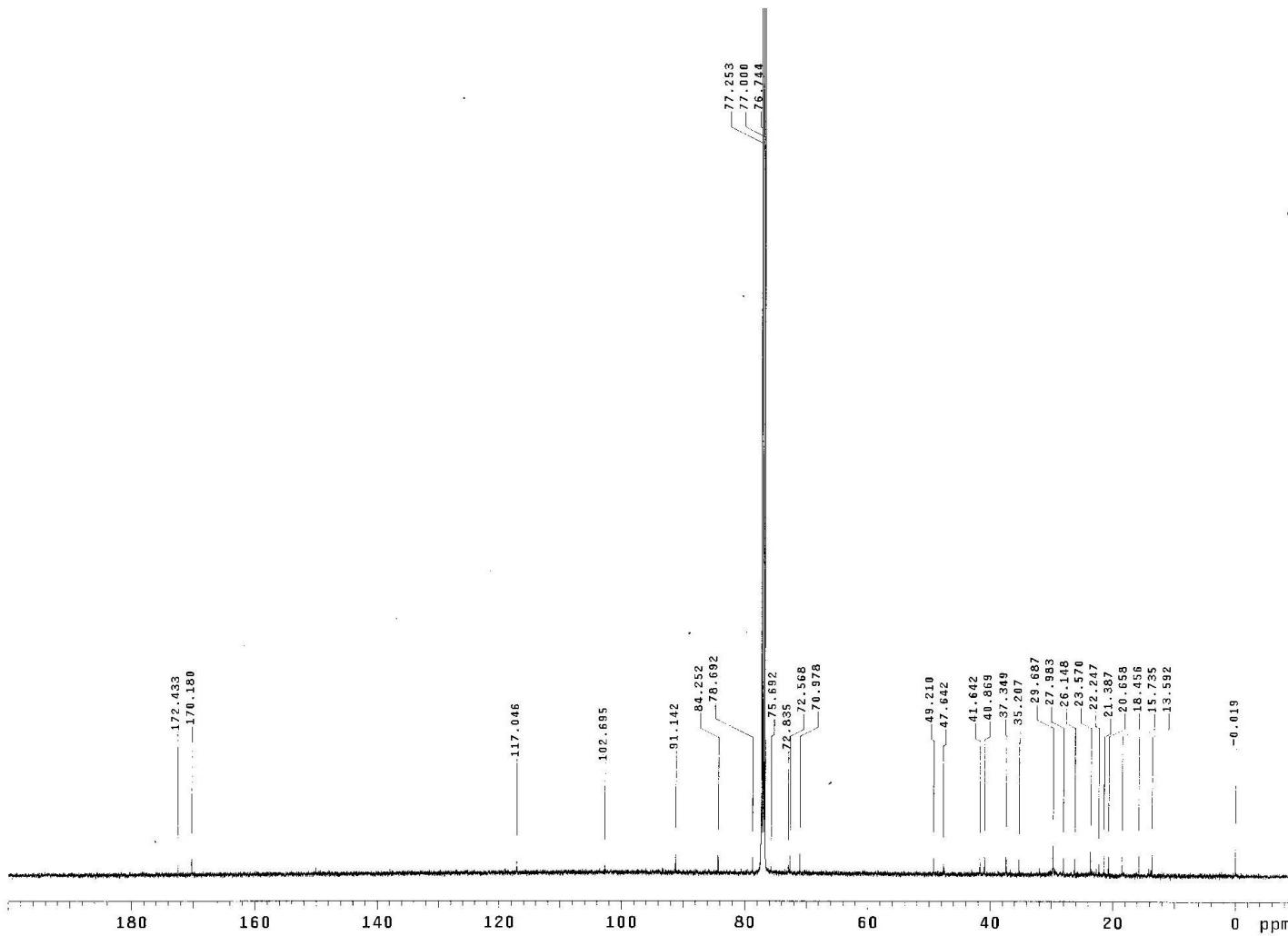


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**S15** HRESIMS spectrum of **5**.



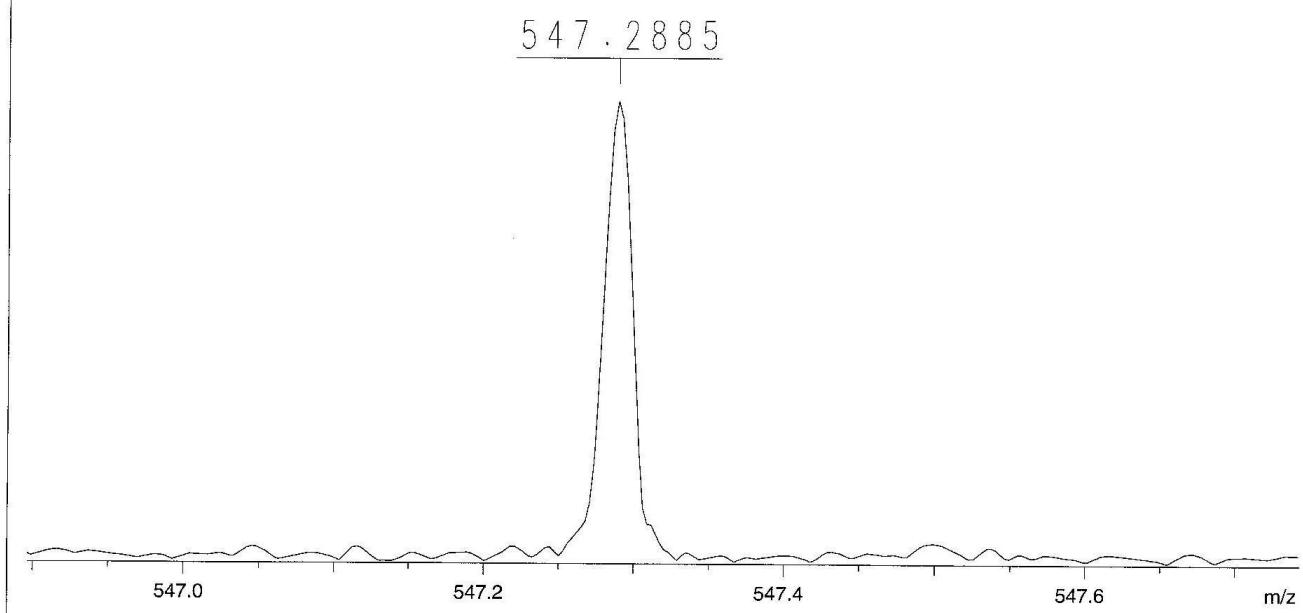
**S16.** <sup>1</sup>H NMR spectrum of **6** in CDCl<sub>3</sub> at 500 MHz.



