

## **Supplementary material**

# ***Design, Synthesis and Biological Evaluation of Lophanic acid derivatives as Antifungal Agents and Antibacterial Agents***

Xiang Yu <sup>1,†</sup>, Xun Song <sup>2,3,†</sup>, Yi Zhang <sup>1,†</sup>, Yemeng Yang <sup>3,†</sup>, Jianghai Ye <sup>1</sup>, Yahua Liu <sup>1</sup>, Lutai Pan <sup>1,\*</sup> and Hongjie Zhang <sup>3,\*</sup>

<sup>1</sup>The Key Laboratory of Miao Medicine of Guizhou Province, Guizhou University of Traditional Chinese Medicine, Guiyang 550025, China;

<sup>2</sup>College of Pharmacy, Shenzhen Technology University, Shenzhen 518118, People's Republic of China

<sup>3</sup>School of Chinese Medicine, Hong Kong Baptist University, Hong Kong, People's Republic of China.

<sup>†</sup>These authors contributed equally to this work.

\*Corresponding Author: Lutai Pan, Email: ltpan@sina.cn;  
Hongjie Zhang, Email: zhanghj@hkbu.edu.hk

## Contents

**Figure S1.**  $^1\text{H}$  NMR spectrum of the compound 3a.

**Figure S2.**  $^{13}\text{C}$  NMR spectrum of the compound 3a.

**Figure S3.** HRMS spectrum of the compound 3a.

**Figure S4.**  $^1\text{H}$  NMR spectrum of the compound 3b.

**Figure S5.**  $^{13}\text{C}$  NMR spectrum of the compound 3b.

**Figure S6.** HRMS spectrum of the compound 3b.

**Figure S7.**  $^1\text{H}$  NMR spectrum of the compound 3c.

**Figure S8.**  $^{13}\text{C}$  NMR spectrum of the compound 3c.

**Figure S9.** HRMS spectrum of the compound 3c.

**Figure S10.**  $^1\text{H}$  NMR spectrum of the compound 3d.

**Figure S11.**  $^{13}\text{C}$  NMR spectrum of the compound 3d.

**Figure S12.** HRMS spectrum of the compound 3d.

**Figure S13.**  $^1\text{H}$  NMR spectrum of the compound 3e.

**Figure S14.**  $^{13}\text{C}$  NMR spectrum of the compound 3e.

**Figure S15.** HRMS spectrum of the compound 3e.

**Figure S16.**  $^1\text{H}$  NMR spectrum of the compound 3f.

**Figure S17.**  $^{13}\text{C}$  NMR spectrum of the compound 3f.

**Figure S18.** HRMS spectrum of the compound 3f.

**Figure S19.**  $^1\text{H}$  NMR spectrum of the compound 3g.

**Figure S20.**  $^{13}\text{C}$  NMR spectrum of the compound 3g.

**Figure S21.** HRMS spectrum of the compound 3g.

**Figure S22.**  $^1\text{H}$  NMR spectrum of the compound **3h**.

**Figure S23.**  $^{13}\text{C}$  NMR spectrum of the compound **3h**.

**Figure S24.** HRMS spectrum of the compound **3h**.

**Figure S25.**  $^1\text{H}$  NMR spectrum of the compound **3i**.

**Figure S26.**  $^{13}\text{C}$  NMR spectrum of the compound **3i**.

**Figure S27.** HRMS spectrum of the compound **3i**.

**Figure S28.**  $^1\text{H}$  NMR spectrum of the compound **3j**.

**Figure S29.**  $^{13}\text{C}$  NMR spectrum of the compound **3j**.

**Figure S30.** HRMS spectrum of the compound **3j**.

**Figure S31.**  $^1\text{H}$  NMR spectrum of the compound **3k**.

**Figure S32.**  $^{13}\text{C}$  NMR spectrum of the compound **3k**.

**Figure S33.** HRMS spectrum of the compound **3k**.

**Figure S34.**  $^1\text{H}$  NMR spectrum of the compound **3l**.

**Figure S35.**  $^{13}\text{C}$  NMR spectrum of the compound **3l**.

**Figure S36.** HRMS spectrum of the compound **3l**.

**Figure S37.**  $^1\text{H}$  NMR spectrum of the compound **3m**.

**Figure S38.**  $^{13}\text{C}$  NMR spectrum of the compound **3m**.

**Figure S39.** HRMS spectrum of the compound **3m**.

**Figure S40.**  $^1\text{H}$  NMR spectrum of the compound **3n**.

**Figure S41.**  $^{13}\text{C}$  NMR spectrum of the compound **3n**.

**Figure S42.** HRMS spectrum of the compound **3n**.

**Figure S43.**  $^1\text{H}$  NMR spectrum of the compound **4**.

**Figure S44.**  $^{13}\text{C}$  NMR spectrum of the compound 4.

**Figure S45.** HRMS spectrum of the compound 4.

**Figure S46.**  $^1\text{H}$  NMR spectrum of the compound 5a.

**Figure S47.**  $^{13}\text{C}$  NMR spectrum of the compound 5a.

**Figure S48.** HRMS spectrum of the compound 5a.

**Figure S49.**  $^1\text{H}$  NMR spectrum of the compound 5b.

**Figure S50.**  $^{13}\text{C}$  NMR spectrum of the compound 5b.

**Figure S51.** HRMS spectrum of the compound 5b.

**Figure S52.**  $^1\text{H}$  NMR spectrum of the compound 5c.

**Figure S53.**  $^{13}\text{C}$  NMR spectrum of the compound 5c.

**Figure S54.** HRMS spectrum of the compound 5c.

**Figure S55.**  $^1\text{H}$  NMR spectrum of the compound 5d.

**Figure S56.**  $^{13}\text{C}$  NMR spectrum of the compound 5d.

**Figure S57.** HRMS spectrum of the compound 5d.

**Figure S58.**  $^1\text{H}$  NMR spectrum of the compound 5e.

**Figure S59.**  $^{13}\text{C}$  NMR spectrum of the compound 5e.

**Figure S60.** HRMS spectrum of the compound 5e.

**Figure S61.**  $^1\text{H}$  NMR spectrum of the compound 5f.

**Figure S62.**  $^{13}\text{C}$  NMR spectrum of the compound 5f.

**Figure S63.** HRMS spectrum of the compound 5f.

**Figure S64.**  $^1\text{H}$  NMR spectrum of the compound 5g.

**Figure S65.**  $^{13}\text{C}$  NMR spectrum of the compound 5g.

**Figure S66.** HRMS spectrum of the compound **5g**.

**Figure S67.**  $^1\text{H}$  NMR spectrum of the compound **5h**.

**Figure S68.**  $^{13}\text{C}$  NMR spectrum of the compound **5h**.

**Figure S69.** HRMS spectrum of the compound **5h**.

**Figure S70.**  $^1\text{H}$  NMR spectrum of the compound **6a**.

**Figure S71.**  $^{13}\text{C}$  NMR spectrum of the compound **6a**.

**Figure S72.** HRMS spectrum of the compound **6a**.

**Figure S73.**  $^1\text{H}$  NMR spectrum of the compound **6b**.

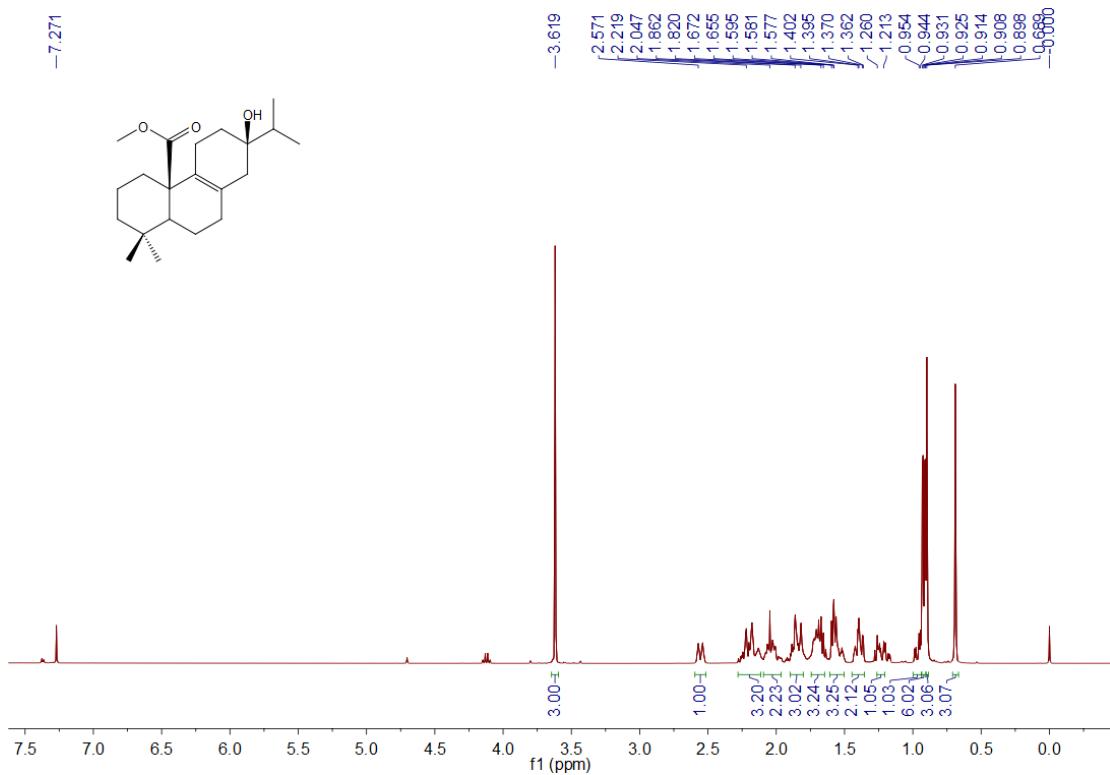
**Figure S74.**  $^{13}\text{C}$  NMR spectrum of the compound **6b**.

**Figure S75.** HRMS spectrum of the compound **6b**.

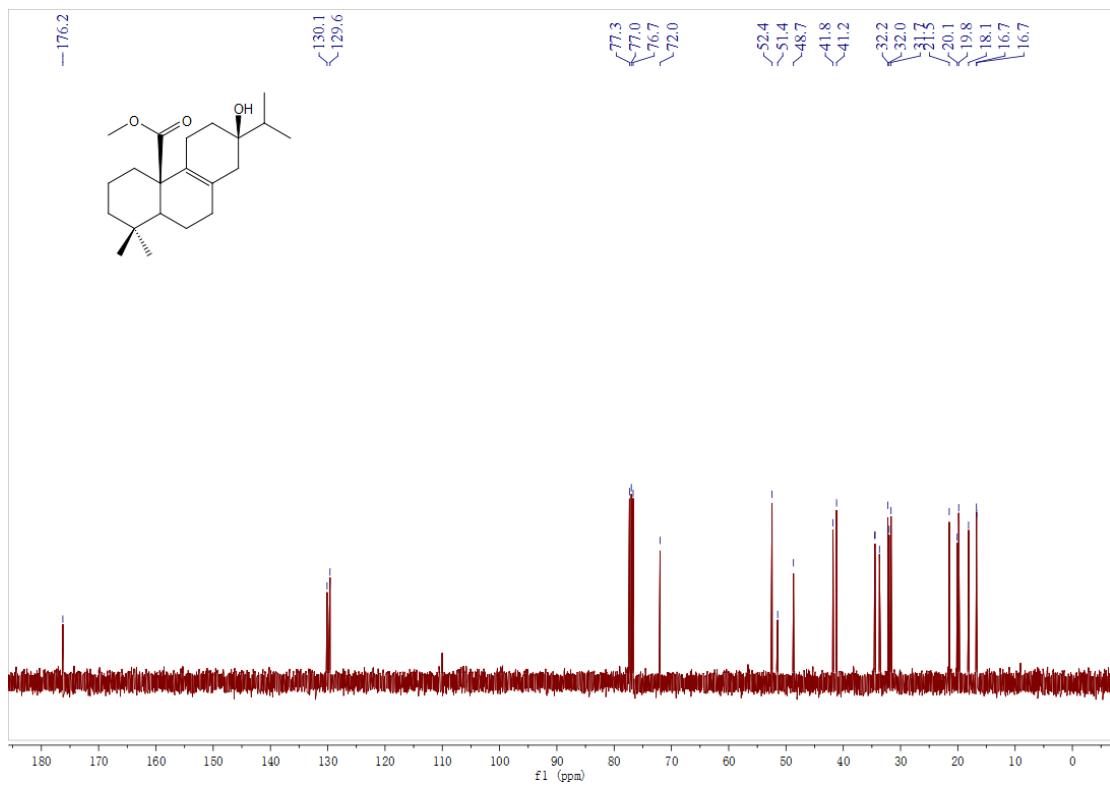
**Figure S76.**  $^1\text{H}$  NMR spectrum of the compound **6c**.

**Figure S77.**  $^{13}\text{C}$  NMR spectrum of the compound **6c**.

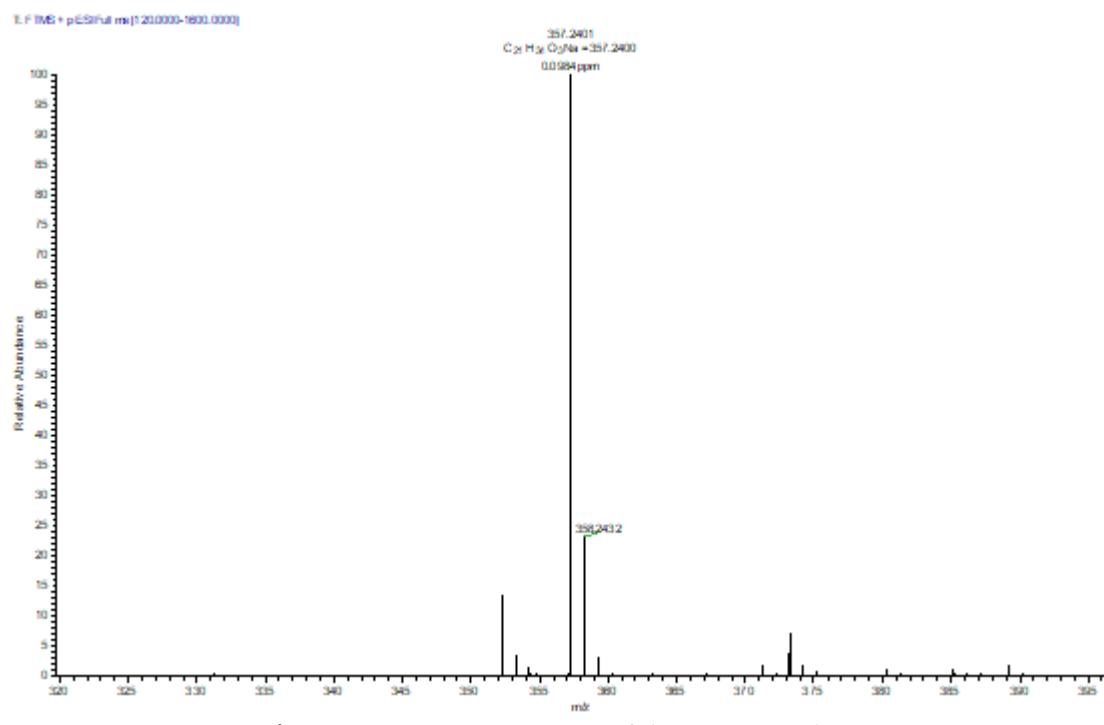
**Figure S78.** HRMS spectrum of the compound **6c**.



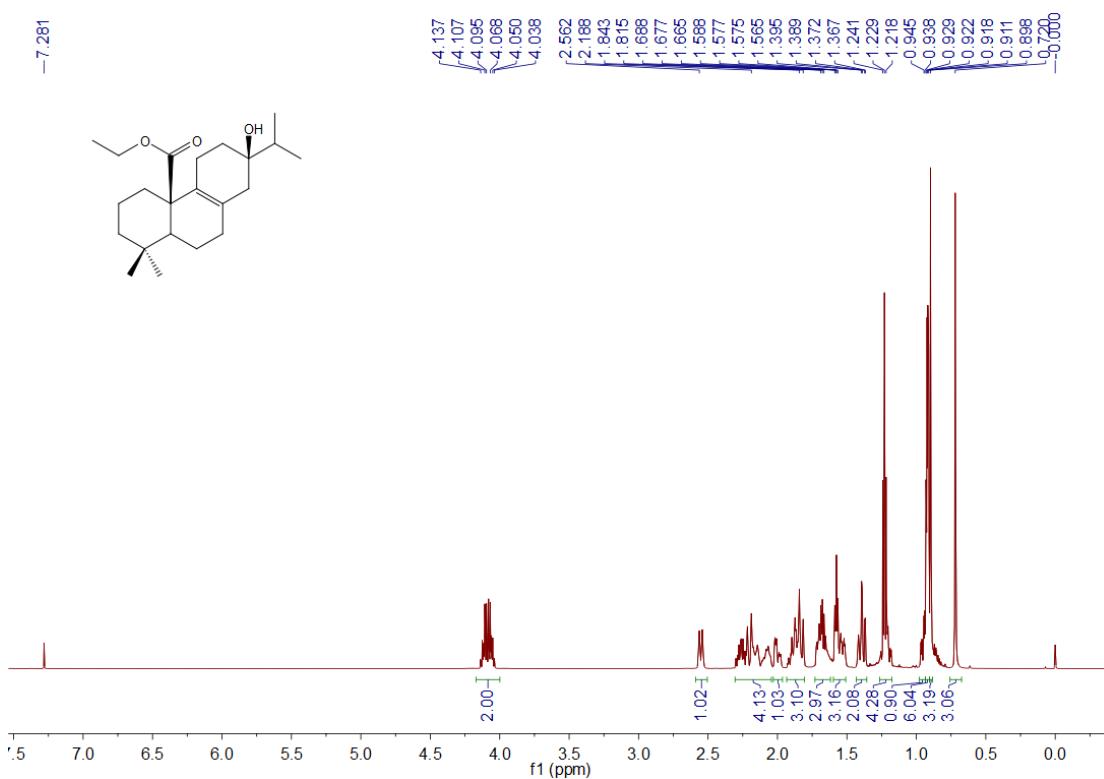
**Figure S1.** <sup>1</sup>H NMR spectrum of the compound 3a.



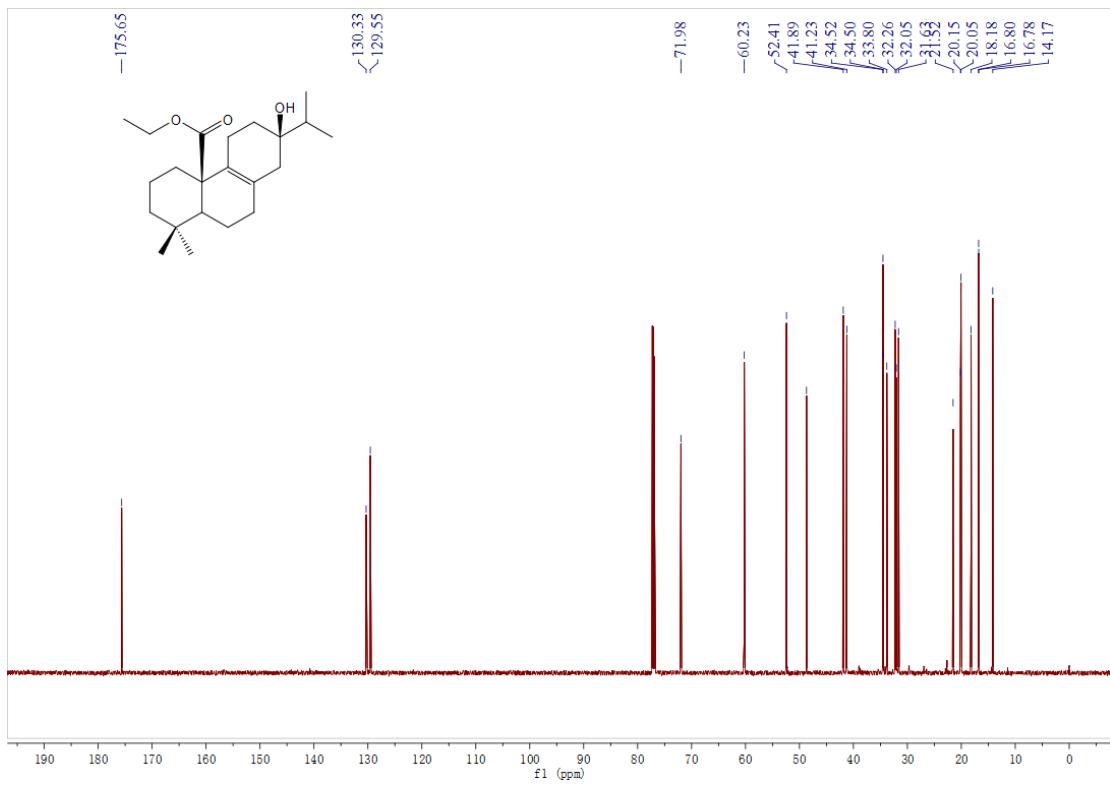
**Figure S2.** <sup>13</sup>C NMR spectrum of the compound 3a.



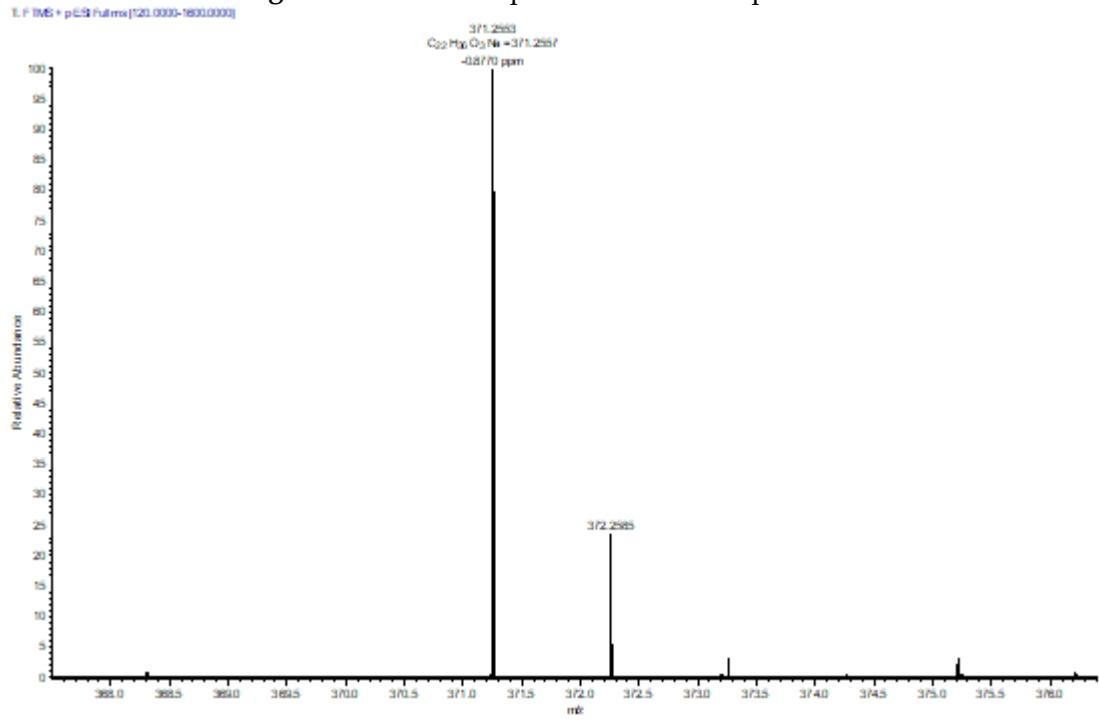
**Figure S3.** HRMS spectrum of the compound **3a**.



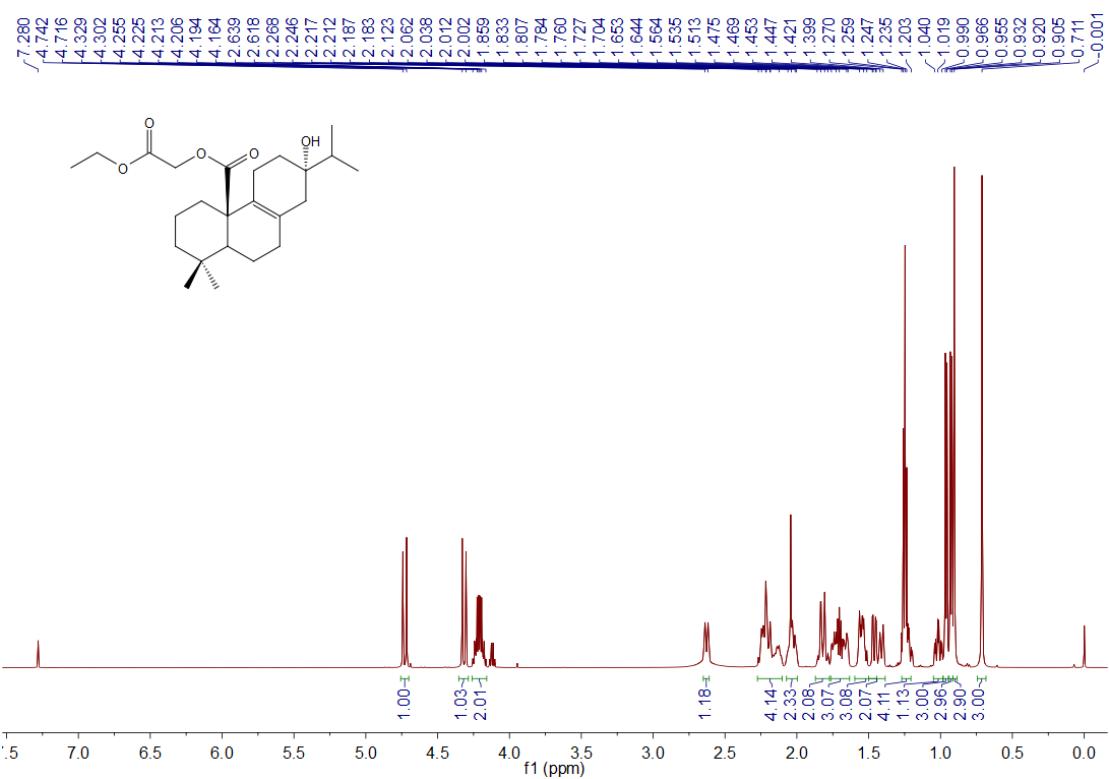
**Figure S4.**  $^1\text{H}$  NMR spectrum of the compound **3b**.



