

# Supplementary Information

## **Biflavonoids from *Selaginella doederleinii* as potential antitumor agents for intervention of non-small-cell lung cancer**

Fenghua Kang,<sup>1,2,3</sup> Sha Zhang,<sup>1,2,3</sup> Dekun Chen,<sup>1,2,3</sup> Jianbing Tan,<sup>1,2,3</sup> Min Kuang,<sup>1,2,3</sup>  
Jinlin Zhang,<sup>1,2,3</sup> Guangyuan Zeng,<sup>1,2,3</sup> Kangping Xu,<sup>1,2,3</sup> Zhenxing Zou<sup>1,2,3\*</sup> and  
Guishan Tan<sup>1,2,3\*</sup>

<sup>1</sup> *Xiangya School of Pharmaceutical Sciences, Central South University, Changsha 410013, PR China.*

<sup>2</sup> *Xiangya Hospital of Central South University, Changsha 410008, PR China.*

<sup>3</sup> *Hunan Key laboratory of Diagnostic and Therapeutic Drug Research for Chronic Diseases, Central South University, Changsha, 410013, Hunan, China.*

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**7-O-methyldelicaflavone (3)**

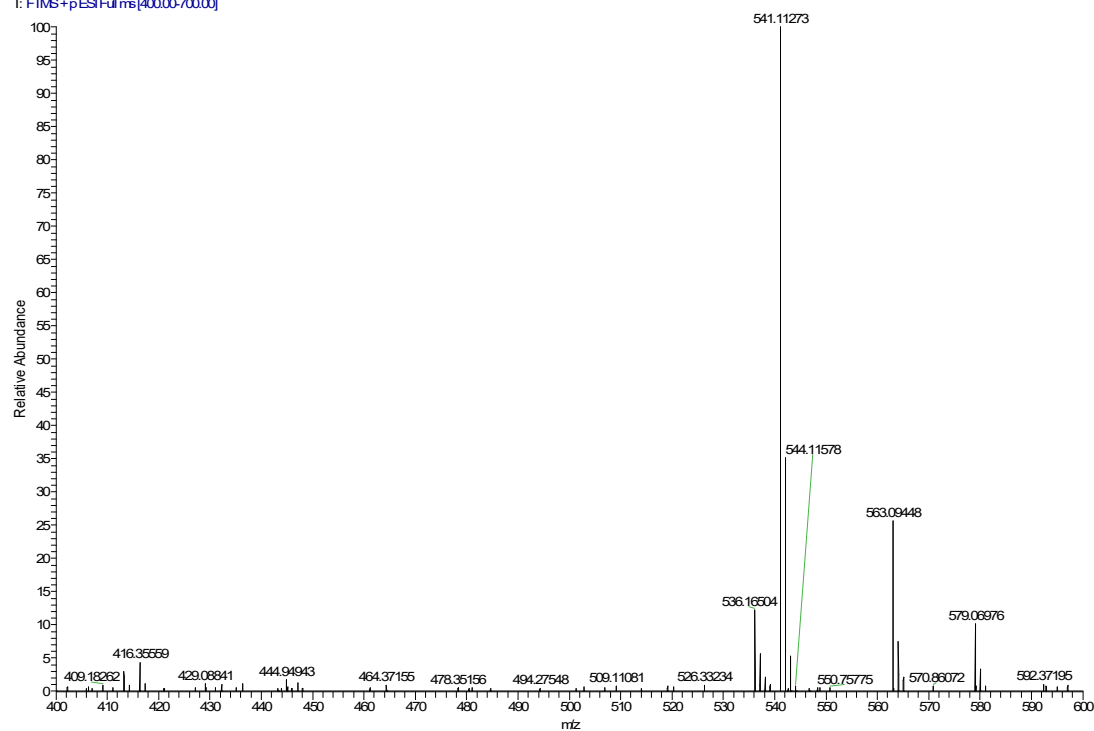
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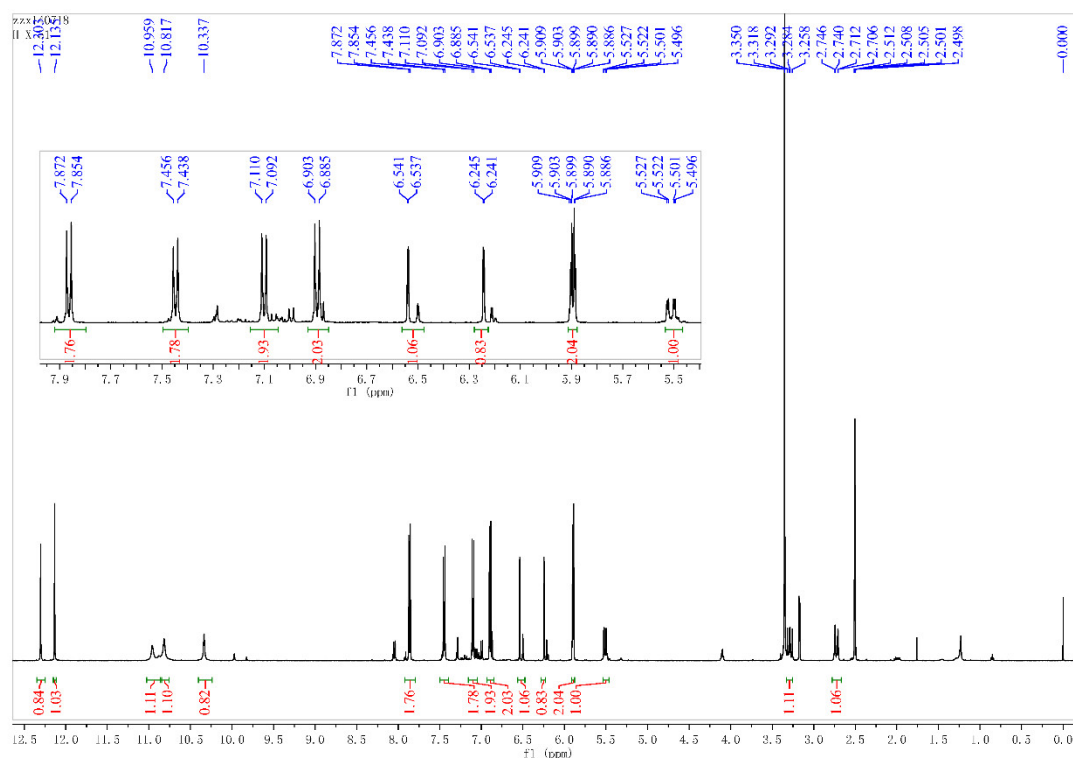
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x51#82 RT: 0.61 AV: 1 NL: 1.19E6  
T: FIMS+pESI Full ms [400.00-700.00]

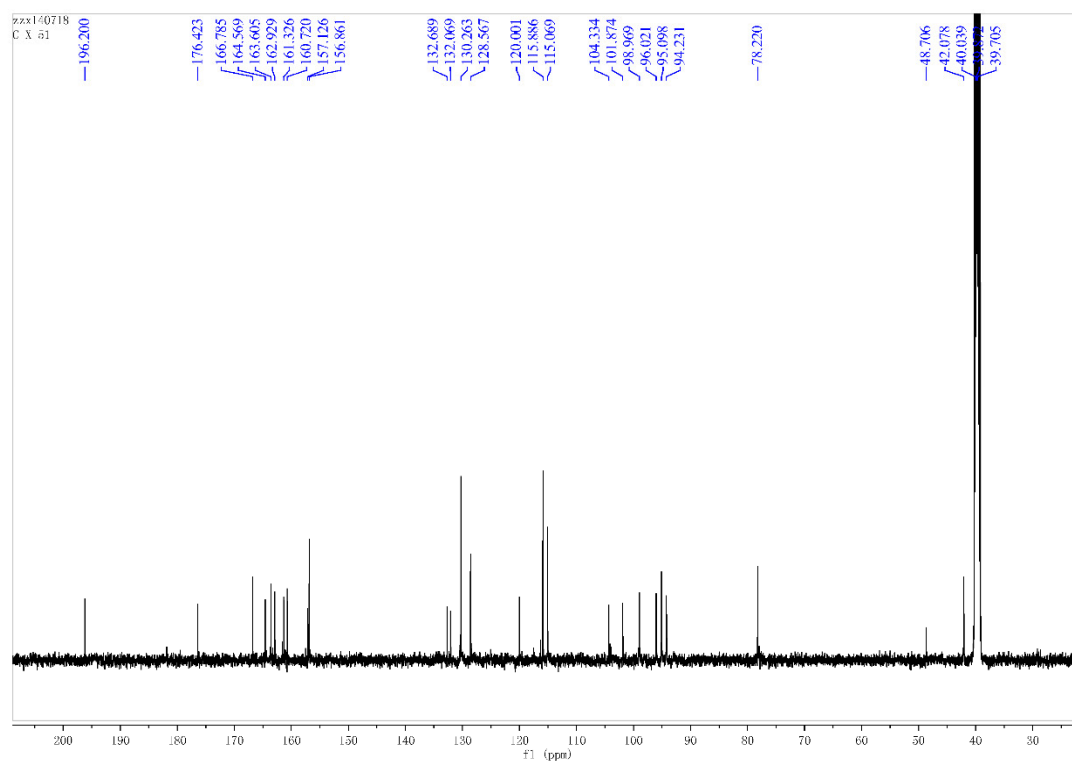


m/z Theo.	Mass	Delta (mmu)	RDB equiv.	Composition
541.11273	541.11292	-0.19	20.5	C <sub>30</sub> H <sub>21</sub> O <sub>10</sub>