**S17.**  $^{13}\text{C}$  NMR spectrum of **6** in  $\text{CDCl}_3$  at 125 MHz.

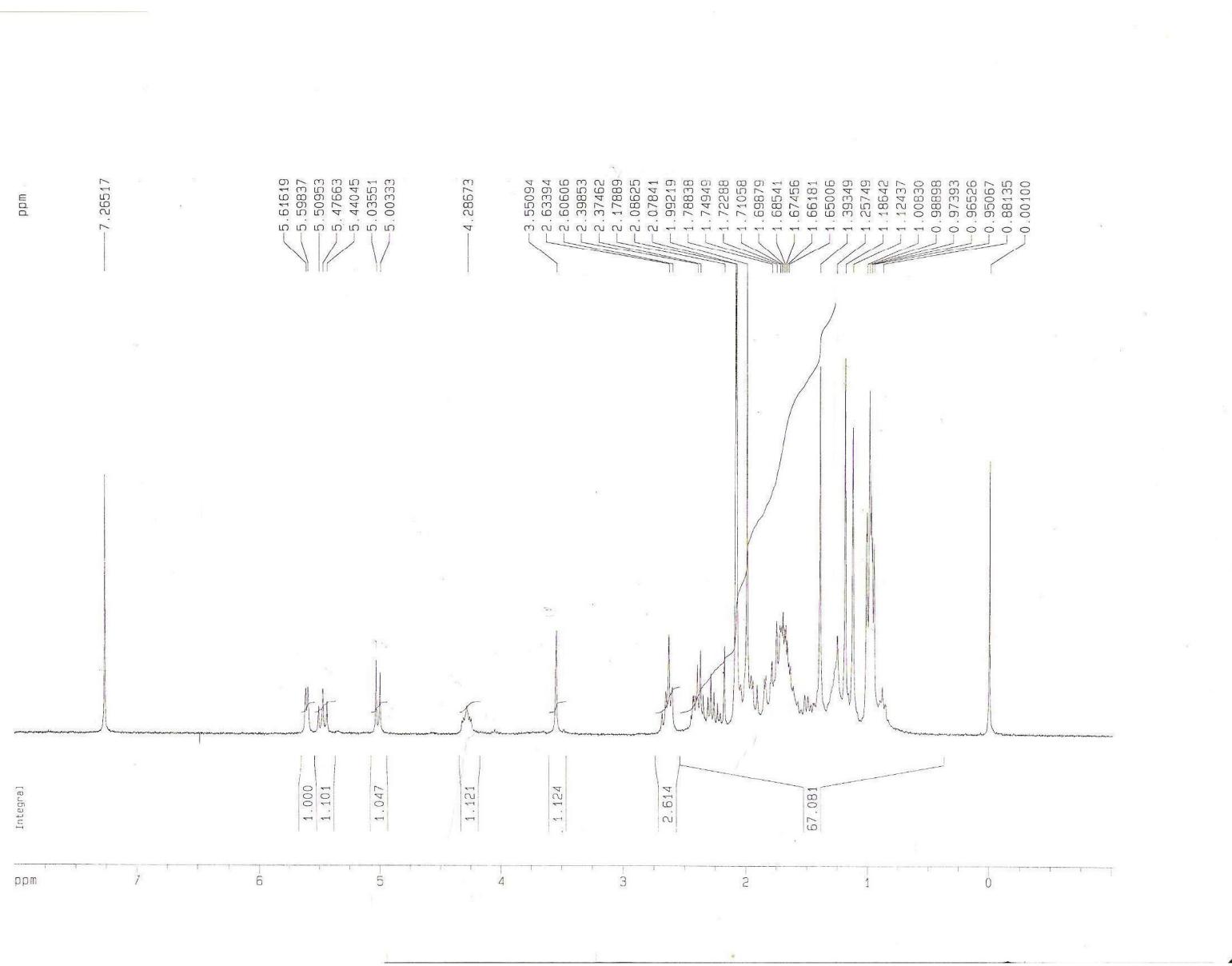
ESI+

Molecular Formula: C<sub>28</sub>H<sub>44</sub>O<sub>9</sub>Na  
Exact Mass: 547.2883  
Measured Mass: 547.2885

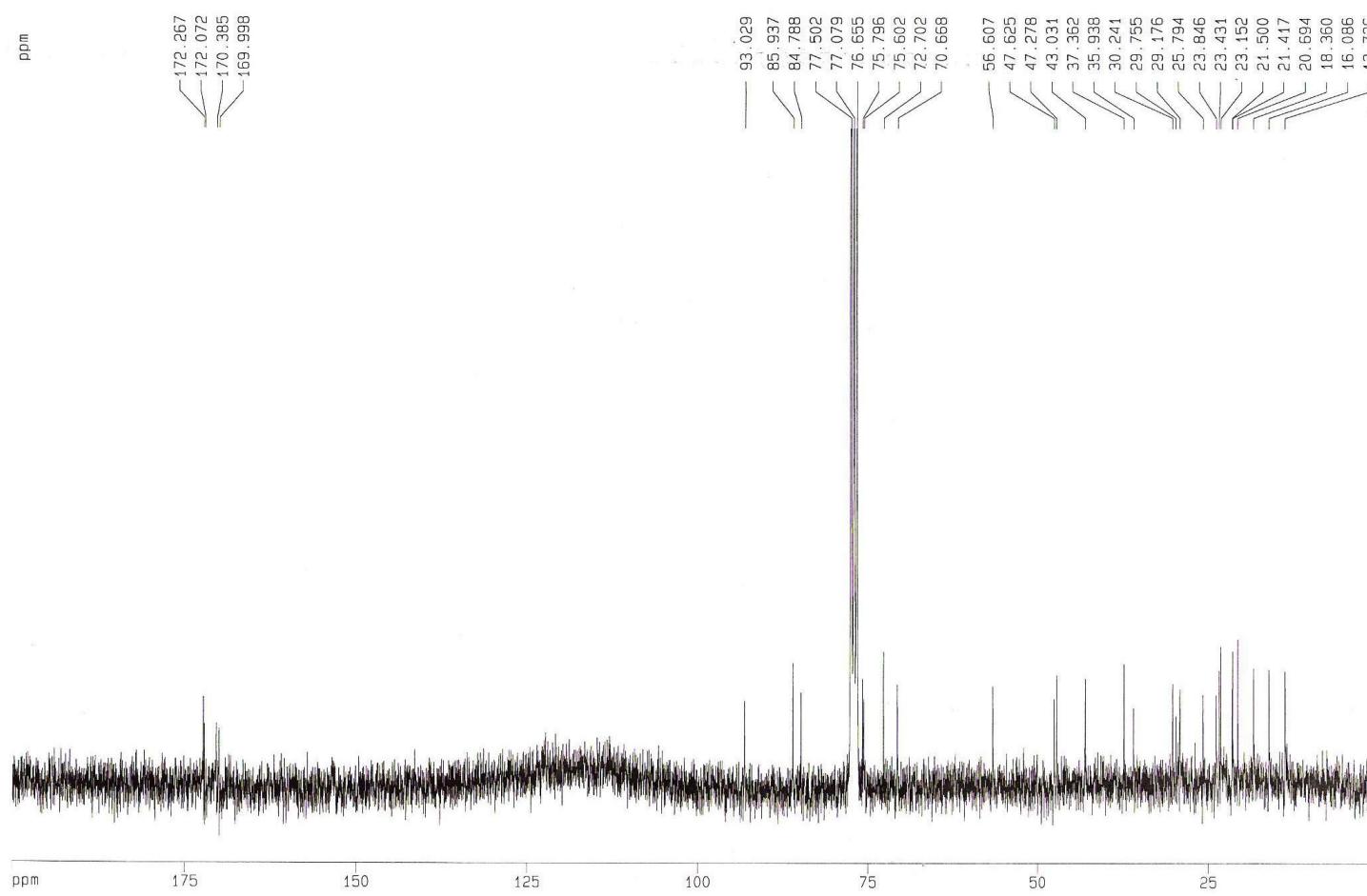


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**S18** HRESIMS spectrum of **6**.



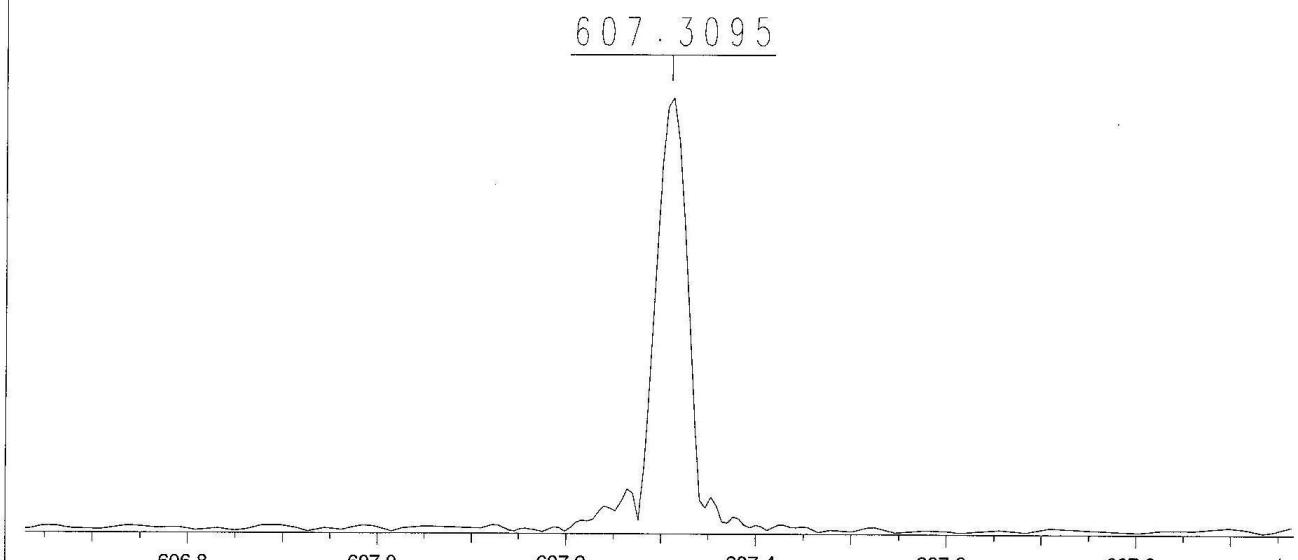
**S19.**  $^1\text{H}$  NMR spectrum of **7** in  $\text{CDCl}_3$  at 300 MHz.



