

## Supporting Information

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

### Diterpenoids from the Roots of *Clerodendrum bungei*

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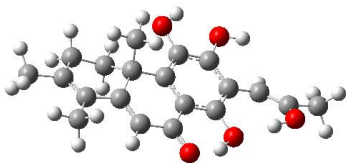
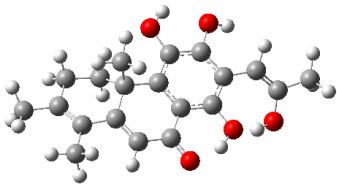
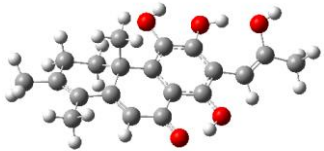
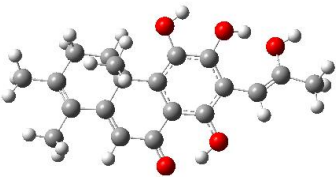
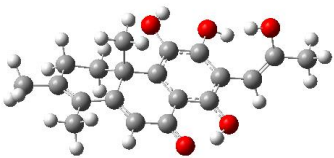
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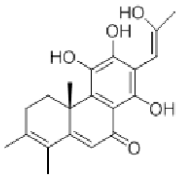
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Table of Contents	Page
<b>Table S1:</b> Re-optimized conformers, energies and proportions for <b>1</b> .	3
<b>Figure S1:</b> <sup>1</sup> H NMR spectrum of <b>1</b> in CDCl <sub>3</sub> .	4
<b>Figure S2:</b> <sup>13</sup> C and DEPT NMR spectra of <b>1</b> in CDCl <sub>3</sub> .	4
<b>Figure S3:</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>1</b> in CDCl <sub>3</sub> .	5
<b>Figure S4:</b> HSQC spectrum of <b>1</b> in CDCl <sub>3</sub> .	5
<b>Figure S5:</b> HMBC spectrum of <b>1</b> in CDCl <sub>3</sub> .	6
<b>Figure S6:</b> NOESY spectrum of <b>1</b> in CDCl <sub>3</sub> .	6
<b>Figure S7:</b> (+)-HR-ESIMS spectrum of <b>1</b> .	7
<b>Figure S8:</b> The UV spectrum of <b>1</b> .	7
<b>Figure S9:</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CD <sub>3</sub> OD.	8
<b>Figure S10:</b> <sup>13</sup> C NMR spectrum of <b>2</b> in CD <sub>3</sub> OD.	8
<b>Figure S11:</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>2</b> in CD <sub>3</sub> OD.	9
<b>Figure S12:</b> HSQC spectrum of <b>2</b> in CD <sub>3</sub> OD.	9
<b>Figure S13:</b> HMBC spectrum of <b>2</b> in CD <sub>3</sub> OD.	10
<b>Figure S14:</b> NOESY spectrum of <b>2</b> in CD <sub>3</sub> OD.	10
<b>Figure S15:</b> (+)-HR-ESIMS spectrum of <b>2</b> .	11
<b>Figure S16:</b> The UV spectrum of <b>2</b> .	11
<b>Figure S17:</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CDCl <sub>3</sub> .	12
<b>Figure S18:</b> <sup>13</sup> C and DEPT NMR spectra of <b>2</b> in CDCl <sub>3</sub> .	12
<b>Figure S19:</b> <sup>1</sup> H NMR spectrum of <b>2a</b> in CDCl <sub>3</sub> .	13

<b>Figure S20:</b> $^1\text{H}$ NMR spectrum of <b>2b</b> in $\text{CDCl}_3$ .	13
<b>Figure S21:</b> $^1\text{H}$ NMR spectrum of <b>3</b> in $\text{CDCl}_3$ .	14
<b>Figure S22:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>3</b> in $\text{CDCl}_3$ .	14
<b>Figure S23:</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of <b>3</b> in $\text{CDCl}_3$ .	15
<b>Figure S24:</b> HSQC spectrum of <b>3</b> in $\text{CDCl}_3$ .	15
<b>Figure S25:</b> HMBC spectrum of <b>3</b> in $\text{CDCl}_3$ .	16
<b>Figure S26:</b> NOESY spectrum of <b>3</b> in $\text{CDCl}_3$ .	16
<b>Figure S27:</b> Linear correlation between the experimental $^{13}\text{C}$ NMR data for <b>3</b> and the calculated data for ( <i>Z</i> )- $\Delta^{15}$ (left) and ( <i>E</i> )- $\Delta^{15}$ (right) isomers, respectively.	17
<b>Figure S28:</b> SciFinder search report for compound <b>1</b> .	17
<b>Figure S29:</b> SciFinder search report for compound <b>2</b> .	18
<b>Figure S30:</b> $^1\text{H}$ NMR spectrum of <b>4</b> in $\text{CDCl}_3$ .	19
<b>Figure S31:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>4</b> in $\text{CDCl}_3$ .	19
<b>Figure S32:</b> $^1\text{H}$ NMR spectrum of <b>5</b> in $\text{CDCl}_3$ .	20
<b>Figure S33:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>5</b> in $\text{CDCl}_3$ .	20
<b>Figure S34:</b> $^1\text{H}$ NMR spectrum of <b>6</b> in $\text{CD}_3\text{OD}$ .	21
<b>Figure S35:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>6</b> in $\text{CD}_3\text{OD}$ .	21
<b>Figure S36:</b> $^1\text{H}$ NMR spectrum of <b>7</b> in $\text{CDCl}_3$ .	22
<b>Figure S37:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>7</b> in $\text{CDCl}_3$ .	22
<b>Figure S38:</b> $^1\text{H}$ NMR spectrum of <b>8</b> in $\text{CDCl}_3$ .	23
<b>Figure S39:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>8</b> in $\text{CDCl}_3$ .	23
<b>Figure S40:</b> $^1\text{H}$ NMR spectrum of <b>9</b> in $\text{CDCl}_3$ .	24
<b>Figure S41:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>9</b> in $\text{CDCl}_3$ .	24
<b>Figure S42:</b> $^1\text{H}$ NMR spectrum of <b>10</b> in $\text{CDCl}_3$ .	25
<b>Figure S43:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>10</b> in $\text{CDCl}_3$ .	25
<b>Figure S44:</b> $^1\text{H}$ NMR spectrum of <b>11</b> in $\text{CDCl}_3$ .	26
<b>Figure S45:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>11</b> in $\text{CDCl}_3$ .	26
<b>Figure S46:</b> $^1\text{H}$ NMR spectrum of <b>12</b> in $\text{CDCl}_3$ .	27
<b>Figure S47:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>12</b> in $\text{CDCl}_3$ .	27
<b>Figure S48:</b> $^1\text{H}$ NMR spectrum of <b>13</b> in $\text{CDCl}_3$ .	28
<b>Figure S49:</b> $^{13}\text{C}$ and DEPT NMR spectra of <b>13</b> in $\text{CDCl}_3$ .	28

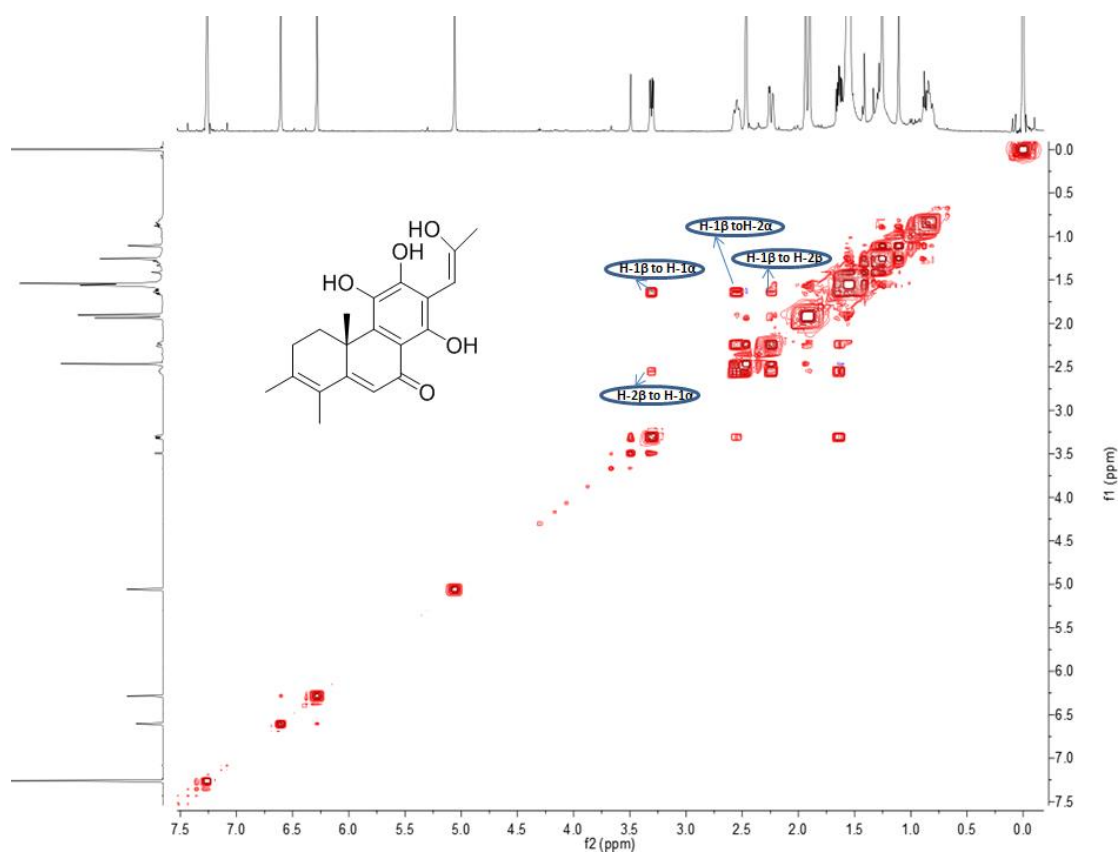
**Table S1.** Re-optimized conformers, energies and proportions for **1**.

No.	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1151.8059374	-722769.743777874	52.57
2		-1151.8058152	-722769.667096152	46.18
3		-1151.8022875	-722767.453429125	1.10
4		-1151.7997953	-722765.889548703	0.08
5		-1151.7996883	-722765.822405133	0.07

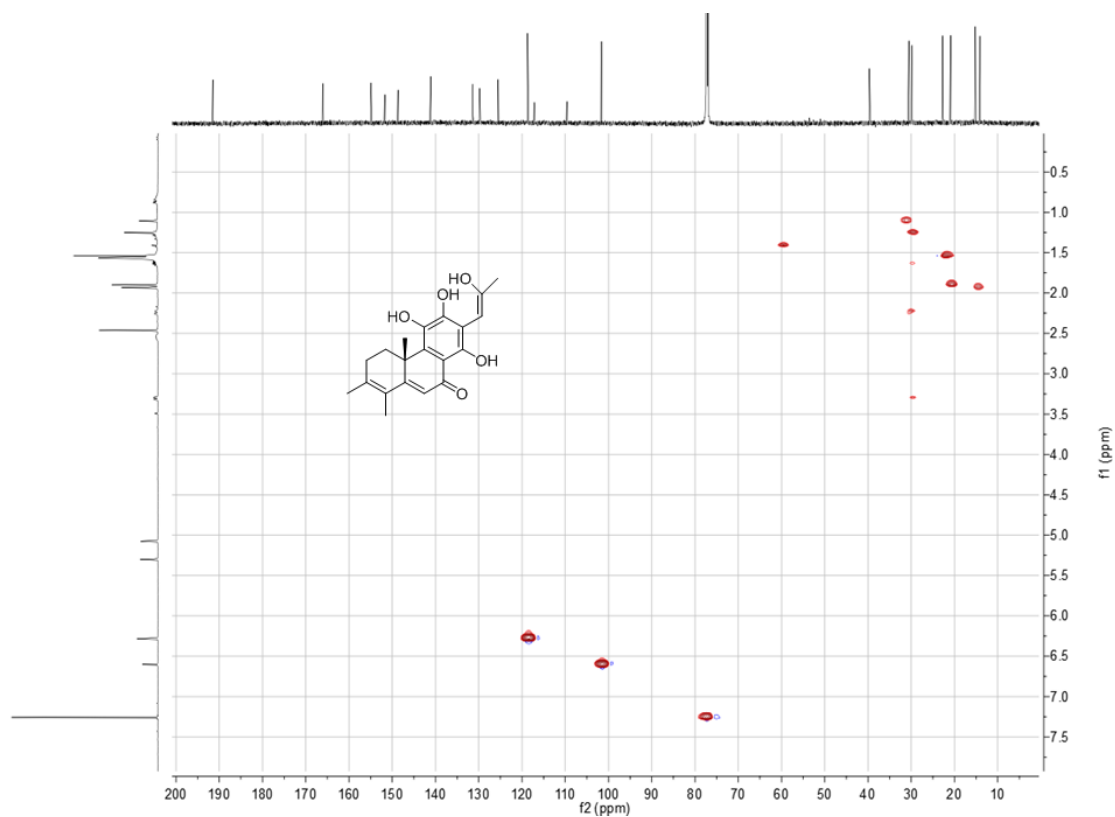


Chemical structure of compound 10a is shown. The  $^{13}\text{C}$  NMR spectrum (f1 (ppm)) displays peaks at the following chemical shifts (ppm): 191.50, 166.09, 154.88, 151.72, 148.68, 141.05, 131.36, 129.80, 125.52, 118.70, 117.19, 109.63, 101.66, 77.37, 77.46, 76.95, 39.67, 30.55, 29.92, 22.69, 20.90, 15.17, and 14.15.

