

## Supporting Information

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### Chemical Constituents from the Roots of *Rehmannia glutinosa*

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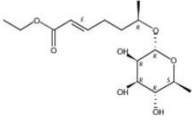
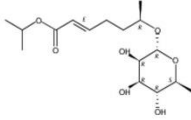
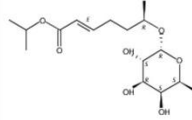
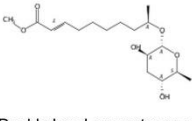
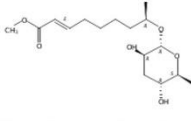
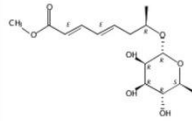
<p>Score: 95</p> <p>1. <b>2563912-22-9</b></p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p><b>C<sub>15</sub> H<sub>26</sub> O<sub>7</sub></b> INDEX NAME NOT YET ASSIGNED</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 318.36 <b>Boiling Point (Predicted)</b> Value: 470.0±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.21±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 13.04±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 2 References Reactions</p>	<p>Score: 95</p> <p>2. <b>2563912-27-4</b></p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p><b>C<sub>16</sub> H<sub>28</sub> O<sub>7</sub></b> INDEX NAME NOT YET ASSIGNED</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 332.39 <b>Boiling Point (Predicted)</b> Value: 475.5±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.19±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 13.04±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References</p>	<p>Score: 95</p> <p>3. <b>2566620-10-6</b></p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p><b>C<sub>16</sub> H<sub>28</sub> O<sub>7</sub></b> INDEX NAME NOT YET ASSIGNED</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 332.39 <b>Boiling Point (Predicted)</b> Value: 475.5±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.19±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 13.04±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References Reactions</p>
<p>Score: 94</p> <p>4. <b>1186217-51-5</b></p>  <p>Double bond geometry as shown., Absolute stereochemistry.</p> <p><b>C<sub>17</sub> H<sub>30</sub> O<sub>8</sub></b> 2-Decenoic acid, 9-[(3,6-dideoxy-α-L-arabino-hexopyranosyl)oxy]-, methyl ester, (2E,9R)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 330.42 <b>Boiling Point (Predicted)</b> Value: 474.0±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.11±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 13.56±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References Reactions</p>	<p>Score: 94</p> <p>5. <b>1355684-04-6</b></p>  <p>Absolute stereochemistry., Rotation (-), Double bond geometry as shown.</p> <p><b>C<sub>16</sub> H<sub>28</sub> O<sub>8</sub></b> 2-Nonenoic acid, 8-[(3,6-dideoxy-α-L-arabino-hexopyranosyl)oxy]-, methyl ester, (2E,8R)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 316.39 <b>Boiling Point (Predicted)</b> Value: 462.5±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.12±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 13.56±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 6 References Reactions</p>	<p>Score: 94</p> <p>6. <b>1413812-28-8</b></p>  <p>Double bond geometry as shown., Rotation (+), Absolute stereochemistry.</p> <p><b>C<sub>15</sub> H<sub>24</sub> O<sub>7</sub></b> 2,4-Octadienoic acid, 7-[(6-deoxy-α-L-mannopyranosyl)oxy]-, methyl ester, (2E,4E,7R)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 316.35 <b>Boiling Point (Predicted)</b> Value: 482.3±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.23±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 13.03±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References Reactions</p>

Figure S1: SciFinder search report of the new compound with 94-95% similarity

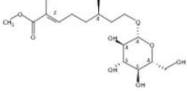
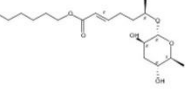
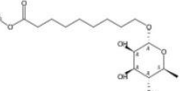
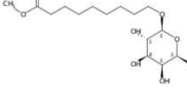
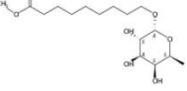
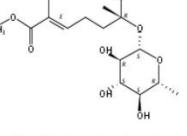
<p>Score: 93</p> <p>7.</p> <p><b>158921-24-5</b></p>  <p>Double bond geometry as shown., Rotation (-)., Absolute stereochemistry.</p> <p><b>C<sub>17</sub> H<sub>30</sub> O<sub>8</sub></b> 2-Octenoic acid, 8-(β-D-glucopyranosyloxy)-2,6-dimethyl-, methyl ester, (2E,6R)-</p> <p><b>Key Physical Properties:</b></p> <p><b>Molecular Weight</b> 362.42</p> <p><b>Boiling Point (Predicted)</b> Value: 546.7±50.0 °C   Condition: Press: 760 Torr</p> <p><b>Density (Predicted)</b> Value: 1.24±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>pKa (Predicted)</b> Value: 12.94±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 3 References</p>	<p>Score: 93</p> <p>8.</p> <p><b>2563912-50-3</b></p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p><b>C<sub>19</sub> H<sub>34</sub> O<sub>8</sub></b> INDEX NAME NOT YET ASSIGNED</p> <p><b>Key Physical Properties:</b></p> <p><b>Molecular Weight</b> 358.47</p> <p><b>Boiling Point (Predicted)</b> Value: 497.1±45.0 °C   Condition: Press: 760 Torr</p> <p><b>Density (Predicted)</b> Value: 1.08±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>pKa (Predicted)</b> Value: 13.55±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 2 References</p>	<p>Score: 92</p> <p>9.</p> <p><b>74597-40-3</b></p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>16</sub> H<sub>30</sub> O<sub>7</sub></b> Nonanoic acid, 9-[(6-deoxy-α-L-mannopyranosyl)oxy]-, methyl ester</p> <p><b>Key Physical Properties:</b></p> <p><b>Molecular Weight</b> 334.41</p> <p><b>Boiling Point (Predicted)</b> Value: 464.1±45.0 °C   Condition: Press: 760 Torr</p> <p><b>Density (Predicted)</b> Value: 1.17±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>pKa (Predicted)</b> Value: 13.08±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 10 References Reactions</p>
<p>Score: 92</p> <p>10.</p> <p><b>143528-28-3</b></p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>16</sub> H<sub>30</sub> O<sub>7</sub></b> Nonanoic acid, 9-[(6-deoxy-β-L-galactopyranosyl)oxy]-, methyl ester</p> <p><b>Key Physical Properties:</b></p> <p><b>Molecular Weight</b> 334.41</p> <p><b>Boiling Point (Predicted)</b> Value: 464.1±45.0 °C   Condition: Press: 760 Torr</p> <p><b>Density (Predicted)</b> Value: 1.17±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>pKa (Predicted)</b> Value: 13.08±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 4 References</p>	<p>Score: 92</p> <p>11.</p> <p><b>143528-33-0</b></p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>16</sub> H<sub>30</sub> O<sub>7</sub></b> Nonanoic acid, 9-[(6-deoxy-α-L-galactopyranosyl)oxy]-, methyl ester</p> <p><b>Key Physical Properties:</b></p> <p><b>Molecular Weight</b> 334.41</p> <p><b>Boiling Point (Predicted)</b> Value: 464.1±45.0 °C   Condition: Press: 760 Torr</p> <p><b>Density (Predicted)</b> Value: 1.17±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>pKa (Predicted)</b> Value: 13.08±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 2 References</p>	<p>Score: 92</p> <p>12.</p> <p><b>263759-17-7</b></p>  <p>Double bond geometry as shown., Rotation (+)., Absolute stereochemistry.</p> <p><b>C<sub>17</sub> H<sub>28</sub> O<sub>7</sub></b> 2,7-Octadienoic acid, 6-[(6-deoxy-β-D-glucopyranosyl)oxy]-2,6-dimethyl-, methyl ester, (2E,6R)-</p> <p><b>Key Physical Properties:</b></p> <p><b>Molecular Weight</b> 344.40</p> <p><b>Boiling Point (Predicted)</b> Value: 507.1±50.0 °C   Condition: Press: 760 Torr</p> <p><b>Density (Predicted)</b> Value: 1.19±0.1 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>pKa (Predicted)</b> Value: 13.03±0.70   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 3 References</p>

Figure S2: SciFinder search report of the new compound with 92-93% similarity

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

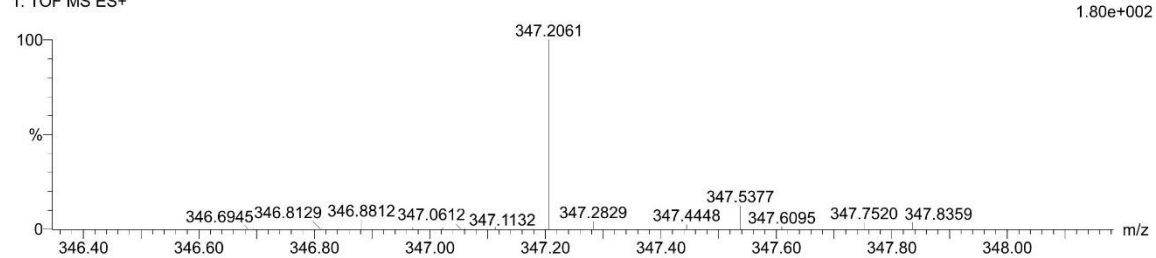
Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

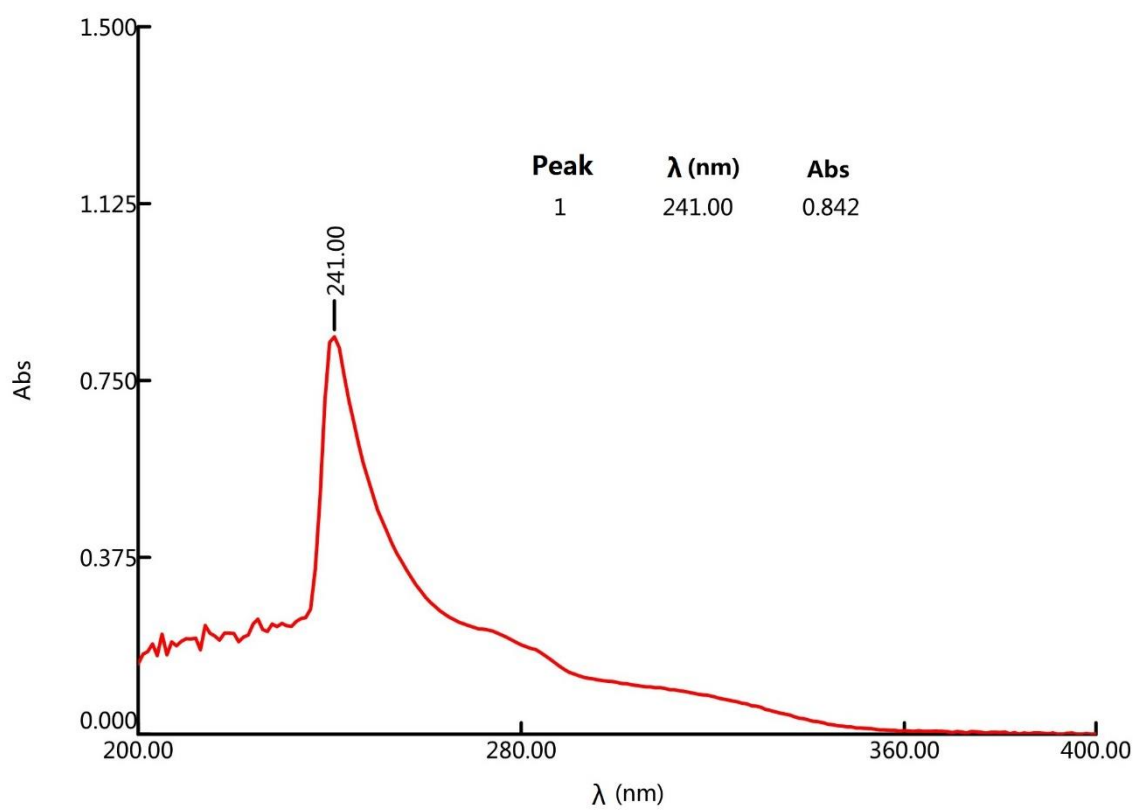
C: 17-17 H: 31-31 O: 0-10 F: 0-5

1: TOF MS ES+

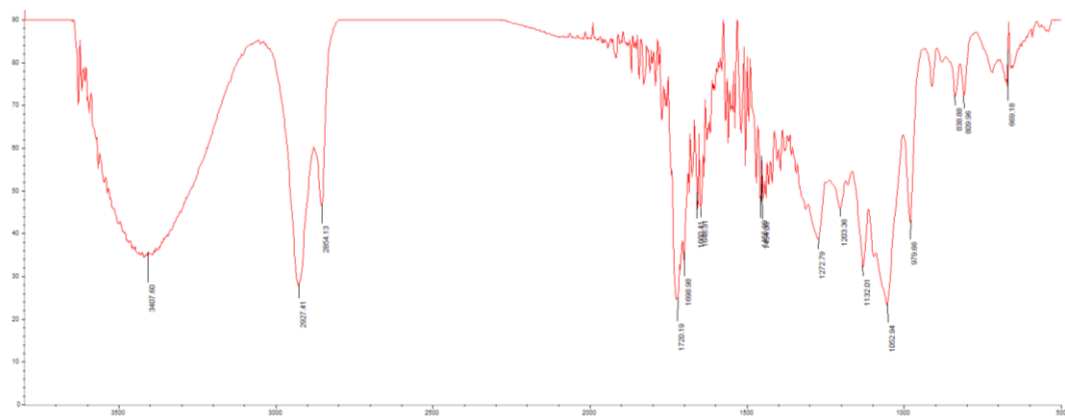
Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
347.2061	347.2070	-0.9	-2.6	2.5	66.0	n/a	n/a	C17 H31 O7

