

## SUPPORTING INFORMATION

### **Triterpenoids from *Ganoderma lucidum* and their Potential Anti-inflammatory Effects**

Yan-Li Wu,<sup>†,‡</sup> Fei Han,<sup>†,‡</sup> Shan-Shan Luan,<sup>‡,‡</sup> Rui Ai,<sup>†</sup> Peng Zhang,<sup>†</sup> Hua Li,<sup>\*,†,‡</sup> and

Li-Xia Chen<sup>\*,†</sup>

<sup>†</sup> Wuya College of Innovation, School of Pharmacy, Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China.

<sup>‡</sup> School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan, 430030, China.

#### **Corresponding Authors**

\* Tel: +86-24-23986463. E-mail: [syzyclx@163.com](mailto:syzyclx@163.com). (Li-Xia Chen)

Tel: +86-24-23986463. E-mail: [li\\_hua@hust.edu.cn](mailto:li_hua@hust.edu.cn). (Hua Li)

### List of supporting information

- Figure S1.** <sup>1</sup>H-NMR spectrum of **1** (400 MHz, CD<sub>3</sub>OD)  
**Figure S2.** <sup>13</sup>C-NMR spectrum of **1** (100 MHz, CD<sub>3</sub>OD)  
**Figure S3.** HSQC spectrum of **1** (600 MHz, CD<sub>3</sub>OD)  
**Figure S4.** HMBC spectrum of **1** (600 MHz, CD<sub>3</sub>OD)  
**Figure S5.** NOESY spectrum of **1** (600 MHz, CD<sub>3</sub>OD)  
**Figure S6.** HRESIMS spectrum of **1**  
**Figure S7.** UV spectrum of compound **1**  
**Figure S8.** IR spectrum of compound **1**  
**Figure S9.** <sup>1</sup>H-NMR spectrum of **2** (400 MHz, CD<sub>3</sub>OD)  
**Figure S10.** <sup>13</sup>C-NMR spectrum of **2** (100 MHz, CD<sub>3</sub>OD)  
**Figure S11.** HSQC spectrum of **2** (600 MHz, CD<sub>3</sub>OD)  
**Figure S12.** HMBC spectrum of **2** (600 MHz, CD<sub>3</sub>OD)  
**Figure S13.** H-<sup>1</sup>H COSY spectrum of compound **2**(600 MHz, CD<sub>3</sub>OD)  
**Figure S14.** NOESY spectrum of compound **2** (600 MHz, CD<sub>3</sub>OD)  
**Figure S15.** HRESIMS spectrum of compound **2**  
**Figure S16.** UV spectrum of compound **2**  
**Figure S17.** IR spectrum of **2**  
**Figure S18.** <sup>1</sup>H-NMR spectrum of **3** (400 MHz, CDCl<sub>3</sub>)  
**Figure S19.** <sup>13</sup>C-NMR spectrum of **3** (100 MHz, CDCl<sub>3</sub>)  
**Figure S20.** HSQC spectrum of **3** (600 MHz, CDCl<sub>3</sub>)  
**Figure S21.** HMBC spectrum of **3** (600 MHz, CDCl<sub>3</sub>)  
**Figure S22.** NOESY spectrum of **3** (600 MHz, CDCl<sub>3</sub>)  
**Figure S23.** HRESIMS spectrum of **3**  
**Figure S24.** UV spectrum of **3**  
**Figure S25.** IR spectrum of **3**  
**Figure S26.** <sup>1</sup>H-NMR spectrum of **4** (600 MHz, CDCl<sub>3</sub>)  
**Figure S27.** <sup>13</sup>C-NMR spectrum of **4** (150 MHz, CDCl<sub>3</sub>)  
**Figure S28.** HSQC spectrum of **4** (600 MHz, CDCl<sub>3</sub>)  
**Figure S29.** HMBC spectrum of **4** (600 MHz, CDCl<sub>3</sub>)  
**Figure S30.** NOESY spectrum of **4** (600 MHz, CDCl<sub>3</sub>)  
**Figure S31.** HRESIMS spectrum of **4**  
**Figure S32.** UV spectrum of **4**  
**Figure S33.** IR spectrum of **4**  
**Figure S34.** <sup>1</sup>H-NMR spectrum of **5** (600 MHz, CD<sub>3</sub>OD)  
**Figure S35.** <sup>13</sup>C-NMR spectrum of **5** (150 MHz, CD<sub>3</sub>OD)  
**Figure S36.** HSQC spectrum of **5** (600 MHz, CD<sub>3</sub>OD)  
**Figure S37.** HMBC spectrum of **5** (600 MHz, CD<sub>3</sub>OD)  
**Figure S38.** NOESY spectrum of **5** (600 MHz, CD<sub>3</sub>OD)  
**Figure S39.** HRESIMS spectrum of **5**  
**Figure S40.** UV spectrum of **5**  
**Figure S41.** IR spectrum of **5**  
**Figure S42.** <sup>1</sup>H-NMR spectrum of **6** (600 MHz, CD<sub>3</sub>OD)  
**Figure S43.** <sup>13</sup>C-NMR spectrum of **6** (150 MHz, CD<sub>3</sub>OD)

- Figure S44.** HSQC spectrum of **6** (600 MHz, CD<sub>3</sub>OD)
- Figure S45.** HMBC spectrum of **6** (600 MHz, CD<sub>3</sub>OD)
- Figure S46.** NOESY spectrum of **6** (600 MHz, CD<sub>3</sub>OD)
- Figure S47.** HRESIMS spectrum of **6**
- Figure S48.** UV spectrum of **6**
- Figure S49.** IR spectrum of **6**
- Figure S50.** <sup>1</sup>H-NMR (600 MHz, C<sub>5</sub>D<sub>5</sub>N) spectrum of the (*R*)-MTPA ester of **6**
- Figure S51.** <sup>1</sup>H-NMR (600 MHz, C<sub>5</sub>D<sub>5</sub>N) spectrum of the (*S*)-MTPA ester of **6**
- Table S1** The inhibition rate against NO production of all compounds at 50 μM.

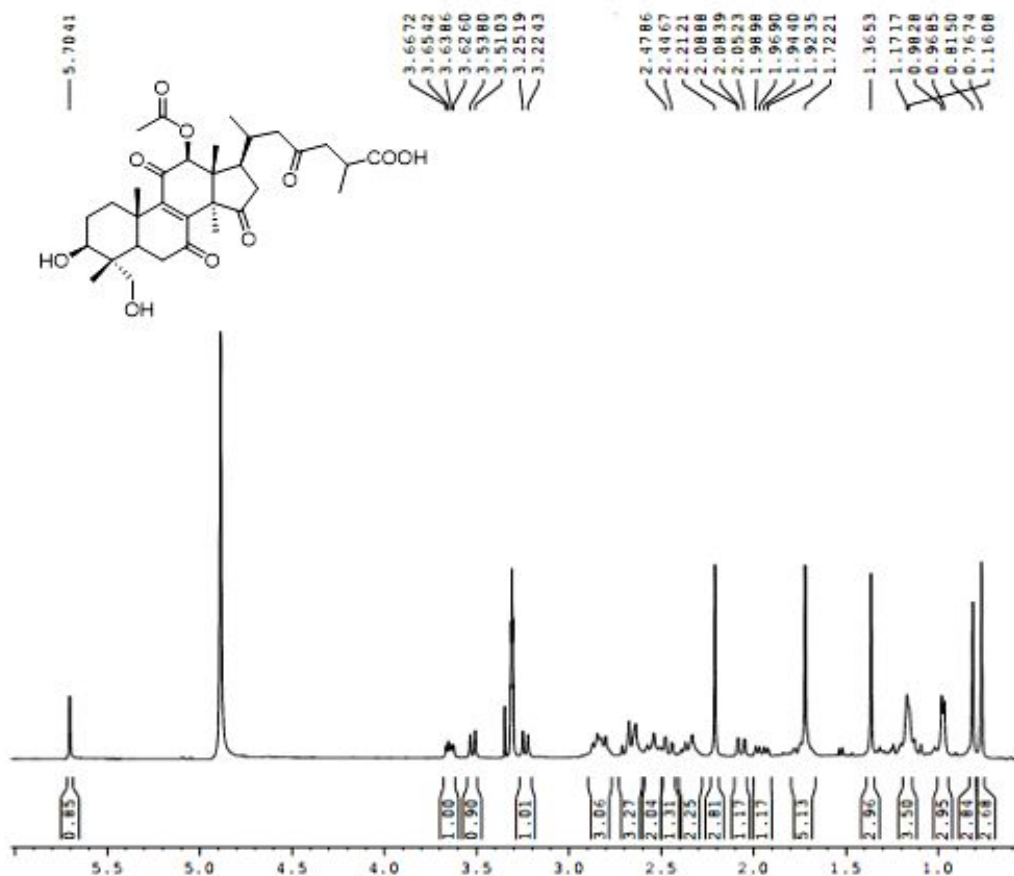


Figure S1. <sup>1</sup>H-NMR spectrum of **1** (400 MHz, CD<sub>3</sub>OD)

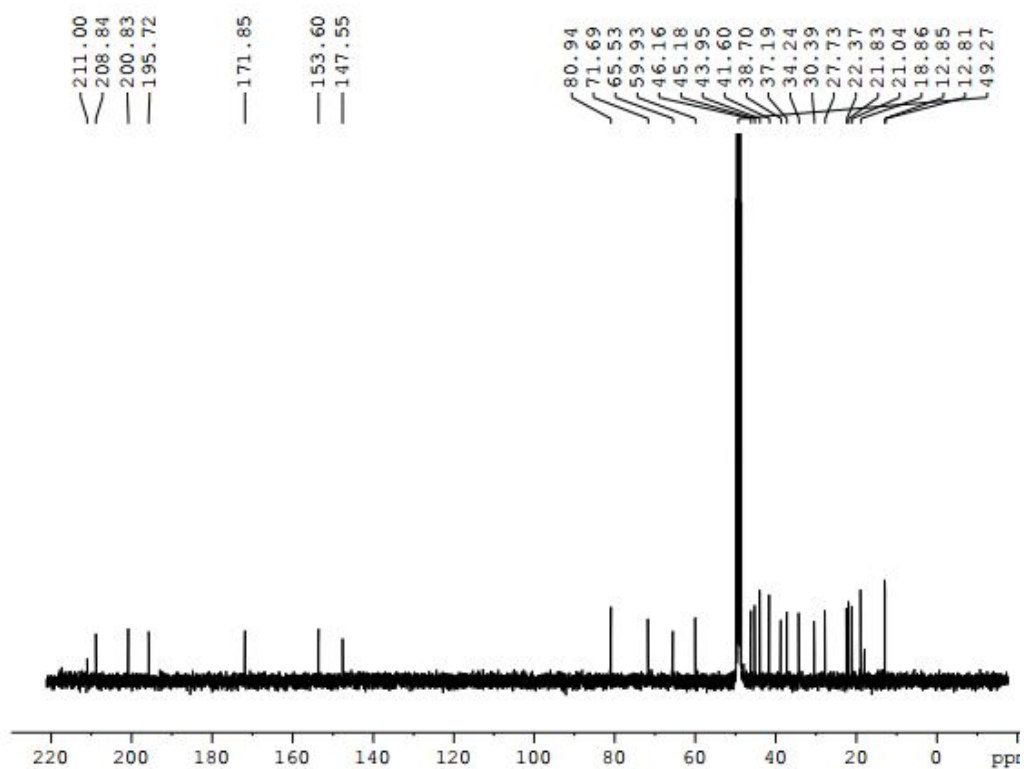
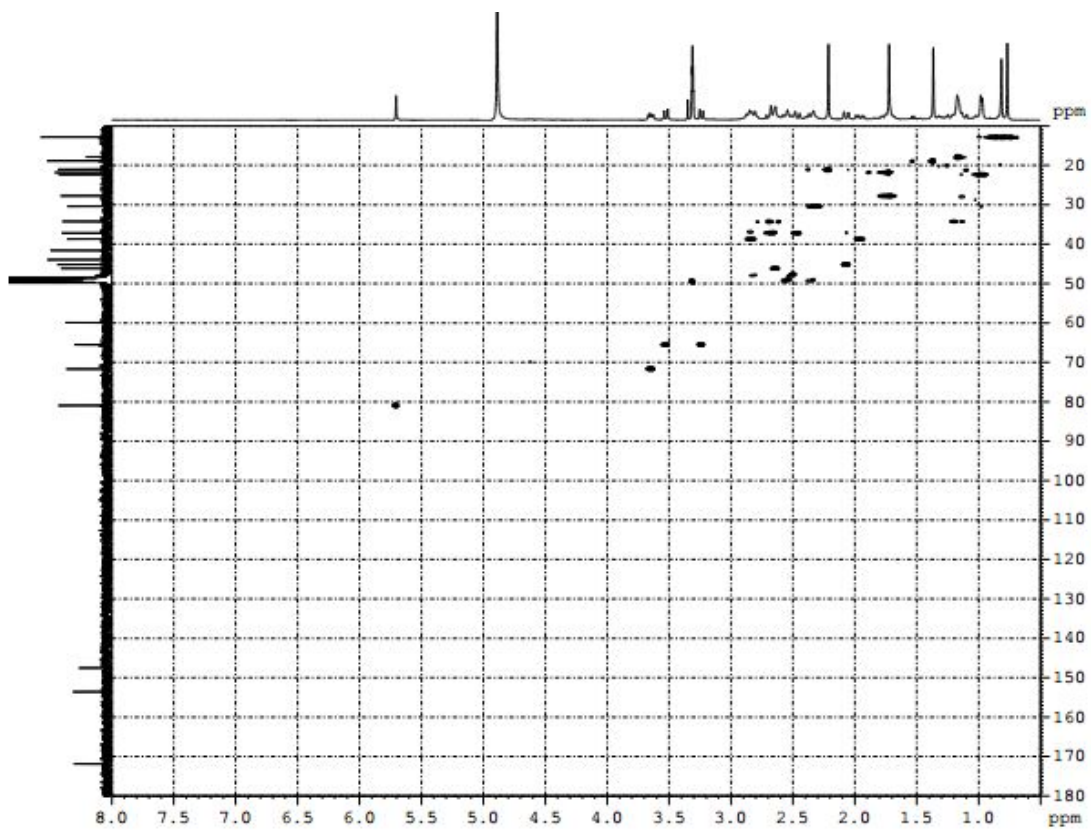
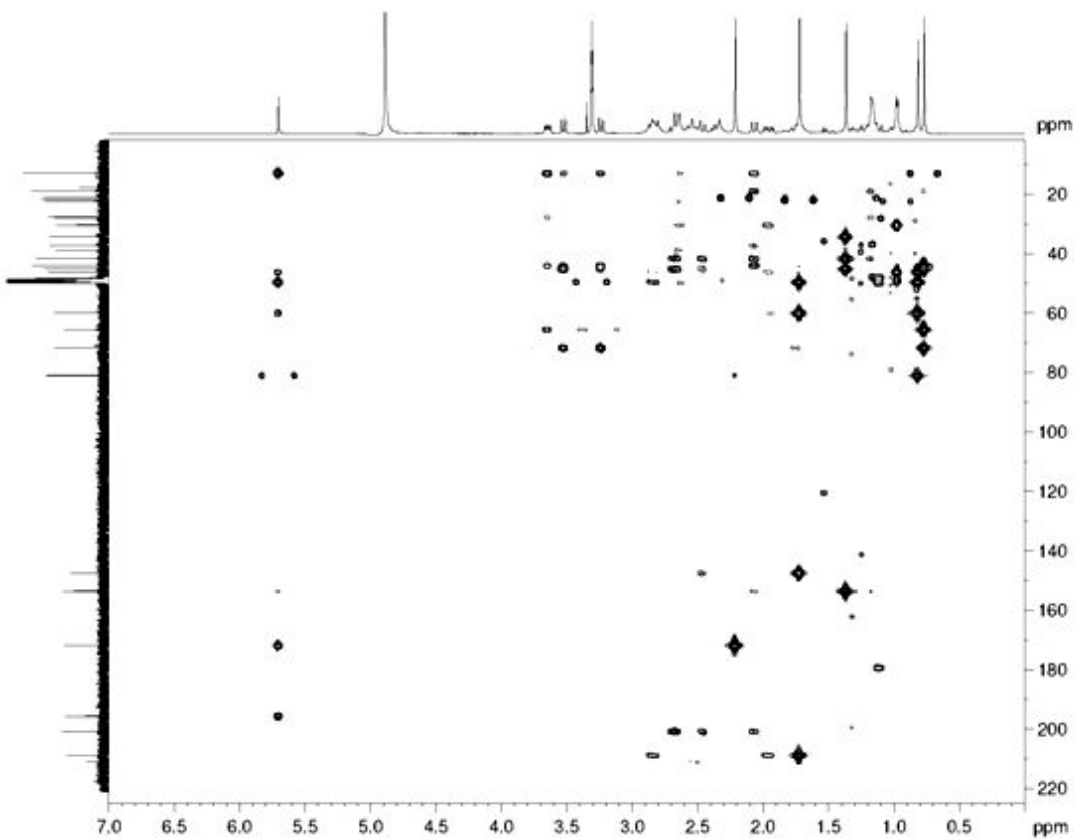


