

Supporting Information

Rec. Nat. Prod. X:X (202X) XX-XX

Chemical Constituents from the Roots of *Rehmannia glutinosa*

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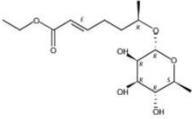
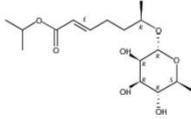
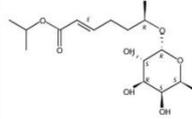
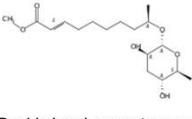
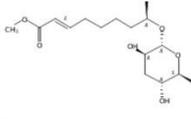
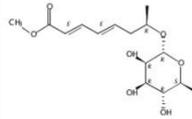
<p>Score: 95</p> <p>1. 2563912-22-9</p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p>C₁₅ H₂₆ O₇ INDEX NAME NOT YET ASSIGNED</p> <p>Key Physical Properties: Molecular Weight 318.36 Boiling Point (Predicted) Value: 470.0±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.21±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.04±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 2 References Reactions</p>	<p>Score: 95</p> <p>2. 2563912-27-4</p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p>C₁₆ H₂₈ O₇ INDEX NAME NOT YET ASSIGNED</p> <p>Key Physical Properties: Molecular Weight 332.39 Boiling Point (Predicted) Value: 475.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.19±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.04±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References</p>	<p>Score: 95</p> <p>3. 2566620-10-6</p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p>C₁₆ H₂₈ O₇ INDEX NAME NOT YET ASSIGNED</p> <p>Key Physical Properties: Molecular Weight 332.39 Boiling Point (Predicted) Value: 475.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.19±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.04±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References Reactions</p>
<p>Score: 94</p> <p>4. 1186217-51-5</p>  <p>Double bond geometry as shown., Absolute stereochemistry.</p> <p>C₁₇ H₃₀ O₈ 2-Decenoic acid, 9-[(3,6-dideoxy-α-L-arabino-hexopyranosyl)oxy]-, methyl ester, (2E,9R)-</p> <p>Key Physical Properties: Molecular Weight 330.42 Boiling Point (Predicted) Value: 474.0±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.11±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.56±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References Reactions</p>	<p>Score: 94</p> <p>5. 1355684-04-6</p>  <p>Absolute stereochemistry., Rotation (-), Double bond geometry as shown.</p> <p>C₁₆ H₂₈ O₈ 2-Nonenic acid, 8-[(3,6-dideoxy-α-L-arabino-hexopyranosyl)oxy]-, methyl ester, (2E,8R)-</p> <p>Key Physical Properties: Molecular Weight 316.39 Boiling Point (Predicted) Value: 462.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.12±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.56±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 6 References Reactions</p>	<p>Score: 94</p> <p>6. 1413812-28-8</p>  <p>Double bond geometry as shown., Rotation (+), Absolute stereochemistry.</p> <p>C₁₅ H₂₄ O₇ 2,4-Octadienoic acid, 7-[(6-deoxy-α-L-mannopyranosyl)oxy]-, methyl ester, (2E,4E,7R)-</p> <p>Key Physical Properties: Molecular Weight 316.35 Boiling Point (Predicted) Value: 482.3±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.23±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.03±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References Reactions</p>

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

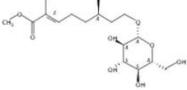
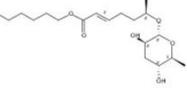
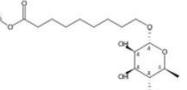
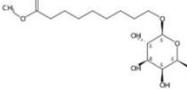
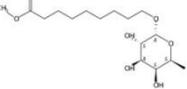
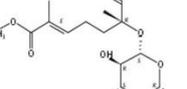
<p>Score: 93</p> <p>7.</p> <p>158921-24-5</p>  <p>Double bond geometry as shown., Rotation (-)., Absolute stereochemistry.</p> <p>C₁₇ H₃₀ O₈ 2-Octenoic acid, 8-((β-D-glucopyranosyloxy)-2,6-dimethyl-, methyl ester), (2E,6R)-</p> <p>Key Physical Properties:</p> <p>Molecular Weight 362.42</p> <p>Boiling Point (Predicted) Value: 546.7±50.0 °C Condition: Press: 760 Torr</p> <p>Density (Predicted) Value: 1.24±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr</p> <p>pKa (Predicted) Value: 12.94±0.70 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 3 References</p>	<p>Score: 93</p> <p>8.</p> <p>2563912-50-3</p>  <p>Absolute stereochemistry., Double bond geometry as shown.</p> <p>C₁₉ H₃₄ O₈ INDEX NAME NOT YET ASSIGNED</p> <p>Key Physical Properties:</p> <p>Molecular Weight 358.47</p> <p>Boiling Point (Predicted) Value: 497.1±45.0 °C Condition: Press: 760 Torr</p> <p>Density (Predicted) Value: 1.08±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr</p> <p>pKa (Predicted) Value: 13.55±0.70 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 2 References</p>	<p>Score: 92</p> <p>9.</p> <p>74597-40-3</p>  <p>Absolute stereochemistry.</p> <p>C₁₆ H₃₀ O₇ Nonanoic acid, 9-[(6-deoxy-α-L-mannopyranosyl)oxy]-, methyl ester</p> <p>Key Physical Properties:</p> <p>Molecular Weight 334.41</p> <p>Boiling Point (Predicted) Value: 464.1±45.0 °C Condition: Press: 760 Torr</p> <p>Density (Predicted) Value: 1.17±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr</p> <p>pKa (Predicted) Value: 13.08±0.70 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 10 References Reactions</p>
<p>Score: 92</p> <p>10.</p> <p>143528-28-3</p>  <p>Absolute stereochemistry.</p> <p>C₁₆ H₃₀ O₇ Nonanoic acid, 9-[(β-D-galactopyranosyl)oxy]-, methyl ester</p> <p>Key Physical Properties:</p> <p>Molecular Weight 334.41</p> <p>Boiling Point (Predicted) Value: 464.1±45.0 °C Condition: Press: 760 Torr</p> <p>Density (Predicted) Value: 1.17±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr</p> <p>pKa (Predicted) Value: 13.08±0.70 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 4 References</p>	<p>Score: 92</p> <p>11.</p> <p>143528-33-0</p>  <p>Absolute stereochemistry.</p> <p>C₁₆ H₃₀ O₇ Nonanoic acid, 9-[(6-deoxy-α-L-galactopyranosyl)oxy]-, methyl ester</p> <p>Key Physical Properties:</p> <p>Molecular Weight 334.41</p> <p>Boiling Point (Predicted) Value: 464.1±45.0 °C Condition: Press: 760 Torr</p> <p>Density (Predicted) Value: 1.17±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr</p> <p>pKa (Predicted) Value: 13.08±0.70 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 2 References</p>	<p>Score: 92</p> <p>12.</p> <p>263759-17-7</p>  <p>Double bond geometry as shown., Rotation (+)., Absolute stereochemistry.</p> <p>C₁₇ H₂₈ O₇ 2,7-Octadienoic acid, 6-[(6-deoxy-β-D-glucopyranosyl)oxy]-2,6-dimethyl-, methyl ester, (2E,6R)-</p> <p>Key Physical Properties:</p> <p>Molecular Weight 344.40</p> <p>Boiling Point (Predicted) Value: 507.1±50.0 °C Condition: Press: 760 Torr</p> <p>Density (Predicted) Value: 1.19±0.1 g/cm³ Condition: Temp: 20 °C Press: 760 Torr</p> <p>pKa (Predicted) Value: 13.03±0.70 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 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

