

**Hemiacetalmeroterpenoids A-C and Astellolide Q with  
Antimicrobial Activity from the Marine-Derived Fungus  
*Penicillium* sp. N-5**

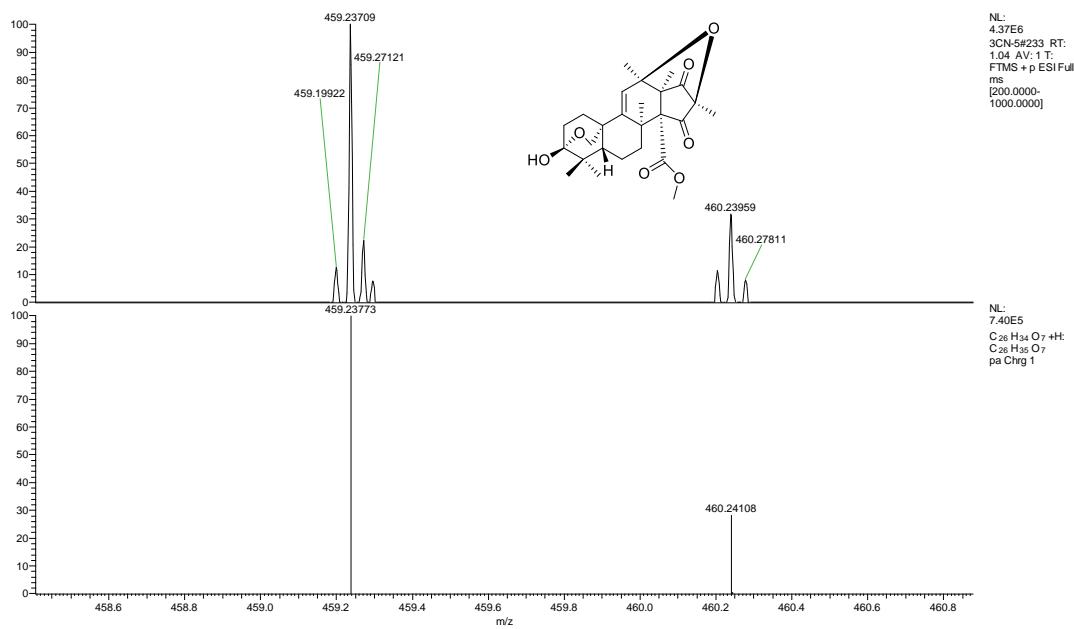
Tao Chen, Wencong Yang, Taobo Li, Yihao Yin, Yufeng Liu, Bo Wang \*,  
Zhigang She \*

School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, China

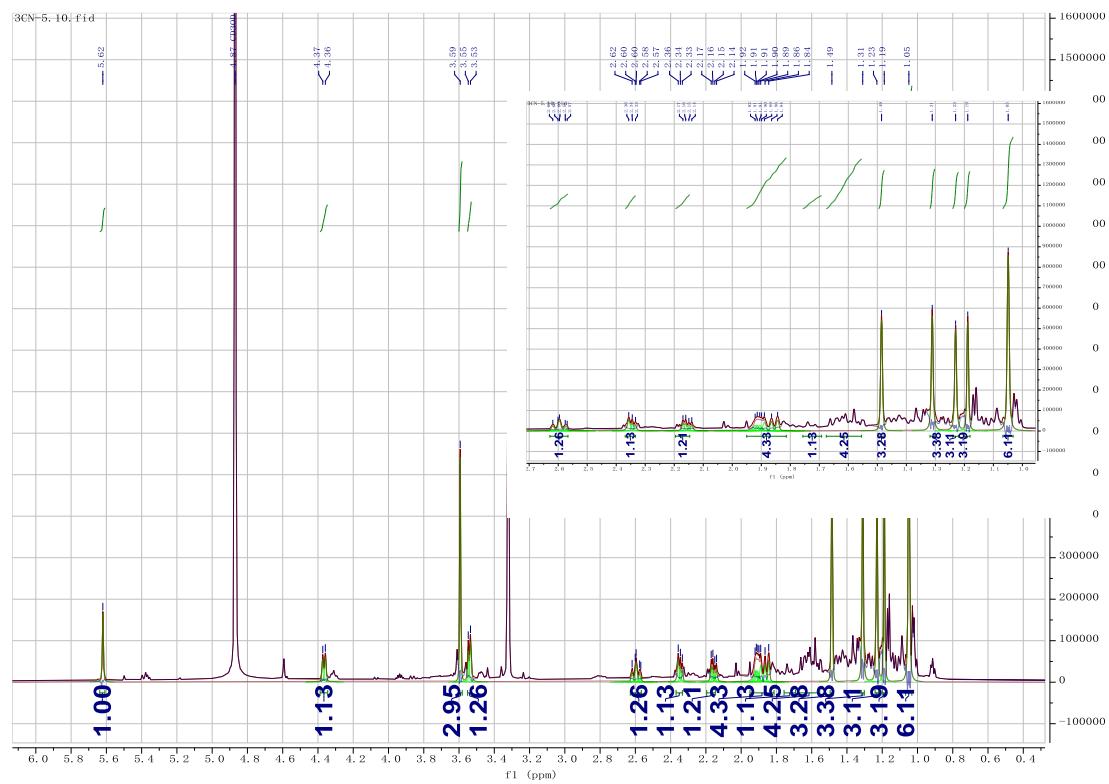
\* Correspondence: ceswb@mail.sysu.edu.cn (B.W.); cesshzg@mail.sysu.edu.cn  
(Z.S.)

## Supporting information

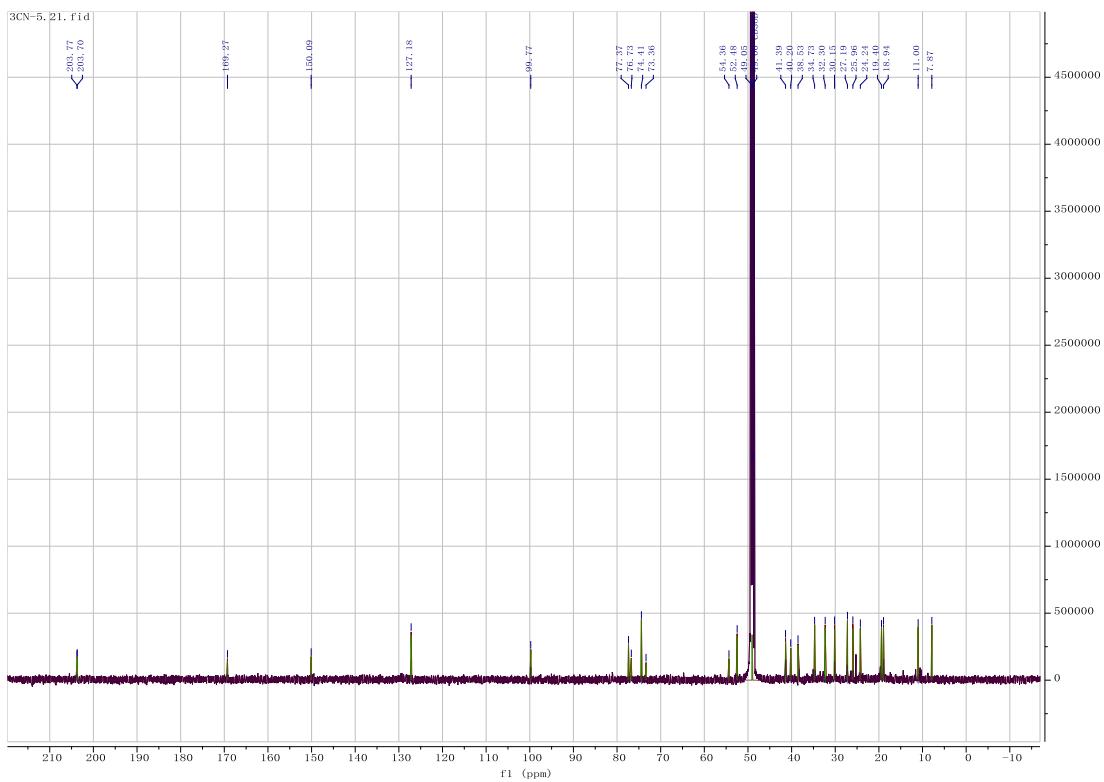
<b>Figure S1.</b> HRESIMS spectrum of compound <b>1</b> .....	3
<b>Figure S2.</b> $^1\text{H}$ NMR spectrum of compound <b>1</b> (600 MHz, CD <sub>3</sub> OD).....	3
<b>Figure S3.</b> $^{13}\text{C}$ NMR spectrum of compound <b>1</b> (150 MHz, CD <sub>3</sub> OD).....	4
<b>Figure S4.</b> DEPT135 spectrum of compound <b>1</b> (150 MHz, CD <sub>3</sub> OD) .....	4
<b>Figure S5.</b> HSQC spectrum of compound <b>1</b> (CD <sub>3</sub> OD).....	5
<b>Figure S6.</b> H, H-COSY spectrum of compound <b>1</b> (CD <sub>3</sub> OD) .....	5
<b>Figure S7.</b> HMBC spectrum of compound <b>1</b> (CD <sub>3</sub> OD).....	6
<b>Figure S8.</b> NOE spectrum of compound <b>1</b> (CD <sub>3</sub> OD).....	6
<b>Figure S9.</b> HRESIMS spectrum of compound <b>2</b> .....	7
<b>Figure S10.</b> $^1\text{H}$ NMR spectrum of compound <b>2</b> (600 MHz, CD <sub>3</sub> OD) .....	7
<b>Figure S11.</b> $^{13}\text{C}$ NMR spectrum of compound <b>2</b> (150 MHz, CD <sub>3</sub> OD) .....	8
<b>Figure S12.</b> DEPT135 spectrum of compound <b>2</b> (150 MHz, CD <sub>3</sub> OD) .....	8
<b>Figure S13.</b> HSQC spectrum of compound <b>2</b> (CD <sub>3</sub> OD) .....	9
<b>Figure S14.</b> H, H-COSY spectrum of compound <b>2</b> (CD <sub>3</sub> OD).....	9
<b>Figure S15.</b> HMBC spectrum of compound <b>2</b> (CD <sub>3</sub> OD) .....	10
<b>Figure S17.</b> HRESIMS spectrum of compound <b>3</b> .....	11
<b>Figure S18.</b> $^1\text{H}$ NMR spectrum of compound <b>3</b> (600 MHz, CD <sub>3</sub> OD) .....	11
<b>Figure S19.</b> $^{13}\text{C}$ NMR spectrum of compound <b>3</b> (150 MHz, CD <sub>3</sub> OD) .....	12
<b>Figure S20.</b> HSQC spectrum of compound <b>3</b> (CD <sub>3</sub> OD) .....	12
<b>Figure S21.</b> H, H-COSY spectrum of compound <b>3</b> (CD <sub>3</sub> OD).....	13
<b>Figure S22.</b> HMBC spectrum of compound <b>3</b> (CD <sub>3</sub> OD) .....	13
<b>Figure S23.</b> NOE spectrum of compound <b>3</b> (CD <sub>3</sub> OD) .....	14
<b>Figure S24.</b> NOE spectrum of compound <b>14</b> (CD <sub>3</sub> OD) .....	14
<b>Figure S25.</b> HRESIMS spectrum of compound <b>15</b> .....	15
<b>Figure S26.</b> $^1\text{H}$ NMR spectrum of compound <b>15</b> (400 MHz, CD <sub>3</sub> OD).....	15
<b>Figure S27.</b> $^{13}\text{C}$ NMR spectrum of compound <b>15</b> (100 MHz, CD <sub>3</sub> OD).....	16
<b>Figure S28.</b> DEPT135 spectrum of compound <b>15</b> (150 MHz, CD <sub>3</sub> OD) .....	16
<b>Figure S29.</b> HSQC spectrum of compound <b>15</b> (CD <sub>3</sub> OD) .....	17
<b>Figure S30.</b> H, H-COSY spectrum of compound <b>15</b> (CD <sub>3</sub> OD) .....	17
<b>Figure S31.</b> HMBC spectrum of compound <b>15</b> (CD <sub>3</sub> OD).....	18
<b>Figure S32.</b> NOE spectrum of compound <b>15</b> (CD <sub>3</sub> OD) .....	18
<b>Figure S33.</b> UV and ECD of compound <b>1</b> (CD <sub>3</sub> OD) .....	19
<b>Figure S34.</b> UV and ECD of compound <b>2</b> (CD <sub>3</sub> OD) .....	19
<b>Figure S35.</b> UV and ECD of compound <b>3</b> (CD <sub>3</sub> OD) .....	19
<b>Figure S36.</b> UV and ECD of compound <b>14</b> (CD <sub>3</sub> OD) .....	20
<b>Figure S37.</b> UV and ECD of compound <b>15</b> (CD <sub>3</sub> OD) .....	20