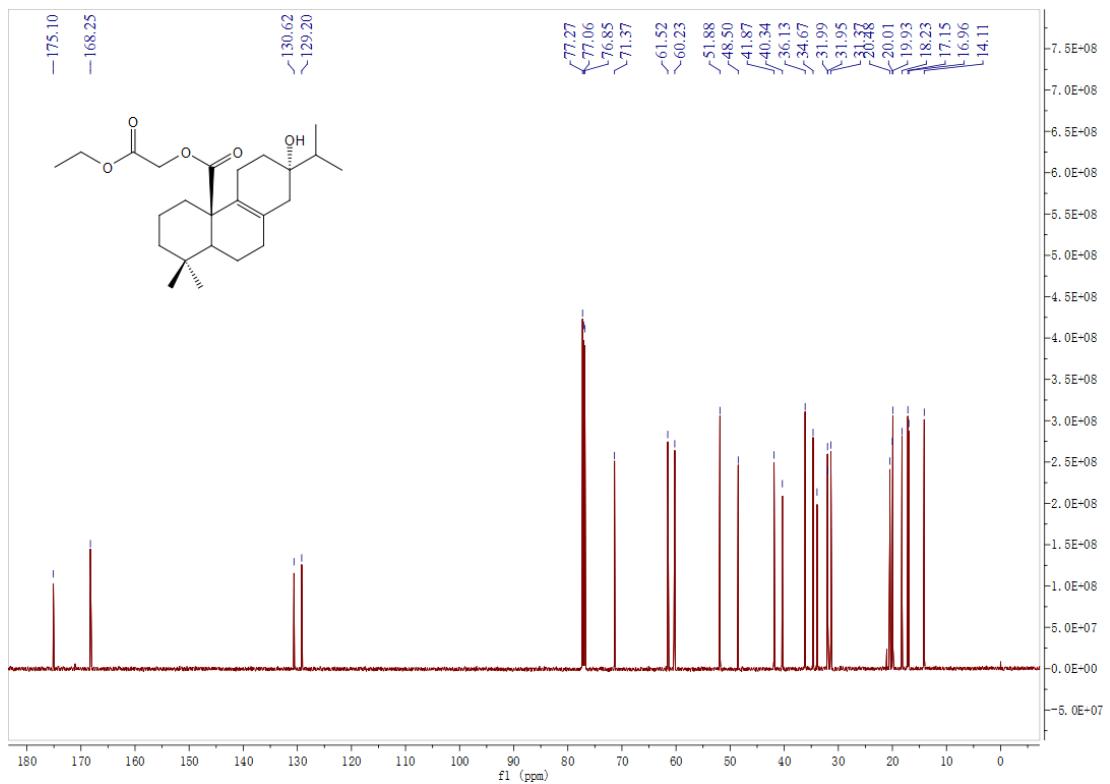
**Figure S5.**  $^{13}\text{C}$  NMR spectrum of the compound **3b**.



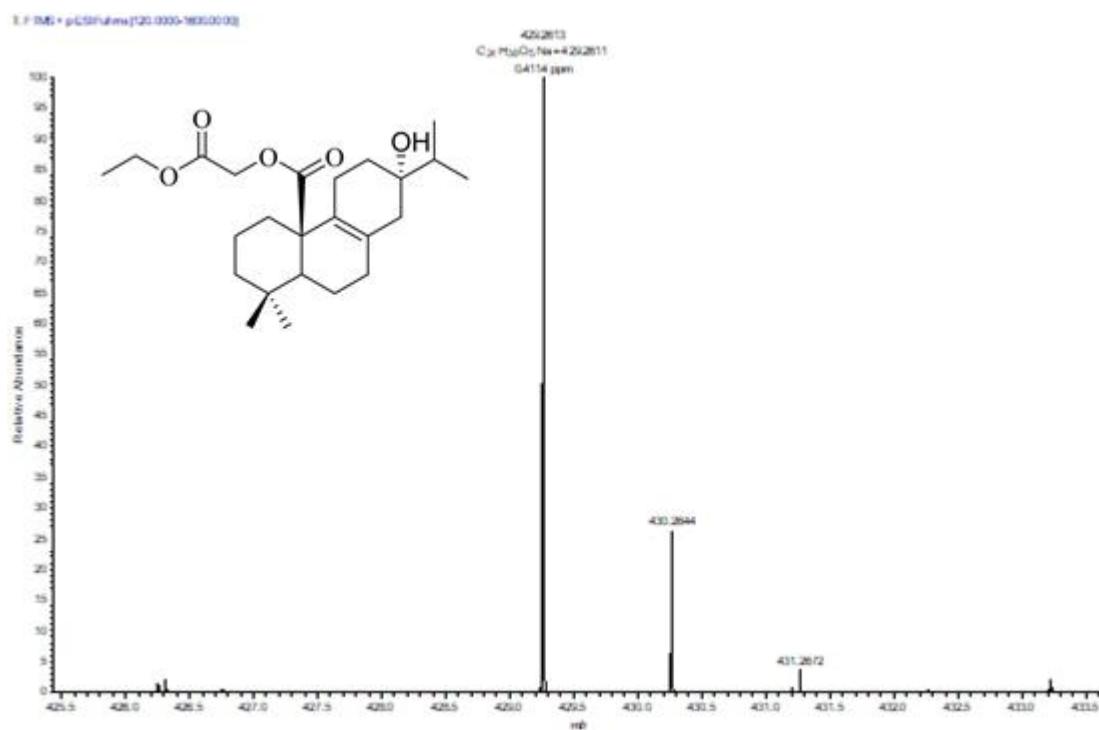
**Figure S6.** HRMS spectrum of the compound **3b**.



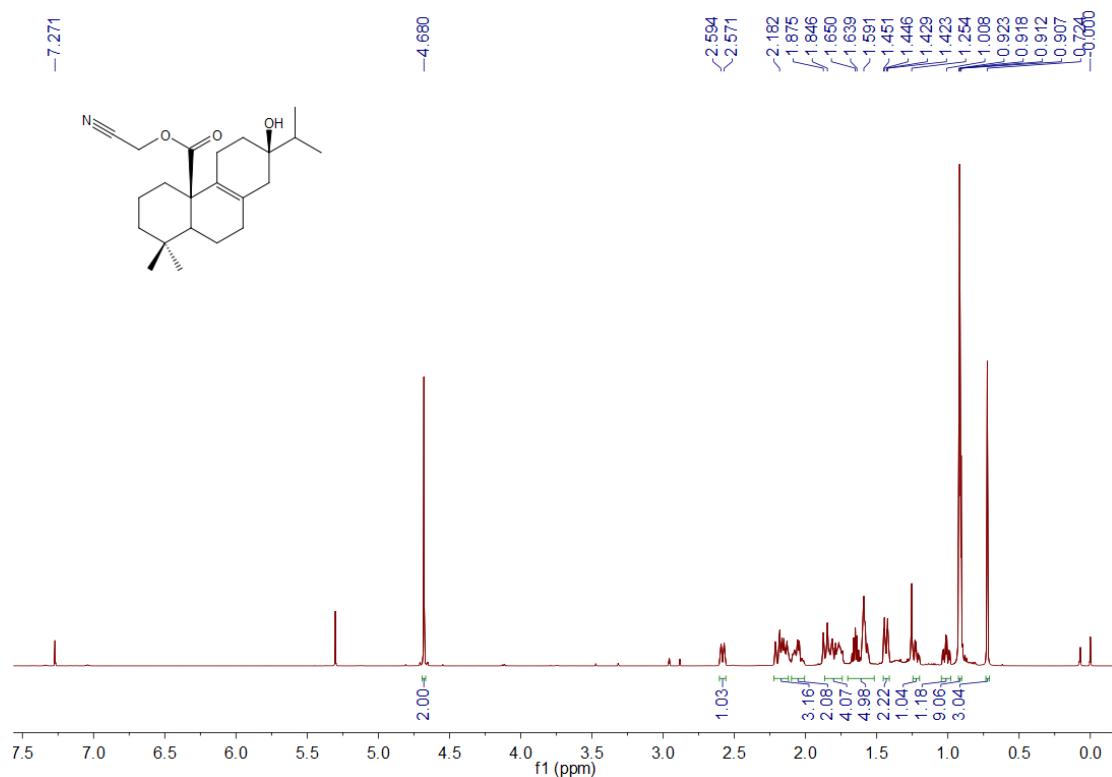
**Figure S7.** <sup>1</sup>H NMR spectrum of the compound 3c.



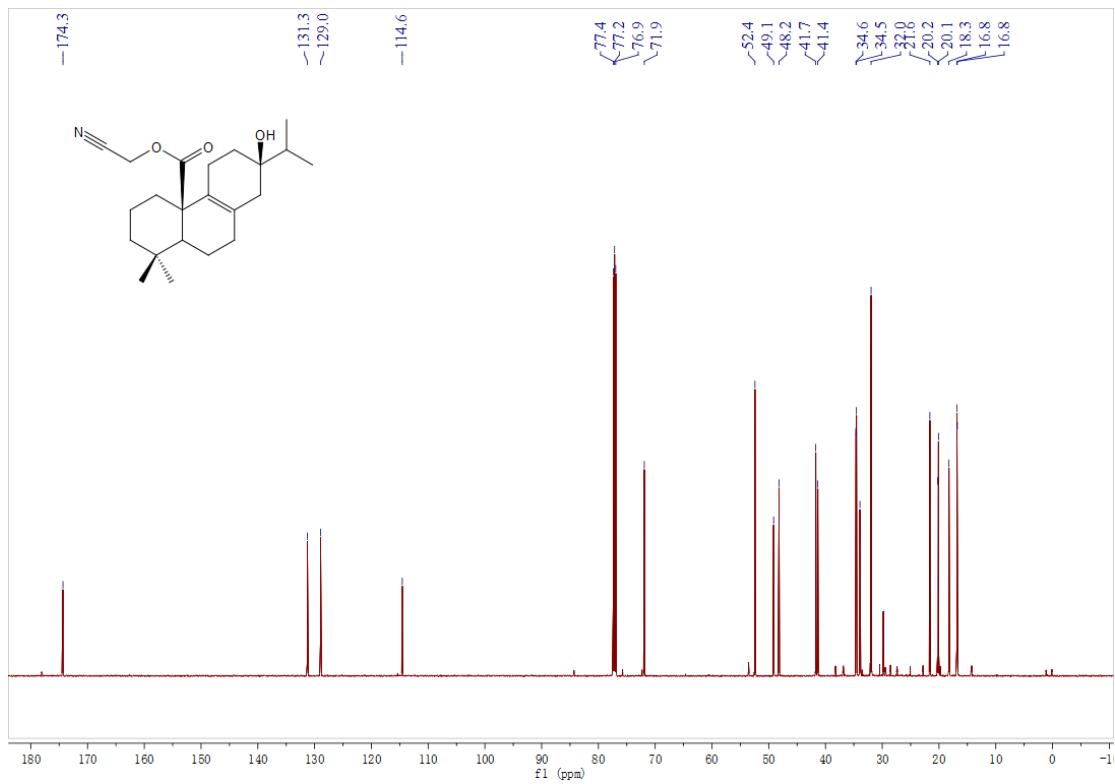
**Figure S8.** <sup>13</sup>C NMR spectrum of the compound 3c.



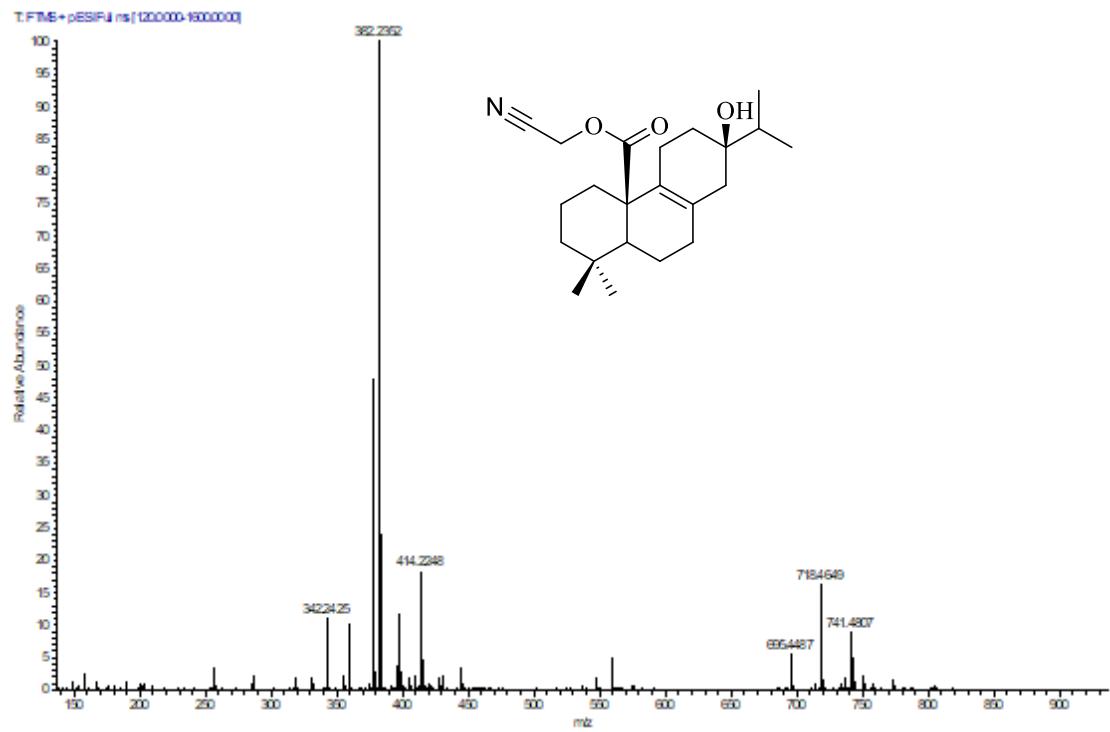
**Figure S9.** HRMS spectrum of the compound **3c**.



**Figure S10.**  $^1\text{H}$  NMR spectrum of the compound **3d**.



**Figure S11.**  $^{13}\text{C}$  NMR spectrum of the compound 3d.



**Figure S12.** HRMS spectrum of the compound 3d.

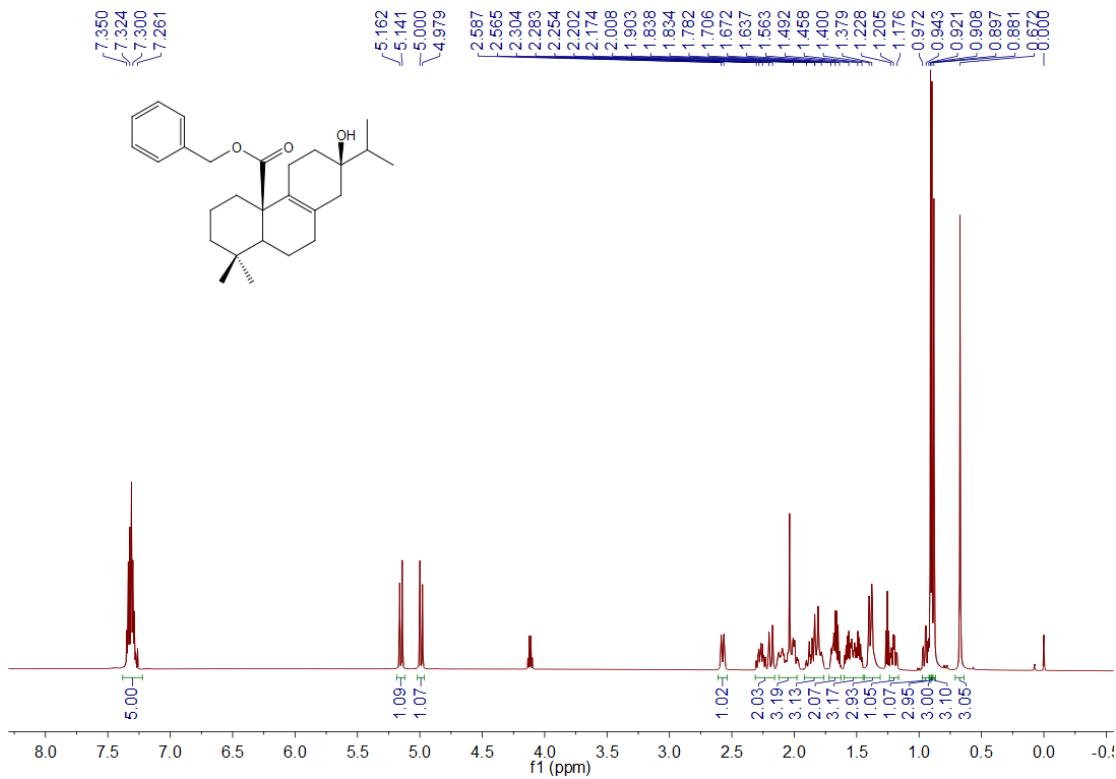


Figure S13. <sup>1</sup>H NMR spectrum of the compound 3e.

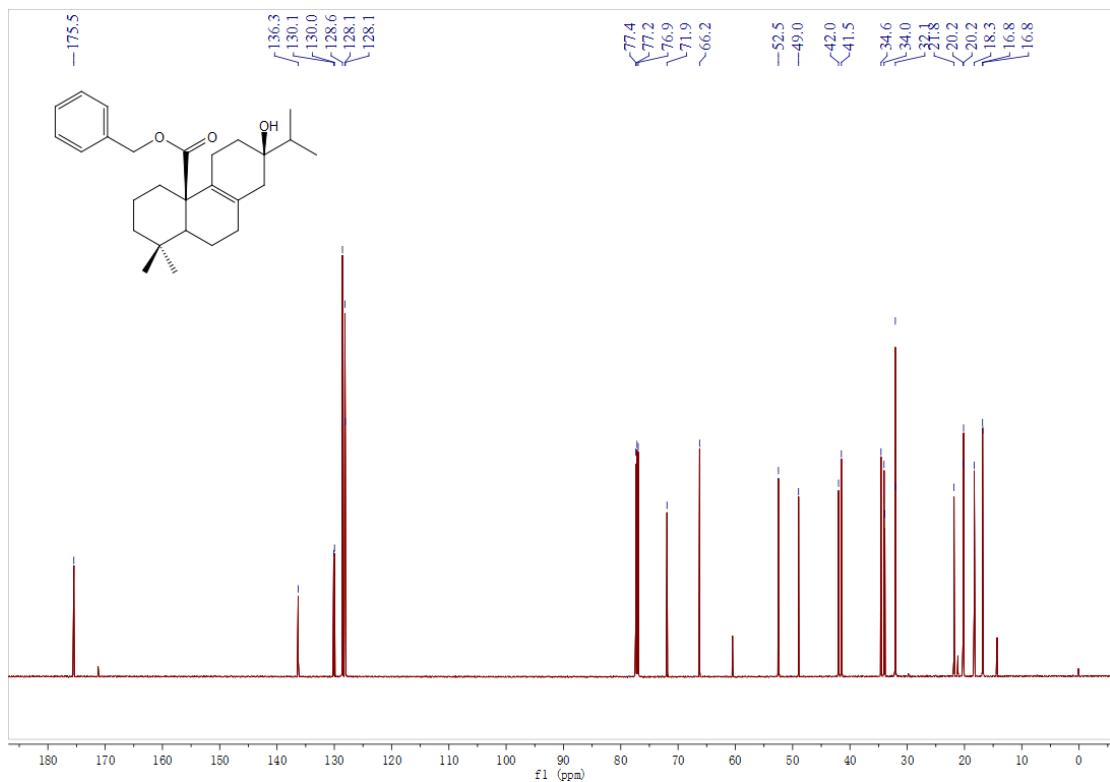


Figure S14. <sup>13</sup>C NMR spectrum of the compound 3e.

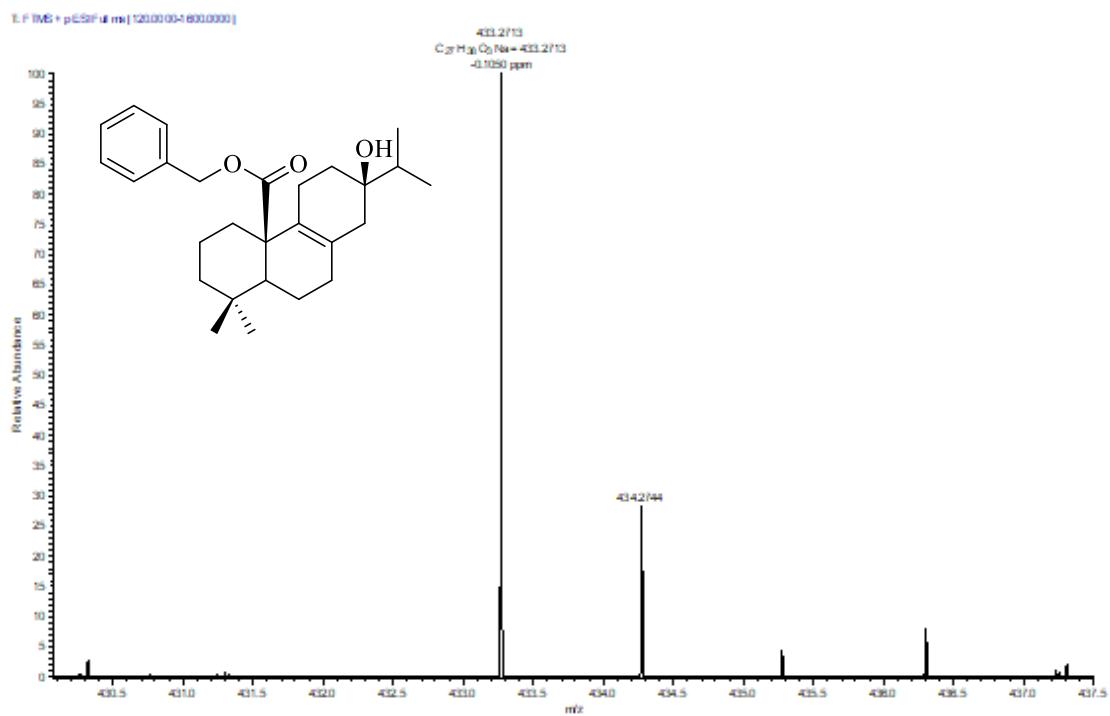


Figure S15. HRMS spectrum of the compound 3e.

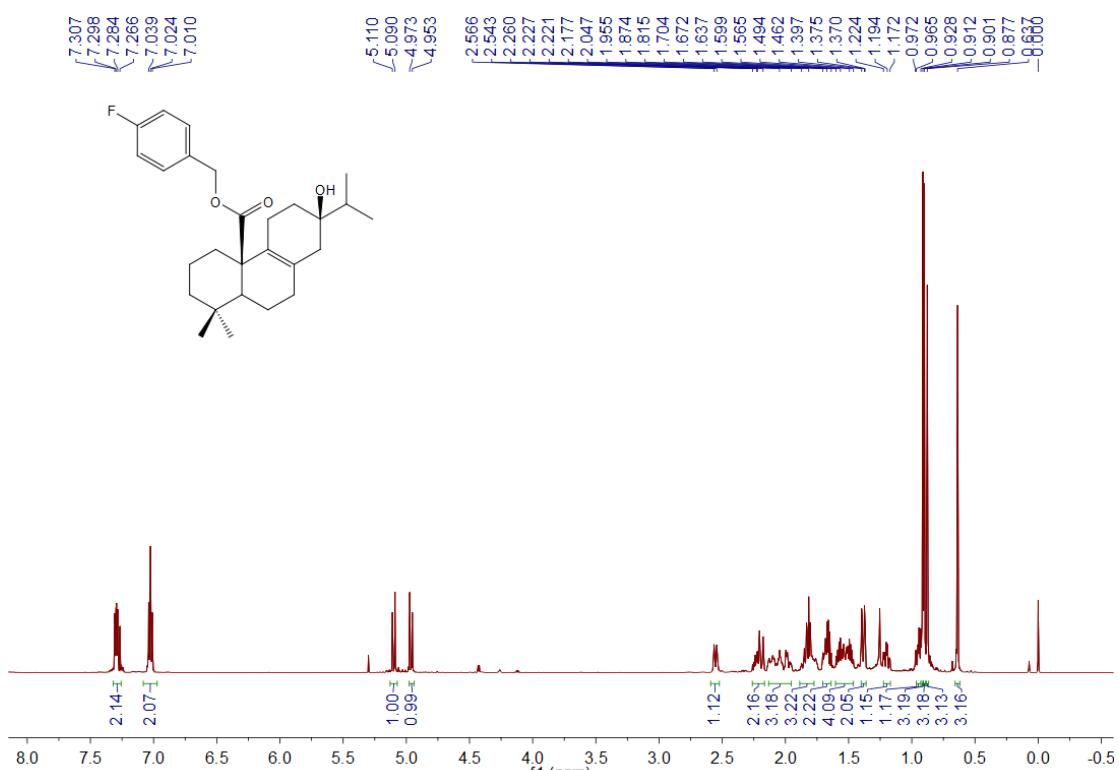
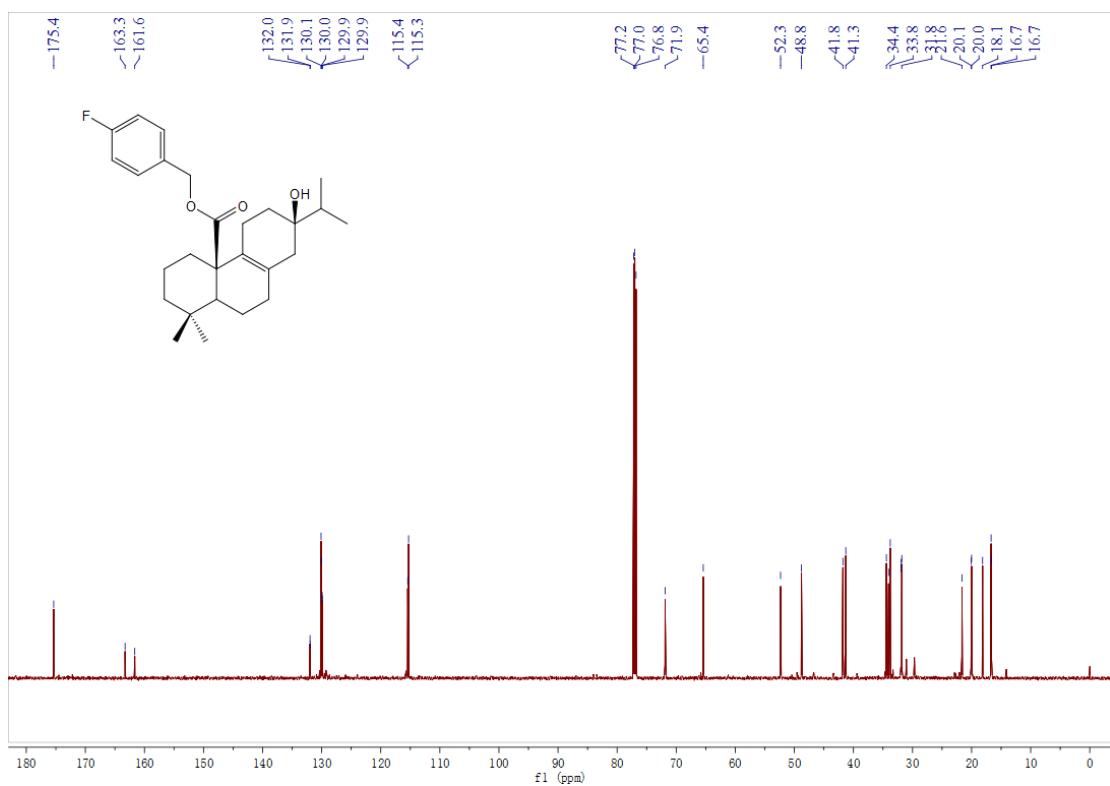
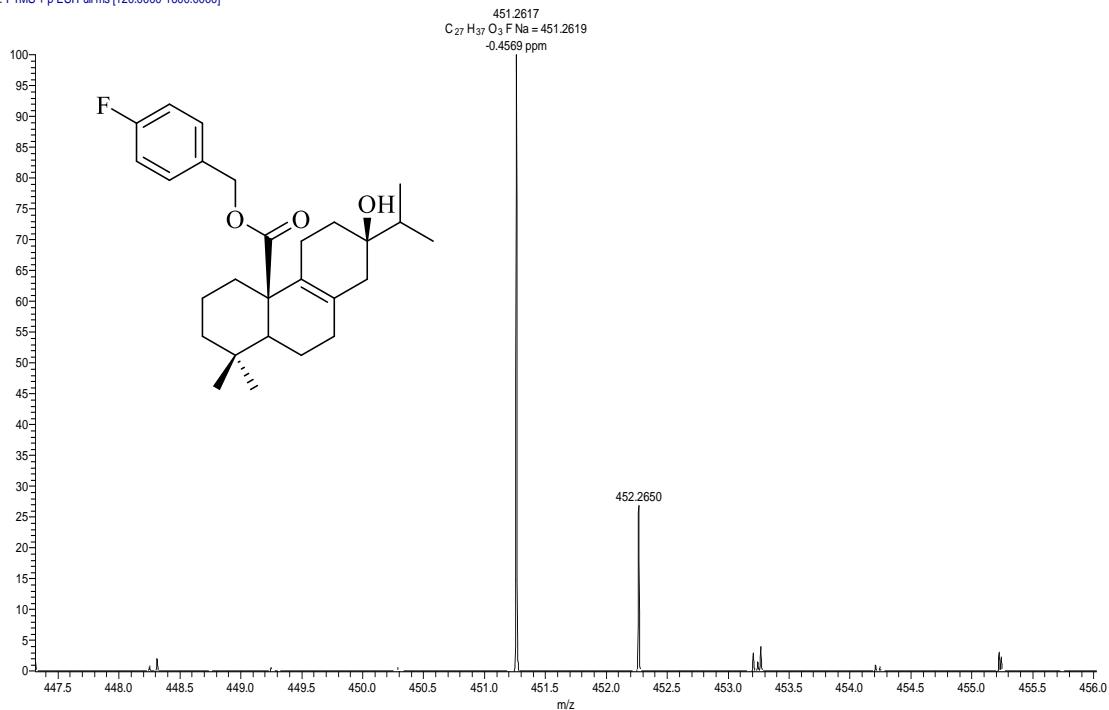


Figure S16.  $^1\text{H}$  NMR spectrum of the compound 3f.