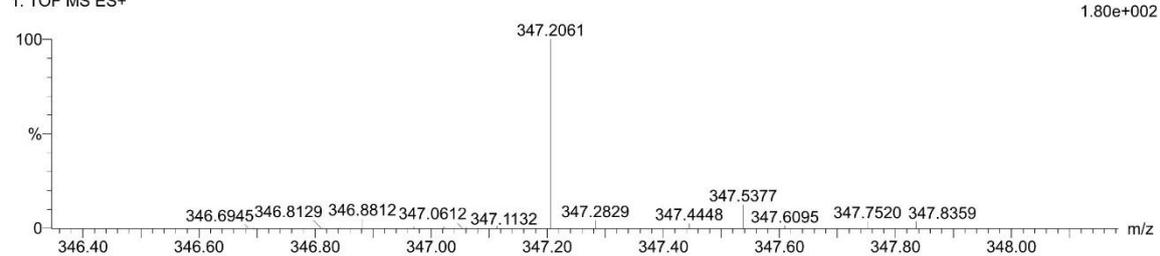
Monoisotopic Mass, Even Electron Ions

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

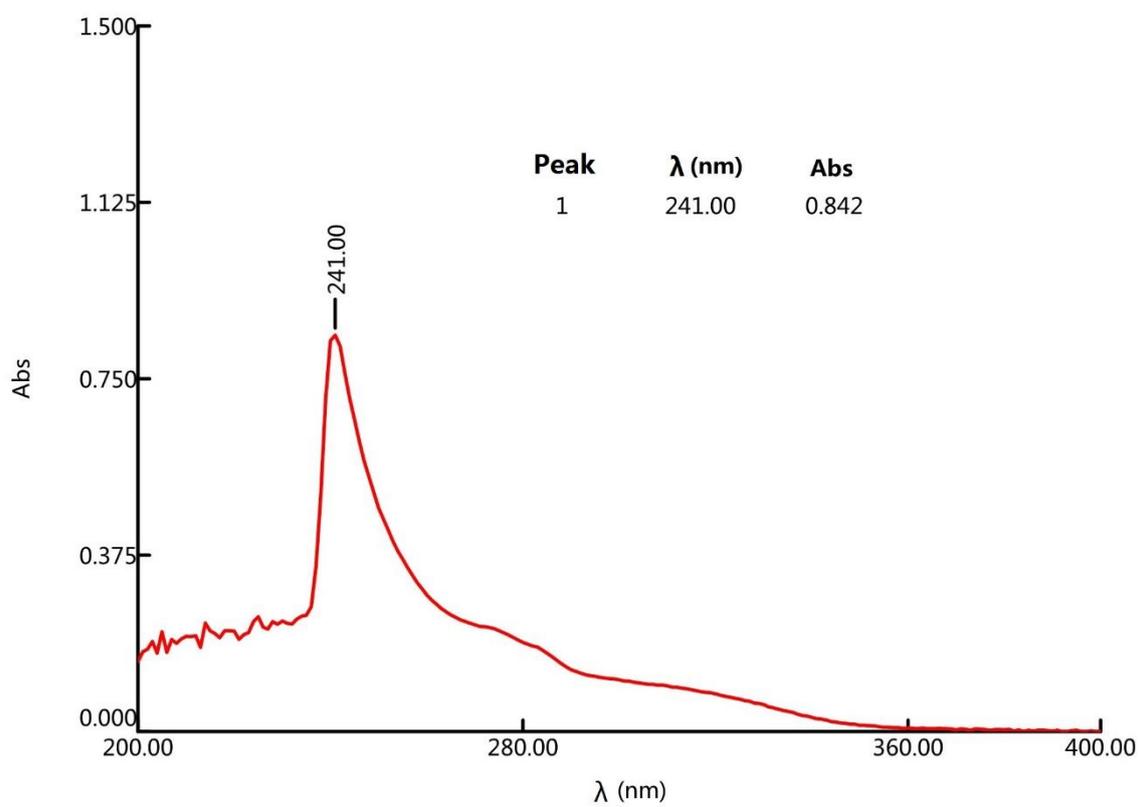


Figure S4: UV spectrum of **1** in CHCl₃

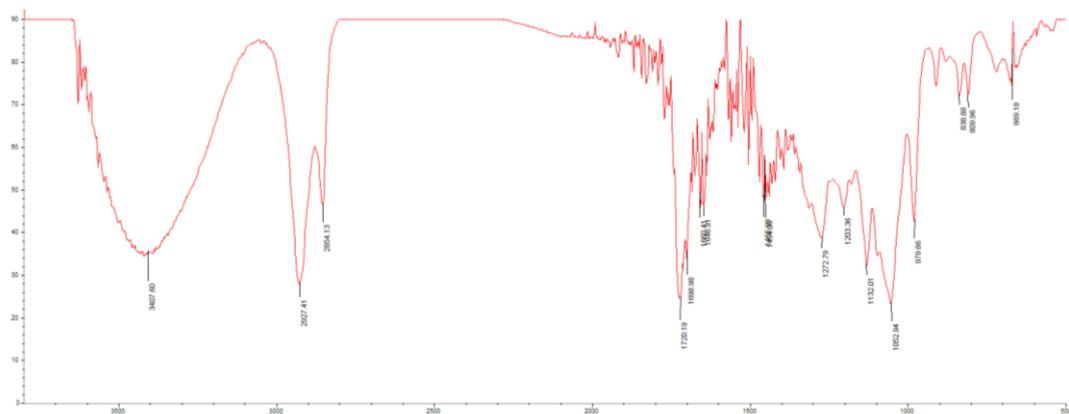


Figure S5: IR spectrum of **1**

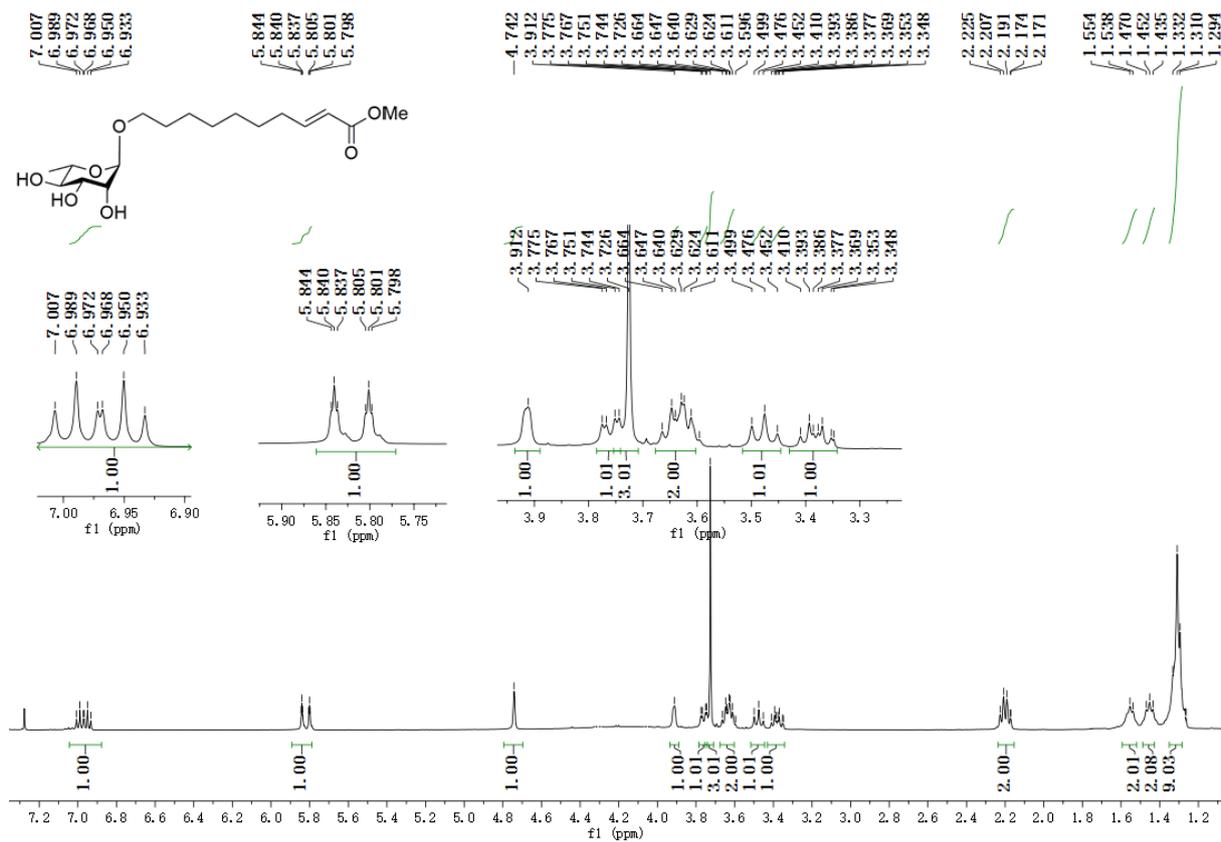


Figure S6: ^1H NMR spectrum (400 MHz) of **1** in CDCl_3

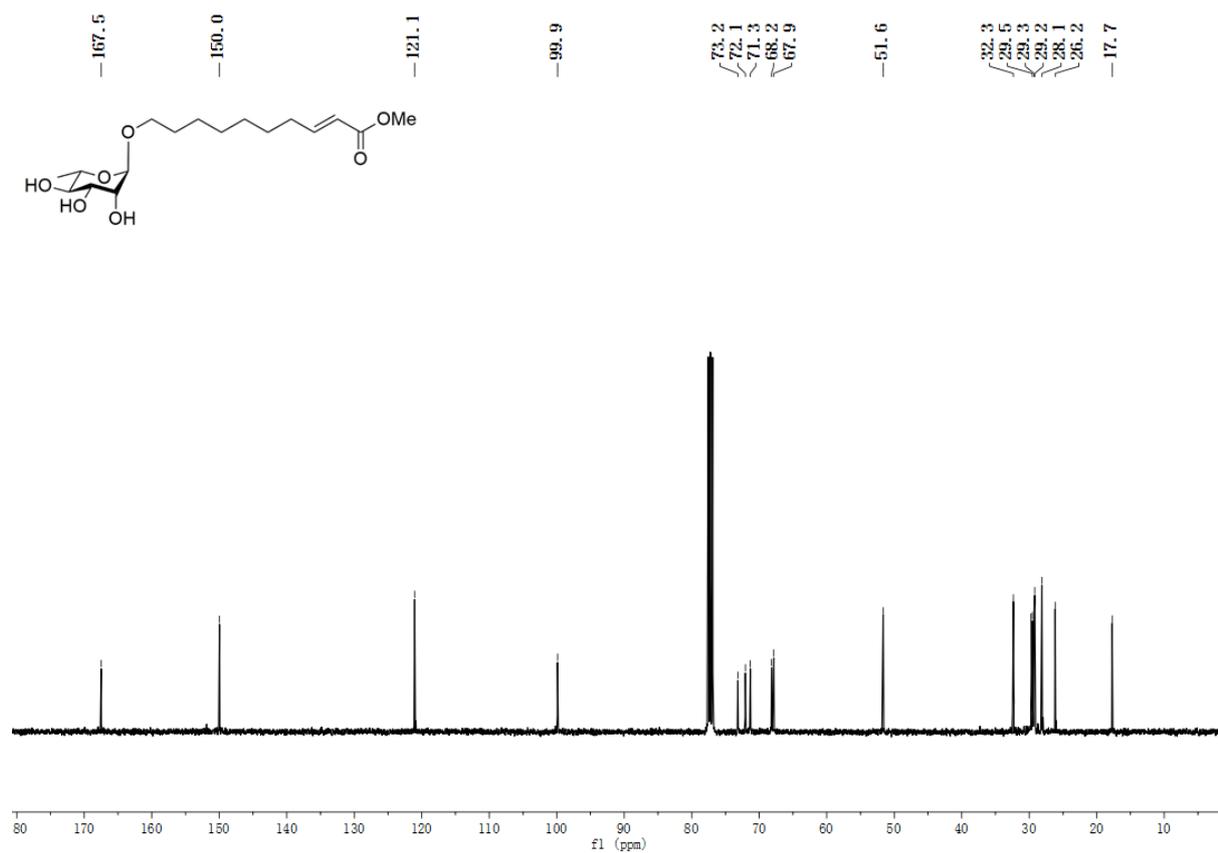