**Figure S2:**  $^{13}\text{C}$  and DEPT NMR spectra of **1** in  $\text{CDCl}_3$ .

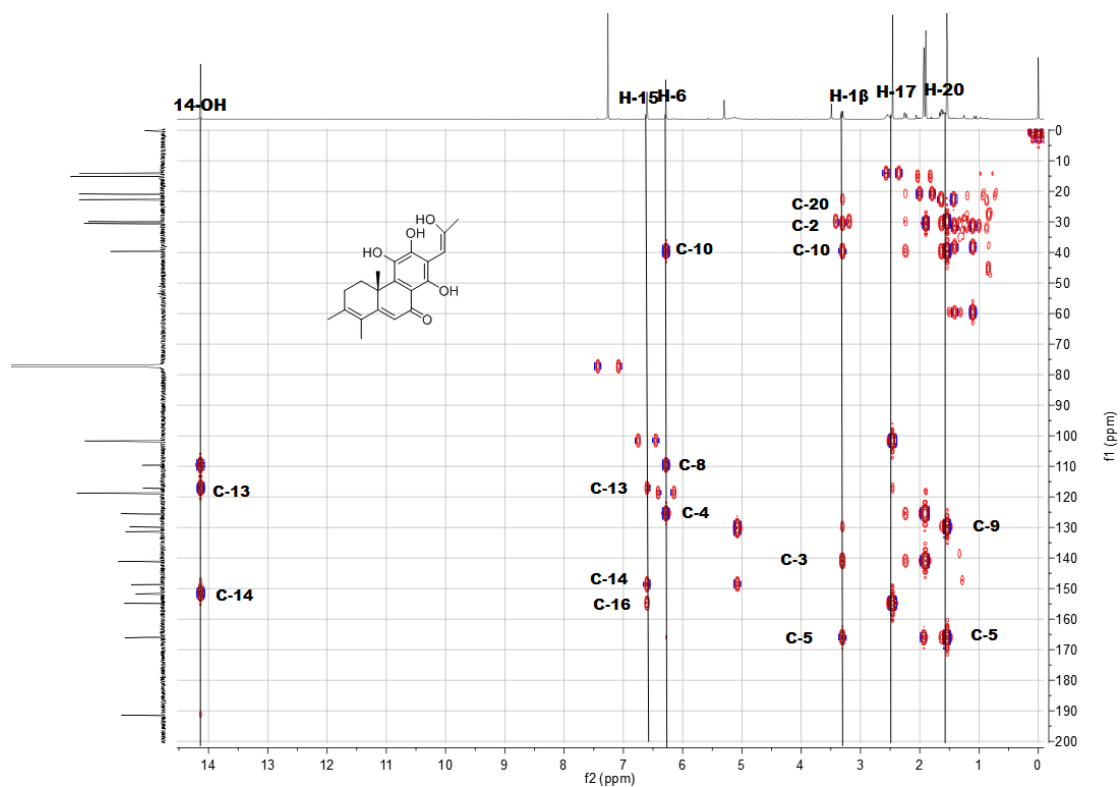


**Figure S3:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{CDCl}_3$ .

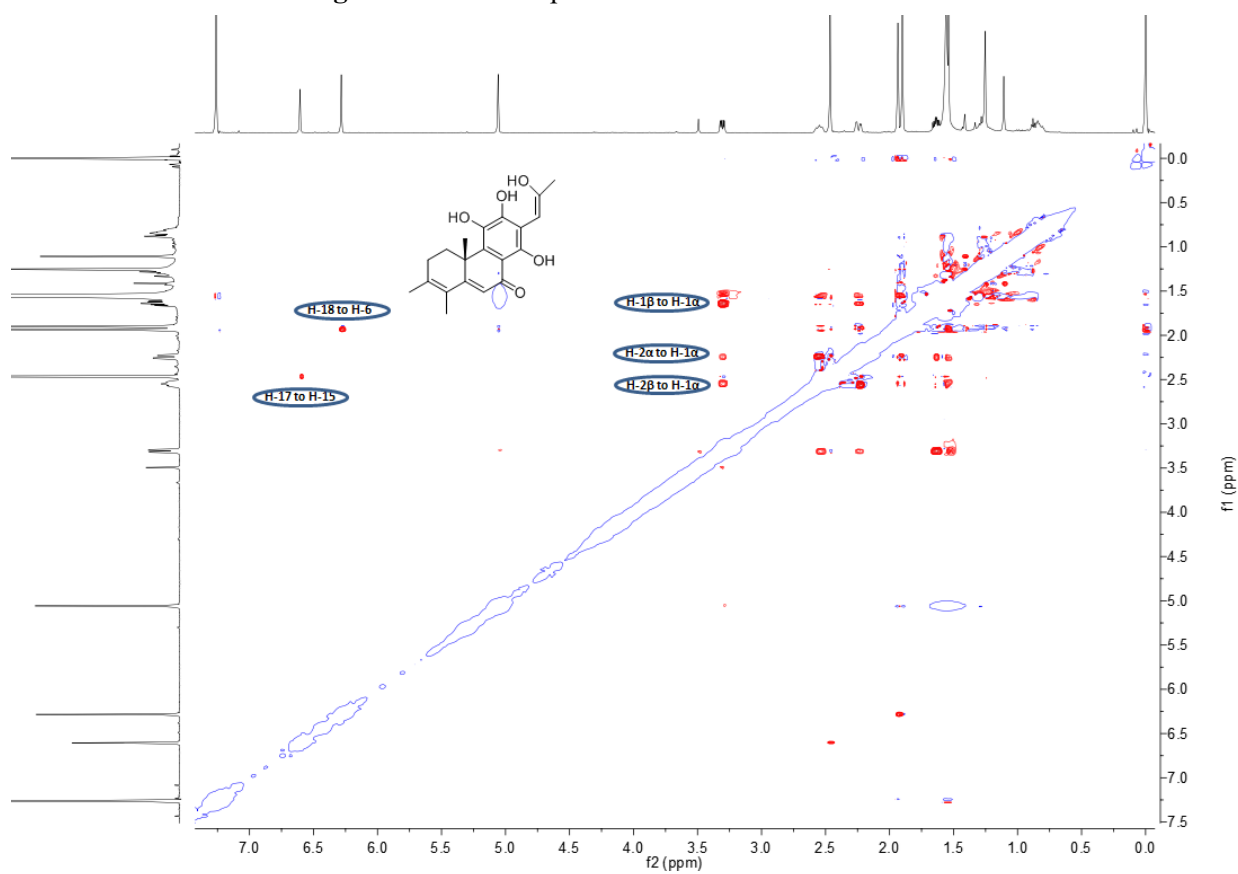


**Figure S4:** HSQC spectrum of **1** in  $\text{CDCl}_3$ .

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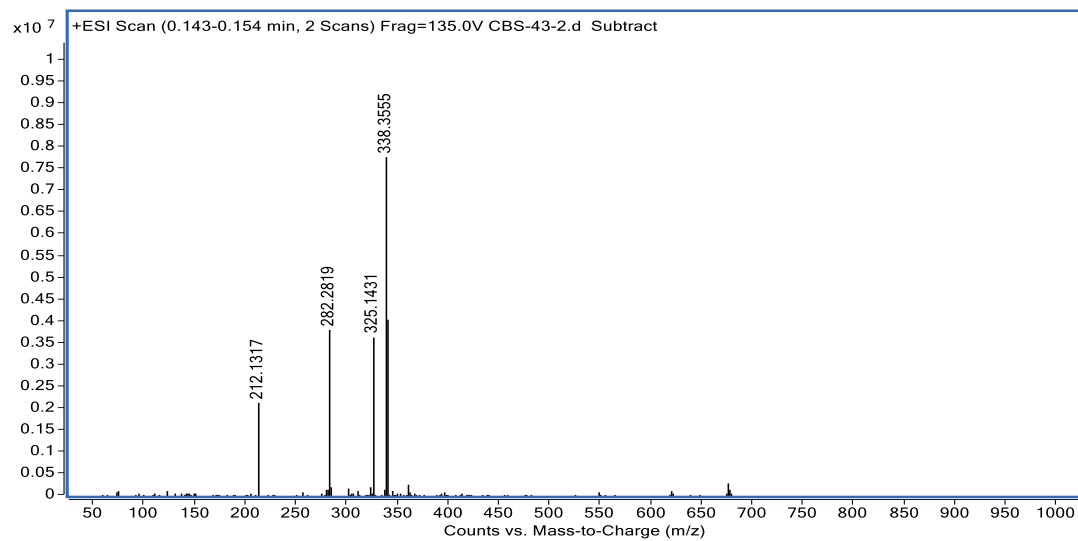


**Figure S5:** HMBC spectrum of **1** in  $\text{CDCl}_3$ .

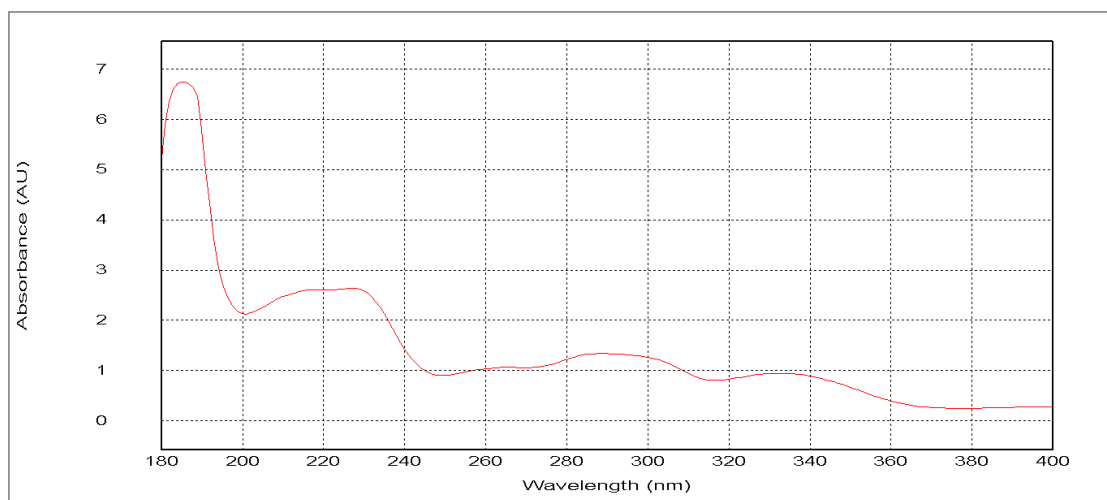


**Figure S6:** NOESY spectrum of **1** in  $\text{CDCl}_3$

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**Figure S7:** (+)-HR-ESIMS spectrum of **1**.



**Figure S8:**The UV spectrum of **1**.

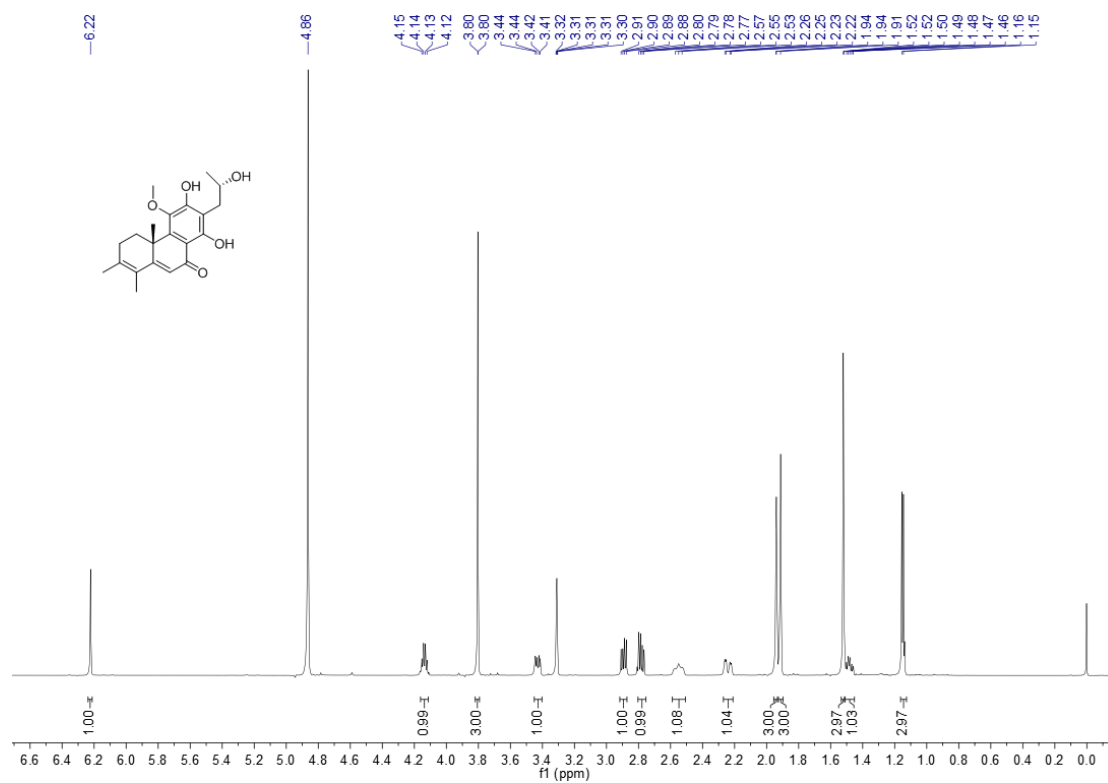


Figure S9: <sup>1</sup>H NMR spectrum of 2 in CD<sub>3</sub>OD.

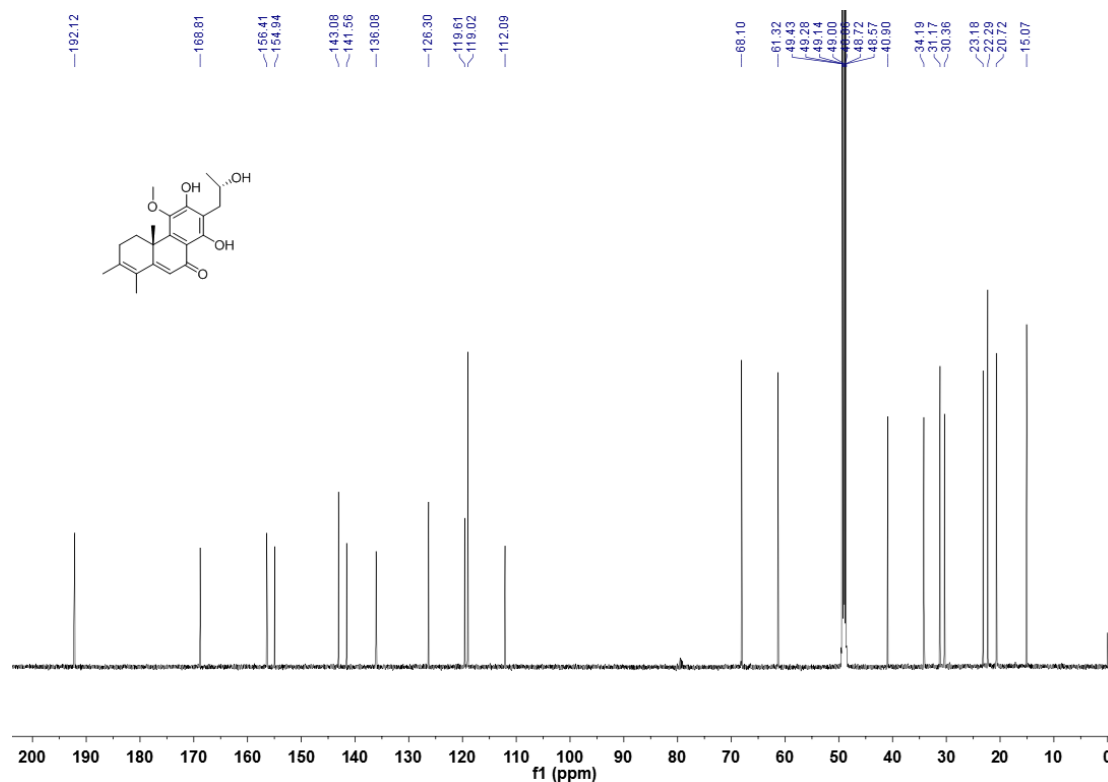
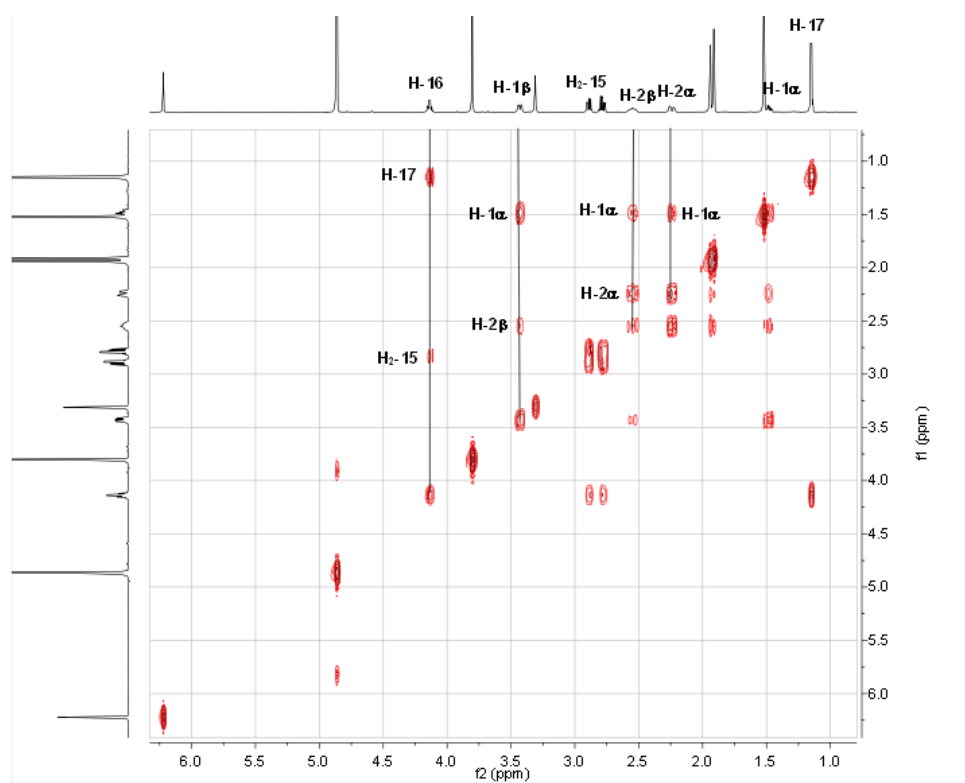
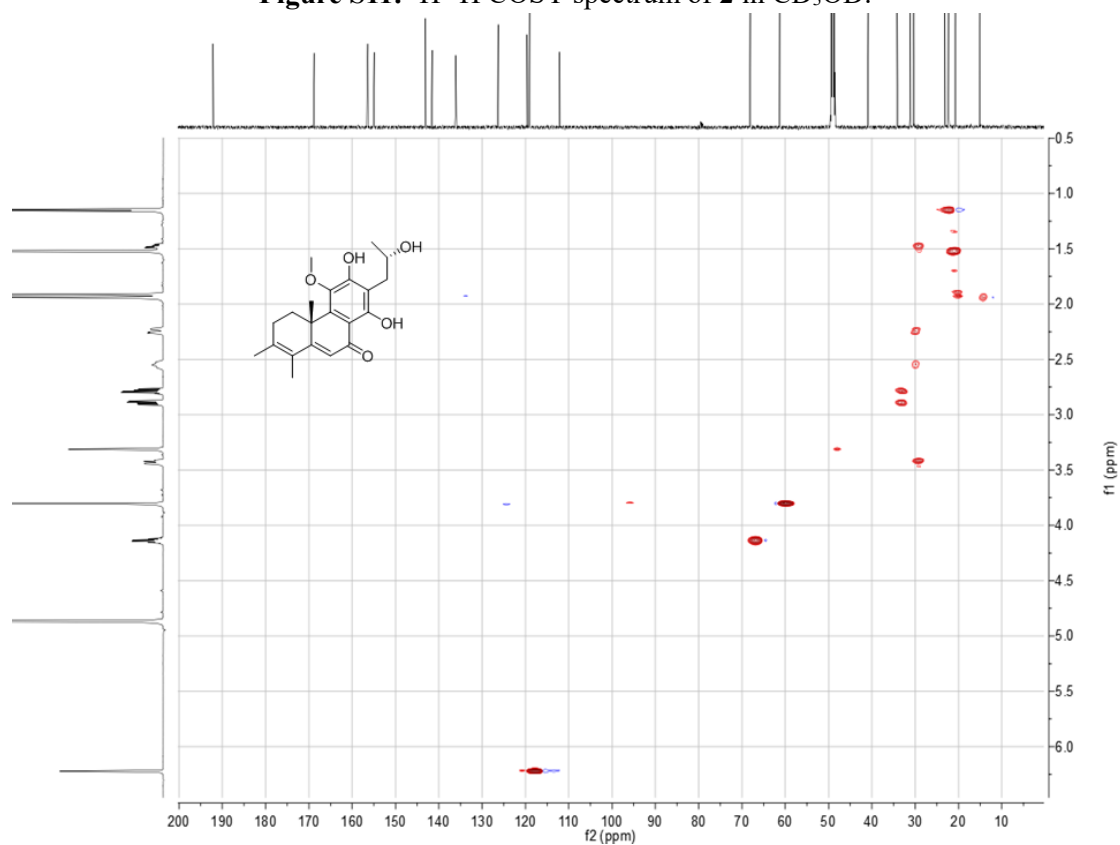