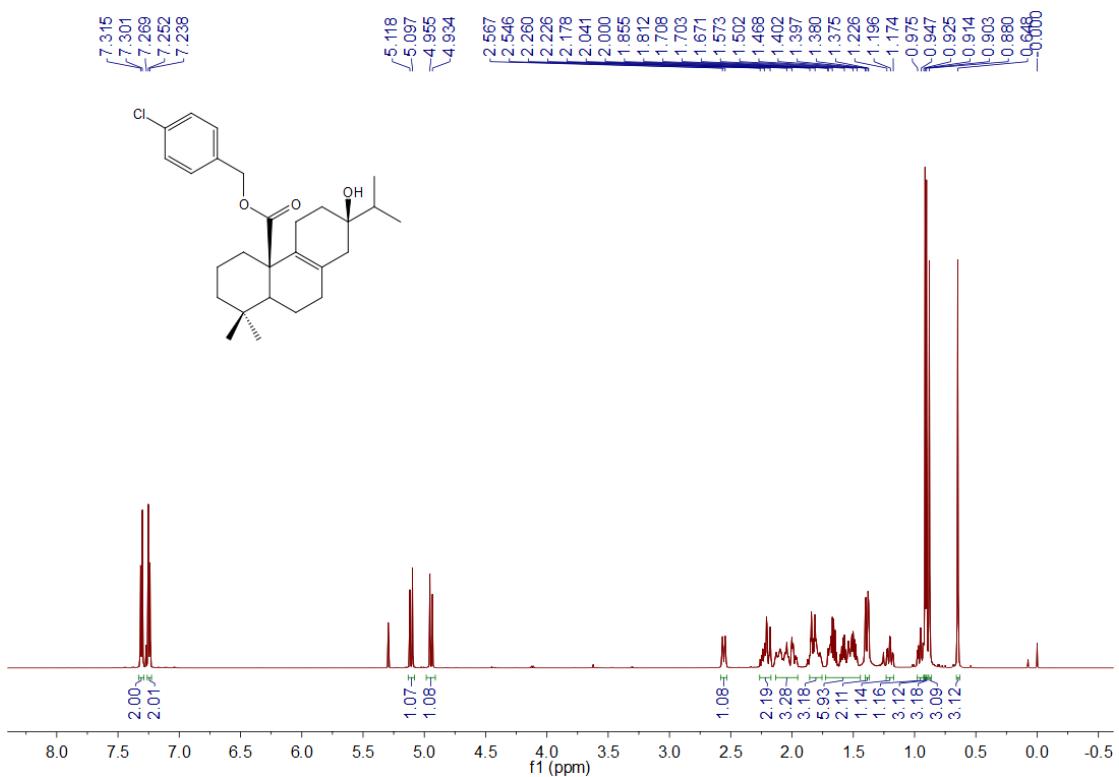


**Figure S17.**  $^{13}\text{C}$  NMR spectrum of the compound 3f.

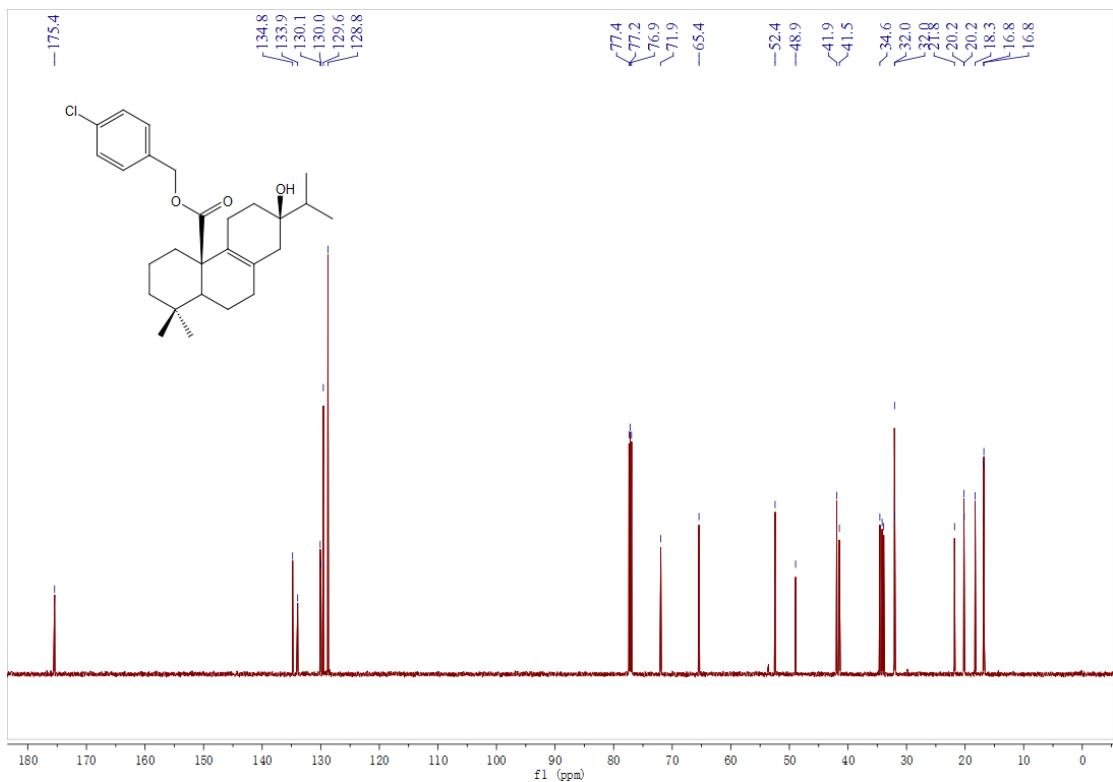
Y-58 #39 RT: 0.17 AV: 1 NL: 6.72E5  
T: FTMS + p ESI Full ms [120.0000-1600.0000]



**Figure S18.** HRMS spectrum of the compound 3f.



**Figure S19.** <sup>1</sup>H NMR spectrum of the compound 3g.



**Figure S20.** <sup>13</sup>C NMR spectrum of the compound 3g.

Y-59#40 RT: 0.18 AV: 1 NL: 6.77E8  
T: FTMS + p ESI Full ms [120.0000-1600.0000]

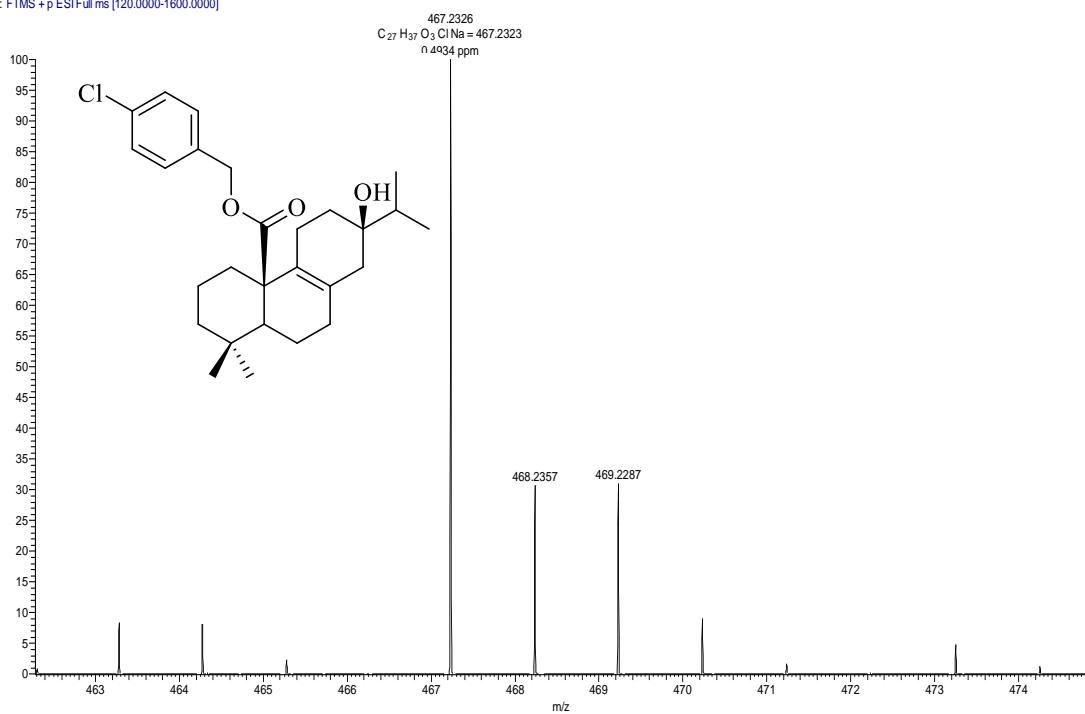


Figure S21. HRMS spectrum of the compound 3g.

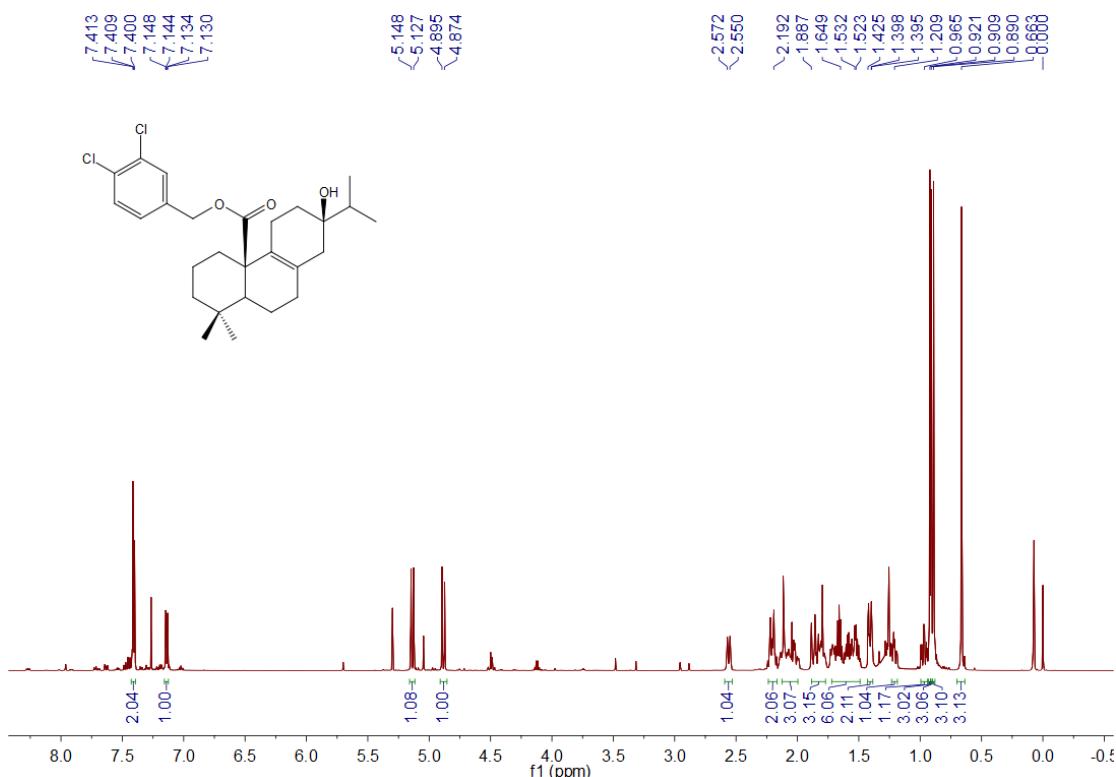
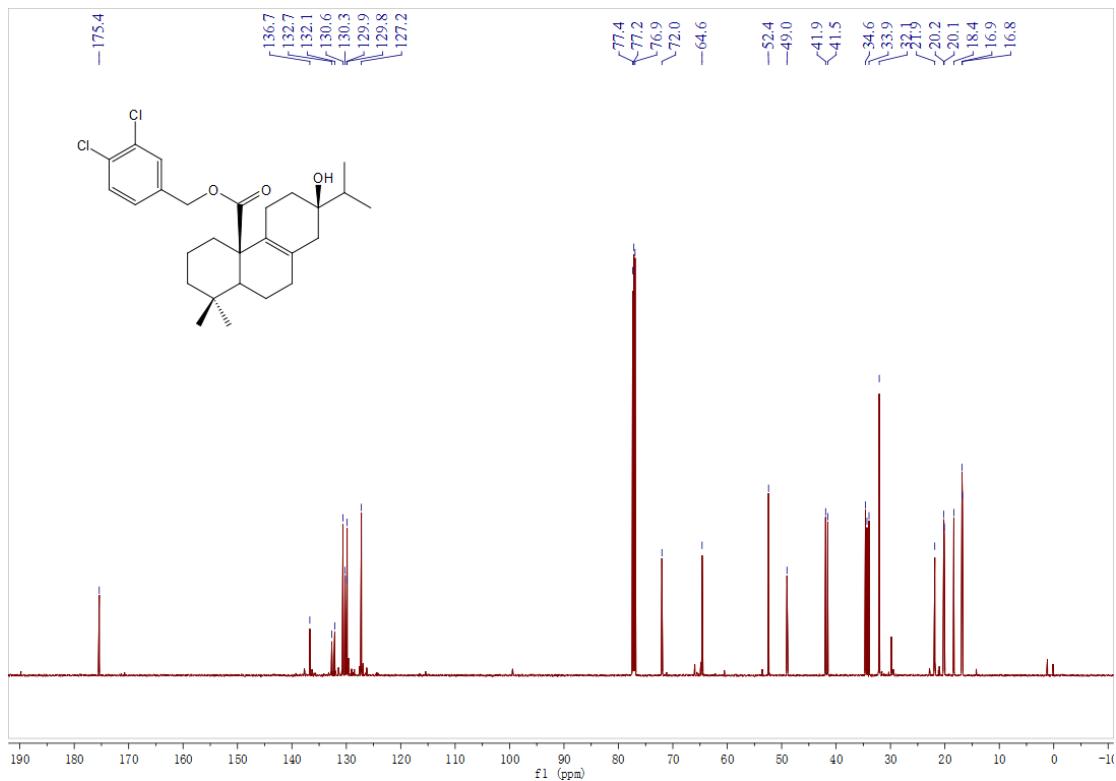
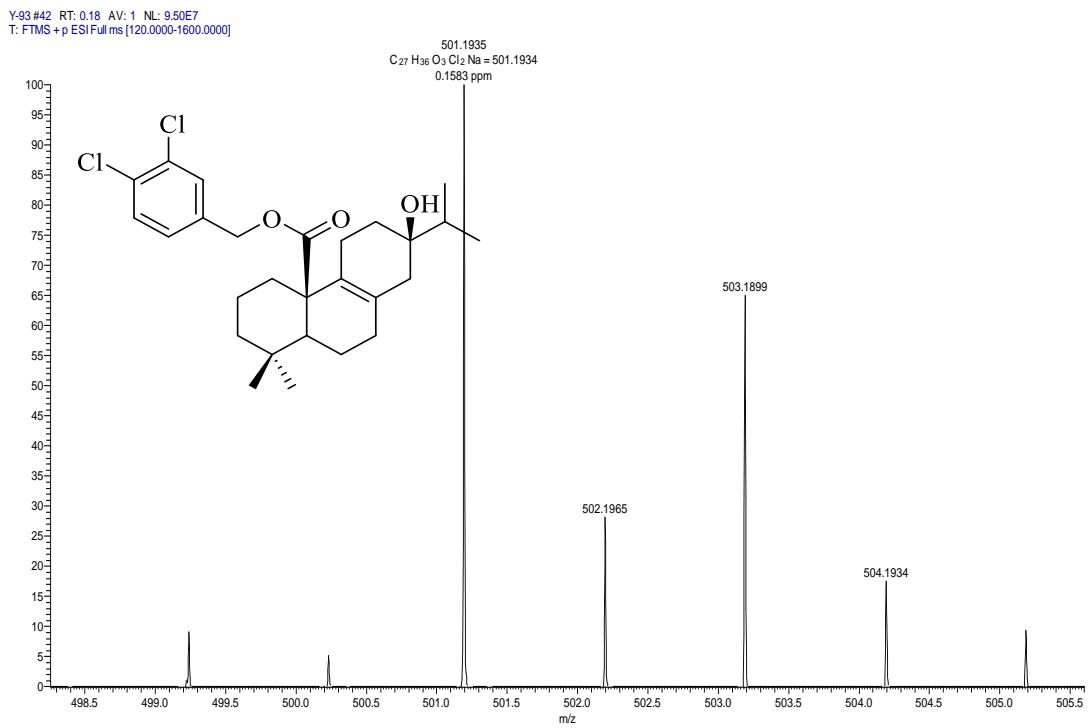


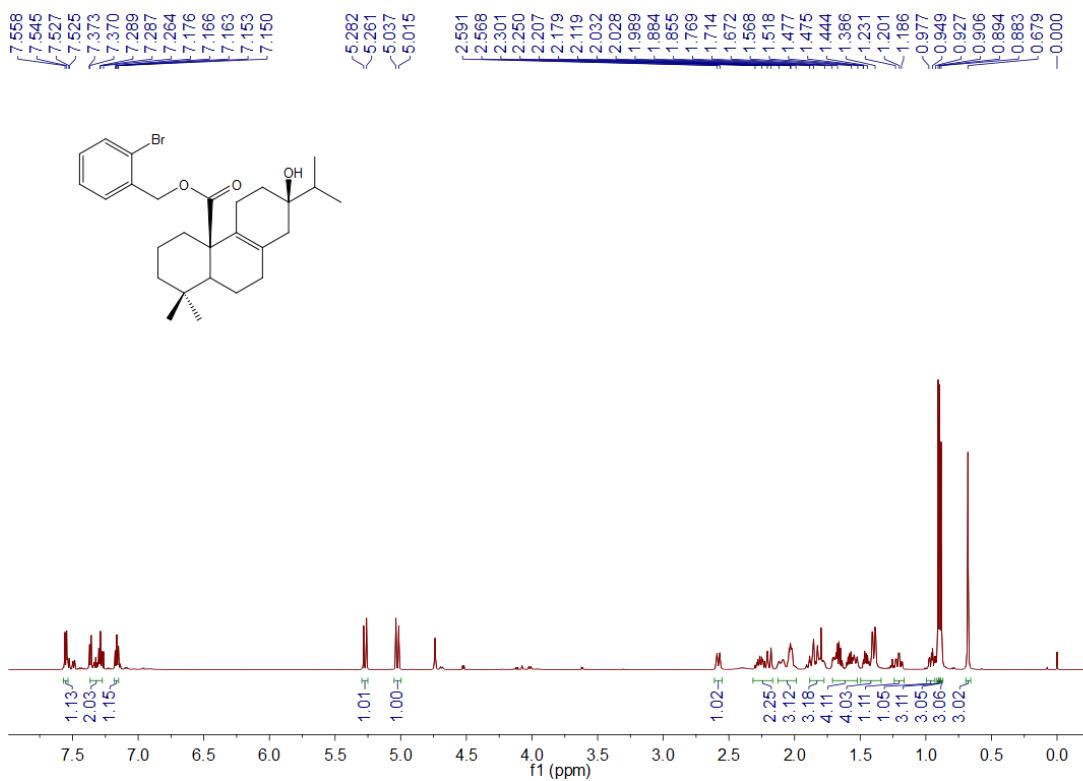
Figure S22.  $^1\text{H}$  NMR spectrum of the compound 3h.



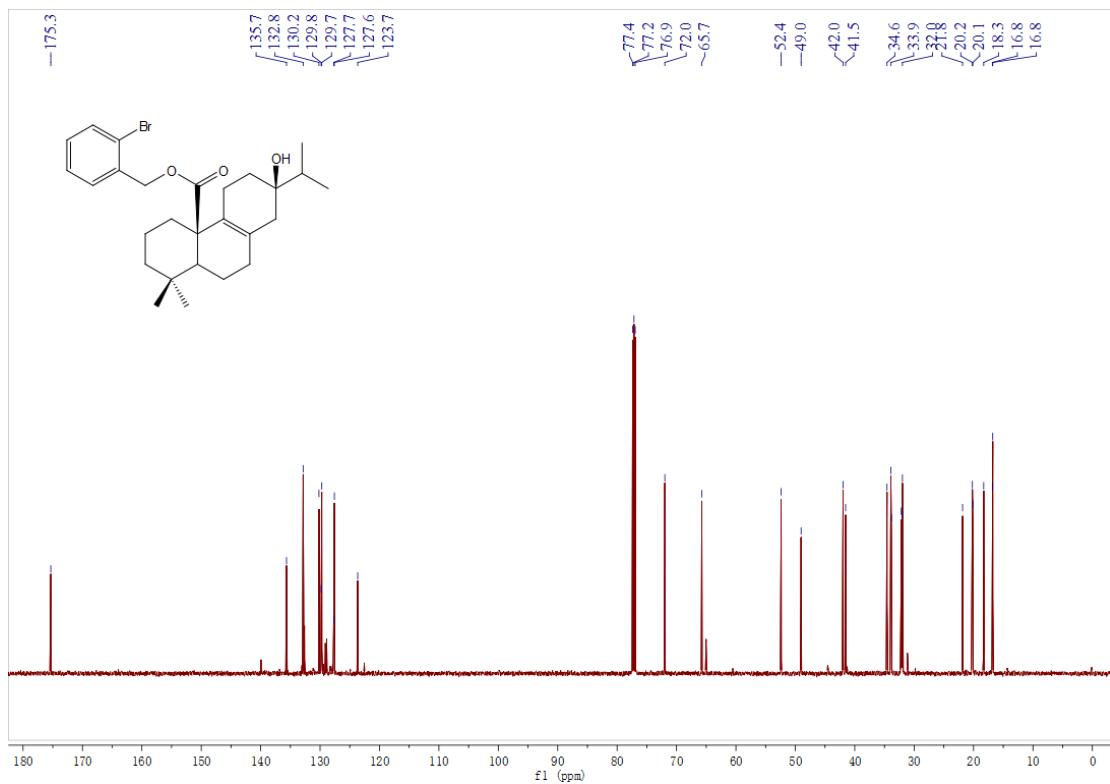
**Figure S23.**  $^{13}\text{C}$  NMR spectrum of the compound **3h**.



**Figure S24.** HRMS spectrum of the compound **3h**.



**Figure S25.** <sup>1</sup>H NMR spectrum of the compound 3i.



**Figure S26.** <sup>13</sup>C NMR spectrum of the compound 3i.

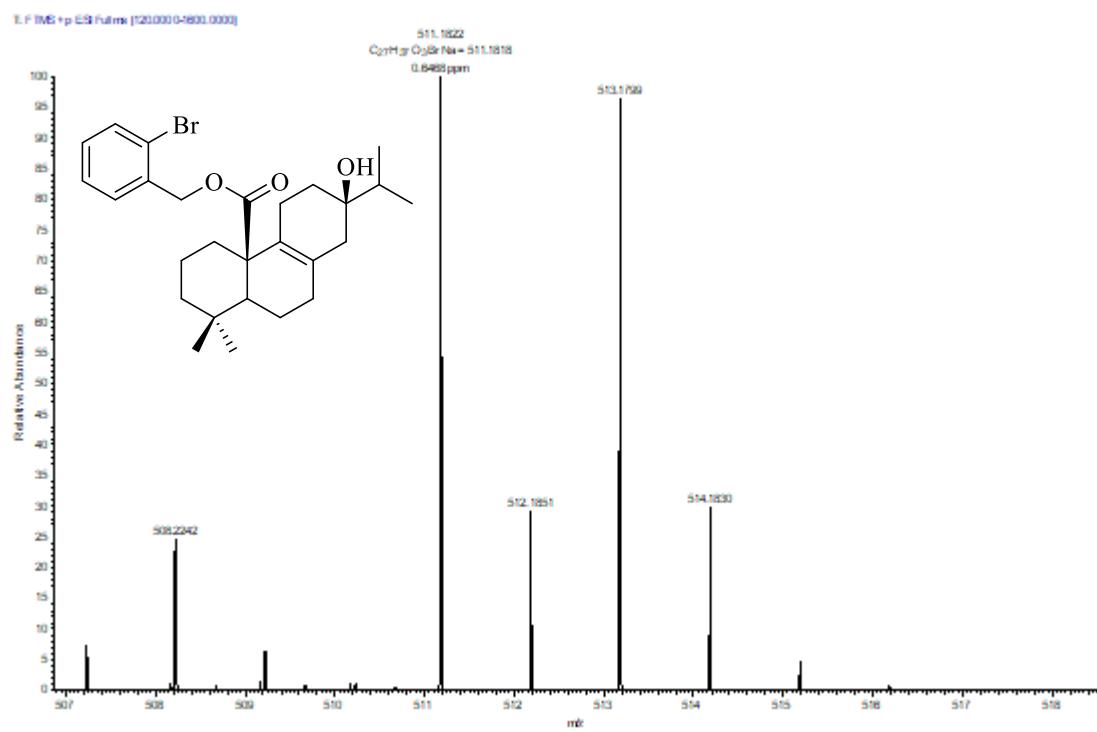


Figure S27. HRMS spectrum of the compound 3i.