Figure S7: ^{13}C NMR spectrum (100 MHz) of **1** in CDCl_3

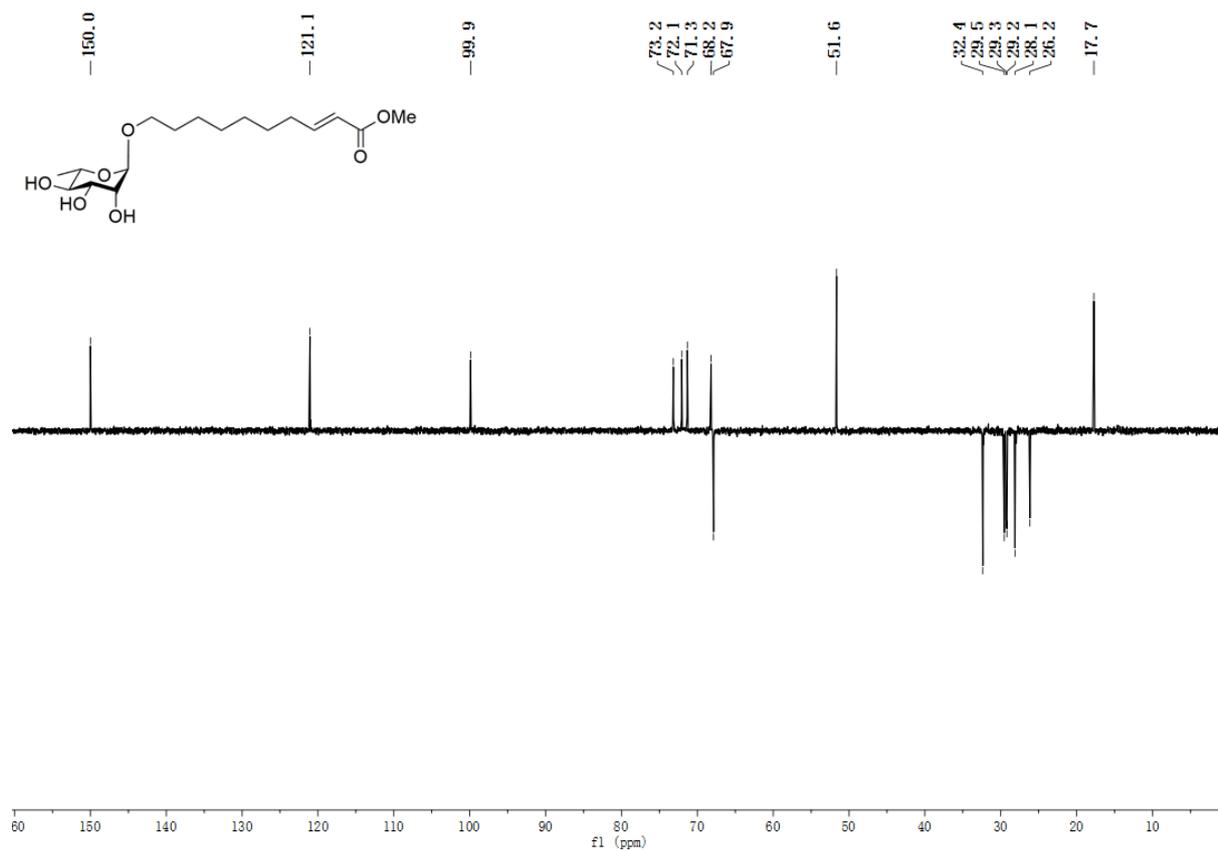


Figure S8: DEPT 135 spectrum of **1** in CDCl₃

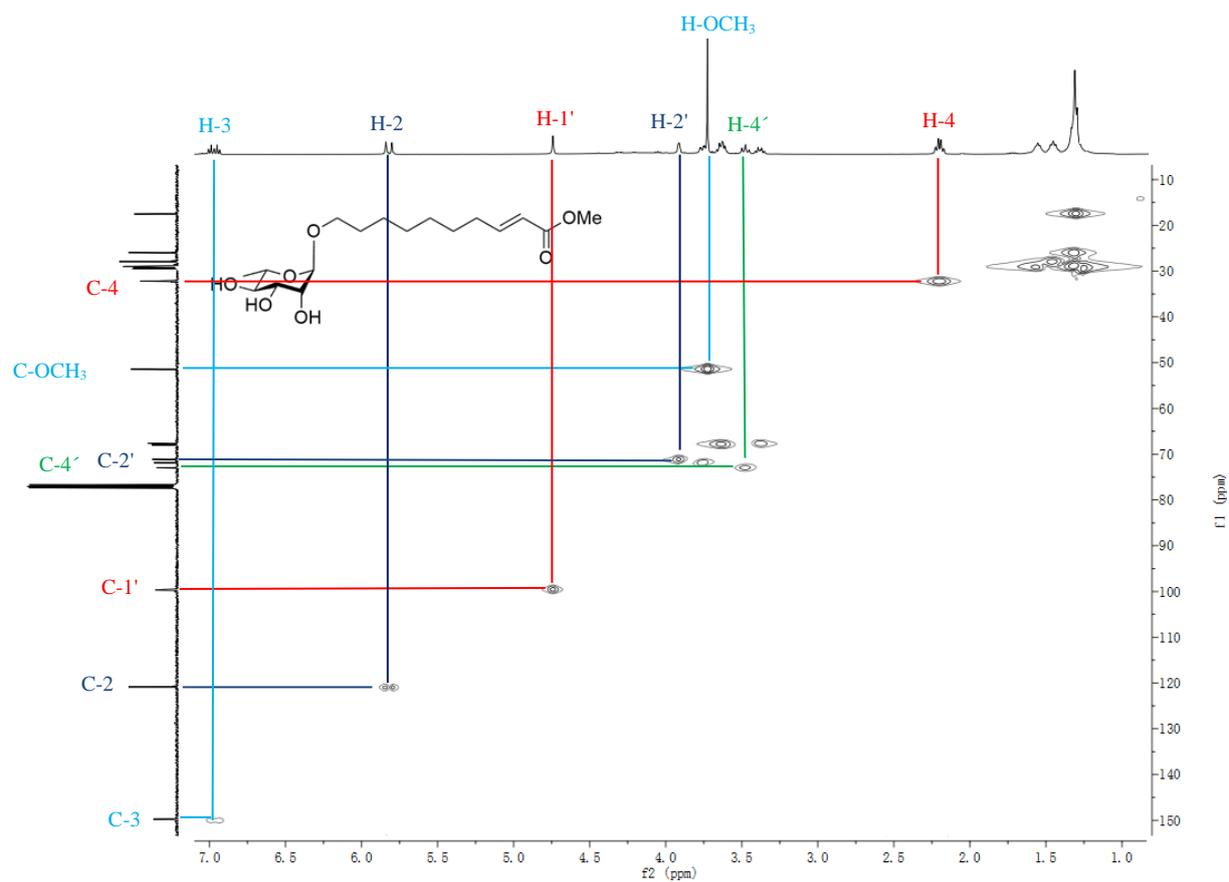


Figure S9: HSQC spectrum of **1** in CDCl_3

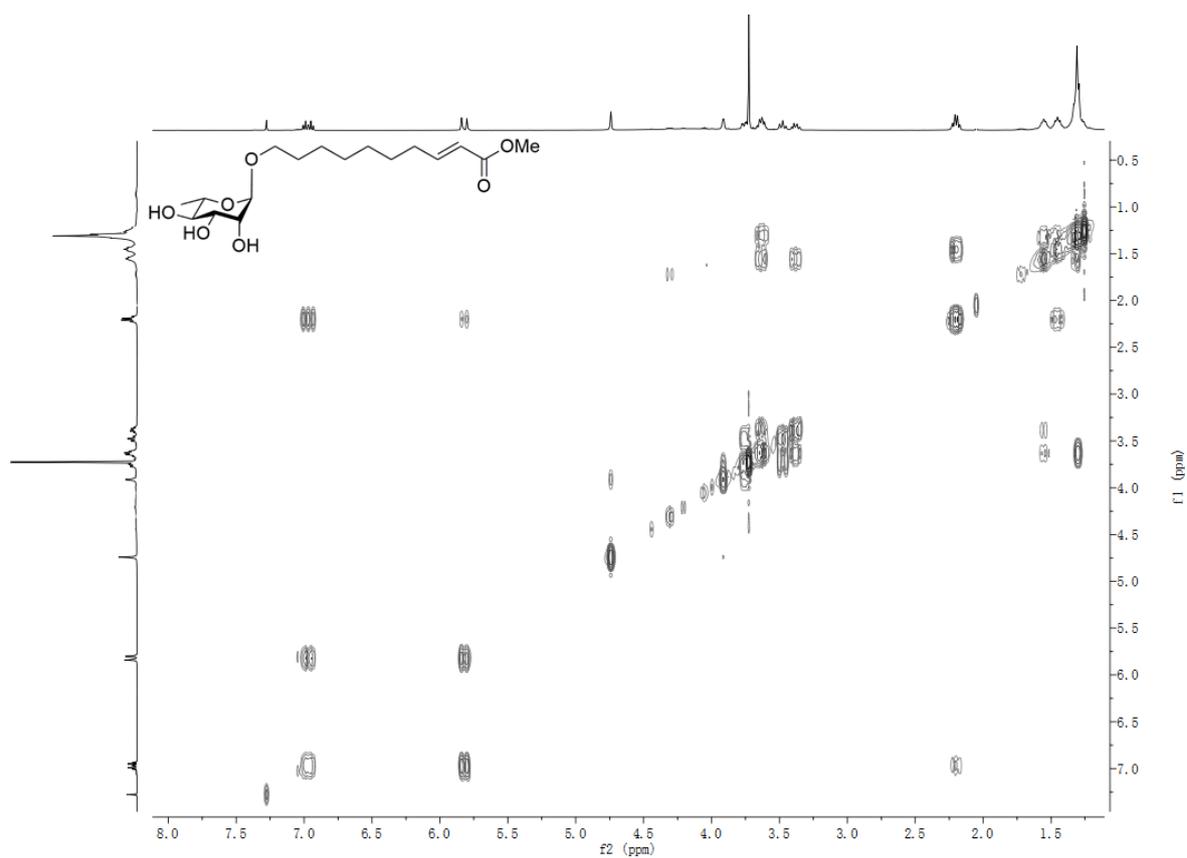


Figure S10: ^1H - ^1H COSY spectrum of **1** in CDCl_3

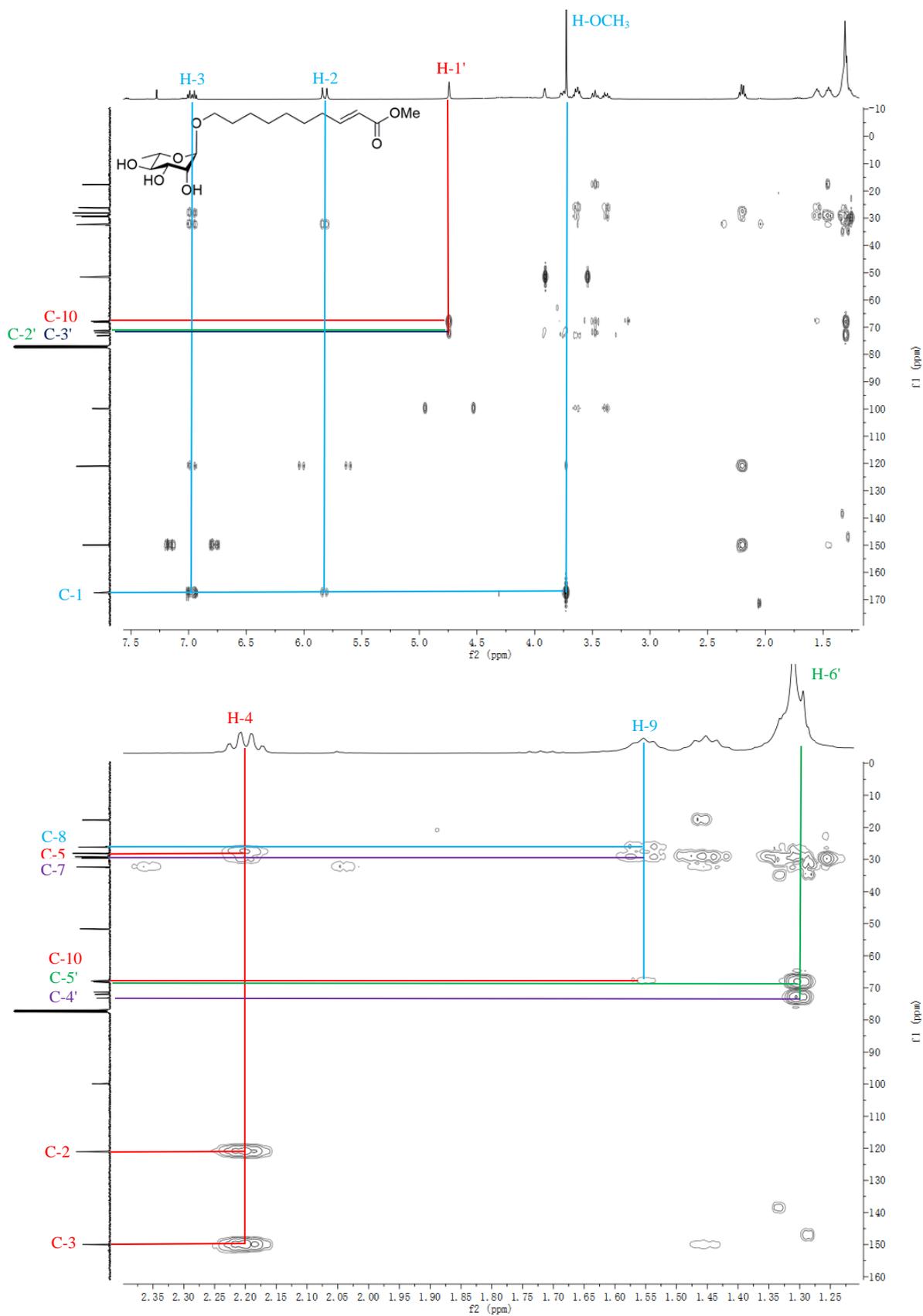


