

## Supplementary Information

### **Hyalodendriellins A-F, new 14-membered resorcylic acid lactones from the endophytic fungus *Hyalodendriella* sp. Ponipodef12**

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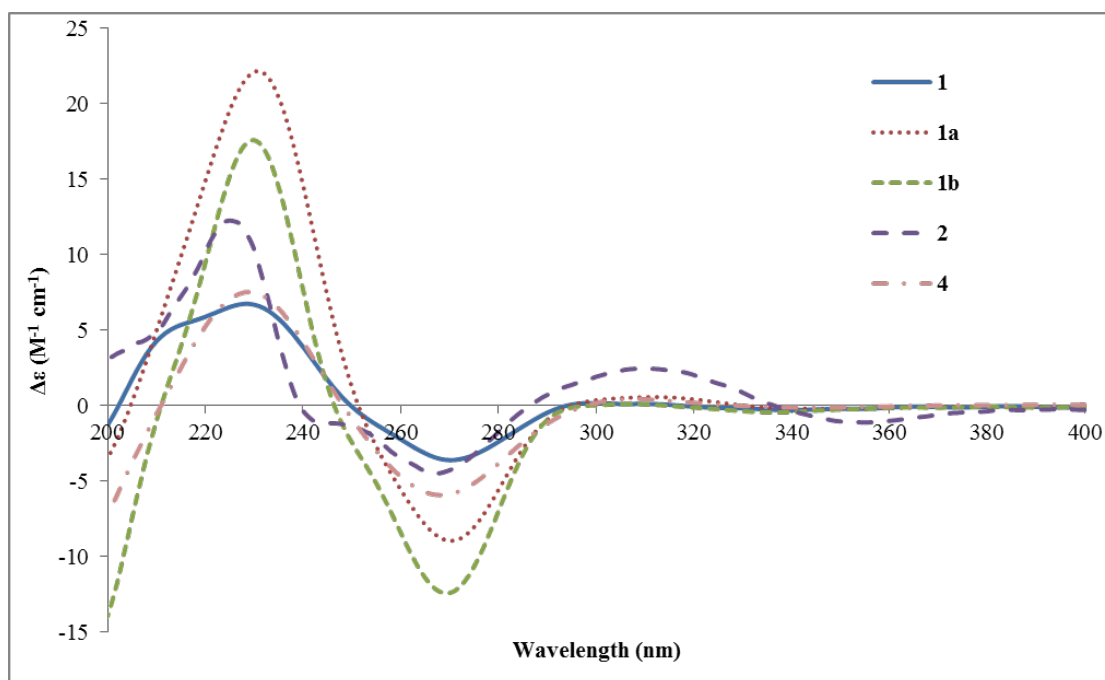
‡ These authors contributed equally.

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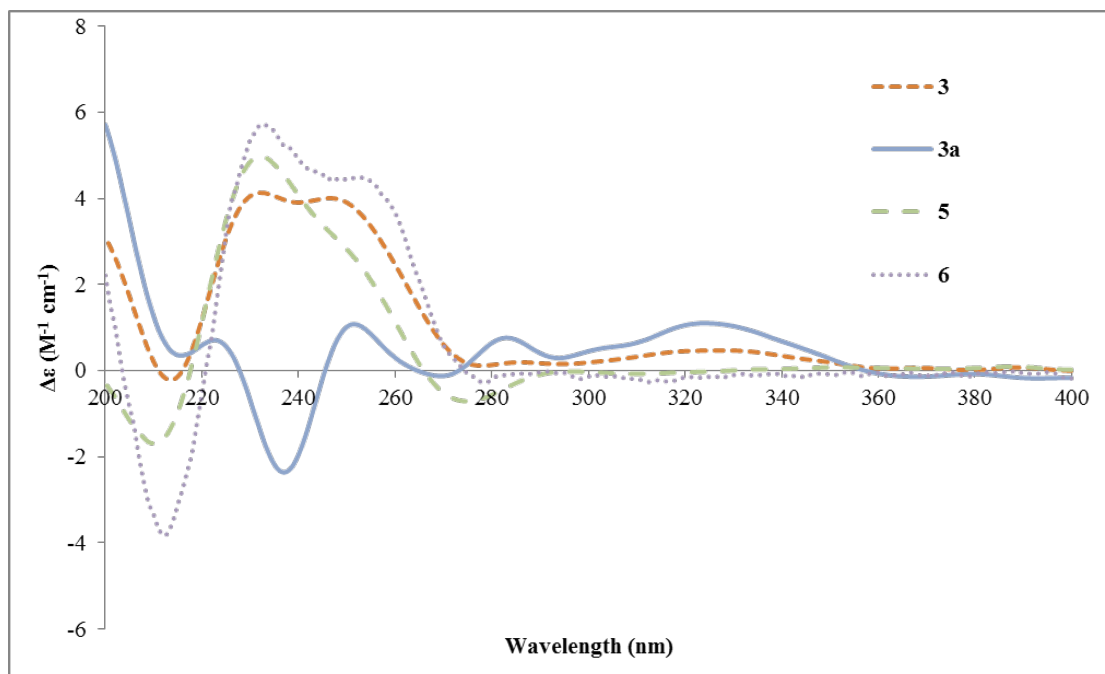
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## 1. CD spectra of 1-6, 1a-1b, and 3a