Figure S2. <sup>13</sup>C-NMR spectrum of **1** (100 MHz, CD<sub>3</sub>OD)



**Figure S3.** HSQC spectrum of **1** (600 MHz, CD<sub>3</sub>OD)



**Figure S4.** HMBC spectrum of **1** (600 MHz, CD<sub>3</sub>OD)

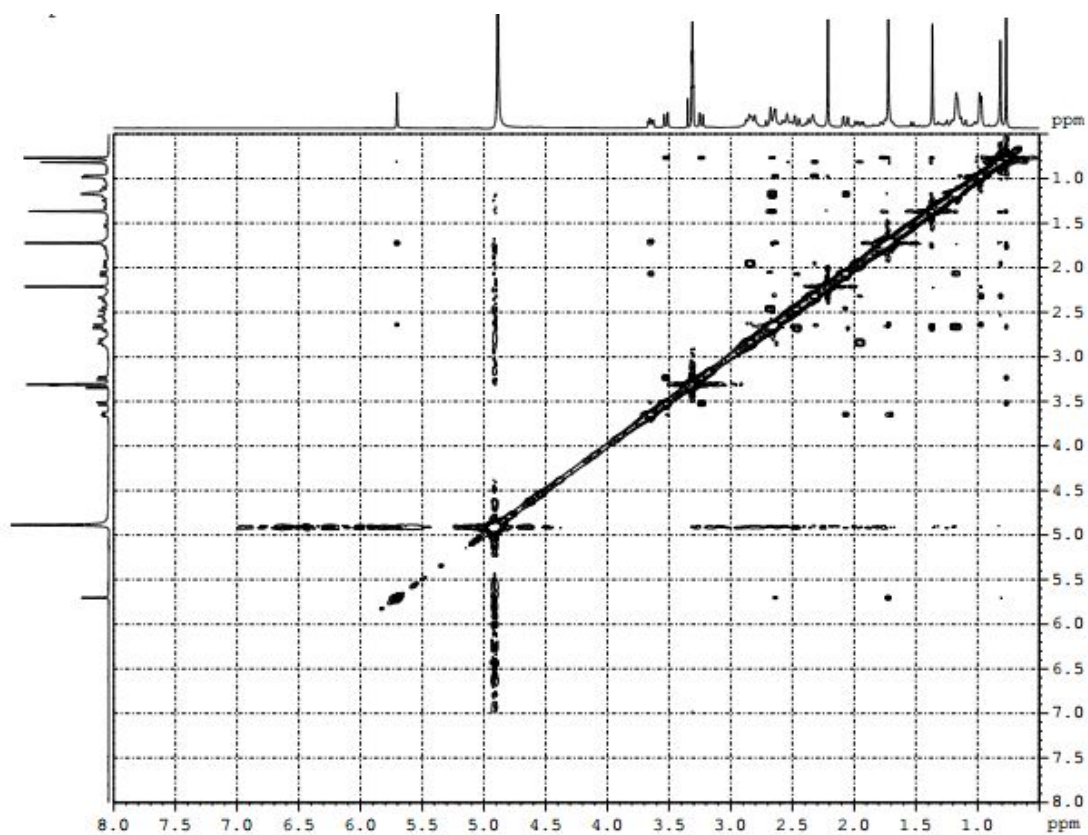
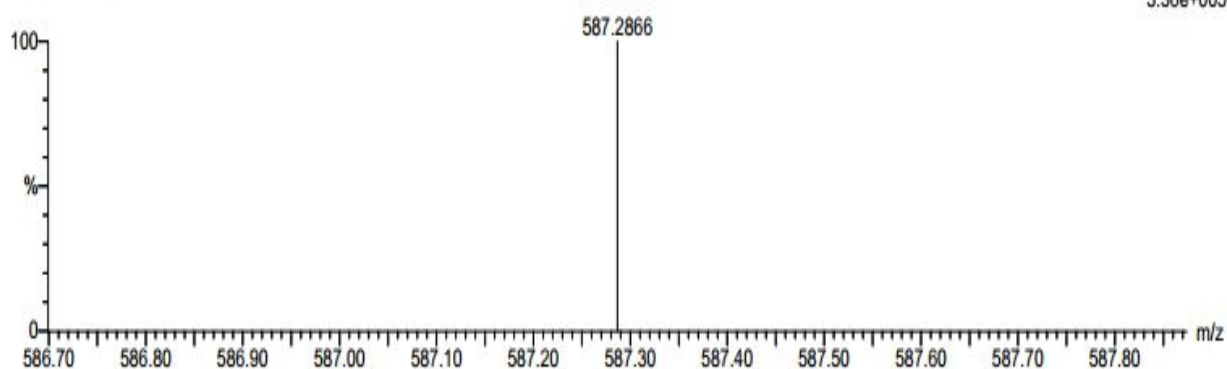


Figure S5. NOESY spectrum of **1** (600 MHz, CD<sub>3</sub>OD)

SY0923neg5 26 (0.116)  
1: TOF MS ES-

3.36e+005



Minimum: 3.0  
Maximum: 4.0 2.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
587.2866	587.2856	1.0	1.7	11.5	40.2	n/a	n/a	C <sub>32</sub> H <sub>43</sub> O <sub>10</sub>

Figure S6. HRMS spectrum of **1**

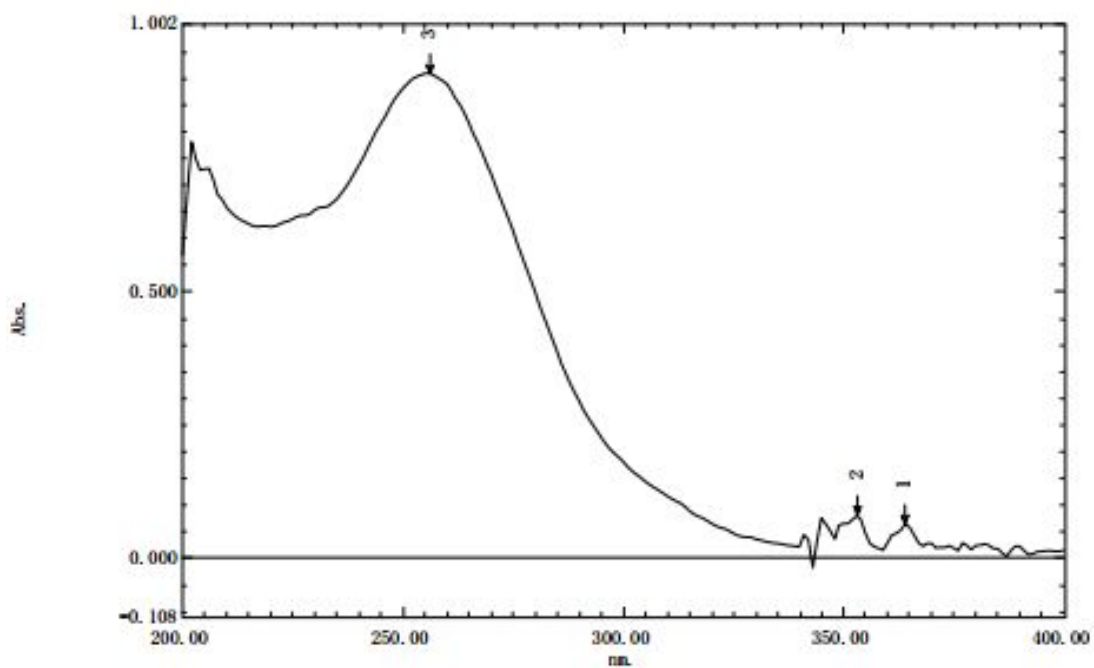


Figure S7. UV spectrum of **1**

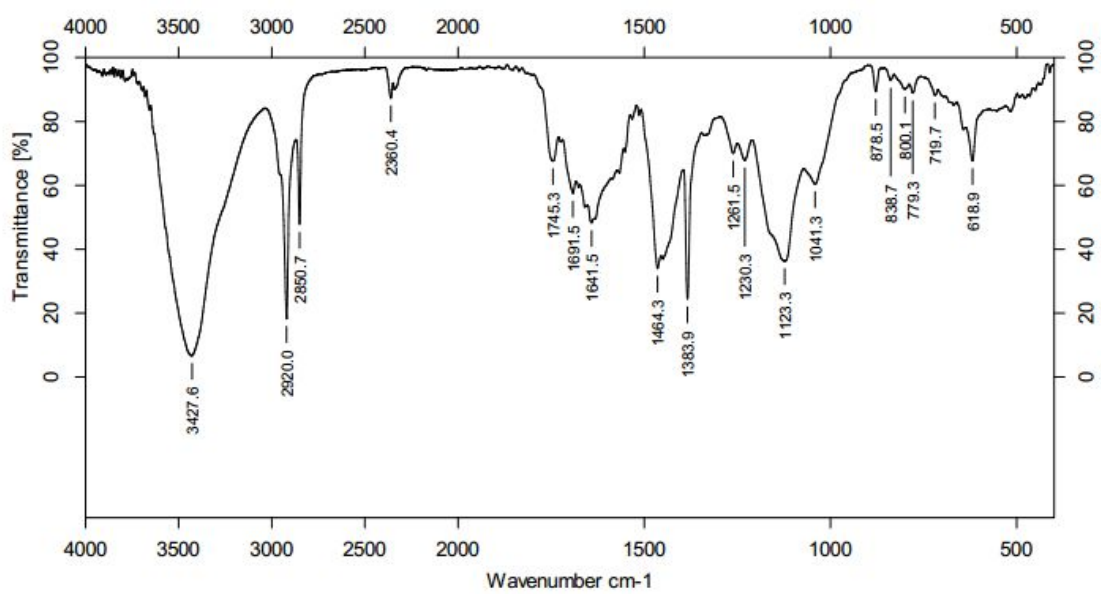


Figure S8. IR spectrum of **1**

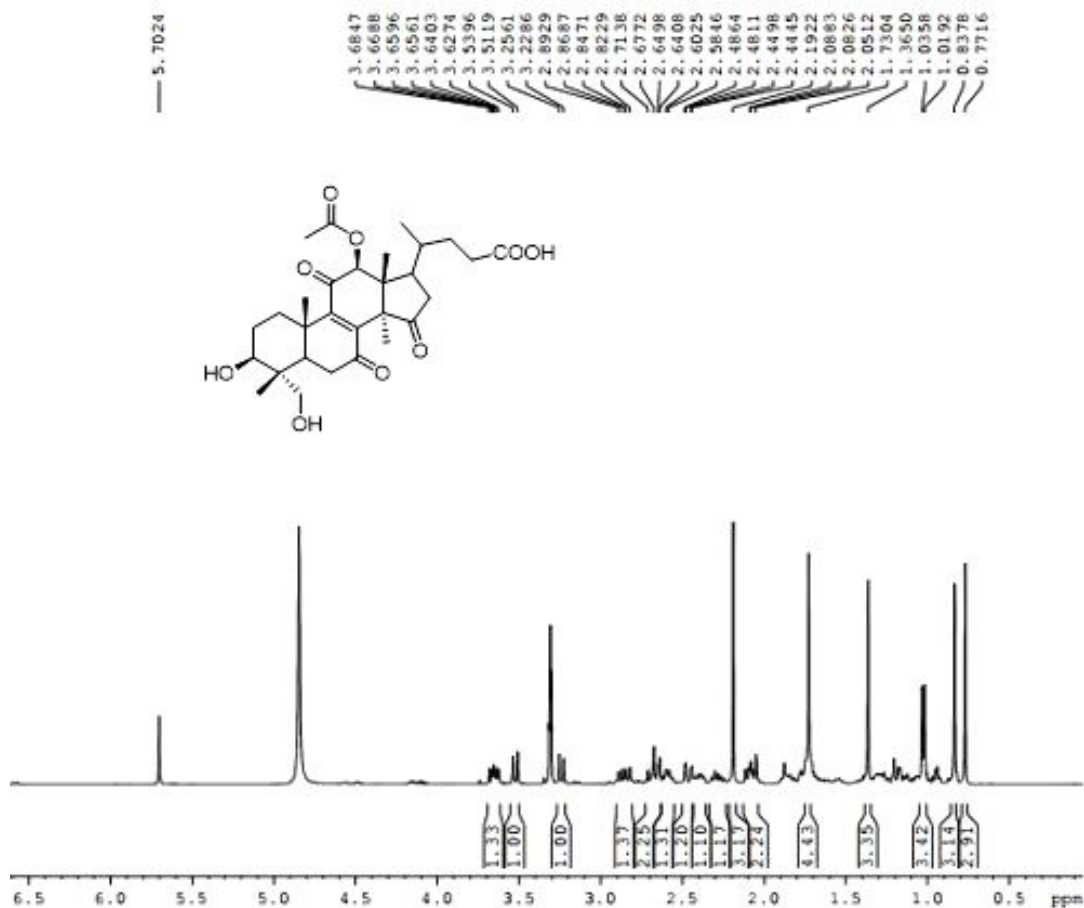


Figure S9.  $^1\text{H-NMR}$  spectrum of **2** (400 MHz,  $\text{CD}_3\text{OD}$ )

