

# Bioactivities of steroids and sesquiterpenes from the branches and leaves of *Aglaia lawii*

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## ECD calculation details of 1–6

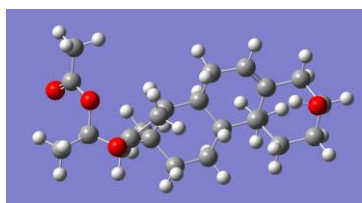
**Table S1** ECD analysis parameters of 1–6.

No.	half-bandwidth (eV)	UV correction (nm)
<b>1</b>	0.16	0
<b>2</b>	0.16	0
<b>3</b>	0.16	0
<b>4</b>	0.16	0
<b>5</b>	0.16	0
<b>6</b>	0.16	0

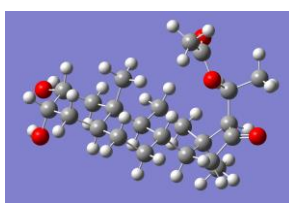
**Table S2** Important thermodynamic parameters for 1–6 at B3LYP/6-31G(d) level of theory.

NO.	E <sup>a</sup> (Hartree)	C <sup>b</sup> (Hartree)	G <sup>c</sup> (kcal/mol)
<b>1</b>	-1197.831564	0.484682	-751347.141924
<b>2</b>	-1273.563122	0.510408	-798853.308562
<b>3</b>	-1359.620929	0.666449	-852757.525745
<b>4</b>	-1433.643746	0.647647	-898703.503488
<b>5</b>	-1433.631309	0.648259	-898695.319807
<b>6</b>	-851.037260	0.352475	-533813.209435

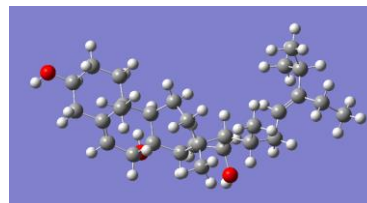
a Electronic energy; b Thermal correction to Gibbs free energy obtained; c Gibbs free energy (E + C).



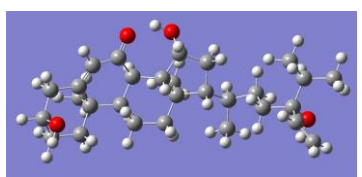
**1**



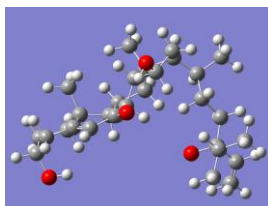
**2**



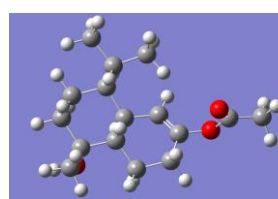
**3**



**4**



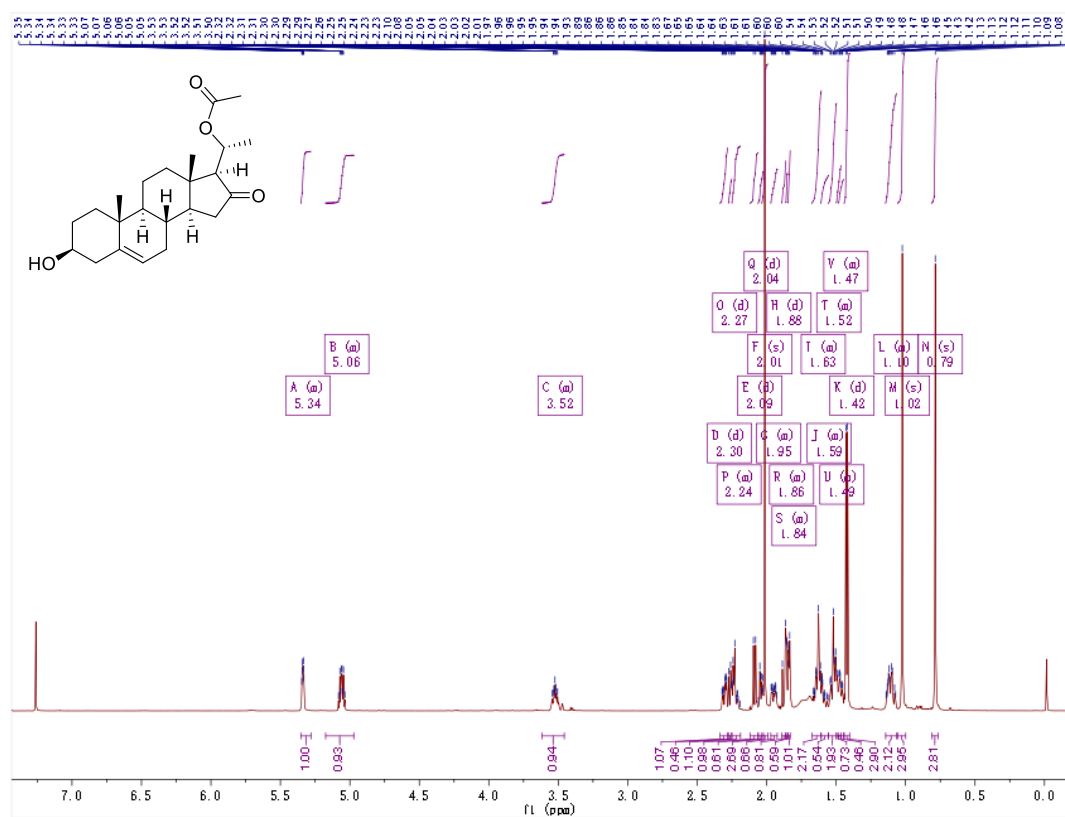
**5**



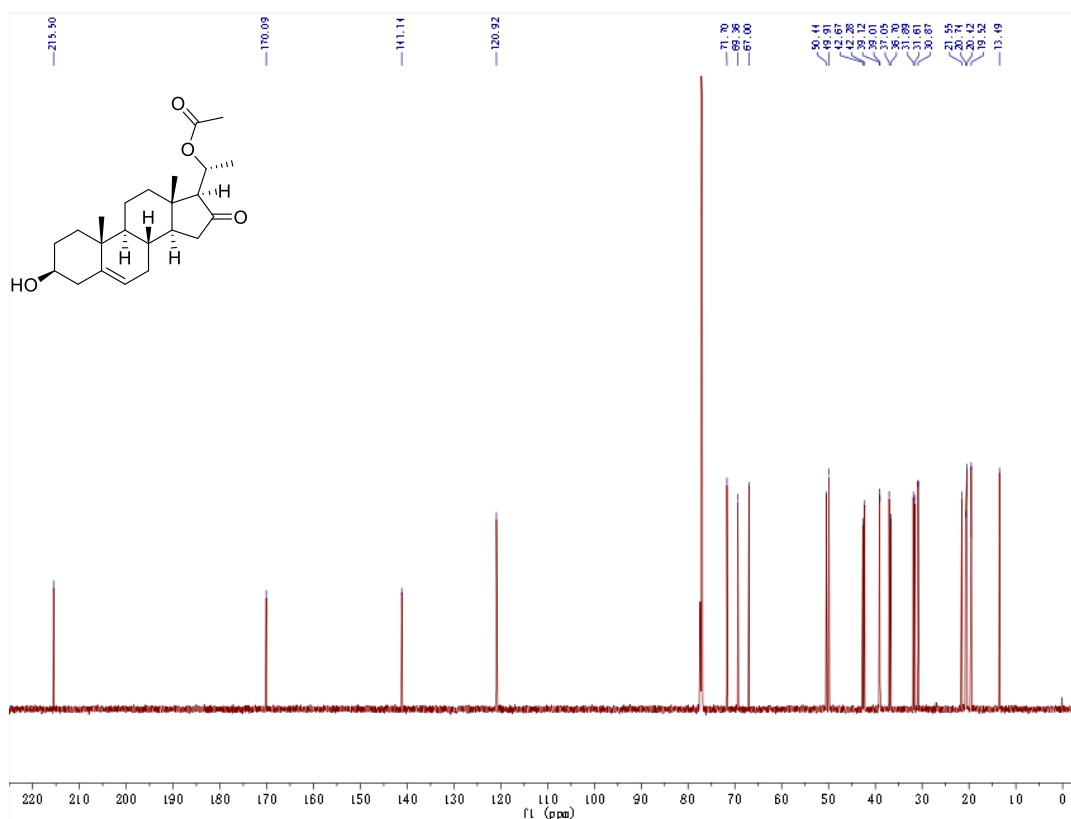
**6**

**Table S3** Crystal data and structure refinement for compound **1**

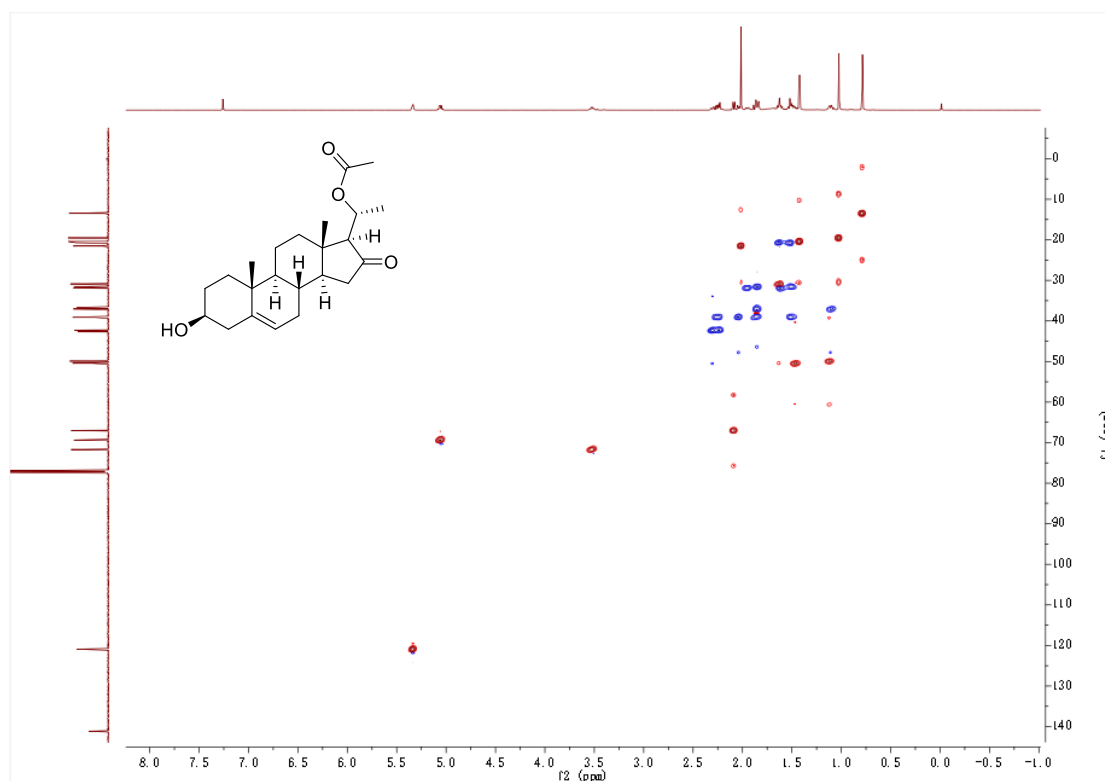
Identification code	<b>1</b>
Empirical formula	C <sub>23</sub> H <sub>34</sub> O <sub>4</sub>
Formula weight	374.50
Temperature/K	99.96 (13)
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	5.70310(10)
b/Å	10.8236(2)
c/Å	33.1051(4)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/Å <sup>3</sup>	2043.51(6)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.217
$\mu/\text{mm}^{-1}$	0.647
F(000)	816.0
Crystal size/mm <sup>3</sup>	0.6 × 0.06 × 0.04
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
2 $\Theta$ range for data collection/	5.338 to 148.786
Index ranges	-6 ≤ h ≤ 6, -12 ≤ k ≤ 13, -40 ≤ l ≤ 41
Reflections collected	19741
Independent reflections	4094 [ $R_{\text{int}}$ = 0.0454, $R_{\text{sigma}}$ = 0.0289]
Data/restraints/parameters	4094/0/249
Goodness-of-fit on F <sup>2</sup>	1.044
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ = 0.0328, $wR_2$ = 0.0838
Final R indexes [all data]	$R_1$ = 0.0347, $wR_2$ = 0.0850
Largest diff. peak/hole / e Å <sup>-3</sup>	0.23/-0.23
Flack parameter	0.05(8)



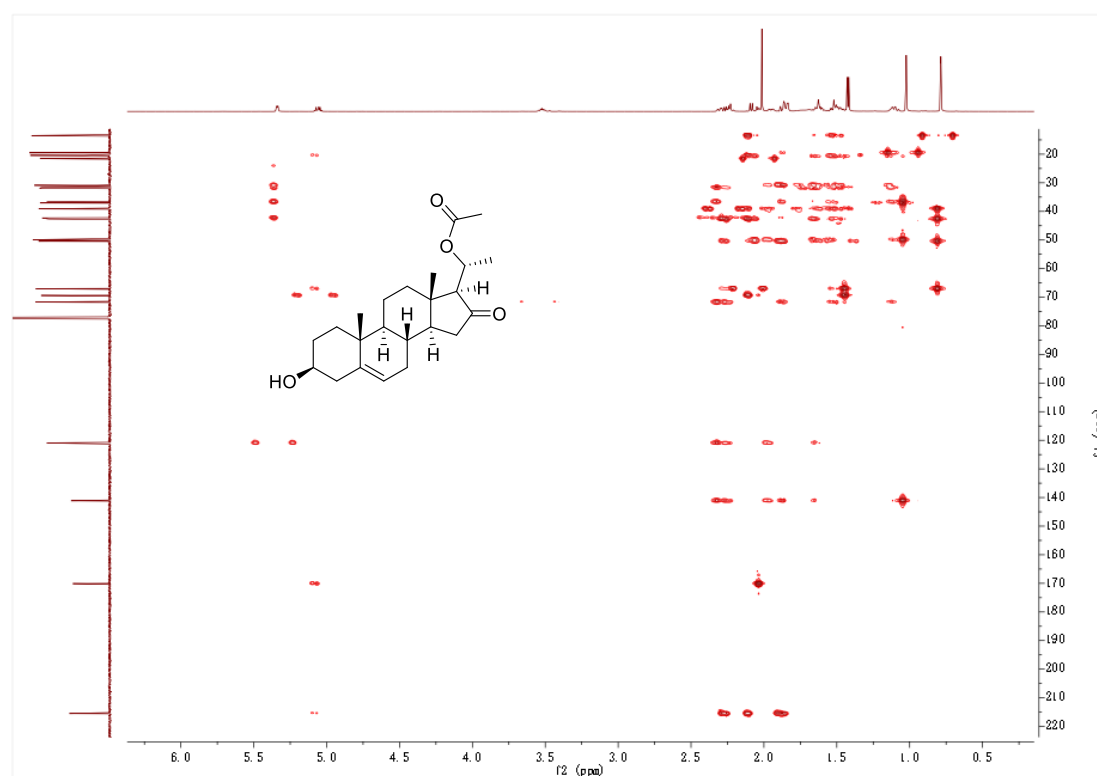
**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{CDCl}_3$  (600 MHz)



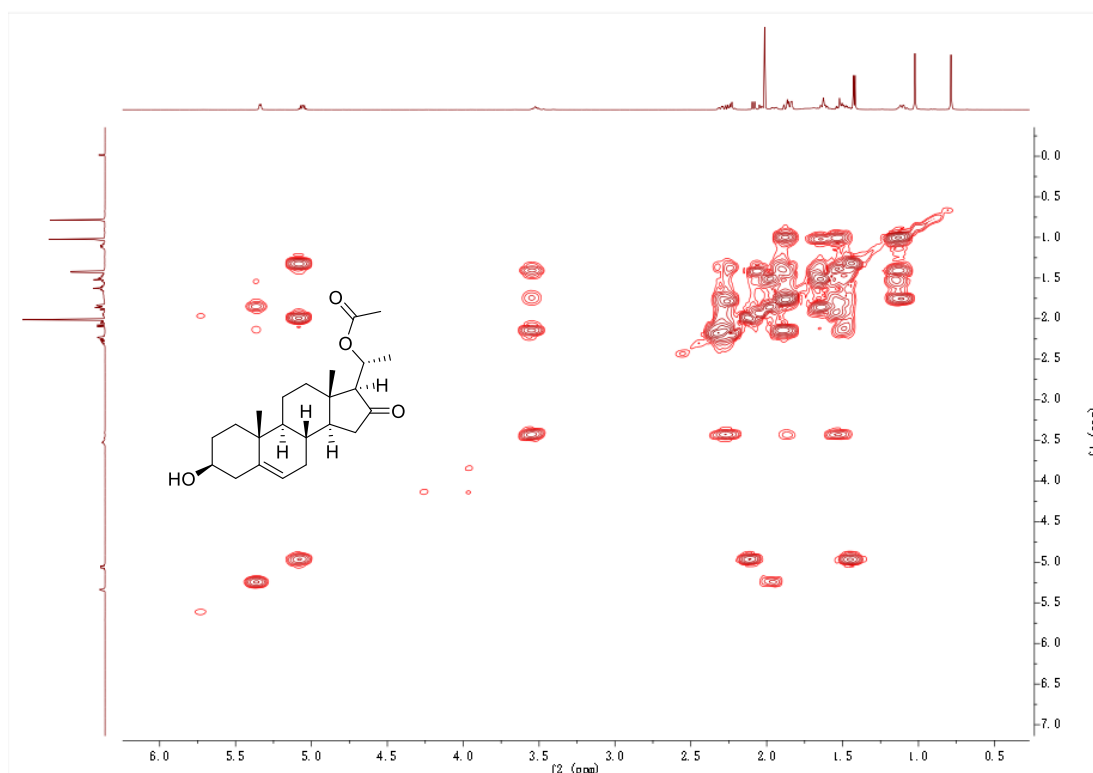
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of compound **1** in  $\text{CDCl}_3$  (150 MHz)



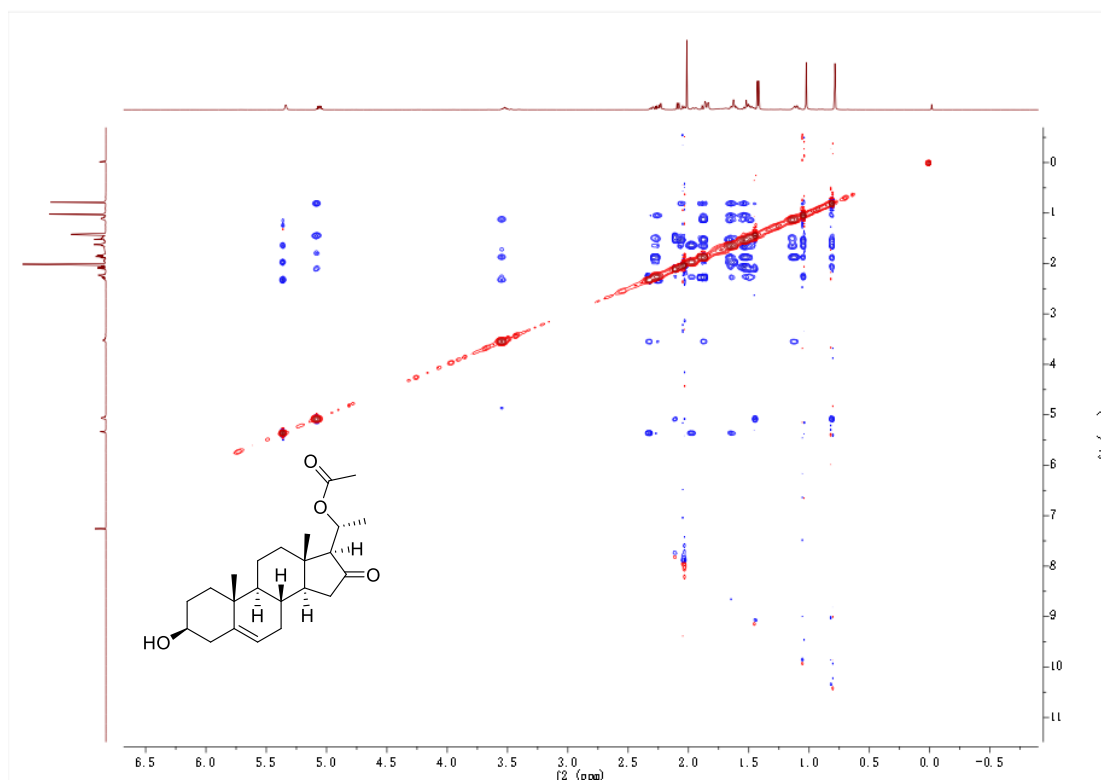
**Figure S3.** HSQC spectrum of compound **1** in  $\text{CDCl}_3$