Figure S11: HMBC spectrum of **1** in CDCl₃

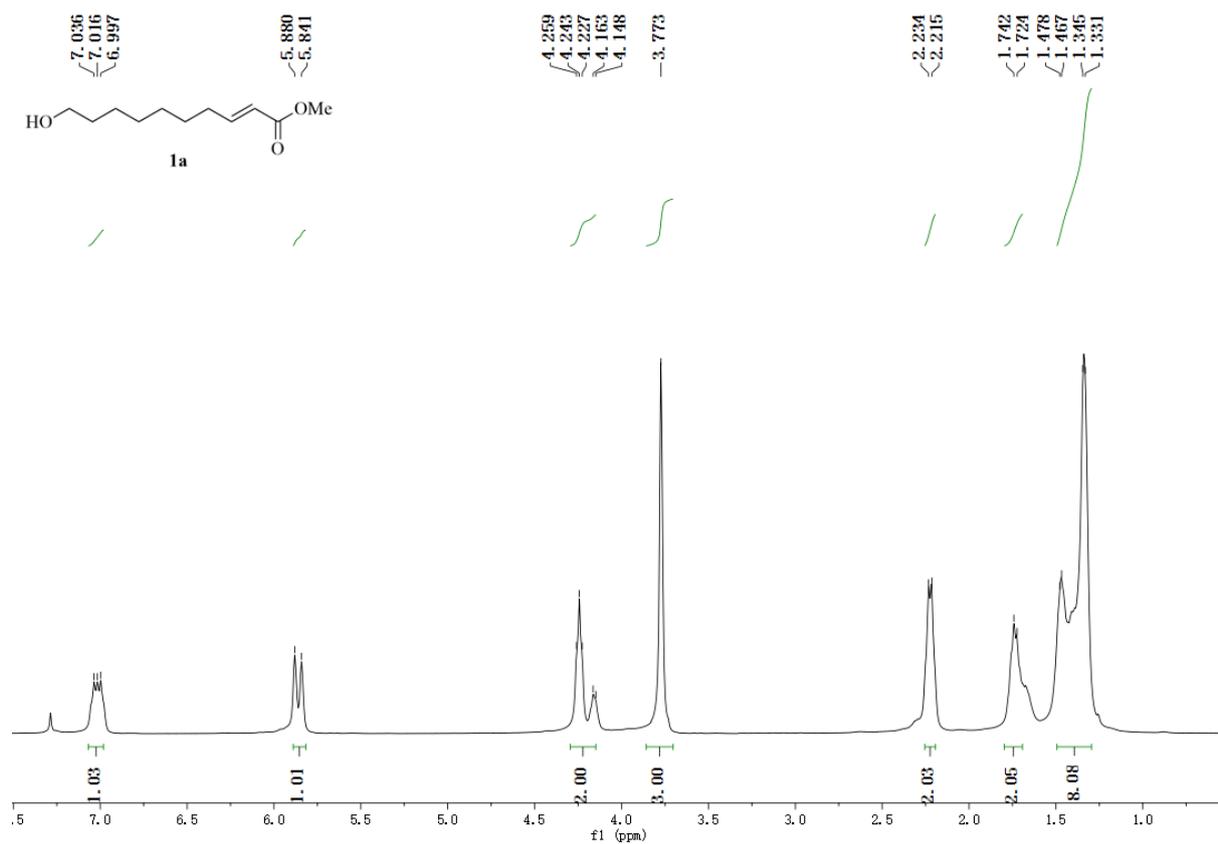


Figure S12: ^1H NMR spectrum (400 MHz) of **1a** in CDCl_3

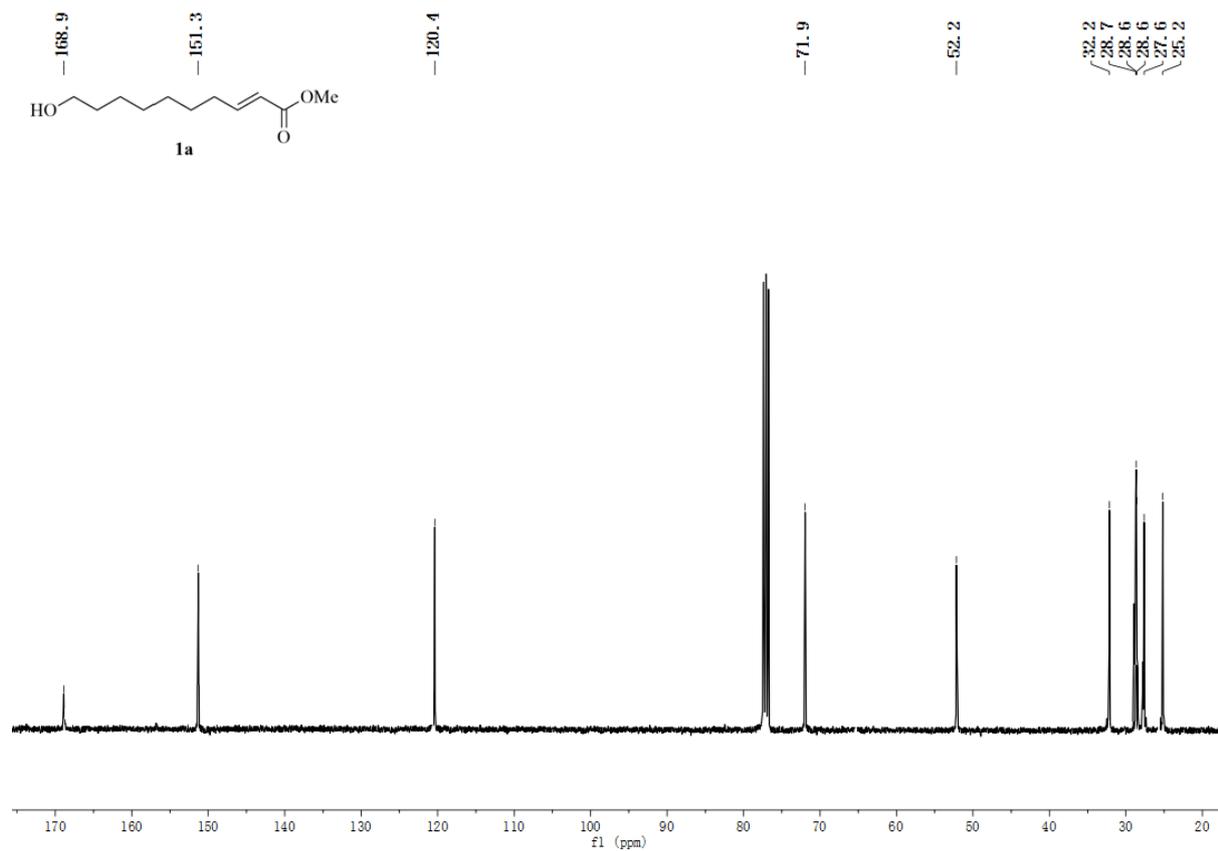


Figure S13: ^{13}C NMR spectrum (100 MHz) of **1a** in CDCl_3

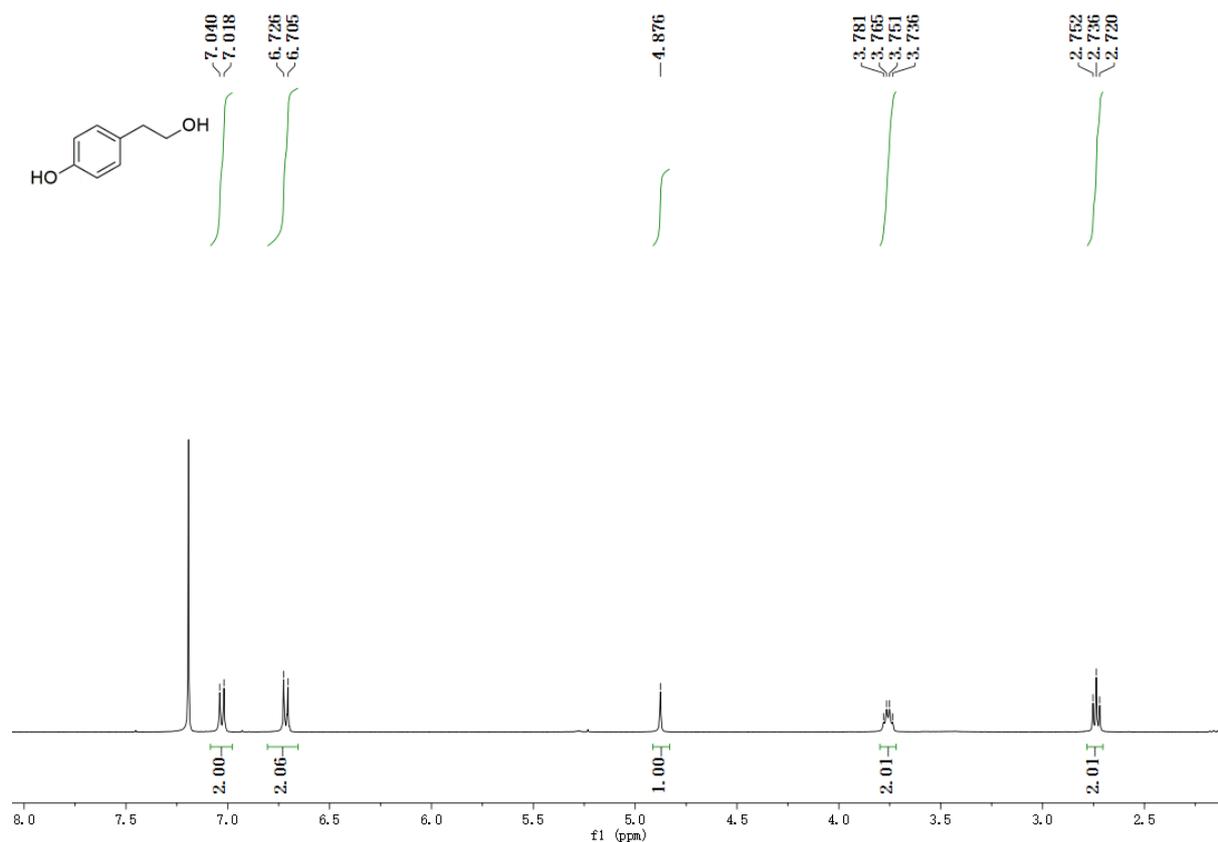


Figure S14: ¹H NMR spectrum (400 MHz) of **2** in CDCl₃

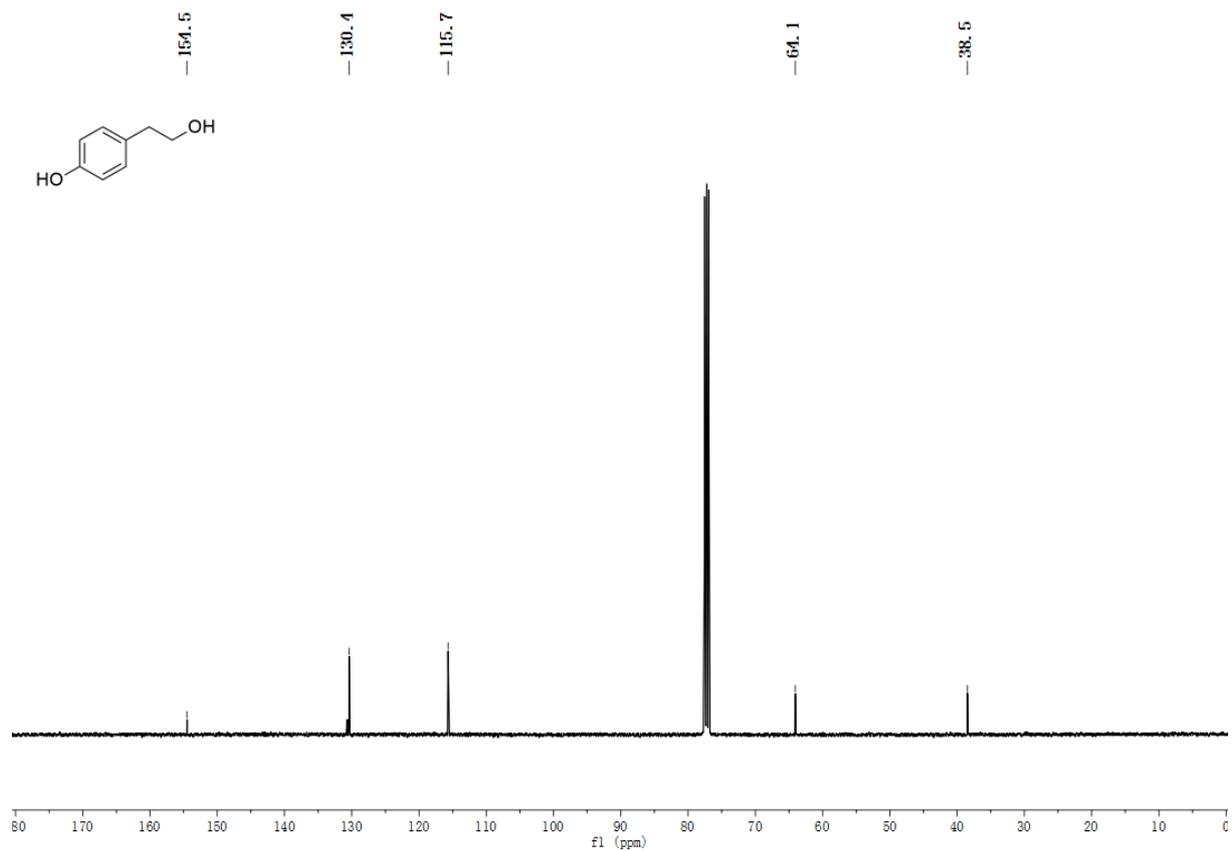


Figure S15: ¹³C NMR spectrum (100 MHz) of **2** in CDCl₃

