

# **Bioactive Steroids with Structural Diversity from the South China Sea soft coral *Lobophytum* sp. and sponge *Xestospongia* sp.**

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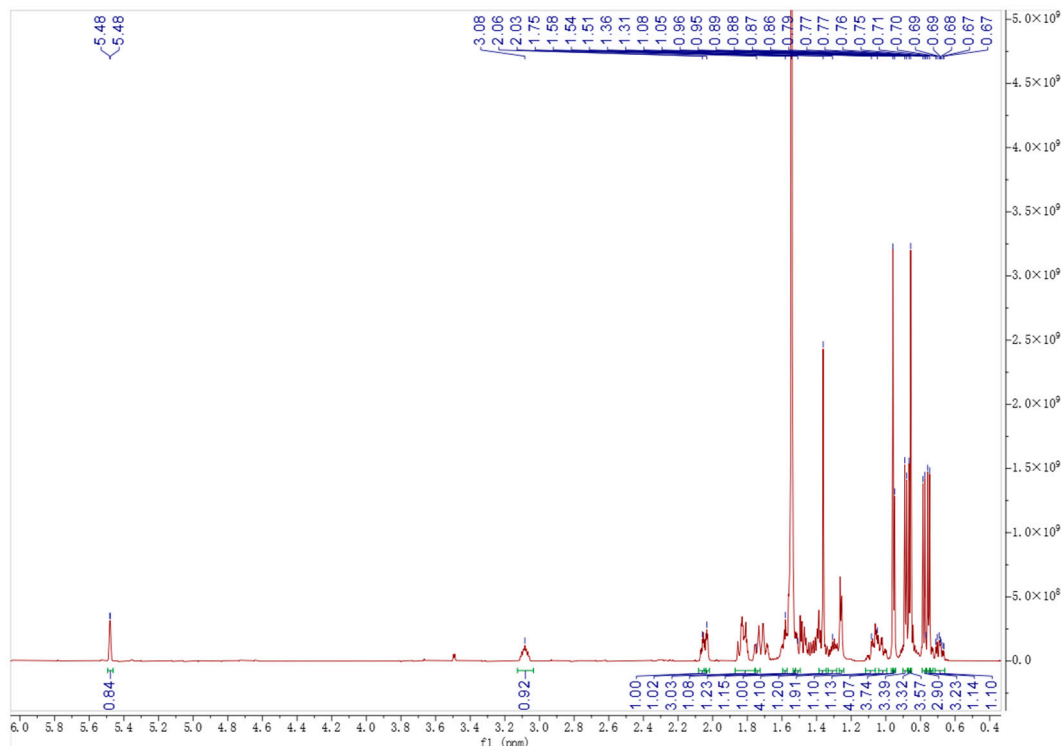
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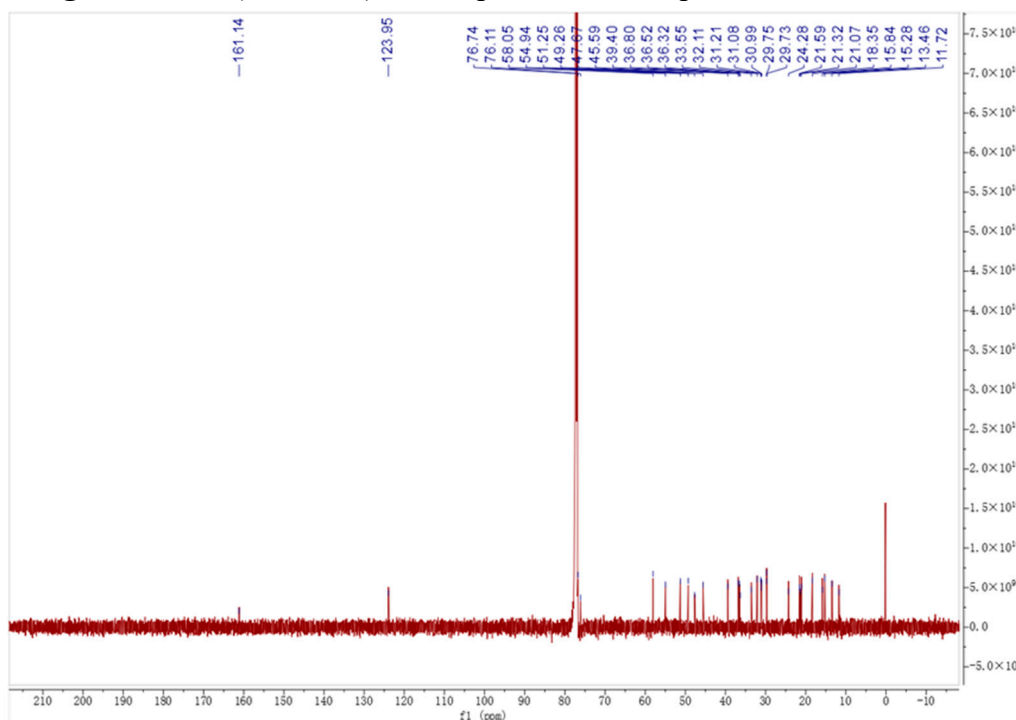
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## Original spectra of 1

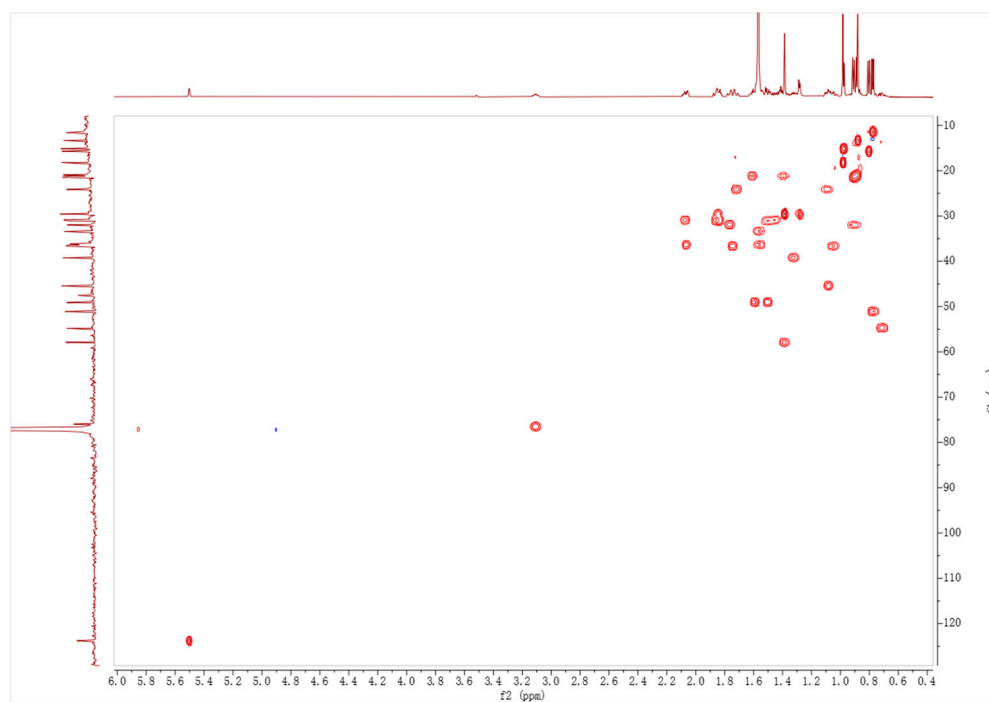
**Figure S1.**  $^1\text{H}$  (600 MHz) NMR spectrum of compound **1** in  $\text{CDCl}_3$ .