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

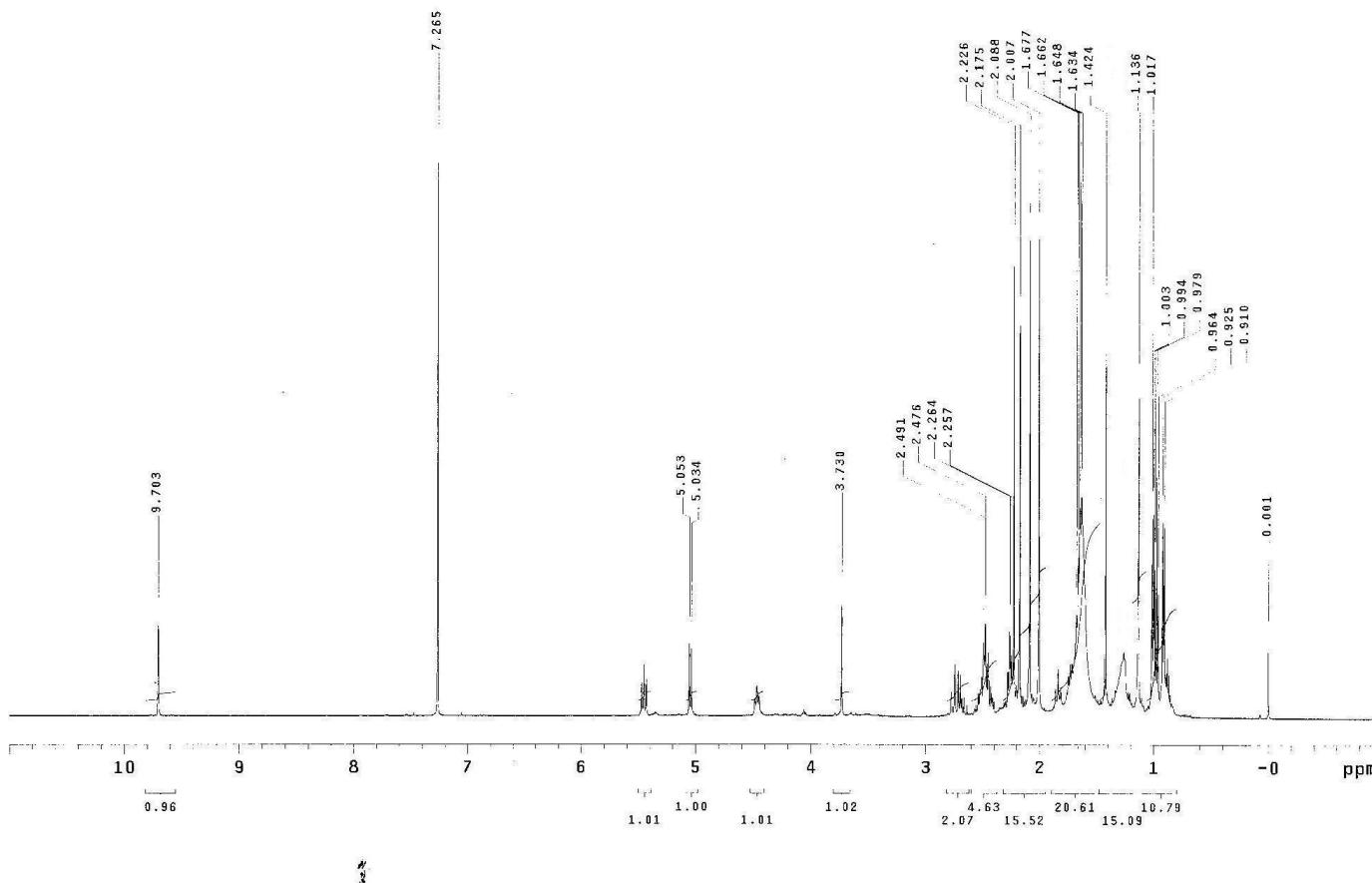
ESI+

Molecular Formula: C<sub>30</sub>H<sub>48</sub>O<sub>11</sub>Na  
Exact Mass: 607.3094  
Measured Mass: 607.3095