Figure S10: <sup>13</sup>C NMR spectrum of 2 in CD<sub>3</sub>OD.





**Figure S11:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{CD}_3\text{OD}$ .



**Figure S12:** HSQC spectrum of **2** in  $\text{CD}_3\text{OD}$ .

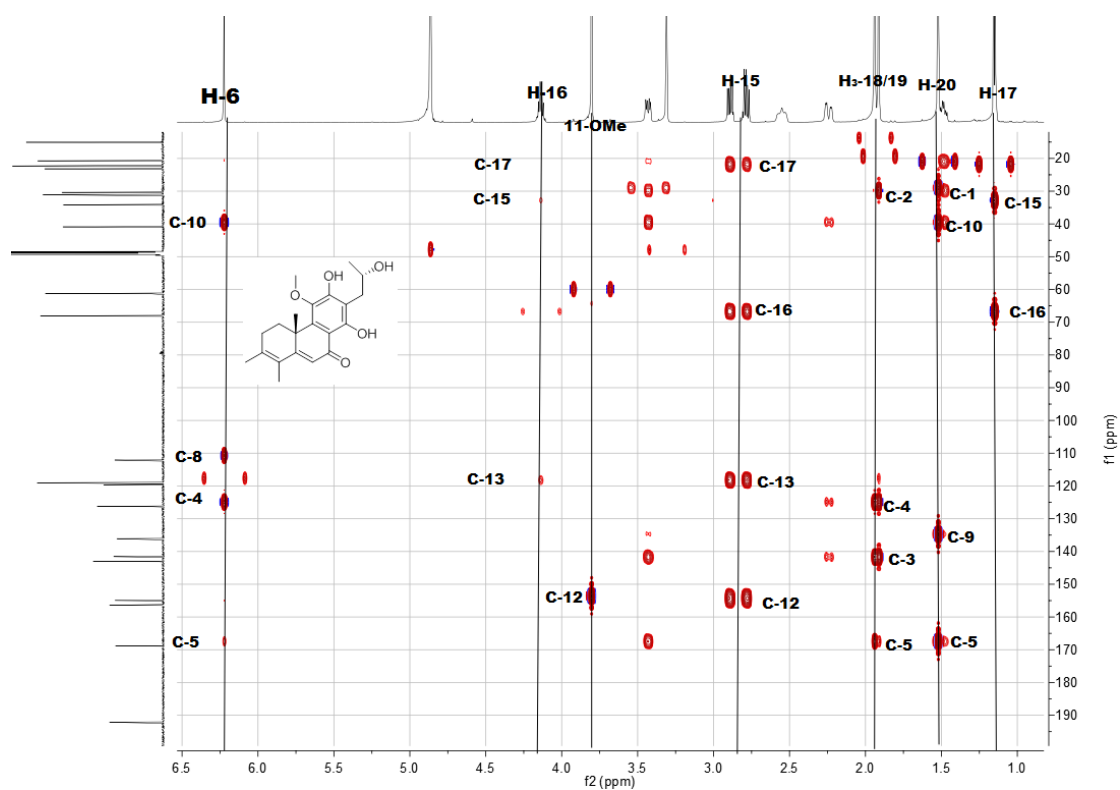


Figure S13: HMBC spectrum of **2** in CD<sub>3</sub>OD.

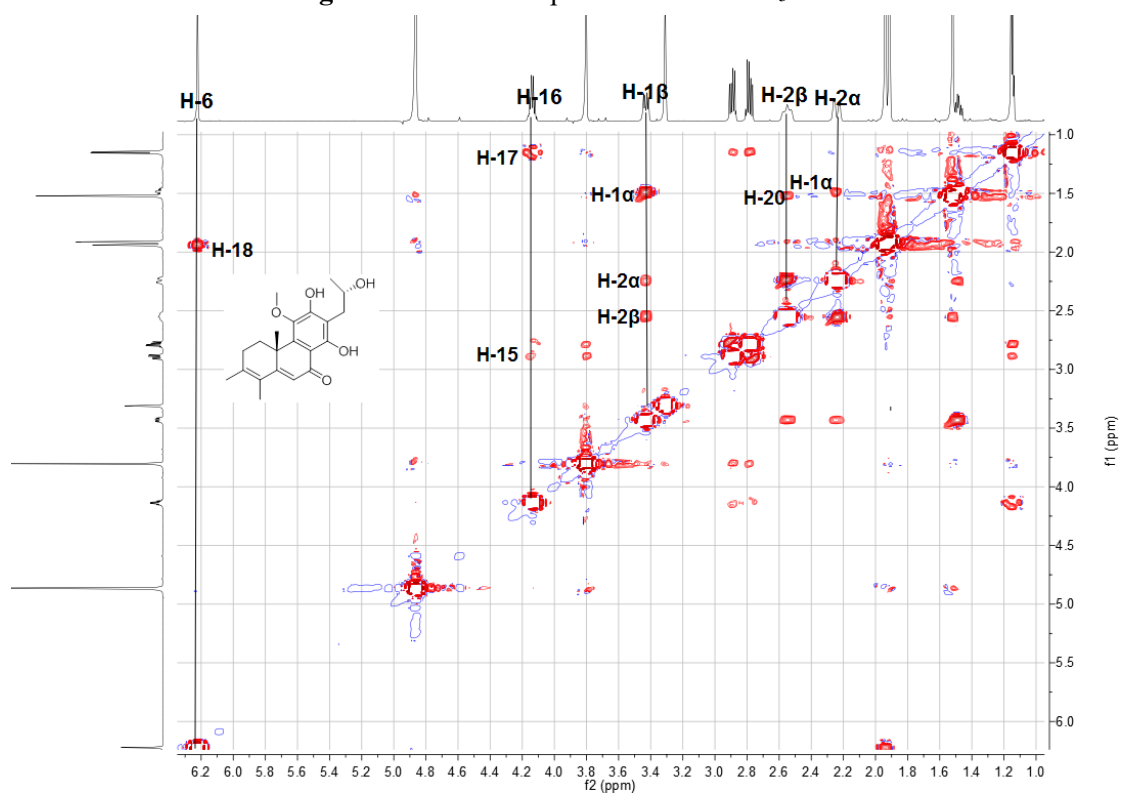
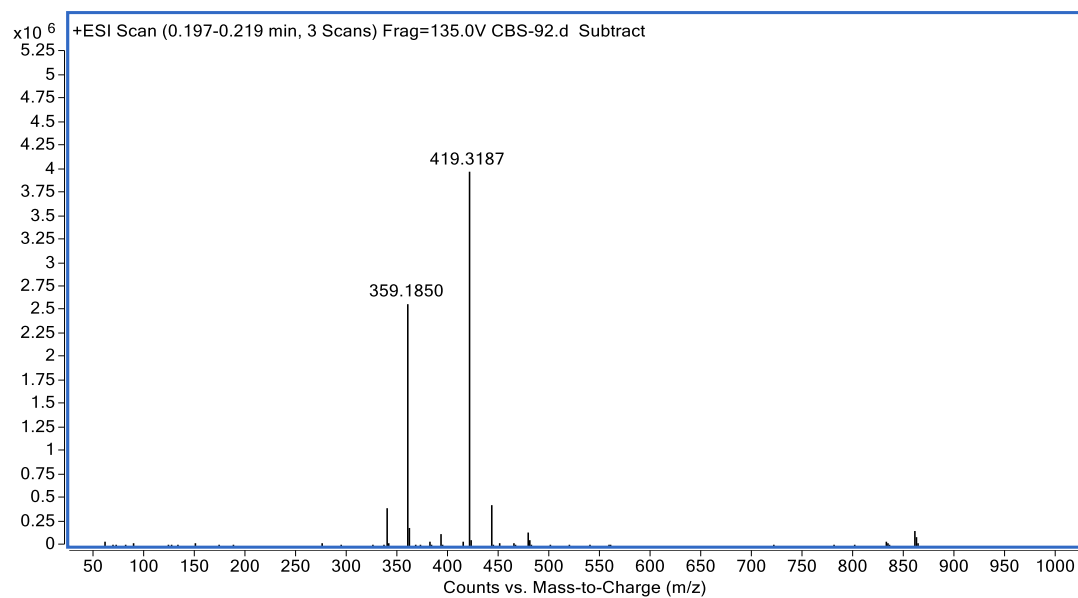
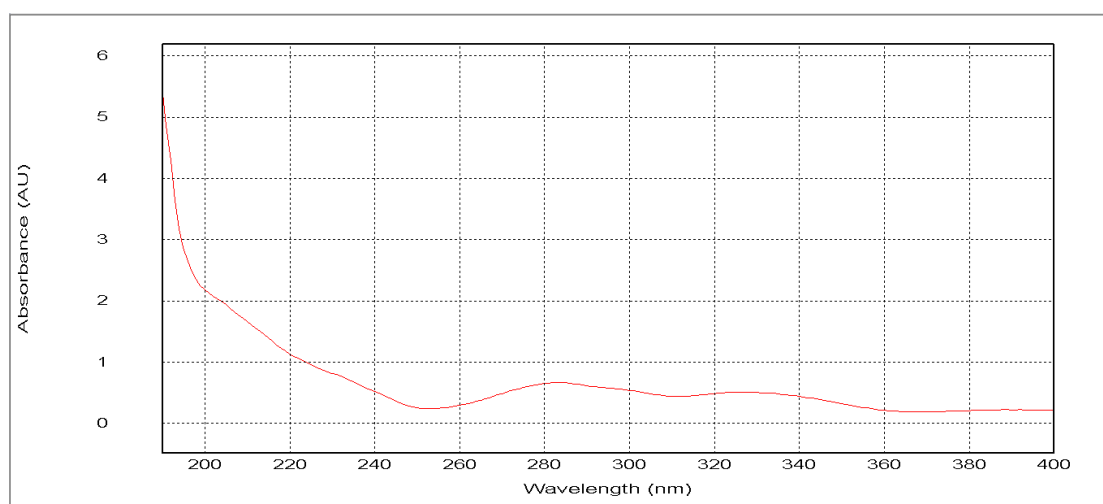


Figure S14: NOESY spectrum of **2** in CD<sub>3</sub>OD.



**Figure S15:** (+)-HR-ESIMS spectrum of **2**.



**Figure S16:** The UV spectrum of **2**.

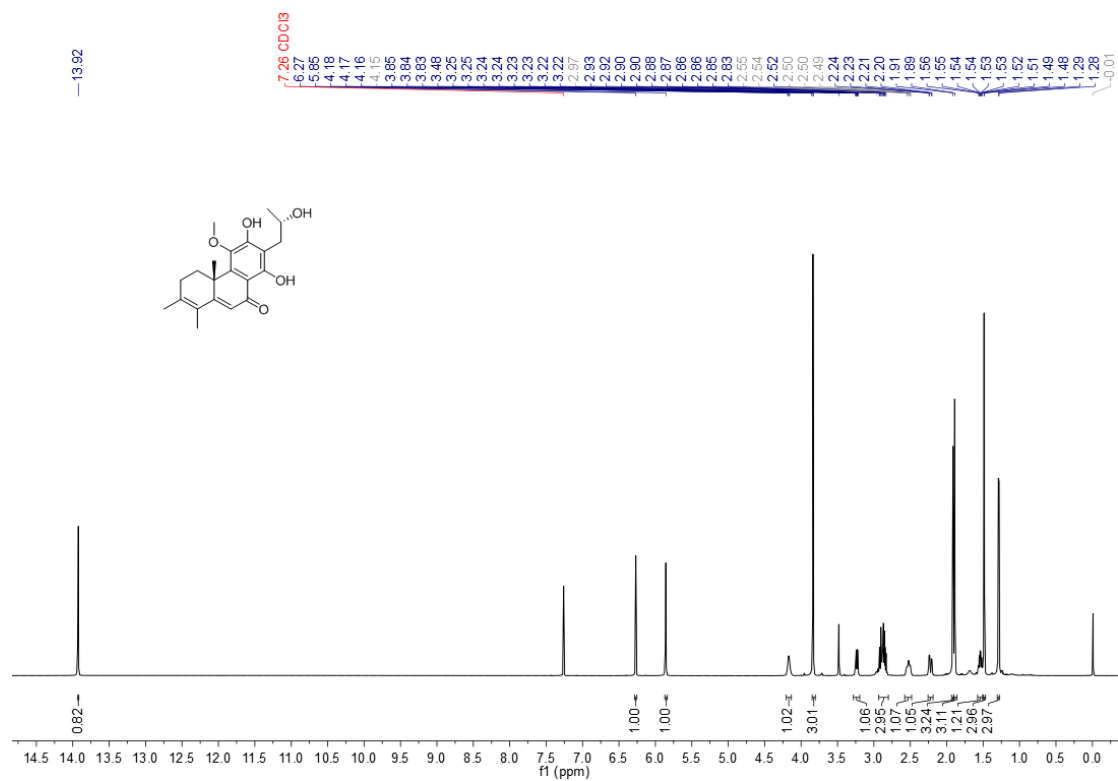


Figure S17: <sup>1</sup>H NMR spectrum of **2** in CDCl<sub>3</sub>.