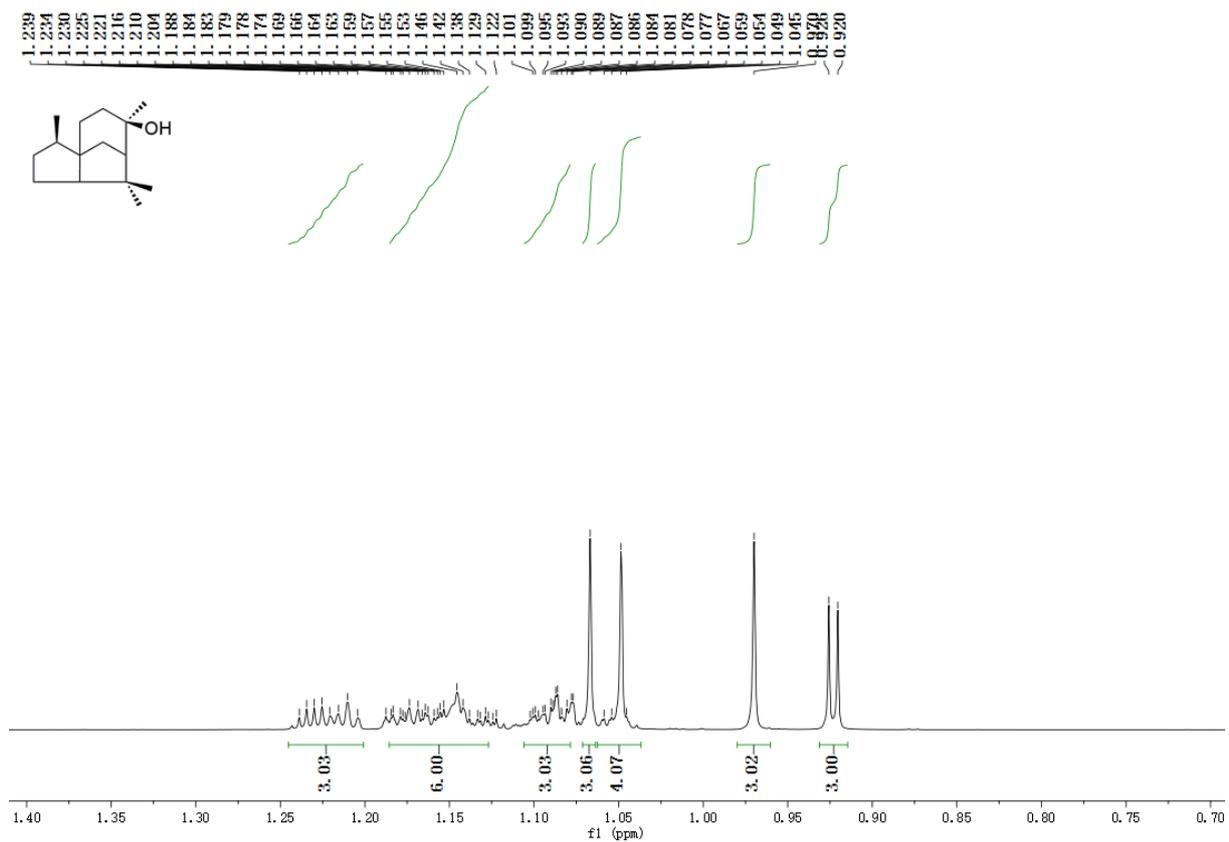


Figure S16: ¹H NMR spectrum (400 MHz) of 3 in CDCl₃

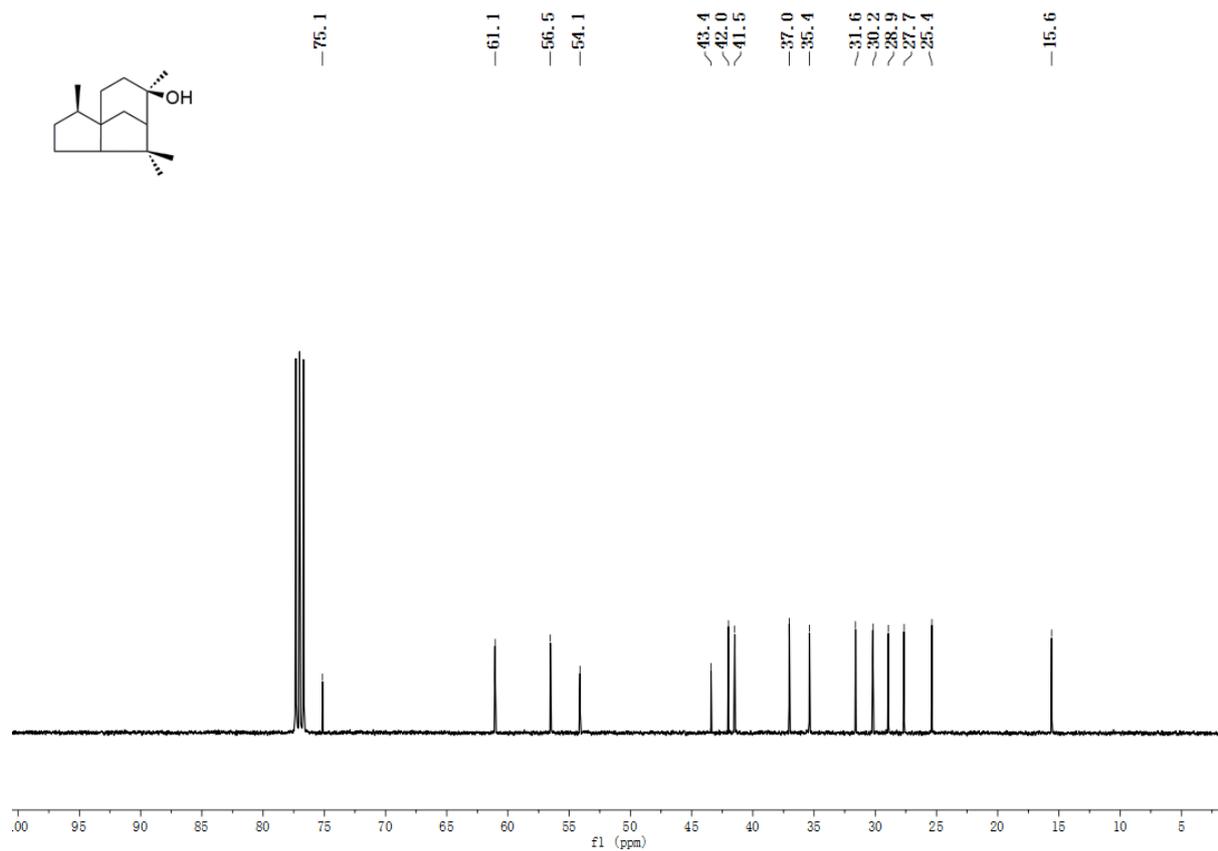


Figure S17: ^{13}C NMR spectrum (100 MHz) of **3** in CDCl_3

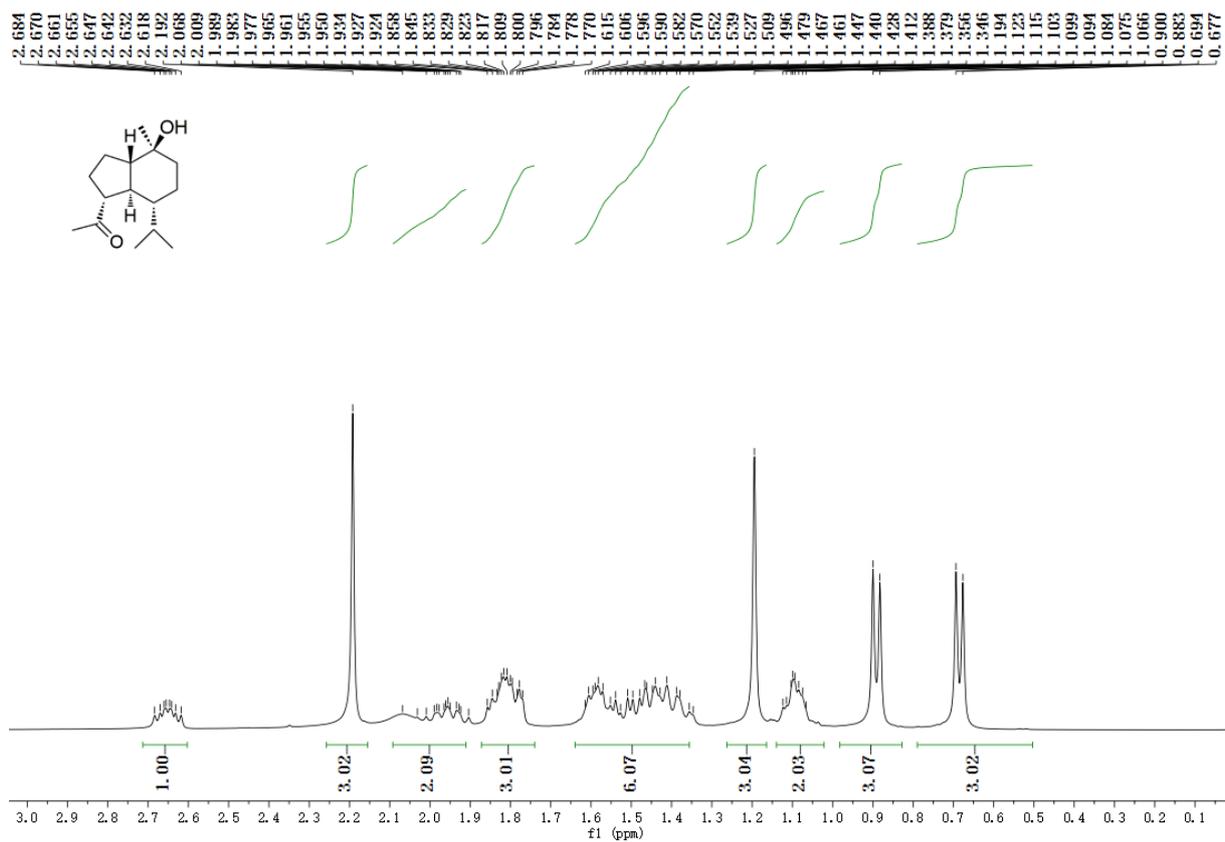


Figure S18: ¹H NMR spectrum (400 MHz) of **4** in CDCl₃

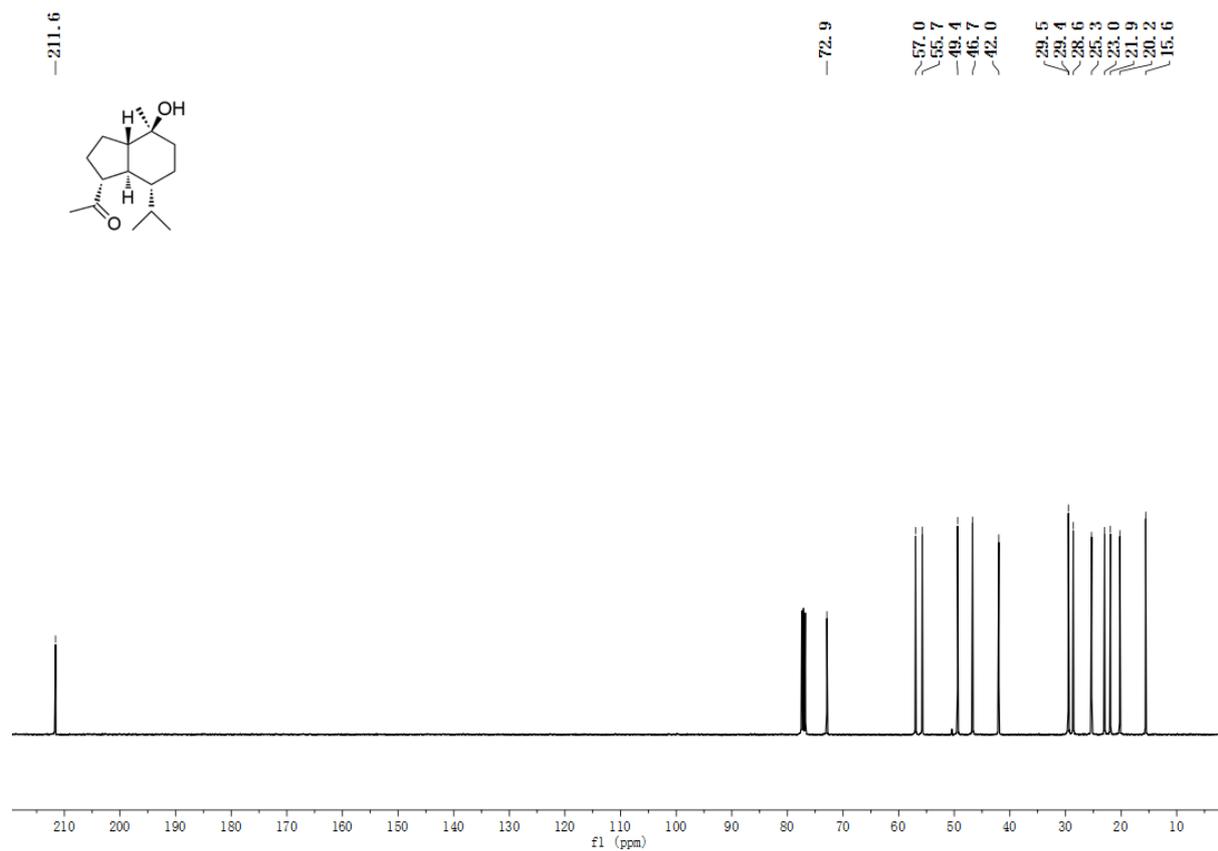


Figure S19: ^{13}C NMR spectrum (100 MHz) of **4** in CDCl_3