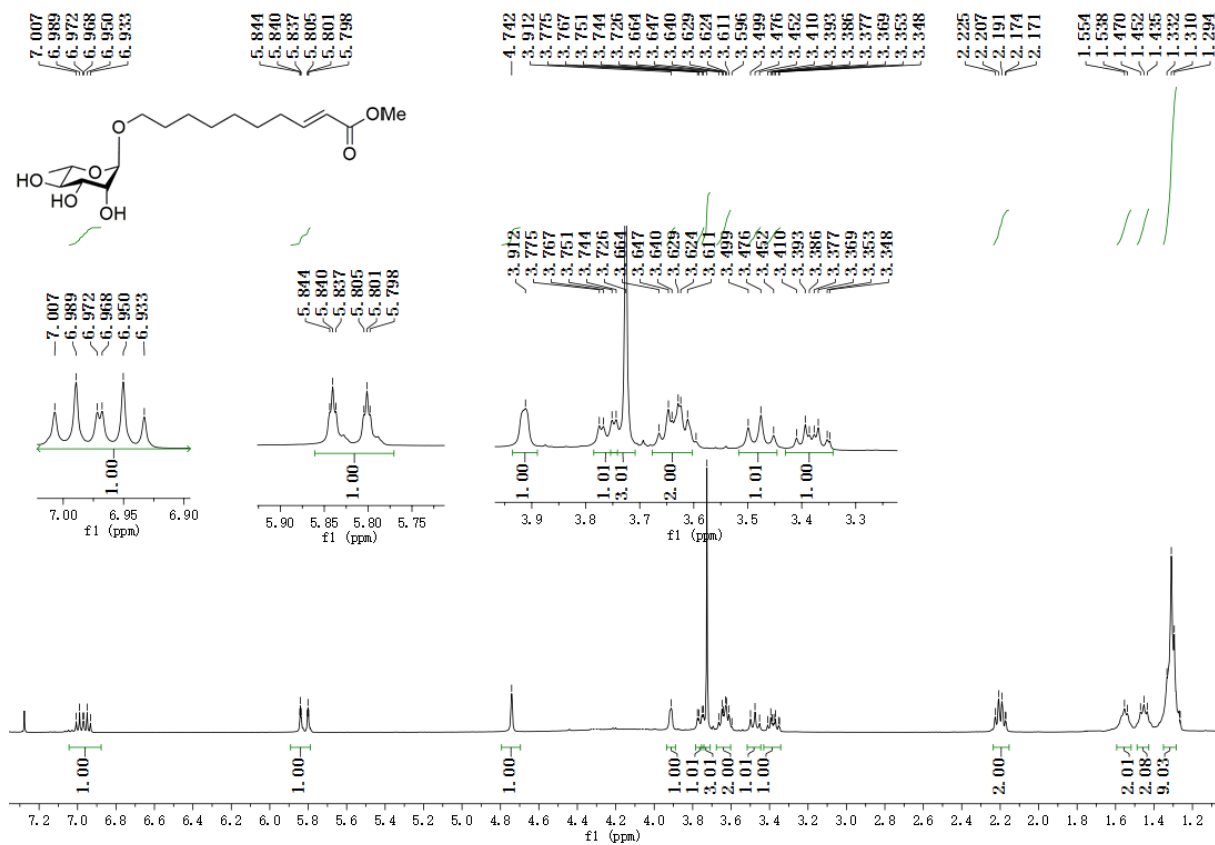
Figure S3: HR-ESI-MS spectrum of 1



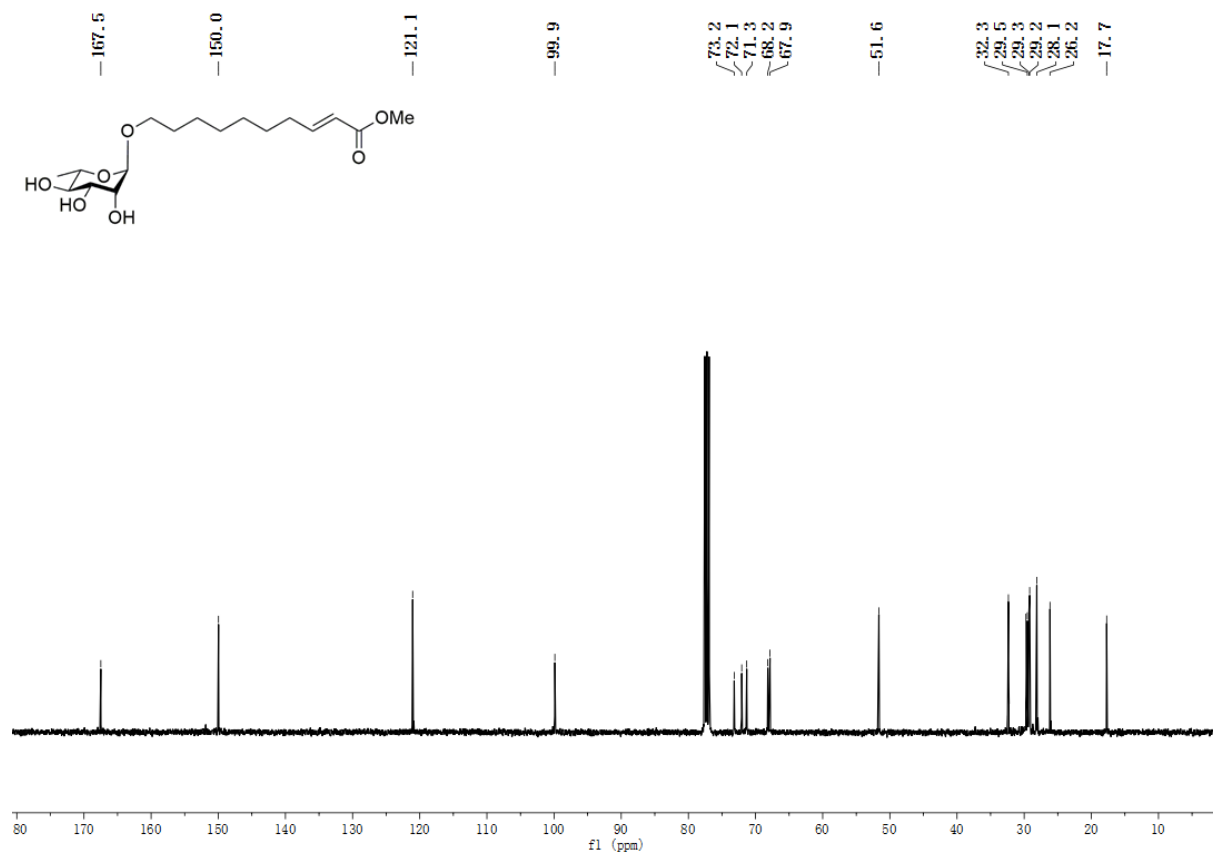
**Figure S4:** UV spectrum of **1** in CHCl<sub>3</sub>



