

**Przewalcyrones A–F, Epoxychromene-Containing Polycyclic  
Polyprenylated Acylphloroglucinols with Immunosuppressive Activity  
from *Hypericum przewalskii* Maxim.**

Yulin Duan,<sup>a</sup> Shuangshuang Xie,<sup>a</sup> Yi Guo,<sup>a</sup> Yuben Qiao,<sup>a</sup> Zhengyi Shi,<sup>a</sup> Li Tao,<sup>a</sup> Mengyi Deng,<sup>a</sup>

Yunfang Cao,<sup>a</sup> Yongbo Xue,<sup>b,\*</sup> Changxing Qi,<sup>a,\*</sup> and Yonghui Zhang<sup>a,\*</sup>

<sup>a</sup> *Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy,  
Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, People's  
Republic of China*

<sup>b</sup> *School of Pharmaceutical Sciences (Shenzhen), Sun Yat-Sen University, Guangzhou 510275, People's  
Republic of China*

\*Corresponding author

*E-mail addresses:* xueyb@mail.sysu.edu.cn (Y. Xue); qichangxing@hust.edu.cn (C. Qi);  
zhangyh@mails.tjmu.edu.cn (Y. Zhang).

<b>Contents</b>	<b>Pages</b>
<b>Figure S1.</b> <sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD) spectrum of compound <b>1</b>	5
<b>Figure S2.</b> <sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD) spectrum of compound <b>1</b>	5
<b>Figure S3.</b> HSQC spectrum of compound <b>1</b>	6
<b>Figure S4.</b> HMBC spectrum of compound <b>1</b>	6
<b>Figure S5.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of compound <b>1</b>	7
<b>Figure S6.</b> NOESY spectrum of compound <b>1</b>	7
<b>Figure S7.</b> HR-ESI-MS spectrum of compound <b>1</b>	8
<b>Figure S8.</b> UV spectrum of compound <b>1</b>	8
<b>Figure S9.</b> IR spectrum of compound <b>1</b>	9
<b>Figure S10.</b> <sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD) spectrum of compound <b>2</b>	9
<b>Figure S11.</b> <sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD) spectrum of compound <b>2</b>	10
<b>Figure S12.</b> HSQC spectrum of compound <b>2</b>	10
<b>Figure S13.</b> HMBC spectrum of compound <b>2</b>	11
<b>Figure S14.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of compound <b>2</b>	11
<b>Figure S15.</b> NOESY spectrum of compound <b>2</b>	12
<b>Figure S16.</b> HR-ESI-MS spectrum of compound <b>2</b>	12
<b>Figure S17.</b> UV spectrum of compound <b>2</b>	13
<b>Figure S18.</b> IR spectrum of compound <b>2</b>	13
<b>Figure S19.</b> <sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD) spectrum of compound <b>3</b>	14
<b>Figure S20.</b> <sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD) spectrum of compound <b>3</b>	14
<b>Figure S21.</b> HSQC spectrum of compound <b>3</b>	15
<b>Figure S22.</b> HMBC spectrum of compound <b>3</b>	15
<b>Figure S23.</b> <sup>1</sup> H- <sup>1</sup> H COSY spectrum of compound <b>3</b>	16
<b>Figure S24.</b> NOESY spectrum of compound <b>3</b>	16
<b>Figure S25.</b> HR-ESI-MS spectrum of compound <b>3</b>	17
<b>Figure S26.</b> UV spectrum of compound <b>3</b>	17
<b>Figure S27.</b> IR spectrum of compound <b>3</b>	18
<b>Figure S28.</b> <sup>1</sup> H-NMR (600 MHz, CD <sub>3</sub> OD) spectrum of compound <b>4</b>	18

<b>Figure S29.</b> <sup>13</sup> C-NMR (150 MHz, CD <sub>3</sub> OD) spectrum of compound <b>4</b>	19
<b>Figure S30.</b> HSQC spectrum of compound <b>4</b>	19
<b>Figure S31.</b> HMBC spectrum of compound <b>4</b>	20
<b>Figure S32.</b> <sup>1</sup> H– <sup>1</sup> H COSY spectrum of compound <b>4</b>	20
<b>Figure S33.</b> ROESY spectrum of compound <b>4</b>	21
<b>Figure S34.</b> HR-ESI-MS spectrum of compound <b>4</b>	21
<b>Figure S35.</b> UV spectrum of compound <b>4</b>	22
<b>Figure S36.</b> IR spectrum of compound <b>4</b>	22
<b>Figure S37.</b> <sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD) spectrum of compound <b>5</b>	23
<b>Figure S38.</b> <sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD) spectrum of compound <b>5</b>	23
<b>Figure S39.</b> HSQC spectrum of compound <b>5</b>	24
<b>Figure S40.</b> HMBC spectrum of compound <b>5</b>	24
<b>Figure S41.</b> <sup>1</sup> H– <sup>1</sup> H COSY spectrum of compound <b>5</b>	25
<b>Figure S42.</b> NOESY spectrum of compound <b>5</b>	25
<b>Figure S43.</b> HR-ESI-MS spectrum of compound <b>5</b>	26
<b>Figure S44.</b> UV spectrum of compound <b>5</b>	26
<b>Figure S45.</b> IR spectrum of compound <b>5</b>	27
<b>Figure S46.</b> <sup>1</sup> H-NMR (800 MHz, CD <sub>3</sub> OD) spectrum of compound <b>6</b>	27
<b>Figure S47.</b> <sup>13</sup> C-NMR (200 MHz, CD <sub>3</sub> OD) spectrum of compound <b>6</b>	28
<b>Figure S48.</b> HSQC spectrum of compound <b>6</b>	28
<b>Figure S49.</b> HMBC spectrum of compound <b>6</b>	29
<b>Figure S50.</b> <sup>1</sup> H– <sup>1</sup> H COSY spectrum of compound <b>6</b>	29
<b>Figure S51.</b> ROESY spectrum of compound <b>6</b>	30
<b>Figure S52.</b> HR-ESI-MS spectrum of compound <b>6</b>	30
<b>Figure S53.</b> UV spectrum of compound <b>6</b>	31
<b>Figure S54.</b> IR spectrum of compound <b>6</b>	31
<b>Figure S55.</b> <sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD) spectrum of compound <b>7</b>	32
<b>Figure S56.</b> <sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD) spectrum of compound <b>7</b>	32
<b>Figure S57.</b> <sup>1</sup> H-NMR (600 MHz, CD <sub>3</sub> OD) spectrum of compound <b>5a</b>	33

<b>Figure S58.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of compound <b>5a</b>	33
<b>Figure S59.</b> HR-ESI-MS spectrum of compound <b>5a</b>	34
<b>Figure S60.</b> $^1\text{H}$ -NMR (600 MHz, $\text{CD}_3\text{OD}$ ) spectrum of compound <b>5b</b>	34
<b>Figure S61.</b> $^1\text{H}$ - $^1\text{H}$ COSY spectrum of compound <b>5b</b>	35
<b>Figure S62.</b> HR-ESI-MS spectrum of compound <b>5b</b>	35

Figure S1.  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**

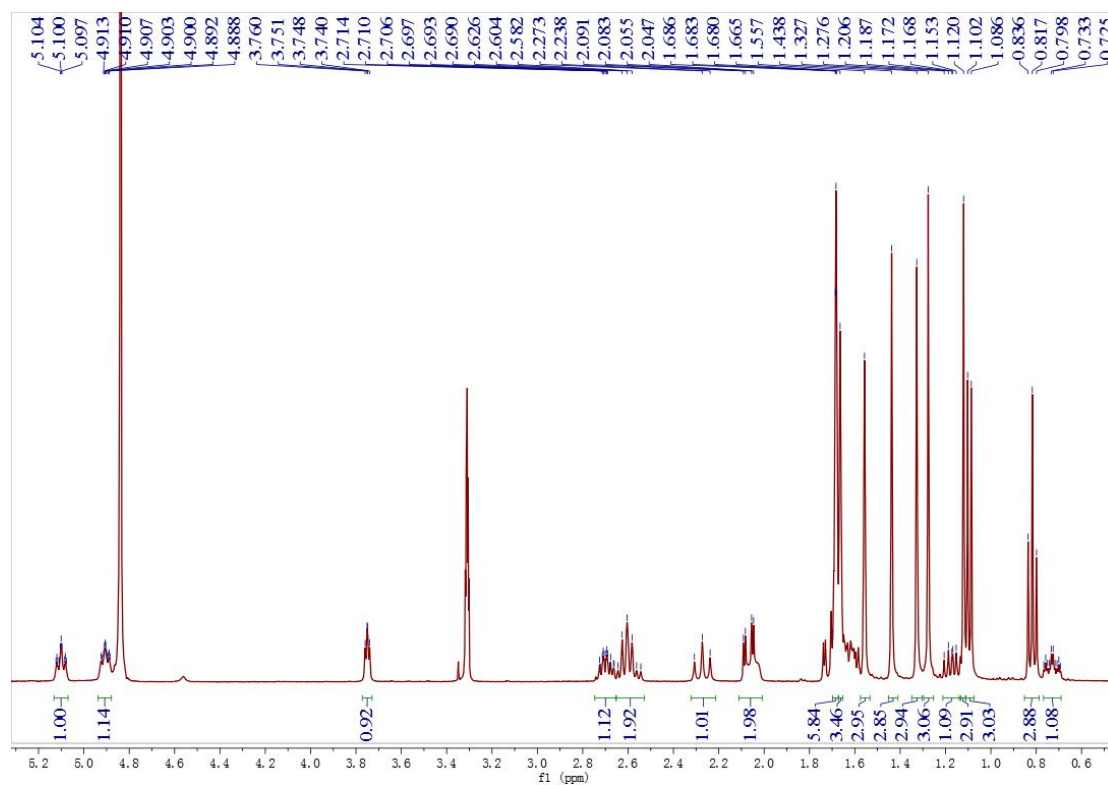
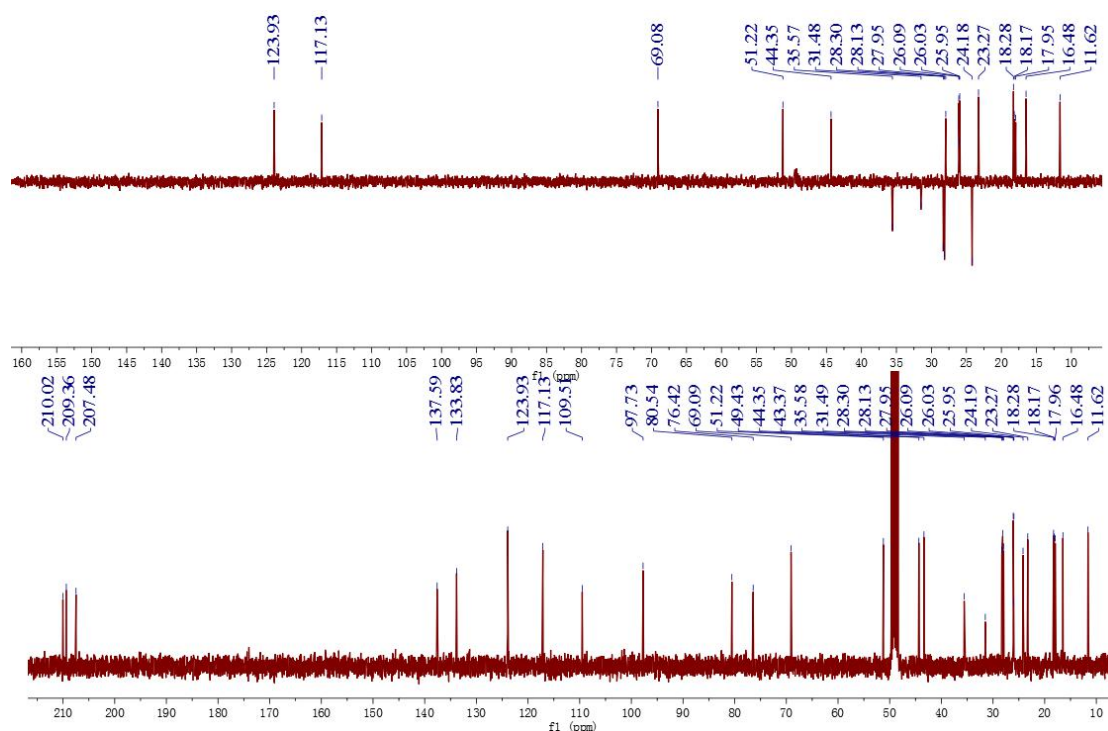
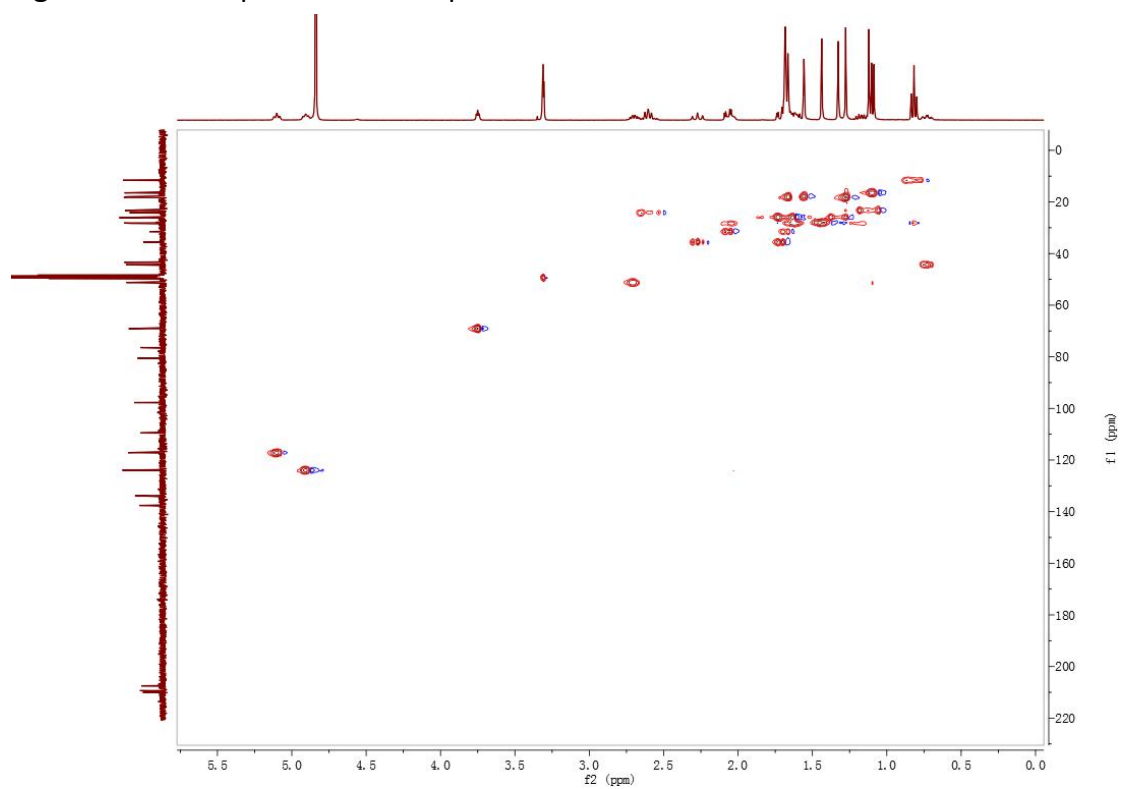