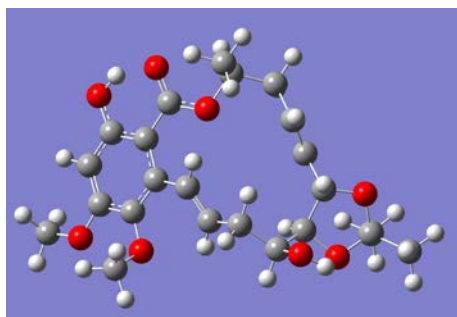


**Figure S1.** The CD spectra of **1**, **1a**, **1b**, **2**, and **4** (in MeOH).

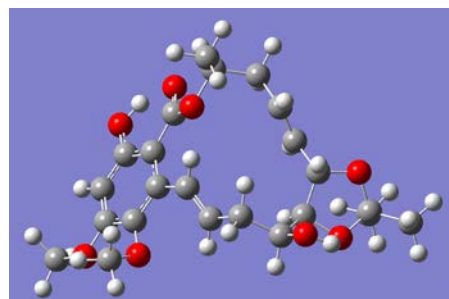


**Figure S2.** The CD spectra of **3**, **3a**, **5**, and **6** (in MeOH).

## 2. Computation Data for 1a, 2, 3b, and 4



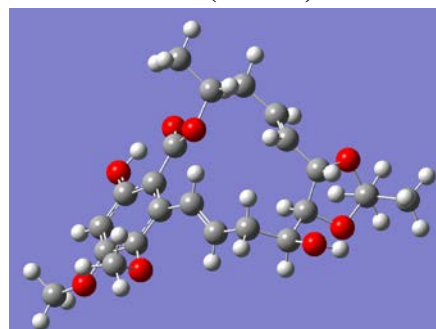
**1a-1 (47.0%)**



**1a-2 (24.0%)**



**1a-3 (11.7%)**

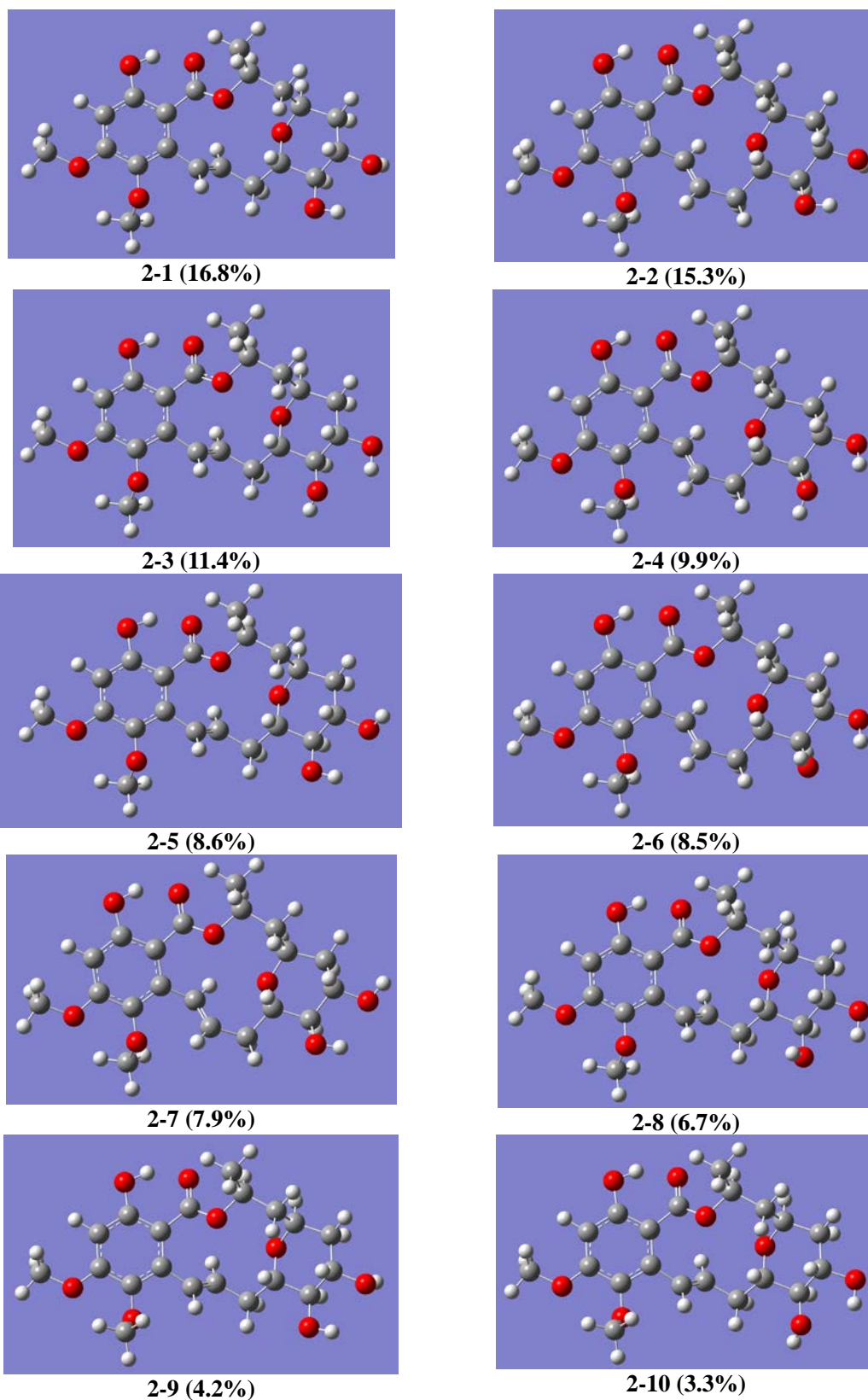


**1a-4 (11.2%)**

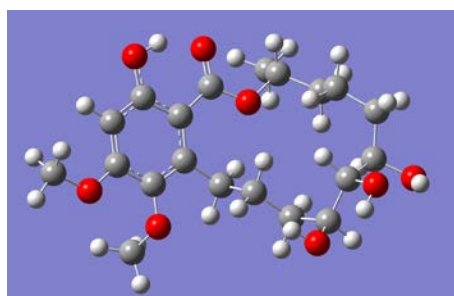


**1a-5 (1.8%)**

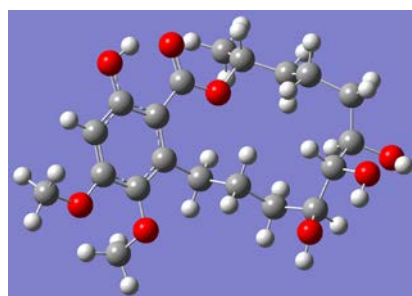
**Figure S3.** The stable conformers of (3*S*, 7*S*, 8*S*, 9*S*)-**1a** with populations greater than 1%.



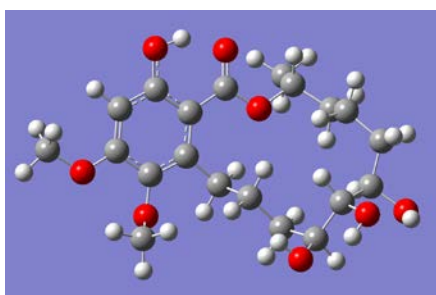
**Figure S4.** The stable conformers of (3*S*, 5*R*, 7*S*, 8*R*, 9*S*)-2 with populations greater than 2%.