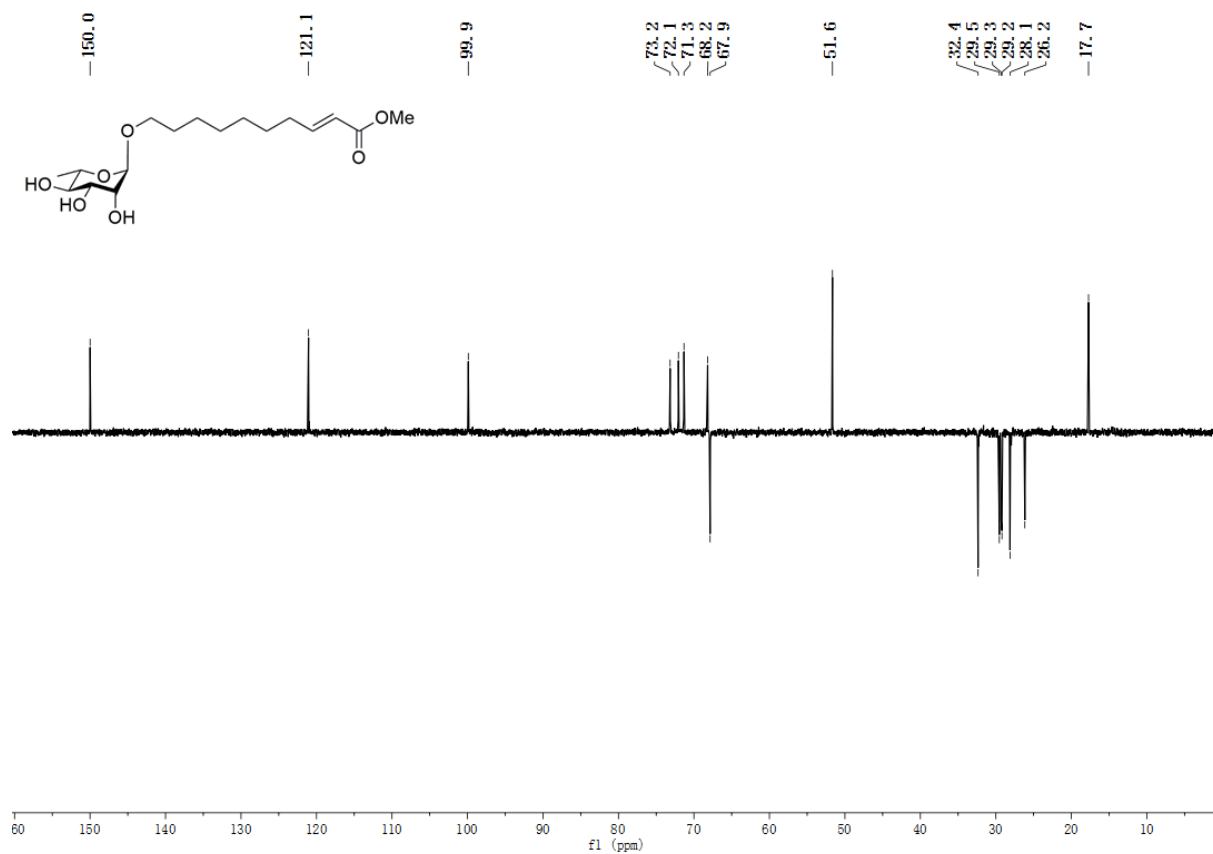
**Figure S5:** IR spectrum of **1**



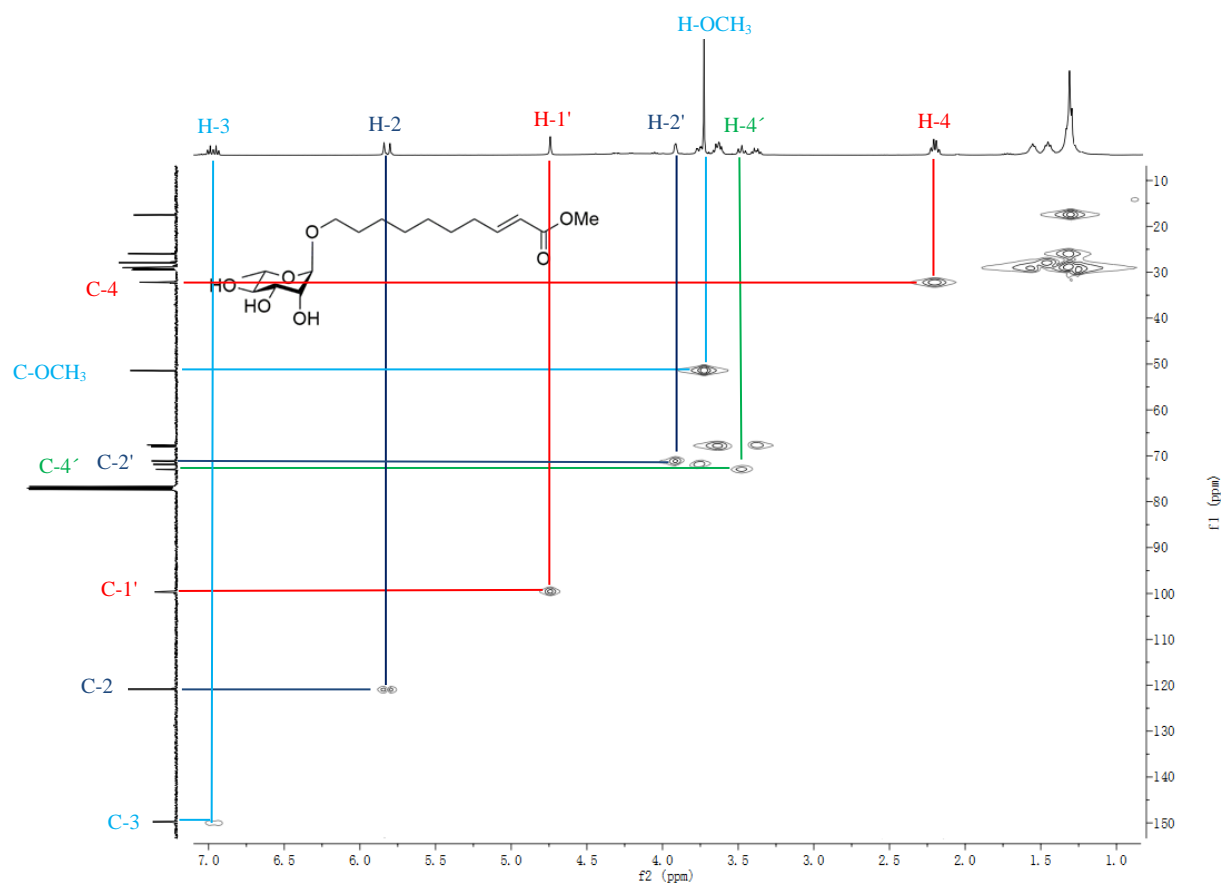




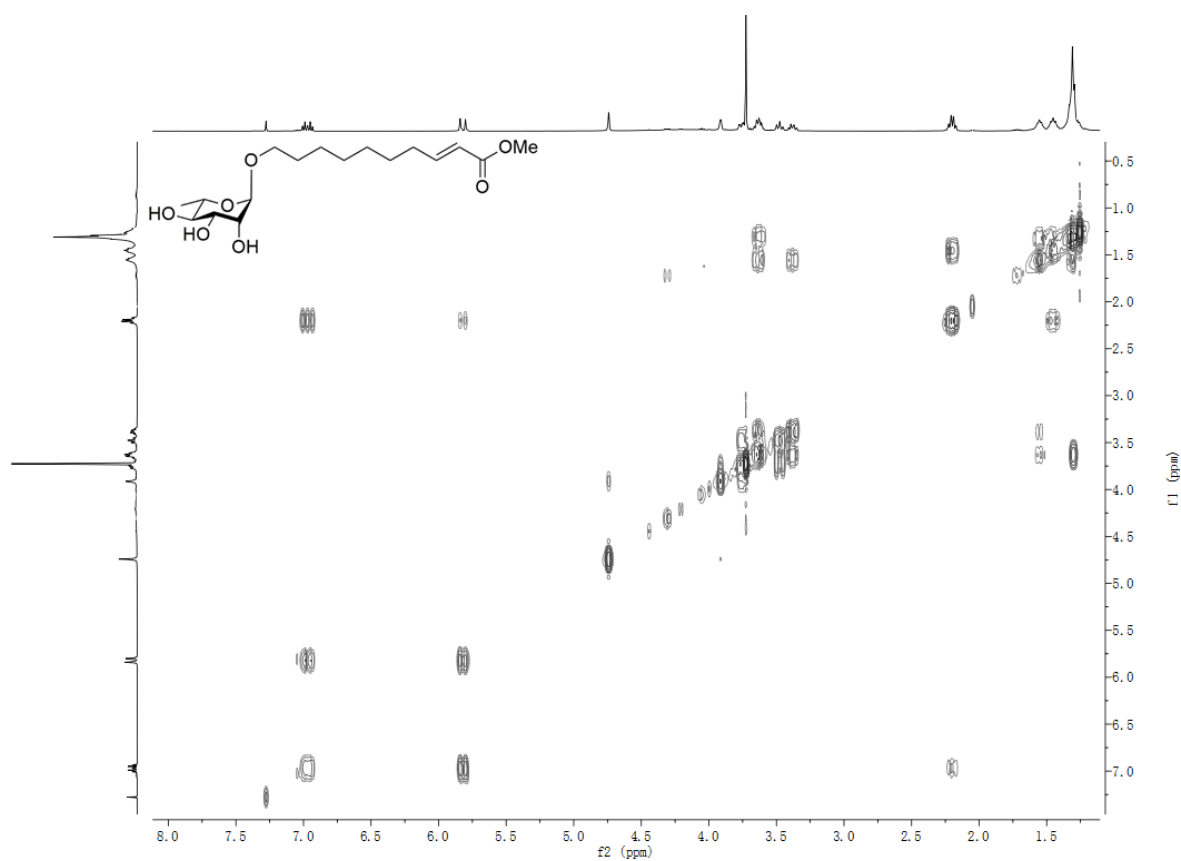
**Figure S7:**  $^{13}\text{C}$  NMR spectrum (100 MHz) of **1** in  $\text{CDCl}_3$



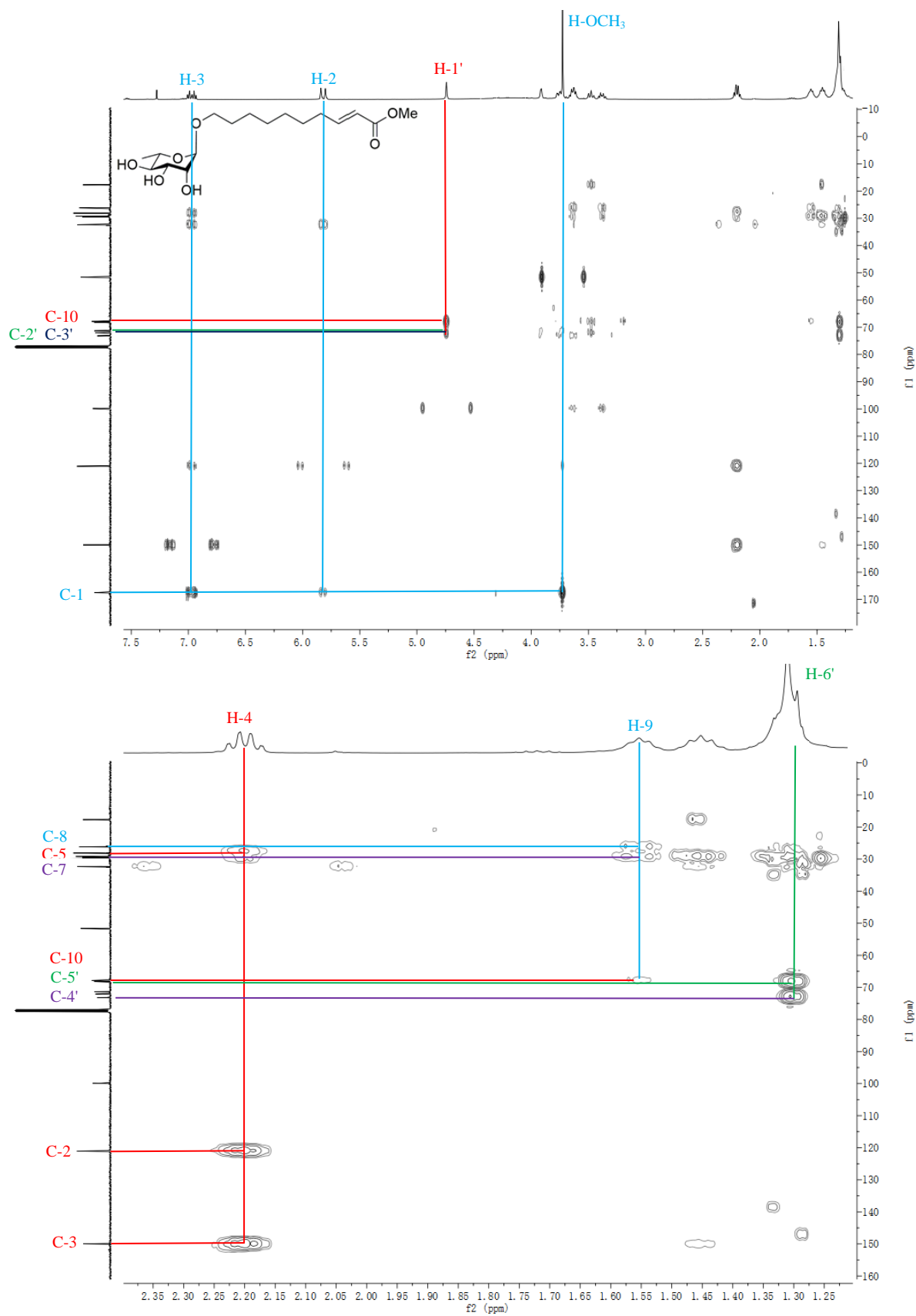
**Figure S8:** DEPT 135 spectrum of **1** in CDCl<sub>3</sub>



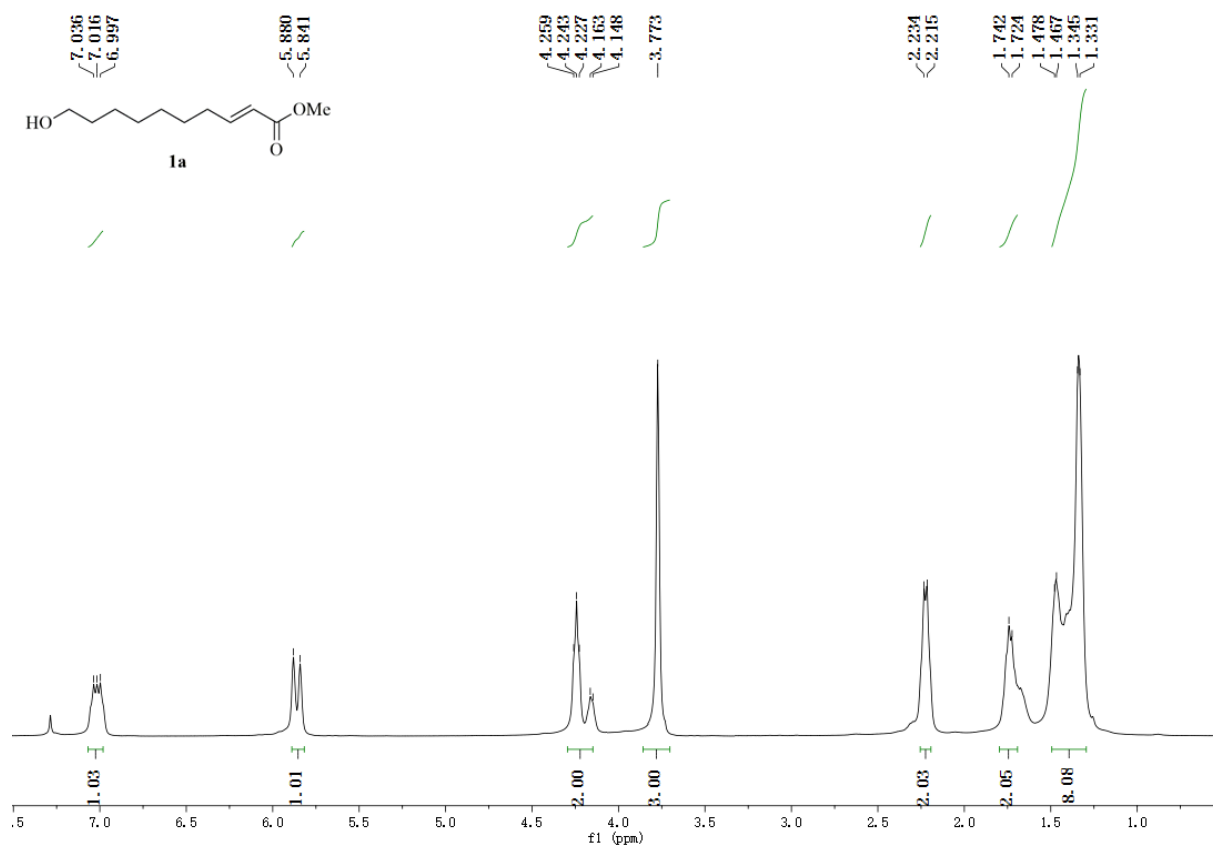
**Figure S9:** HSQC spectrum of **1** in  $\text{CDCl}_3$