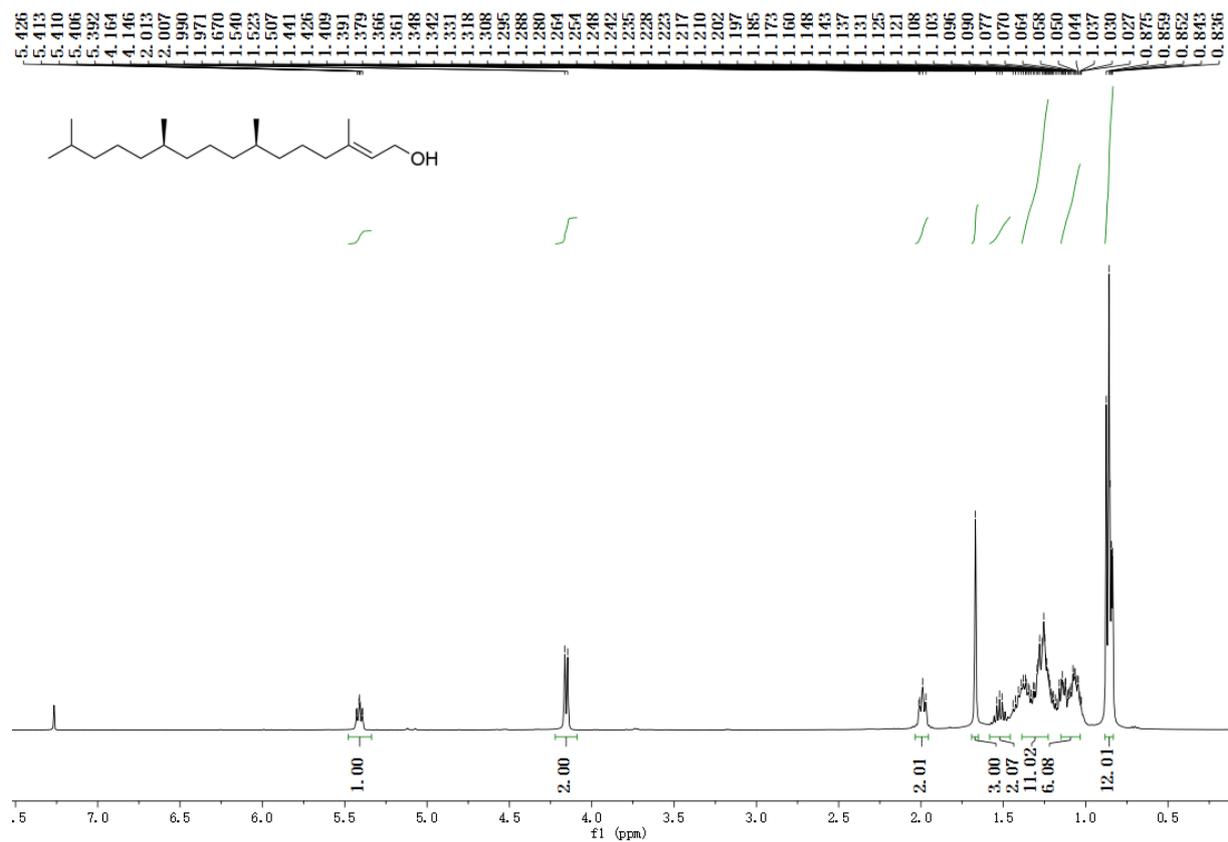


Figure S20: ^1H NMR spectrum (400 MHz) of **5** in CDCl_3

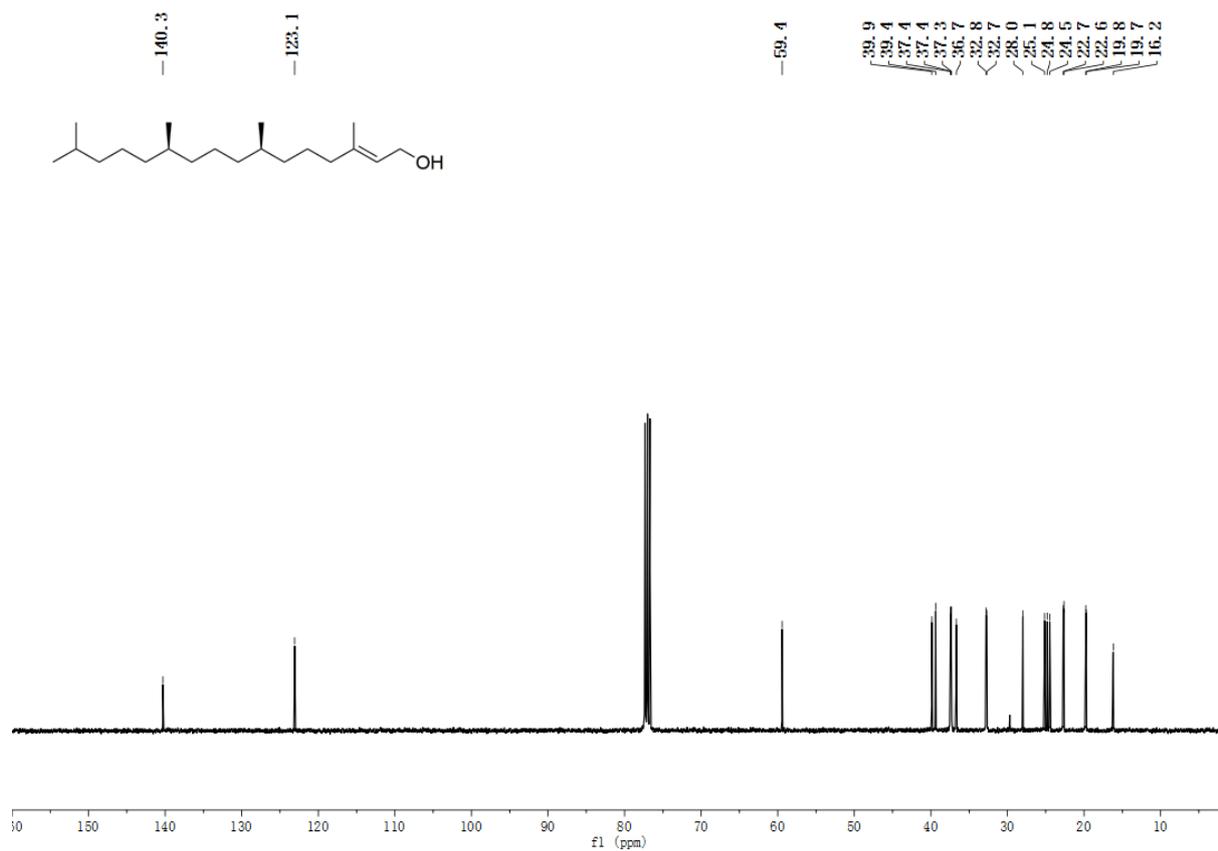


Figure S21: ^{13}C NMR spectrum (100 MHz) of **5** in CDCl_3

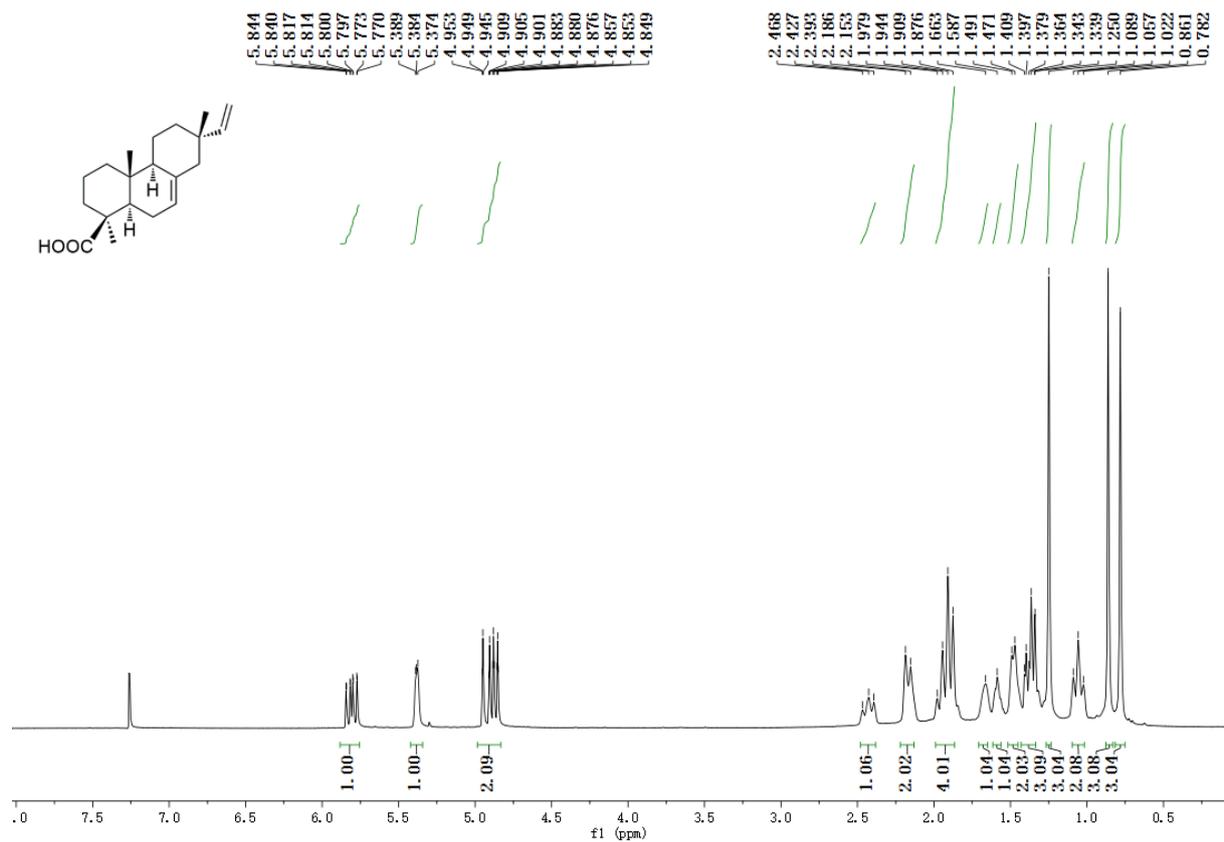


Figure S22: ^1H NMR spectrum (400 MHz) of **6** in CDCl_3

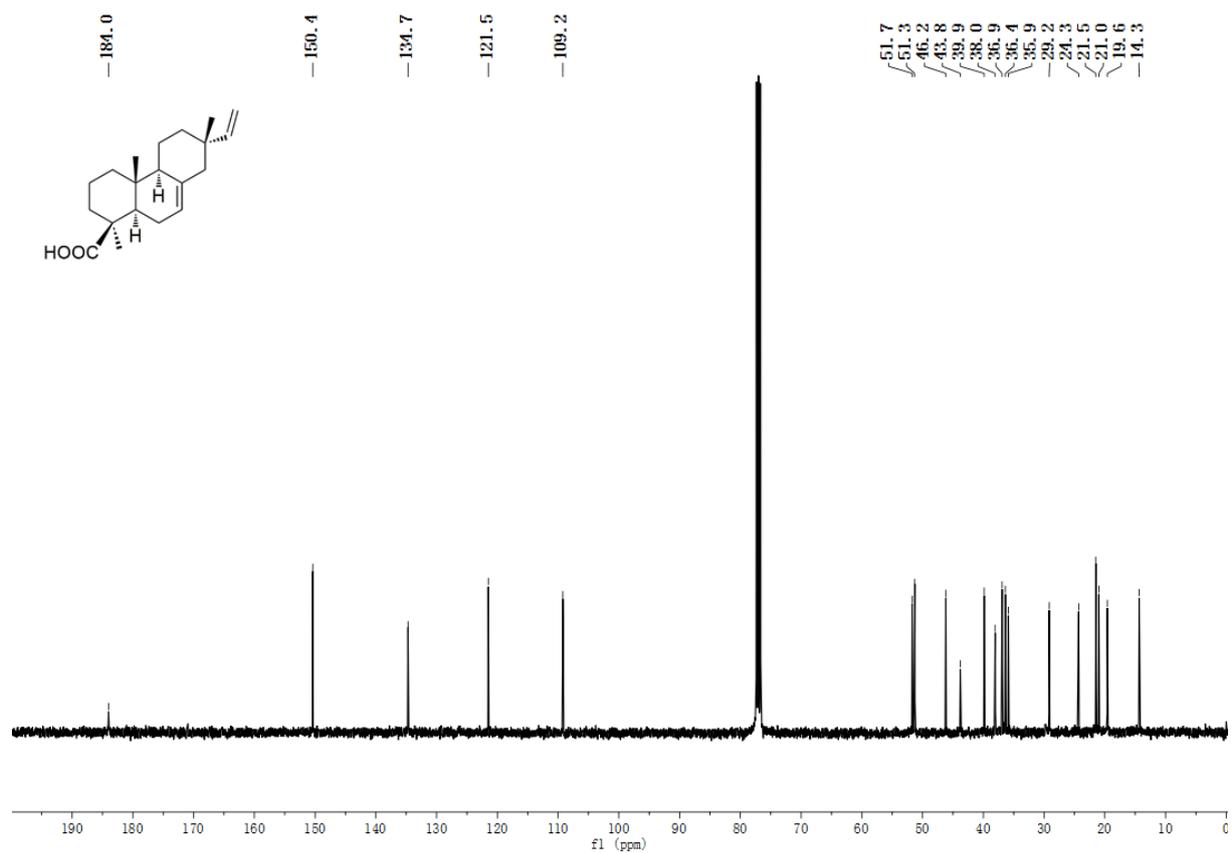


Figure S23: ^{13}C NMR spectrum (100 MHz) of **6** in CDCl_3