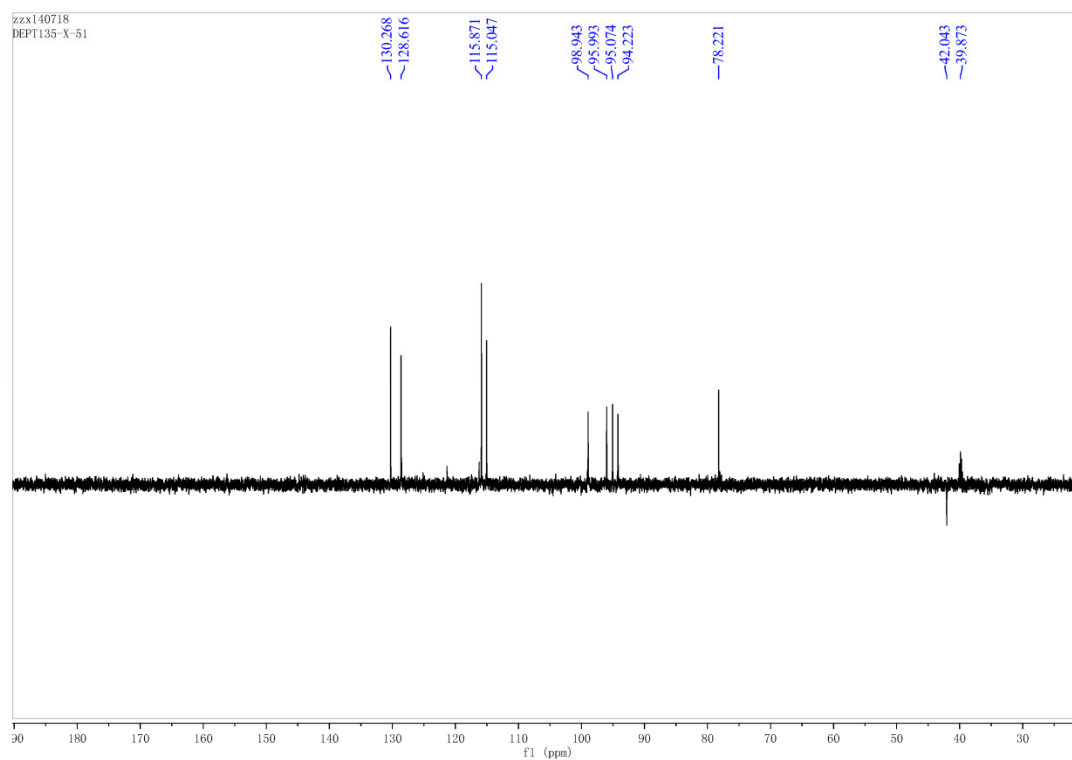
Figure S1. HRESIMS spectrum of 1



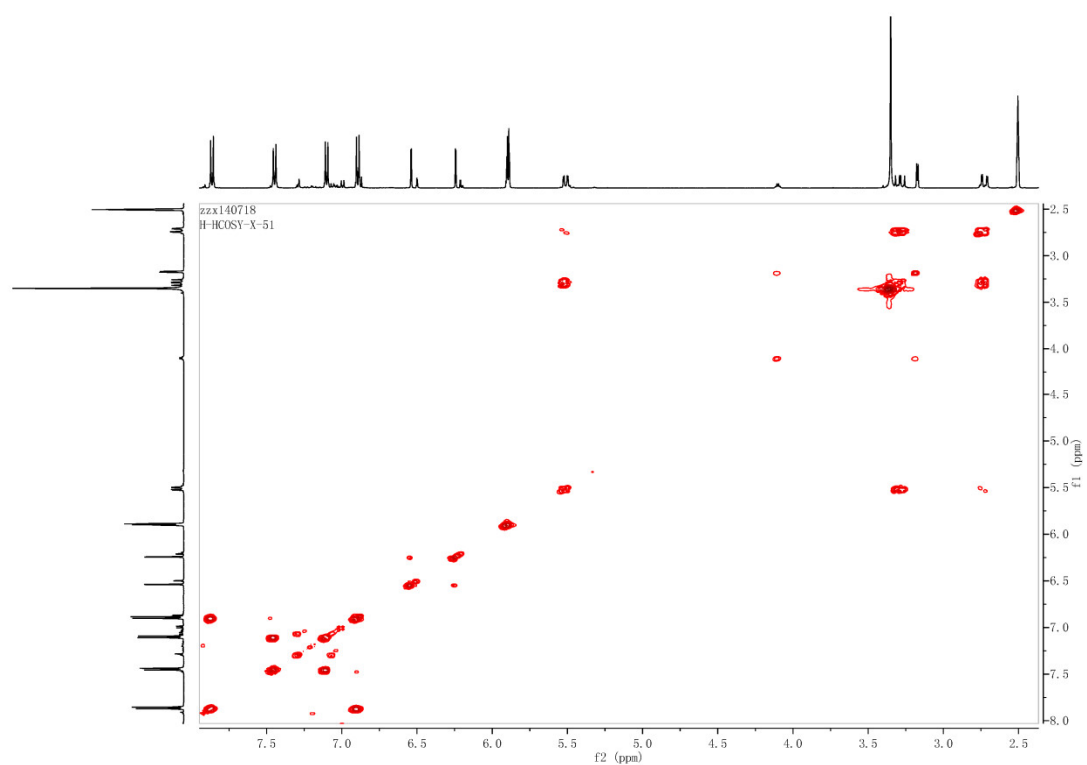
**Figure S2.**  $^1\text{H}$  NMR spectrum (500 MHz) of **1** in  $\text{DMSO-}d_6$



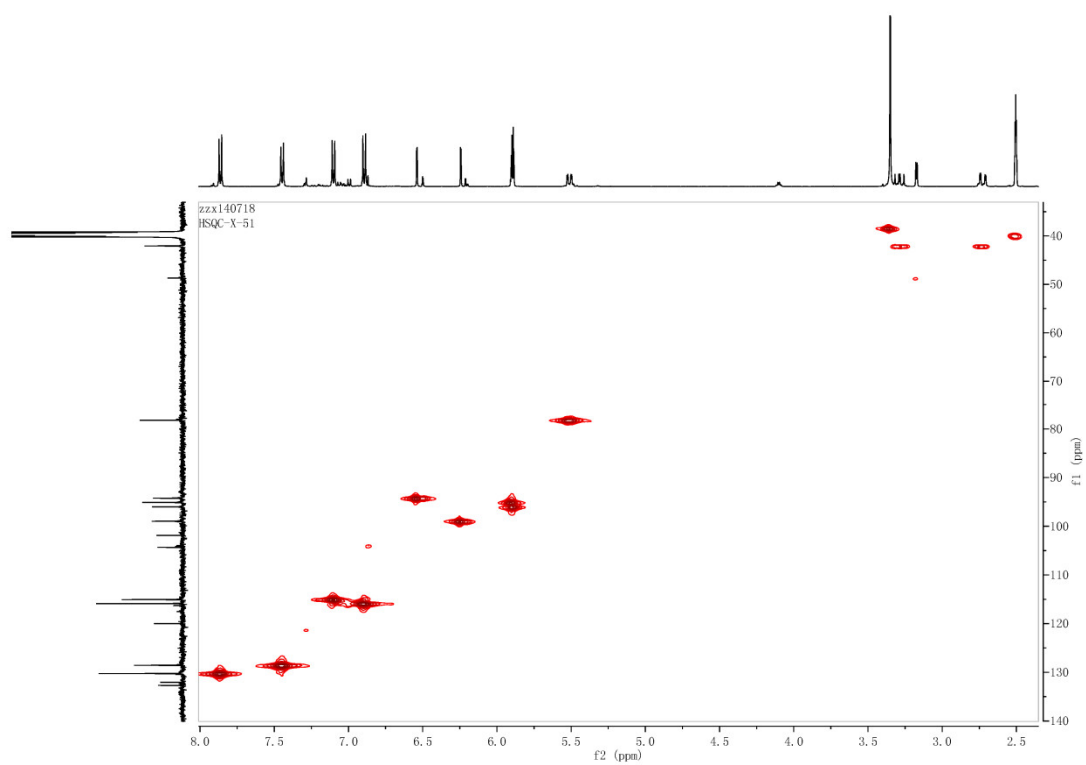
**Figure S3.**  $^{13}\text{C}$  NMR spectrum (125 MHz) of **1** in  $\text{DMSO-}d_6$



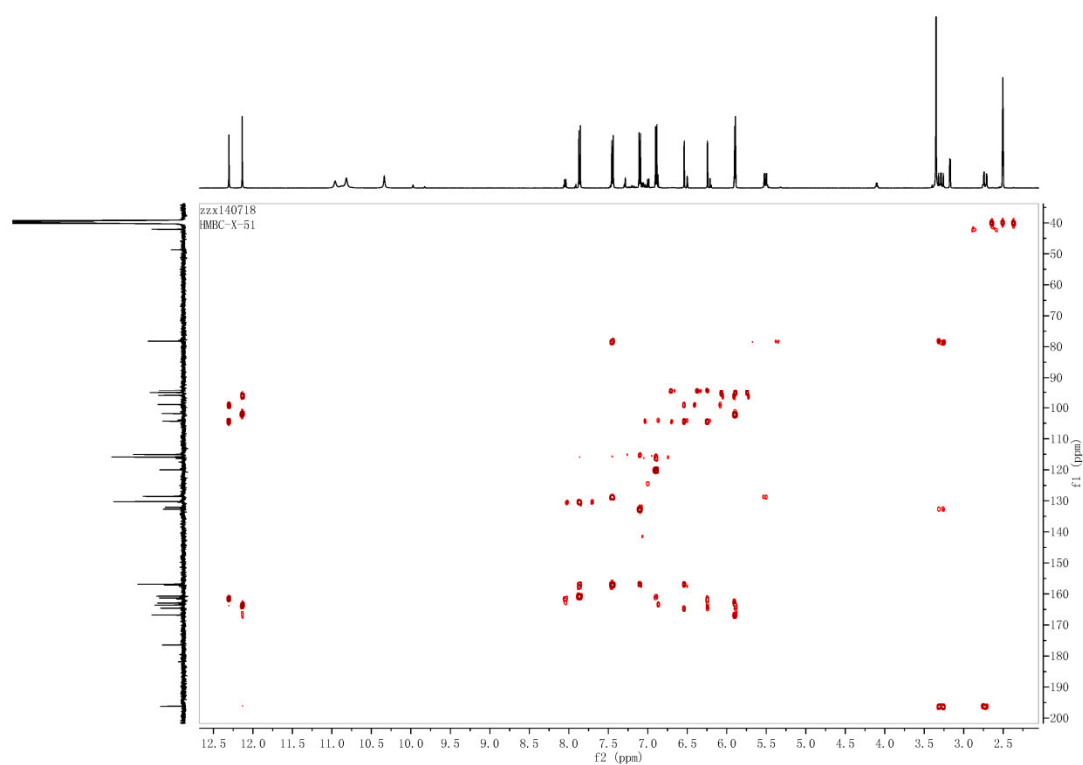
**Figure S4.** DEPT 135 spectrum (125 MHz) of **1** in  $\text{DMSO-}d_6$