Figure S2.  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **1**



**Figure S3.** HSQC spectrum of compound **1**



**Figure S4.** HMBC spectrum of compound **1**

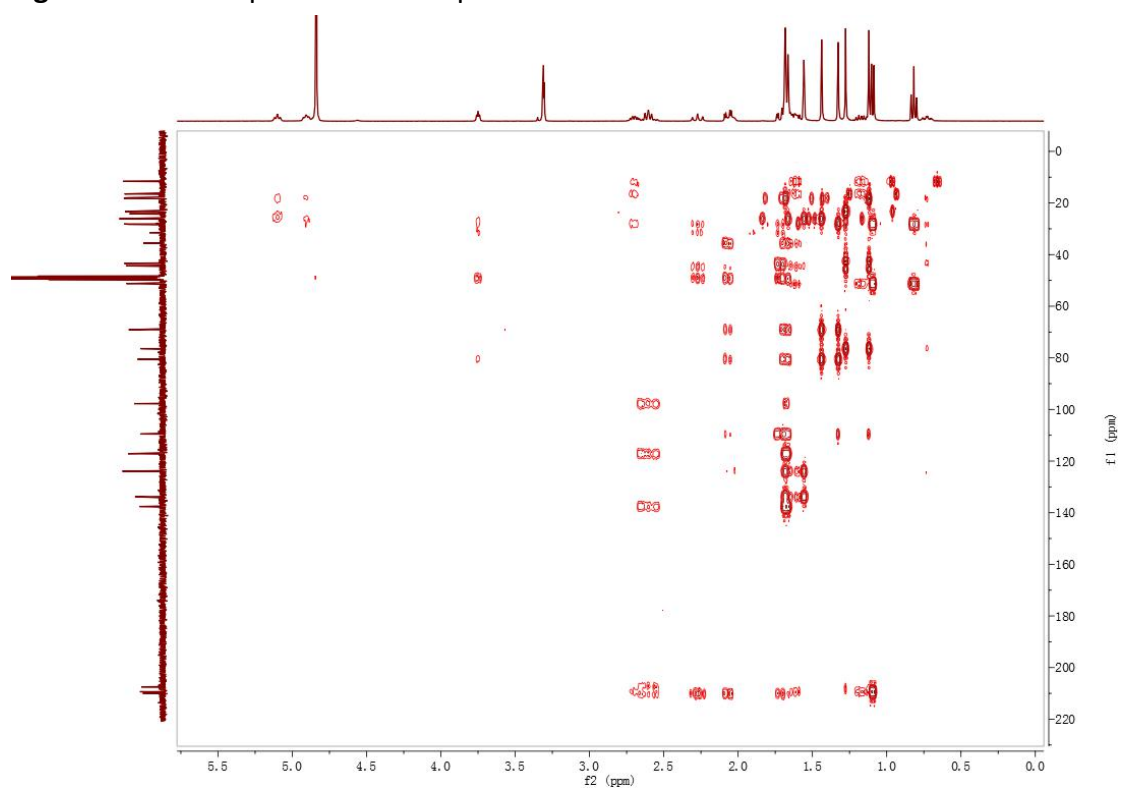


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**

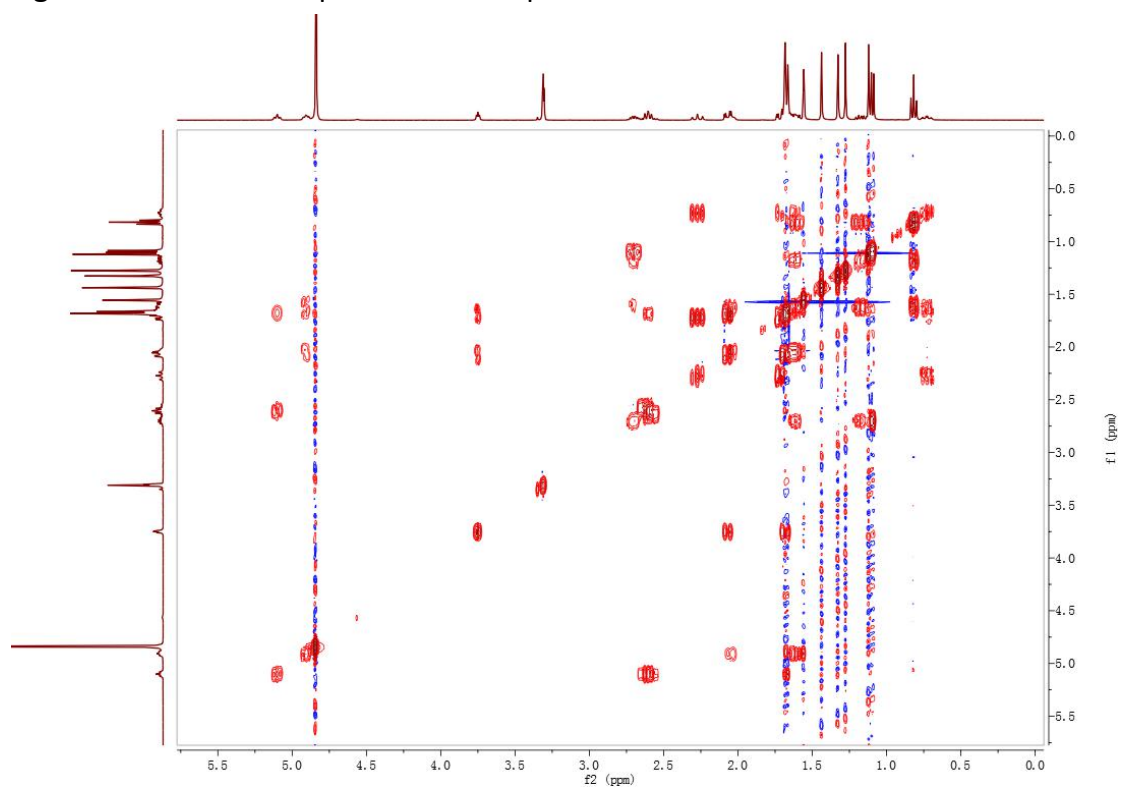
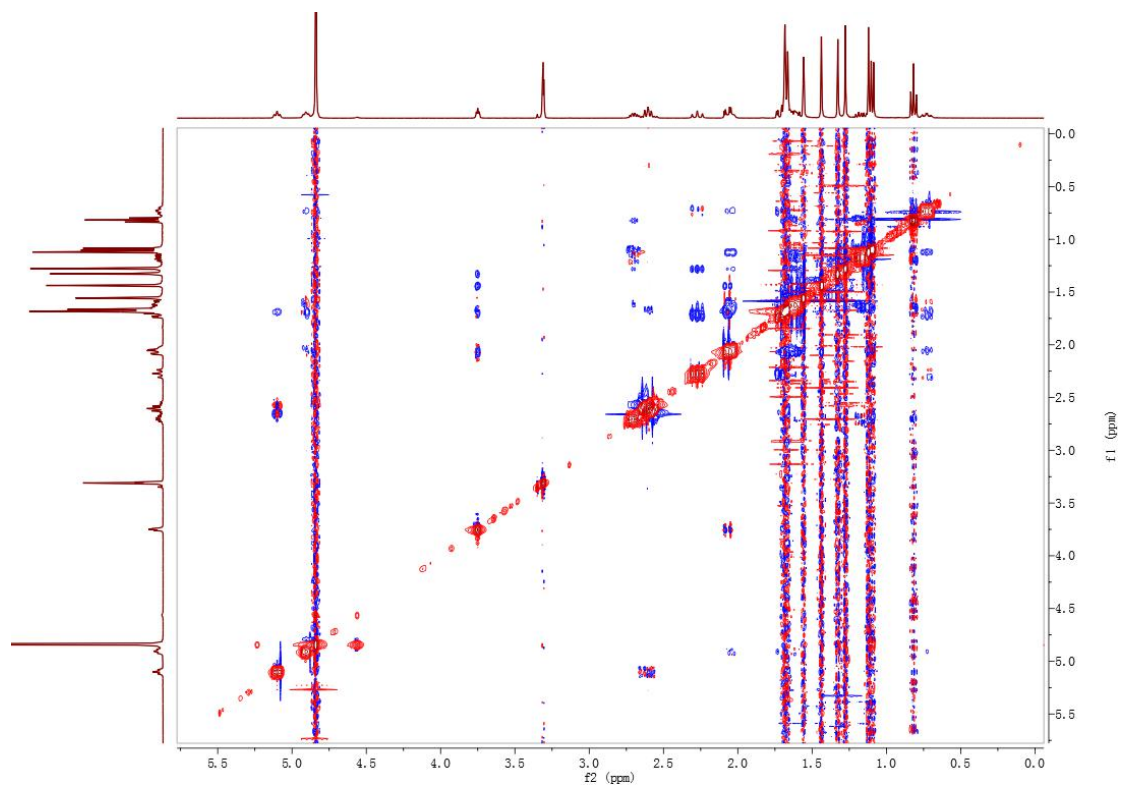
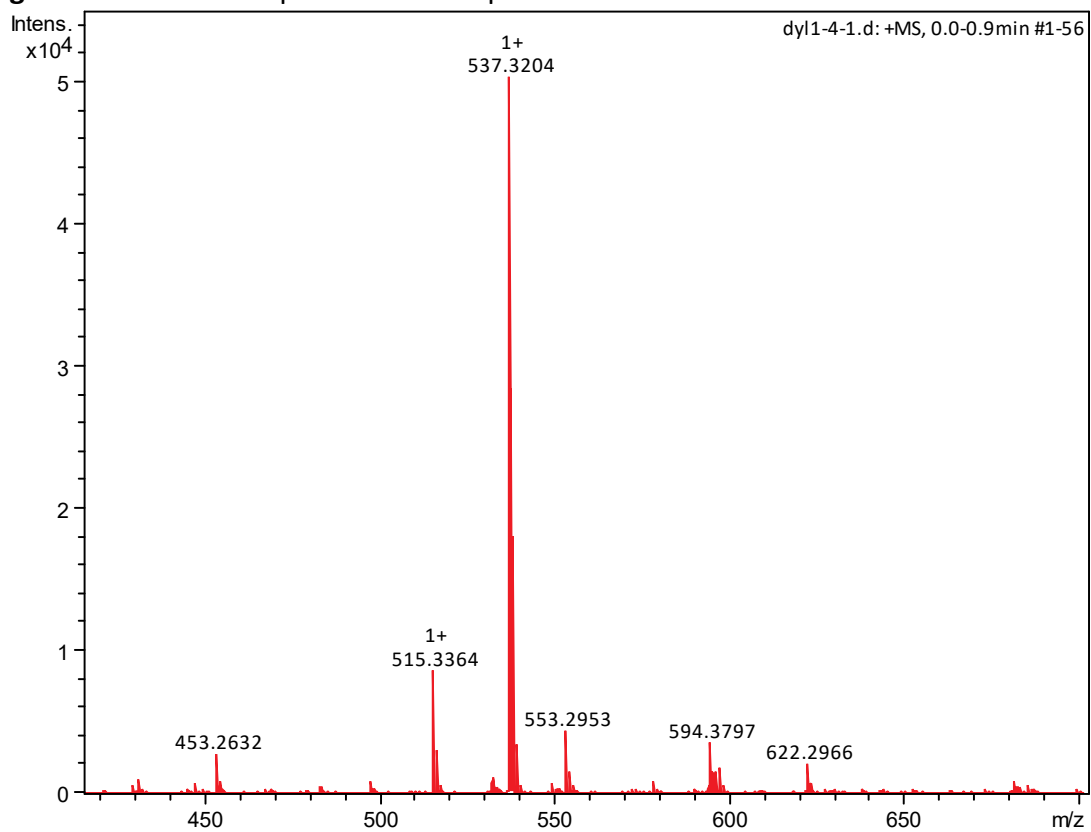