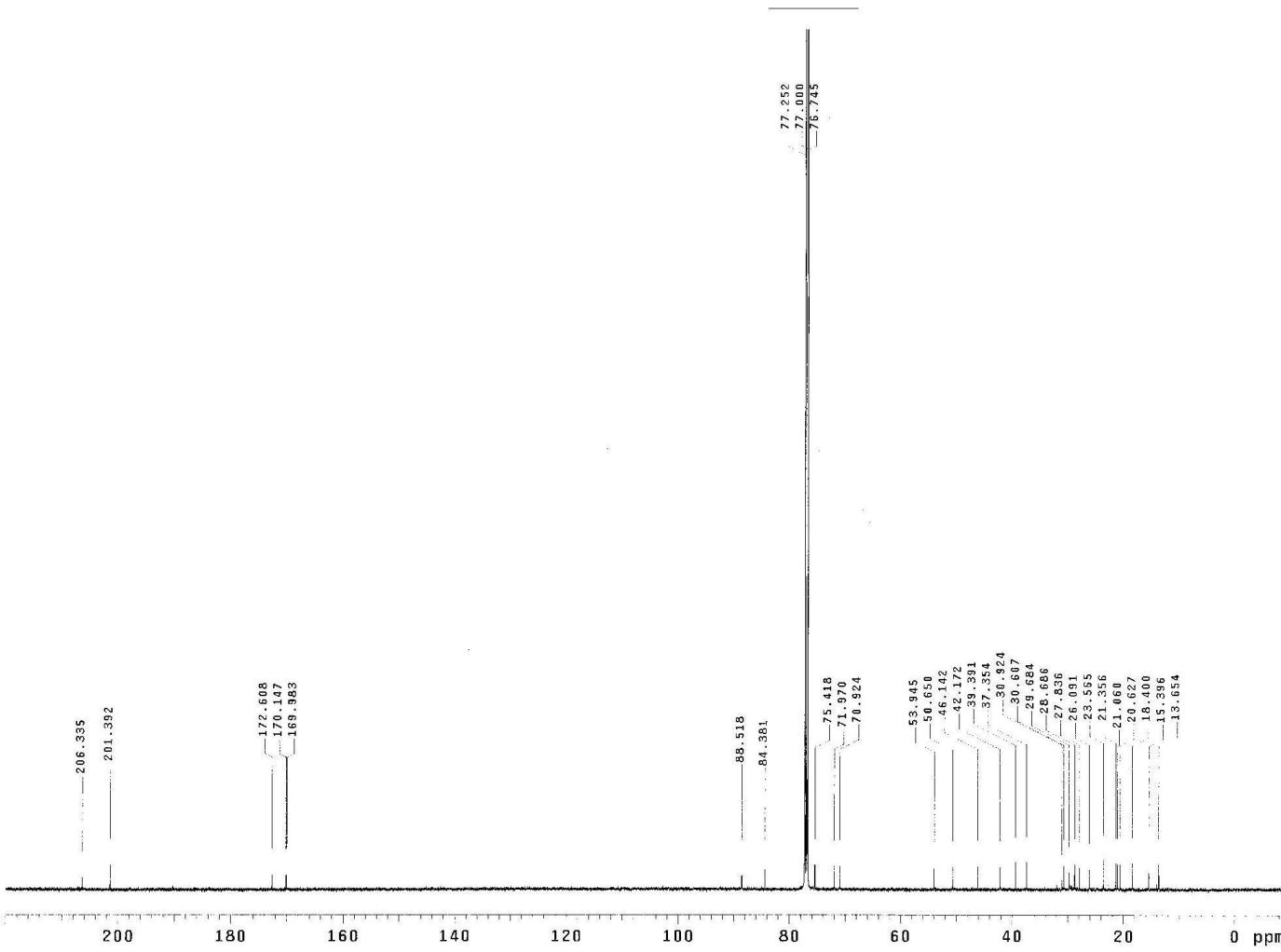


/d=/Data/yu/FSC4275I/1/pdata/1 Administrator Wed Jul 18 12:44:45 2007

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



**S22.**  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{CDCl}_3$  at 500 MHz.



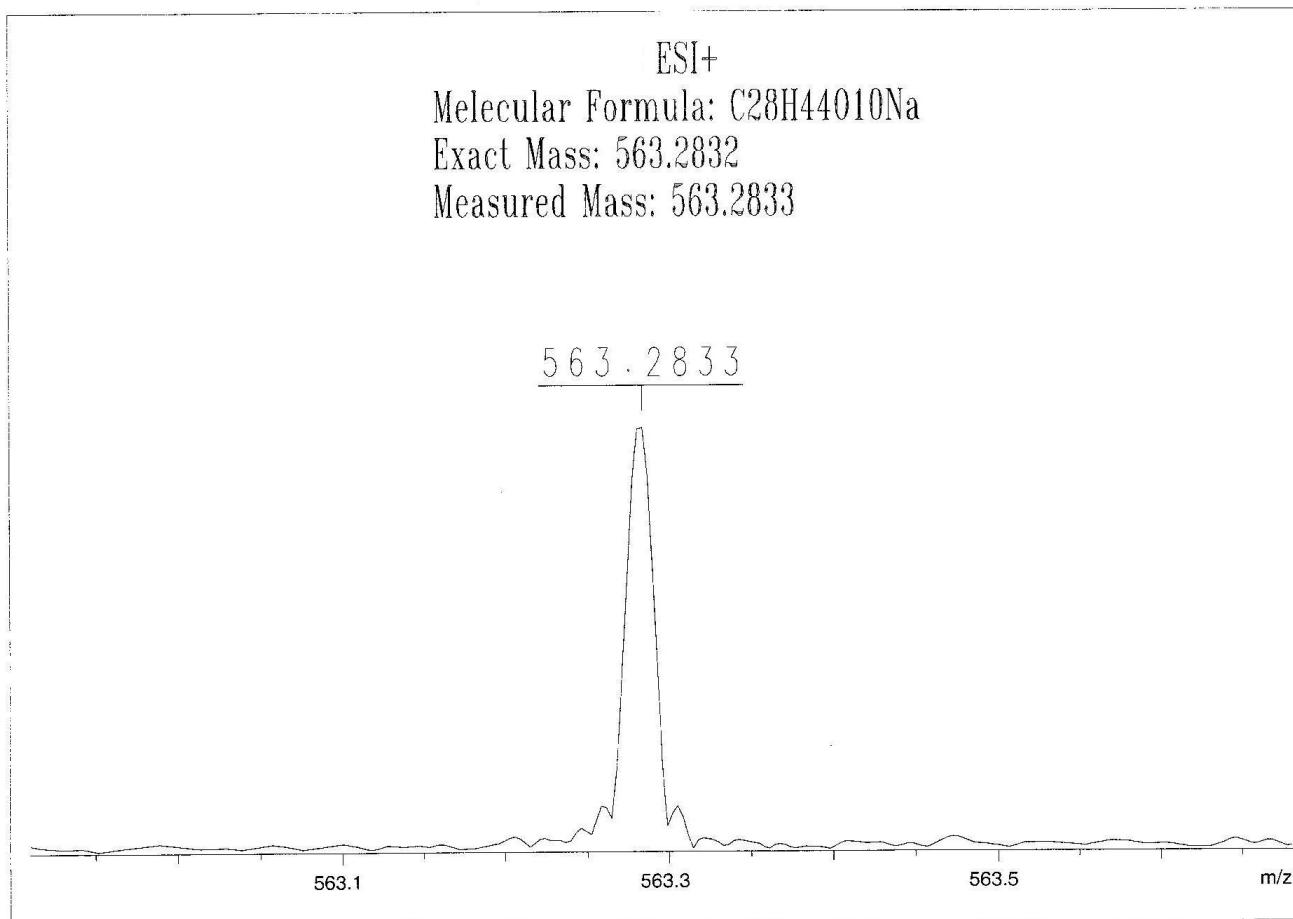
S23.  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{CDCl}_3$  at 125 MHz.