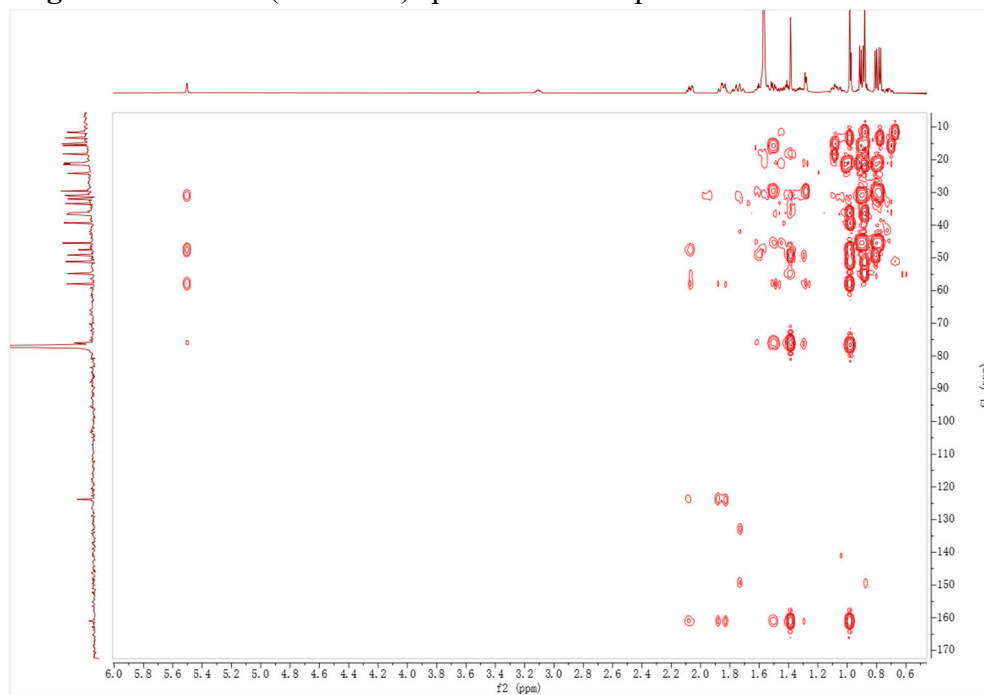
**Figure S2.**  $^{13}\text{C}$  (150 MHz) NMR spectrum of compound **1** in  $\text{CDCl}_3$ .



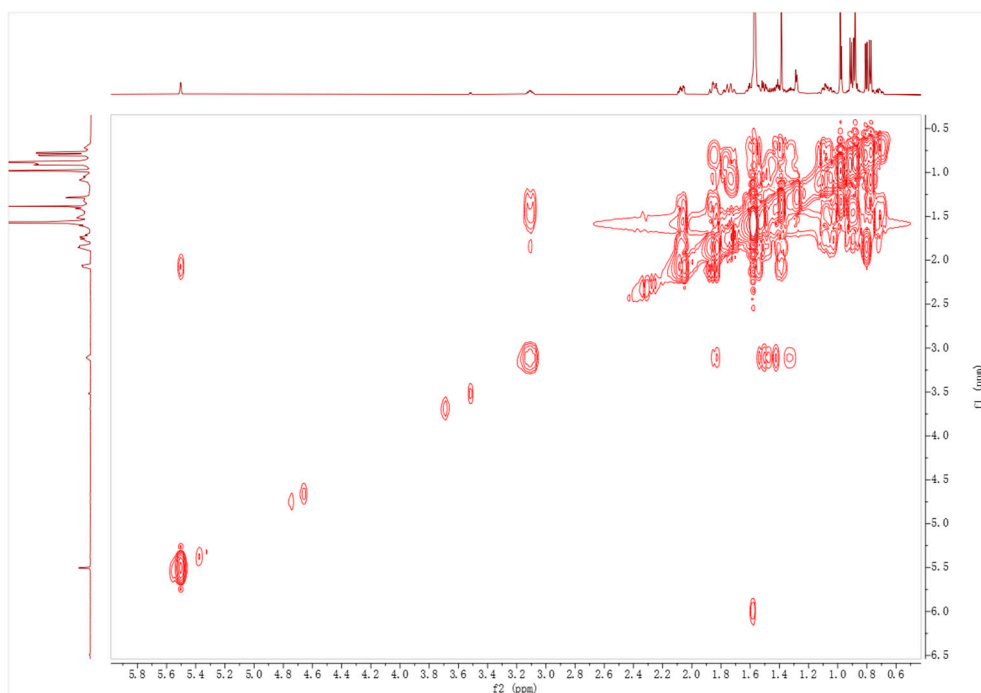
**Figure S3.** HSQC (600 MHz) spectrum of compound **1** in CDCl<sub>3</sub>