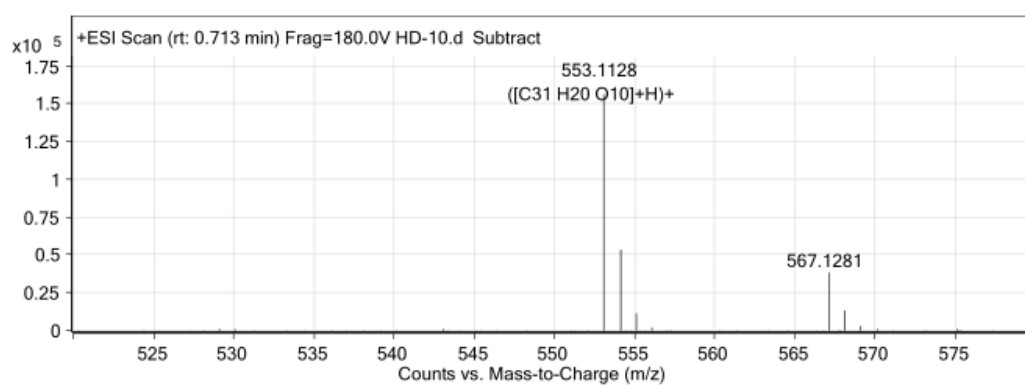
**Figure S5.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{DMSO-}d_6$



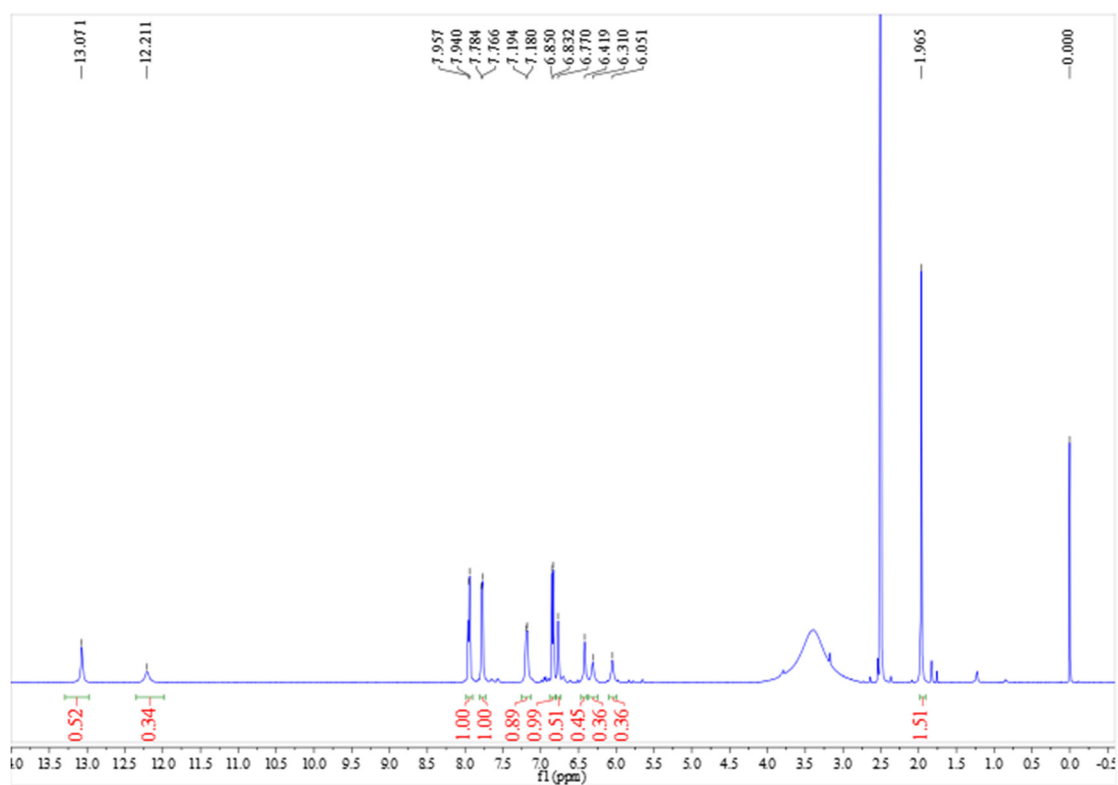
**Figure S6.** HSQC spectrum of **1** in  $\text{DMSO-}d_6$



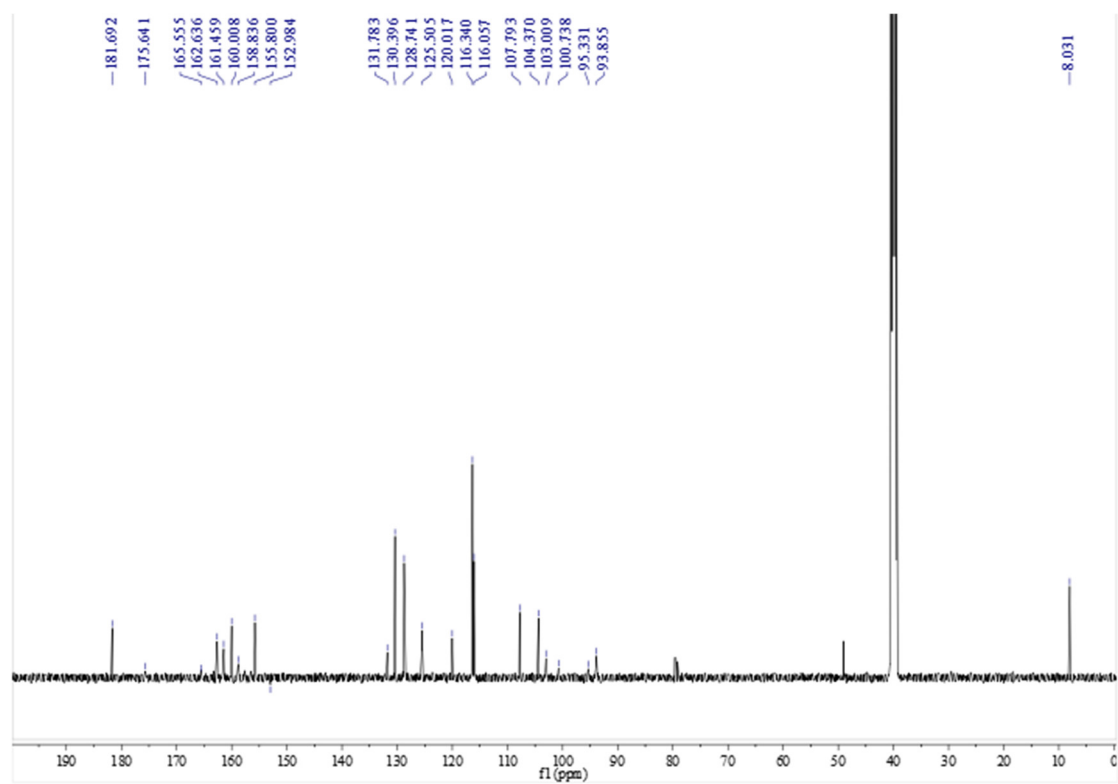
**Figure S7.** HMBC spectrum of **1** in DMSO-*d*<sub>6</sub>