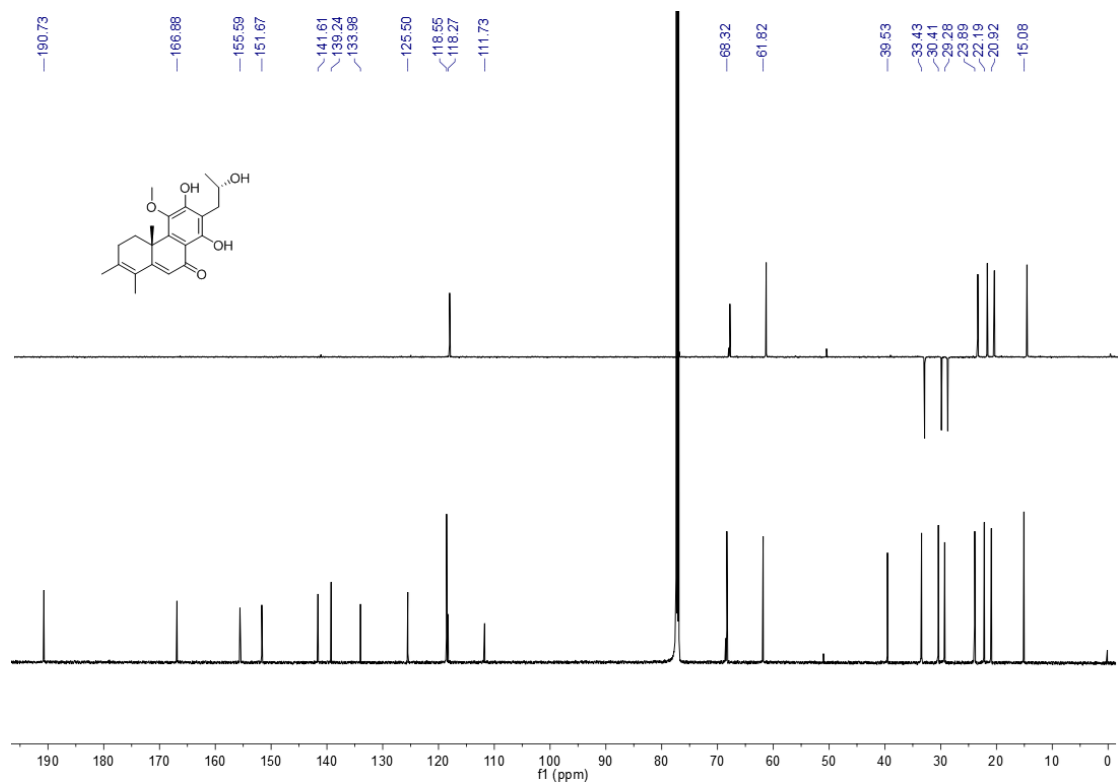
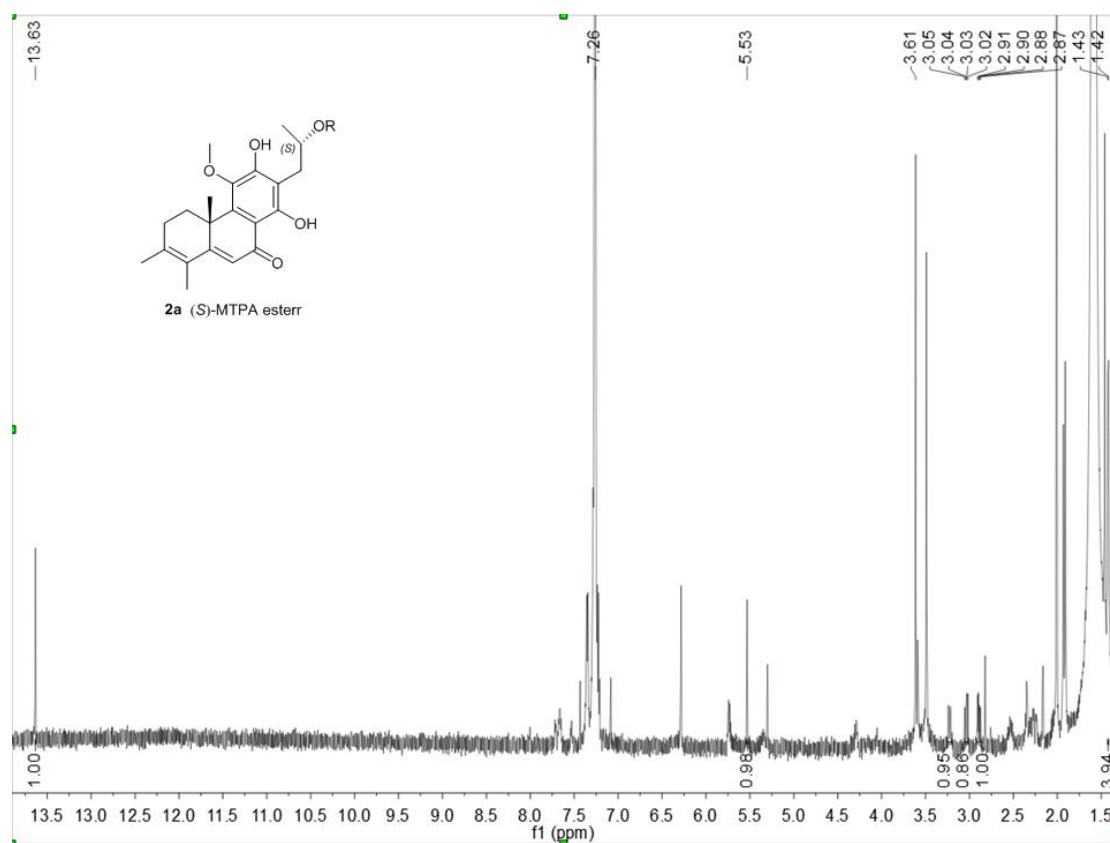
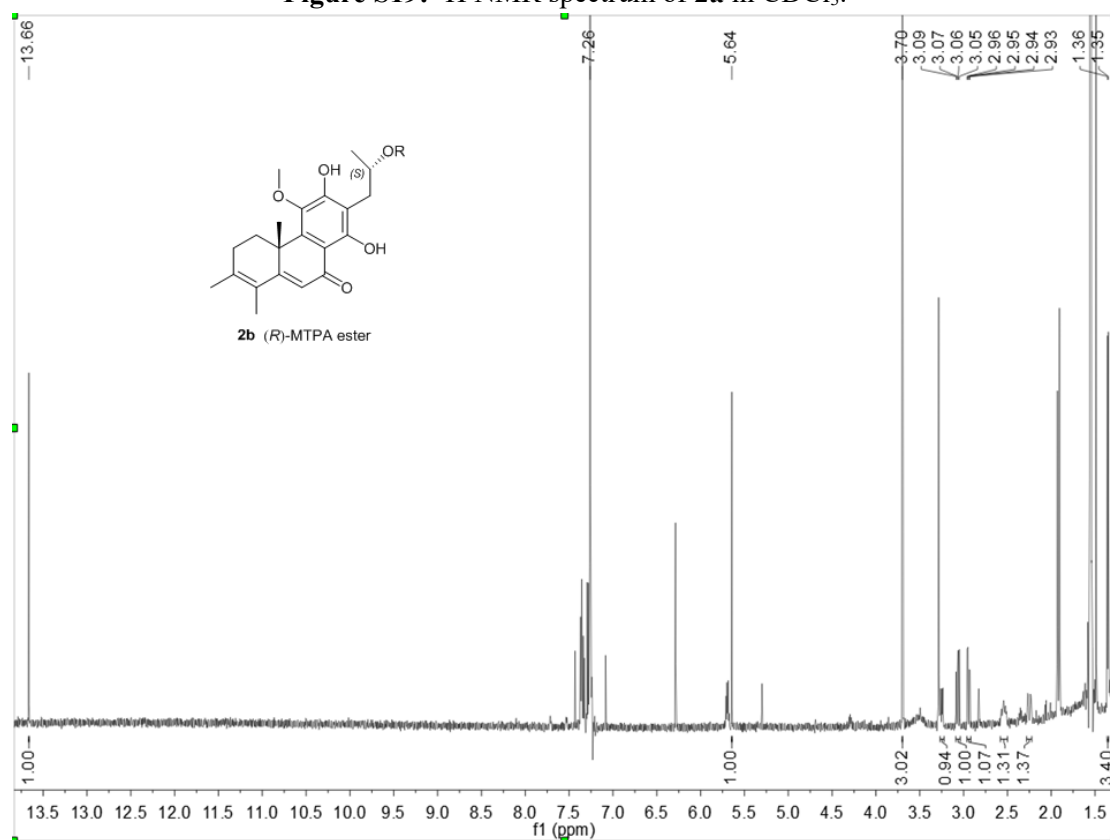


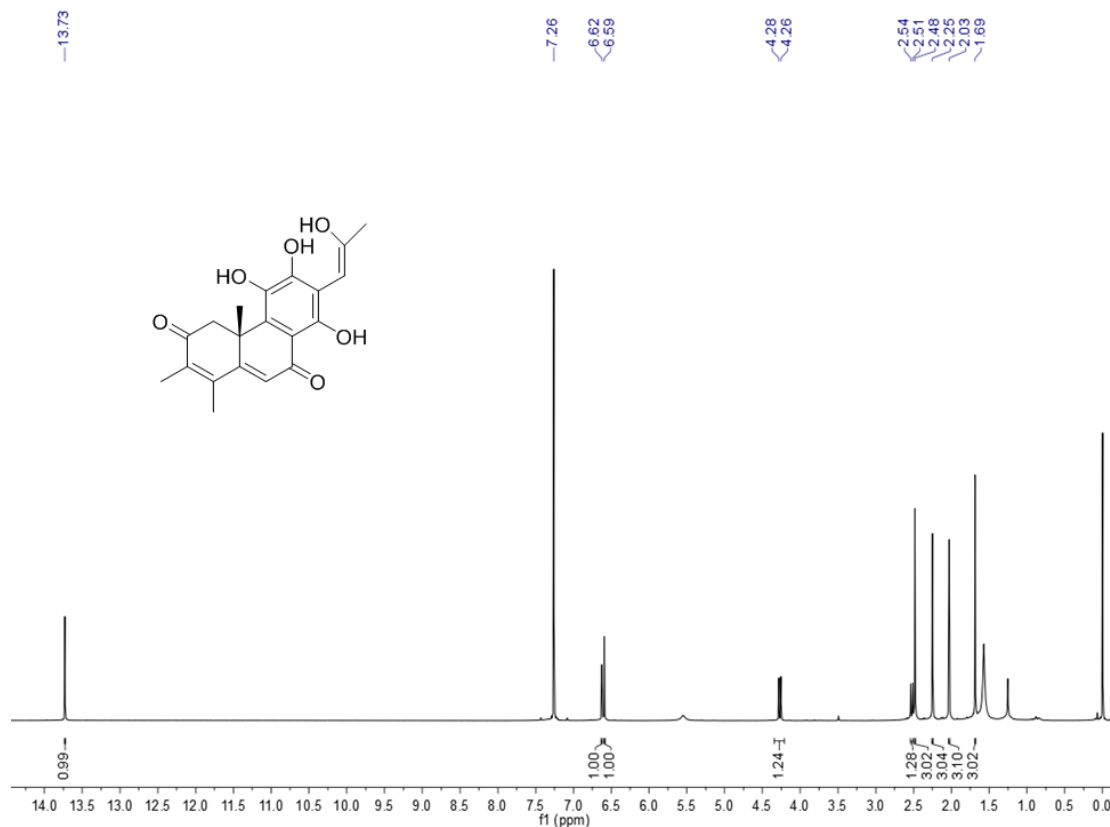
Figure S18: <sup>13</sup>C and DEPT NMR spectra of **2** in CDCl<sub>3</sub>.



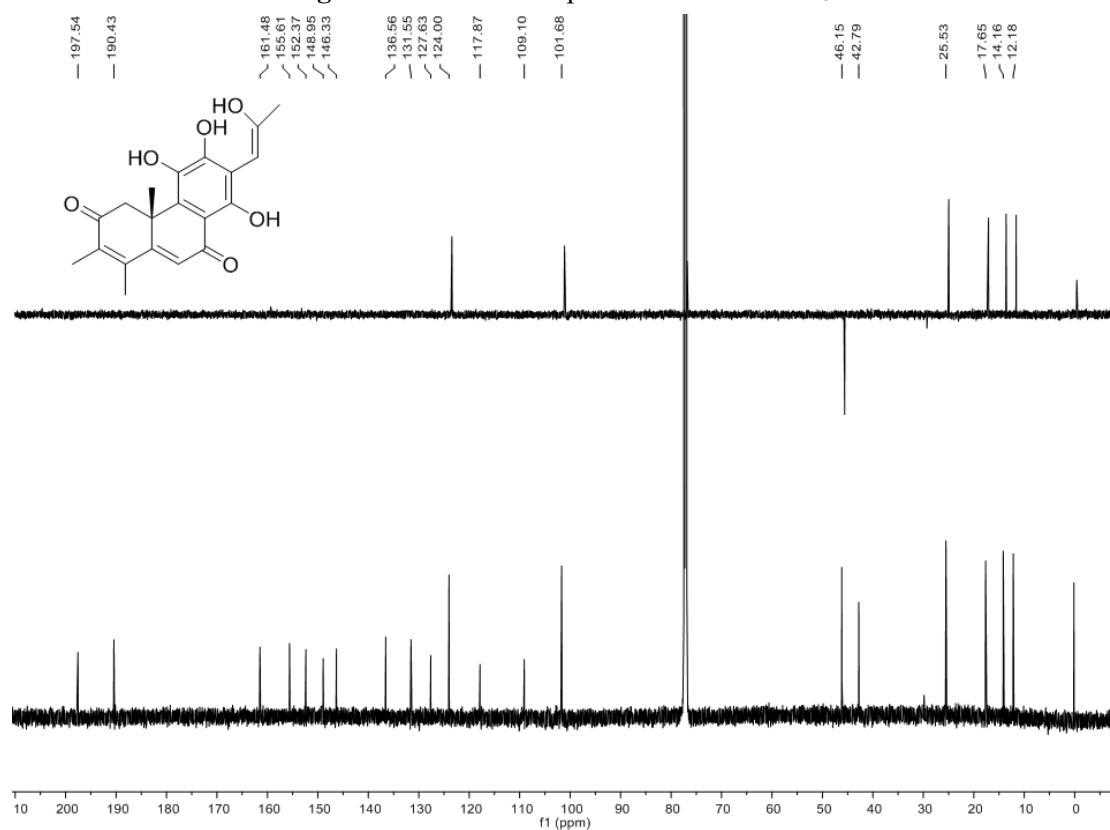
**Figure S19:**  $^1\text{H}$  NMR spectrum of **2a** in CDCl<sub>3</sub>.



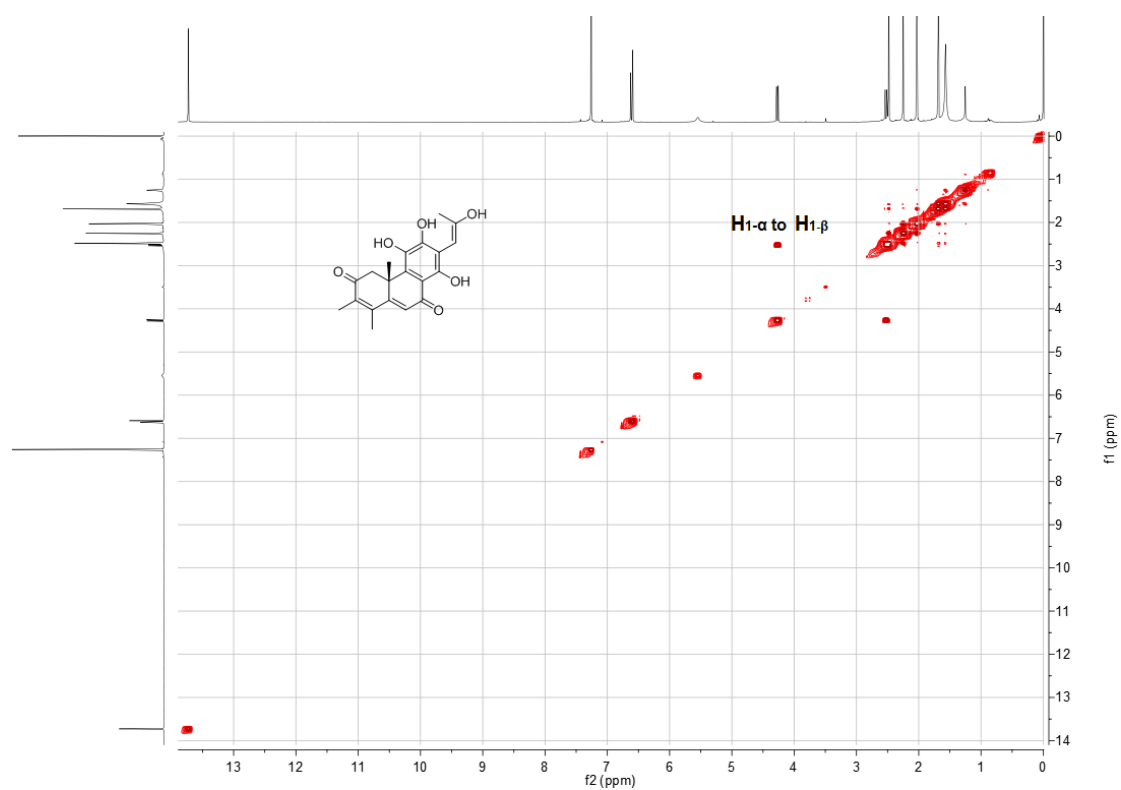
**Figure S20:**  $^1\text{H}$  NMR spectrum of **2b** in CDCl<sub>3</sub>.