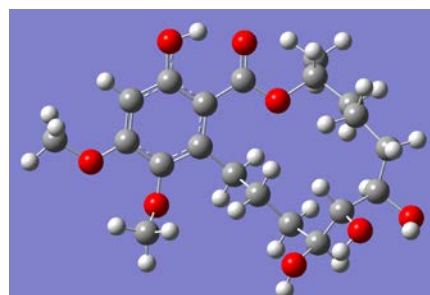
**3b-1 (50.2%)**



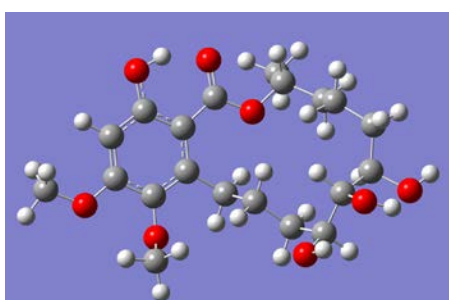
**3b-2 (23.6%)**



**3b-3 (9.3%)**

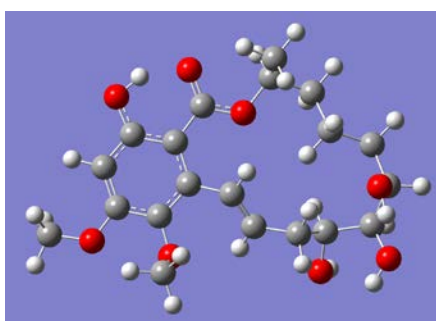


**3b-4 (8.7%)**

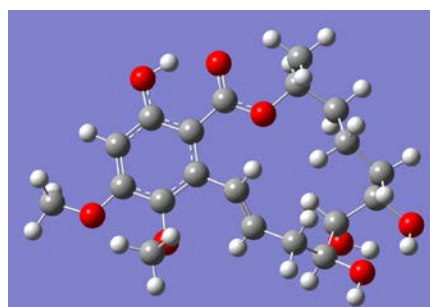


**3b-5 (6.1%)**

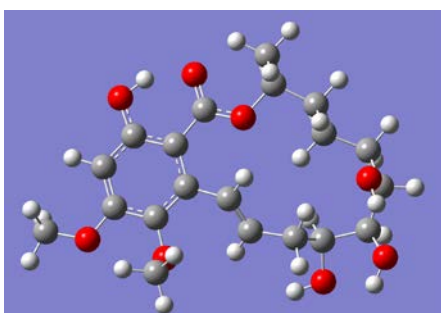
**Figure S5.** The stable conformers of (3*R*, 7*R*, 8*R*, 9*S*)-**3b** with populations greater than 1%.



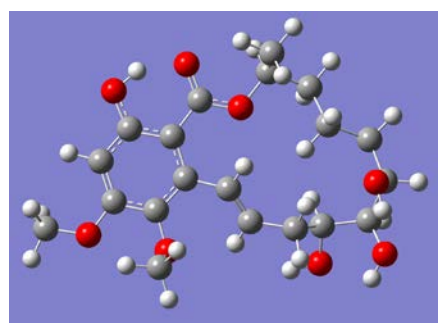
**4-1 (27.2%)**



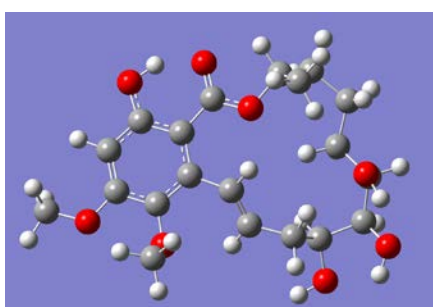
**4-2 (23.5%)**



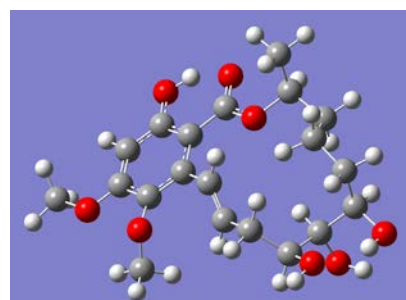
**4-3 (20.1%)**



**4-4 (19.9%)**



**4-5 (3.3%)**



**4-6 (2.0%)**

**Figure S6.** The stable conformers of (3*S*, 7*R*, 8*R*, 9*S*)-**4** with populations greater than 1%.



### 3. (1D, 2D) NMR, IR, and HRESIMS spectra

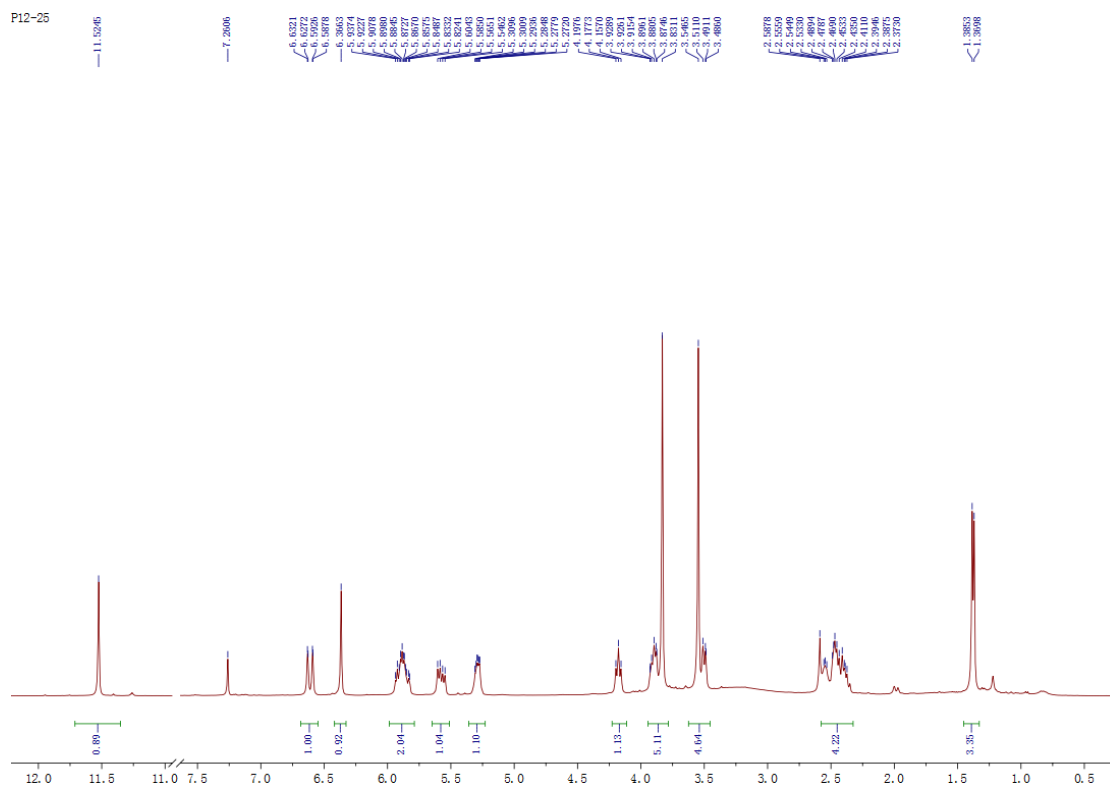


Figure S7.  $^1\text{H}$  NMR spectrum of **1** ( $\text{CDCl}_3$ , 400MHz)