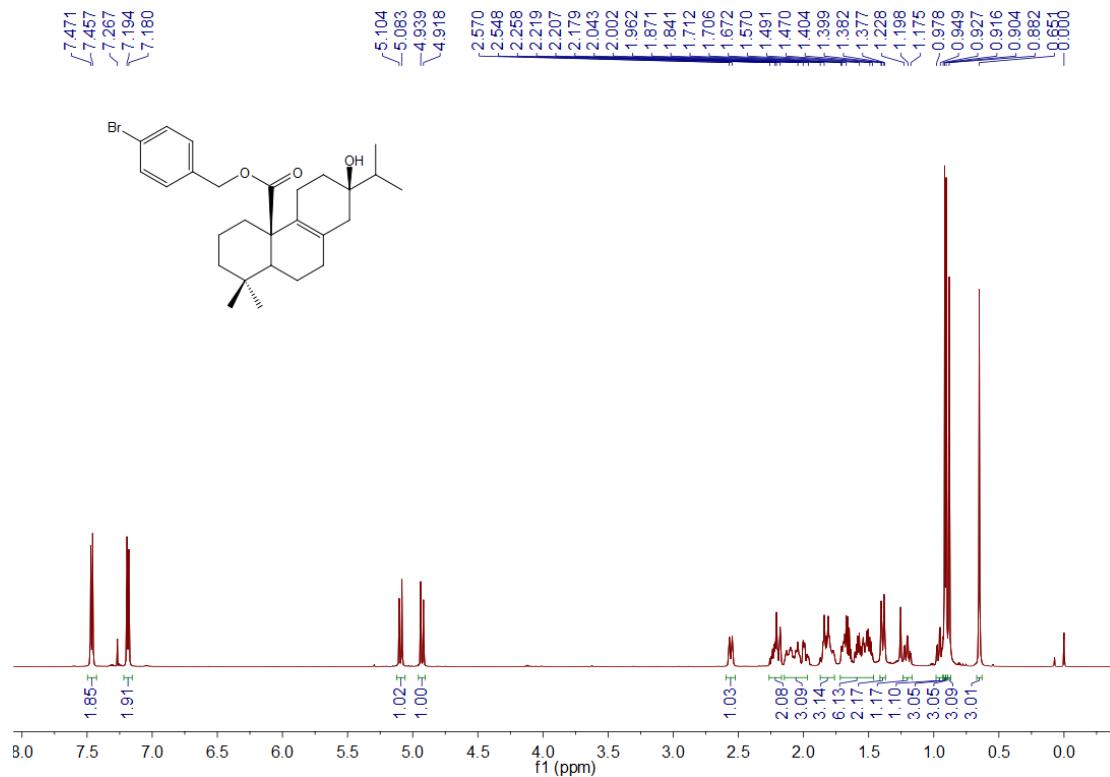
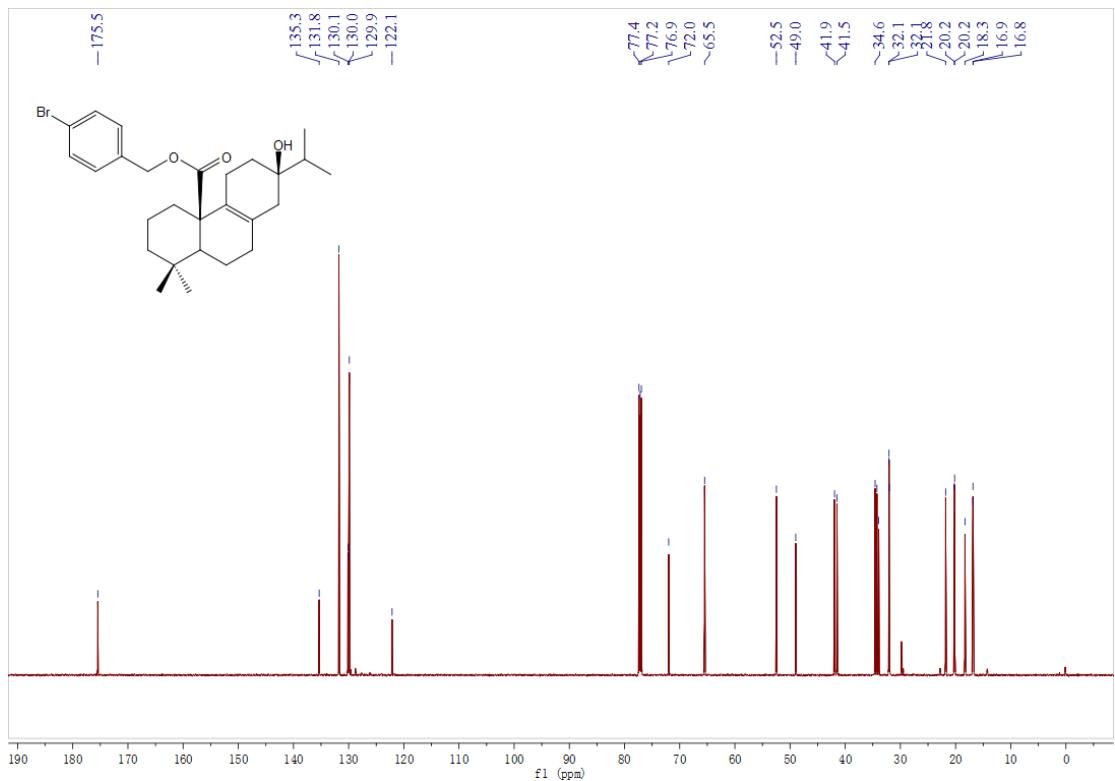
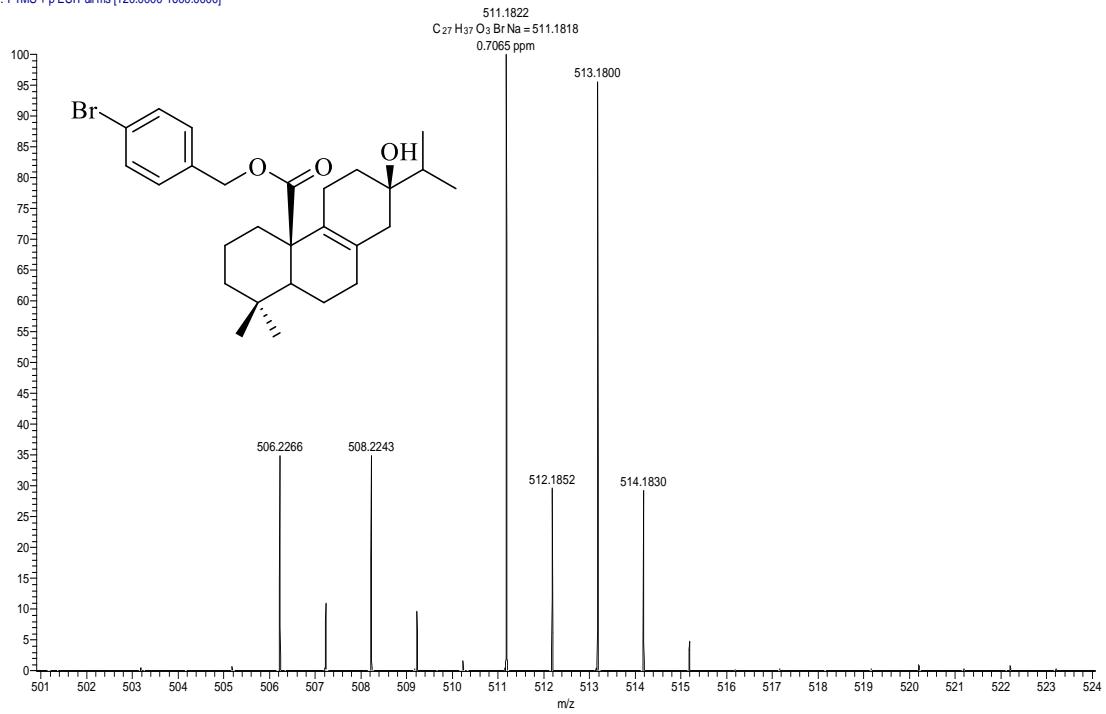


Figure S28.  $^1\text{H}$  NMR spectrum of the compound 3j.

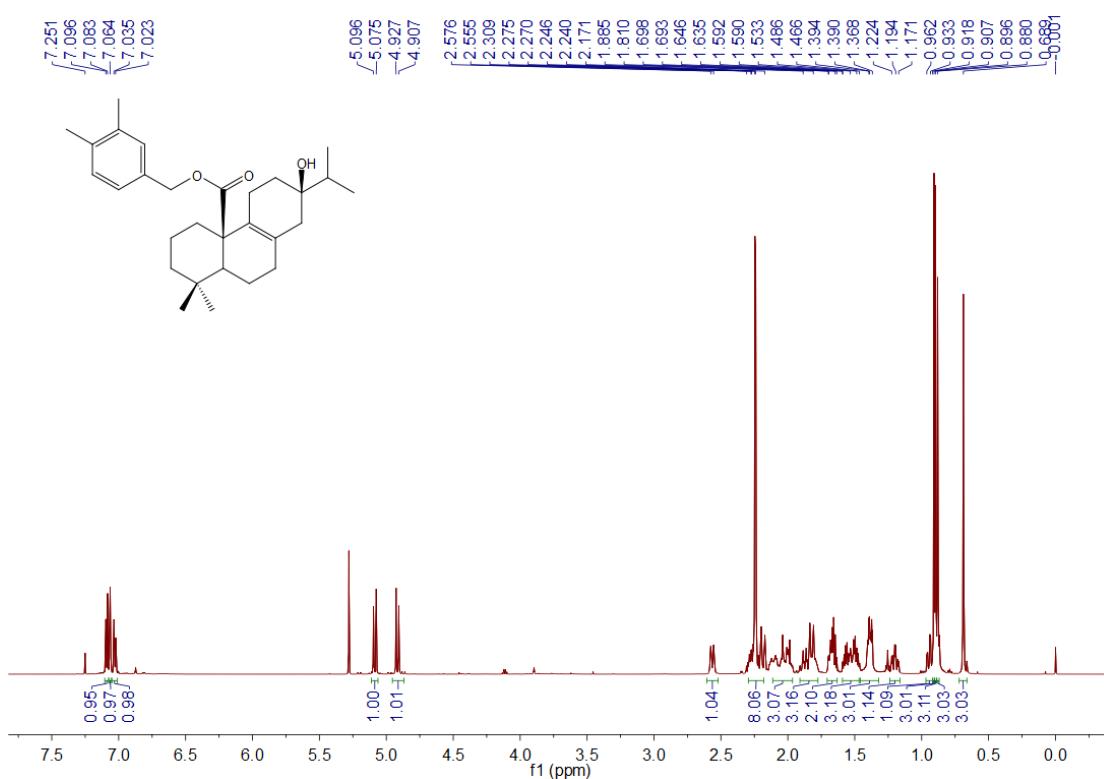


**Figure S29.**  $^{13}\text{C}$  NMR spectrum of the compound 3j.

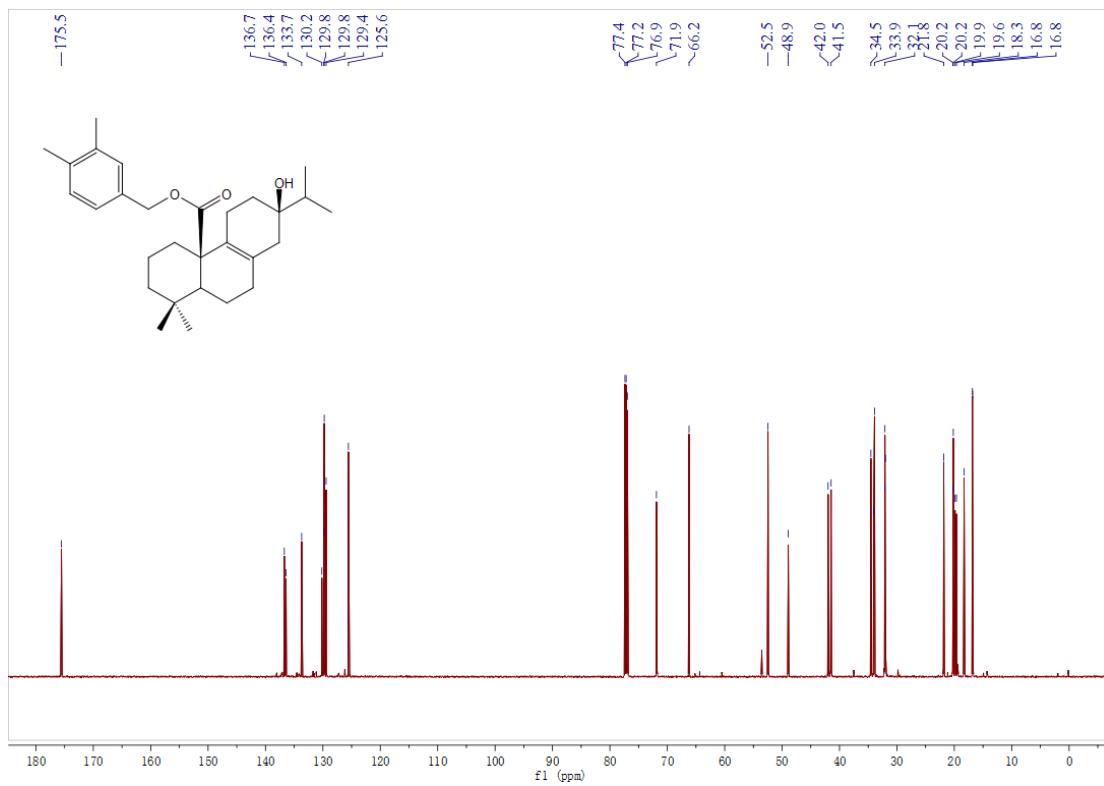
Y-73 #41 RT: 0.18 AV: 1 NL: 1.87E8  
T: FTMS + p ESI Full ms [120.000-1600.000]



**Figure S30.** HRMS spectrum of the compound 3j.



**Figure S31.**  $^1\text{H}$  NMR spectrum of the compound **3k**.



**Figure S32.**  $^{13}\text{C}$  NMR spectrum of the compound **3k**.

Y-55 #44 RT: 0.19 AV: 1 NL: 2.03E8  
T: FTMS + p ESI Full ms [120.0000-1600.0000]

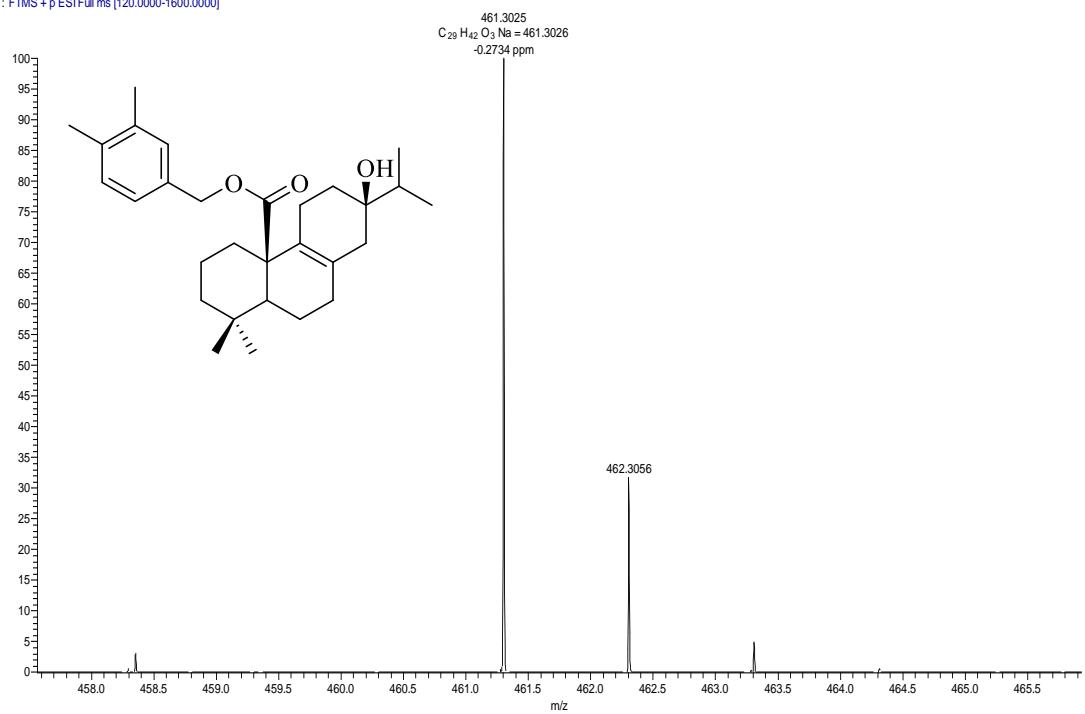


Figure S33. HRMS spectrum of the compound 3k.

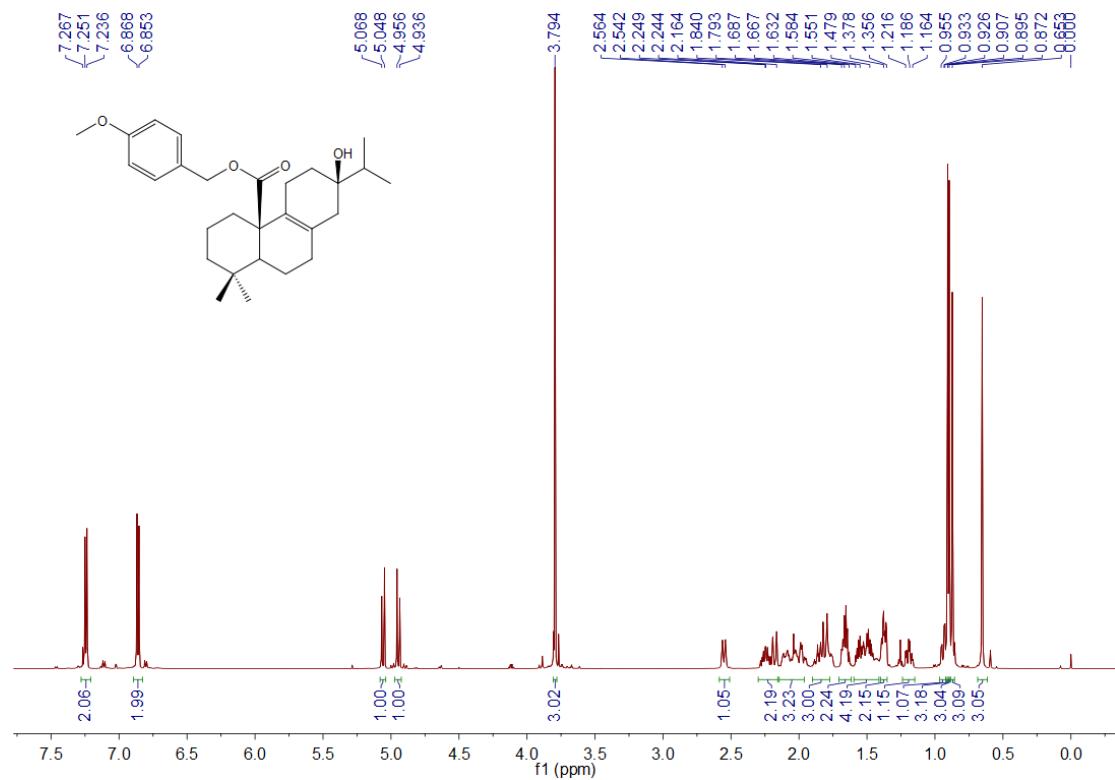
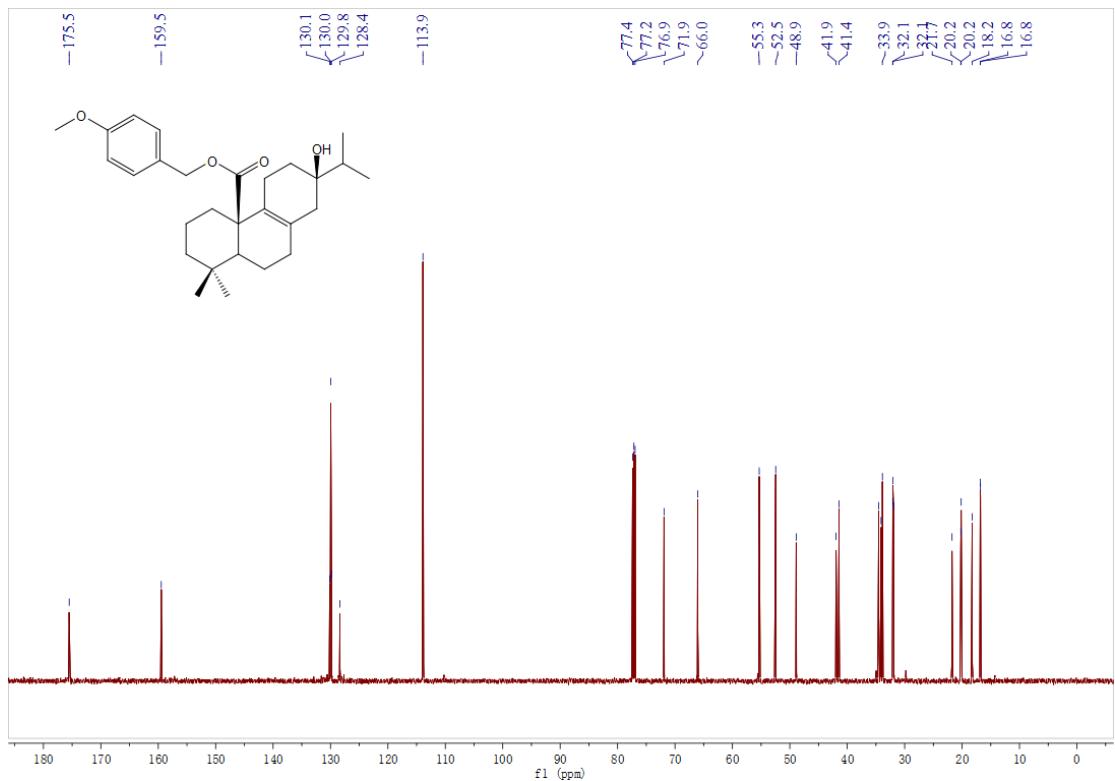
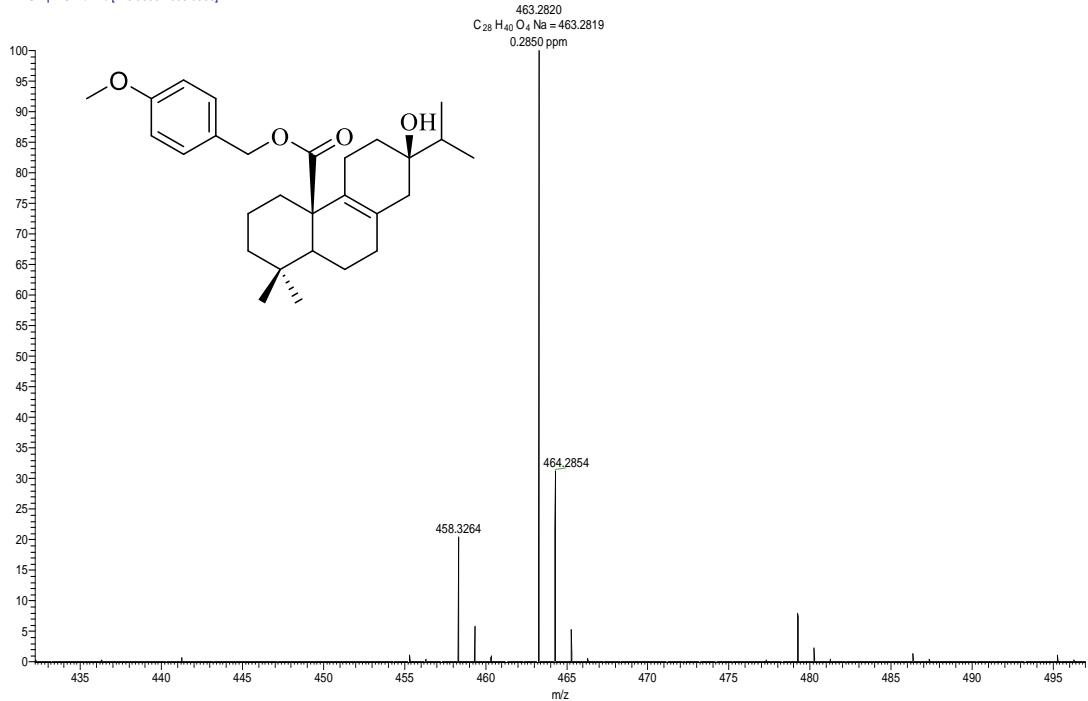


Figure S34.  $^1H$  NMR spectrum of the compound 3l.

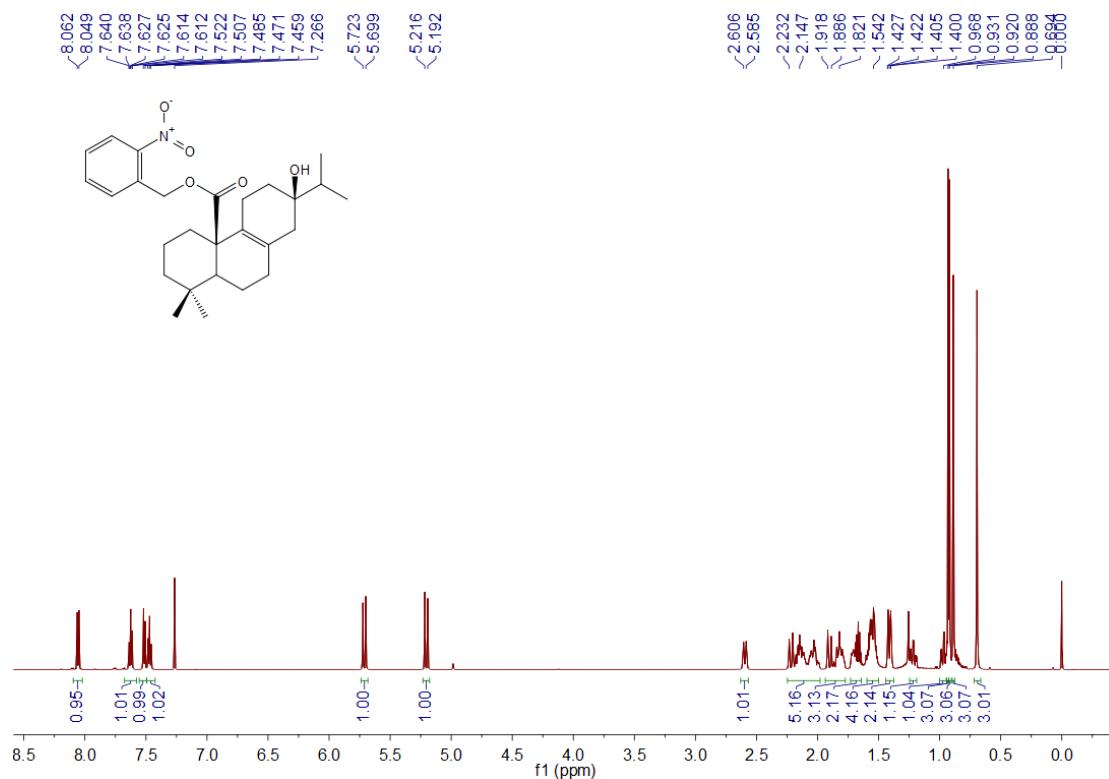


**Figure S35.**  $^{13}\text{C}$  NMR spectrum of the compound 31.

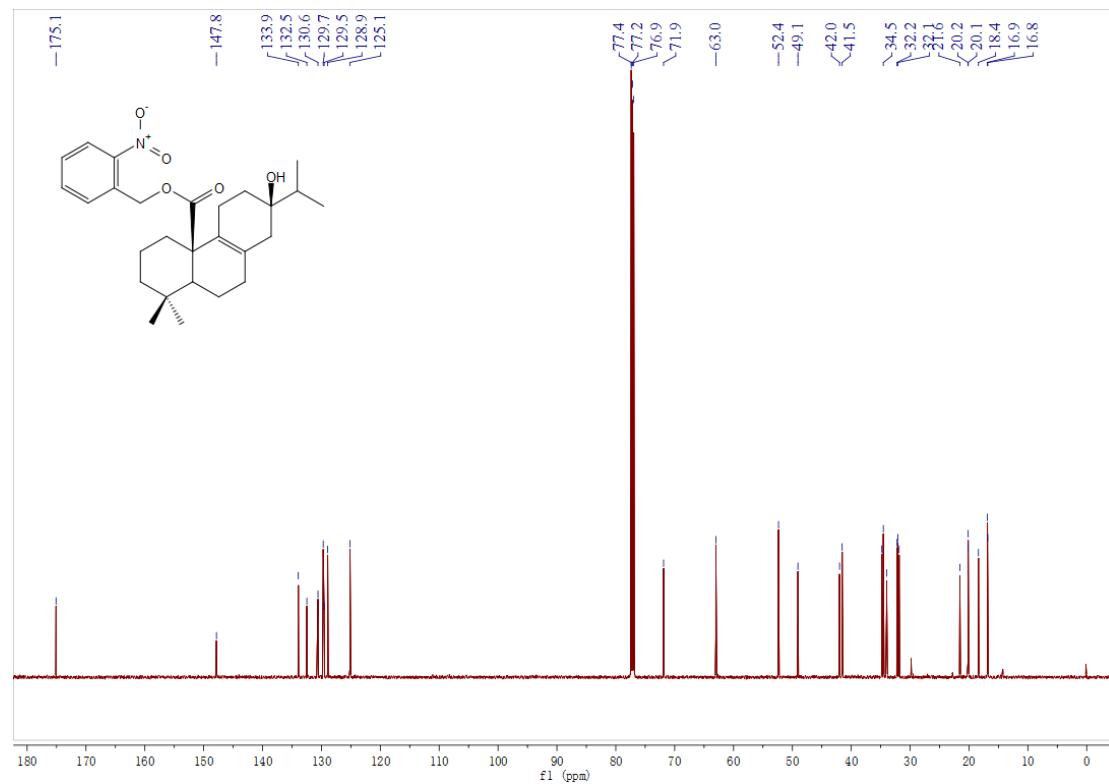
Y-53 #43 RT: 0.19 AV: 1 NL: 8.70E8  
T: FTMS + p ESI Full ms [120.0000-1600.0000]



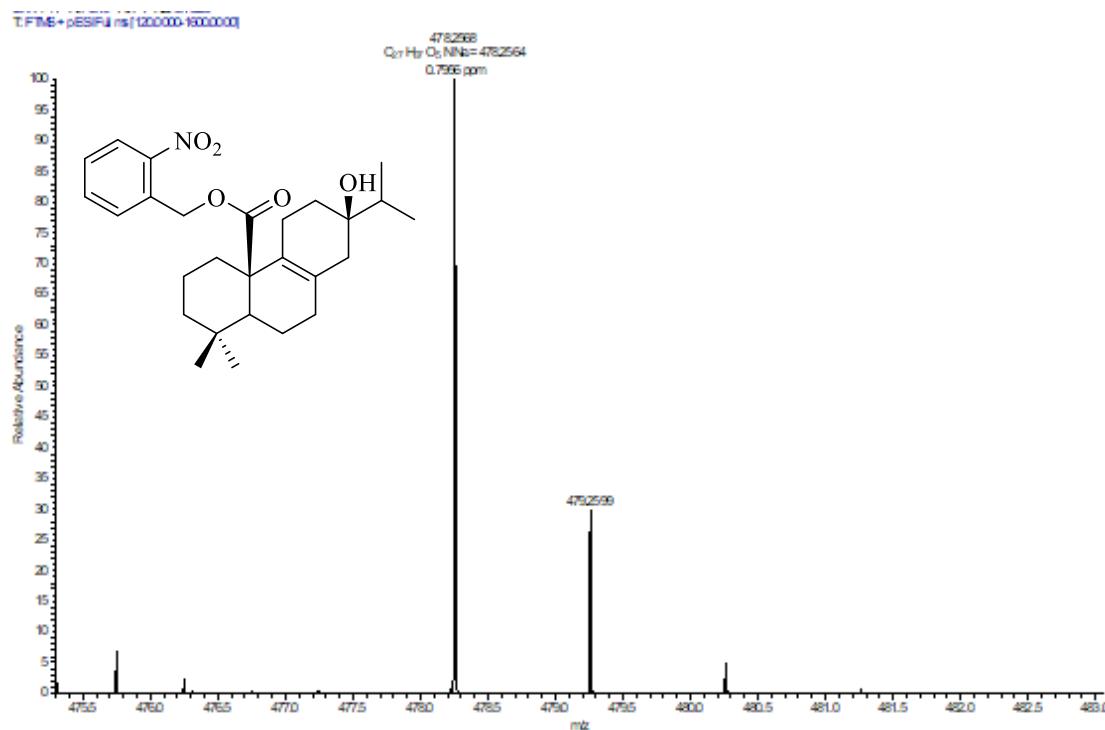
**Figure S36.** HRMS spectrum of the compound 31.