ESI+

Molecular Formula: C<sub>28</sub>H<sub>44</sub>O<sub>10</sub>Na

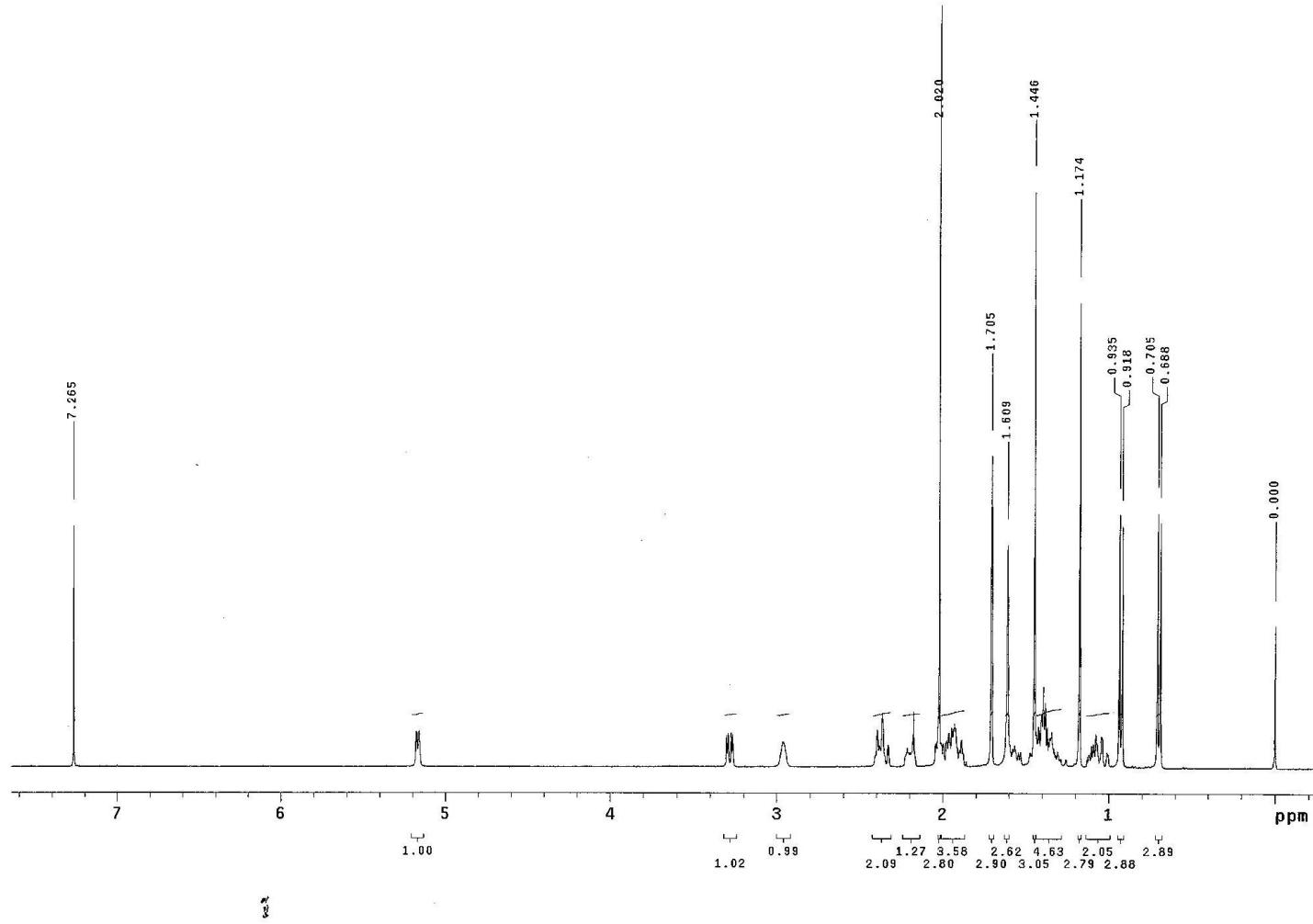
Exact Mass: 563.2832

Measured Mass: 563.2833

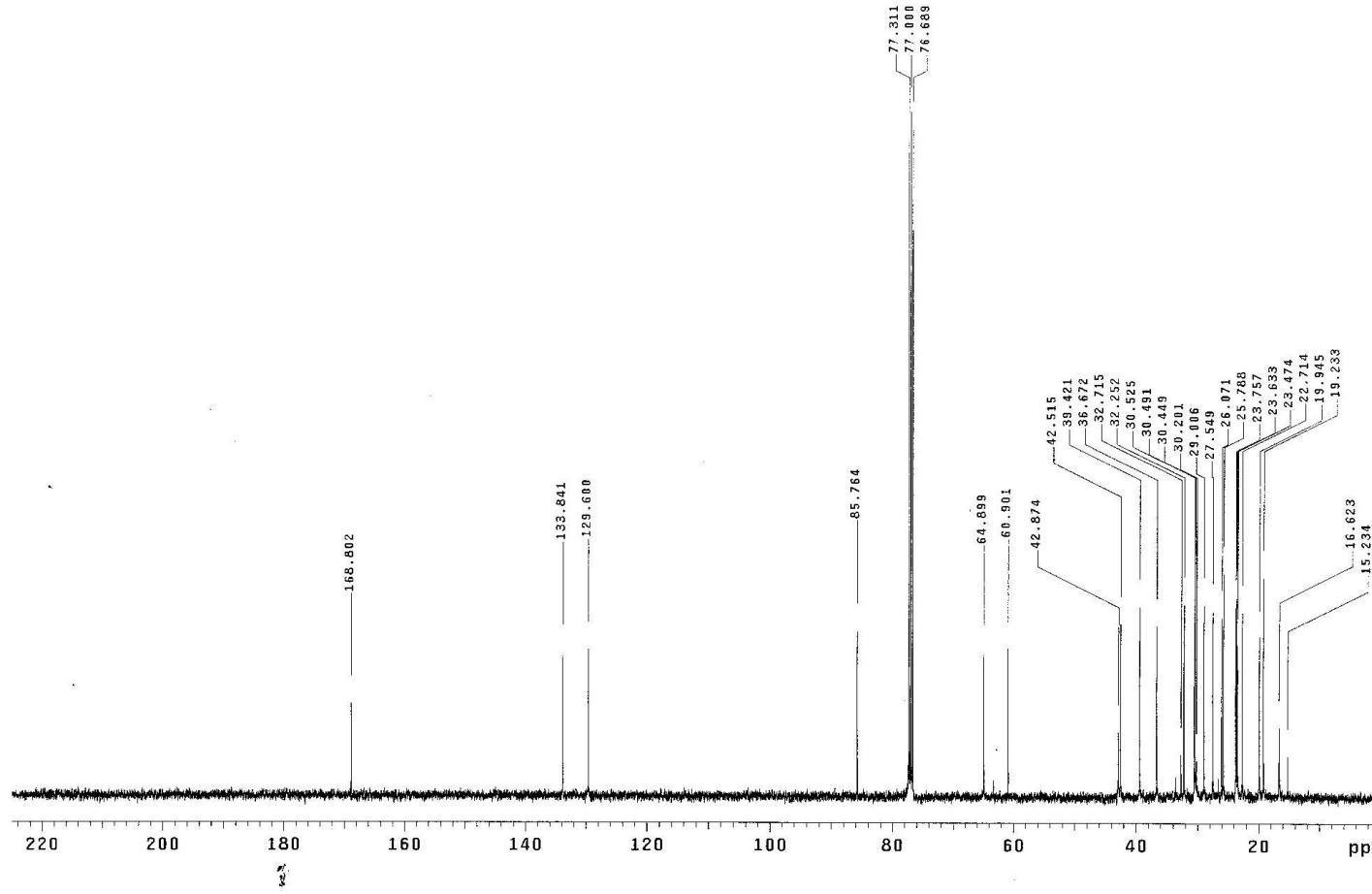


/d=/Data/yu/fsc427ai2/2/pdata/1 Administrator Fri Jan 19 12:01:30 2007

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

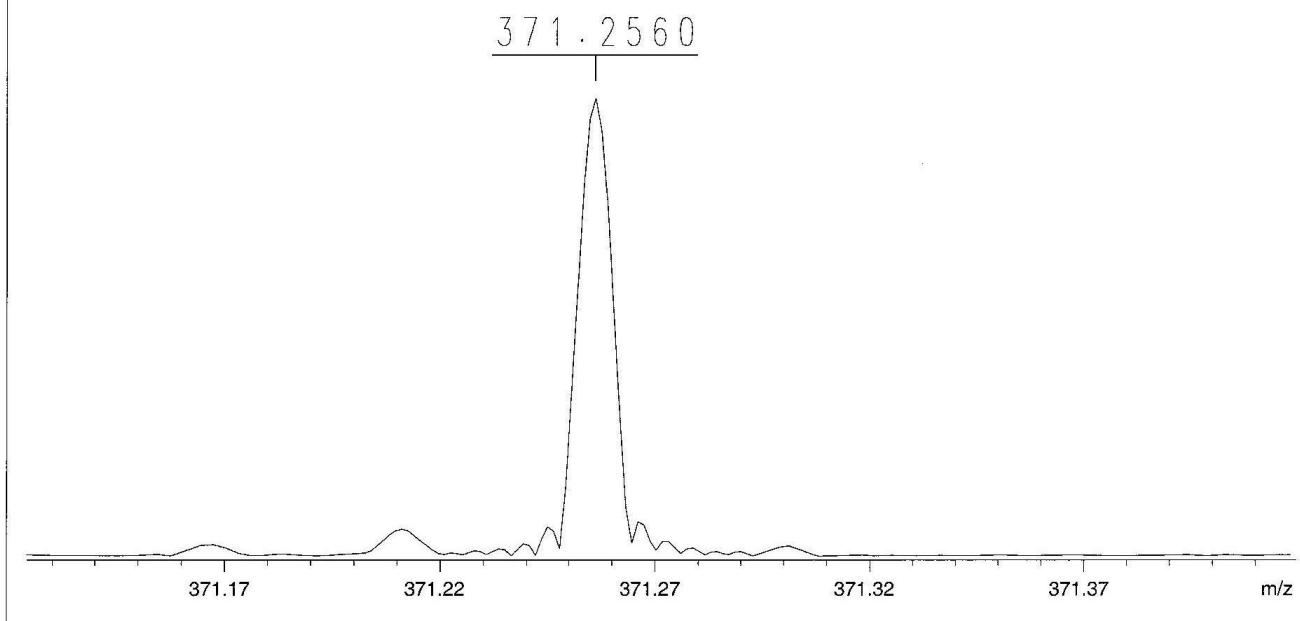


S25.  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{CDCl}_3$  at 400 MHz.



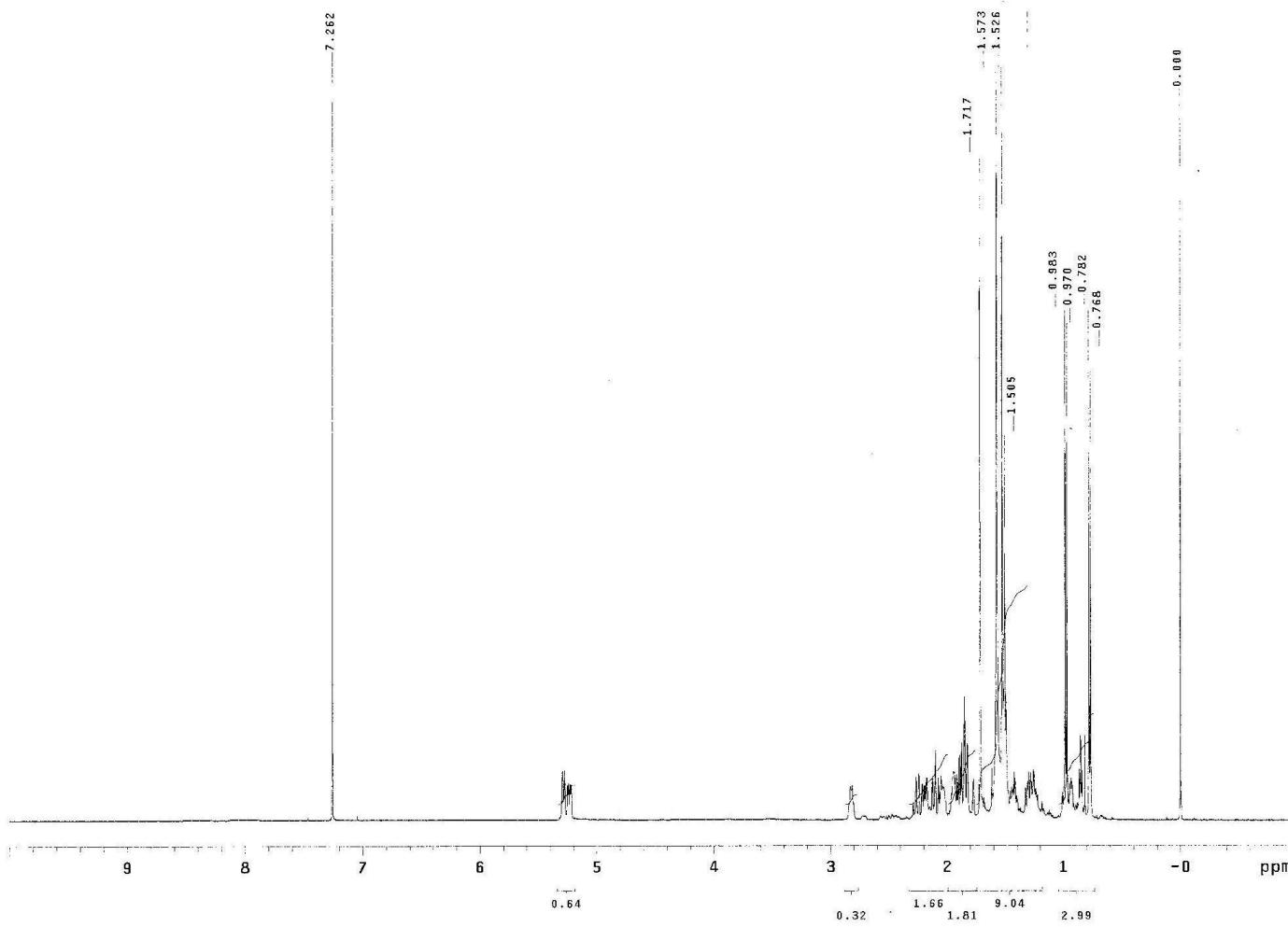
**S26.**  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{CDCl}_3$  at 100 MHz.

ESI+  
Molecular Formula : C<sub>22</sub>H<sub>36</sub>O<sub>3</sub>Na  
Exact Mass : 371.2562  
Measured Mass : 371.2560