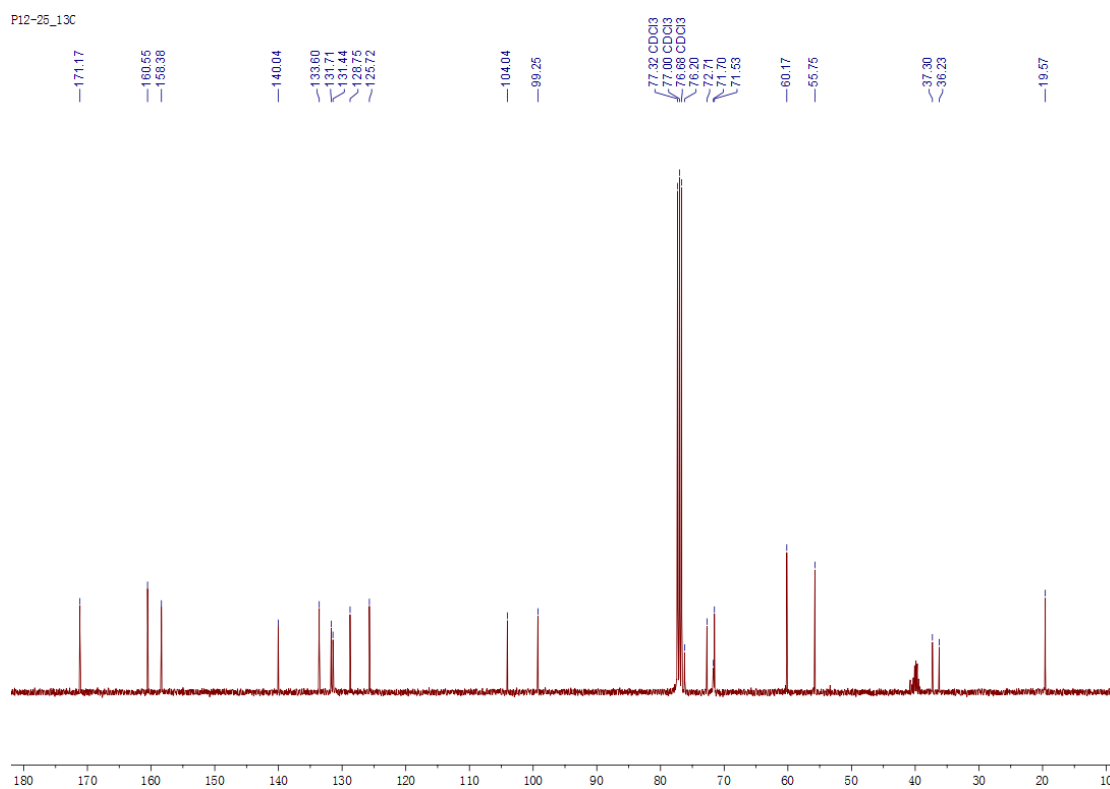
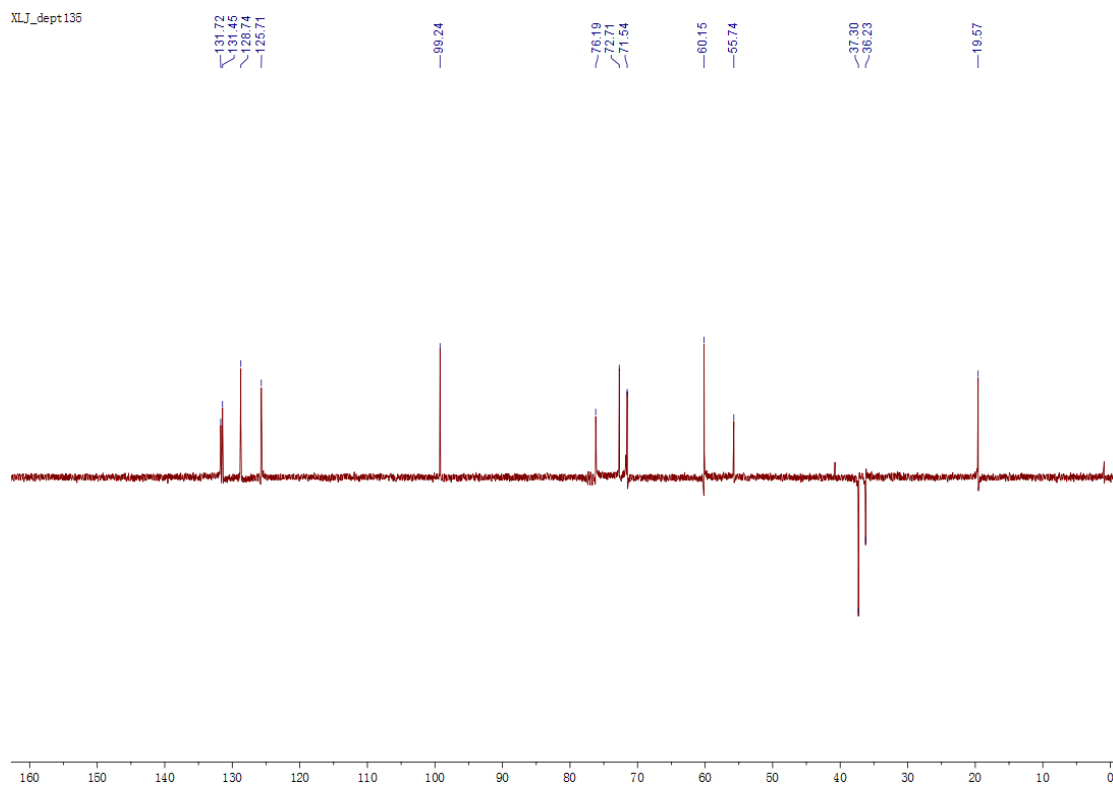
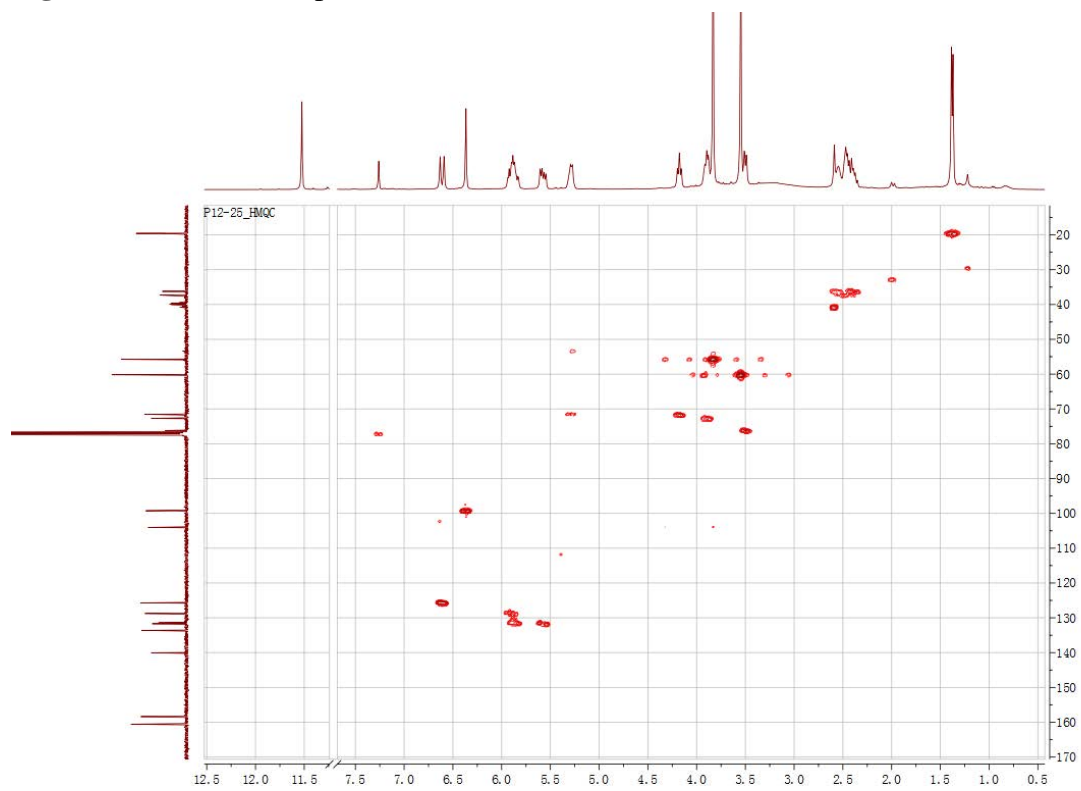