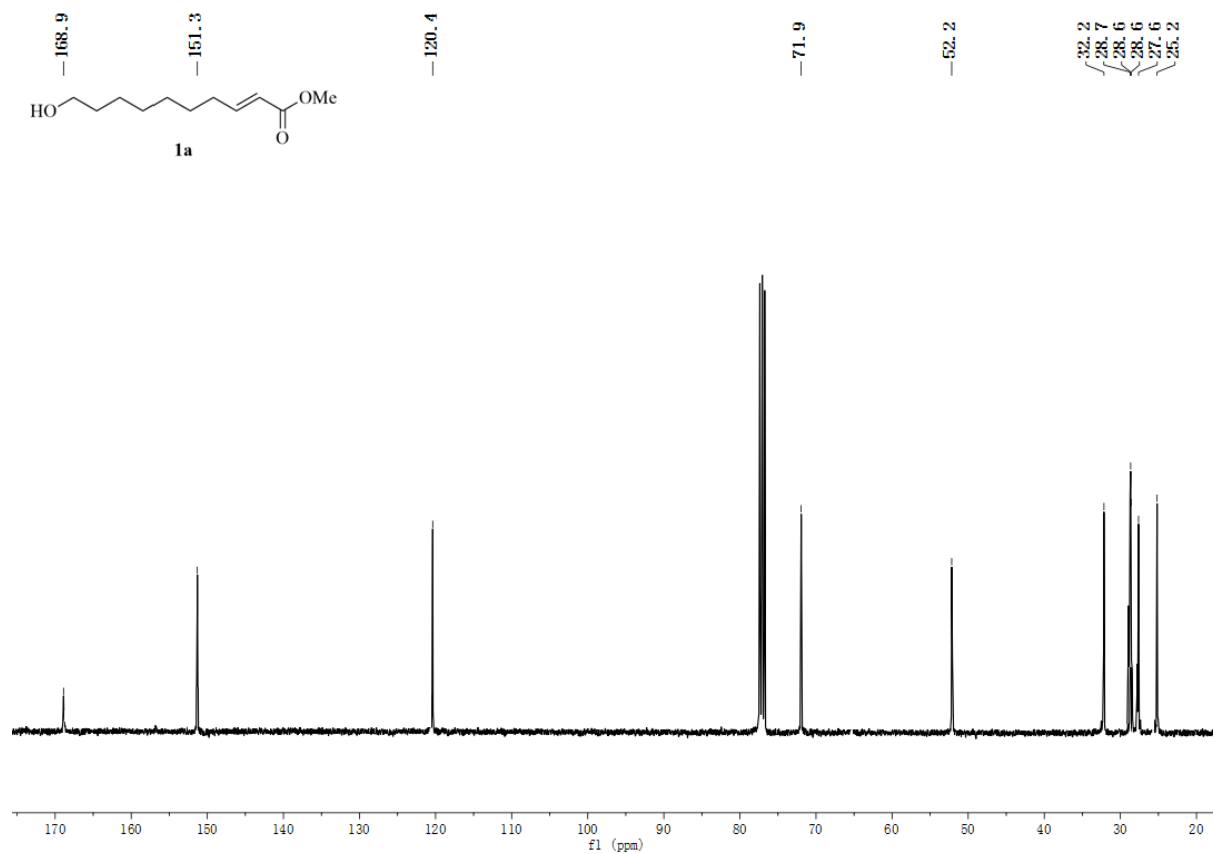
**Figure S10:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{CDCl}_3$



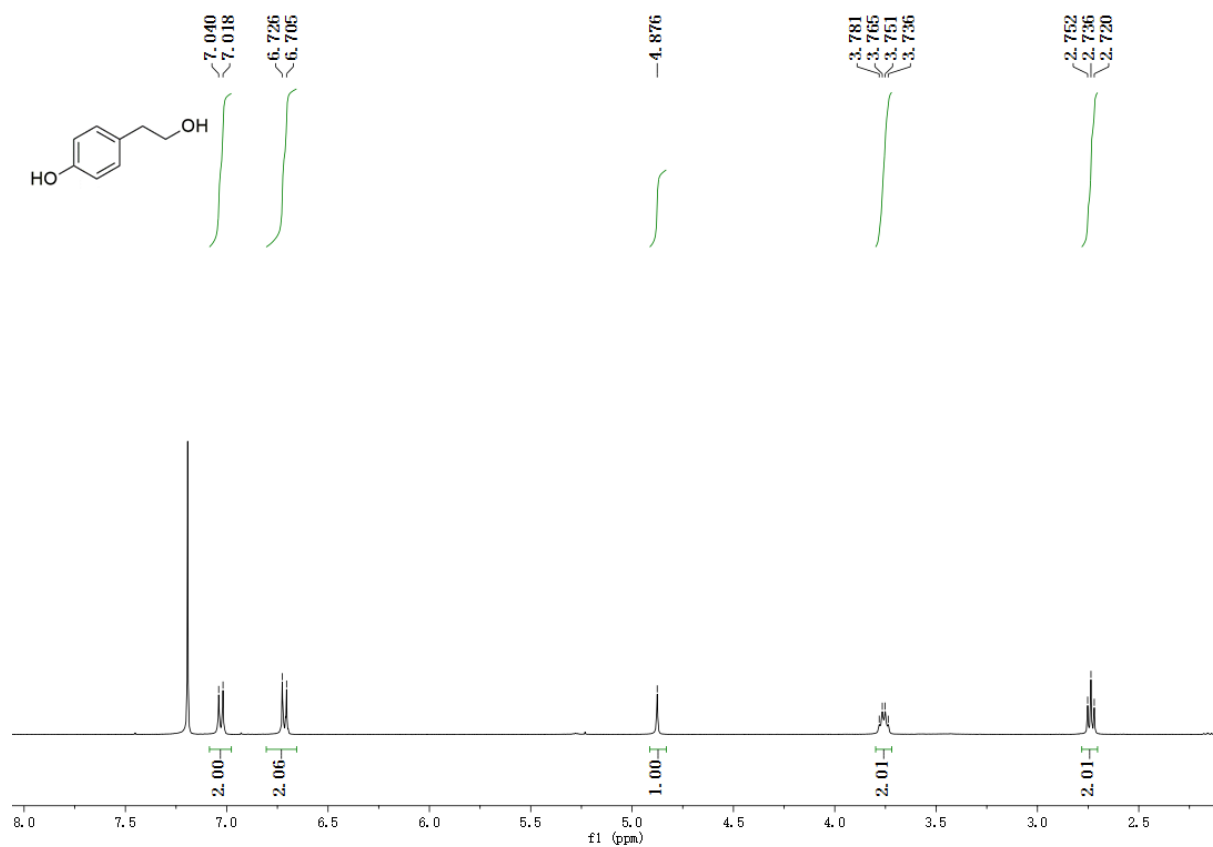
**Figure S11:** HMBC spectrum of **1** in CDCl<sub>3</sub>