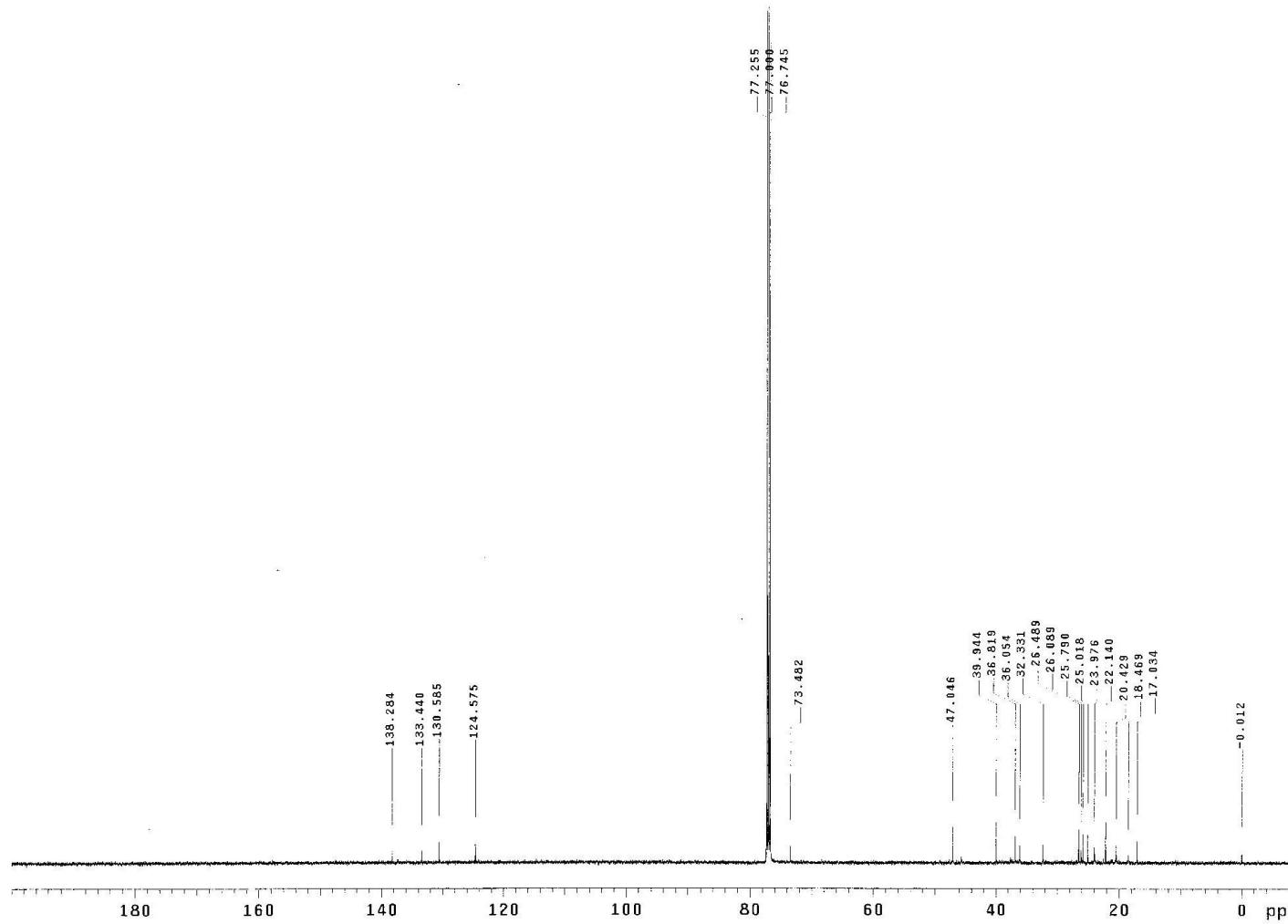


/d=/Data/yu/FSC4LOW1/1/pdata/1 Administrator Fri Aug 15 16:40:04 2008

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

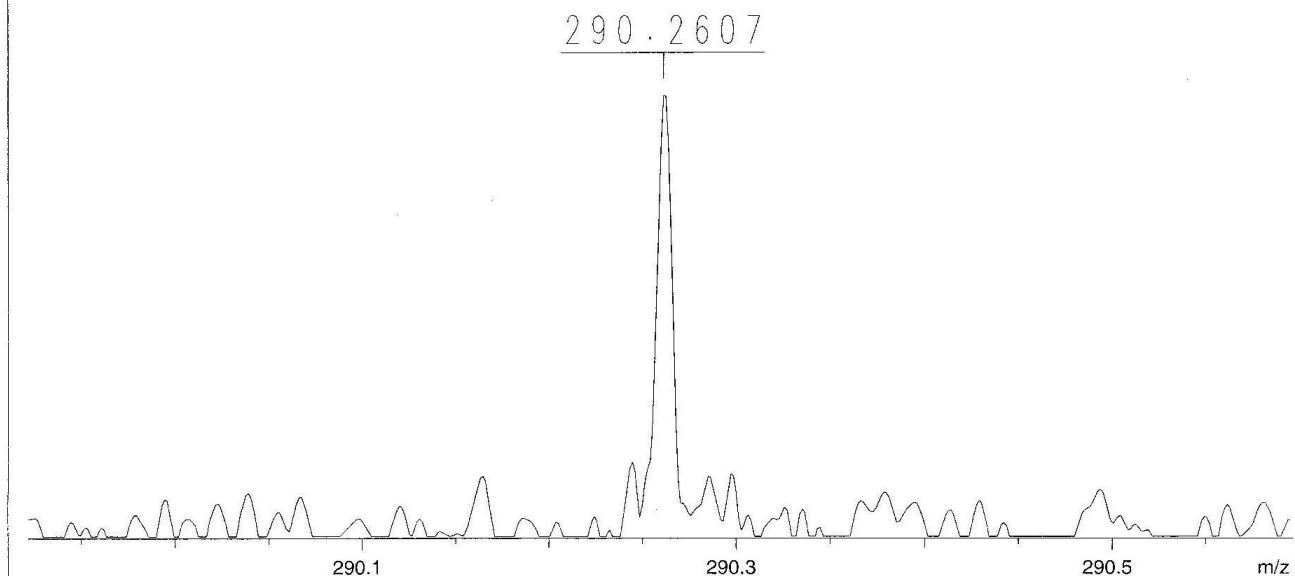


**S28.**  $^{13}\text{C}$  NMR spectrum of **10** in  $\text{CDCl}_3$  at 500 MHz.



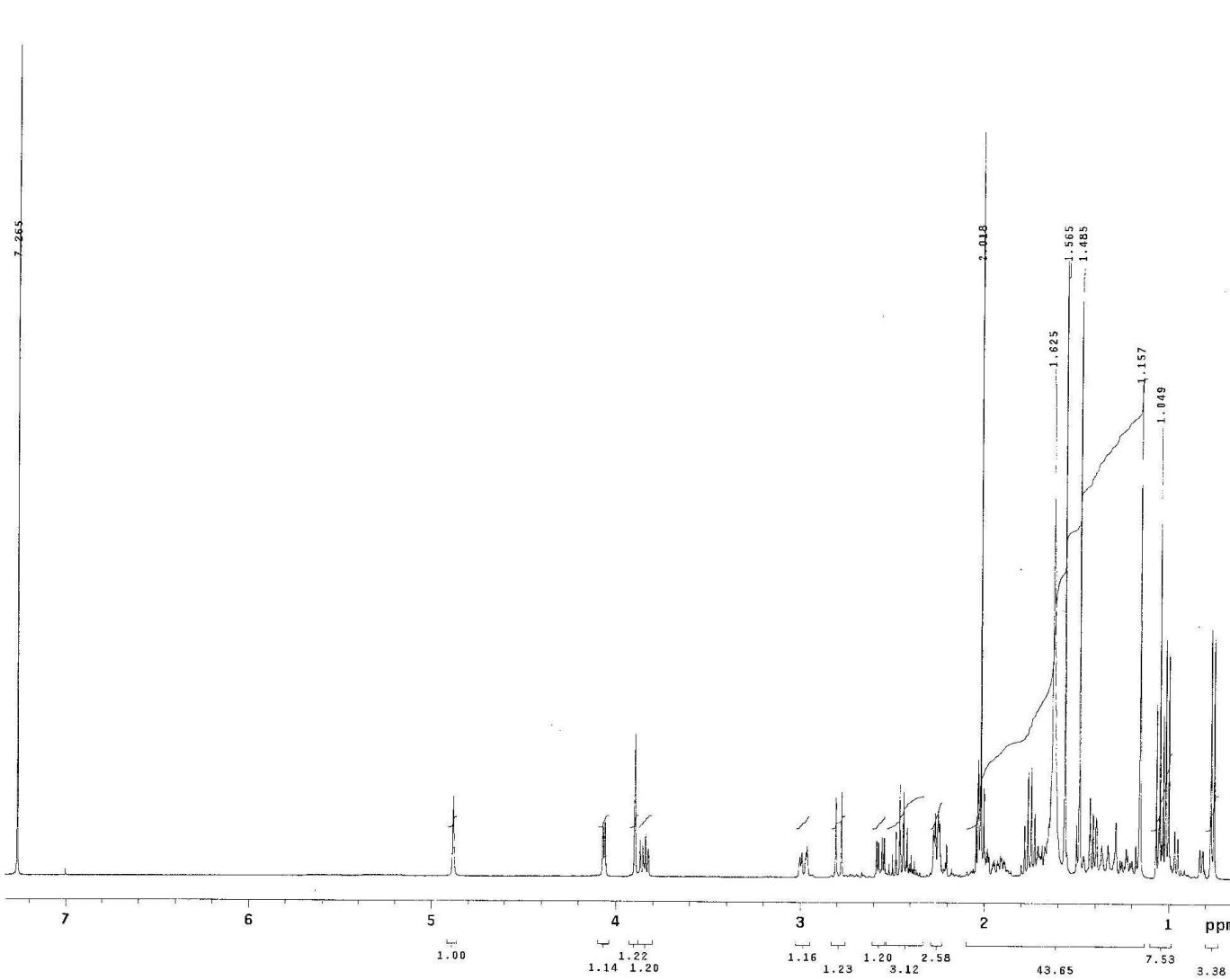
**S29.** <sup>13</sup>C NMR spectrum of **10** in CDCl<sub>3</sub> at 125 MHz.