**Figure S4.** HMBC spectrum of compound **1** in  $\text{CDCl}_3$

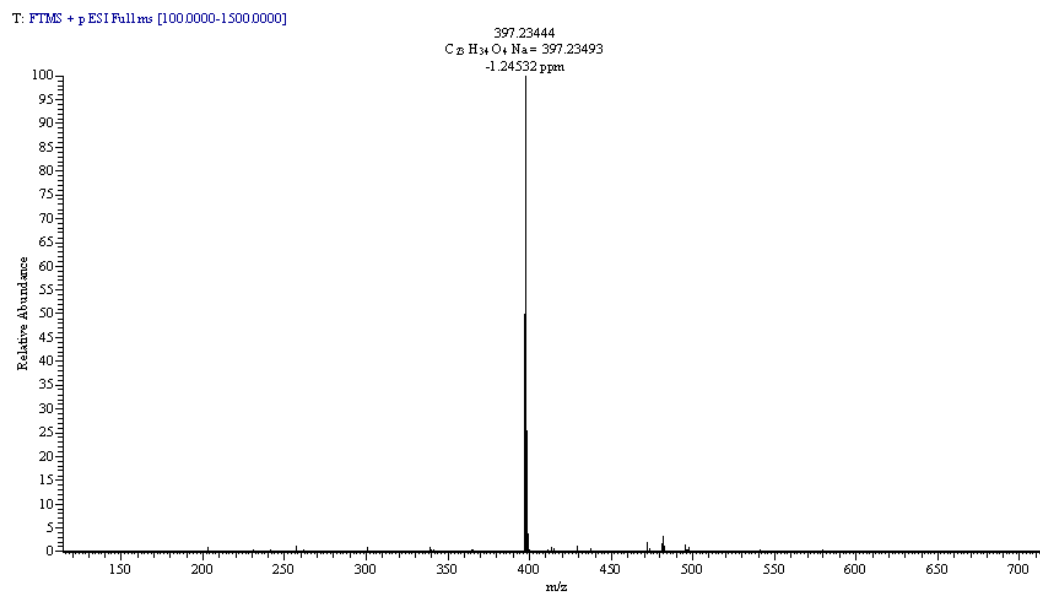


**Figure S5.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1** in  $\text{CDCl}_3$

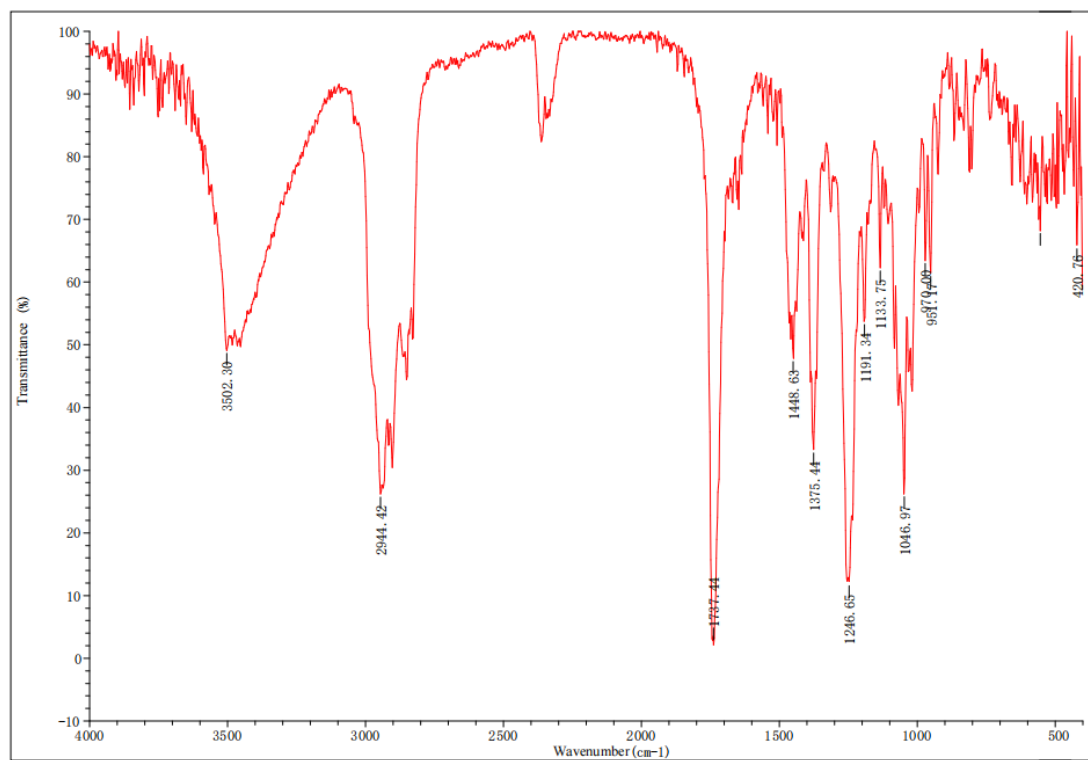


**Figure S6.** NOESY spectrum of compound **1** in  $\text{CDCl}_3$

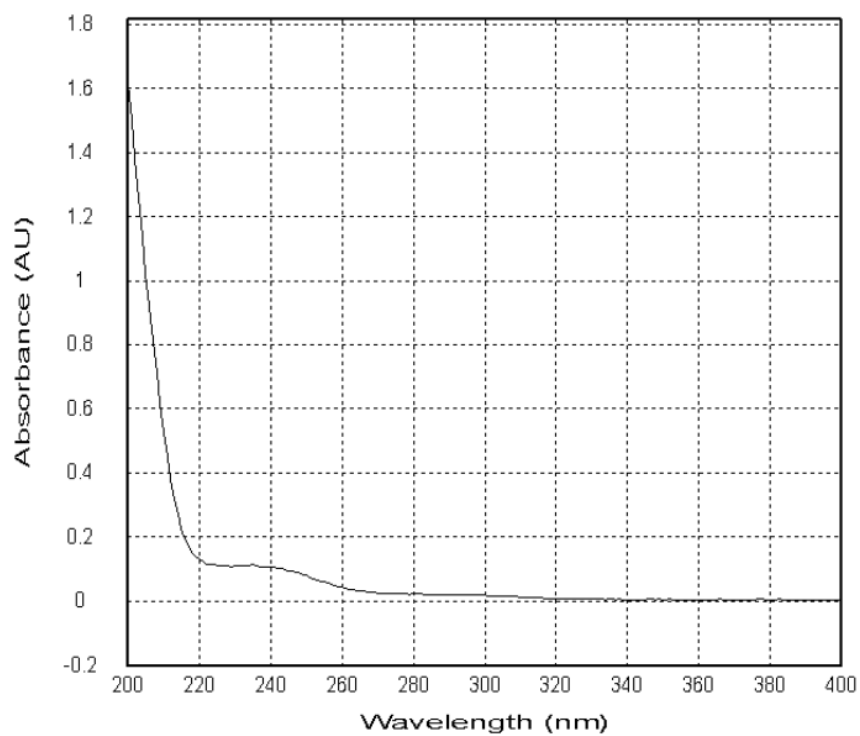




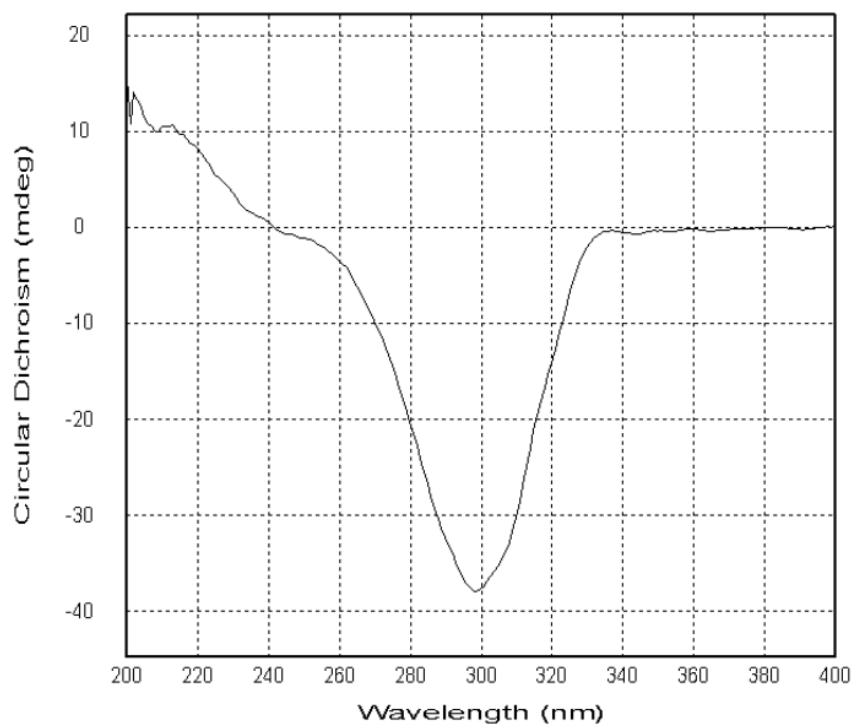
**Figure S7.** HRESIMS spectrum of compound **1**



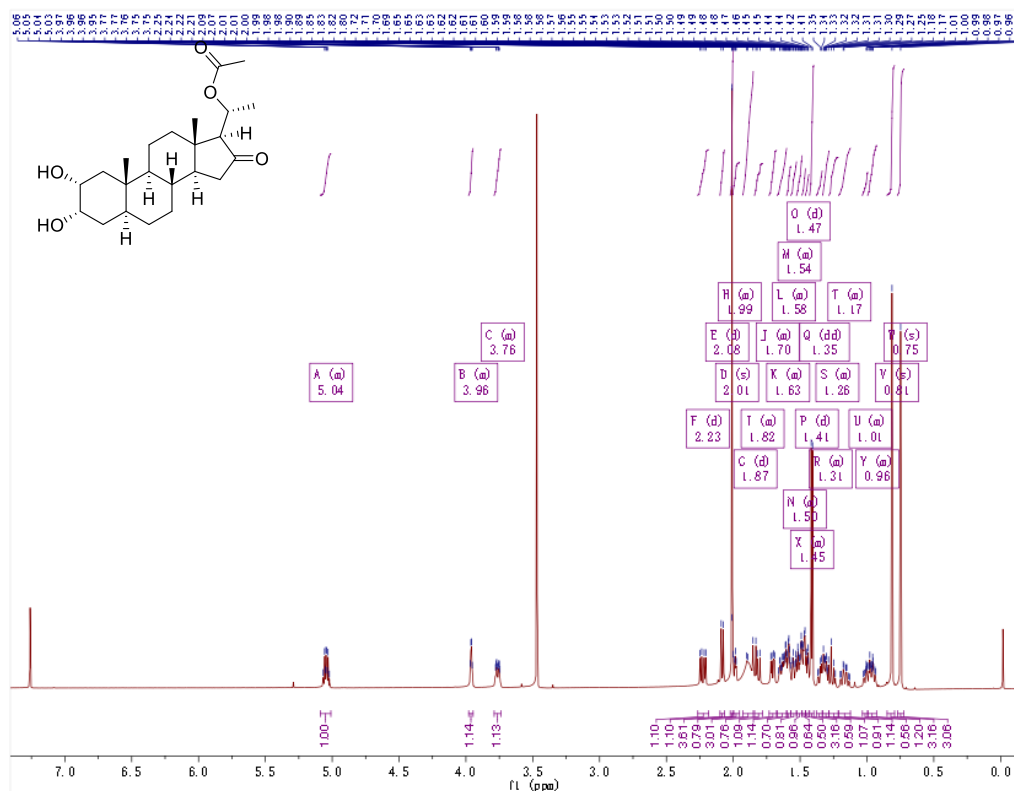
**Figure S8.** IR spectrum of compound **1**



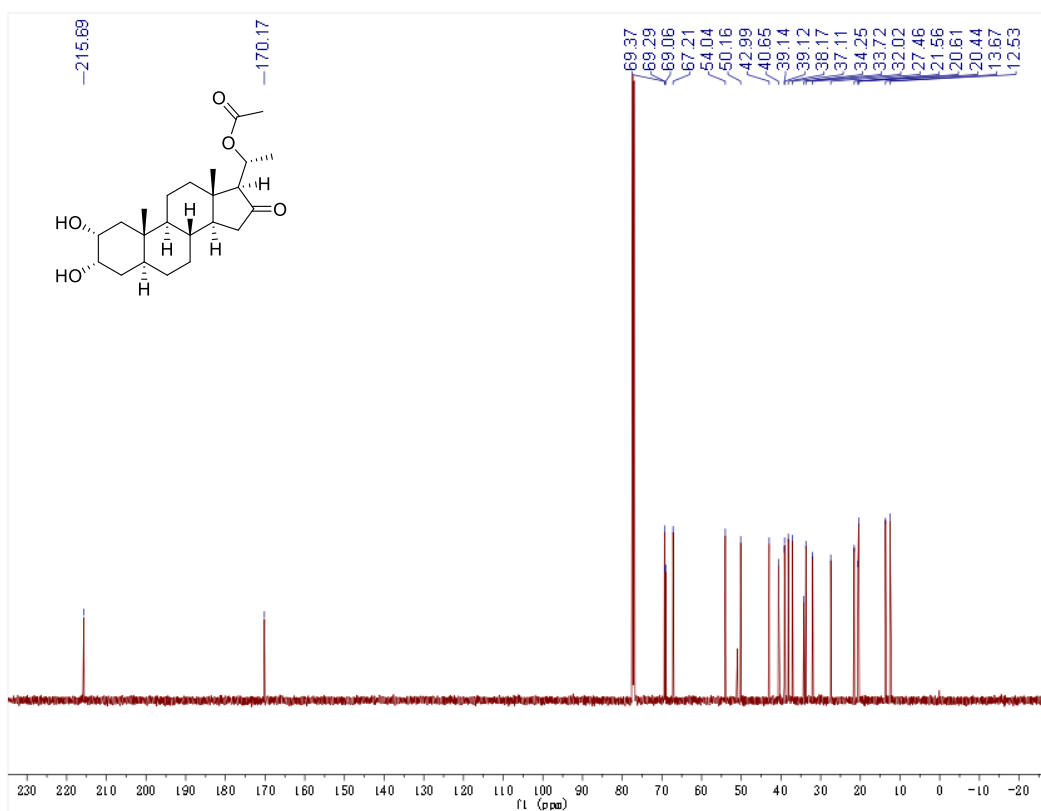
**Figure S9.** UV spectrum of compound **1**



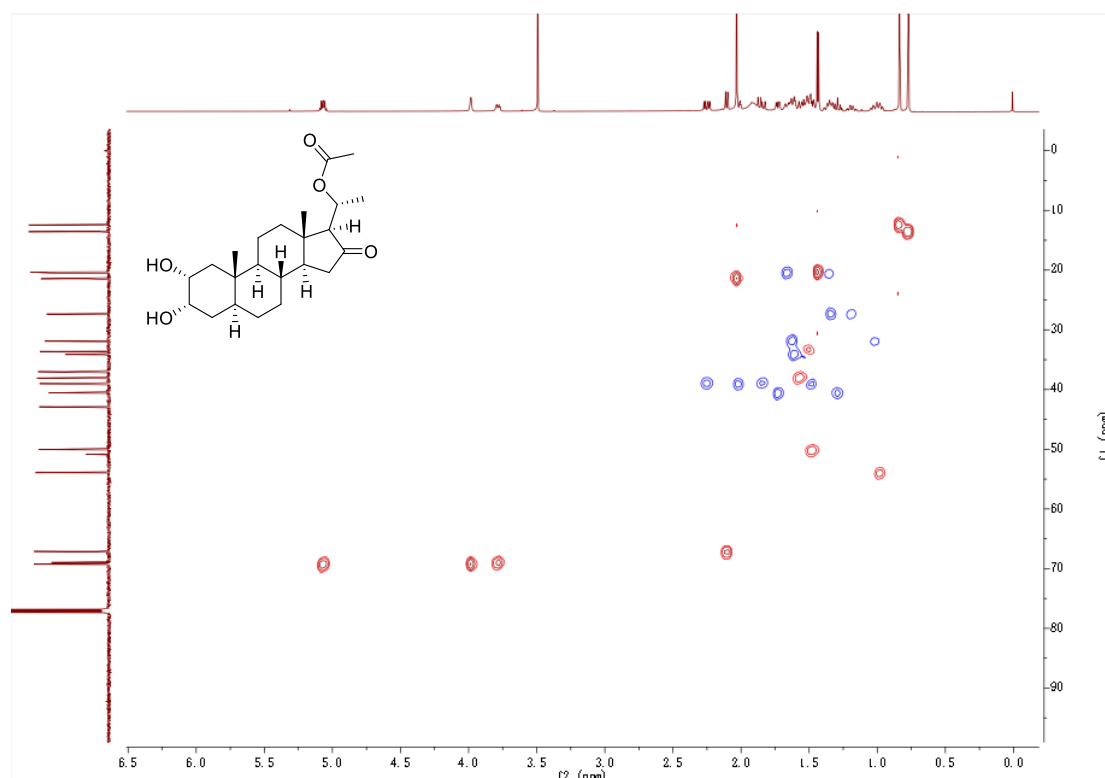
**Figure S10.** CD spectrum of compound **1**



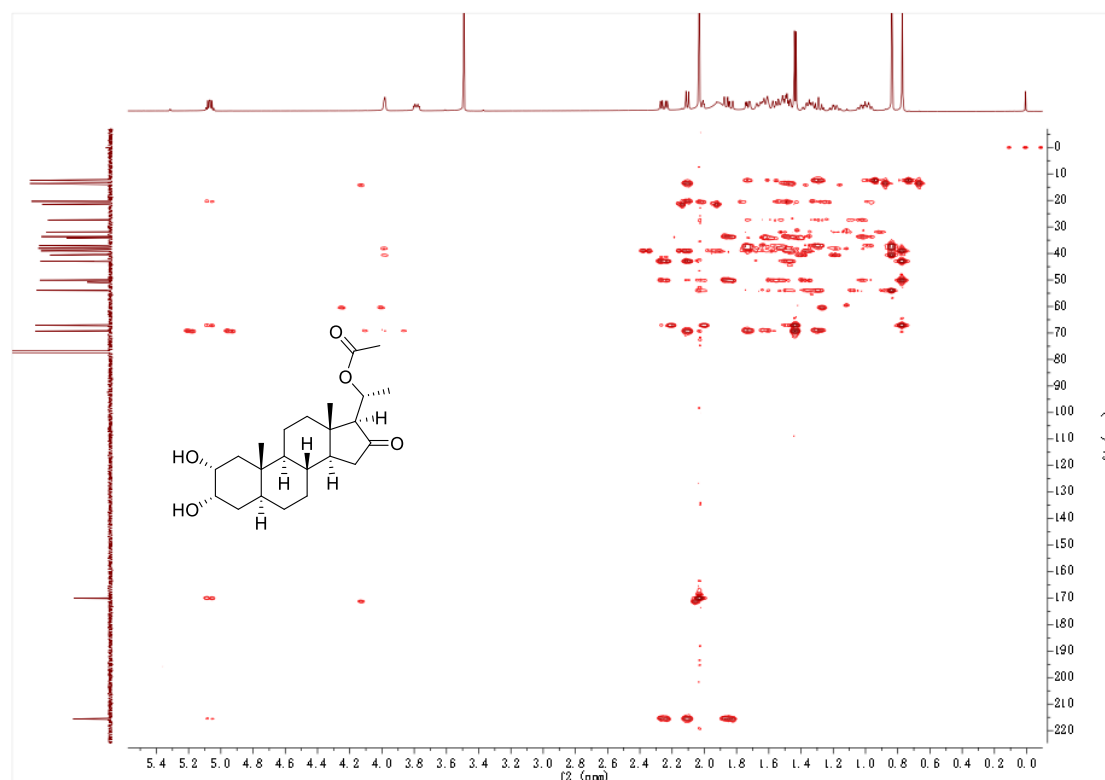
**Figure S11.** <sup>1</sup>H NMR spectrum of compound **2** in CDCl<sub>3</sub> (600 MHz)



