

## Supporting Information

### ***ent*-Rosane diterpenoids from the aerial parts of *Euphorbia milii* with activity against Epstein-Barr virus lytic replication**

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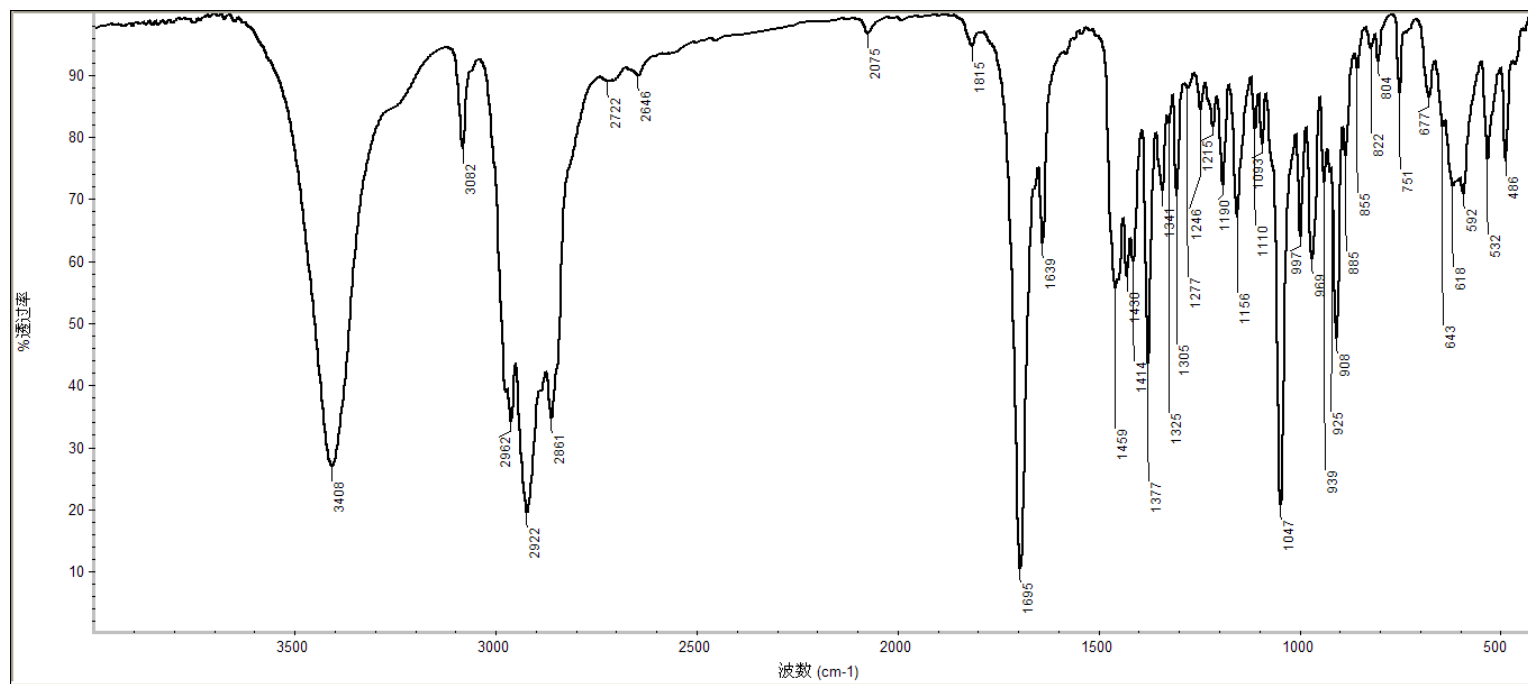
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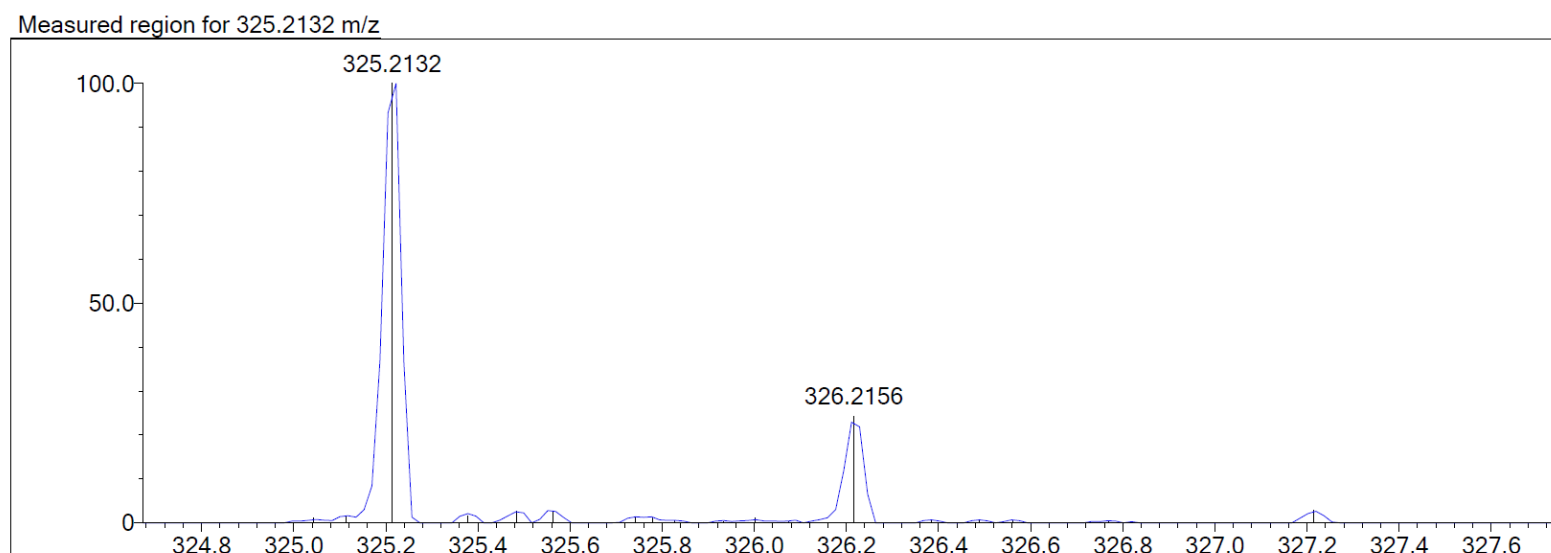
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**Figure S1.** The IR Spectra of Compound **1**




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SPECTRUM -

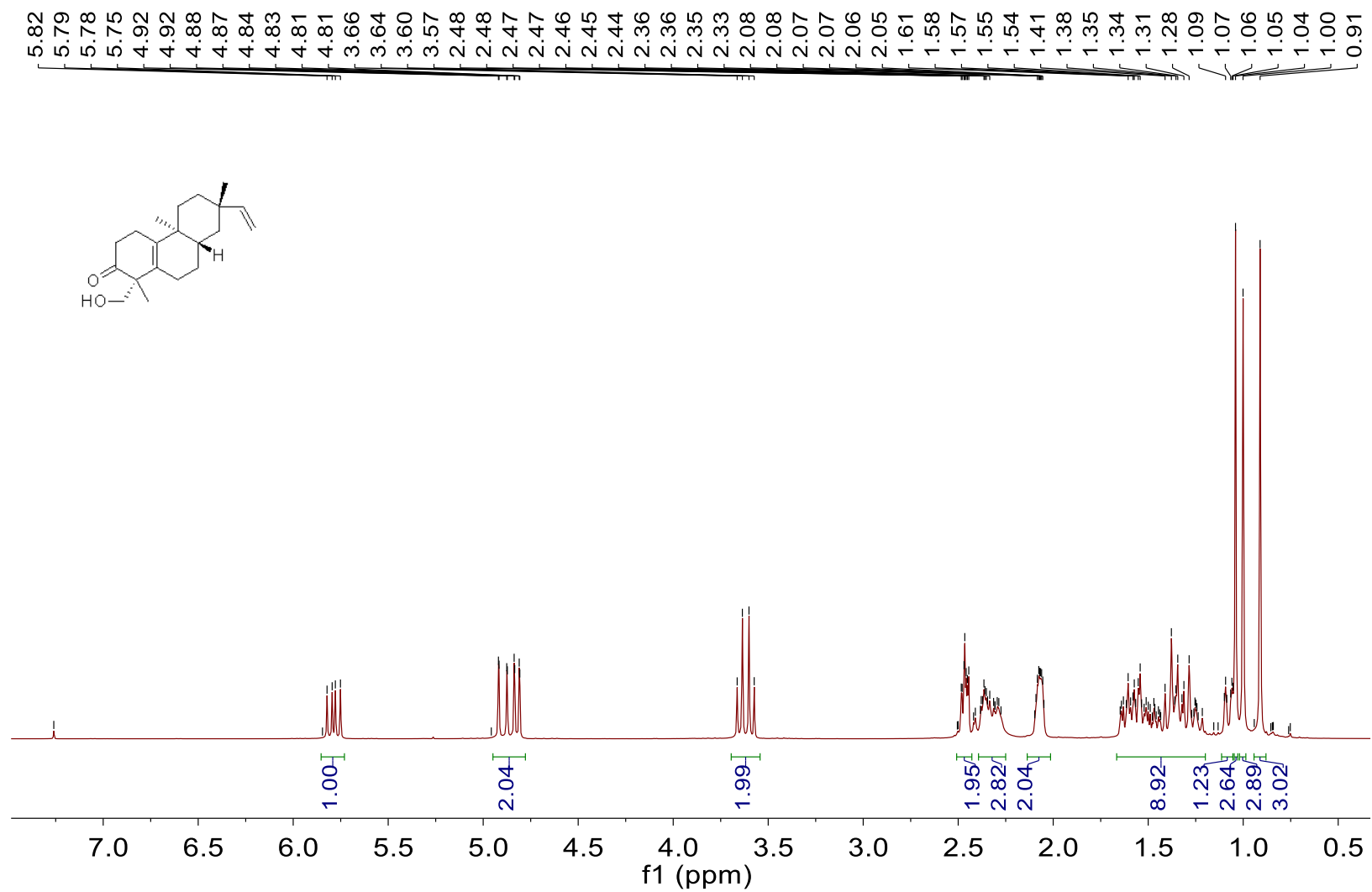
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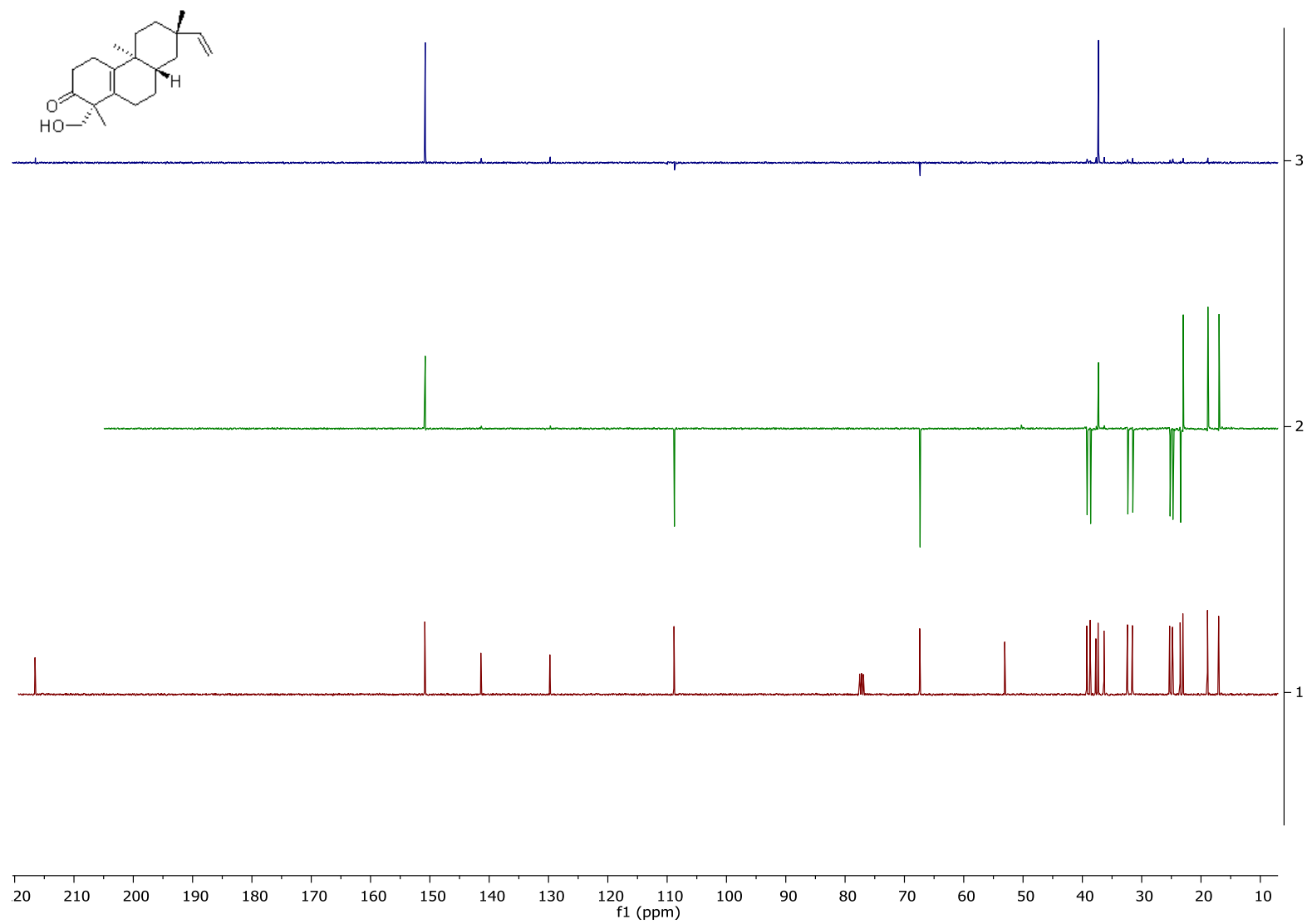
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
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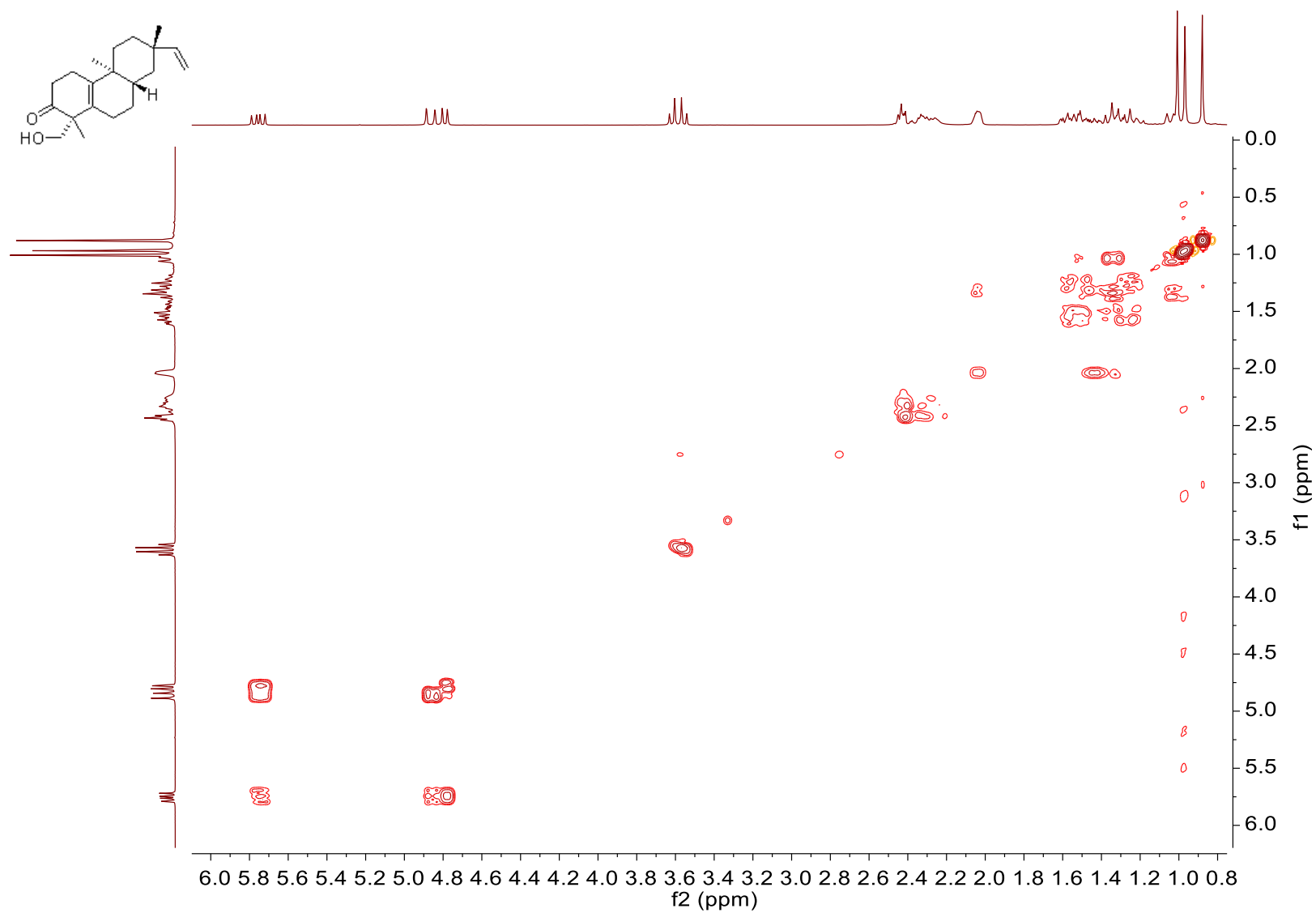
**Figure S2.** The HRESIMS Spectroscopic Data of Compound **1**



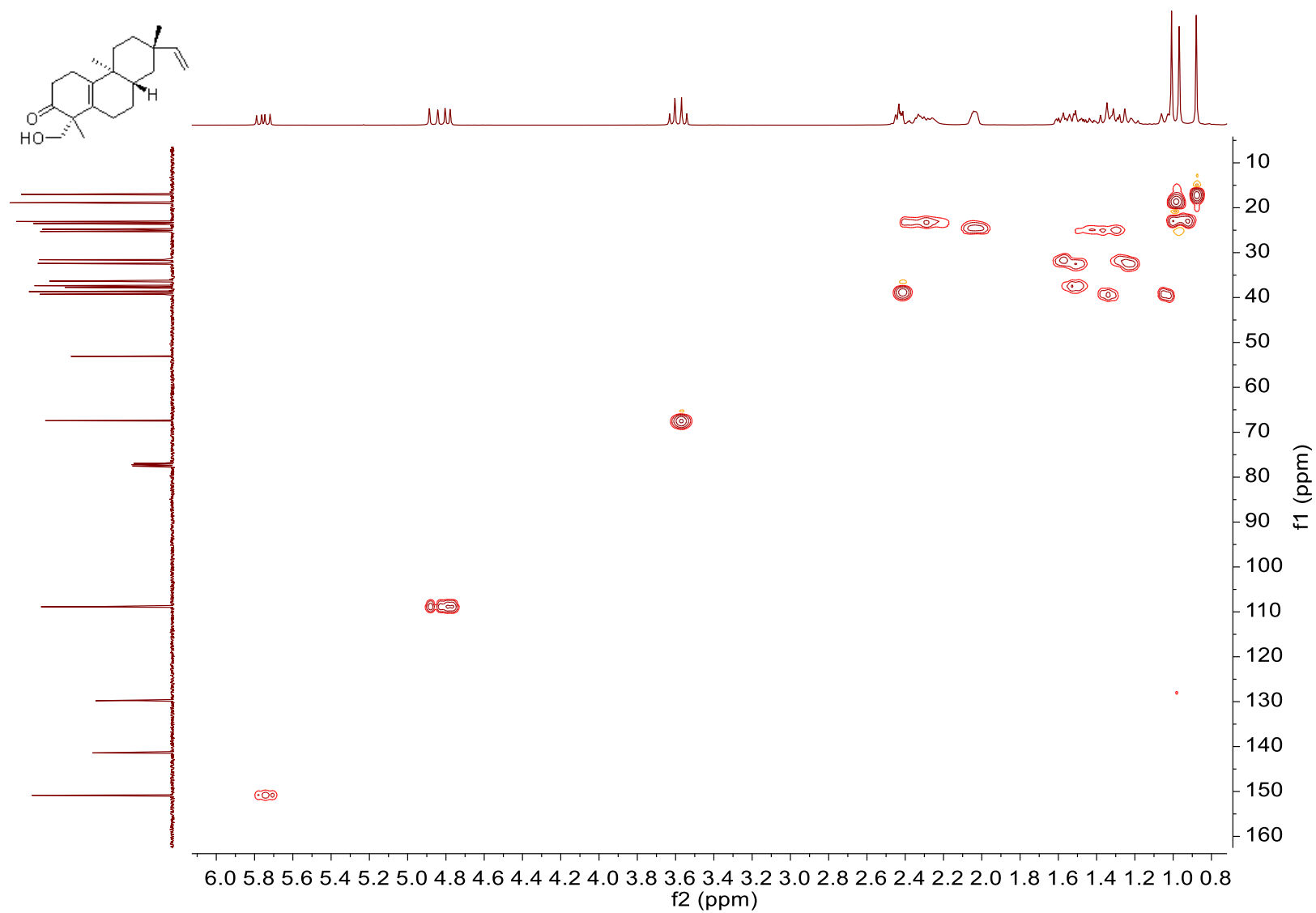
**Figure S3.** The <sup>1</sup>H NMR Spectrum of Compound **1** in CDCl<sub>3</sub>



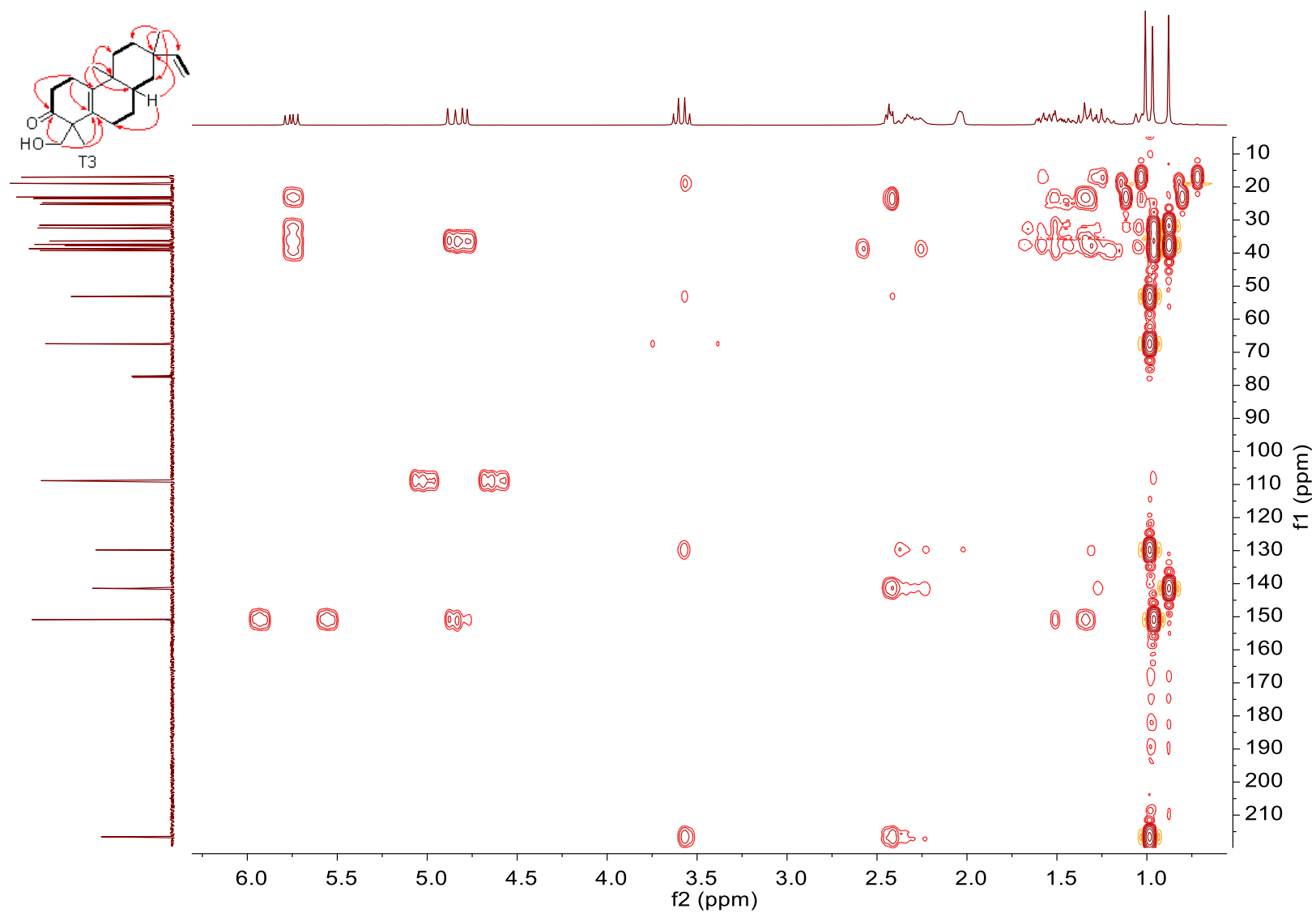
**Figure S4.** The  $^{13}\text{C}$  NMR Spectrum of Compound **1** in  $\text{CDCl}_3$



**Figure S5.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **1** in  $\text{CDCl}_3$

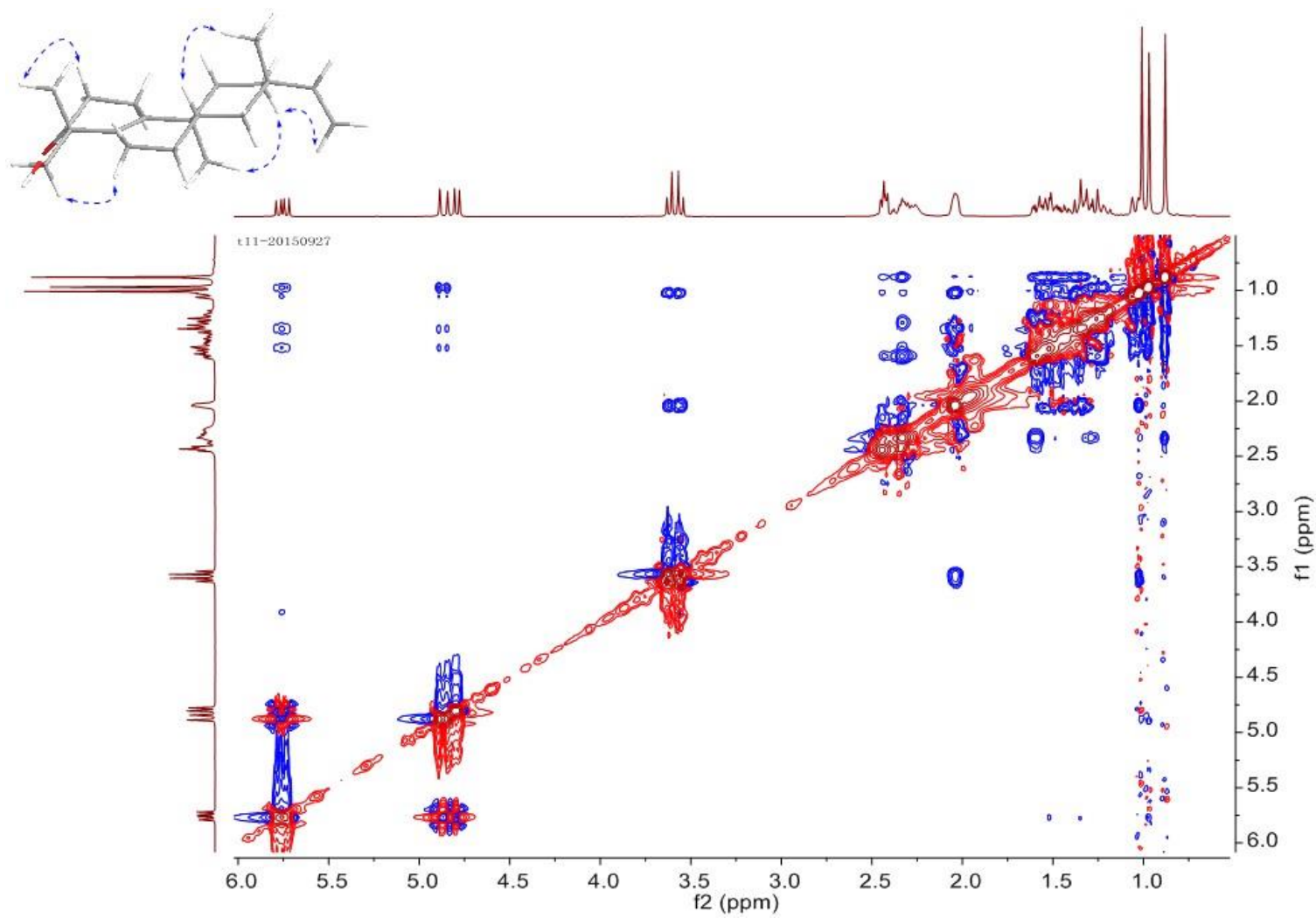


**Figure S6.** The HSQC Spectrum of Compound **1** in CDCl<sub>3</sub>

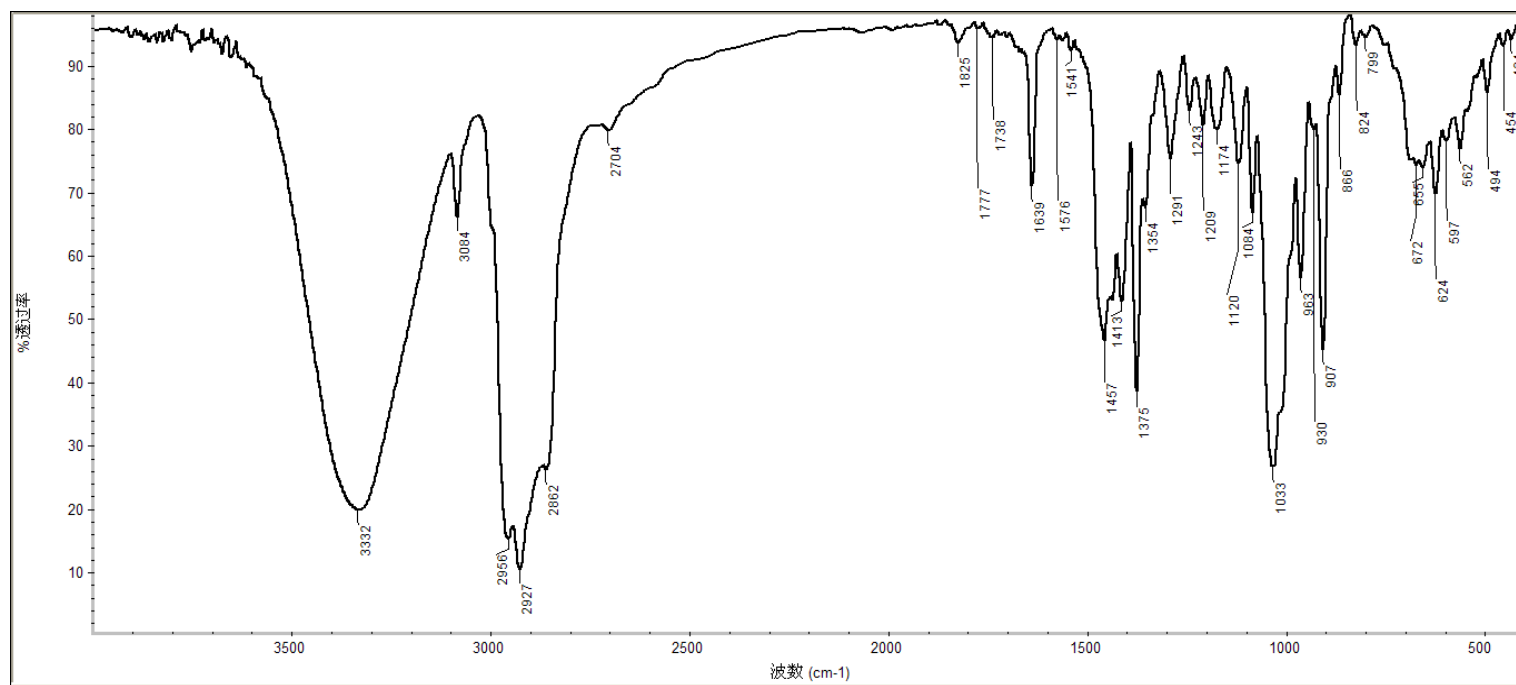


**Figure S7.** The HMBC Spectrum of Compound **1** in  $\text{CDCl}_3$

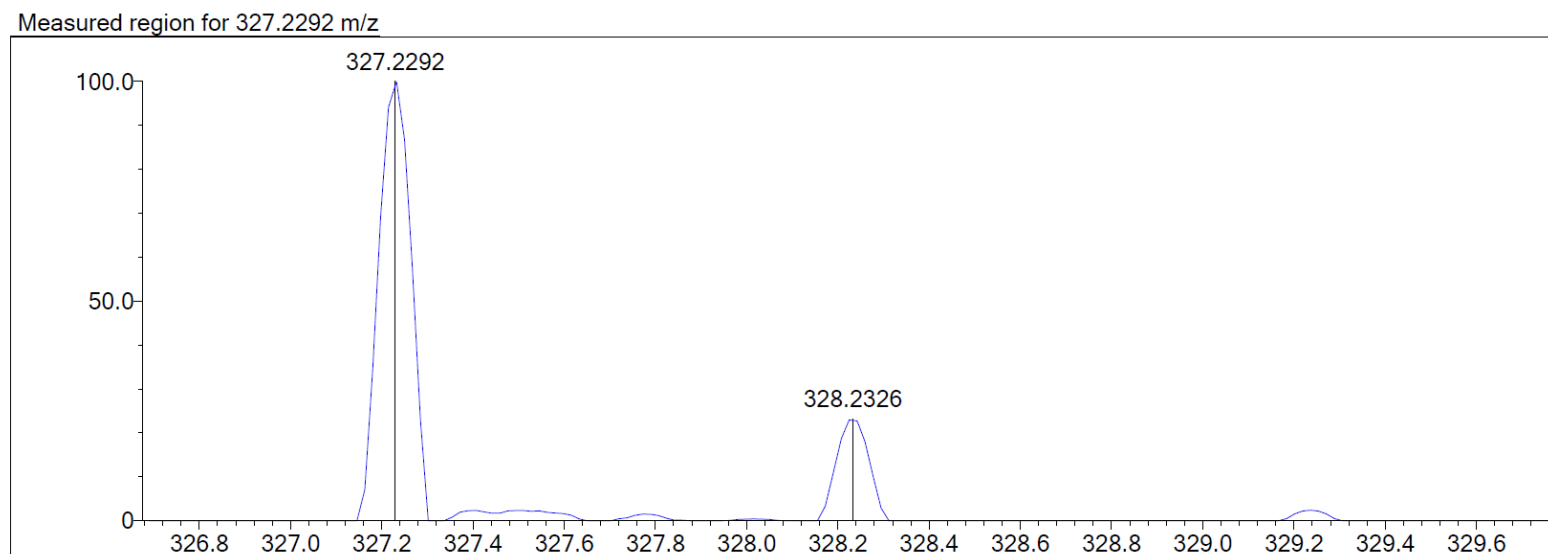




**Figure S8.** The NOESY Spectrum of Compound **1** in CDCl<sub>3</sub>



**Figure S9.** The IR Spectra of Compound 2




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SPECTRUM -

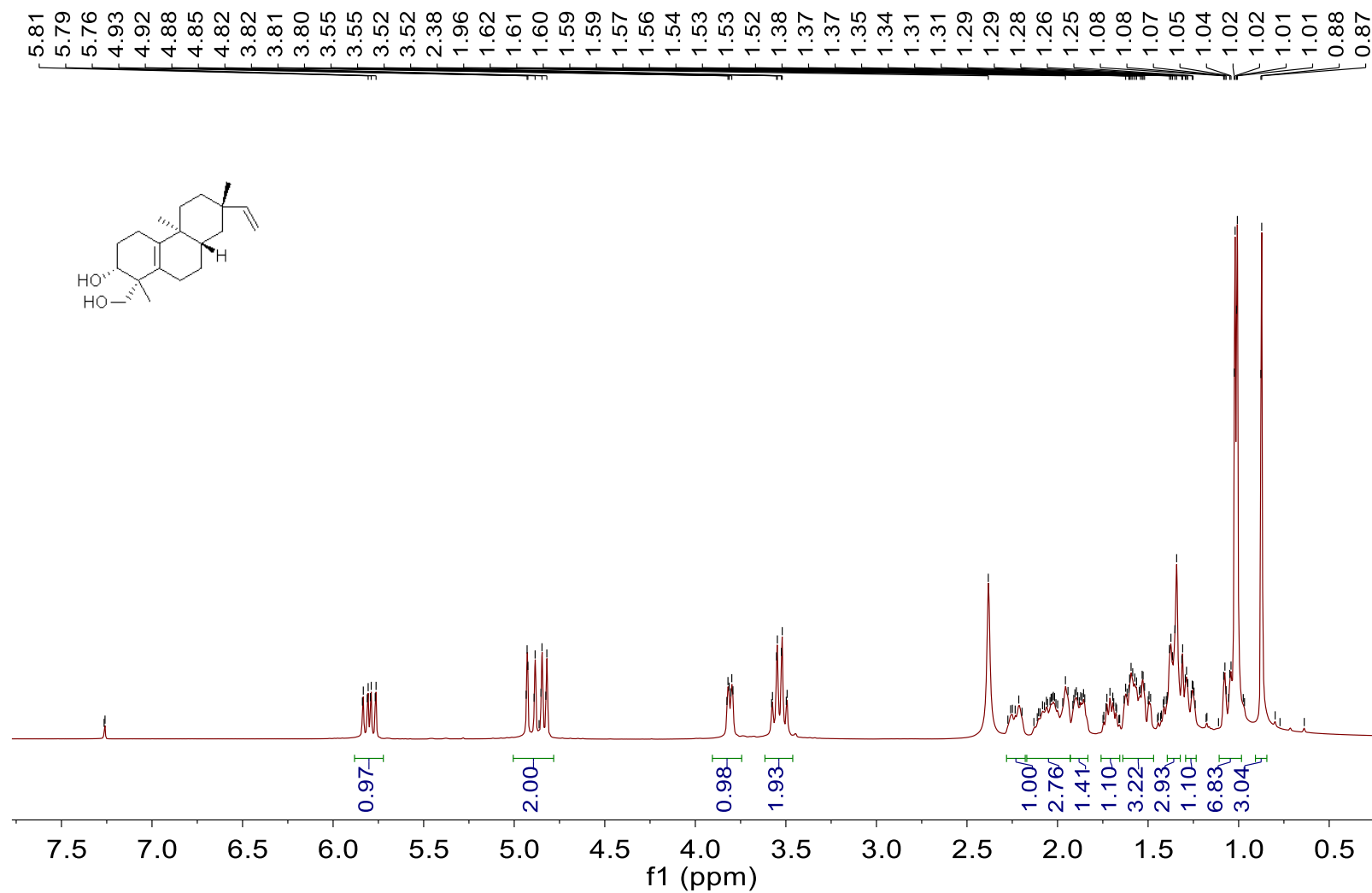
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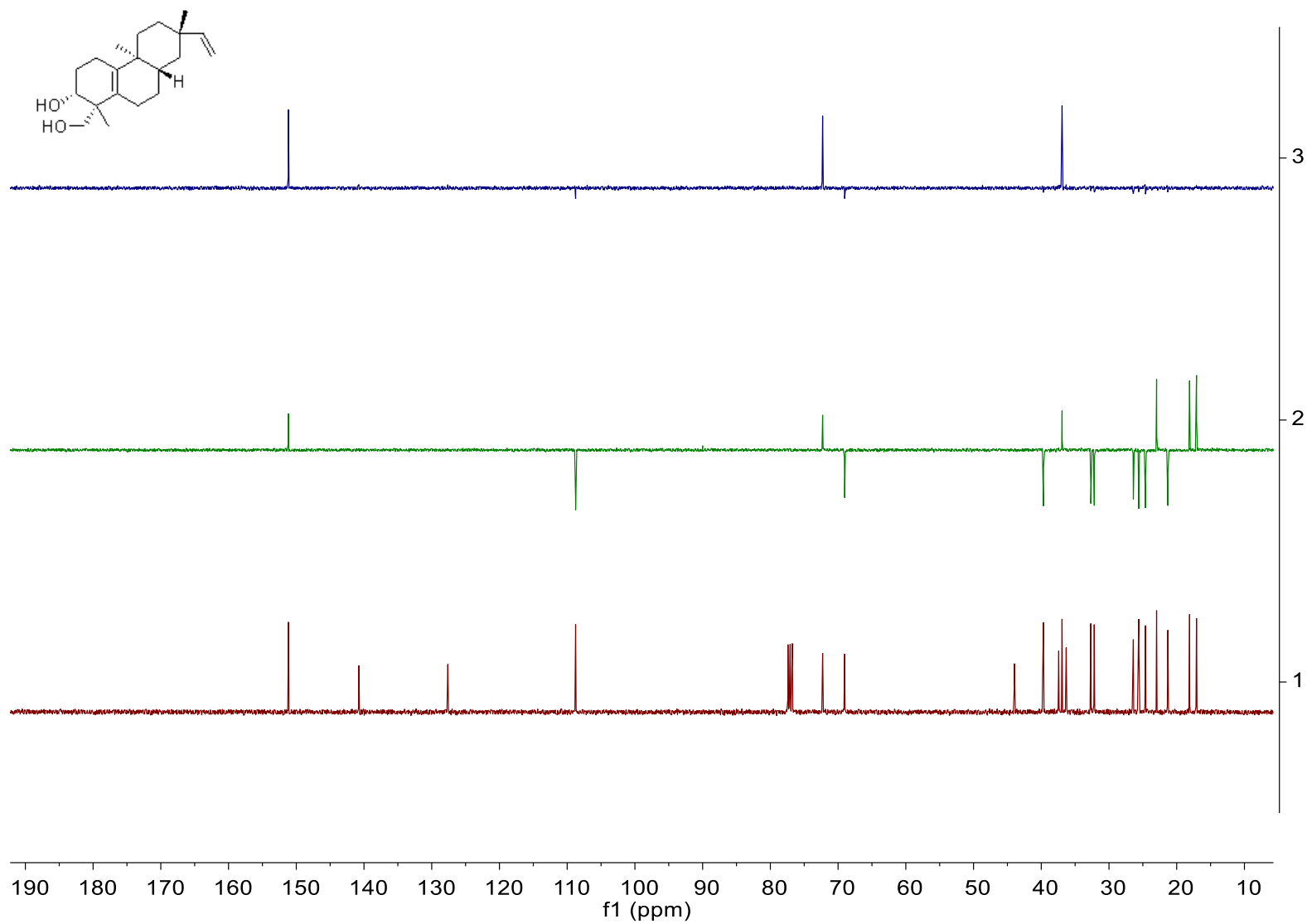
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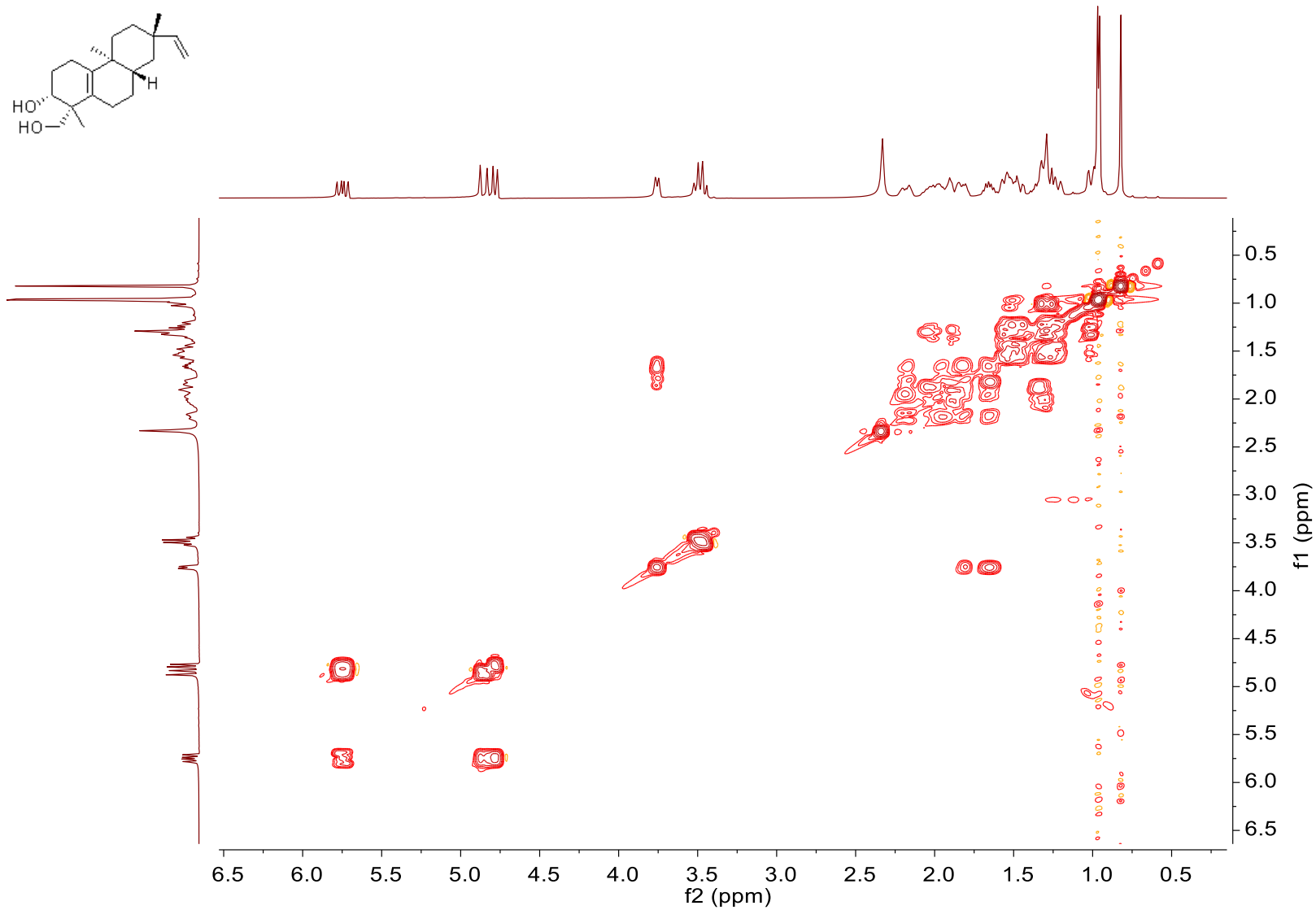
**Figure S10.** The HRESIMS Spectroscopic Data of Compound **2**