**Figure S12:**  $^1\text{H}$  NMR spectrum (400 MHz) of **1a** in  $\text{CDCl}_3$

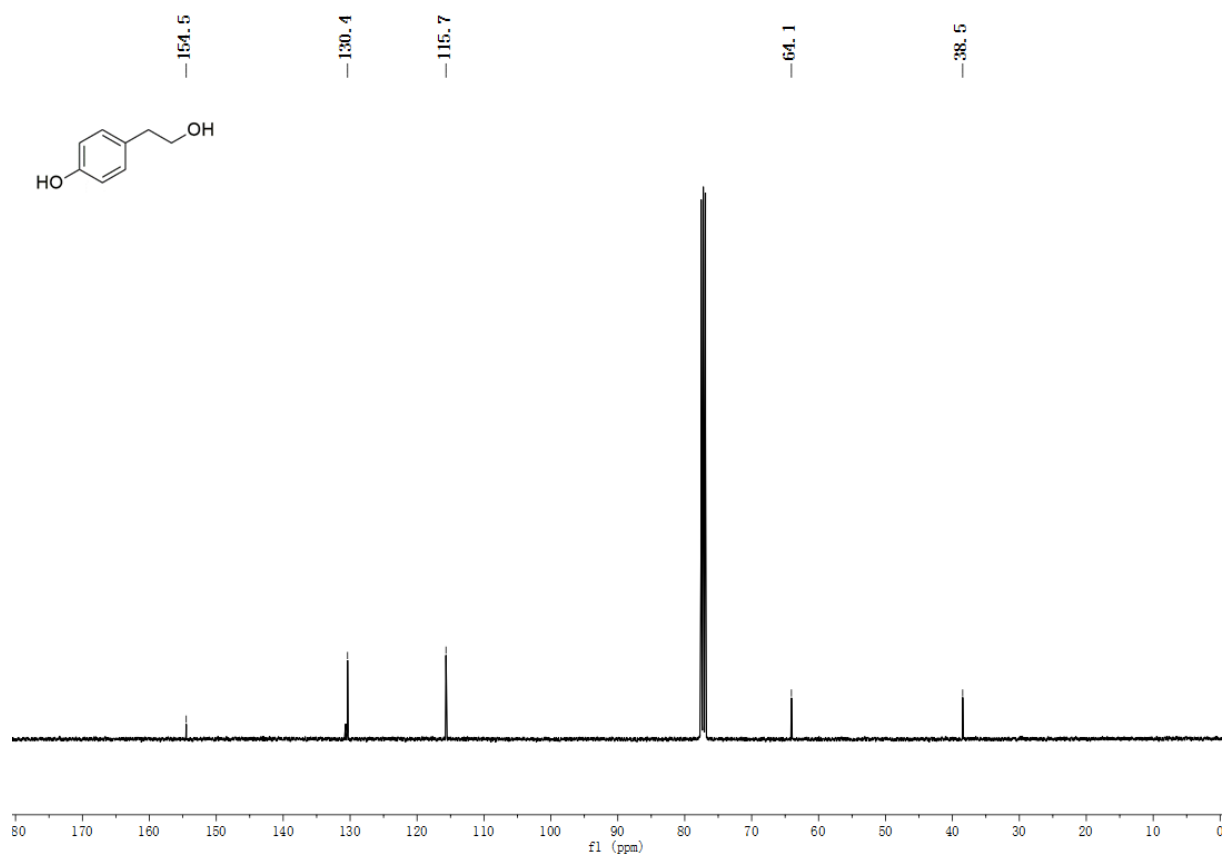


**Figure S13:** <sup>13</sup>C NMR spectrum (100 MHz) of **1a** in CDCl<sub>3</sub>

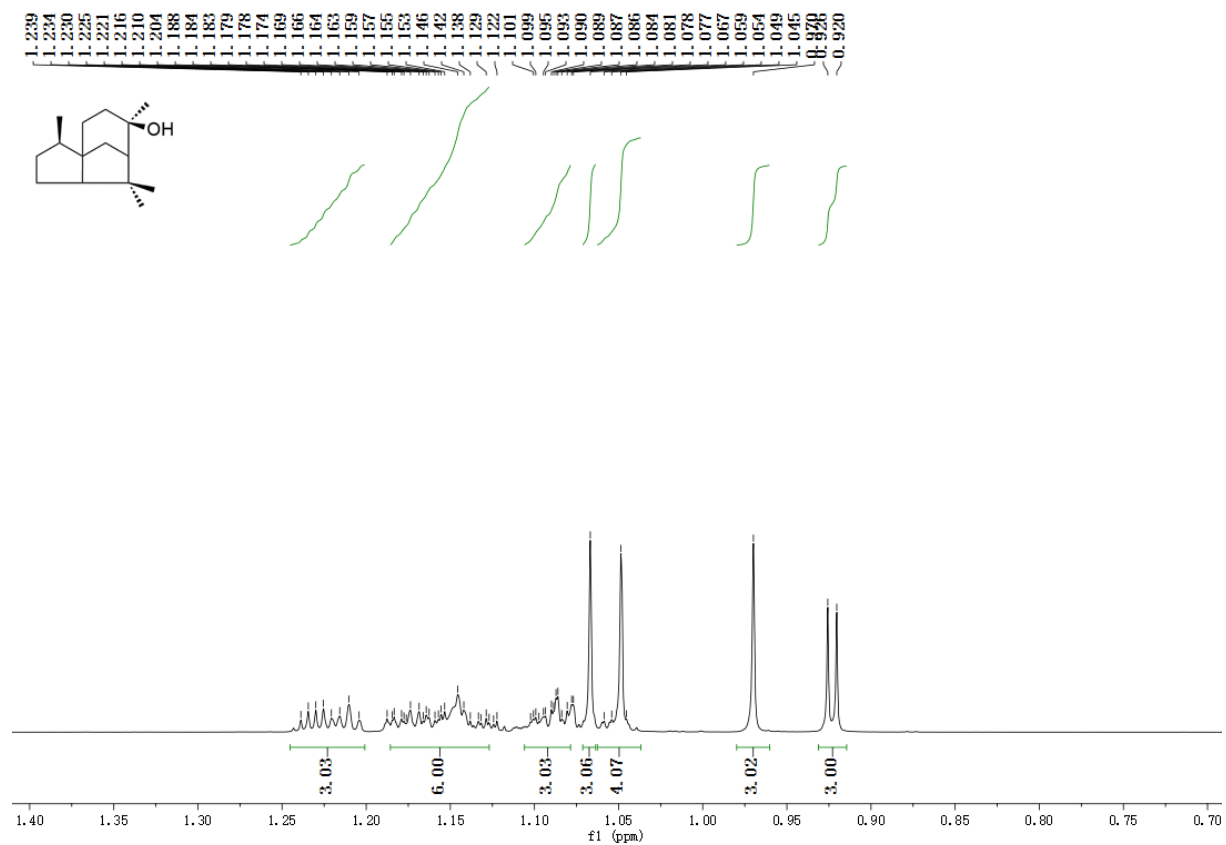


**Figure S14:** <sup>1</sup>H NMR spectrum (400 MHz) of **2** in CDCl<sub>3</sub>

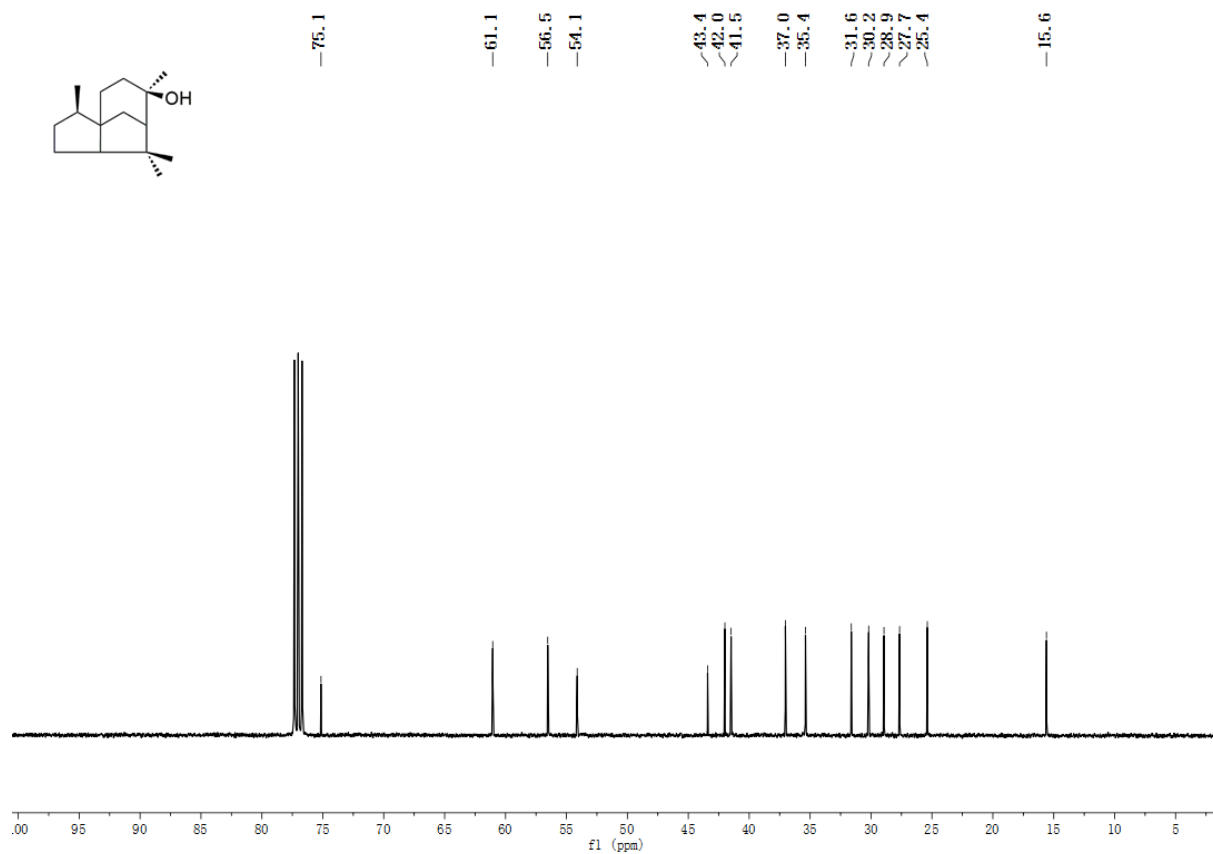




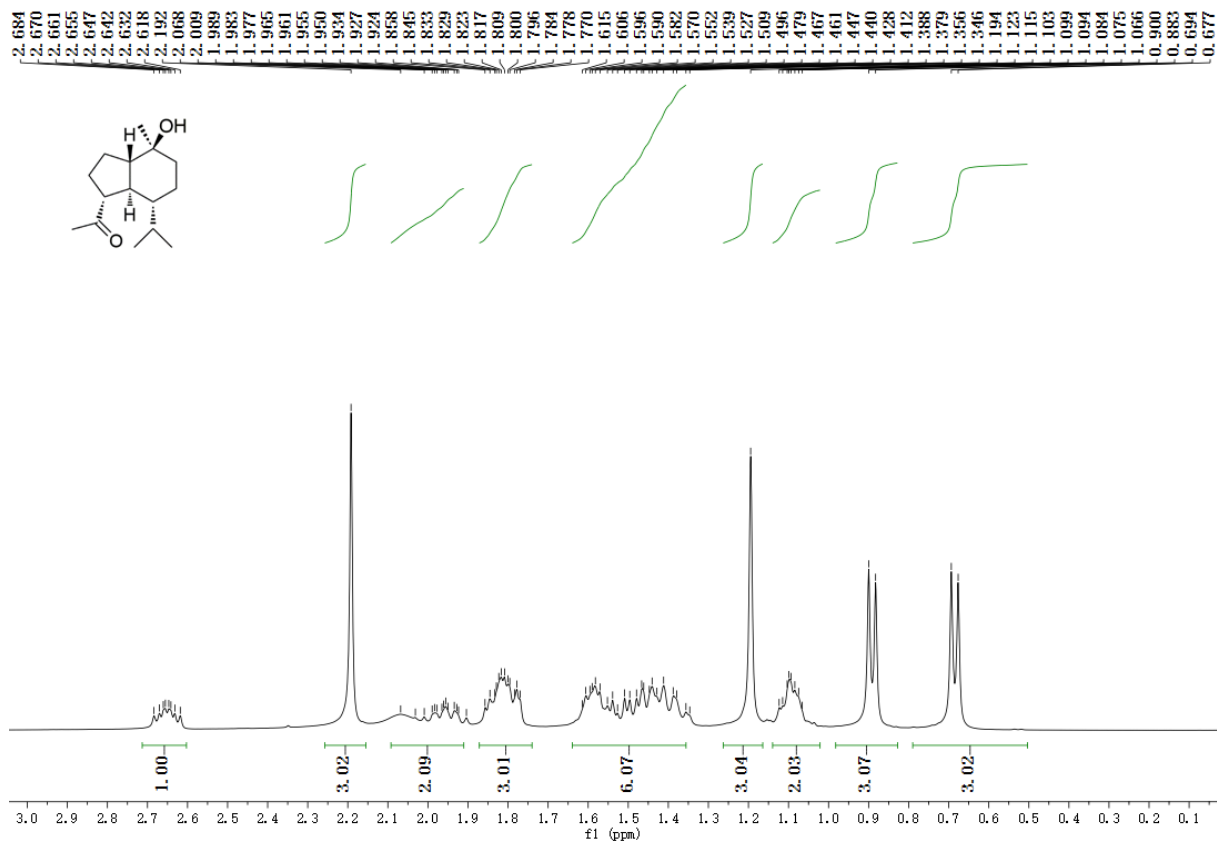
**Figure S15:** <sup>13</sup>C NMR spectrum (100 MHz) of **2** in CDCl<sub>3</sub>



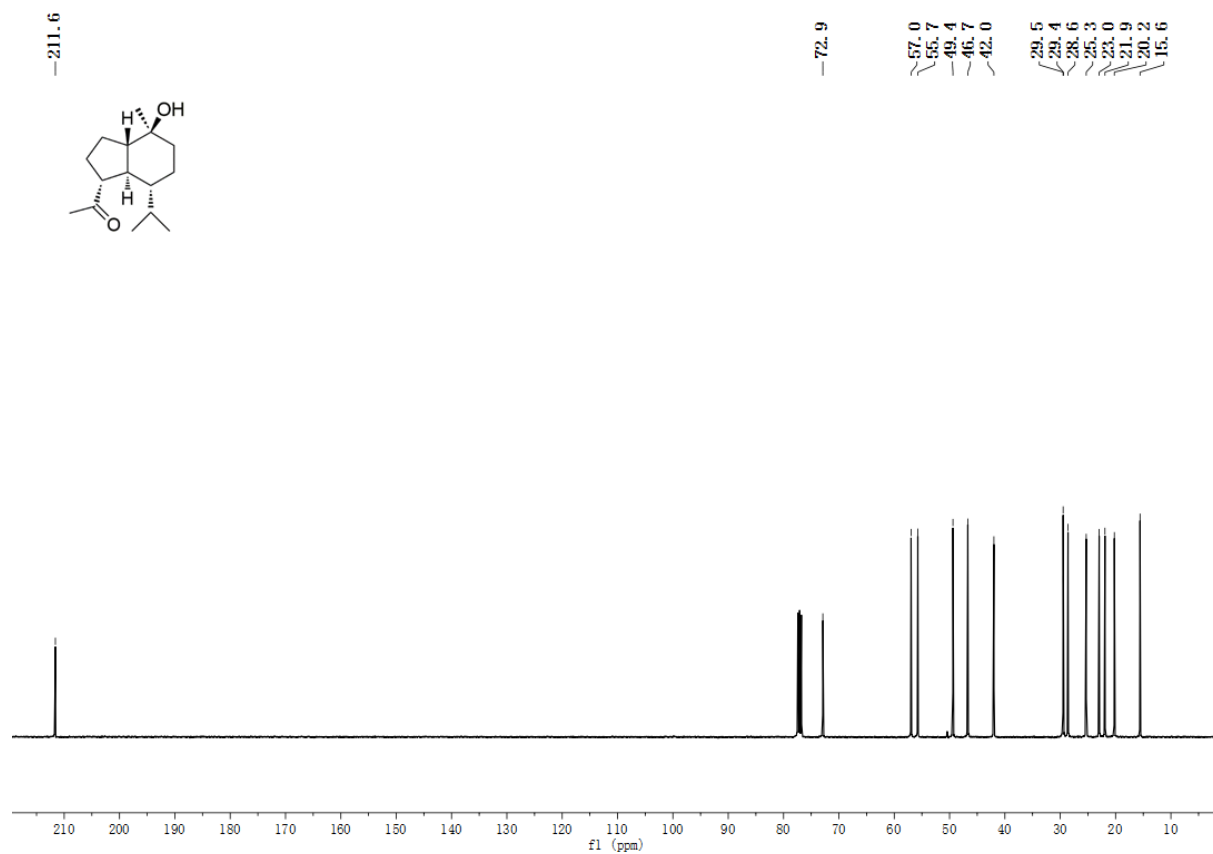
**Figure S16:**  $^1\text{H}$  NMR spectrum (400 MHz) of **3** in  $\text{CDCl}_3$