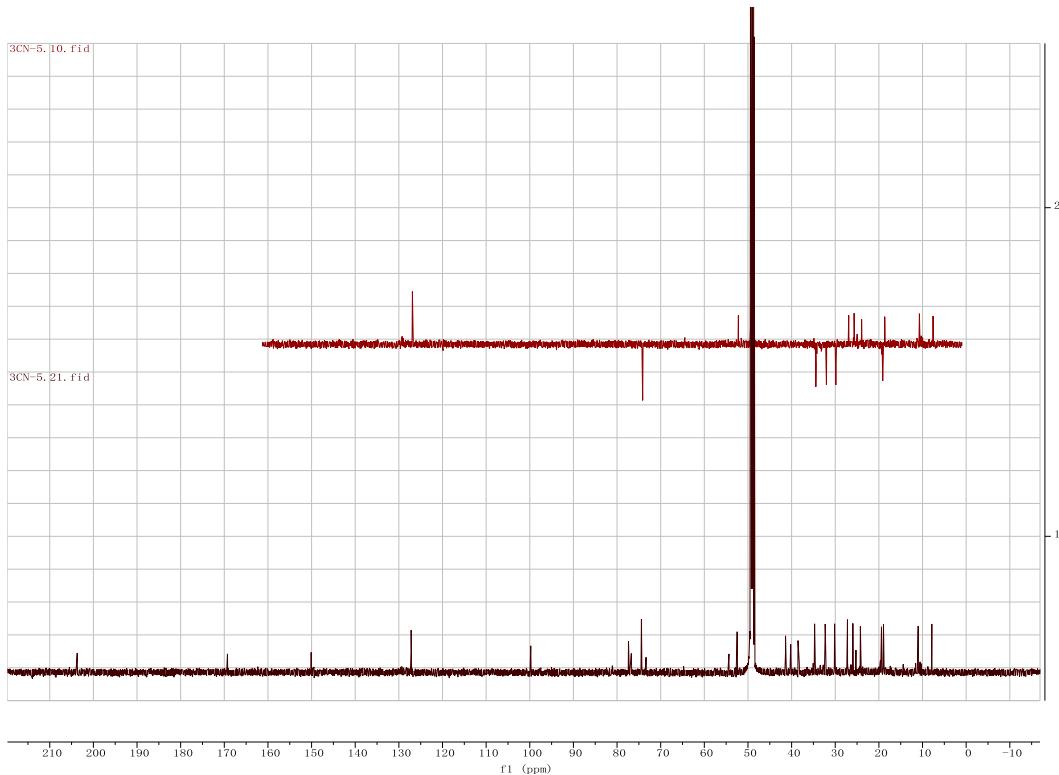
**Figure S1.** HRESIMS spectrum of compound 1



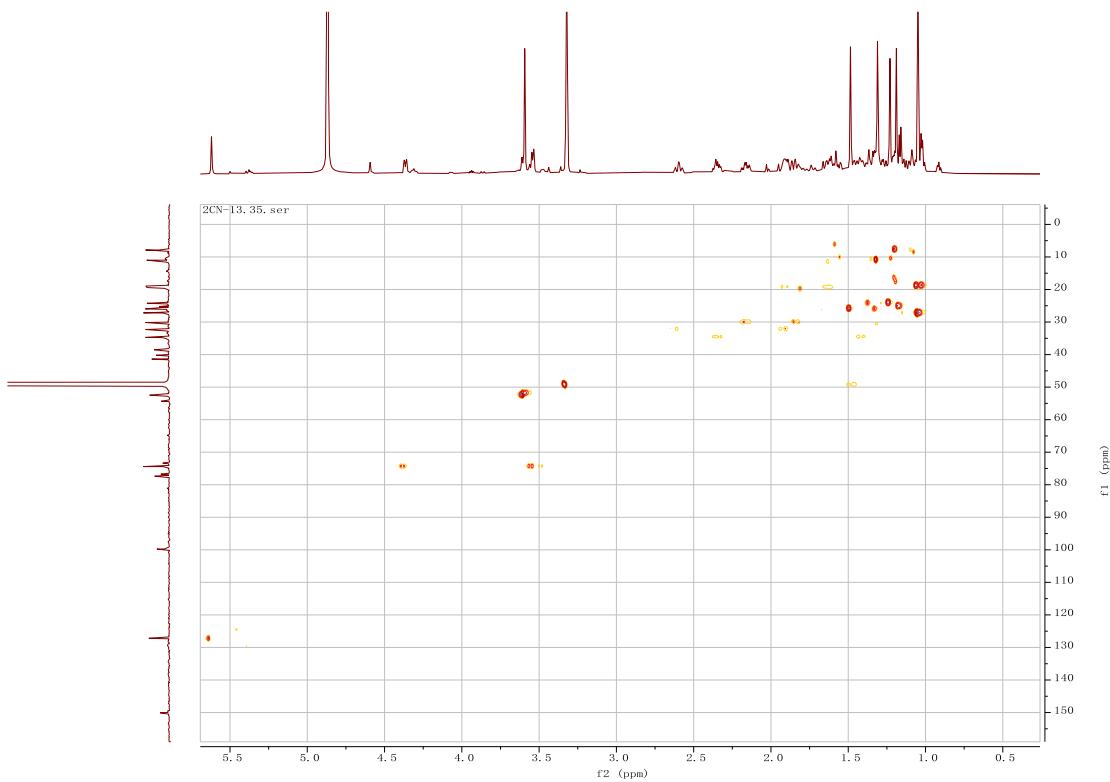
**Figure S2.** <sup>1</sup>H NMR spectrum of compound 1 (600 MHz, CD<sub>3</sub>OD)



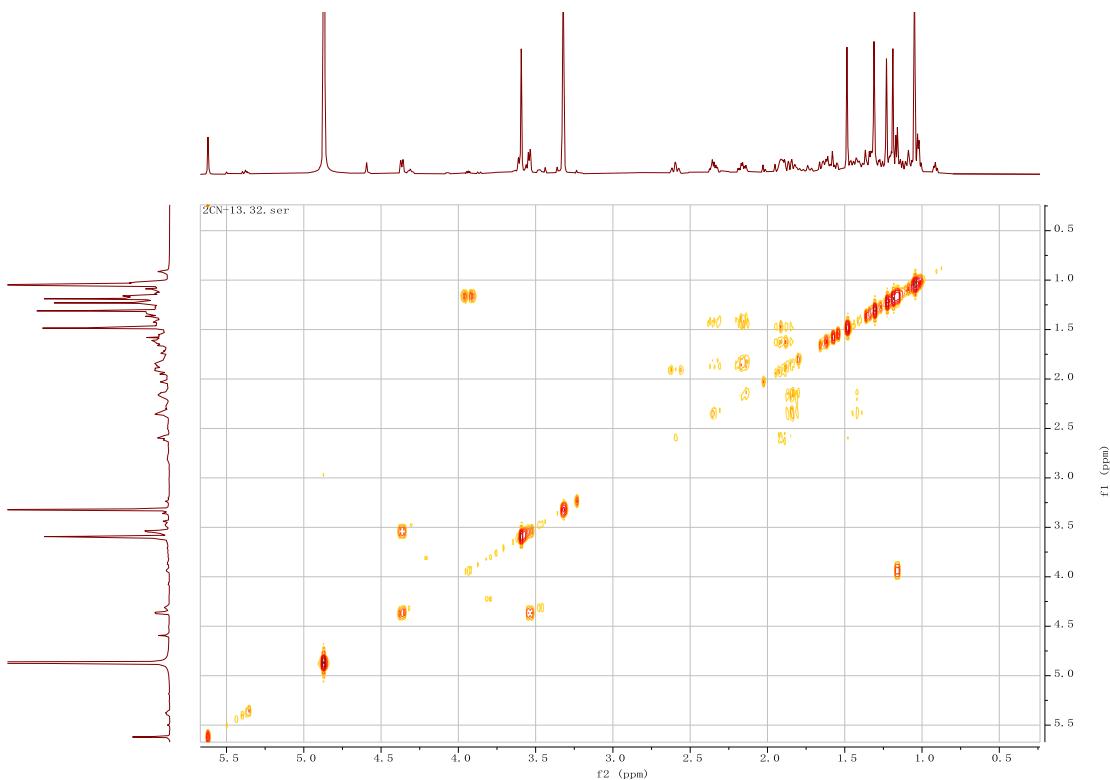
**Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound **1** (150 MHz,  $\text{CD}_3\text{OD}$ )



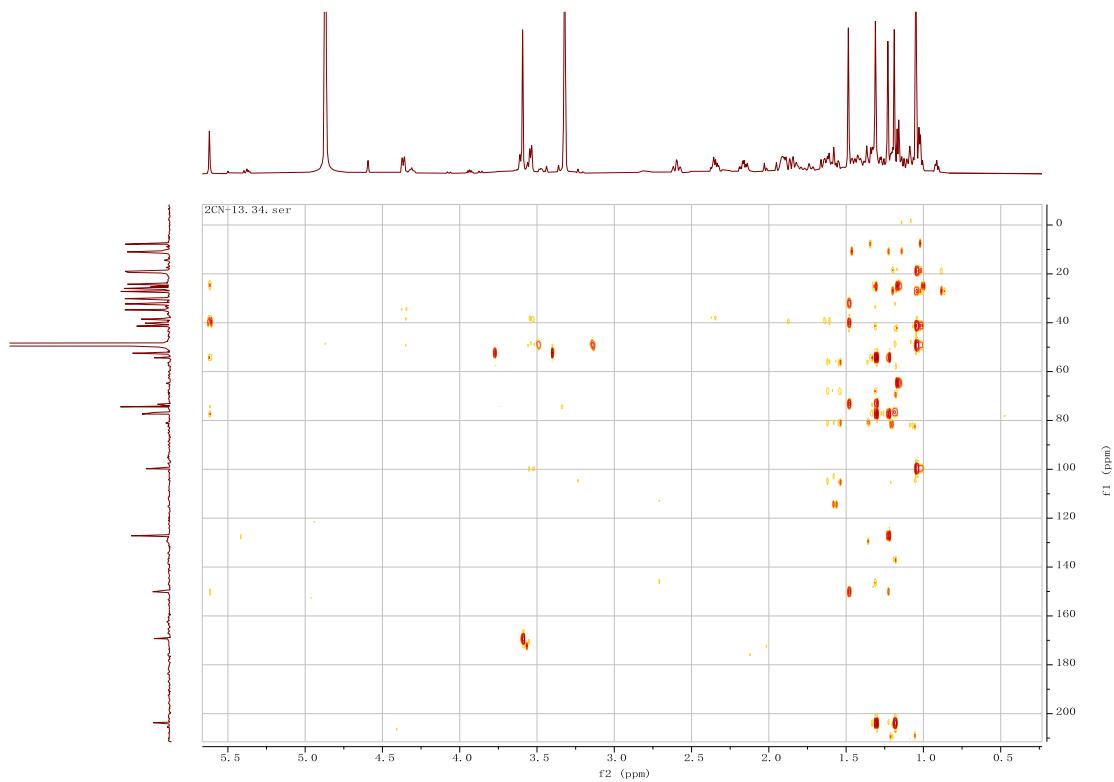
**Figure S4.** DEPT135 spectrum of compound **1** (150 MHz,  $\text{CD}_3\text{OD}$ )