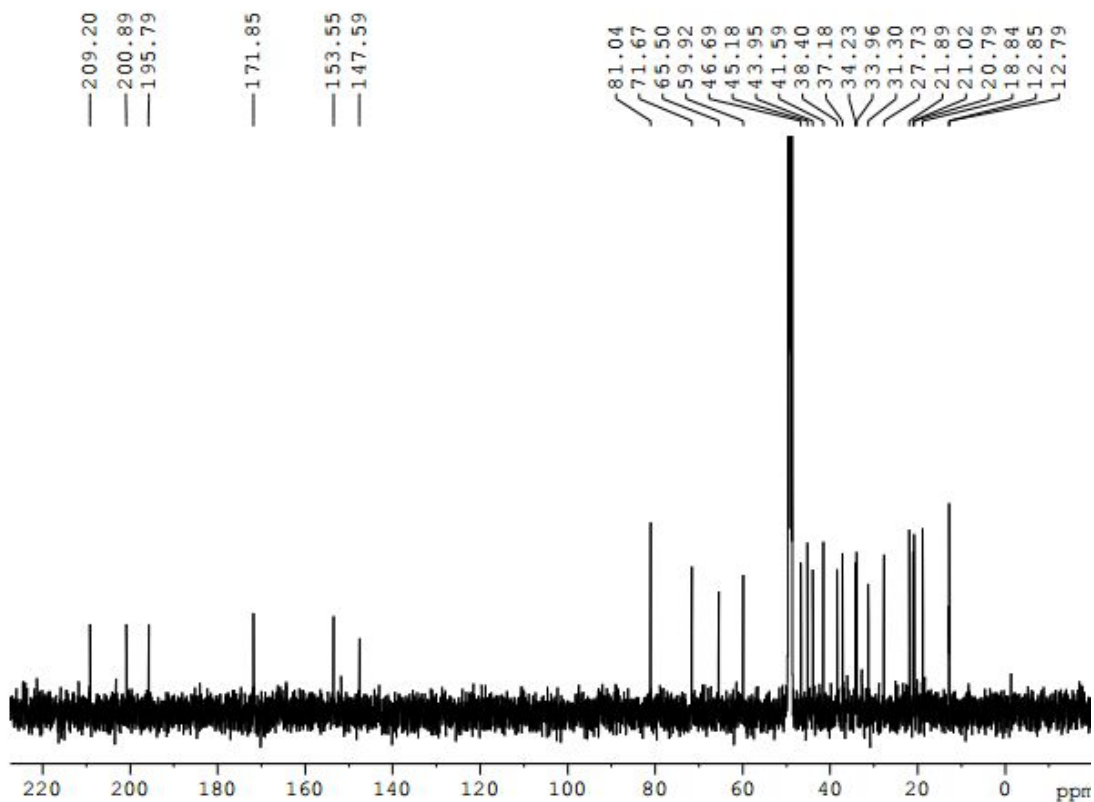
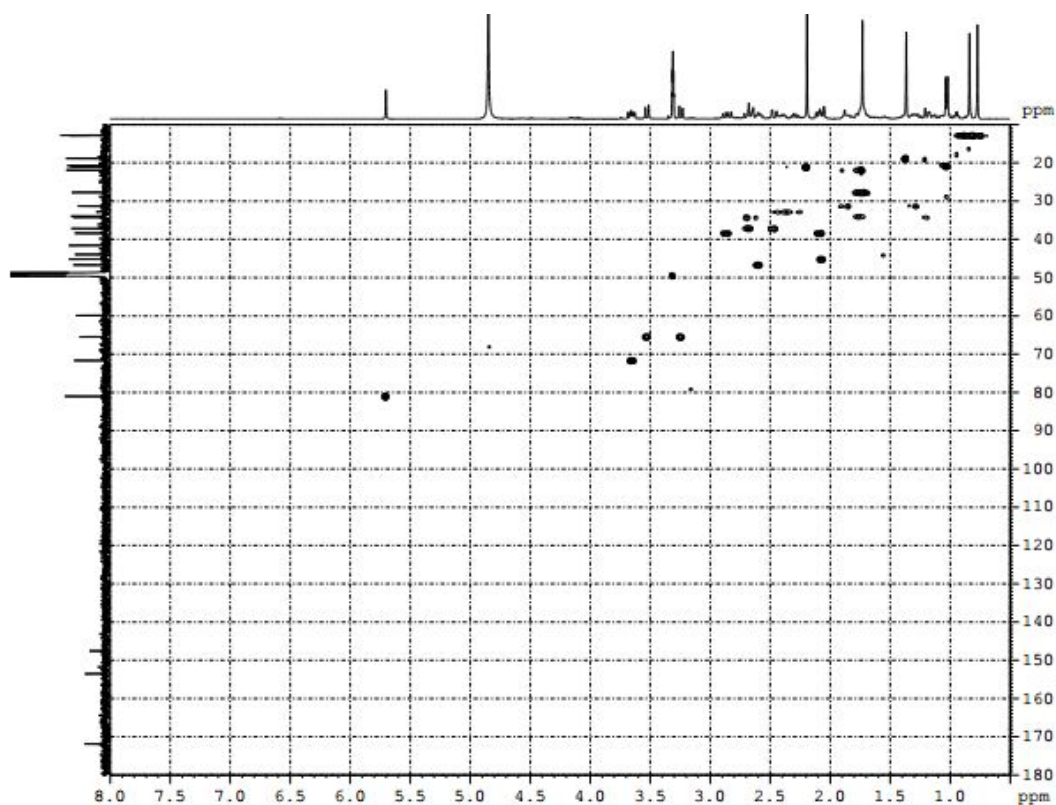
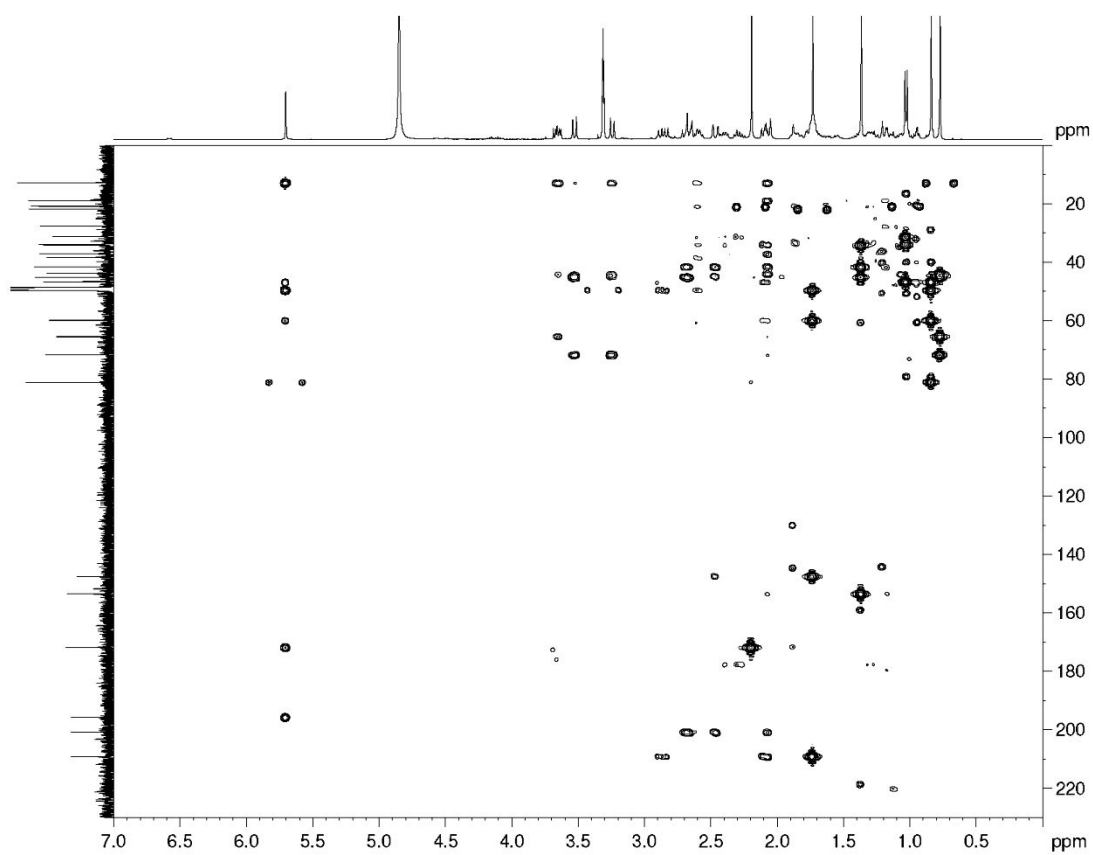


Figure S10.  $^{13}\text{C-NMR}$  spectrum of **2** (100 MHz,  $\text{CD}_3\text{OD}$ )

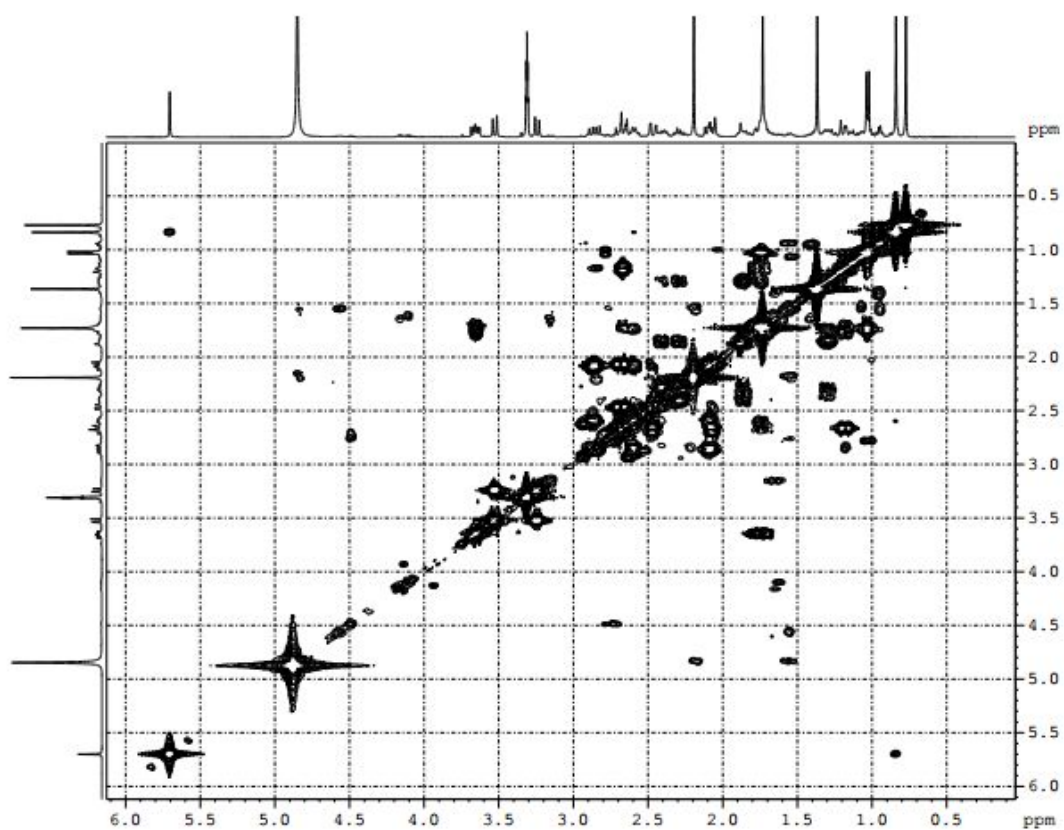




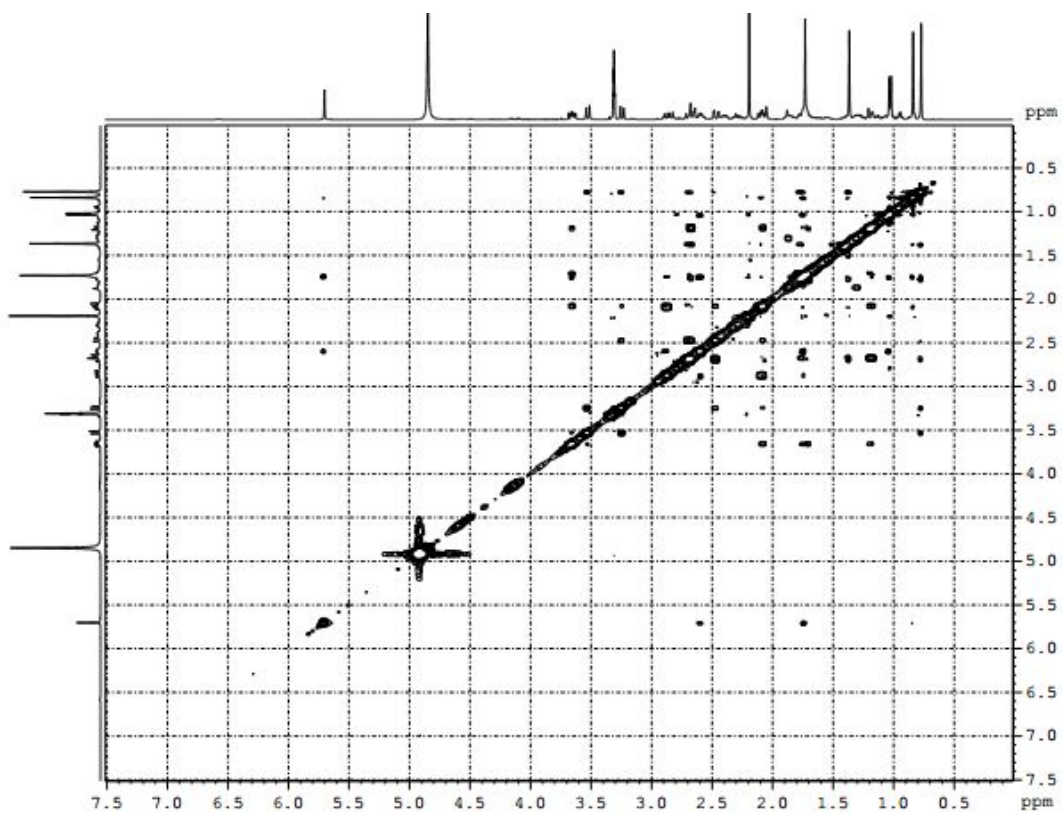
**Figure S11.** HSQC spectrum of **2** (600 MHz, CD<sub>3</sub>OD)