**Figure S4.** HMBC (600 MHz) spectrum of compound **1** in CDCl<sub>3</sub>.



**Figure S5.**  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz) spectrum of compound **1** in  $\text{CDCl}_3$ .



**Figure S6.** NOESY (600 MHz) spectrum of compound **1** in  $\text{CDCl}_3$ .

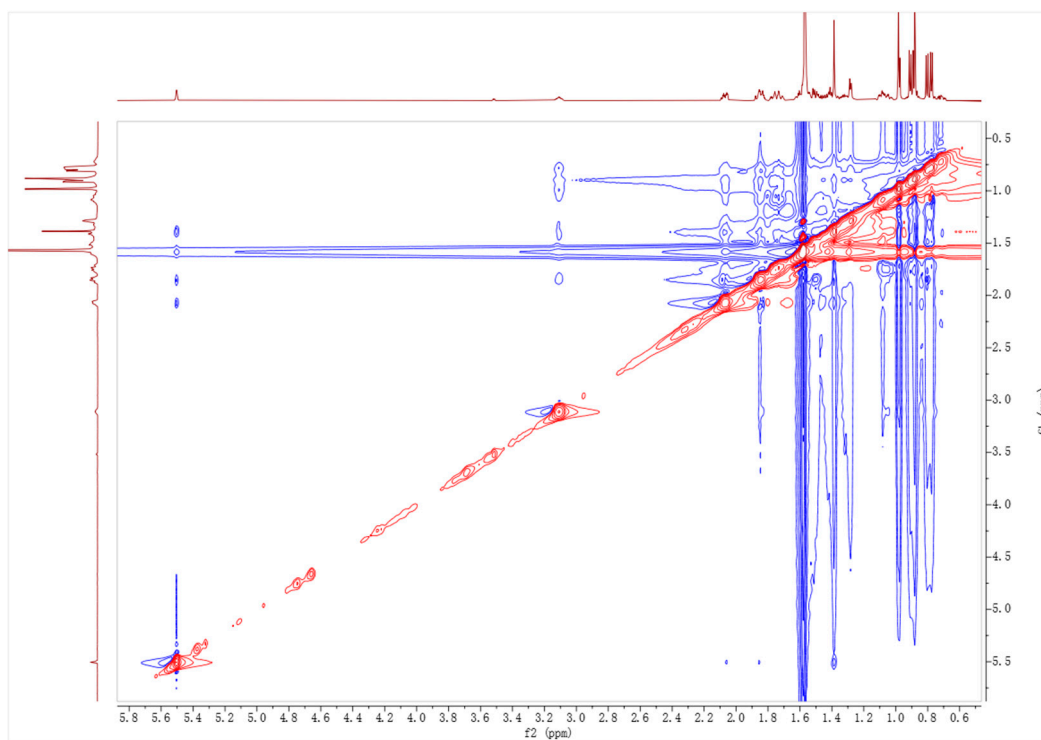
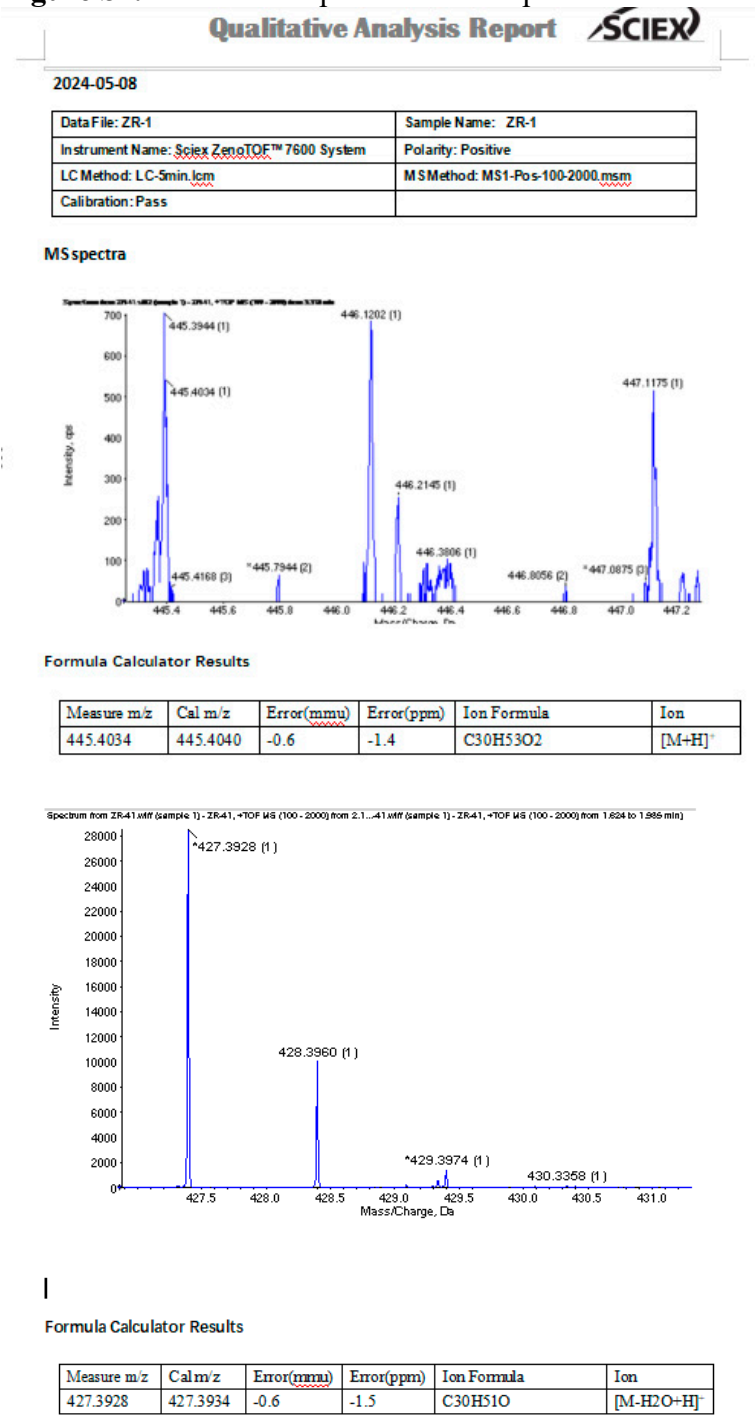
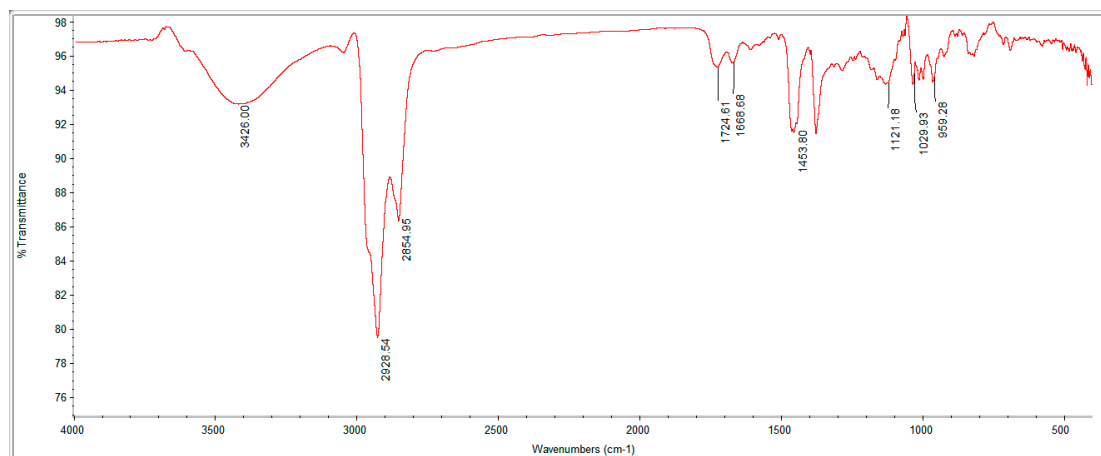