Figure S8.  $^{13}\text{C}$  NMR spectrum of **1** ( $\text{CDCl}_3$ , 100MHz)



**Figure S9.** DEPT-135 spectrum of **1** (CDCl<sub>3</sub>, 100MHz)



**Figure S10.** HMQC spectrum of **1** (CDCl<sub>3</sub>)

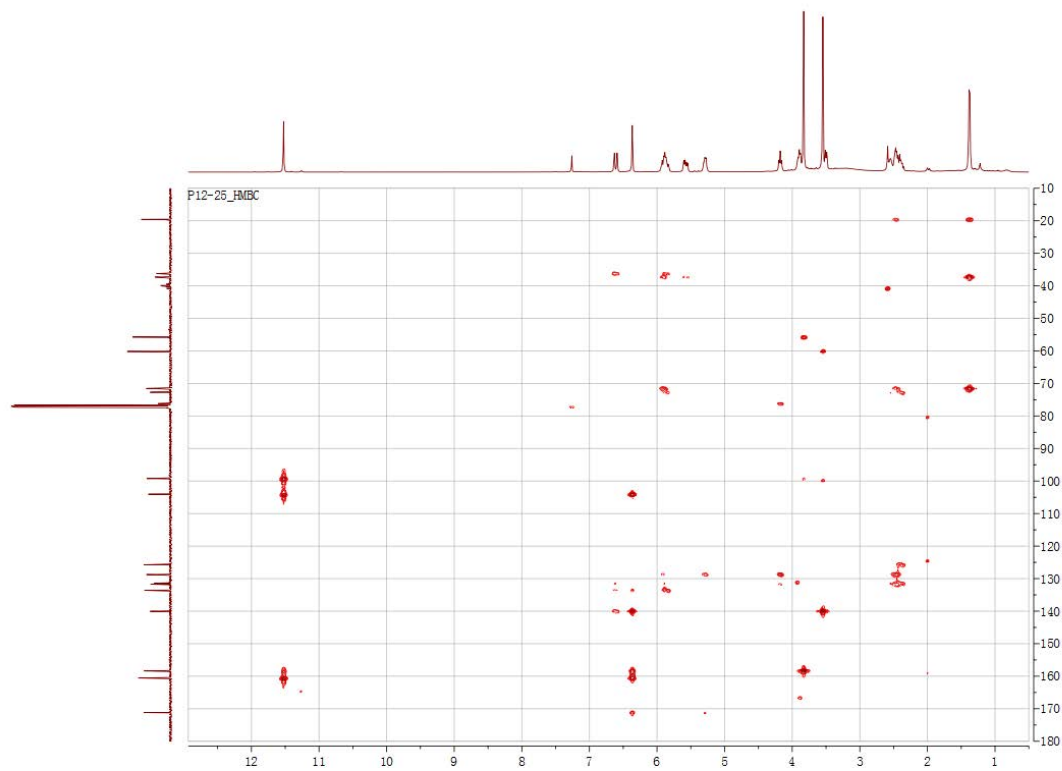


Figure S11. HMBC spectrum of **1** ( $\text{CDCl}_3$ )