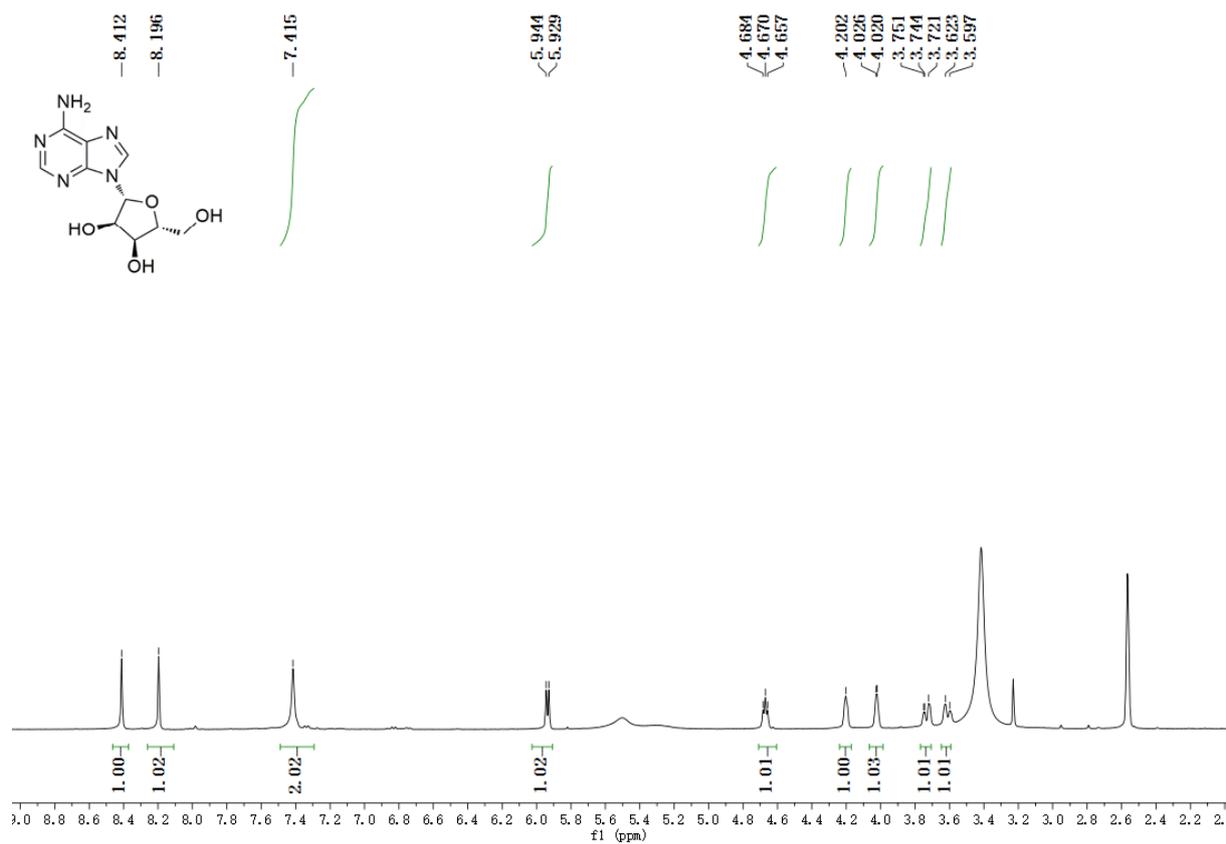


Figure S24: ^1H NMR spectrum (400 MHz) of **7** in $\text{DMSO}-d_6$

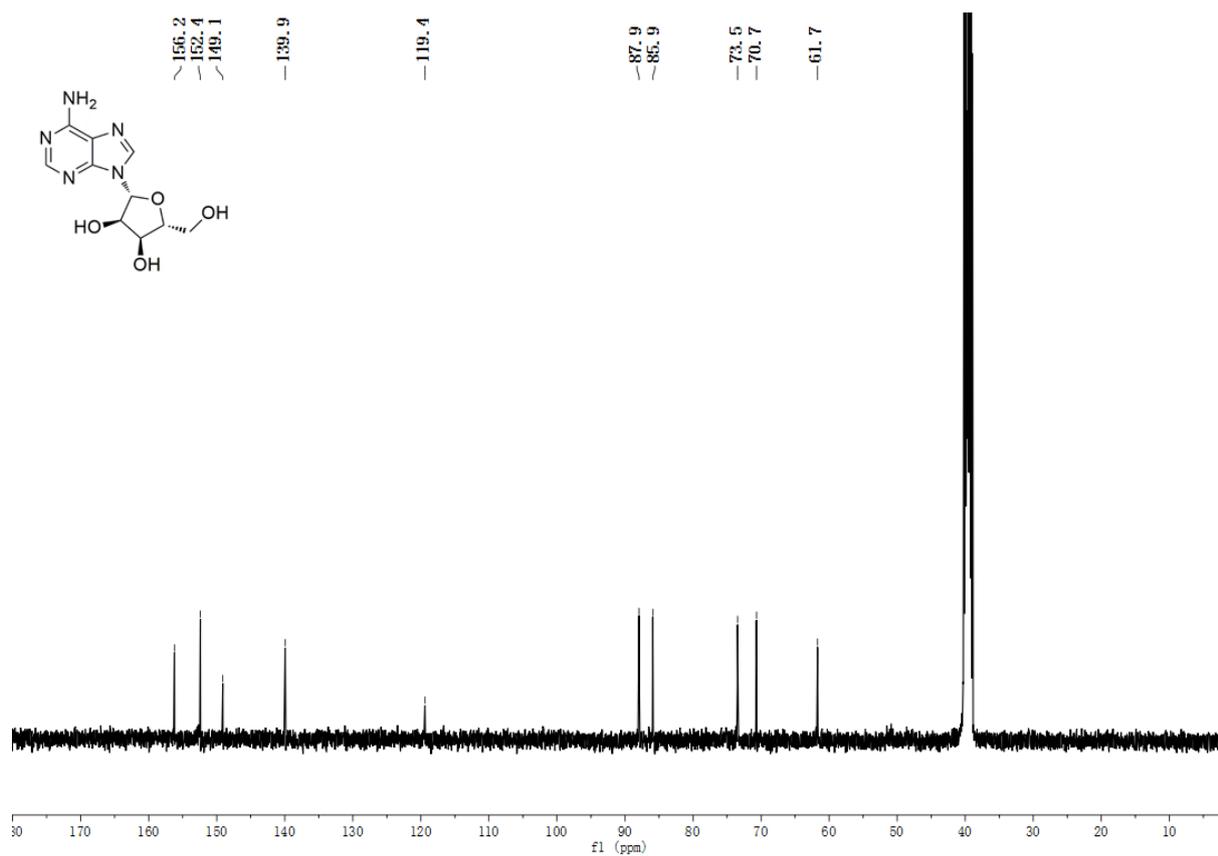


Figure S25: ¹³C NMR spectrum (100 MHz) of **7** in DMSO-*d*₆

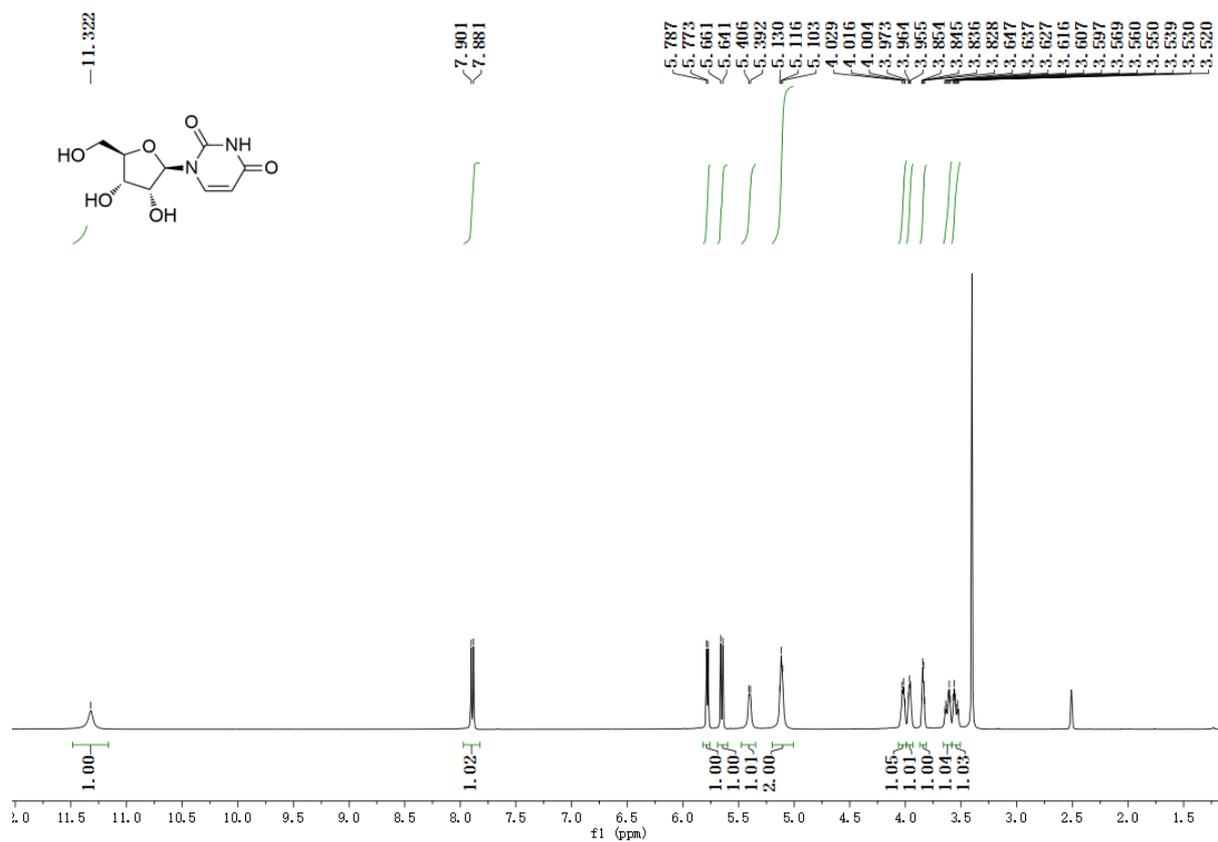


Figure S26: ¹H NMR spectrum (400 MHz) of **8** in DMSO-*d*₆

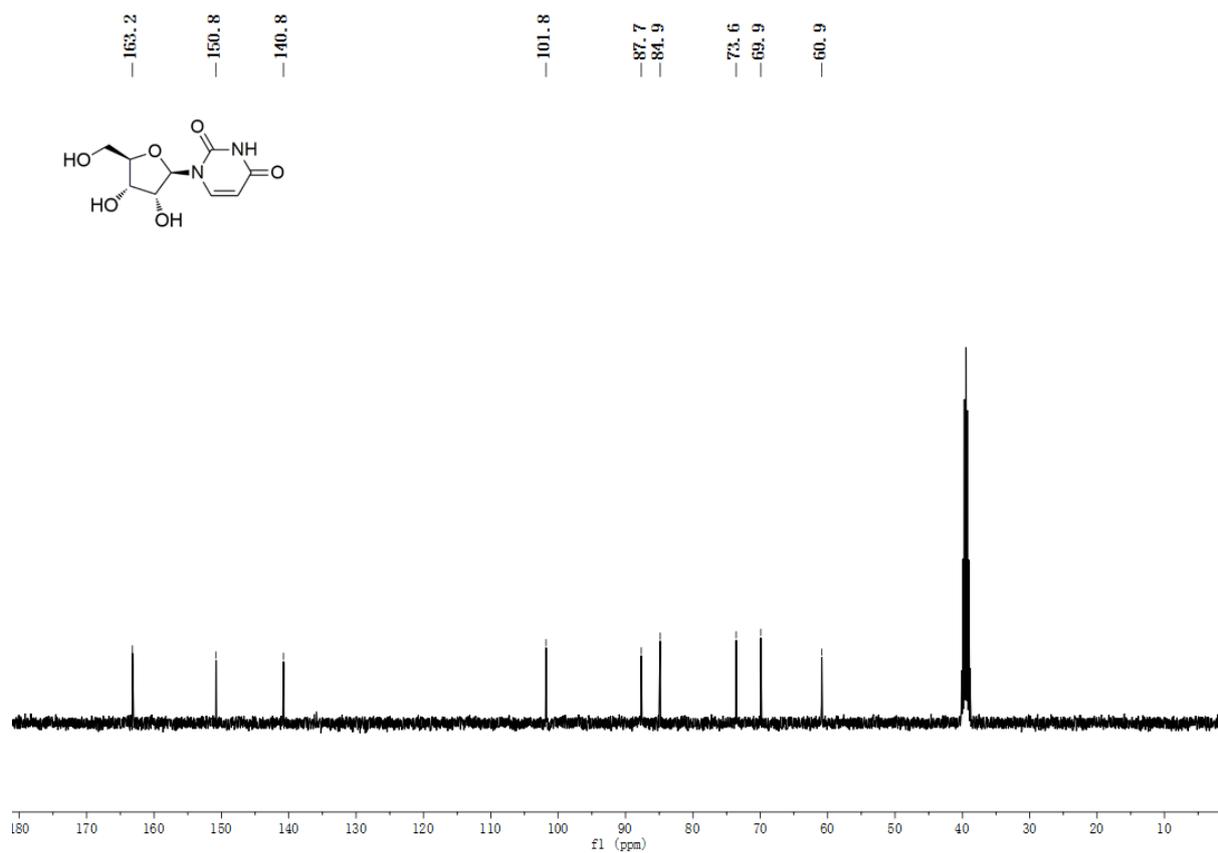


Figure S27: ^{13}C NMR spectrum (100 MHz) of **8** in $\text{DMSO-}d_6$