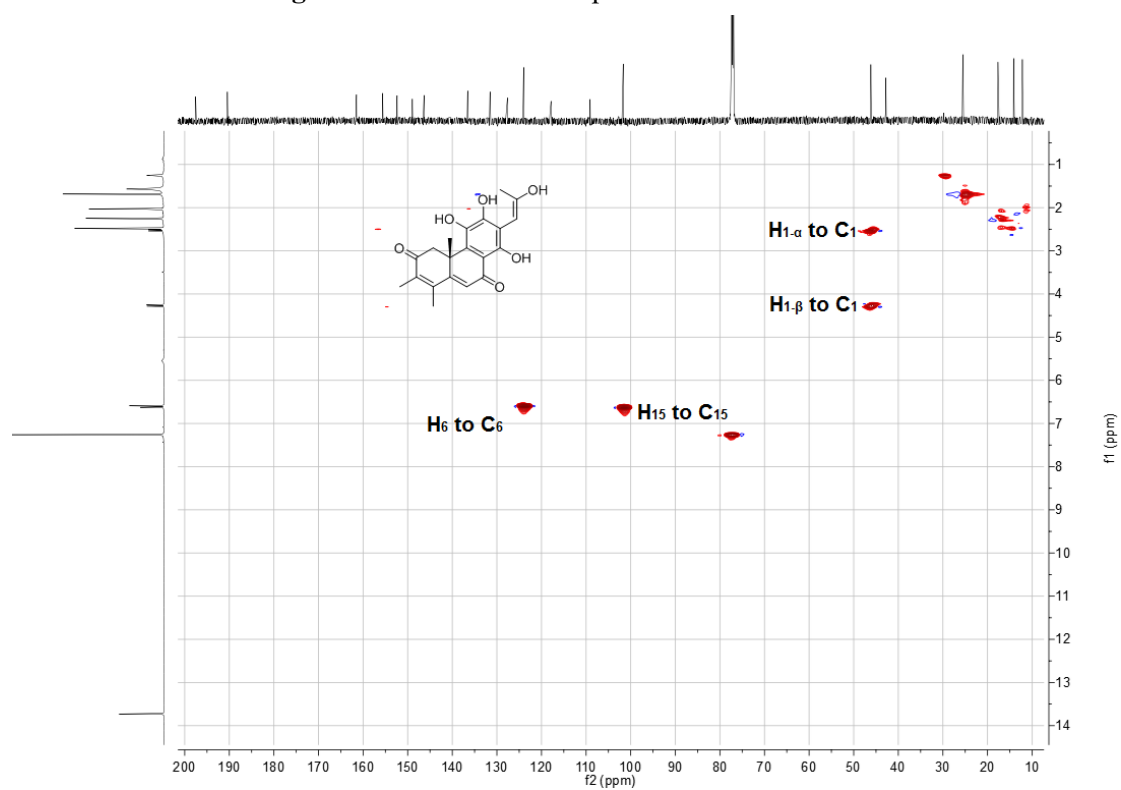
**Figure S21:** <sup>1</sup>H NMR spectrum of **3** in CDCl<sub>3</sub>.



**Figure S22:** <sup>13</sup>C and DEPT NMR spectra of **3** in CDCl<sub>3</sub>.



**Figure S23:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{CDCl}_3$ .



**Figure S24:** HSQC spectrum of **3** in  $\text{CDCl}_3$ .

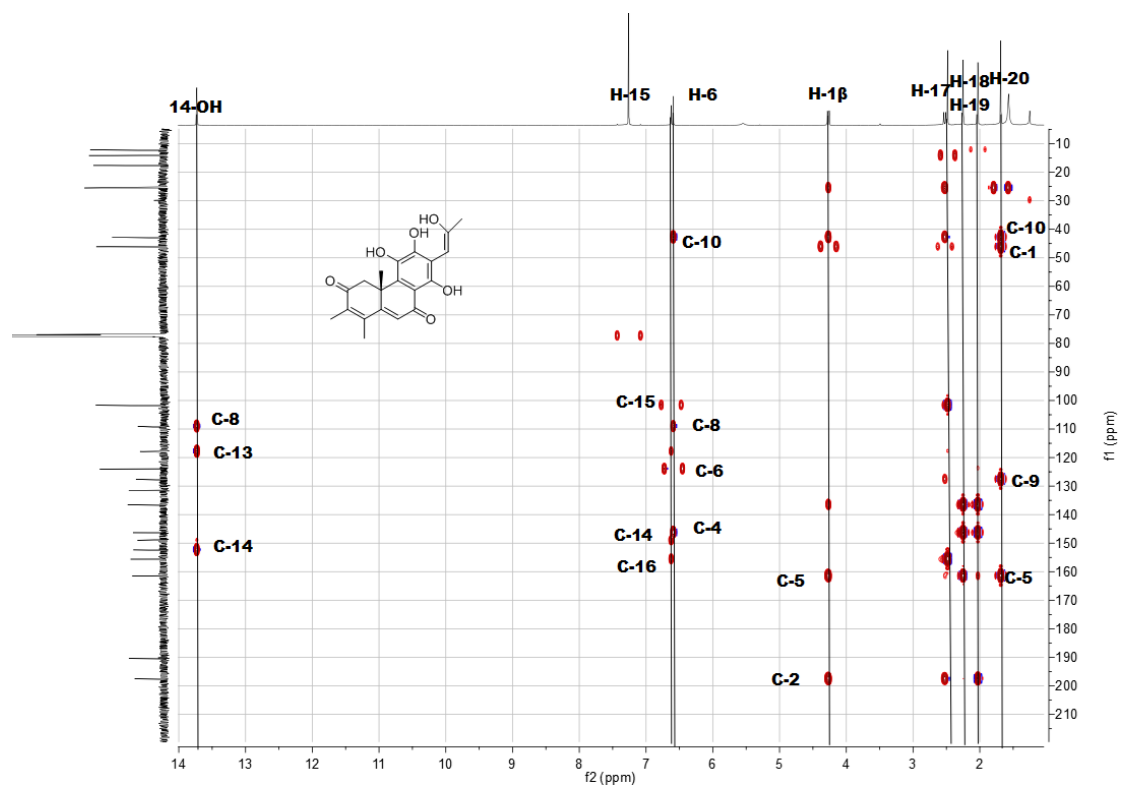


Figure S25: HMBC spectrum of **3** in CDCl<sub>3</sub>.

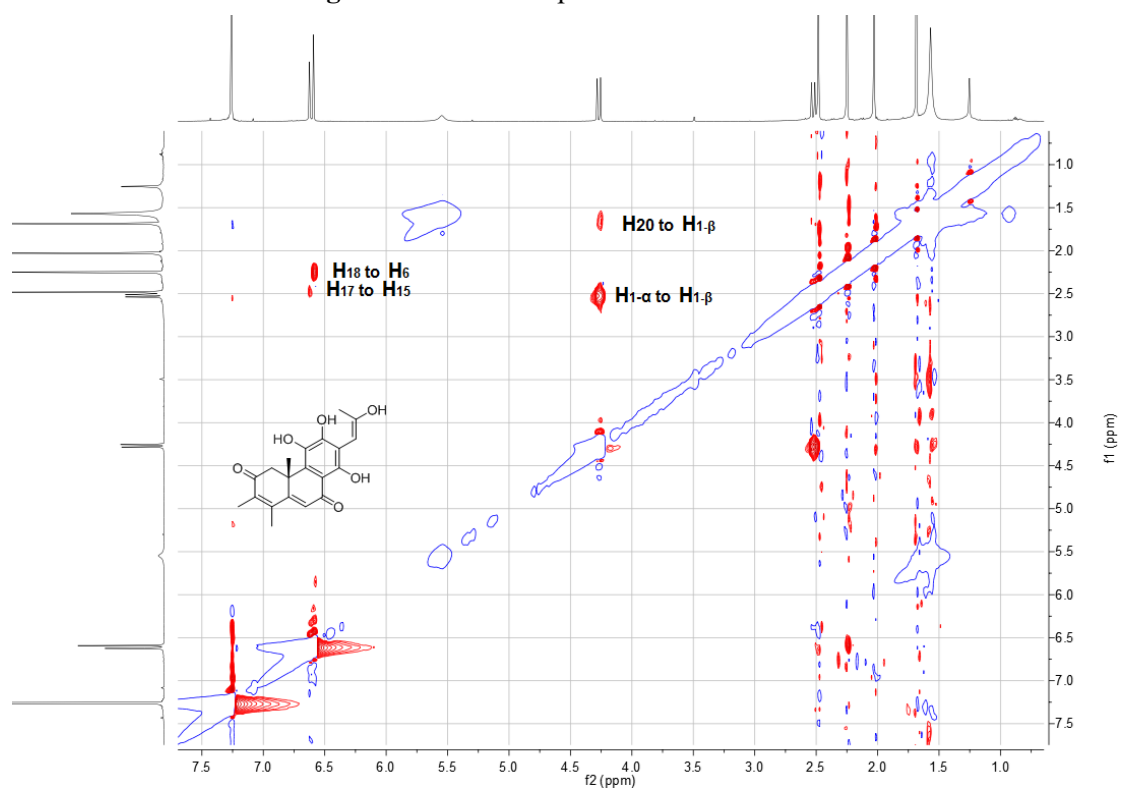
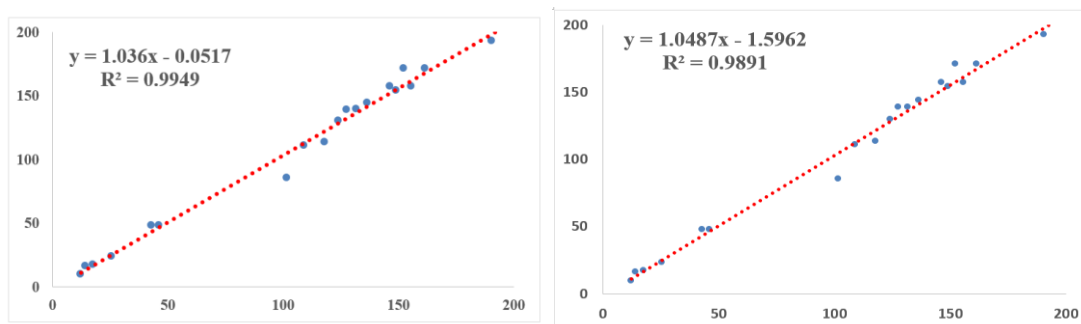


Figure S26: NOESY spectrum of **3** in CDCl<sub>3</sub>.





**Figure S27:** Linear correlation between the experimental  $^{13}\text{C}$  NMR data for **3** and the calculated data for  $(Z)\text{-}\Delta^{15}$  (left) and  $(E)\text{-}\Delta^{15}$  (right) isomers, respectively.

Figure S28 shows the SciFinder search report for compound **1**. The interface displays search results, chemical structures, and physical properties for several compounds. The search results are organized into a table with columns for 'Substances' and 'Similarity'. The table lists 6 of 9 similarity candidates selected, with the top results being:

Similarity	Substances
≥ 99 (most similar)	1
95-98	1
90-94	1
85-89	4
80-84	1
75-79	6
70-74	39
65-69	230
0-64 (least similar)	1045

The search results also include chemical structures and physical properties for the top candidates. The first candidate is a complex polycyclic compound with multiple hydroxyl groups. The second candidate is a similar polycyclic compound with a different substitution pattern. The third candidate is a polycyclic compound with a different substitution pattern. The fourth candidate is a polycyclic compound with a different substitution pattern. The fifth candidate is a polycyclic compound with a different substitution pattern. The sixth candidate is a polycyclic compound with a different substitution pattern. The seventh candidate is a polycyclic compound with a different substitution pattern. The eighth candidate is a polycyclic compound with a different substitution pattern. The ninth candidate is a polycyclic compound with a different substitution pattern.

**Figure S28:** SciFinder search report for compound **1**.



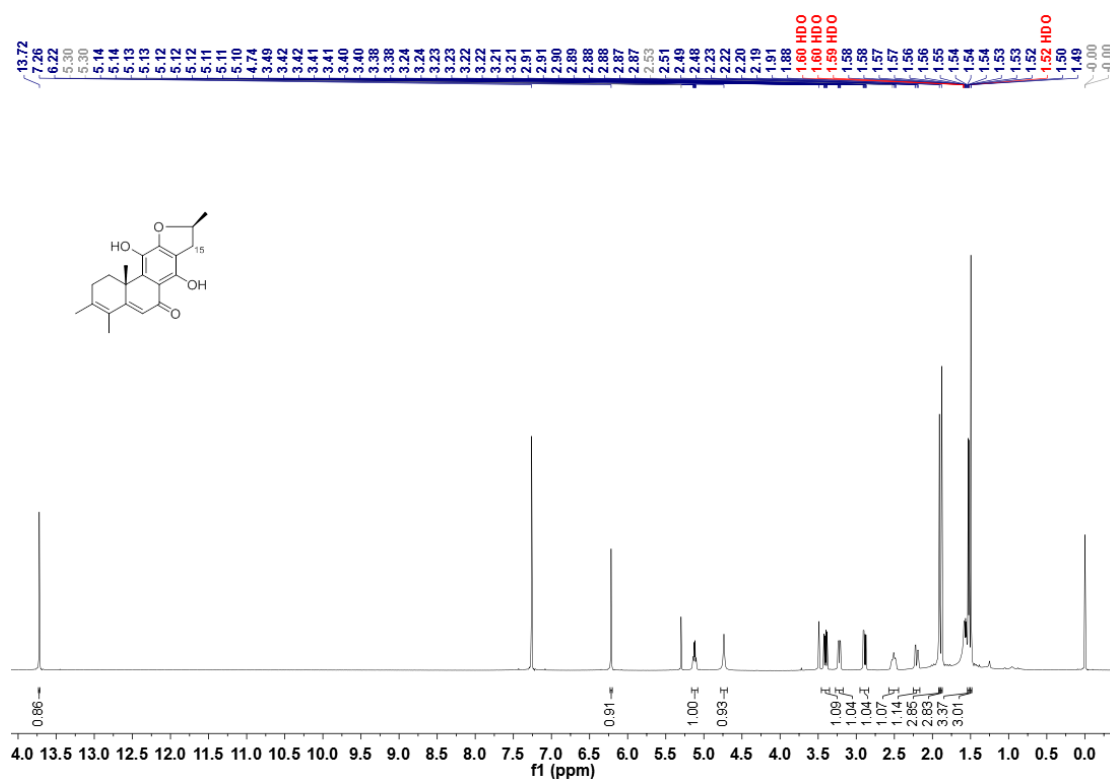


Figure S30: <sup>1</sup>H NMR spectrum of **4** in CDCl<sub>3</sub>.