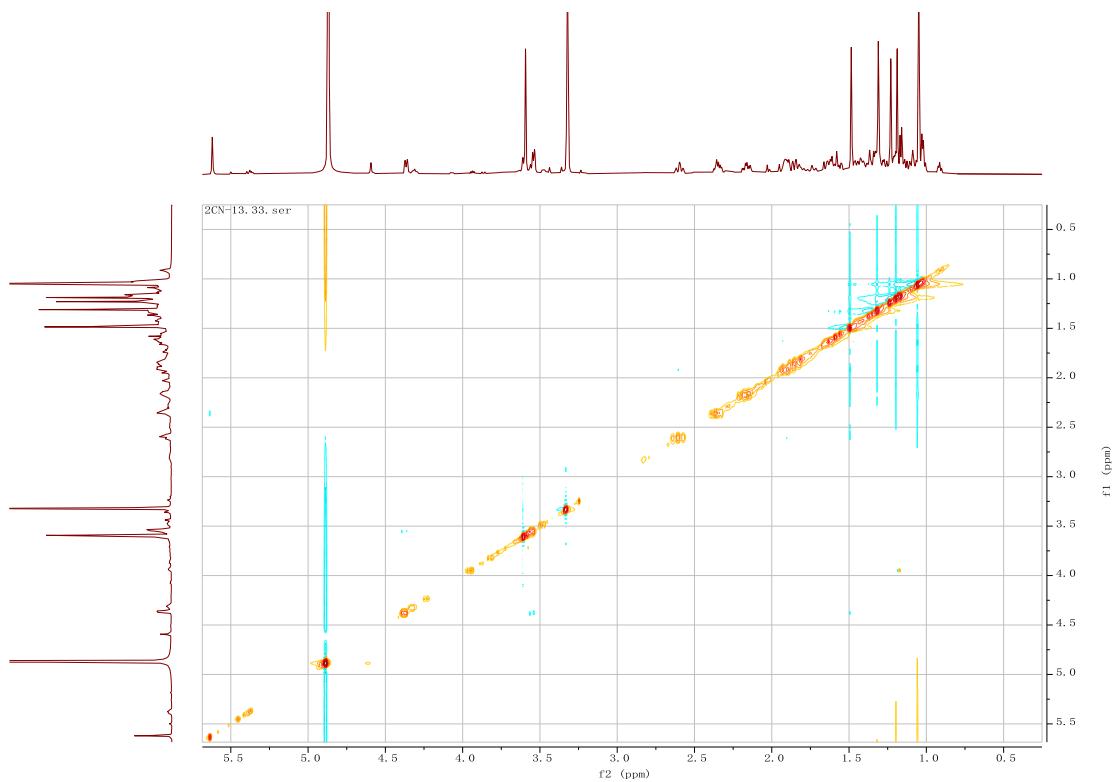
**Figure S5.** HSQC spectrum of compound **1** ( $\text{CD}_3\text{OD}$ )



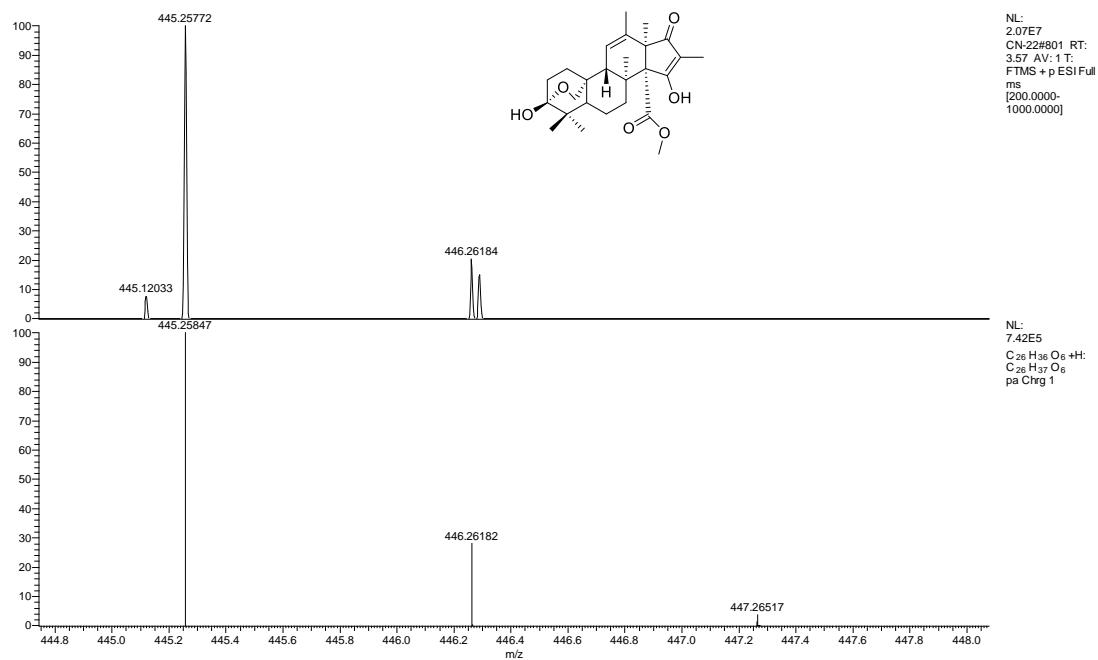
**Figure S6.**  $\text{H}, \text{H}$ -COSY spectrum of compound **1** ( $\text{CD}_3\text{OD}$ )



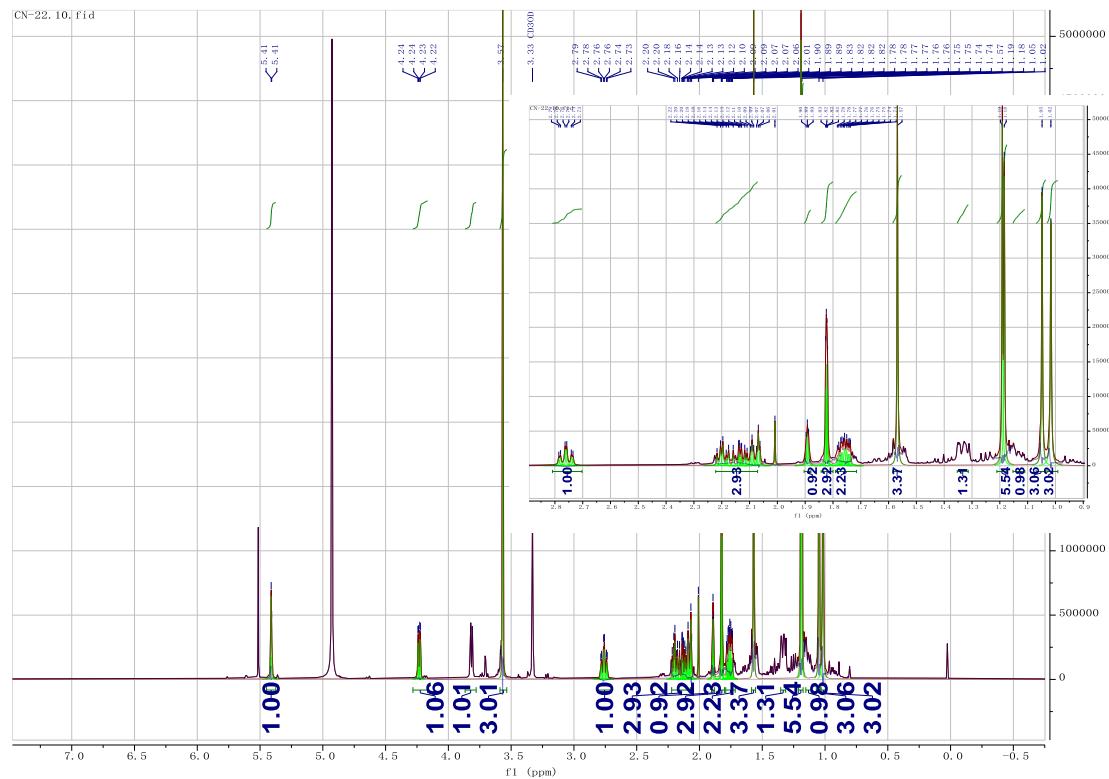
**Figure S7.** HMBC spectrum of compound **1** ( $\text{CD}_3\text{OD}$ )



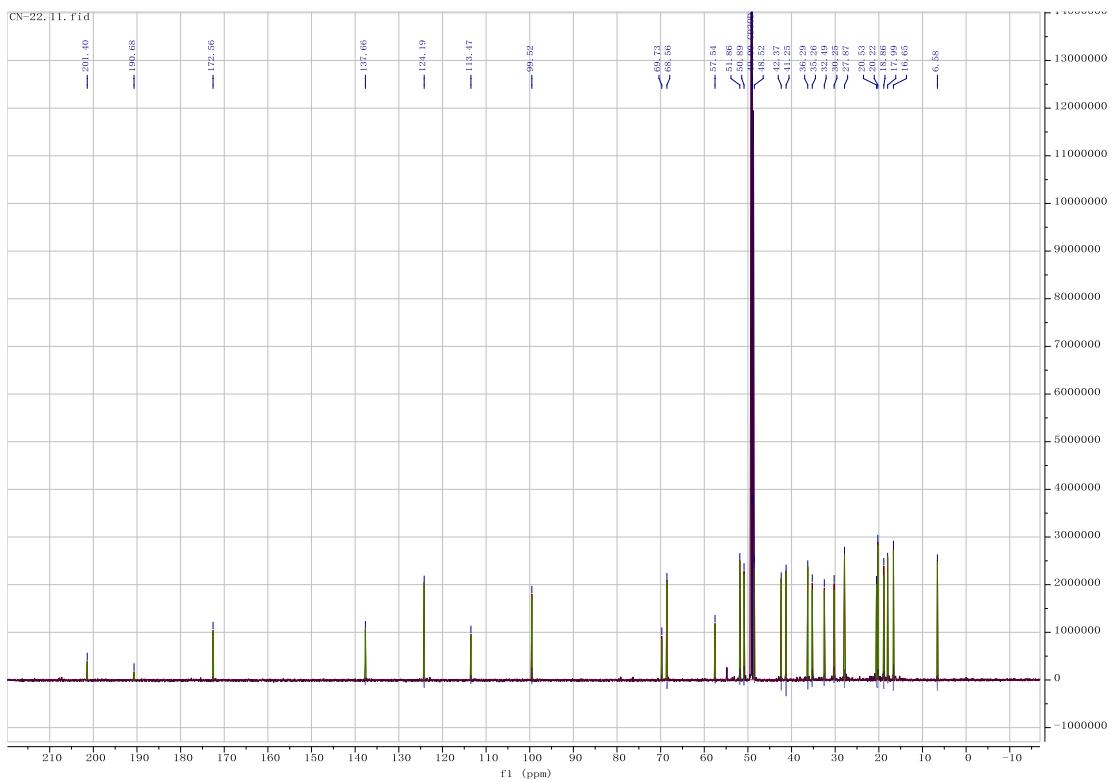
**Figure S8.** NOE spectrum of compound **1** ( $\text{CD}_3\text{OD}$ )



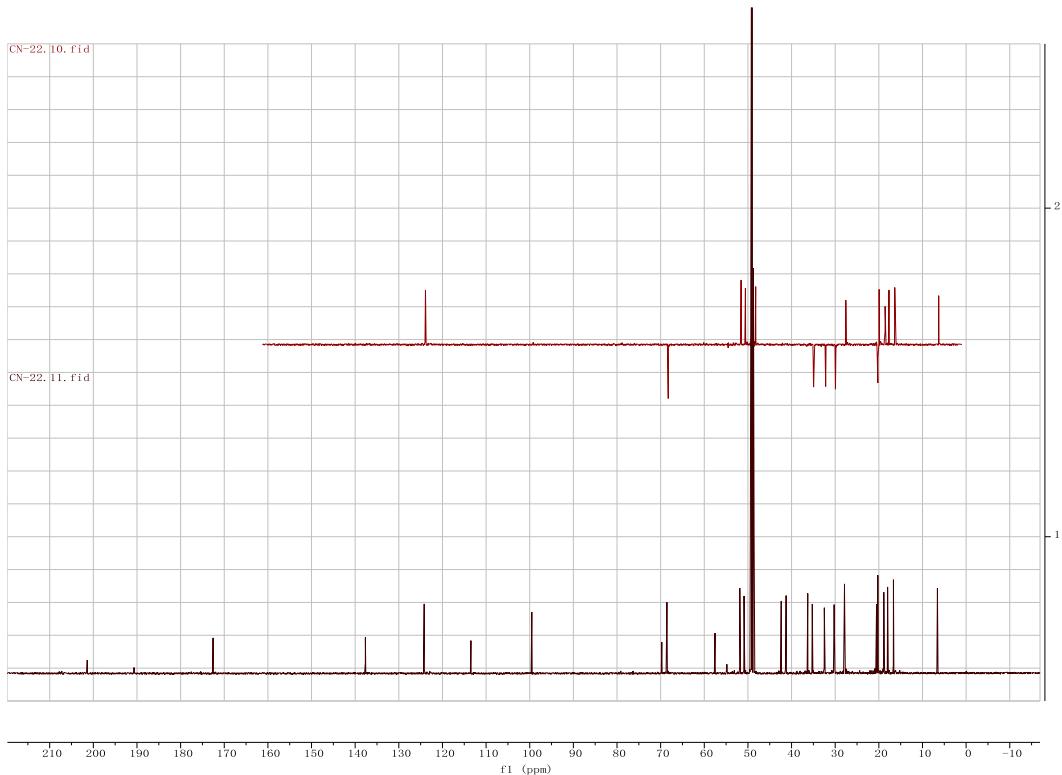
**Figure S9.** HRESIMS spectrum of compound 2