**Figure S8.** HRESIMS spectrum of **2**

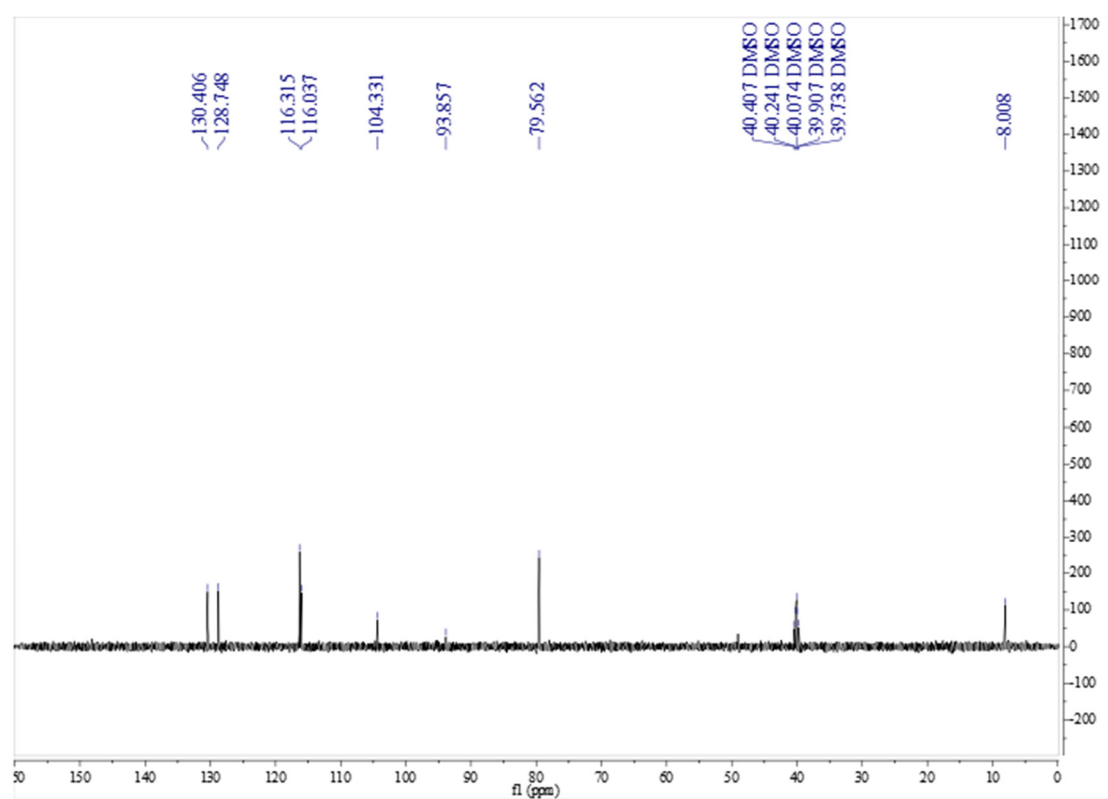


**Figure S9.** <sup>1</sup>H NMR spectrum (500 MHz) of **2** in DMSO-*d*<sub>6</sub>

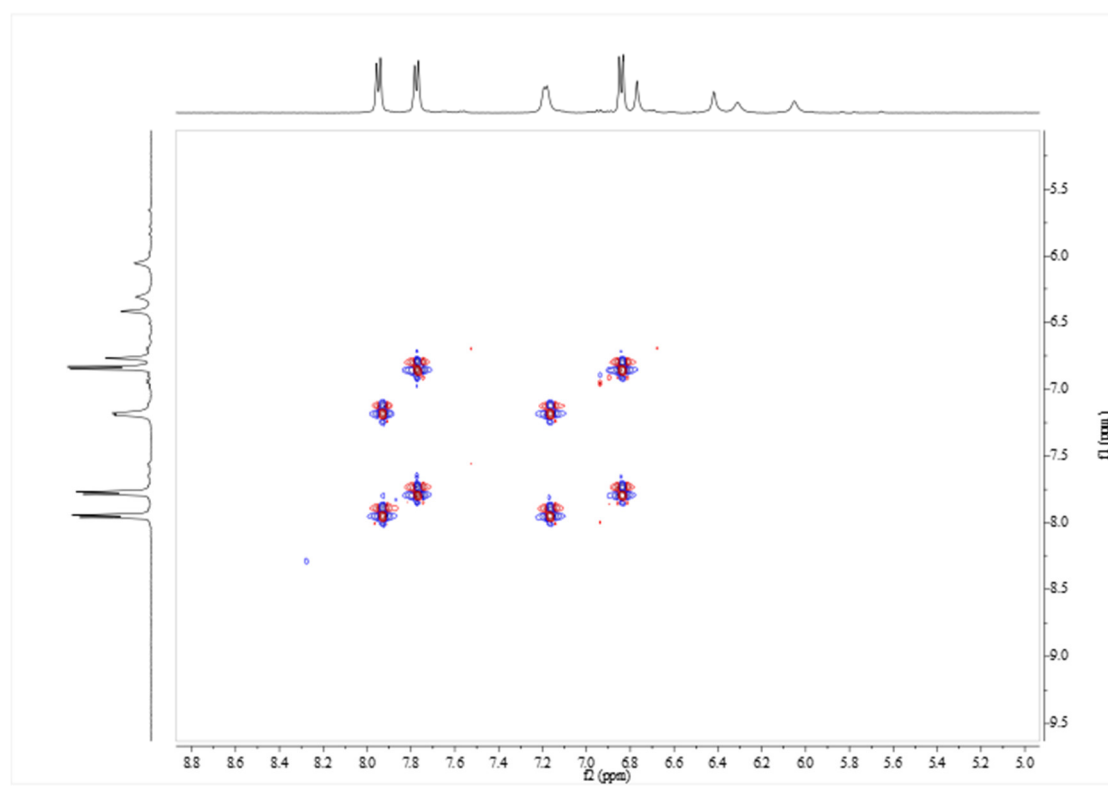


**Figure S10.** <sup>13</sup>C NMR spectrum (125 MHz) of **2** in DMSO-*d*<sub>6</sub>

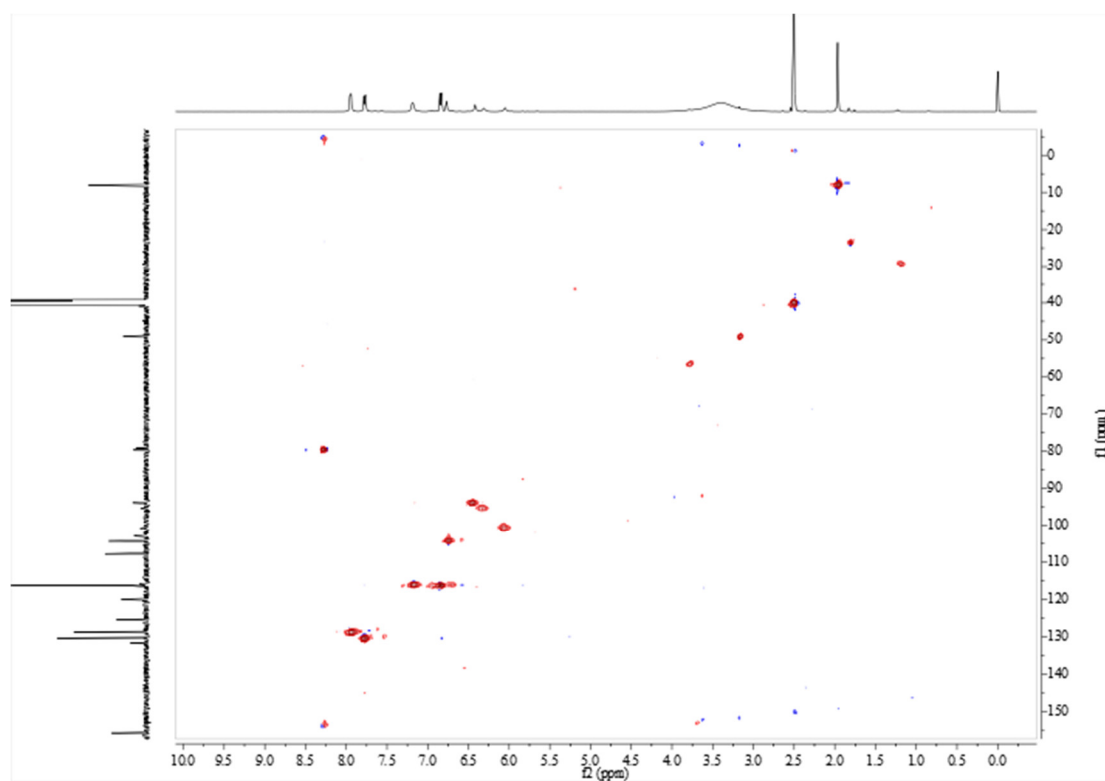




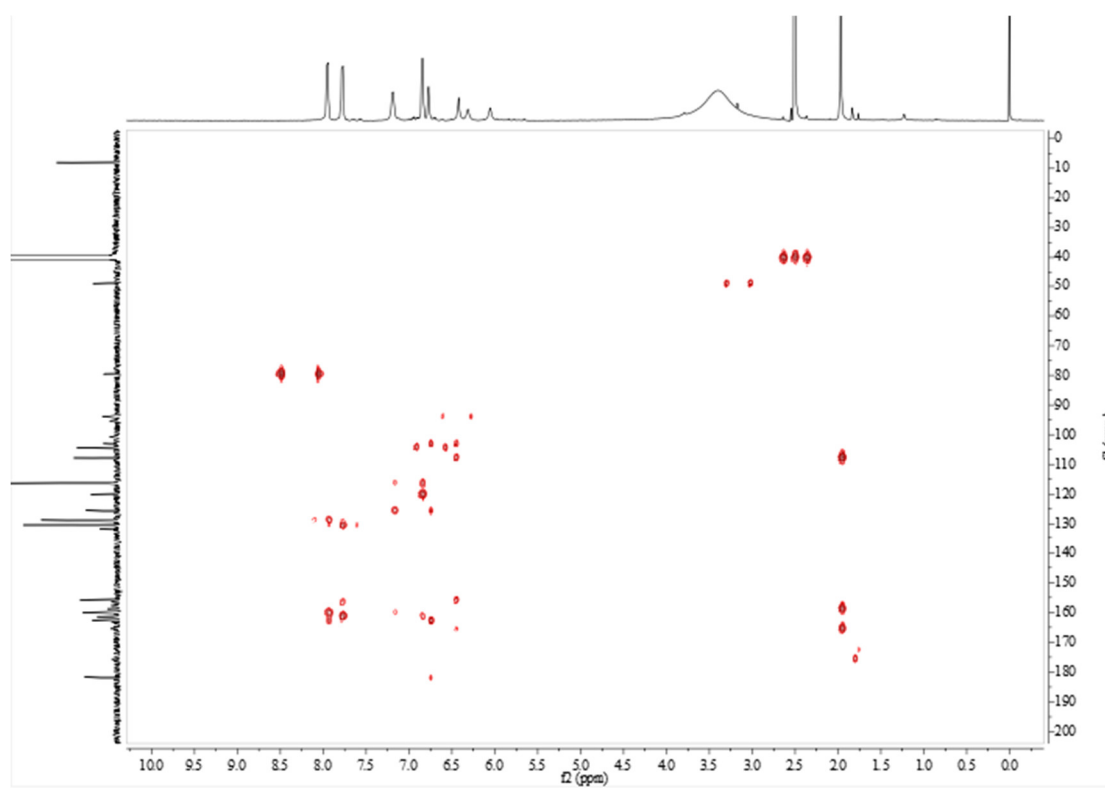
**Figure S11.** DEPT 135 spectrum (125 MHz) of **2** in DMSO-*d*<sub>6</sub>