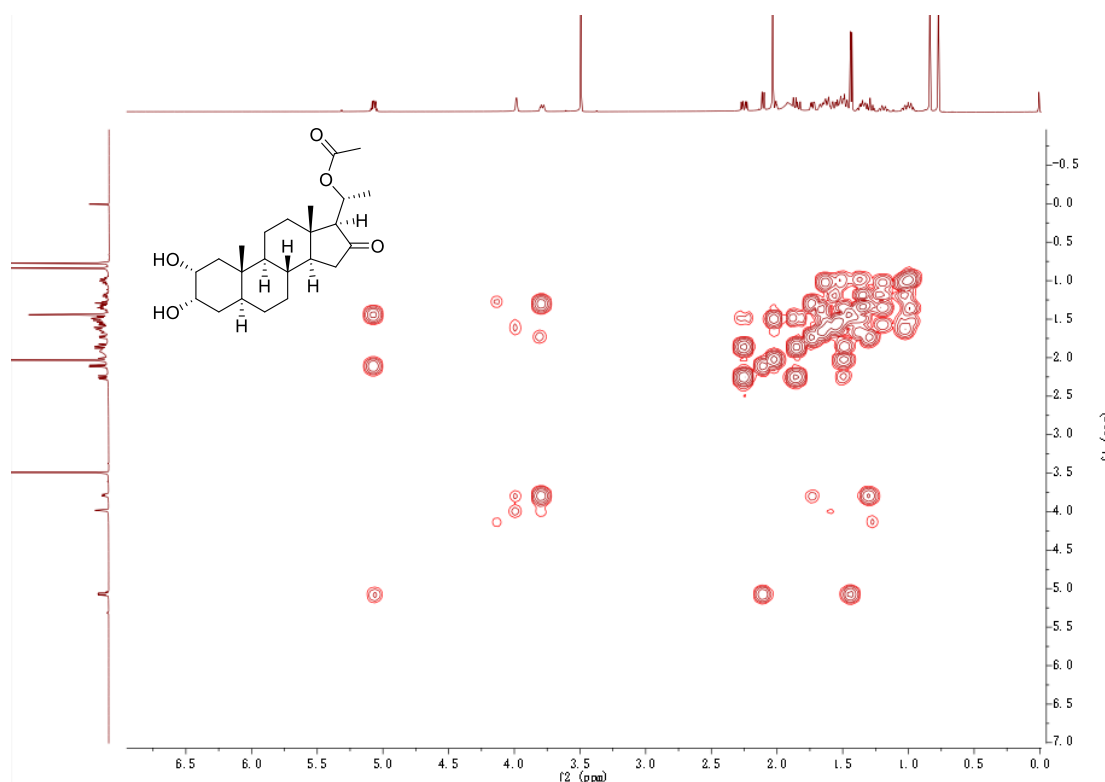
**Figure S12.** <sup>13</sup>C NMR spectrum of compound **2** in CDCl<sub>3</sub> (150 MHz)



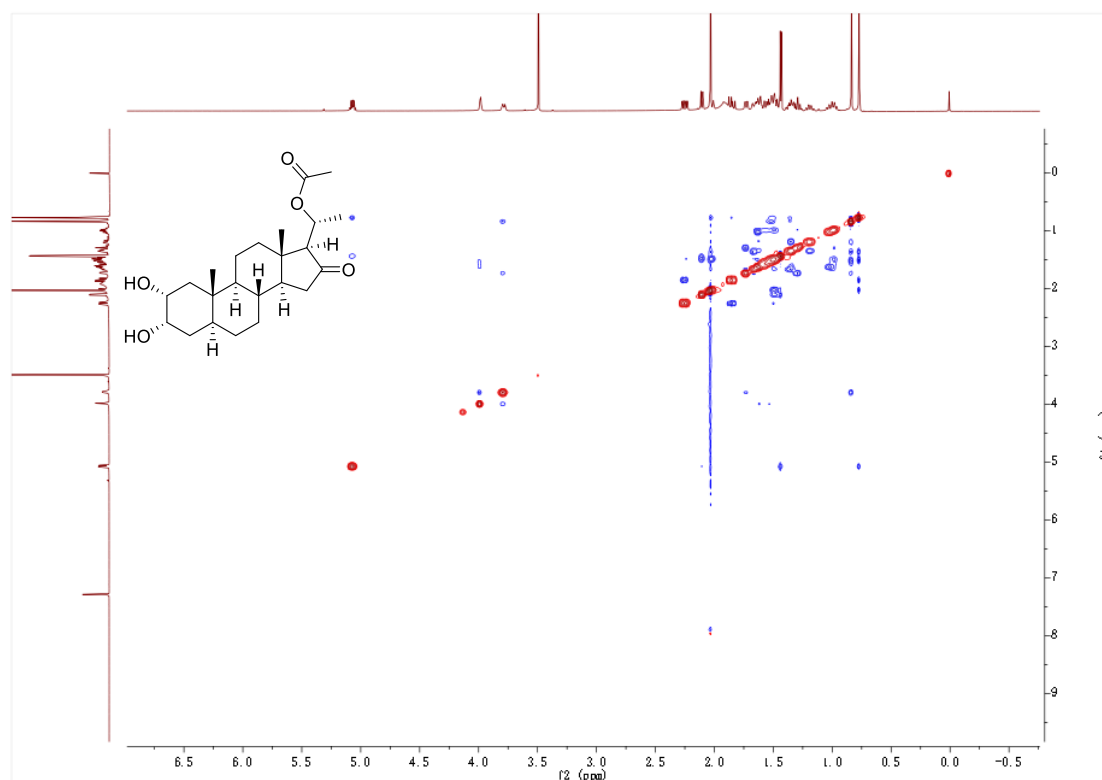
**Figure S13.** HSQC spectrum of compound **2** in  $\text{CDCl}_3$



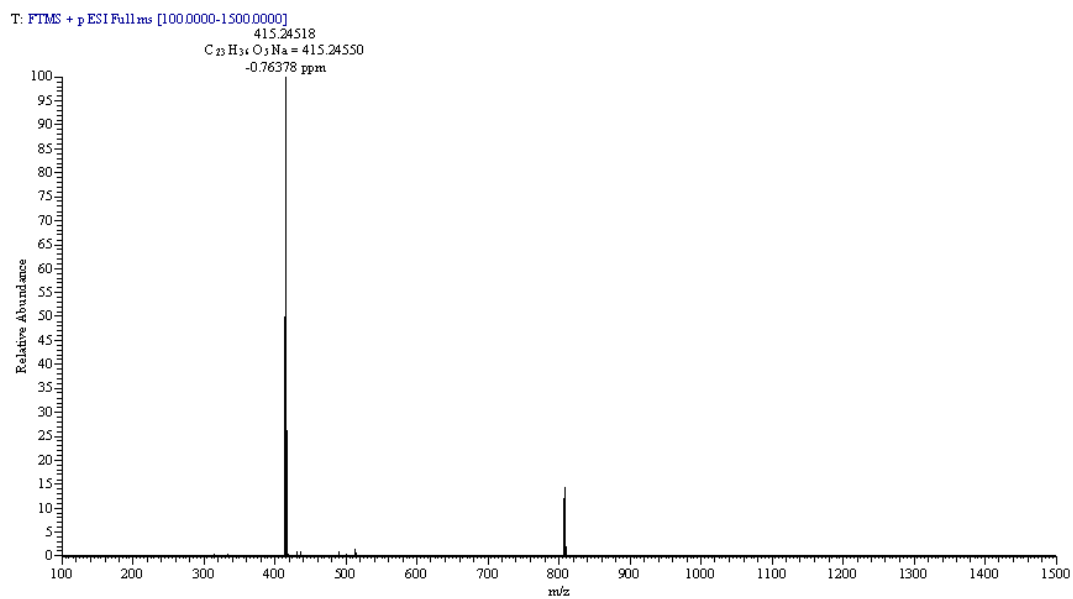
**Figure S14.** HMBC spectrum of compound **2** in  $\text{CDCl}_3$



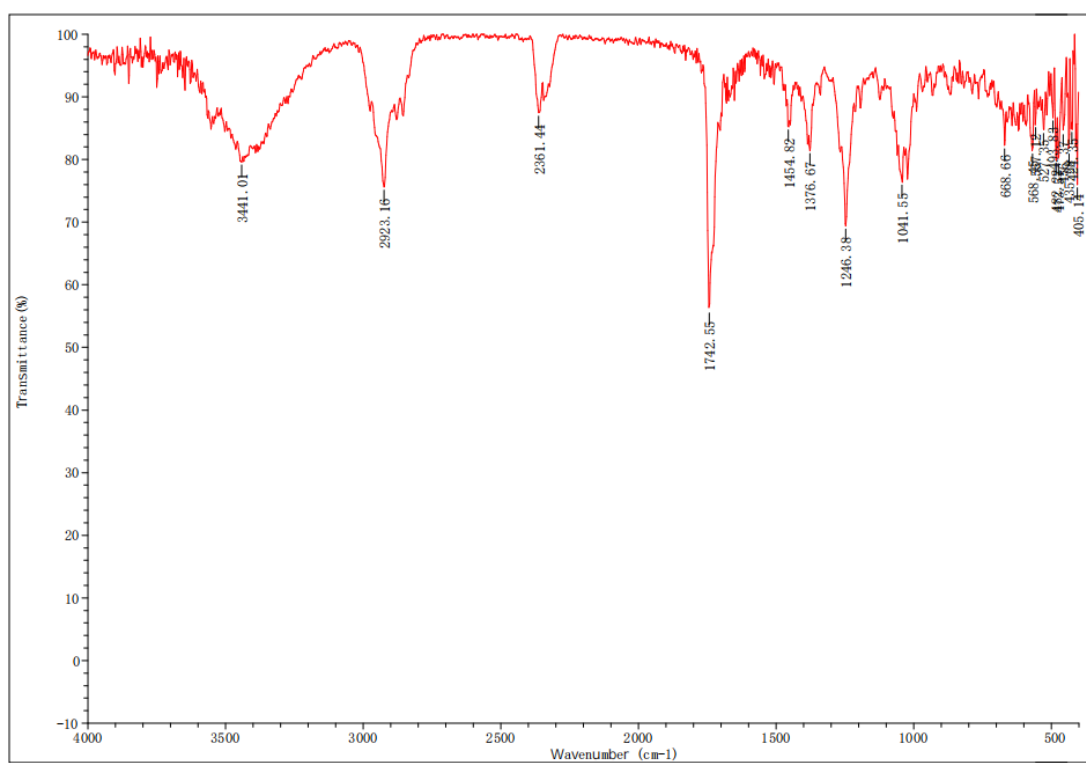
**Figure S15.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in  $\text{CDCl}_3$



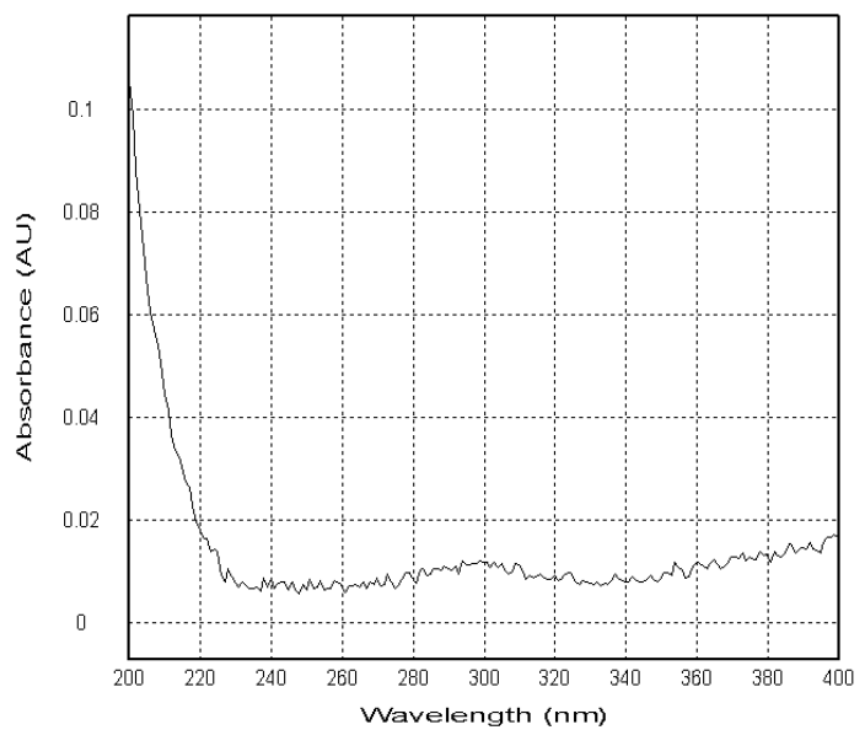
**Figure S16.** NOESY spectrum of compound **2** in  $\text{CDCl}_3$



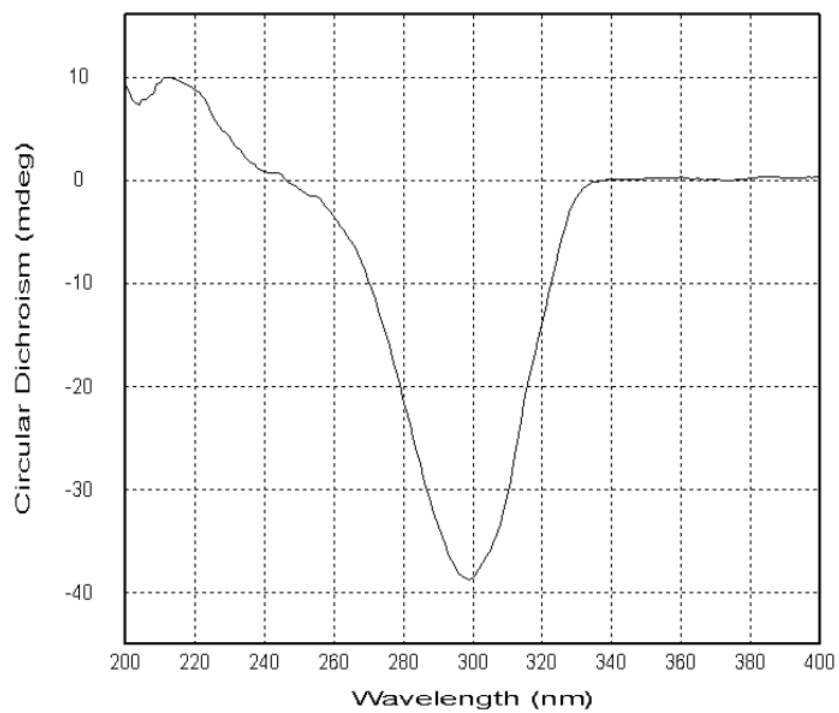
**Figure S17.** HRESIMS spectrum of compound **2**



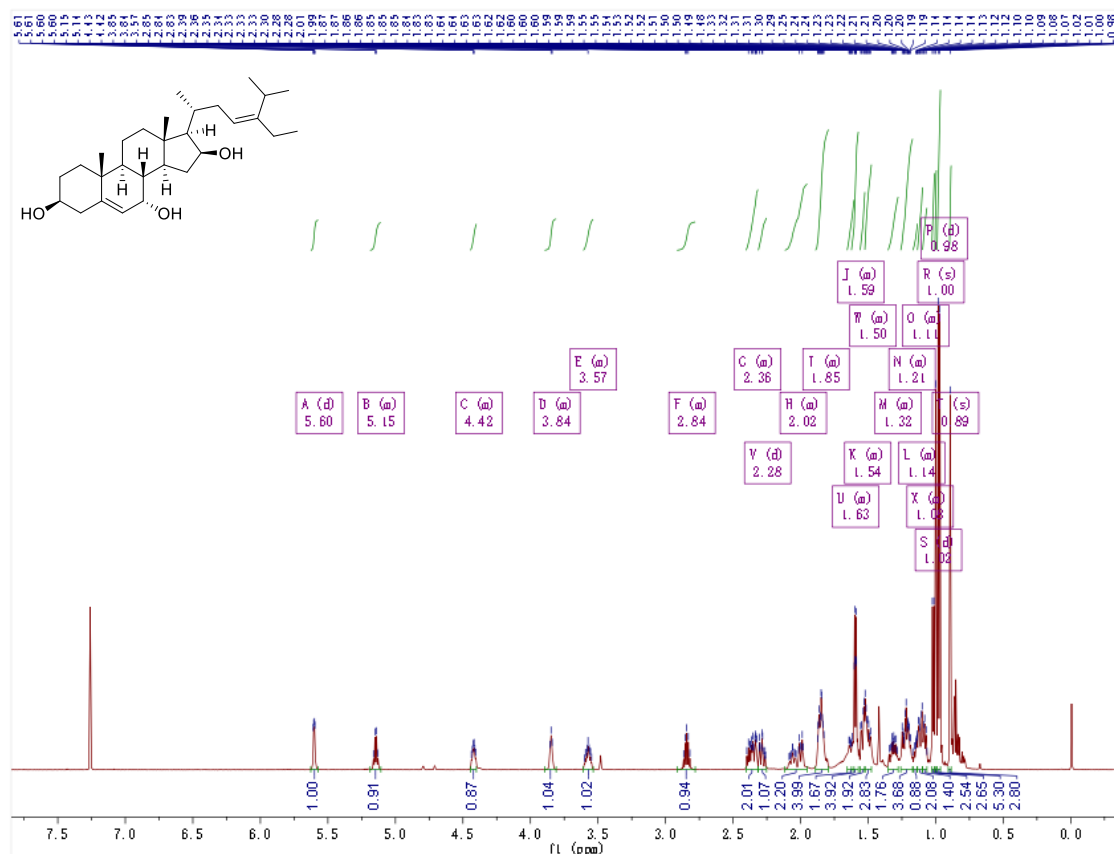
**Figure S18.** IR spectrum of compound **2**



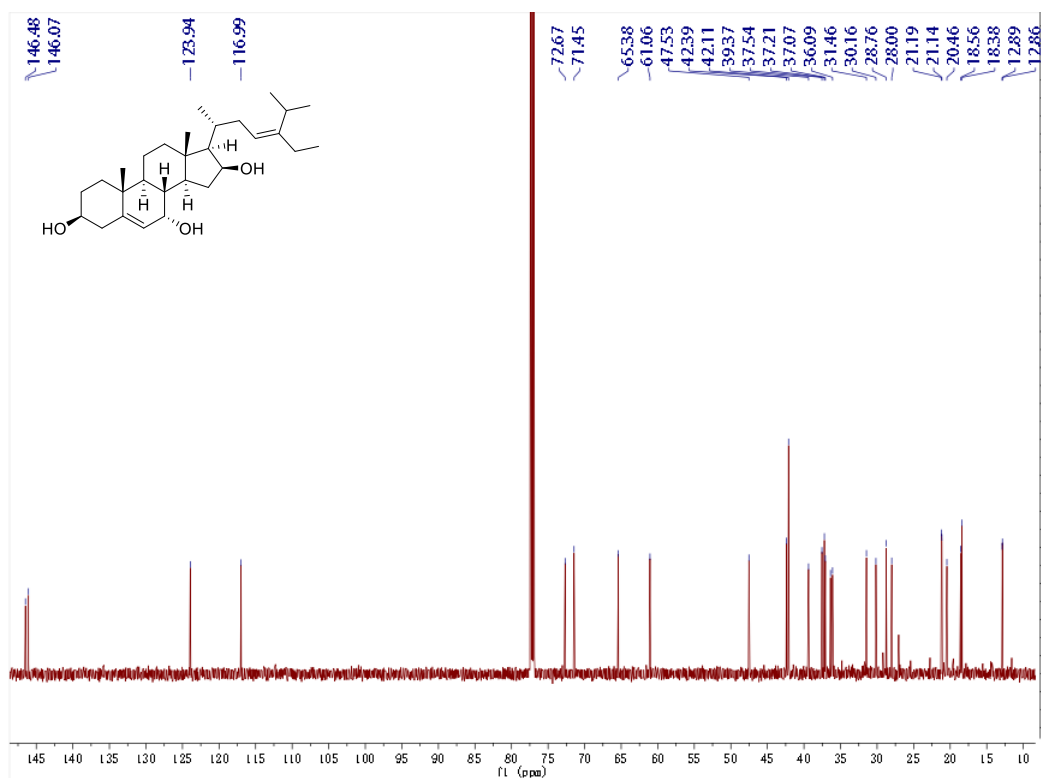
**Figure S19.** UV spectrum of compound **2**