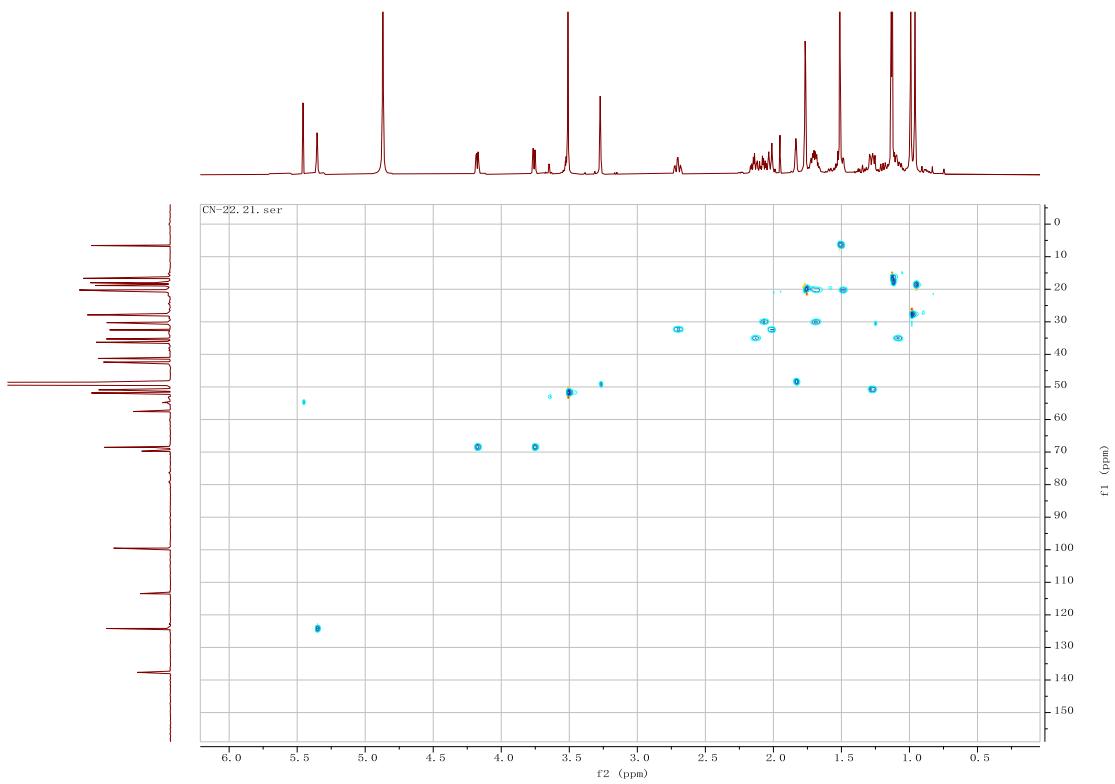
**Figure S10.** <sup>1</sup>H NMR spectrum of compound 2 (600 MHz, CD<sub>3</sub>OD)



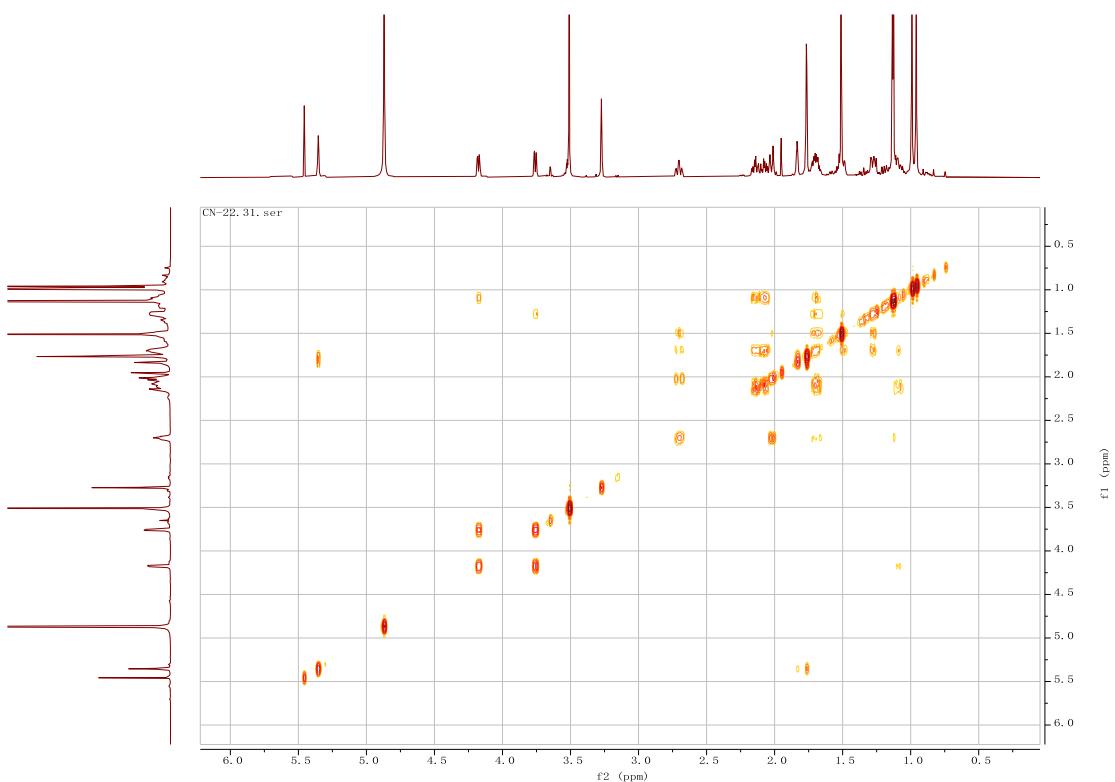
**Figure S11.**  $^{13}\text{C}$  NMR spectrum of compound 2 (150 MHz,  $\text{CD}_3\text{OD}$ )



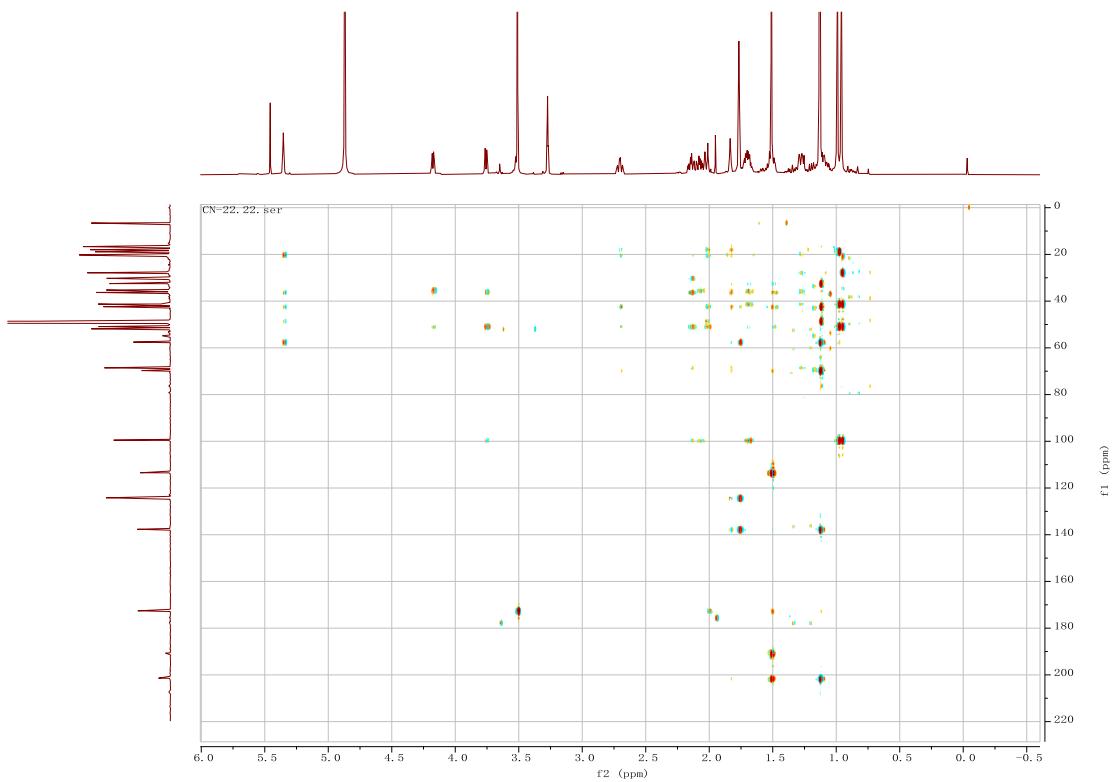
**Figure S12.** DEPT135 spectrum of compound 2 (150 MHz,  $\text{CD}_3\text{OD}$ )



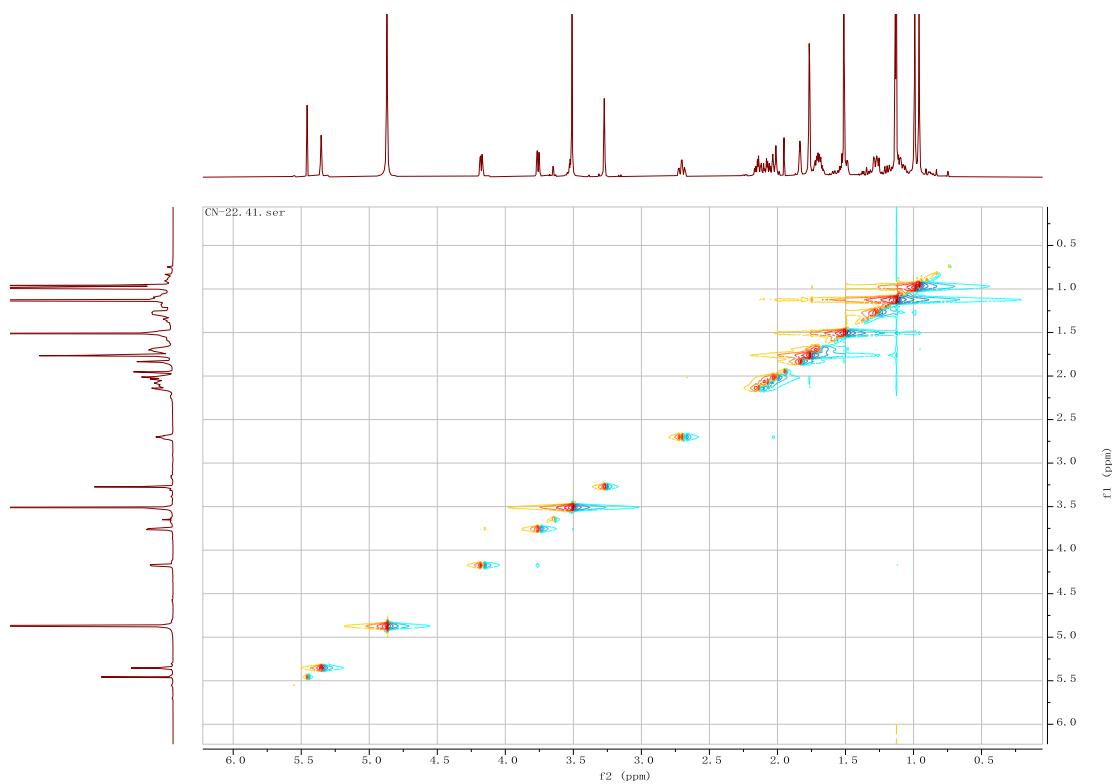
**Figure S13.** HSQC spectrum of compound **2** ( $\text{CD}_3\text{OD}$ )



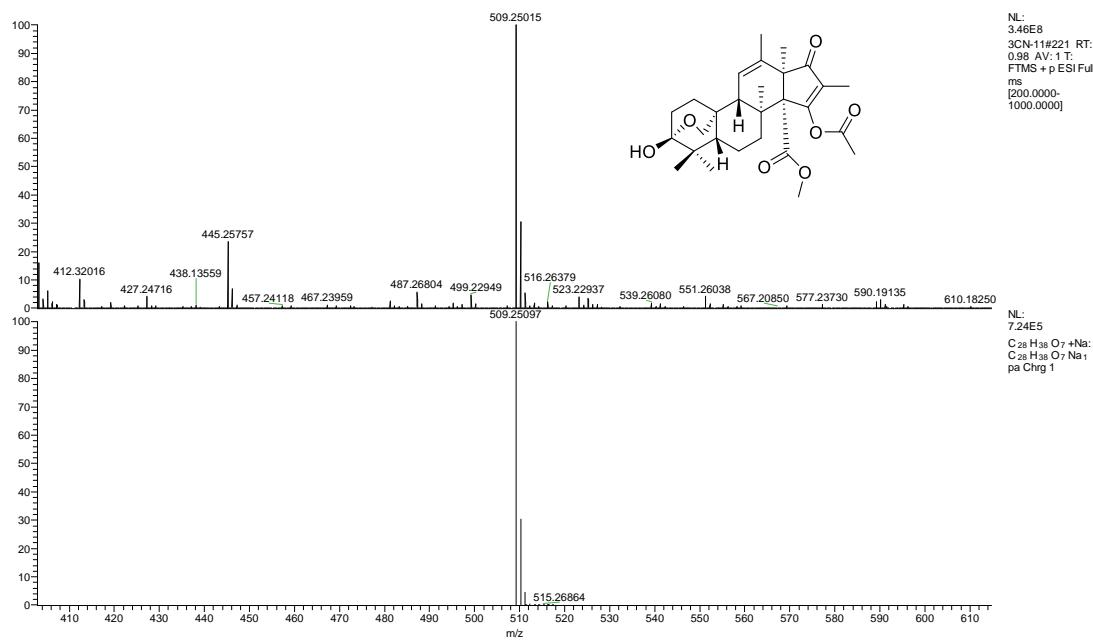
**Figure S14.** H, H-COSY spectrum of compound **2** ( $\text{CD}_3\text{OD}$ )