**Figure S12.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **2** in DMSO-*d*<sub>6</sub>



**Figure S13.** HSQC spectrum of **2** in DMSO-*d*<sub>6</sub>



**Figure S14.** HMBC spectrum of **2** in DMSO-*d*<sub>6</sub>

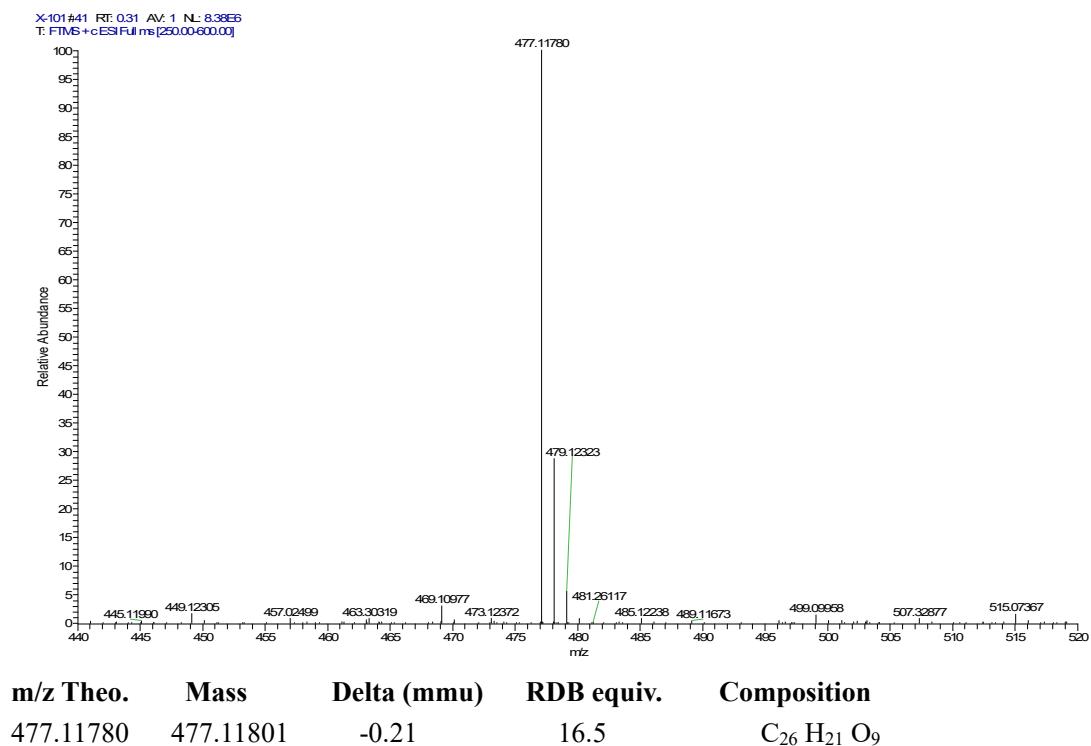


Figure S15. HRESIMS spectrum of **3**

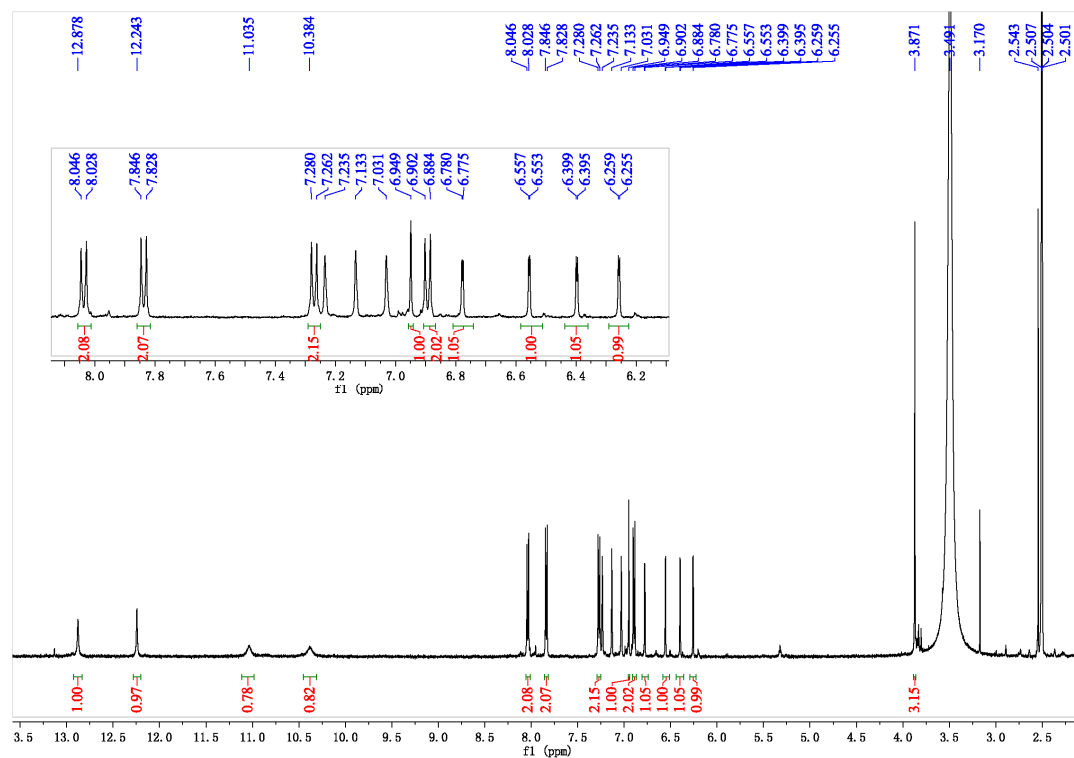


Figure S16. <sup>1</sup>H NMR spectrum (500 MHz) of **3** in DMSO-*d*<sub>6</sub>

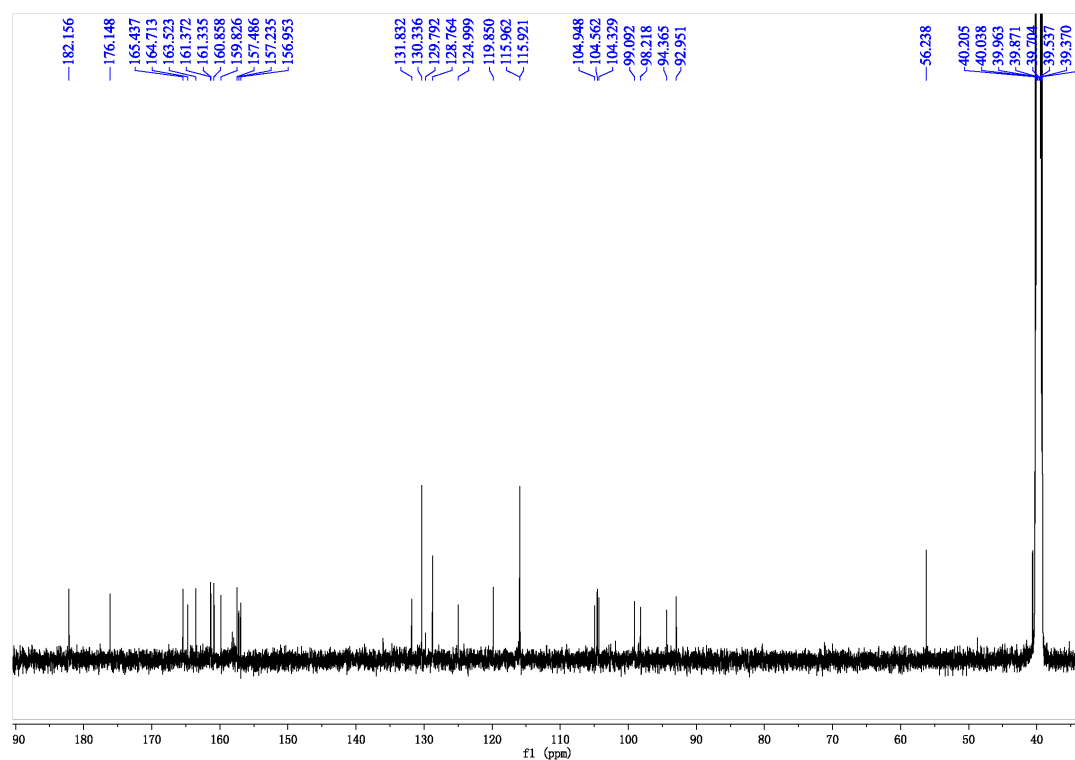


Figure S17.  $^{13}\text{C}$  NMR spectrum (125 MHz) of **3** in  $\text{DMSO-}d_6$