**Figure S12.** HMBC spectrum of **2** (600 MHz, CD<sub>3</sub>OD)



**Figure S13.** H-<sup>1</sup>H COSY spectrum of **2** (600 MHz, CD<sub>3</sub>OD)



**Figure S14.** NOESY spectrum of **2** (600 MHz, CD<sub>3</sub>OD)

SY0923neg4 43 (0.177)  
1: TOF MS ES-

3.87e+004

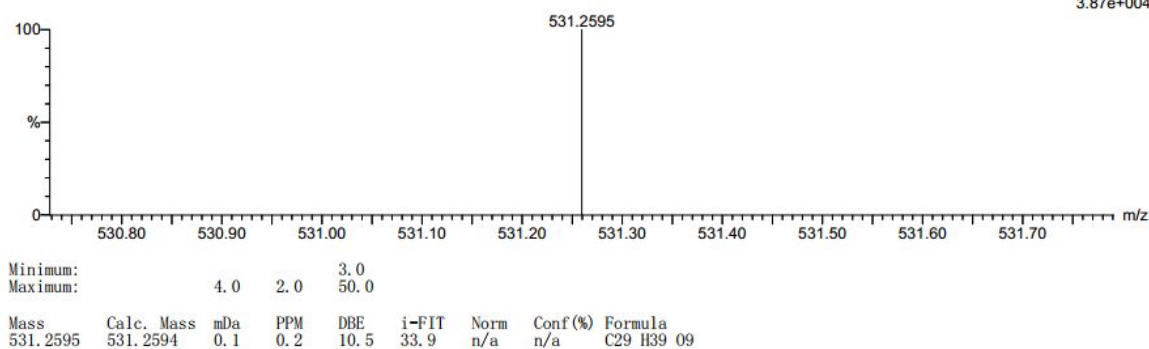


Figure S15. HRESIMS spectrum of 2

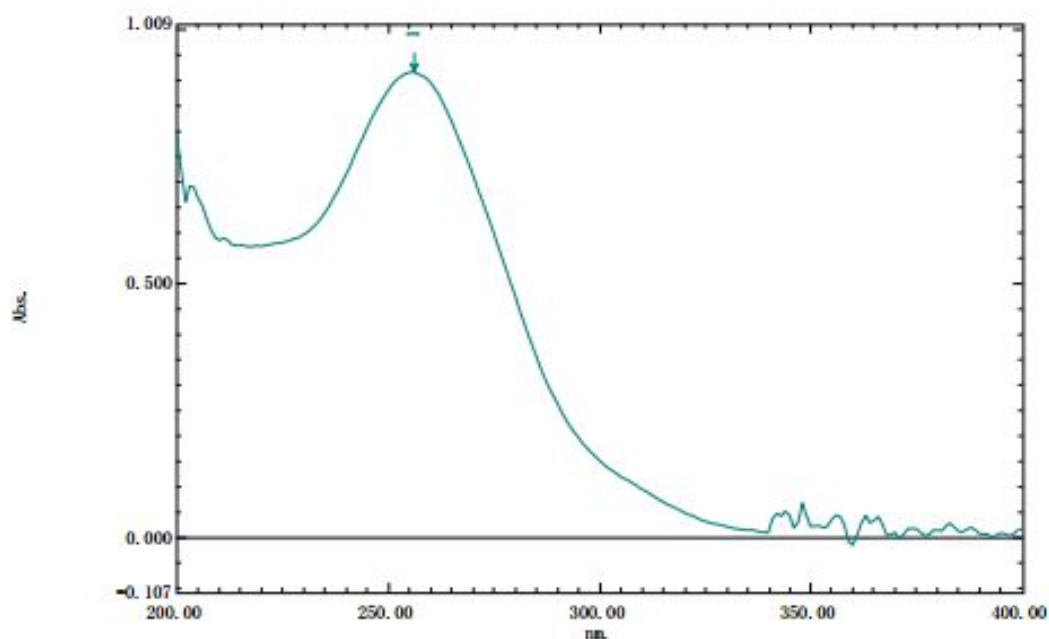


Figure S16. UV spectrum of 2

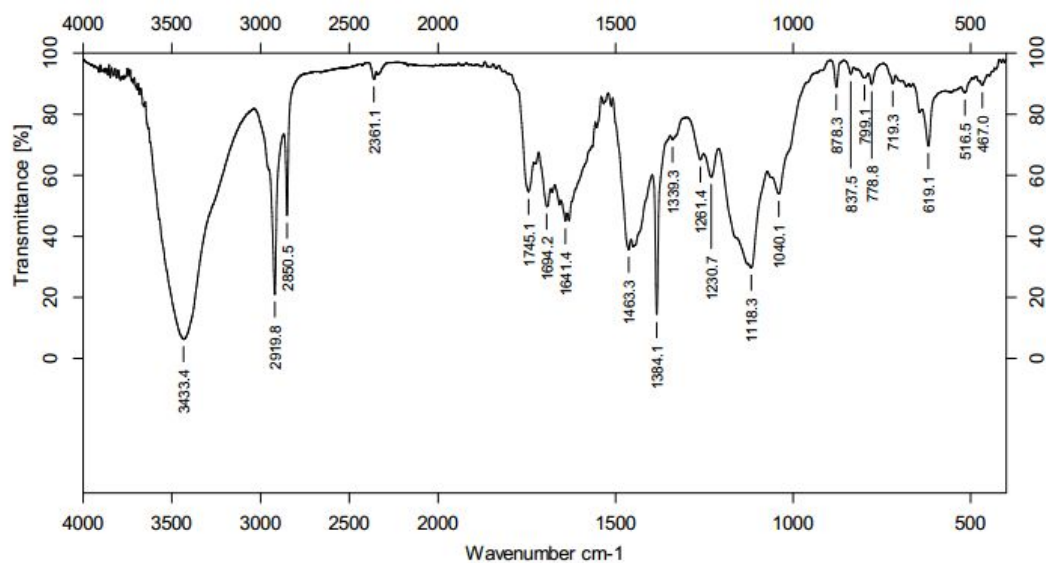


Figure S17. IR spectrum of 2

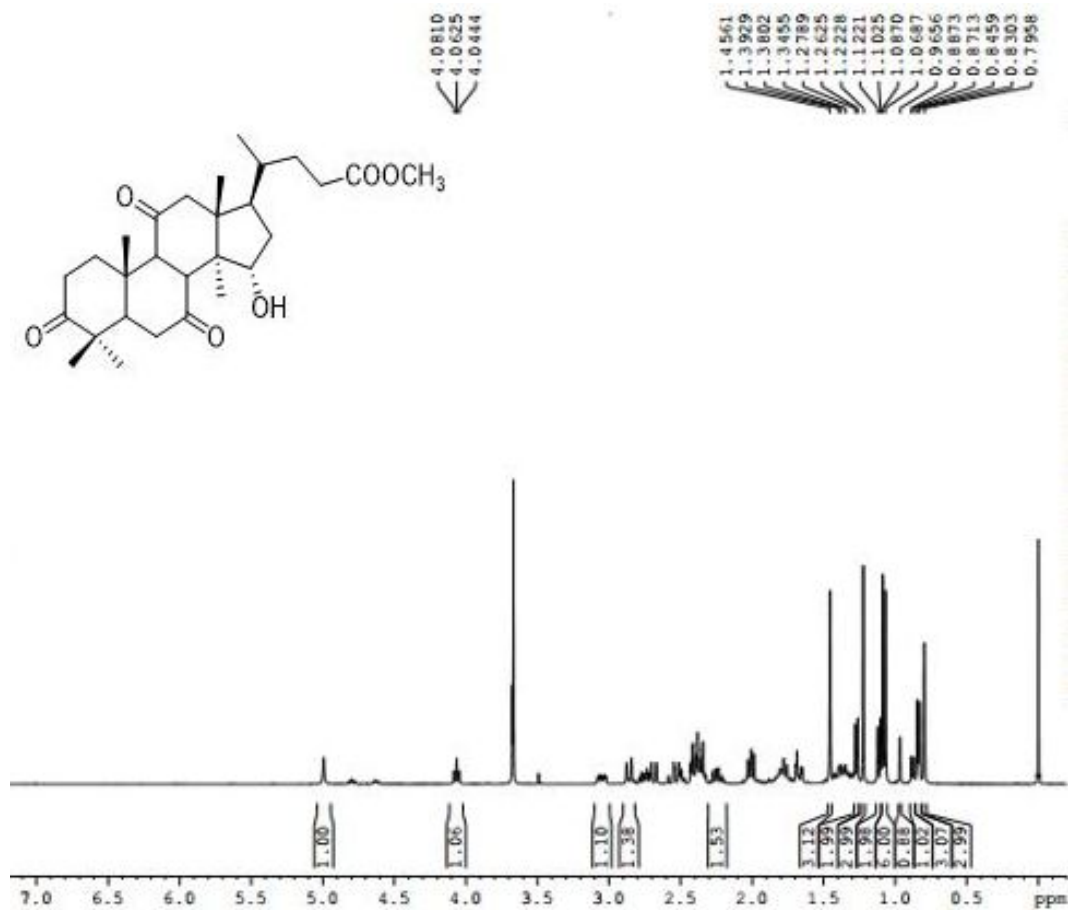


Figure S18.  $^1\text{H-NMR}$  spectrum of **3** (400 MHz,  $\text{CDCl}_3$ )

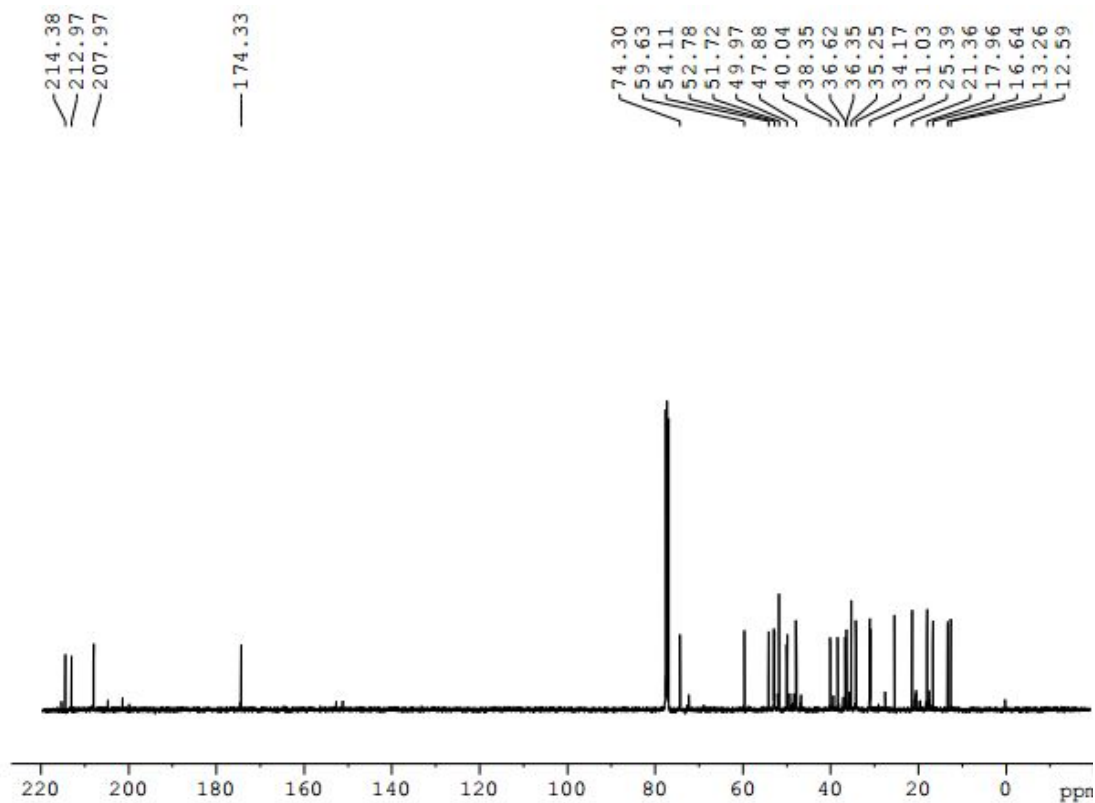
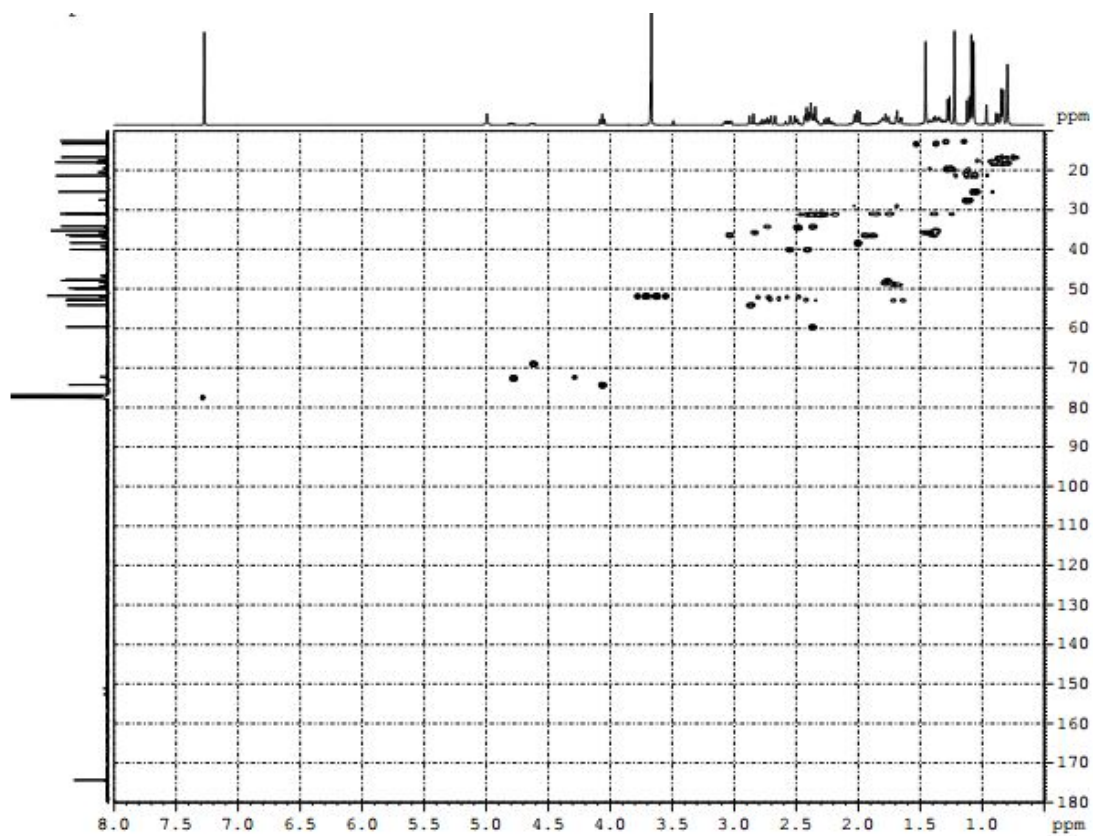
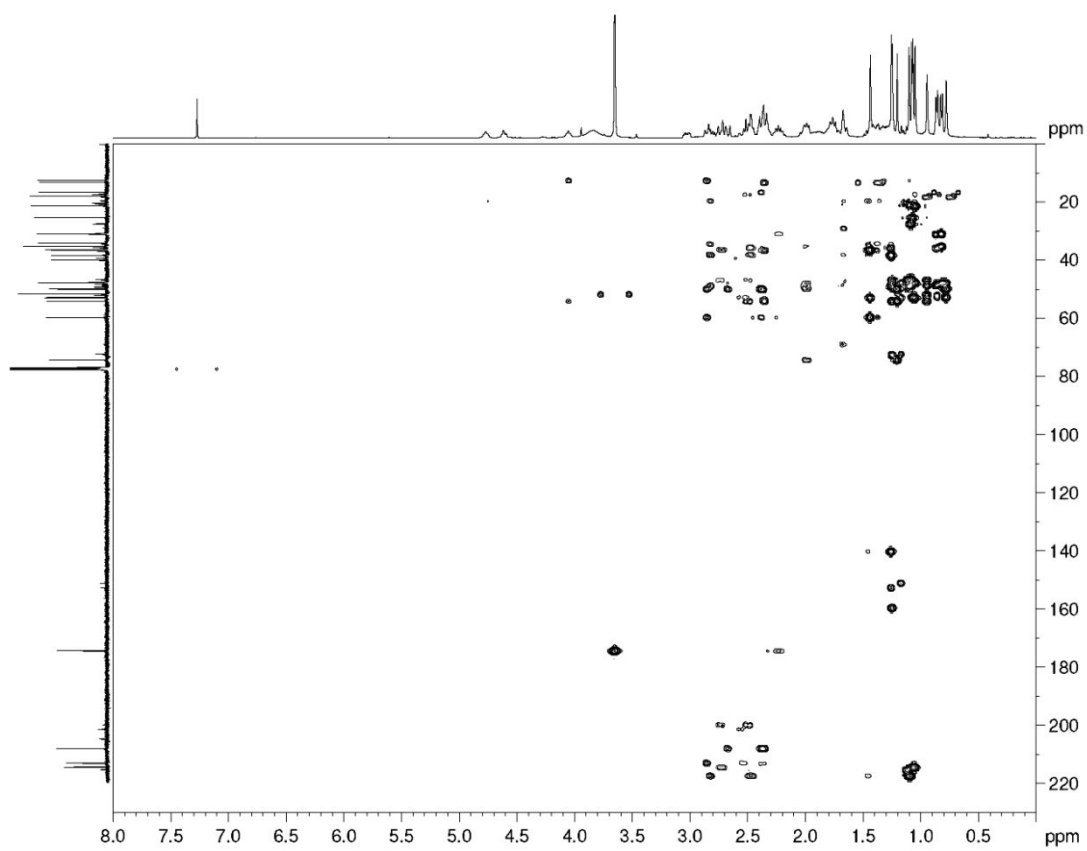


Figure S19.  $^{13}\text{C-NMR}$  spectrum of **3** (100 MHz,  $\text{CDCl}_3$ )



**Figure S20.** HSQC spectrum of **3** (600 MHz, CDCl<sub>3</sub>)



**Figure S21.** HMBC spectrum of **3** (600 MHz, CDCl<sub>3</sub>)

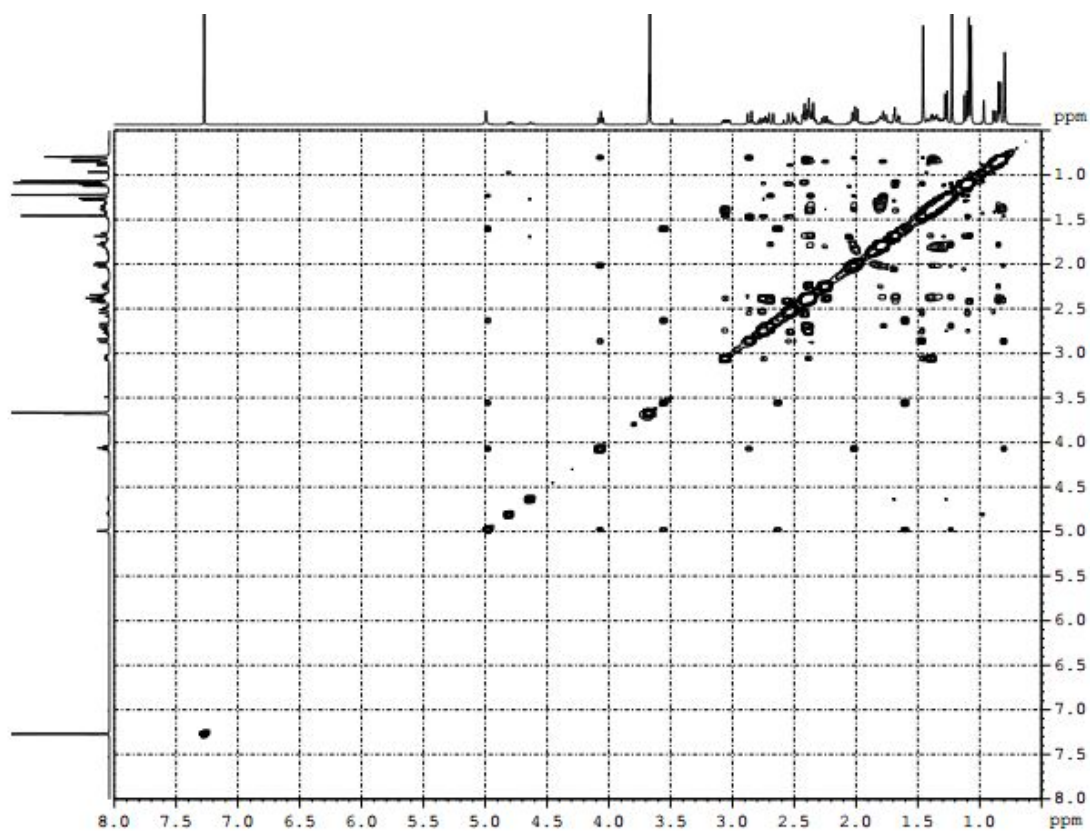


Figure S22. NOESY spectrum of **3** (600 MHz, CDCl<sub>3</sub>)