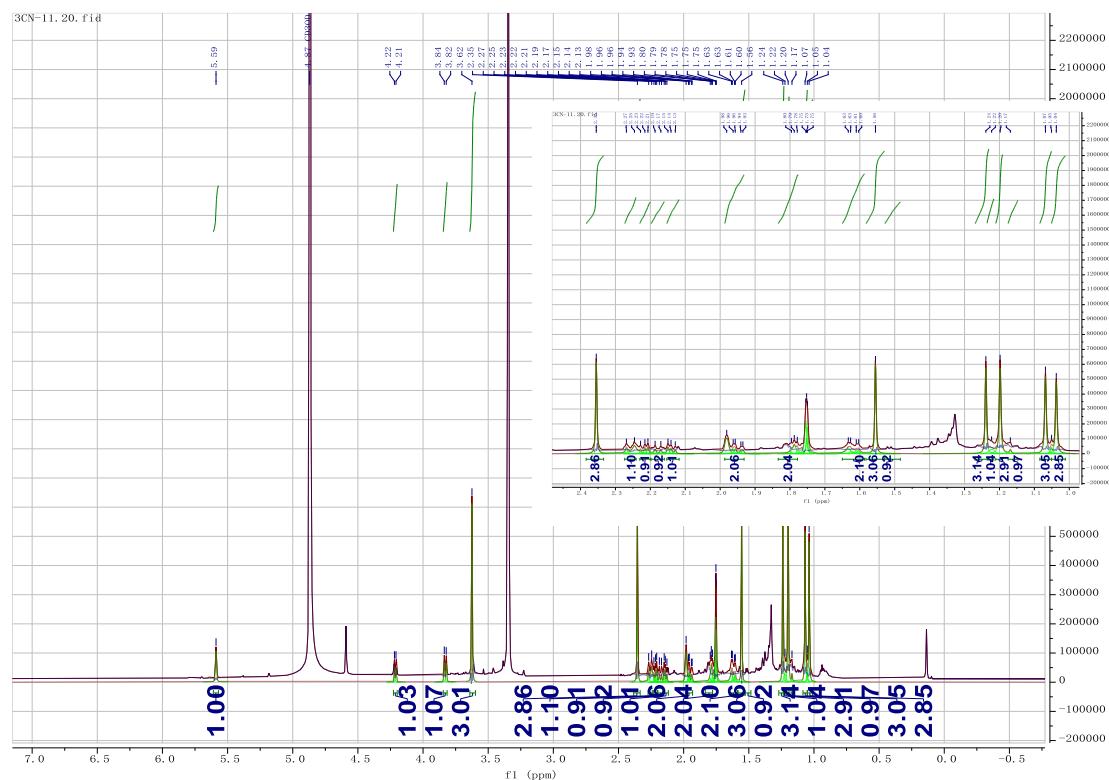
**Figure S15.** HMBC spectrum of compound 2 ( $\text{CD}_3\text{OD}$ )



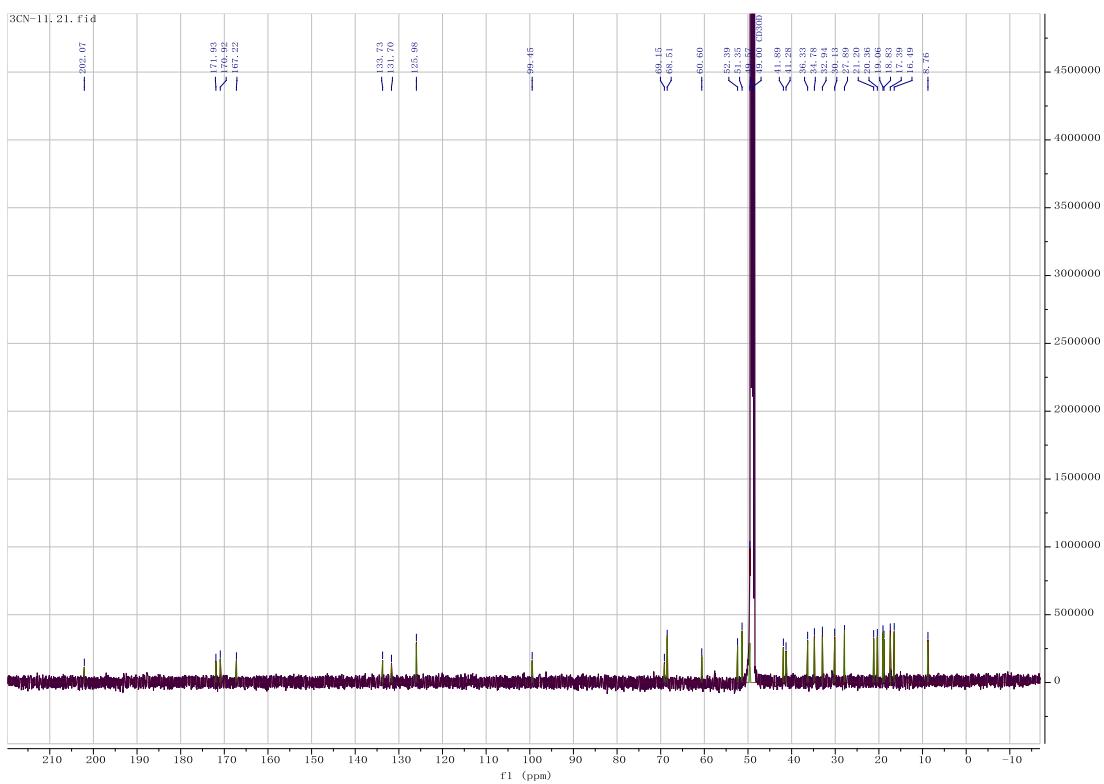
**Figure S16.** NOE spectrum of compound 2 ( $\text{CD}_3\text{OD}$ )



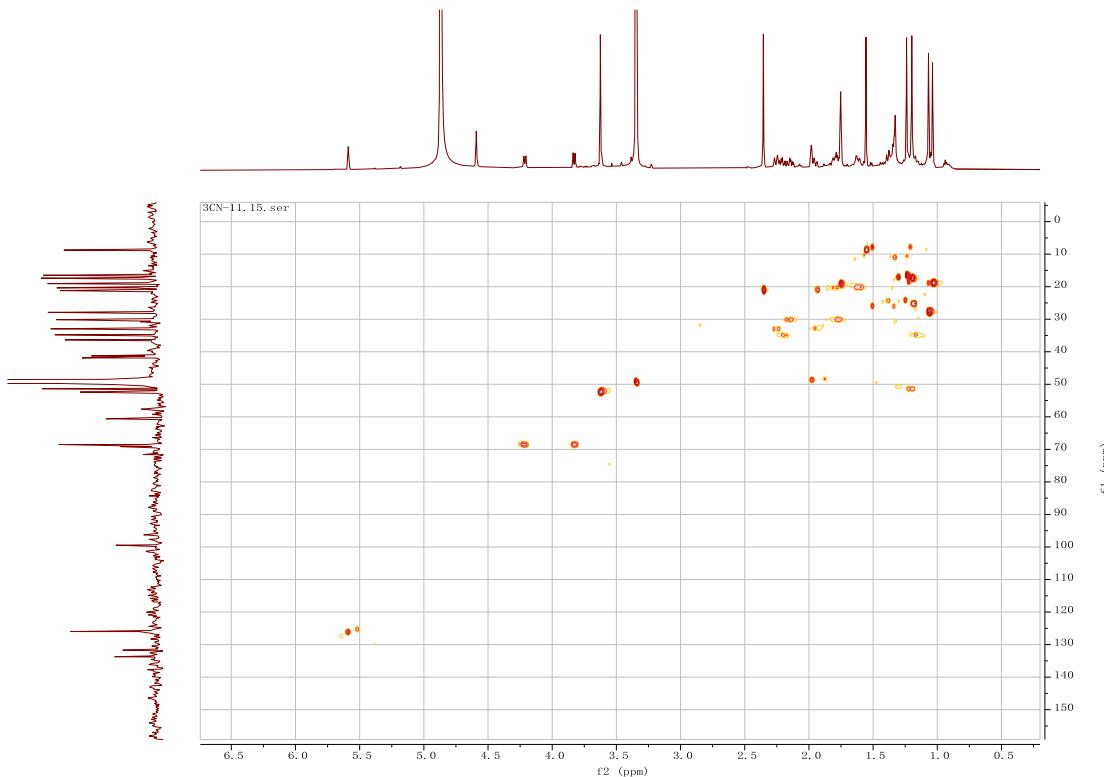
**Figure S17.** HRESIMS spectrum of compound 3



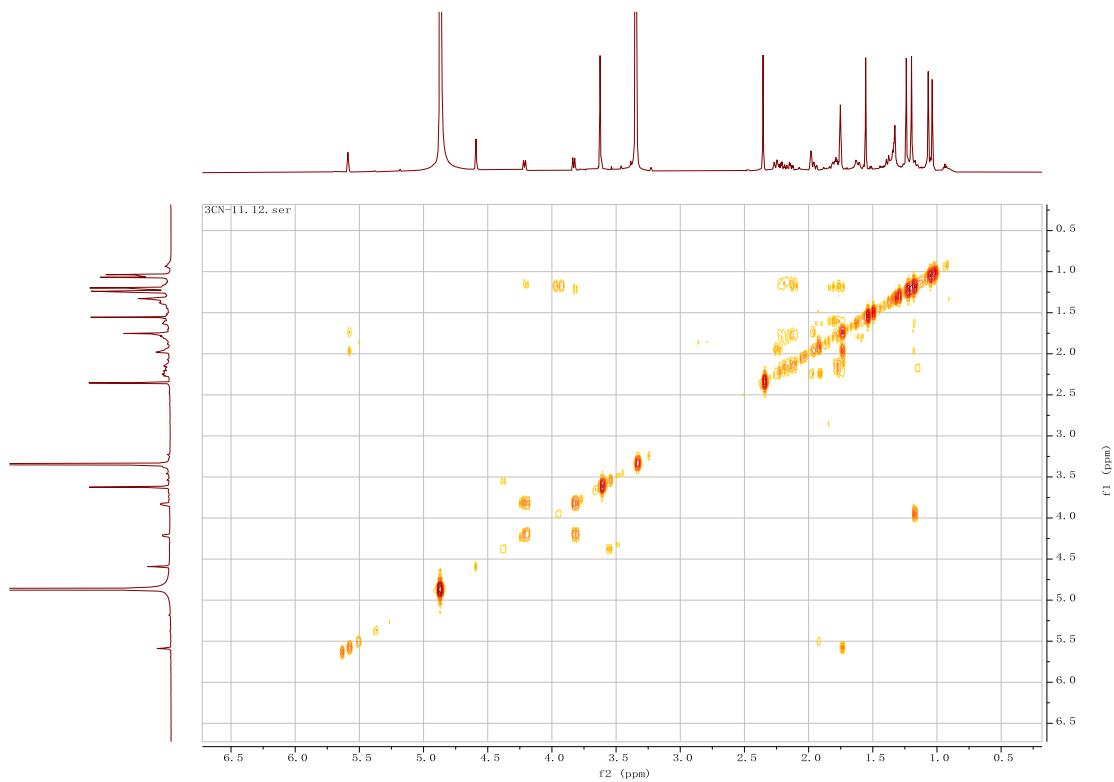
**Figure S18.** <sup>1</sup>H NMR spectrum of compound 3 (600 MHz, CD<sub>3</sub>OD)