Figure S7. HR-ESIMS spectrum of compound 1.

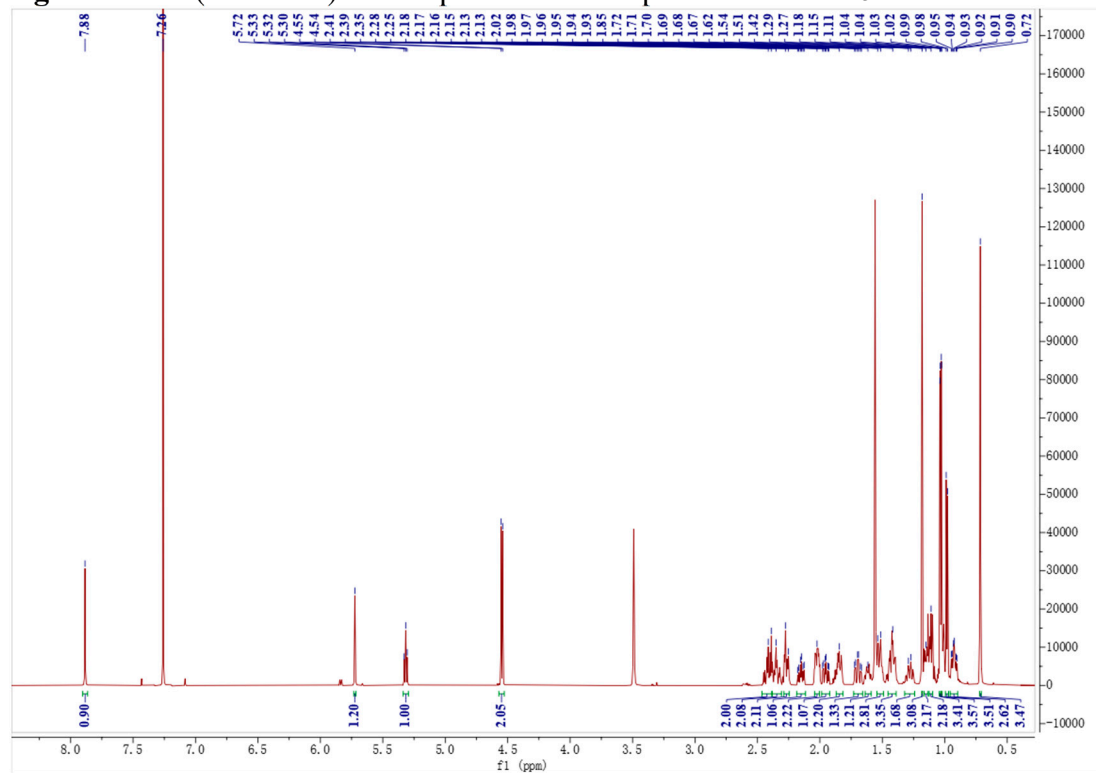


**Figure S8.** IR spectrum of compound **1**.

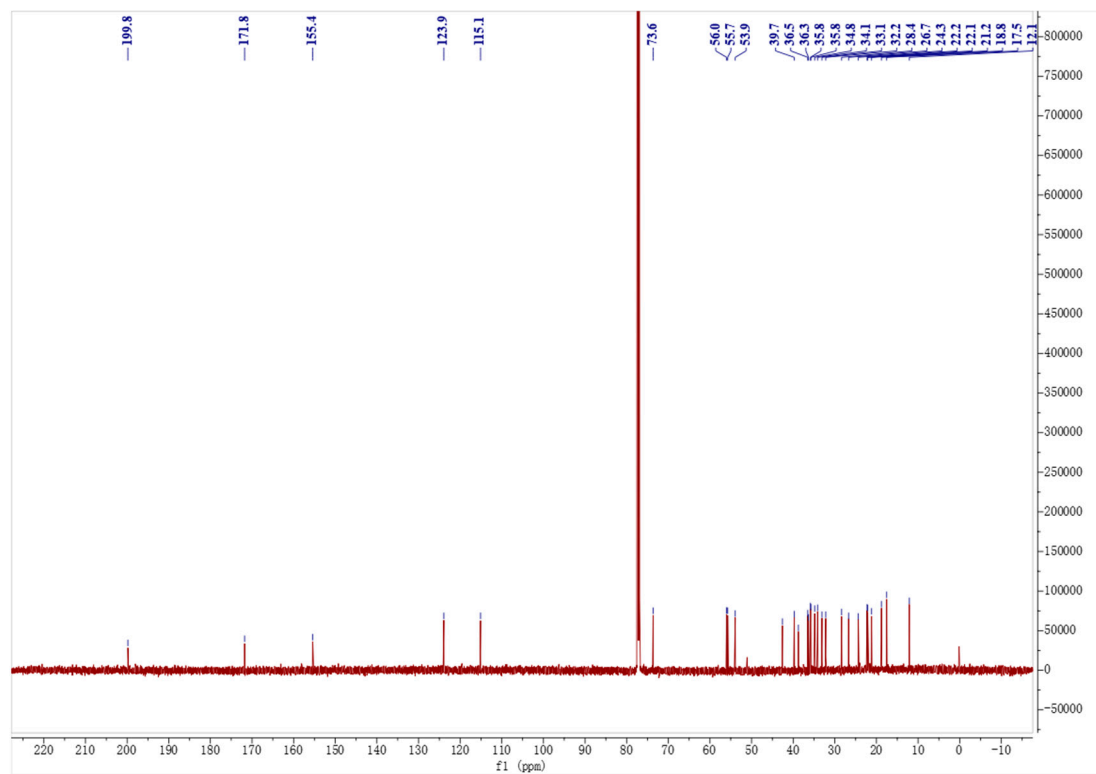


**Original spectra of 4**

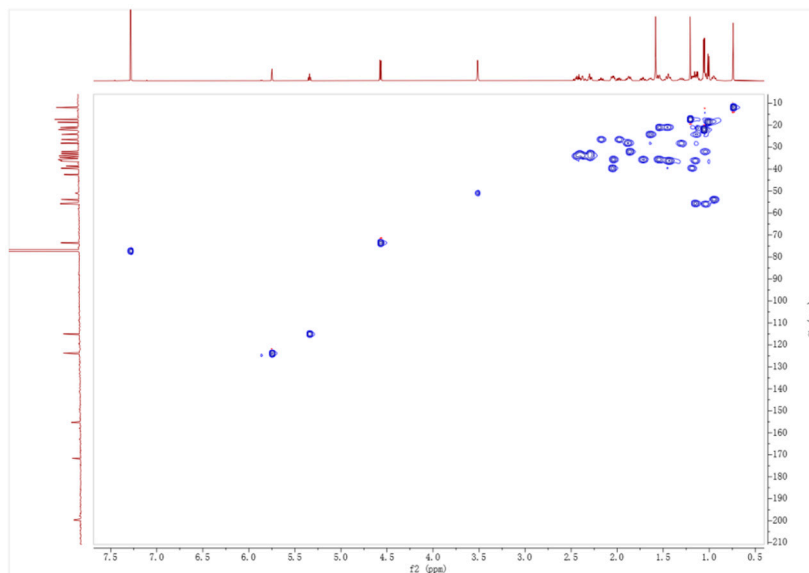
**Figure S9.** <sup>1</sup>H (600 MHz) NMR spectrum of compound **4** in CDCl<sub>3</sub>.