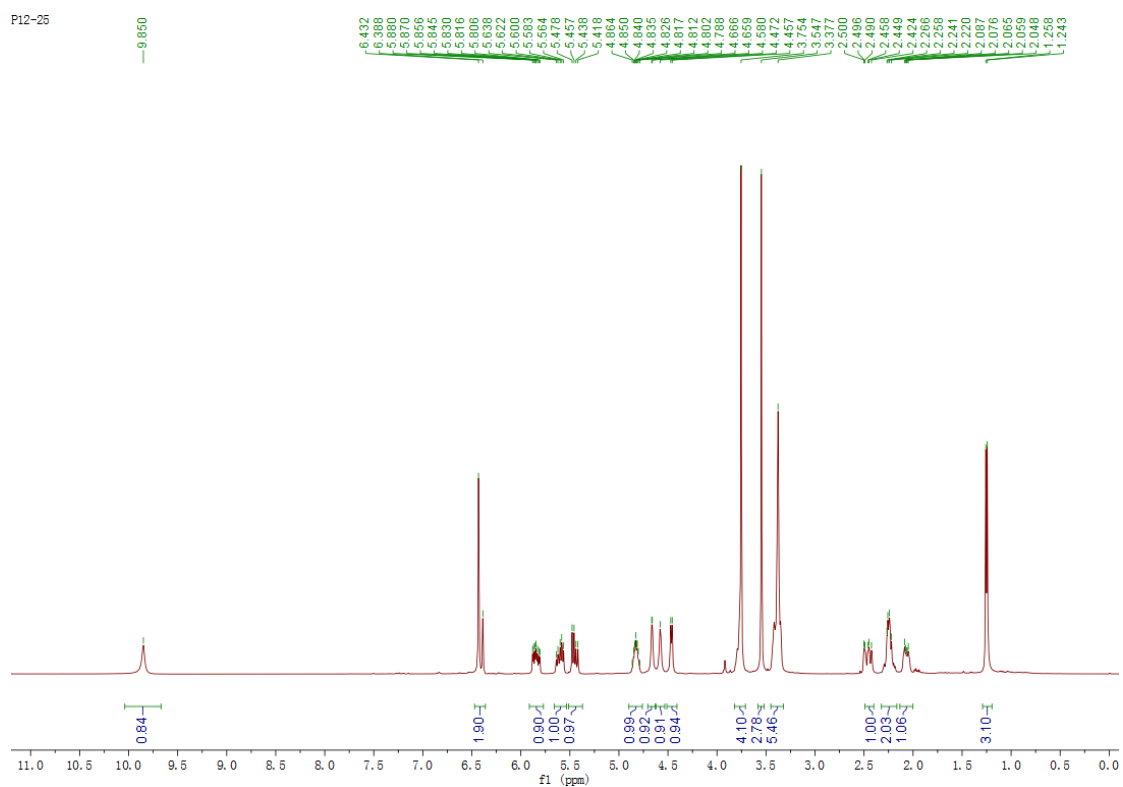
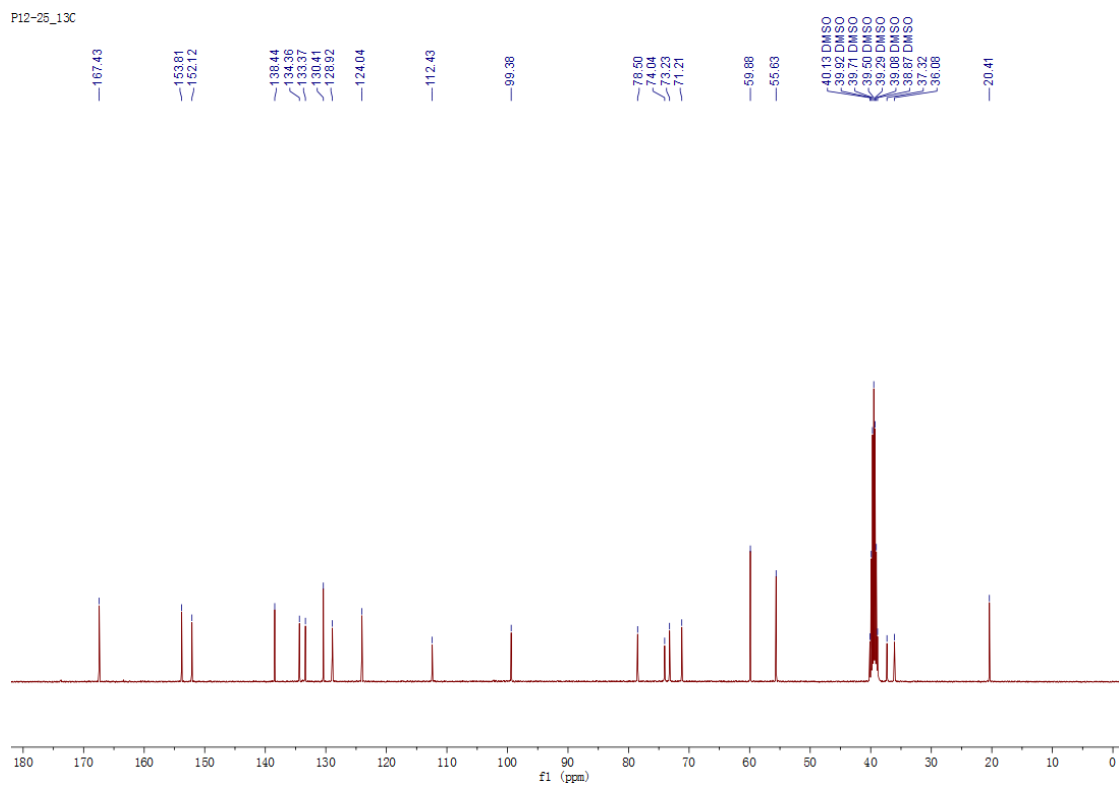
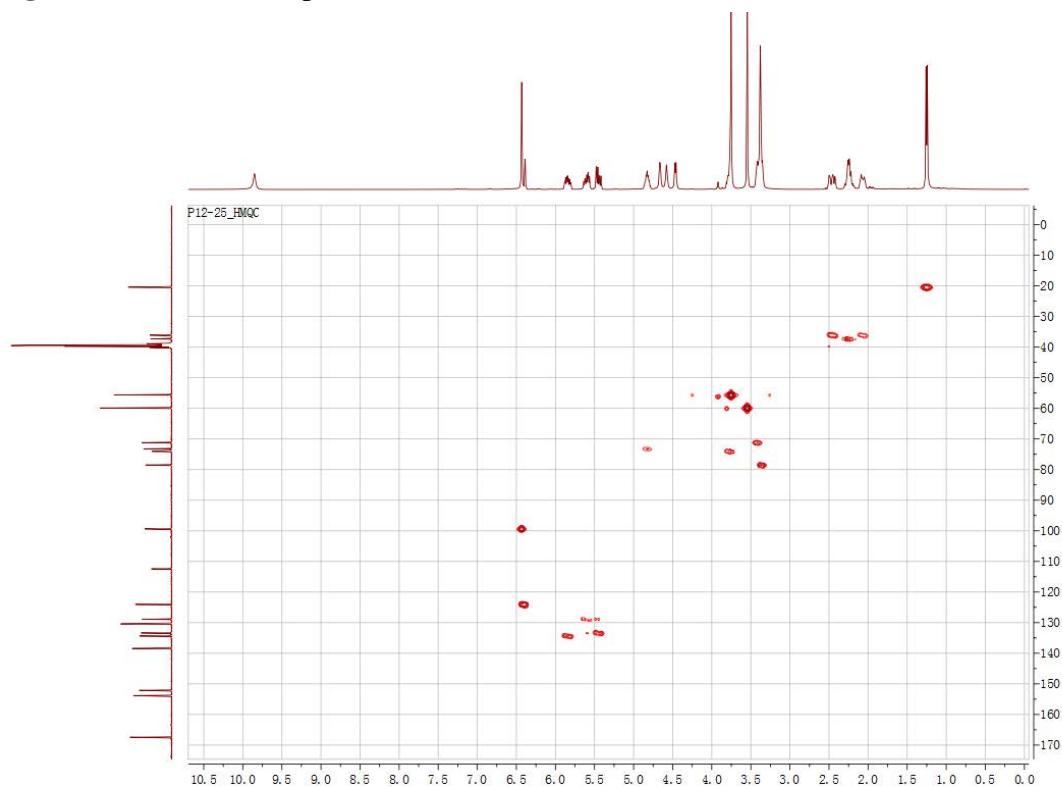