**Figure S17:** <sup>13</sup>C NMR spectrum (100 MHz) of **3** in CDCl<sub>3</sub>



**Figure S18:** <sup>1</sup>H NMR spectrum (400 MHz) of **4** in CDCl<sub>3</sub>



**Figure S19:** <sup>13</sup>C NMR spectrum (100 MHz) of **4** in CDCl<sub>3</sub>

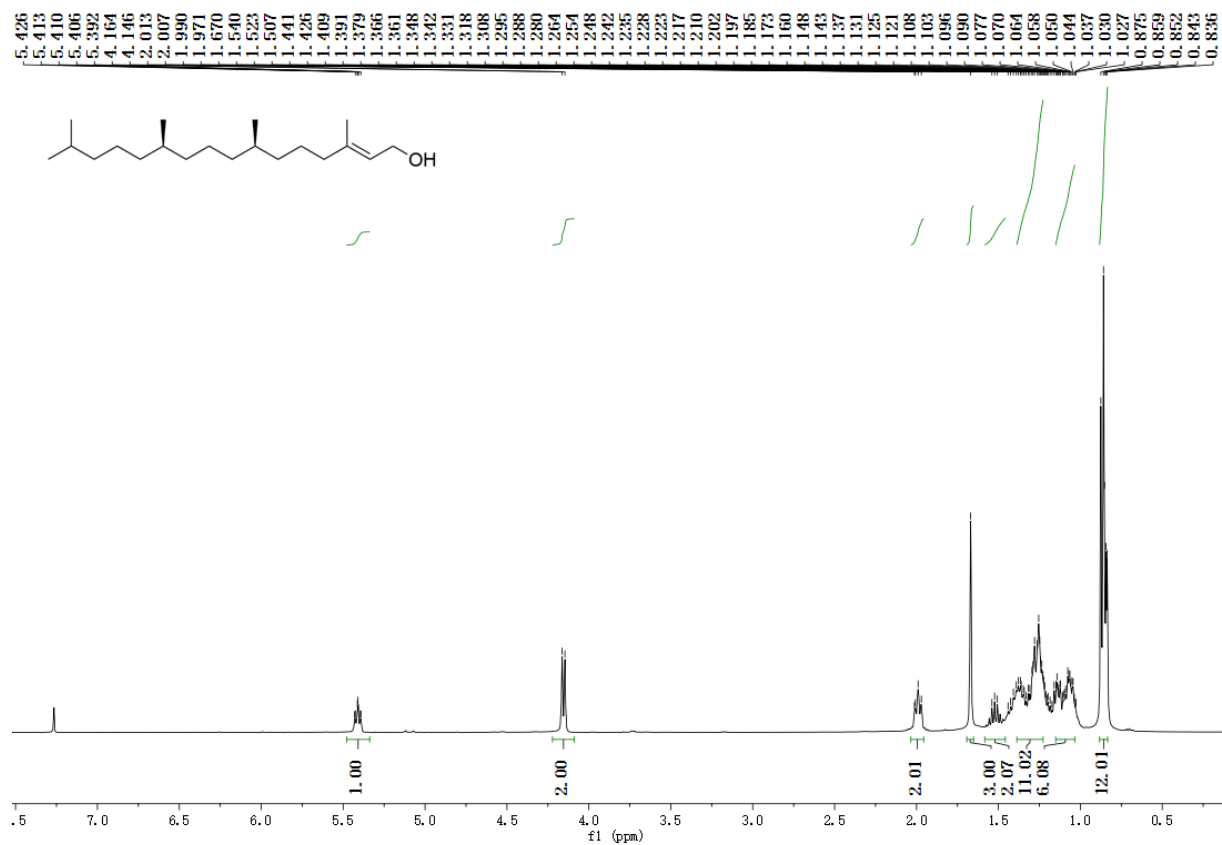
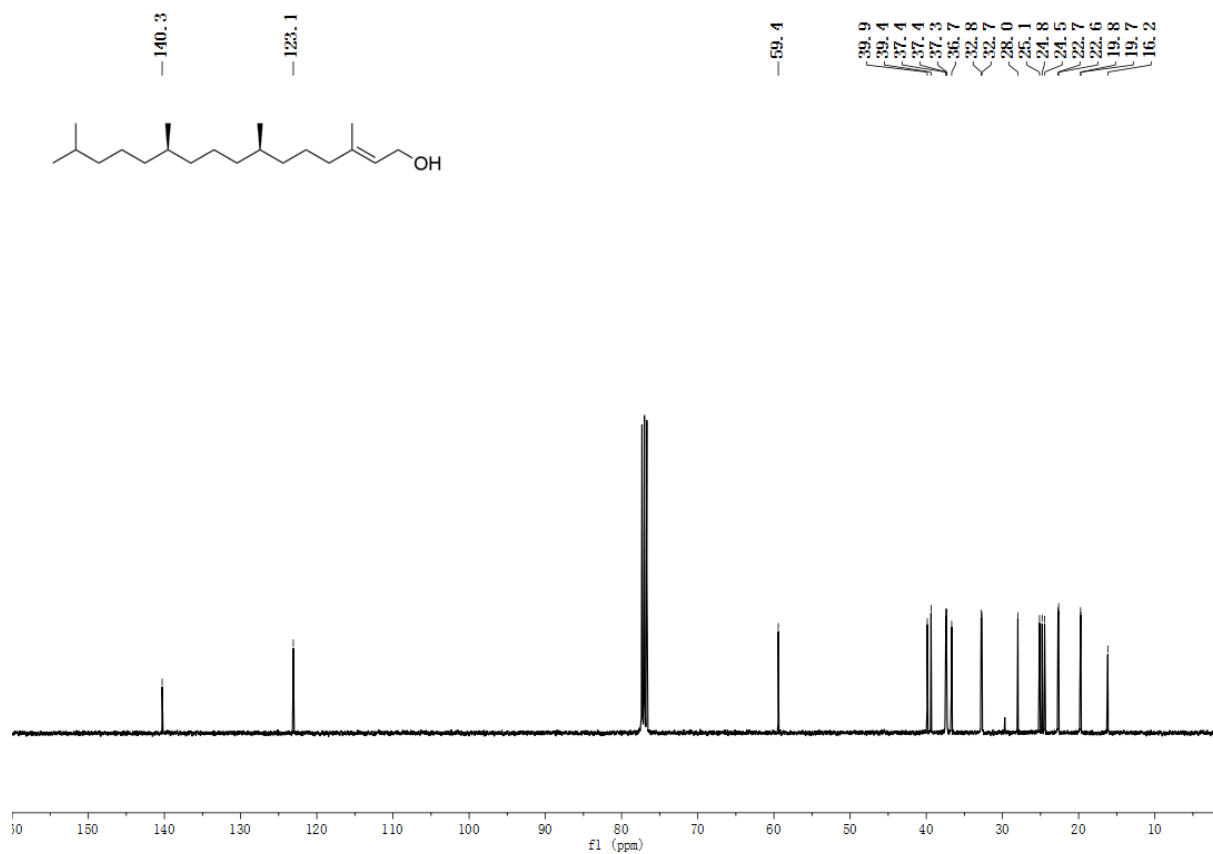
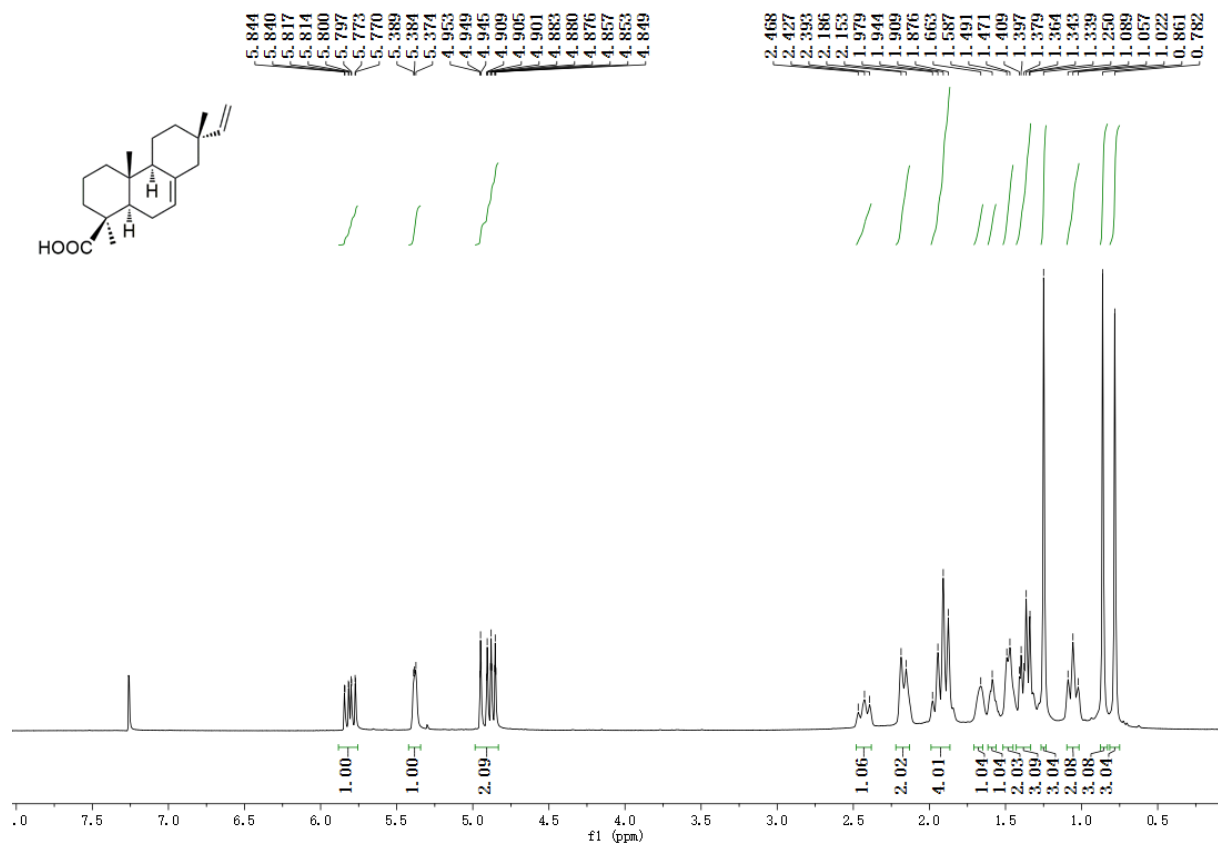