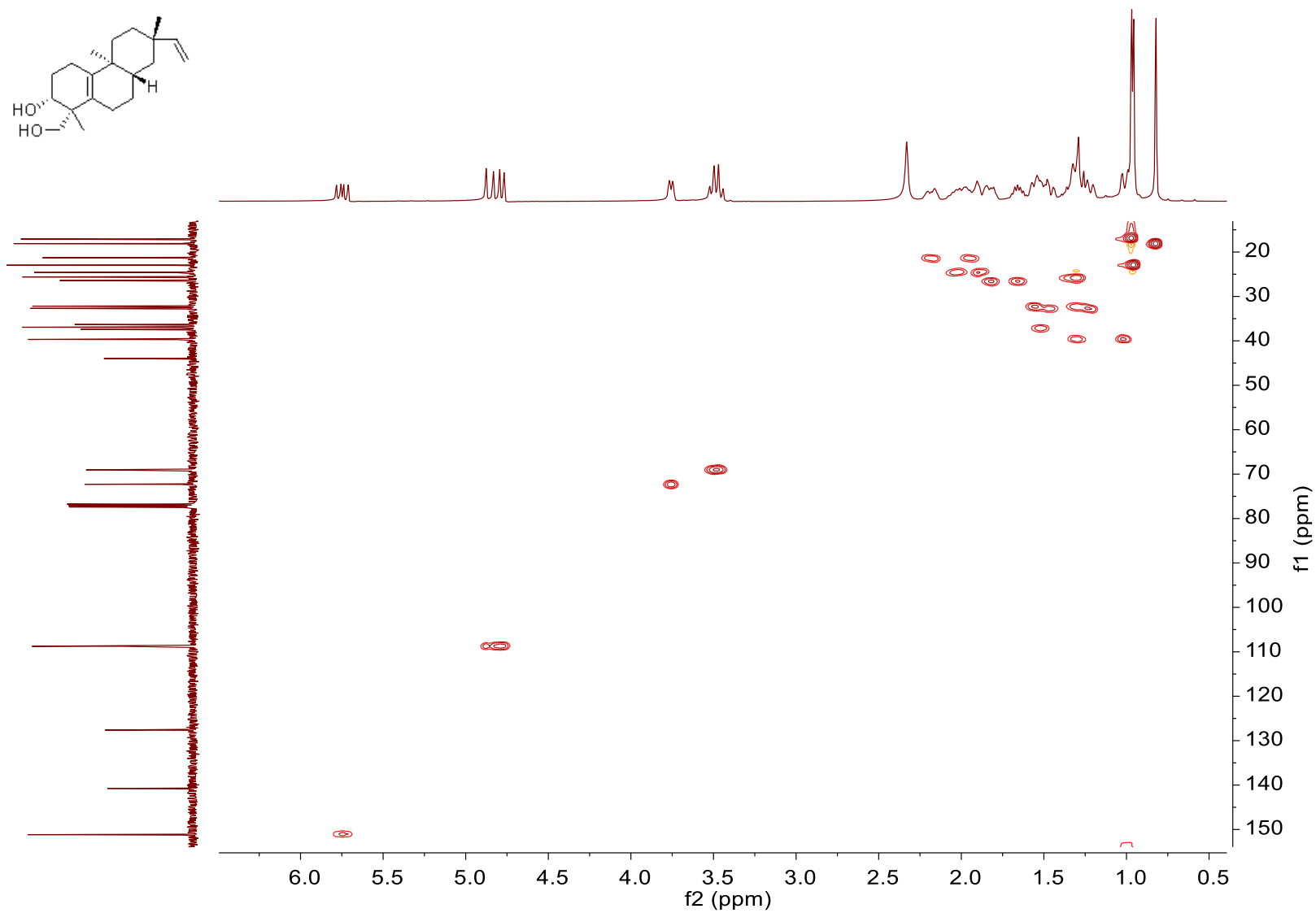
**Figure S11.** The <sup>1</sup>H NMR Spectrum of Compound **2** in CDCl<sub>3</sub>



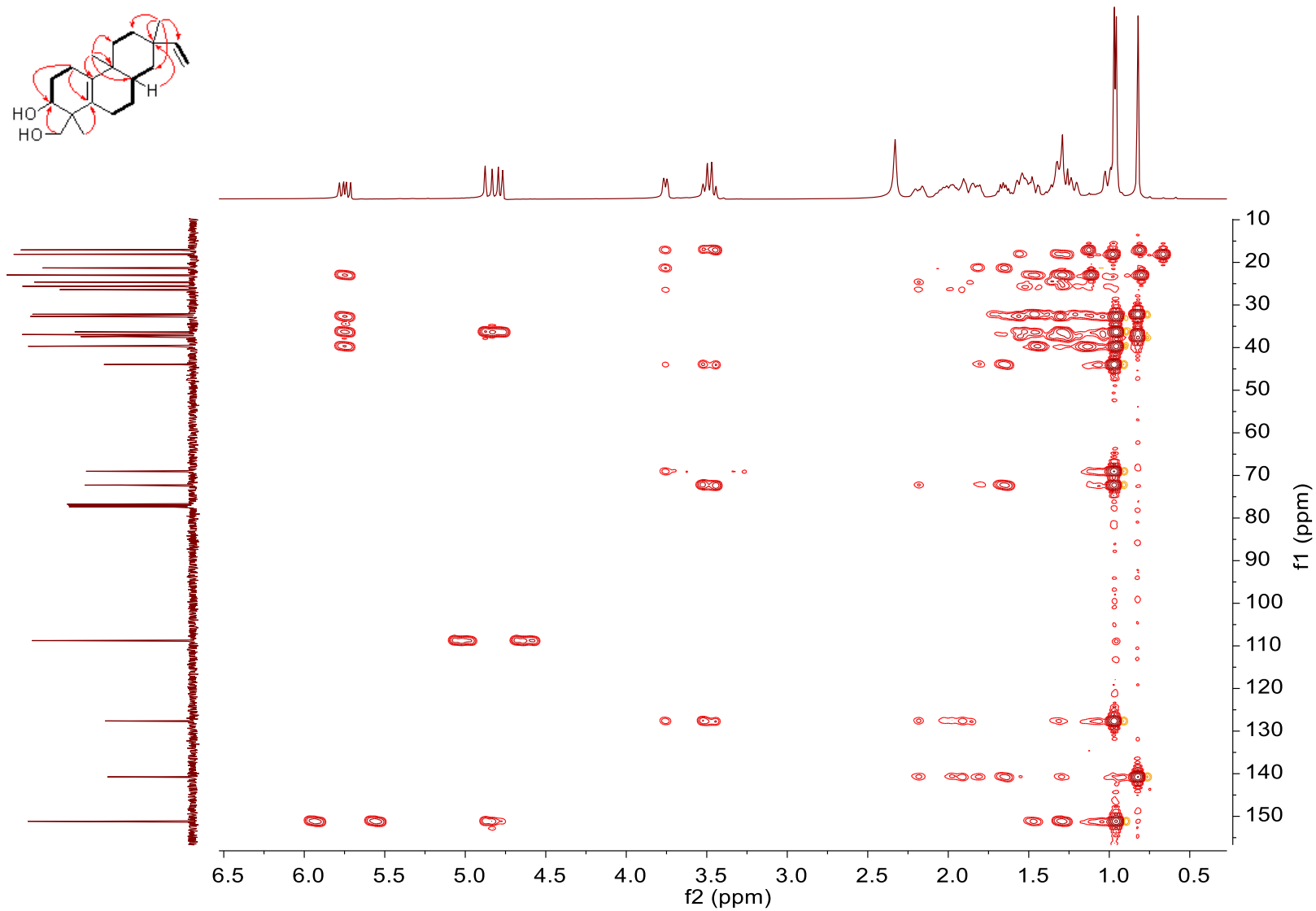
**Figure S12.** The  $^{13}\text{C}$  NMR Spectrum of Compound **2** in  $\text{CDCl}_3$



**Figure S13.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **2** in  $\text{CDCl}_3$

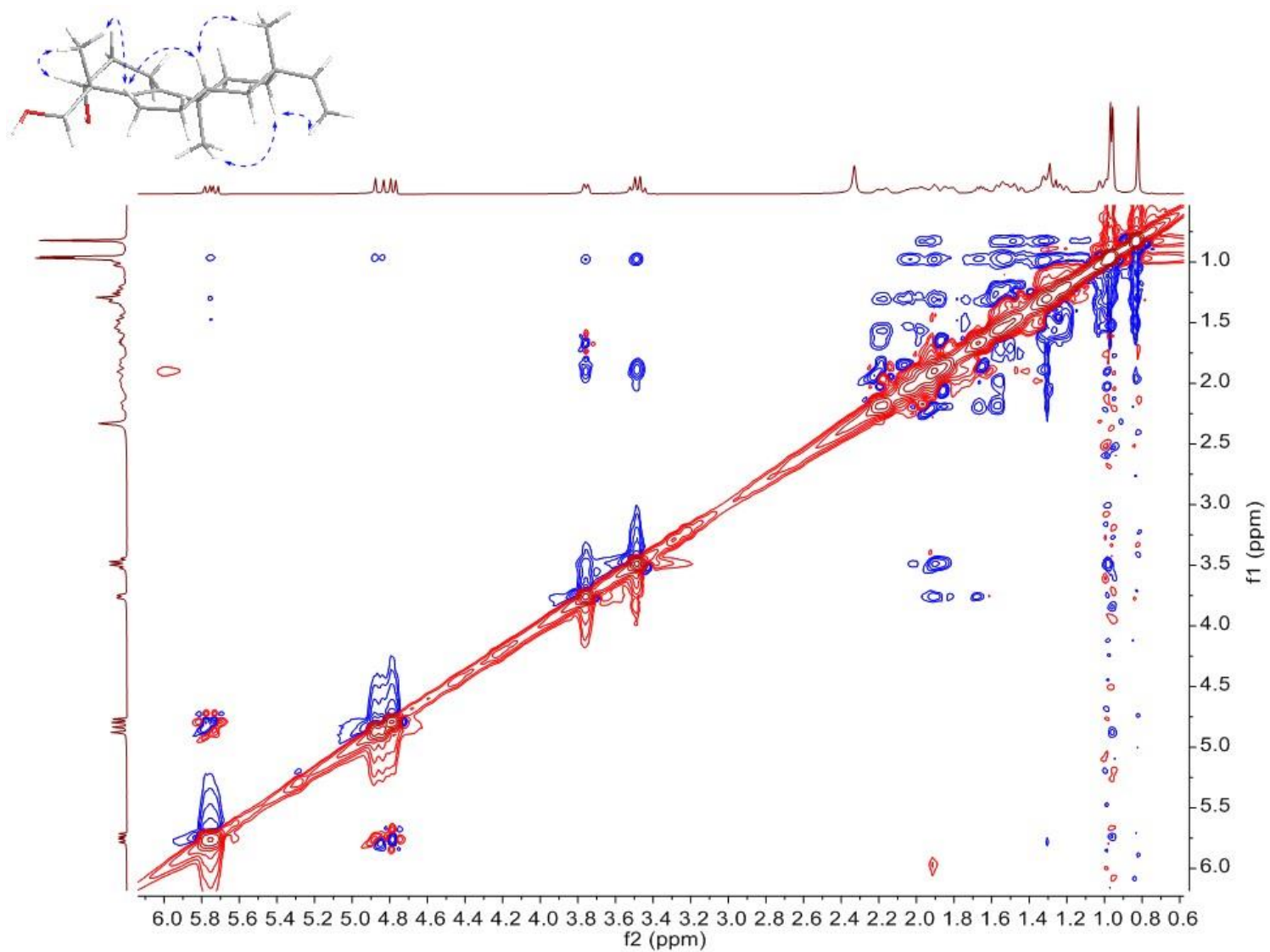


**Figure S14.** The HSQC Spectrum of Compound **2** in CDCl<sub>3</sub>

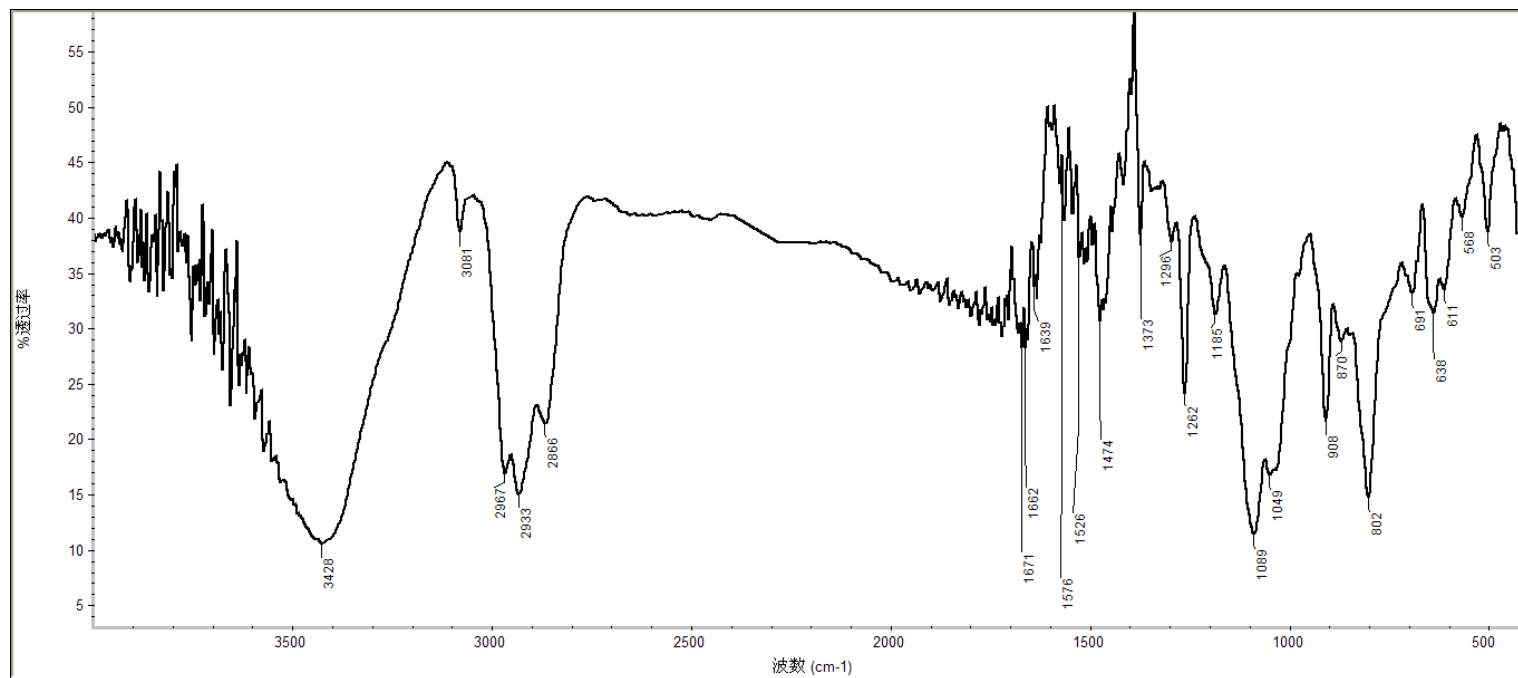


**Figure S15.** The HMBC Spectrum of Compound **2** in  $\text{CDCl}_3$

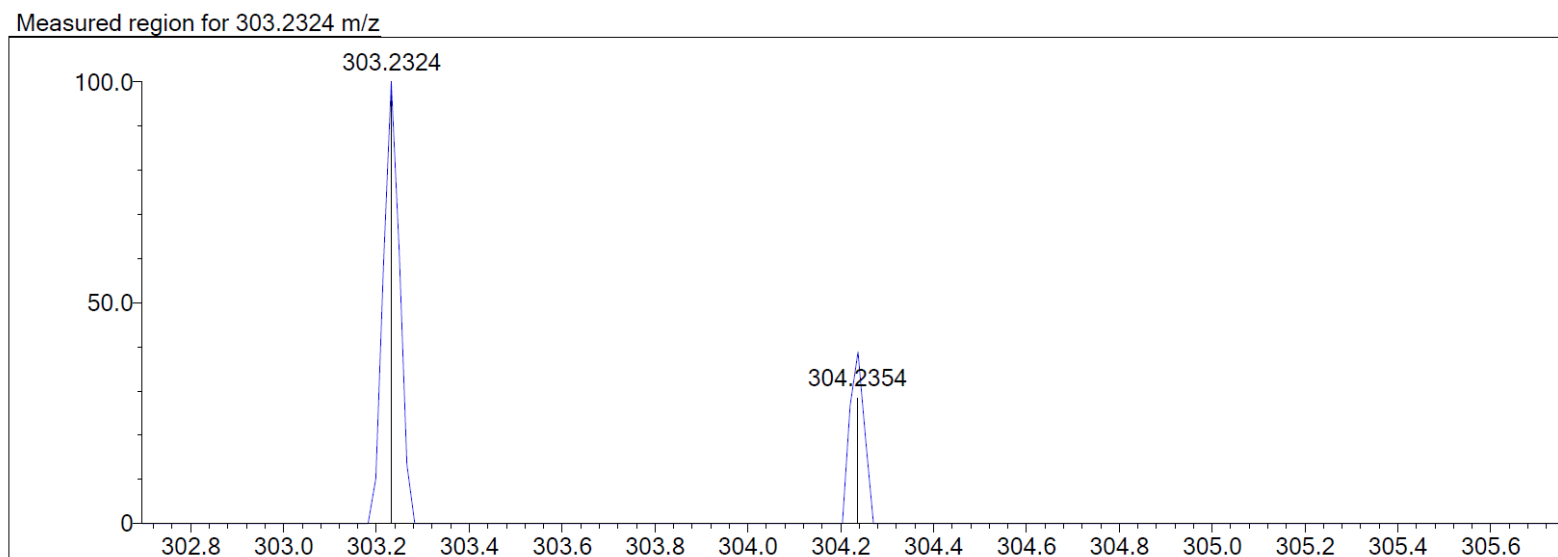




**Figure S16.** The NOESY Spectrum of Compound **2** in CDCl<sub>3</sub>



**Figure S17.** The IR Spectra of Compound **3**




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SPECTRUM -

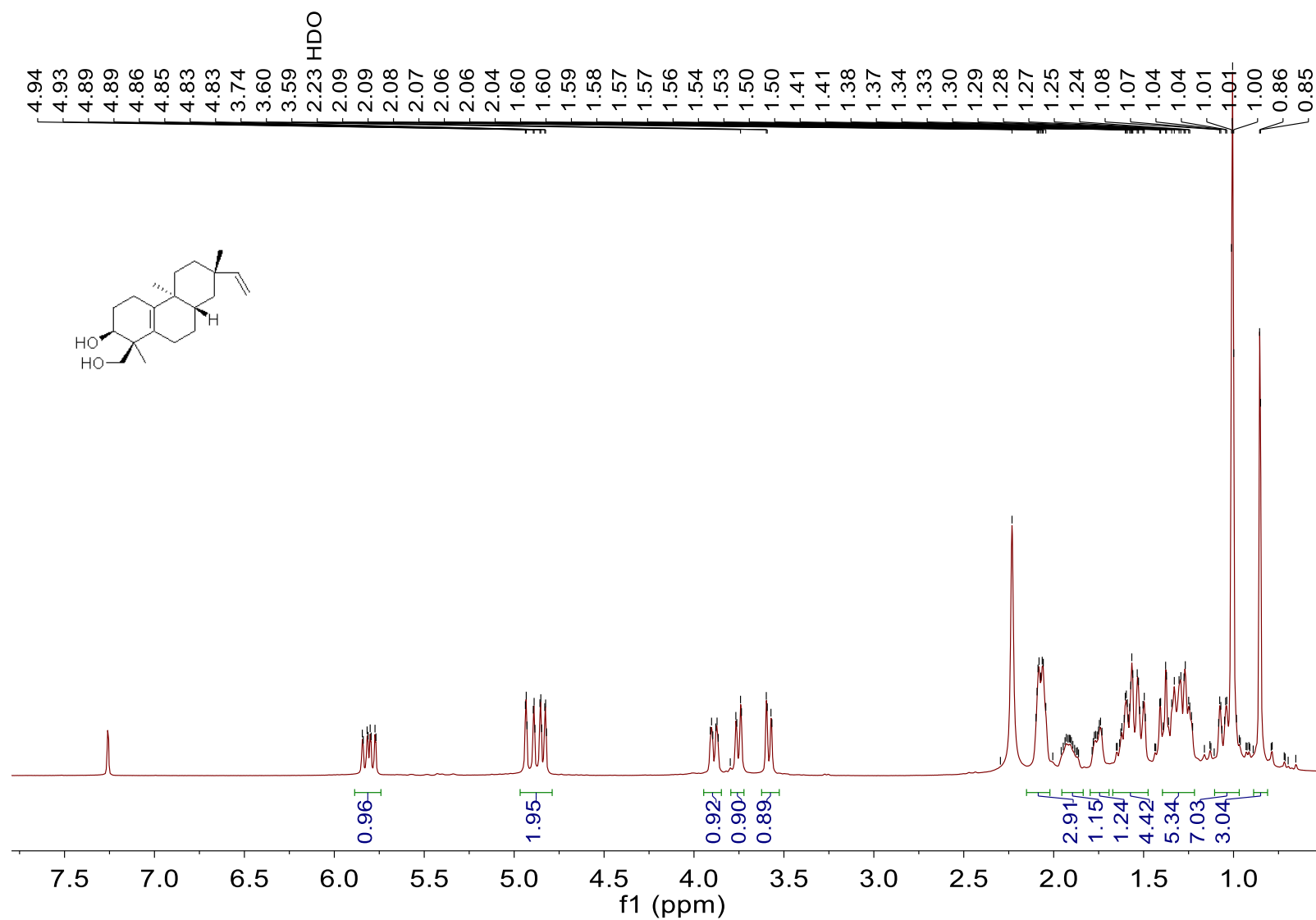
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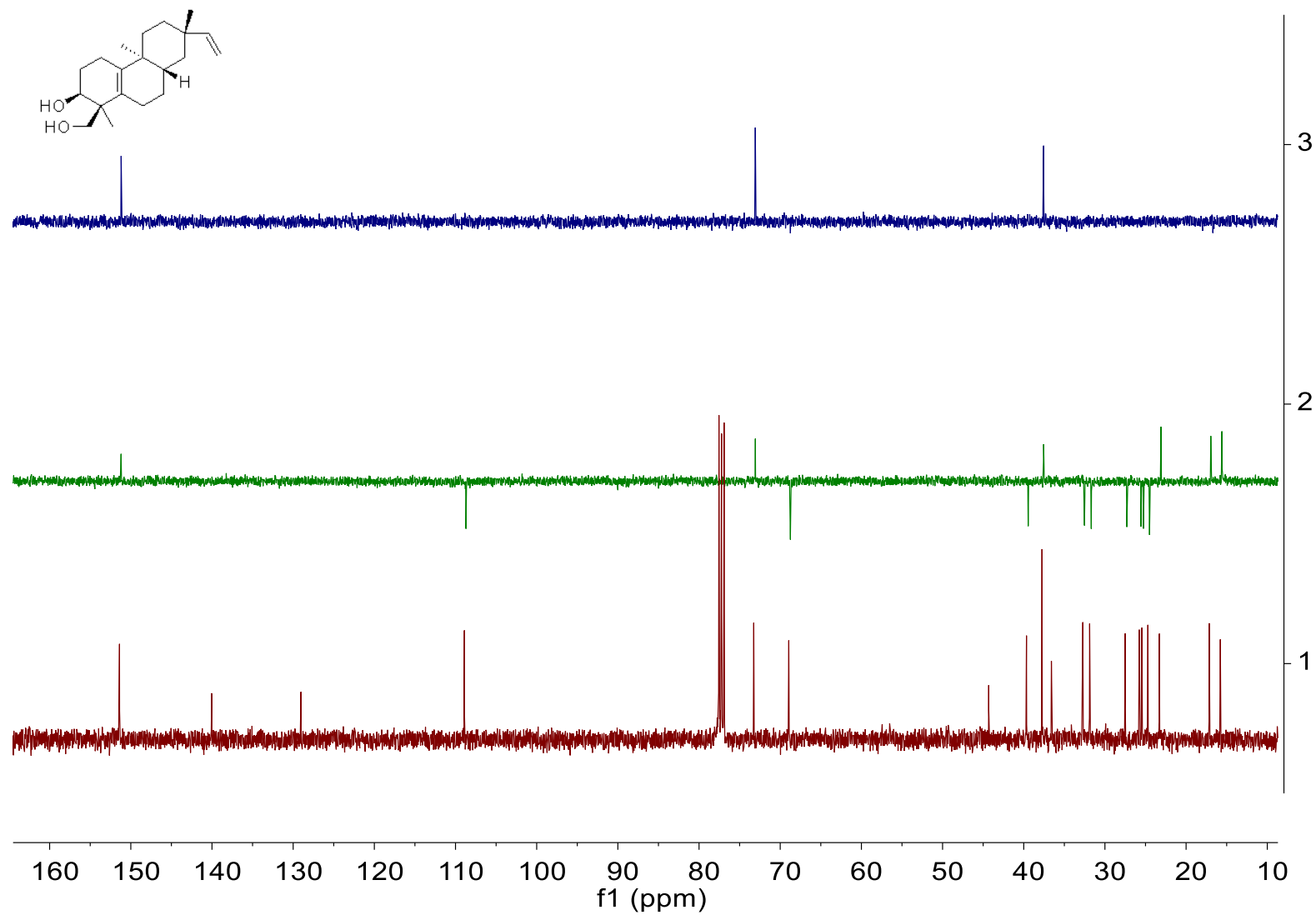
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
303.2324	303.2330	-1.98	5.0	C <sub>20</sub> H <sub>31</sub> O <sub>2</sub>

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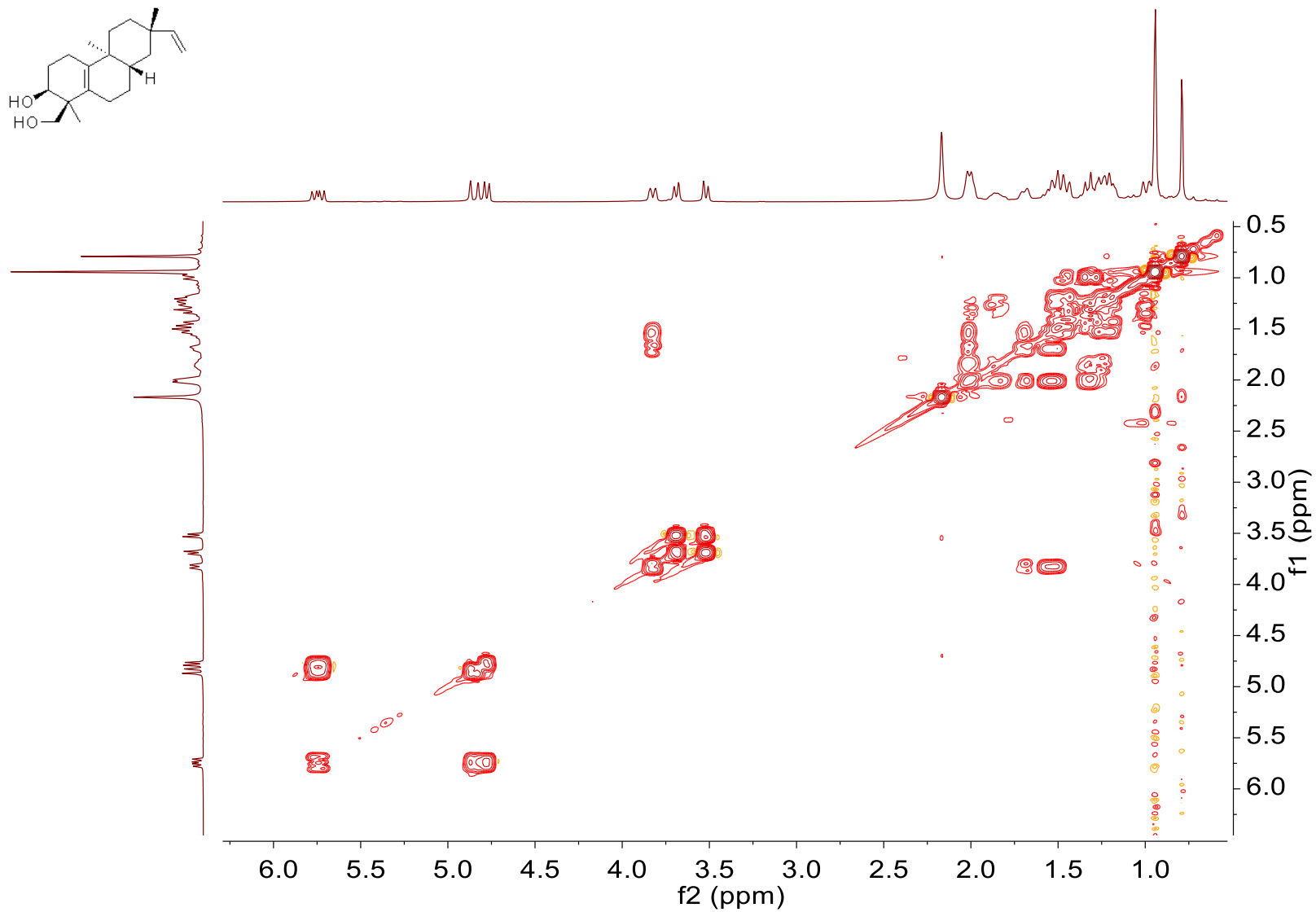
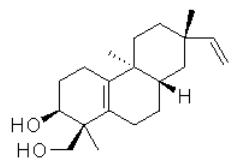
**Figure S18.** The HRESIMS Spectroscopic Data of Compound **3**



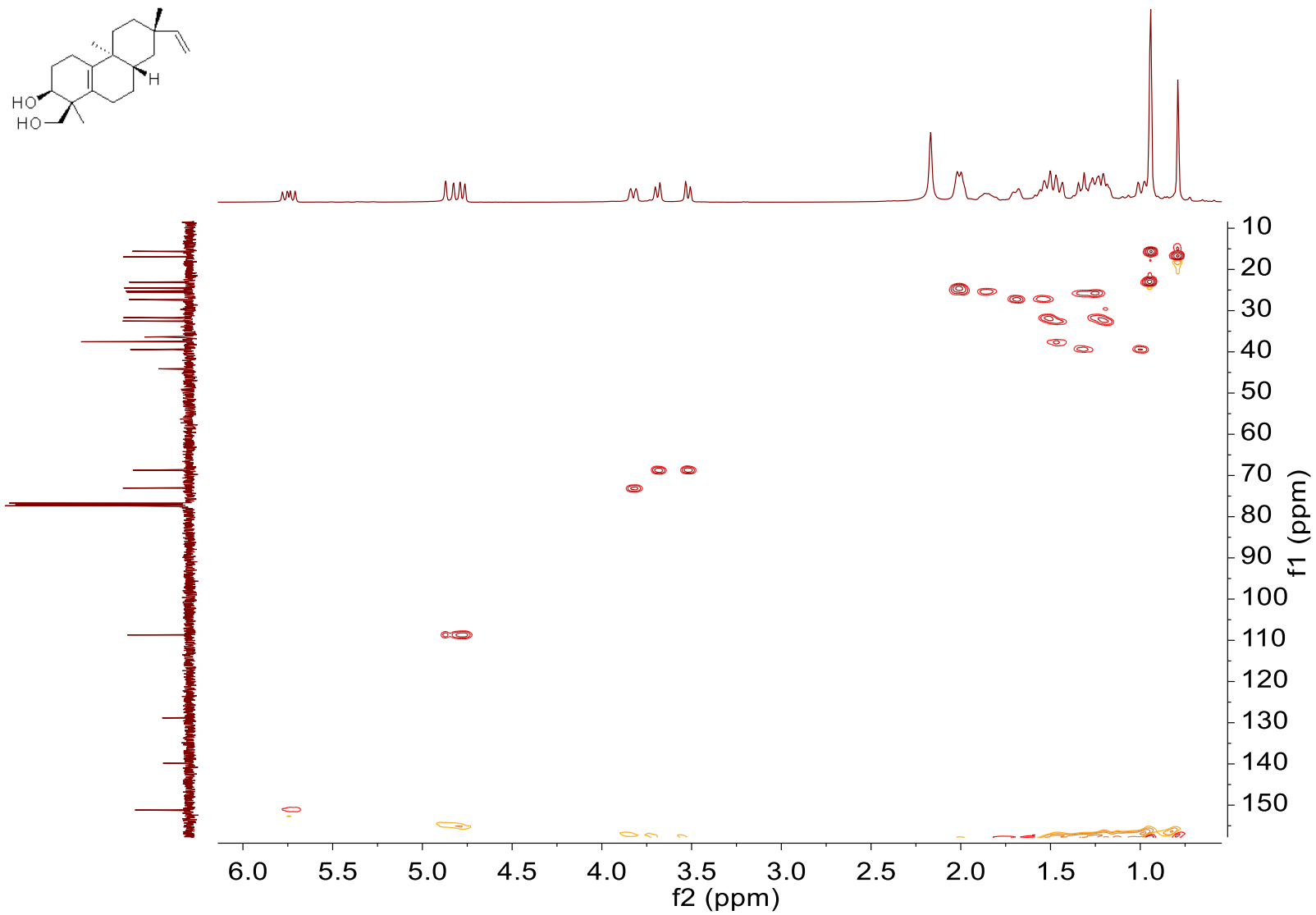
**Figure S19.** The  $^1\text{H}$  NMR Spectrum of Compound **3** in  $\text{CDCl}_3$



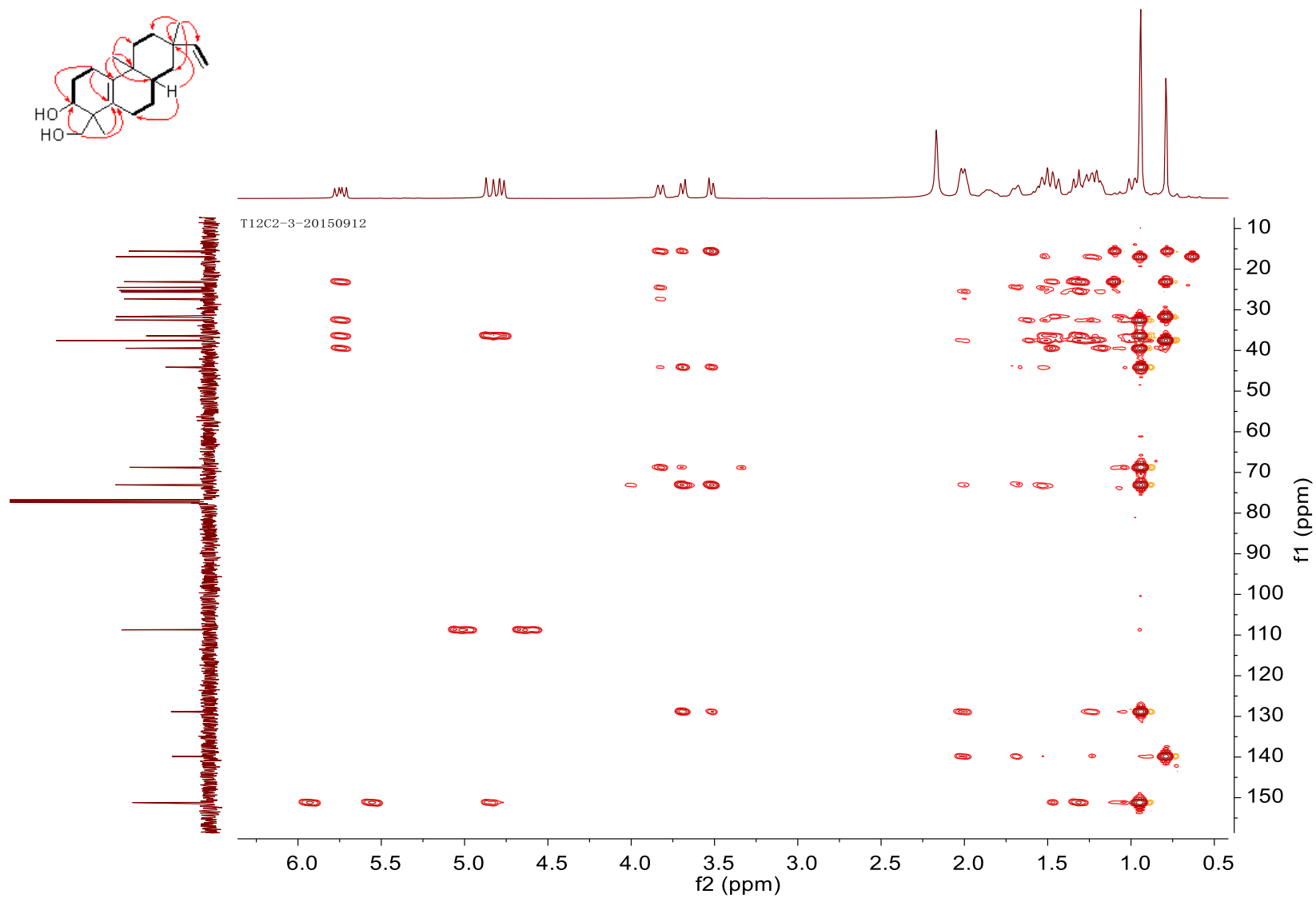
**Figure S20.** The  $^{13}\text{C}$  NMR Spectrum of Compound **3** in  $\text{CDCl}_3$