**Figure S20.** CD spectrum of compound **2**

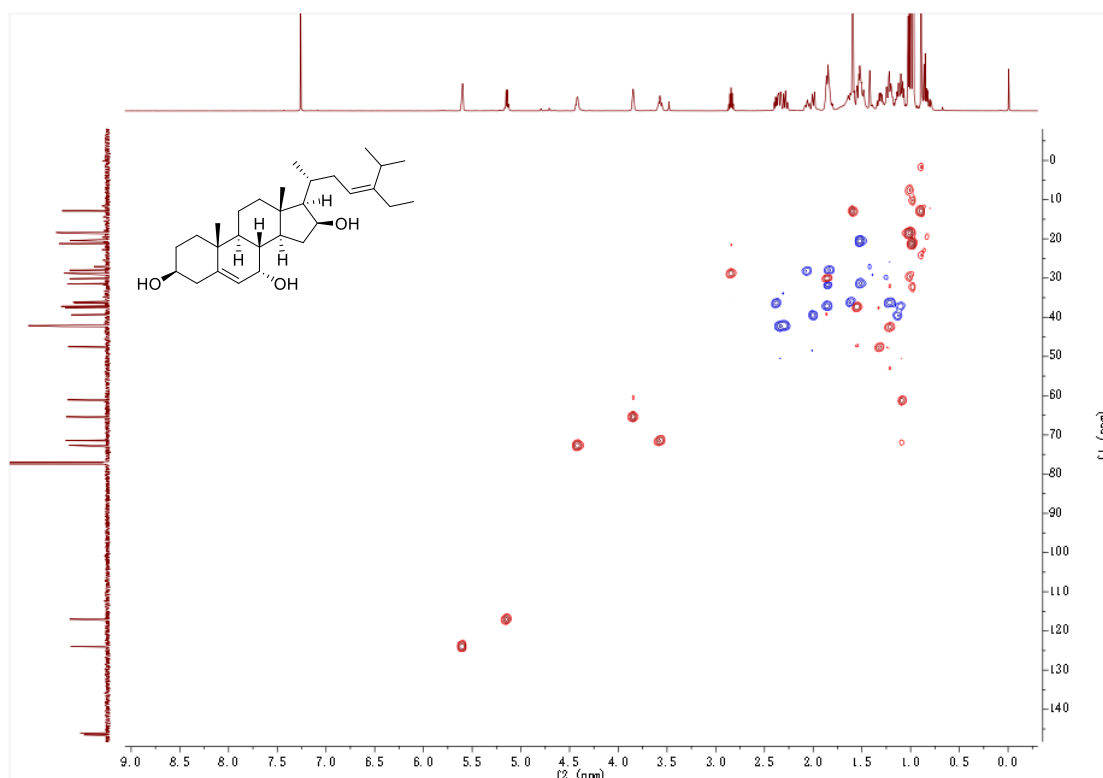


**Figure S21.**  $^1\text{H}$  NMR spectrum of compound **3** in  $\text{CDCl}_3$  (600 MHz)

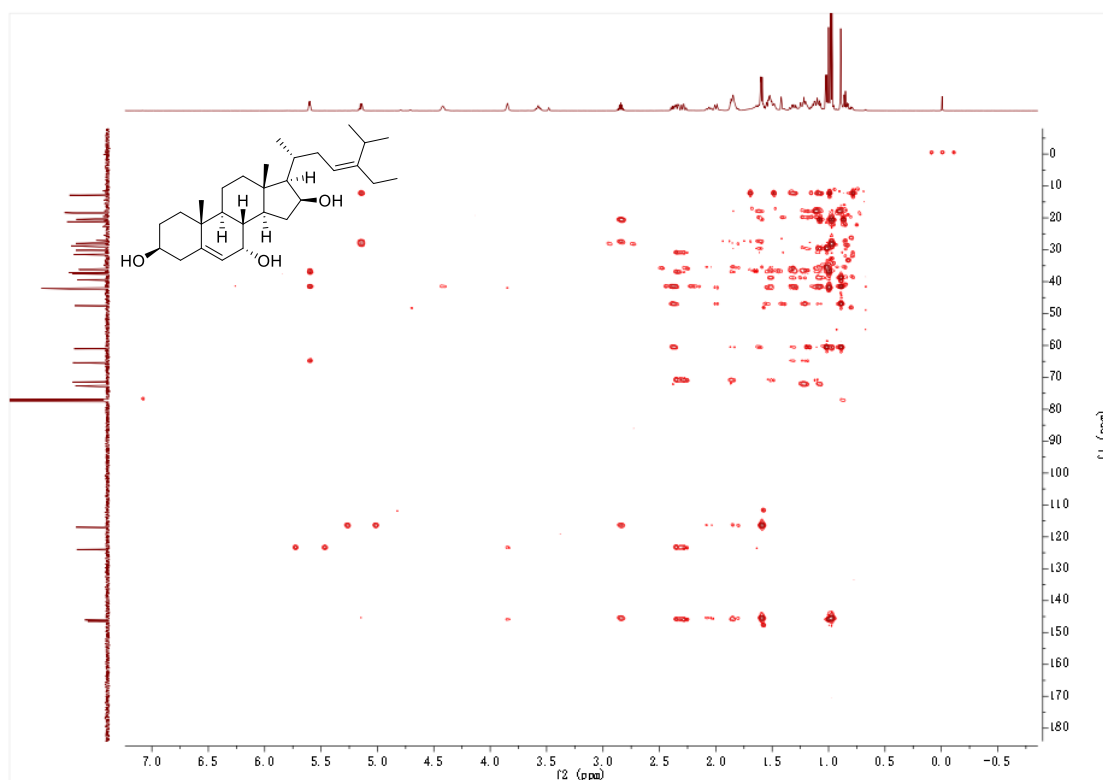


**Figure S22.**  $^{13}\text{C}$  NMR spectrum of compound **3** in  $\text{CDCl}_3$  (150 MHz)

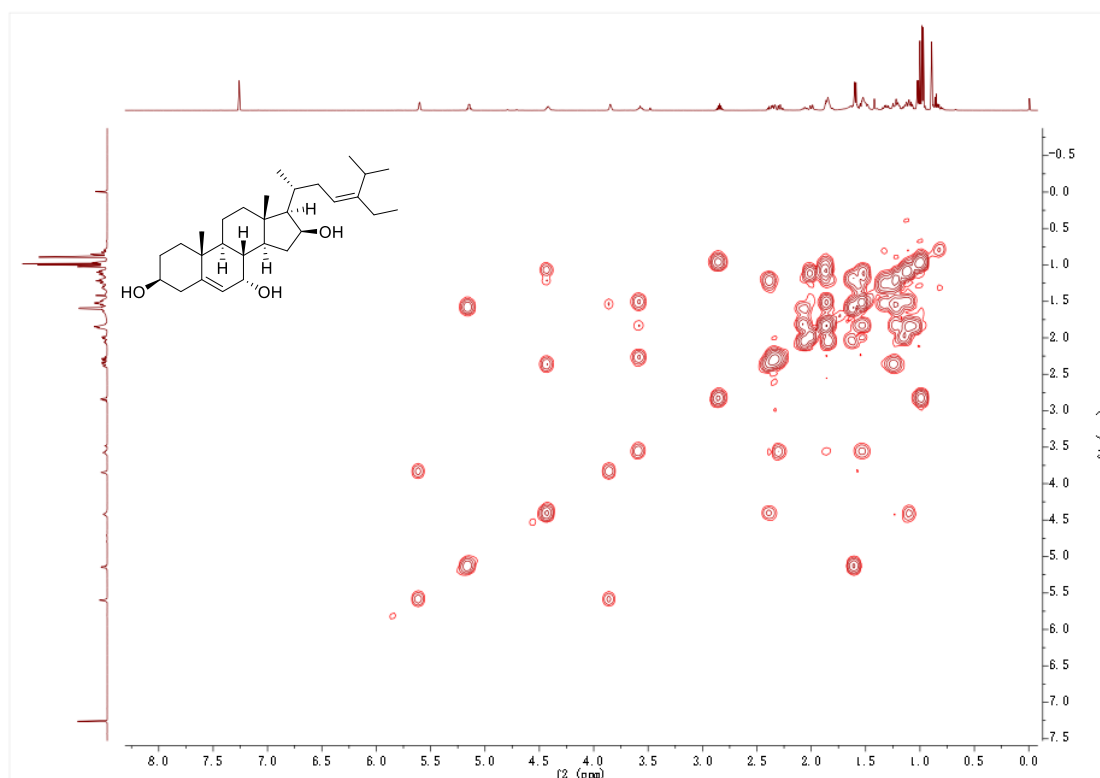




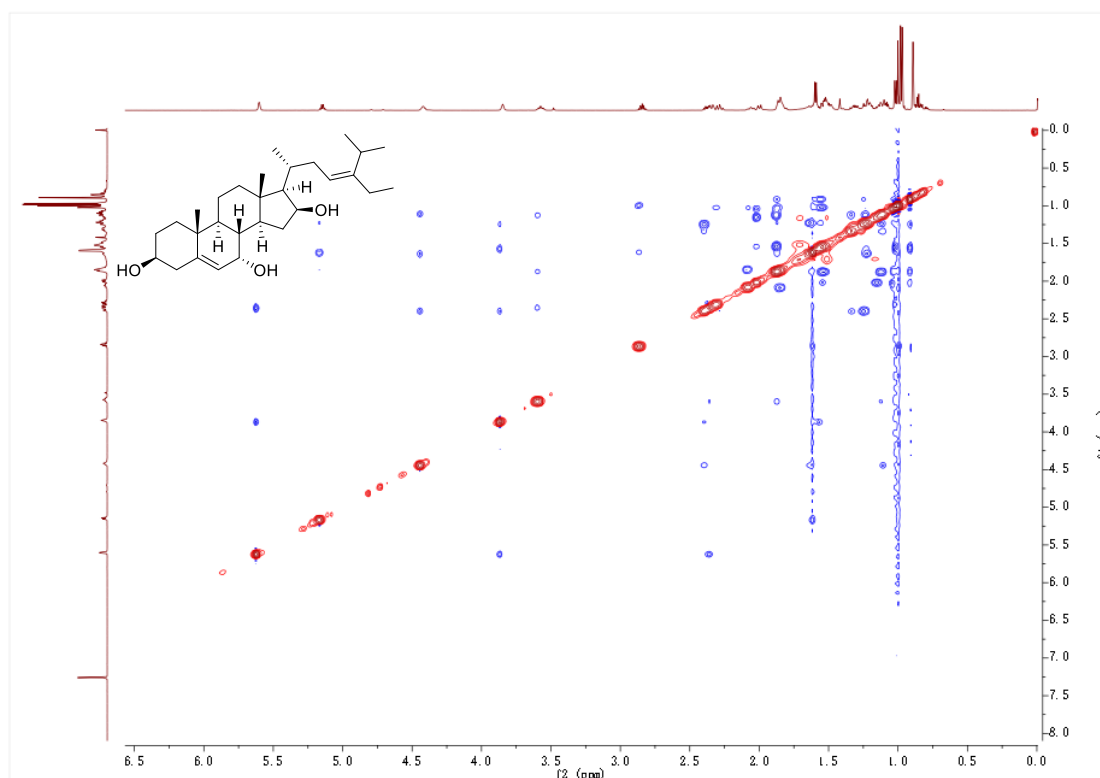
**Figure S23.** HSQC spectrum of compound **3** in  $\text{CDCl}_3$



**Figure S24.** HMBC spectrum of compound **3** in  $\text{CDCl}_3$

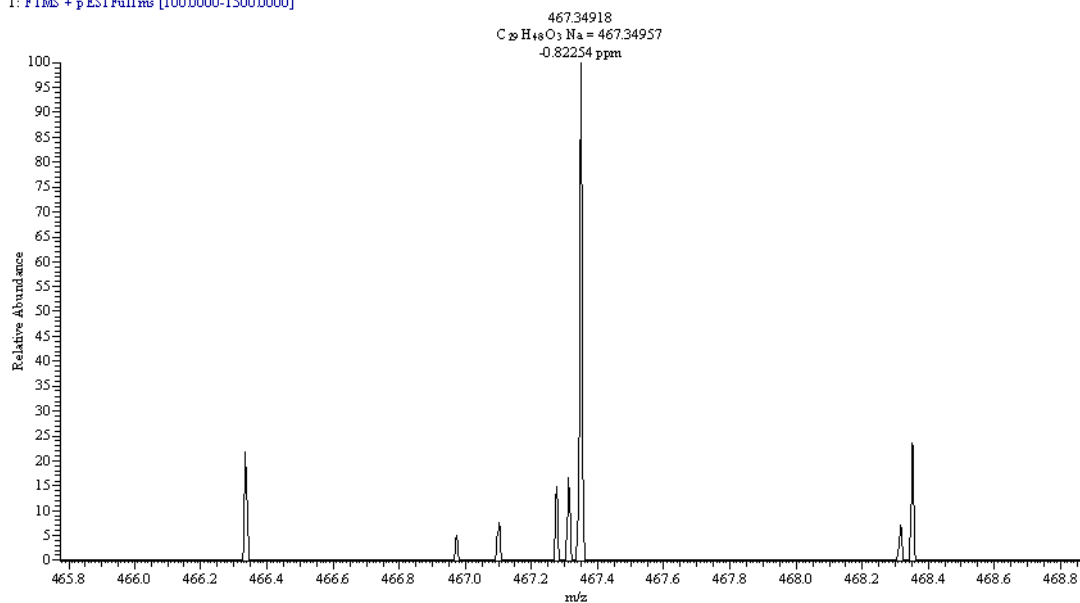


**Figure S25.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3** in  $\text{CDCl}_3$

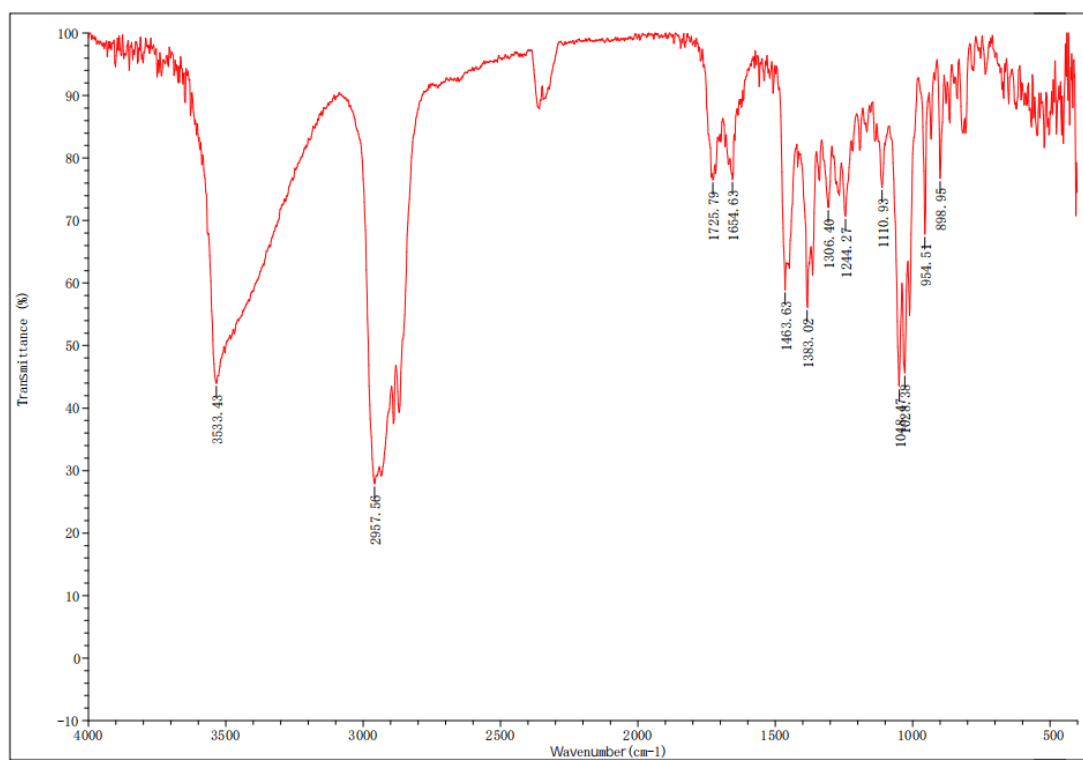


**Figure S26.** NOESY spectrum of compound **3** in  $\text{CDCl}_3$

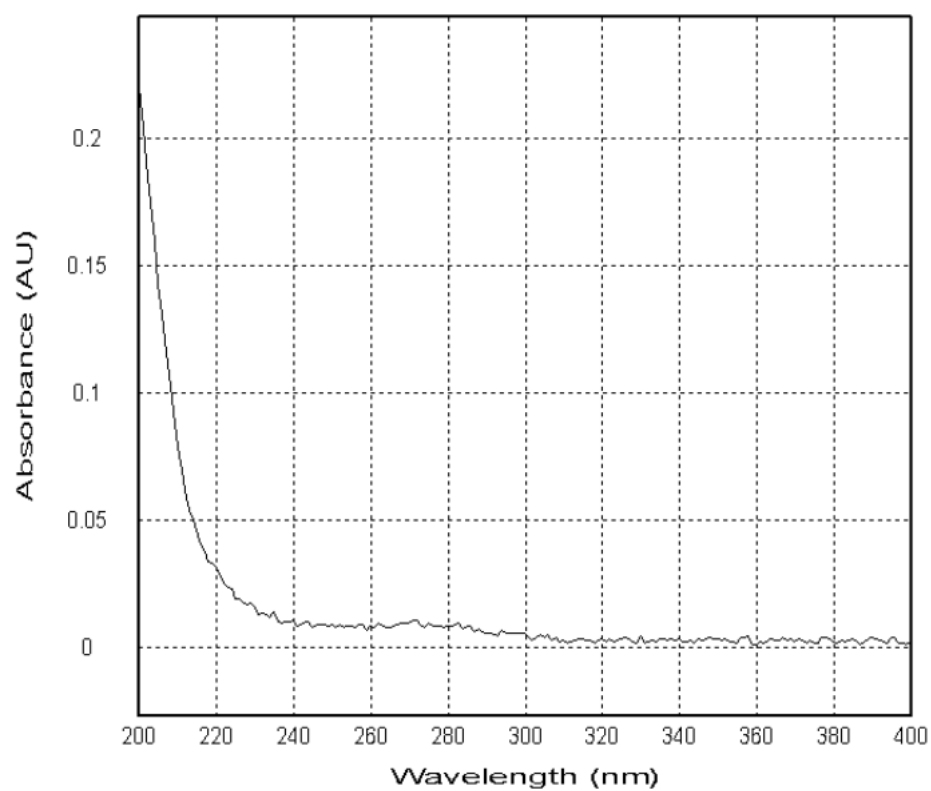
T: FTMS + p ES1 Full ms [100.0000-1500.0000]



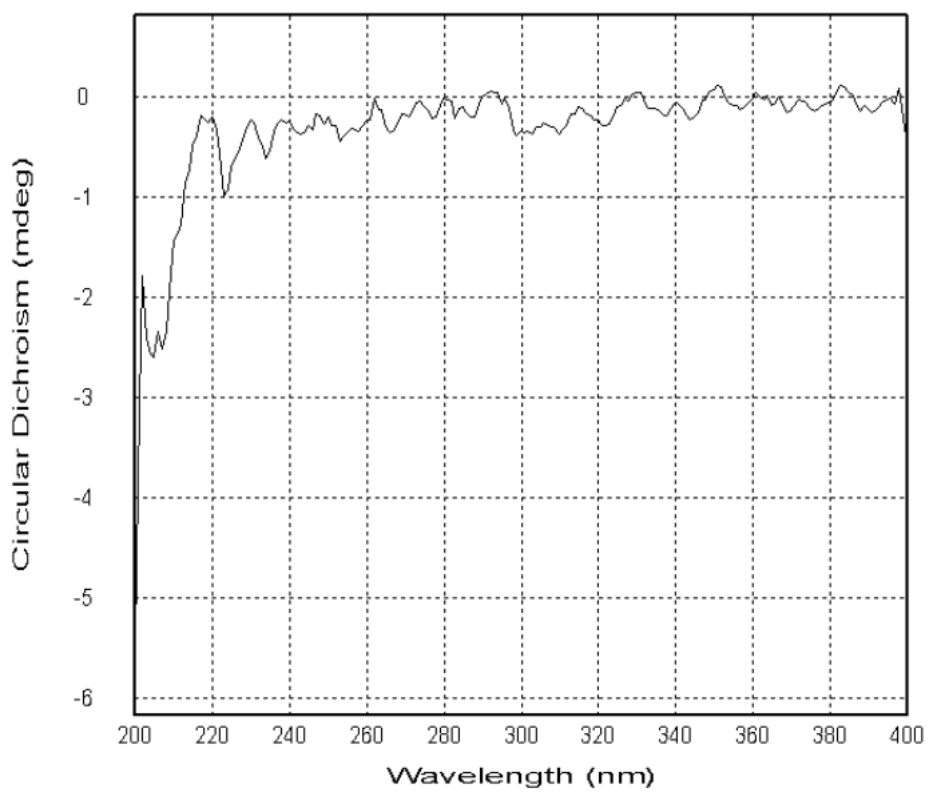
**Figure S27.** HRESIMS spectrum of compound **3**