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

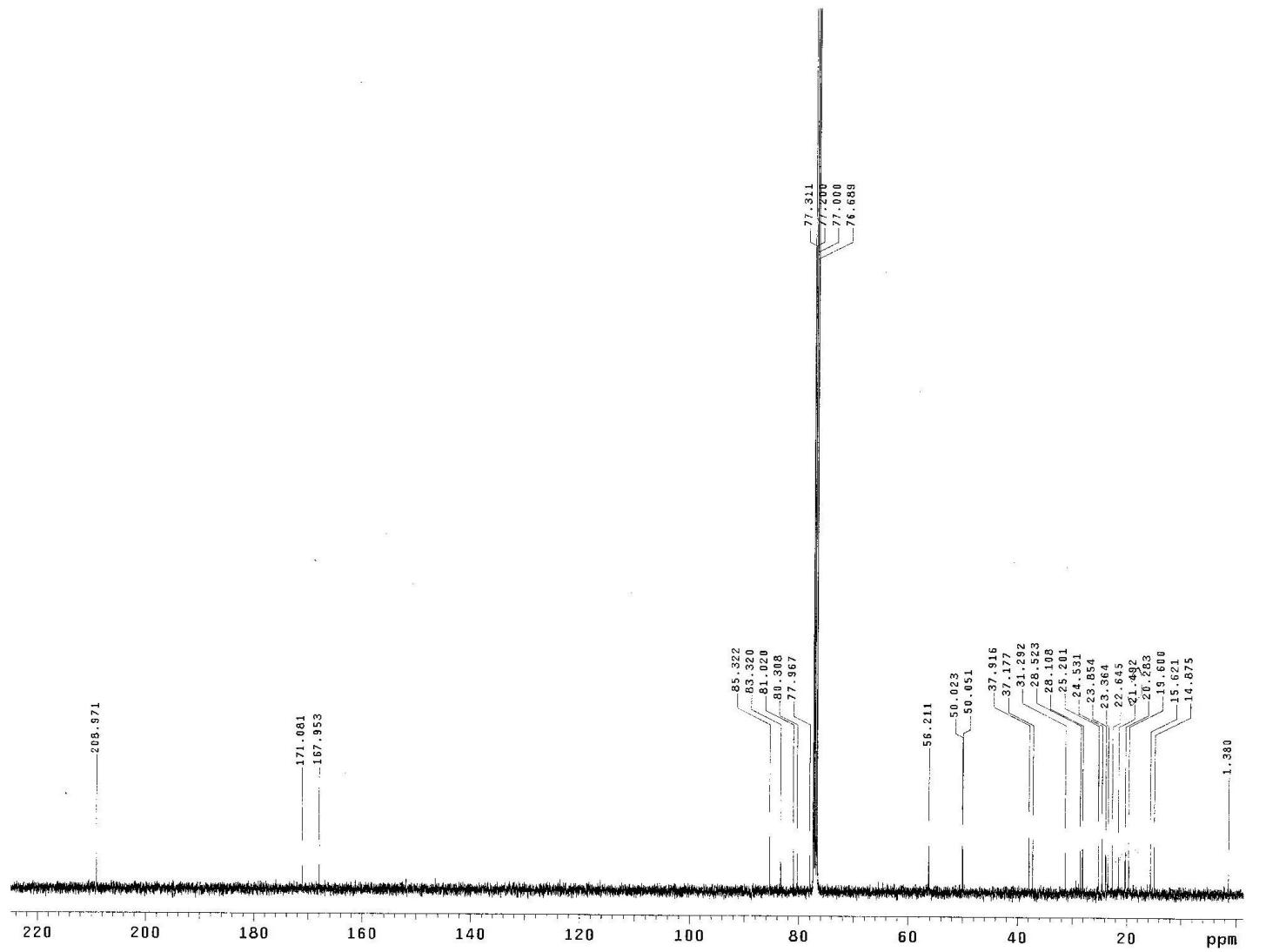


/d=/Data/yu/fsc411e23/11/pdata/1 Administrator Thu Dec 14 17:23:04 2006

**S30** HRESIMS spectrum of **10**.



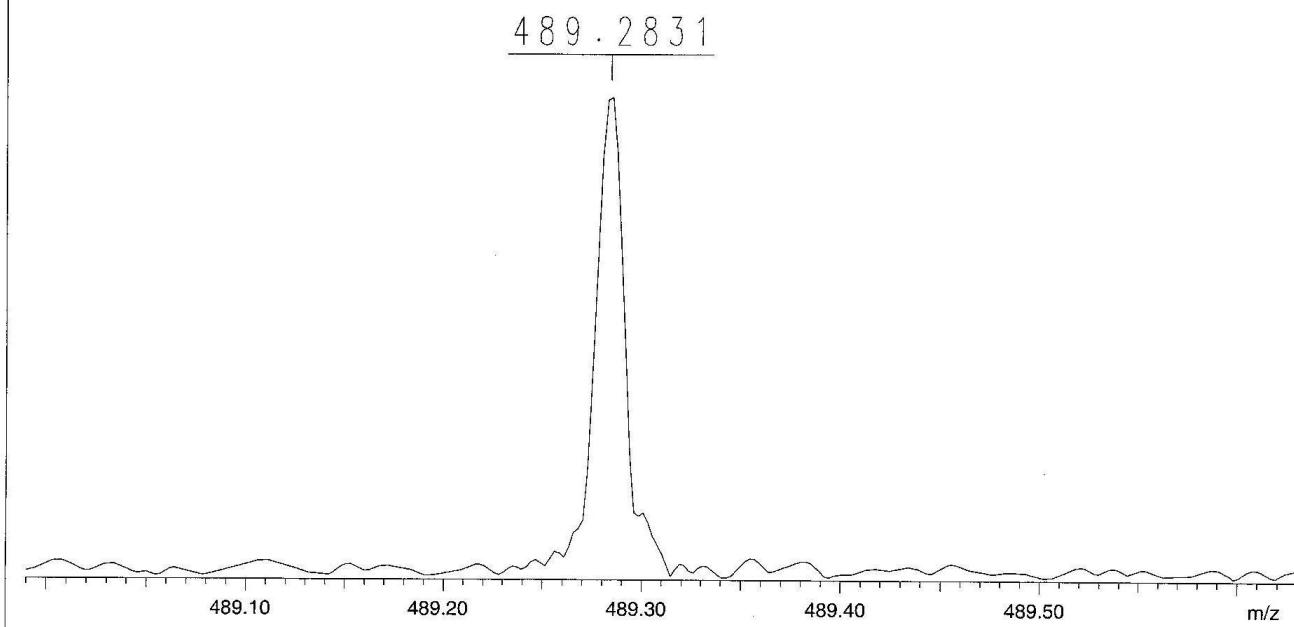
**S31.**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$  at 400 MHz.



S32.  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$  at 100 MHz.