Figure S6. NOESY spectrum of compound **1**



**Figure S7.** HR-ESI-MS spectrum of compound **1**



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

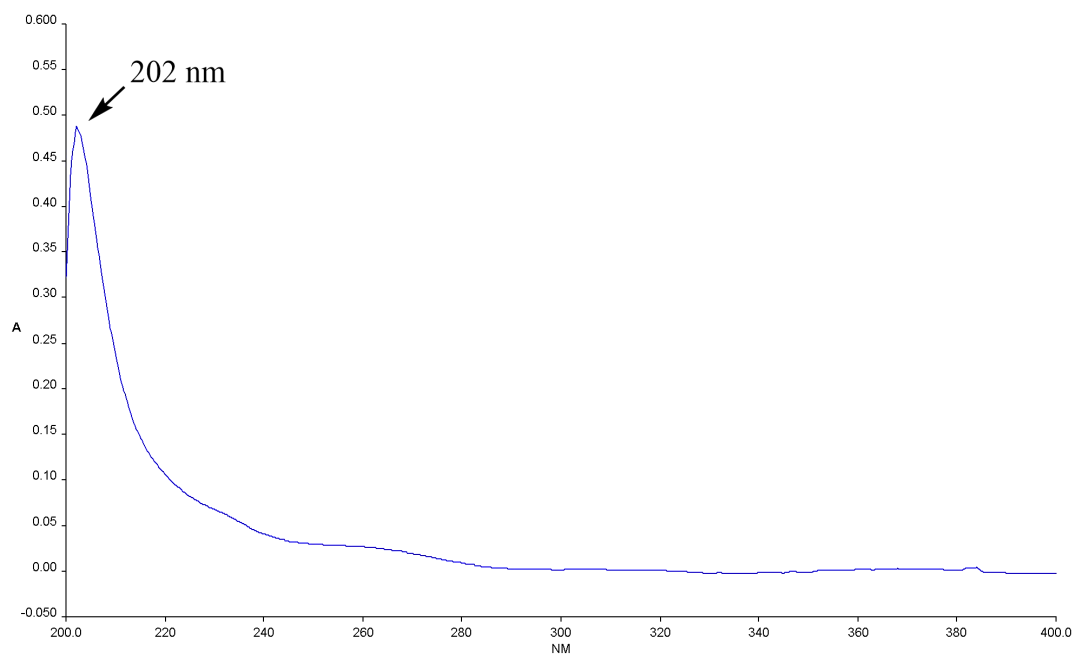




Figure S9. IR spectrum of compound 1

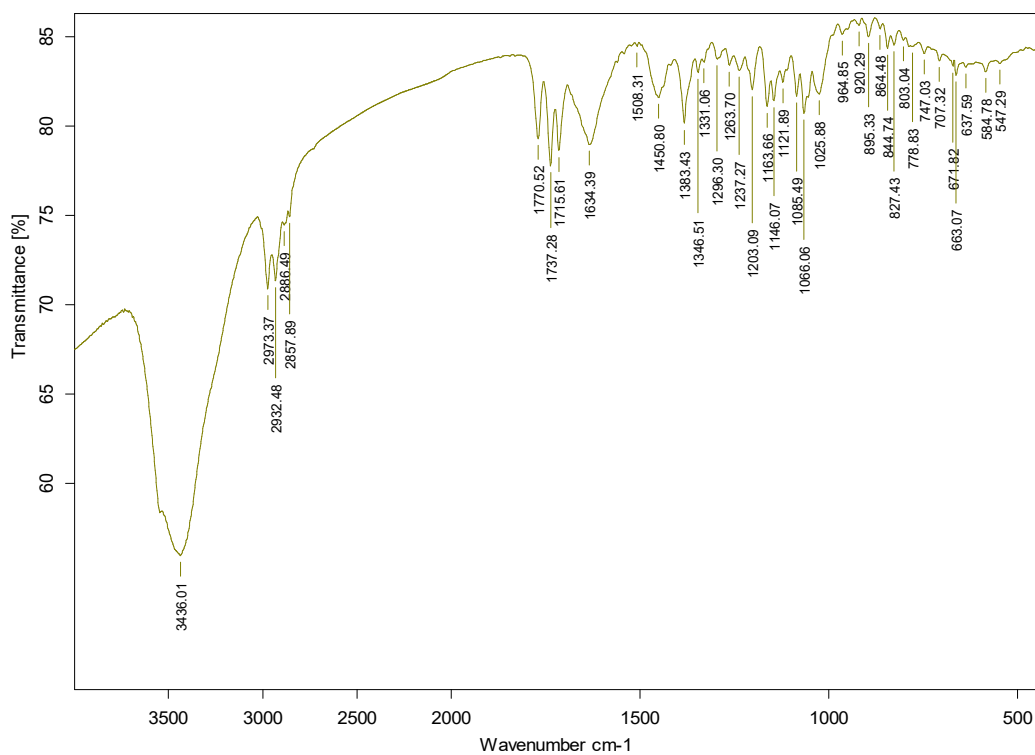


Figure S10.  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2

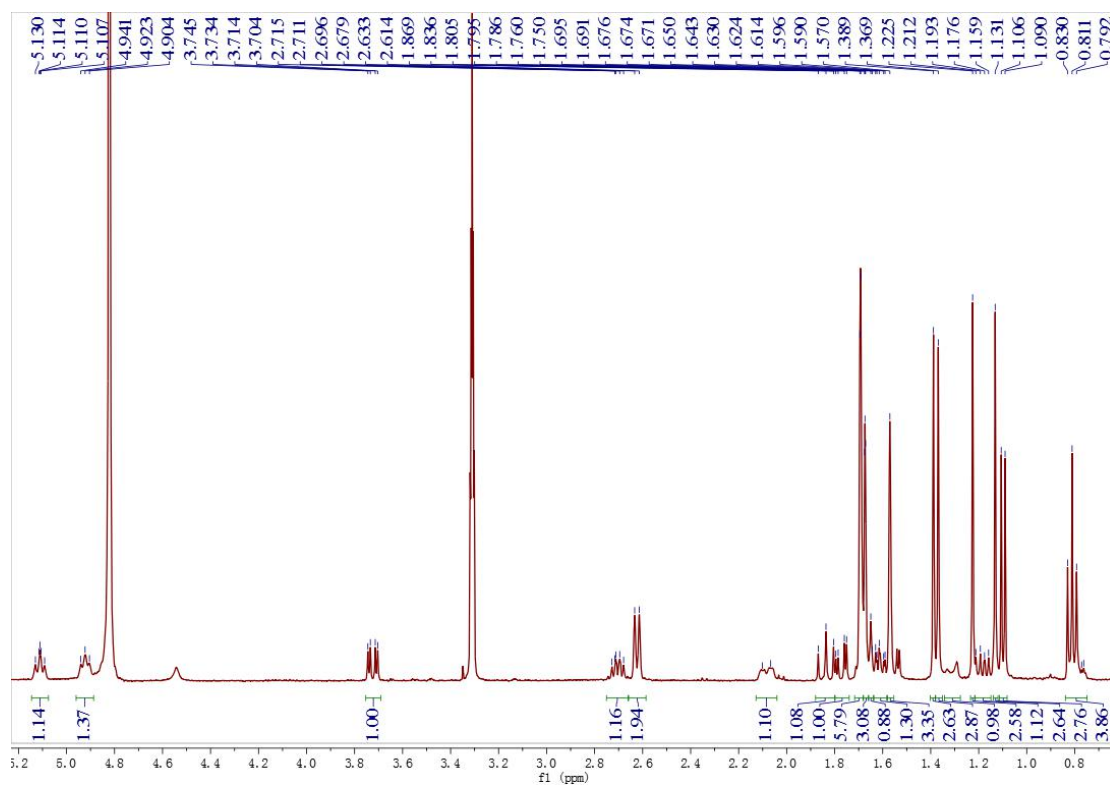


Figure S11.  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 2

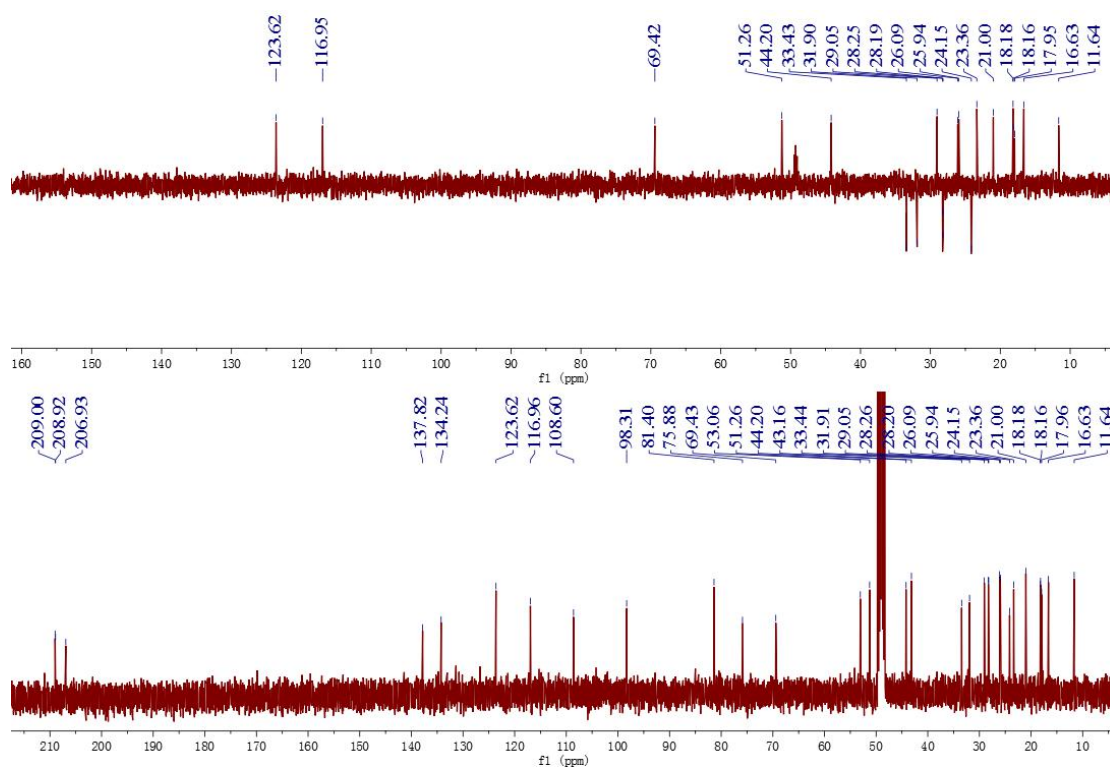


Figure S12. HSQC spectrum of compound 2

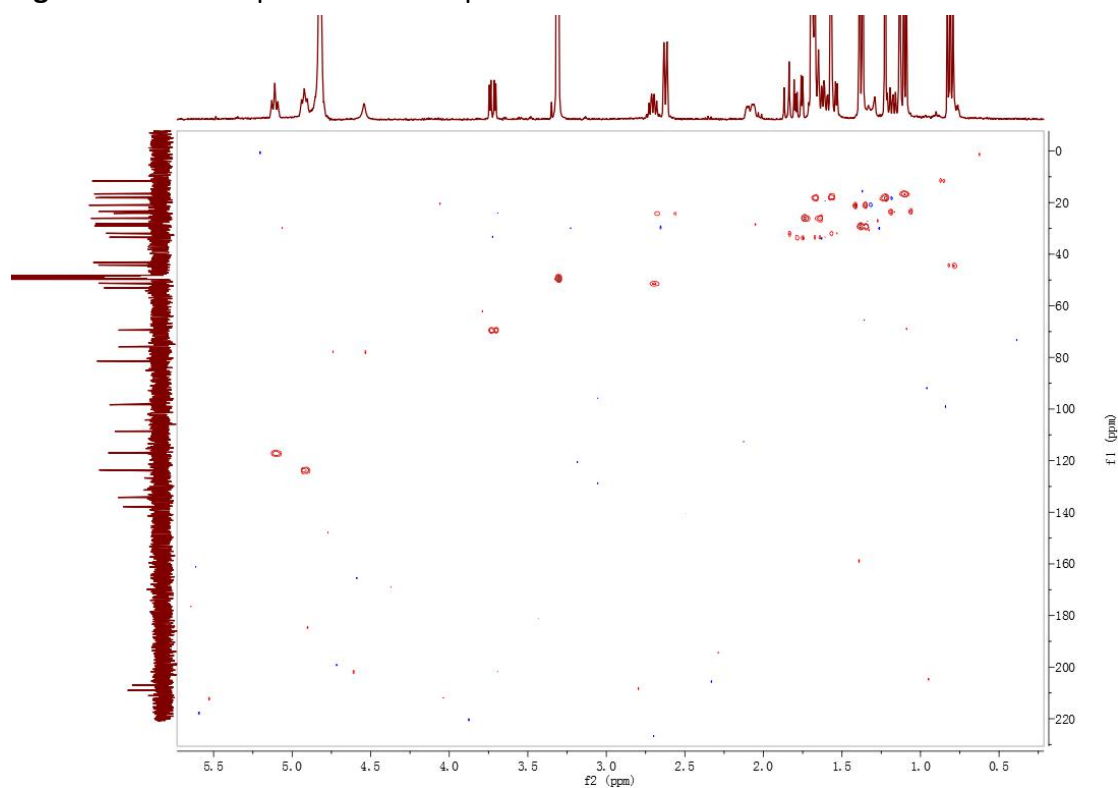


Figure S13. HMBC spectrum of compound 2

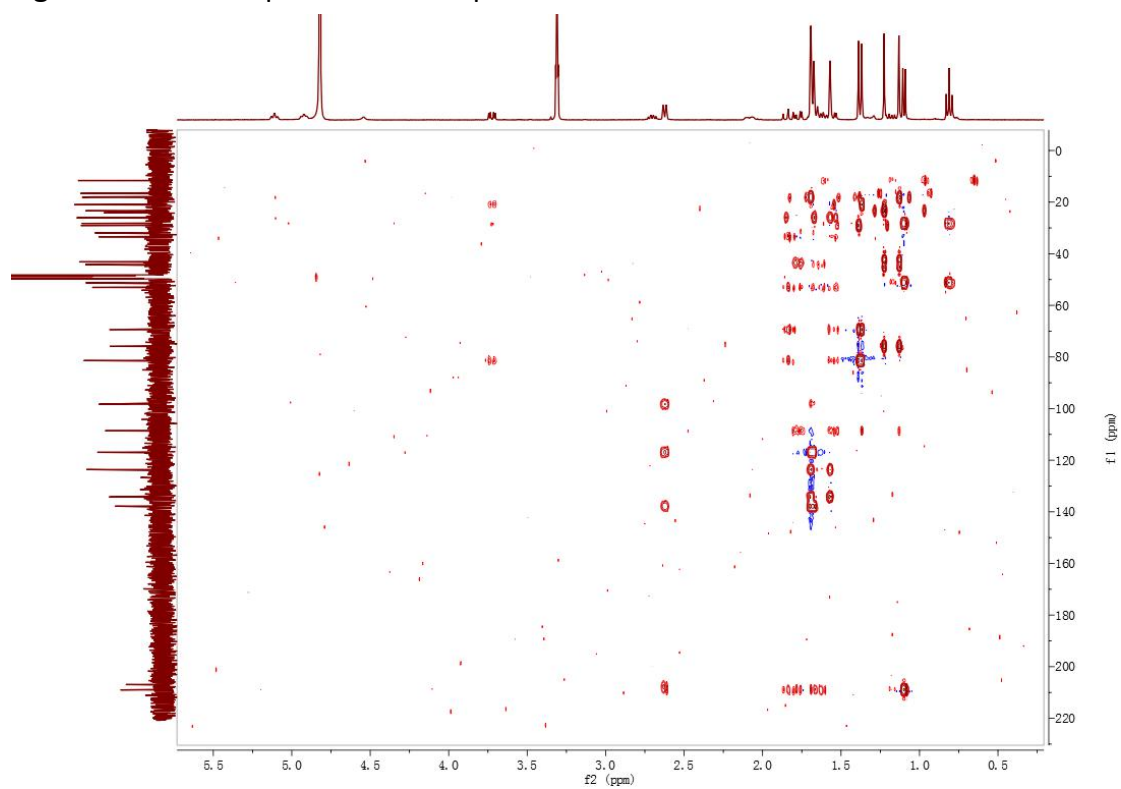


Figure S14.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 2

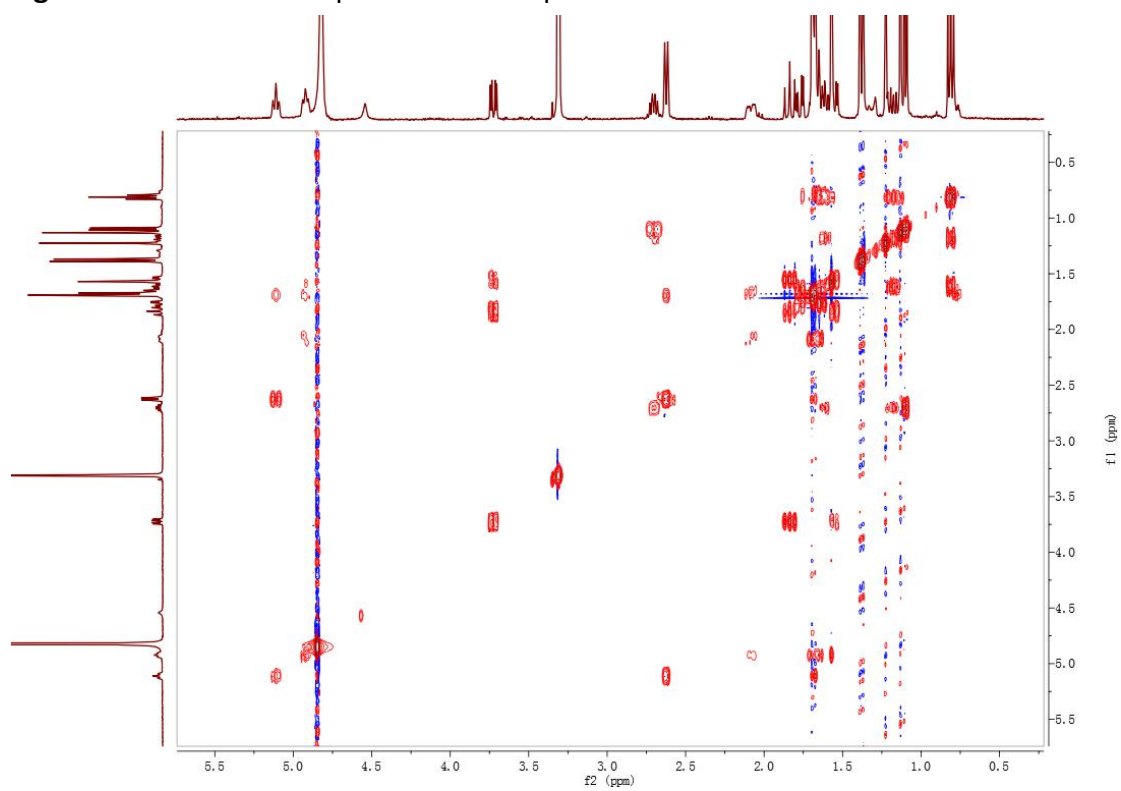


Figure S15. NOESY spectrum of compound 2

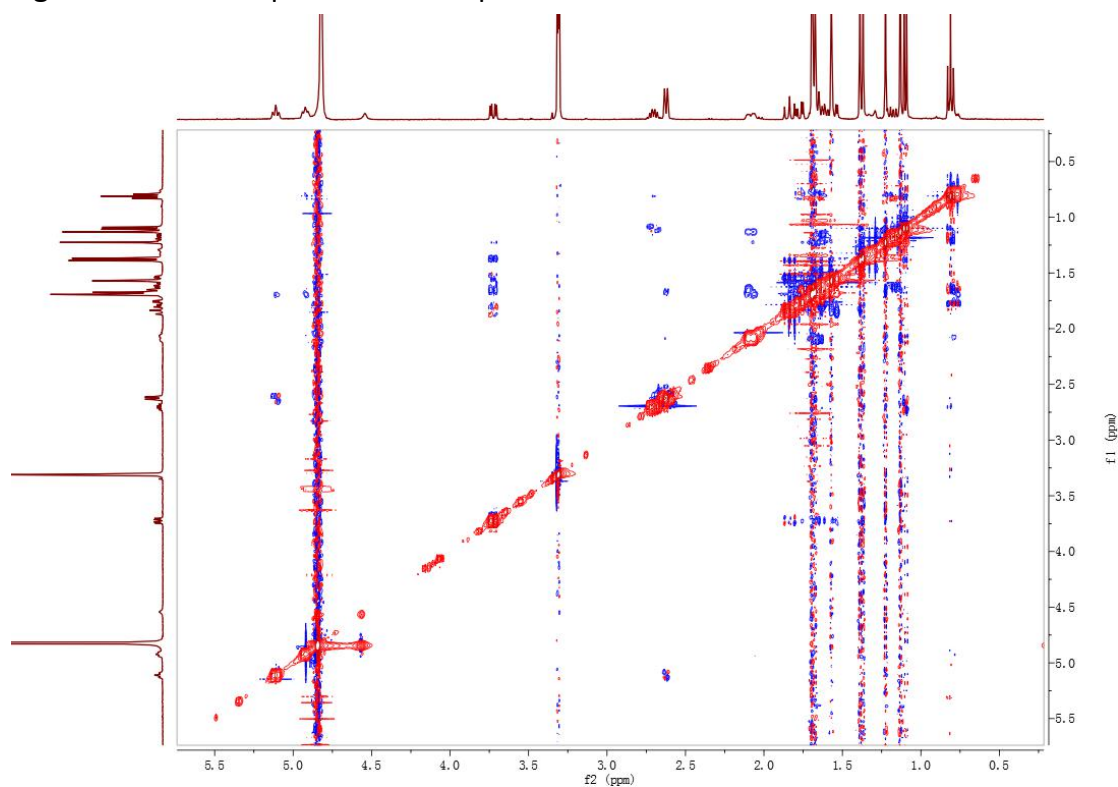
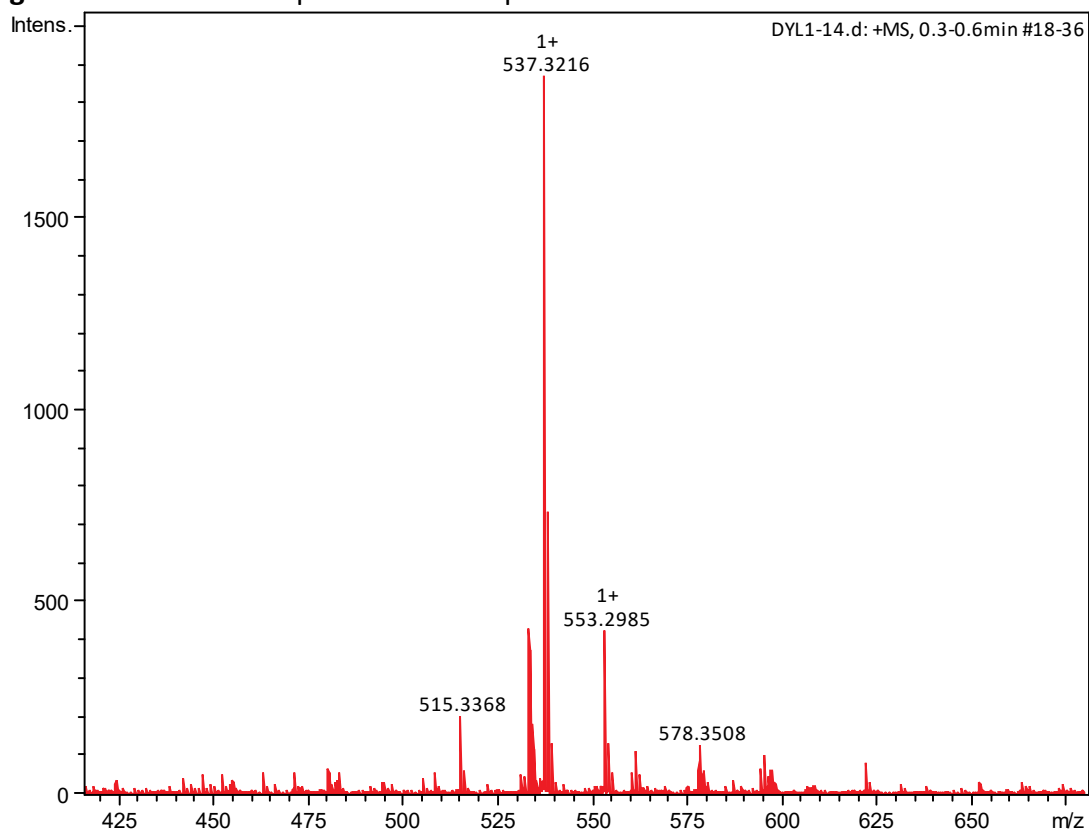
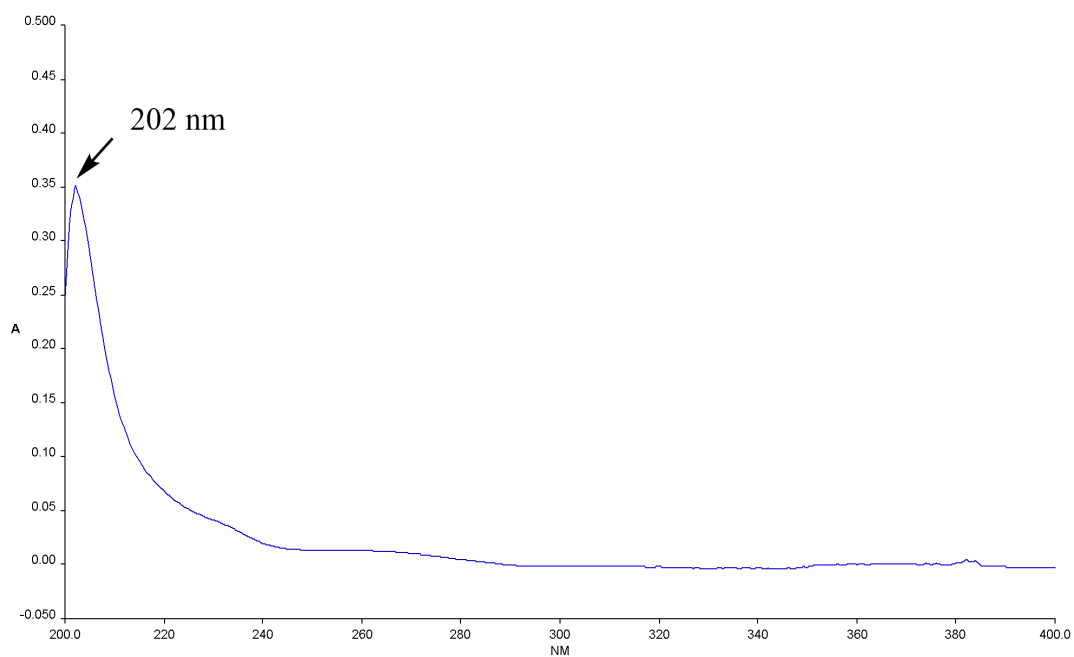