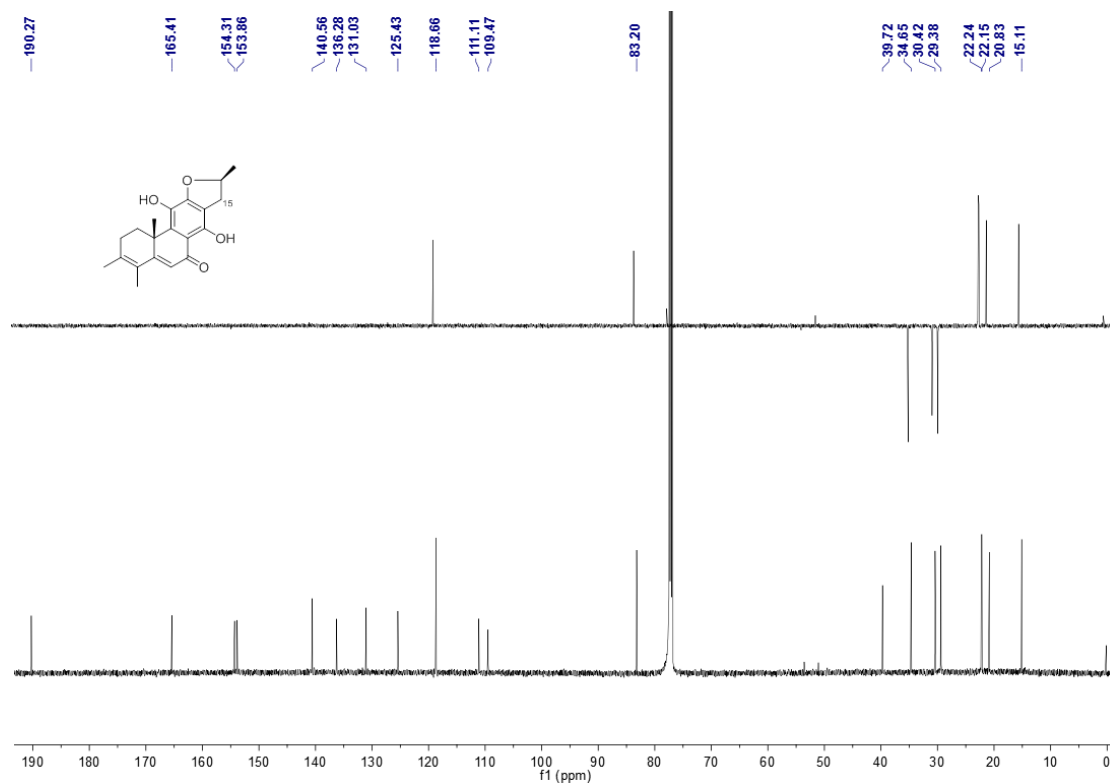


Figure S31: <sup>13</sup>C and DEPT NMR spectra of **4** in CDCl<sub>3</sub>.

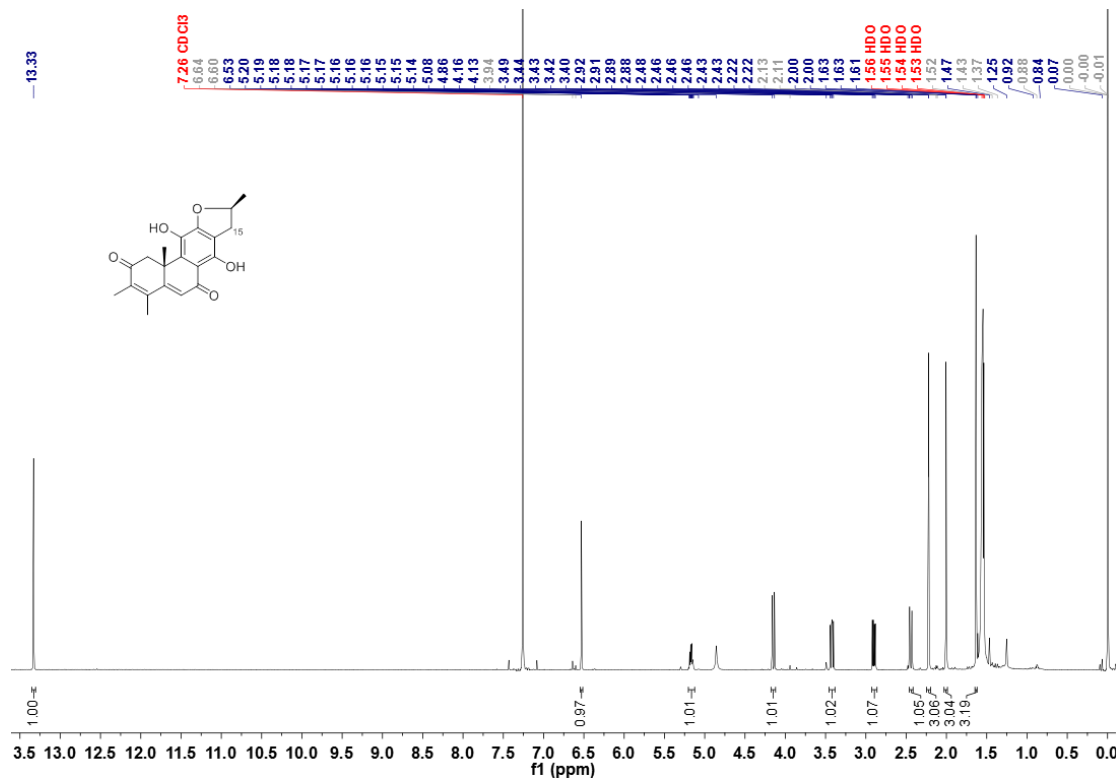


Figure S32: <sup>1</sup>H NMR spectrum of **5** in CDCl<sub>3</sub>.

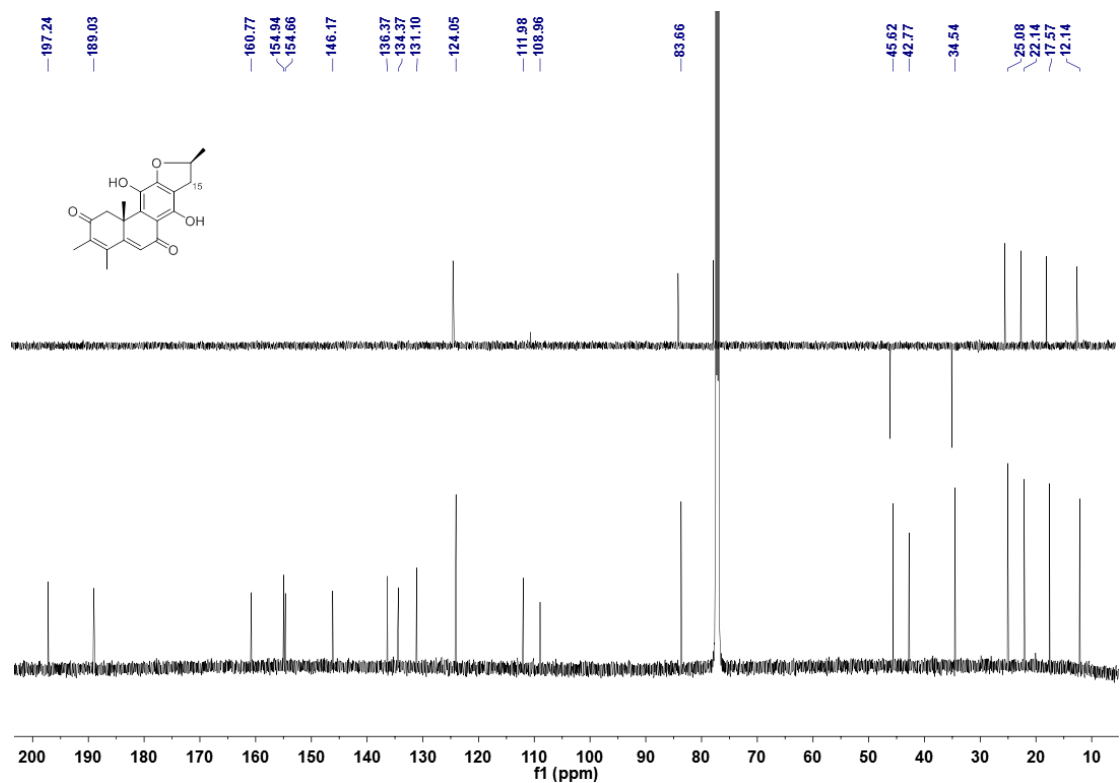


Figure S33: <sup>13</sup>C and DEPT NMR spectra of **5** in CDCl<sub>3</sub>.

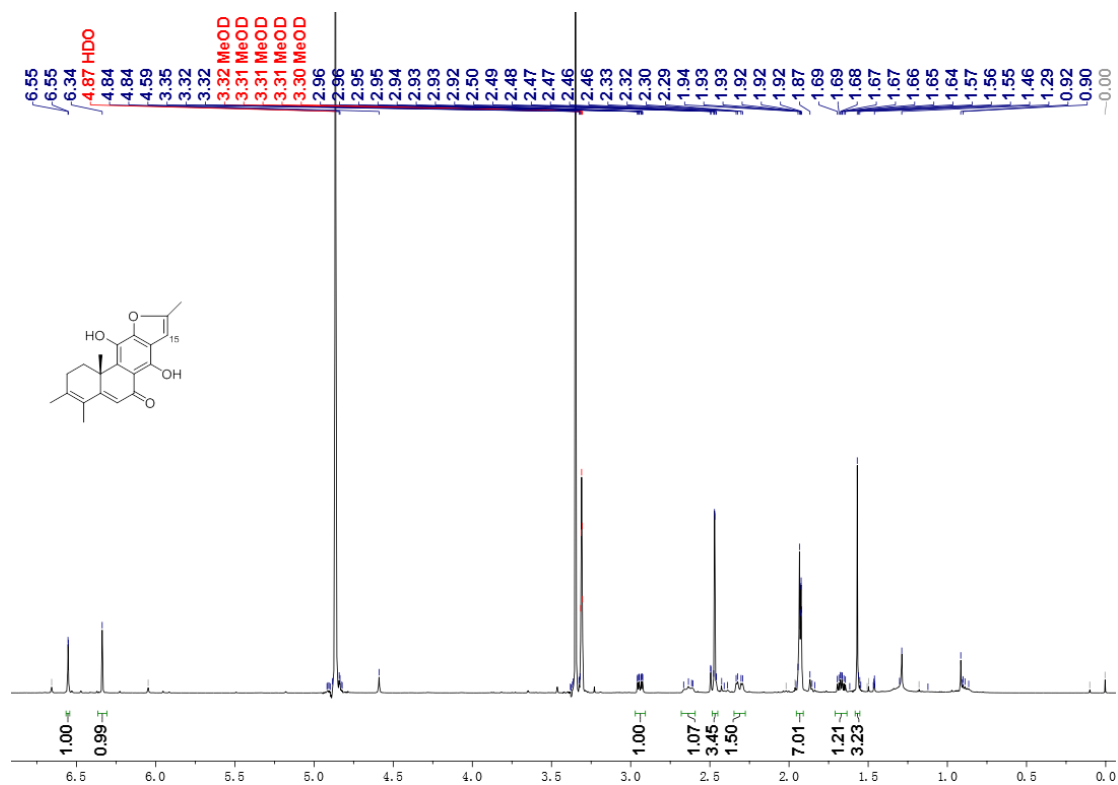


Figure S34: <sup>1</sup>H NMR spectrum of 6 in CD<sub>3</sub>OD.

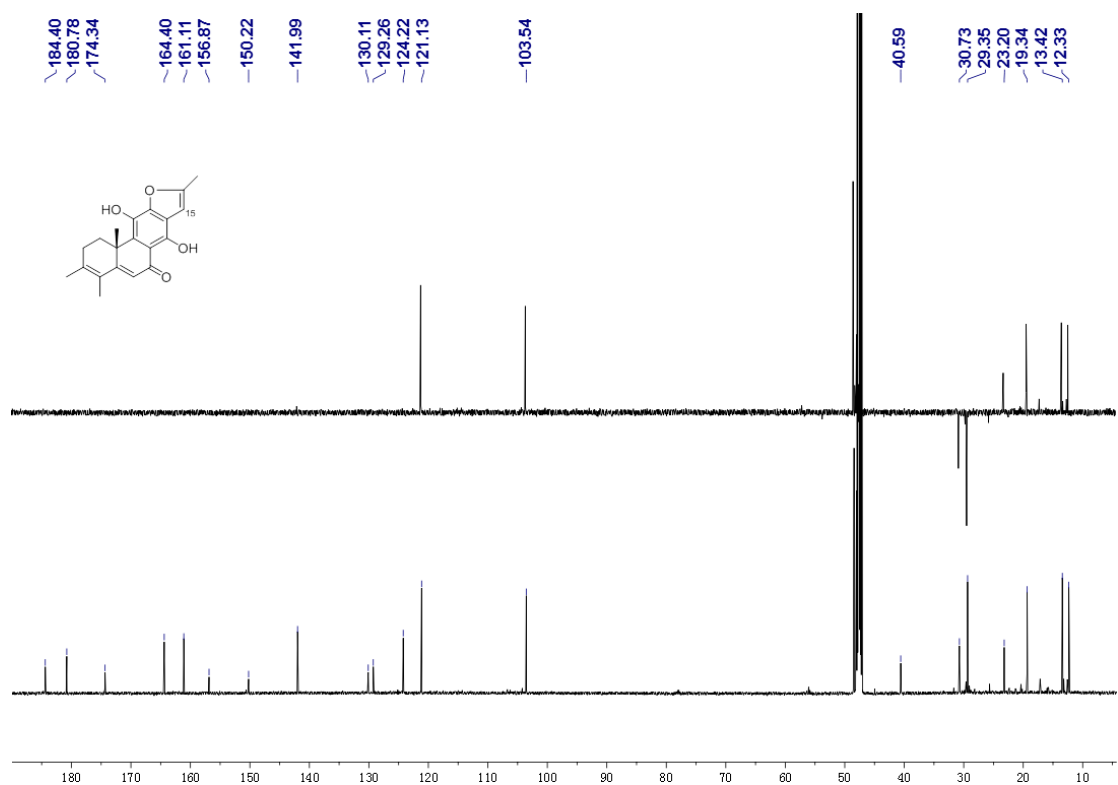


Figure S35: <sup>13</sup>C and DEPT NMR spectra of 6 in CD<sub>3</sub>OD.



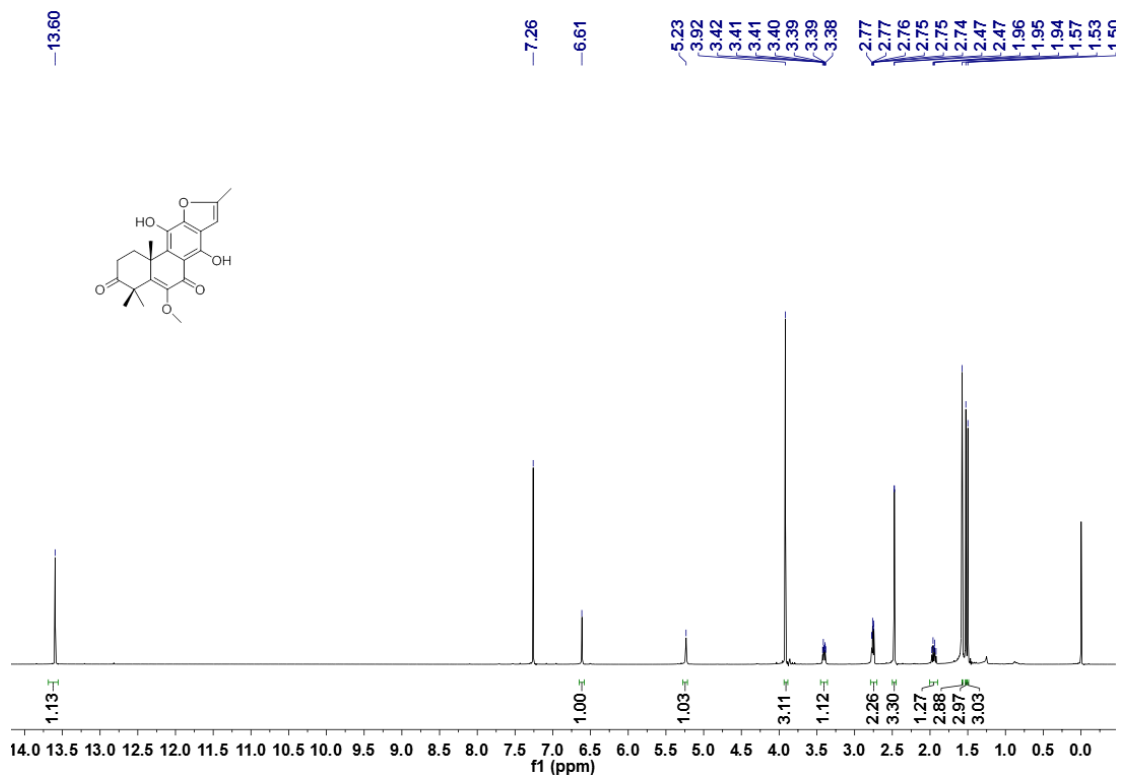


Figure S38:  $^1\text{H}$  NMR spectrum of **8** in CDCl<sub>3</sub>.