Figure S20: <sup>1</sup>H NMR spectrum (400 MHz) of 5 in CDCl<sub>3</sub>

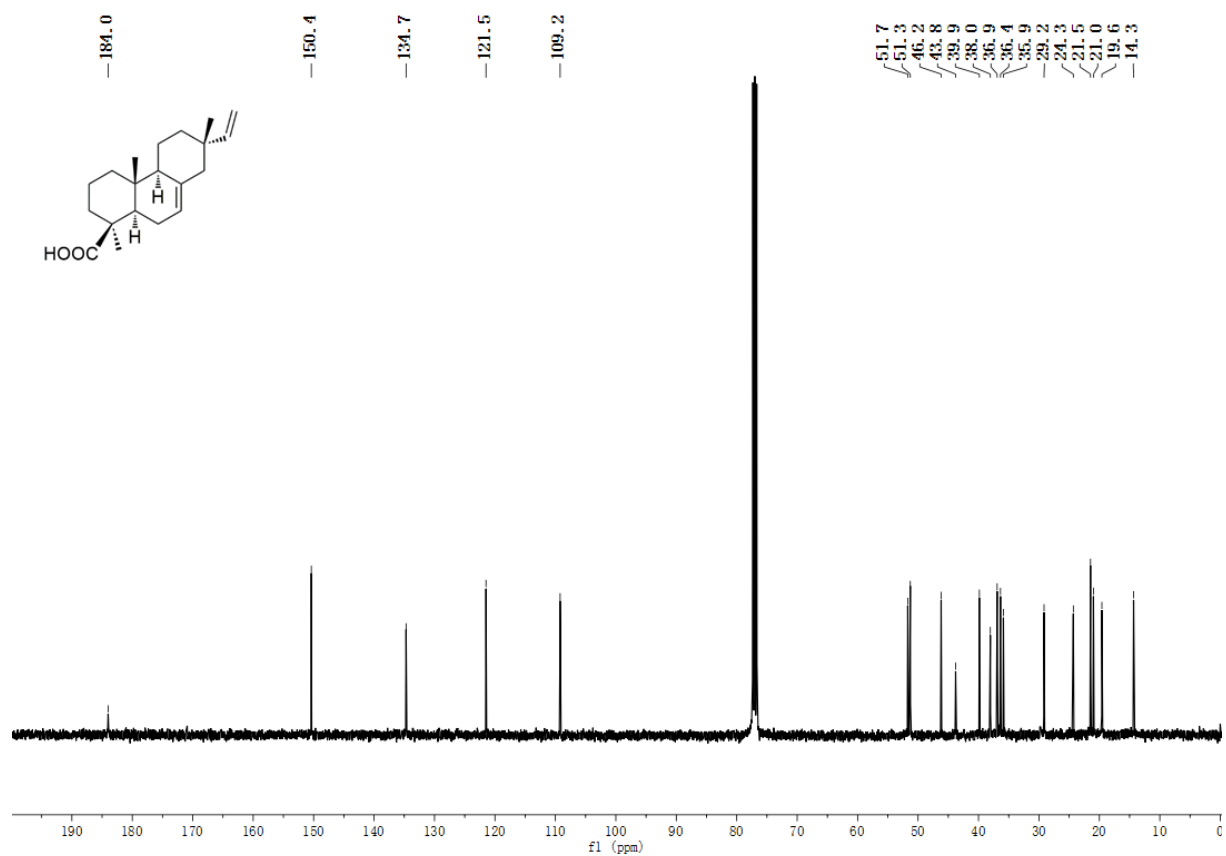


**Figure S21:**  $^{13}\text{C}$  NMR spectrum (100 MHz) of **5** in  $\text{CDCl}_3$

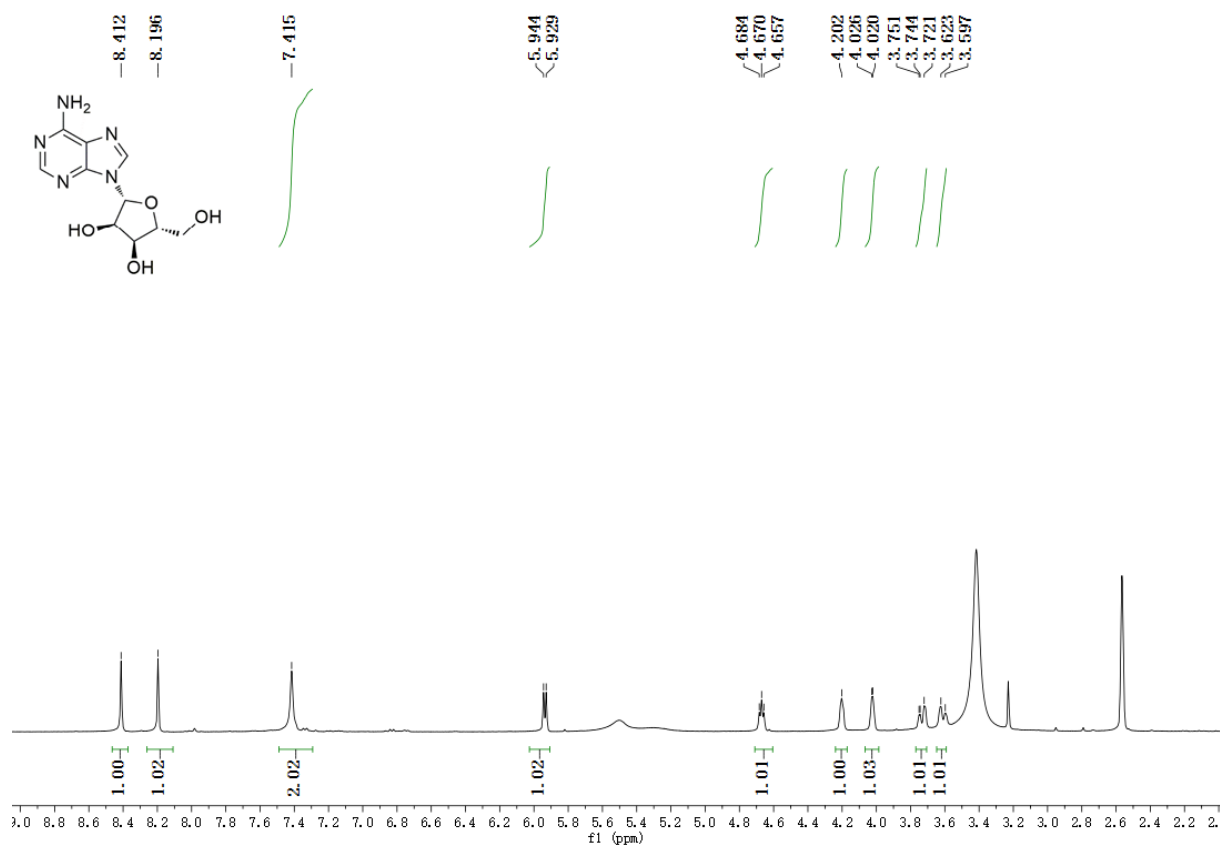


**Figure S22:**  $^1\text{H}$  NMR spectrum (400 MHz) of **6** in  $\text{CDCl}_3$

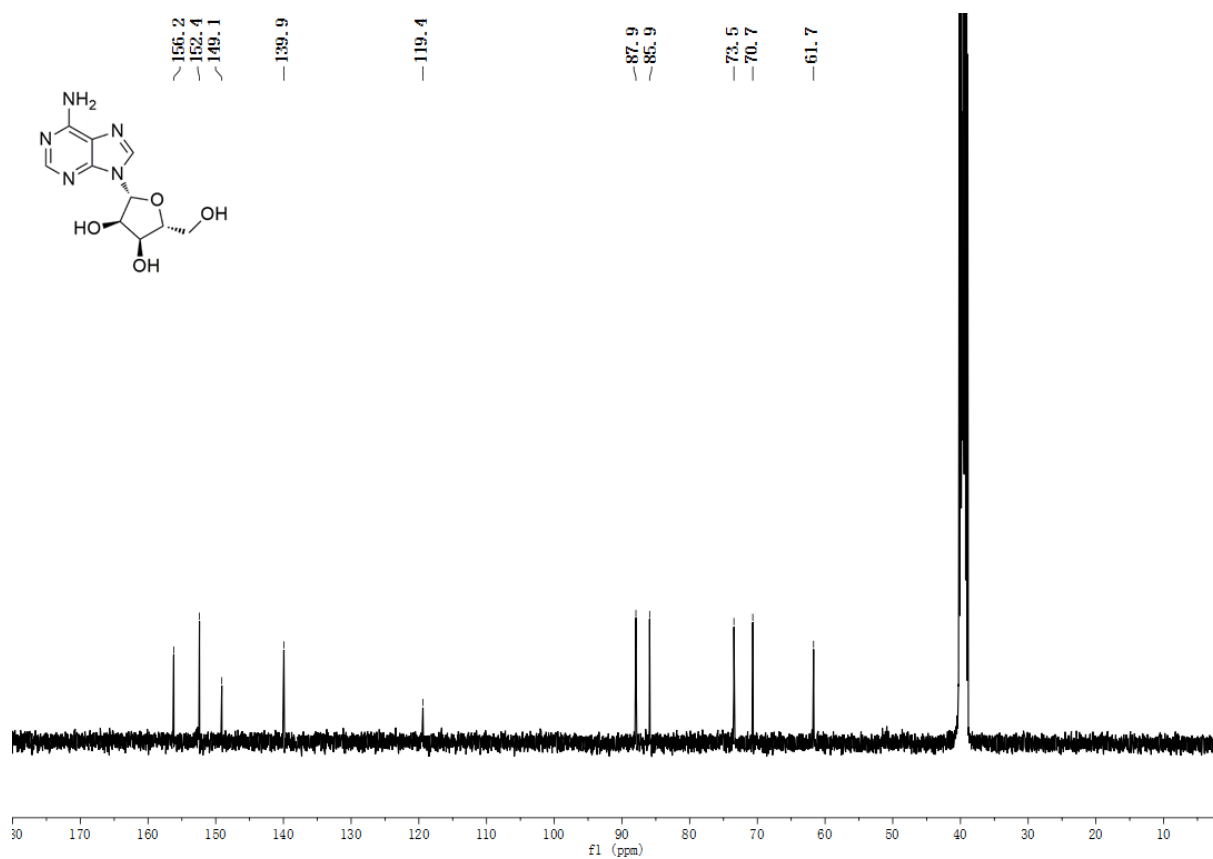




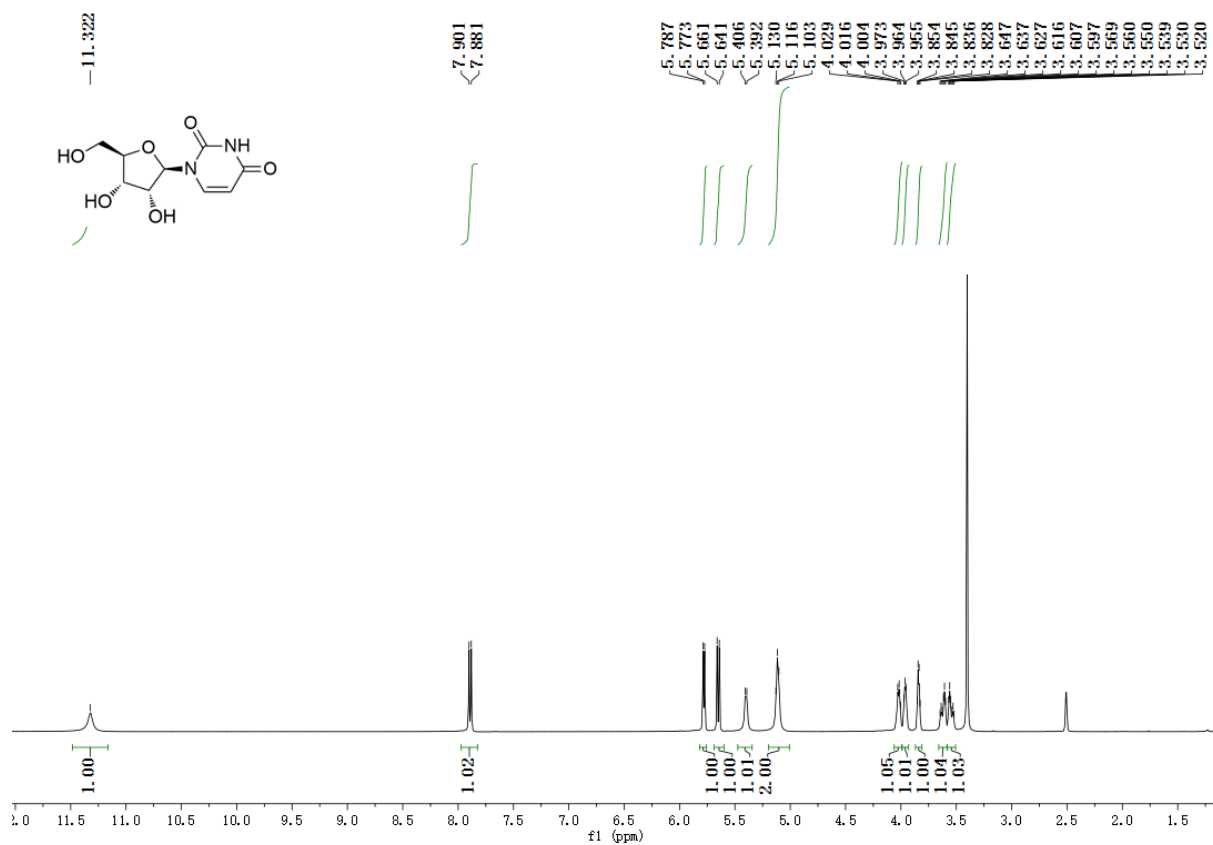
**Figure S23:**  $^{13}\text{C}$  NMR spectrum (100 MHz) of **6** in  $\text{CDCl}_3$



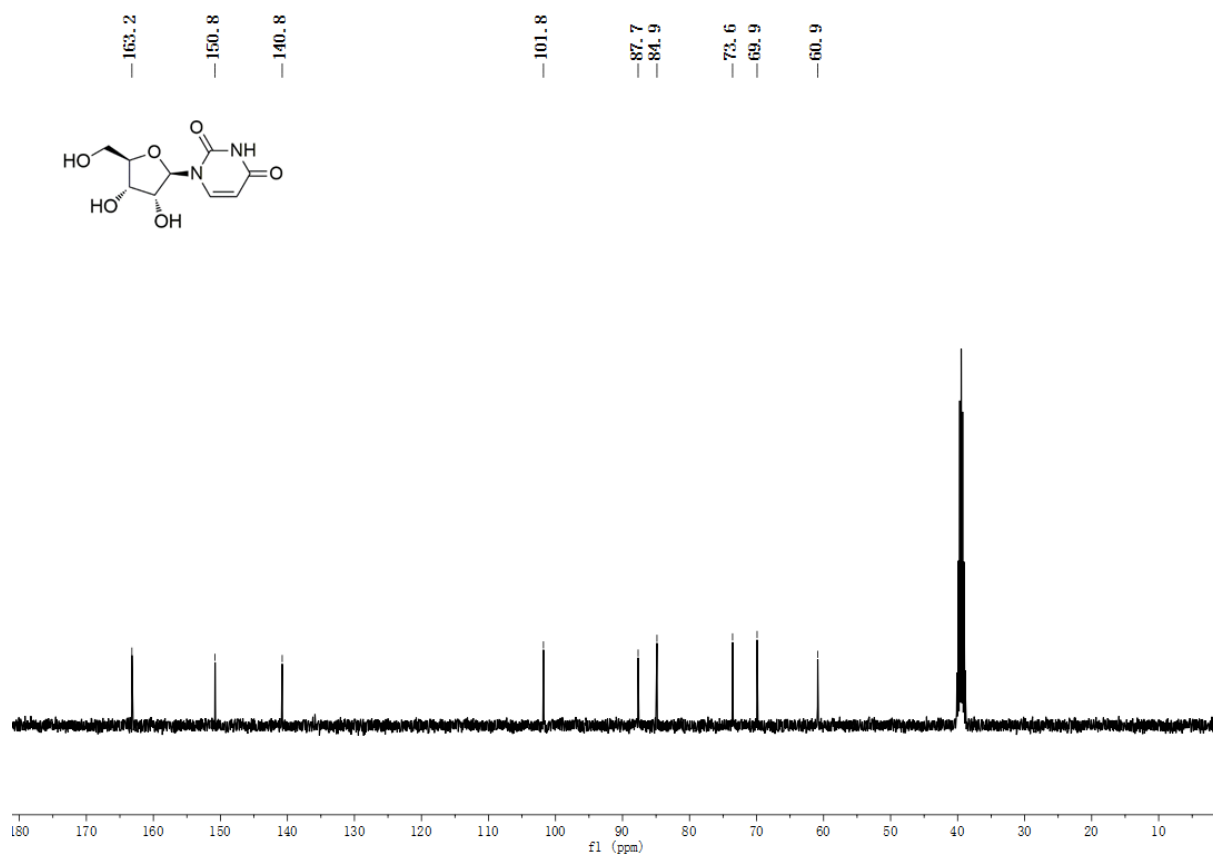
**Figure S24:** <sup>1</sup>H NMR spectrum (400 MHz) of **7** in DMSO-*d*<sub>6</sub>