Figure S12.  $^1\text{H}$  NMR spectrum of **1** ( $\text{DMSO}-d_6$ , 400MHz)



**Figure S13.**  $^{13}\text{C}$  NMR spectrum of **1** (DMSO- $d_6$ , 100MHz)



**Figure S14.** HMQC spectrum of **1** (DMSO- $d_6$ )

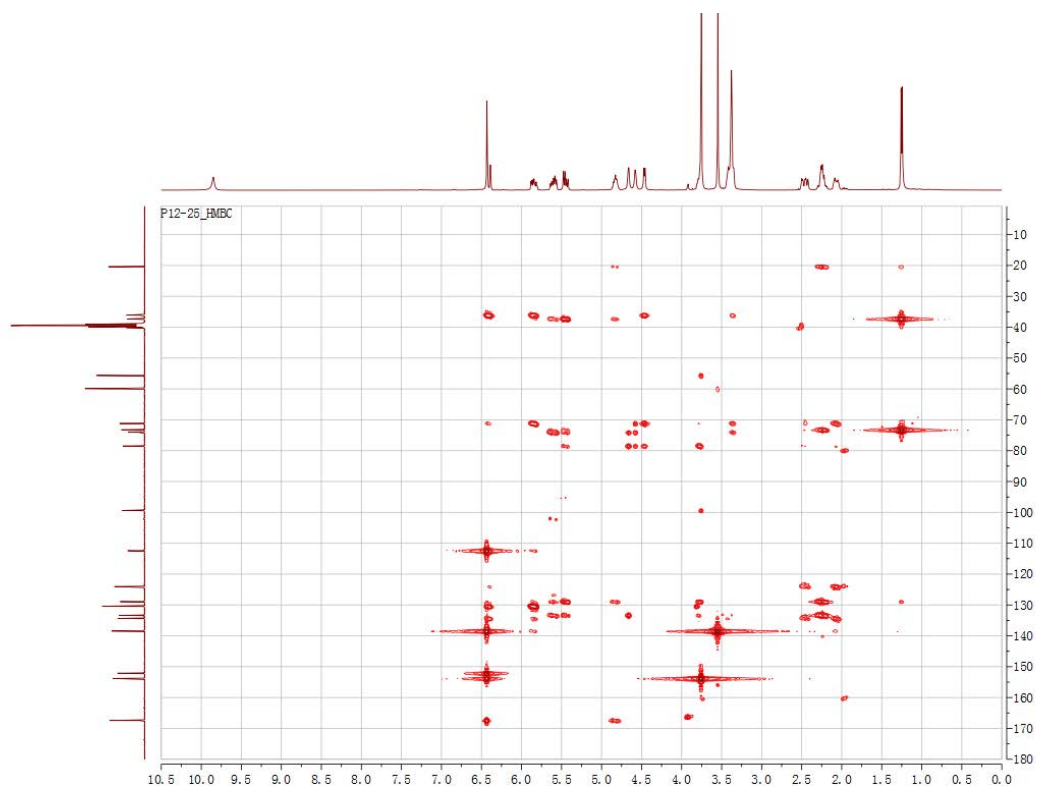


Figure S15. HMBC spectrum of **1** (DMSO- $d_6$ )

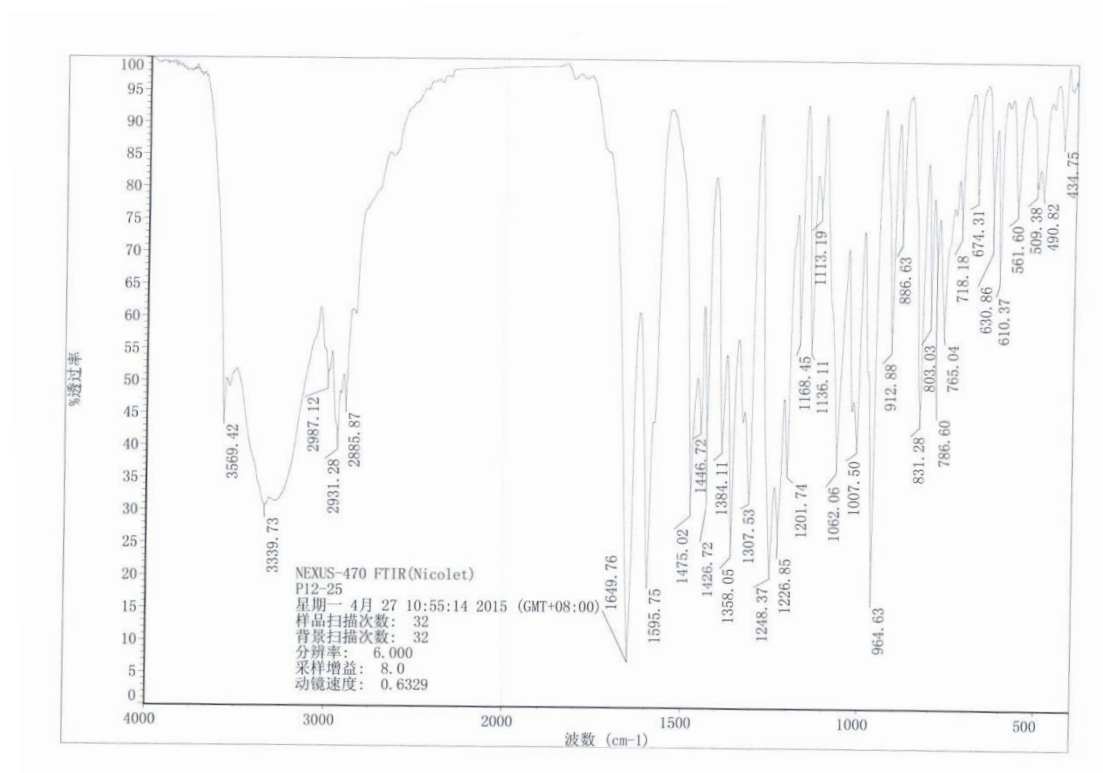


Figure S16. IR spectrum of **1**

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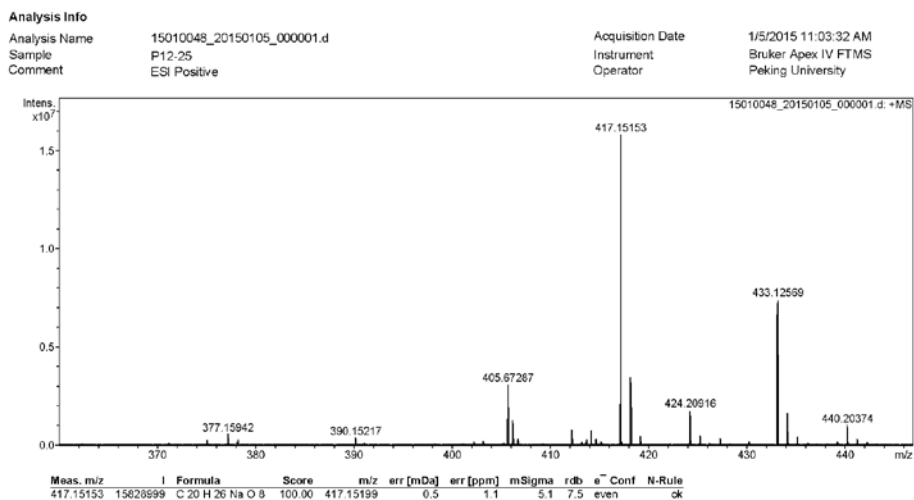