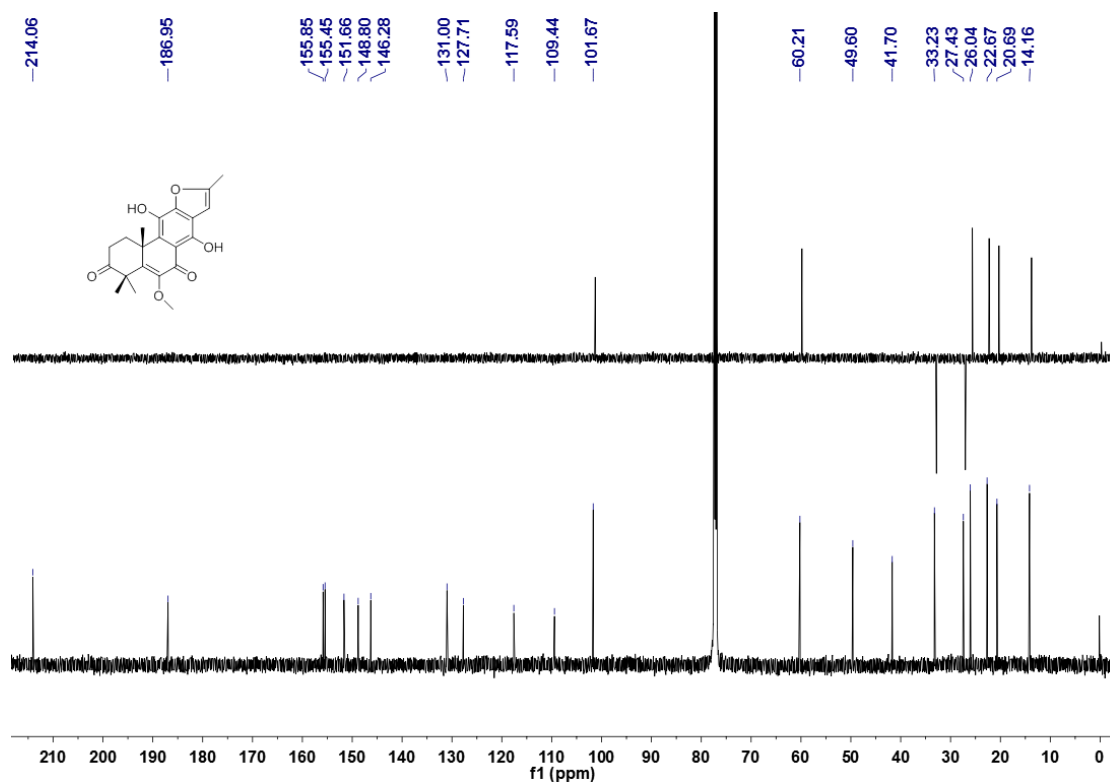


Figure S39:  $^{13}\text{C}$  and DEPT NMR spectra of **8** in CDCl<sub>3</sub>.

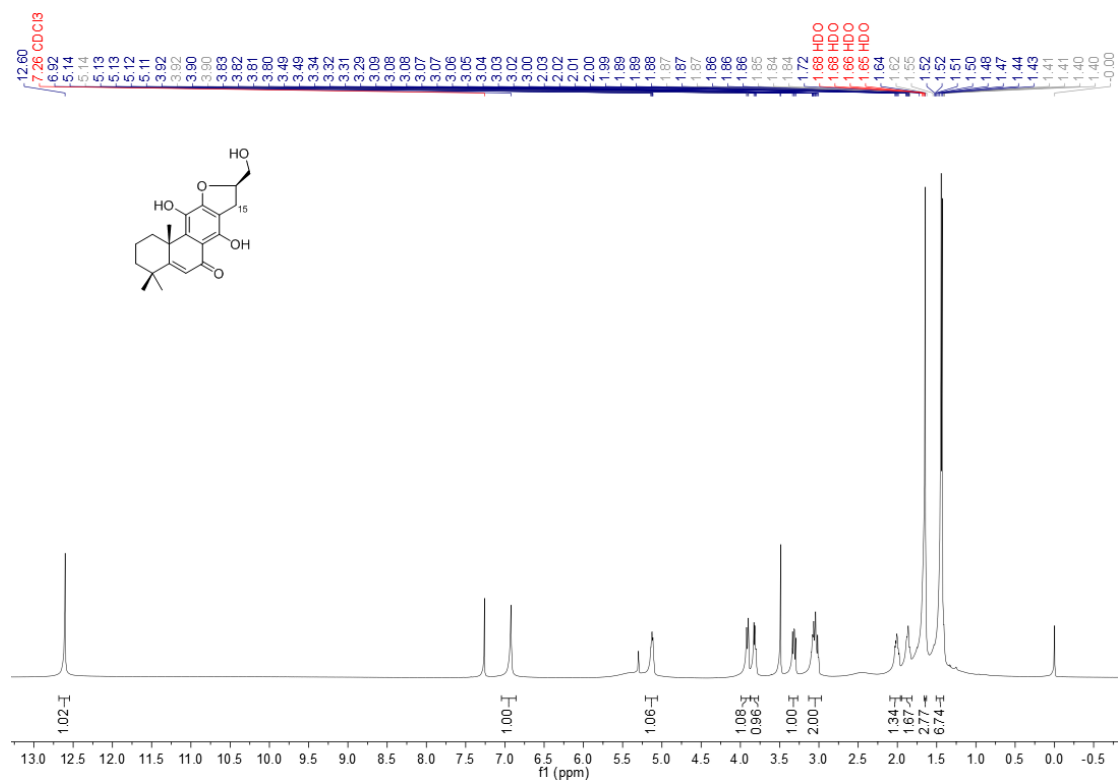


Figure S40: <sup>1</sup>H NMR spectrum of **9** in CDCl<sub>3</sub>.

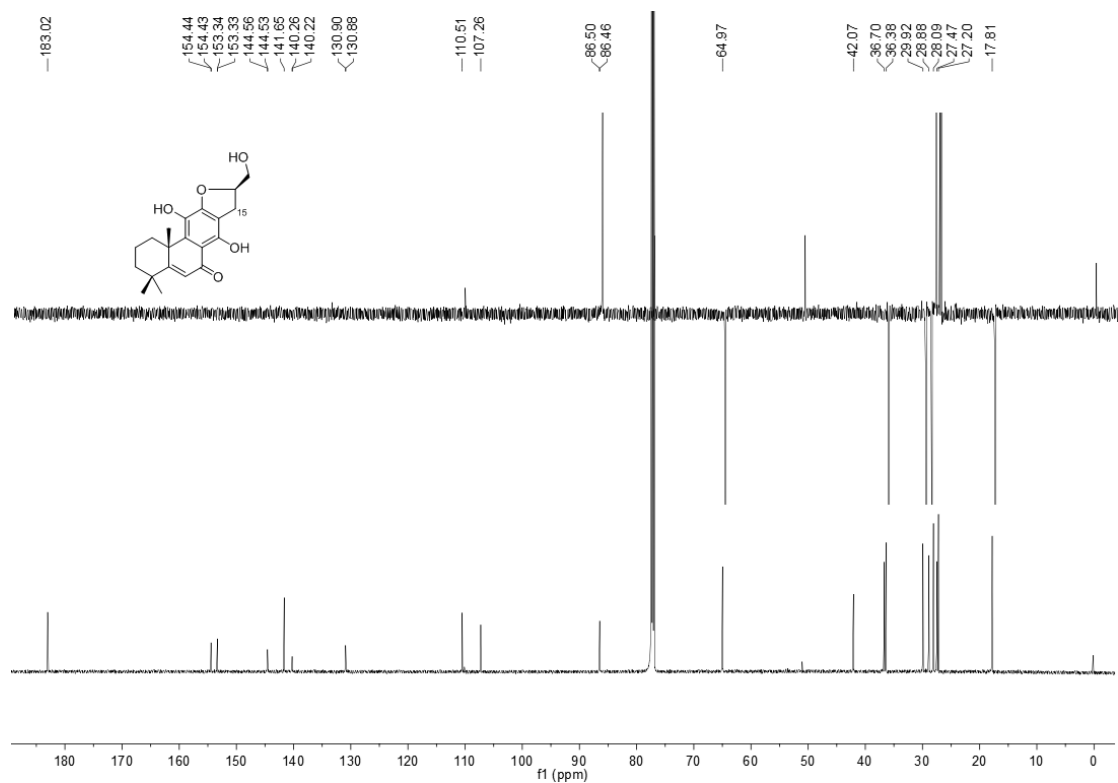


Figure S41: <sup>13</sup>C and DEPT NMR spectra of **9** in CDCl<sub>3</sub>.



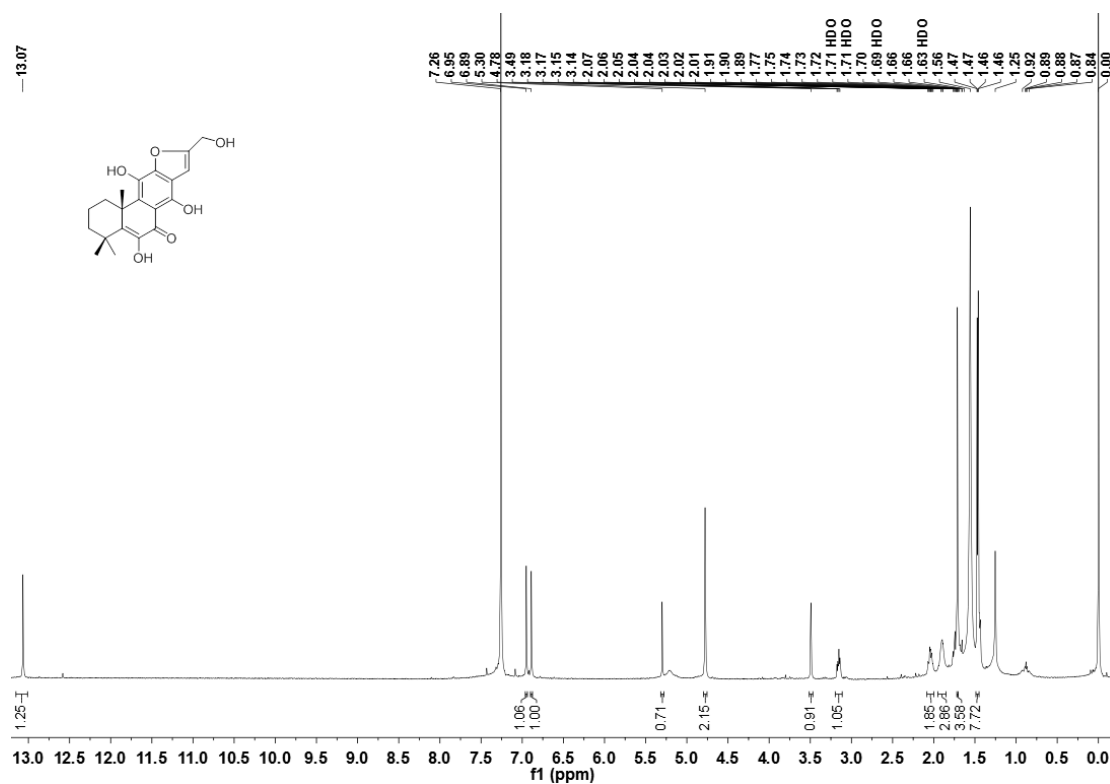


Figure S42: <sup>1</sup>H NMR spectrum of **10** in CDCl<sub>3</sub>.