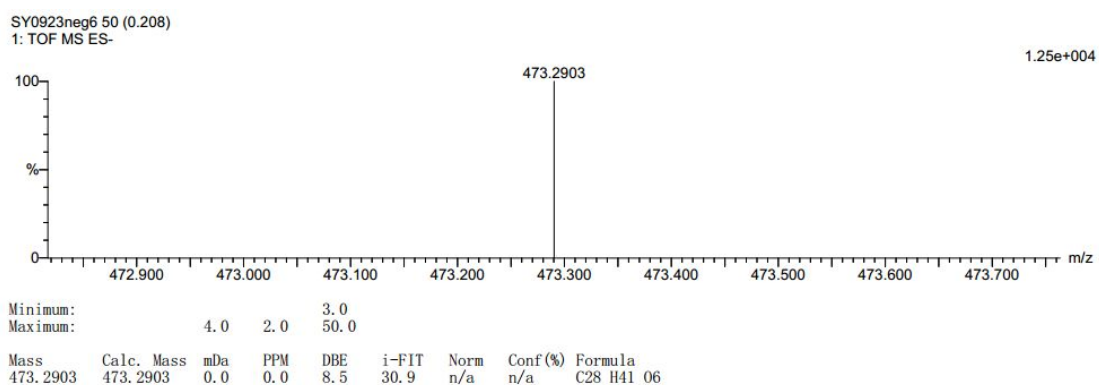
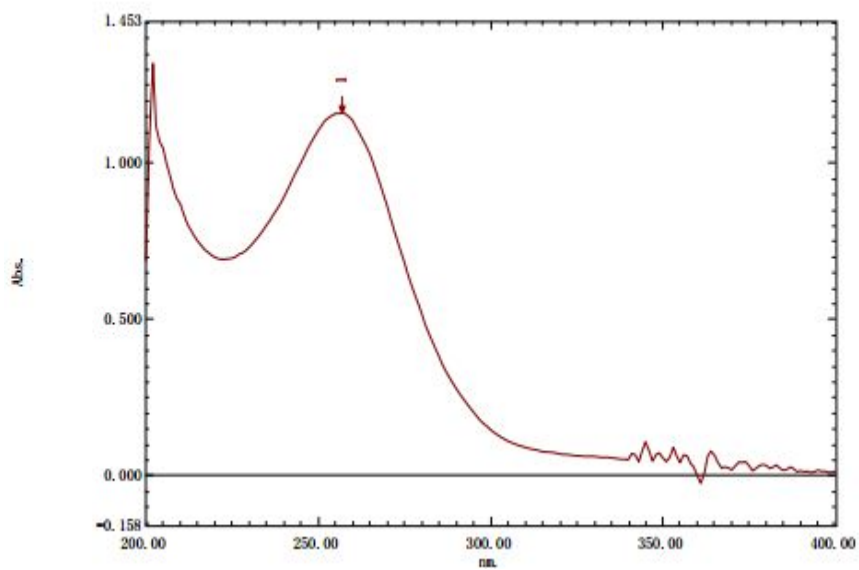
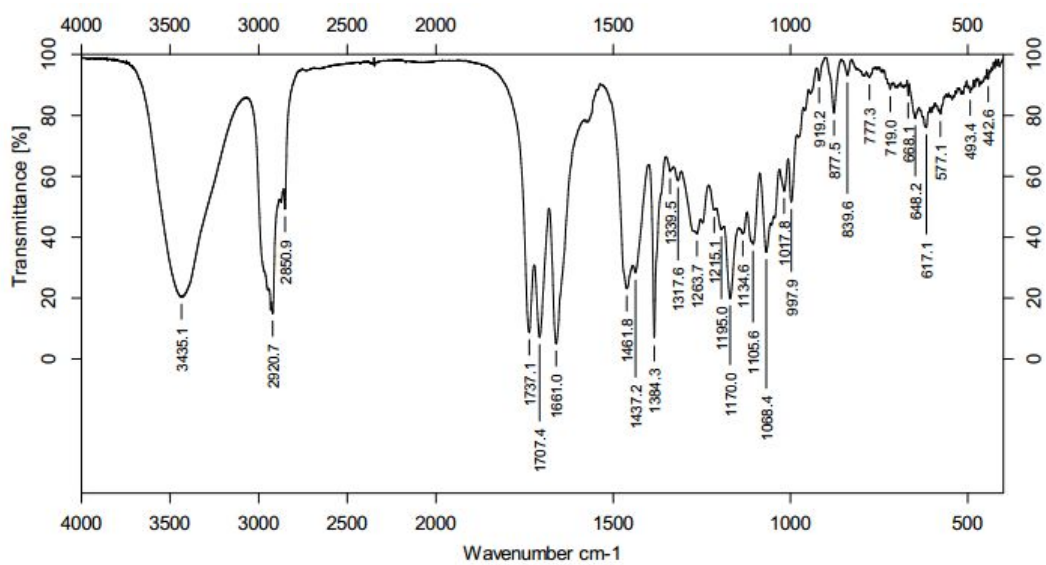


Figure S23. HRESIMS spectrum of **3**



**Figure S24.** UV spectrum of **3**



**Figure S25.** IR spectrum of **3**

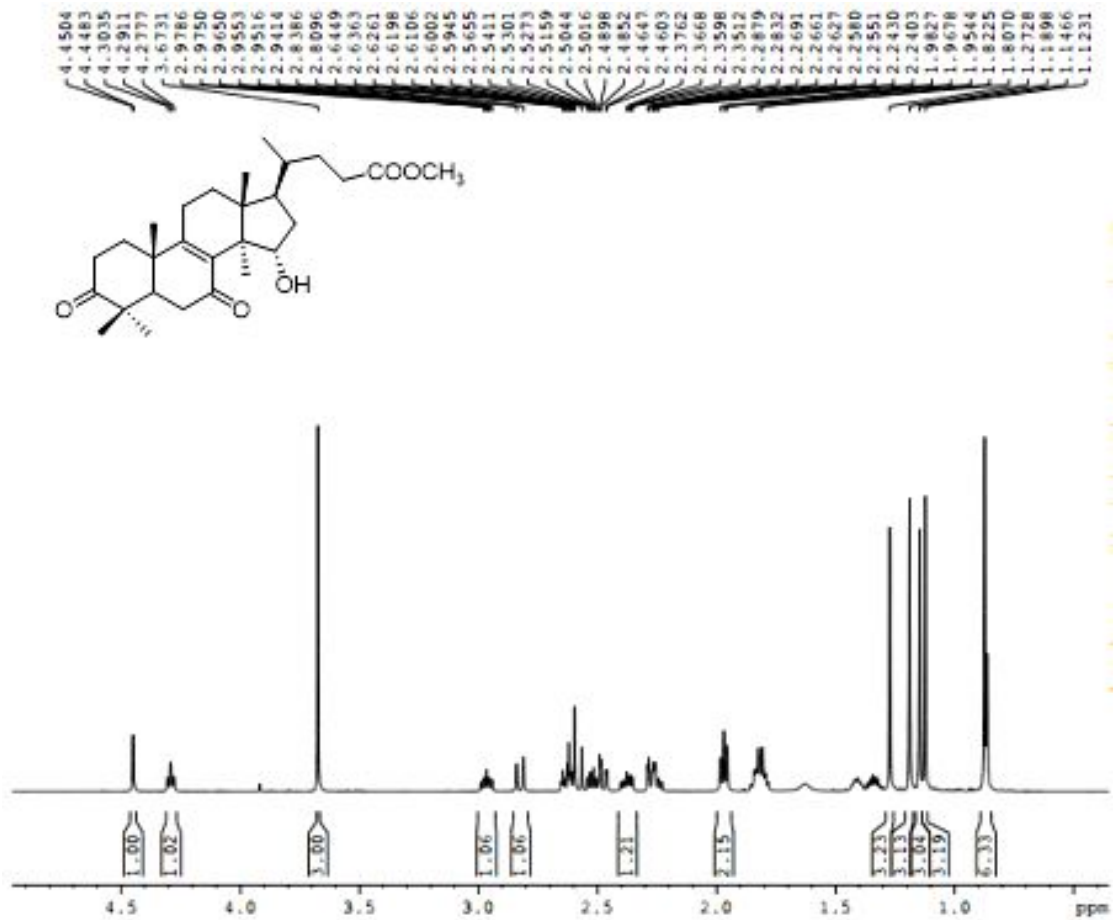


Figure S26. <sup>1</sup>H-NMR spectrum of 4 (600 MHz, CDCl<sub>3</sub>)

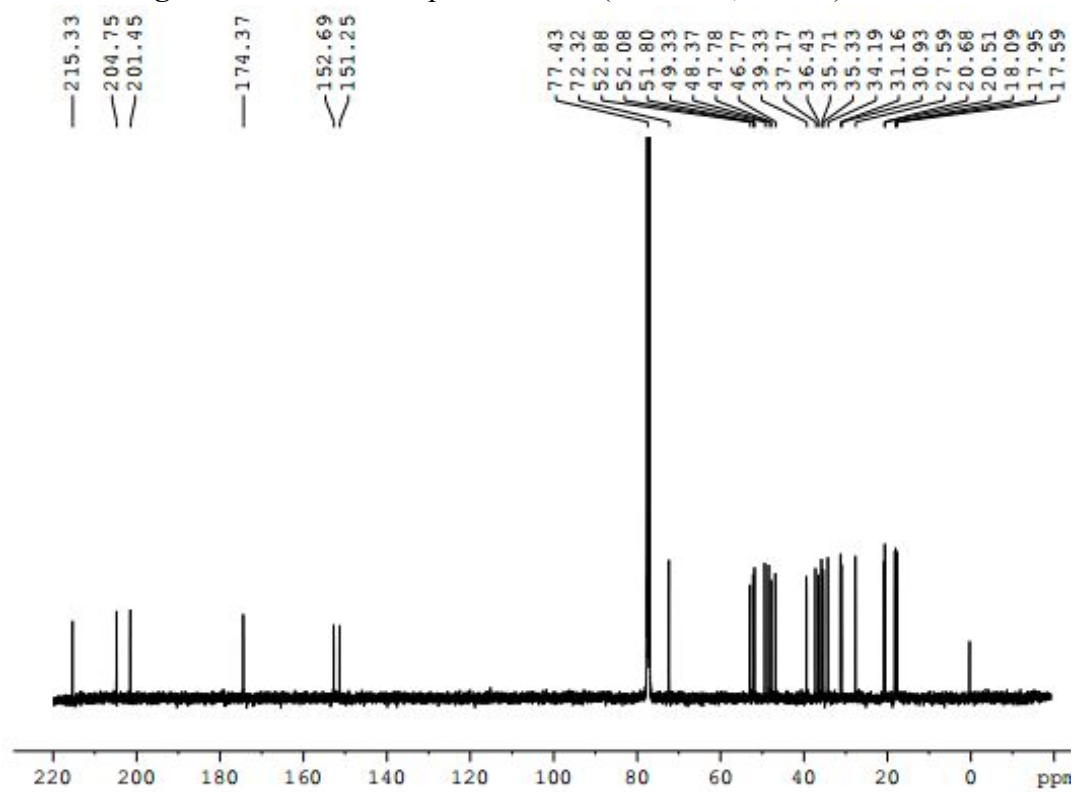
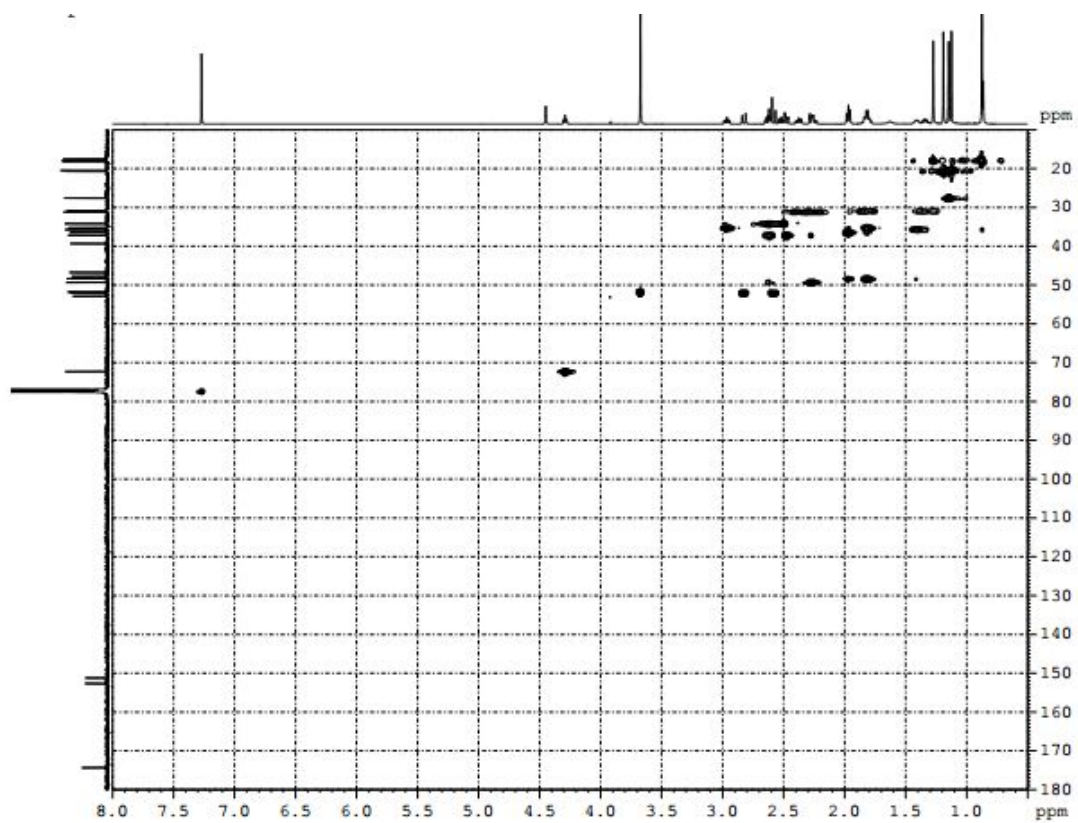
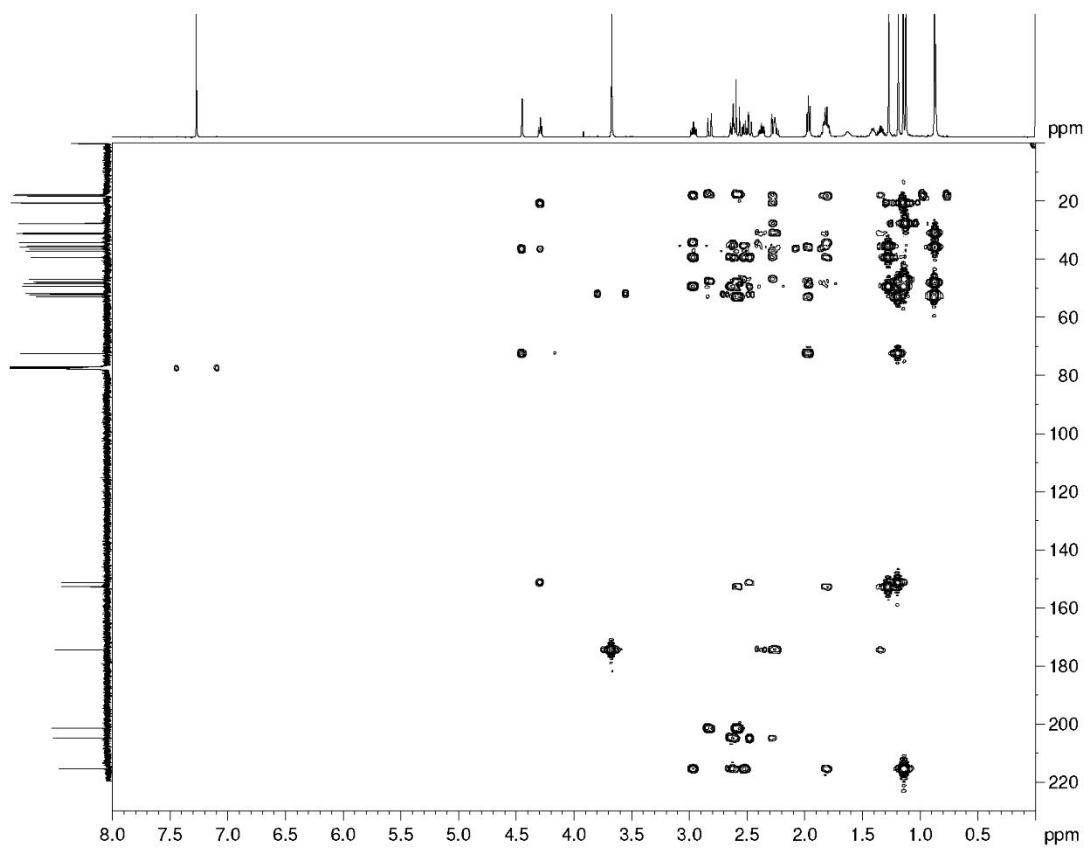


Figure S27. <sup>13</sup>C-NMR spectrum of 4 (150 MHz, CDCl<sub>3</sub>)