**Figure S21.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound 3 in  $\text{CDCl}_3$

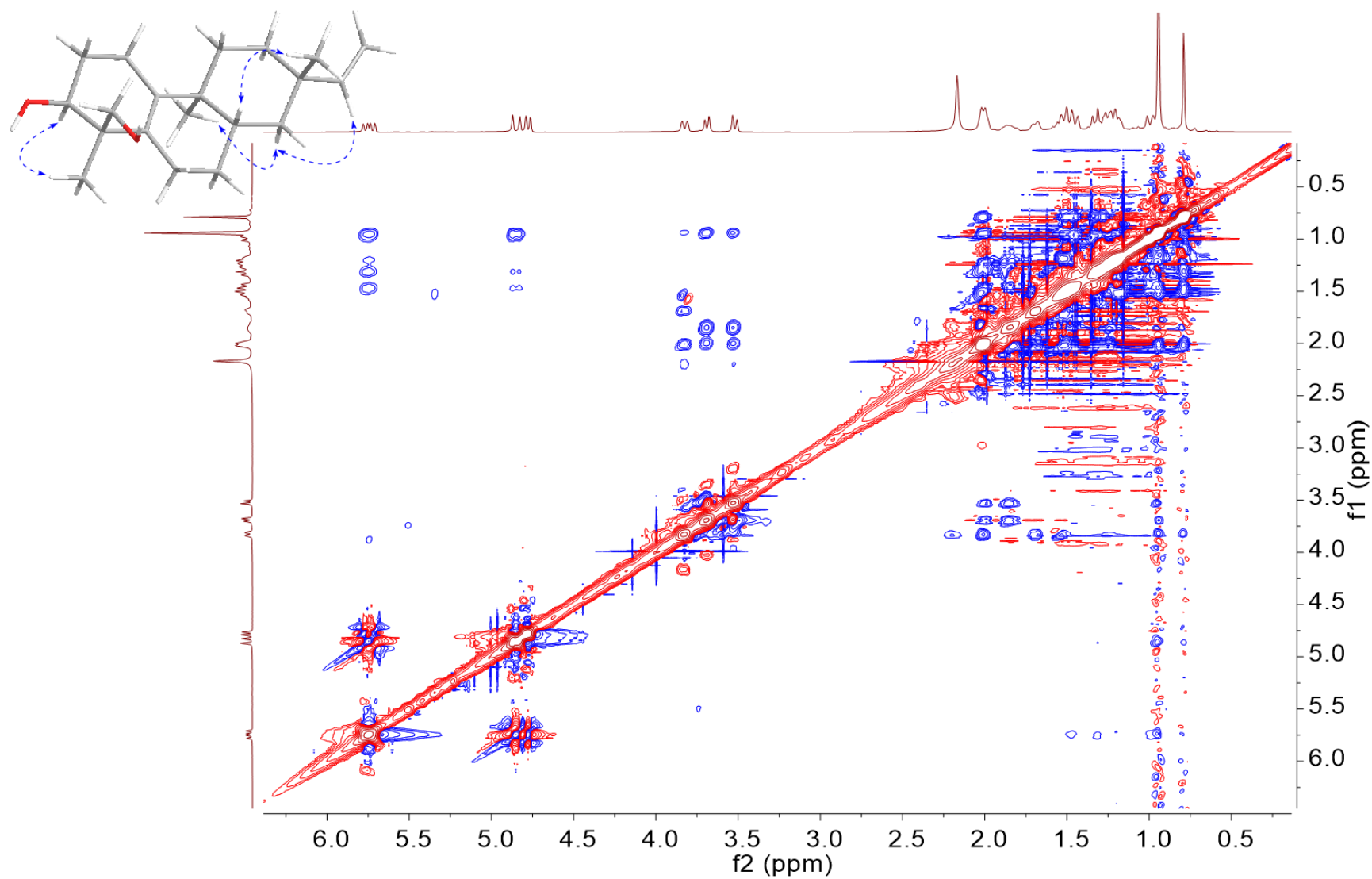


**Figure S22.** The HSQC Spectrum of Compound **3** in  $\text{CDCl}_3$

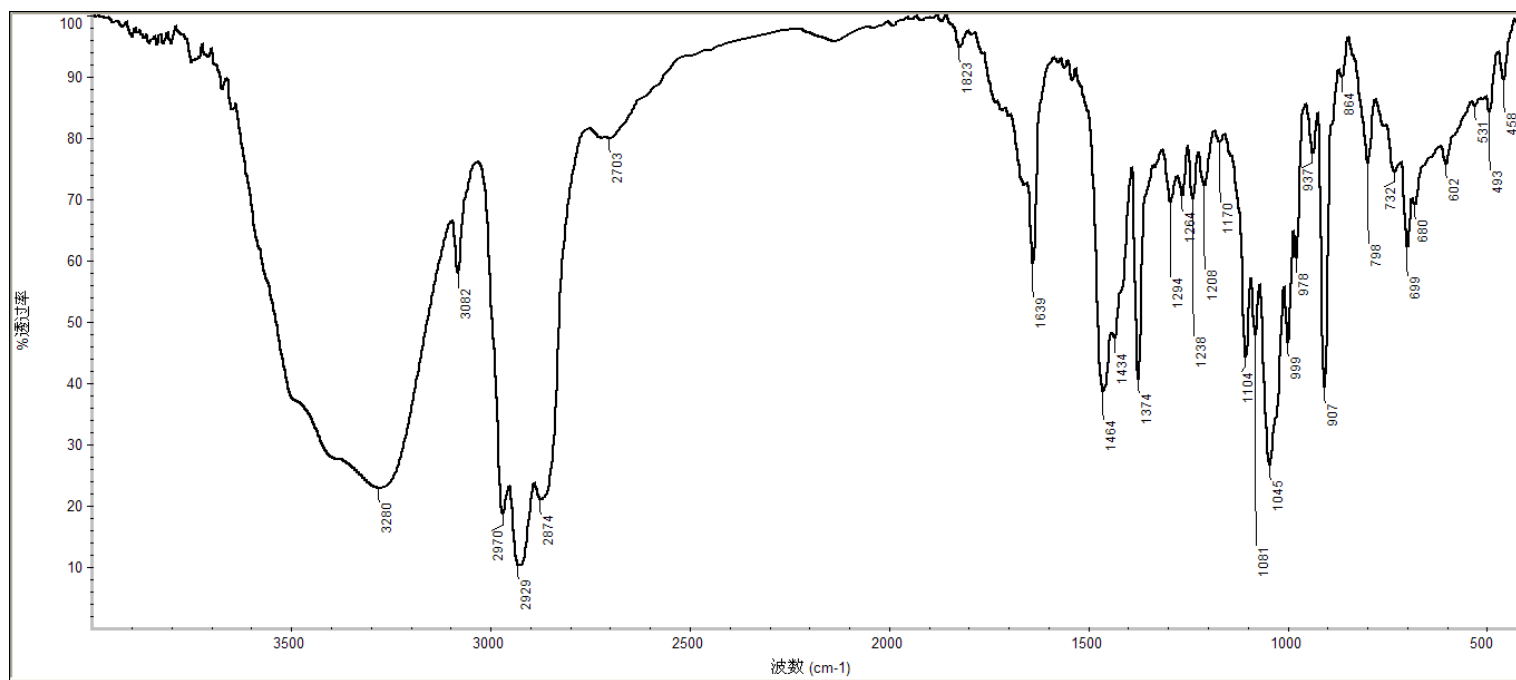


**Figure S23.** The HMBC Spectrum of Compound **3** in  $\text{CDCl}_3$

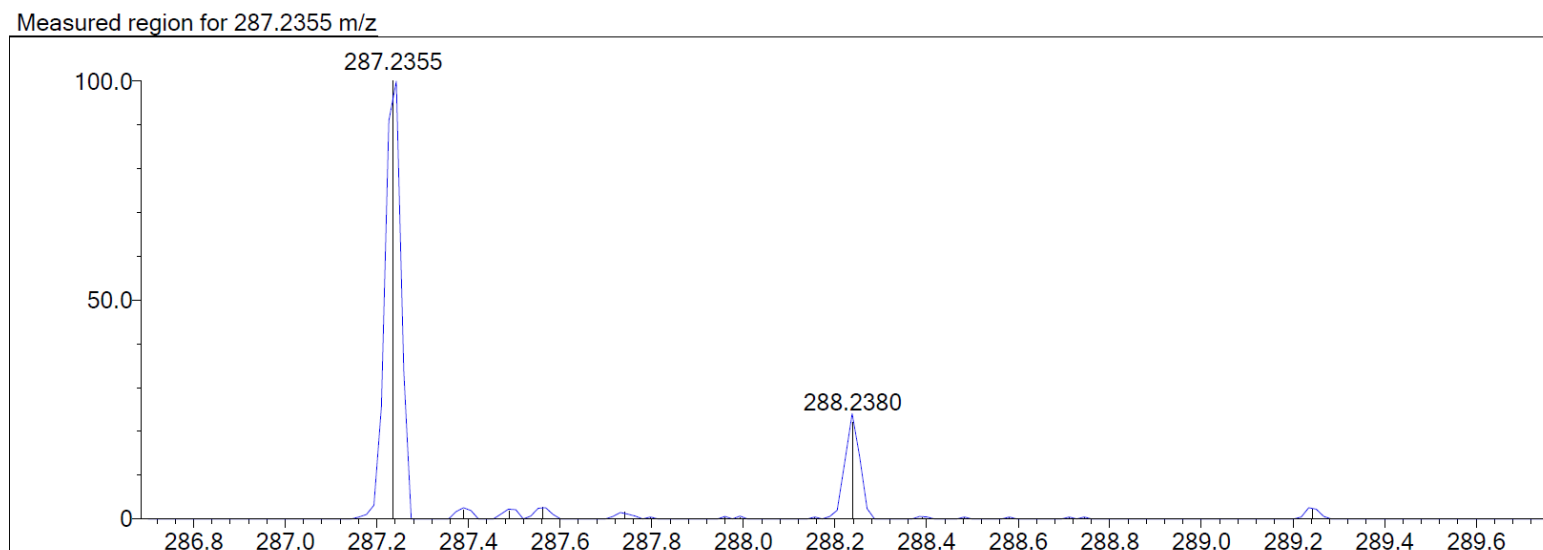




**Figure S24.** The NOESY Spectrum of Compound 3 in CDCl<sub>3</sub>



**Figure S25.** The IR Spectra of Compound **4**




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SPECTRUM -

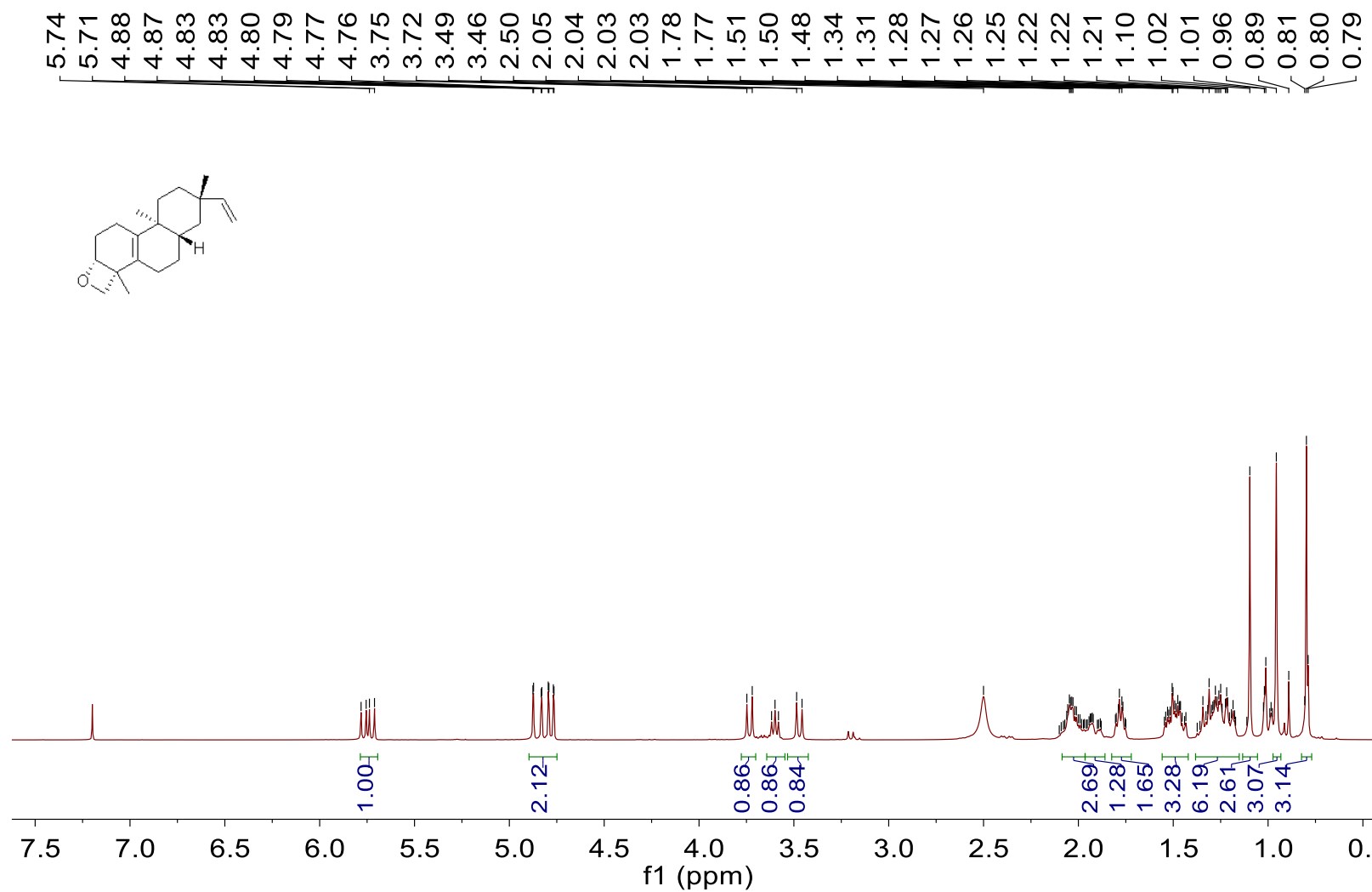
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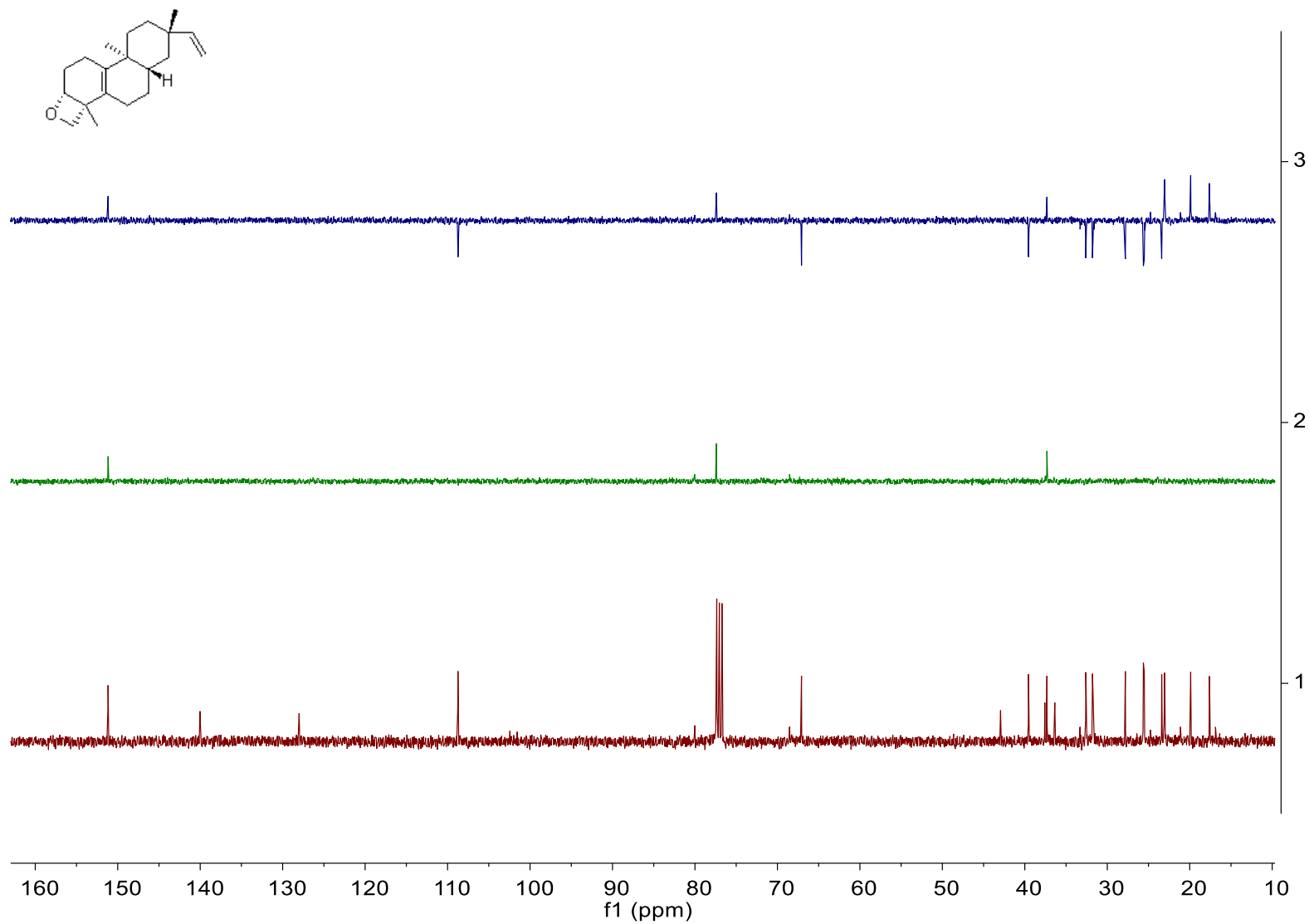
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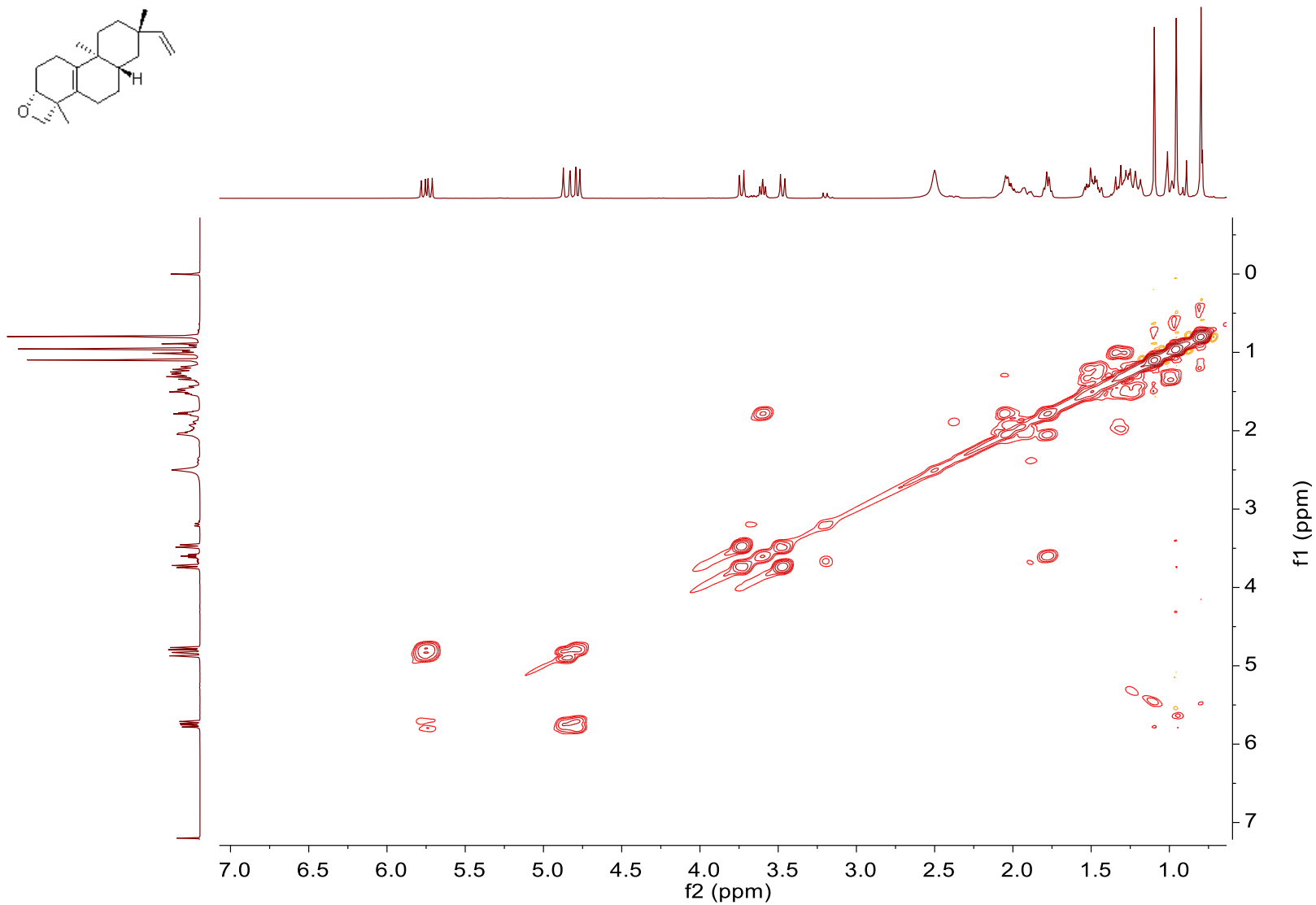
**Figure S26.** The HRESIMS Spectroscopic Data of Compound **4**



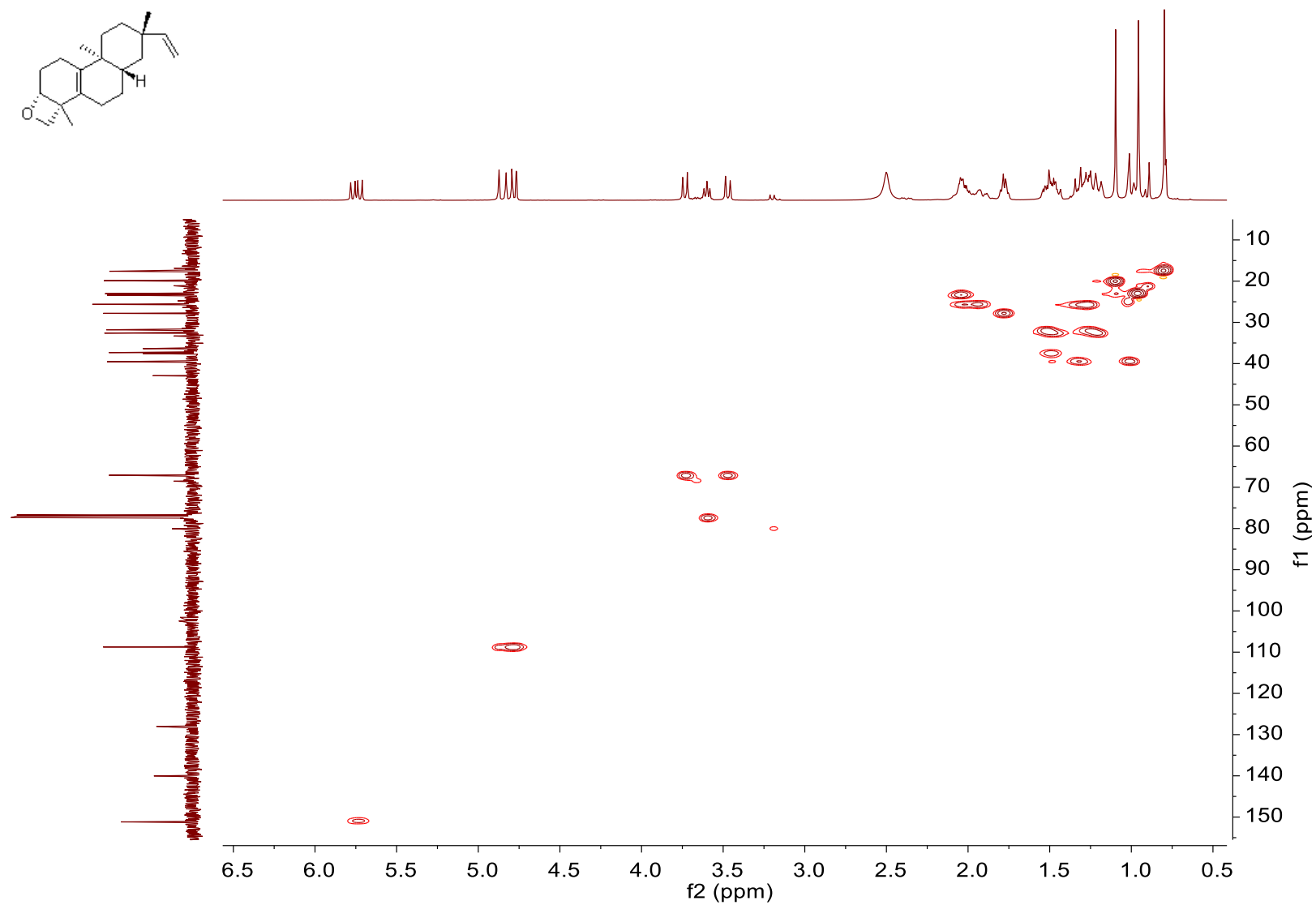
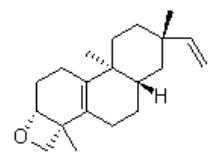
**Figure S27.** The <sup>1</sup>H NMR Spectrum of Compound **4** in CDCl<sub>3</sub>



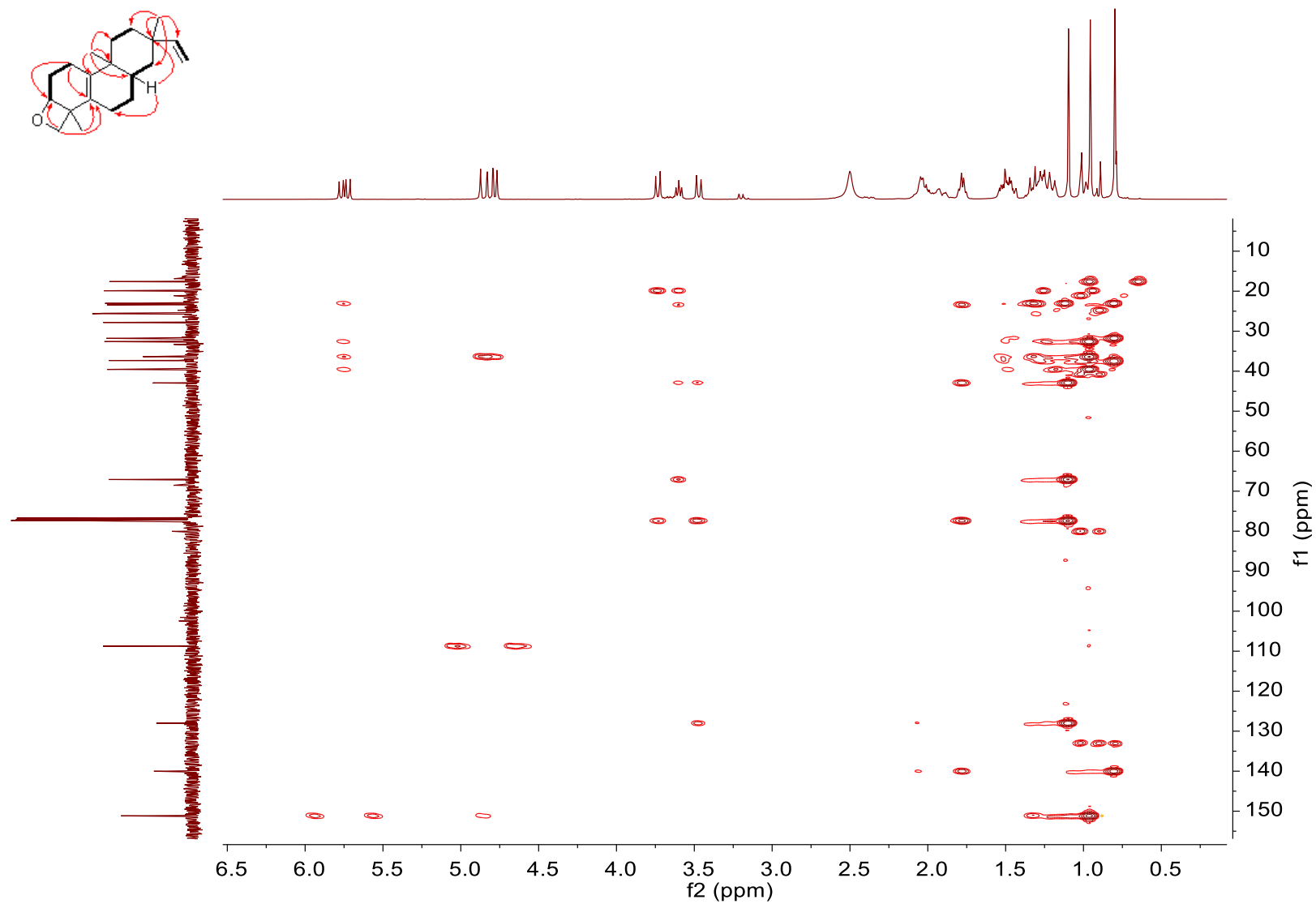
**Figure S28.** The  $^{13}\text{C}$  NMR Spectrum of Compound **4** in  $\text{CDCl}_3$



**Figure S29.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **4** in  $\text{CDCl}_3$

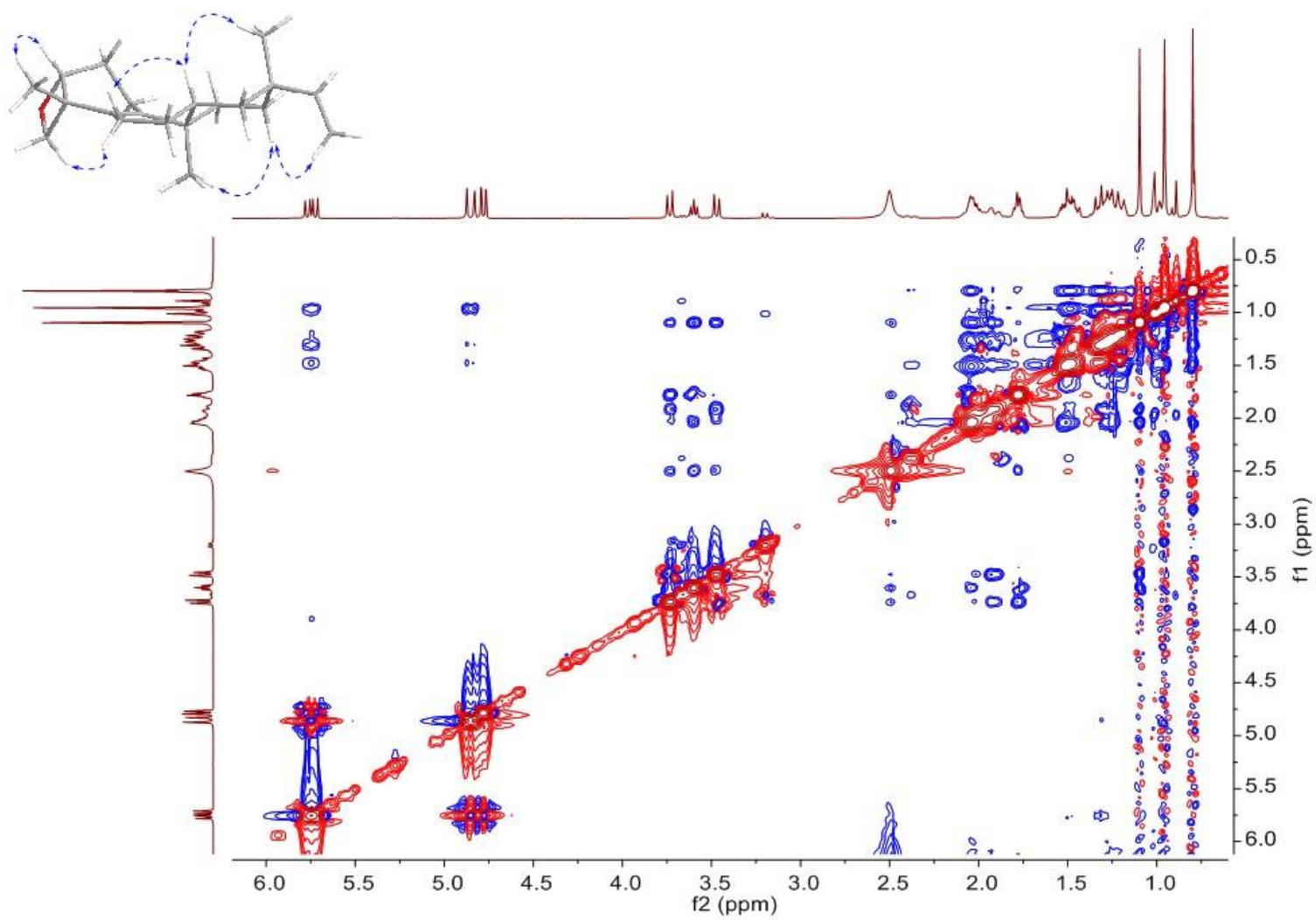


**Figure S30.** The HSQC Spectrum of Compound **4** in CDCl<sub>3</sub>

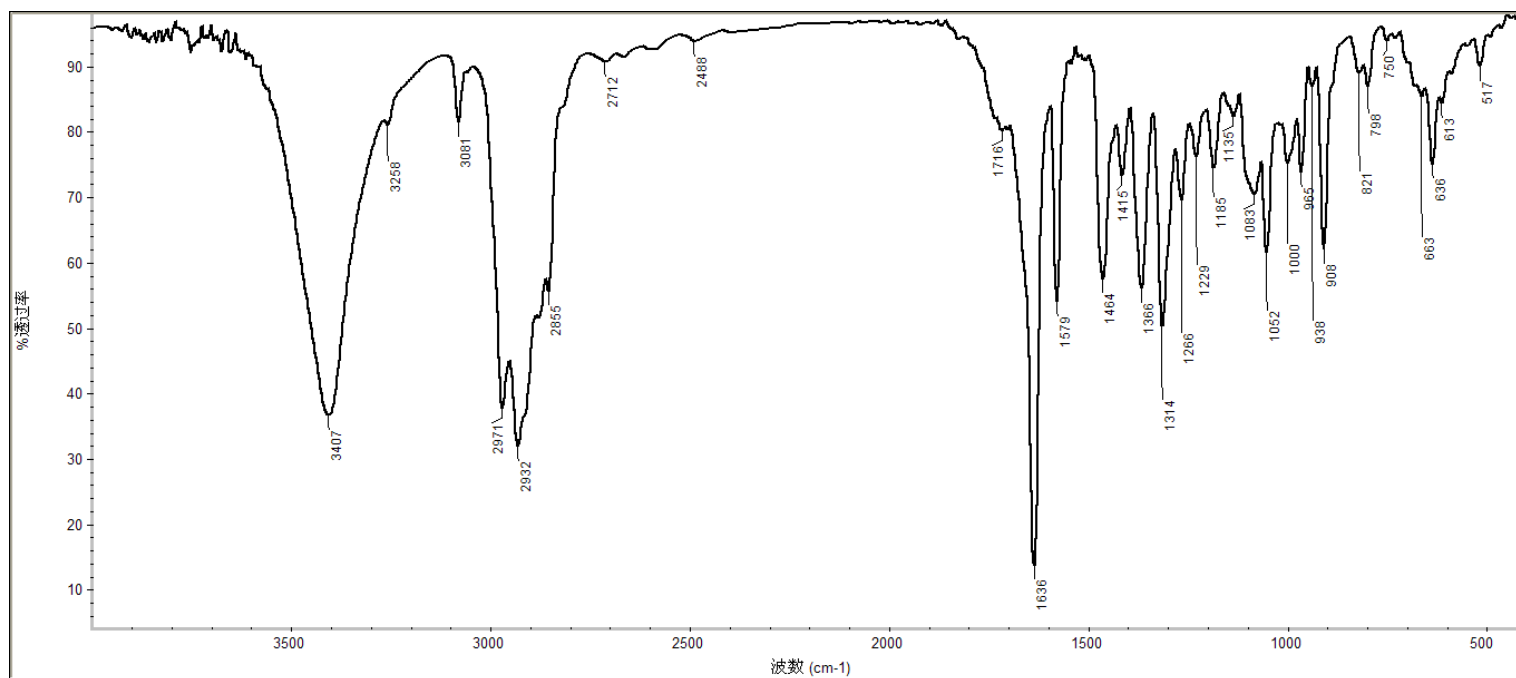


**Figure S31.** The HMBC Spectrum of Compound **4** in  $\text{CDCl}_3$

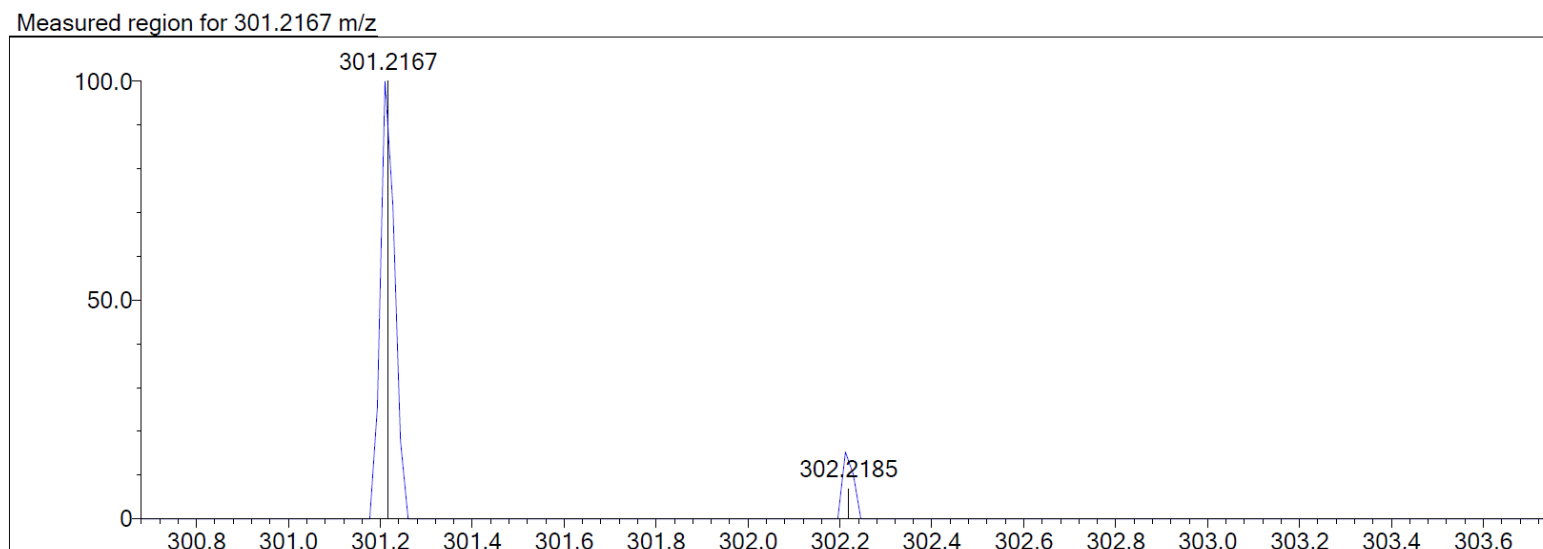




**Figure S32.** The NOESY Spectrum of Compound **4** in CDCl<sub>3</sub>



**Figure S33.** The IR Spectra of Compound **5**




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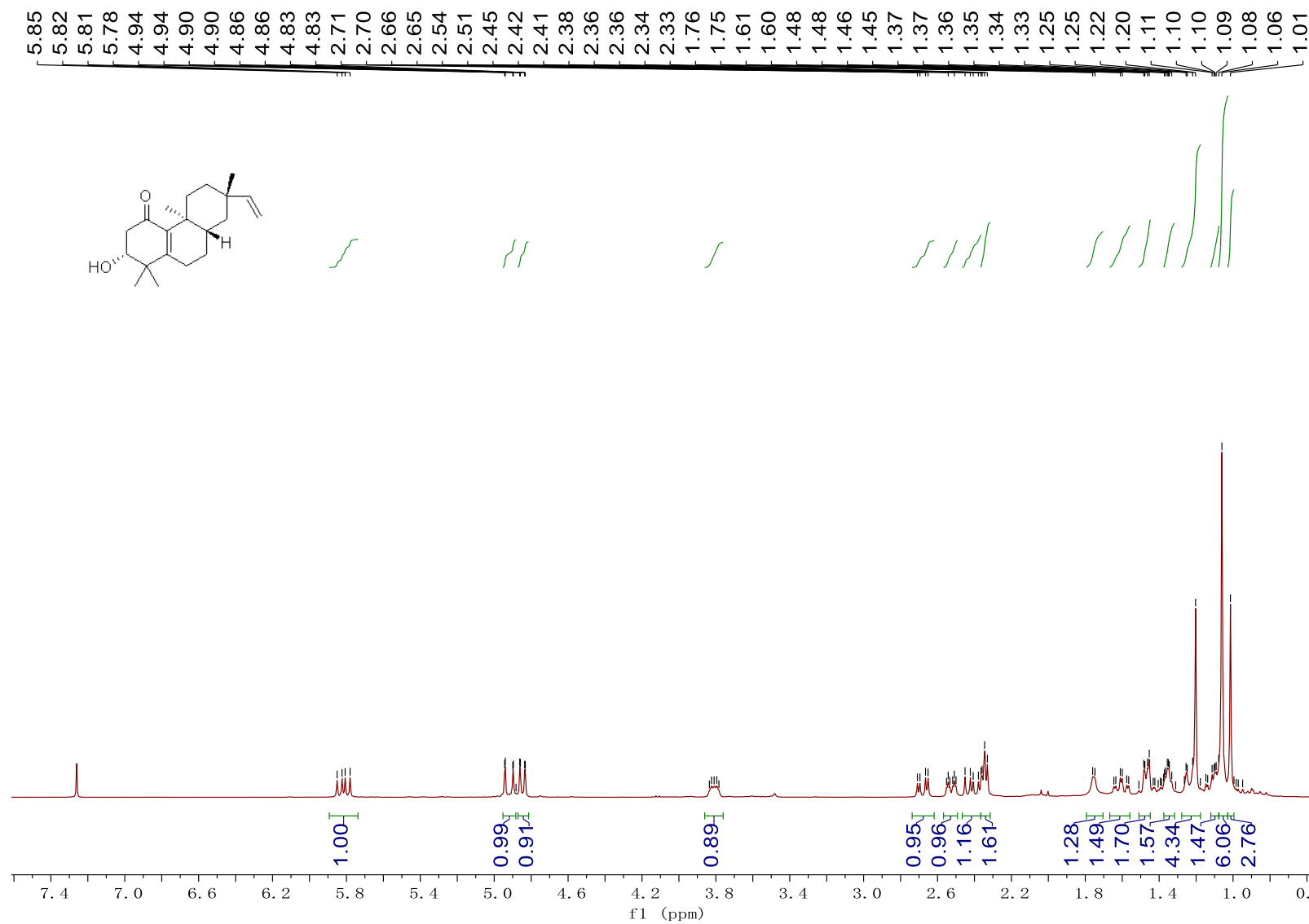
simulation :

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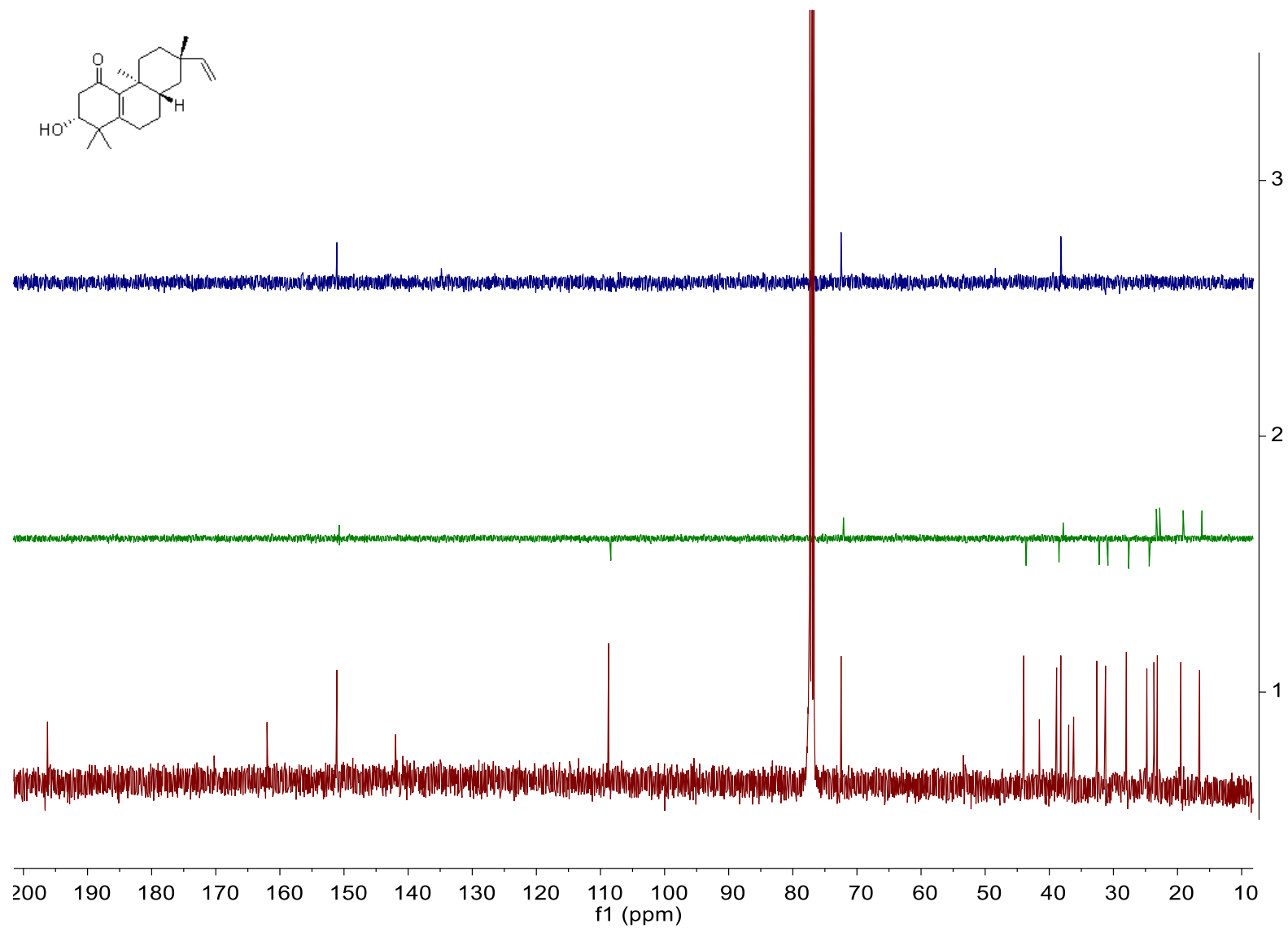
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
301.2167	301.2173	-1.99	6.0	C <sub>20</sub> H <sub>29</sub> O <sub>2</sub>

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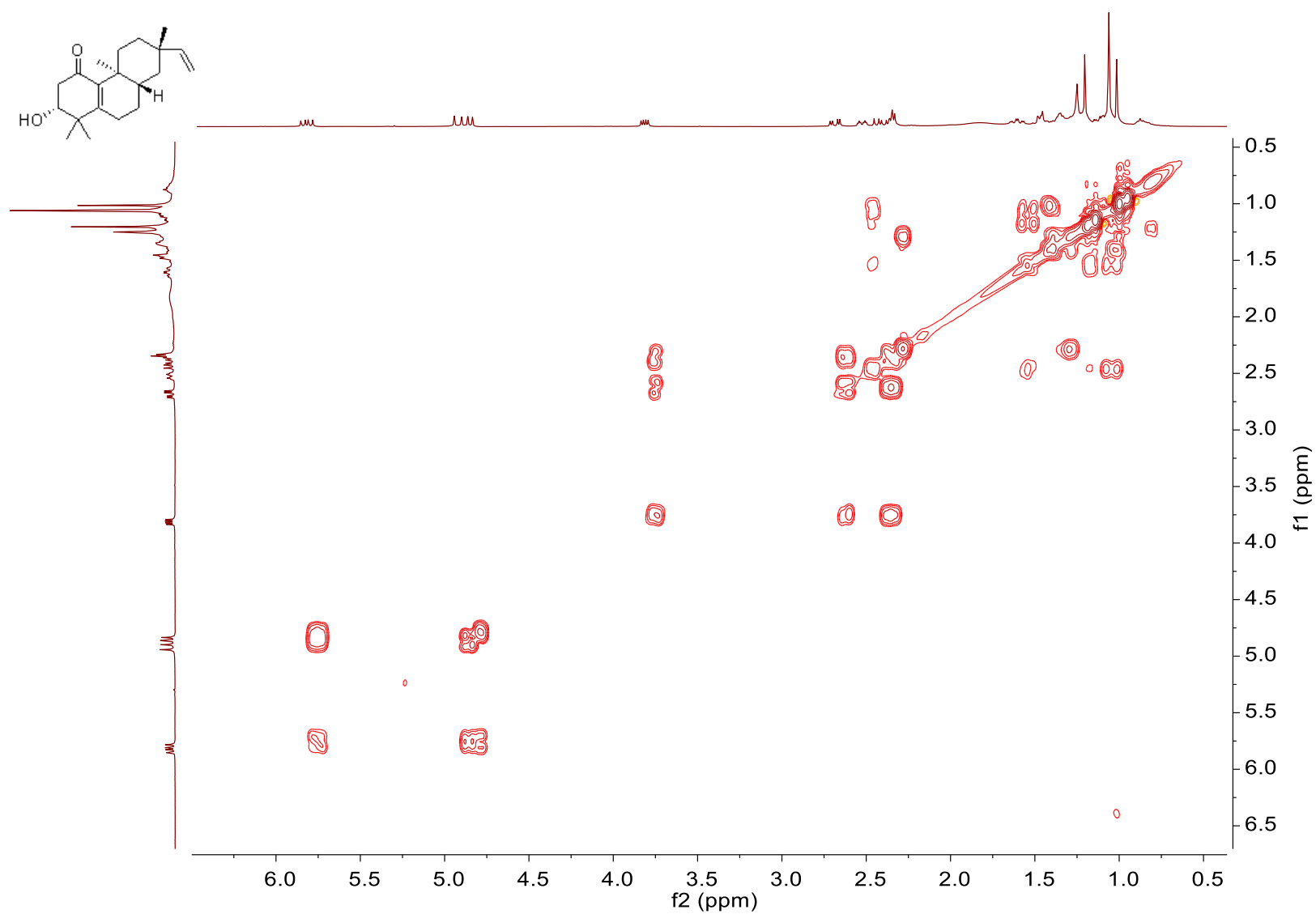
**Figure S34.** The HRESIMS Spectroscopic Data of Compound **5**



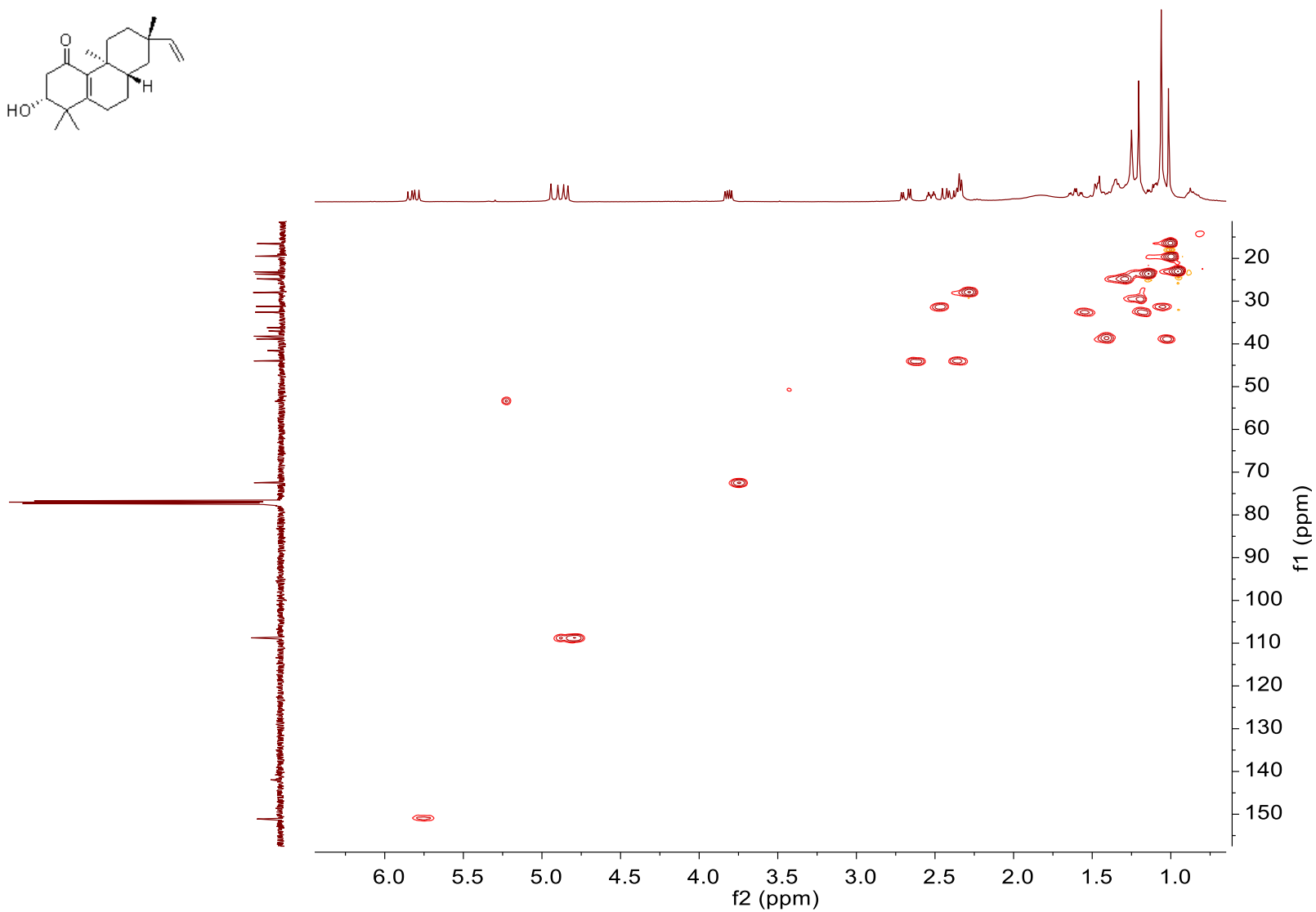
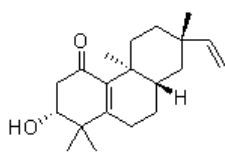
**Figure S35.** The  $^1\text{H}$  NMR Spectrum of Compound 5 in  $\text{CDCl}_3$



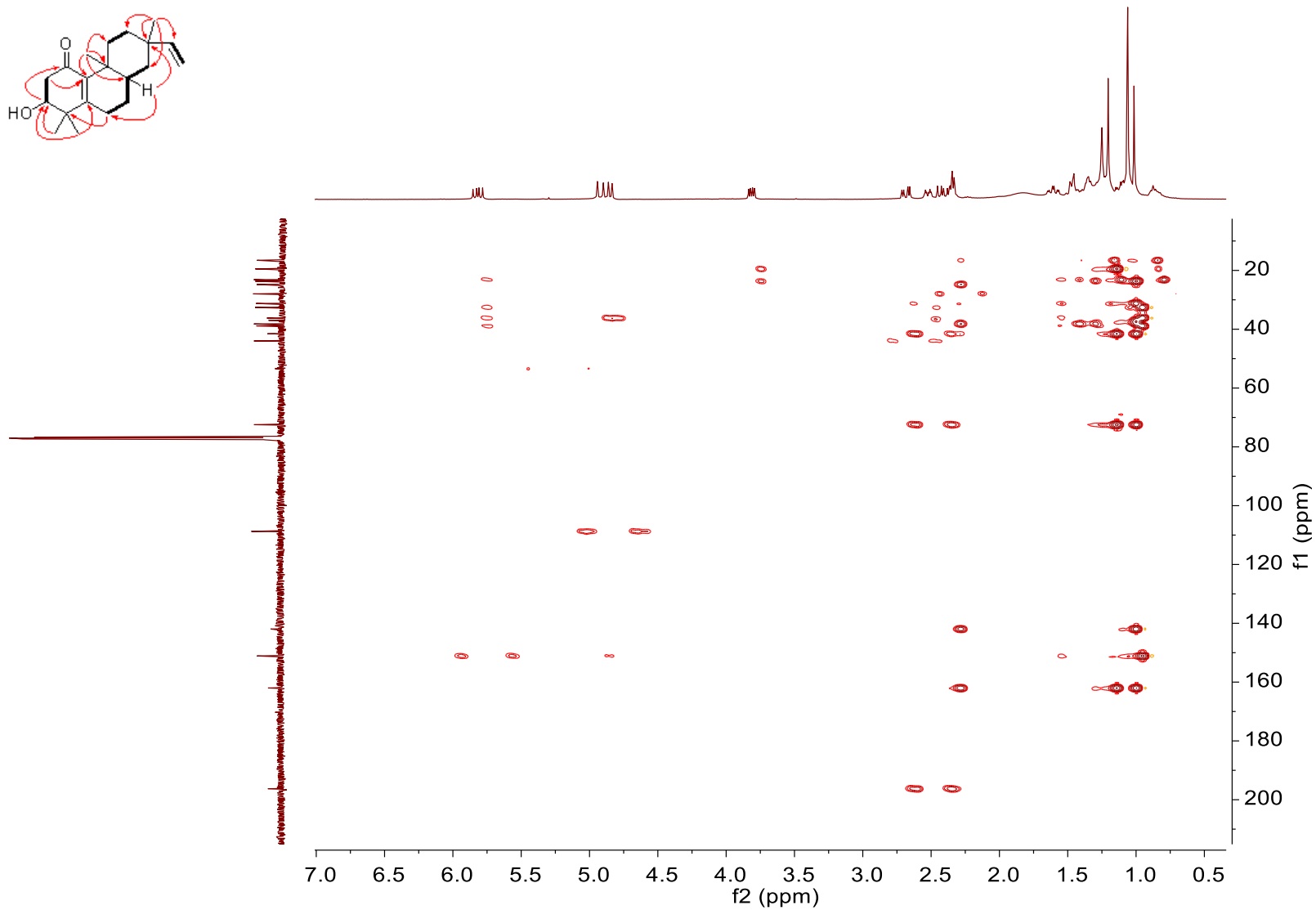
**Figure S36.** The <sup>13</sup>C NMR Spectrum of Compound **5** in CDCl<sub>3</sub>