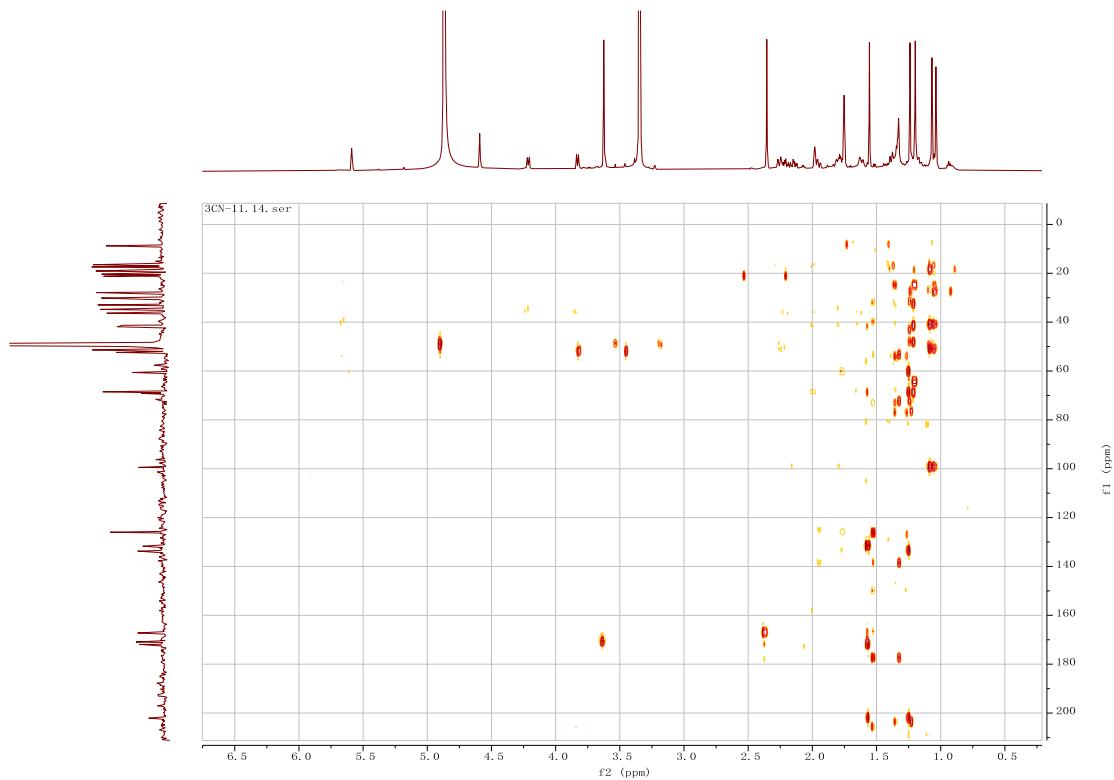
**Figure S19.** <sup>13</sup>C NMR spectrum of compound 3 (150 MHz, CD<sub>3</sub>OD)



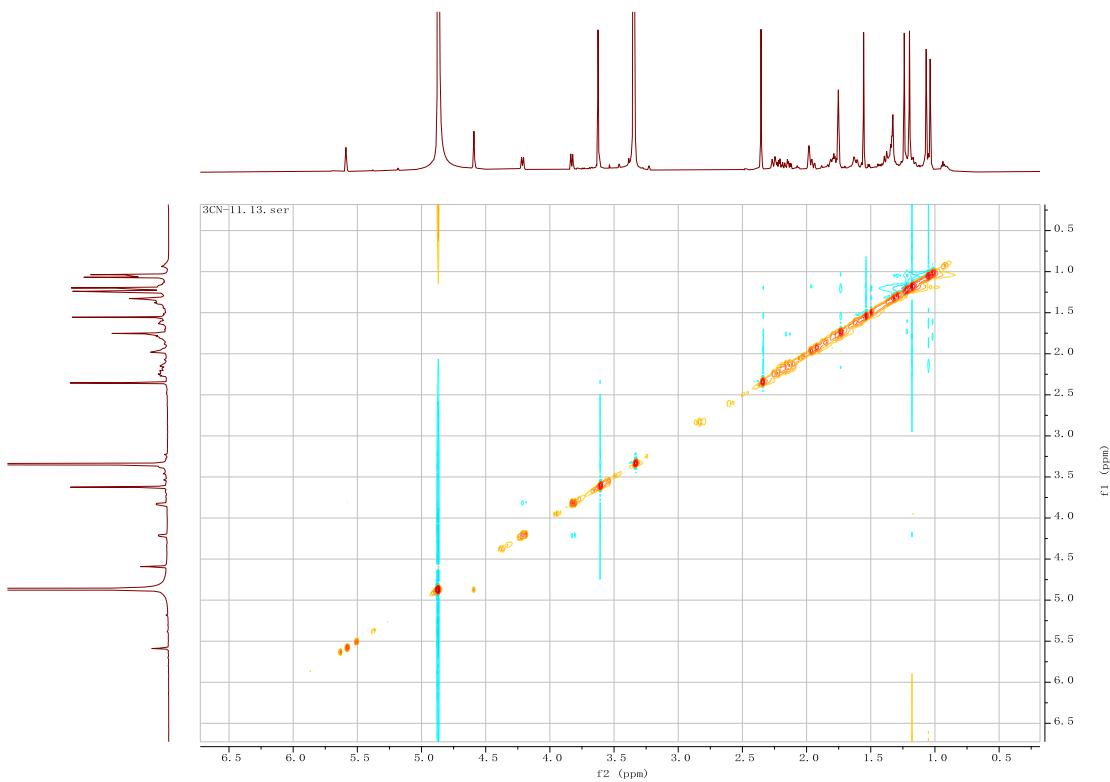
**Figure S20.** HSQC spectrum of compound 3 (CD<sub>3</sub>OD)



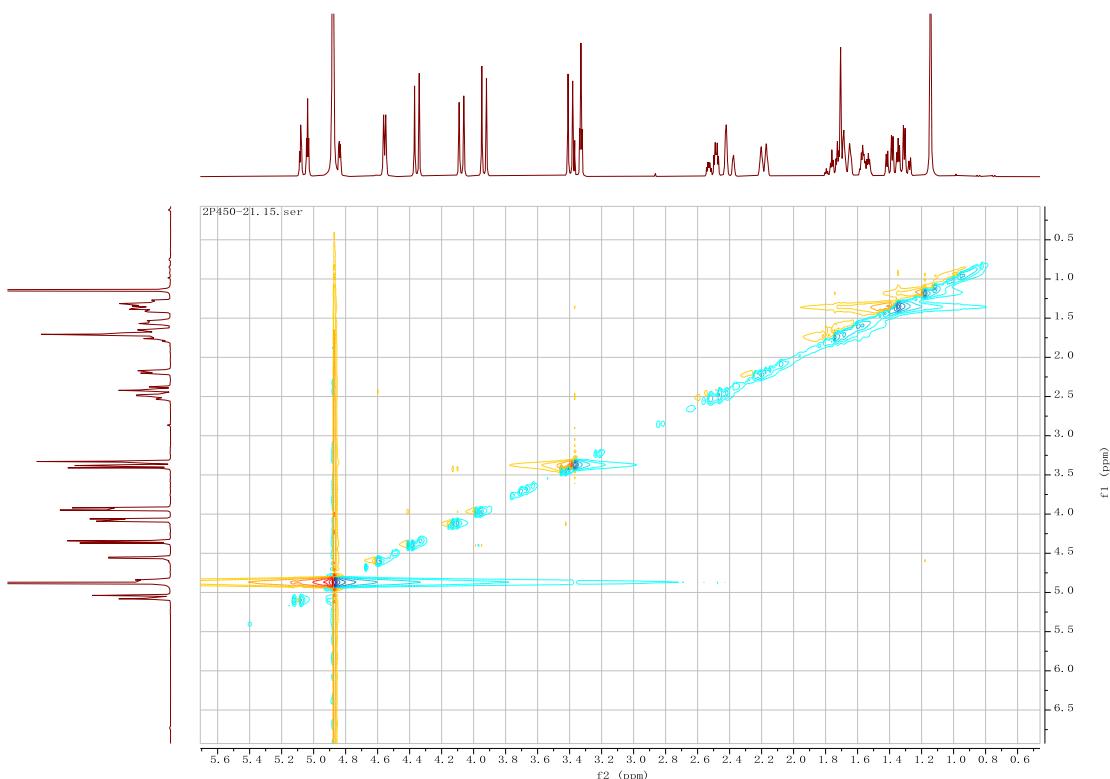
**Figure S21.** H, H-COSY spectrum of compound 3 (CD<sub>3</sub>OD)



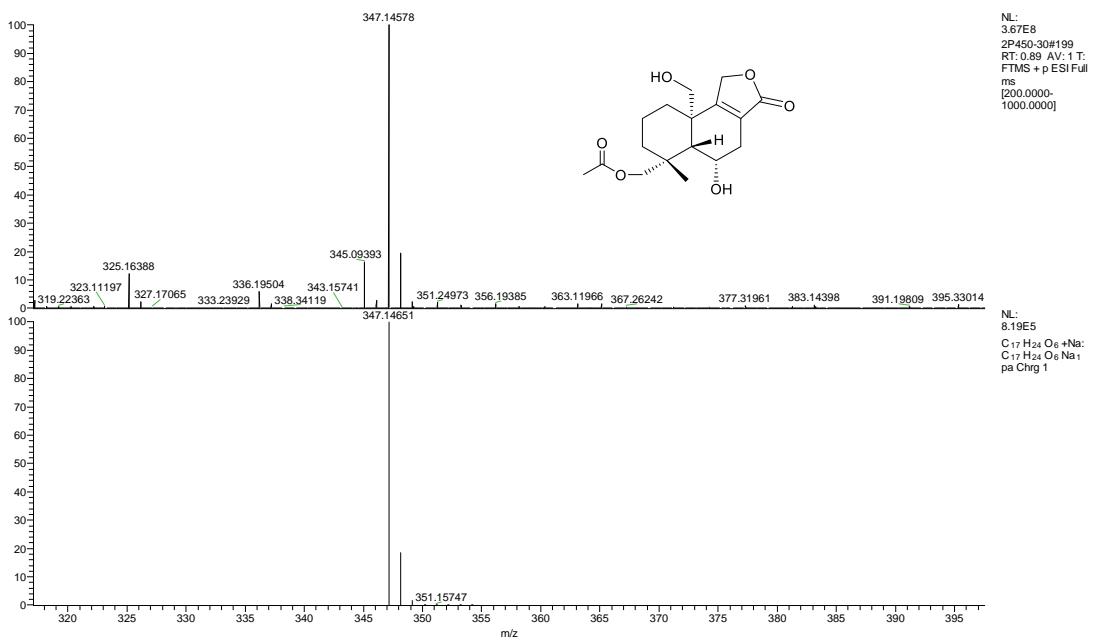
**Figure S22.** HMBC spectrum of compound 3 (CD<sub>3</sub>OD)



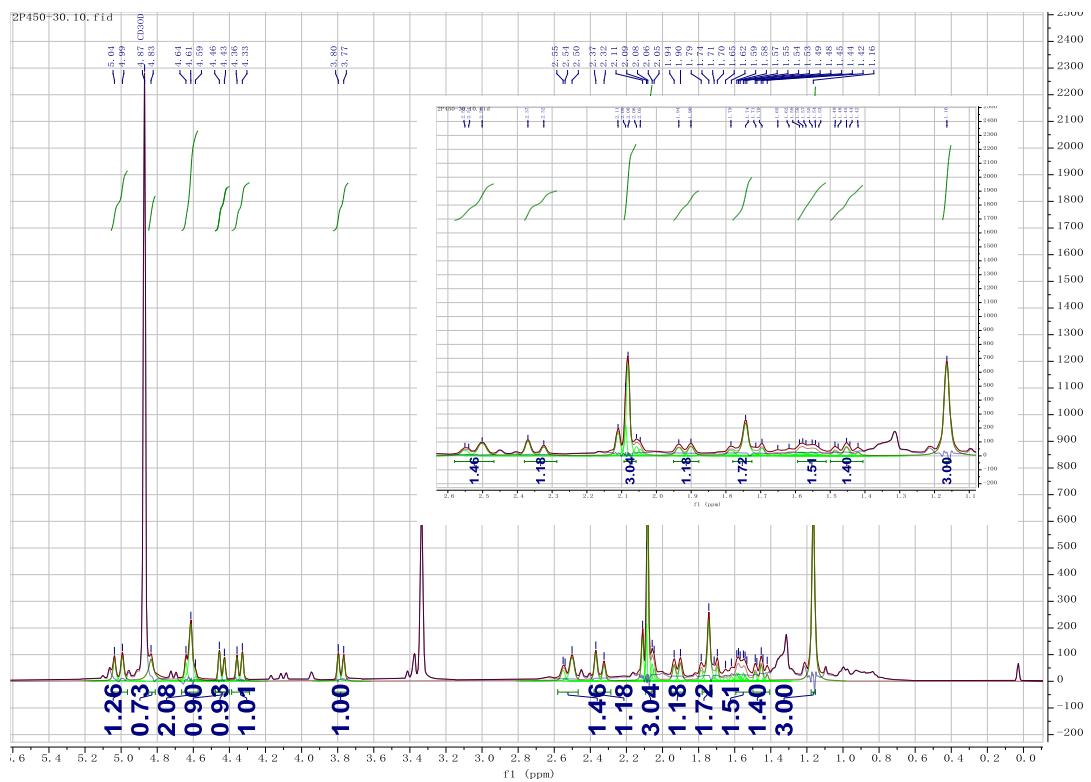
**Figure S23.** NOE spectrum of compound 3 ( $\text{CD}_3\text{OD}$ )