Figure S16. HR-ESI-MS spectrum of compound 2



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



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

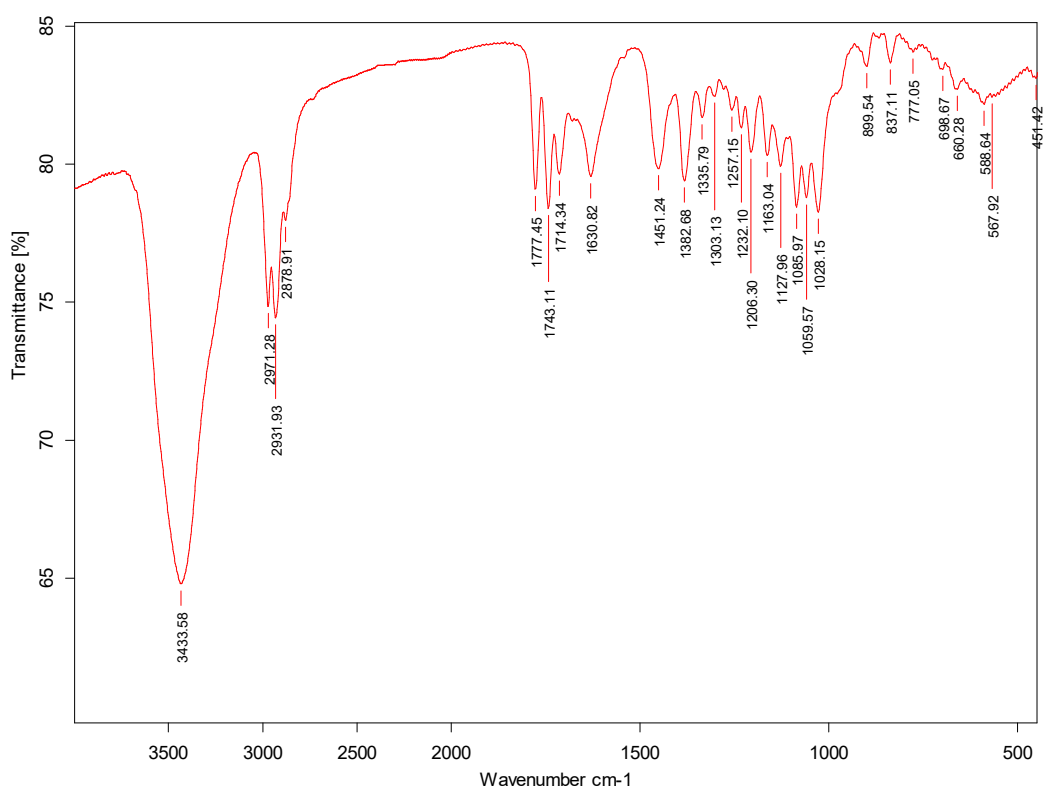


Figure S19.  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **3**

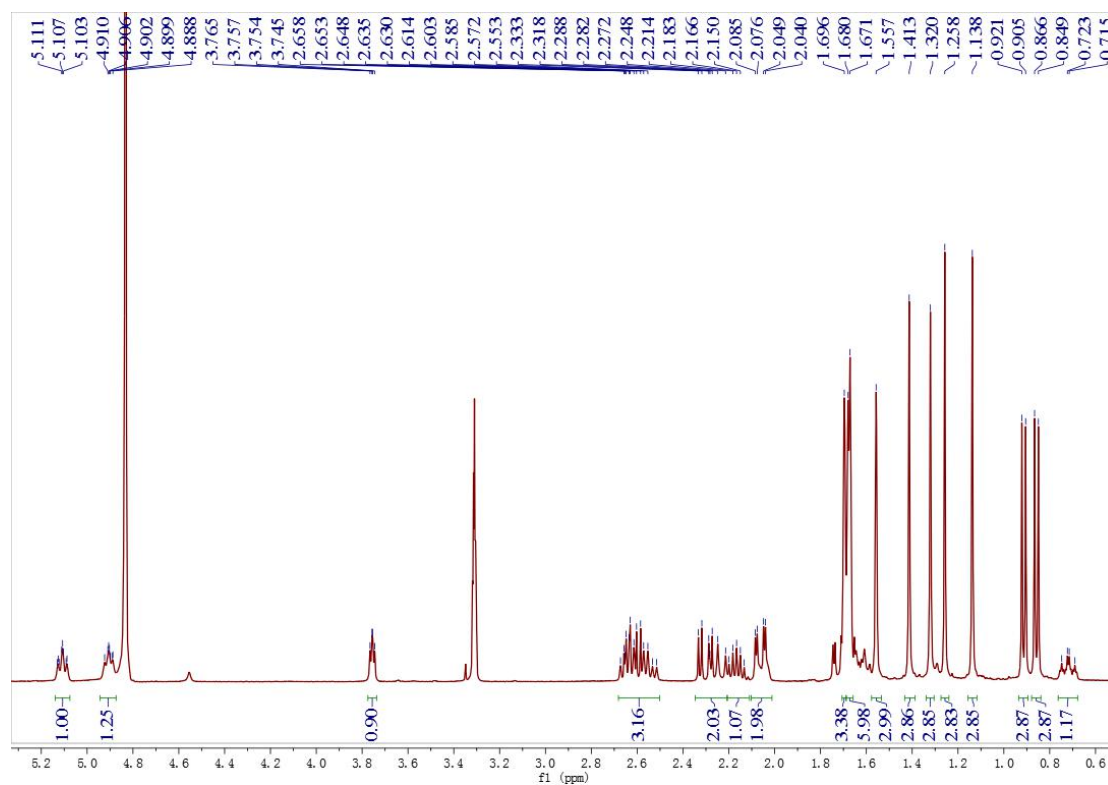


Figure S20.  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **3**

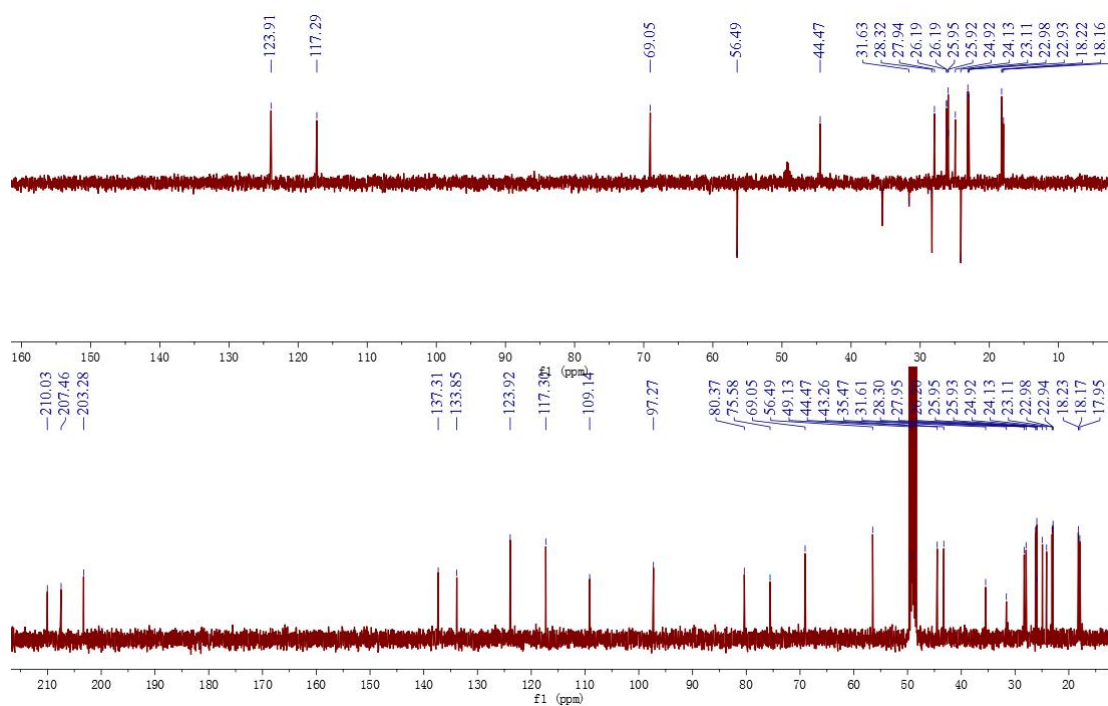


Figure S21. HSQC spectrum of compound 3

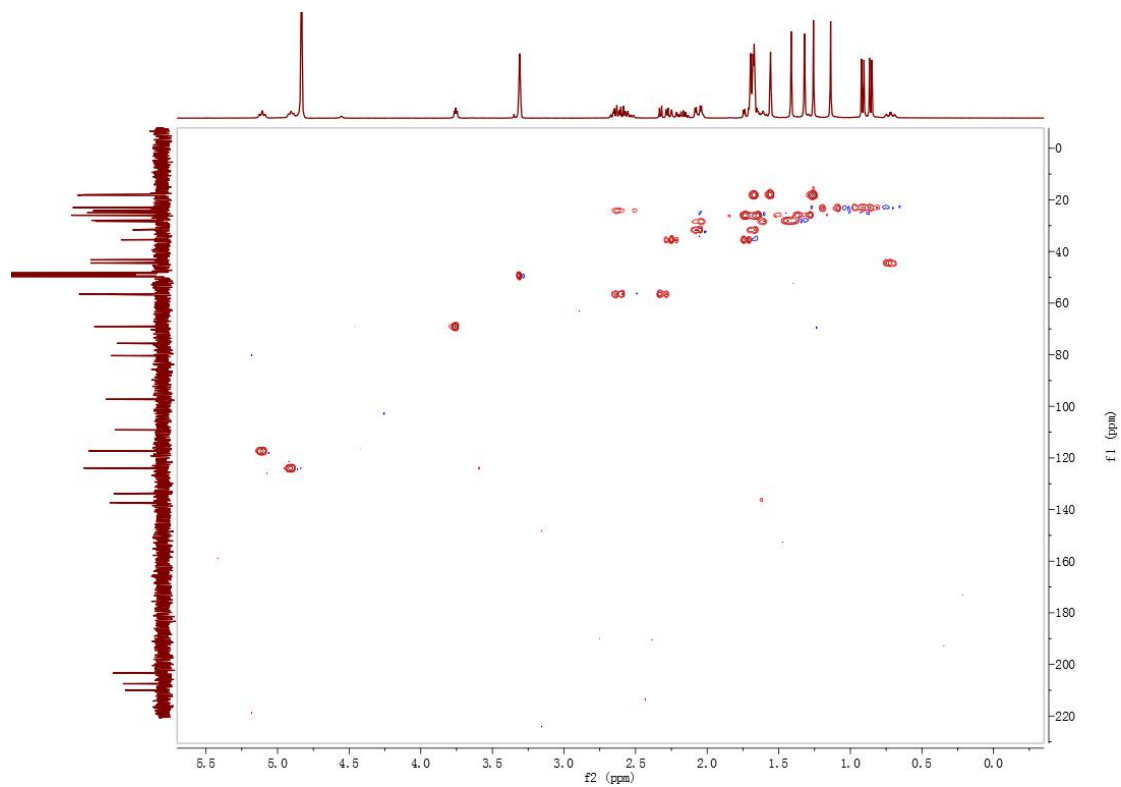


Figure S22. HMBC spectrum of compound 3

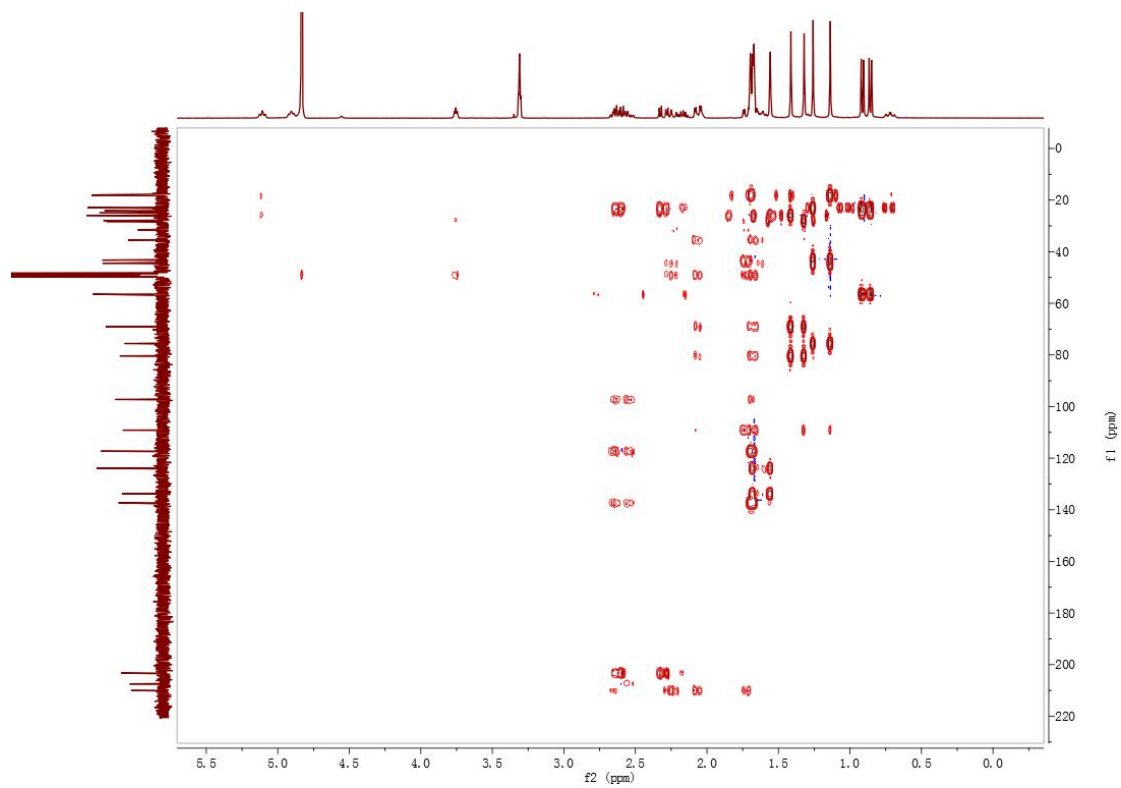


Figure S23.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 3

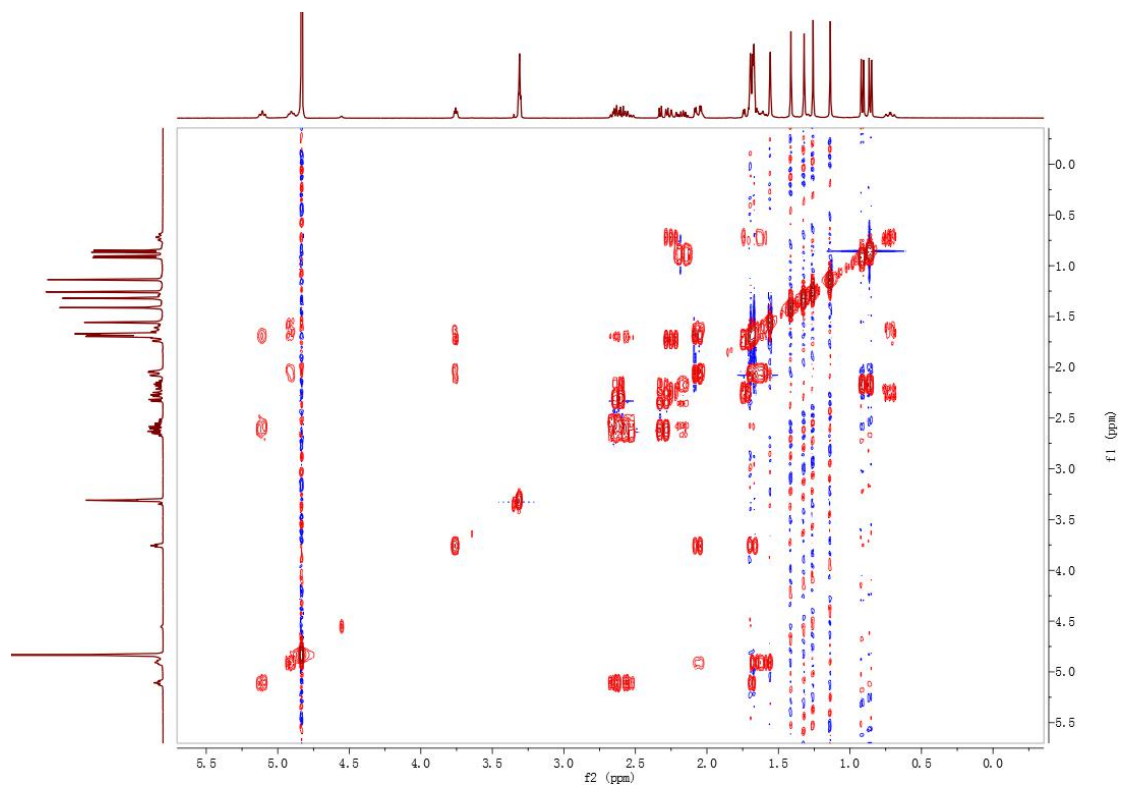
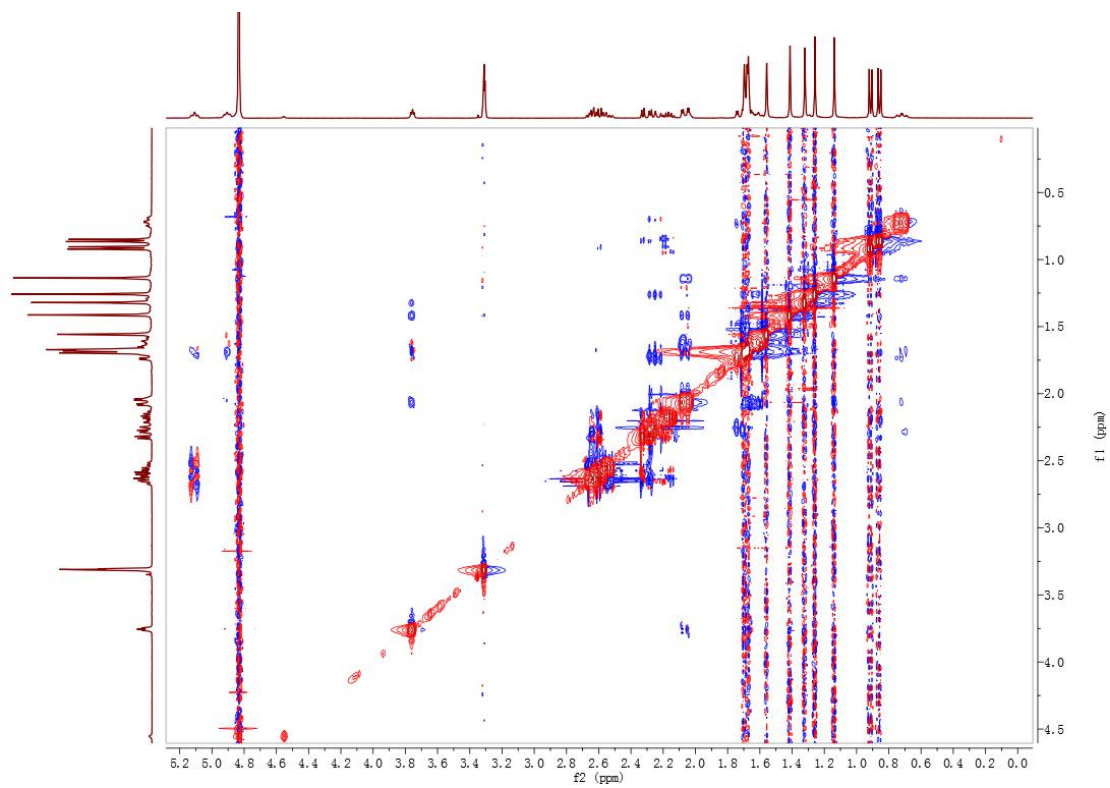
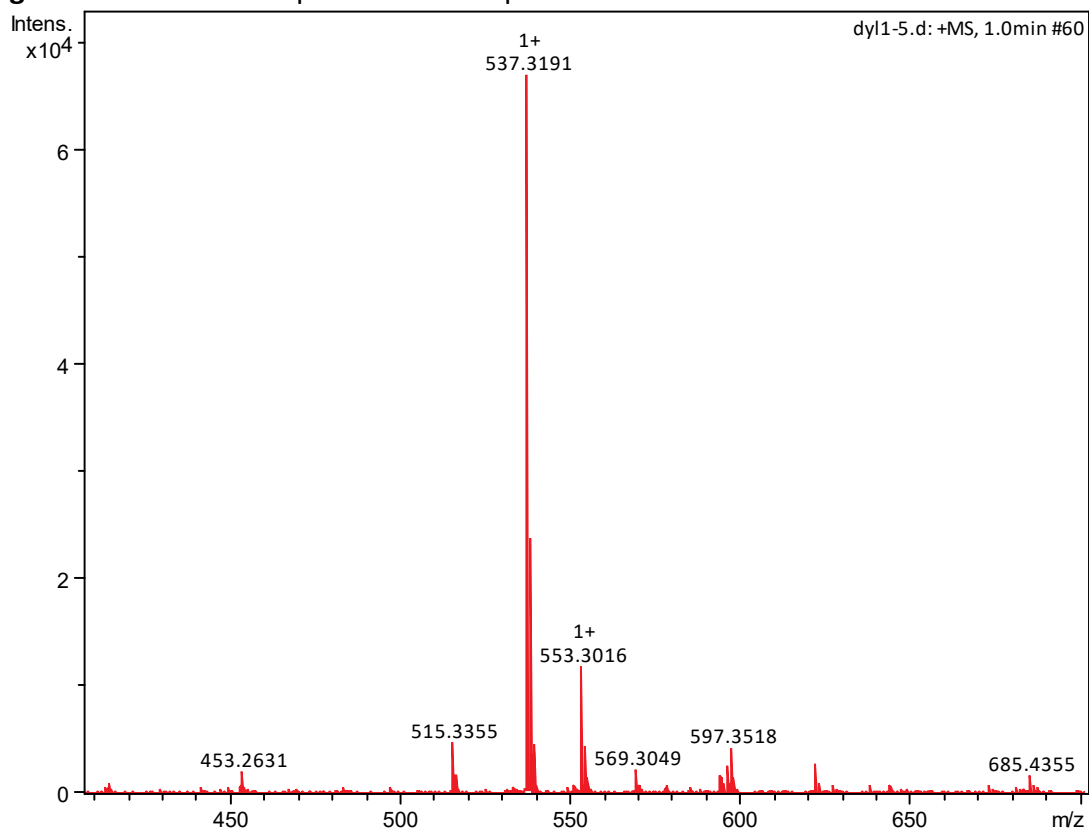