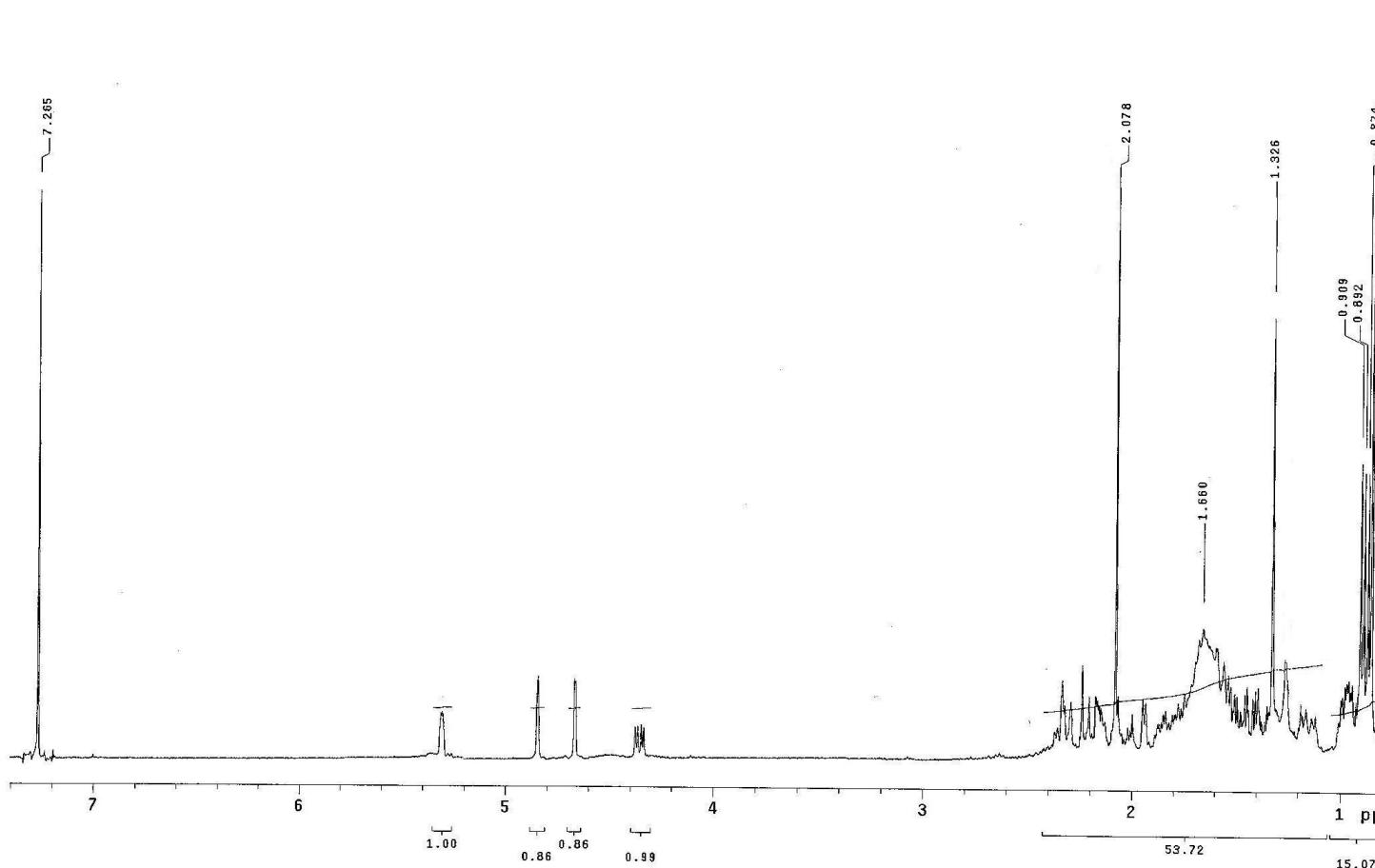
ESI+

Molecular Formula : C<sub>26</sub>H<sub>42</sub>O<sub>7</sub>Na  
Exact Mass : 489.2828  
Measured Mass : 489.2831

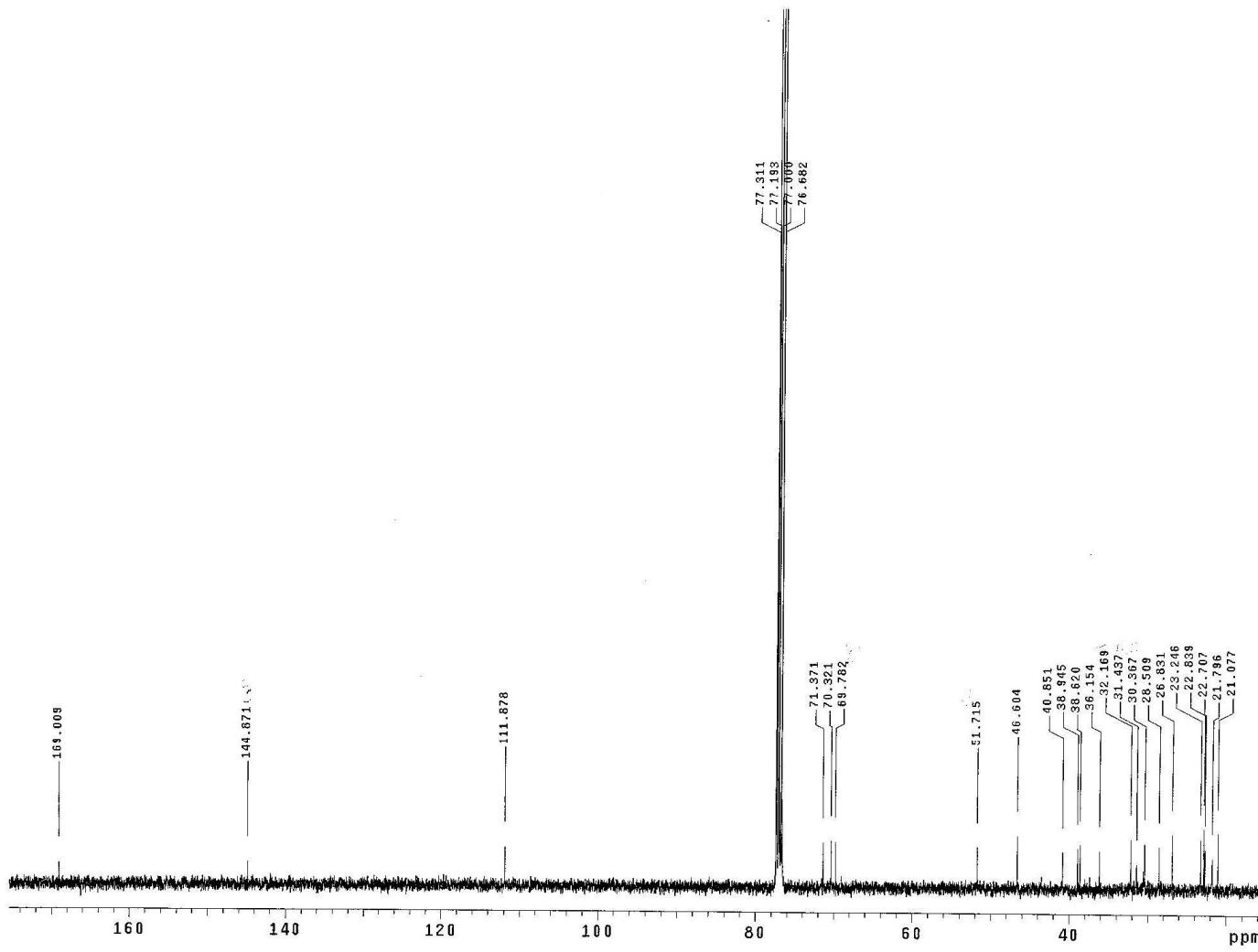


/d=/Data/yu/FSC42331/1/pdata/1 Administrator Thu Mar 20 16:09:13 2008

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

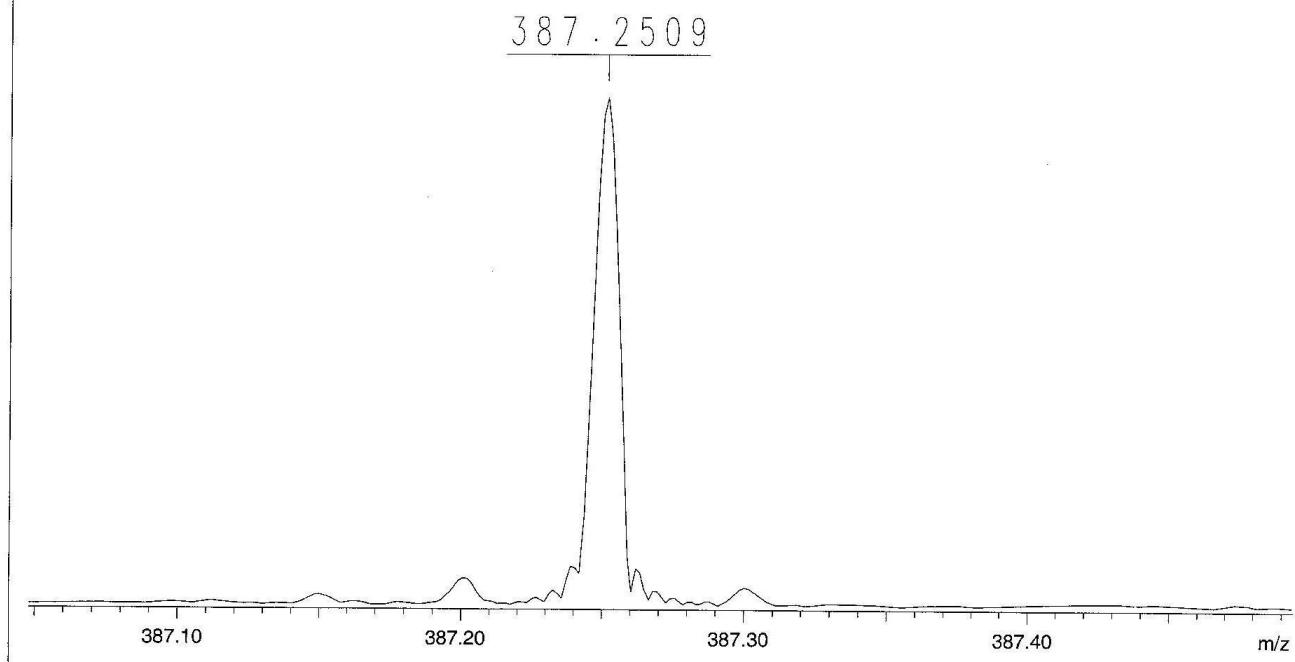


**S34.**  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$  at 400 MHz.



**S35.** <sup>13</sup>C NMR spectrum of **12** in  $\text{CDCl}_3$  at 100 MHz.

ESI+  
Molecular Formula : C<sub>22</sub>H<sub>36</sub>O<sub>4</sub>Na  
Exact Mass : 387.2511  
Measured Mass : 387.2509



/d=/Data/yu/FSC429163min/1/pdata/1 Administrator Fri Aug 15 16:45:27 2008

**S36** HRESIMS spectrum of **12**.