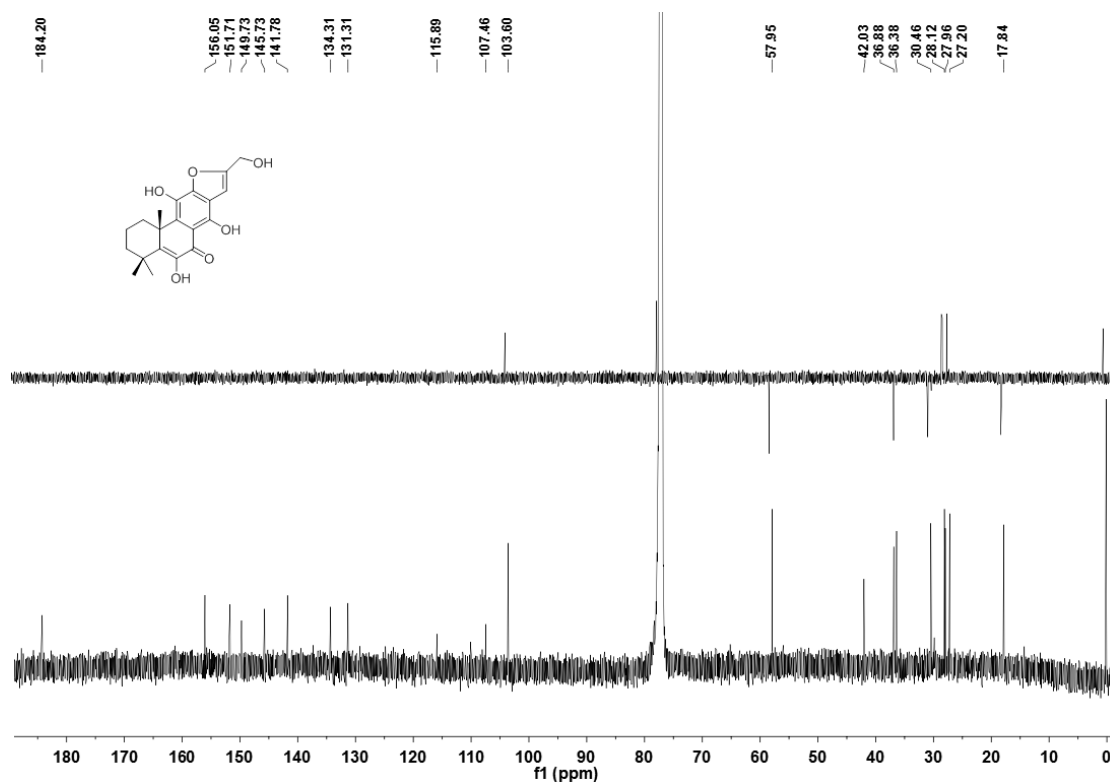
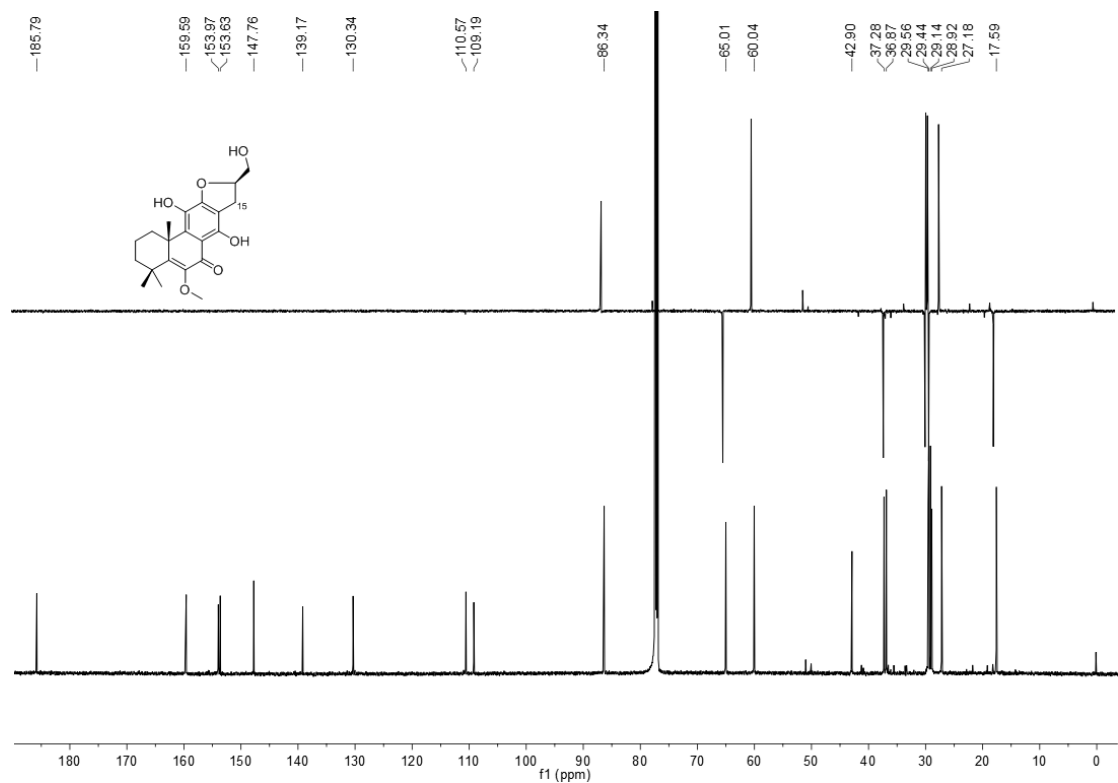
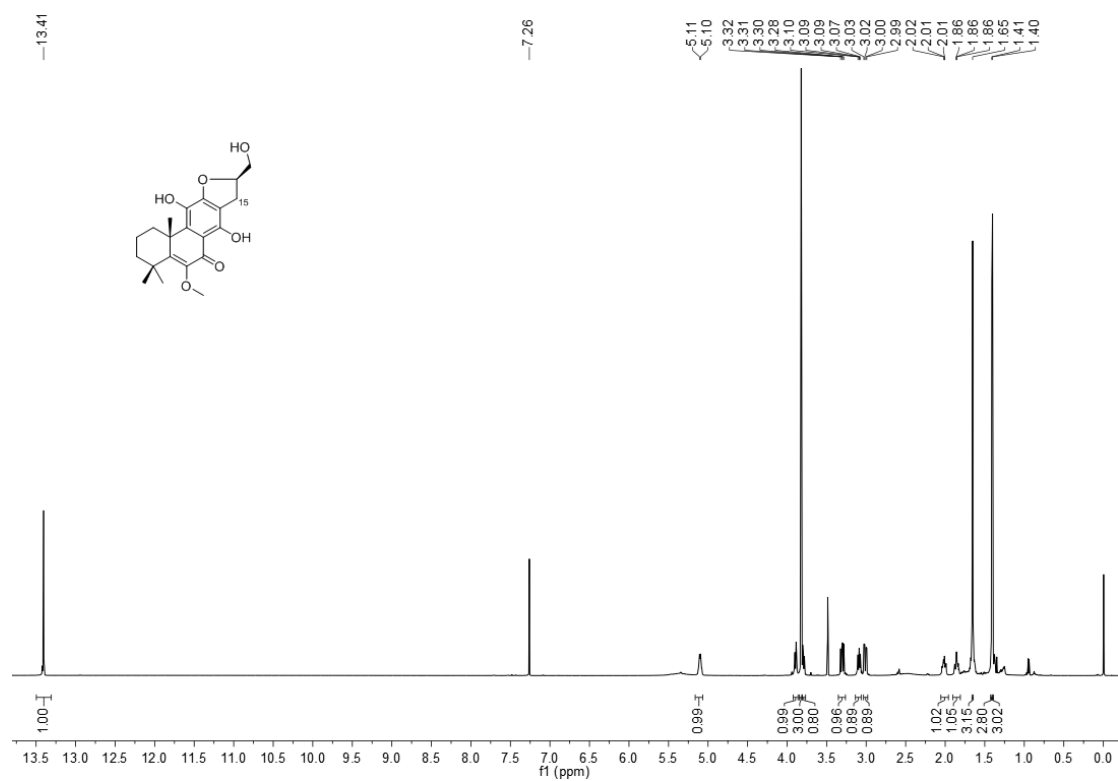


Figure S43: <sup>13</sup>C and DEPT NMR spectra of **10** in CDCl<sub>3</sub>.



**Figure S45:**  $^{13}\text{C}$  and DEPT NMR spectra of **11** in  $\text{CDCl}_3$ .

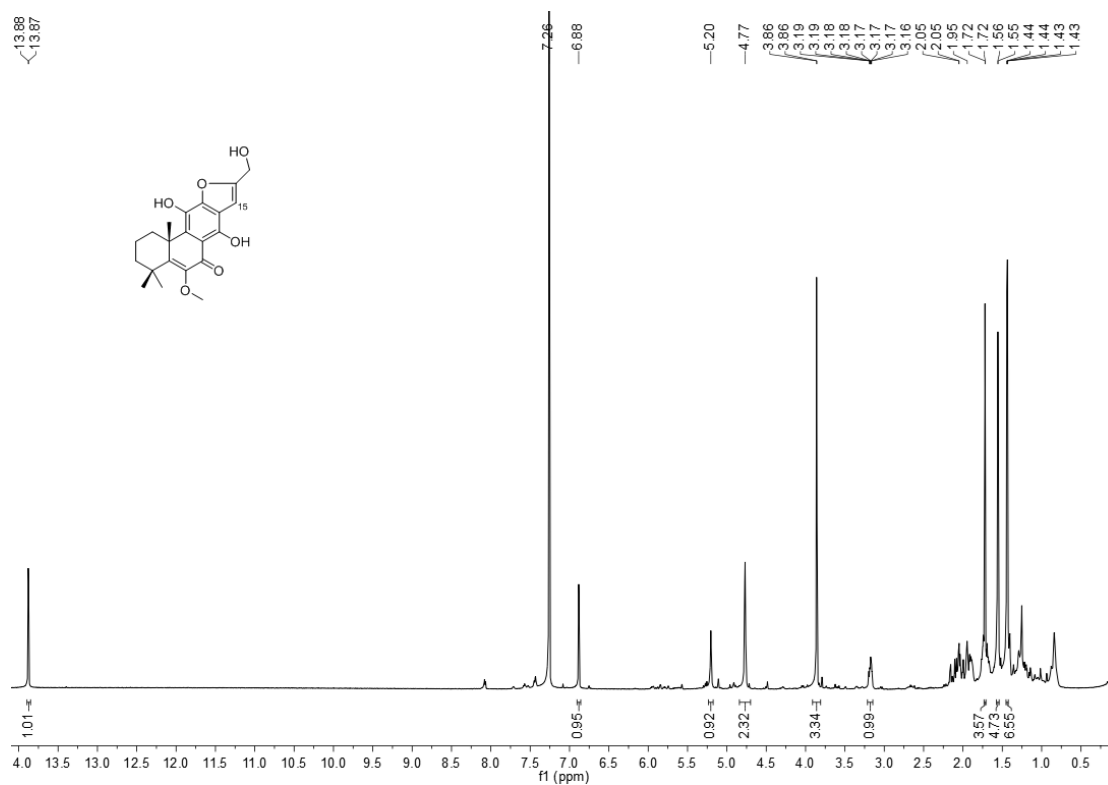


Figure S46: <sup>1</sup>H NMR spectrum of 12 in CDCl<sub>3</sub>.

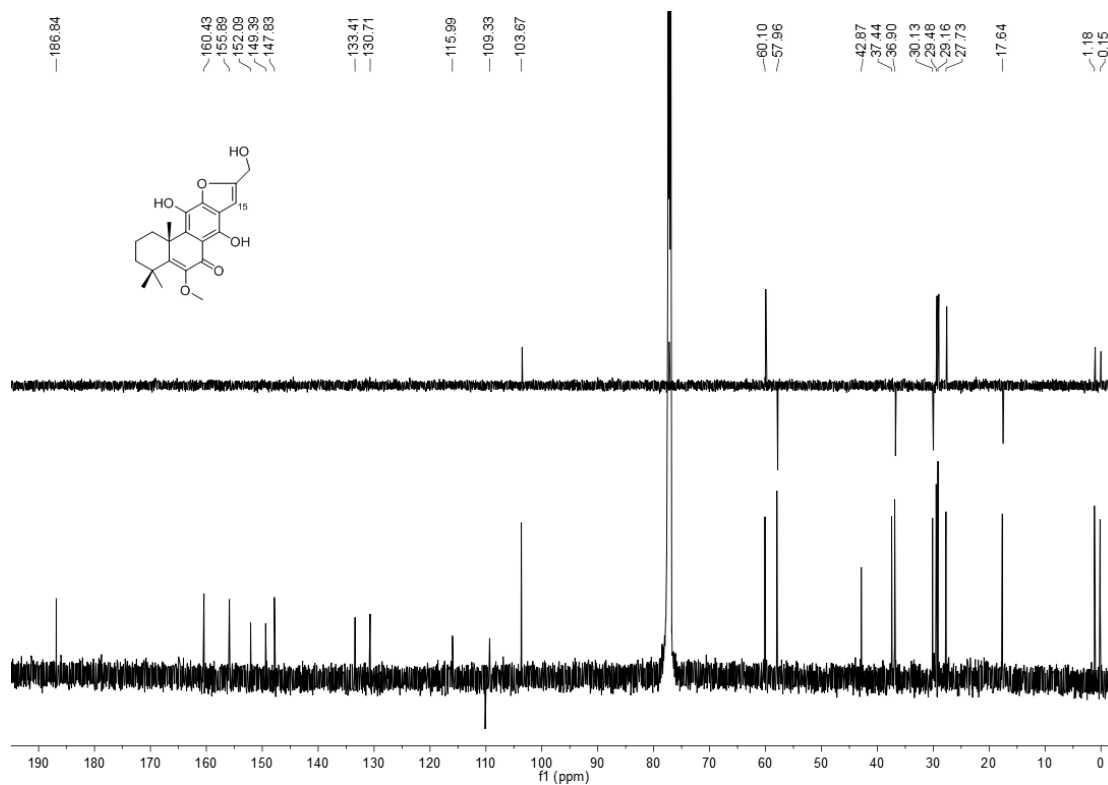
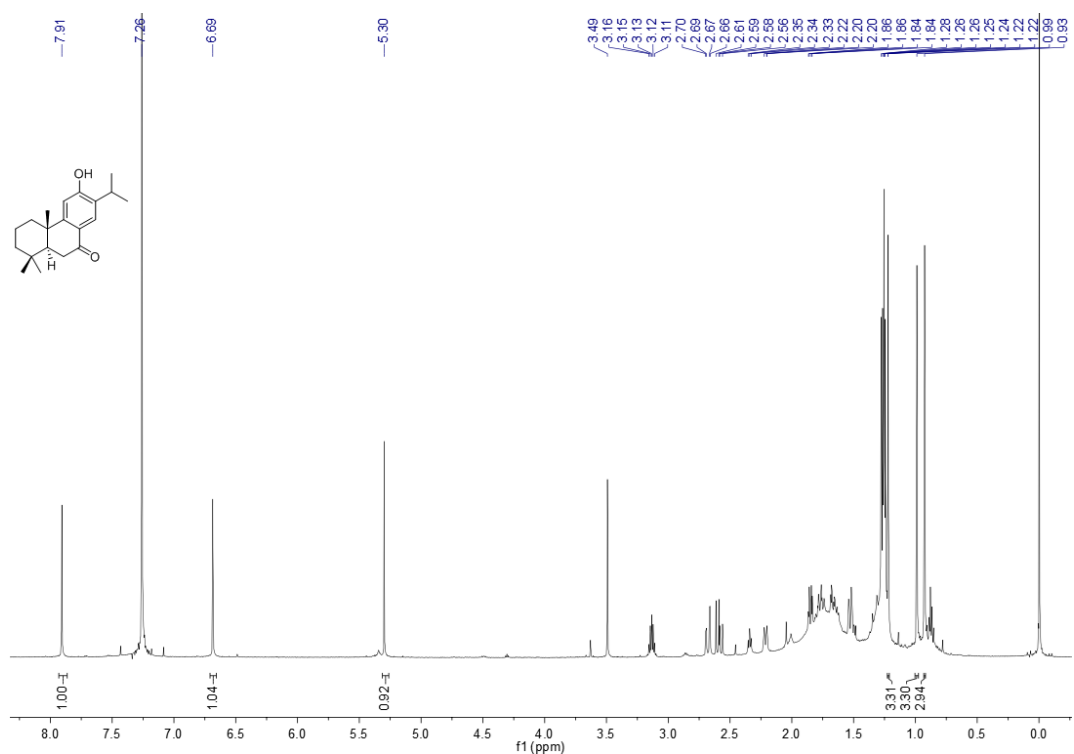
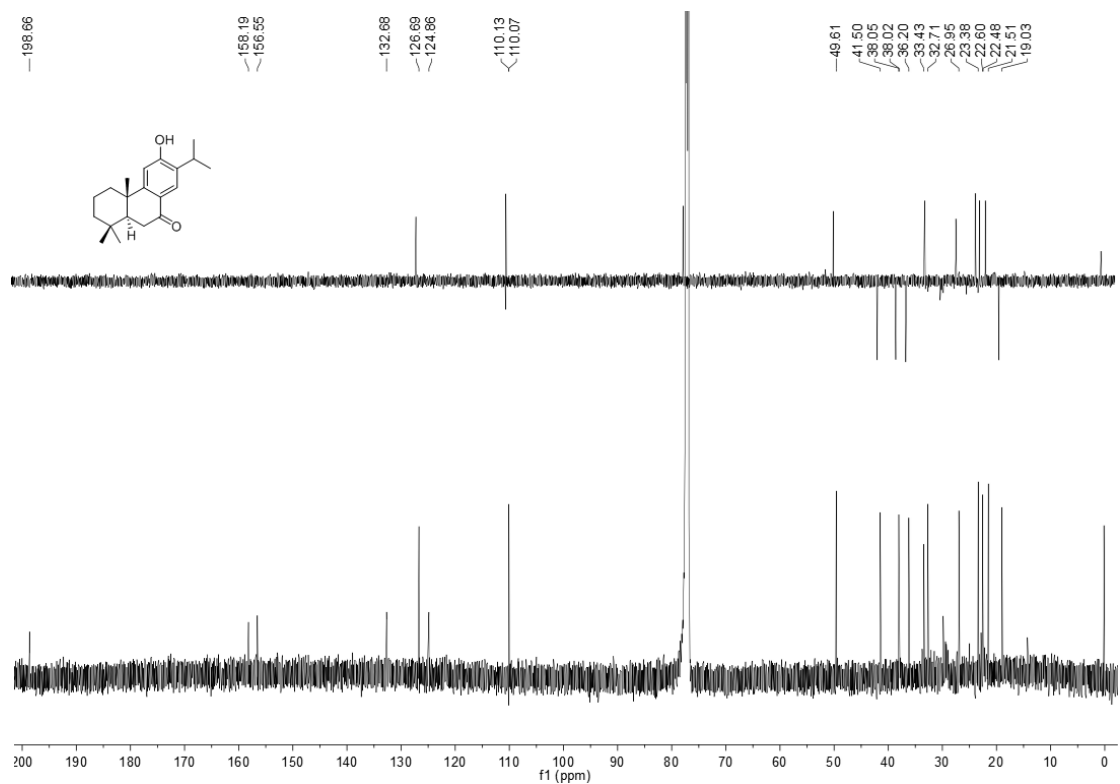


Figure S47: <sup>13</sup>C and DEPT NMR spectra of 12 in CDCl<sub>3</sub>



**Figure S48:** <sup>1</sup>H NMR spectrum of **13** in CDCl<sub>3</sub>.



**Figure S49:** <sup>13</sup>C and DEPT NMR spectra of **13** in CDCl<sub>3</sub>.