Figure S24. NOESY spectrum of compound 3





**Figure S25.** HR-ESI-MS spectrum of compound **3**



**Figure S26.** UV spectrum of compound **3**

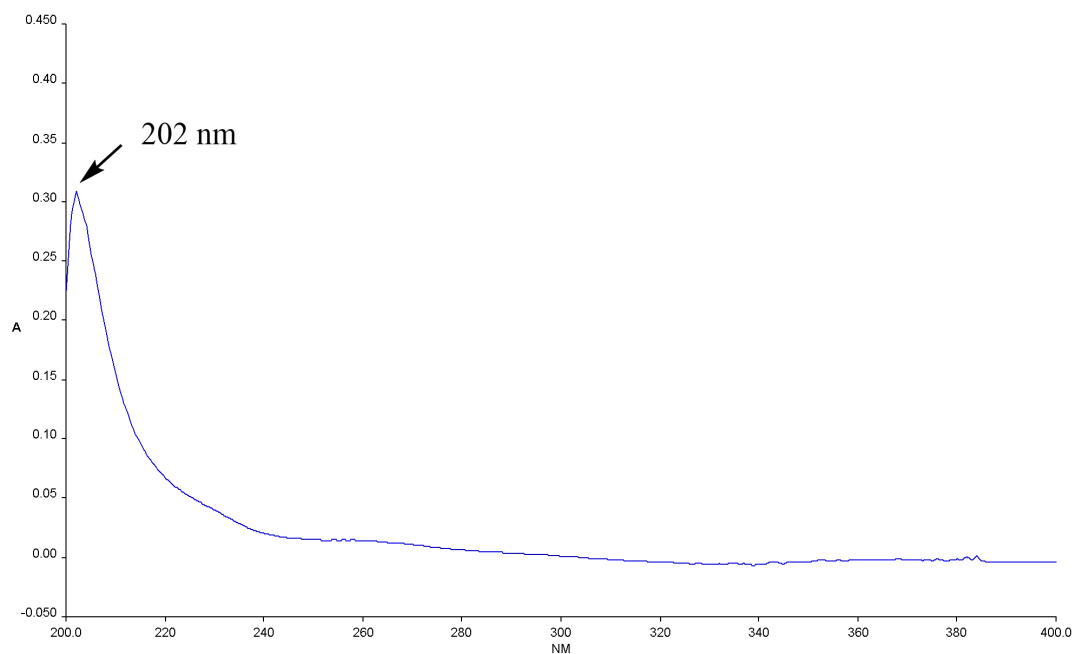


Figure S27. IR spectrum of compound 3

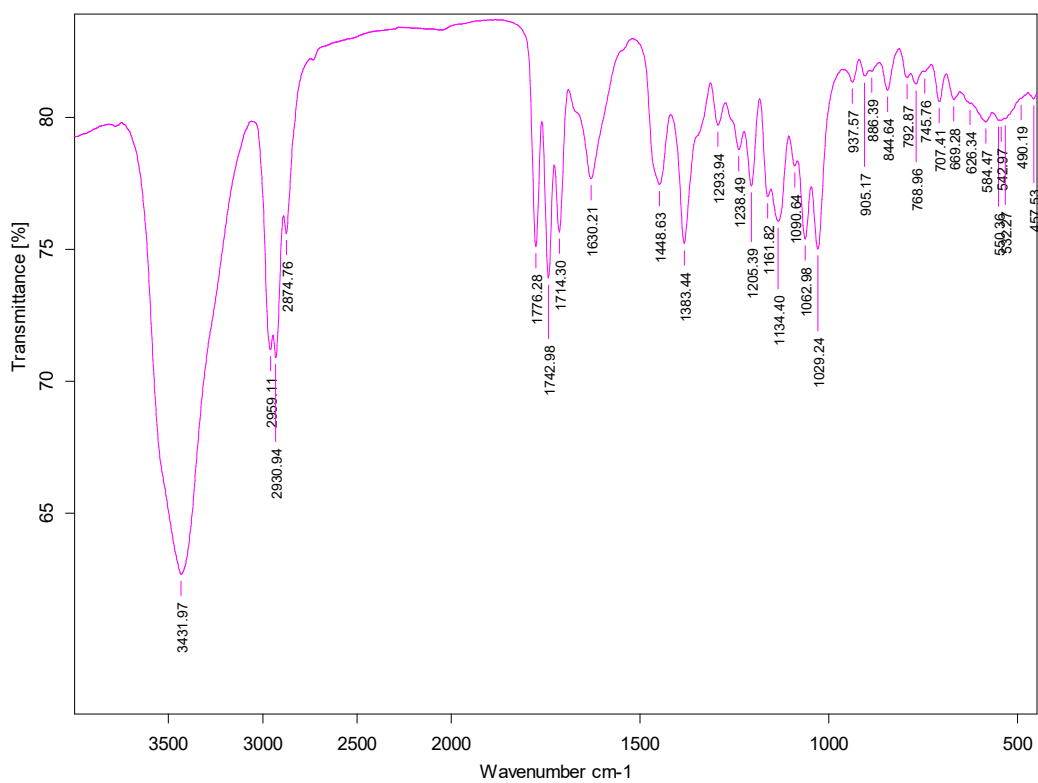


Figure S28. <sup>1</sup>H-NMR (600 MHz, CD<sub>3</sub>OD) spectrum of compound 4

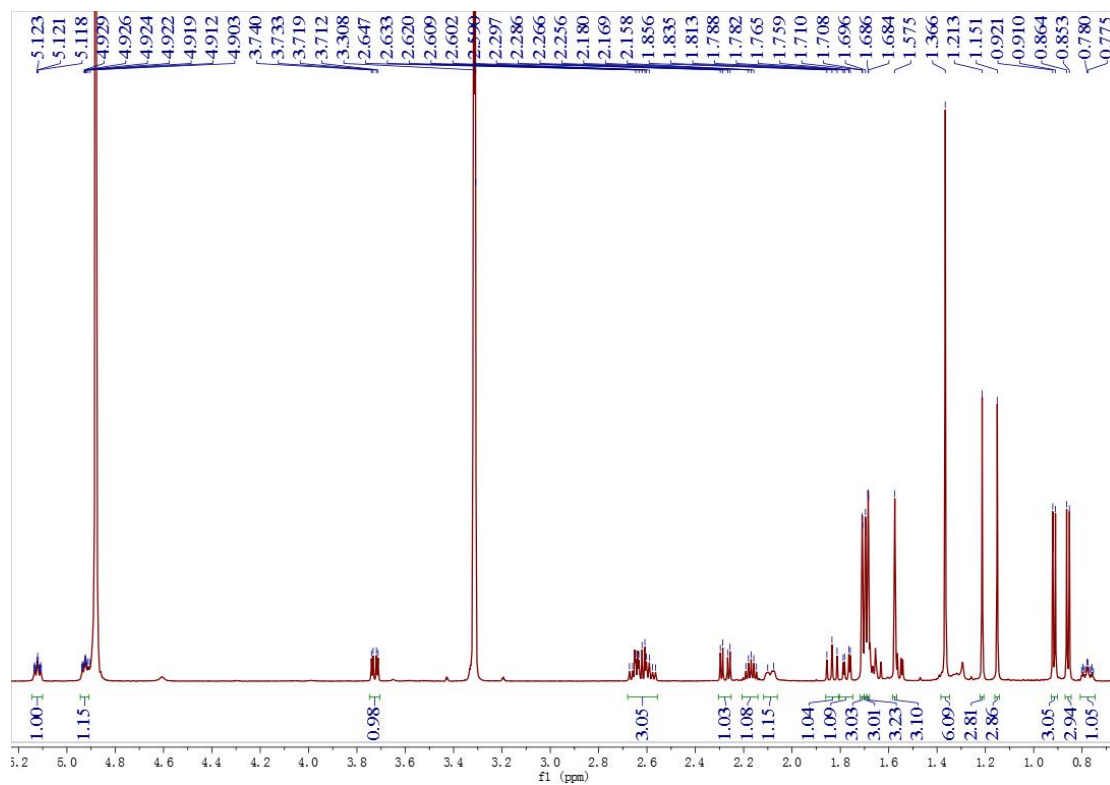


Figure S29.  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 4

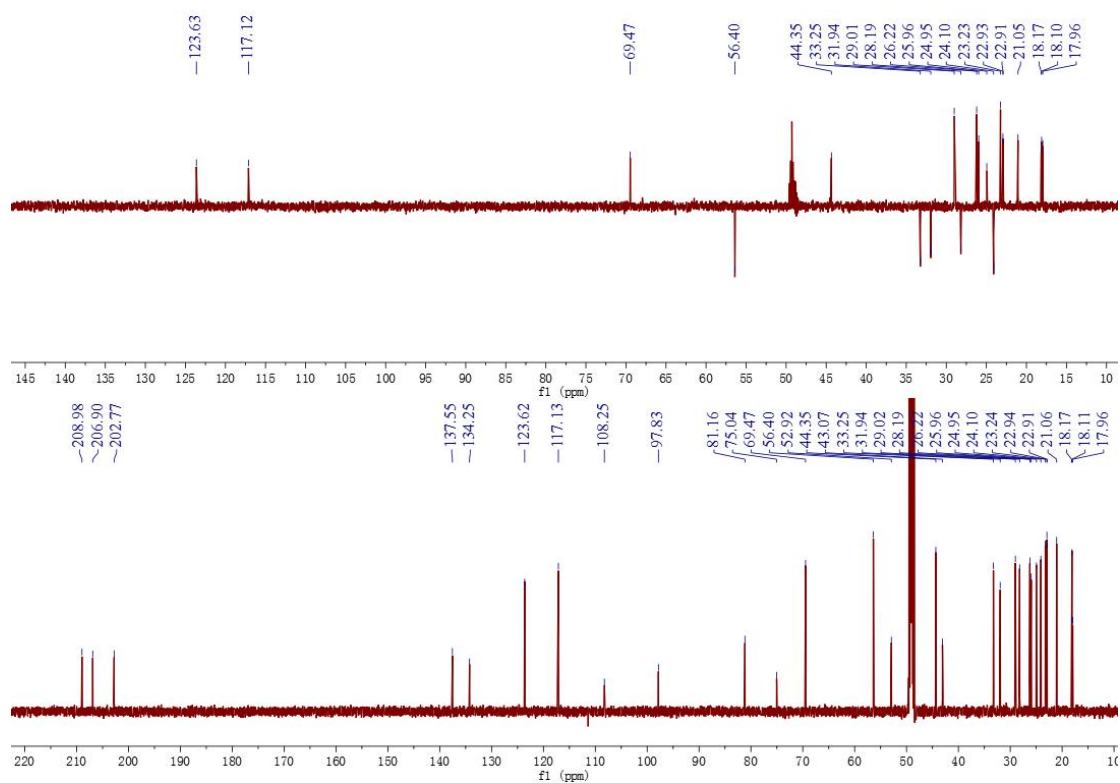


Figure S30. HSQC spectrum of compound 4

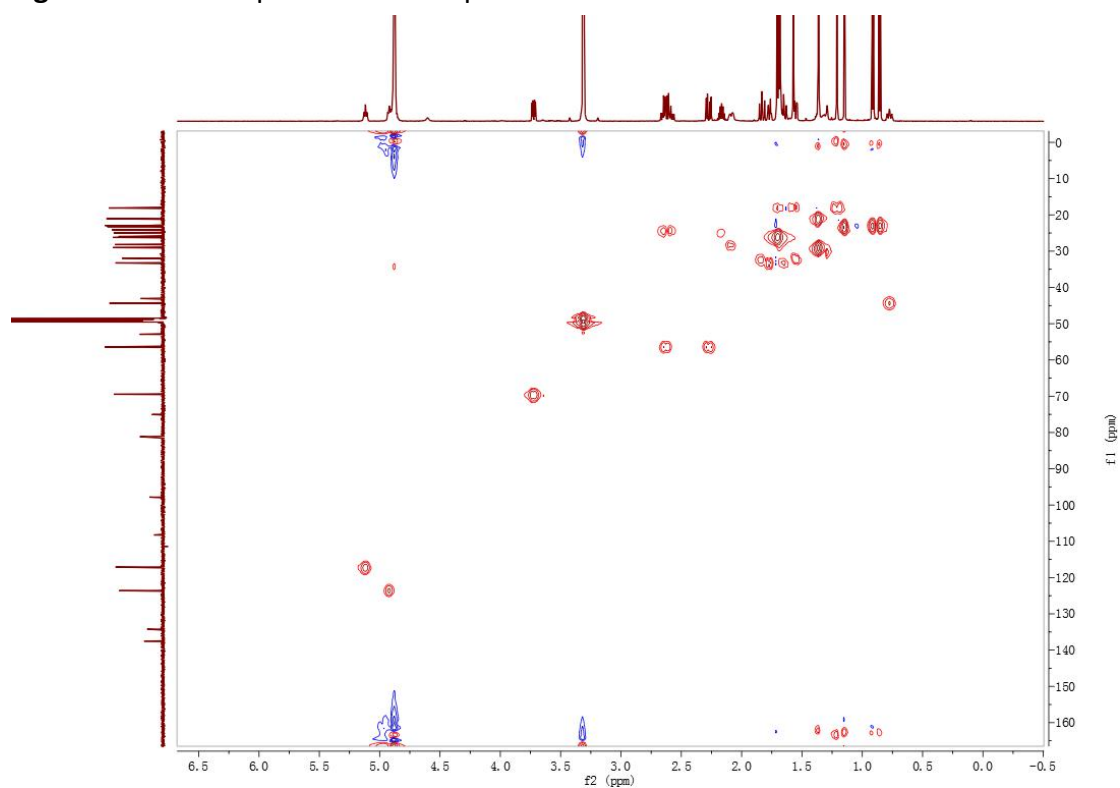


Figure S31. HMBC spectrum of compound 4

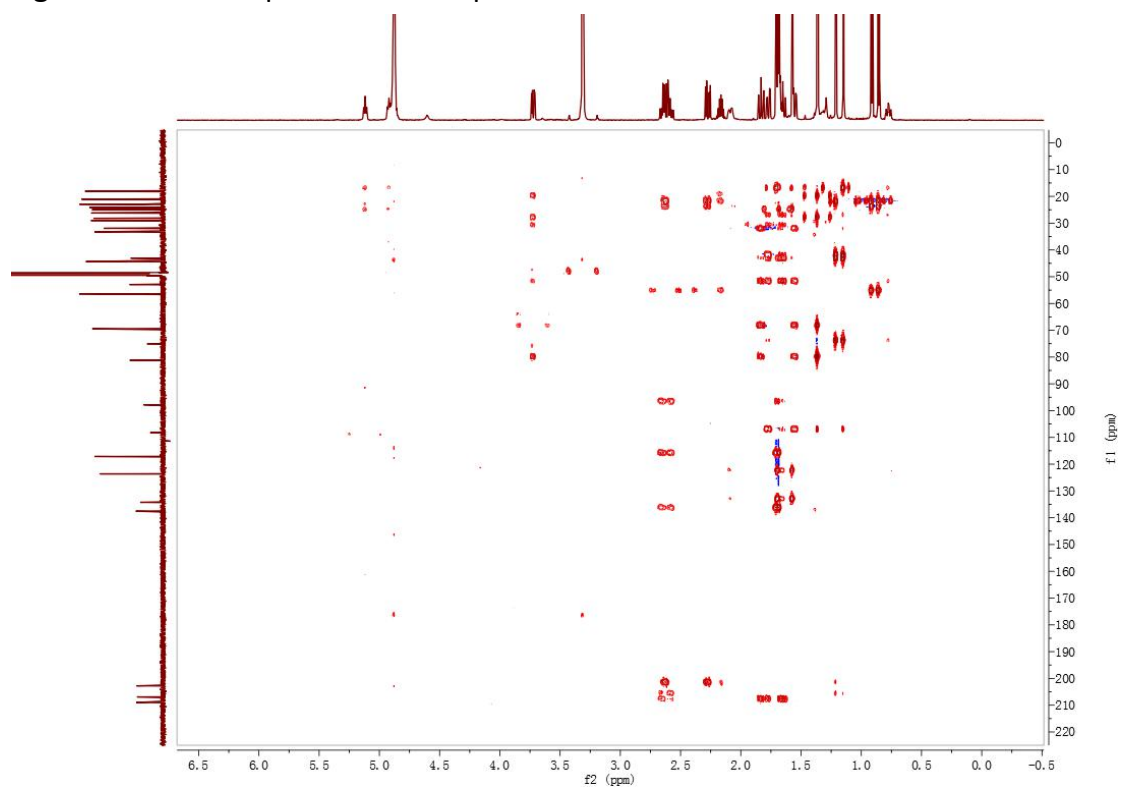


Figure S32.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 4

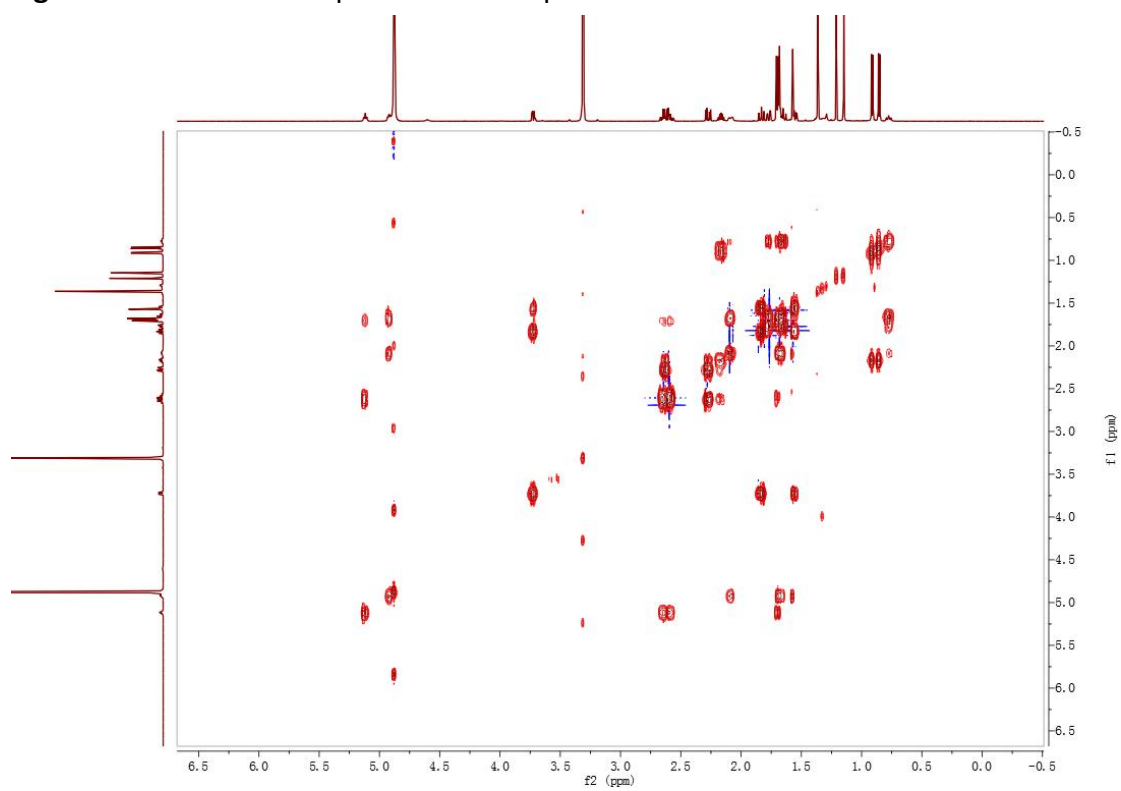


Figure S33. ROESY spectrum of compound 4

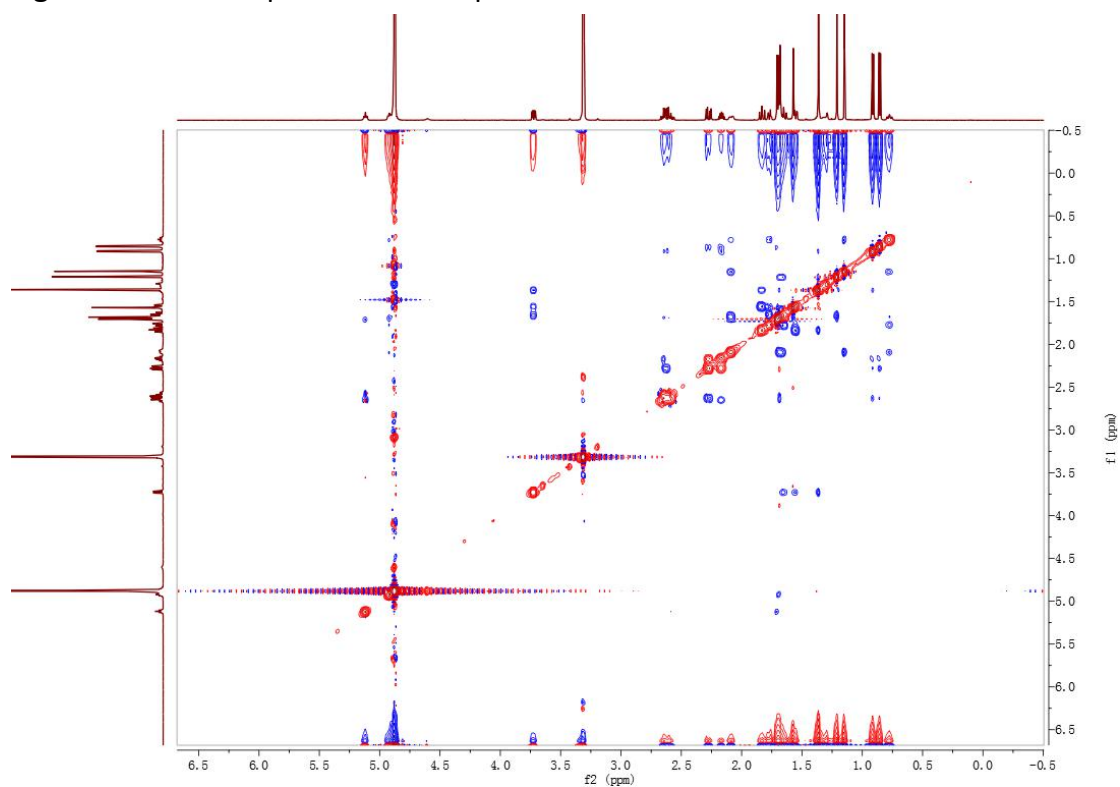


Figure S34. HR-ESI-MS spectrum of compound 4

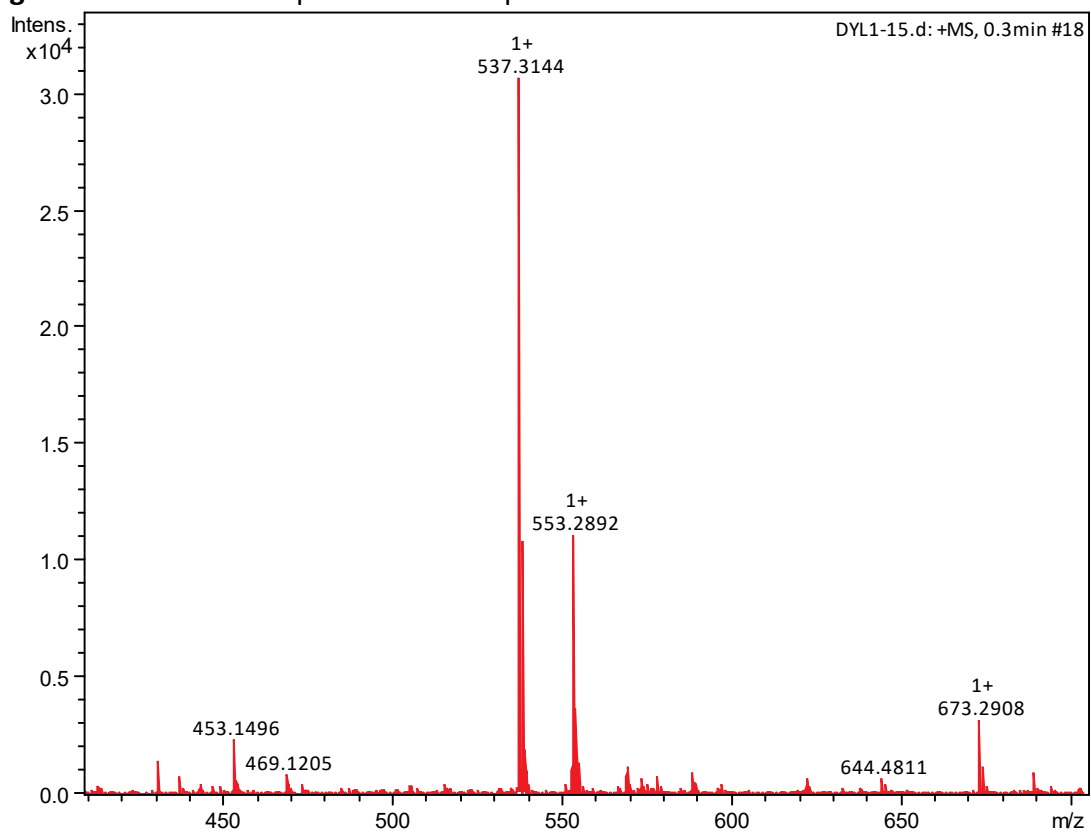


Figure S35. UV spectrum of compound 4

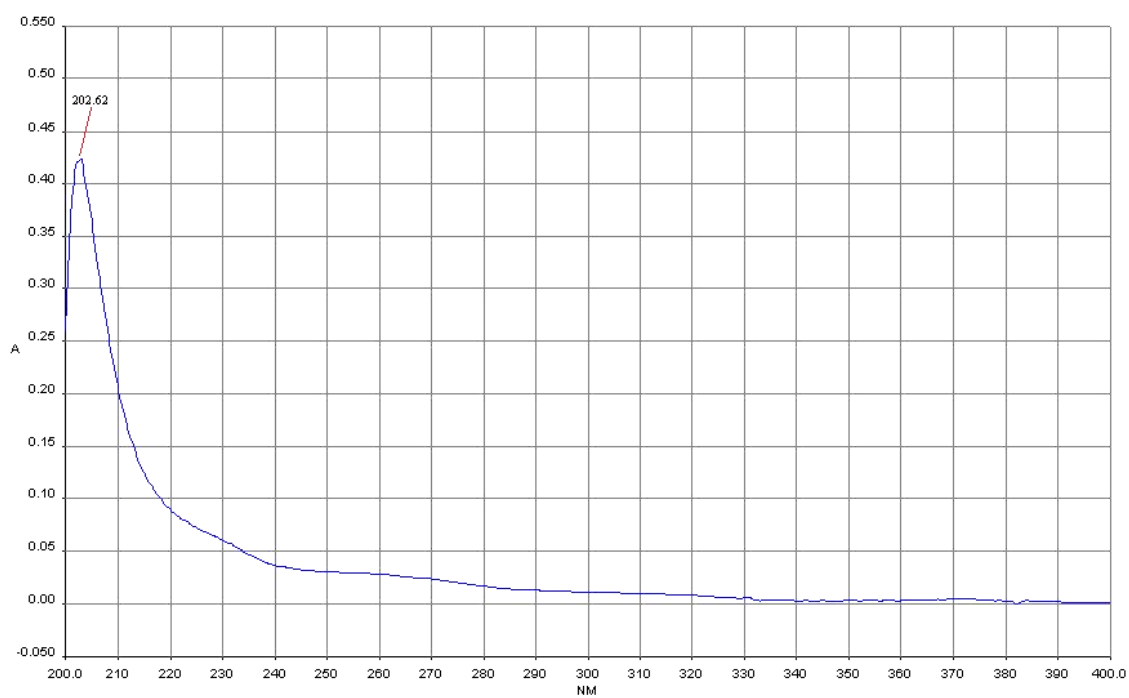
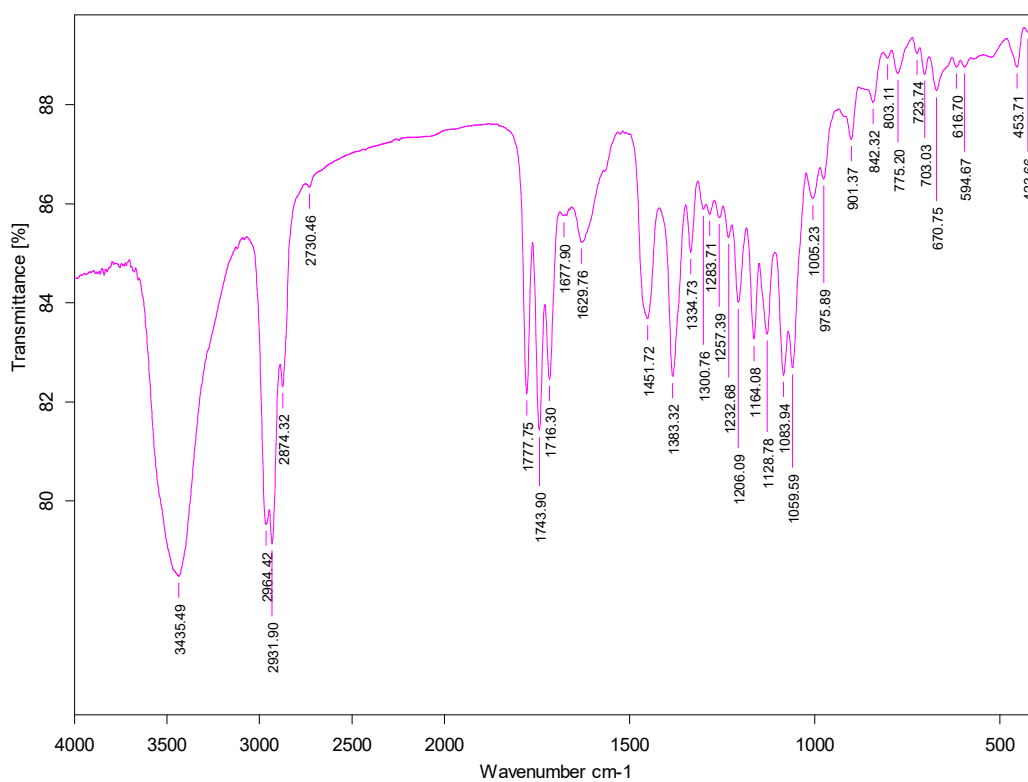
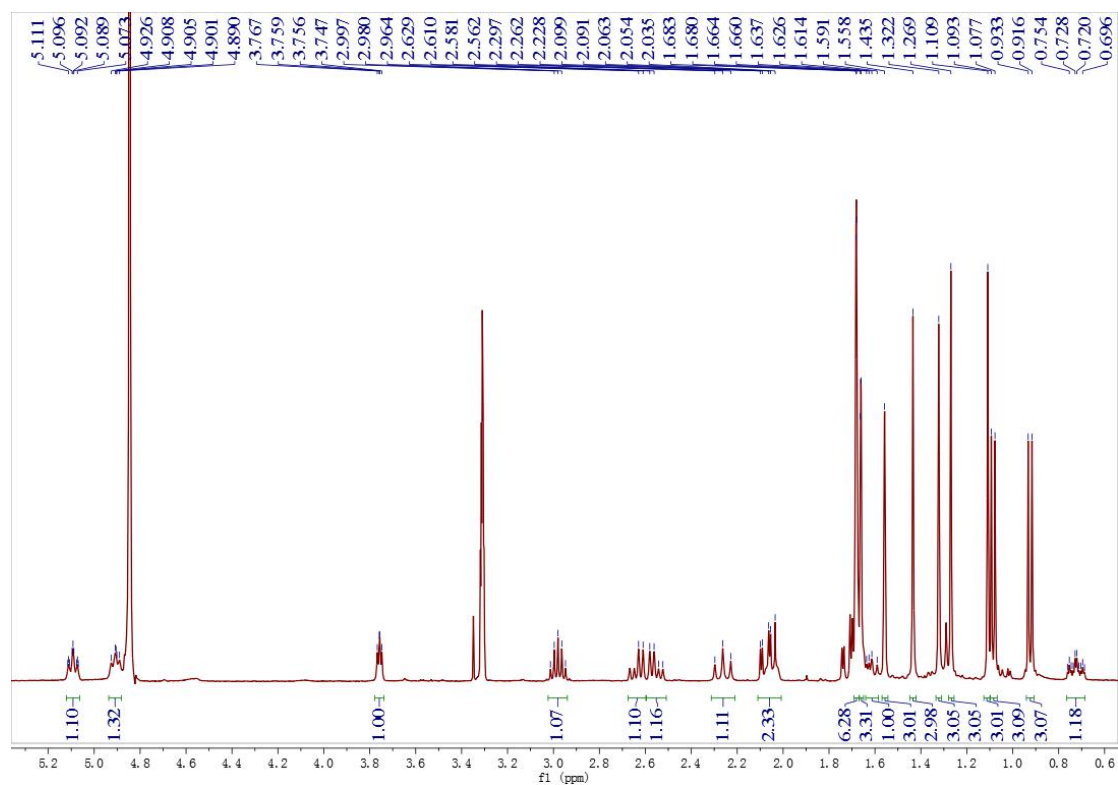