**Figure S10.**  $^{13}\text{C}$  (150 MHz) NMR spectrum of compound **4** in  $\text{CDCl}_3$ .

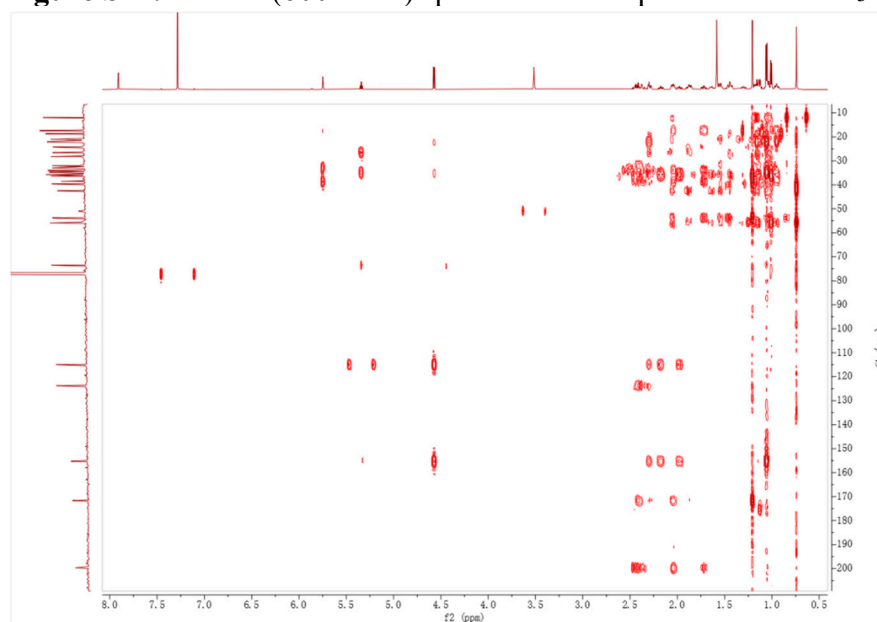


**Figure S11.** HSQC (600 MHz) spectrum of compound **4** in  $\text{CDCl}_3$ .

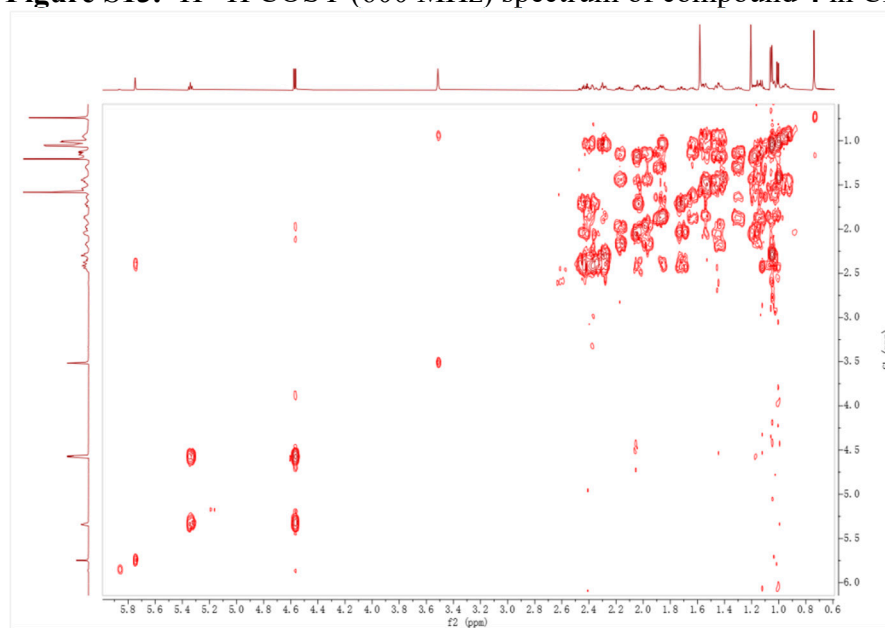




**Figure S12.** HMBC (600 MHz) spectrum of compound **4** in CDCl<sub>3</sub>.

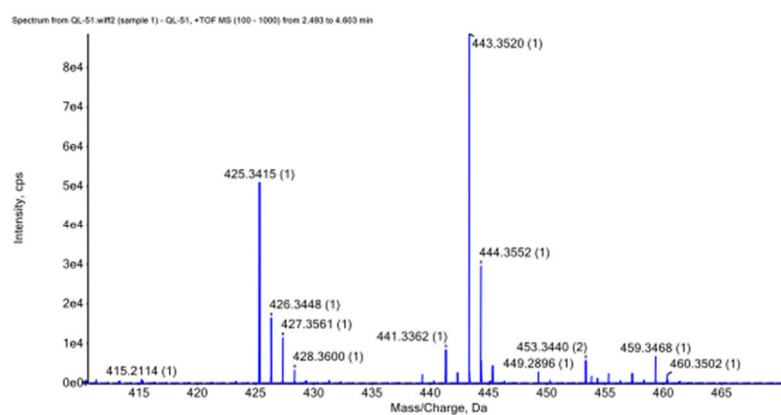
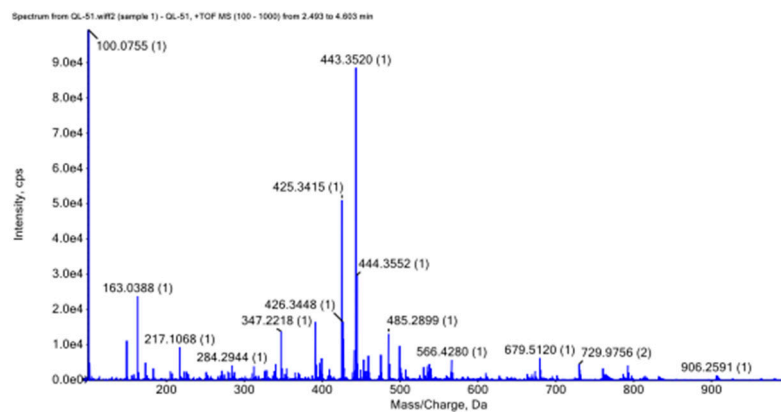