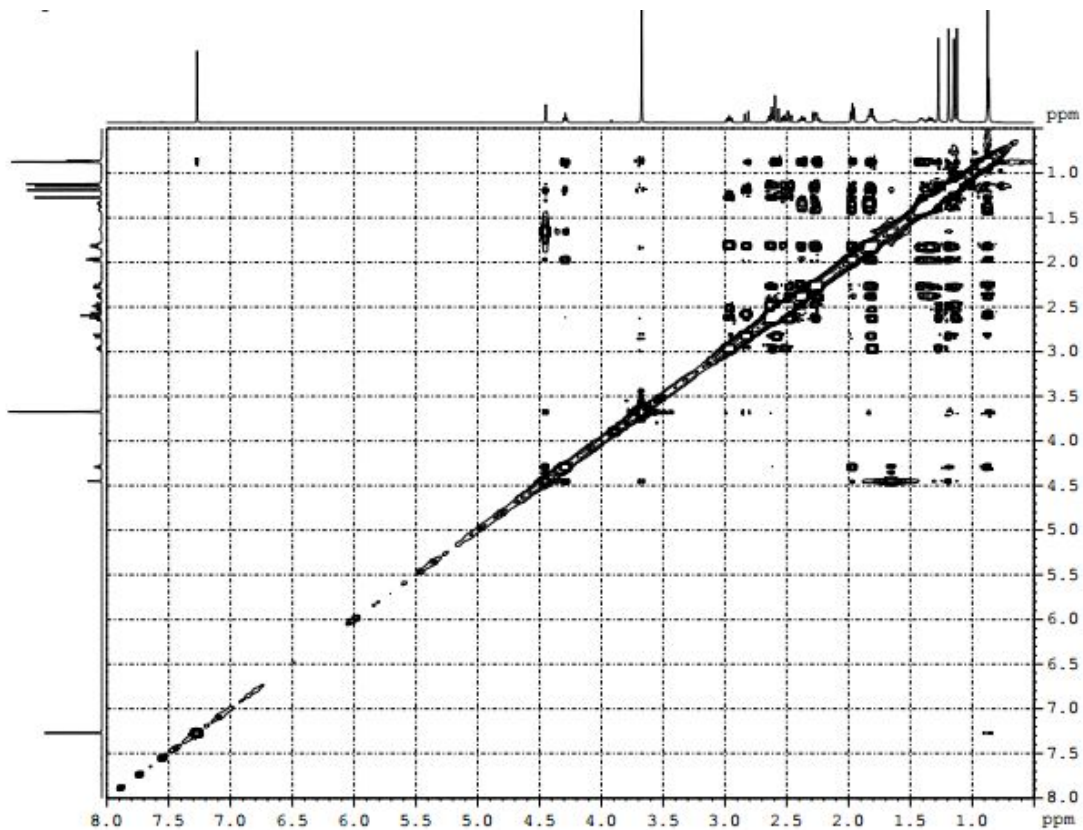




**Figure S28.** HSQC spectrum of **4** (600 MHz, CDCl<sub>3</sub>)

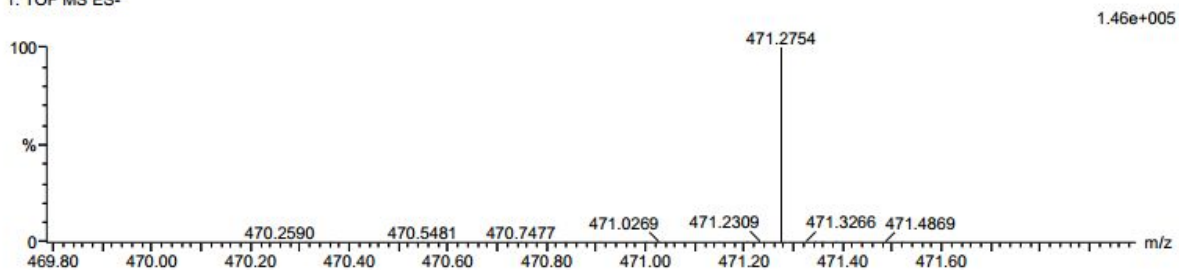


**Figure S29.** HMBC spectrum of **4** (600 MHz, CDCl<sub>3</sub>)



**Figure S30.** NOESY spectrum of **4** (600 MHz,  $\text{CDCl}_3$ )

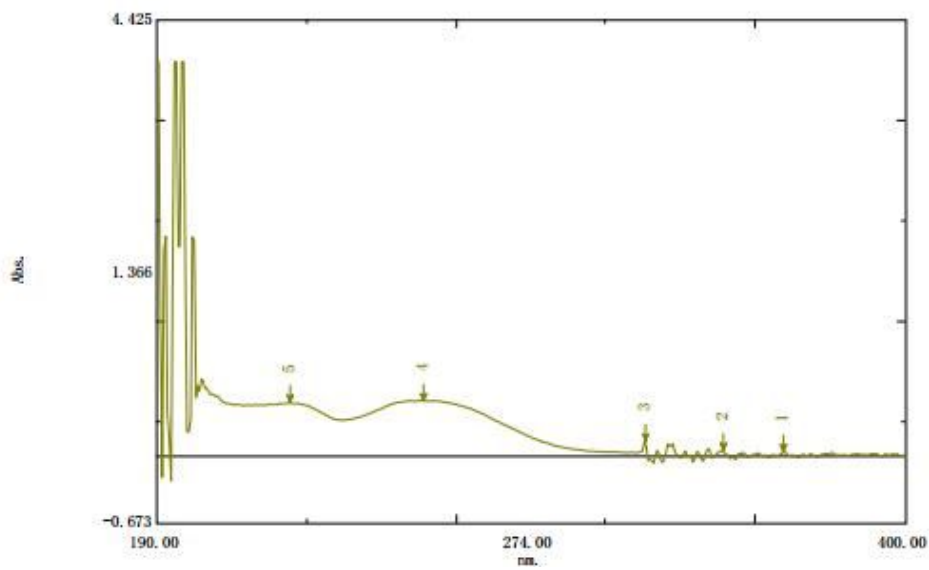
20160519 C9 3608 (13.425)  
1: TOF MS ES-



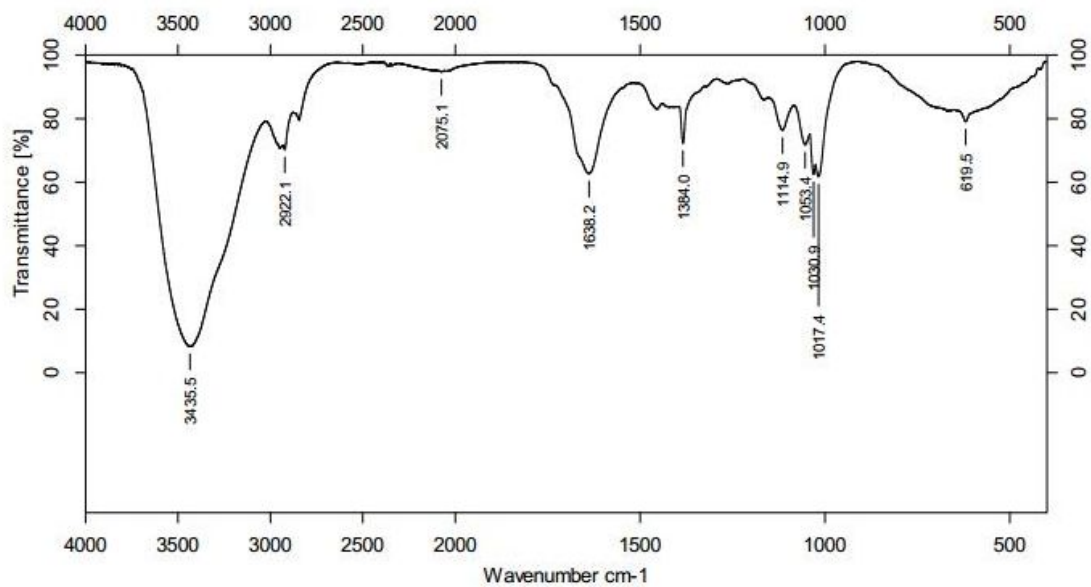
Minimum: 3.0  
Maximum: 4.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
471.2754	471.2747	0.7	1.5	9.5	103.9	n/a	n/a	$\text{C}_{28}\text{H}_{39}\text{O}_6$

**Figure S31.** HRESIMS spectrum of **4**



**Figure S32.** UV spectrum of **4**



**Figure S33.** IR spectrum of **4**

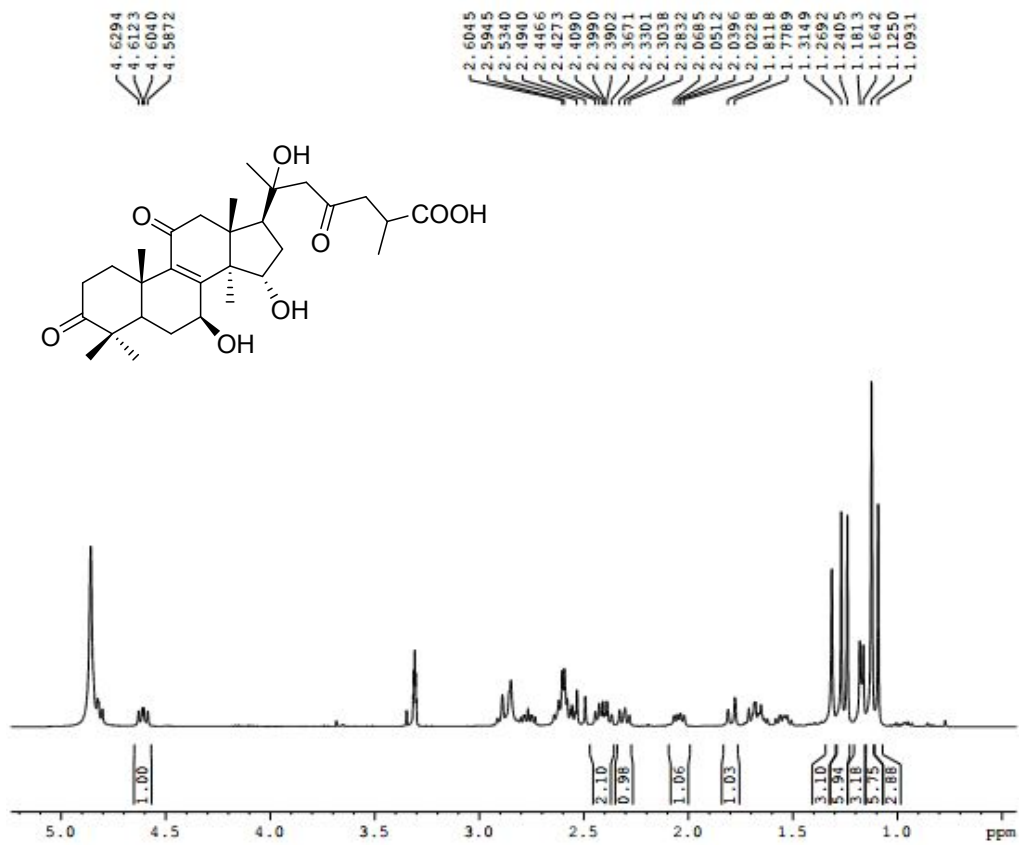


Figure S34.  $^1\text{H}$ -NMR spectrum of **5** (600 MHz,  $\text{CD}_3\text{OD}$ )

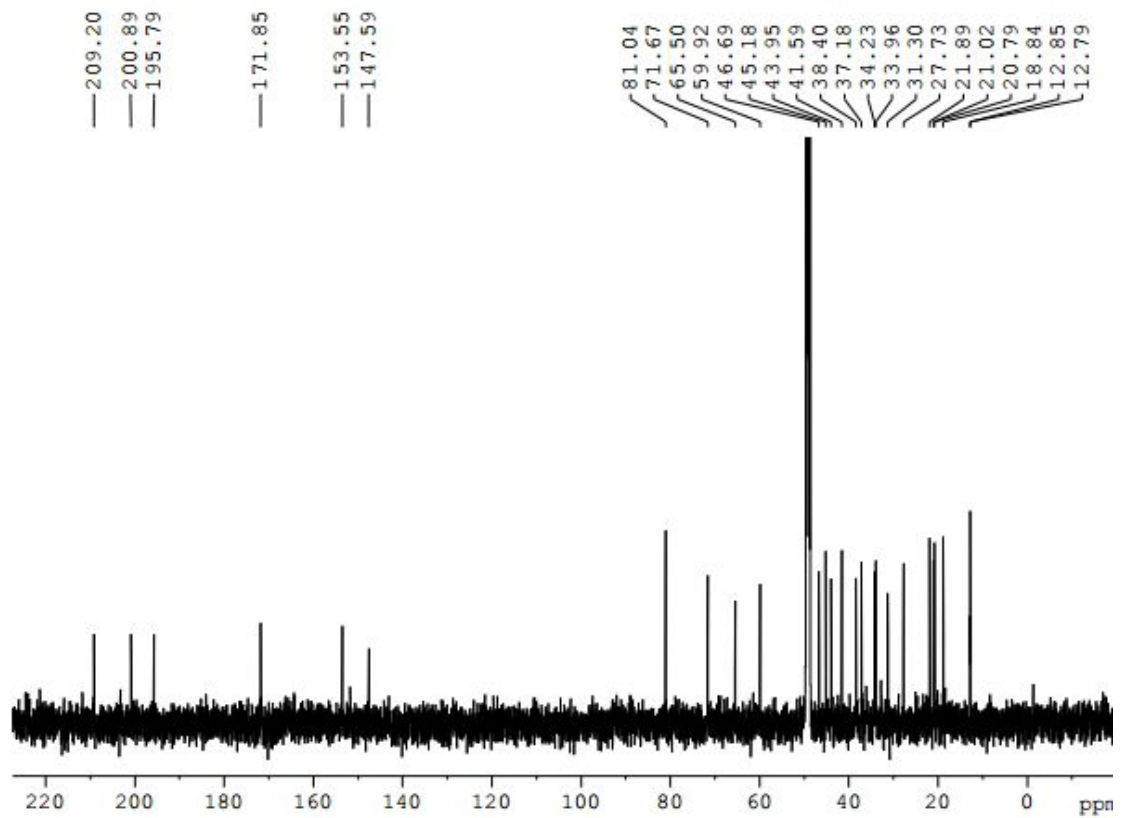
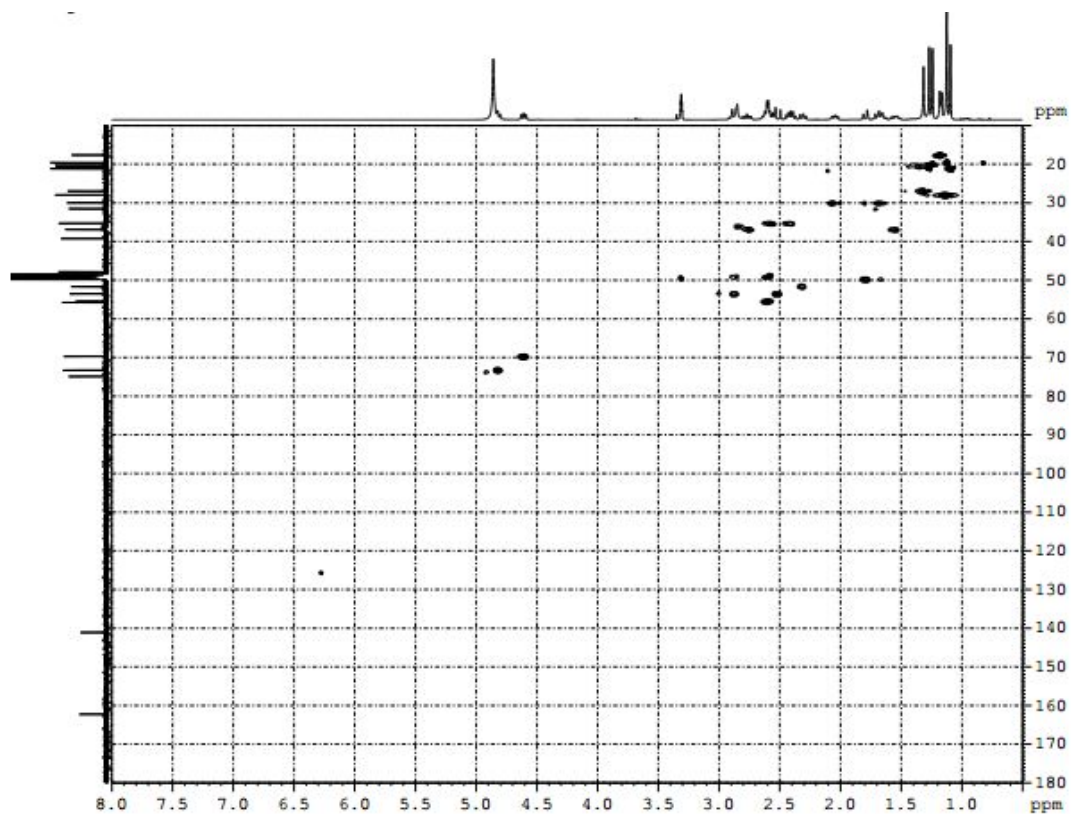
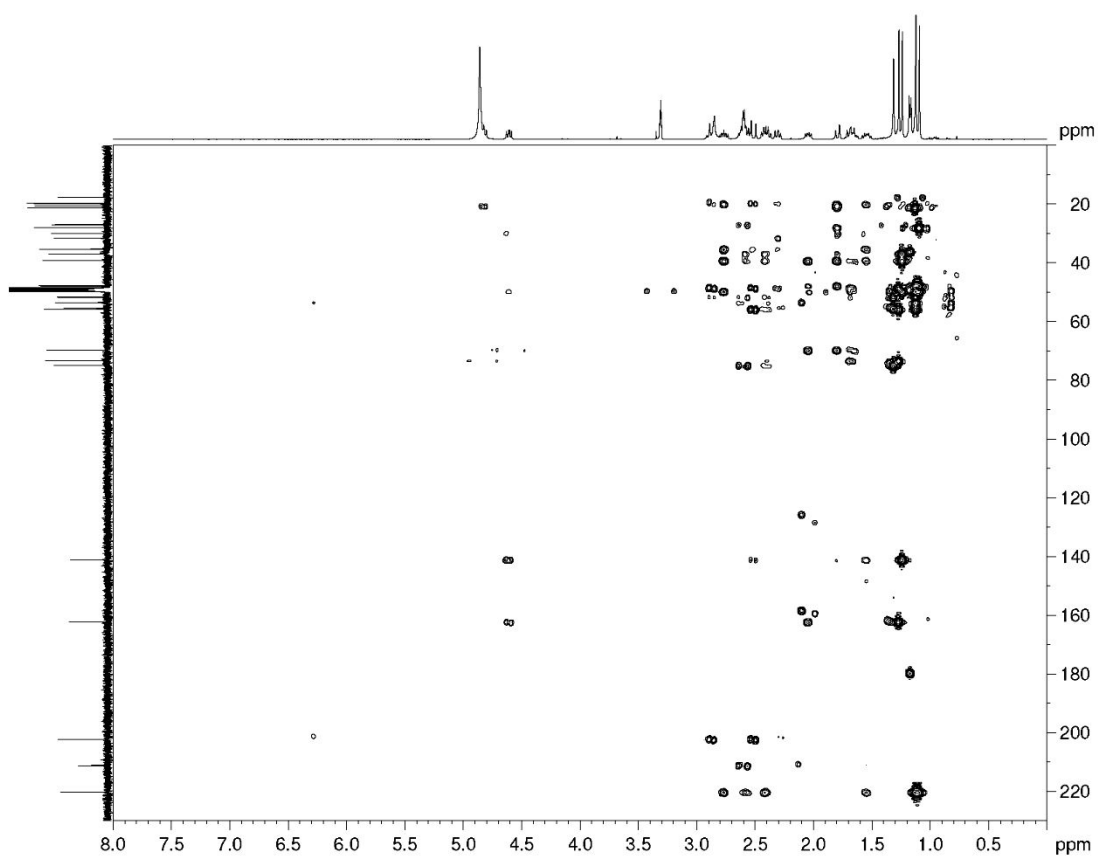