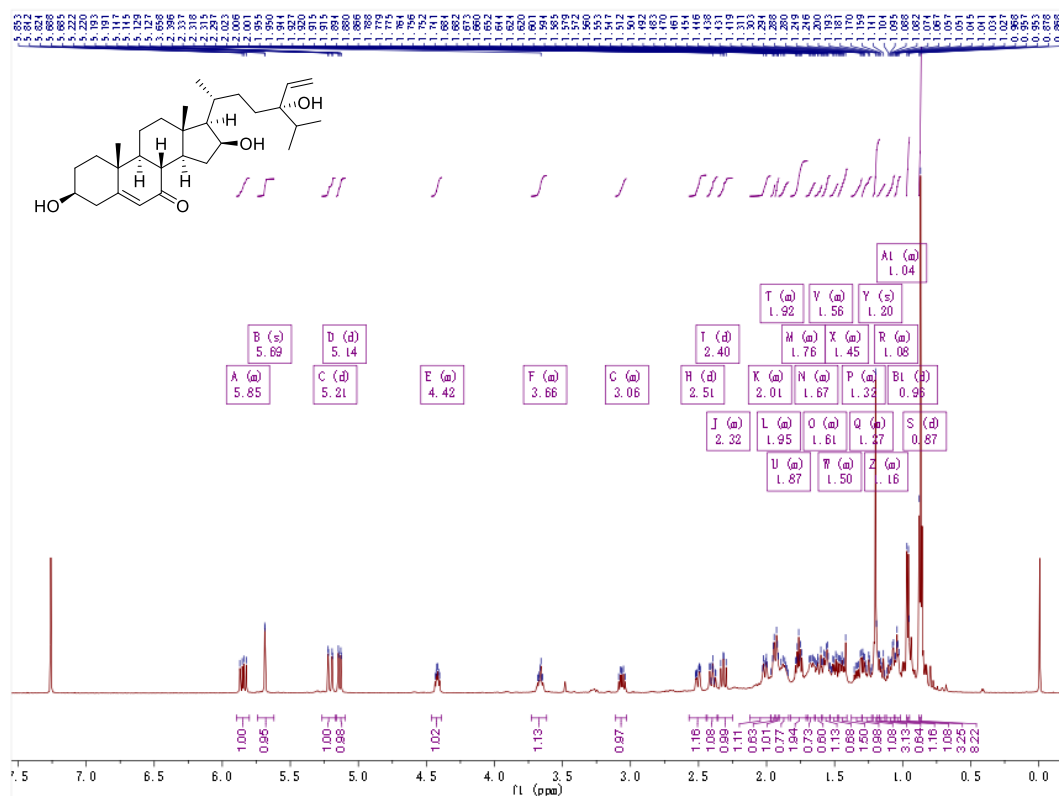
**Figure S28.** IR spectrum of compound **3**



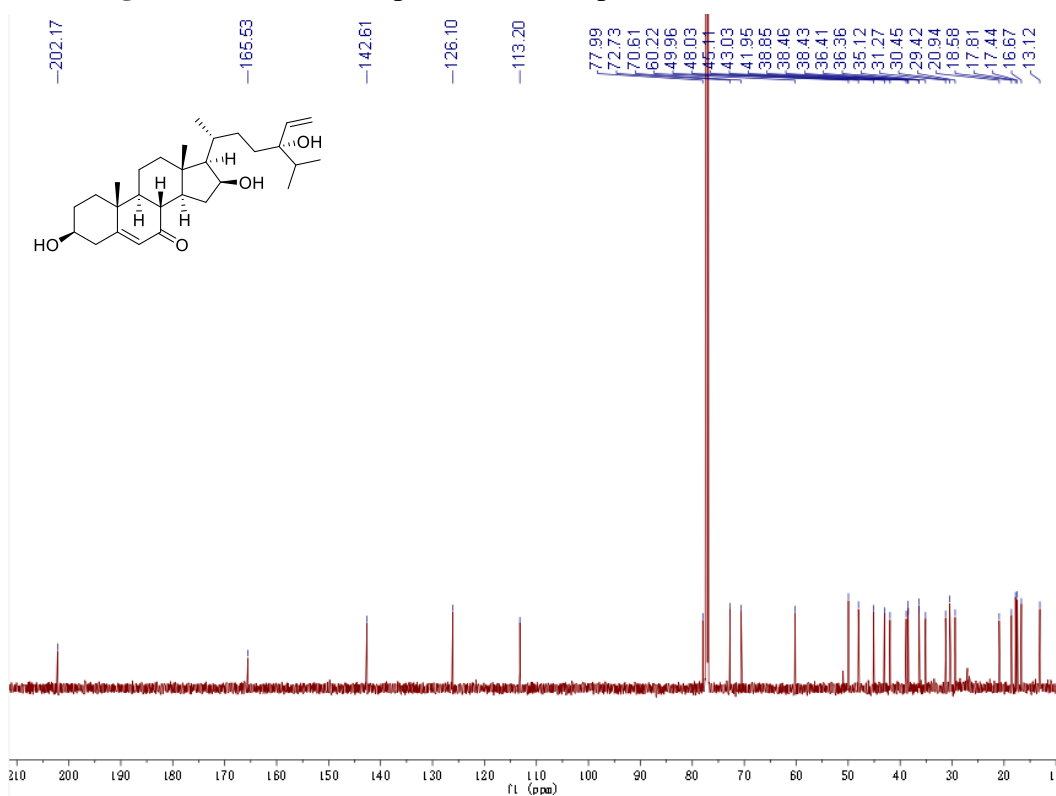
**Figure S29.** UV spectrum of compound **3**



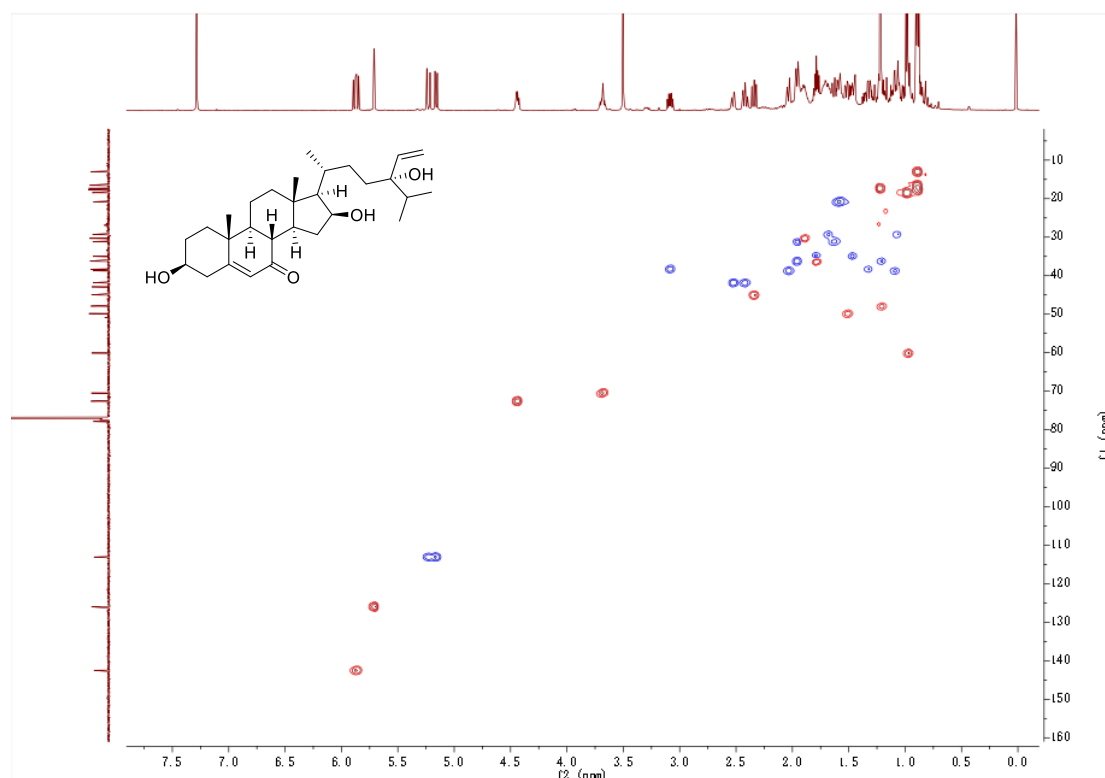
**Figure S30.** CD spectrum of compound **3**



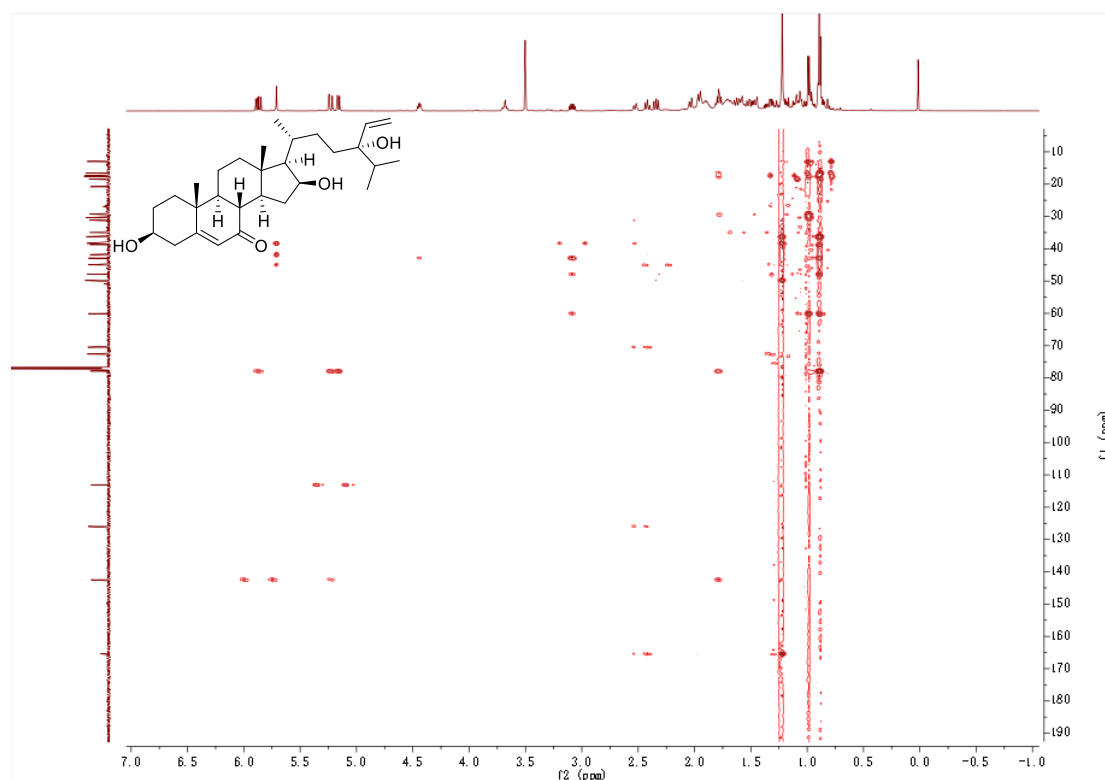
**Figure S31.** <sup>1</sup>H NMR spectrum of compound **4** in CDCl<sub>3</sub> (600 MHz)



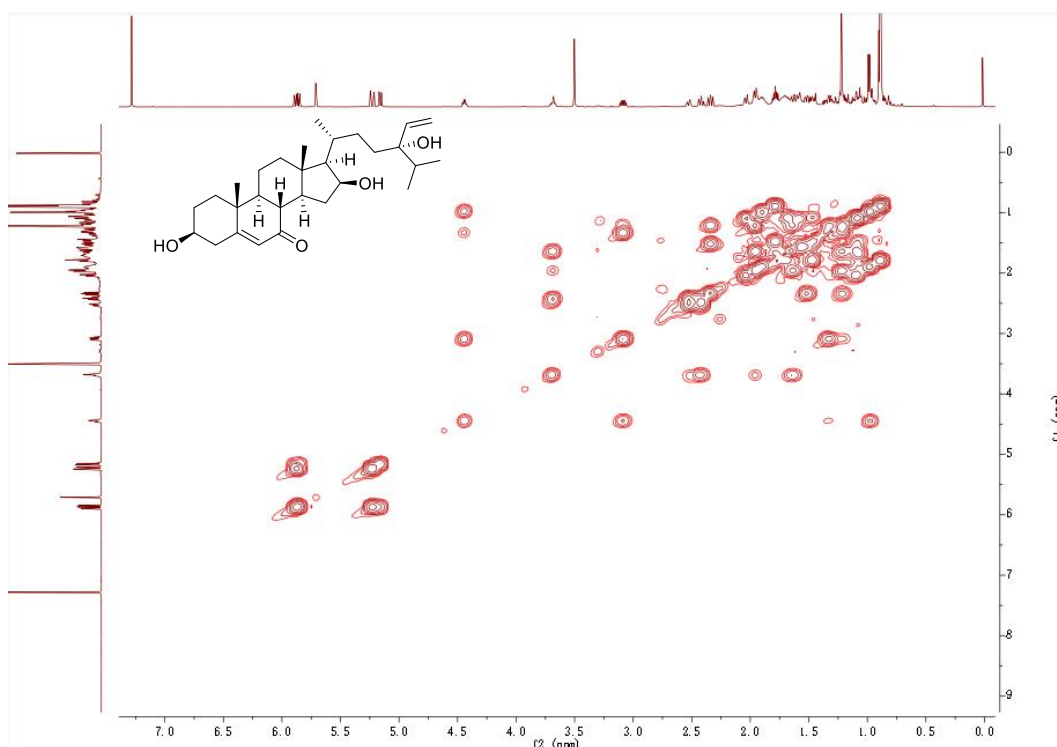
**Figure S32.** <sup>13</sup>C NMR spectrum of compound **4** in CDCl<sub>3</sub> (150 MHz)



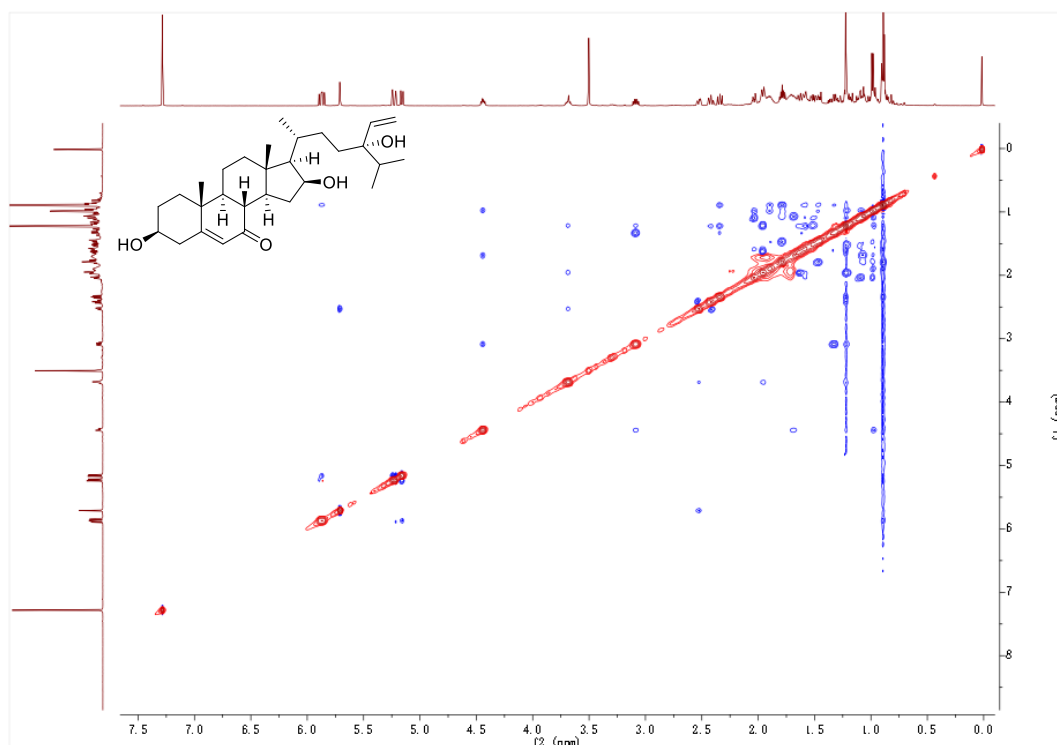
**Figure S33.** HSQC spectrum of compound **4** in  $\text{CDCl}_3$



**Figure S34.** HMBC spectrum of compound **4** in  $\text{CDCl}_3$

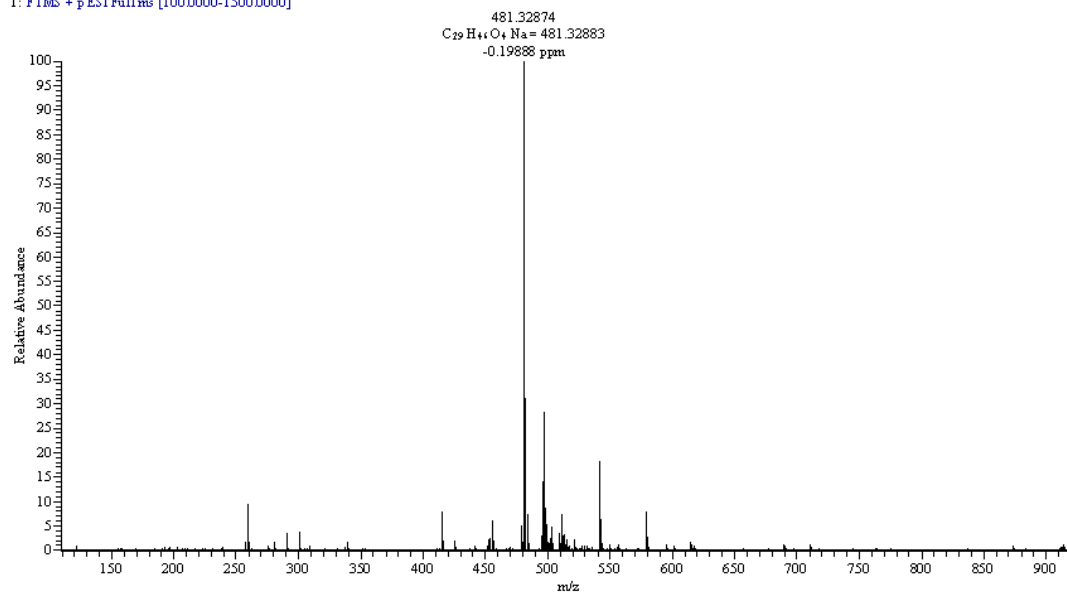


**Figure S35.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4** in  $\text{CDCl}_3$

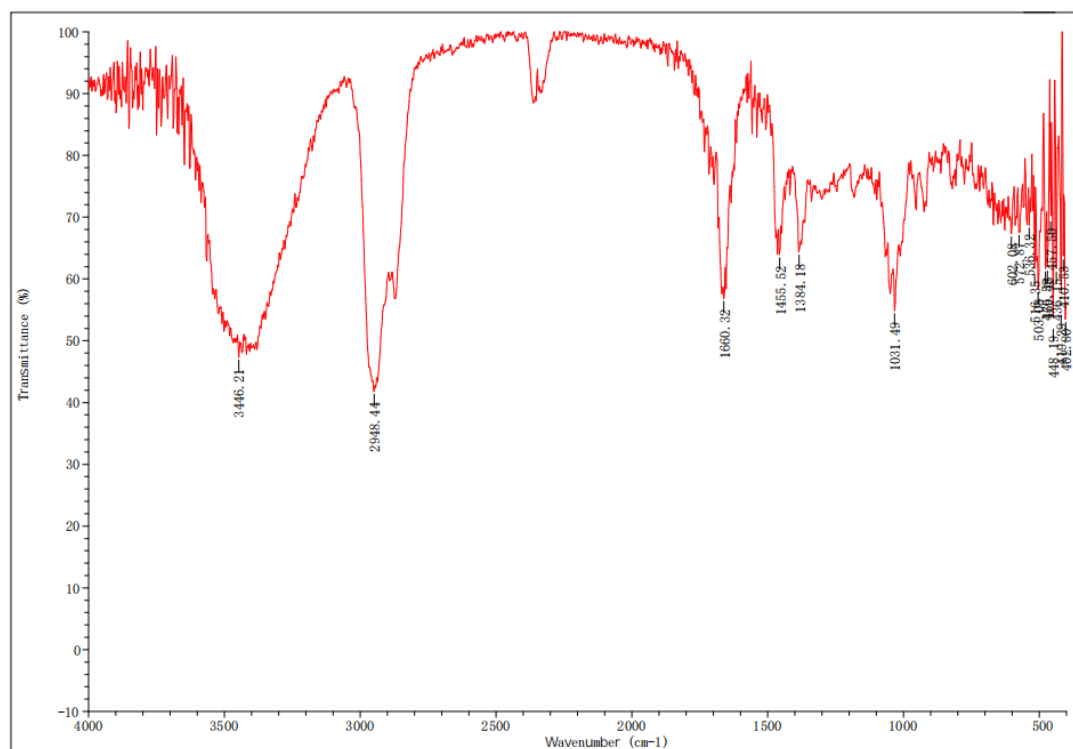


**Figure S36.** NOESY spectrum of compound **4** in  $\text{CDCl}_3$

T: FTMS + p ESI Fullms [100.0000-1500.0000]