**Figure S13.** <sup>1</sup>H-<sup>1</sup>H COSY (600 MHz) spectrum of compound **4** in CDCl<sub>3</sub>.



**Figure S14.** HR-ESIMS spectrum of compound 4.

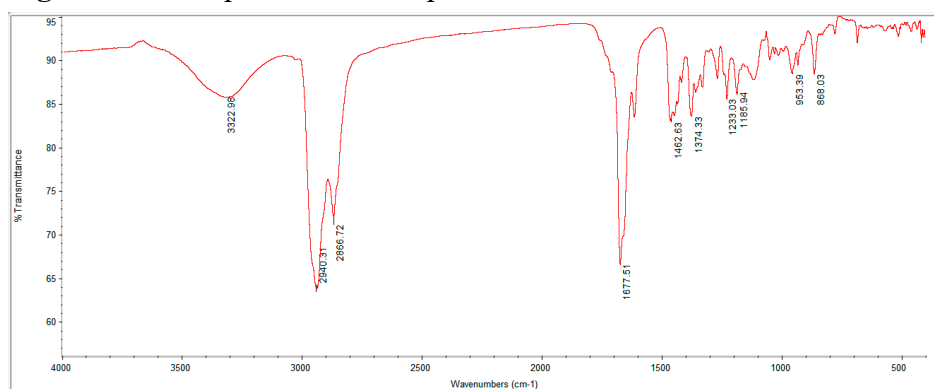
**MS spectra**



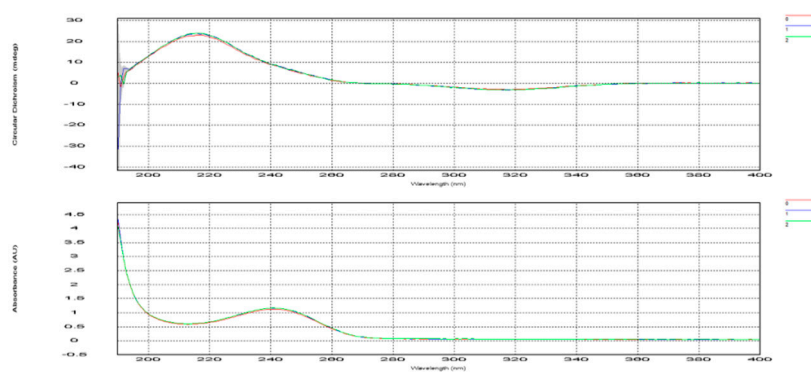
**Formula Calculator Results**

Measured m/z	Cal m/z	Error(mmu)	Error(ppm)	Ion Formula	Ion
443.3520	443.3520	0	0	C <sub>29</sub> H <sub>47</sub> O <sub>3</sub>	[M+H] <sup>+</sup>
425.3415	425.3414	0.1	0.2	C <sub>29</sub> H <sub>45</sub> O <sub>2</sub>	[M+H-H <sub>2</sub> O] <sup>+</sup>