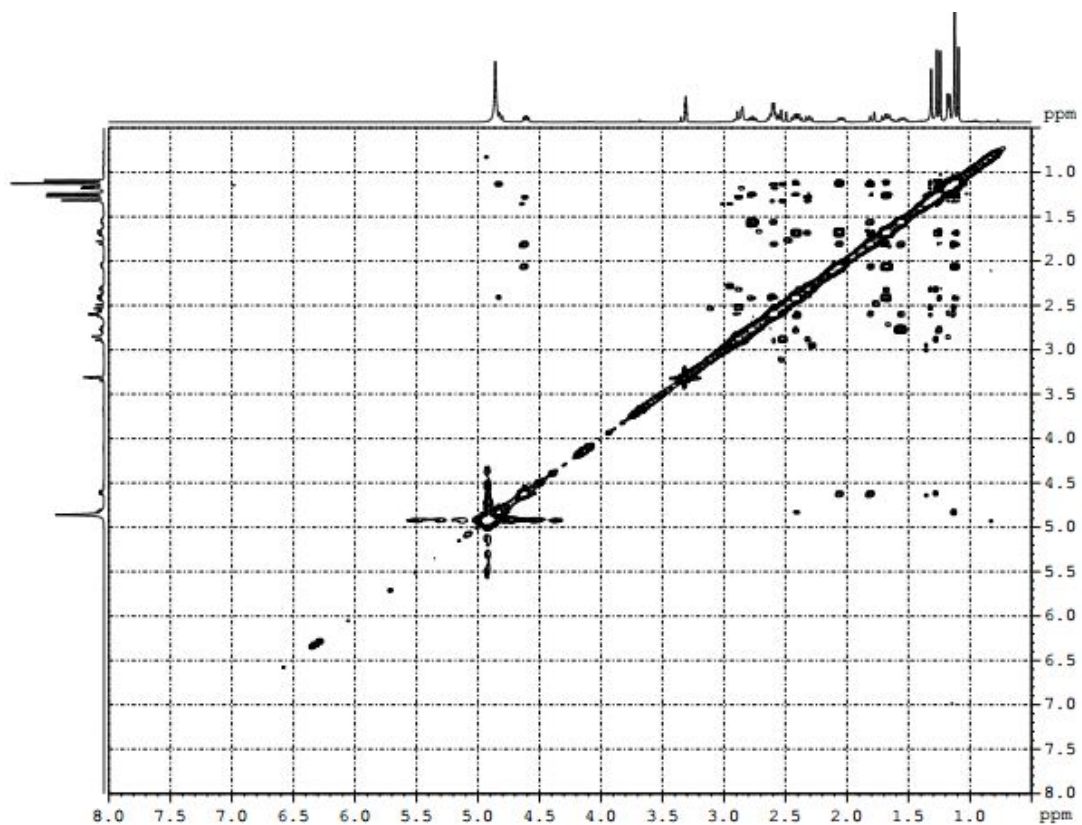
Figure S35.  $^{13}\text{C}$ -NMR spectrum of **5** (150 MHz,  $\text{CD}_3\text{OD}$ )



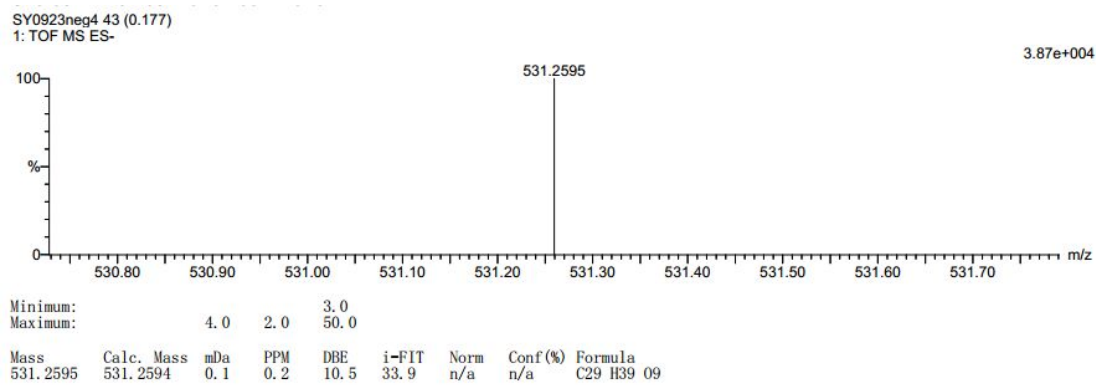
**Figure S36.** HSQC spectrum of **5** (600 MHz, CD<sub>3</sub>OD)



**Figure S37.** HMBC spectrum of **5** (600 MHz, CD<sub>3</sub>OD)



**Figure S38.** NOESY spectrum of **5** (600 MHz, CD<sub>3</sub>OD)



**Figure S39.** HRESIMS spectrum of **5**

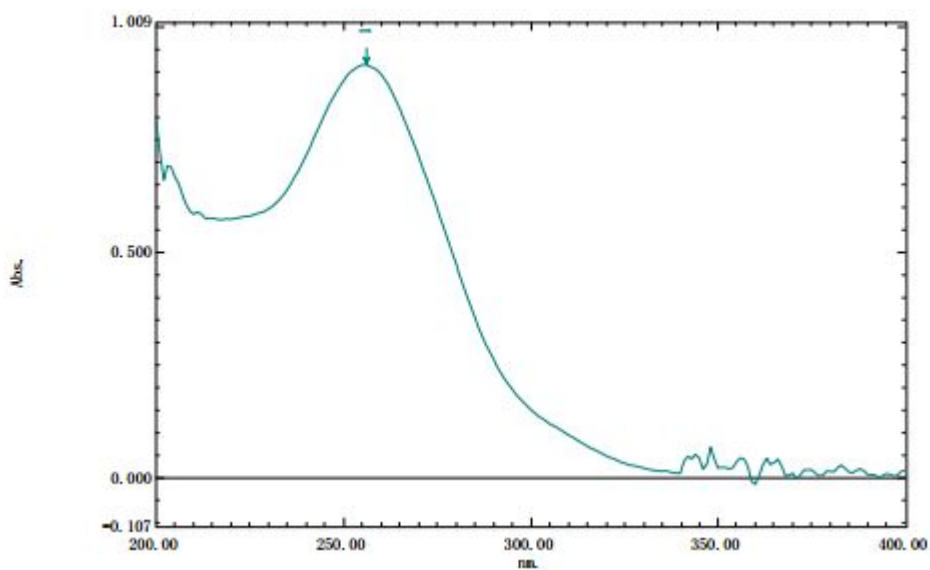


Figure S40. UV spectrum of 5

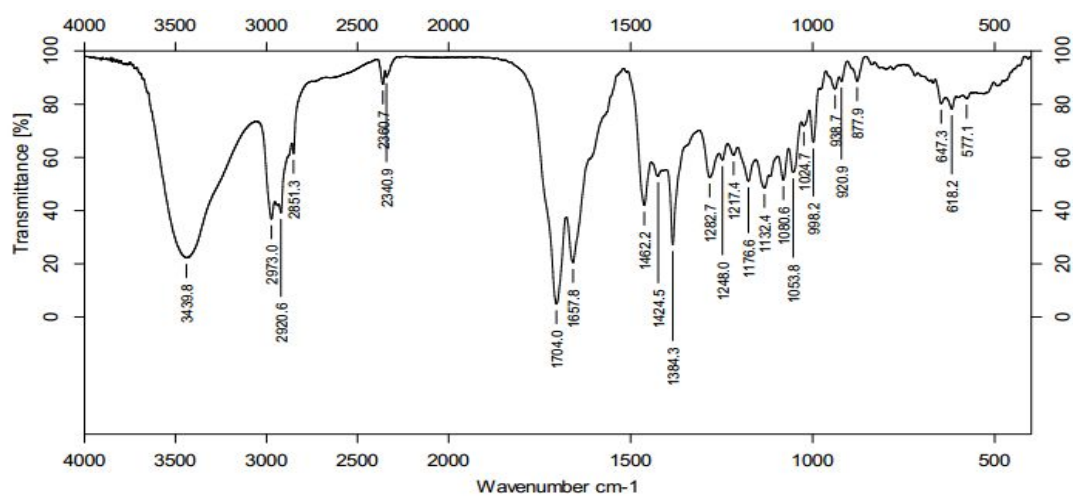
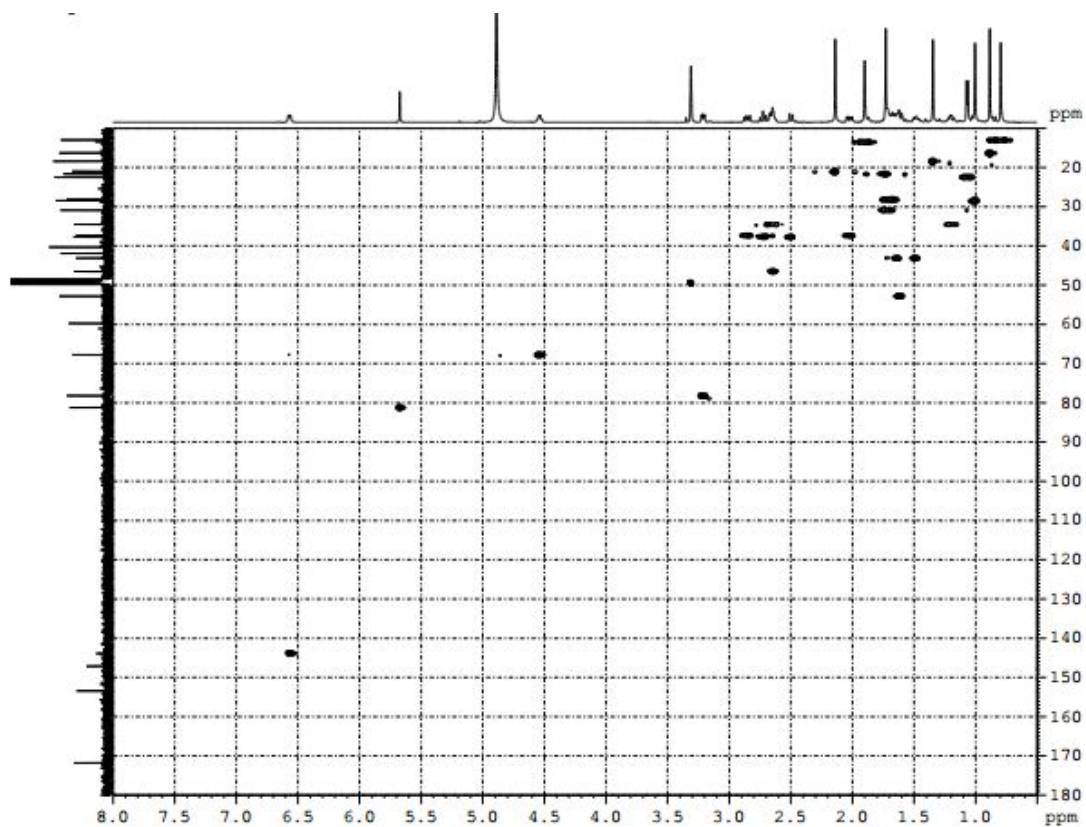