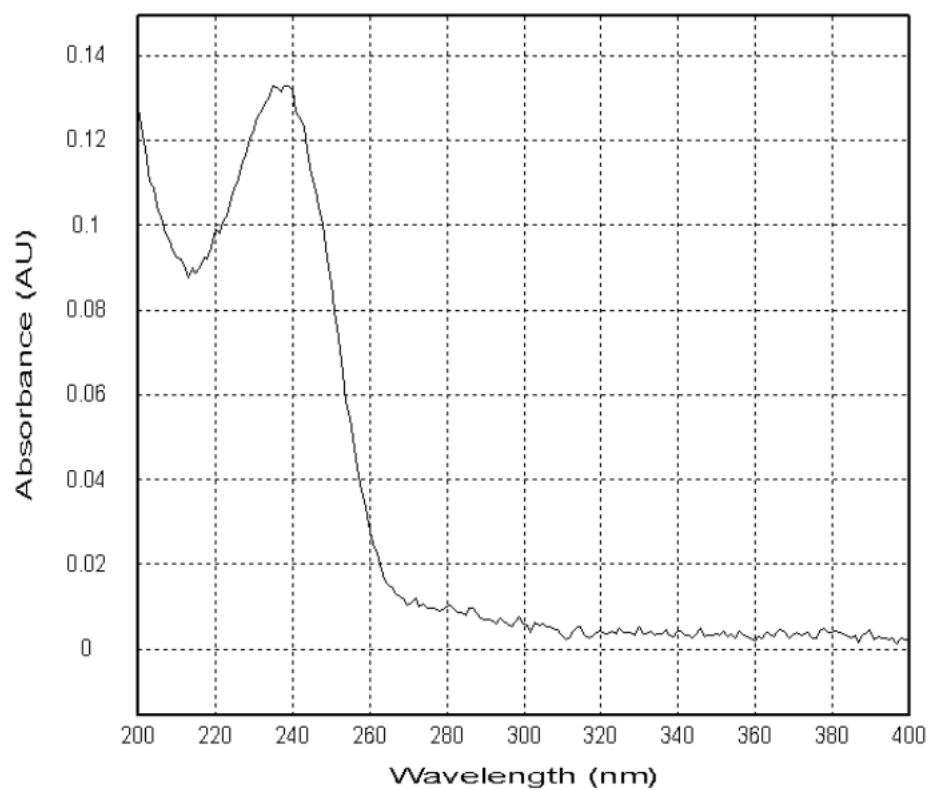


**Figure S37.** HRESIMS spectrum of compound **4**

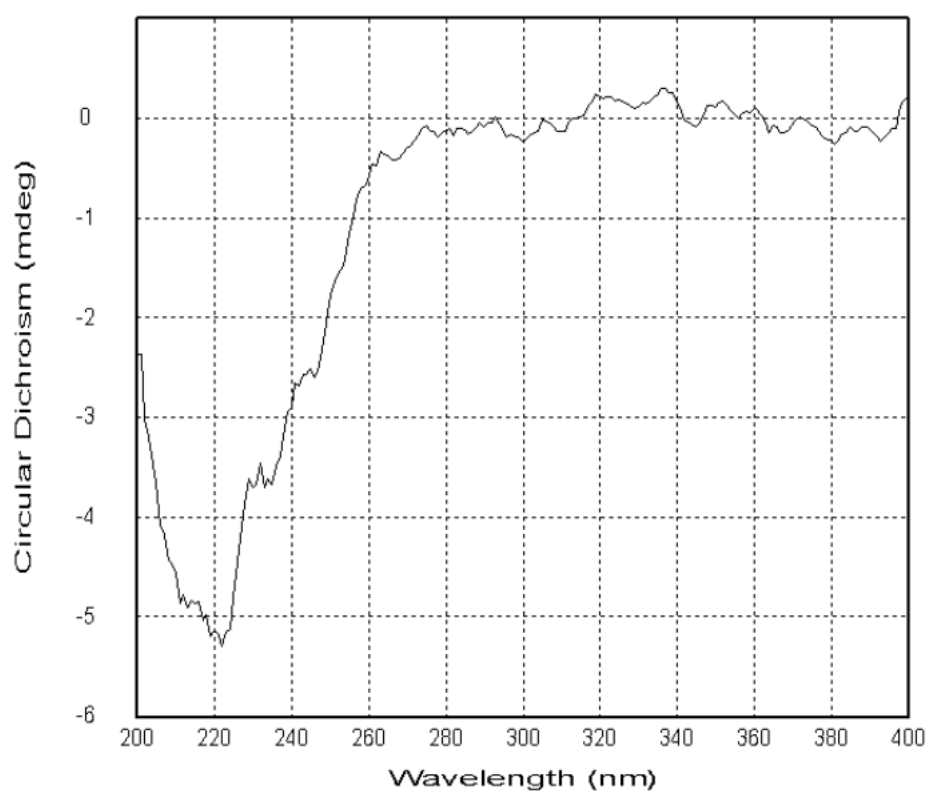


**Figure S38.** IR spectrum of compound **4**

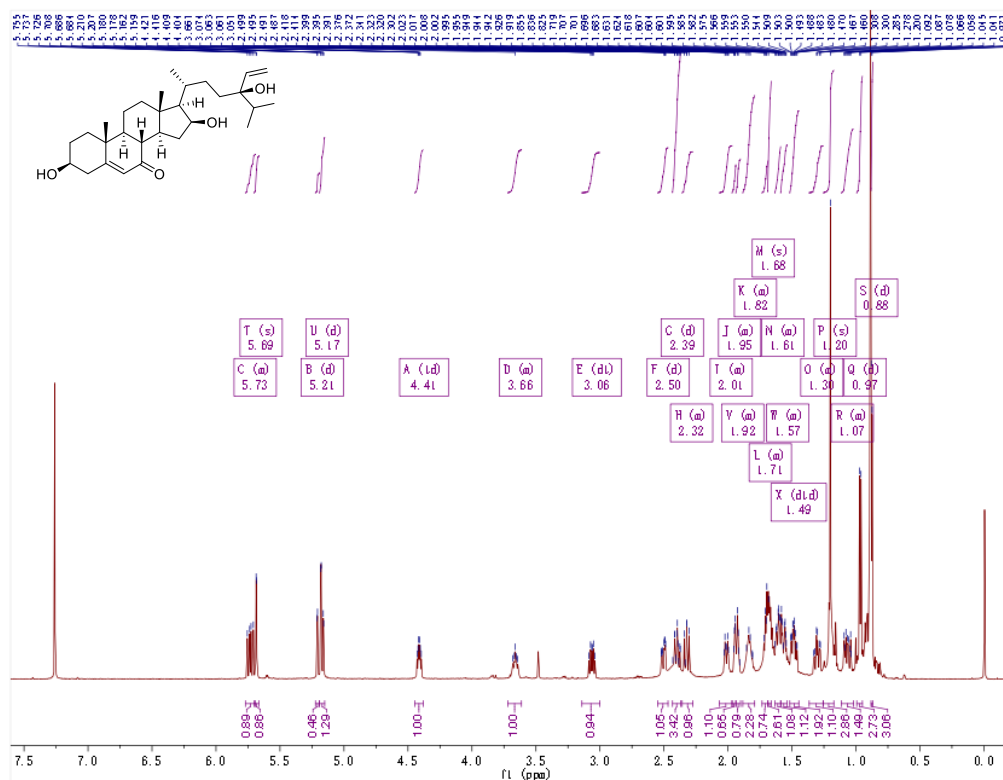




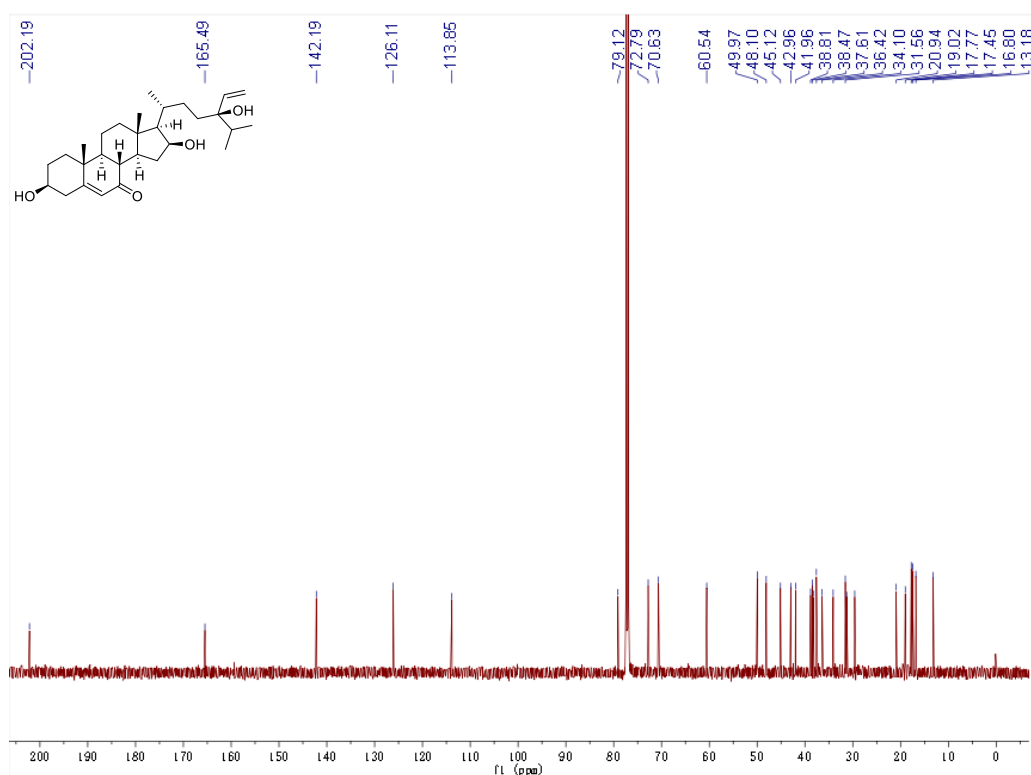
**Figure S39.** UV spectrum of compound **4**



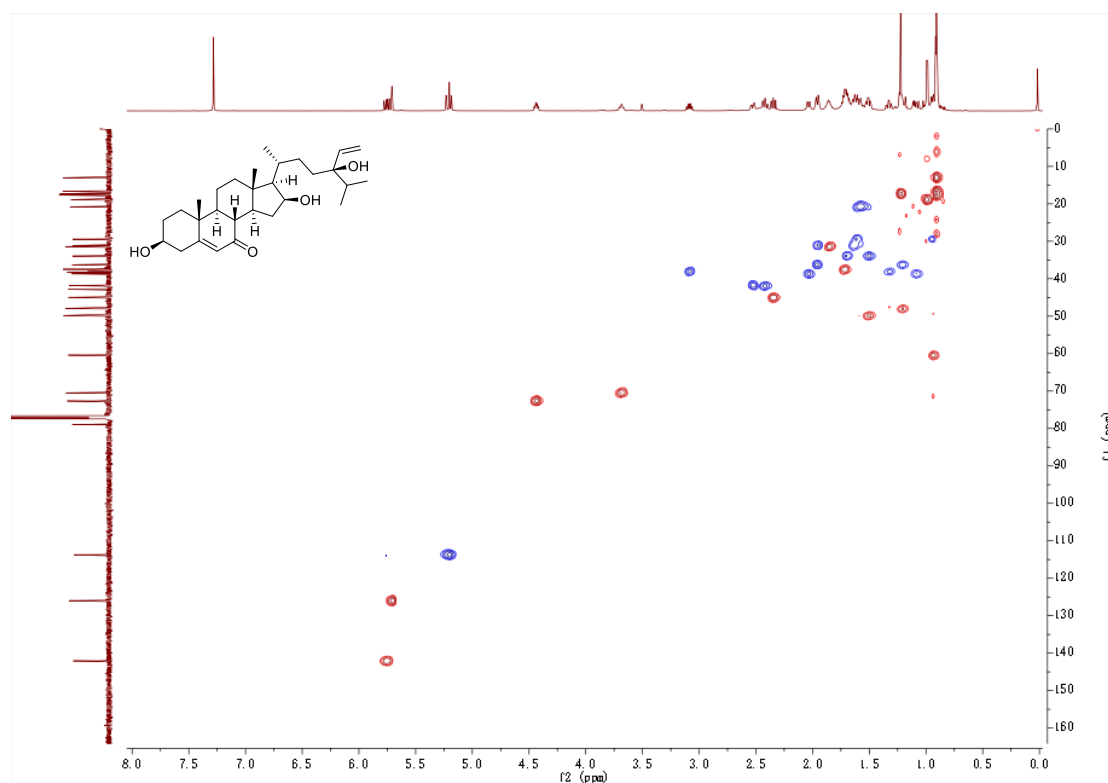
**Figure S40.** CD spectrum of compound **4**



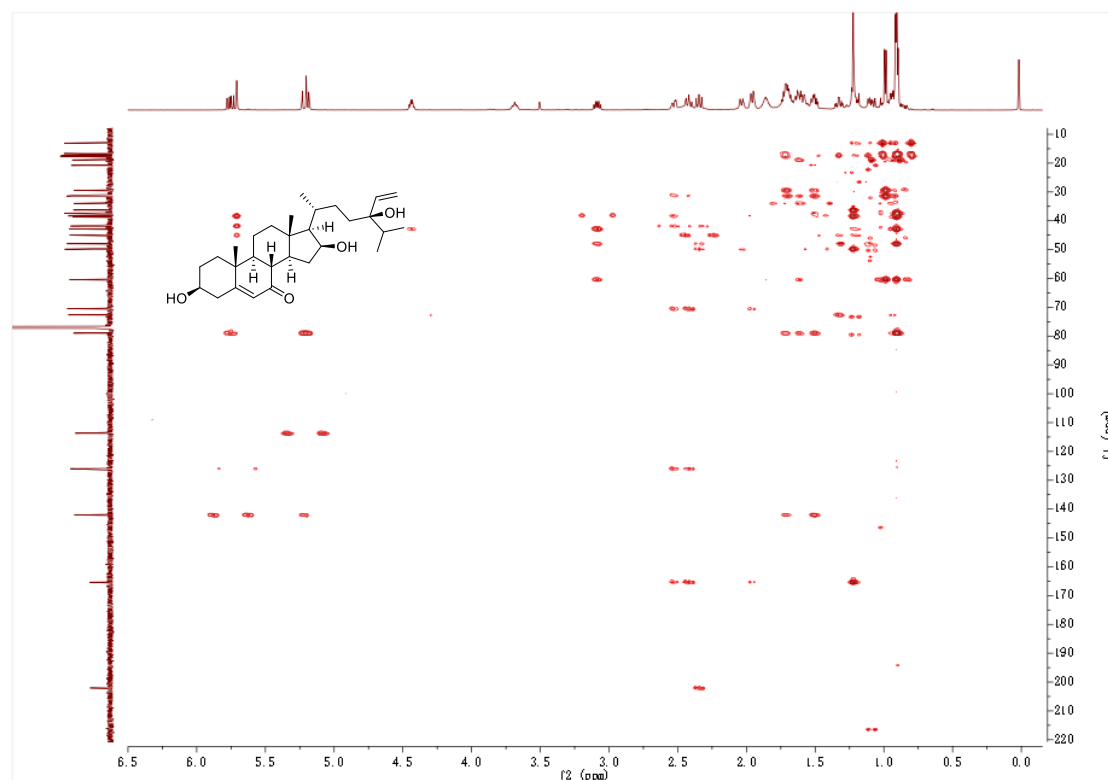
**Figure S41.** <sup>1</sup>H NMR spectrum of compound **5** in CDCl<sub>3</sub> (600 MHz)



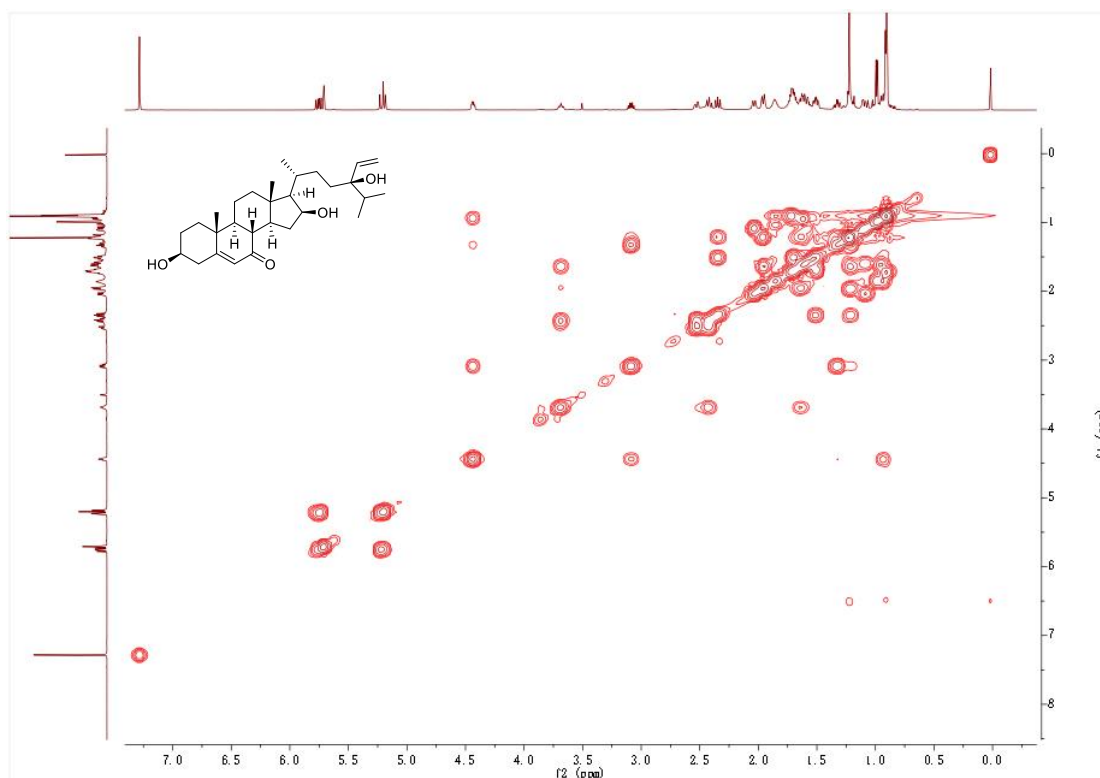
**Figure S42.** <sup>13</sup>C NMR spectrum of compound **5** in CDCl<sub>3</sub> (150 MHz)