Figure S36. IR spectrum of compound 4



**Figure S37.**  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **5**



**Figure S38.**  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound **5**

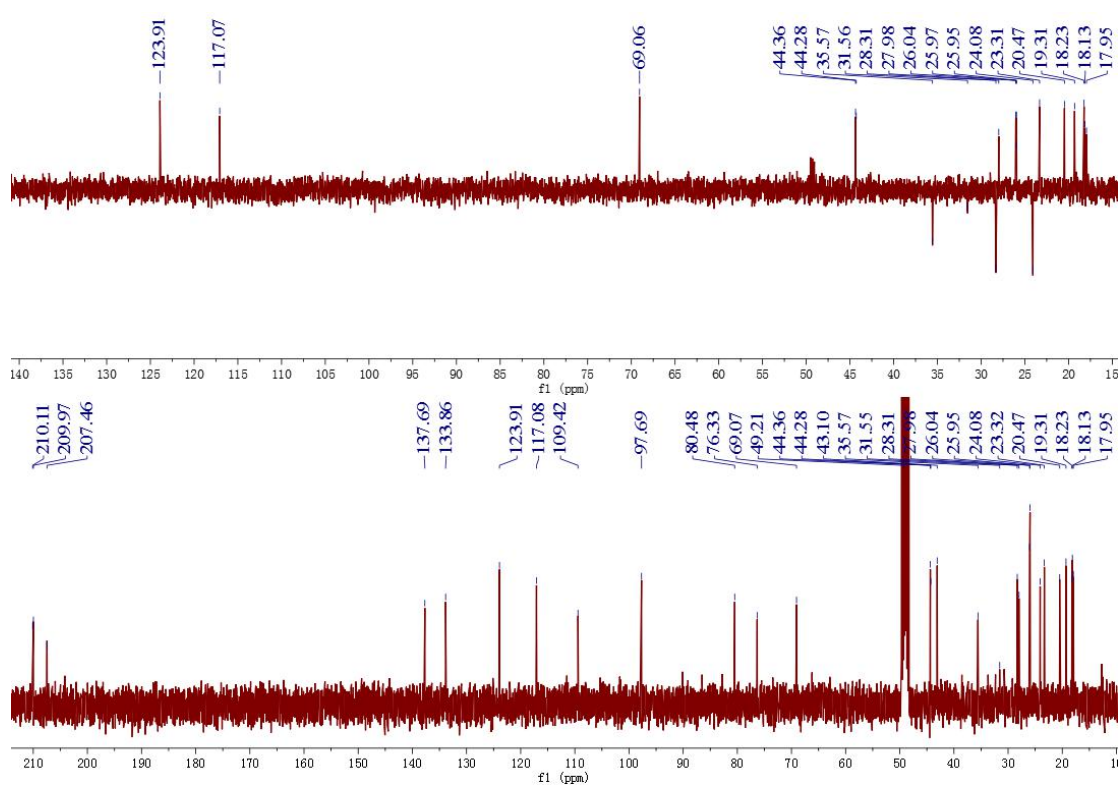


Figure S39. HSQC spectrum of compound 5

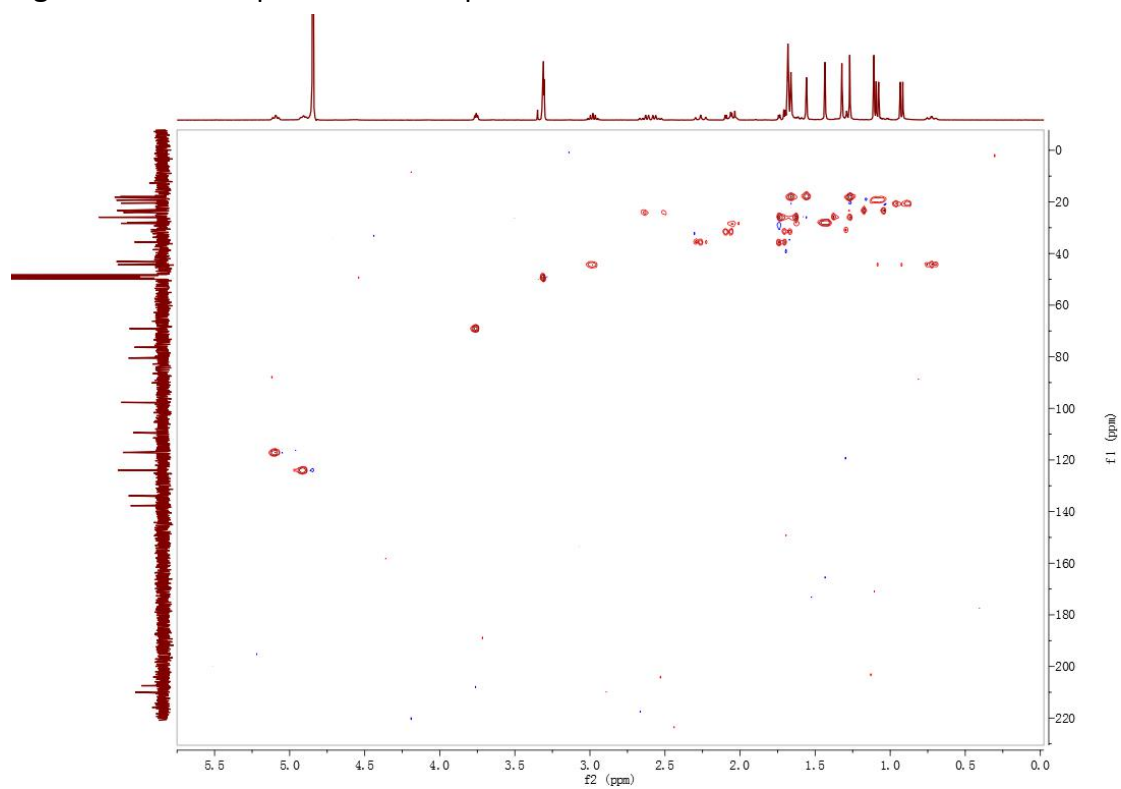


Figure S40. HMBC spectrum of compound 5

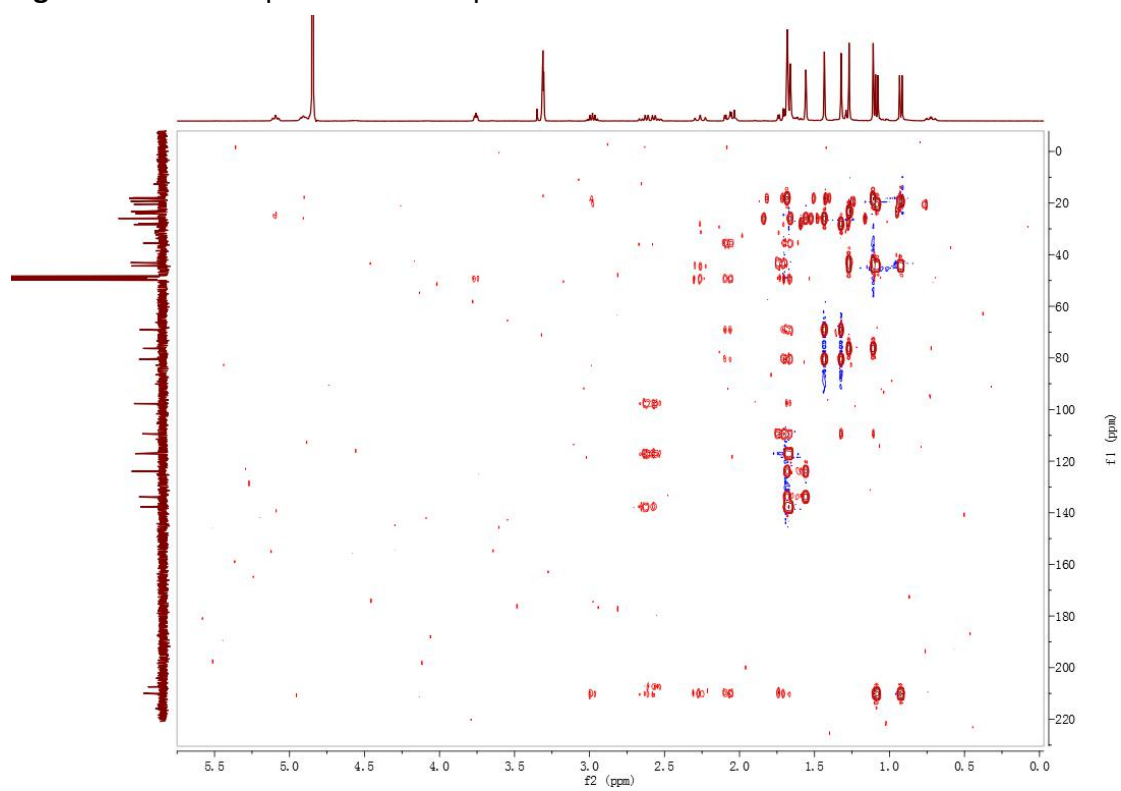




Figure S41.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 5

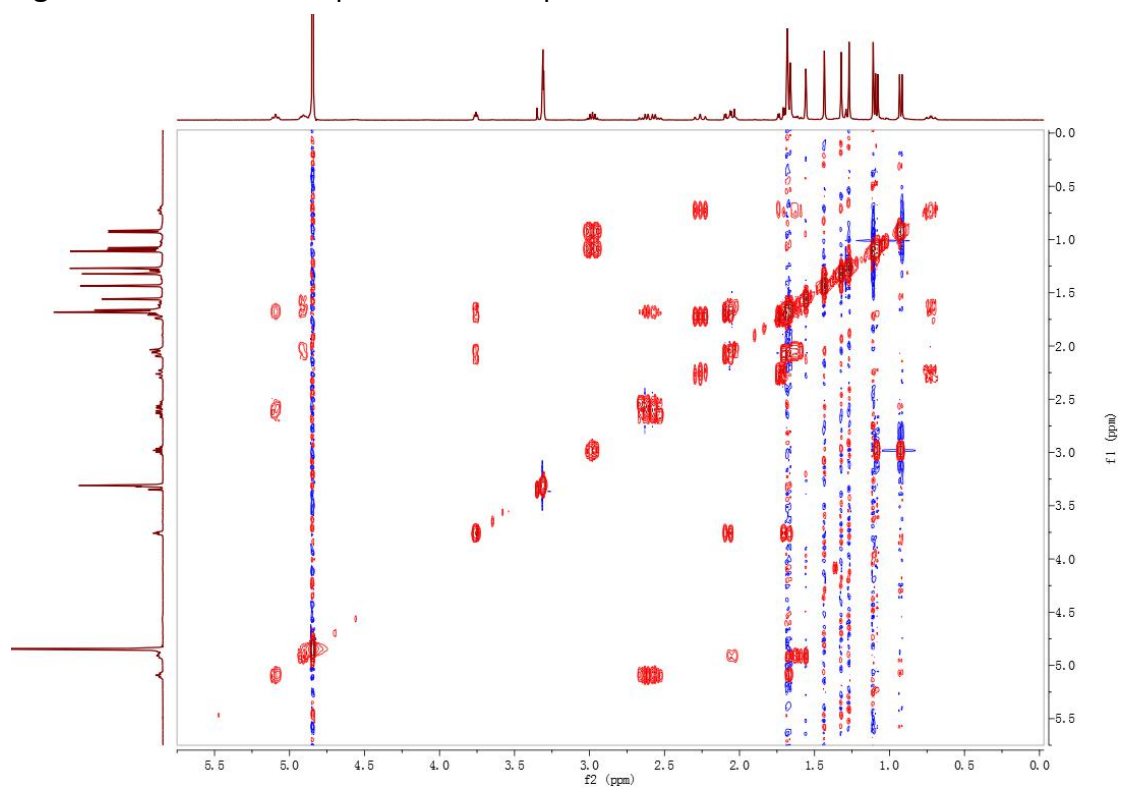
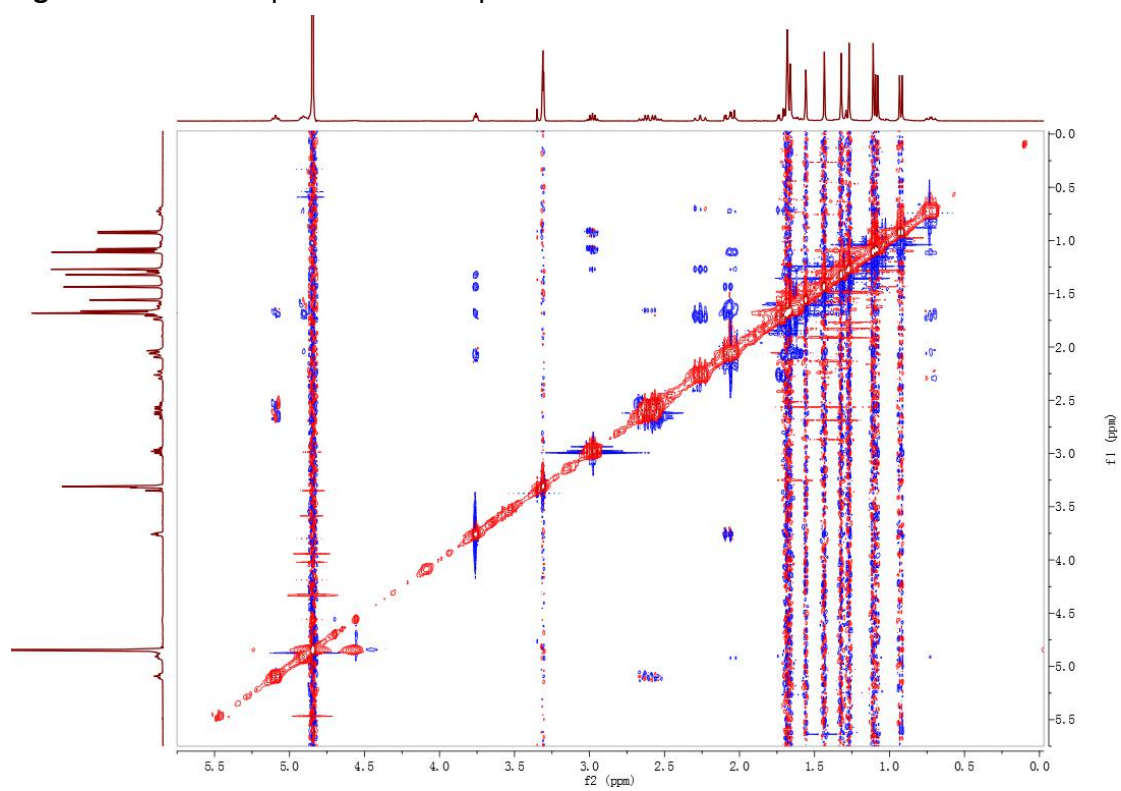
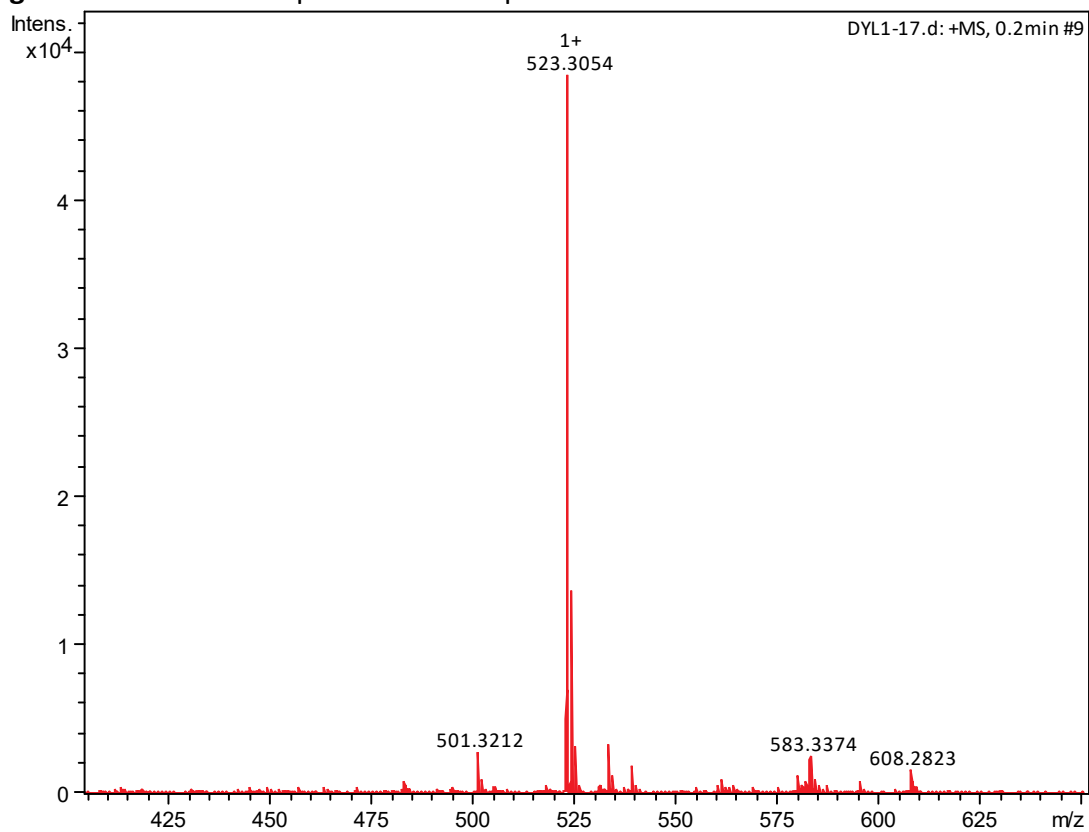


Figure S42. NOESY spectrum of compound 5



**Figure S43.** HR-ESI-MS spectrum of compound **5**



**Figure S44.** UV spectrum of compound **5**

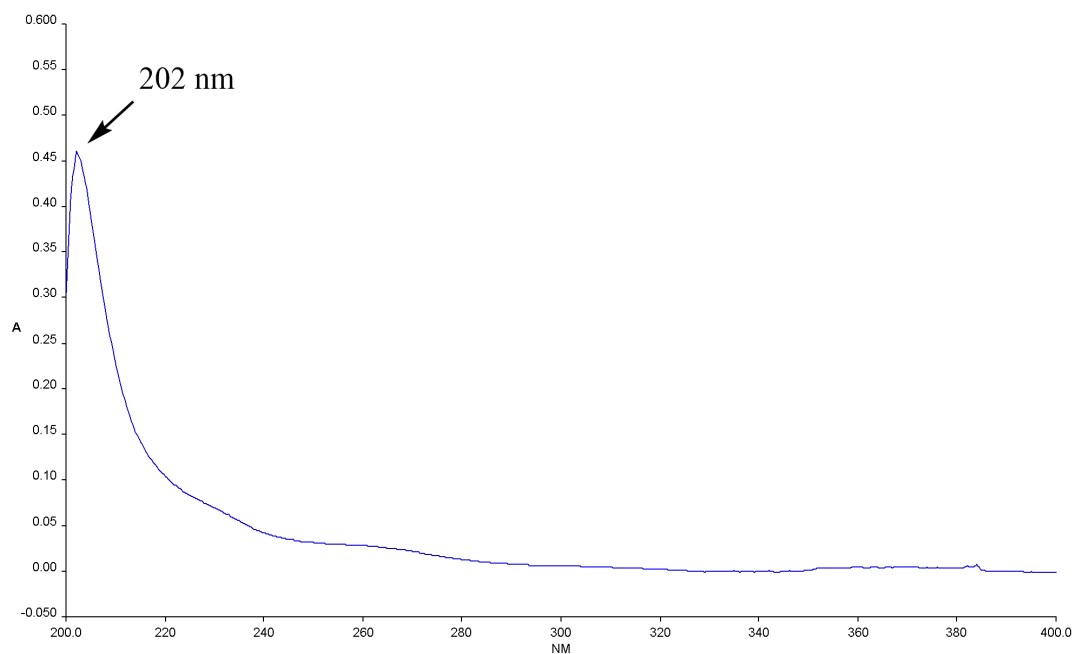


Figure S45. IR spectrum of compound 5

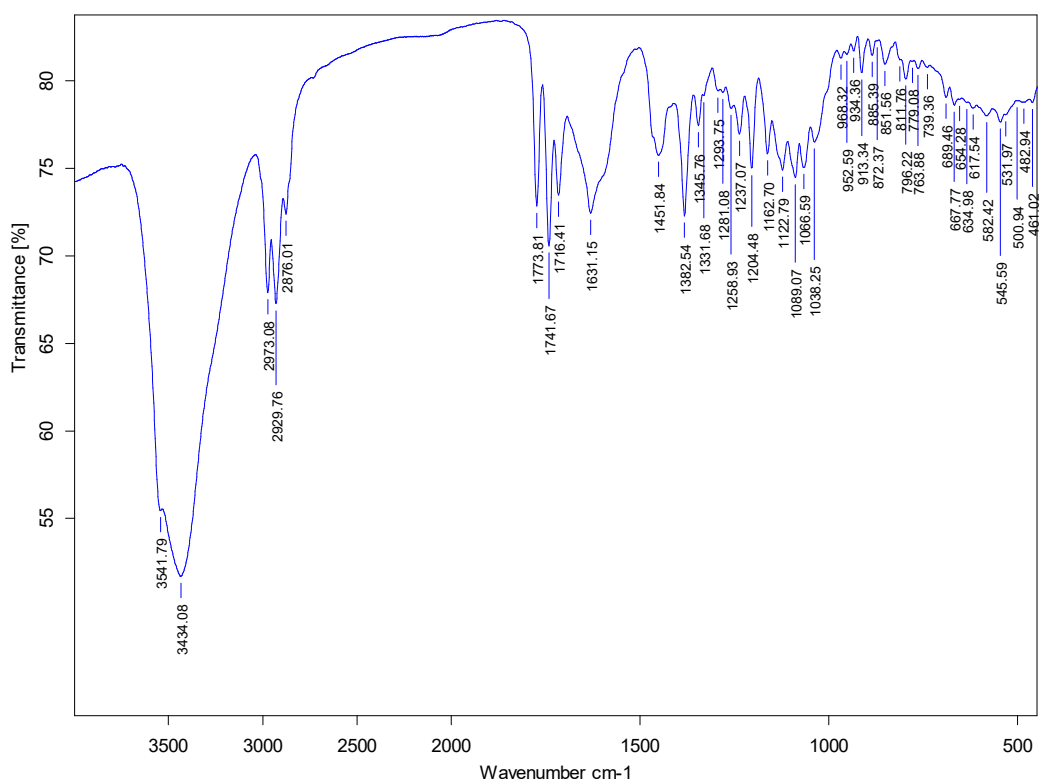


Figure S46. <sup>1</sup>H-NMR (800 MHz, CD<sub>3</sub>OD) spectrum of compound 6

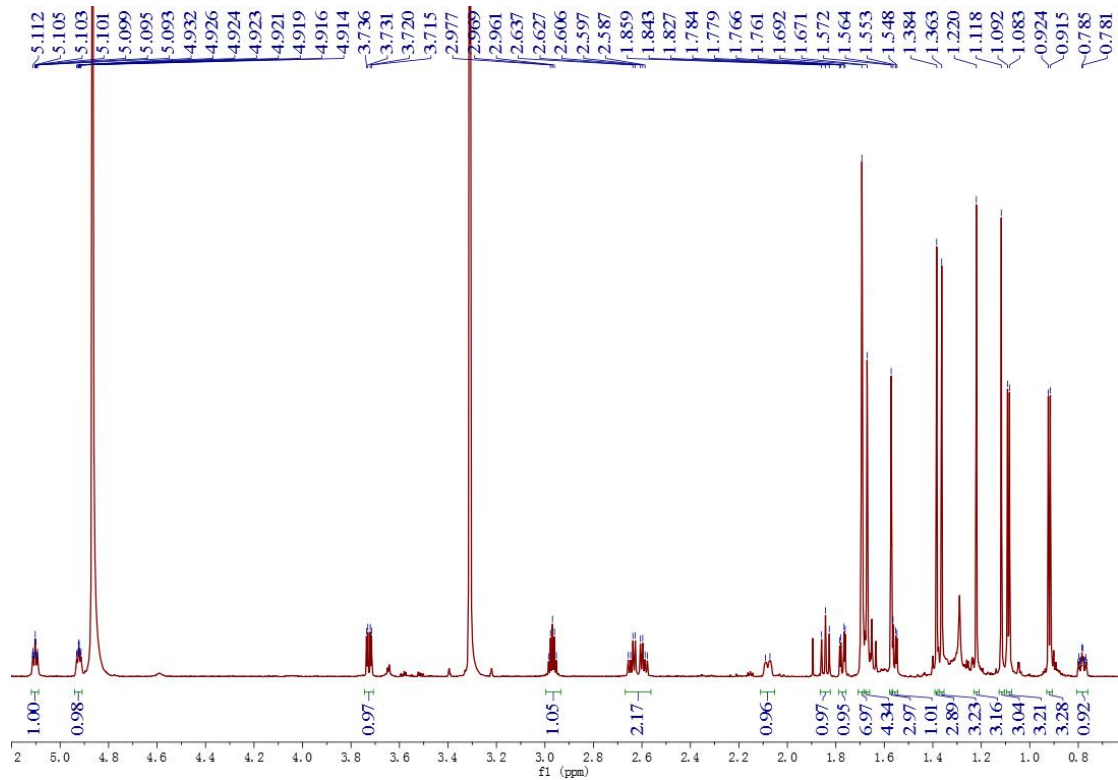


Figure S47.  $^{13}\text{C}$ -NMR (200 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 6