**Figure S37.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **5** in  $\text{CDCl}_3$

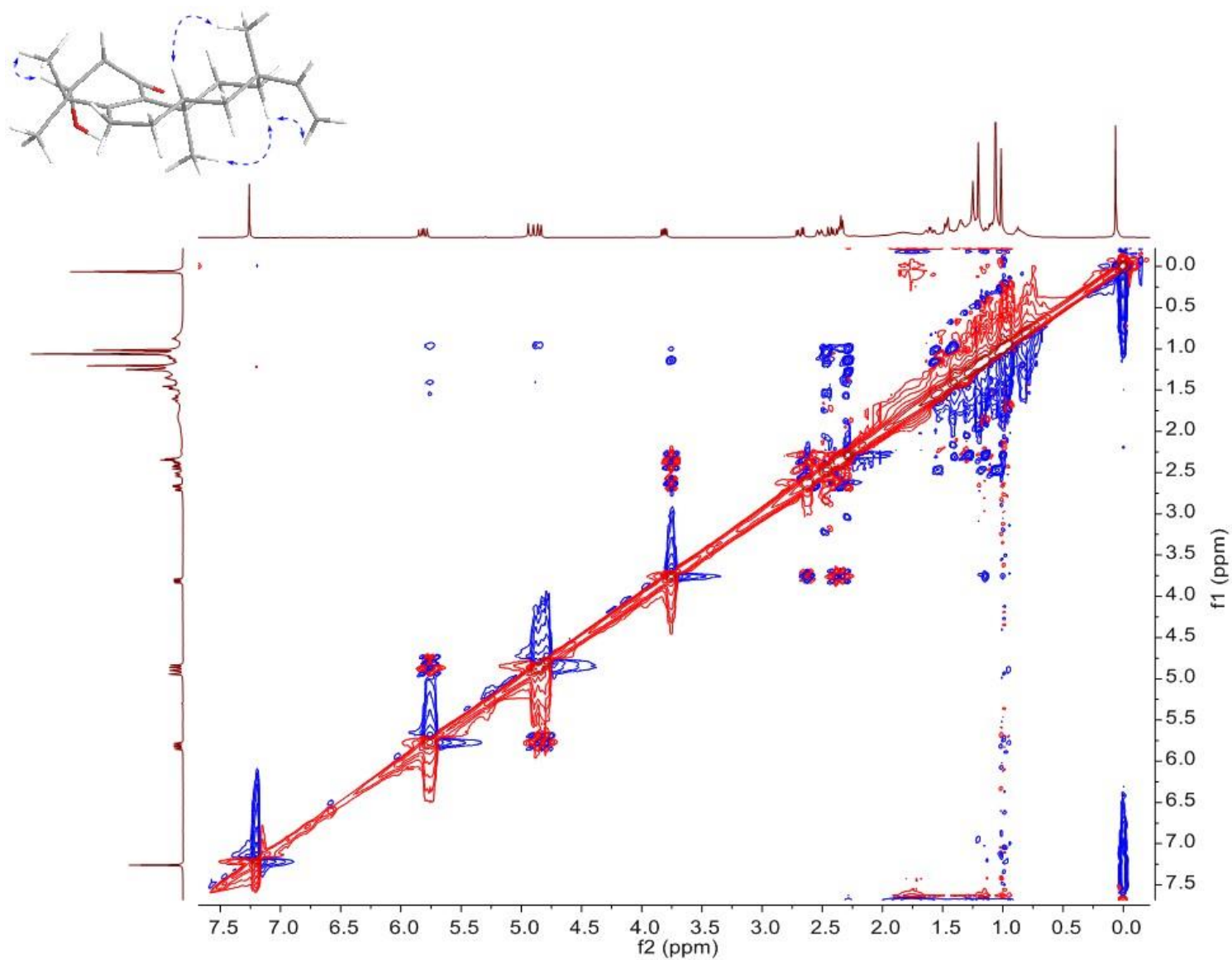


**Figure S38.** The HSQC Spectrum of Compound **5** in  $\text{CDCl}_3$

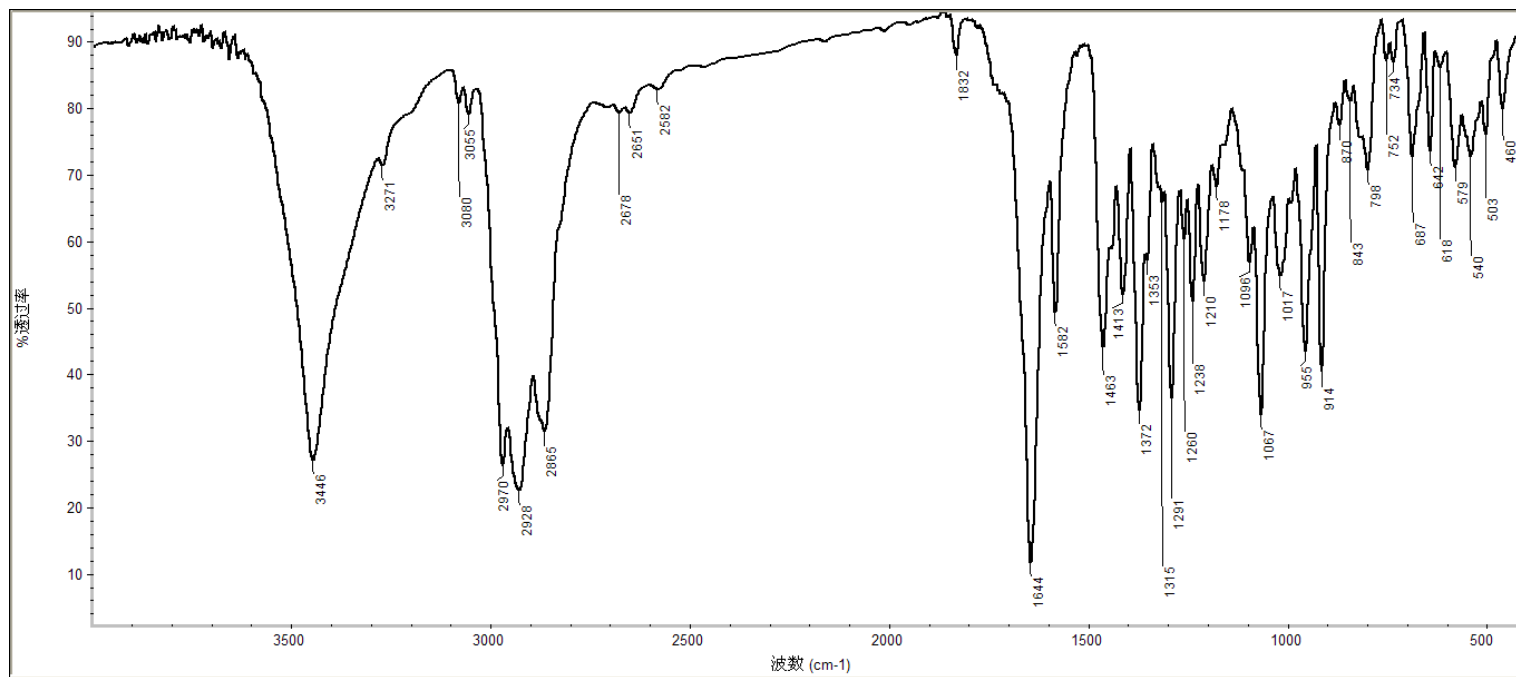


**Figure S39.** The HMBC Spectrum of Compound **5** in  $\text{CDCl}_3$

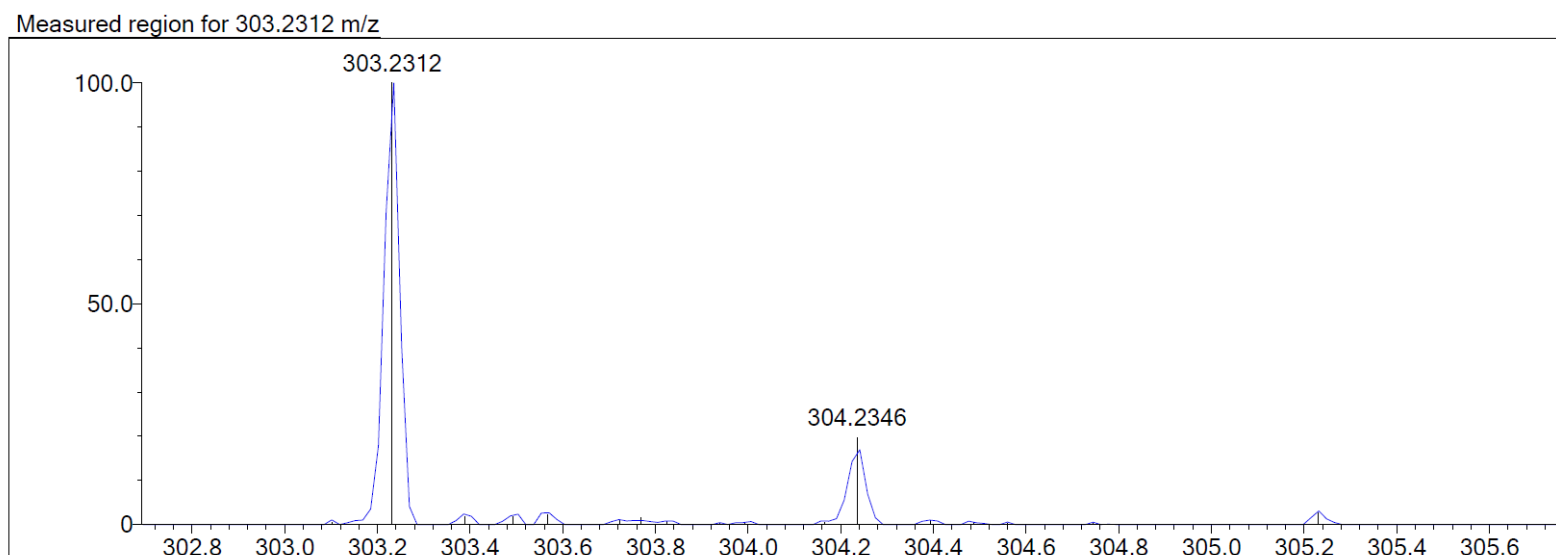




**Figure S40.** The NOESY Spectrum of Compound **5** in CDCl<sub>3</sub>



**Figure S41.** The IR Spectra of Compound **6**

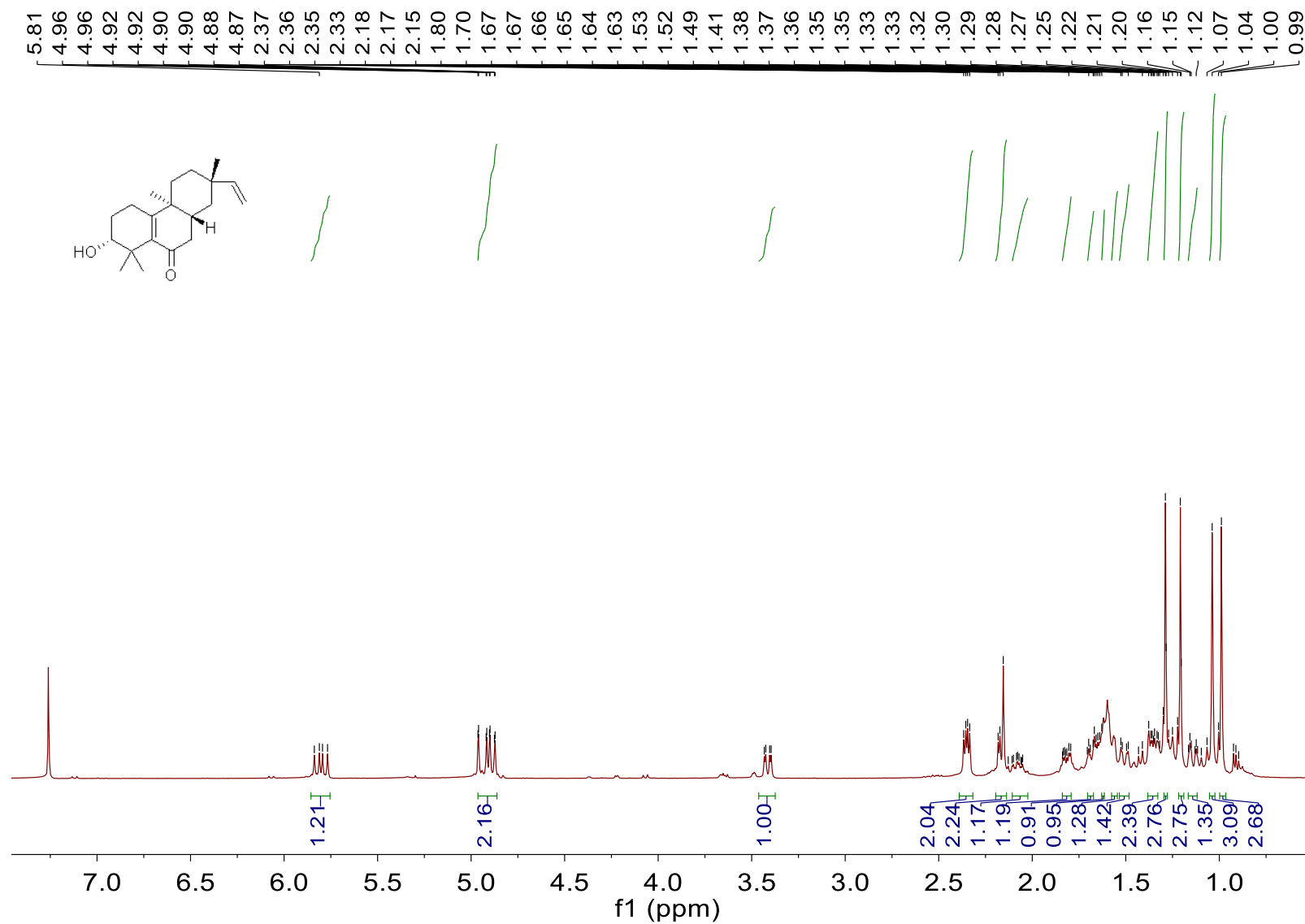


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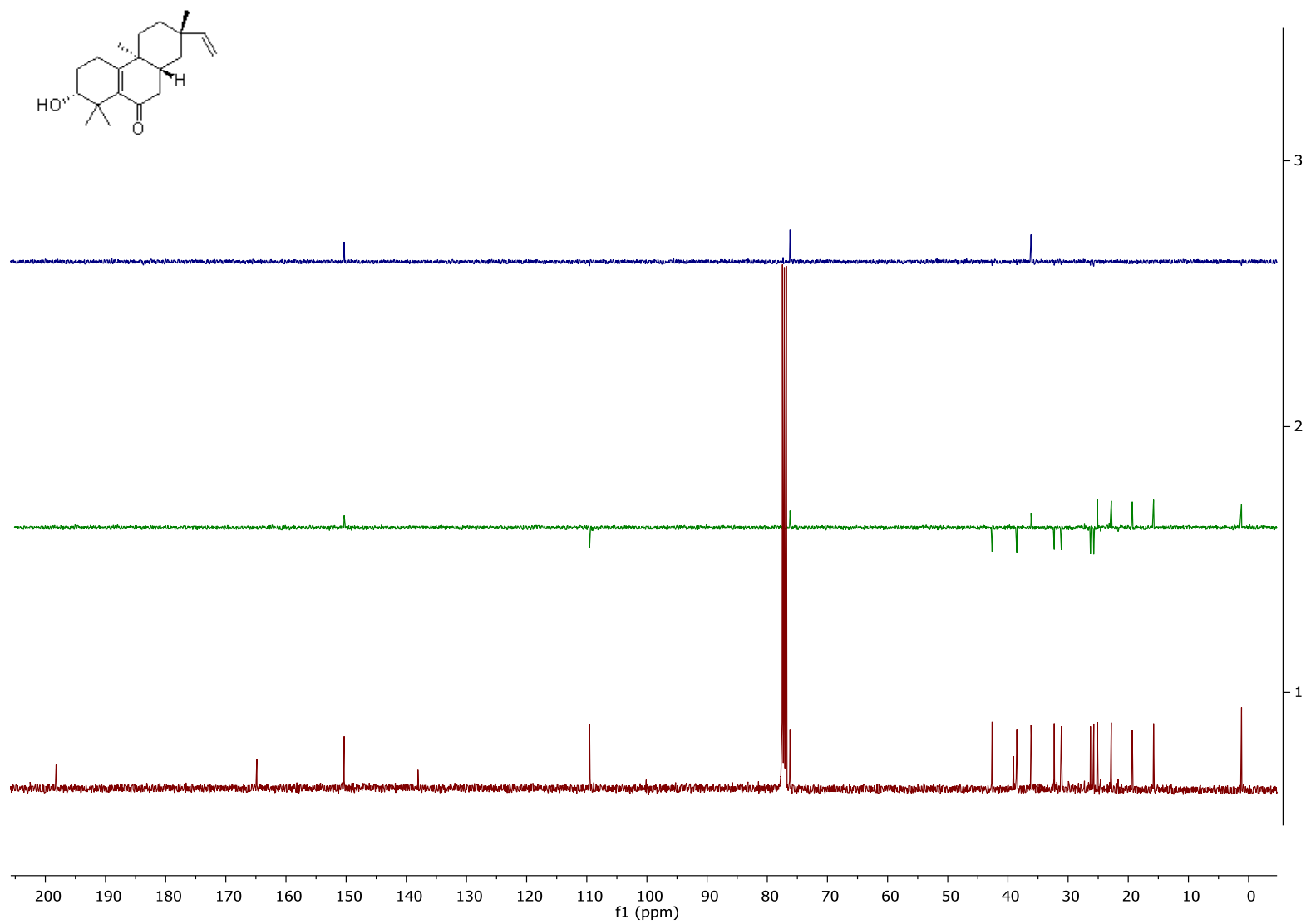
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
303.2312	303.2319	-2.31	6.0	C <sub>20</sub> H <sub>31</sub> O <sub>2</sub>

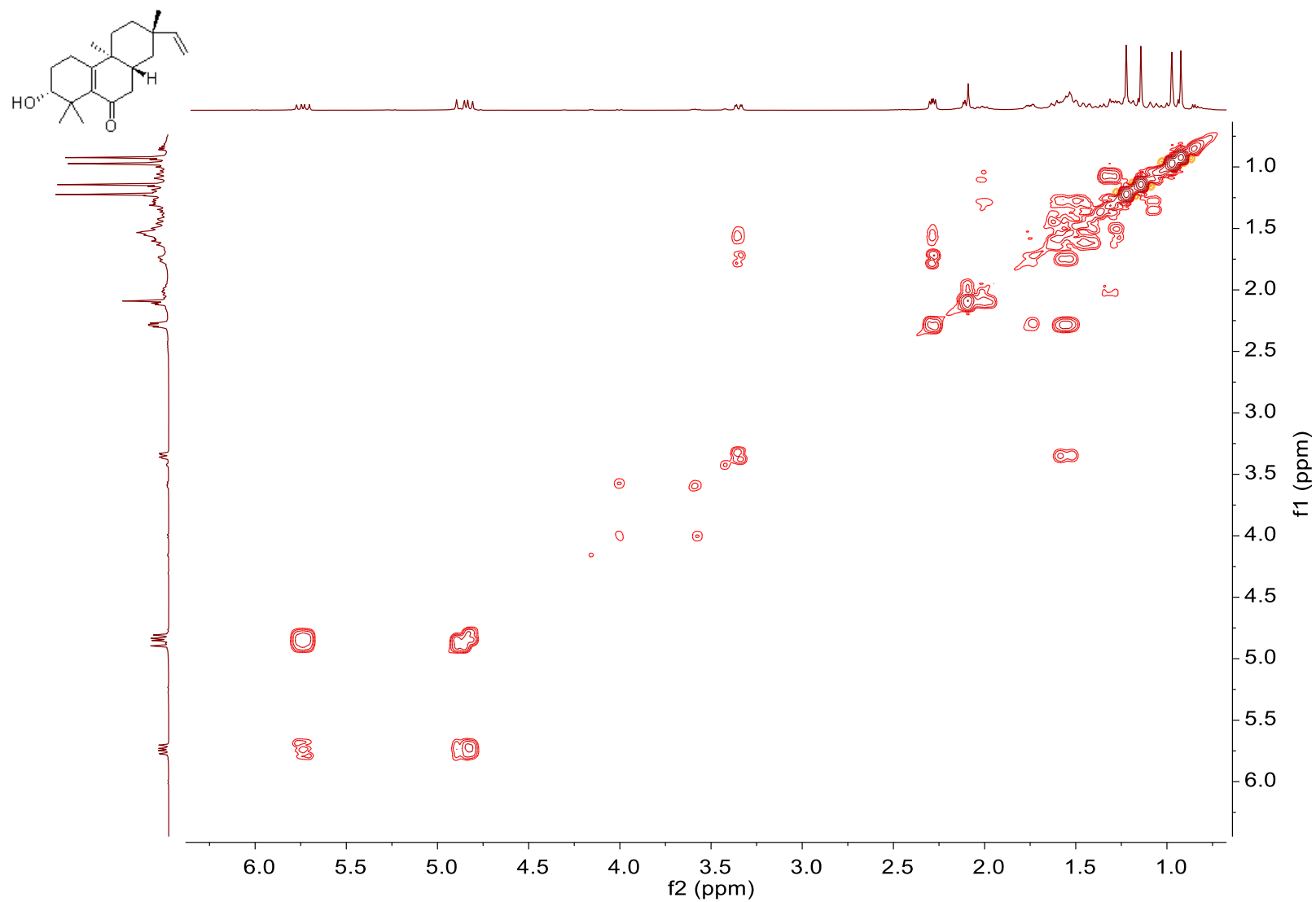
**Figure S42.** The HRESIMS Spectroscopic Data of Compound **6**



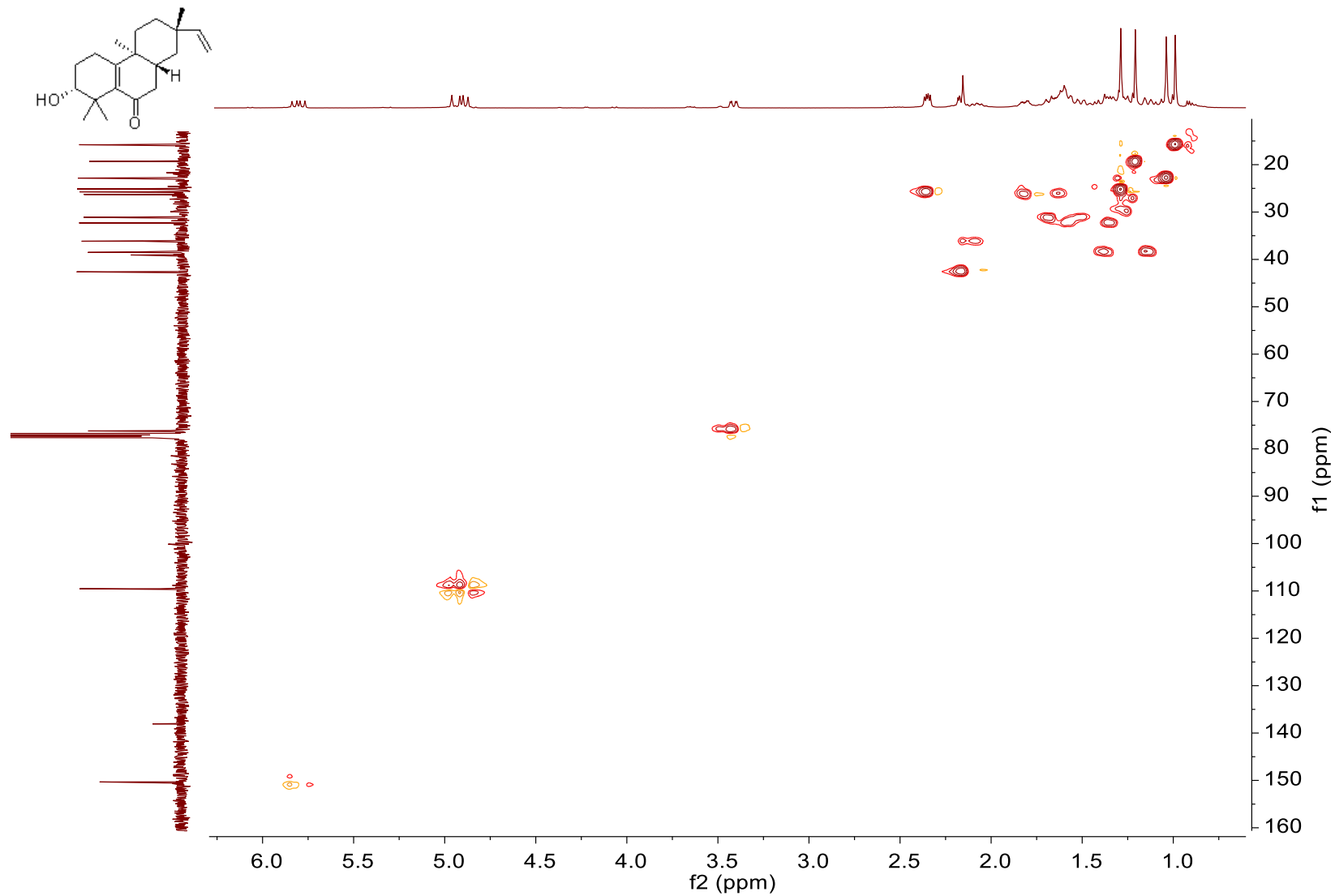
**Figure S43.** The <sup>1</sup>H NMR Spectrum of Compound **6** in CDCl<sub>3</sub>



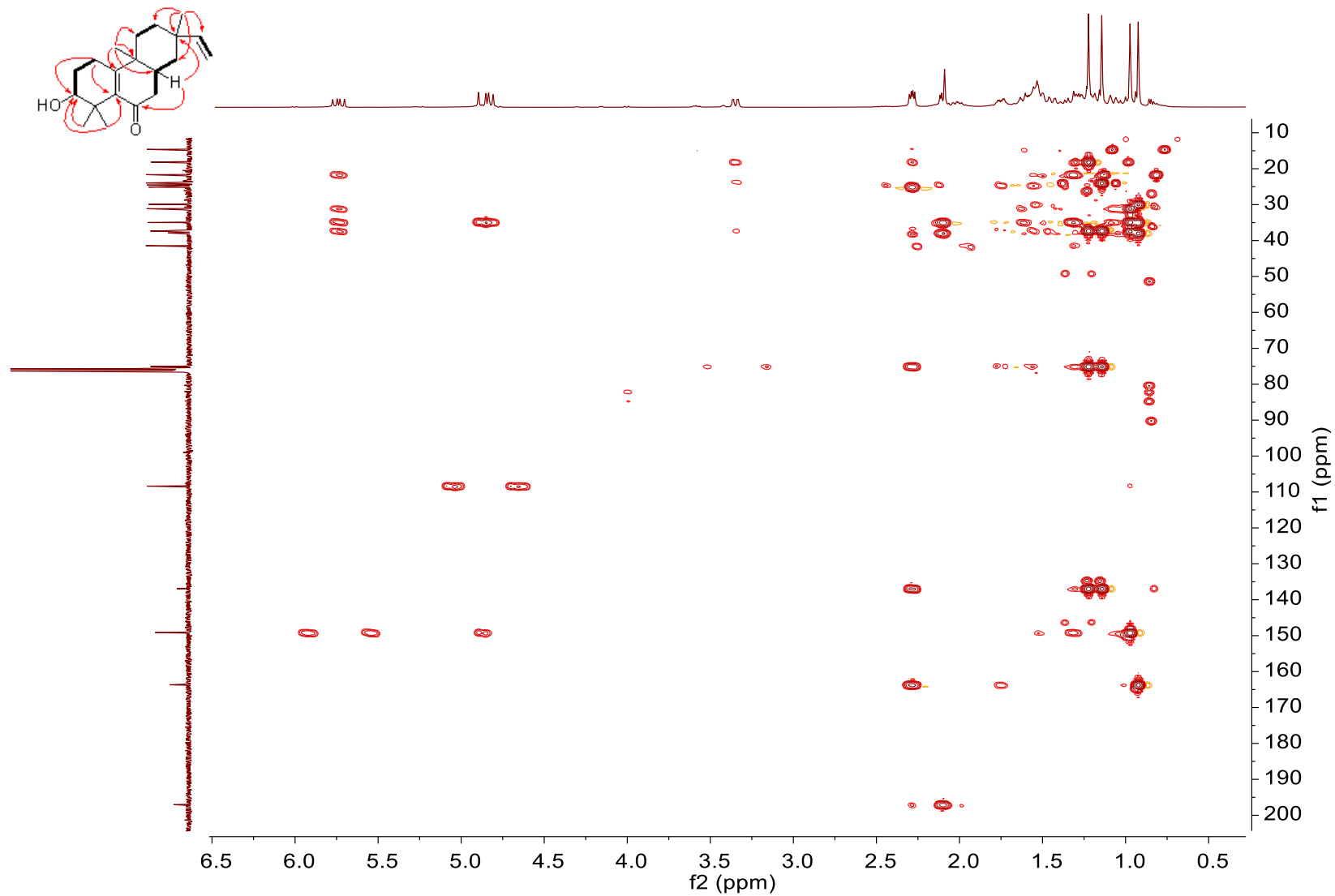
**Figure S44.** The  $^{13}\text{C}$  NMR Spectrum of Compound **6** in  $\text{CDCl}_3$



**Figure S45.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **6** in  $\text{CDCl}_3$

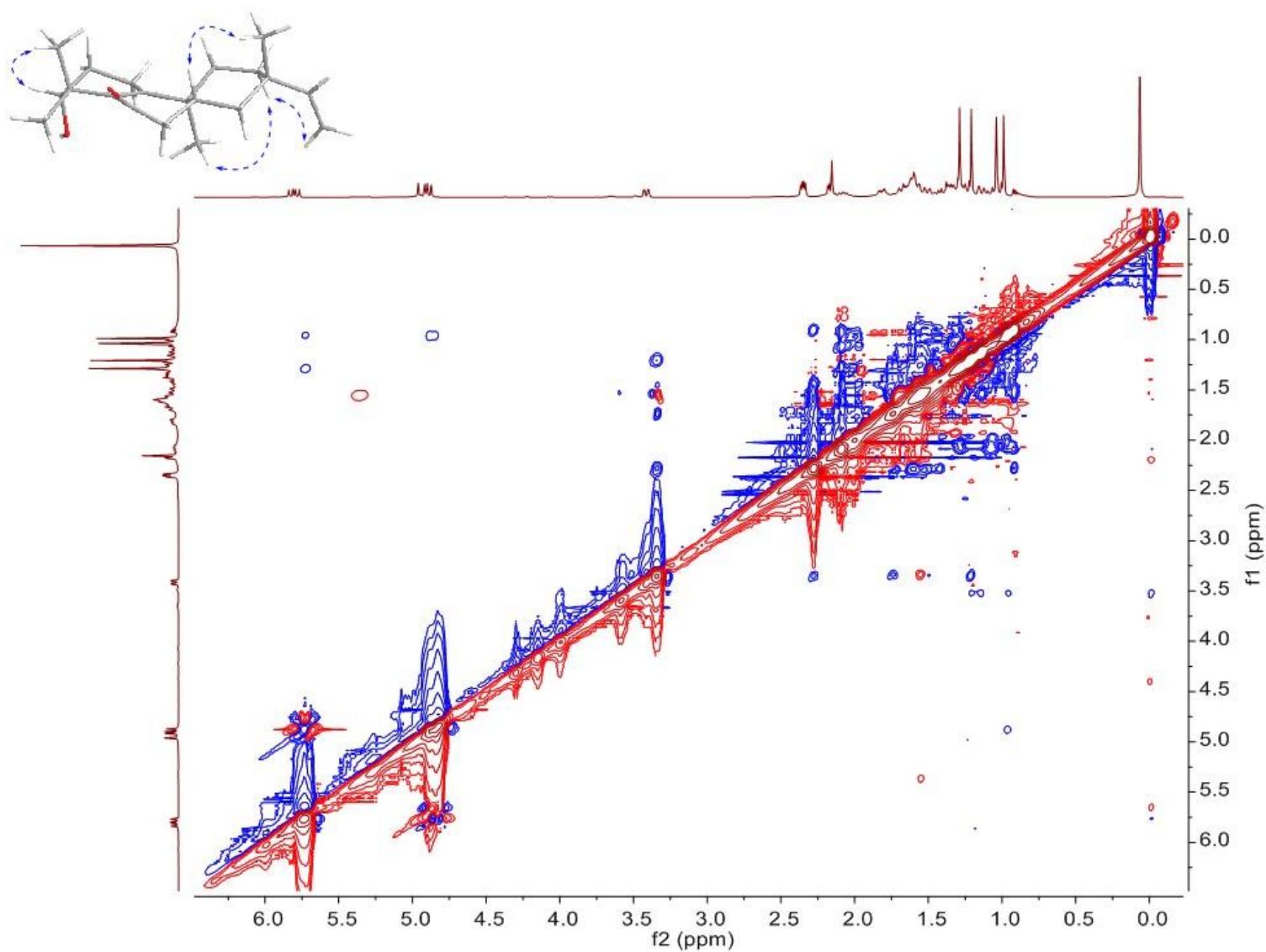


**Figure S46.** The HSQC Spectrum of Compound **6** in CDCl<sub>3</sub>

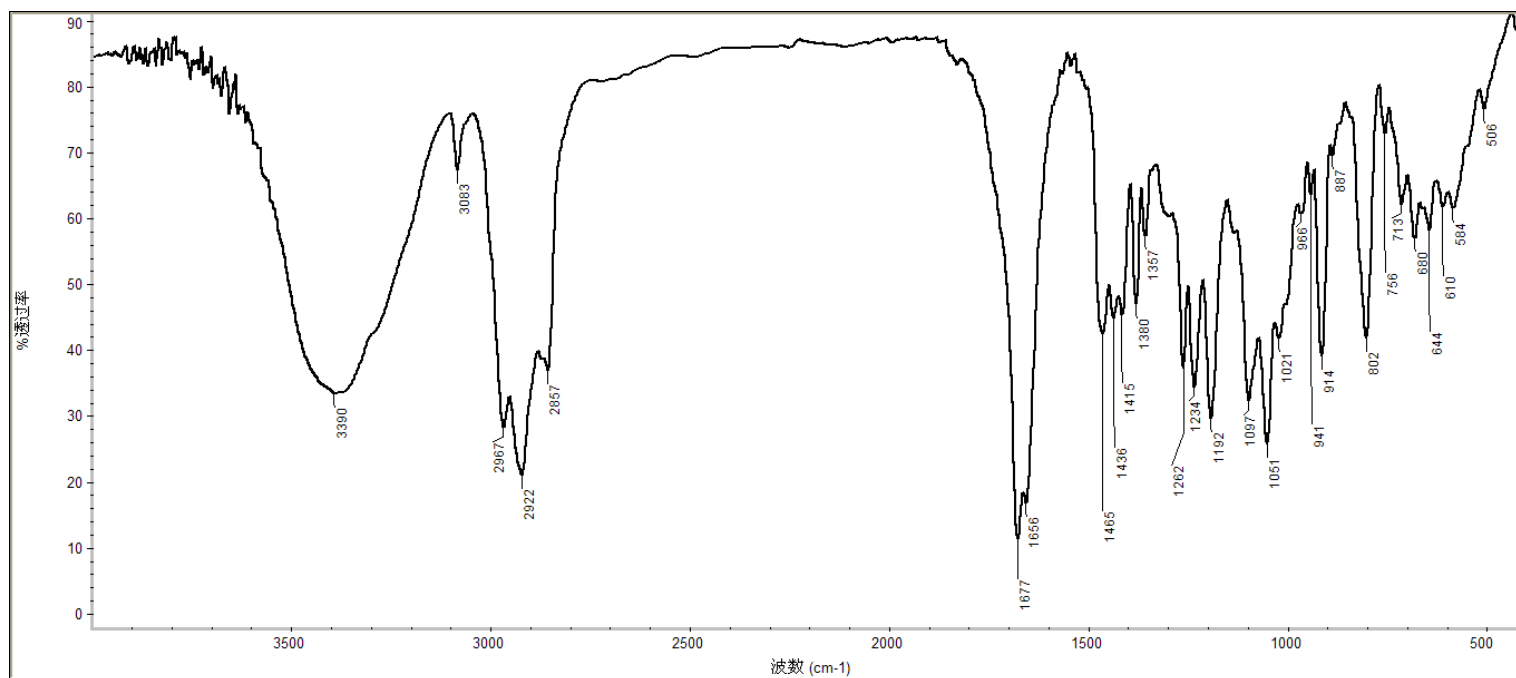


**Figure S47.** The HMBC Spectrum of Compound **6** in  $\text{CDCl}_3$

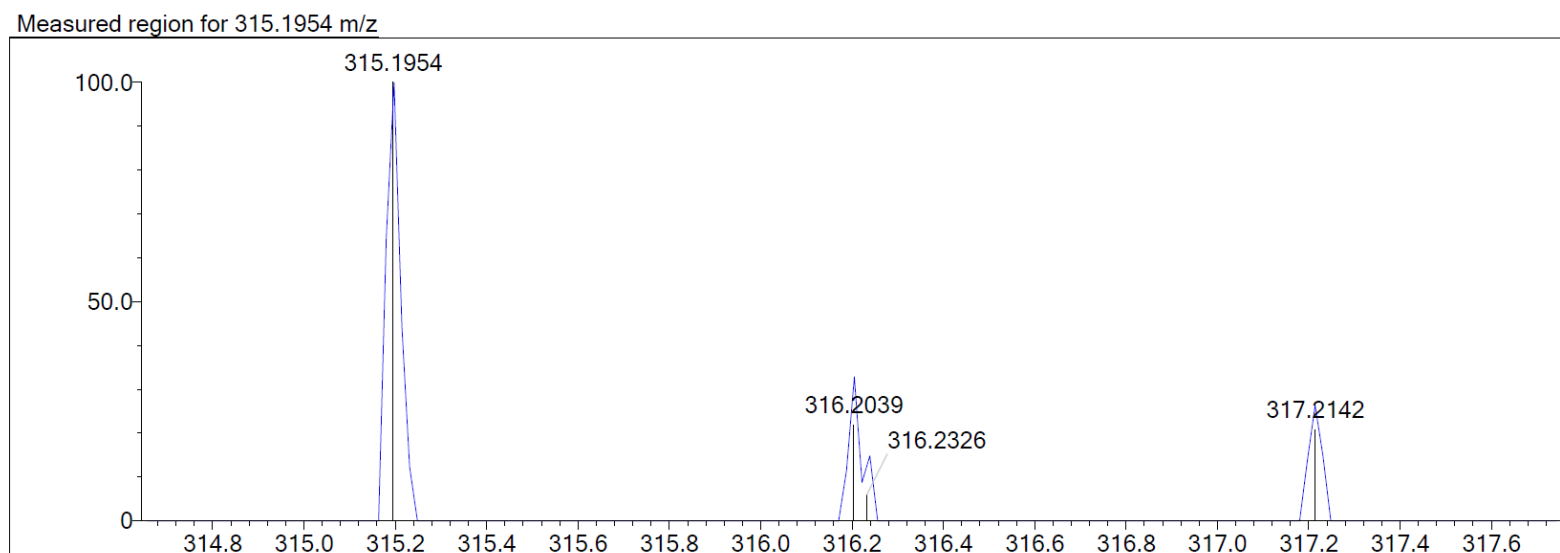




**Figure S48.** The NOESY Spectrum of Compound **6** in CDCl<sub>3</sub>



**Figure S49.** The IR Spectra of Compound **7**




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SPECTRUM -

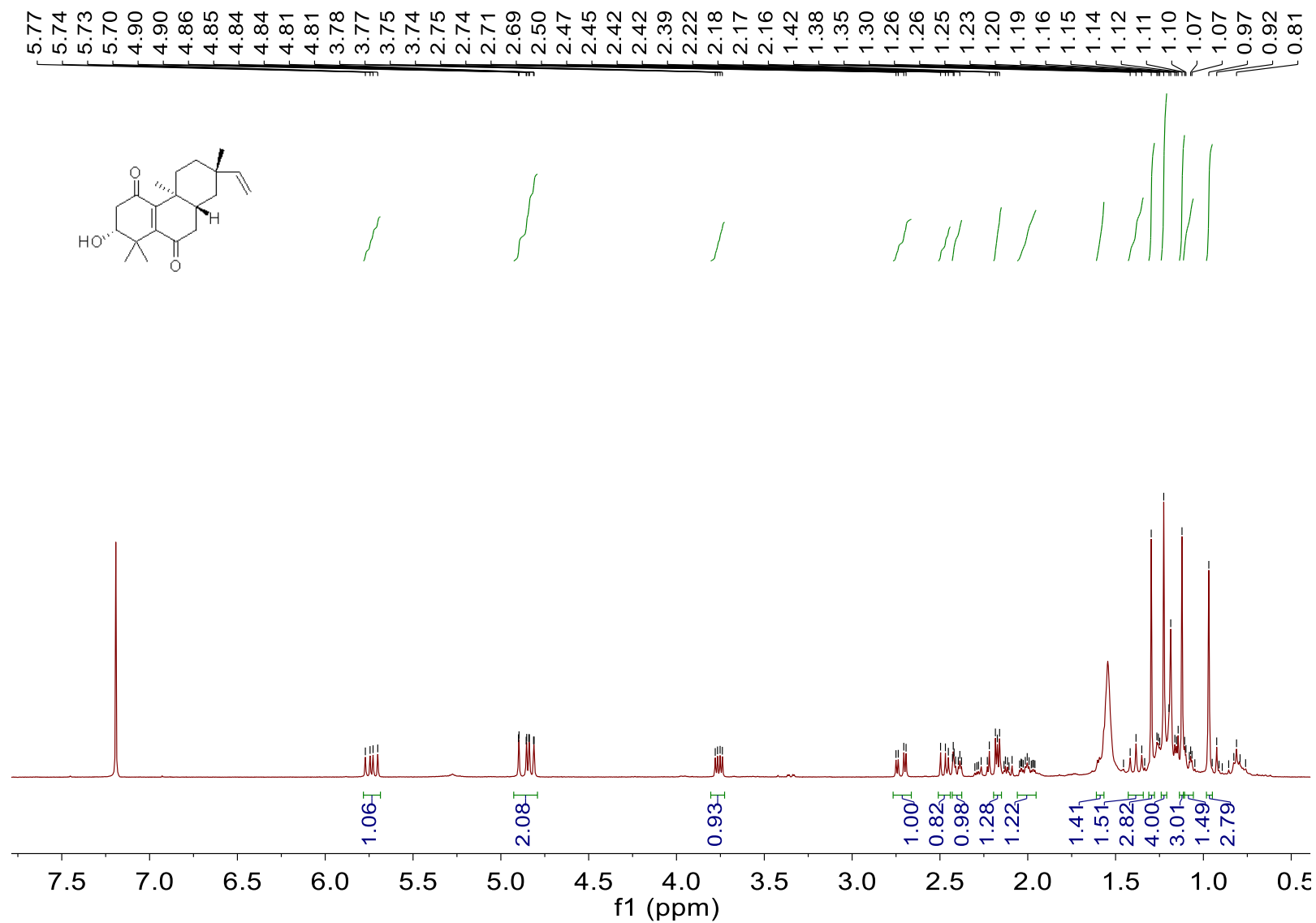
simulation :

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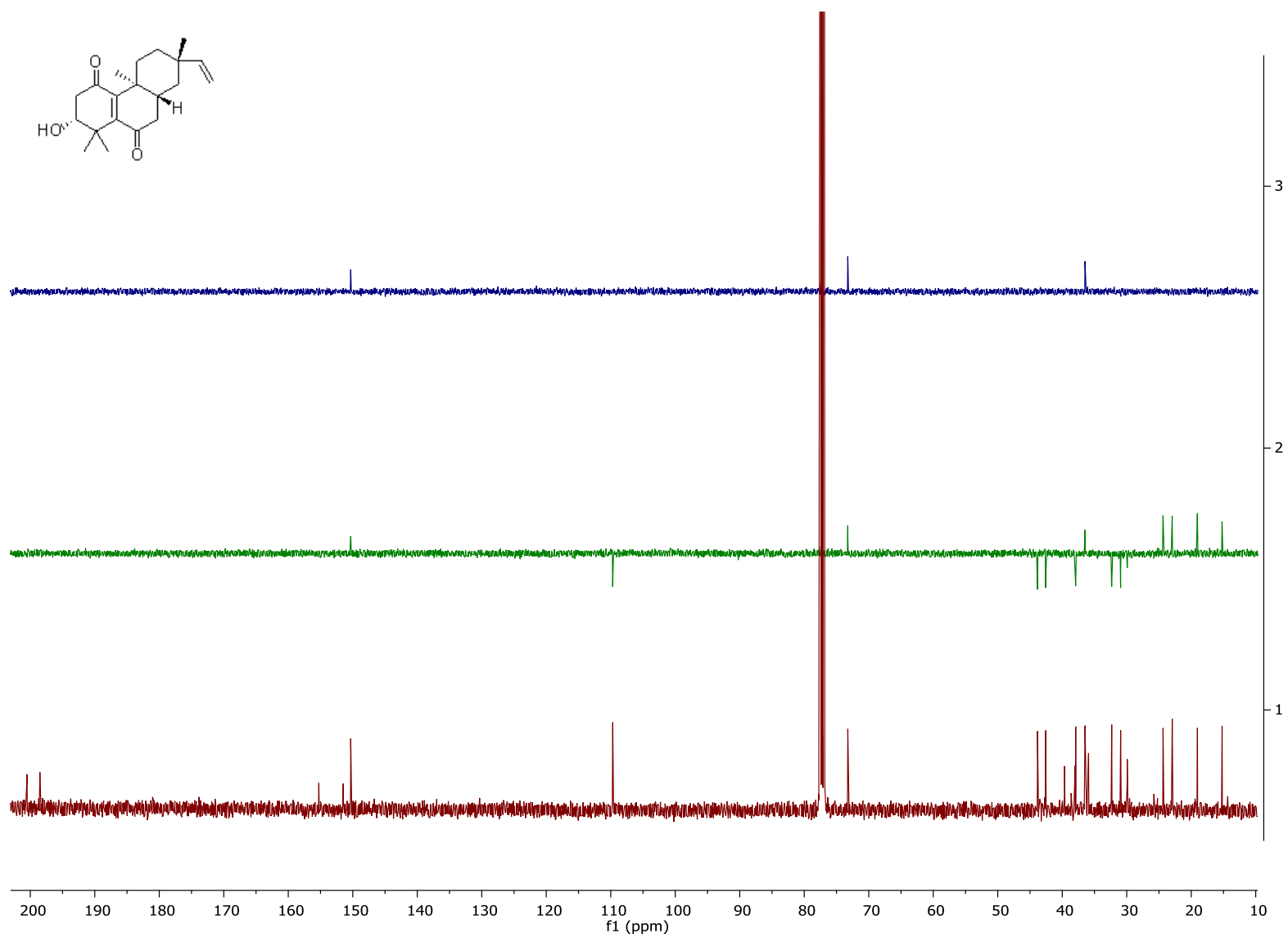
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
315.1954	315.1966	-3.81	7.0	C <sub>20</sub> H <sub>27</sub> O <sub>3</sub>

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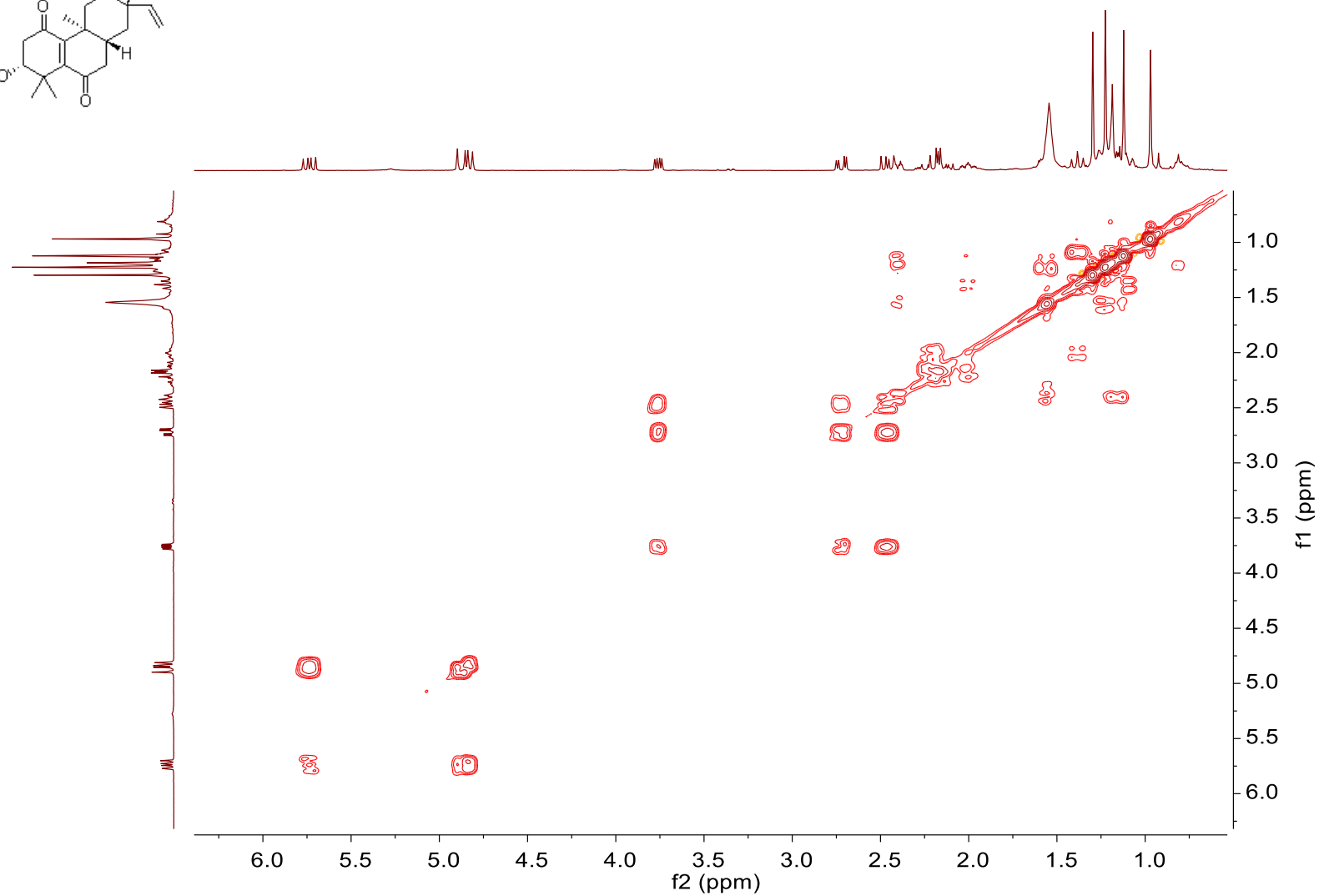
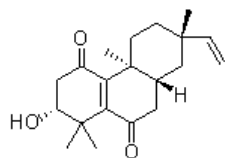
**Figure S50.** The HRESIMS Spectroscopic Data of Compound **7**