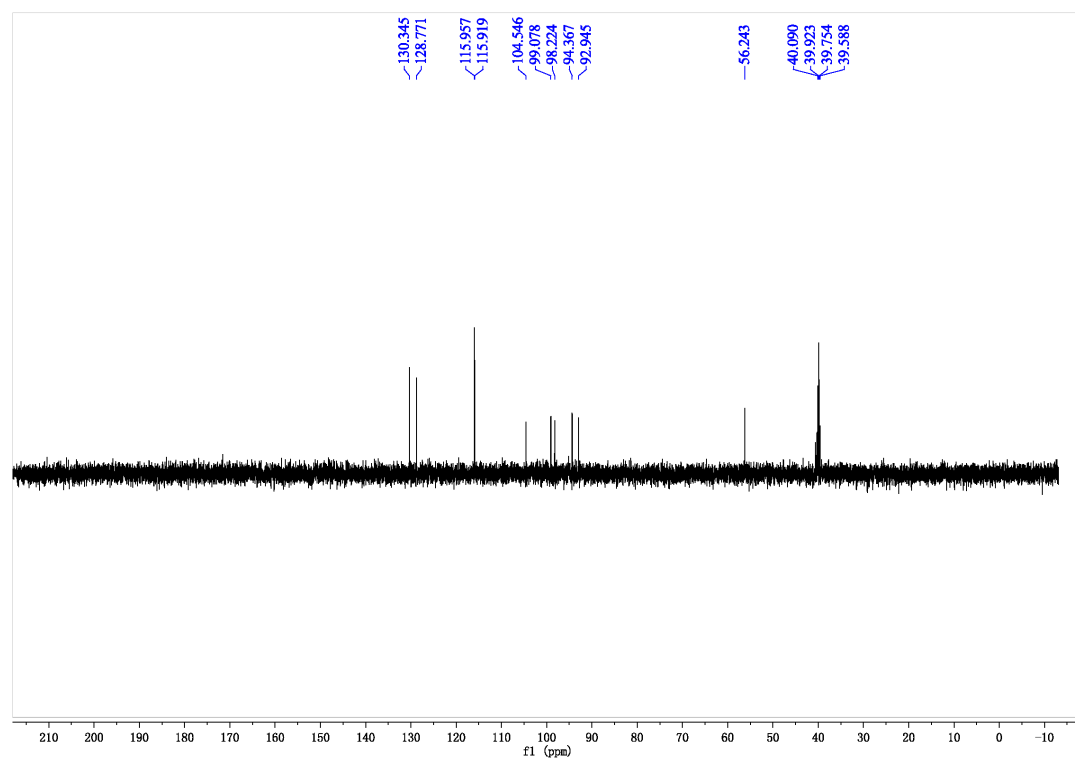
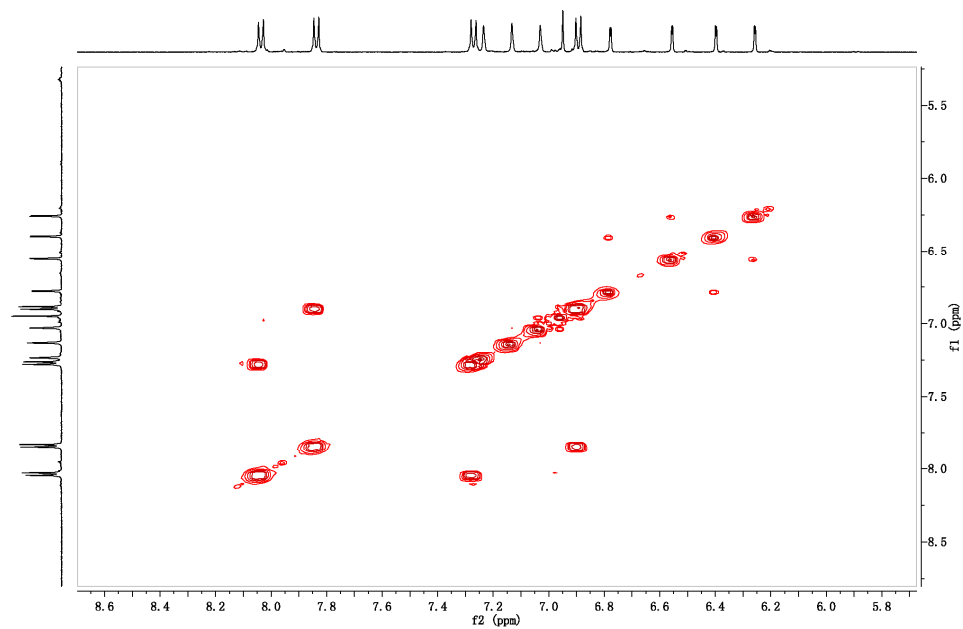
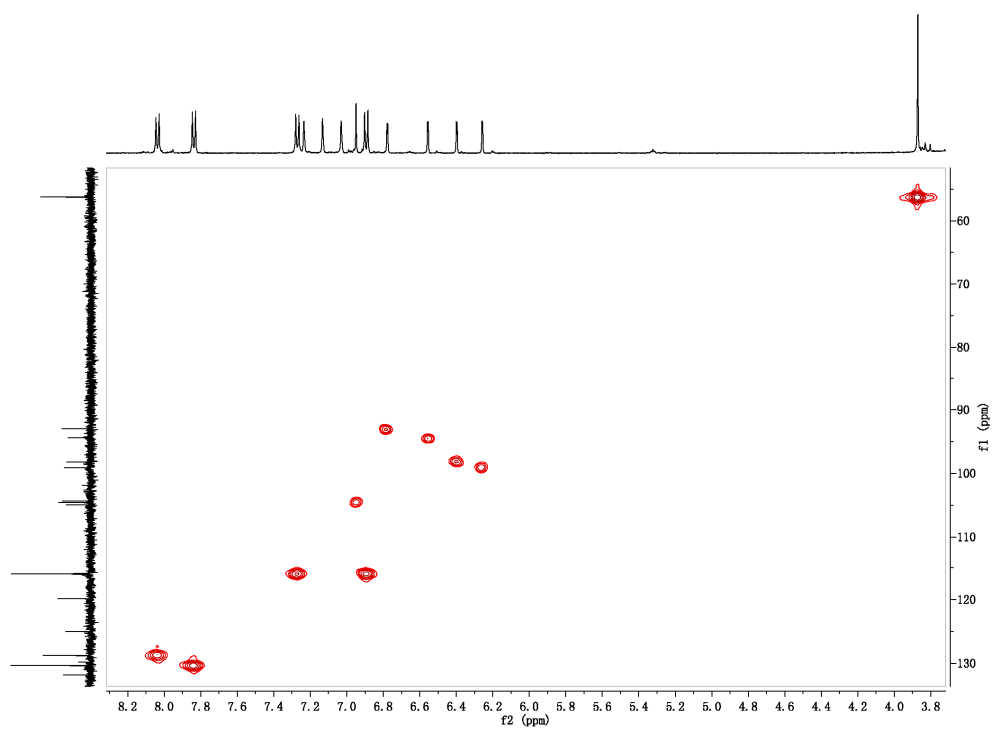


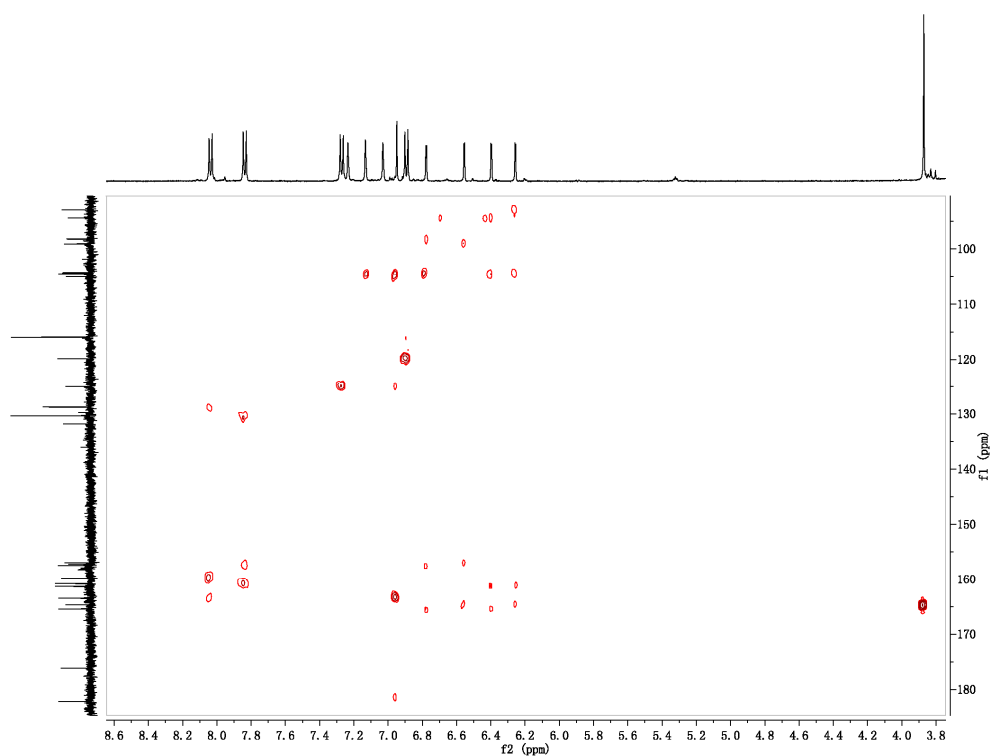
Figure S18. DEPT 135 spectrum (125 MHz) of **3** in  $\text{DMSO-}d_6$