**Figure S15.** IR spectrum of compound **4**.

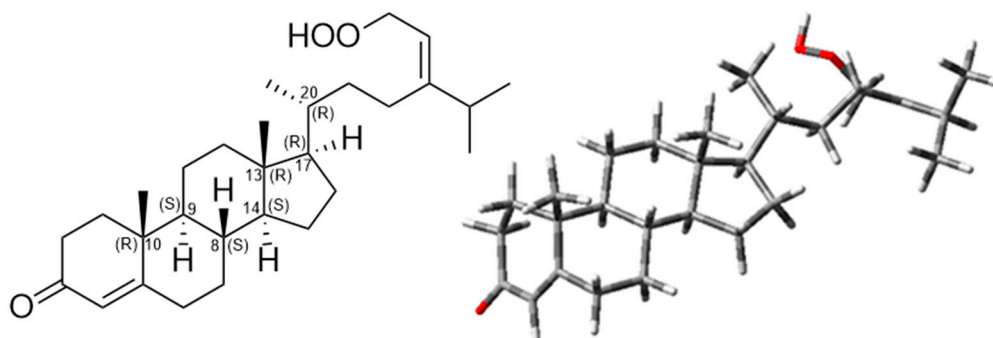


**Figure S16.** UV and ECD spectra of compound **4**.



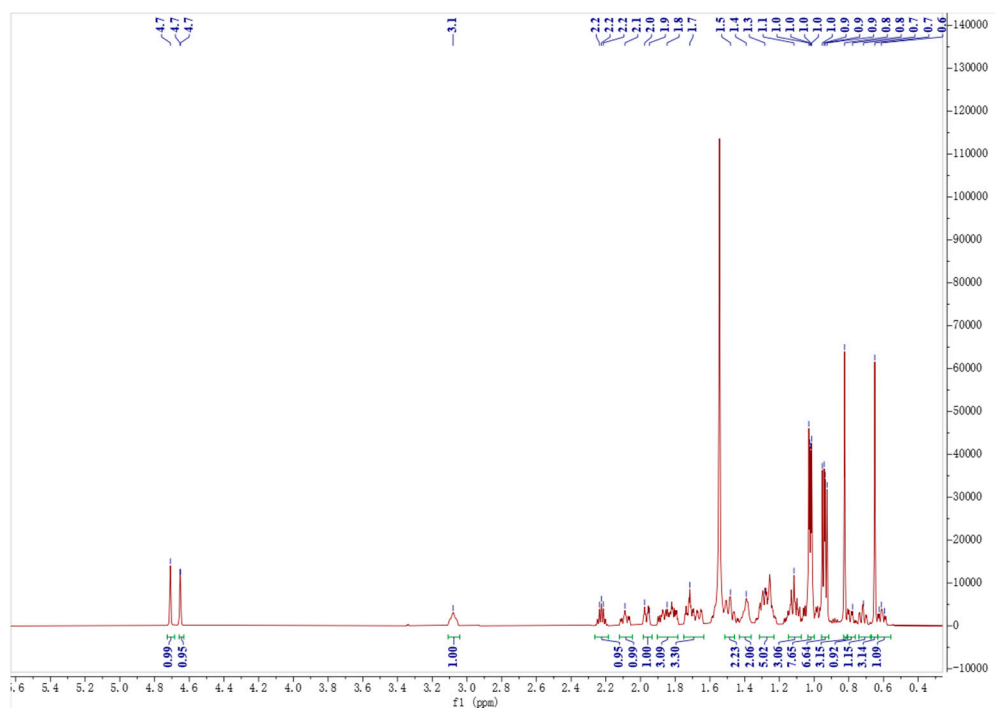
### Computational details (TDDFT-ECD) of **4**

**Figure S17.** Structure of isomer (8*S*,9*S*,10*R*,13*R*,14*S*,17*R*,20*R*)-**4** studied for TDDFT-ECD calculation.

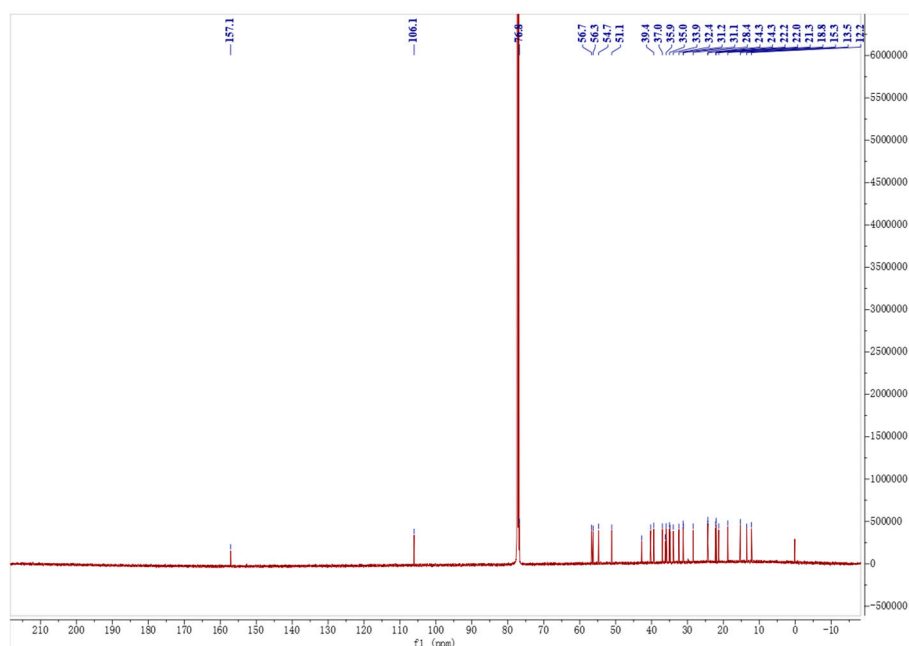


**Original spectra of known compounds 2, 3, and 5**

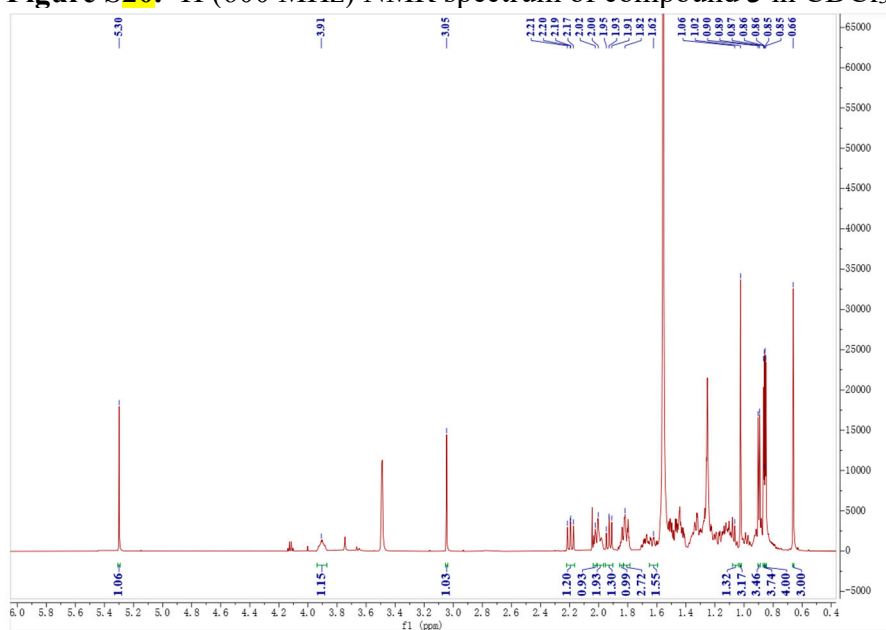
**Figure S18.**  $^1\text{H}$  (600 MHz) NMR spectrum of compound **2** in  $\text{CDCl}_3$ .