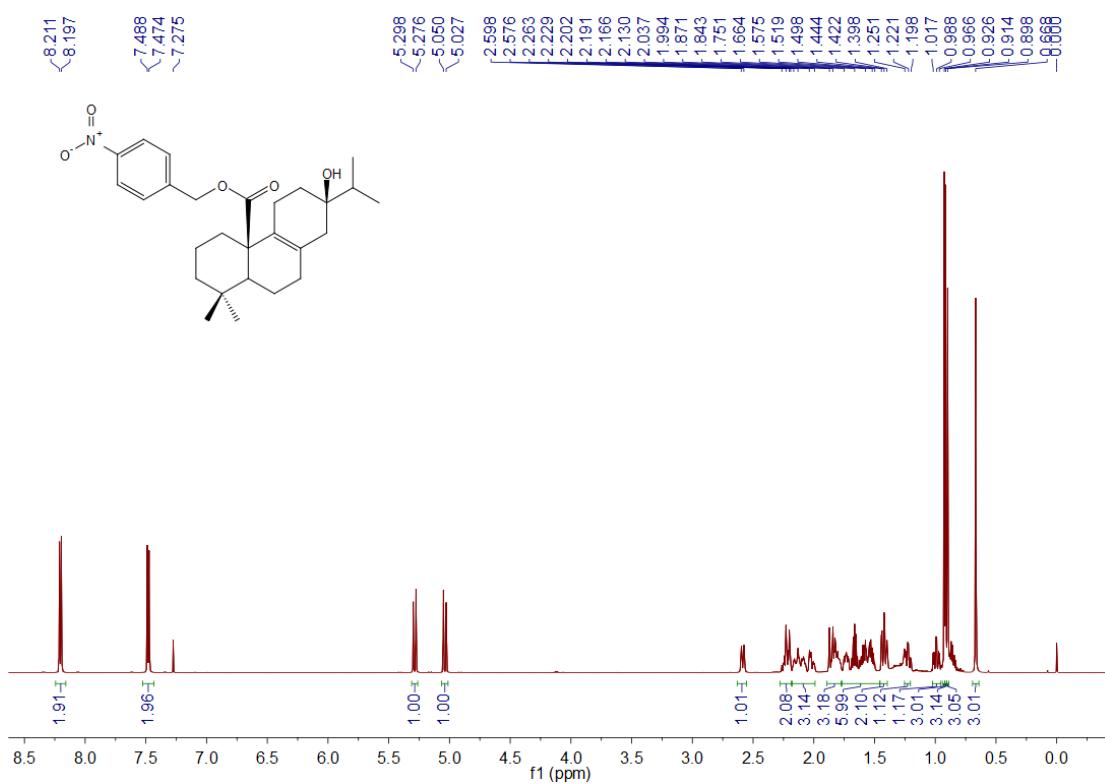
**Figure S37.** <sup>1</sup>H NMR spectrum of the compound 3m.



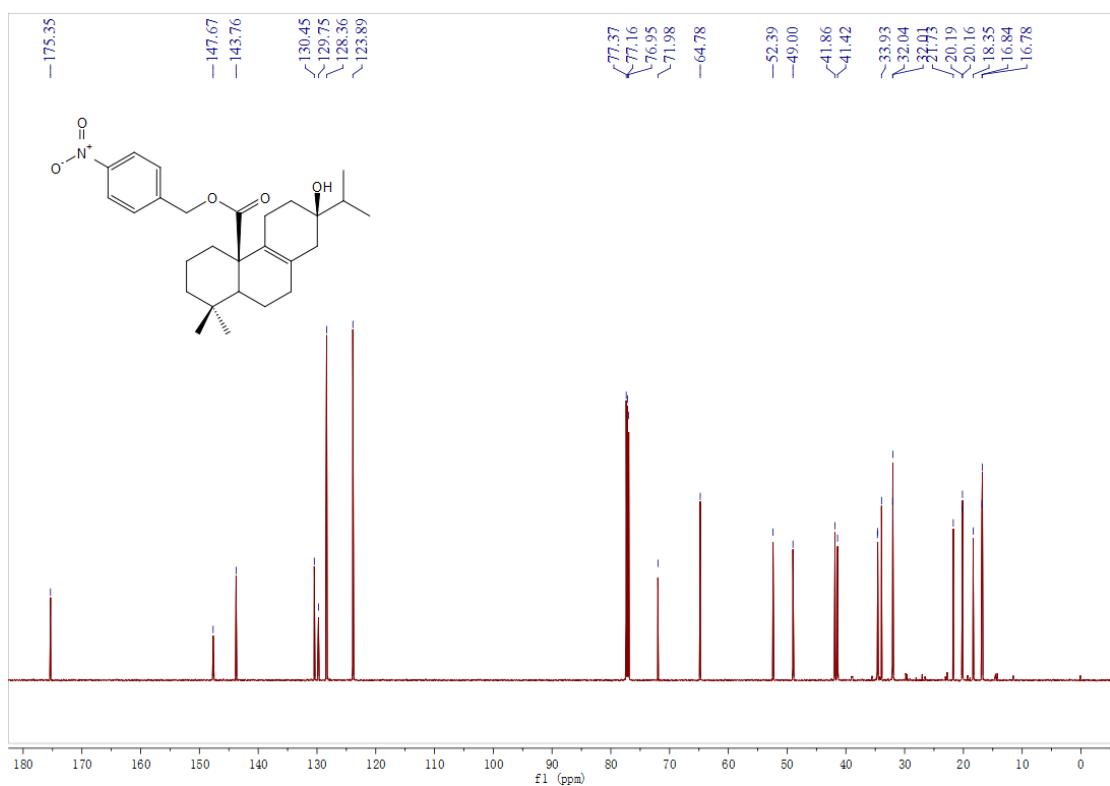
**Figure S38.** <sup>13</sup>C NMR spectrum of the compound 3m.



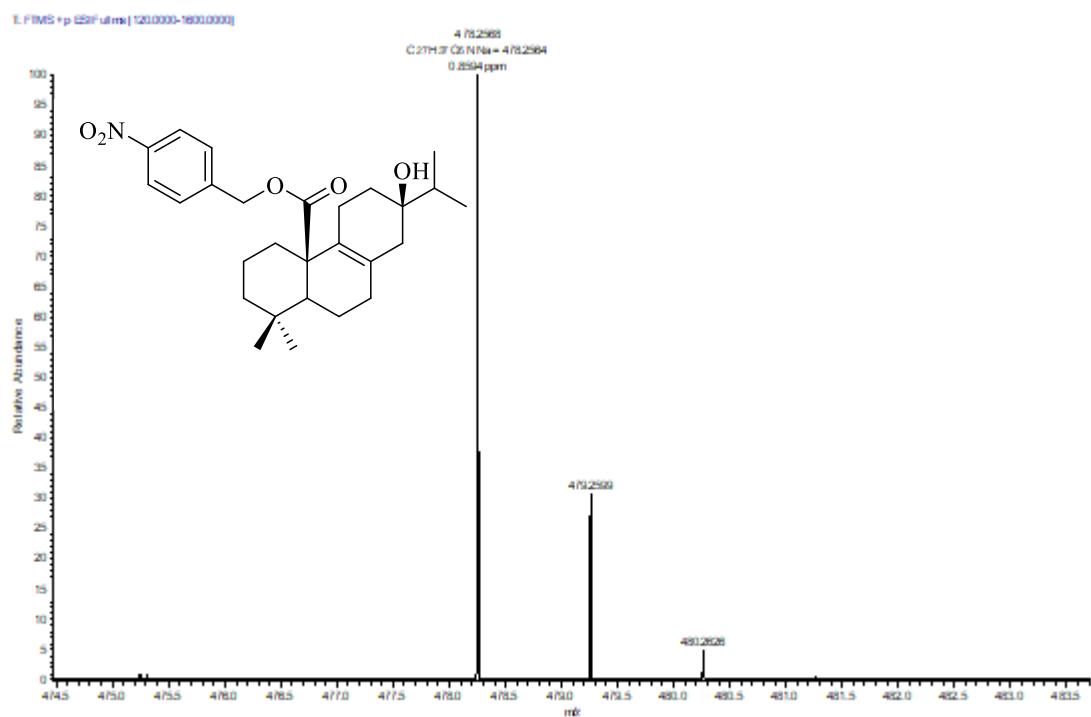
**Figure S39.** HRMS spectrum of the compound **3m**.



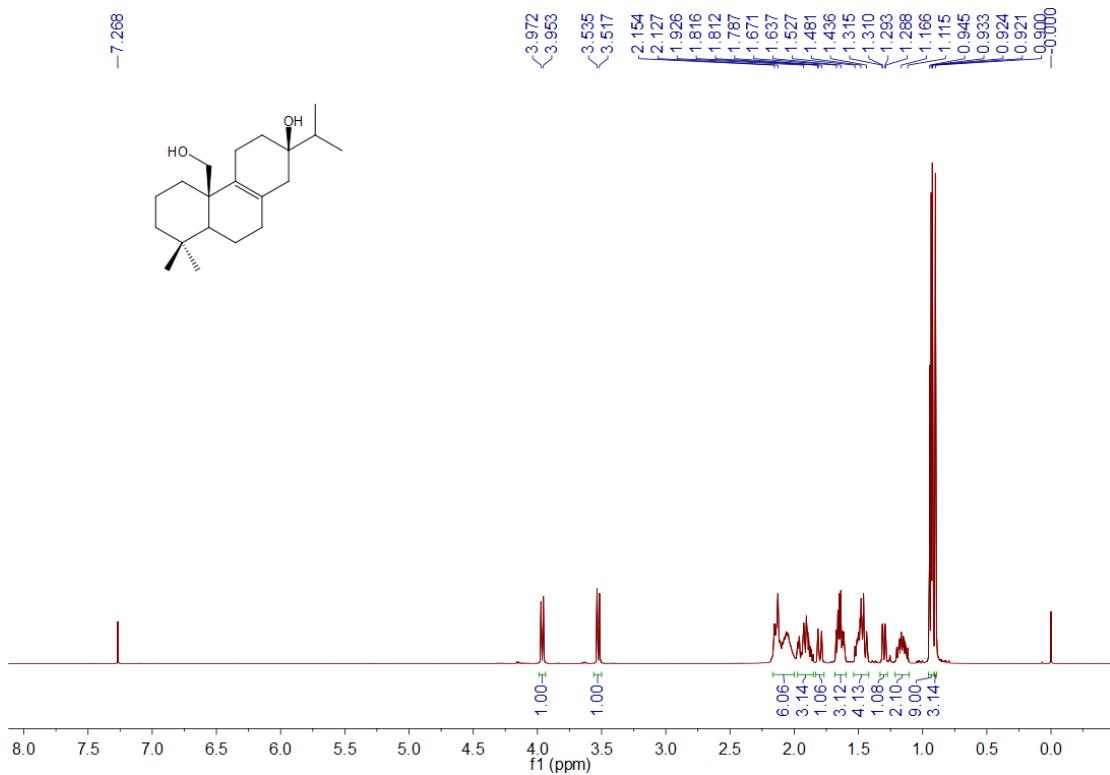
**Figure S40.**  $^1\text{H}$  NMR spectrum of the compound **3n**.



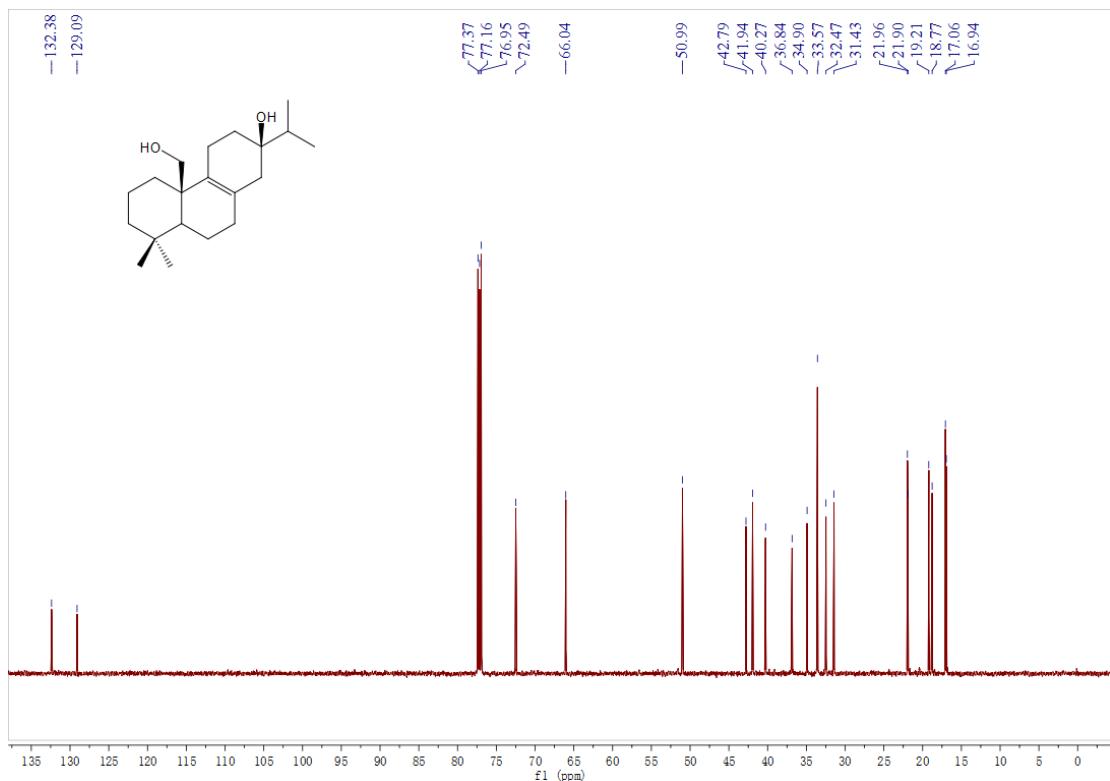
**Figure S41.**  $^{13}\text{C}$  NMR spectrum of the compound **3n**.



**Figure S42.** HRMS spectrum of the compound **3n**.



**Figure S43.** <sup>1</sup>H NMR spectrum of the compound 4.



**Figure S44.** <sup>13</sup>C NMR spectrum of the compound 4.

Y92 #42 RT: 0.18 AV: 1 NL: 1.33E9  
T: FTMS + p ESI Full ms [120.0000-1600.0000]

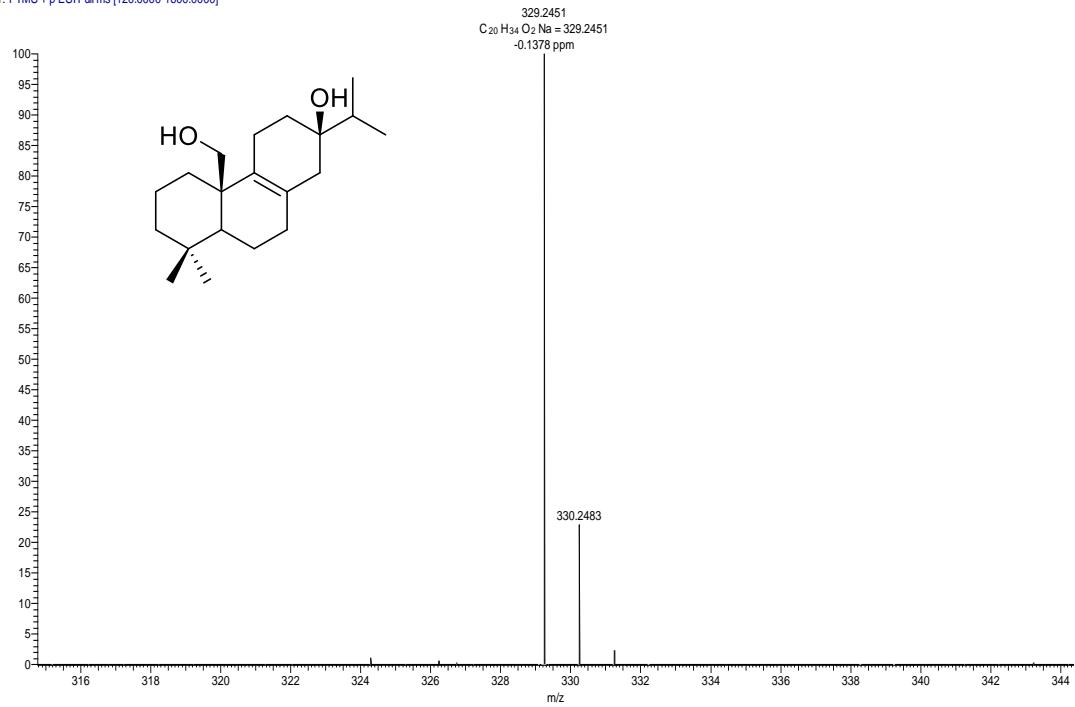


Figure S45. HRMS spectrum of the compound 4.

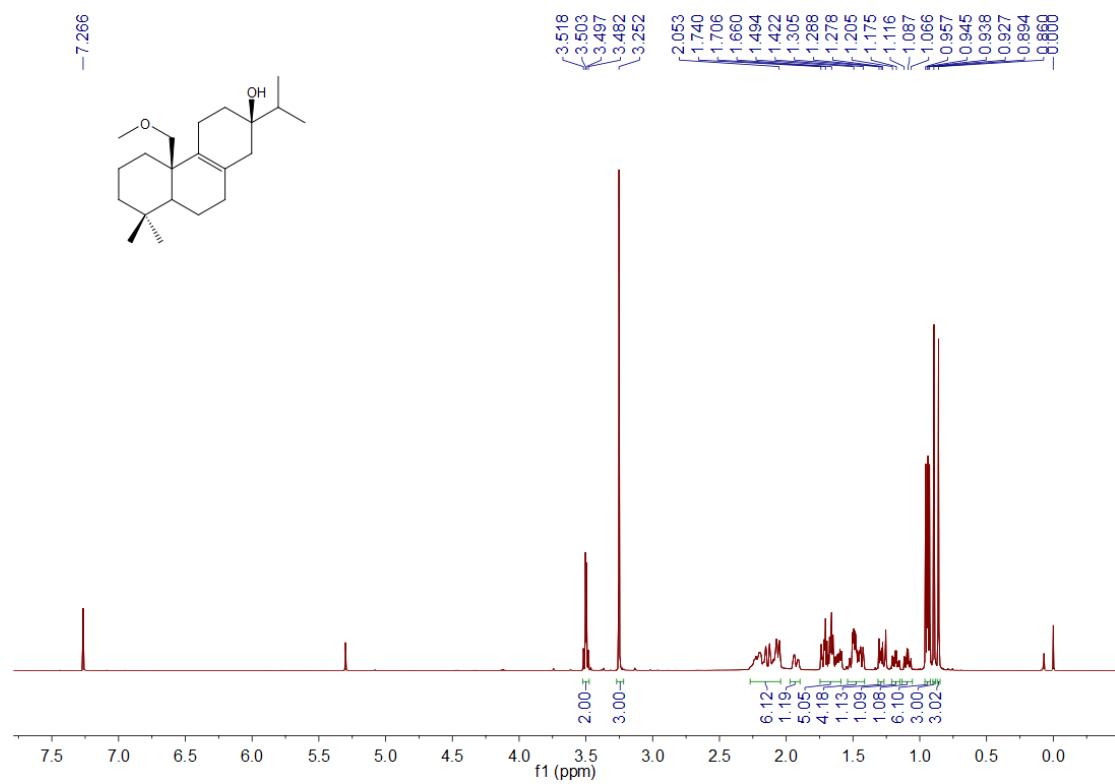
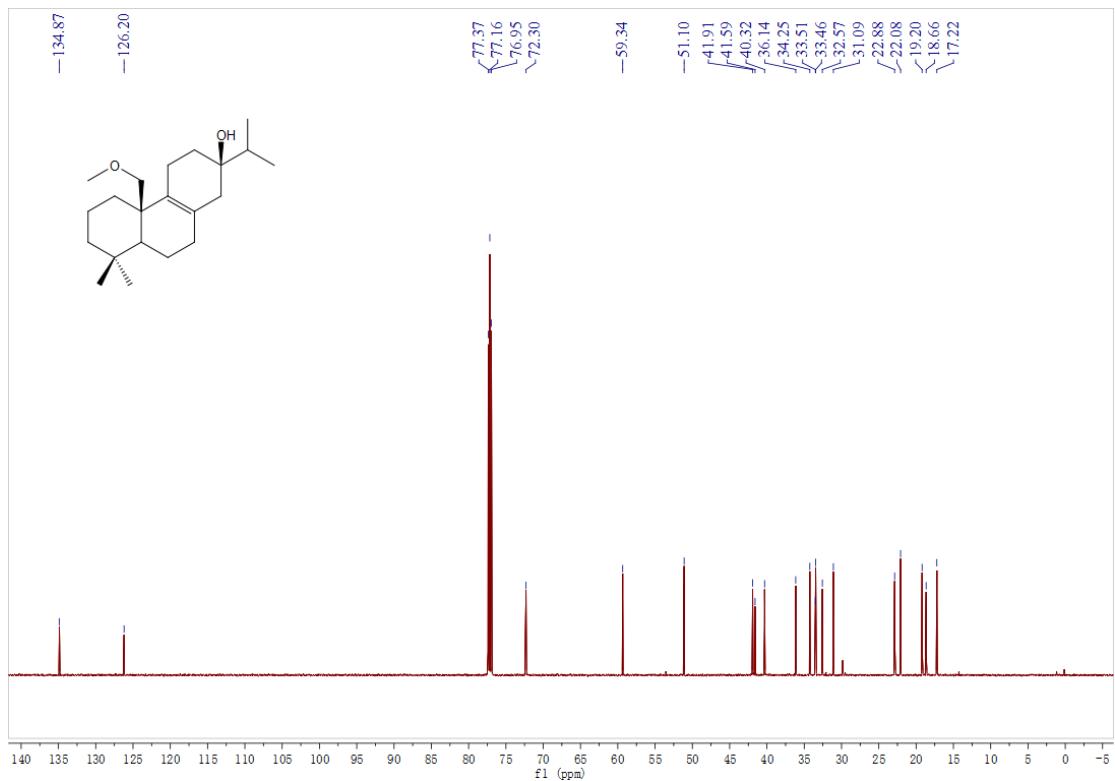
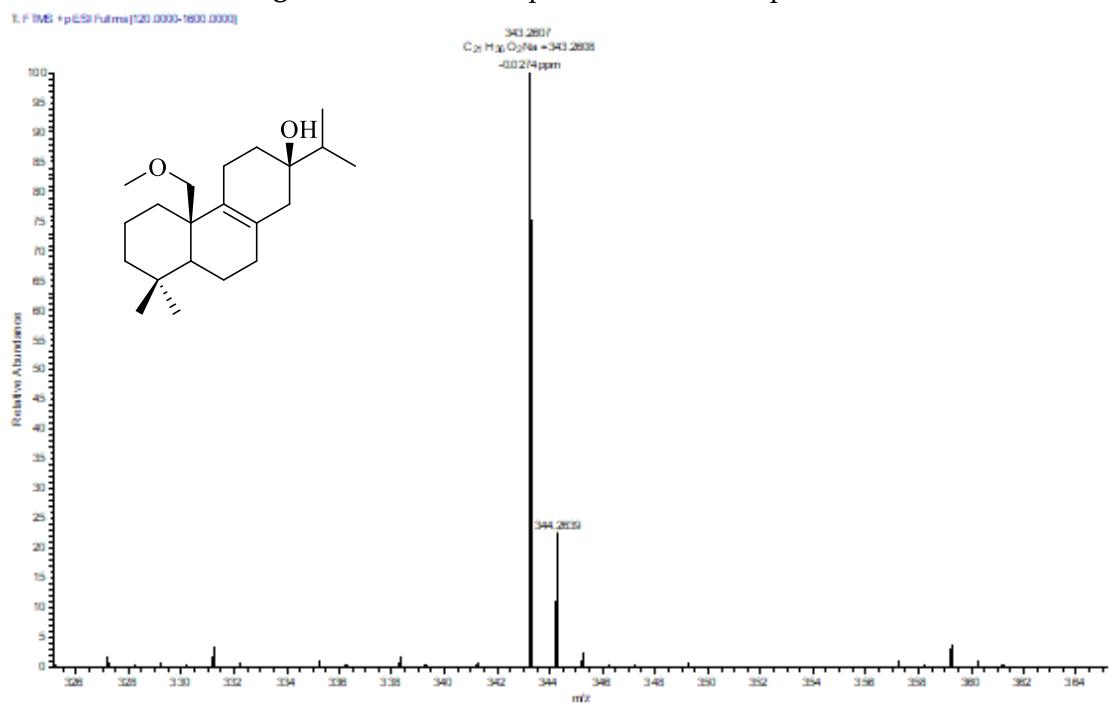


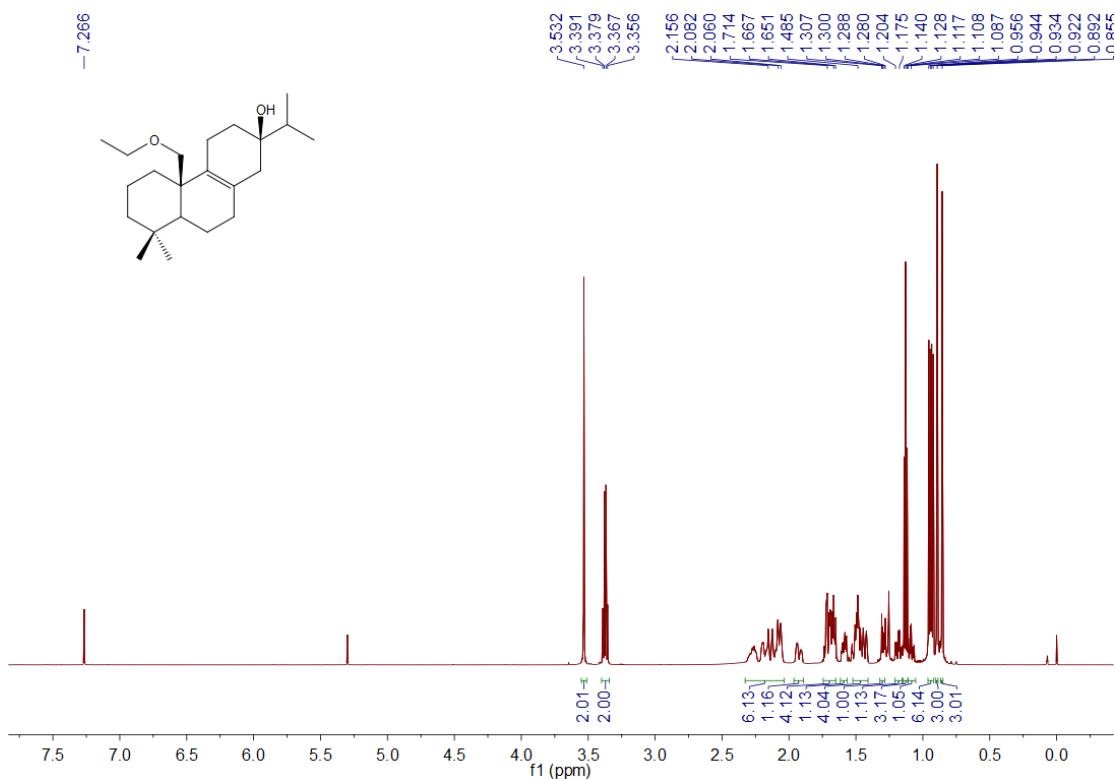
Figure S46.  $^1H$  NMR spectrum of the compound 5a.