**Figure S19.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{DMSO-}d_6$

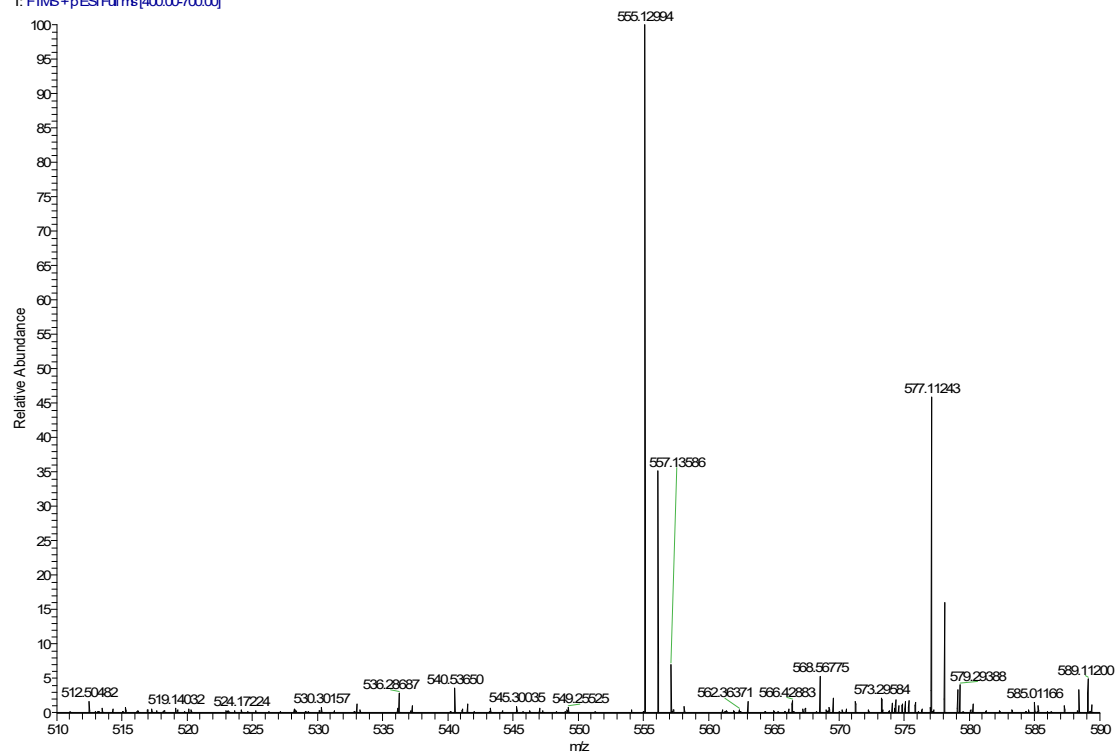


**Figure S20.** HSQC spectrum of **3** in  $\text{DMSO-}d_6$



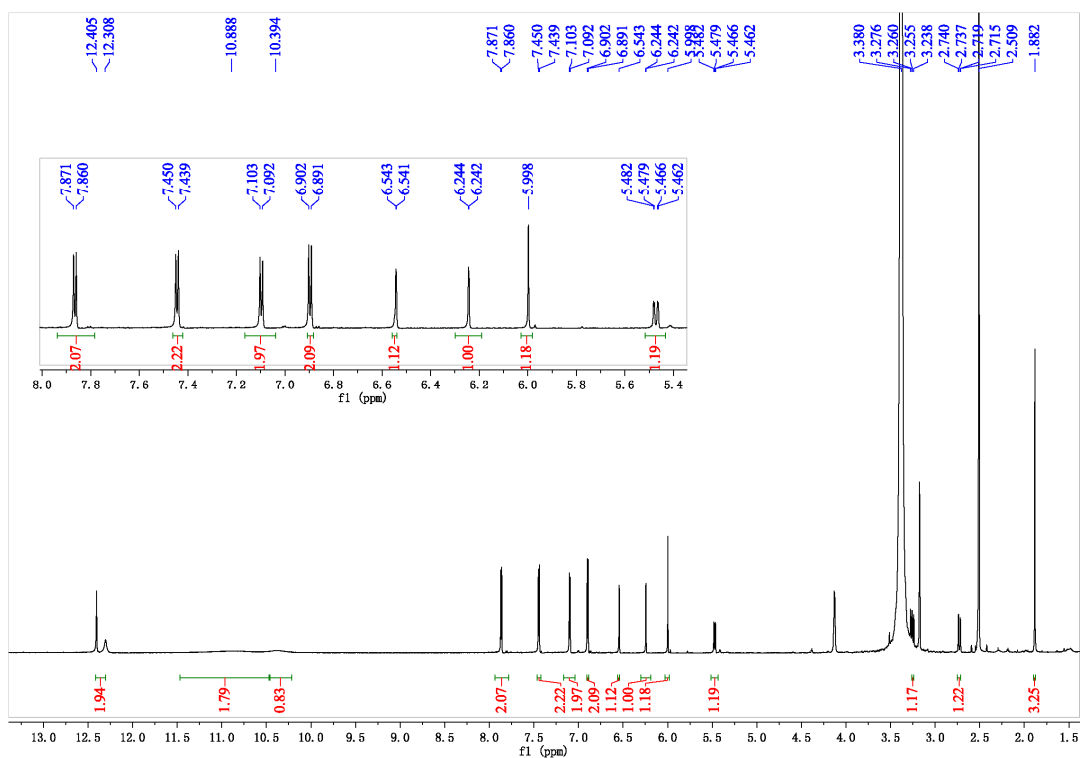
**Figure S21.** HMBC spectrum of **3** in DMSO-*d*<sub>6</sub>

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T: FTMS+pESI Full ms[400.00-700.00]

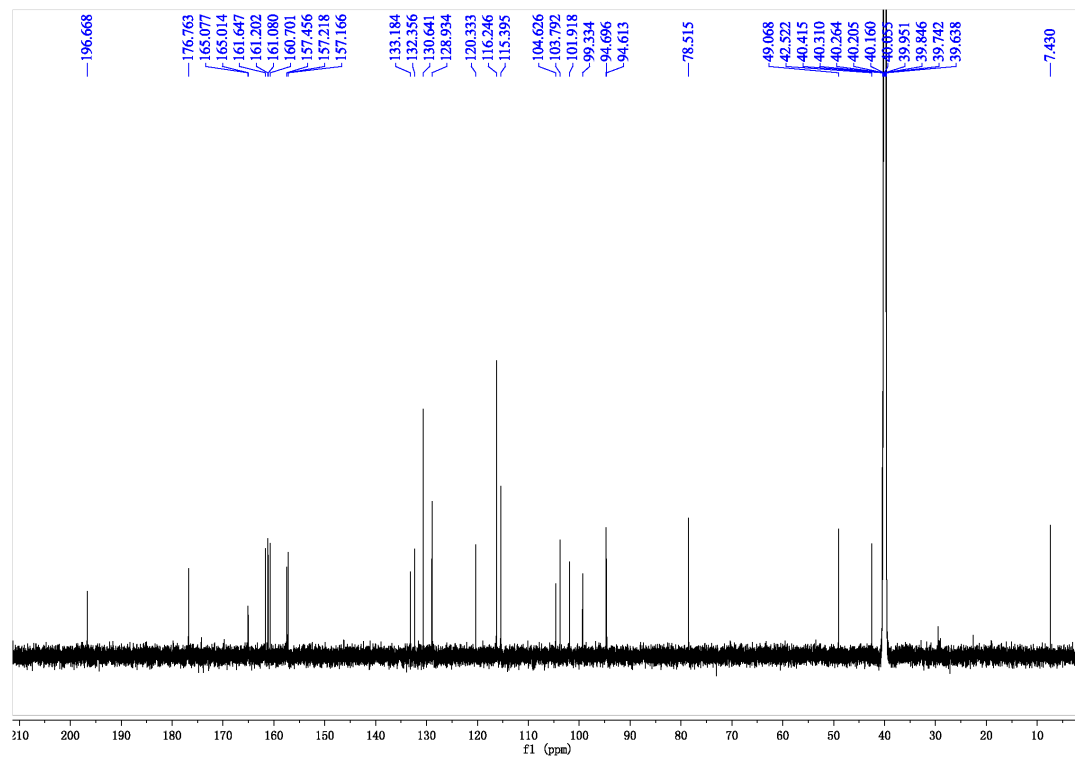


m/z Theo.	Mass	Delta (mmu)	RDB equiv.	Composition
555.12994	555.12857	1.37	20.5	C <sub>31</sub> H <sub>23</sub> O <sub>10</sub>

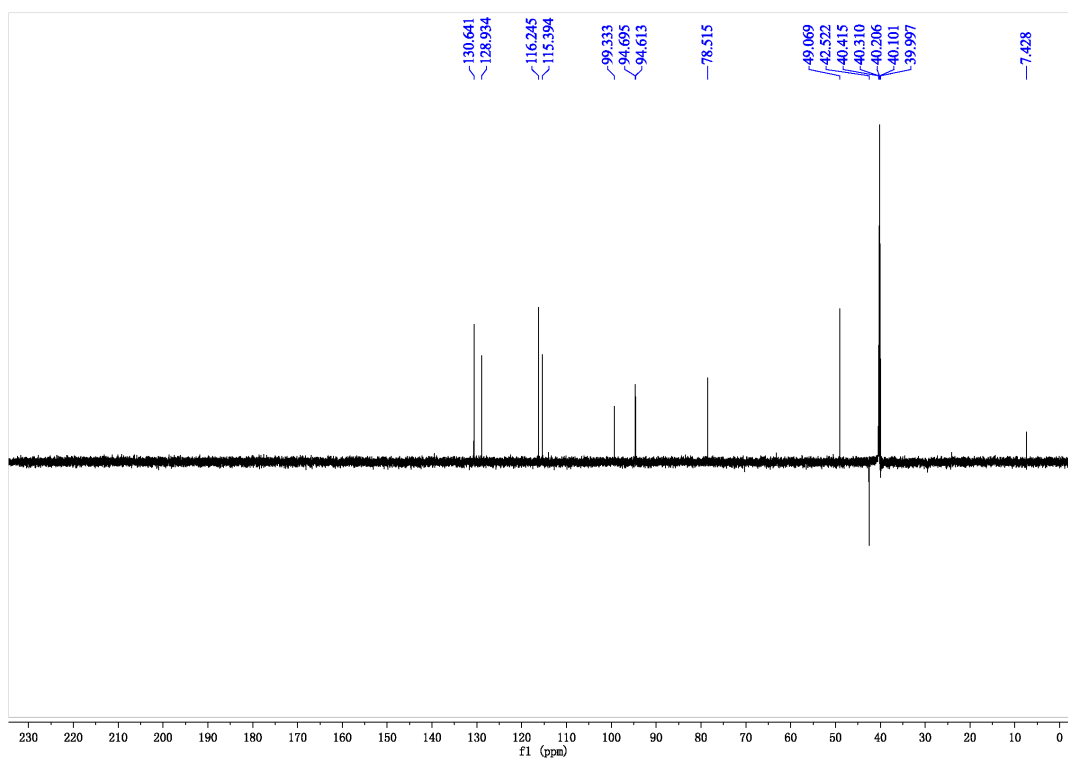
**Figure S22.** HRESIMS spectrum of **4**