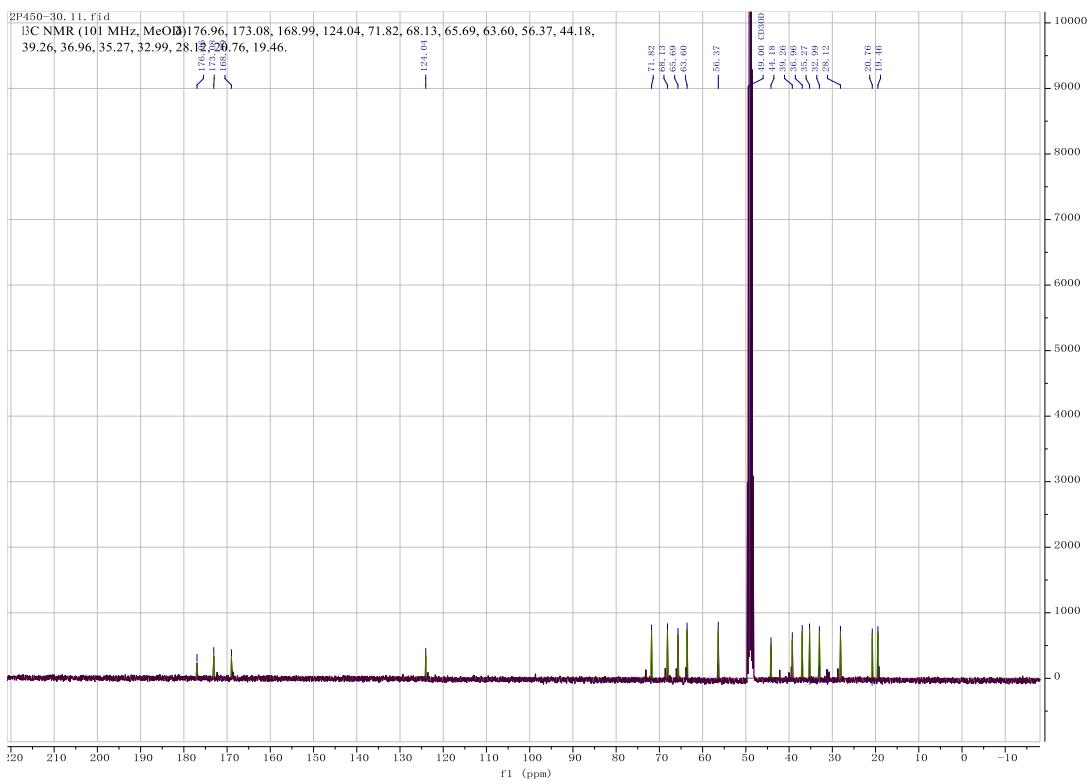
**Figure S24.** NOE spectrum of compound 14 ( $\text{CD}_3\text{OD}$ )



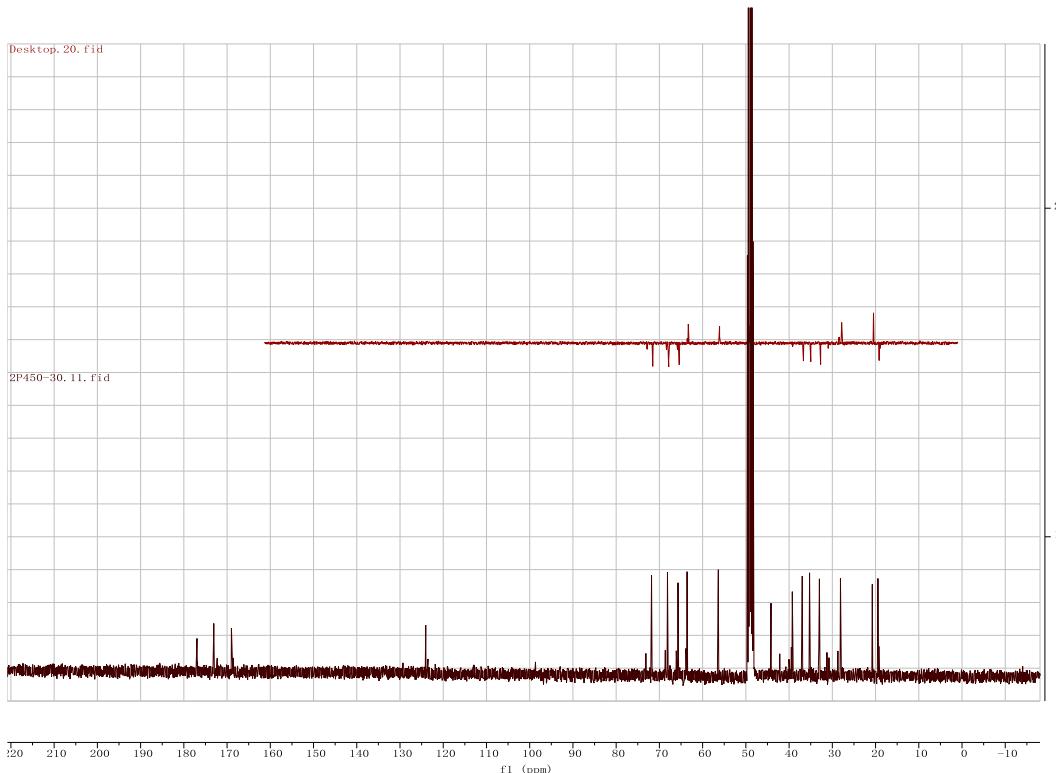
**Figure S25.** HRESIMS spectrum of compound **15**



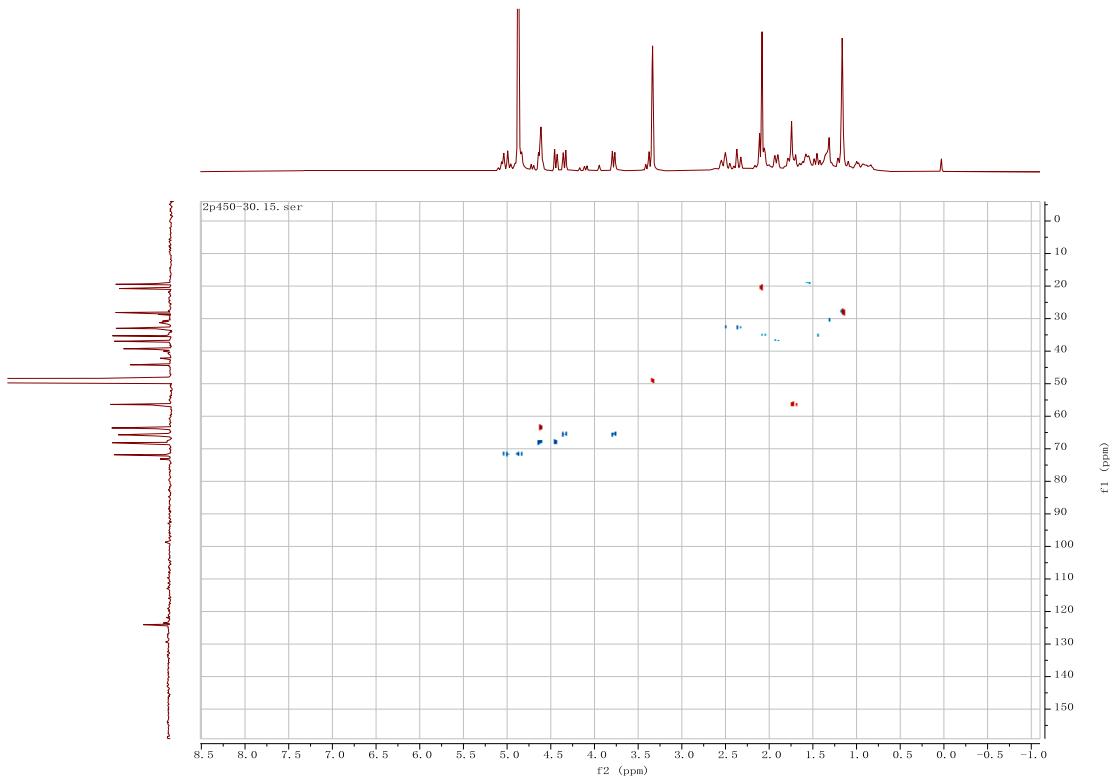
**Figure S26.** <sup>1</sup>H NMR spectrum of compound **15** (400 MHz, CD<sub>3</sub>OD)



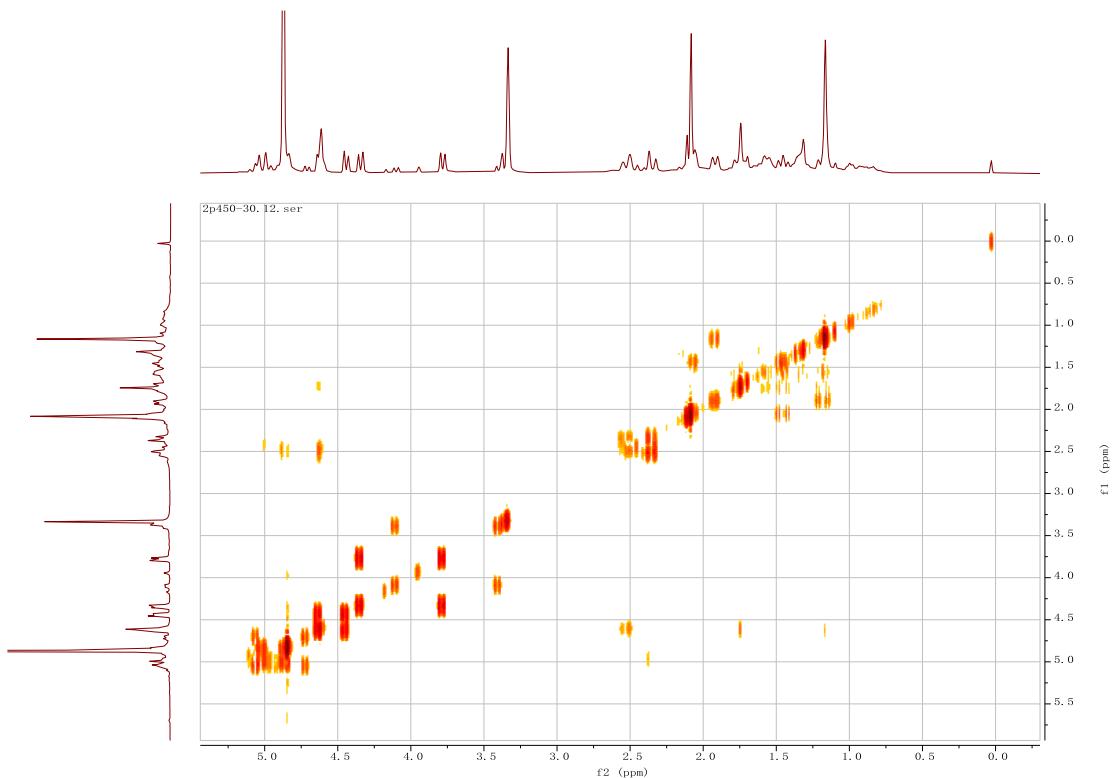
**Figure S27.** <sup>13</sup>C NMR spectrum of compound **15** (100 MHz, CD<sub>3</sub>OD)