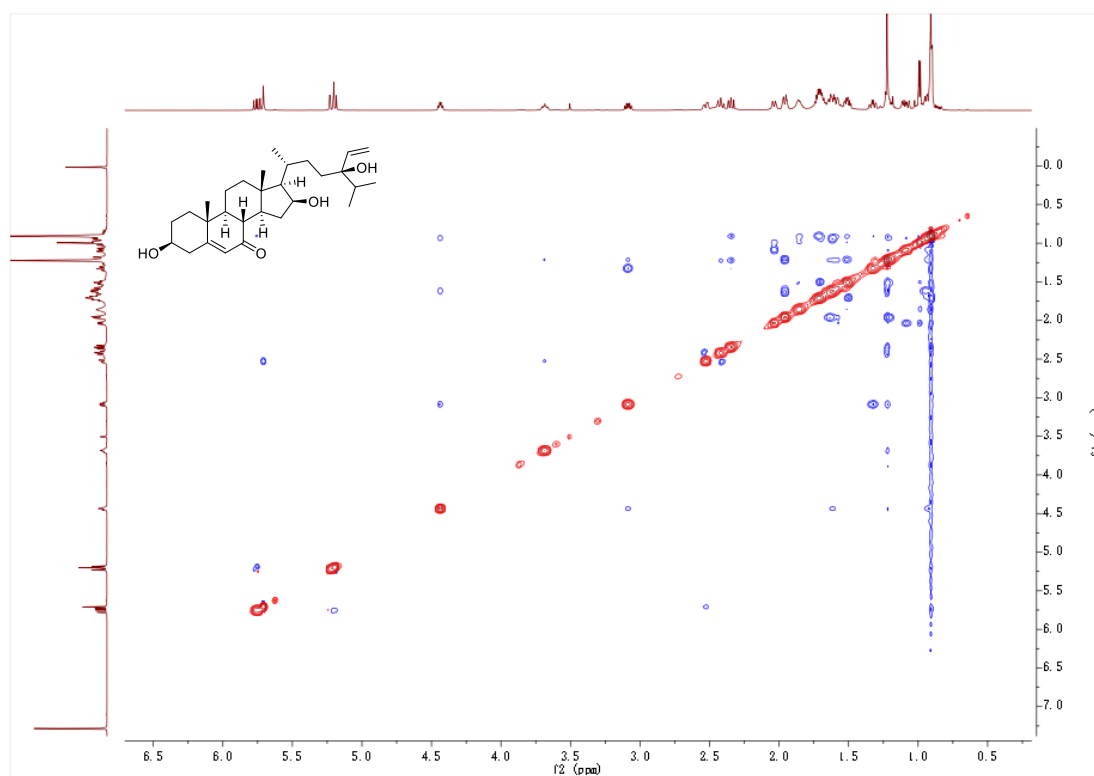
**Figure S43.** HSQC spectrum of compound **5** in  $\text{CDCl}_3$



**Figure S44.** HMBC spectrum of compound **5** in  $\text{CDCl}_3$

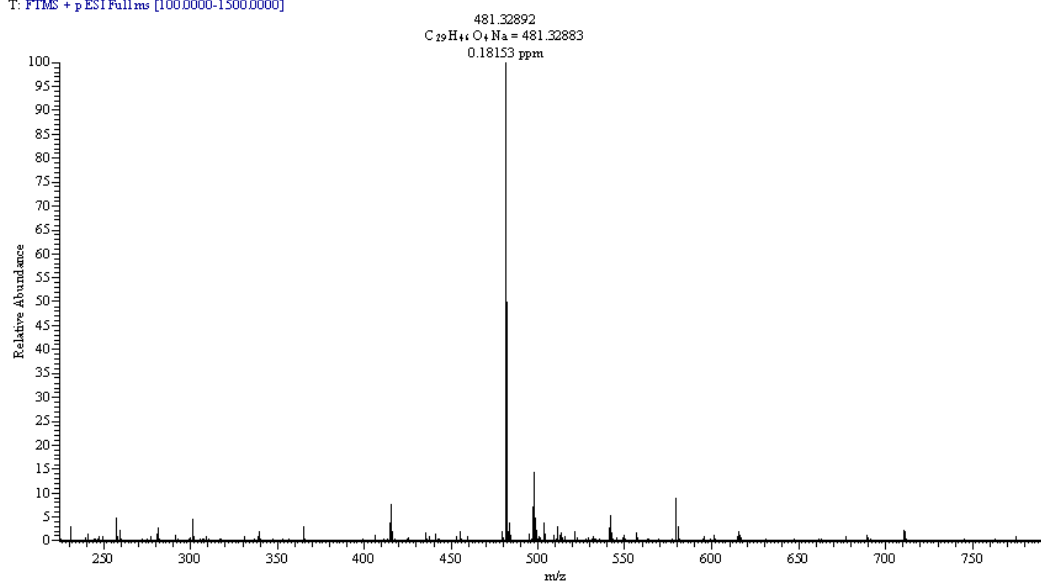


**Figure S45.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **5** in  $\text{CDCl}_3$

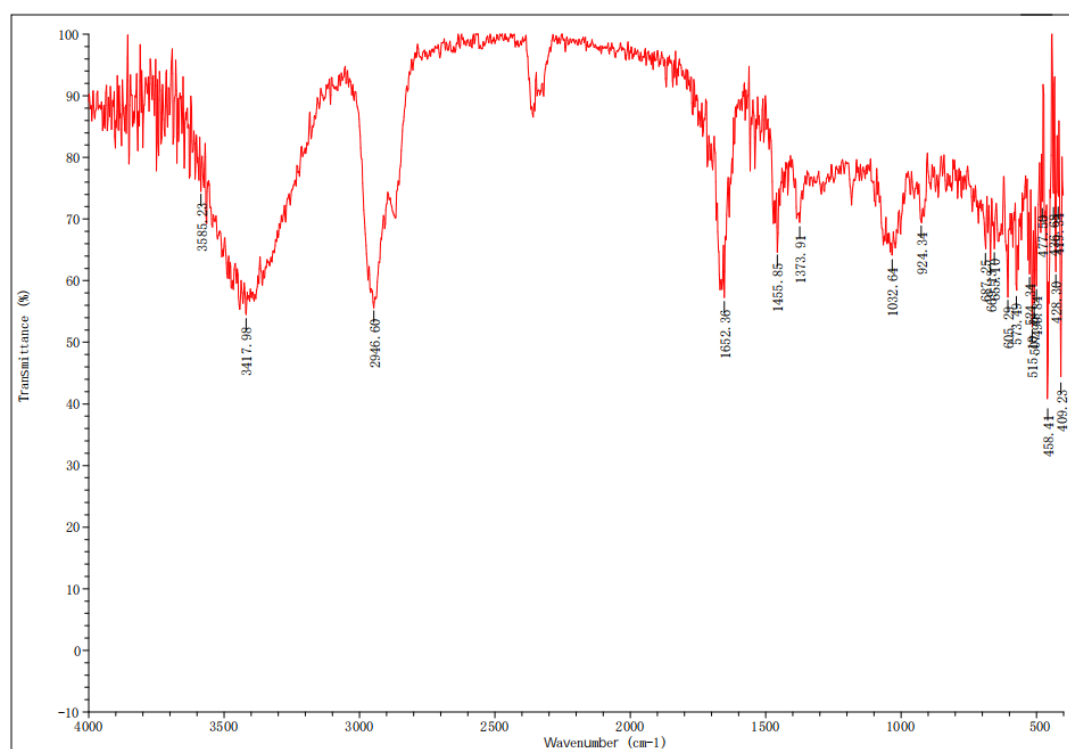


**Figure S46.** NOESY spectrum of compound **5** in  $\text{CDCl}_3$

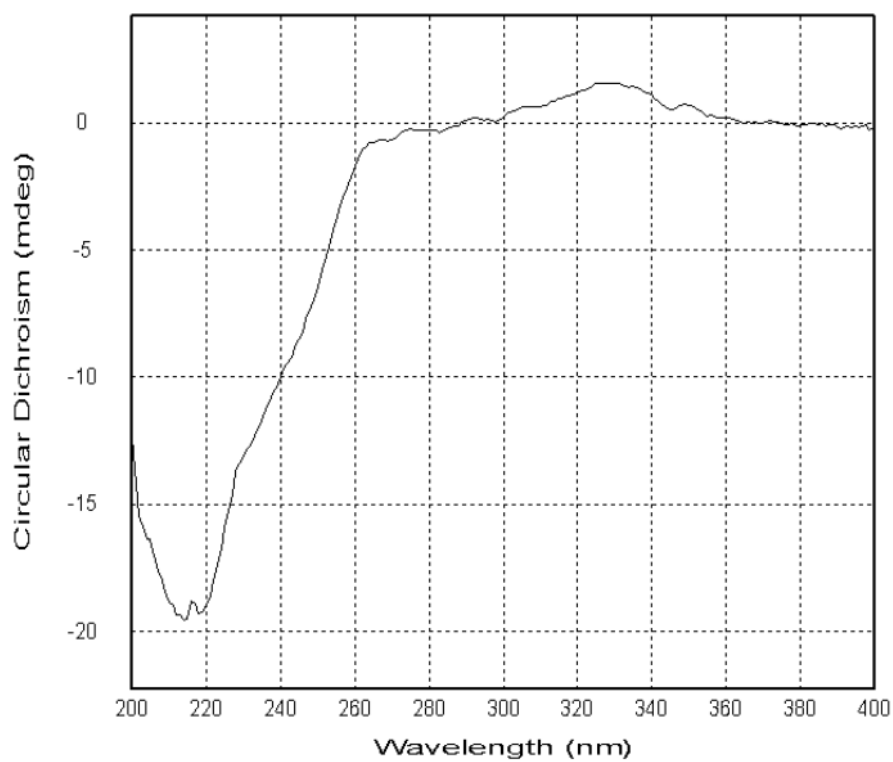
T: FTMS + p ESI Full.ms [100.0000-1500.0000]



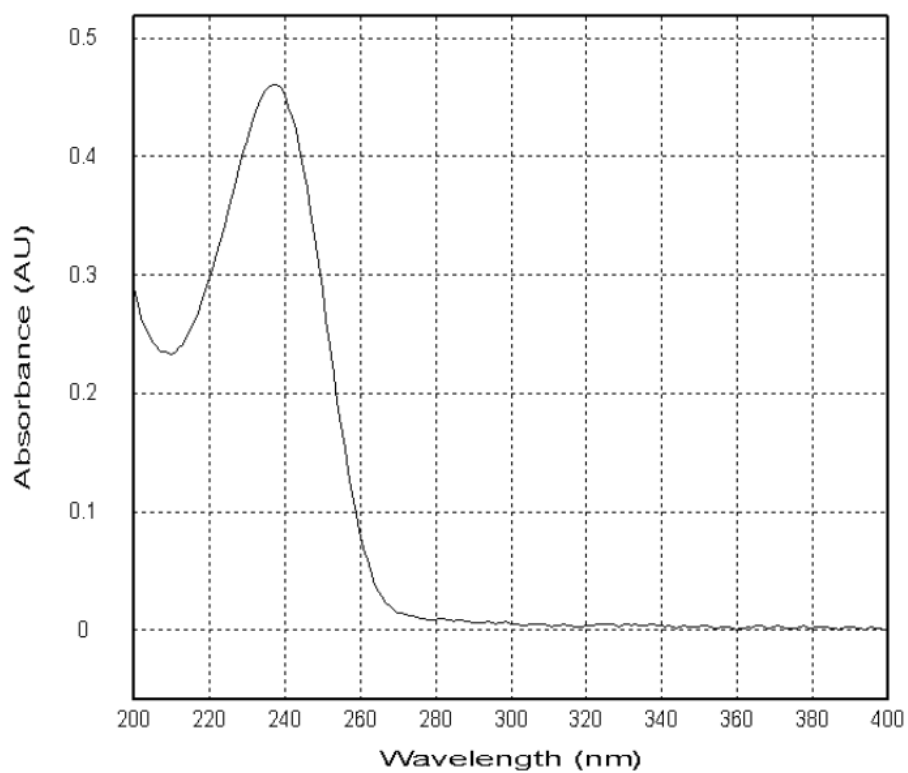
**Figure S47.** HRESIMS spectrum of compound **5**



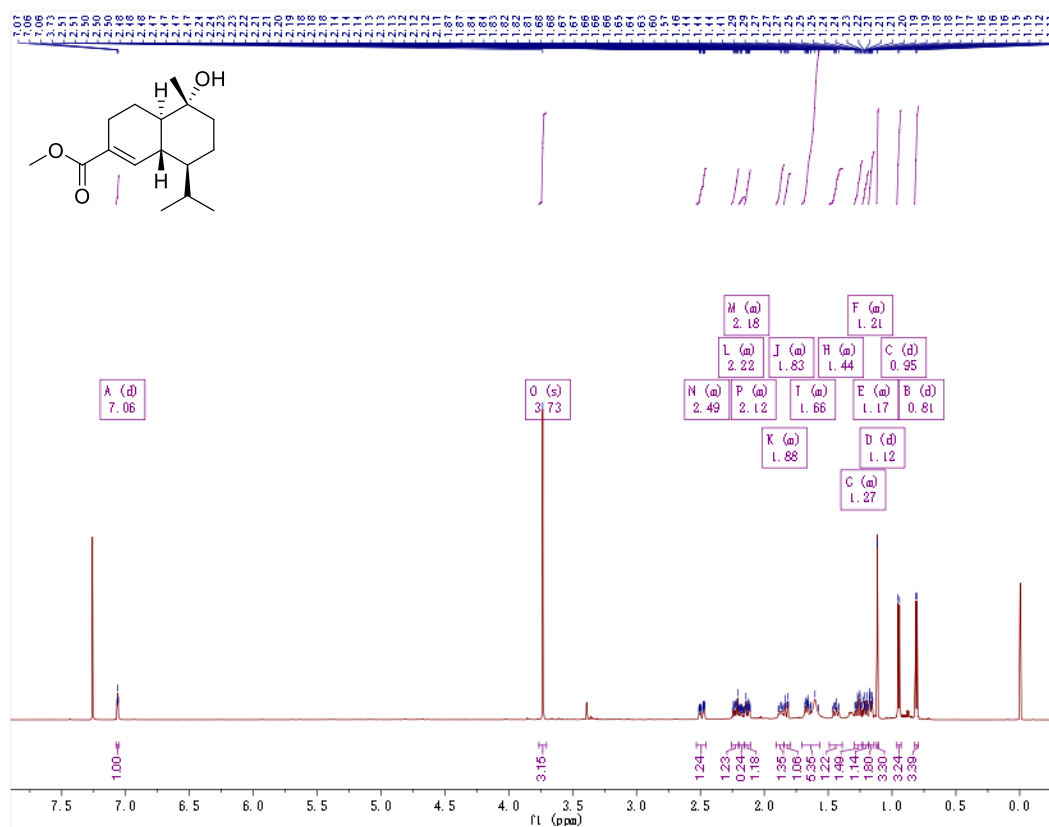
**Figure S48.** IR spectrum of compound **5**



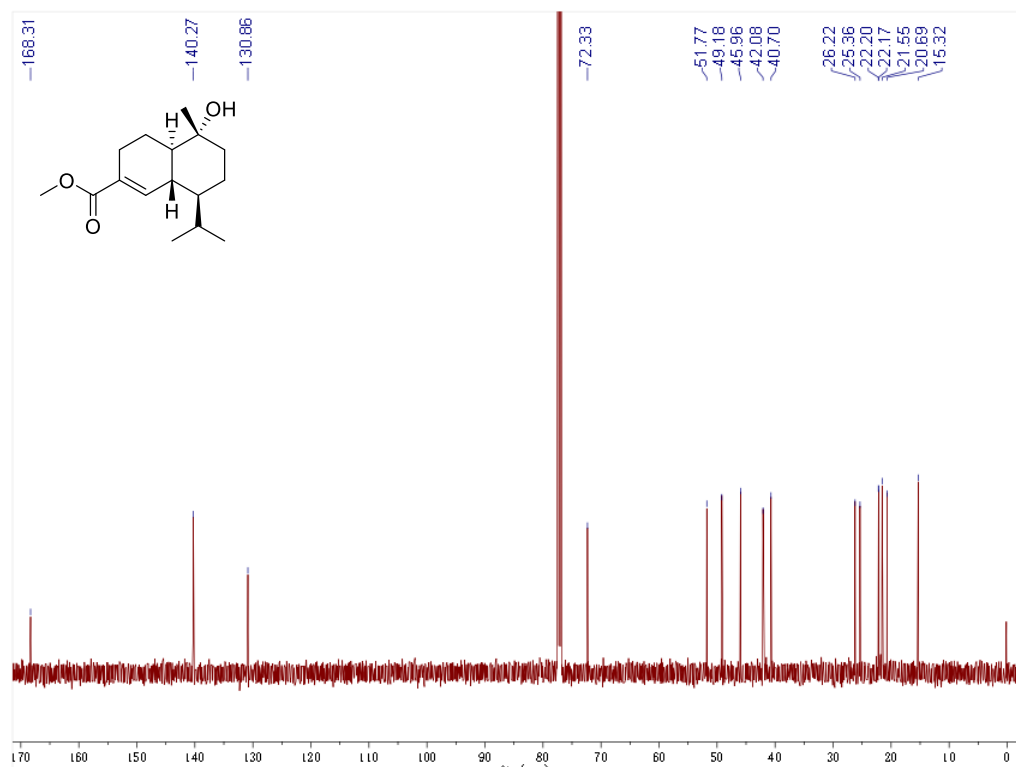
**Figure S49.** UV spectrum of compound **5**



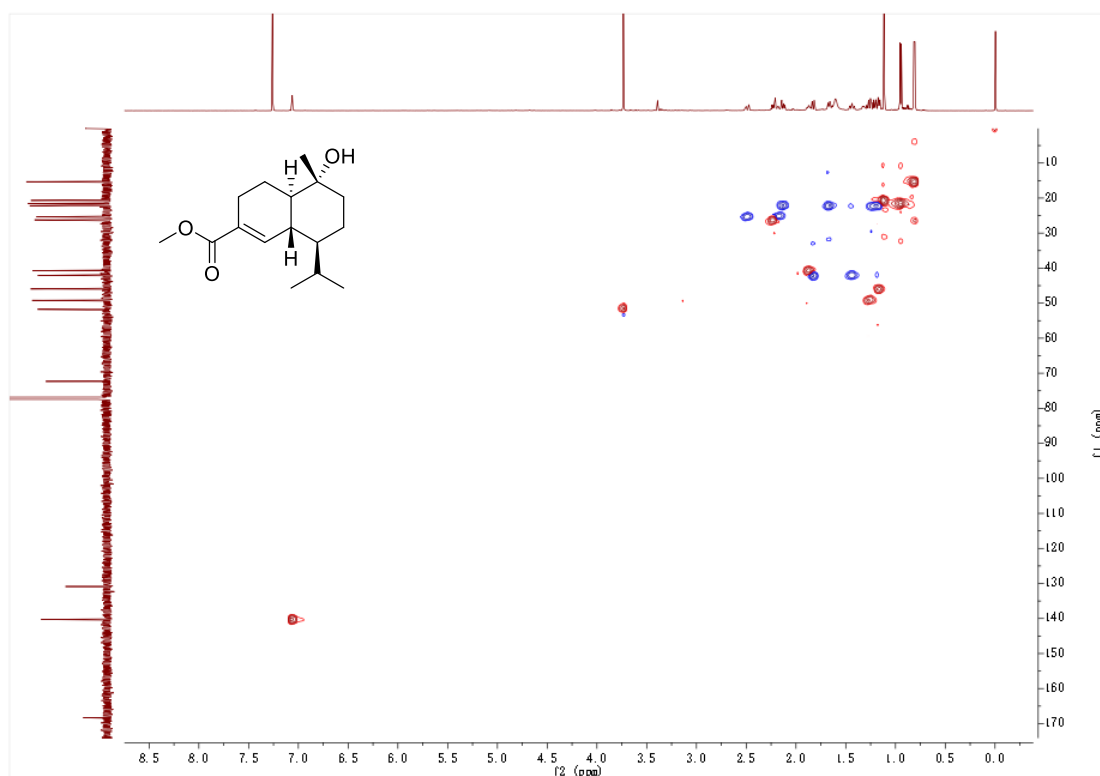
**Figure S50.** CD spectrum of compound **5**