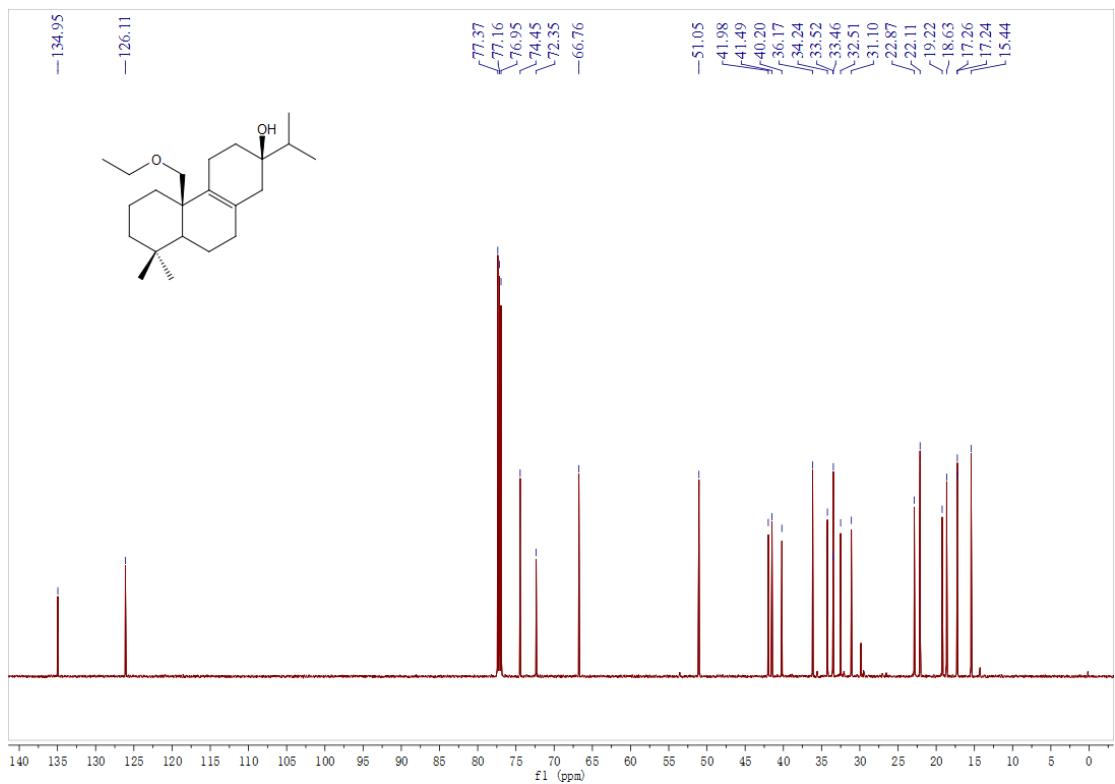
**Figure S47.**  $^{13}\text{C}$  NMR spectrum of the compound **5a**.



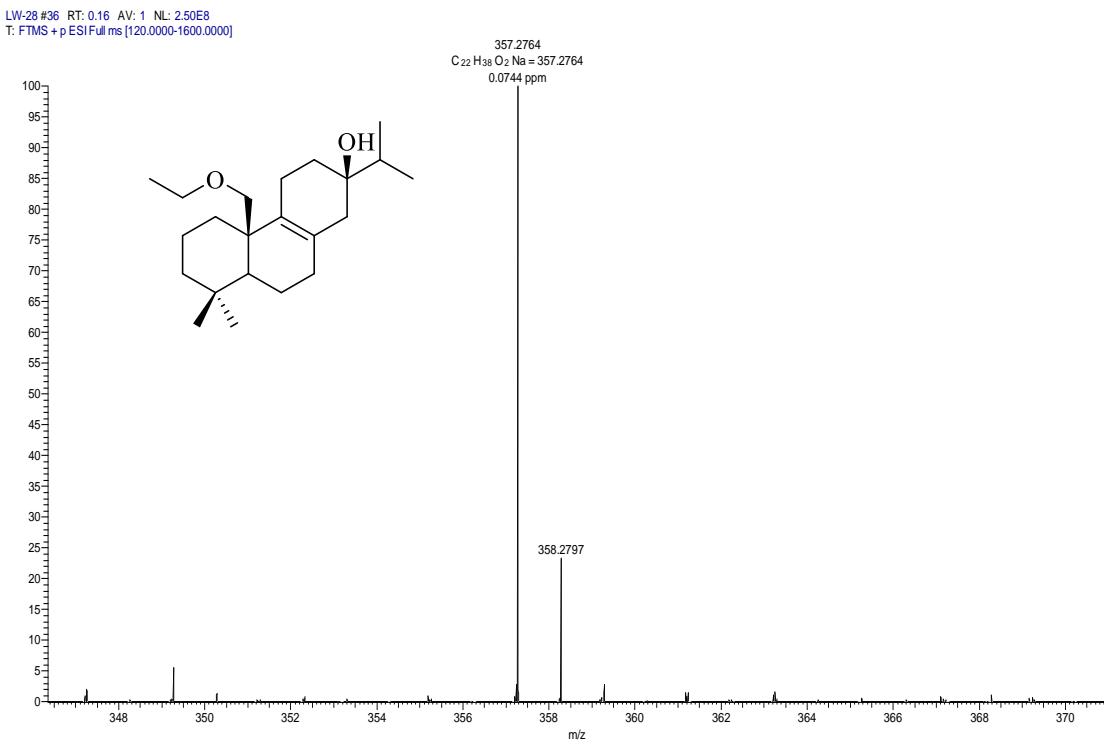
**Figure S48.** HRMS spectrum of the compound **5a**.



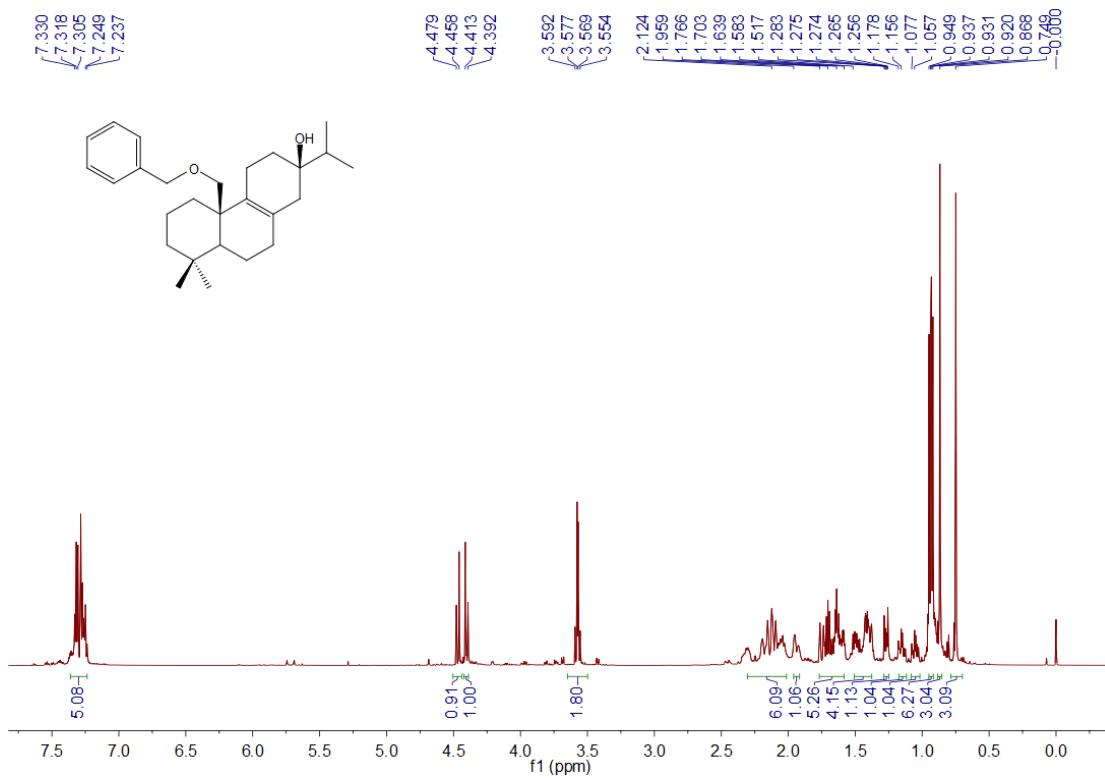
**Figure S49.**  $^1\text{H}$  NMR spectrum of the compound **5b**.



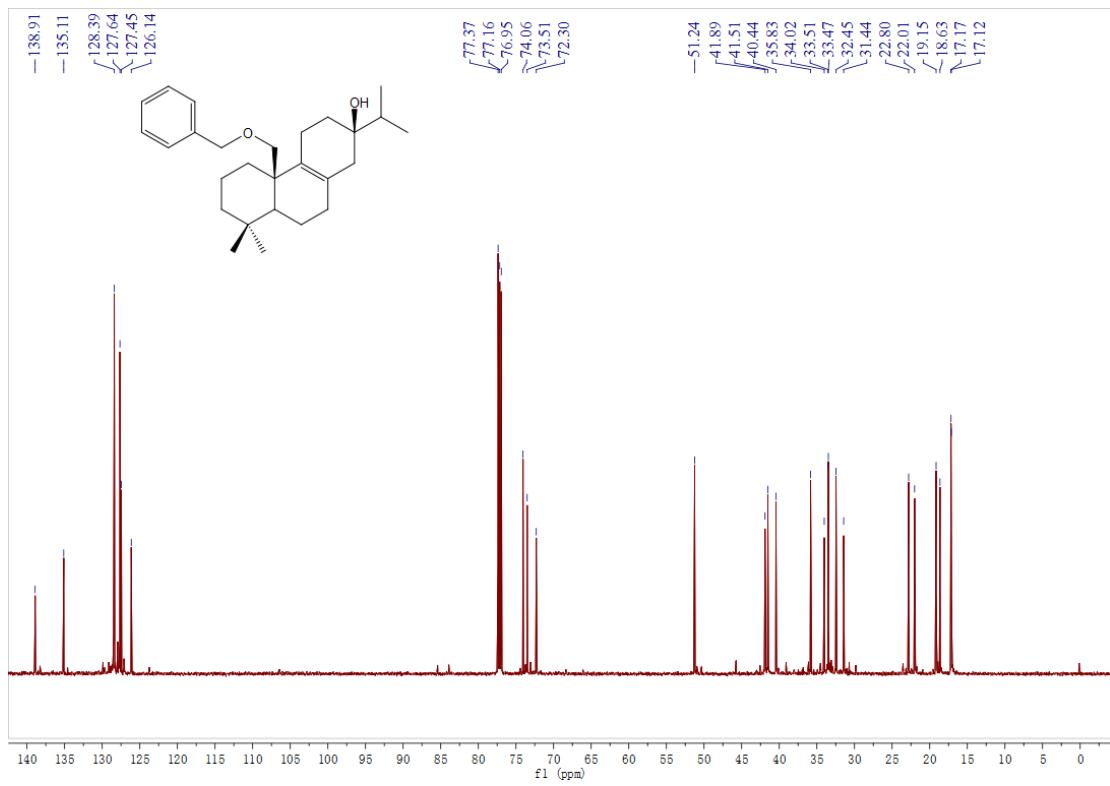
**Figure S50.**  $^{13}\text{C}$  NMR spectrum of the compound **5b**.



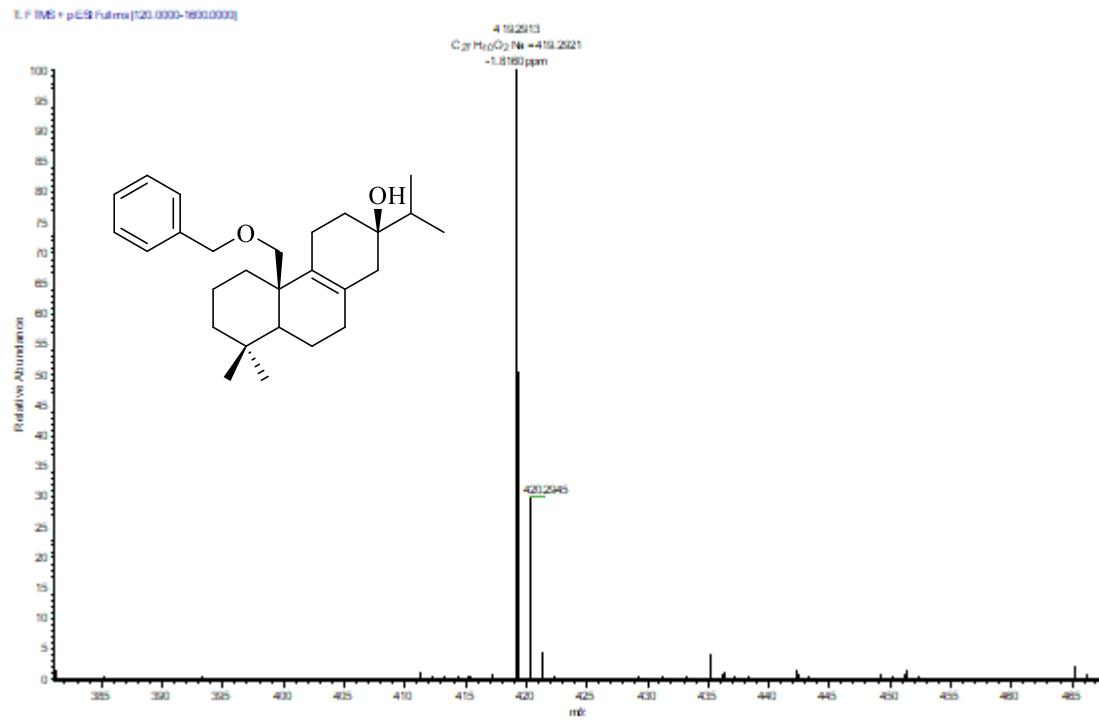
**Figure S51.** HRMS spectrum of the compound **5b**.



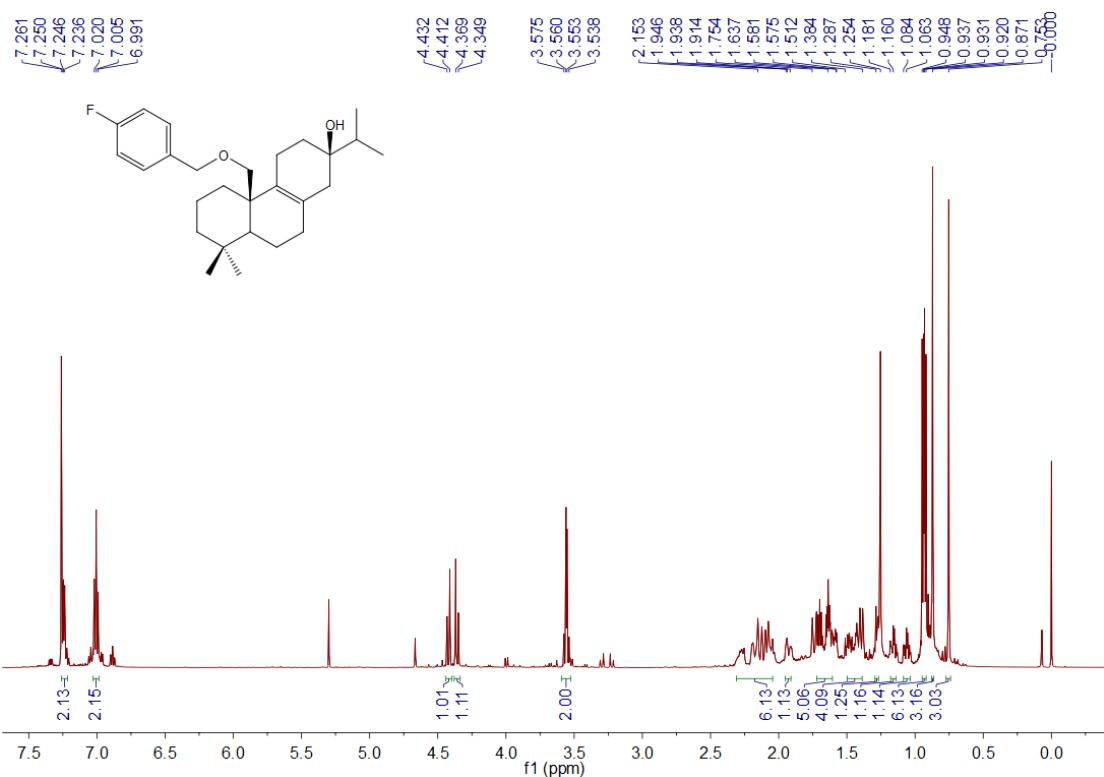
**Figure S52.**  $^1\text{H}$  NMR spectrum of the compound **5c**.



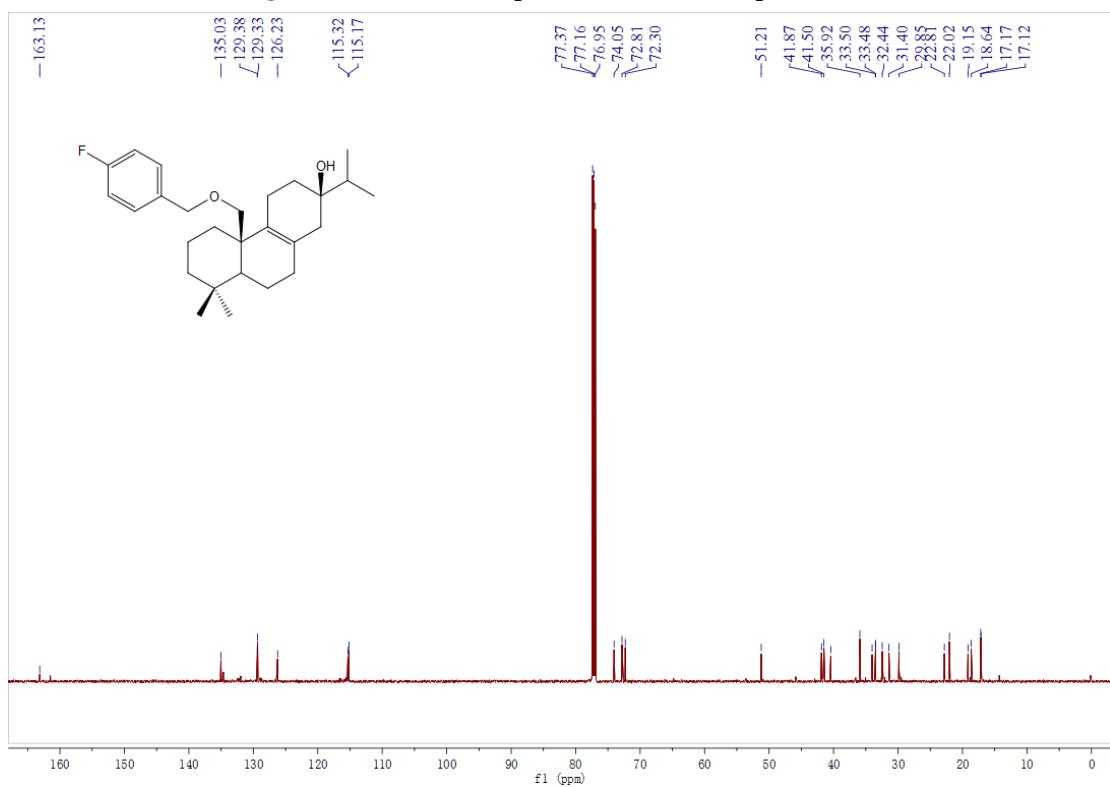
**Figure S53.**  $^{13}\text{C}$  NMR spectrum of the compound 5c.



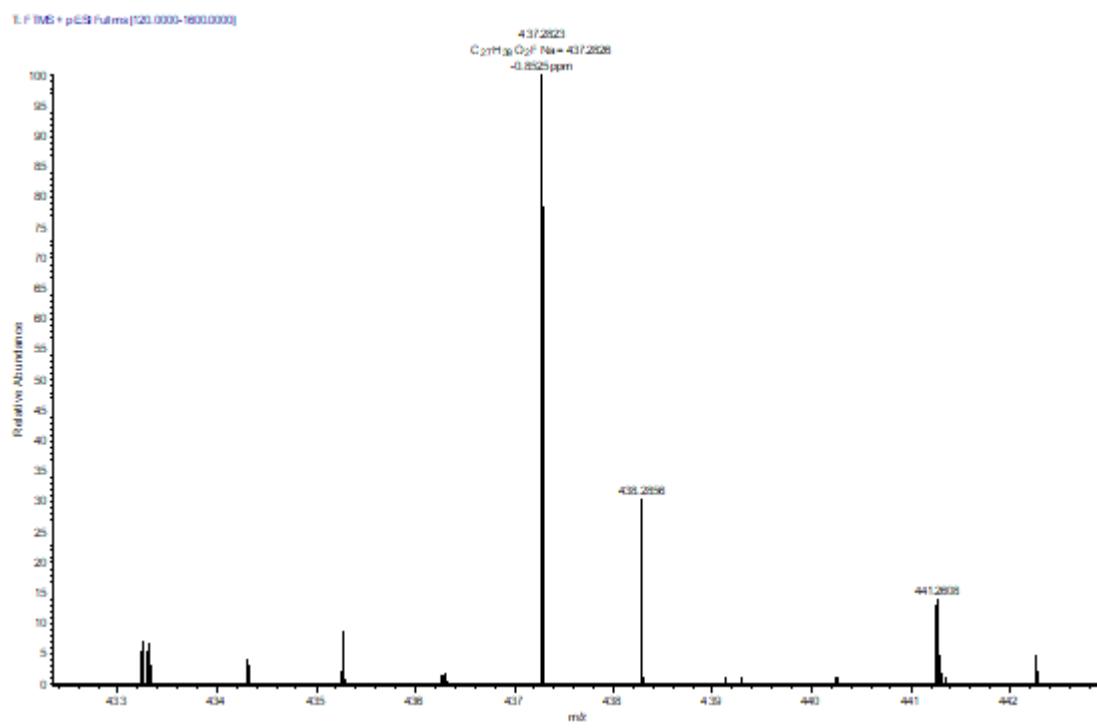
**Figure S54.** HRMS spectrum of the compound 5c.



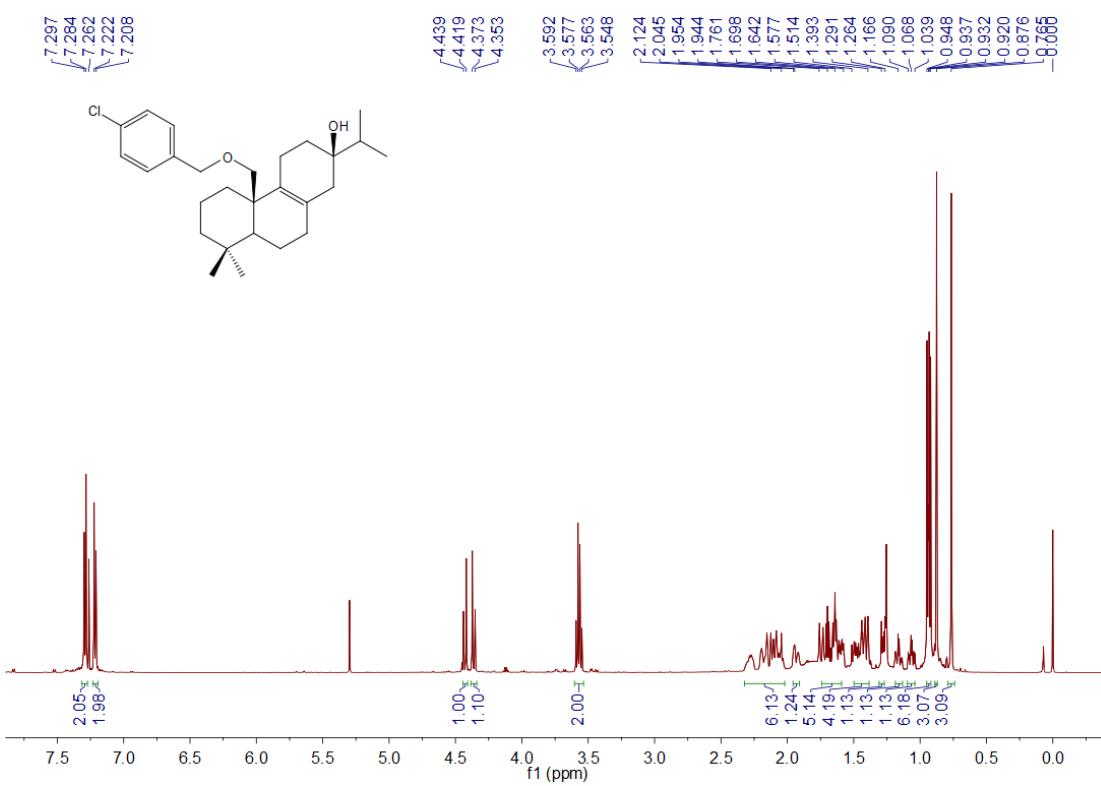
**Figure S55.**  $^1\text{H}$  NMR spectrum of the compound **5d**.