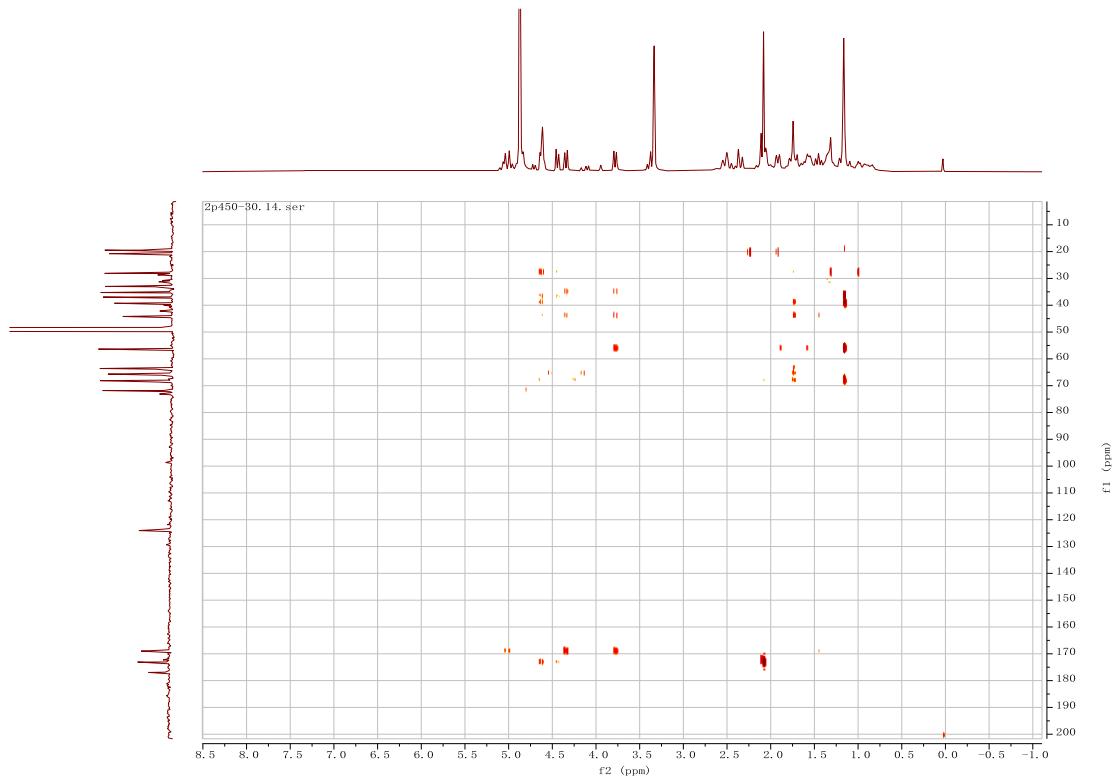
**Figure S28.** DEPT135 spectrum of compound **15** (150 MHz, CD<sub>3</sub>OD)



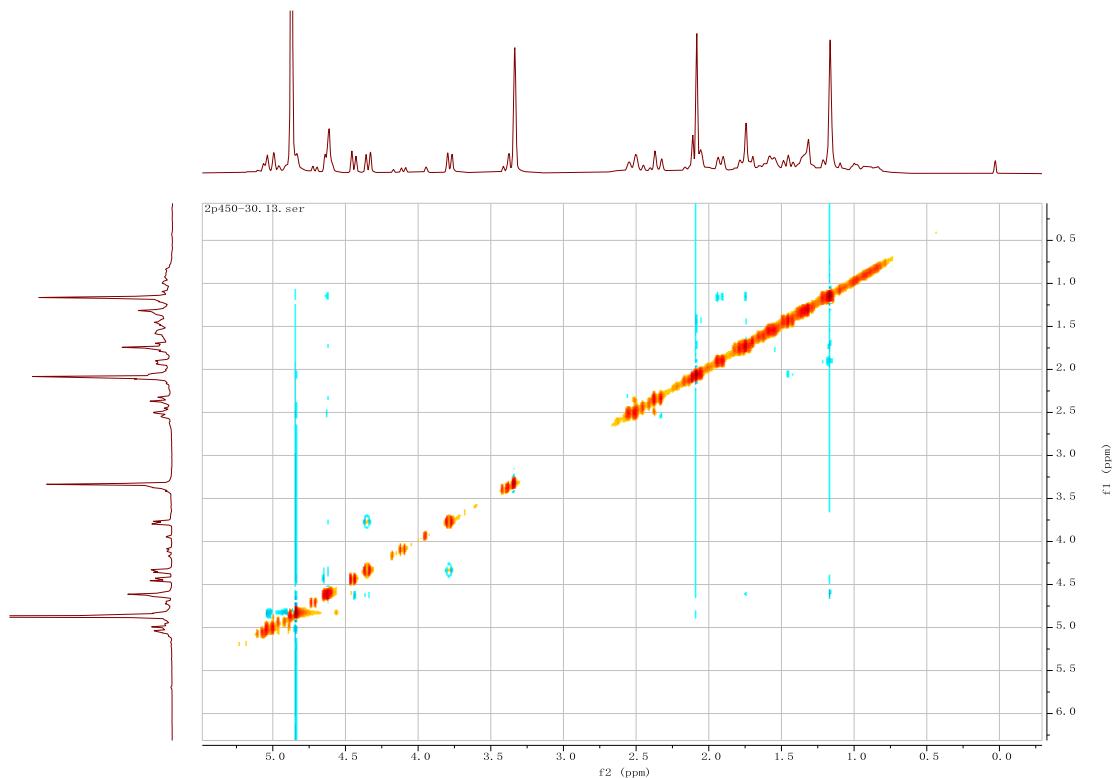
**Figure S29.** HSQC spectrum of compound **15** ( $\text{CD}_3\text{OD}$ )



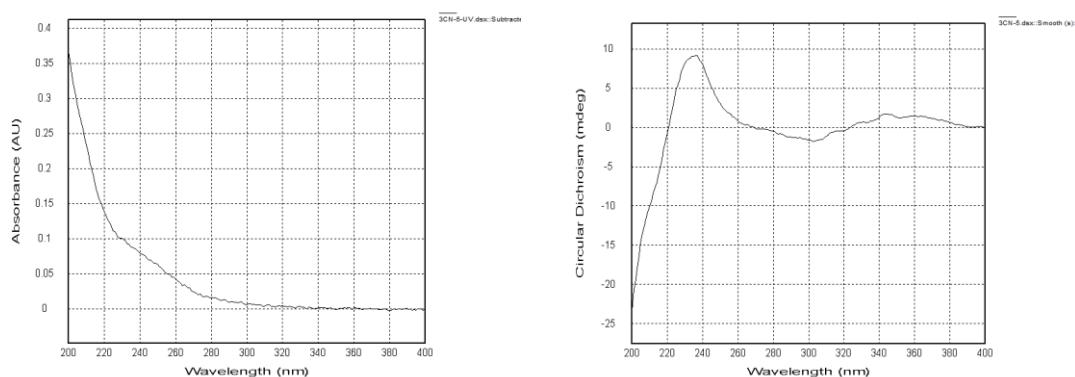
**Figure S30.** H, H-COSY spectrum of compound **15** ( $\text{CD}_3\text{OD}$ )



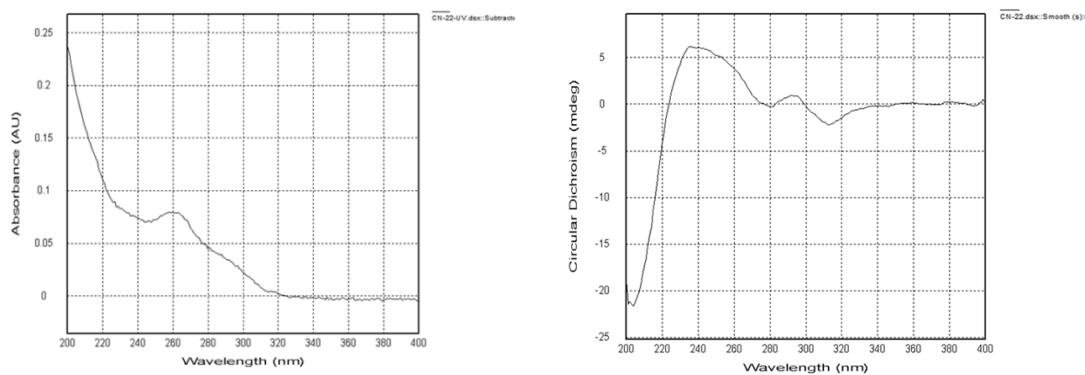
**Figure S31.** HMBC spectrum of compound **15** ( $\text{CD}_3\text{OD}$ )



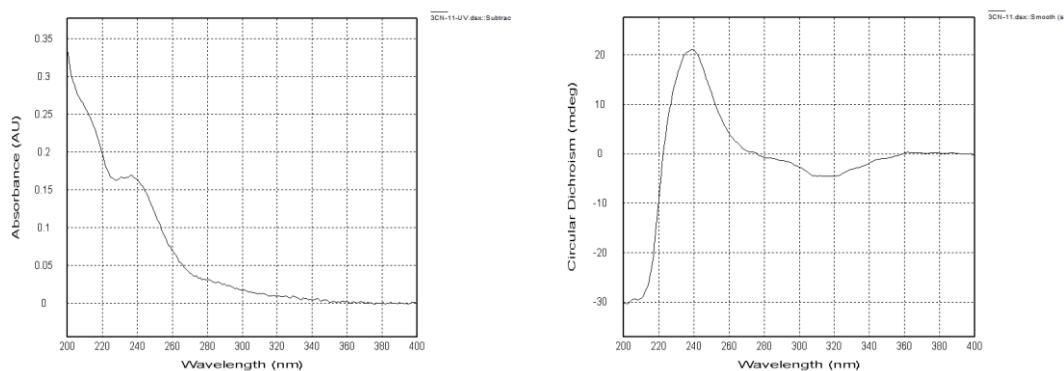
**Figure S32.** NOE spectrum of compound **15** ( $\text{CD}_3\text{OD}$ )



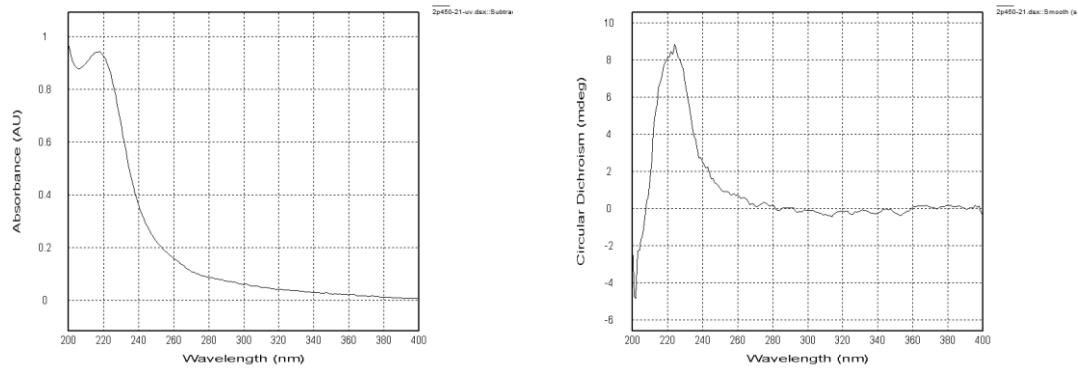
**Figure S33.** UV and ECD of compound **1** ( $\text{CD}_3\text{OD}$ )



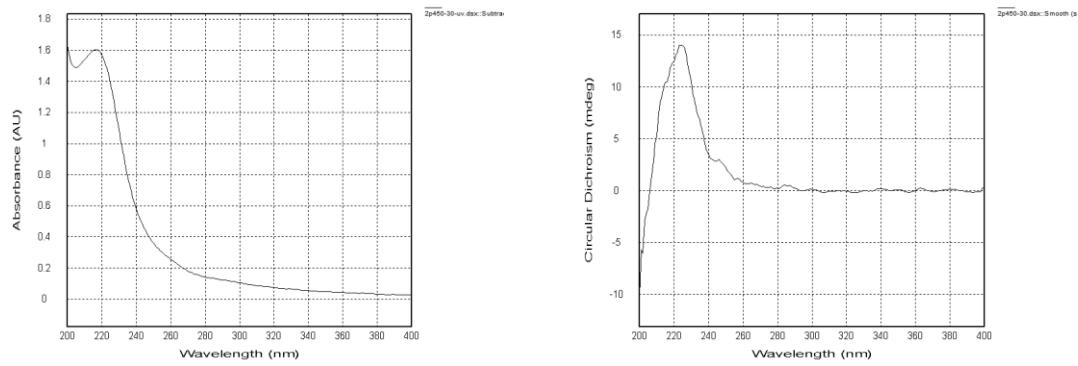
**Figure S34.** UV and ECD of compound **2** ( $\text{CD}_3\text{OD}$ )



**Figure S35.** UV and ECD of compound **3** ( $\text{CD}_3\text{OD}$ )



**Figure S36.** UV and ECD of compound **14** ( $\text{CD}_3\text{OD}$ )



**Figure S37.** UV and ECD of compound **15** ( $\text{CD}_3\text{OD}$ )