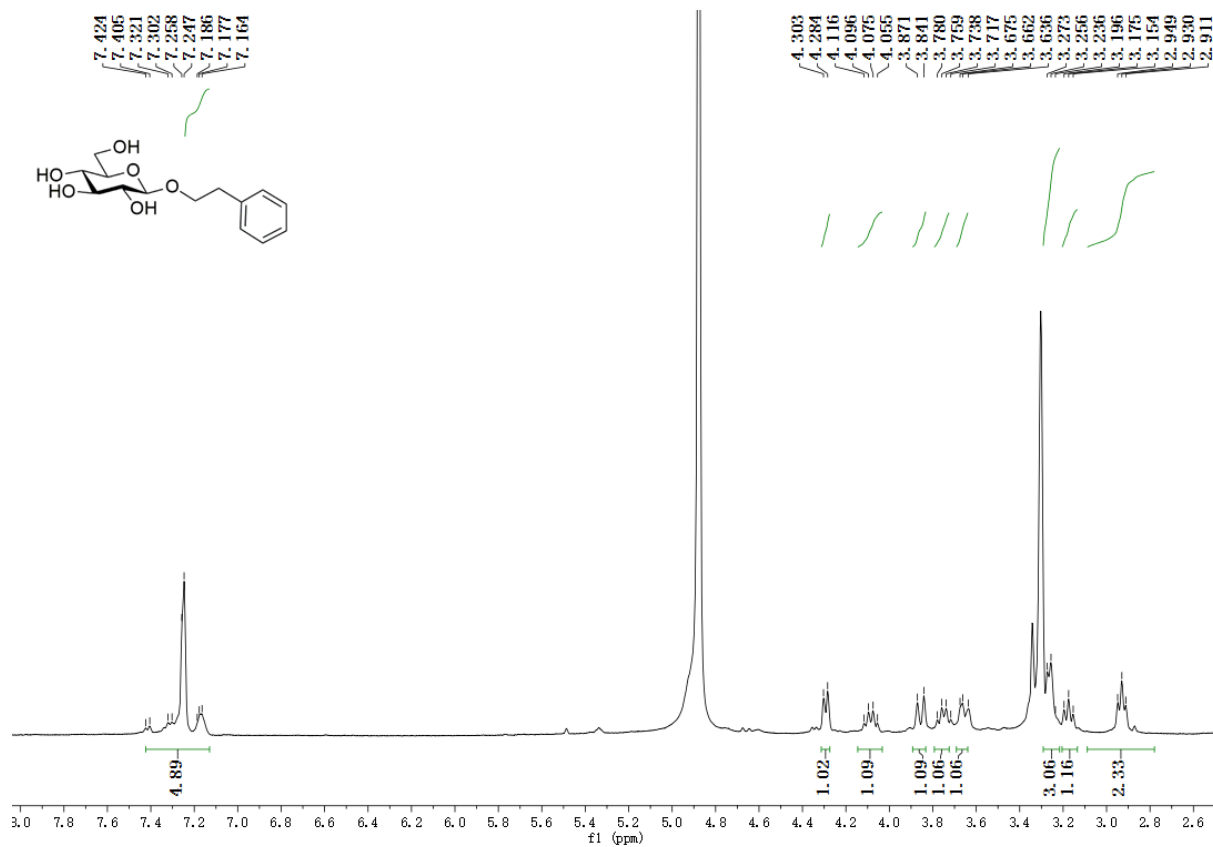
**Figure S25:** <sup>13</sup>C NMR spectrum (100 MHz) of **7** in DMSO-*d*<sub>6</sub>



**Figure S26:** <sup>1</sup>H NMR spectrum (400 MHz) of **8** in DMSO-*d*<sub>6</sub>



**Figure S27:**  $^{13}\text{C}$  NMR spectrum (100 MHz) of **8** in  $\text{DMSO-}d_6$



**Figure S28:** <sup>1</sup>H NMR spectrum (400 MHz) of **9** in CD<sub>3</sub>OD

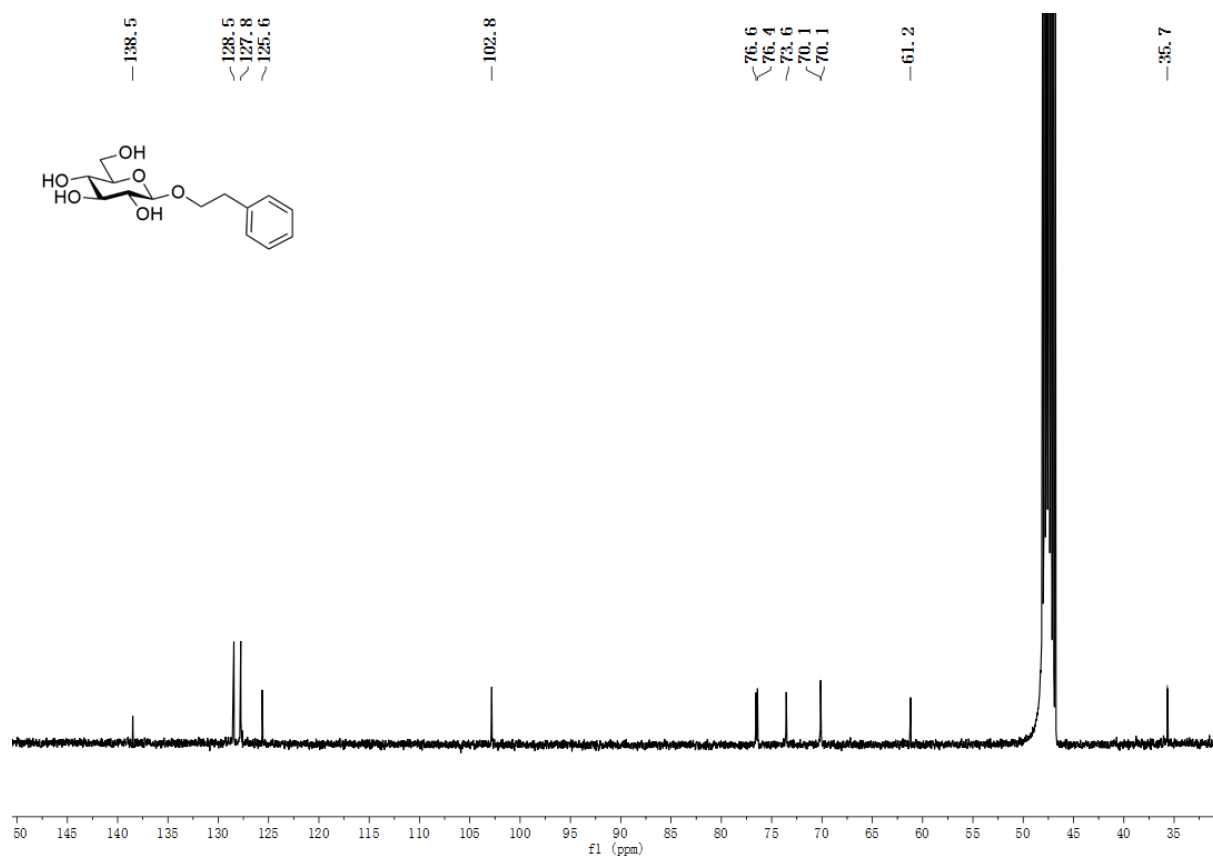
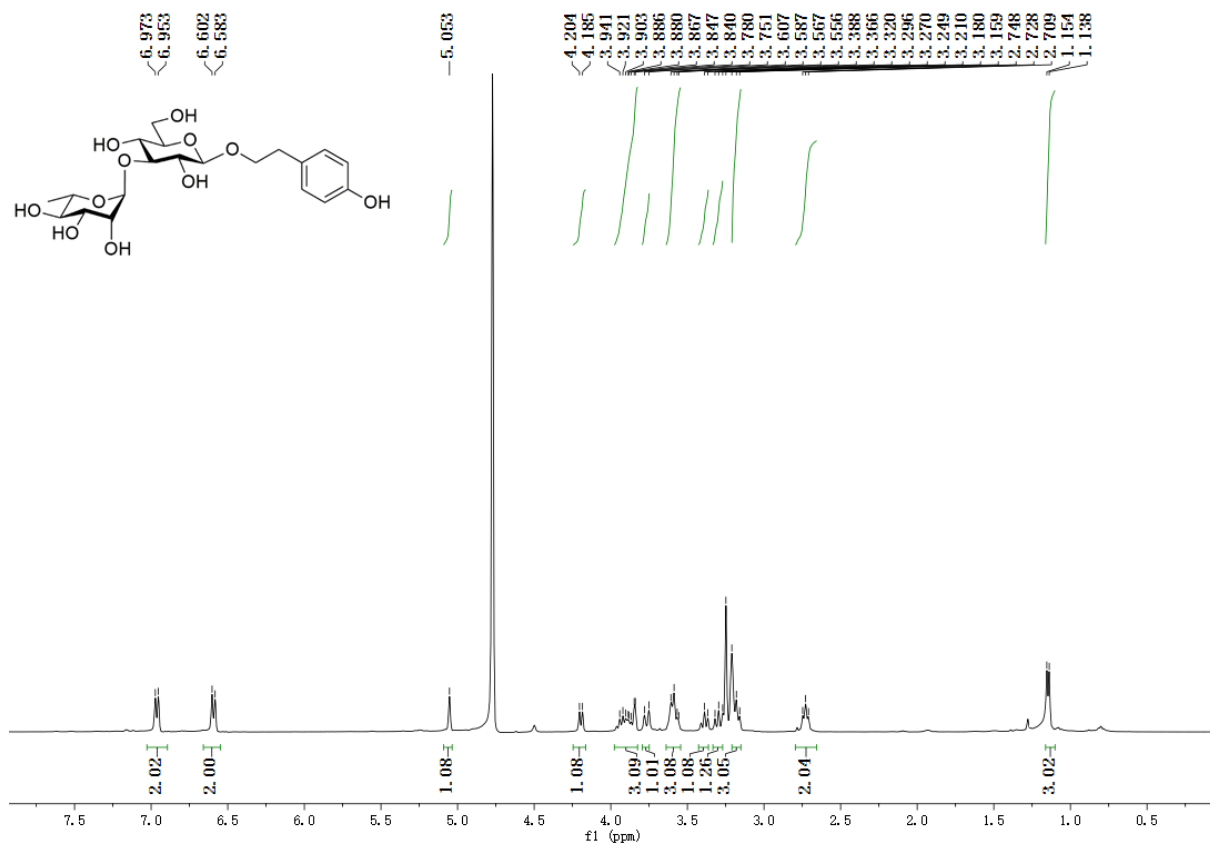
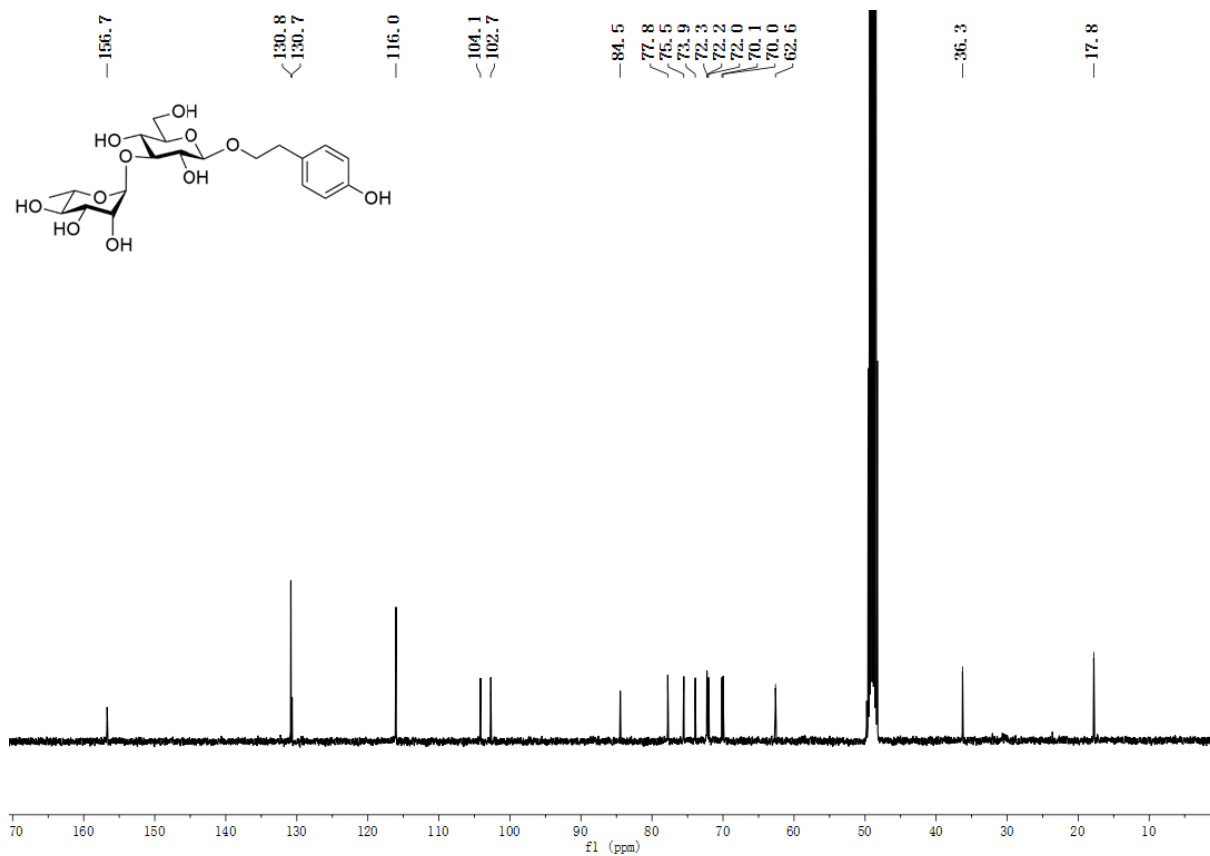


Figure S29: <sup>13</sup>C NMR spectrum (100 MHz) of **9** in CD<sub>3</sub>OD



**Figure S30:** <sup>1</sup>H NMR spectrum (400 MHz) of **10** in CD<sub>3</sub>OD





**Figure S31:** <sup>13</sup>C NMR spectrum (100 MHz) of 10 in CD<sub>3</sub>OD