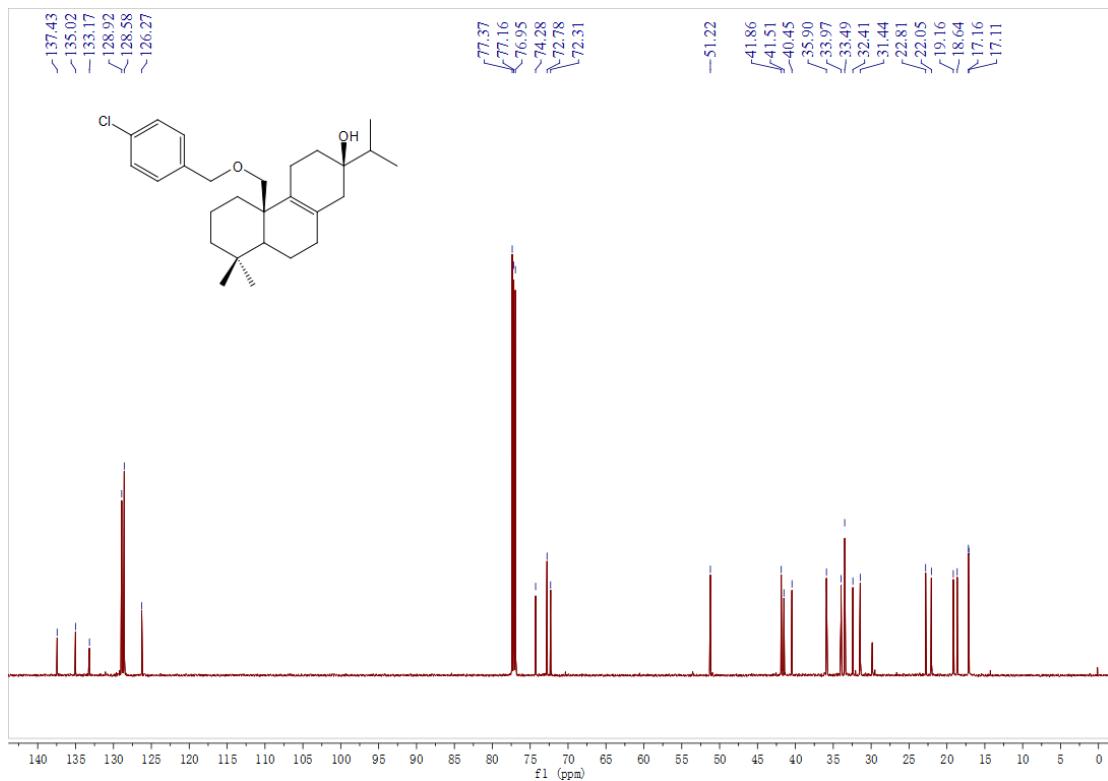
**Figure S56.**  $^{13}\text{C}$  NMR spectrum of the compound **5d**.



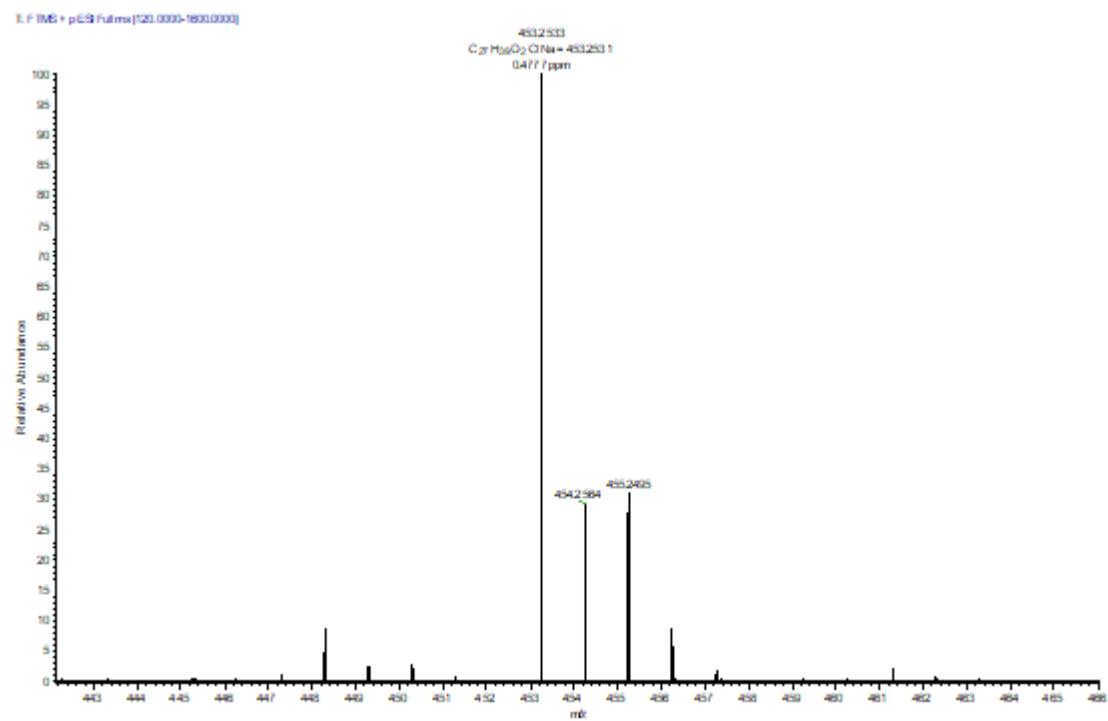
**Figure S57.** HRMS spectrum of the compound **5d**.



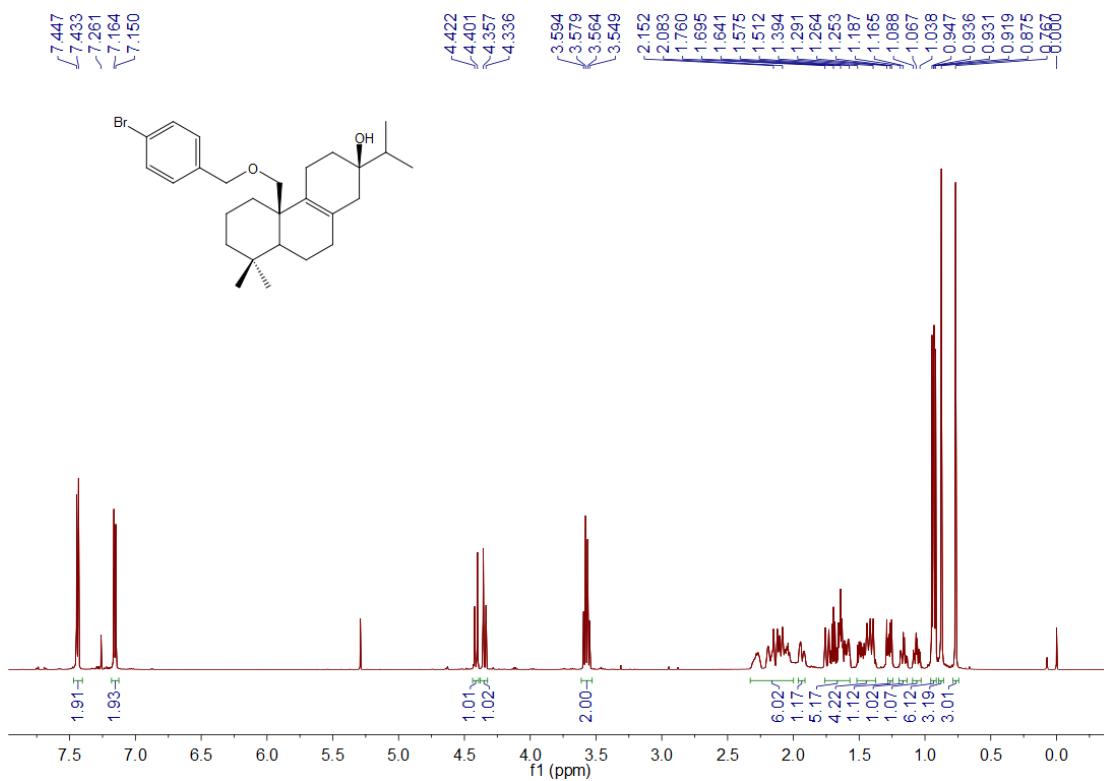
**Figure S58.**  $^{1}\text{H}$  NMR spectrum of the compound **5e**.



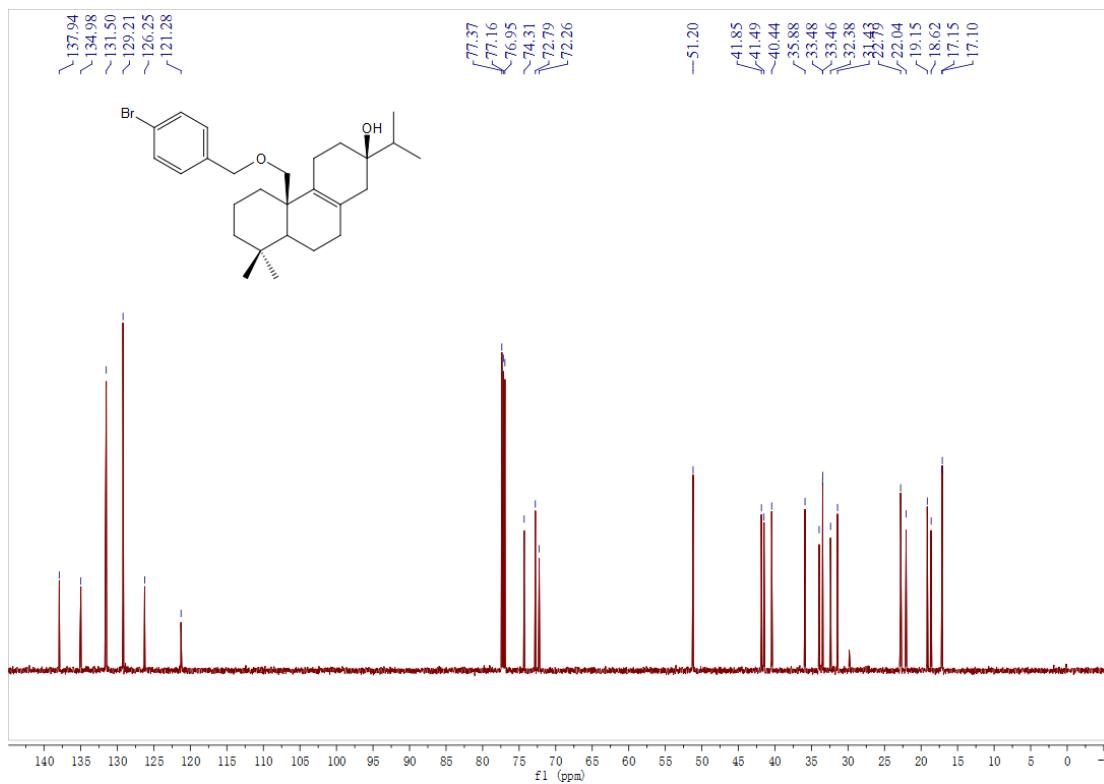
**Figure S59.**  $^{13}\text{C}$  NMR spectrum of the compound 5e.



**Figure S60.** HRMS spectrum of the compound 5e.



**Figure S61.** <sup>1</sup>H NMR spectrum of the compound 5f.



**Figure S62.** <sup>13</sup>C NMR spectrum of the compound 5f.

LW-63 #40 RT: 0.18 AV: 1 NL: 7.53E7  
T: FTMS + p ESI Full ms [120.0000-1600.0000]

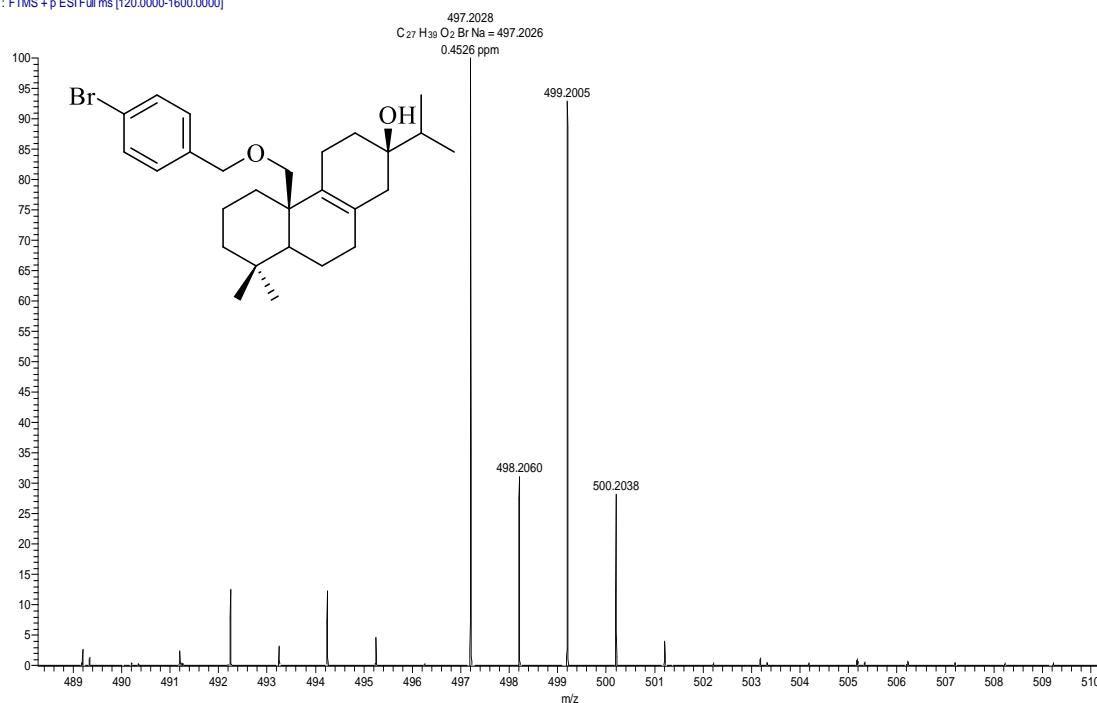


Figure S63. HRMS spectrum of the compound 5f.

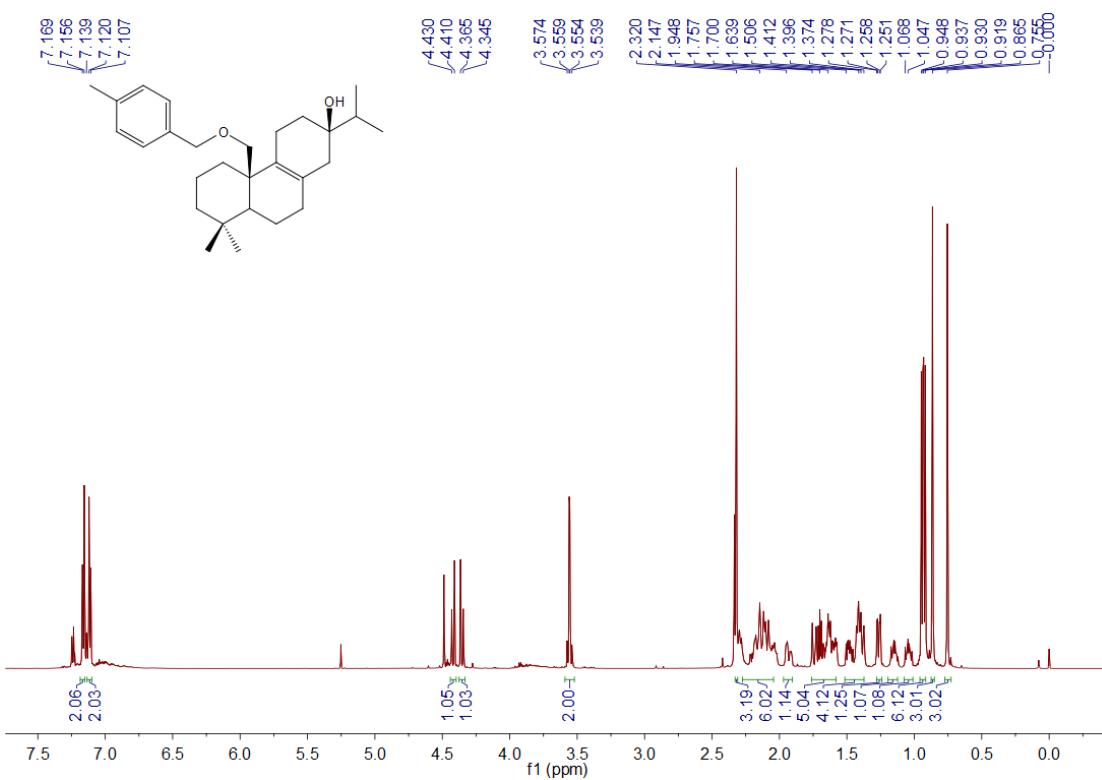
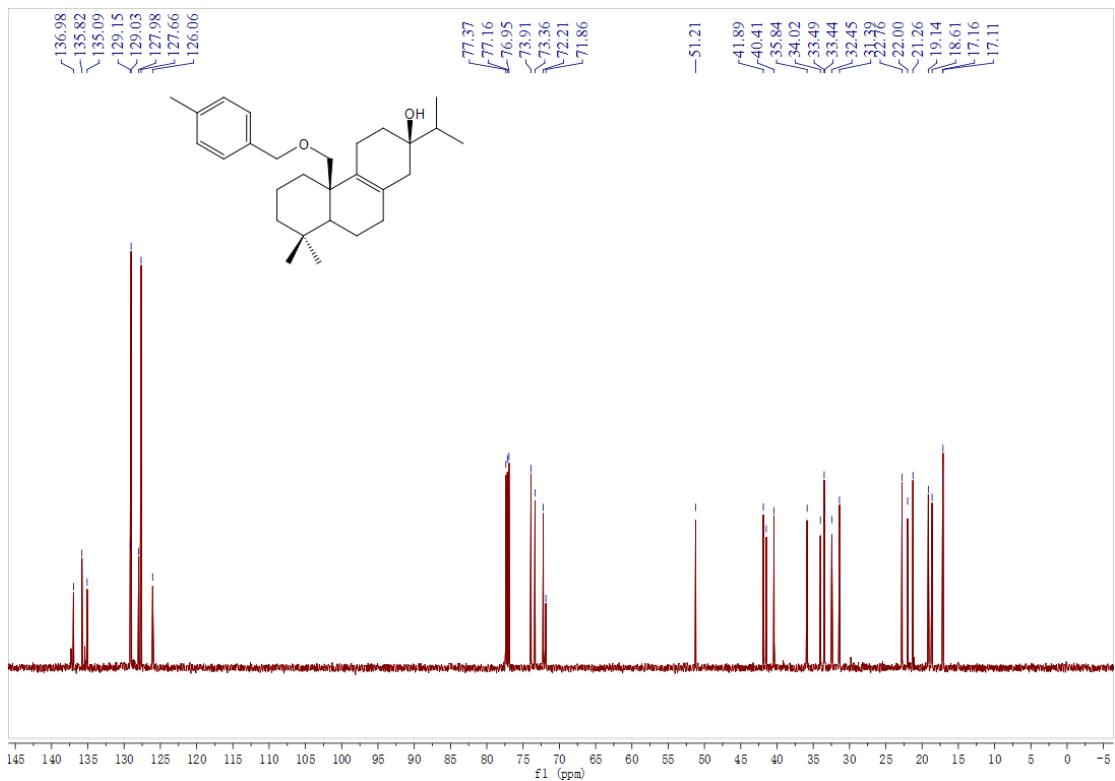
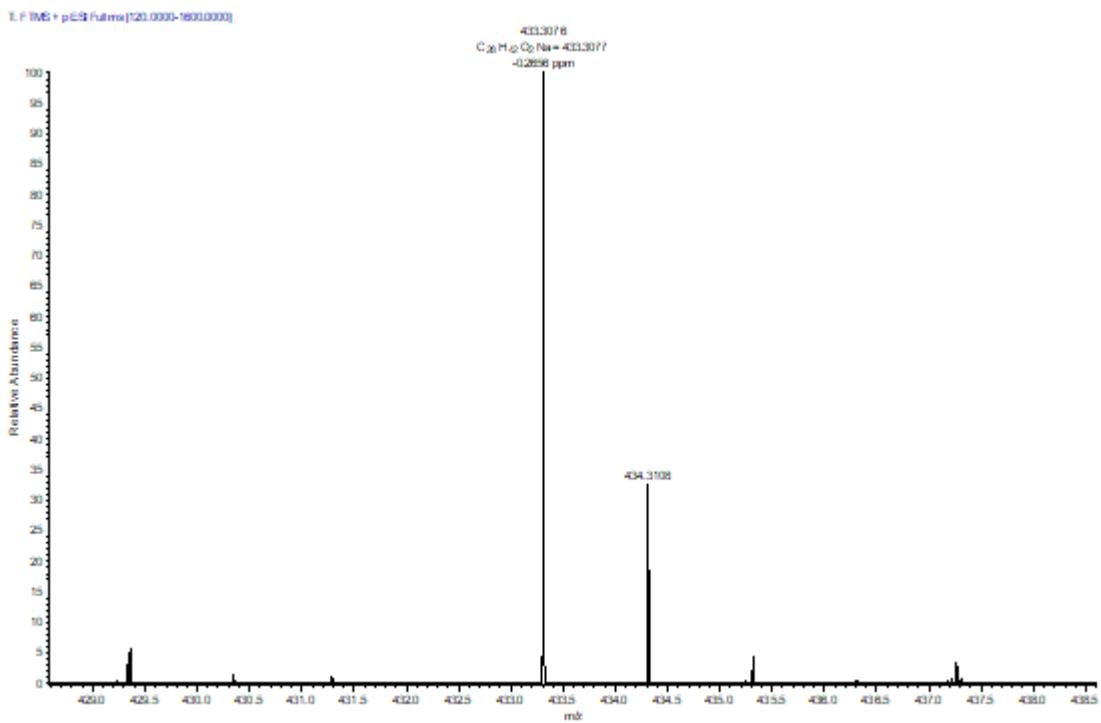


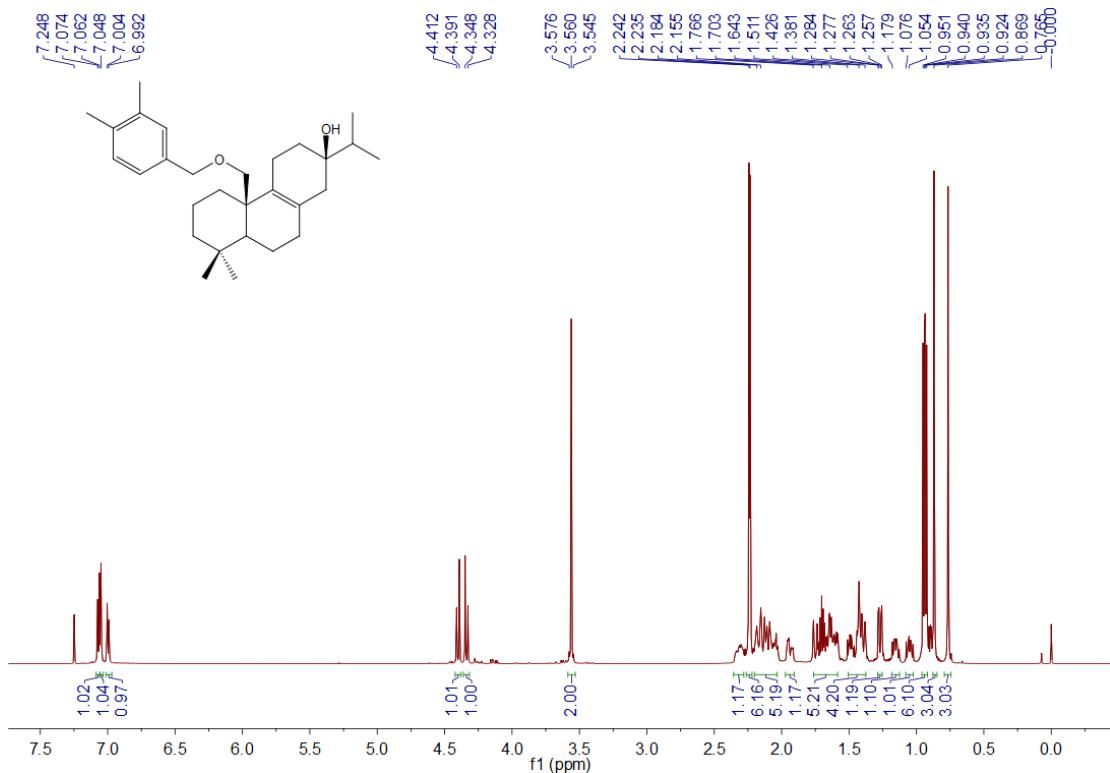
Figure S64.  $^1H$  NMR spectrum of the compound 5g.



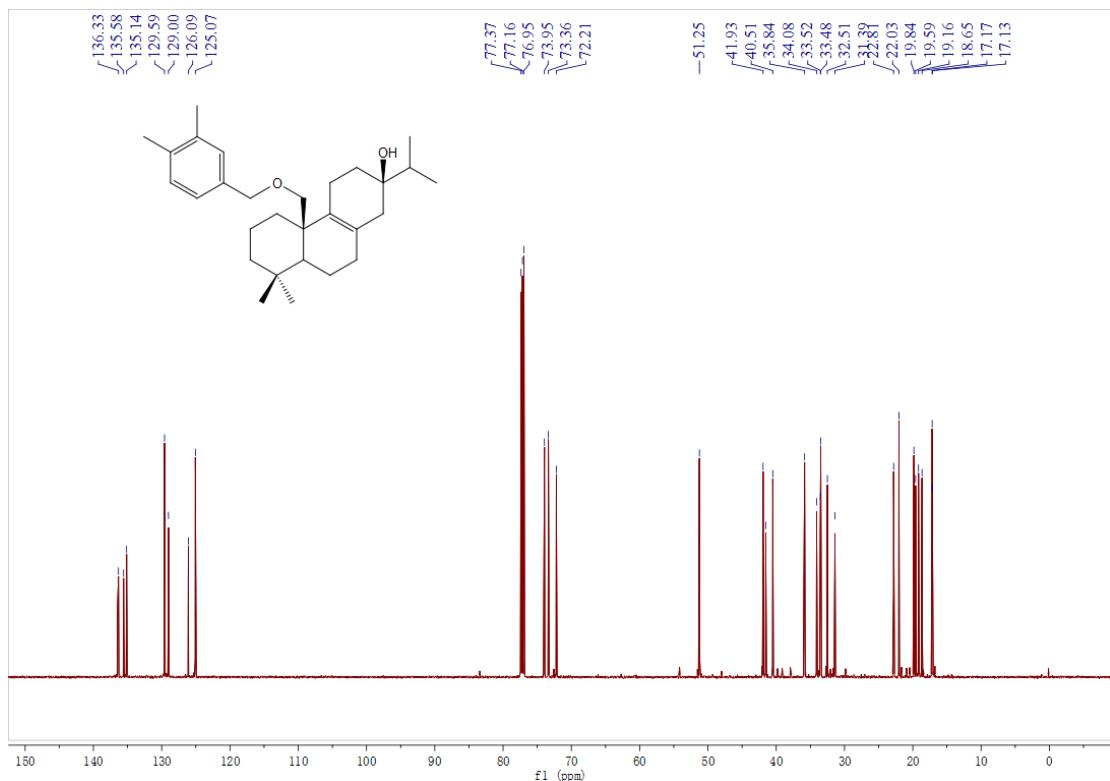
**Figure S65.**  $^{13}\text{C}$  NMR spectrum of the compound **5g**.