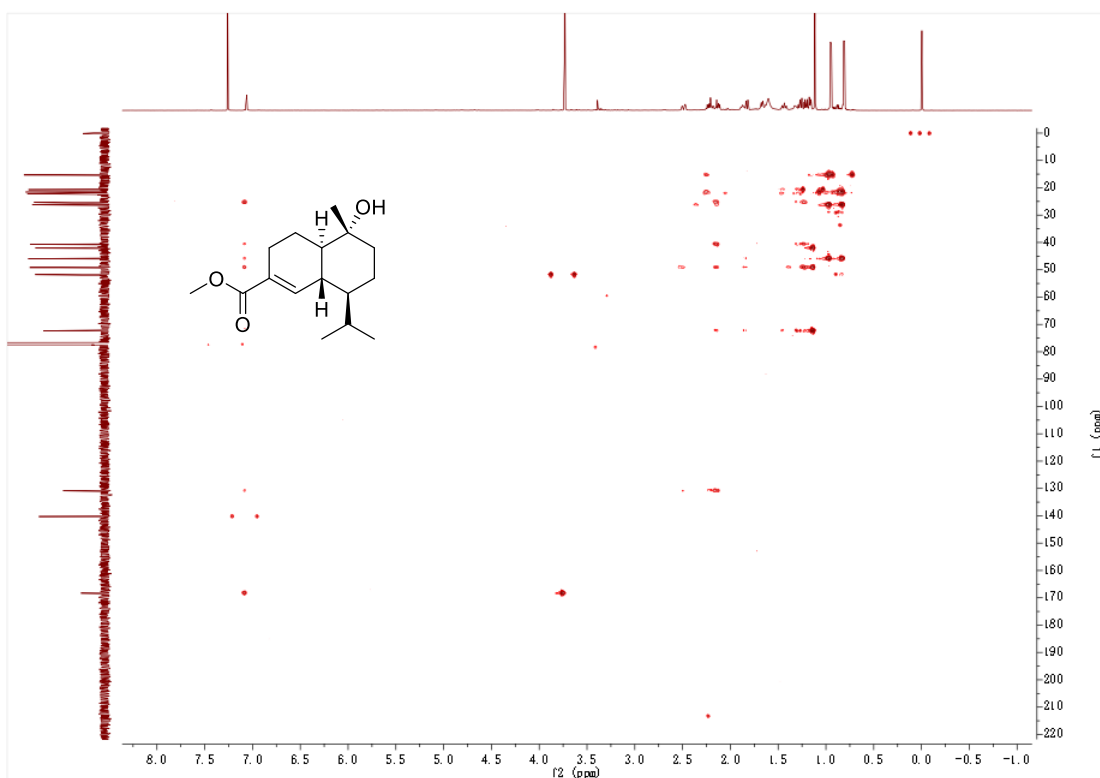
**Figure S51.**  $^1\text{H}$  NMR spectrum of compound **6** in  $\text{CDCl}_3$  (600 MHz)



**Figure S52.**  $^{13}\text{C}$  NMR spectrum of compound **6** in  $\text{CDCl}_3$  (150 MHz)

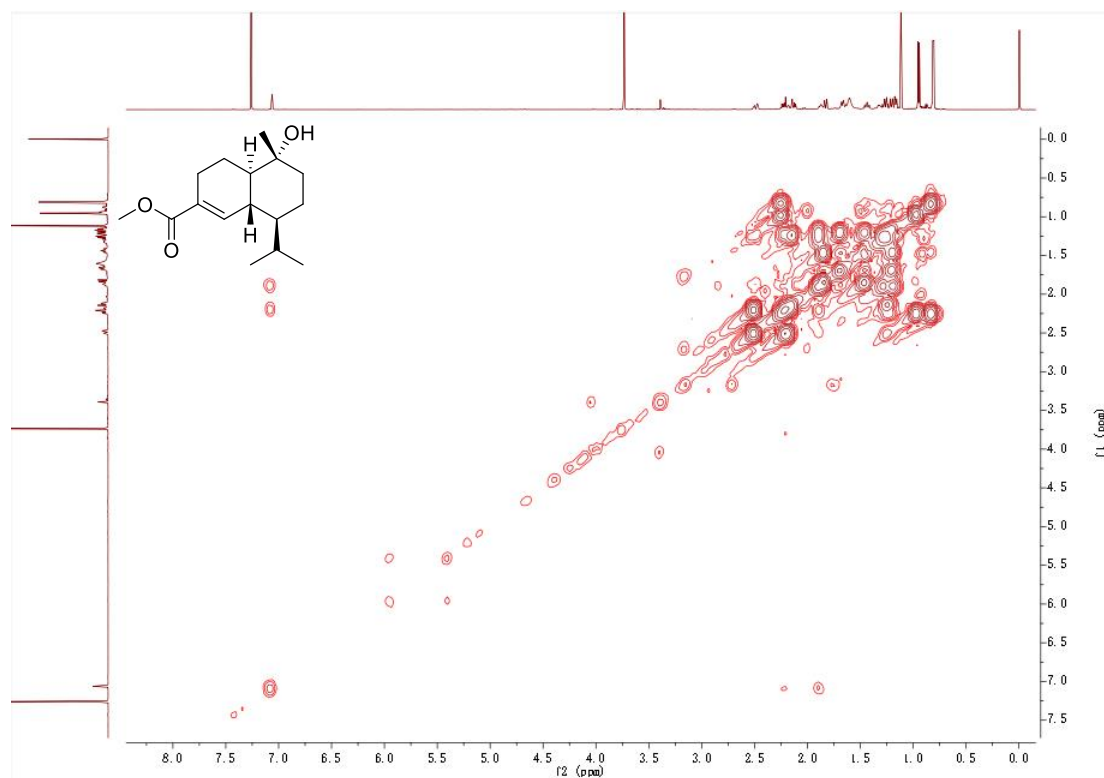


**Figure S53.** HSQC spectrum of compound **6** in CDCl<sub>3</sub>

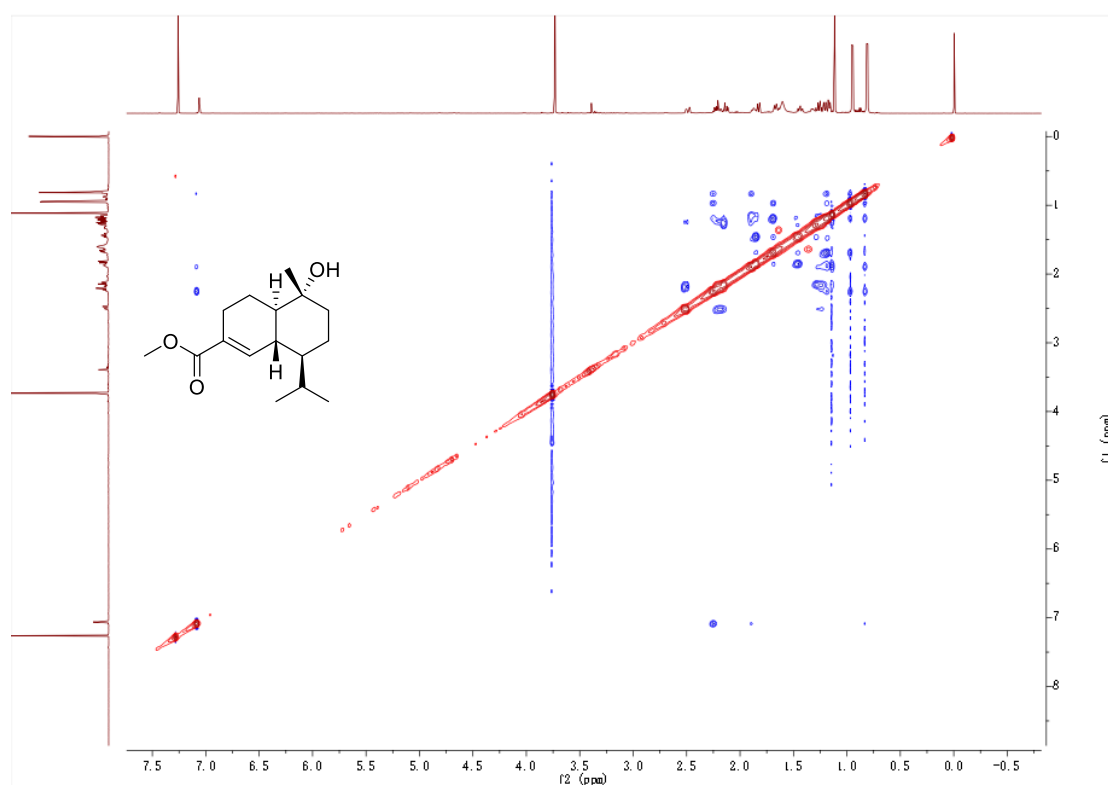


**Figure S54.** HMBC spectrum of compound **6** in CDCl<sub>3</sub>

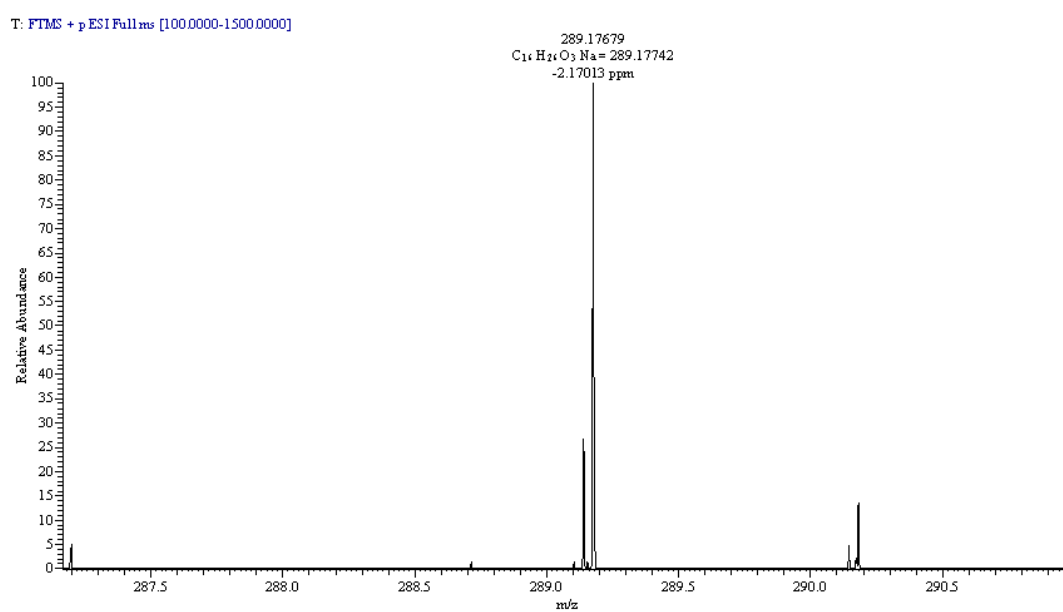
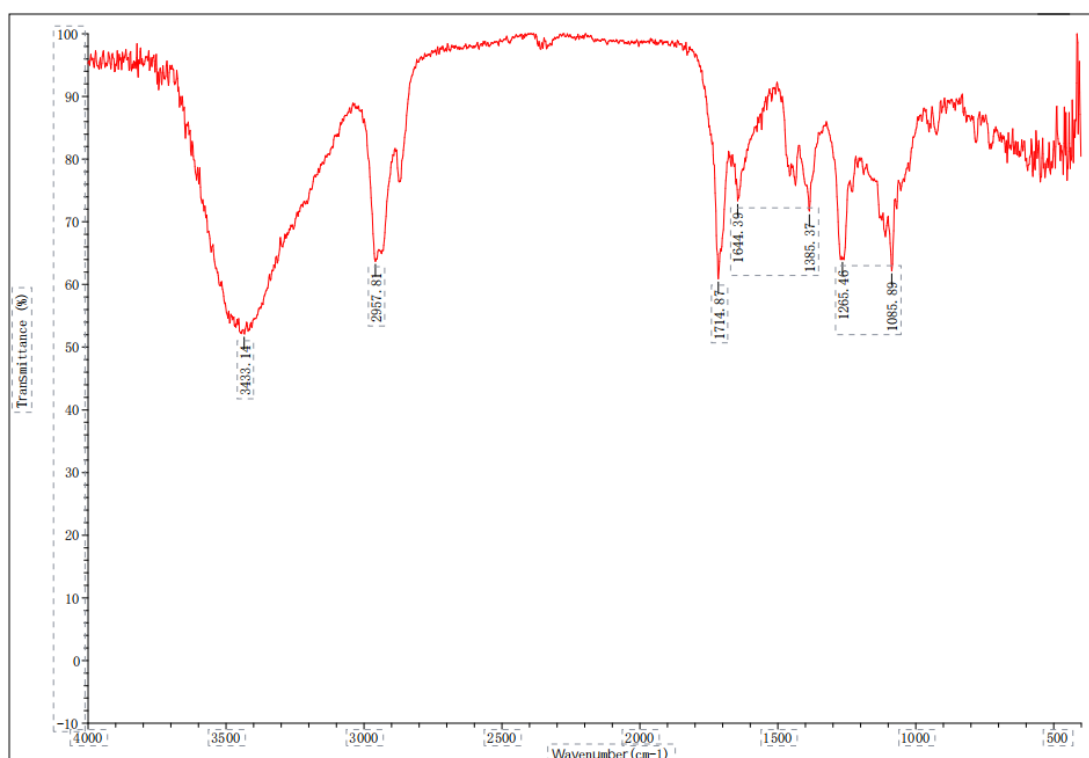


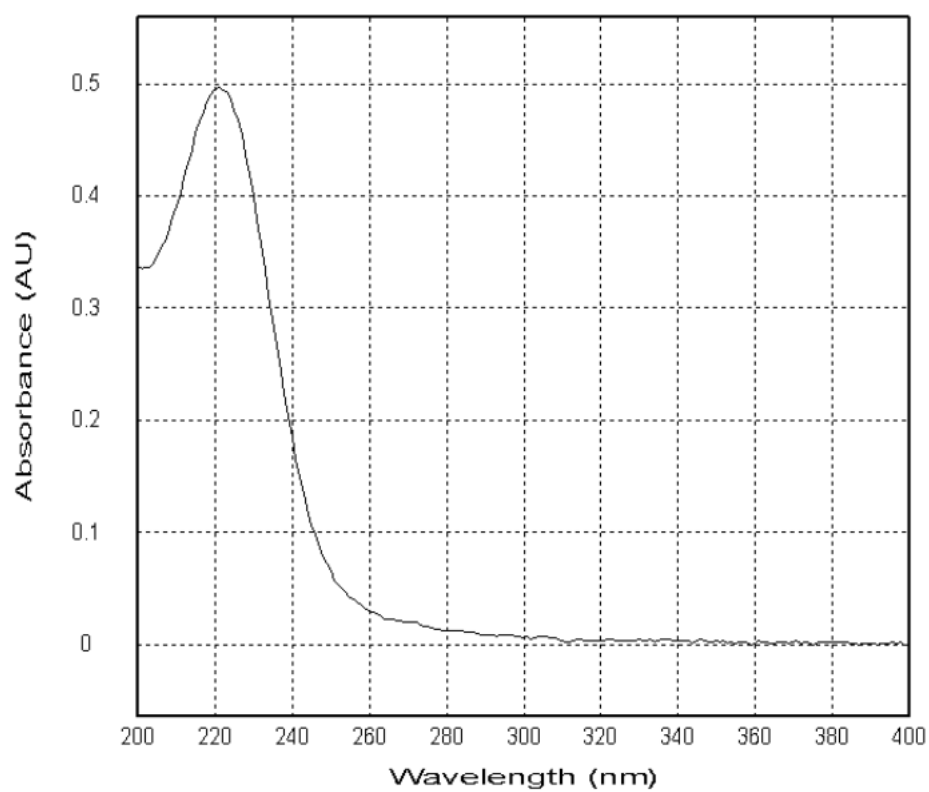


**Figure S55.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **6** in  $\text{CDCl}_3$

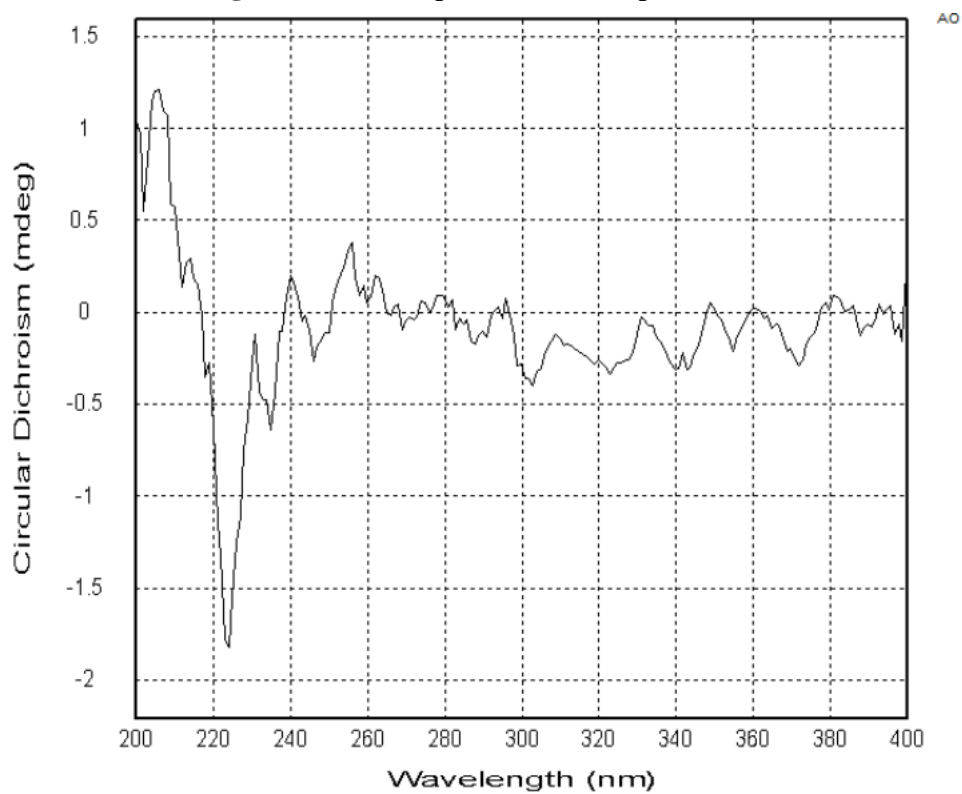


**Figure S56.** NOESY spectrum of compound **6** in  $\text{CDCl}_3$

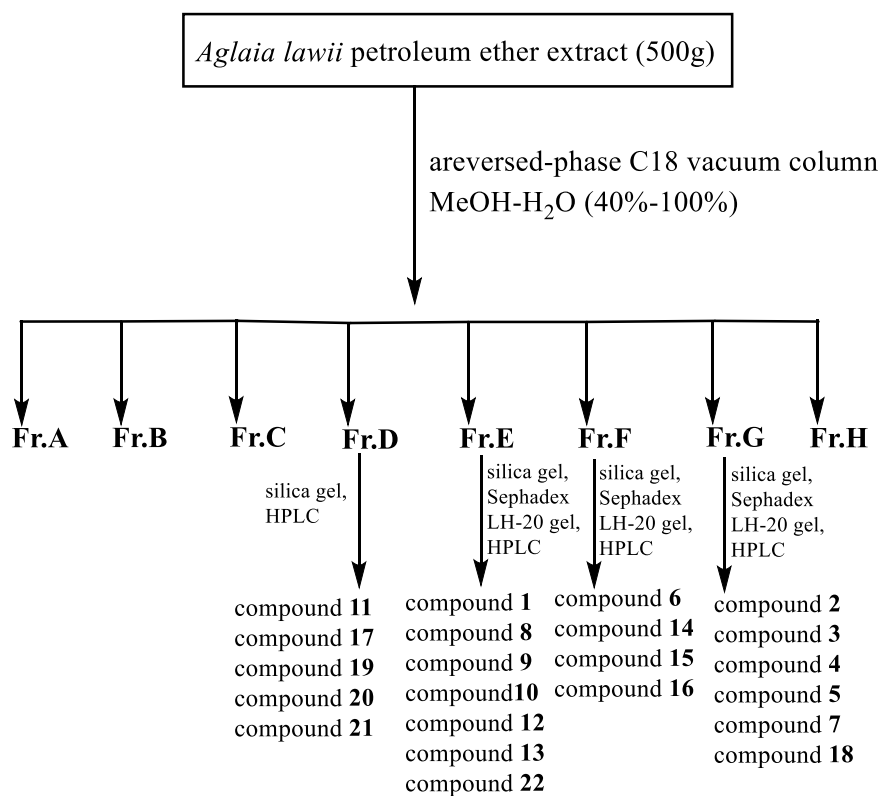




**Figure S59.** UV spectrum of compound **6**



**Figure S60.** CD spectrum of compound **6**



**Figure S61.** Compounds separation flowchart