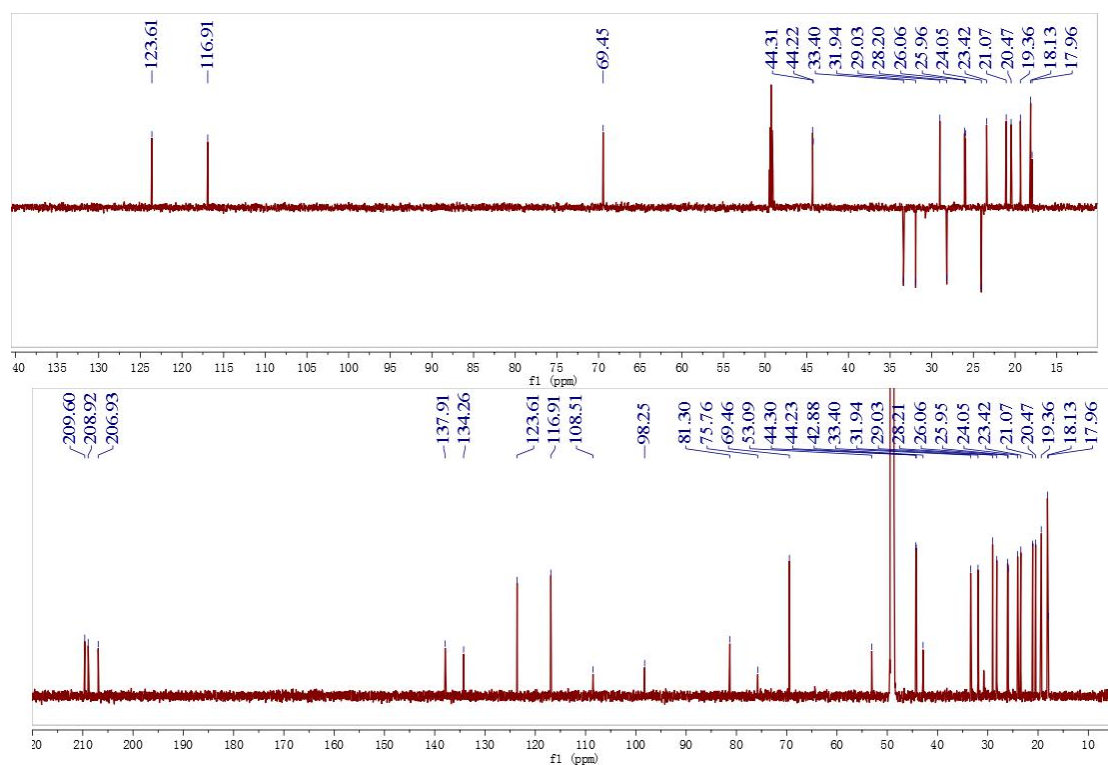


Figure S48. HSQC spectrum of compound 6

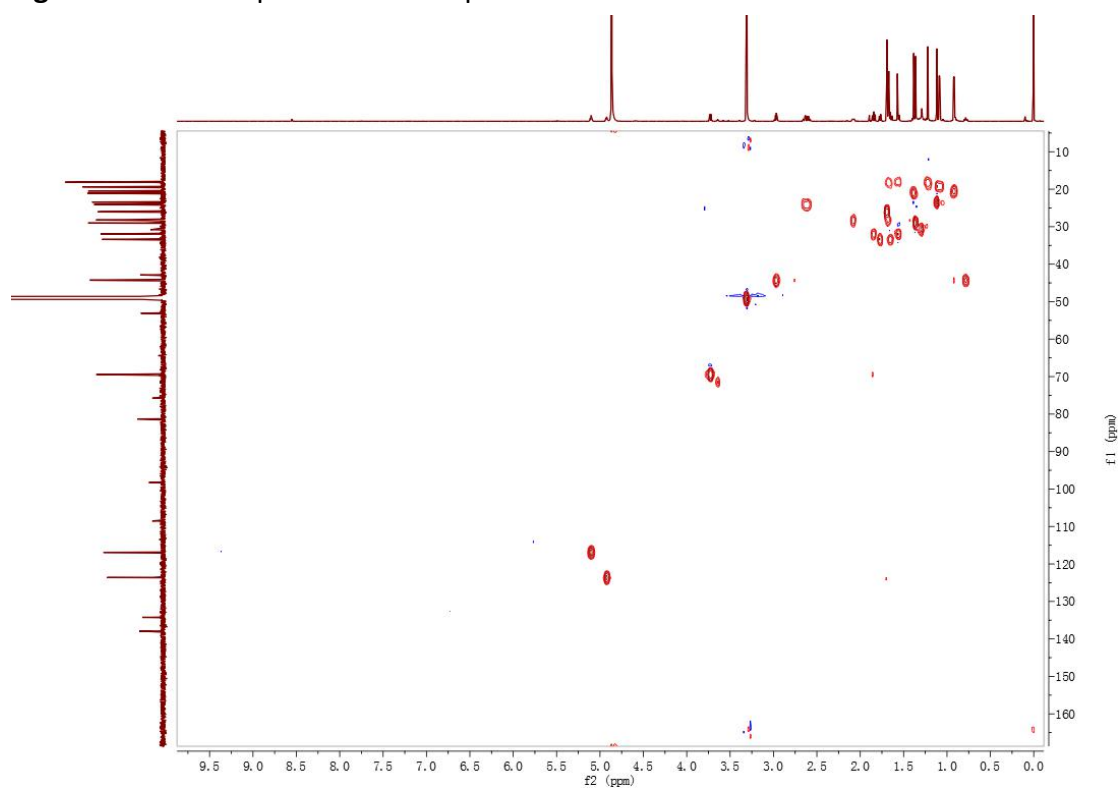


Figure S49. HMBC spectrum of compound 6

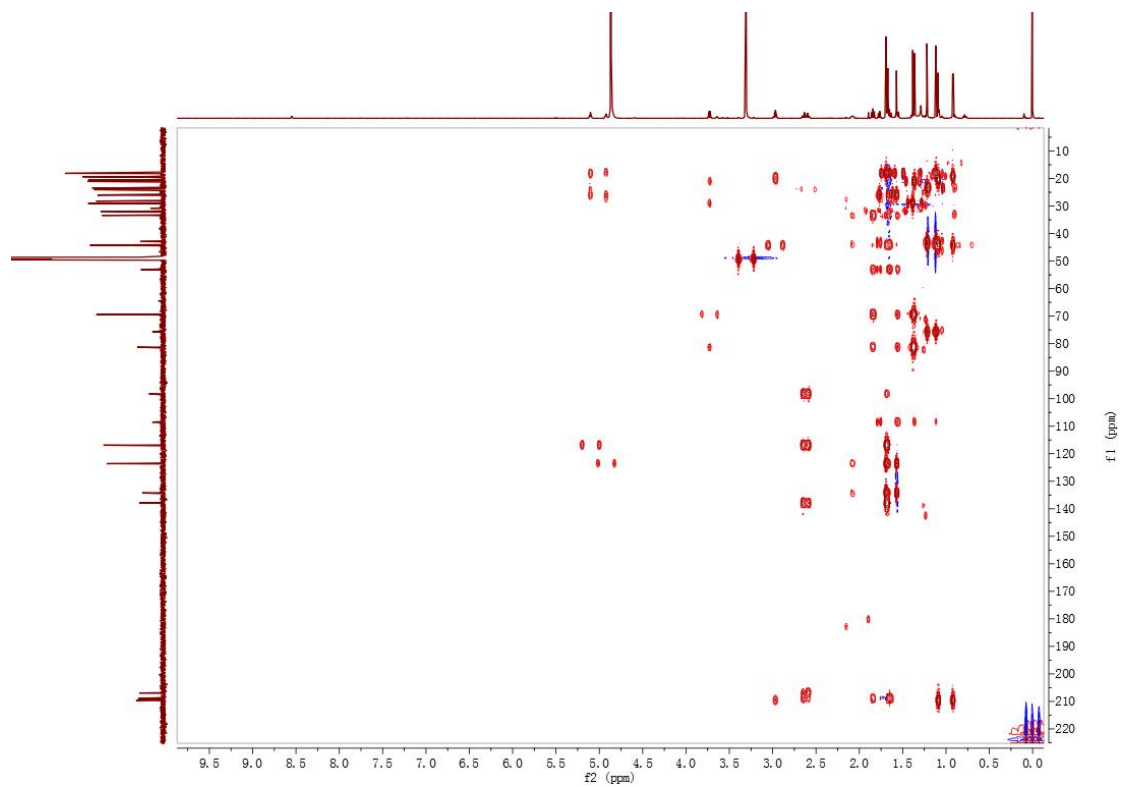


Figure S50.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 6

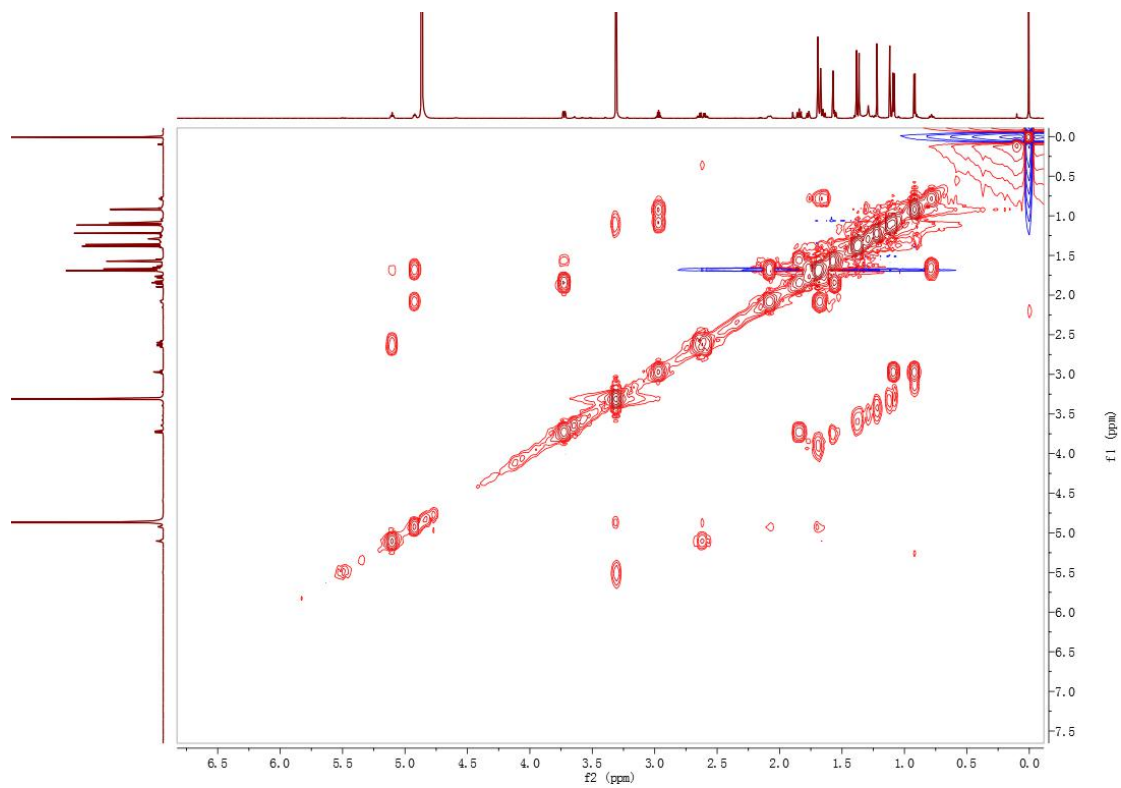


Figure S51. ROESY spectrum of compound 6

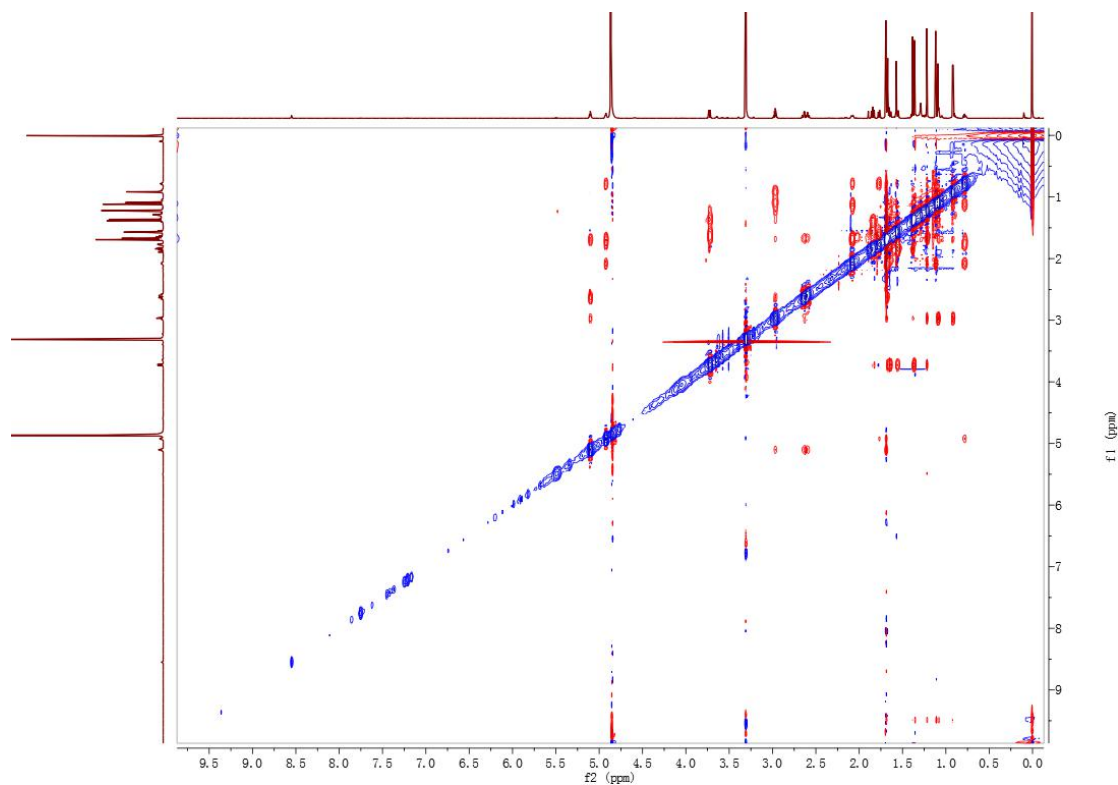


Figure S52. HR-ESI-MS spectrum of compound 6

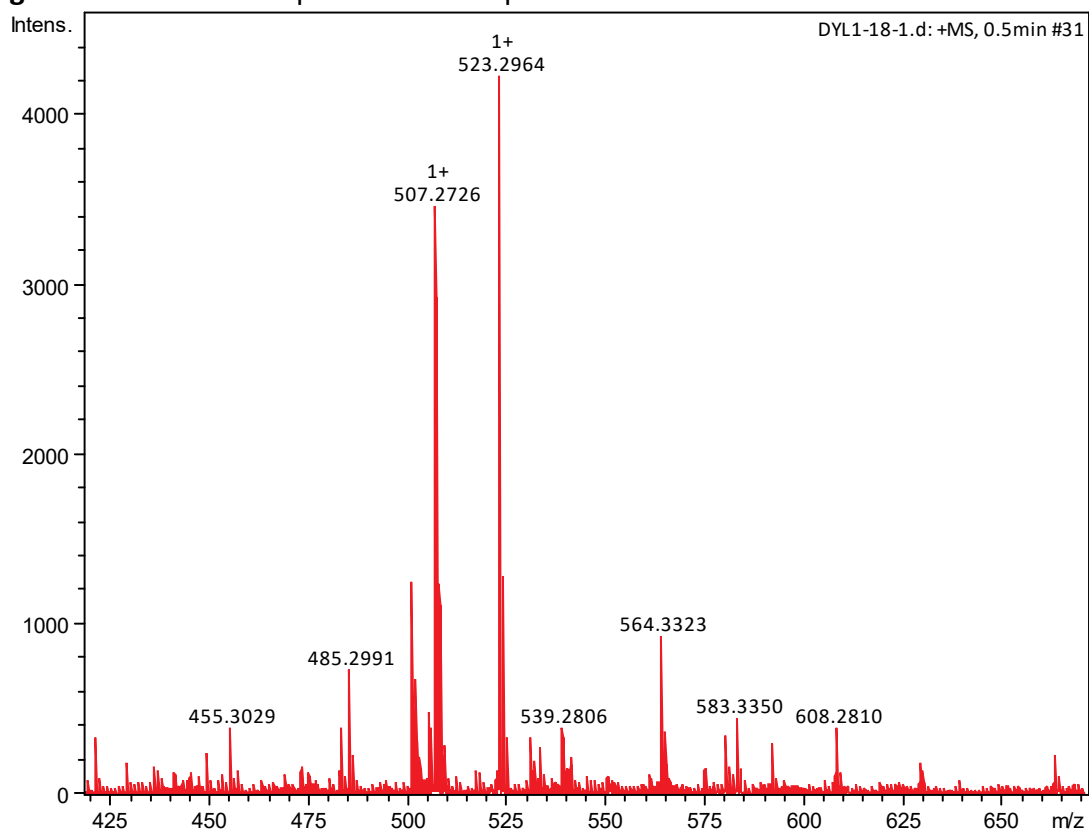


Figure S53. UV spectrum of compound 6

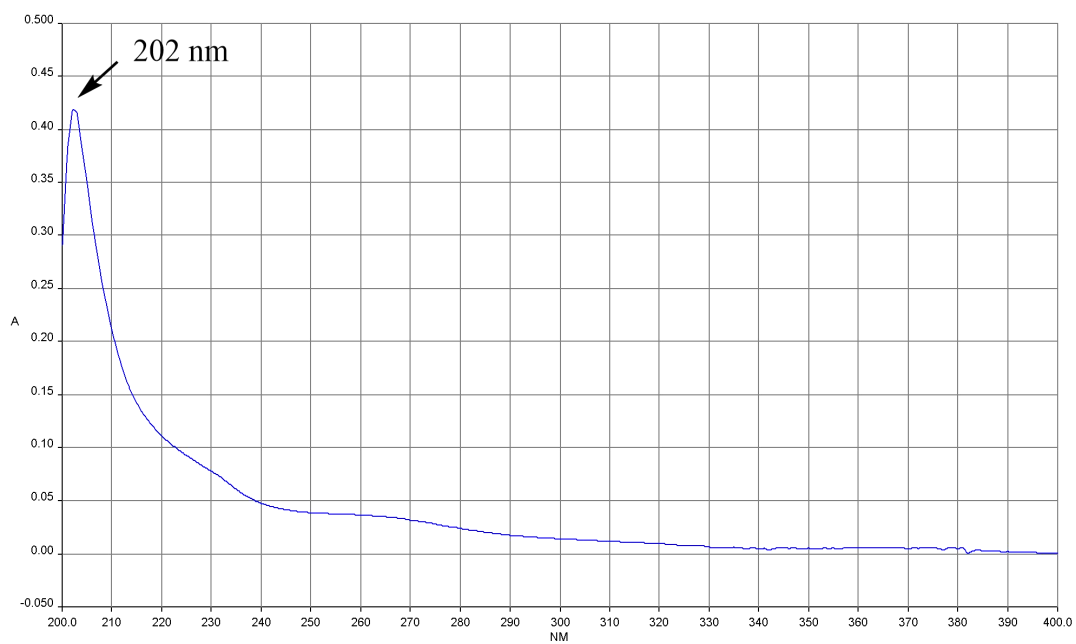


Figure S54. IR spectrum of compound 6

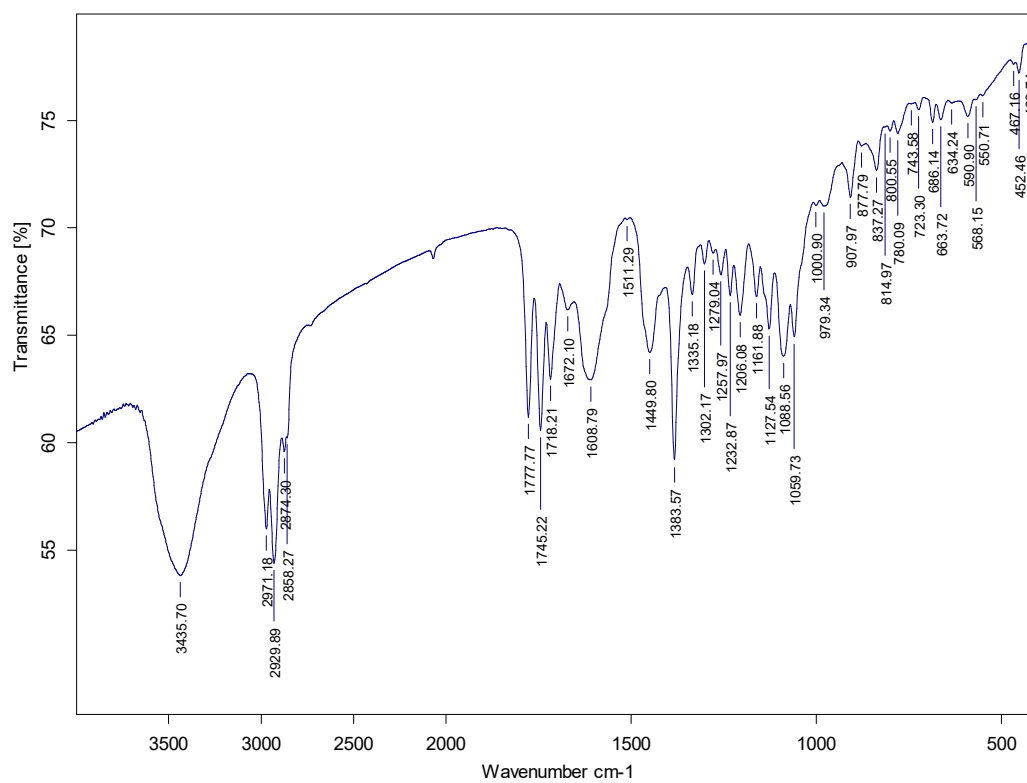


Figure S55. <sup>1</sup>H-NMR (400 MHz, CD<sub>3</sub>OD) spectrum of compound 7

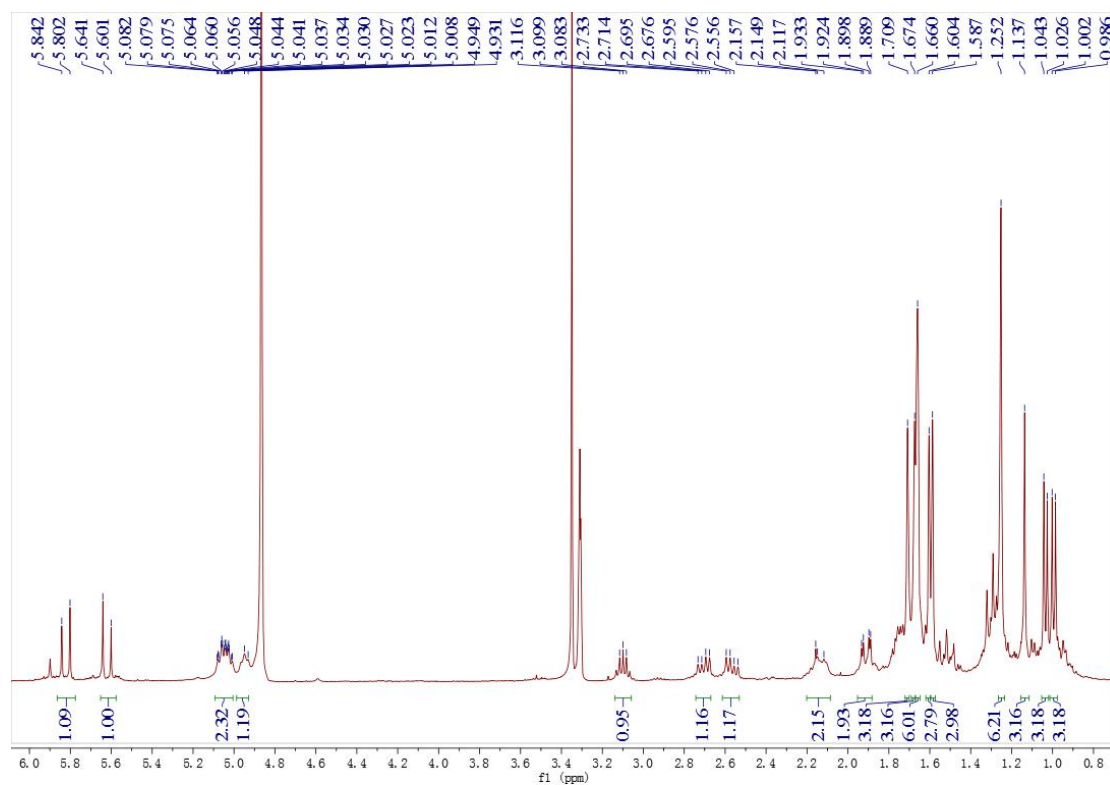