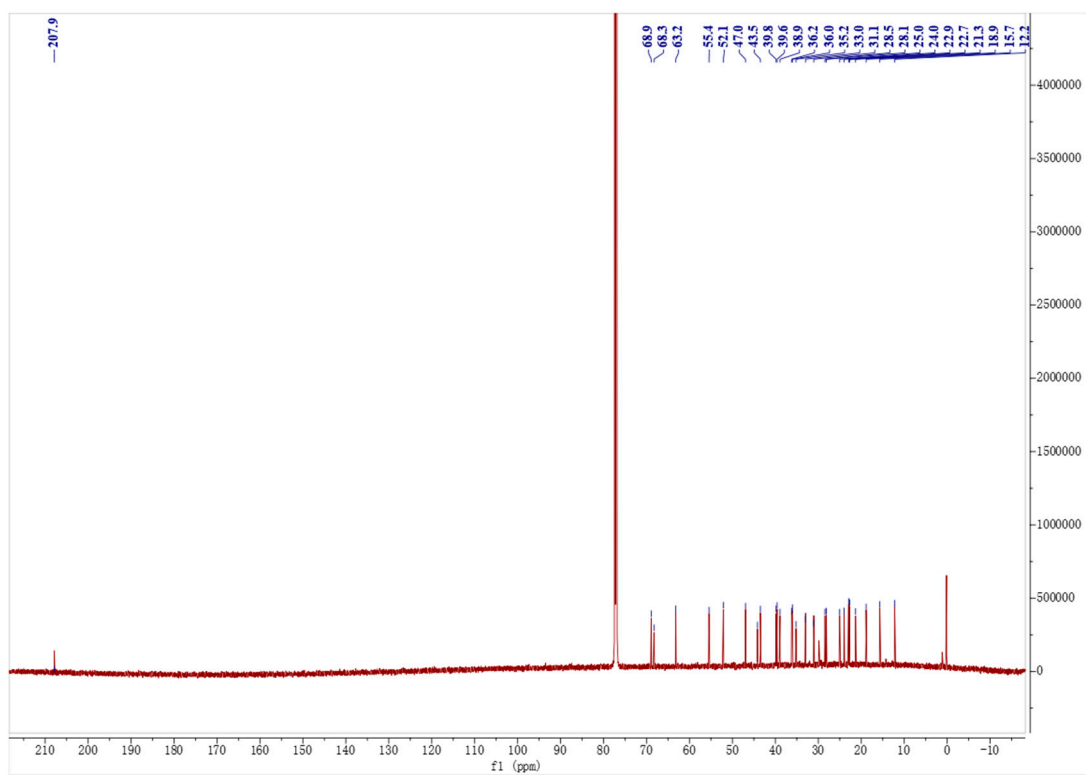
**Figure S19.**  $^{13}\text{C}$  (150 MHz) NMR spectrum of compound **2** in  $\text{CDCl}_3$ .



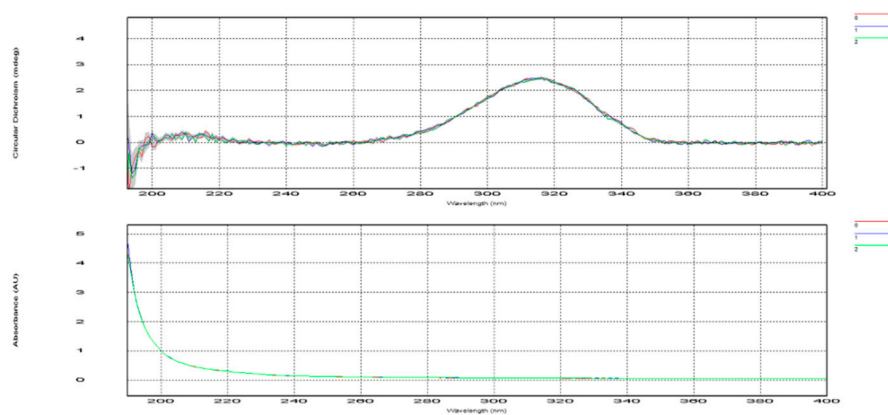
**Figure S20.**  $^1\text{H}$  (600 MHz) NMR spectrum of compound **3** in  $\text{CDCl}_3$ .



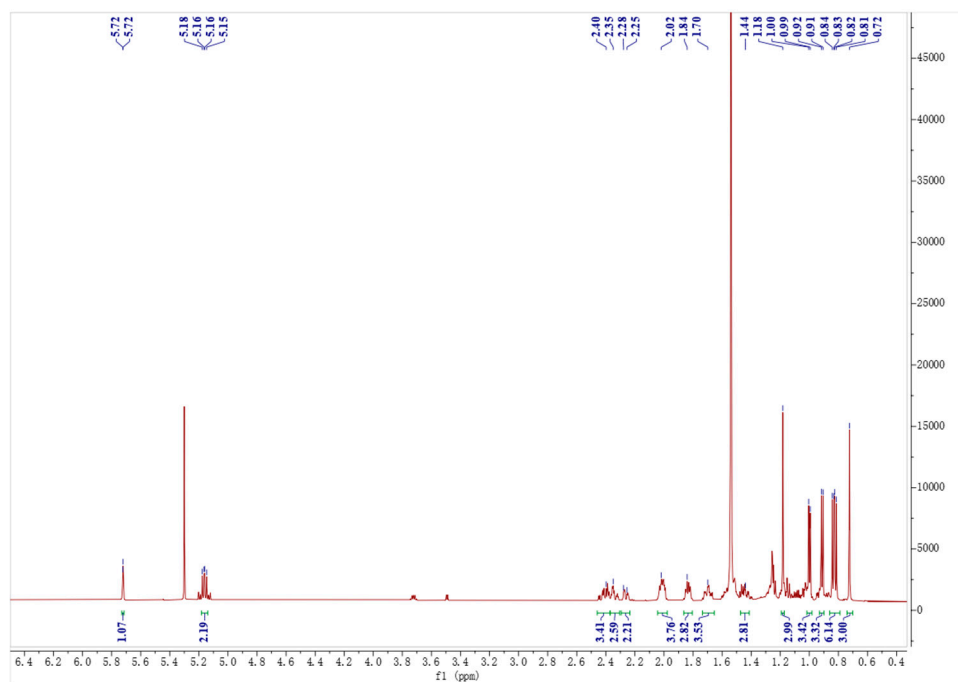
**Figure S21.**  $^{13}\text{C}$  (150 MHz) NMR spectrum of compound **3** in  $\text{CDCl}_3$ .



**Figure S22.** UV and ECD spectra of compound **3**.



**Figure S23.**  $^1\text{H}$  (600 MHz) NMR spectrum of compound **5** in  $\text{CDCl}_3$



**Figure S24.**  $^{13}\text{C}$  (150 MHz) NMR spectrum of compound **5** in  $\text{CDCl}_3$ .