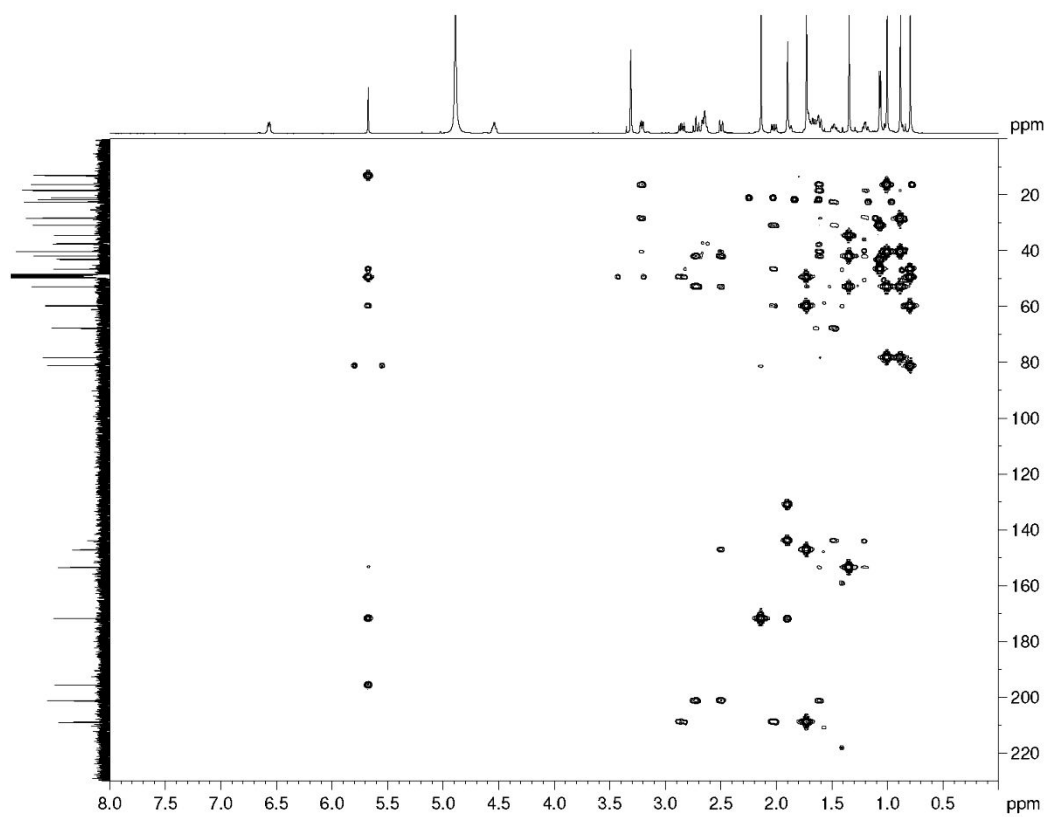
Figure S41. IR spectrum of 5



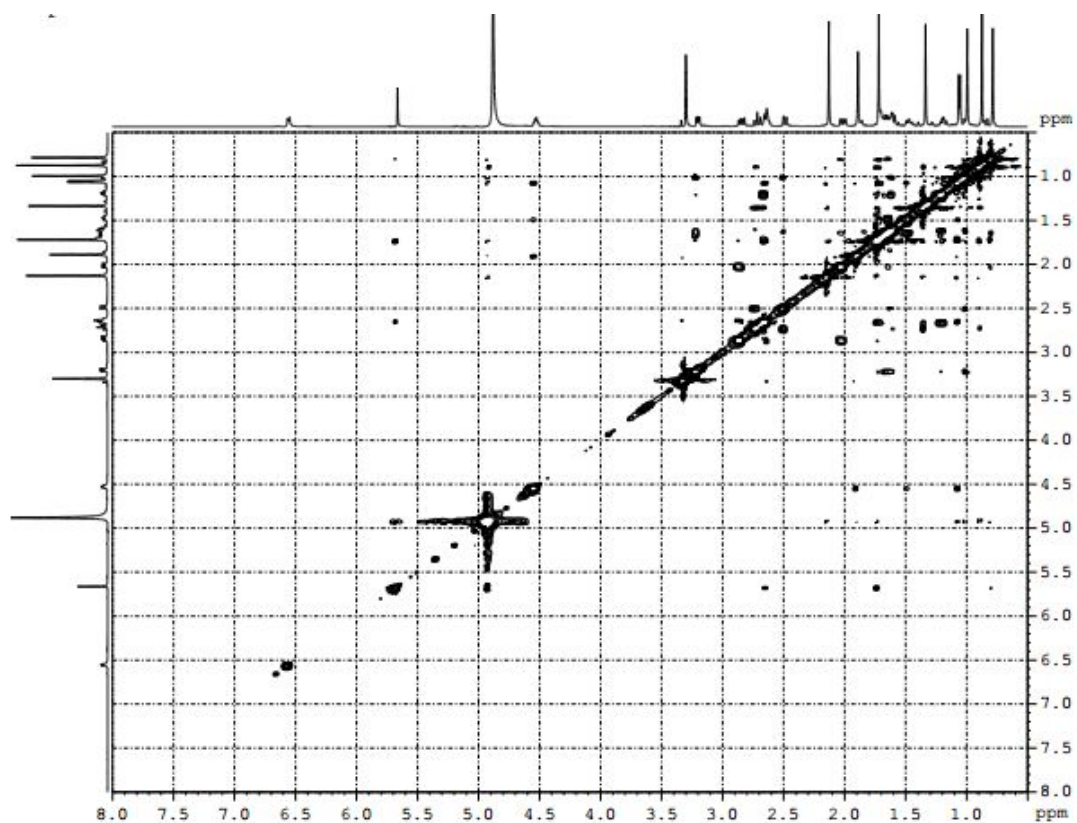




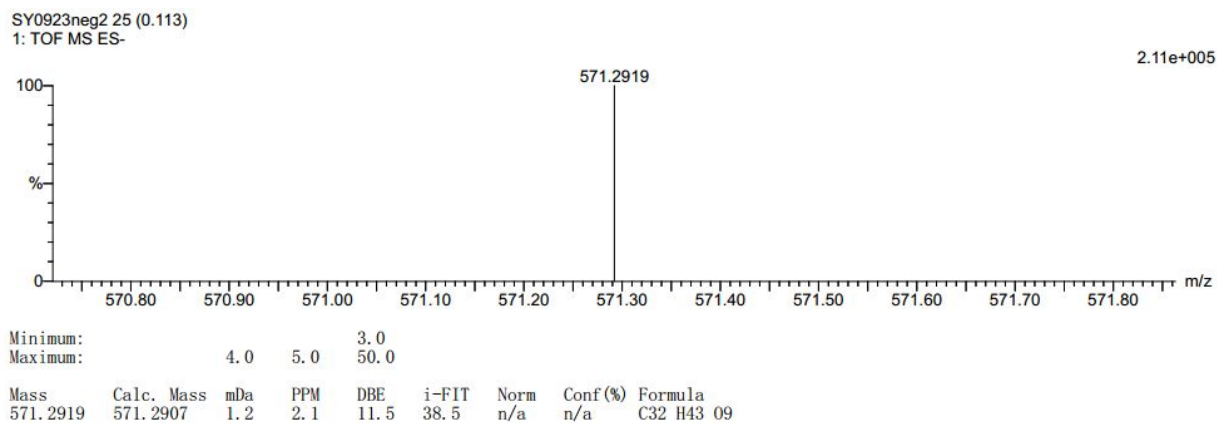
**Figure S44.** HSQC spectrum of **6** (600 MHz, CD<sub>3</sub>OD)



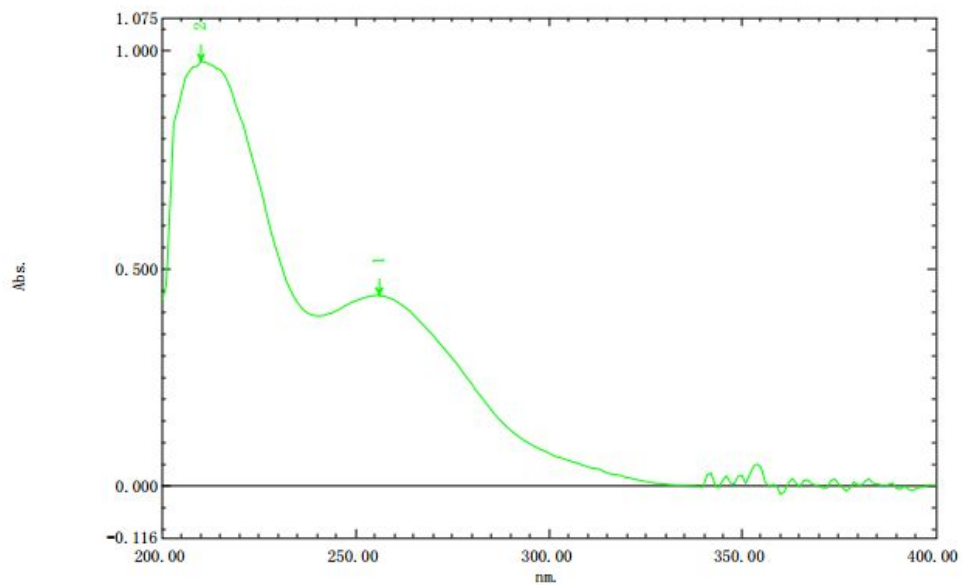
**Figure S45.** HMBC spectrum of **6** (600 MHz, CD<sub>3</sub>OD)



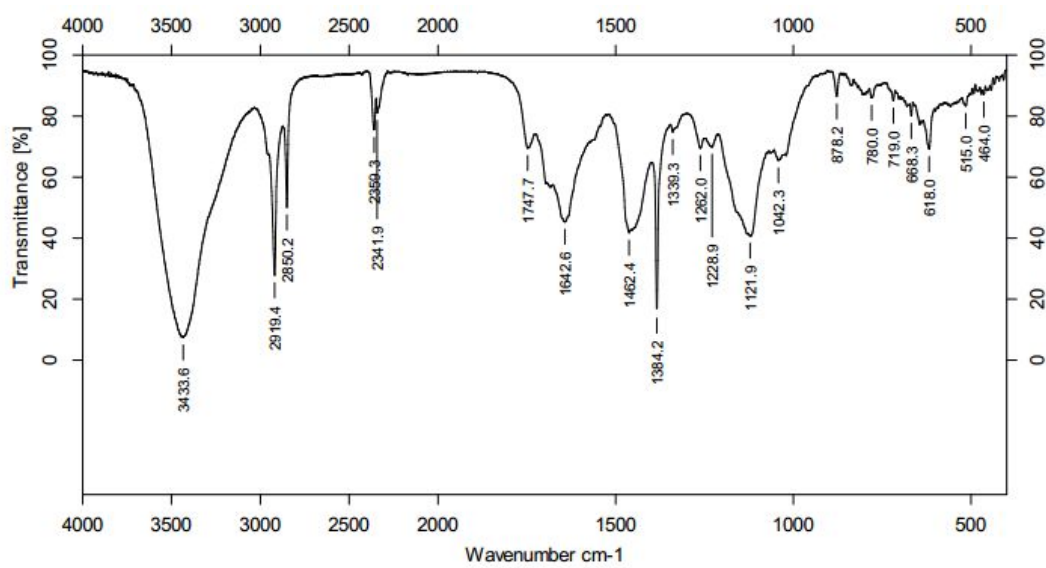
**Figure S46.** NOESY spectrum of **6** (600 MHz, CD<sub>3</sub>OD)



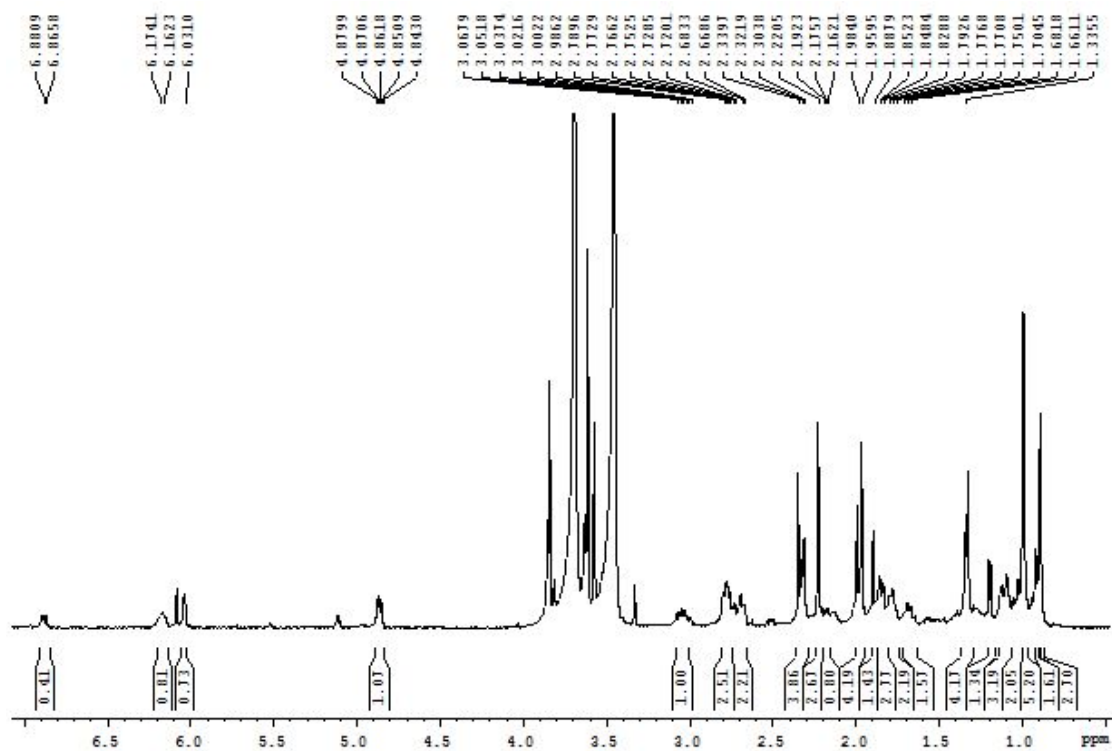
**Figure S47.** HRESIMS spectrum of **6**



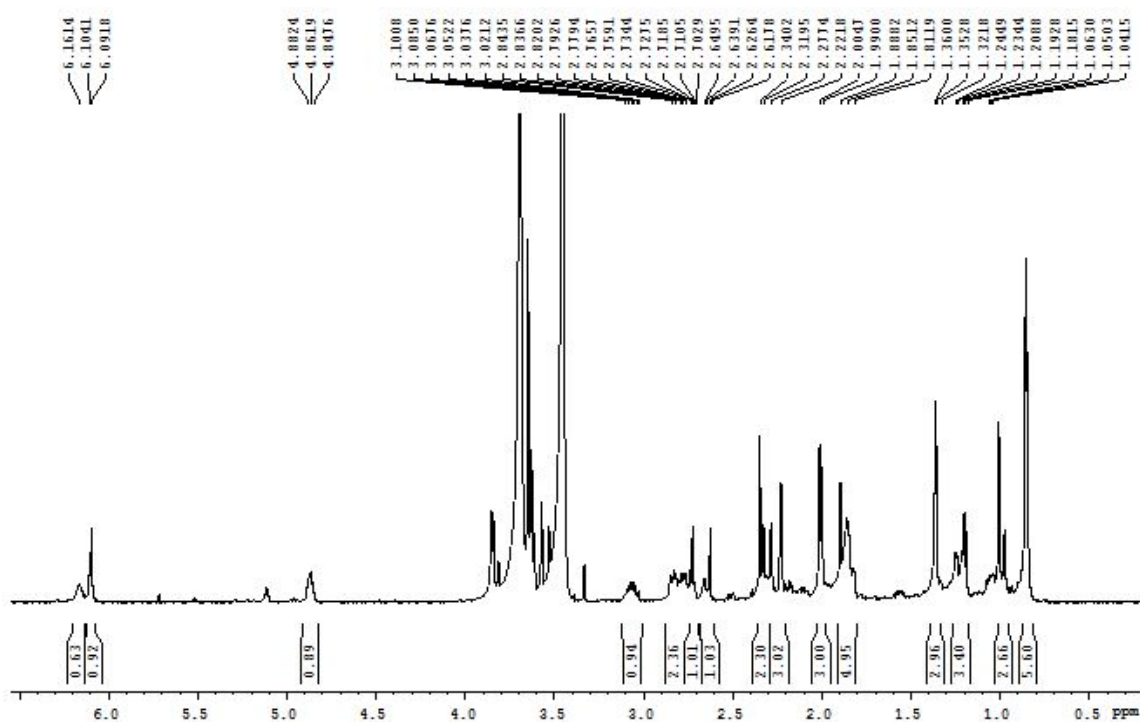
**Figure S48.** UV spectrum of **6**



**Figure S49.** IR spectrum of **6**



**Figure S50.**  $^1\text{H-NMR}$  (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ) spectrum of the (*R*)-MTPA ester of **6**



**Figure S51.**  $^1\text{H-NMR}$  (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ) spectrum of the (*S*)-MTPA ester of **6**

**Table S1** The inhibition rate against NO production of all compounds at 50  $\mu\text{M}$ .<sup>a</sup>

<b>Compounds (50 <math>\mu\text{M}</math>)</b>	<b>No inhibition rate (%)</b>	<b>Compounds (50 <math>\mu\text{M}</math>)</b>	<b>No inhibition rate (%)</b>
<b>1</b>	14.2 $\pm$ 2.7	<b>18</b>	21.7 $\pm$ 2.3
<b>2</b>	16.1 $\pm$ 2.6	<b>19</b>	29.5 $\pm$ 2.7
<b>3</b>	42.1 $\pm$ 2.6	<b>20</b>	24.4 $\pm$ 4.1
<b>4</b>	70.6 $\pm$ 3.3	<b>21</b>	-6.9 $\pm$ 0.8
<b>5</b>	-4.0 $\pm$ 1.9	<b>22</b>	-12.1 $\pm$ 1.9
<b>6</b>	-28.1 $\pm$ 2.9	<b>23</b>	-19.3 $\pm$ 2.0
<b>7</b>	-3.2 $\pm$ 3.1	<b>24</b>	4.4 $\pm$ 1.4
<b>8</b>	13.3 $\pm$ 1.5	<b>25</b>	15.7 $\pm$ 1.9
<b>9</b>	59.8 $\pm$ 3.4	<b>26</b>	16.2 $\pm$ 3.7
<b>10</b>	17.0 $\pm$ 2.6	<b>27</b>	34.3 $\pm$ 2.3
<b>11</b>	14.3 $\pm$ 2.7	<b>28</b>	10.5 $\pm$ 1.7
<b>12</b>	28.9 $\pm$ 3.6	<b>29</b>	-1.5 $\pm$ 2.1
<b>13</b>	3.8 $\pm$ 2.3	<b>30</b>	-14.5 $\pm$ 2.7
<b>14</b>	-8.6 $\pm$ 2.0	<b>31</b>	25.3 $\pm$ 2.3
<b>15</b>	-10.7 $\pm$ 1.2	<b>32</b>	4.0 $\pm$ 2.0
<b>16</b>	-4.0 $\pm$ 1.8	<b>33</b>	-15.7 $\pm$ 1.9
<b>17</b>	20.9 $\pm$ 2.2		

<sup>a</sup> The results were showed as means  $\pm$  SD of at least three independent experiments.