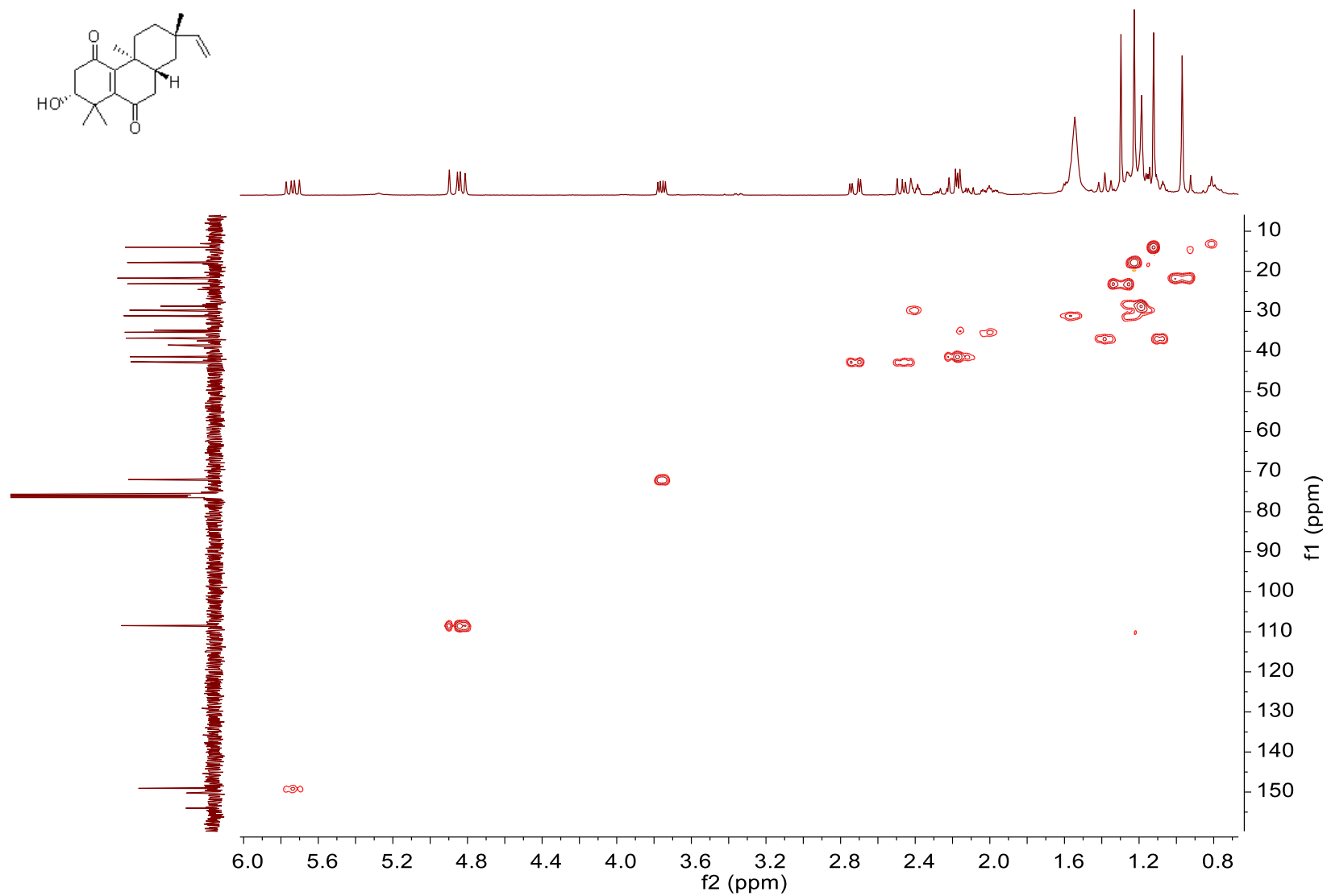
**Figure S51.** The <sup>1</sup>H NMR Spectrum of Compound **7** in CDCl<sub>3</sub>



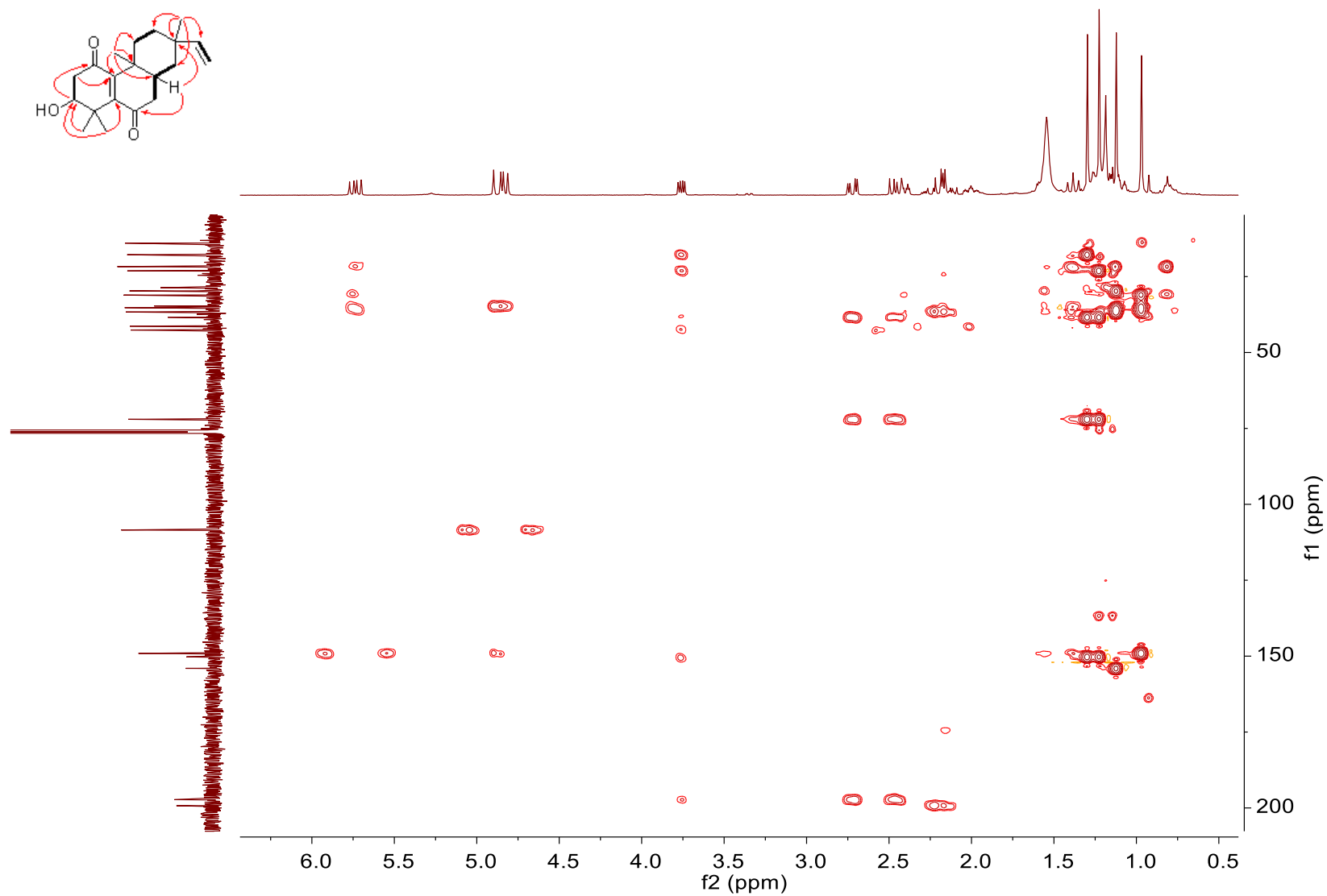
**Figure S52.** The  $^{13}\text{C}$  NMR Spectrum of Compound **7** in  $\text{CDCl}_3$



**Figure S53.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound 7 in  $\text{CDCl}_3$

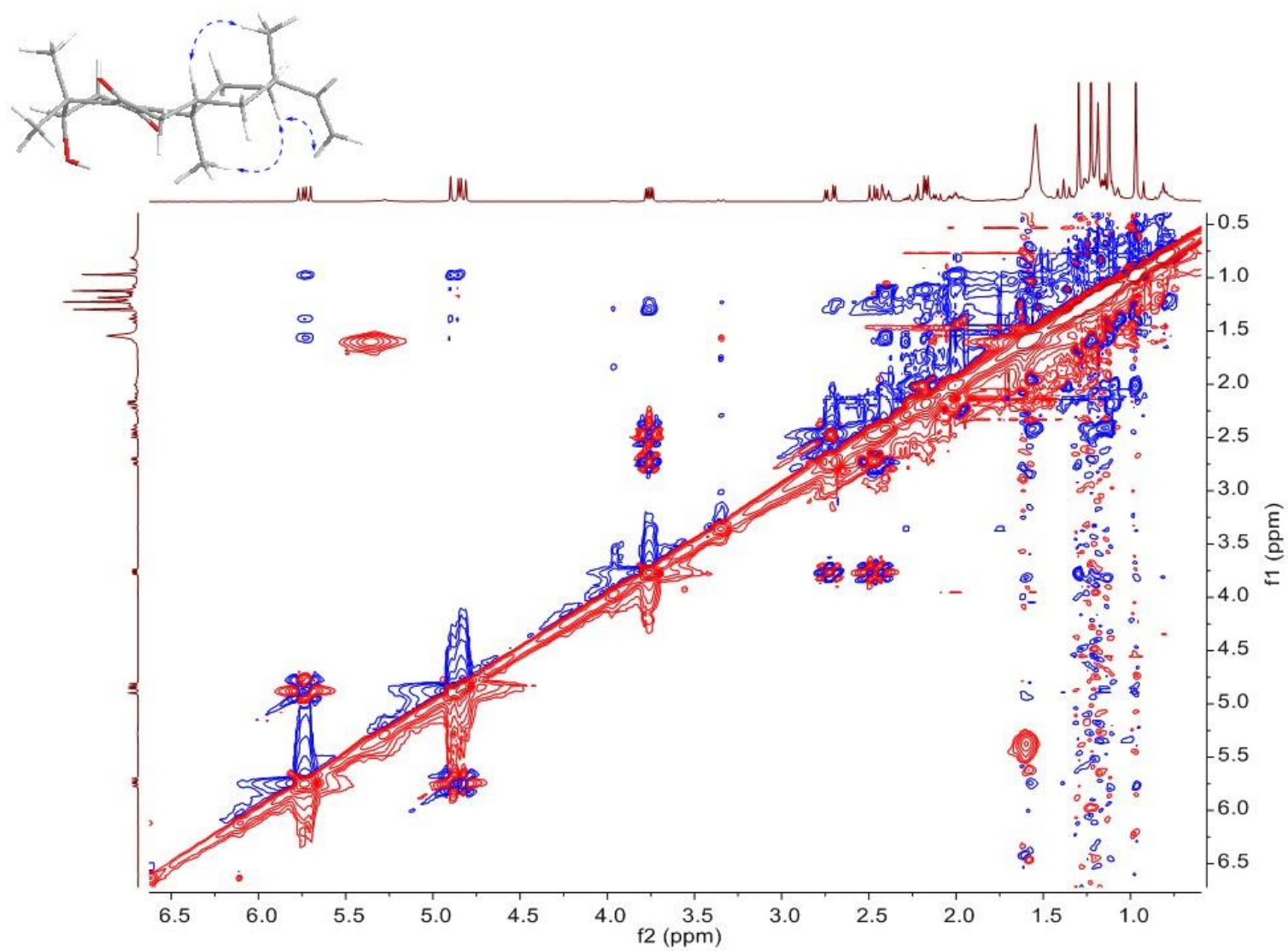


**Figure S54.** The HSQC Spectrum of Compound **7** in CDCl<sub>3</sub>

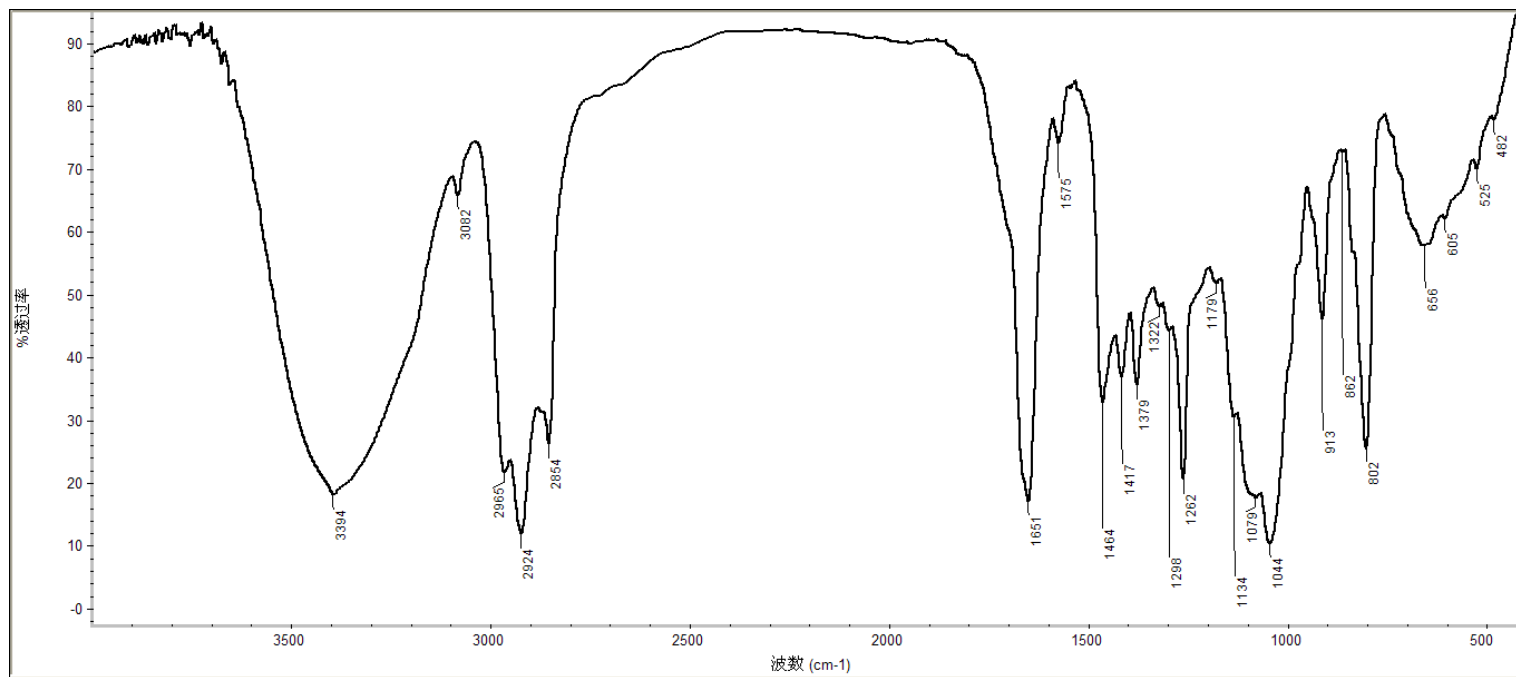


**Figure S55.** The HMBC Spectrum of Compound **7** in  $\text{CDCl}_3$

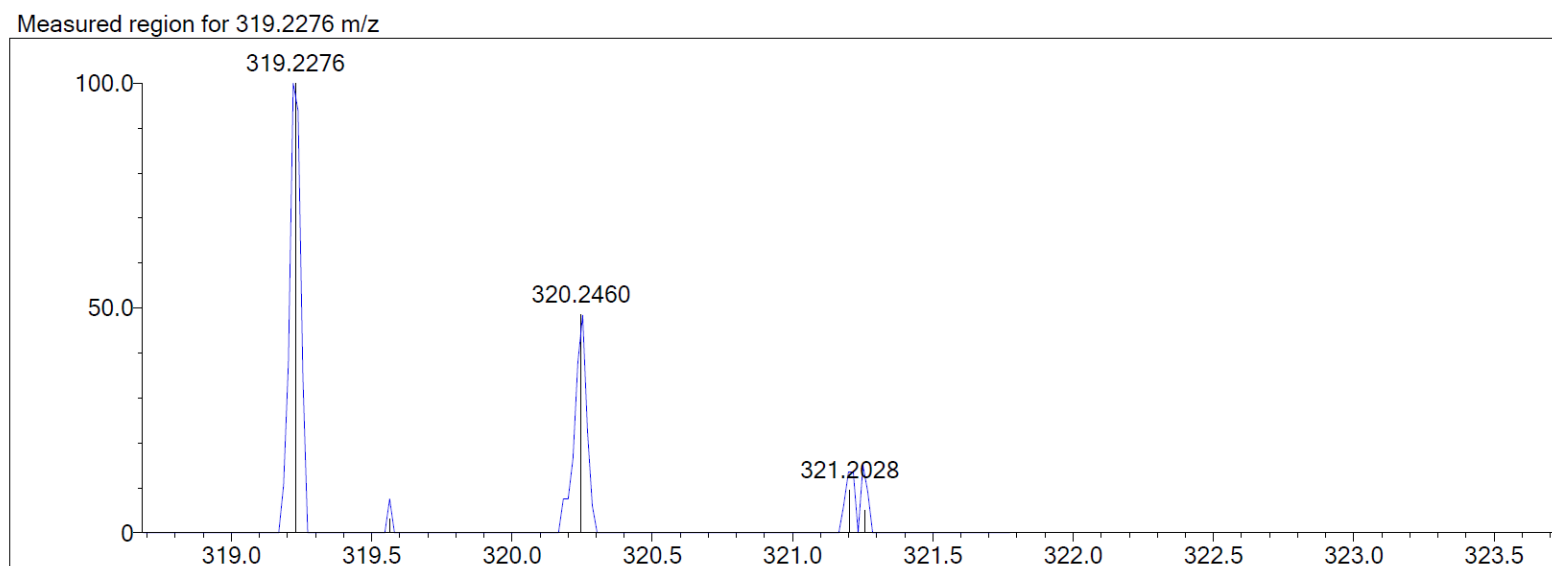




**Figure S56.** The NOESY Spectrum of Compound **7** in CDCl<sub>3</sub>



**Figure S57.** The IR Spectra of Compound **8**

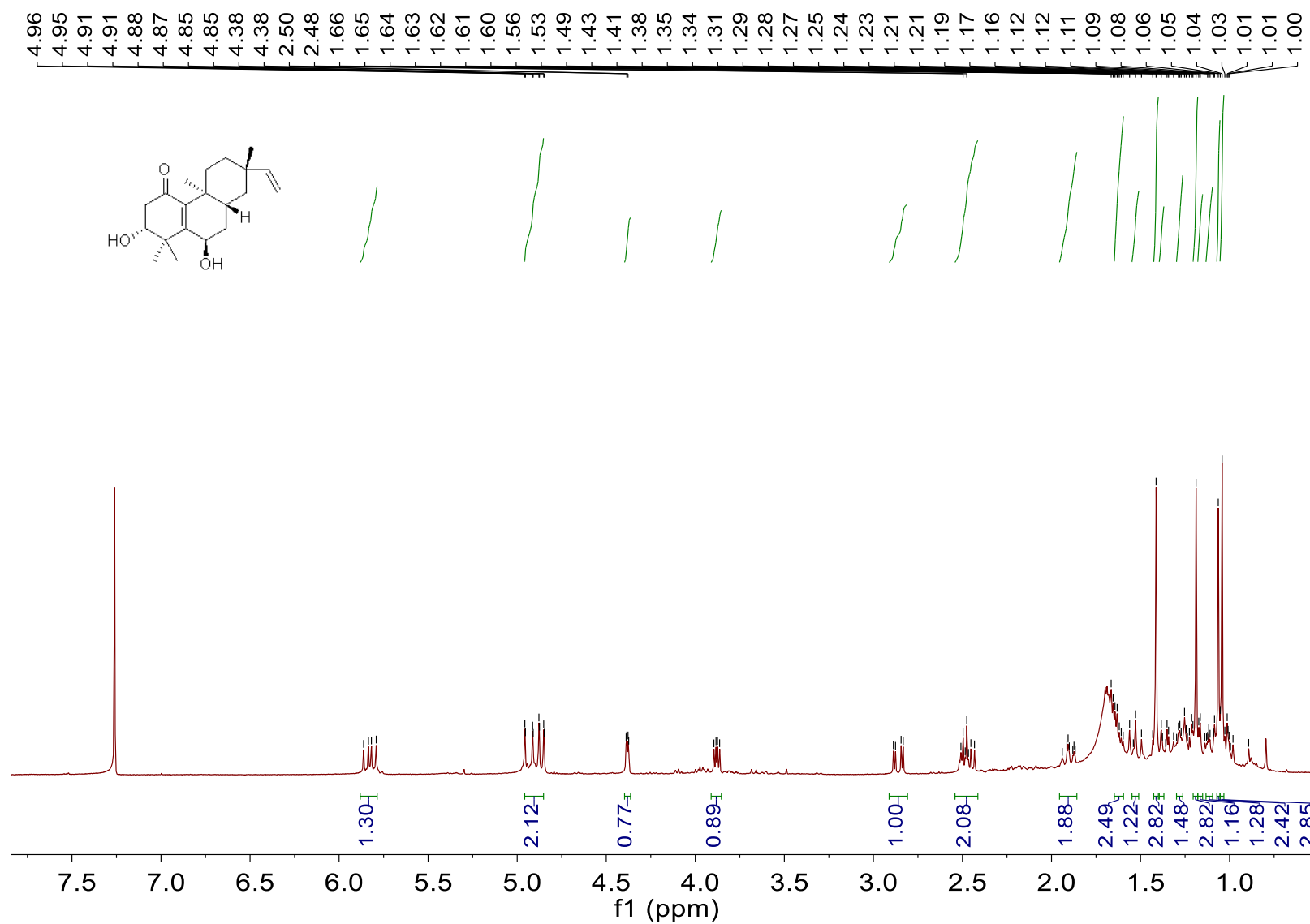


SPECTRUM -

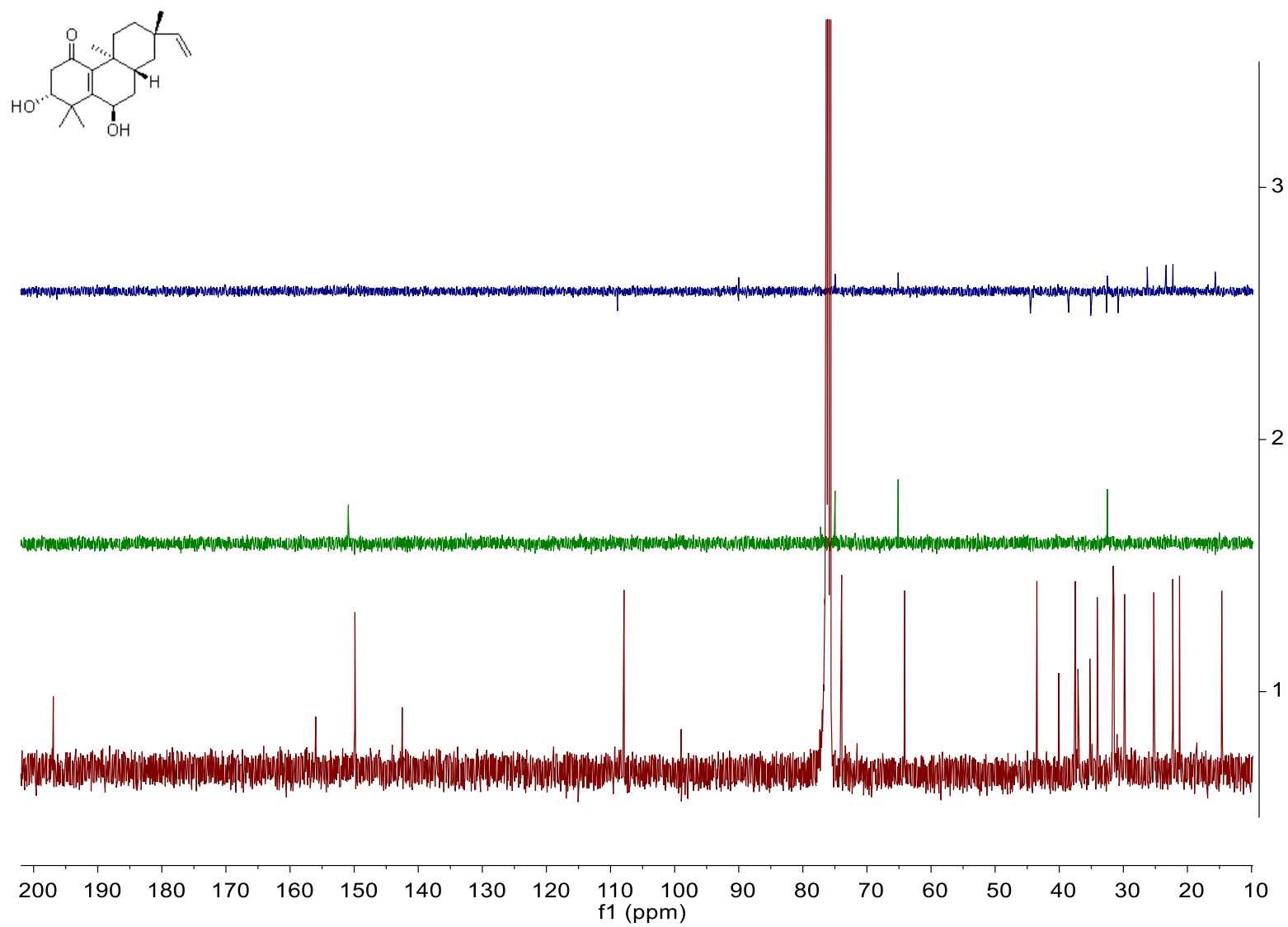
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
319.2276	319.2268	2.51	6.0	C <sub>20</sub> H <sub>31</sub> O <sub>3</sub>

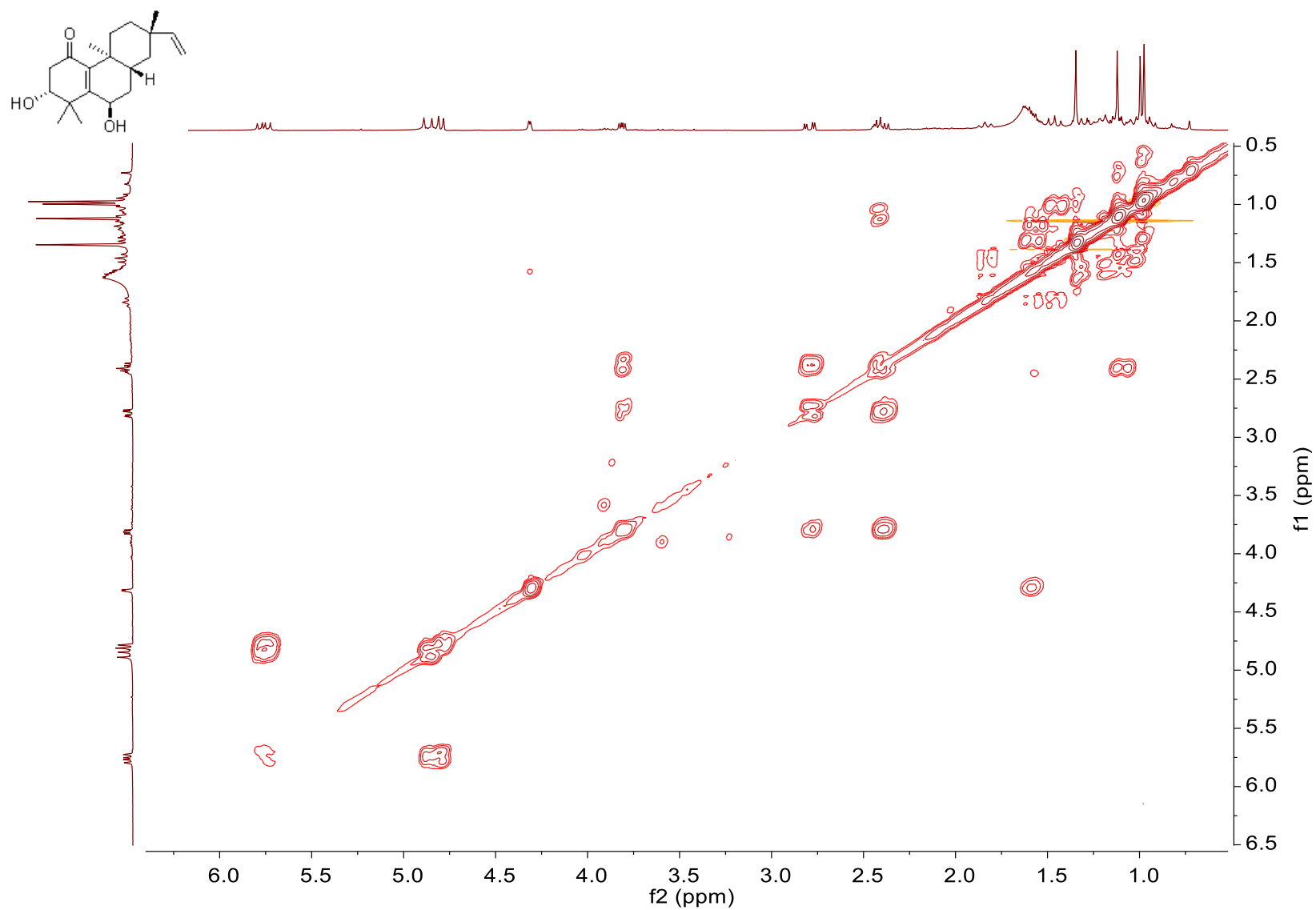
**Figure S58.** The HRESIMS Spectroscopic Data of Compound **8**



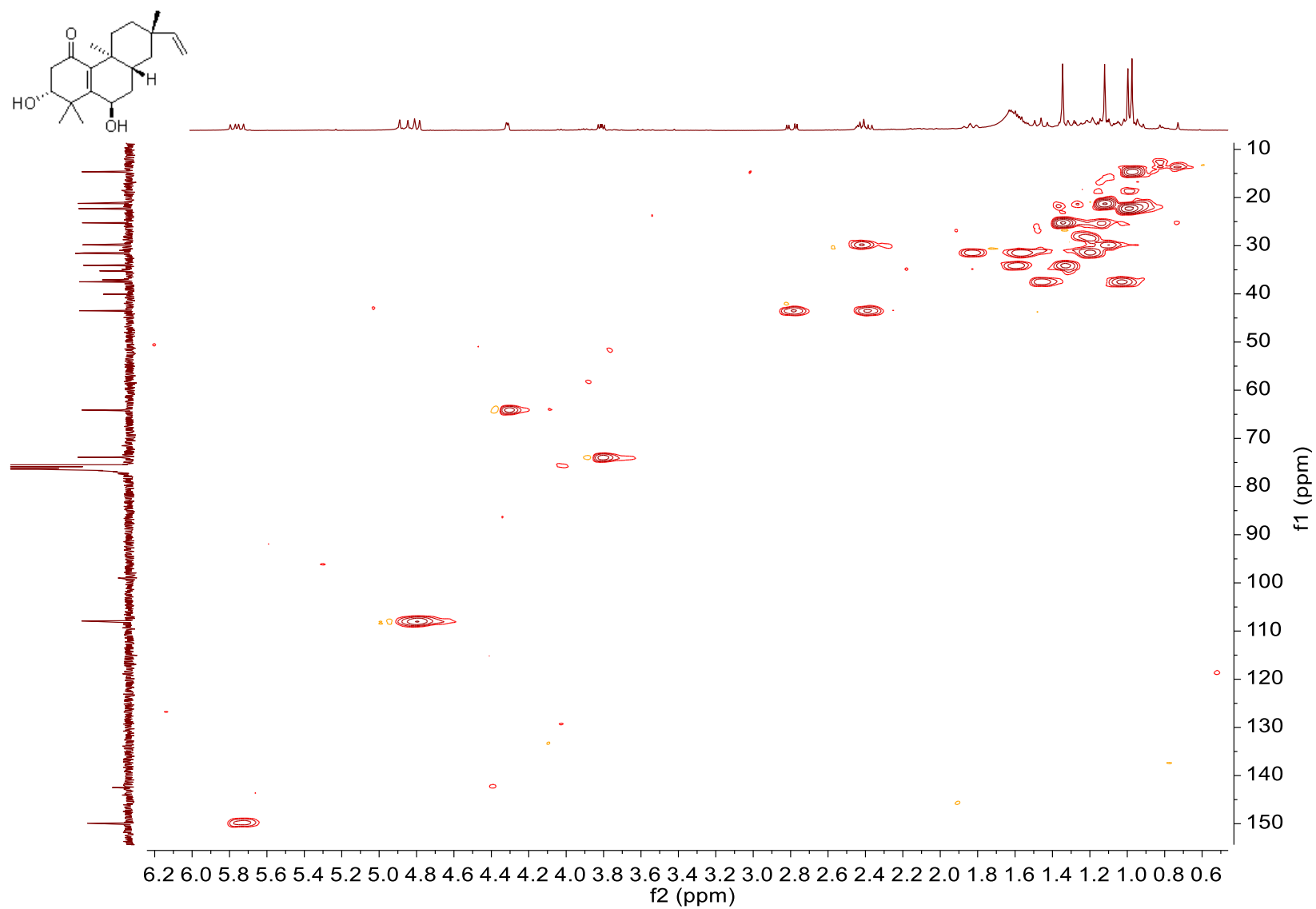
**Figure S59.** The <sup>1</sup>H NMR Spectrum of Compound **8** in CDCl<sub>3</sub>



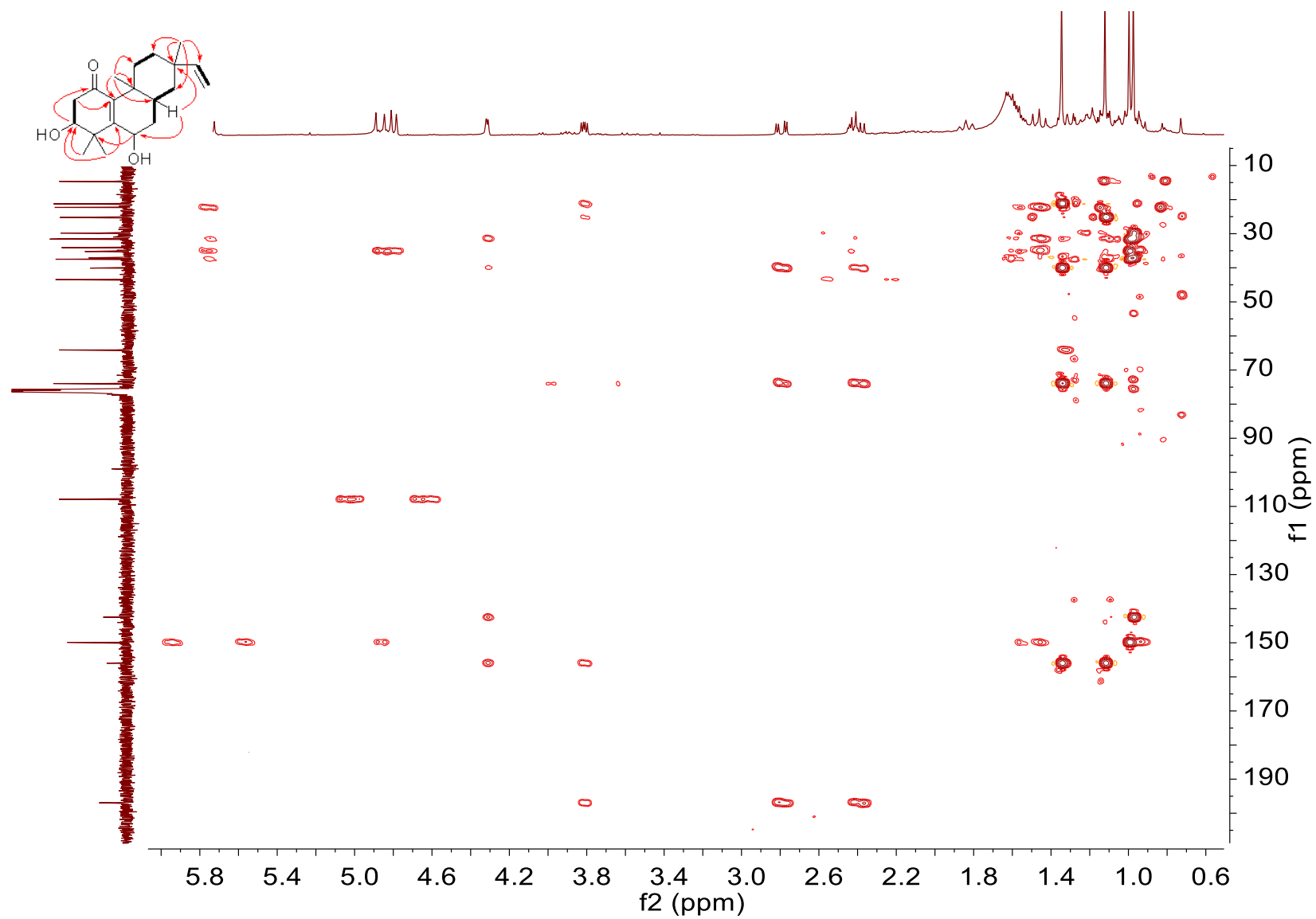
**Figure S60.** The  $^{13}\text{C}$  NMR Spectrum of Compound **8** in  $\text{CDCl}_3$



**Figure S61.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **8** in  $\text{CDCl}_3$

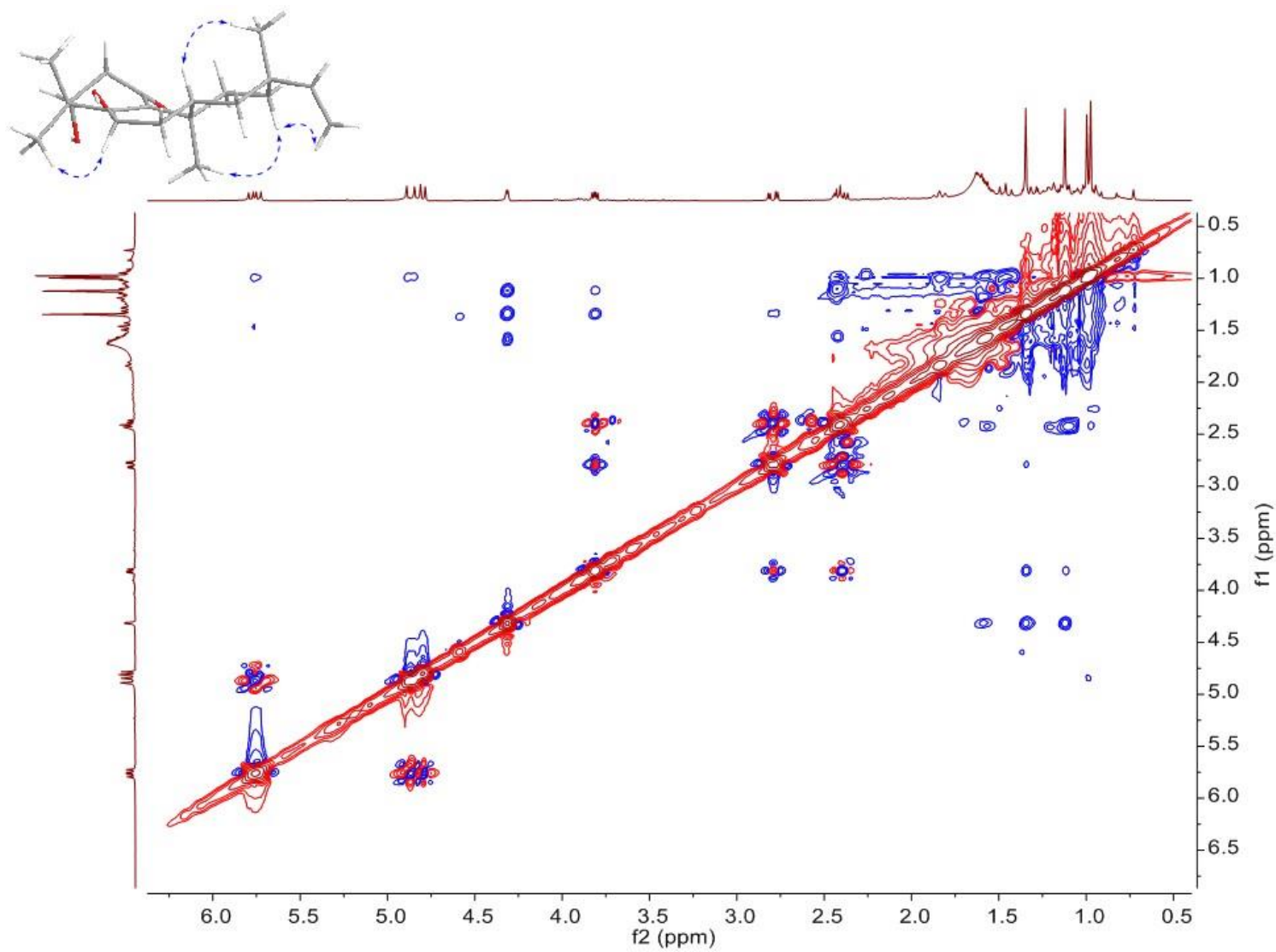


**Figure S62.** The HSQC Spectrum of Compound **8** in CDCl<sub>3</sub>

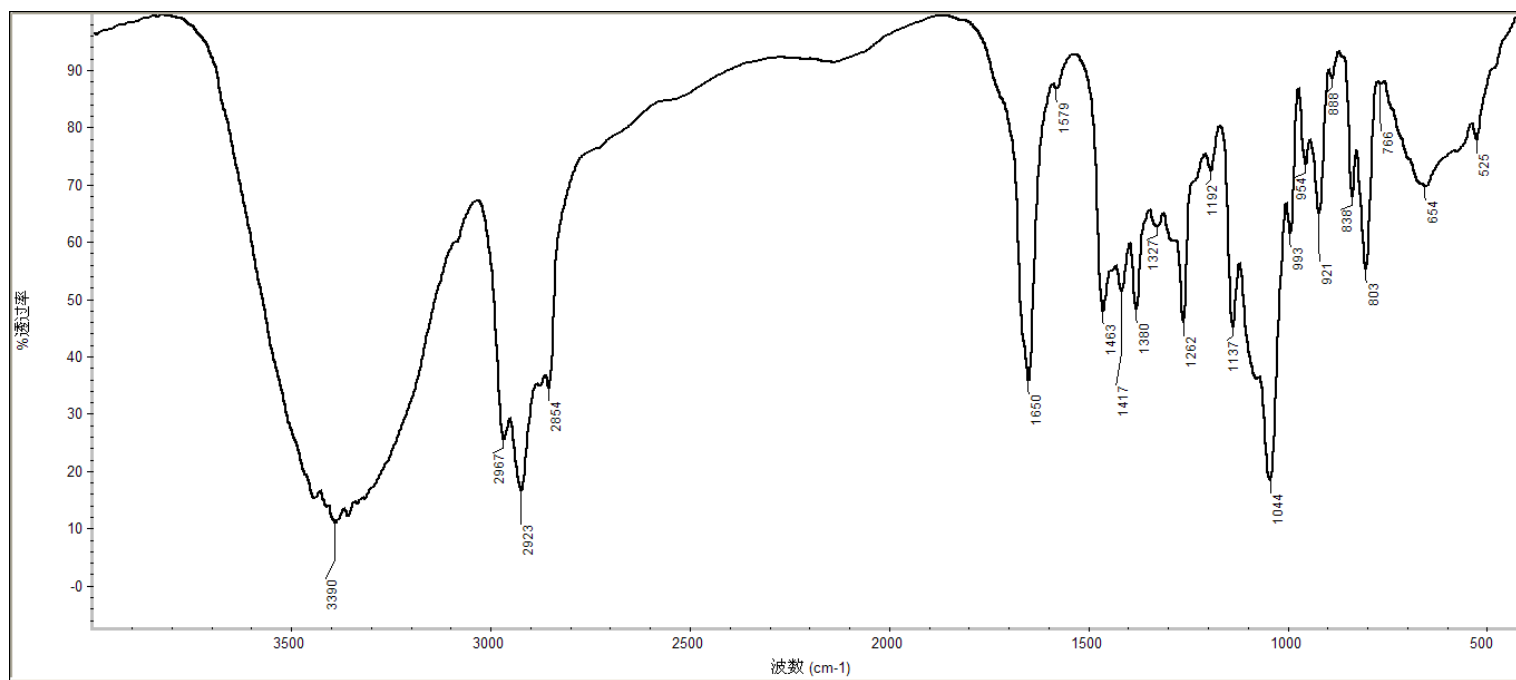


**Figure S63.** The HMBC Spectrum of Compound **8** in CDCl<sub>3</sub>

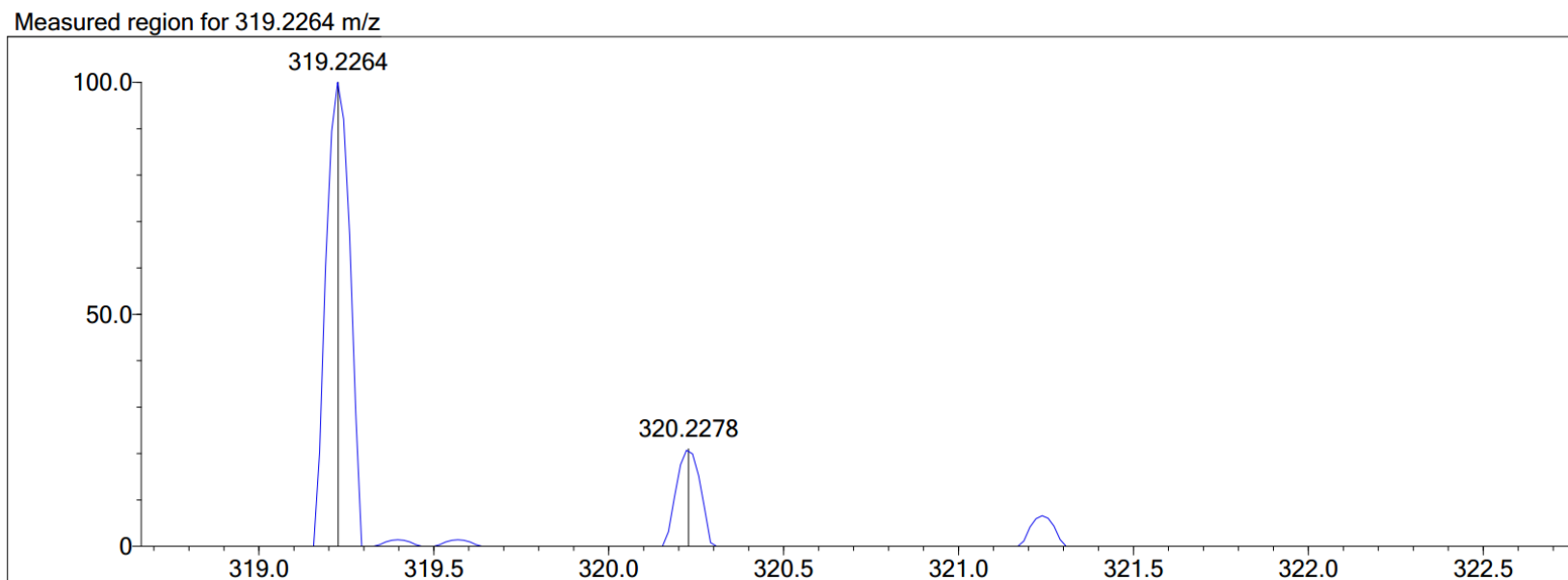




**Figure S64.** The NOESY Spectrum of Compound **8** in CDCl<sub>3</sub>



**Figure S65.** The IR Spectra of Compound **9**

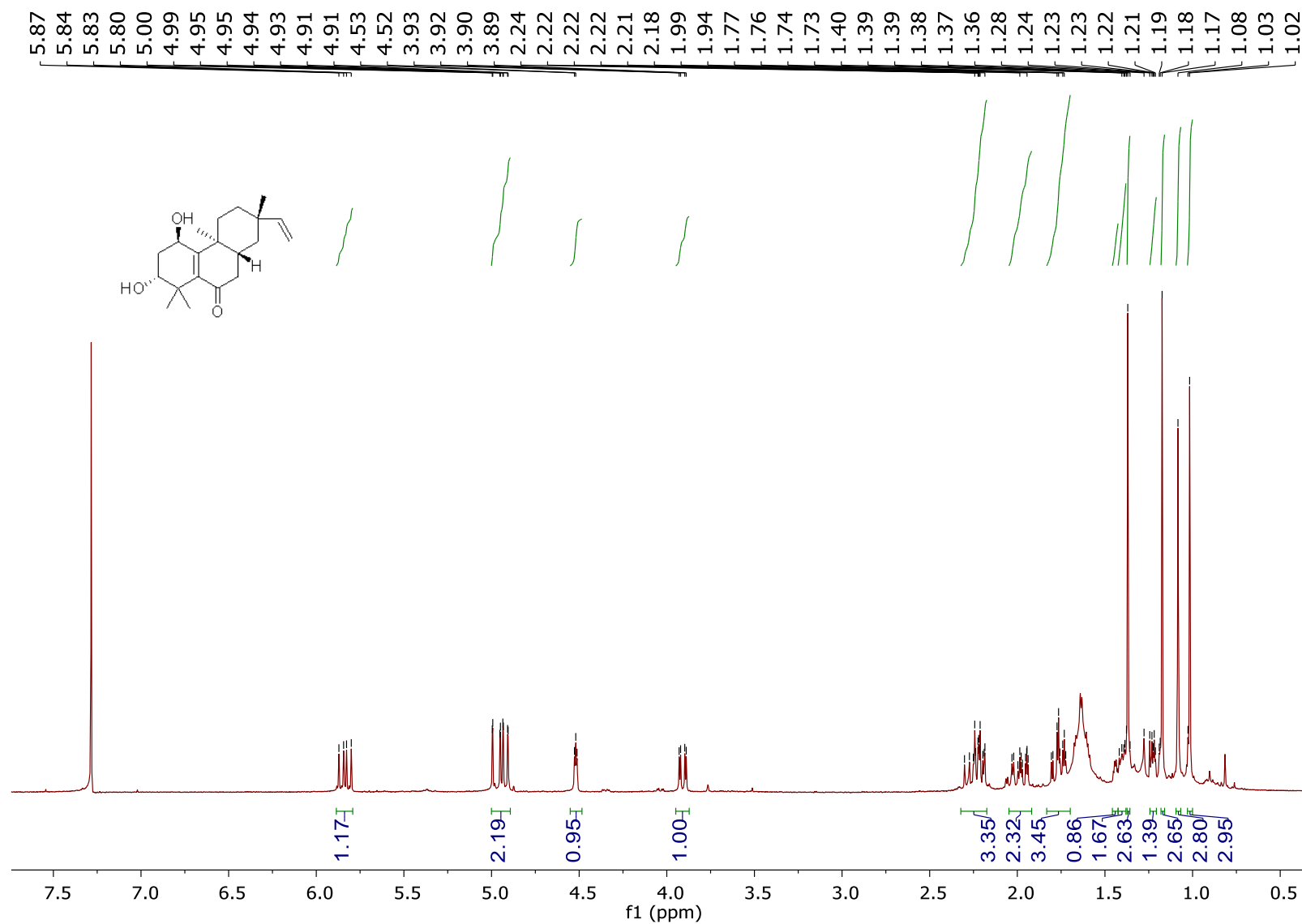


SPECTRUM -

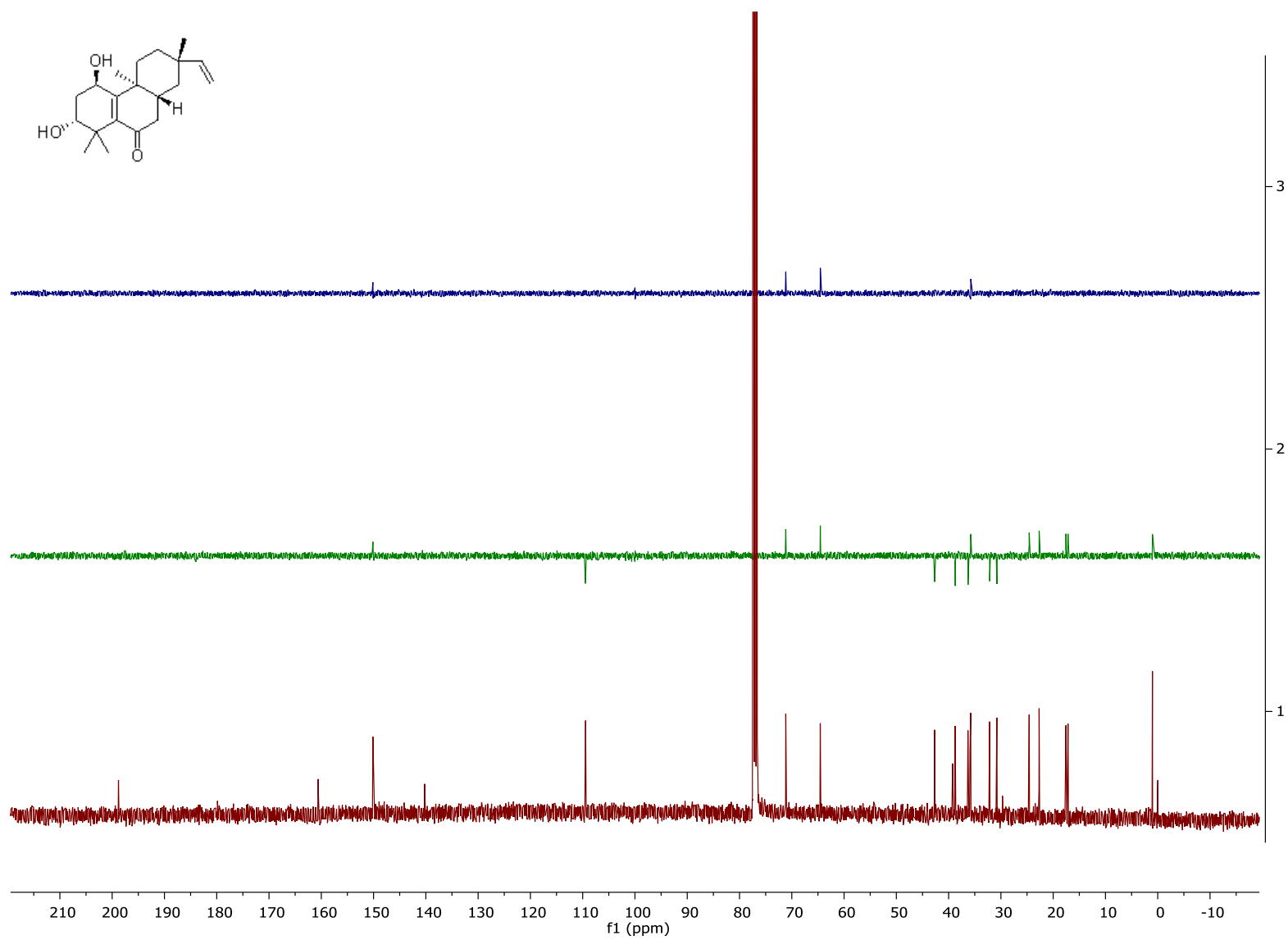
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
319.2264	319.2268	-1.25	6.0	C <sub>20</sub> H <sub>30</sub> O <sub>3</sub>