**Figure S66.** HRMS spectrum of the compound **5g**.



**Figure S67.**  $^1\text{H}$  NMR spectrum of the compound **5h**.



**Figure S68.**  $^{13}\text{C}$  NMR spectrum of the compound **5h**.

LW-67 #44 RT: 0.19 AV: 1 NL: 2.43E7  
T: FTMS + p ESI Full ms [120.0000-1600.0000]

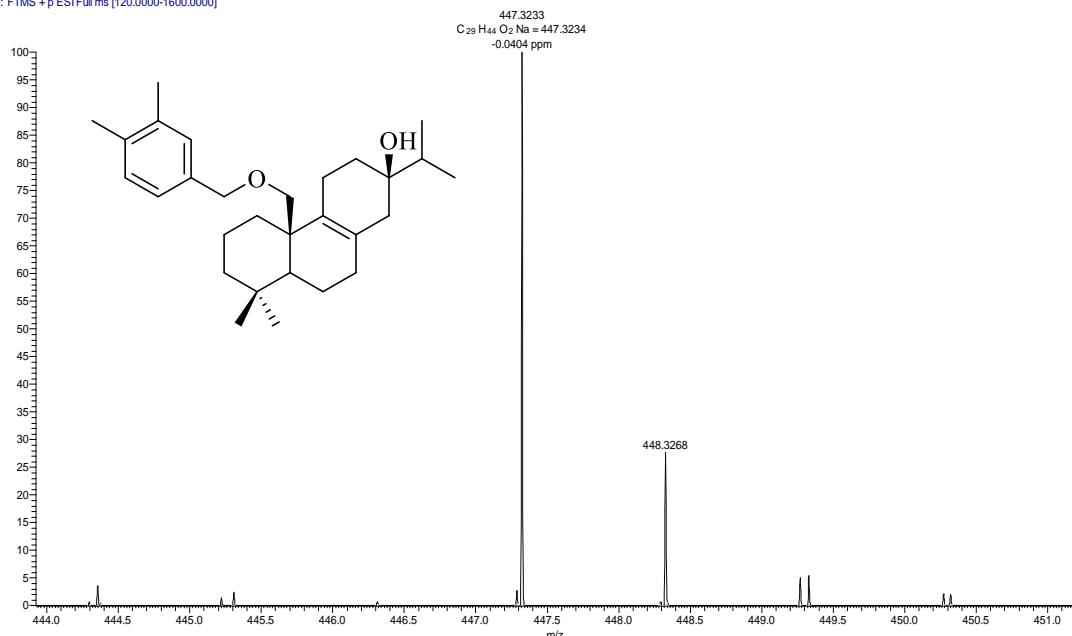


Figure S69. HRMS spectrum of the compound 5h.

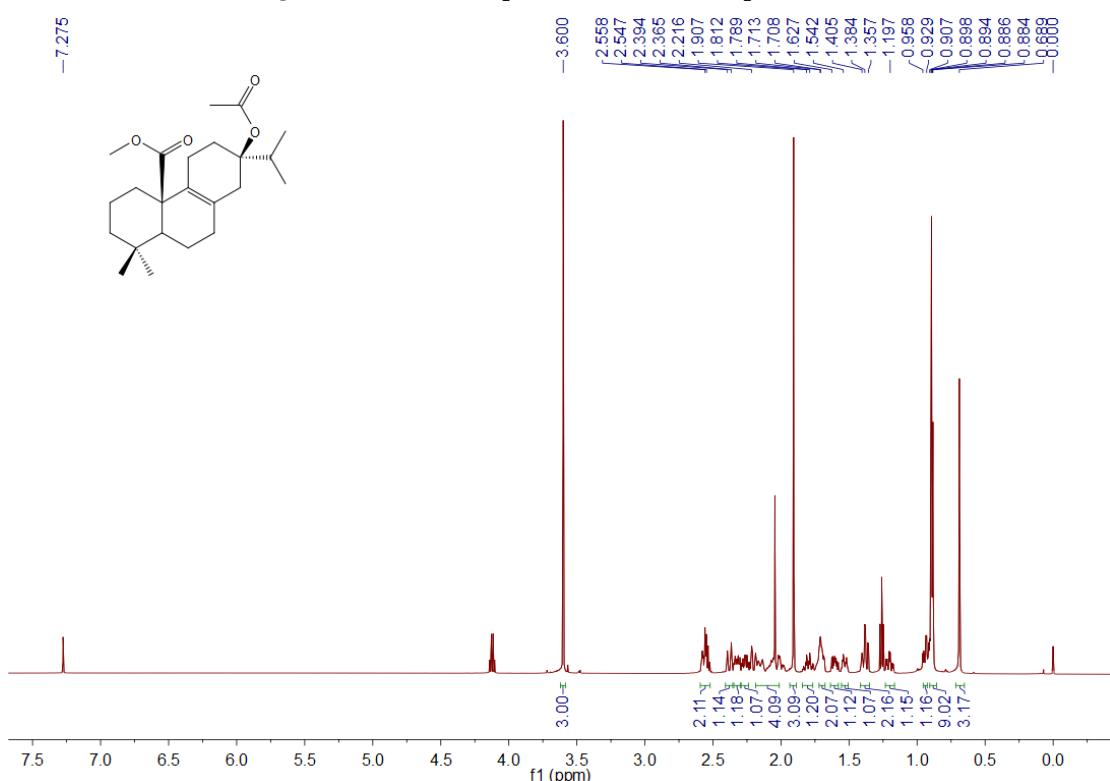
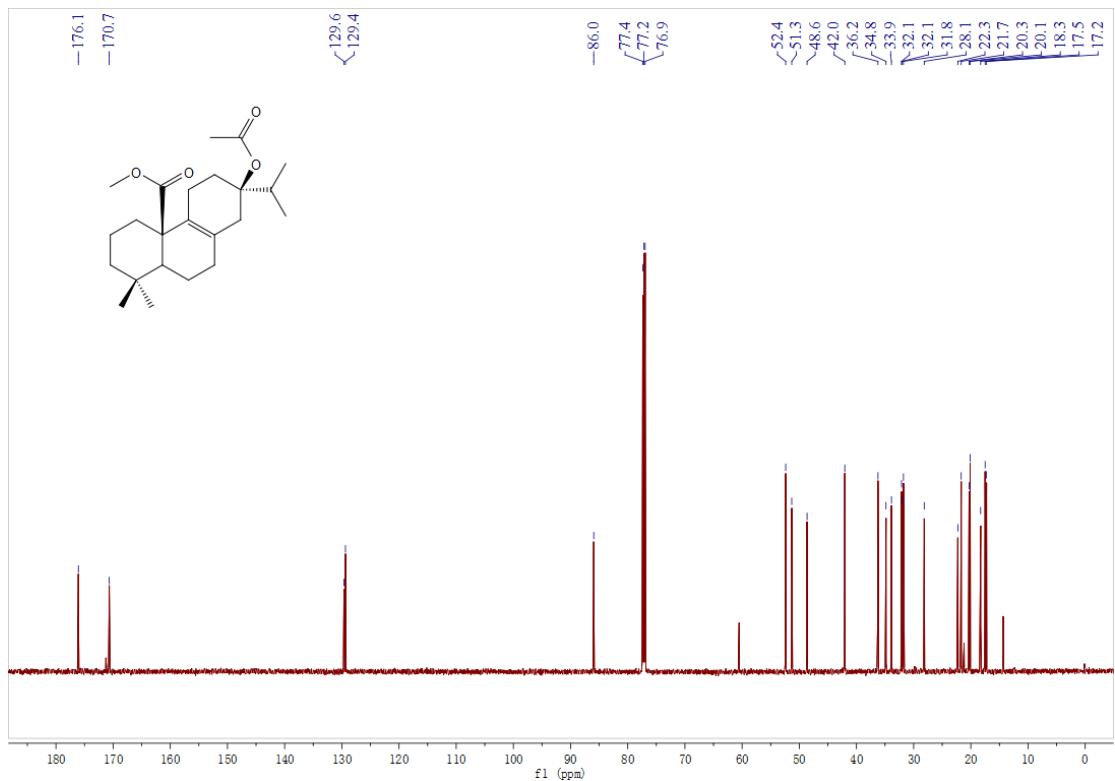
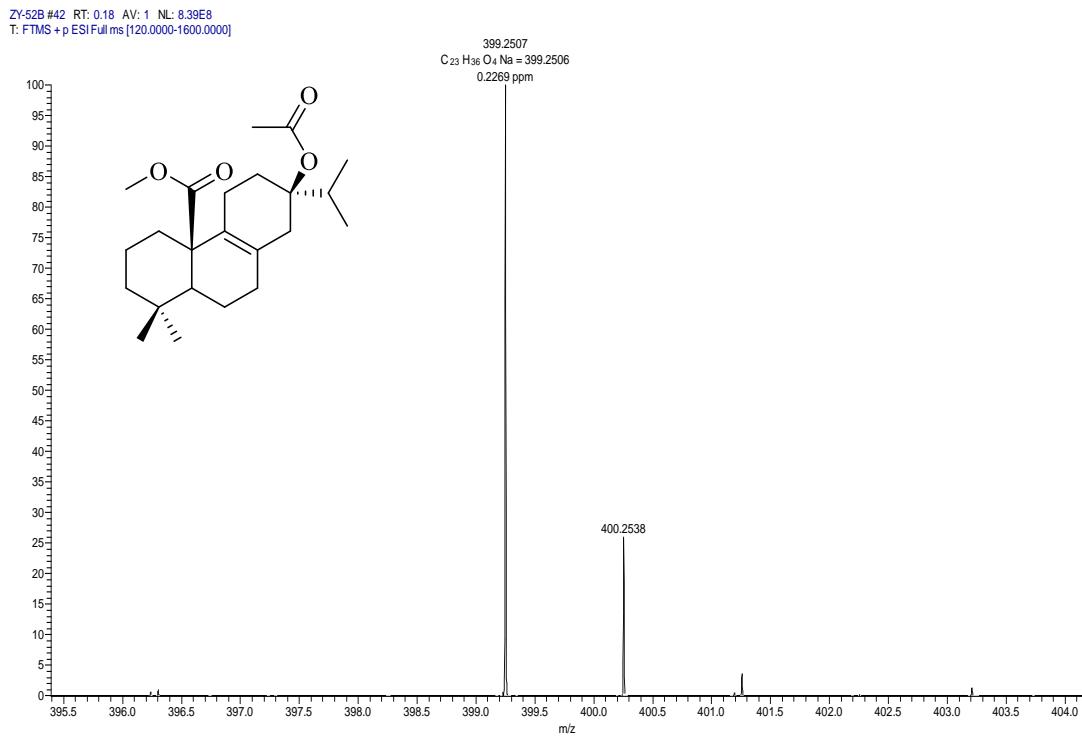


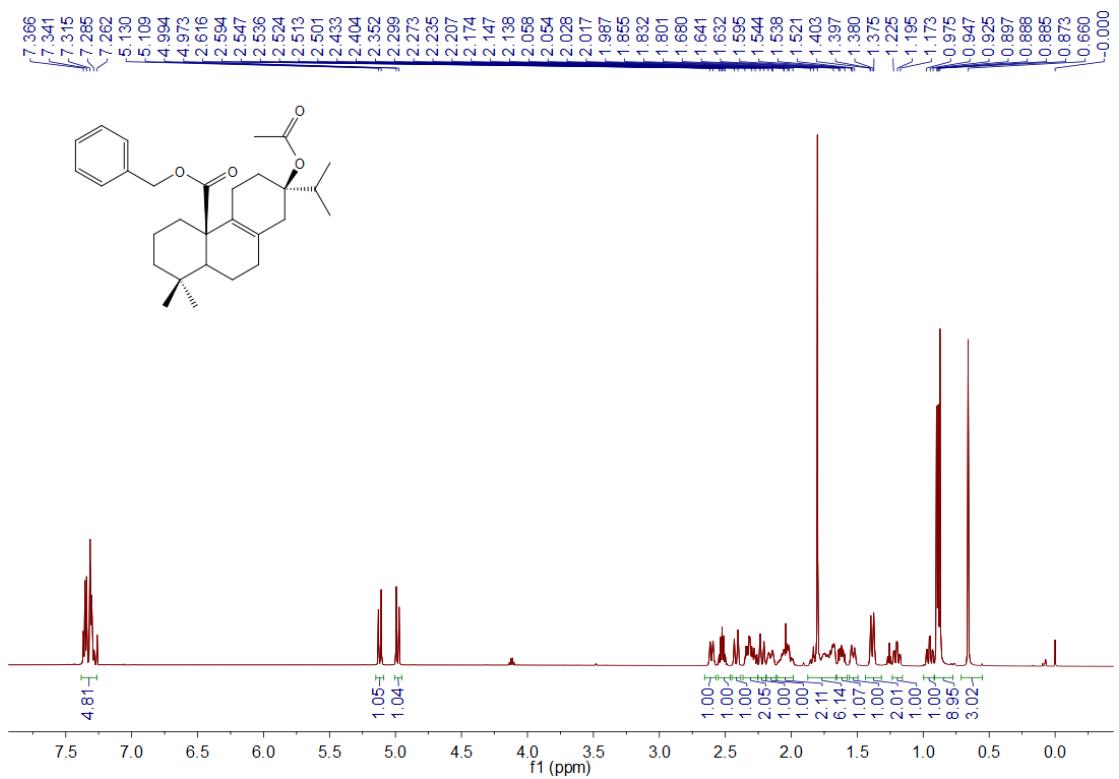
Figure S70. <sup>1</sup>H NMR spectrum of the compound 6a.



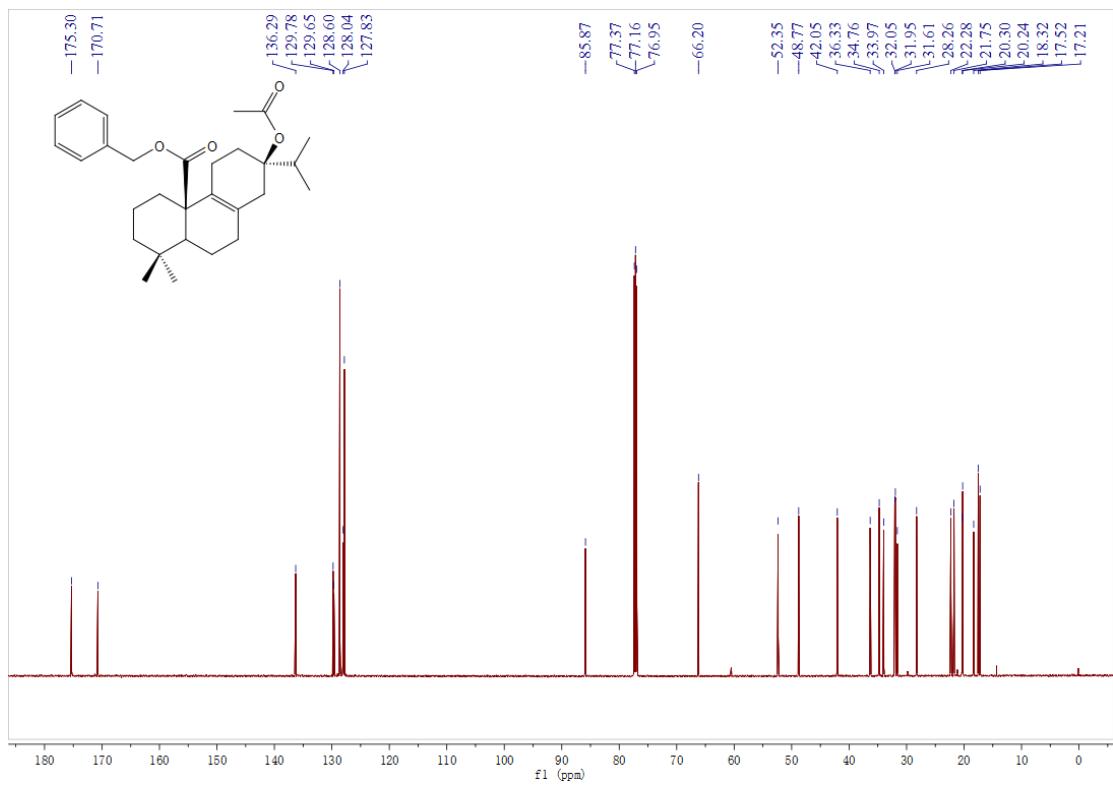
**Figure S71.**  $^{13}\text{C}$  NMR spectrum of the compound **6a**.



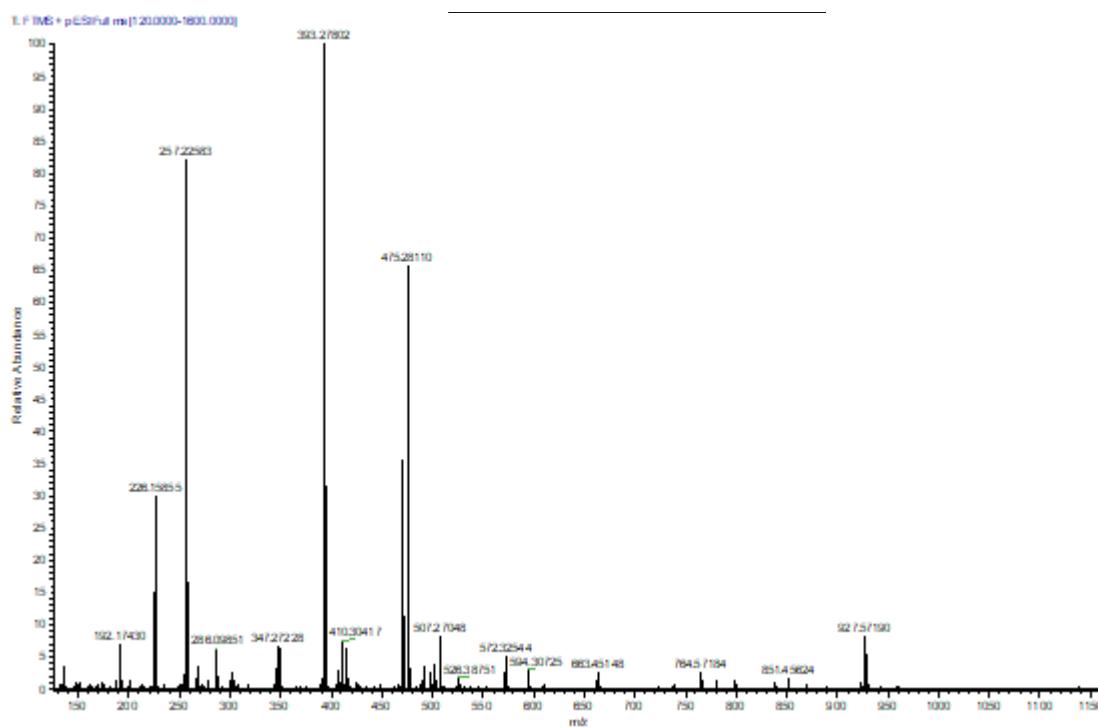
**Figure S72.** HRMS spectrum of the compound **6a**.



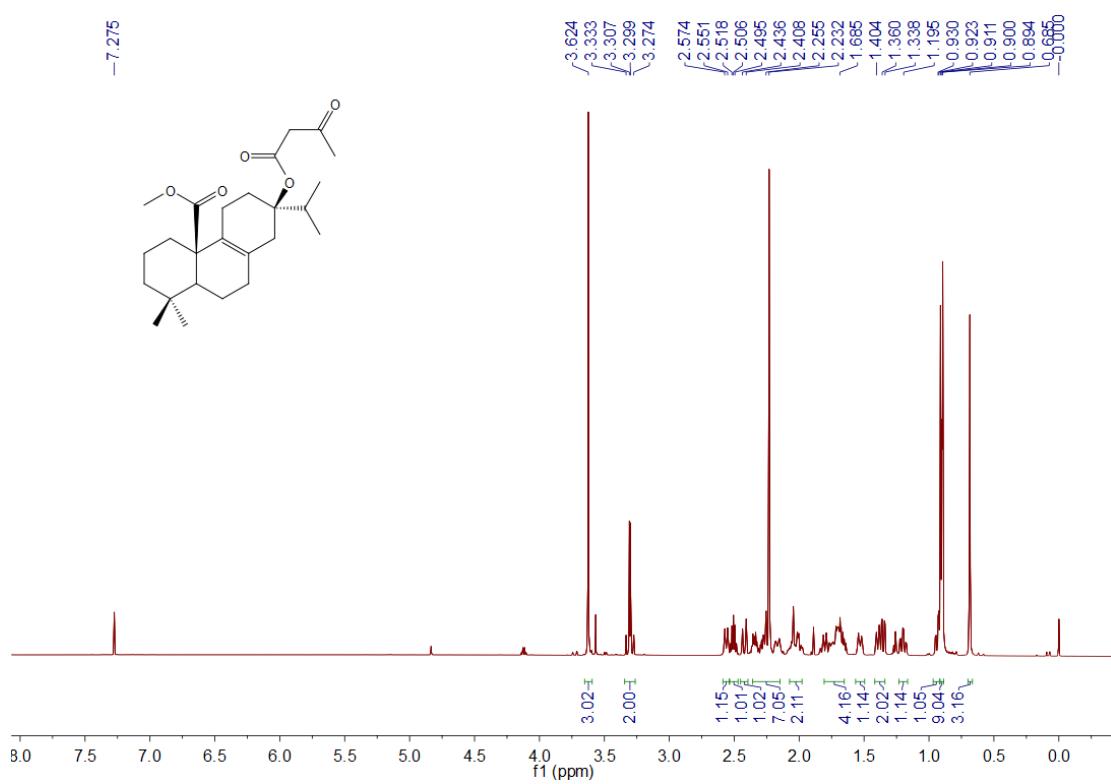
**Figure S73.**  $^1\text{H}$  NMR spectrum of the compound **6b**.



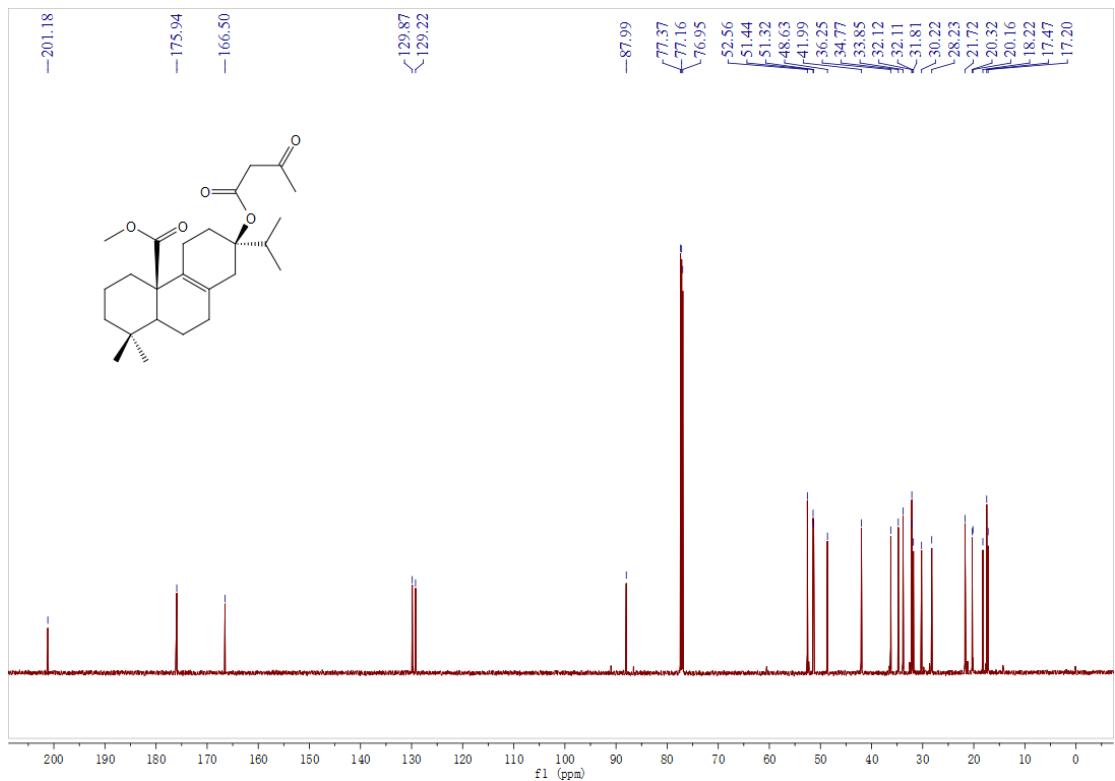
**Figure S74.**  $^{13}\text{C}$  NMR spectrum of the compound **6b**.



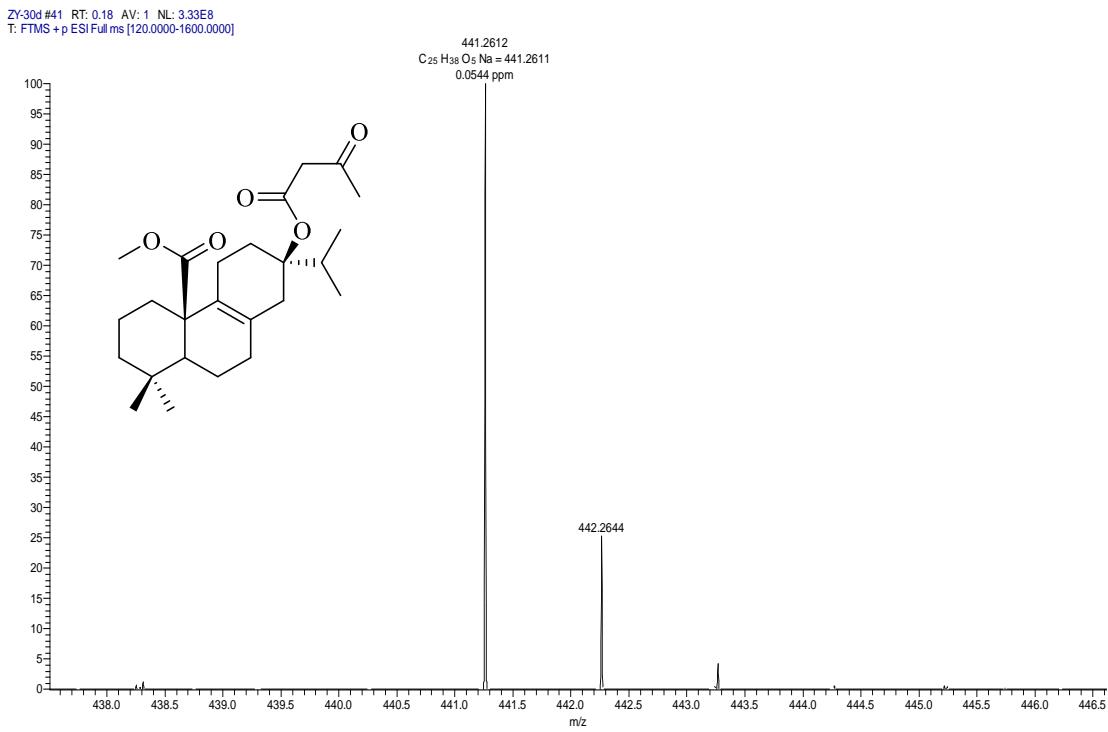
**Figure S75.** HRMS spectrum of the compound **6b**.



**Figure S76.**  $^1\text{H}$  NMR spectrum of the compound **6c**.



**Figure S77.**  $^{13}\text{C}$  NMR spectrum of the compound **6c**.



**Figure S78.** HRMS spectrum of the compound **6c**.