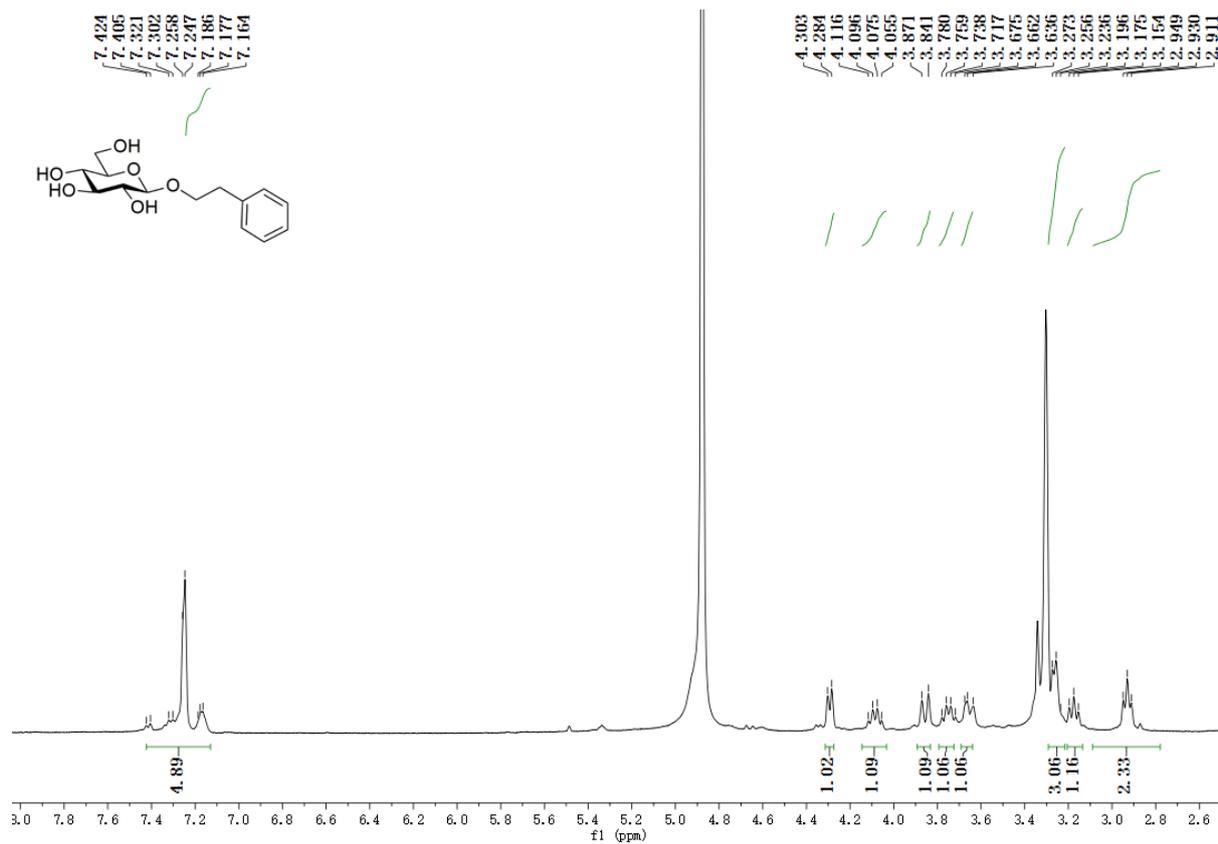


Figure S28: ¹H NMR spectrum (400 MHz) of **9** in CD₃OD

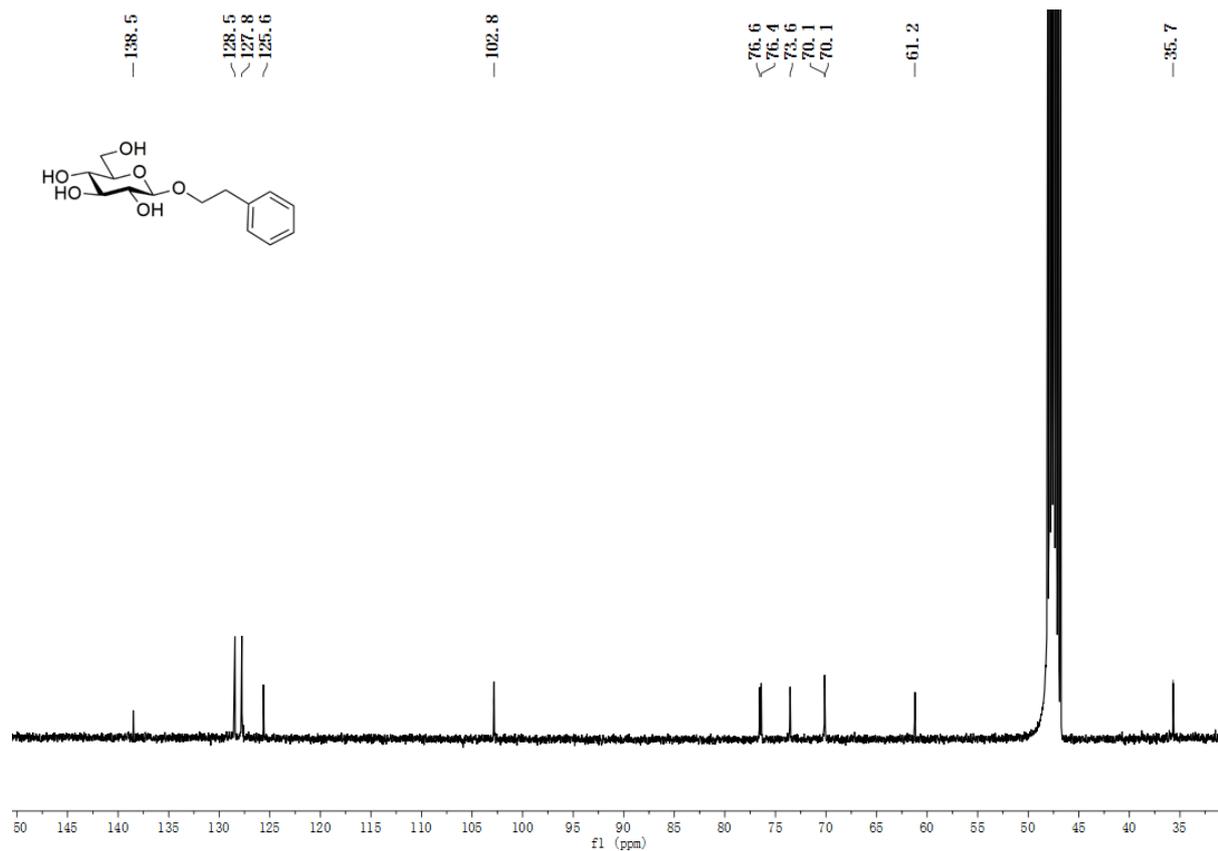


Figure S29: ¹³C NMR spectrum (100 MHz) of **9** in CD₃OD

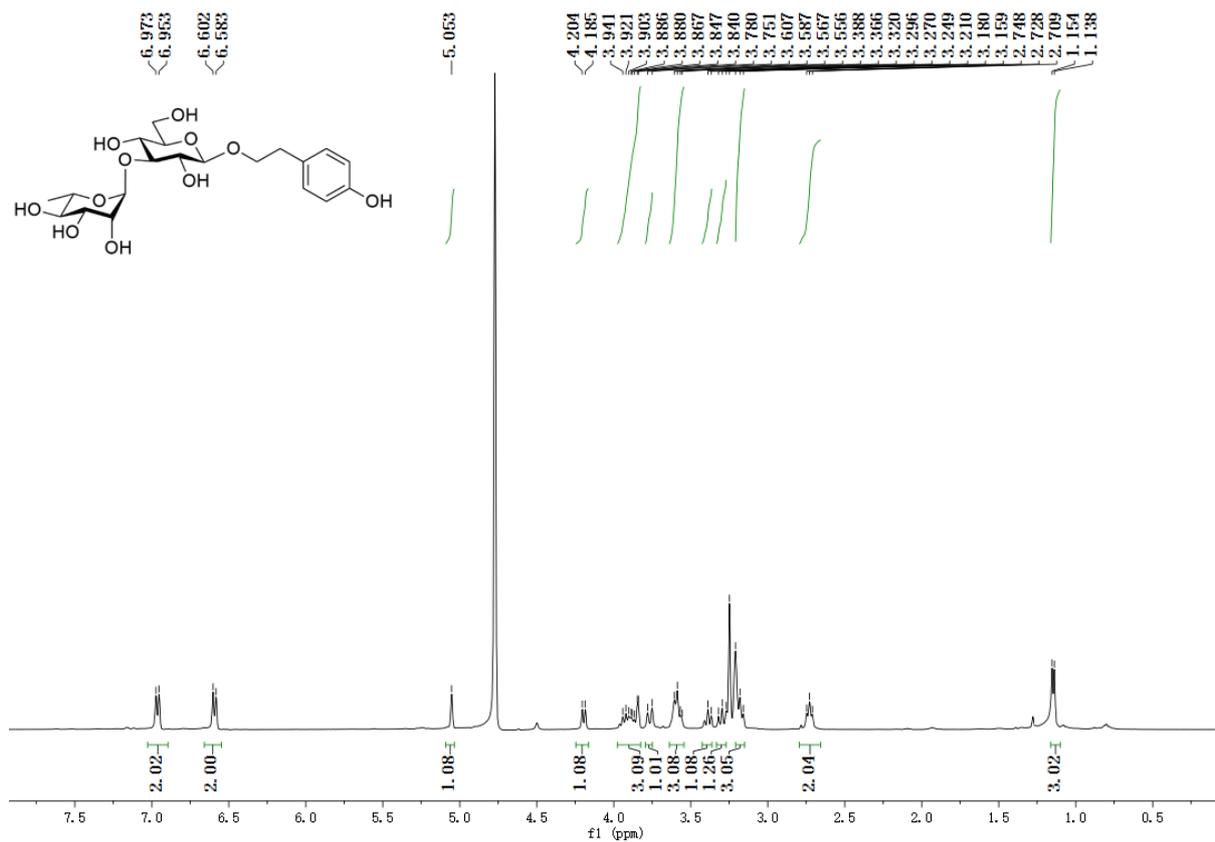


Figure S30: ¹H NMR spectrum (400 MHz) of **10** in CD₃OD

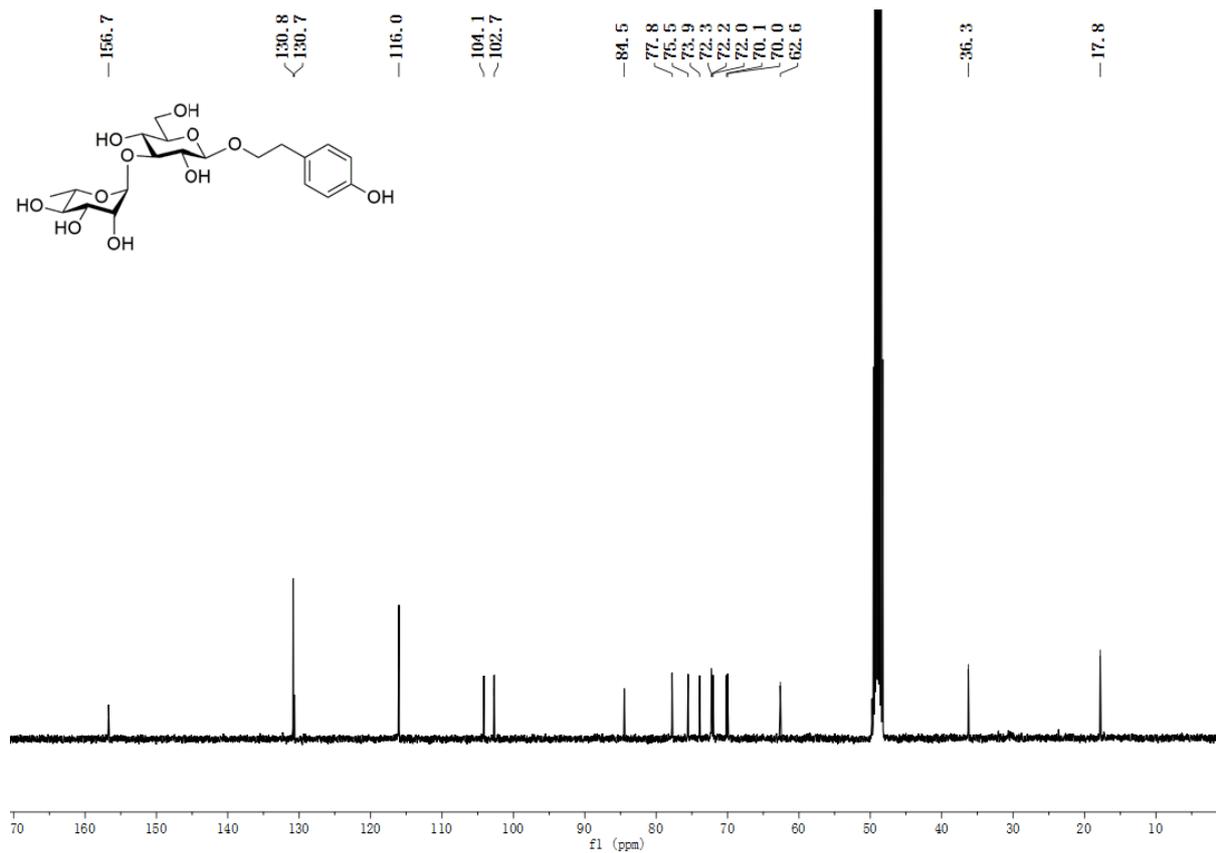


Figure S31: ^{13}C NMR spectrum (100 MHz) of 10 in CD_3OD