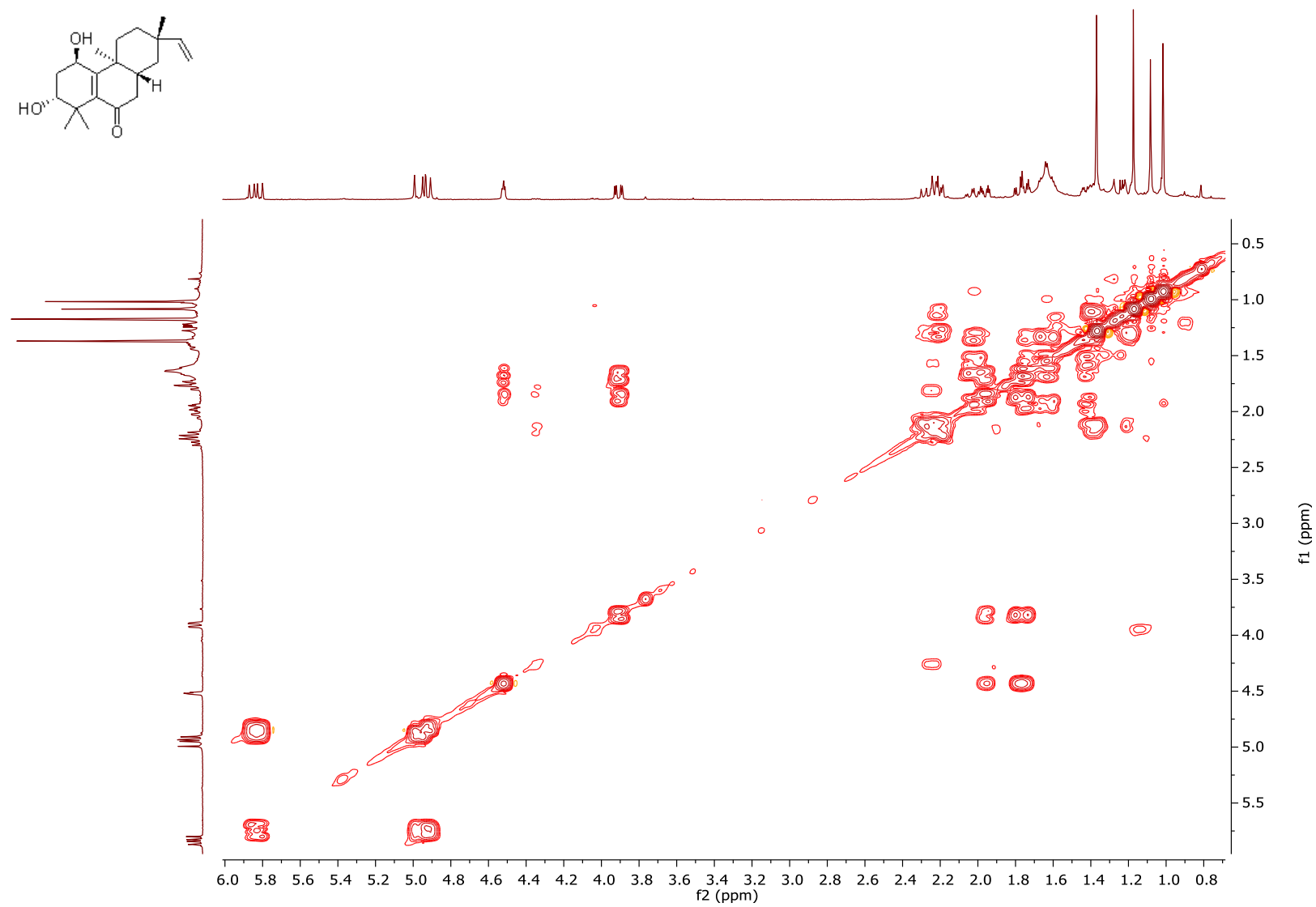
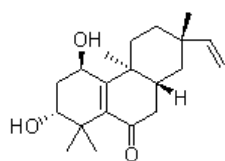
**Figure S66.** The HRESIMS Spectroscopic Data of Compound **9**



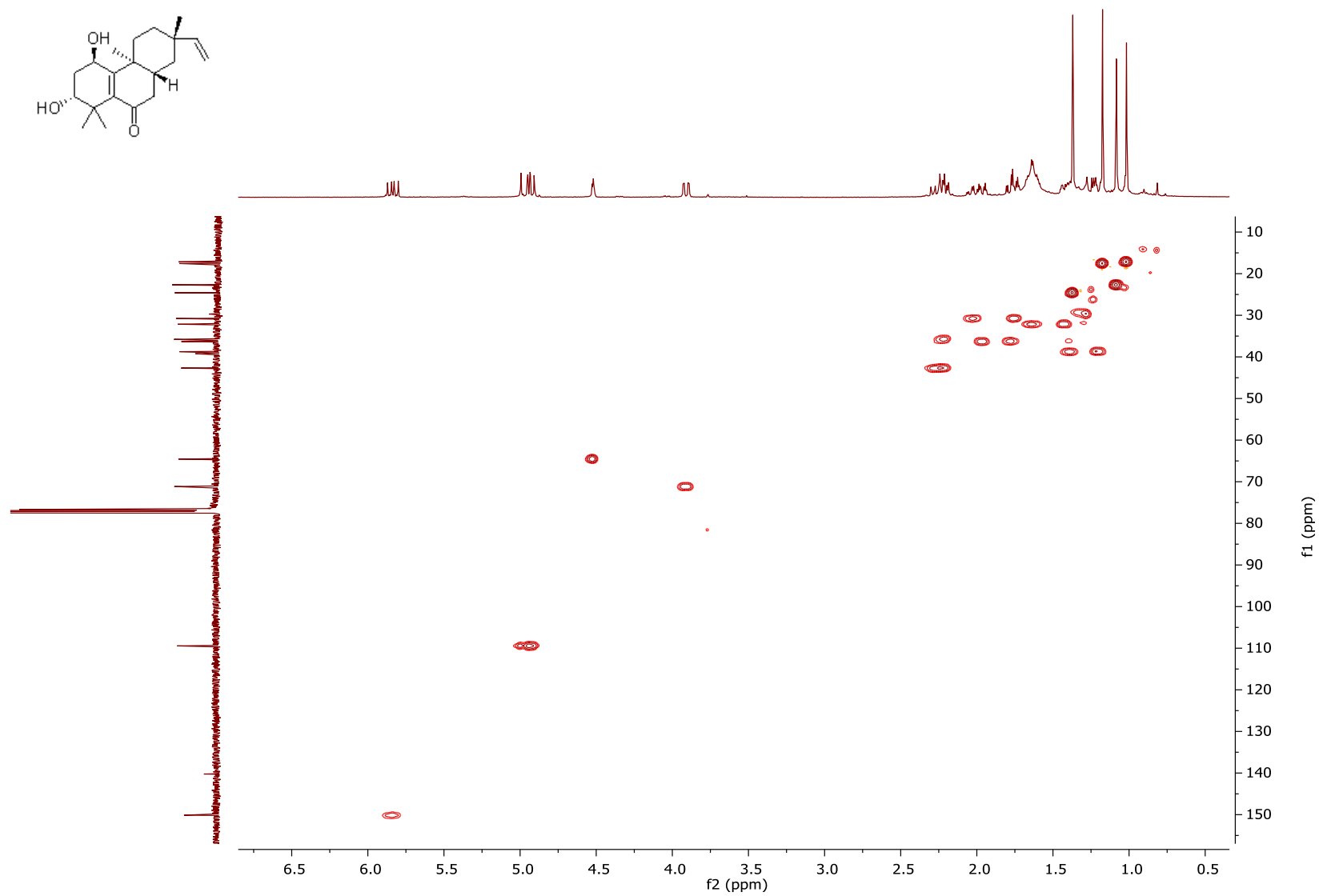
**Figure S67.** The <sup>1</sup>H NMR Spectrum of Compound **9** in CDCl<sub>3</sub>



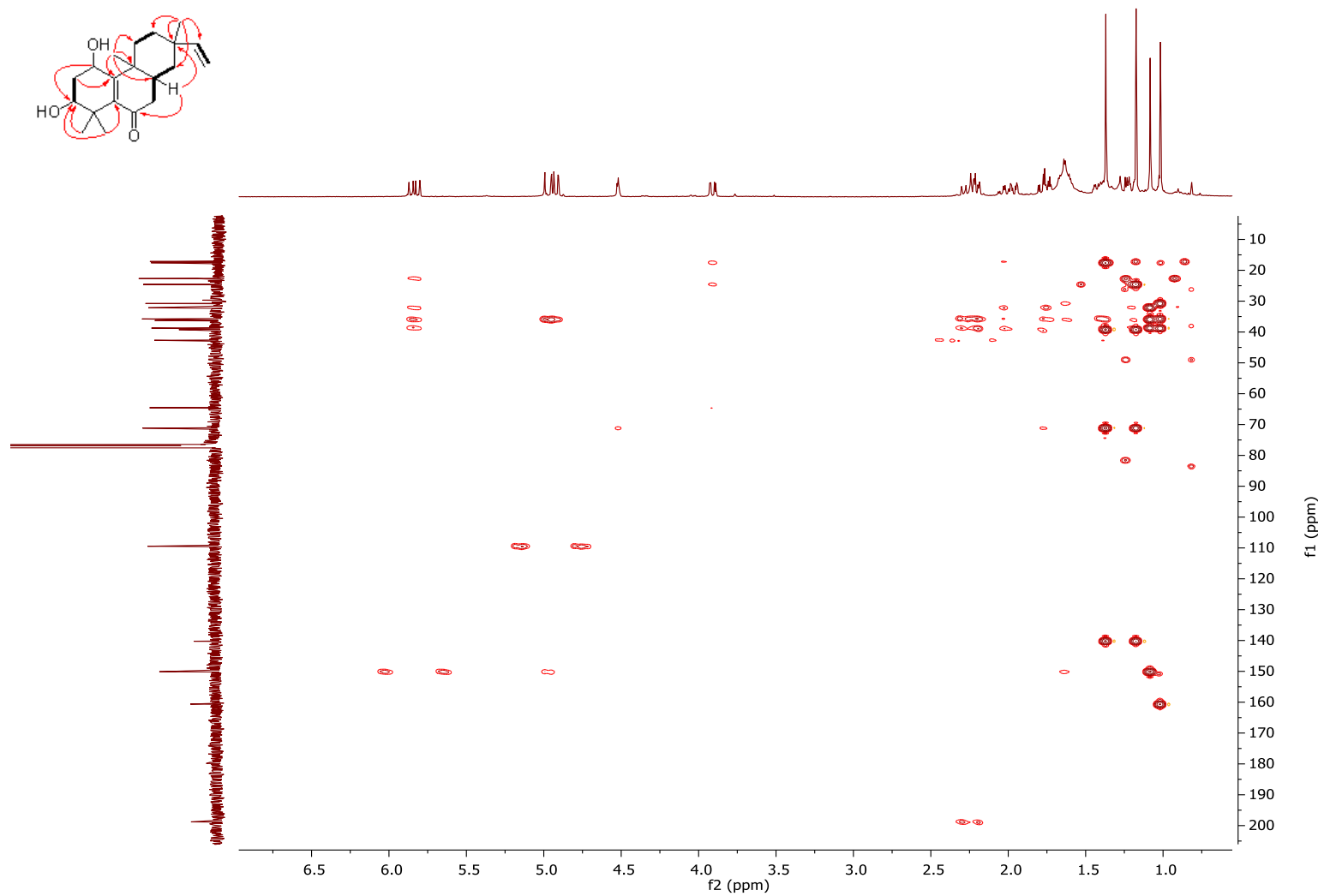
**Figure S68.** The  $^{13}\text{C}$  NMR Spectrum of Compound **9** in  $\text{CDCl}_3$



**Figure S69.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **9** in  $\text{CDCl}_3$

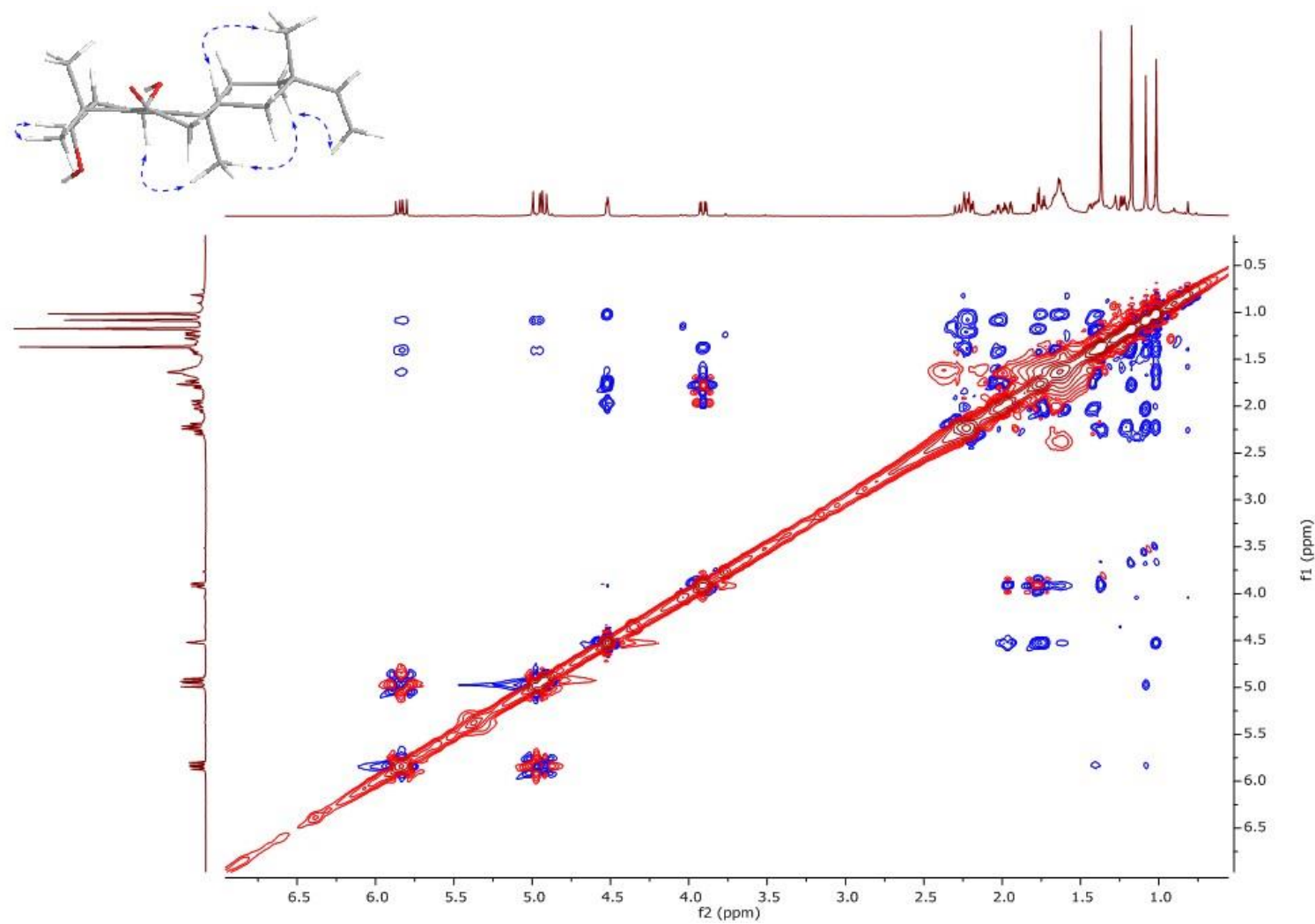


**Figure S70.** The HSQC Spectrum of Compound **9** in CDCl<sub>3</sub>

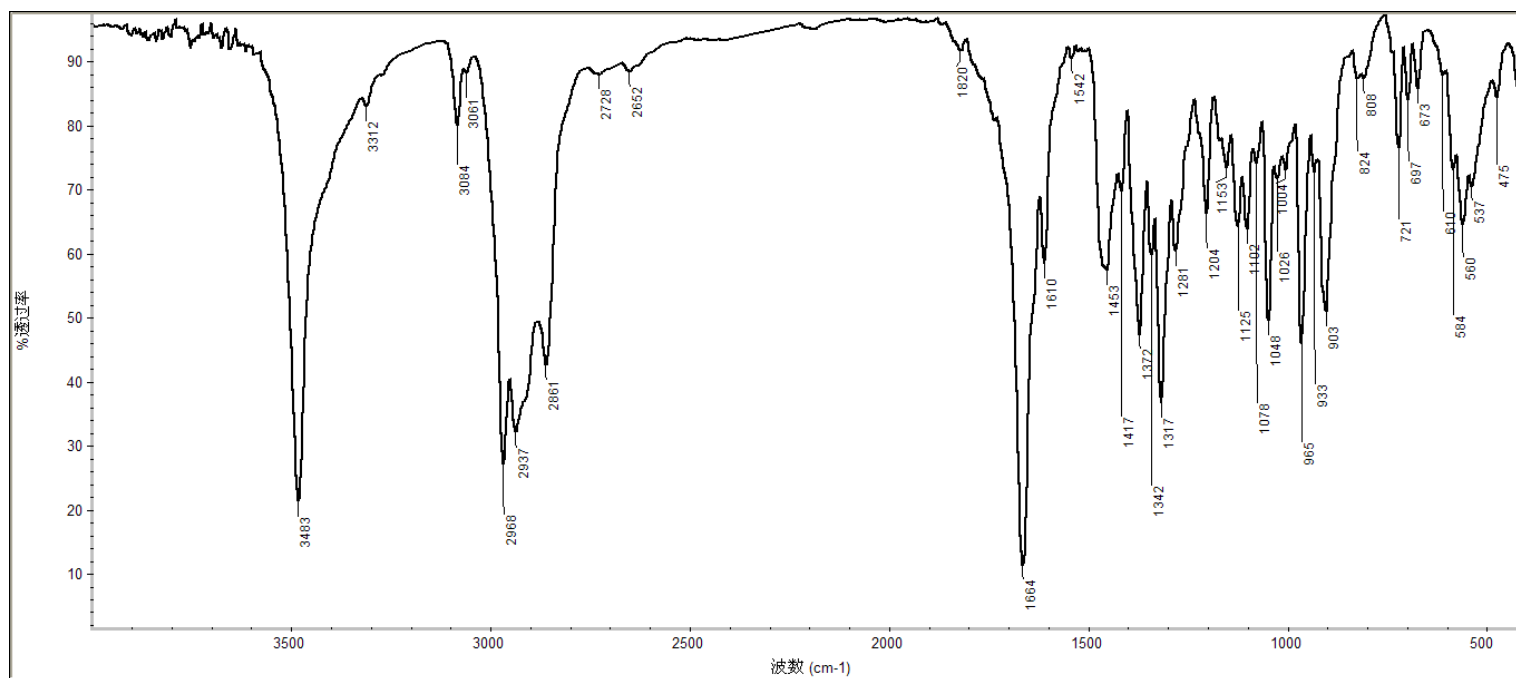


**Figure S71.** The HMBC Spectrum of Compound **9** in CDCl<sub>3</sub>

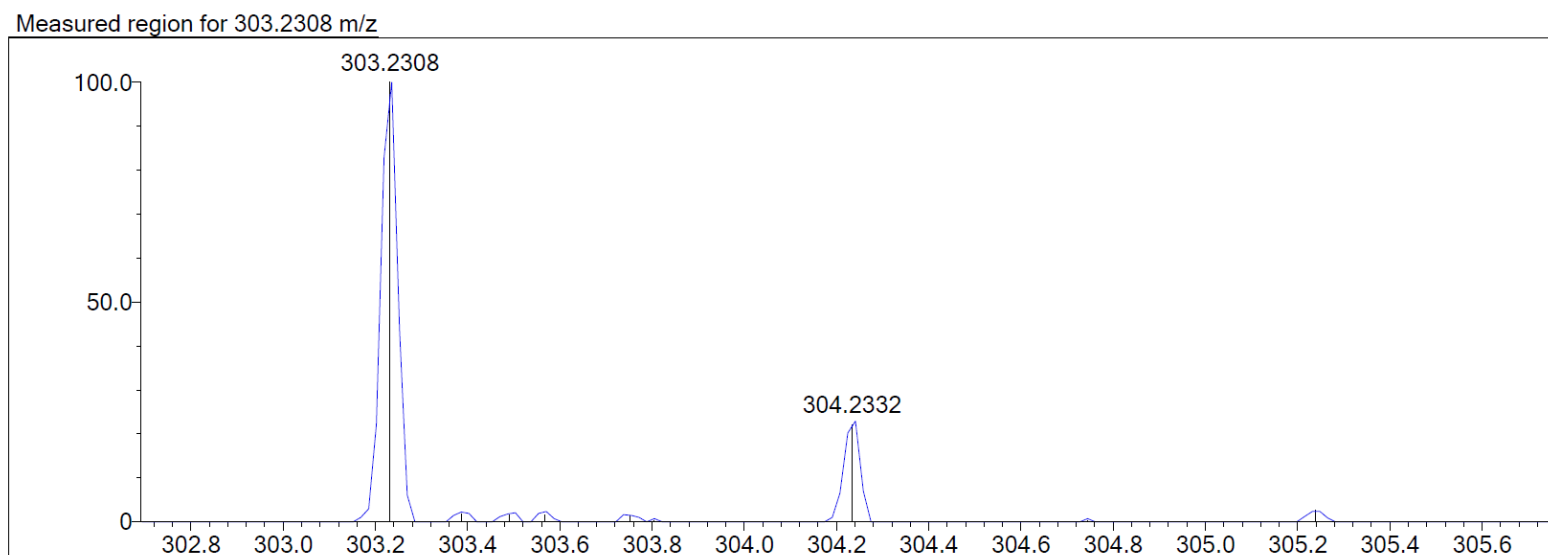




**Figure S72.** The NOESY Spectrum of Compound **9** in CDCl<sub>3</sub>



**Figure S73.** The IR Spectra of Compound **10**




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SPECTRUM -

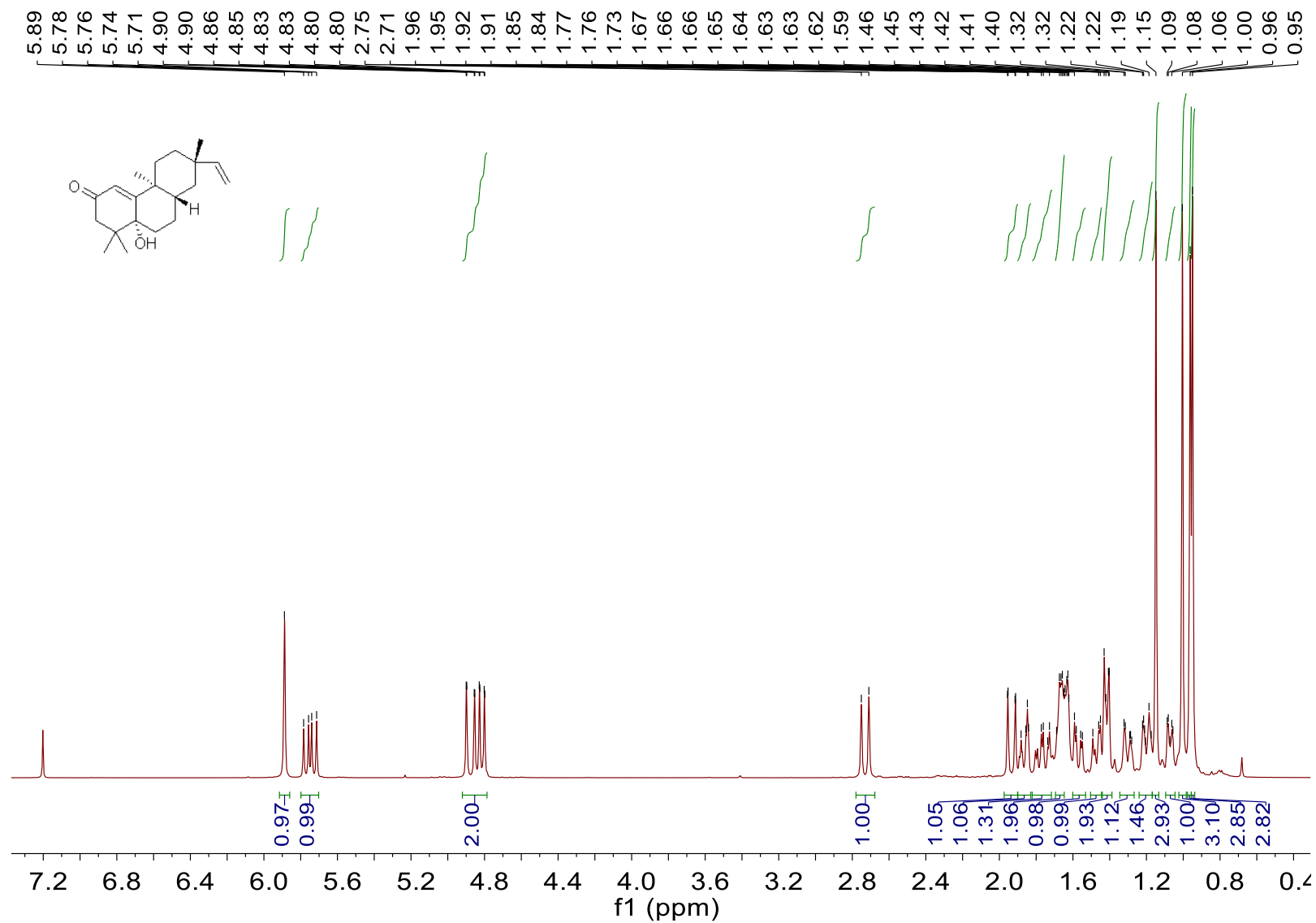
simulation :

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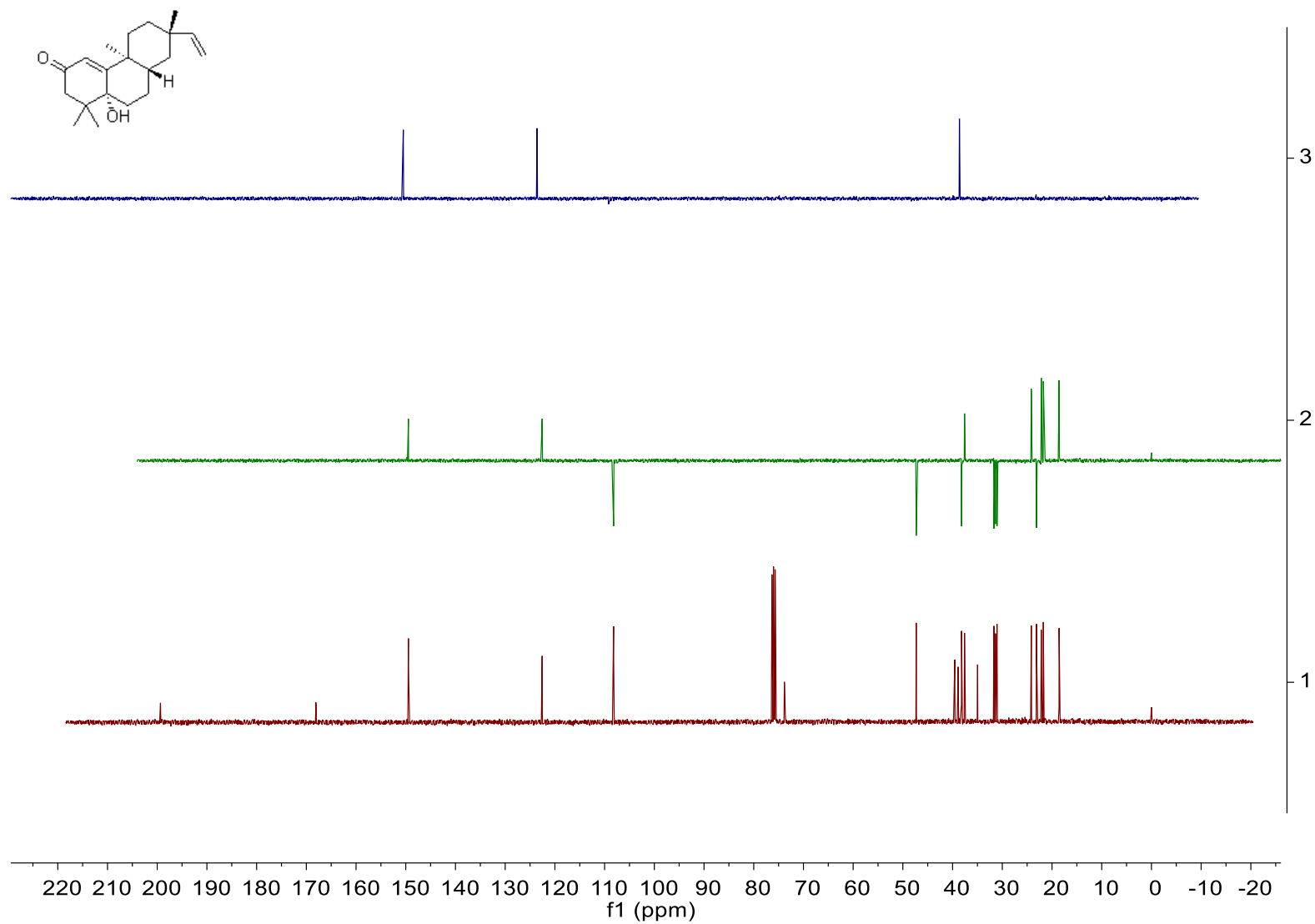
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
303.2308	303.2319	-3.63	6.0	C <sub>20</sub> H <sub>31</sub> O <sub>2</sub>

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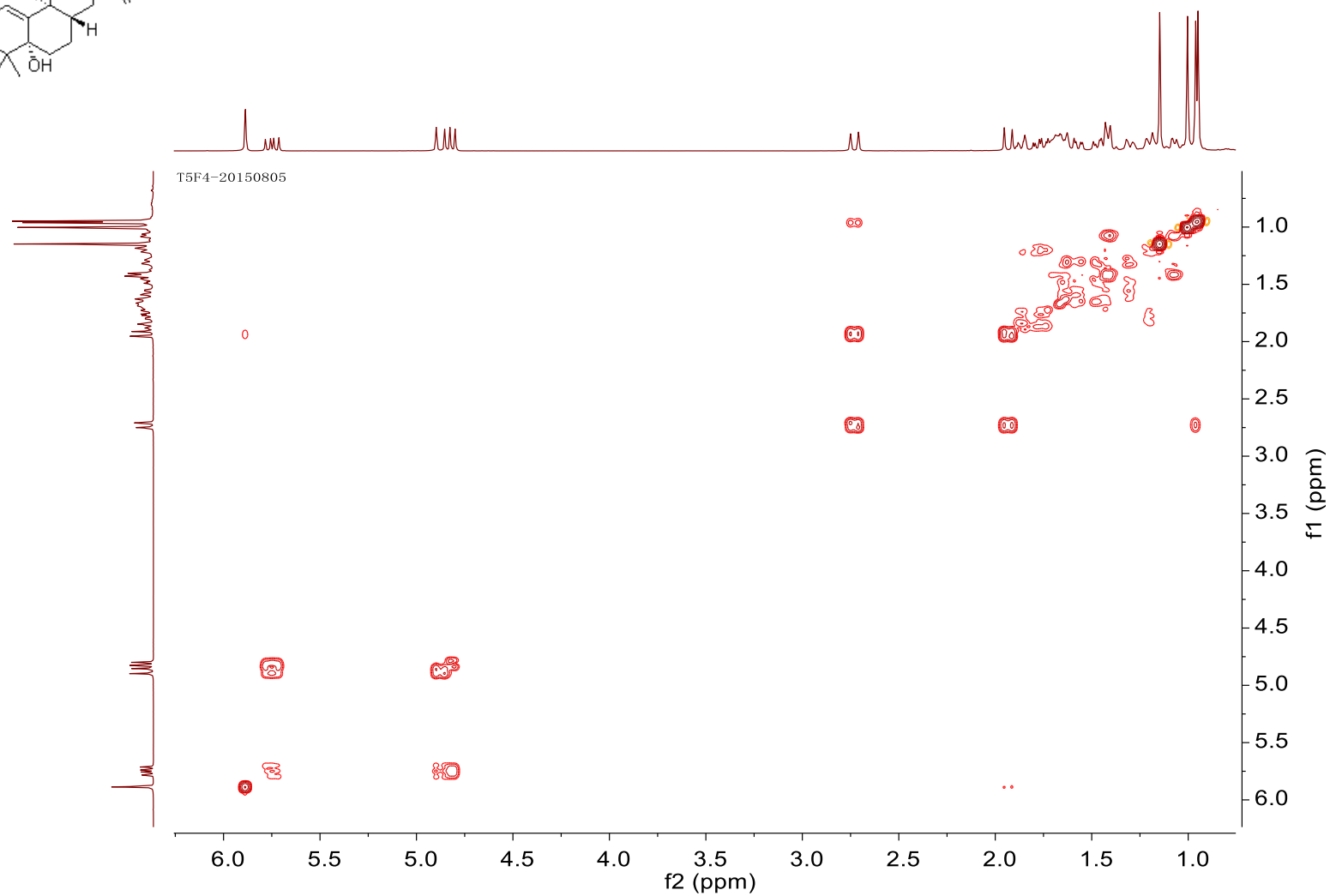
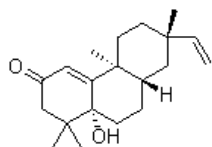
**Figure S74.** The HRESIMS Spectroscopic Data of Compound **10**



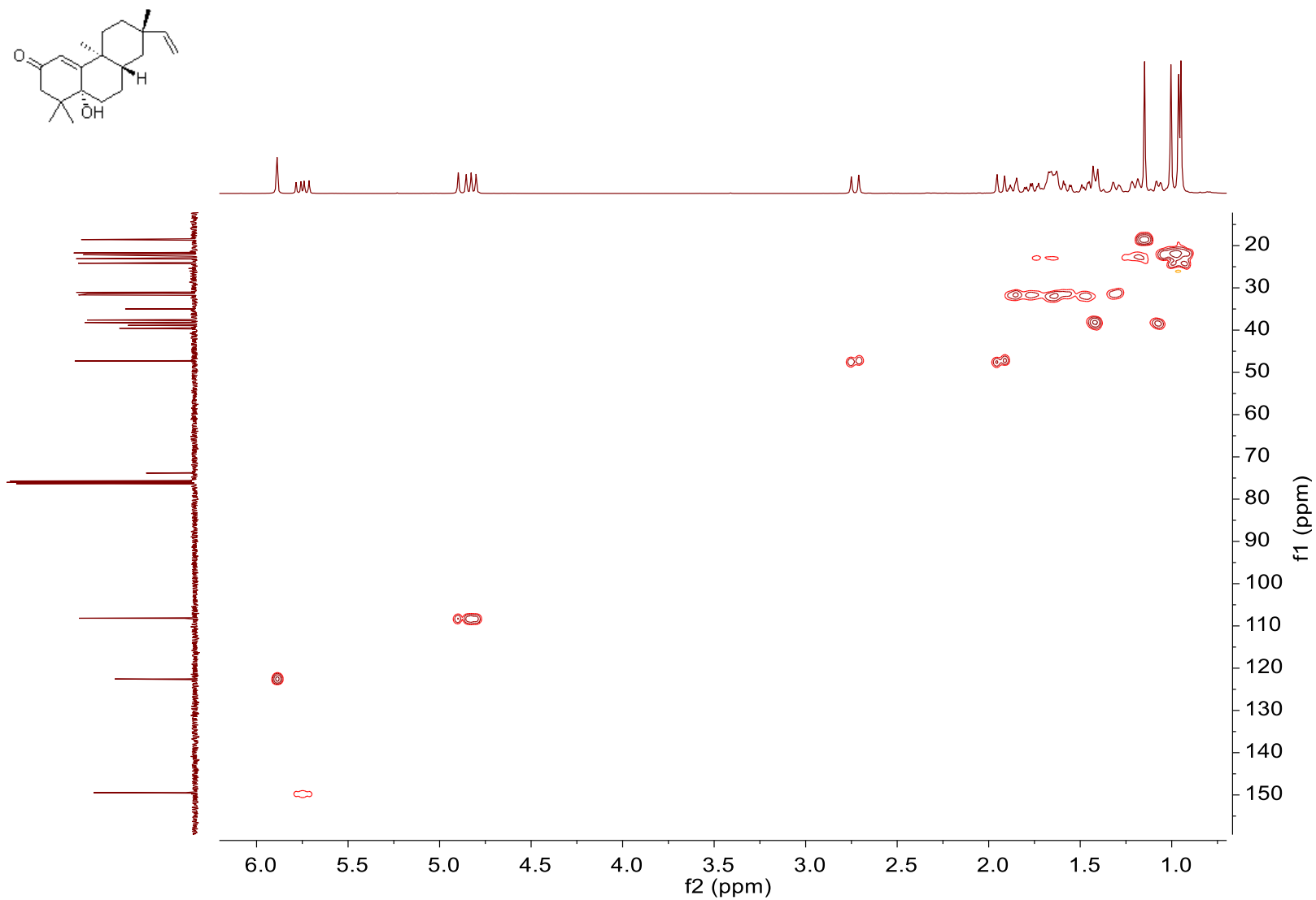
**Figure S75.** The <sup>1</sup>H NMR Spectrum of Compound **10** in CDCl<sub>3</sub>



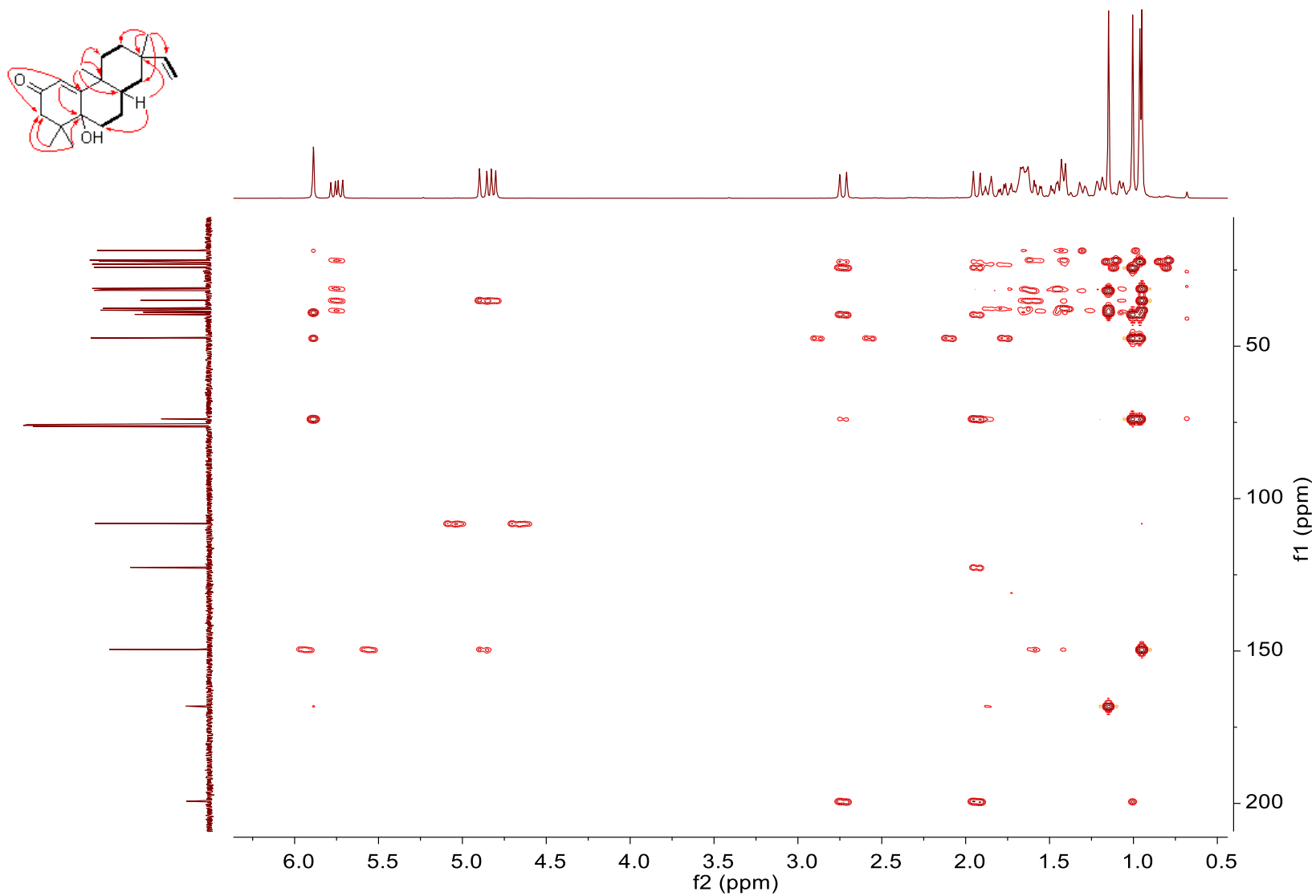
**Figure S76.** The  $^{13}\text{C}$  NMR Spectrum of Compound **10** in  $\text{CDCl}_3$