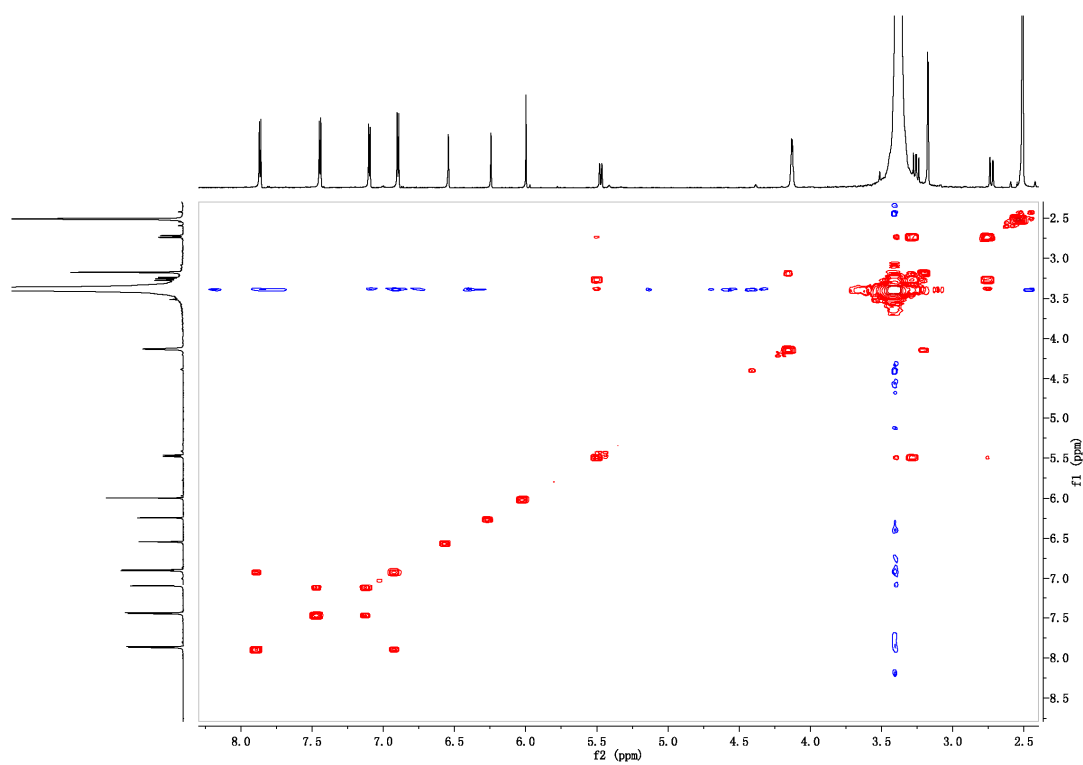
**Figure S23.** <sup>1</sup>H NMR spectrum (800 MHz) of **4** in DMSO-*d*<sub>6</sub>



**Figure S24.** <sup>13</sup>C NMR spectrum (200 MHz) of **4** in DMSO-*d*<sub>6</sub>

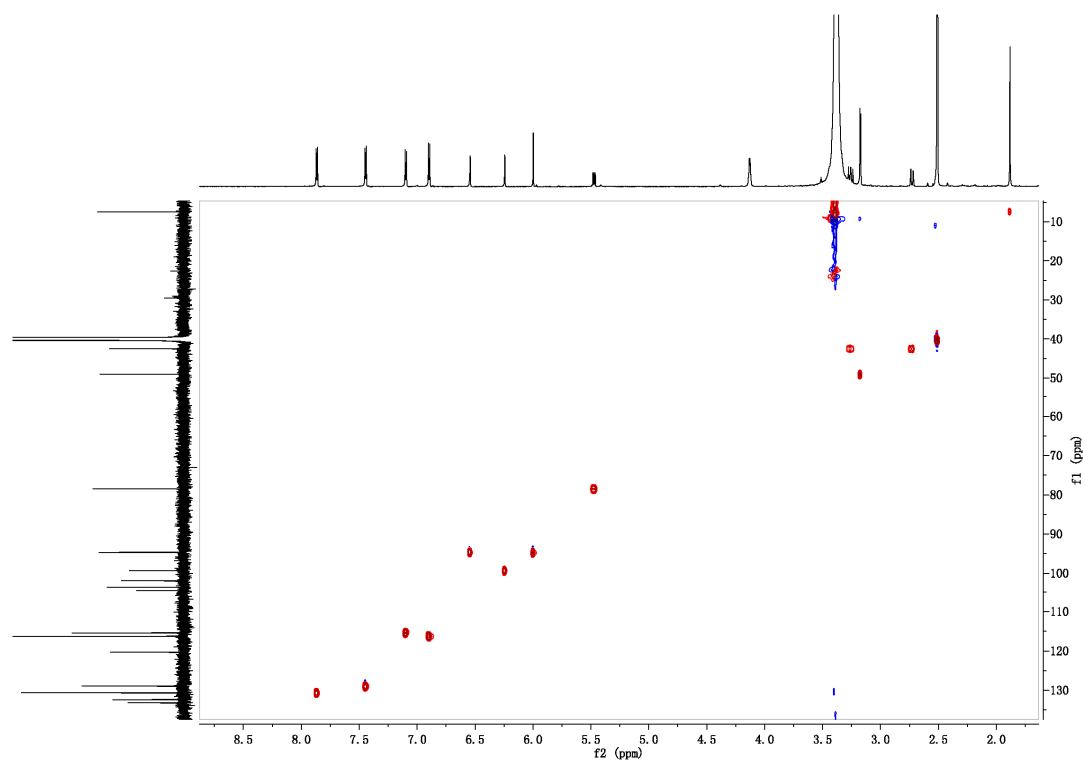


**Figure S25.** DEPT 135 spectrum (125 MHz) of **4** in DMSO-*d*<sub>6</sub>

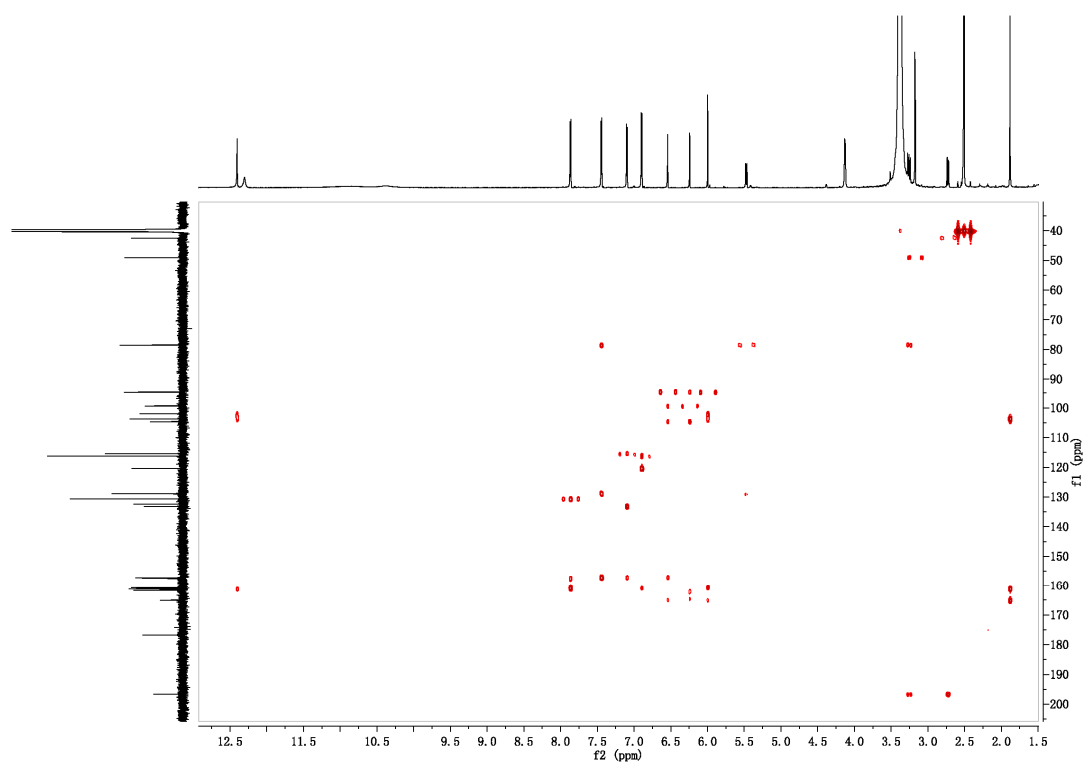


**Figure S26.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **4** in DMSO-*d*<sub>6</sub>

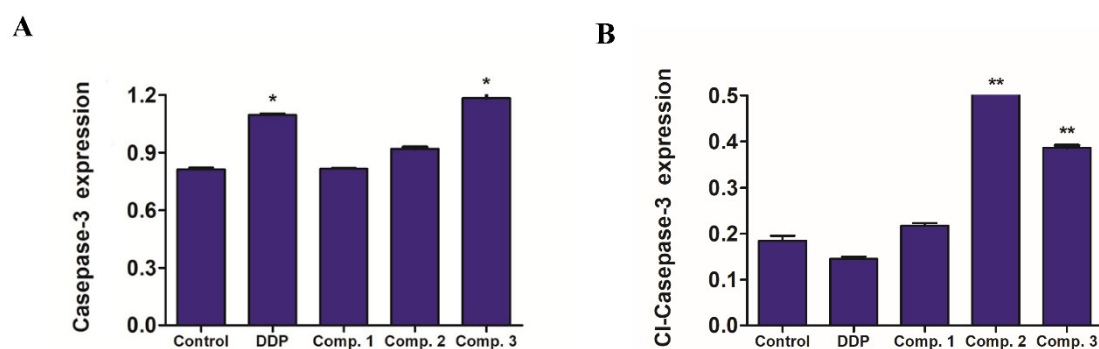




**Figure S27.** HSQC spectrum of **4** in DMSO-*d*<sub>6</sub>



**Figure S28.** HMBC spectrum of **4** in DMSO-*d*<sub>6</sub>



**Figure S29.** Effects of compounds **1-3** on expression of caspase-3 and cleaved caspase-3. A549 cells were treated with vehicle or the indicated compound for 24 h, and the relative levels of caspase-3 and cleaved caspase-3 were determined by western blot assays using  $\beta$ -actin as a control. (A) Quantitative analysis of caspase-3. (B) Quantitative analysis of cleaved caspase-3. Data are expressed as **means** from three independent experiments. \* $P < 0.05$ , \*\* $P < 0.01$  vs control group.