Figure S56. <sup>13</sup>C-NMR (100 MHz, CD<sub>3</sub>OD) spectrum of compound 7

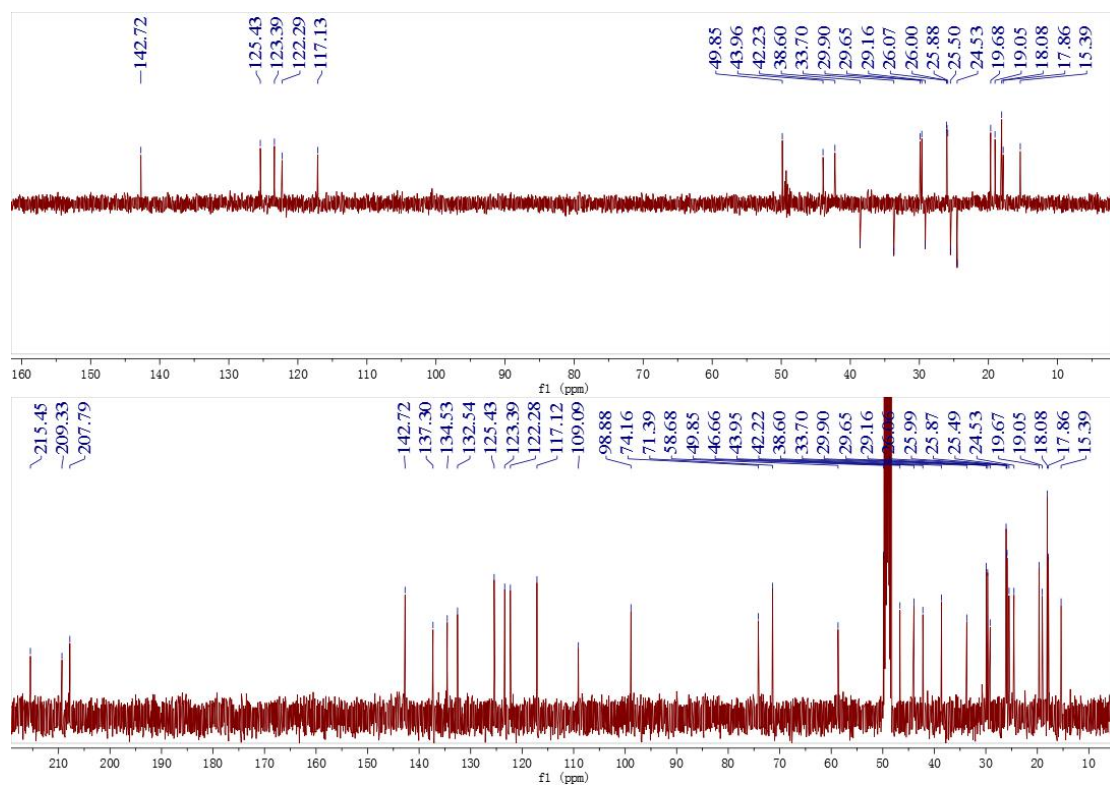




Figure S57.  $^1\text{H}$ -NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 5a

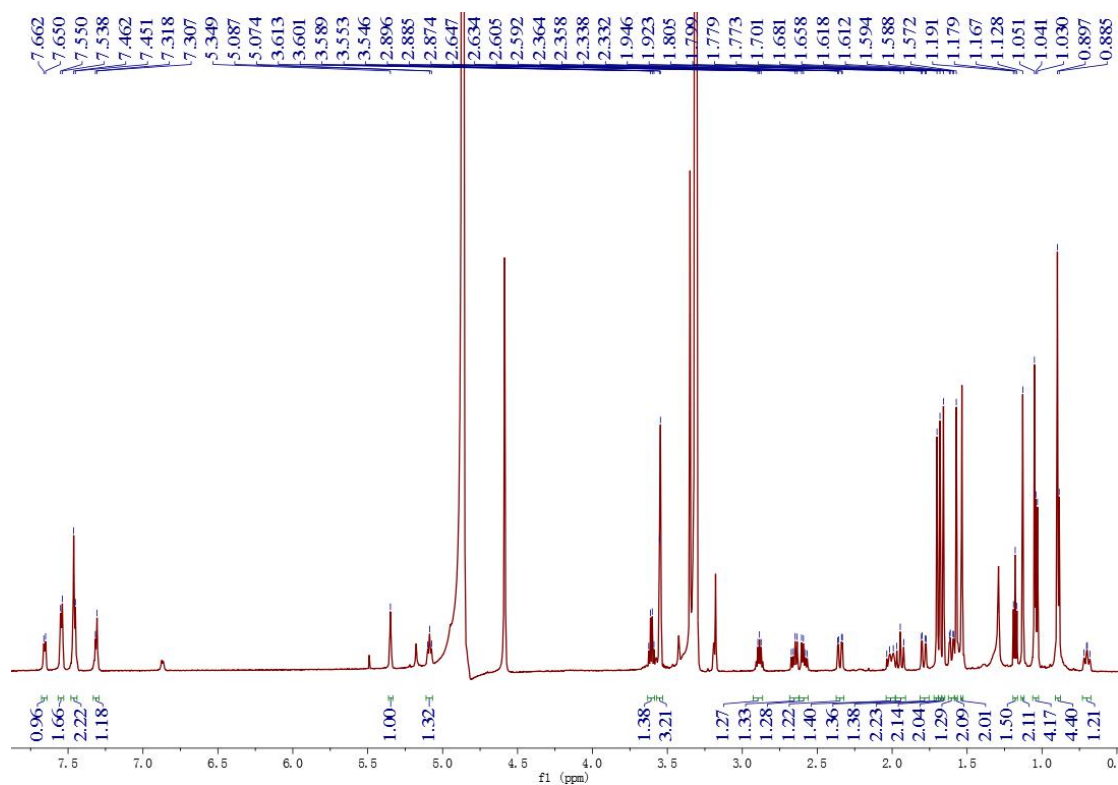


Figure S58.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 5a

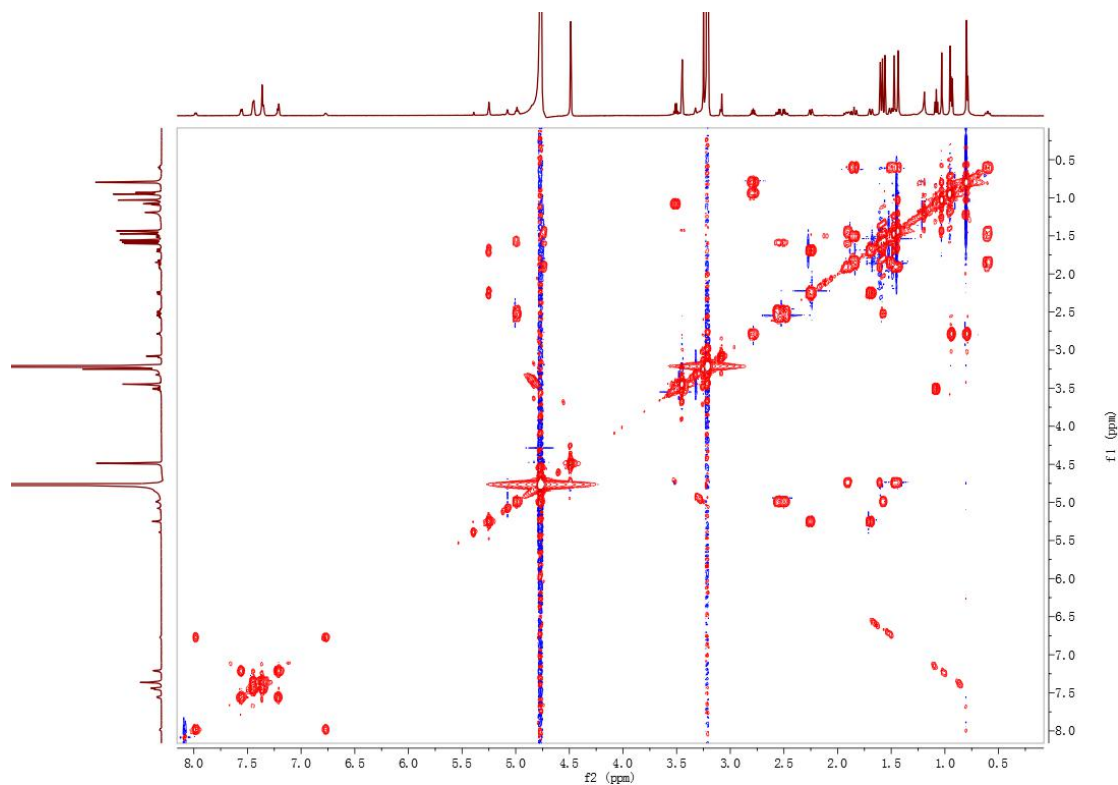


Figure S59. HR-ESI-MS spectrum of compound 5a

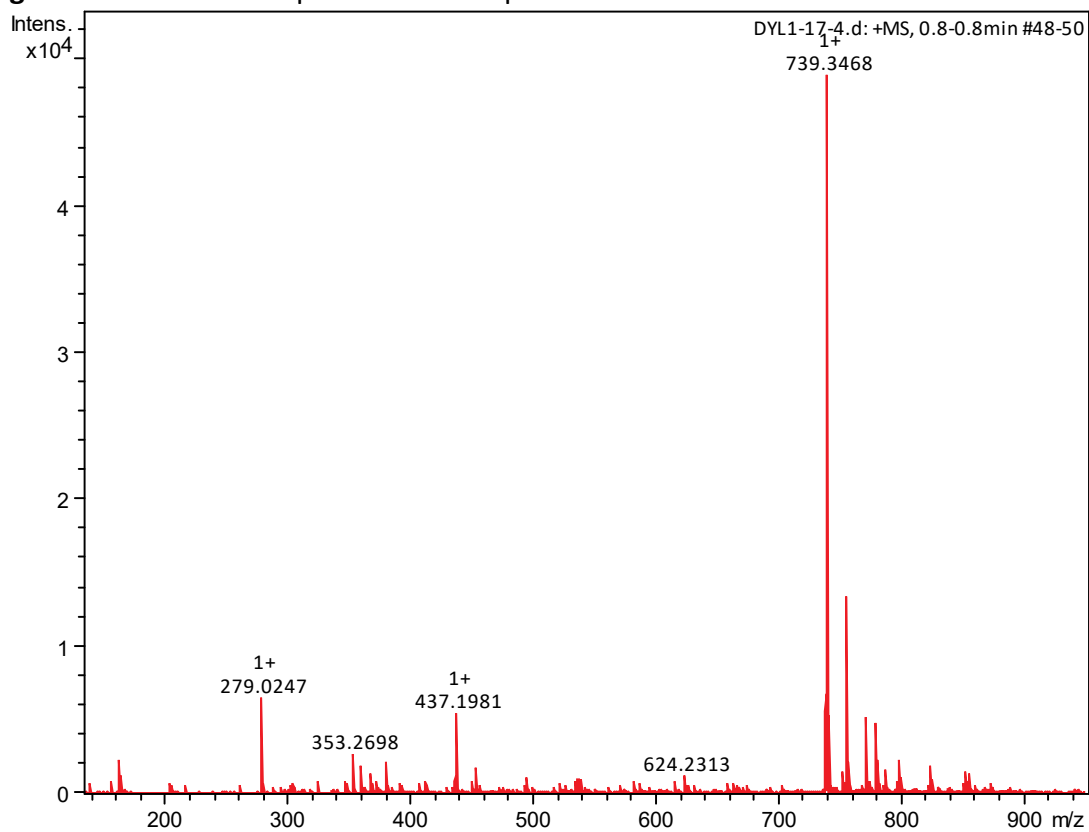
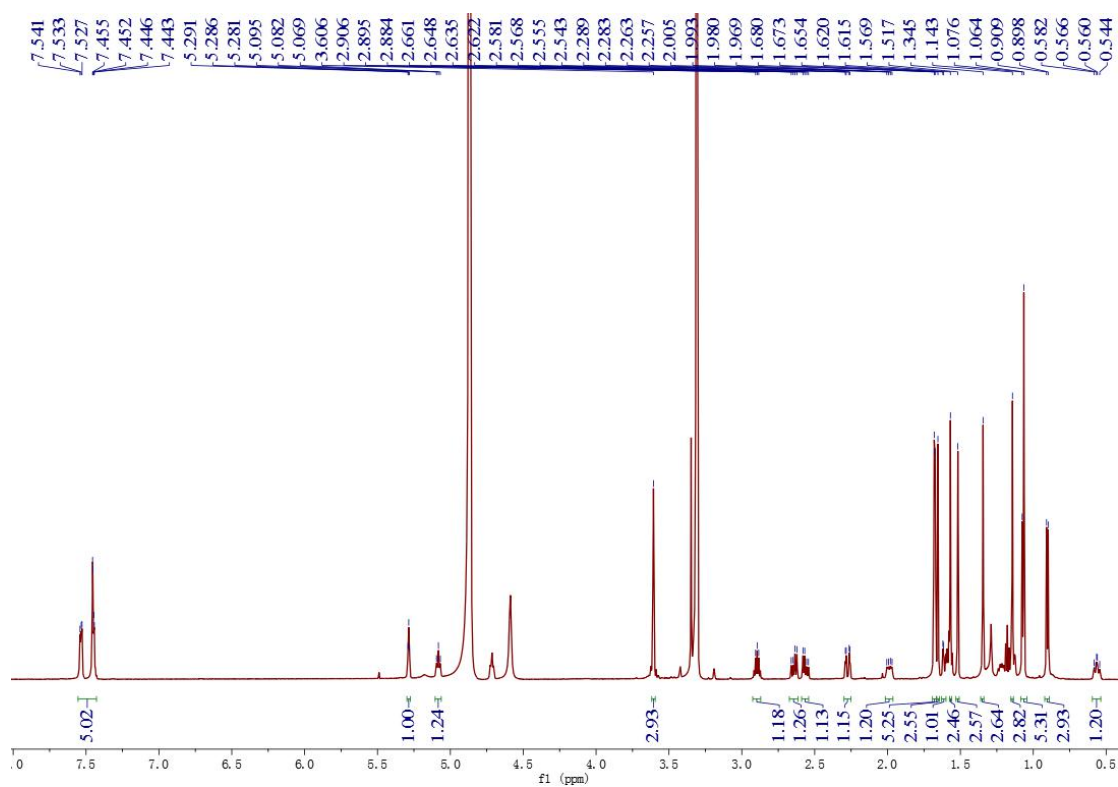
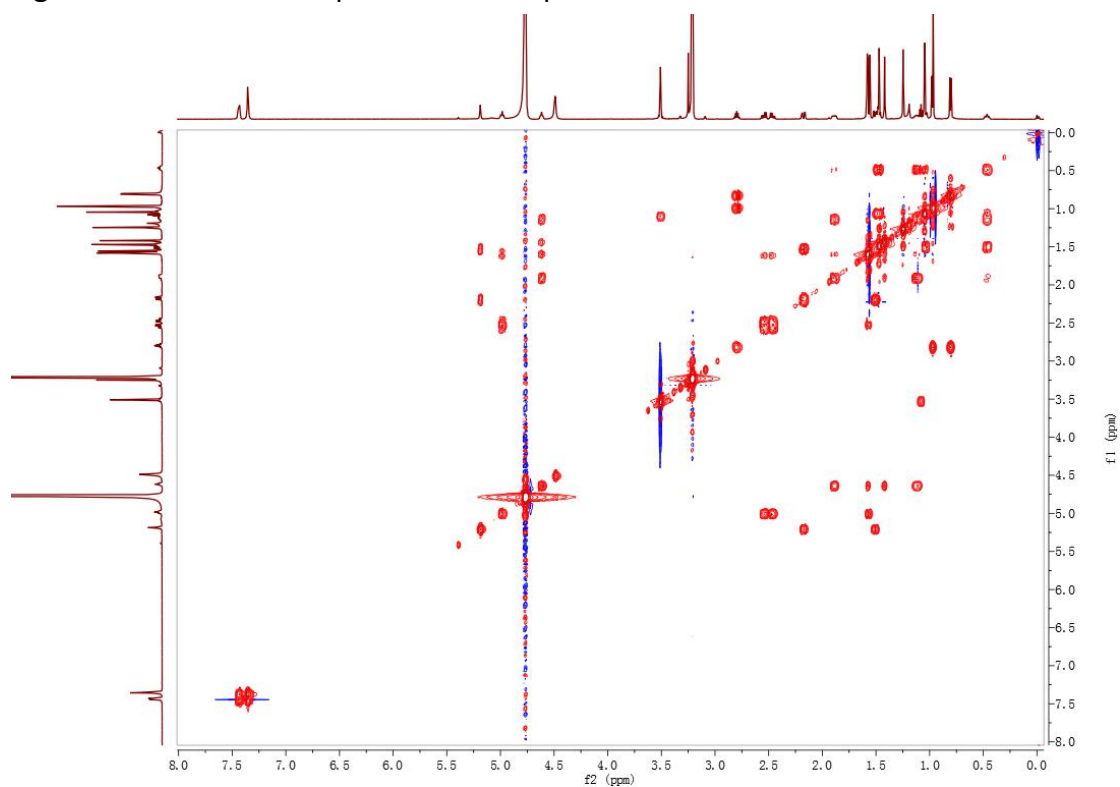


Figure S60. <sup>1</sup>H-NMR (600 MHz, CD<sub>3</sub>OD) spectrum of compound 5b



**Figure S61.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **5b**



**Figure S62.** HR-ESI-MS spectrum of compound **5b**