**Figure S77.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **10** in  $\text{CDCl}_3$

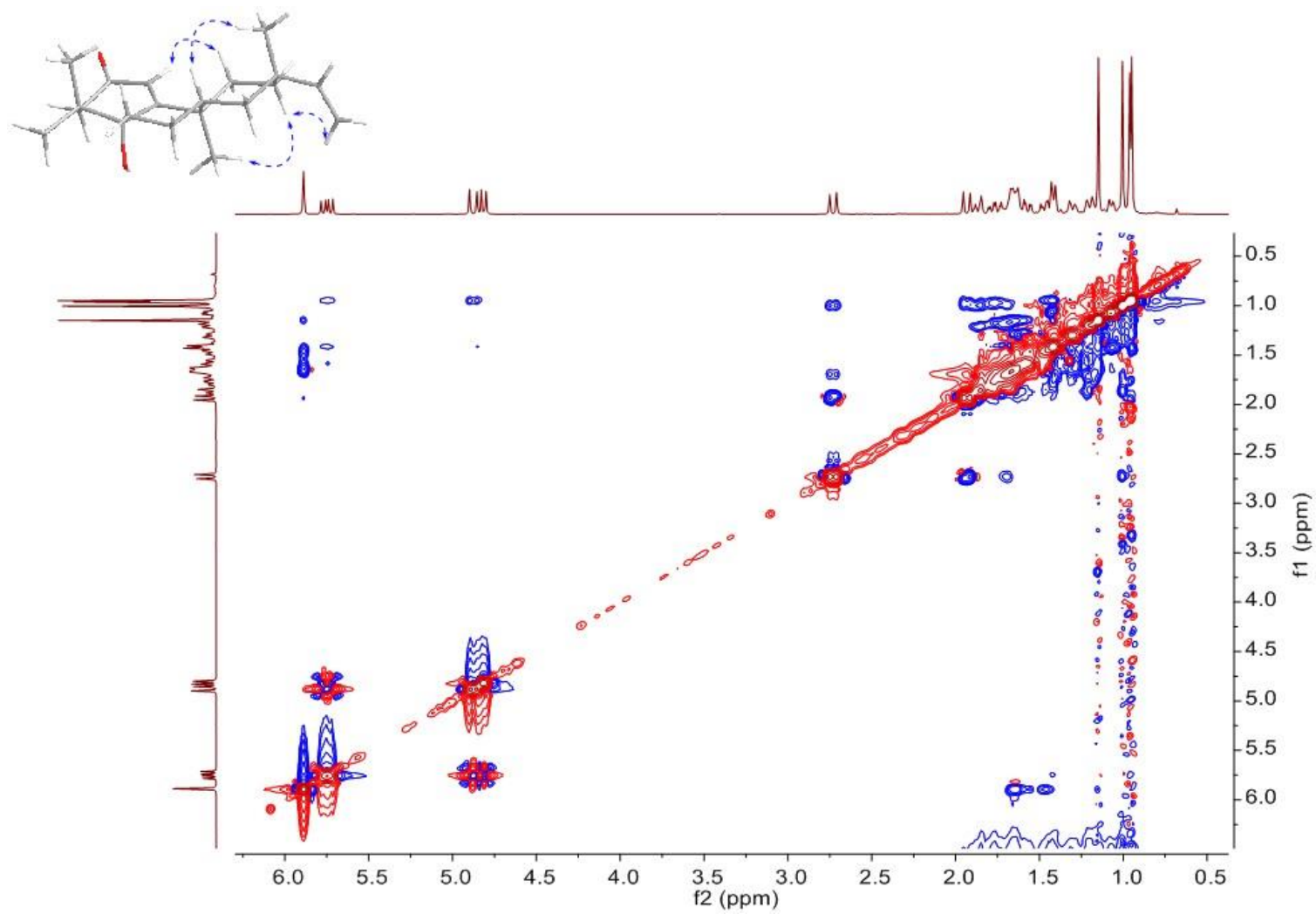


**Figure S78.** The HSQC Spectrum of Compound **10** in  $\text{CDCl}_3$

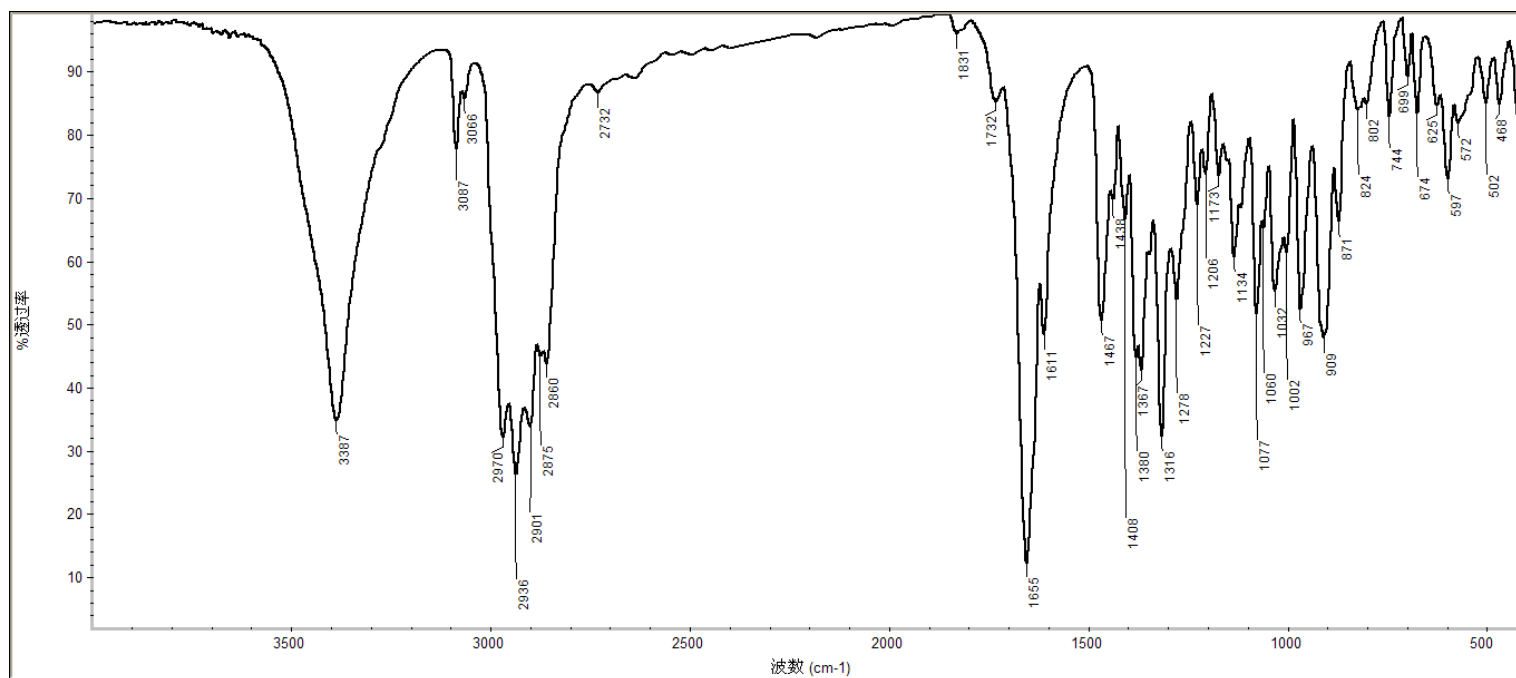


**Figure S79.** The HMBC Spectrum of Compound **10** in  $\text{CDCl}_3$

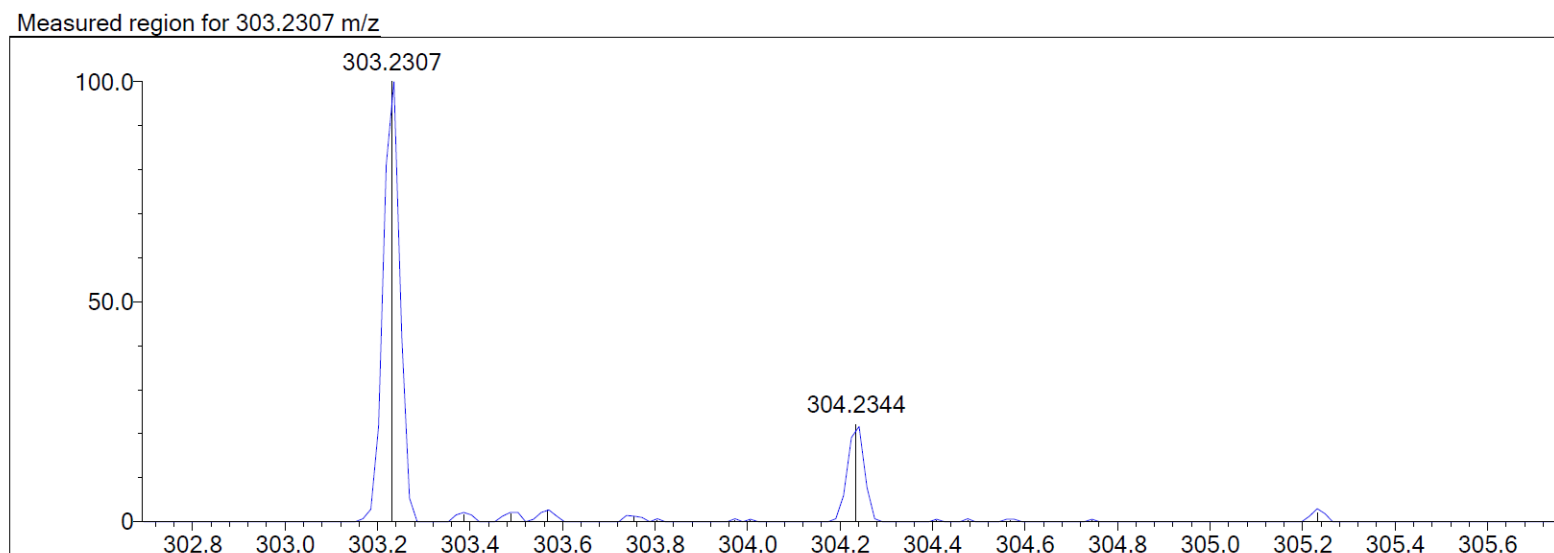




**Figure S80.** The NOESY Spectrum of Compound **10** in CDCl<sub>3</sub>



**Figure S81.** The IR Spectra of Compound **11**




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SPECTRUM -

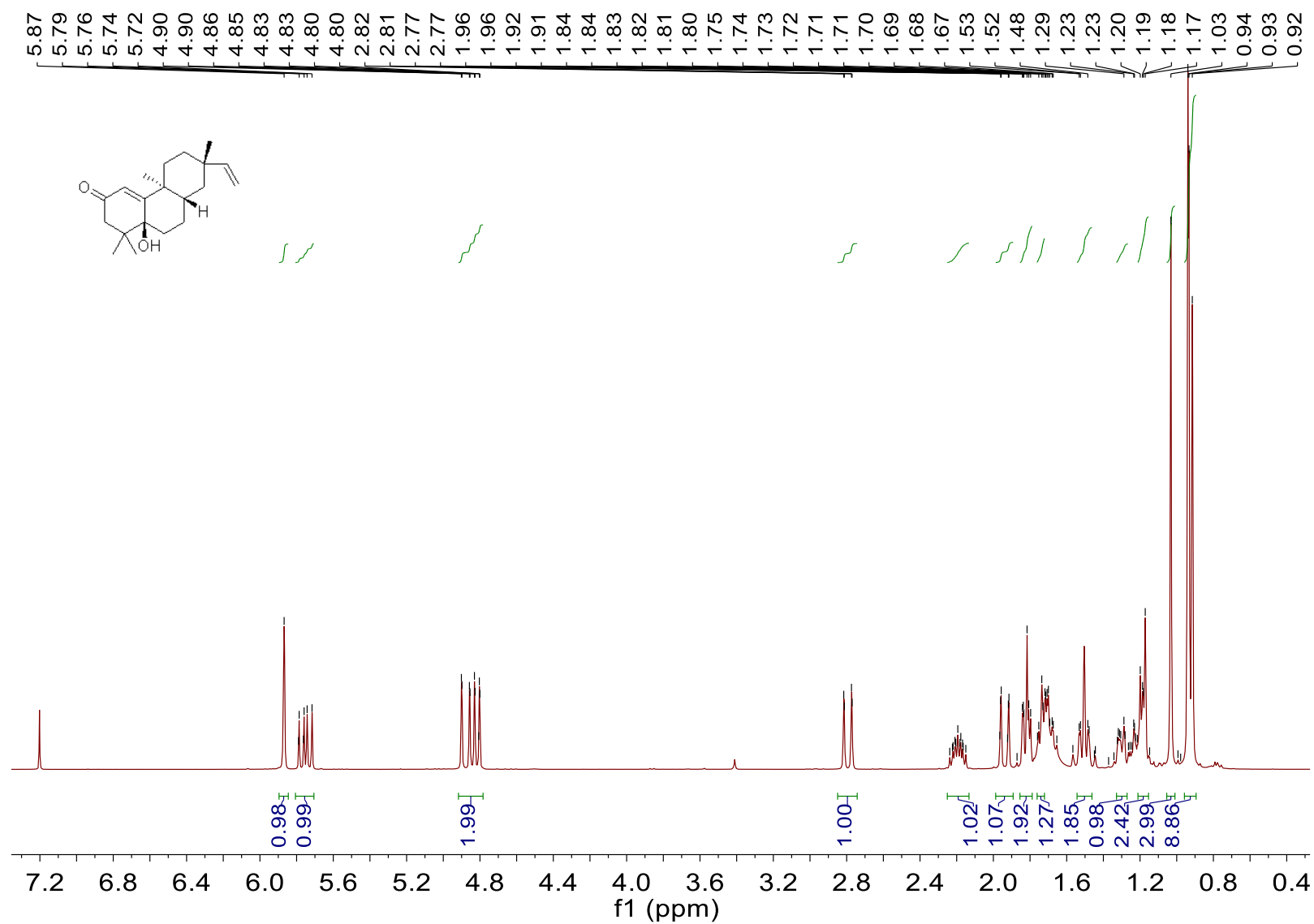
simulation :

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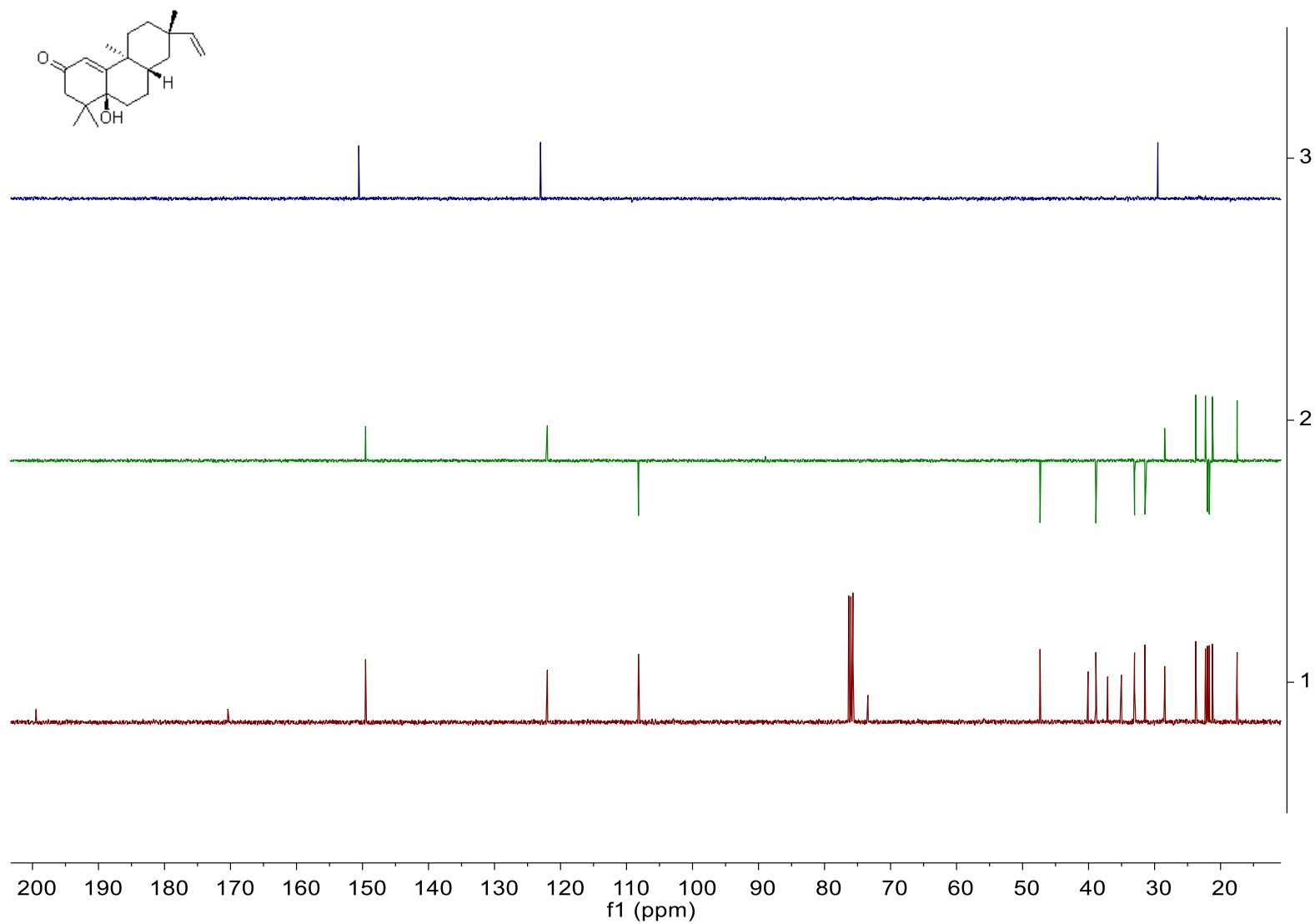
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
303.2307	303.2319	-3.96	6.0	C <sub>20</sub> H <sub>31</sub> O <sub>2</sub>

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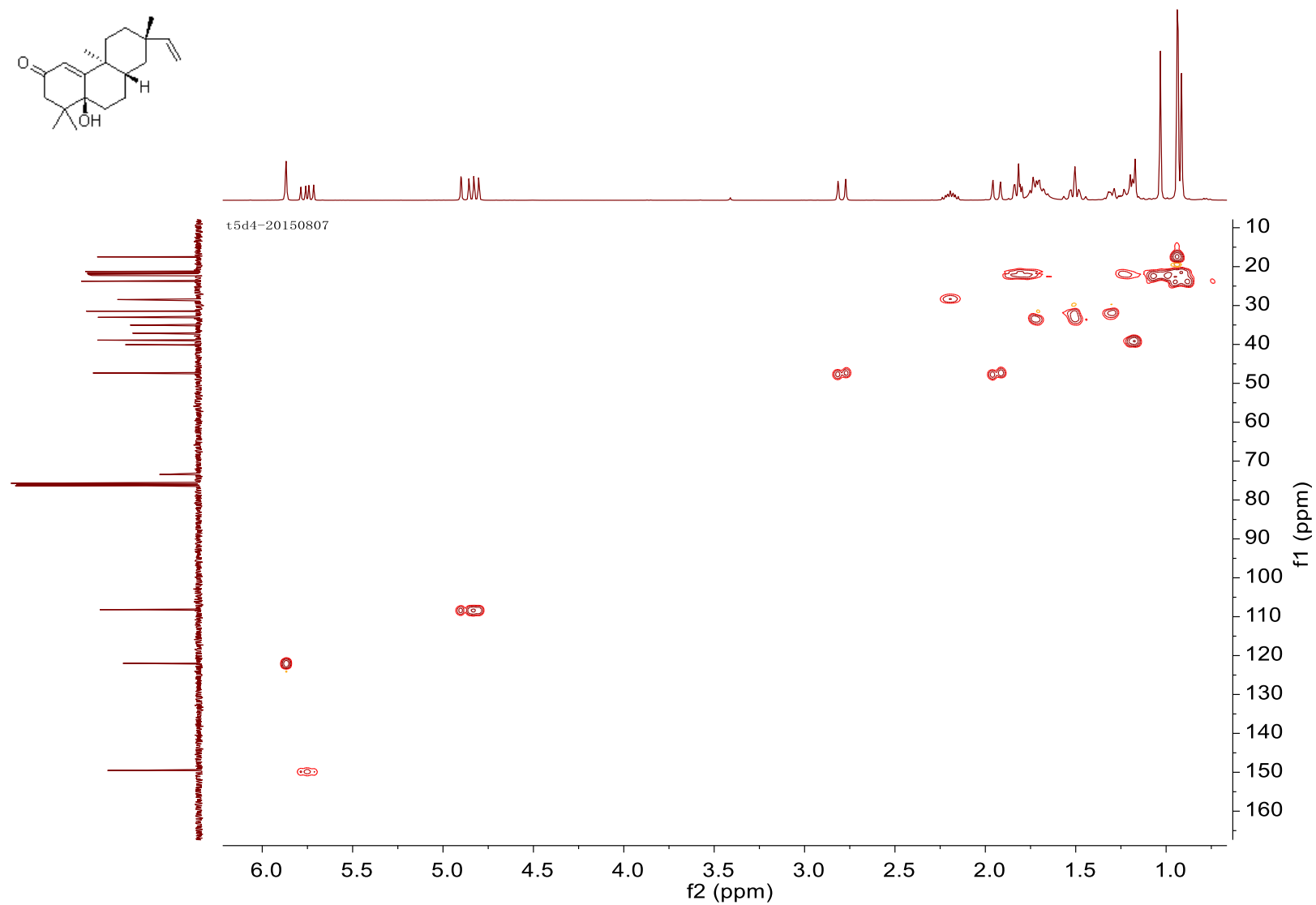
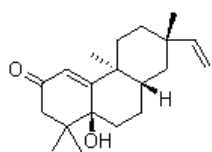
**Figure S82.** The HRESIMS Spectroscopic Data of Compound **11**



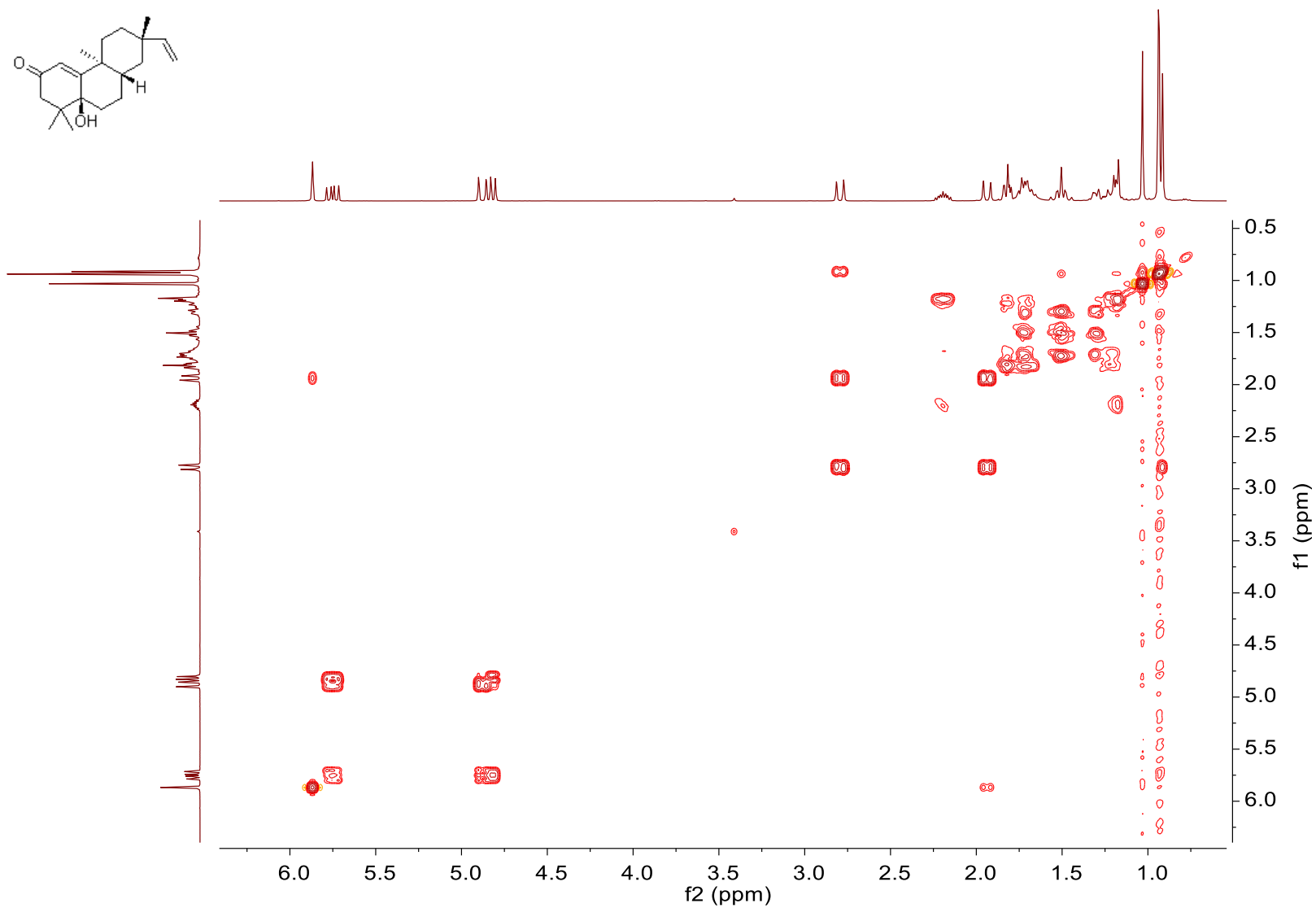
**Figure S83.** The <sup>1</sup>H NMR Spectrum of Compound **11** in CDCl<sub>3</sub>



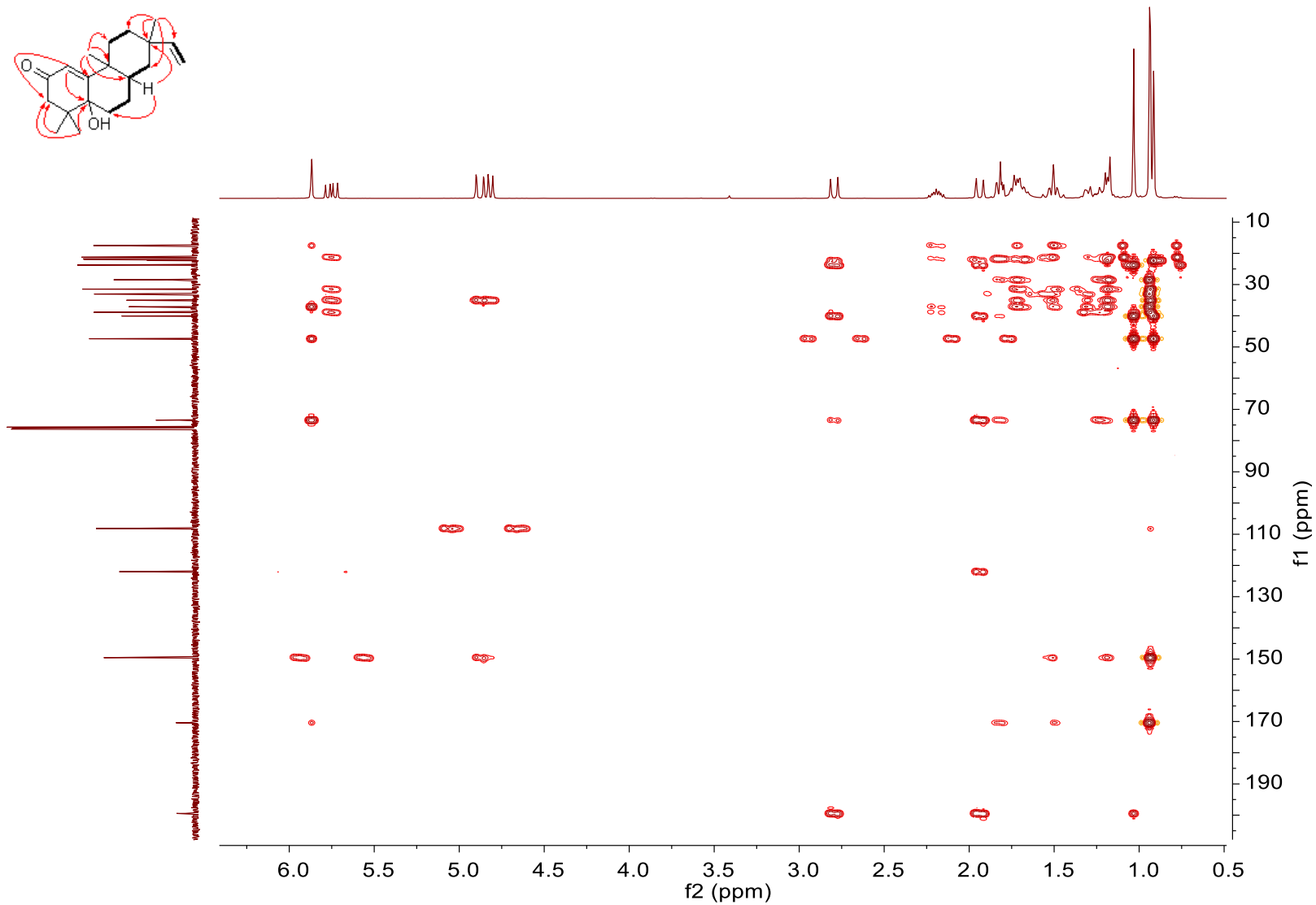
**Figure S84.** The  $^{13}\text{C}$  NMR Spectrum of Compound **11** in  $\text{CDCl}_3$



**Figure S85.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **11** in  $\text{CDCl}_3$

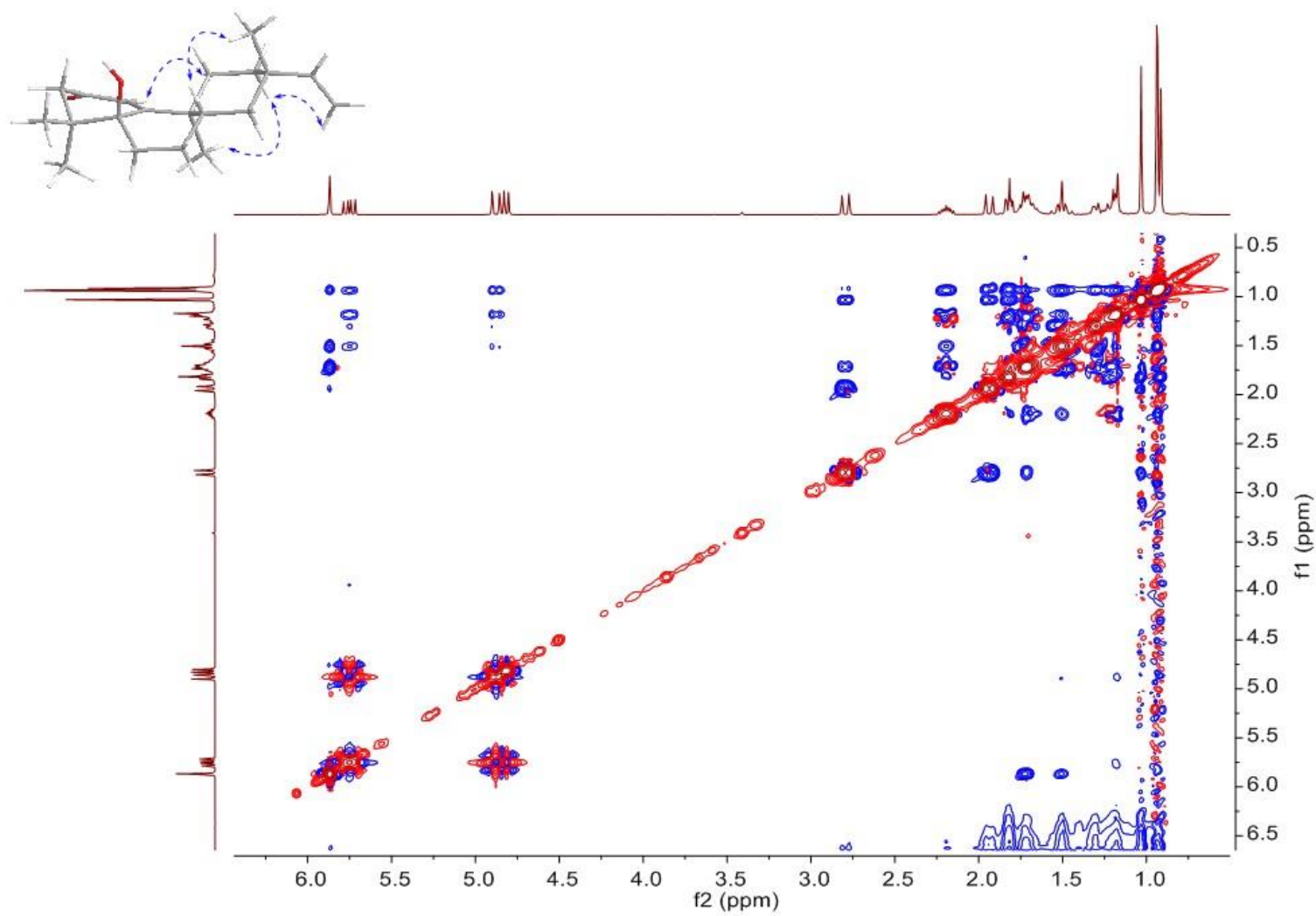


**Figure S86.** The HSQC Spectrum of Compound **11** in  $\text{CDCl}_3$

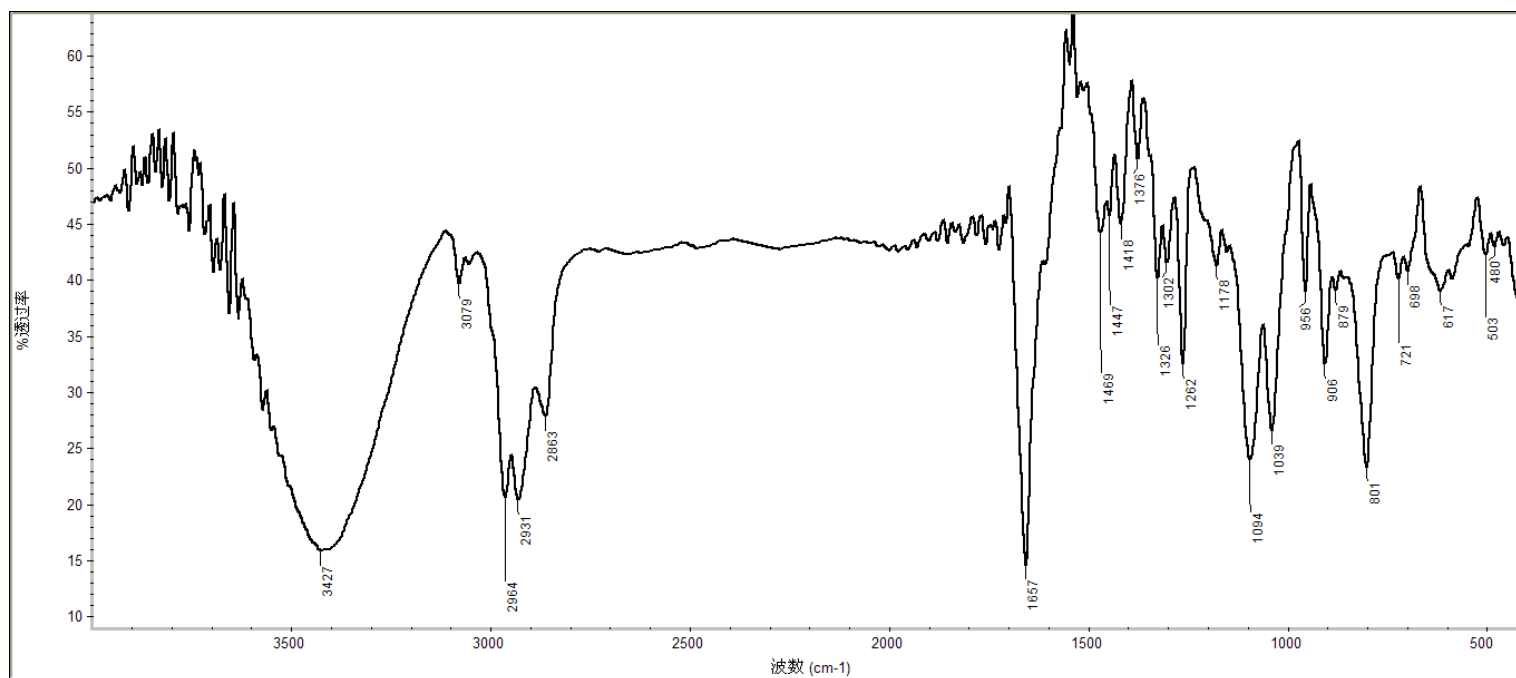


**Figure S87.** The HMBC Spectrum of Compound **11** in  $\text{CDCl}_3$

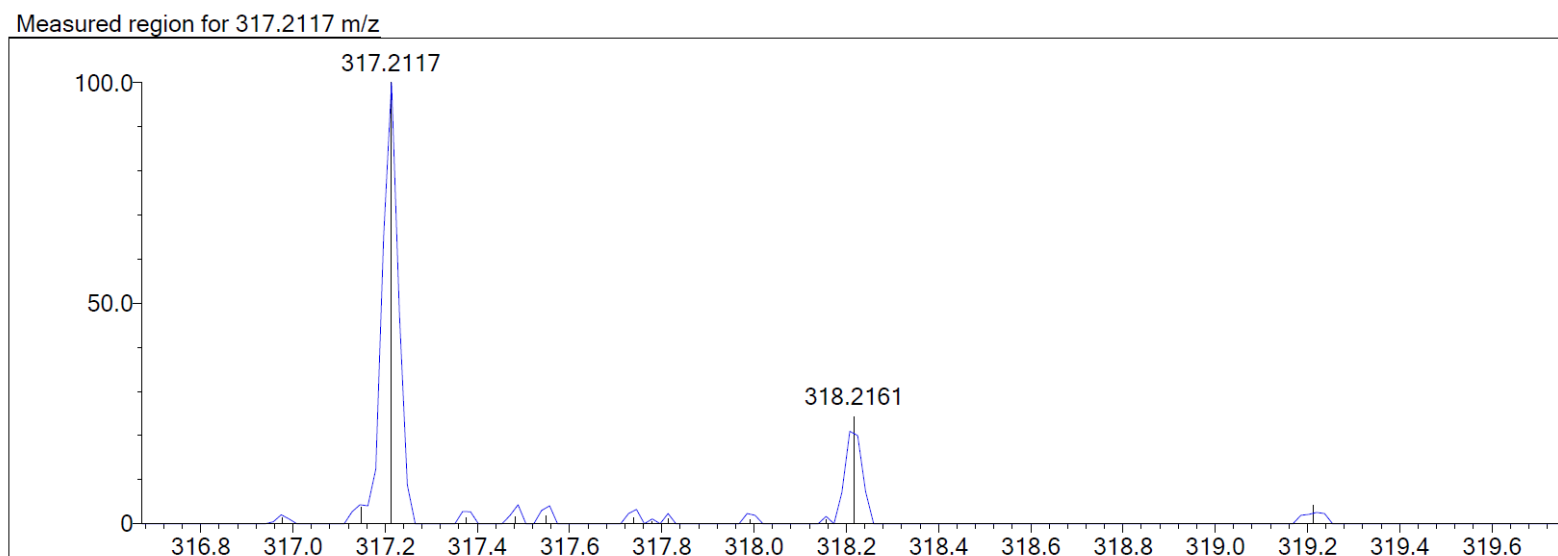




**Figure S88.** The NOESY Spectrum of Compound **11** in CDCl<sub>3</sub>



**Figure S89.** The IR Spectra of Compound **12**




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SPECTRUM -

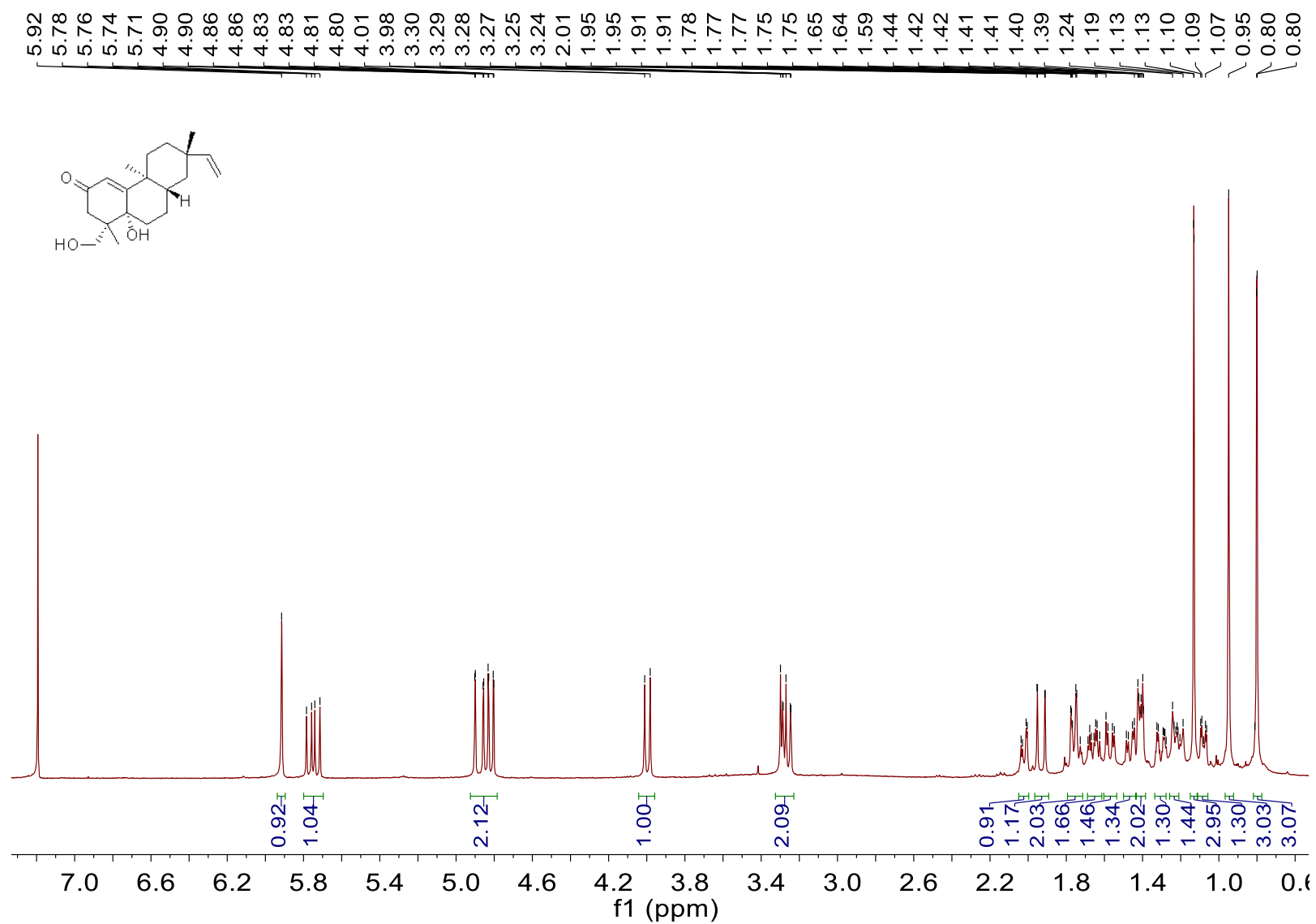
simulation :

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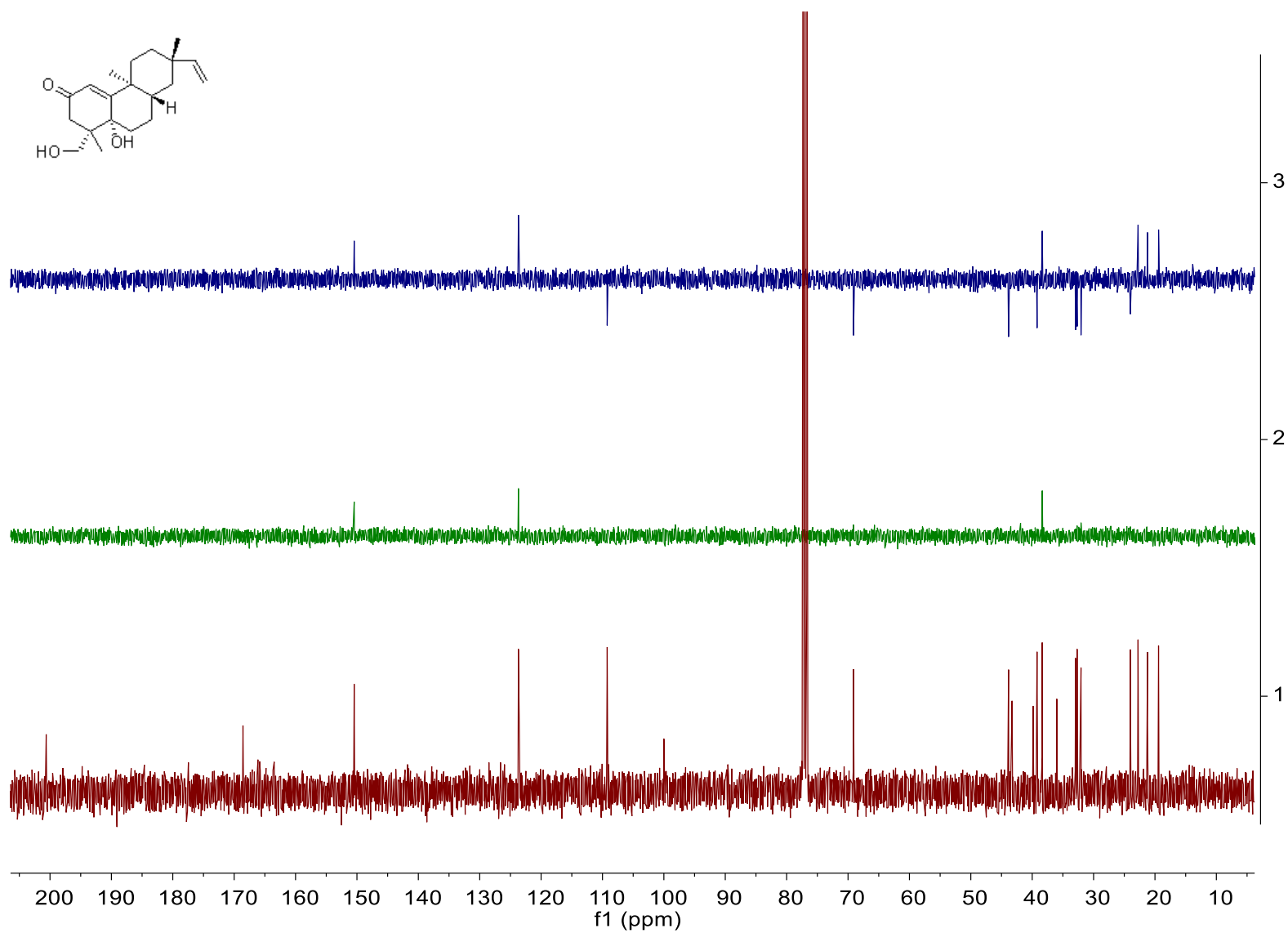
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
317.2117	317.2122	-1.58	6.0	C <sub>20</sub> H <sub>29</sub> O <sub>3</sub>

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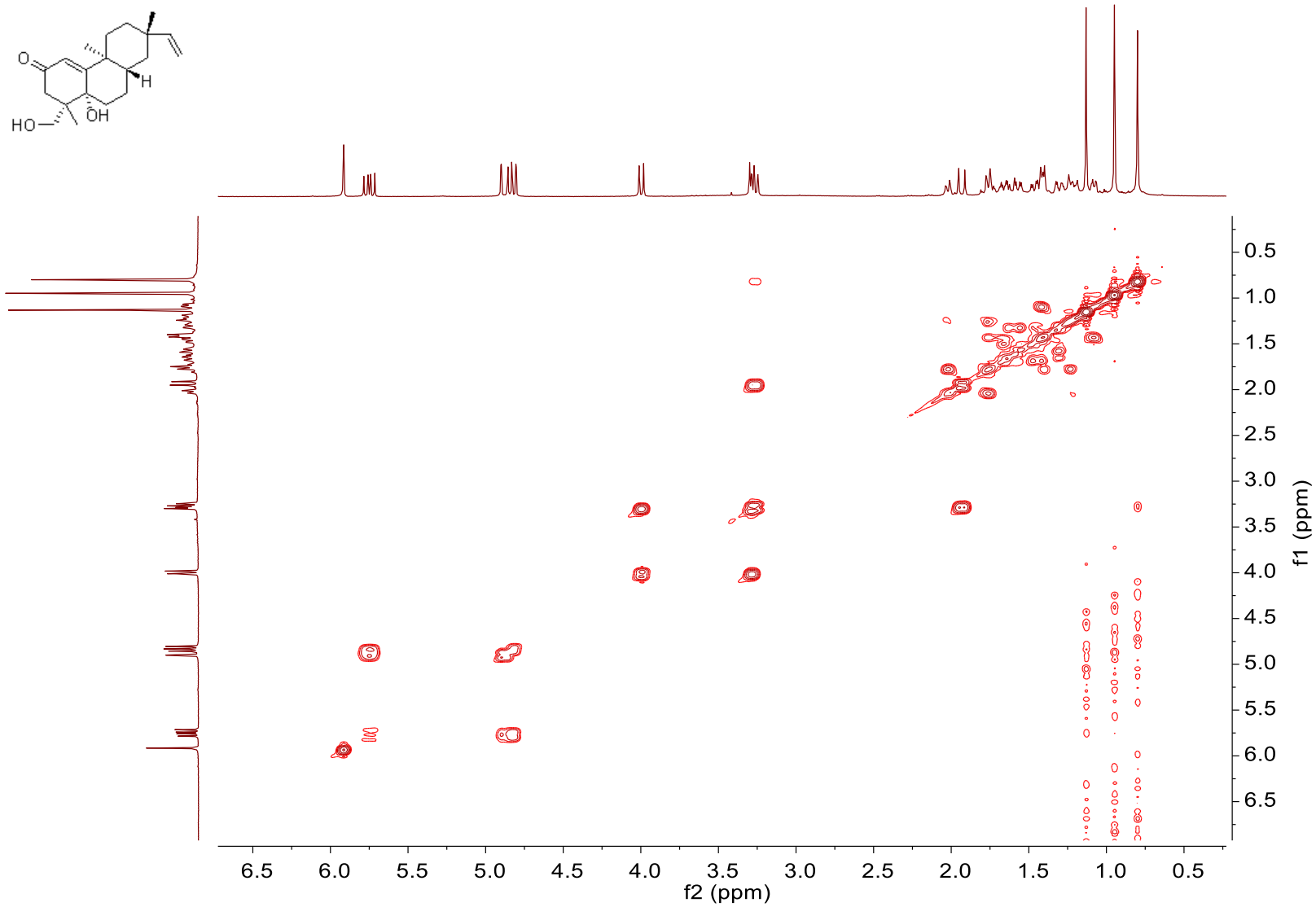
**Figure S90.** The HRESIMS Spectroscopic Data of Compound **12**



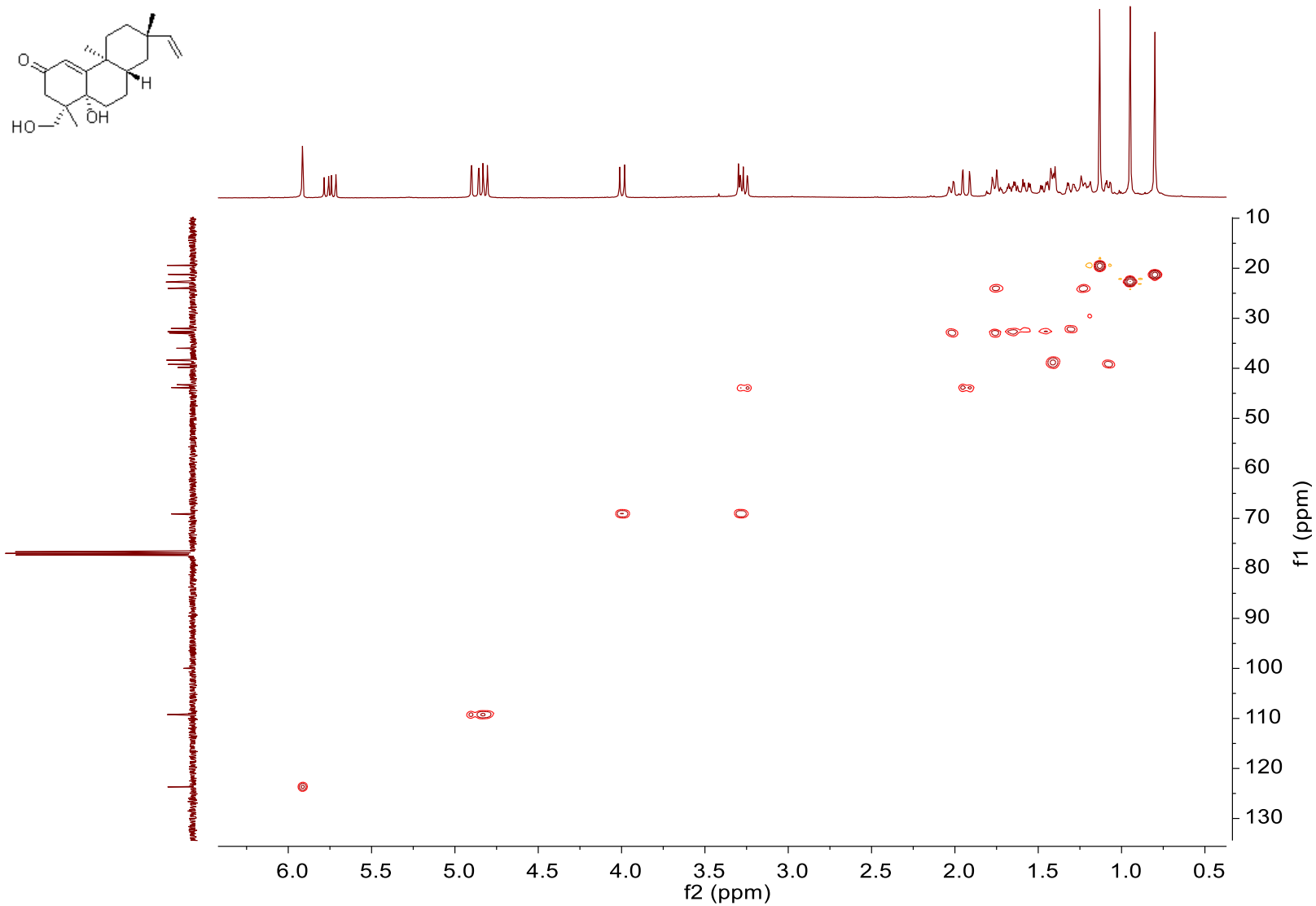
**Figure S91.** The <sup>1</sup>H NMR Spectrum of Compound **12** in CDCl<sub>3</sub>



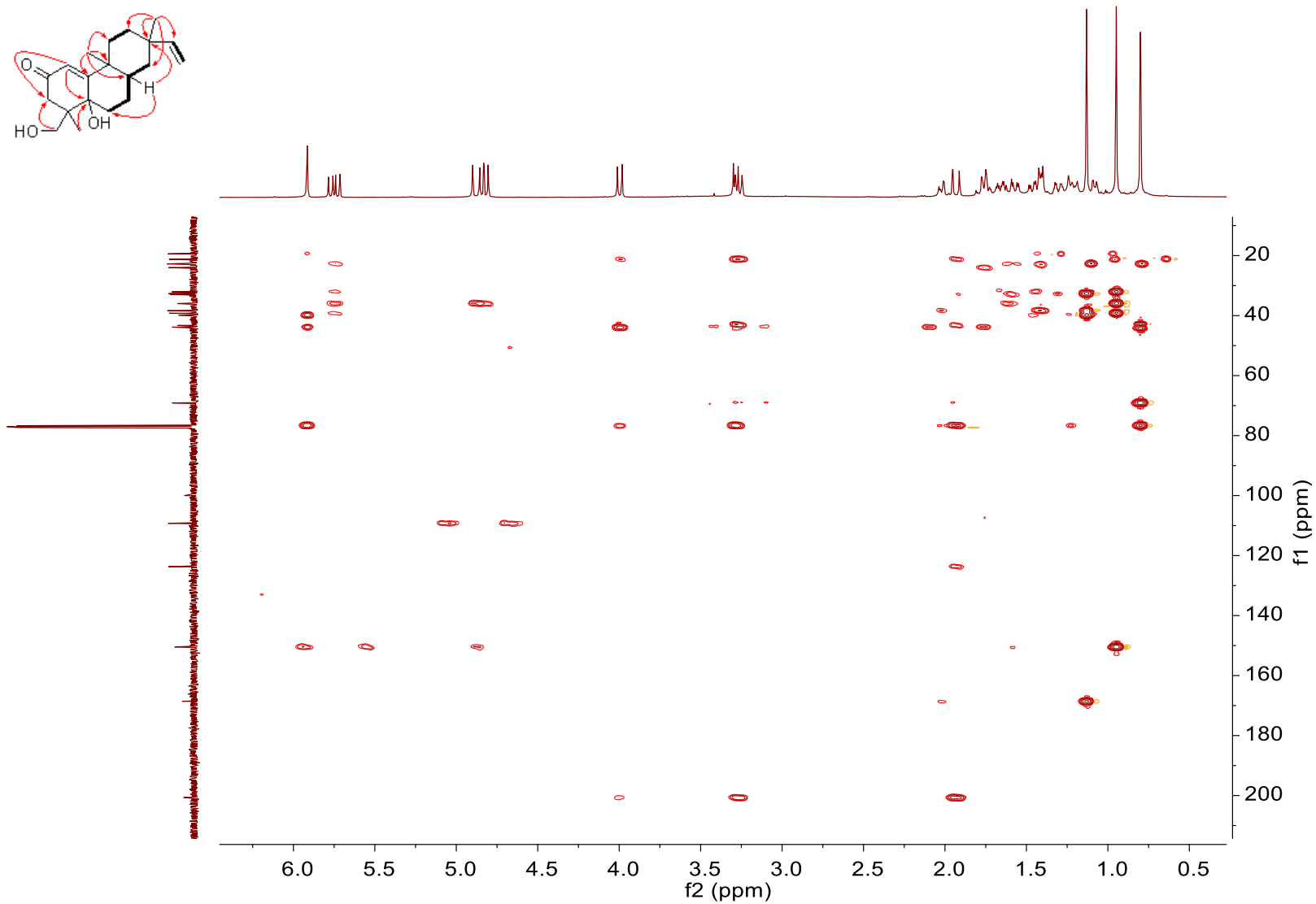
**Figure S92.** The  $^{13}\text{C}$  NMR Spectrum of Compound **12** in  $\text{CDCl}_3$



**Figure S93.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound 12 in  $\text{CDCl}_3$

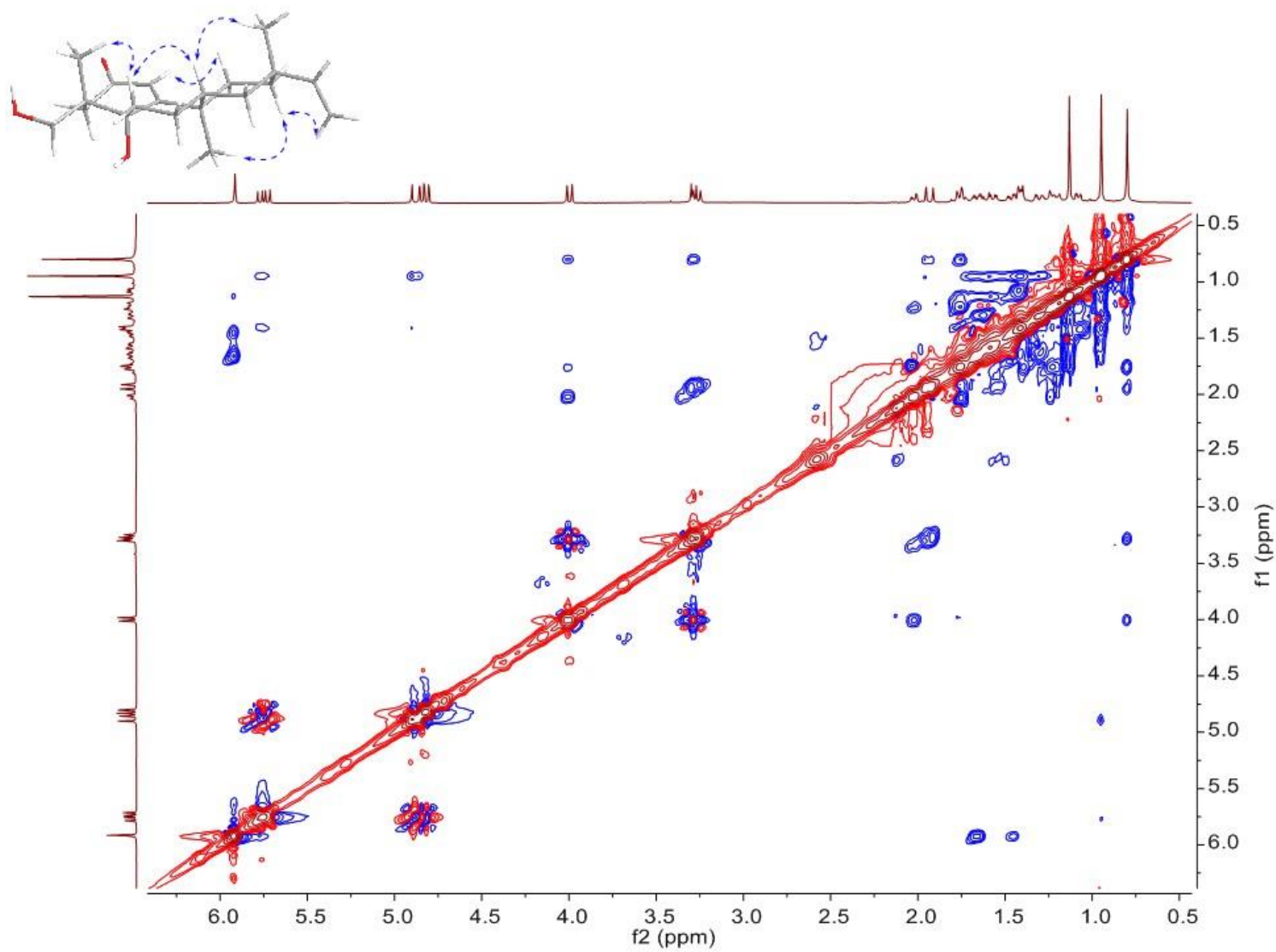


**Figure S94.** The HSQC Spectrum of Compound **12** in  $\text{CDCl}_3$

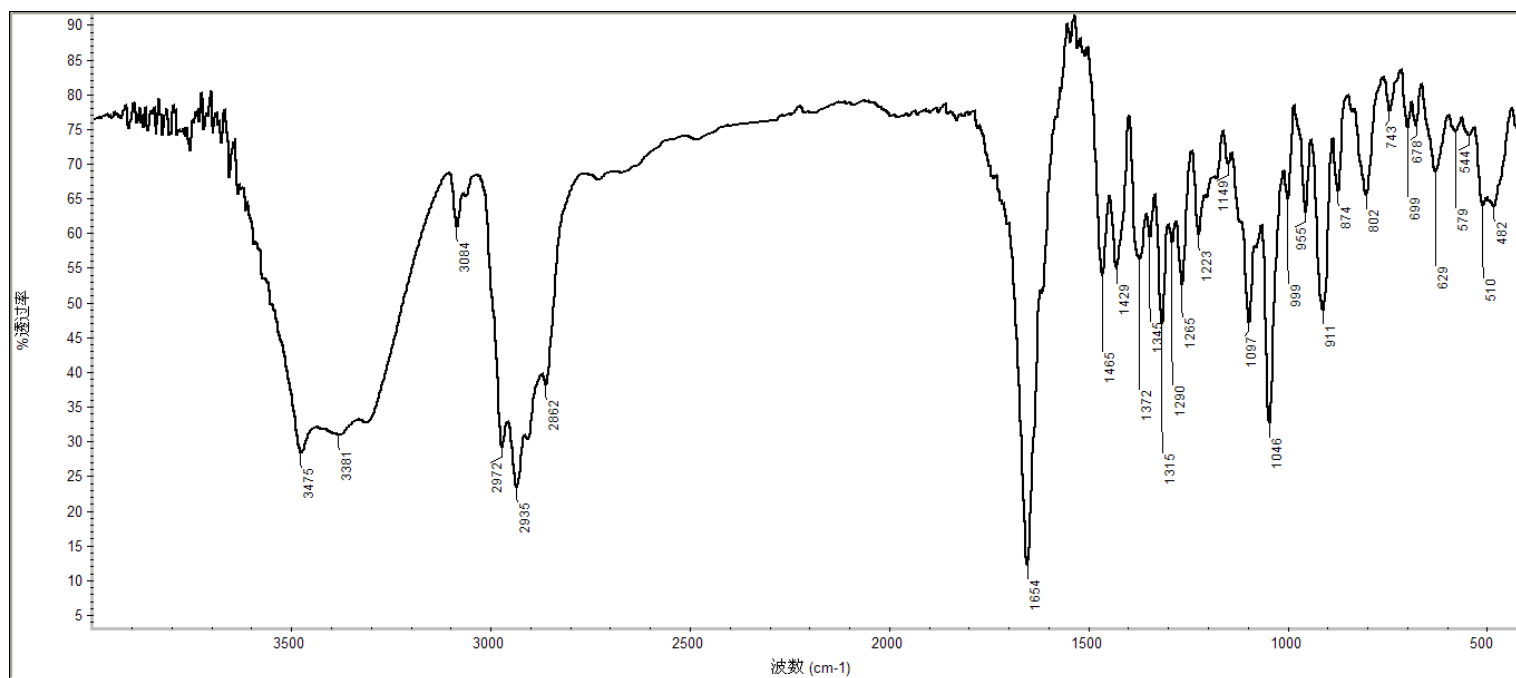


**Figure S95.** The HMBC Spectrum of Compound **12** in  $\text{CDCl}_3$

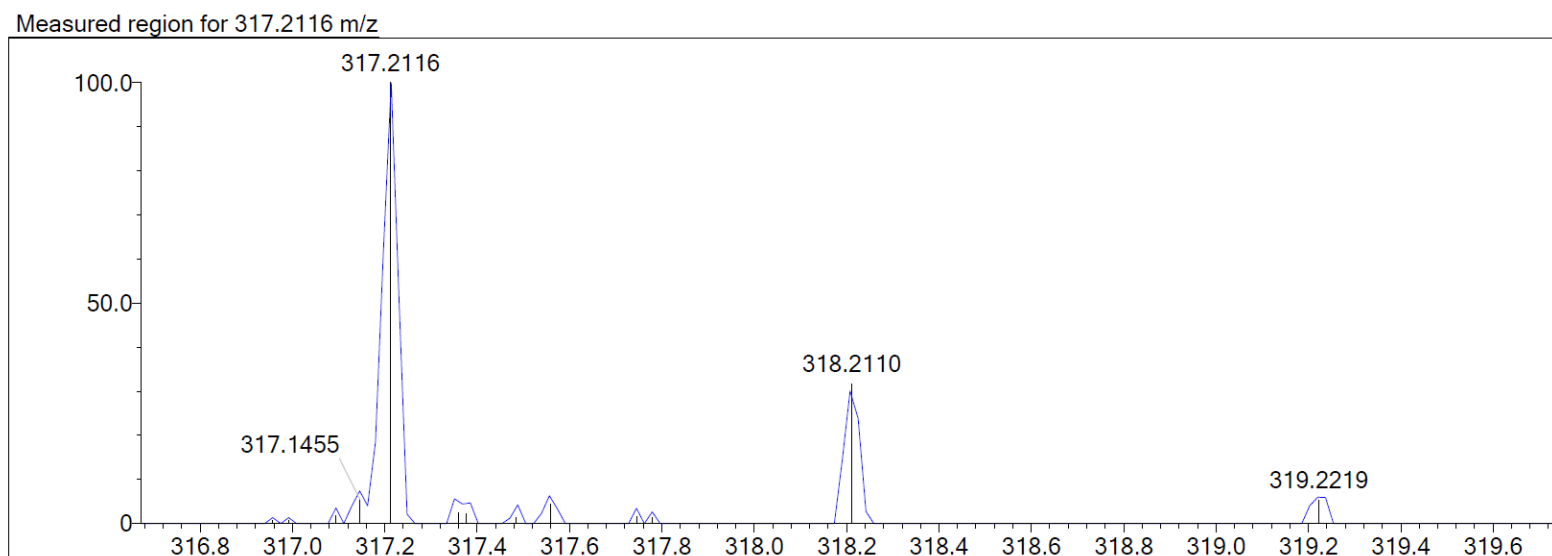




**Figure S96.** The NOESY Spectrum of Compound **12** in CDCl<sub>3</sub>



**Figure S97.** The IR Spectra of Compound **13**

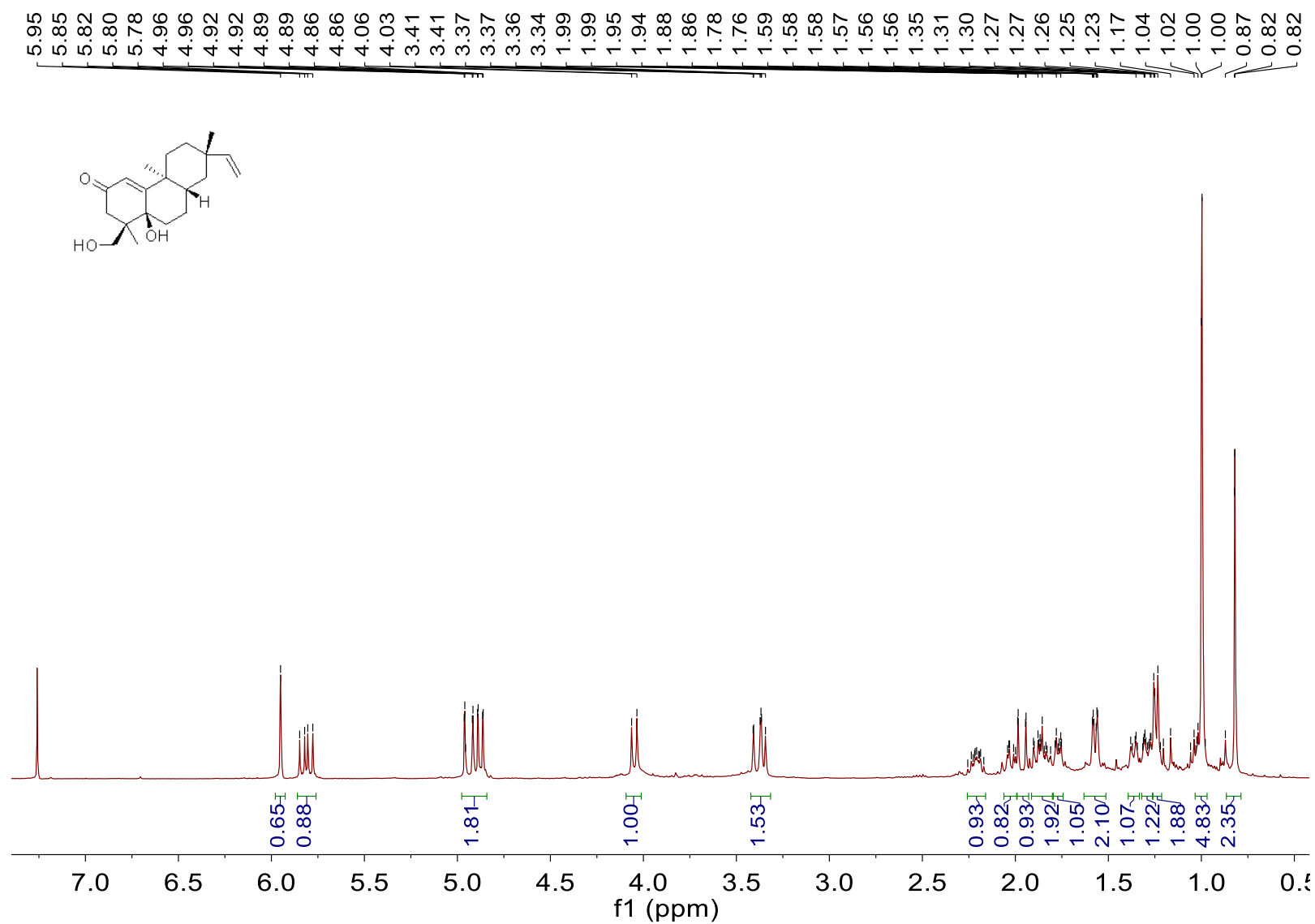


SPECTRUM -

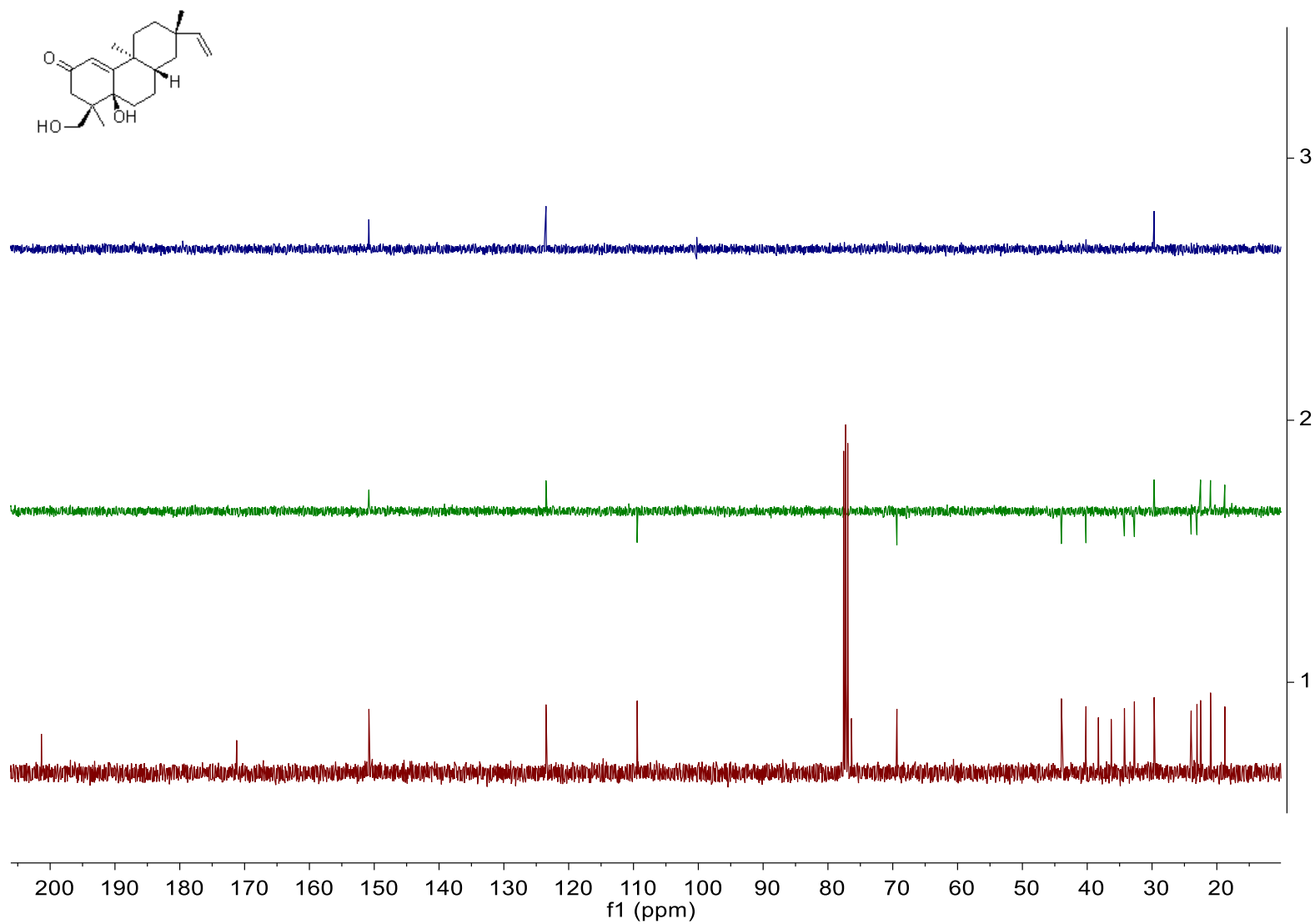
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
317.2116	317.2122	-1.89	6.0	C <sub>20</sub> H <sub>29</sub> O <sub>3</sub>

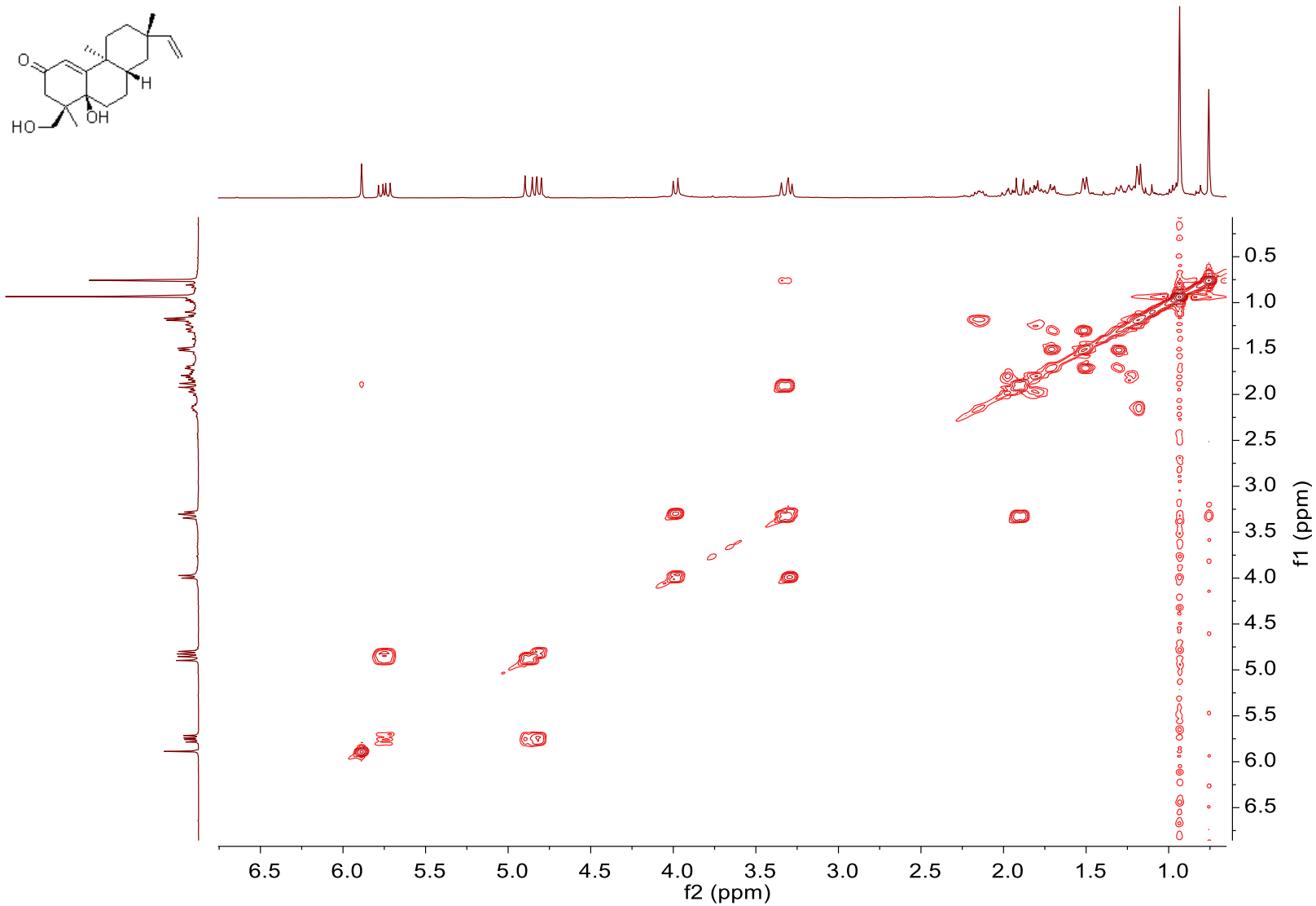
**Figure S98.** The HRESIMS Spectroscopic Data of Compound **13**



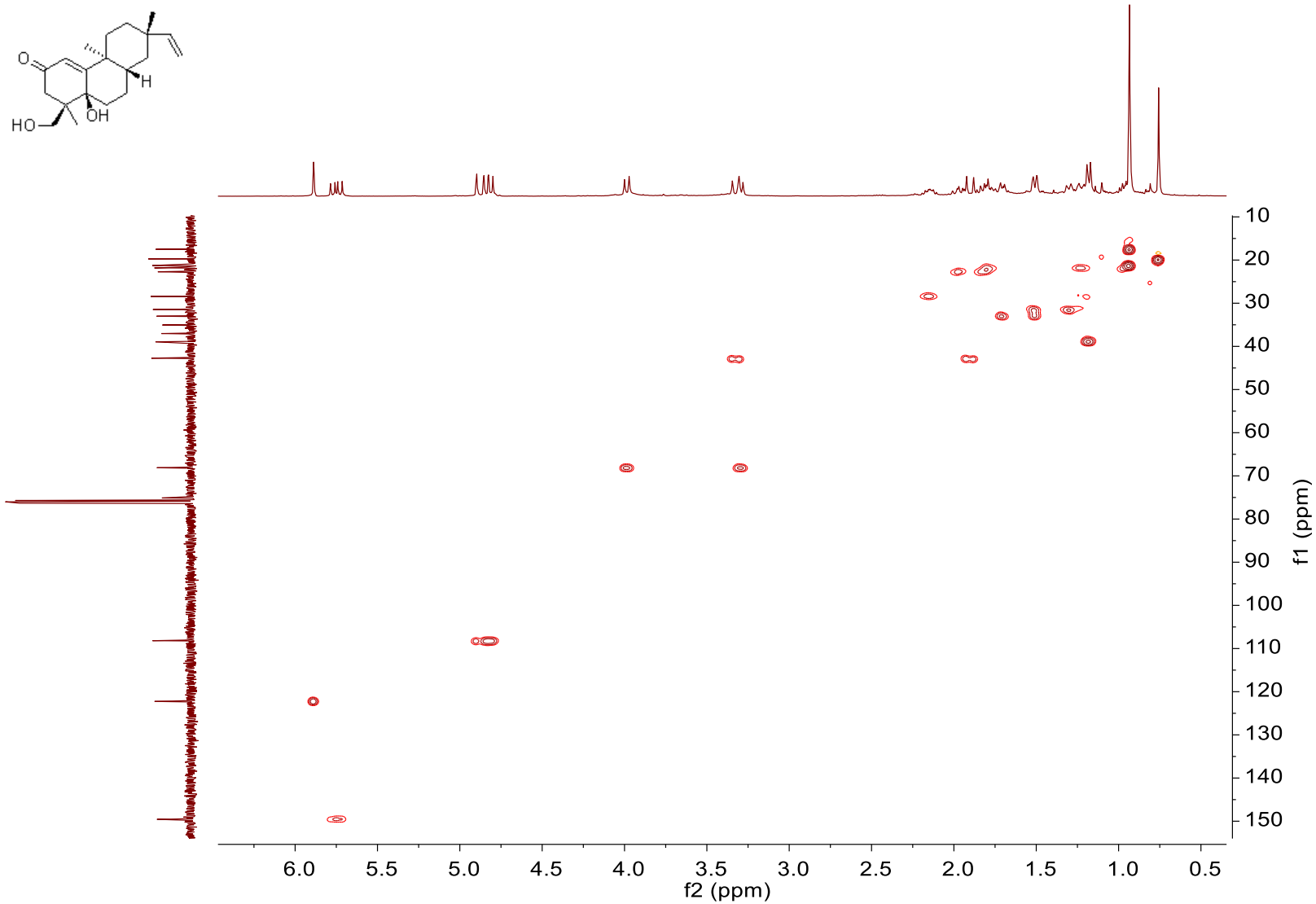
**Figure S99.** The <sup>1</sup>H NMR Spectrum of Compound **13** in CDCl<sub>3</sub>



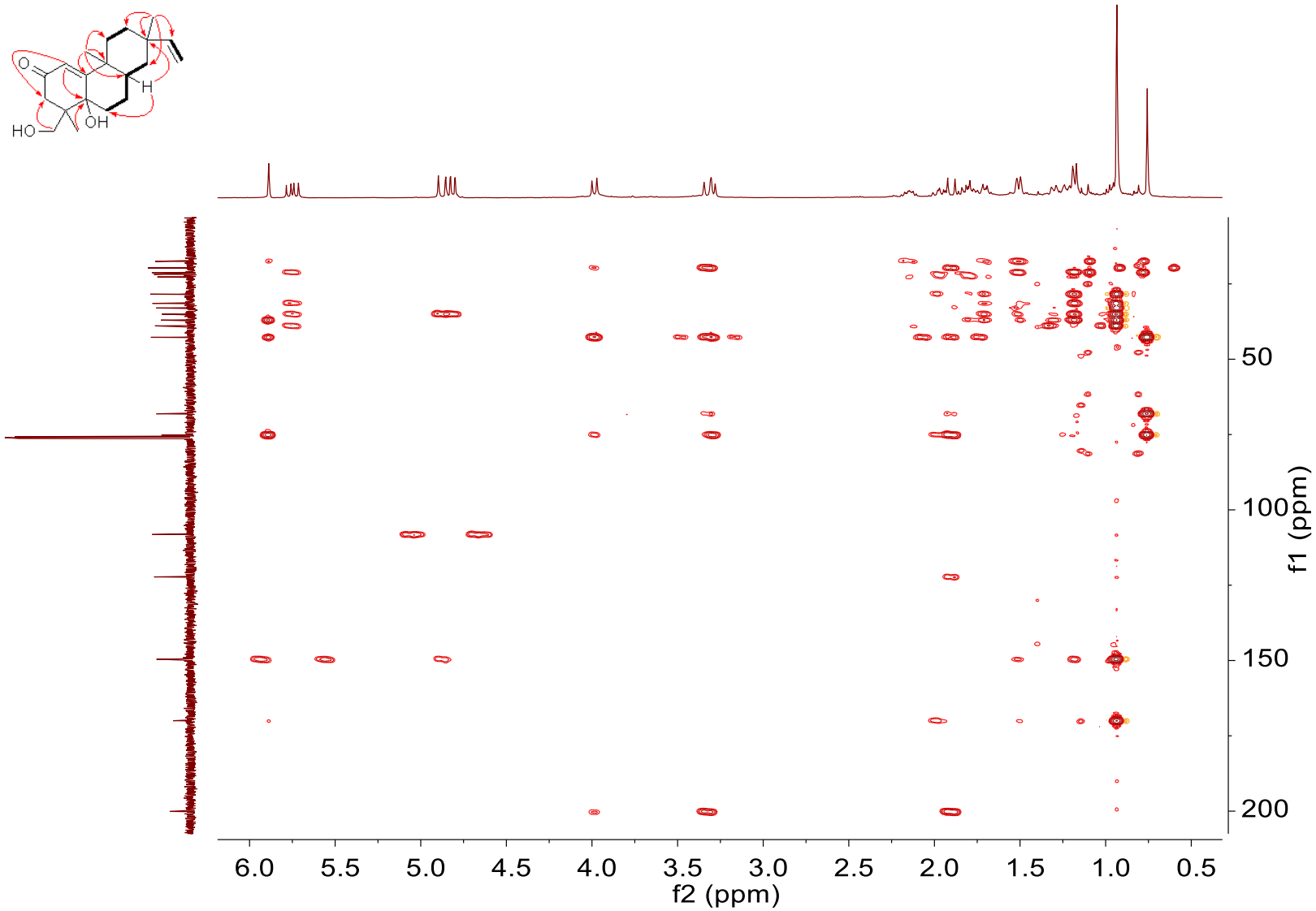
**Figure S100.** The  $^{13}\text{C}$  NMR Spectrum of Compound **13** in  $\text{CDCl}_3$



**Figure S101.** The  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of Compound **13** in  $\text{CDCl}_3$

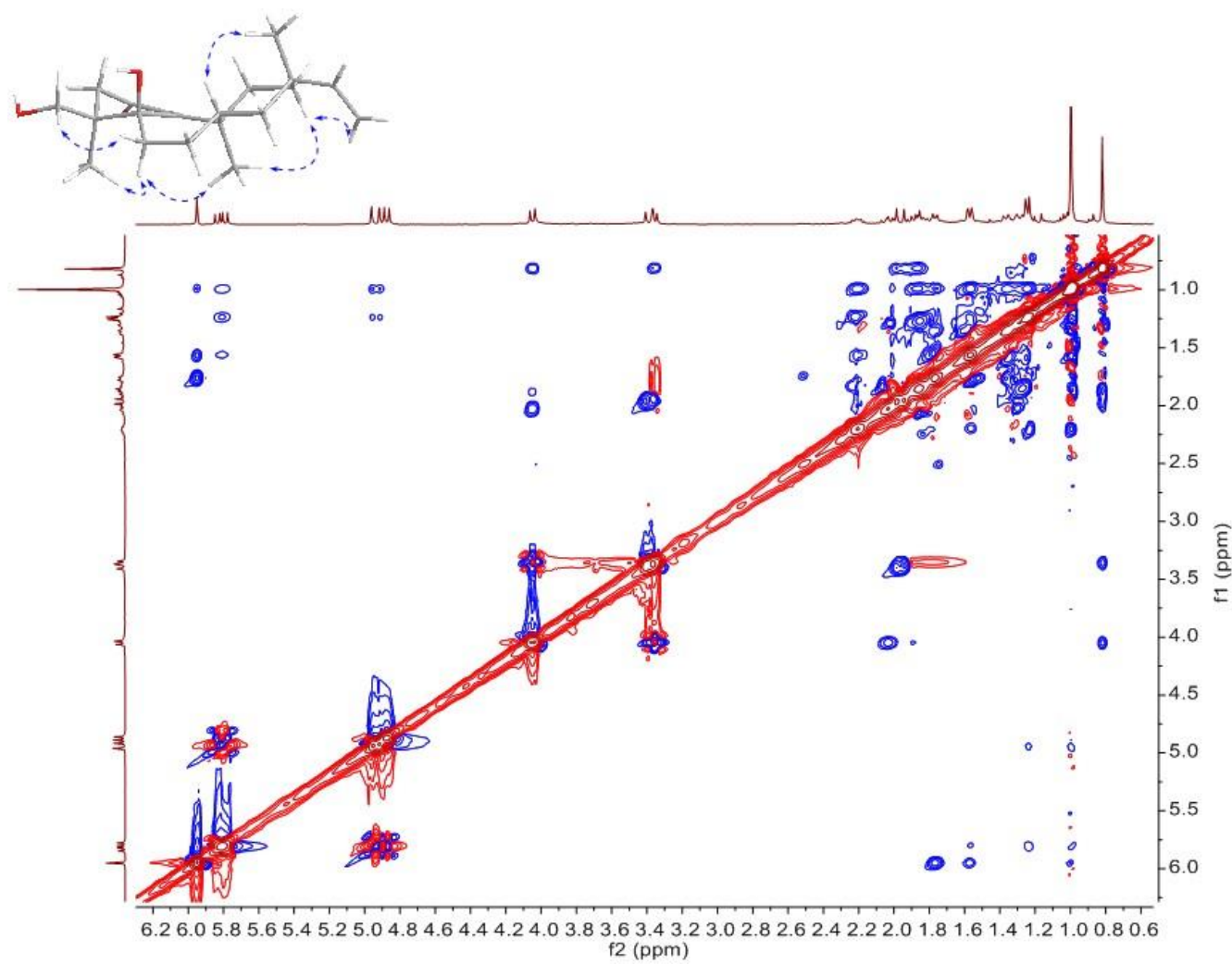


**Figure S102.** The HSQC Spectrum of Compound **13** in CDCl<sub>3</sub>

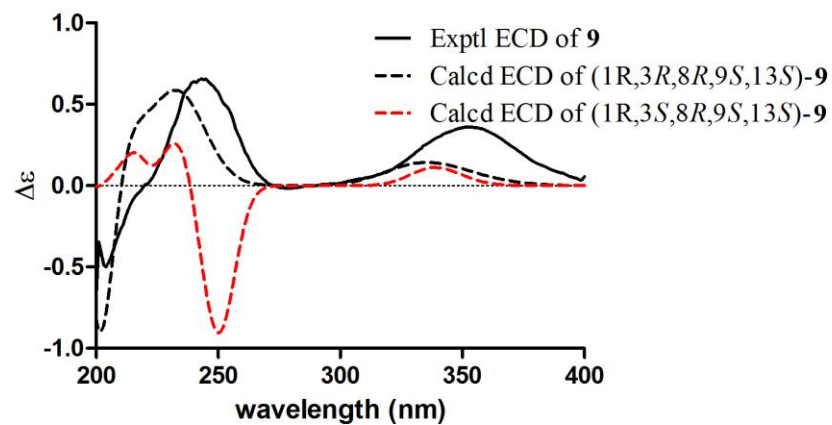
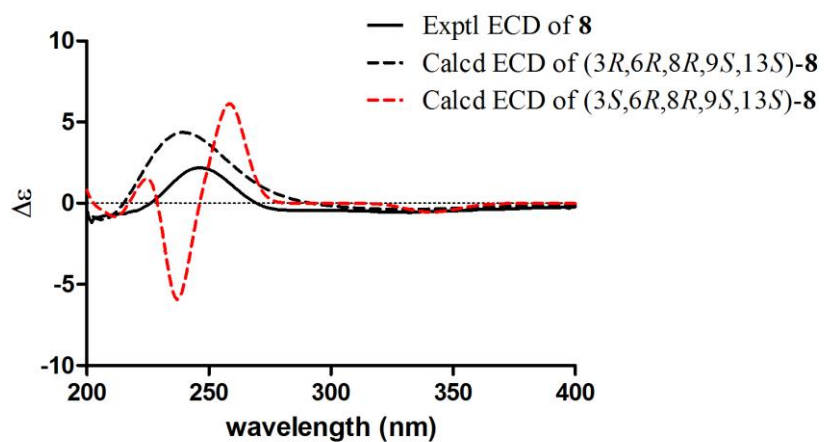
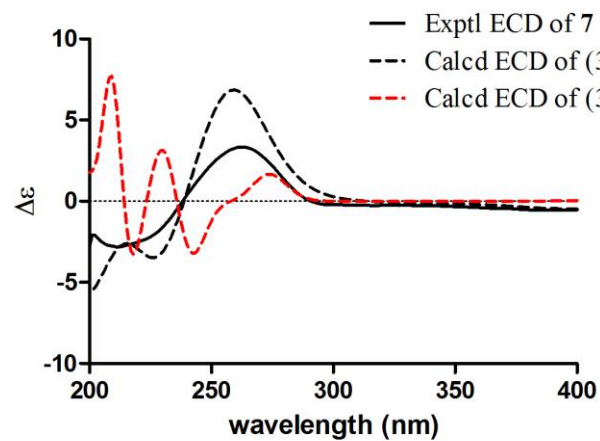
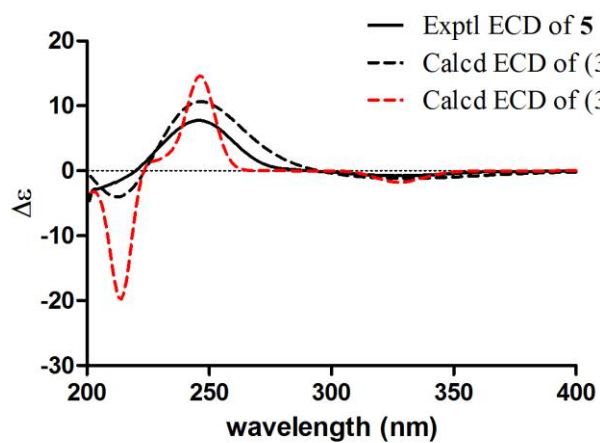


**Figure S103.** The HMBC Spectrum of Compound **13** in  $\text{CDCl}_3$

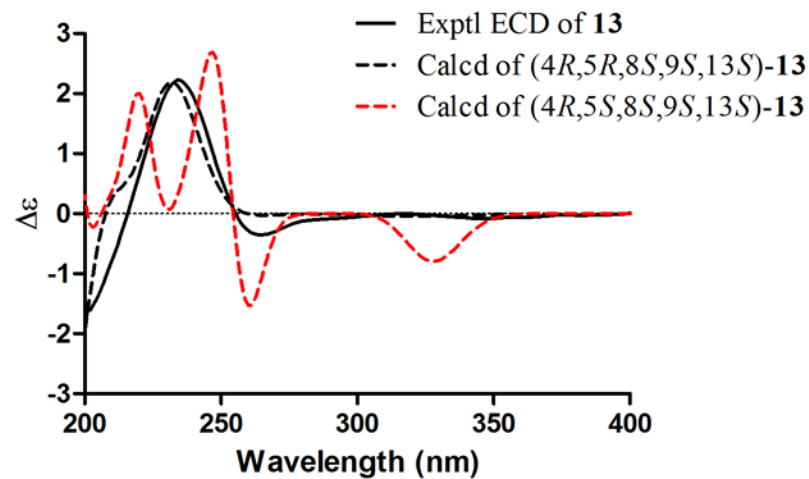
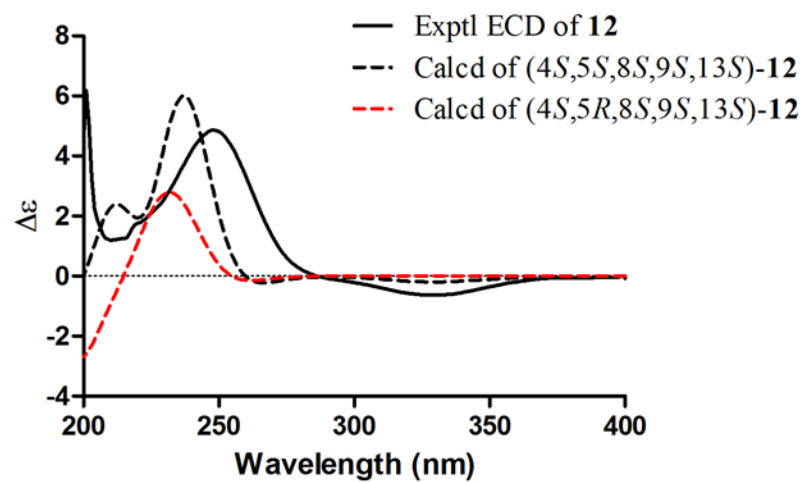




**Figure S104.** The NOESY Spectrum of Compound **13** in CDCl<sub>3</sub>



**Figure S105.** The ECD Spectrum of Compound **5**, **7-9** in MeOH



**Figure S106.** The ECD Spectra of Compounds **12** and **13** in MeOH



**Figure S107.** The Calculated 3D Structures of **12-13**