Figure S17. HRESIMS spectrum of **1**

P12-25a

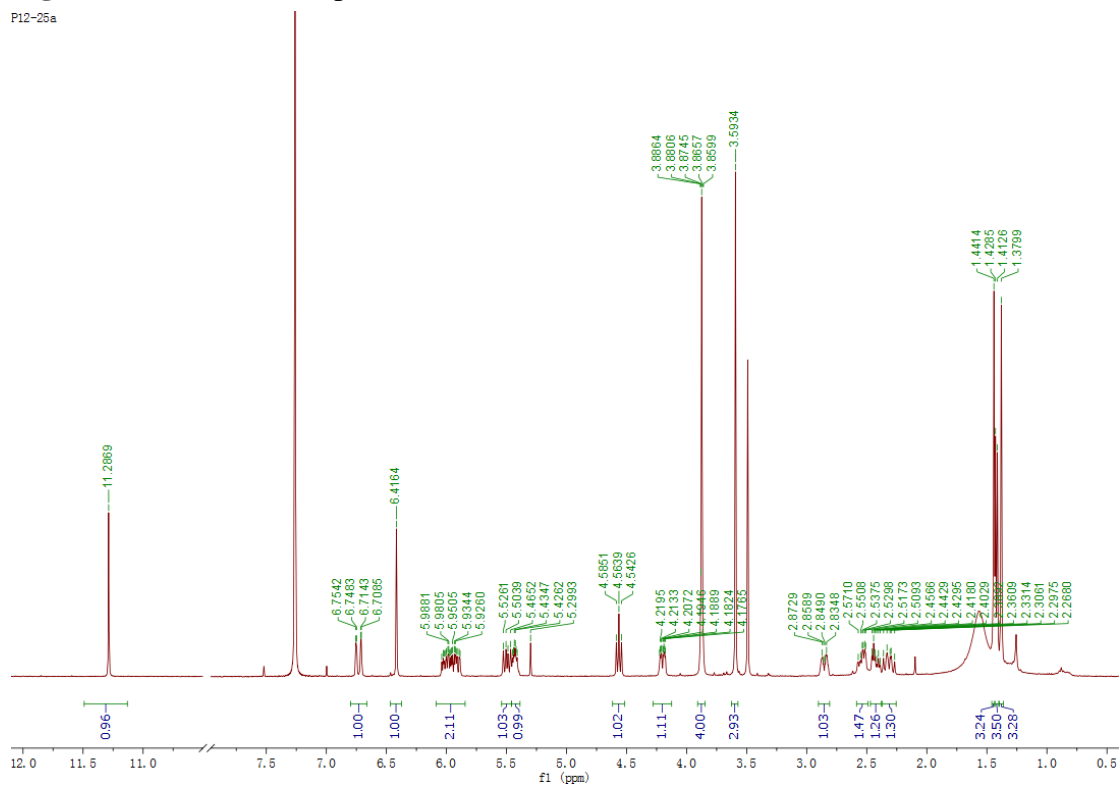


Figure S18. <sup>1</sup>H NMR spectrum of **1a** (CDCl<sub>3</sub>, 400MHz)

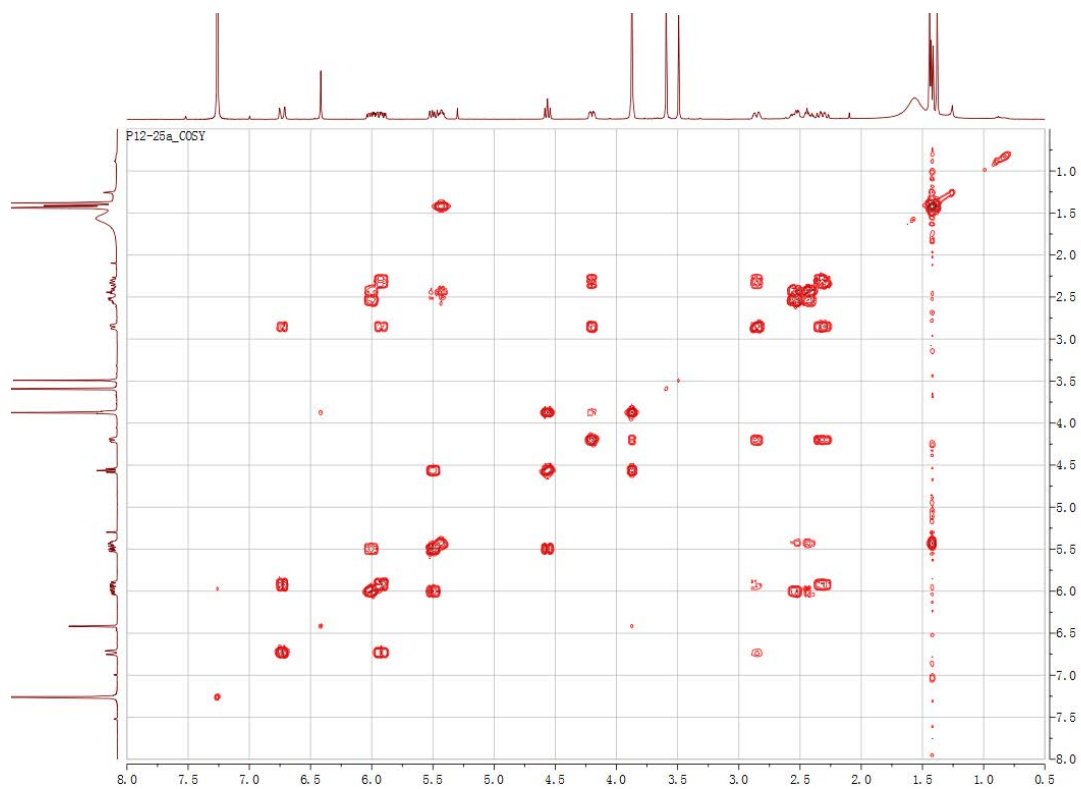


Figure S19.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1a** ( $\text{CDCl}_3$ )

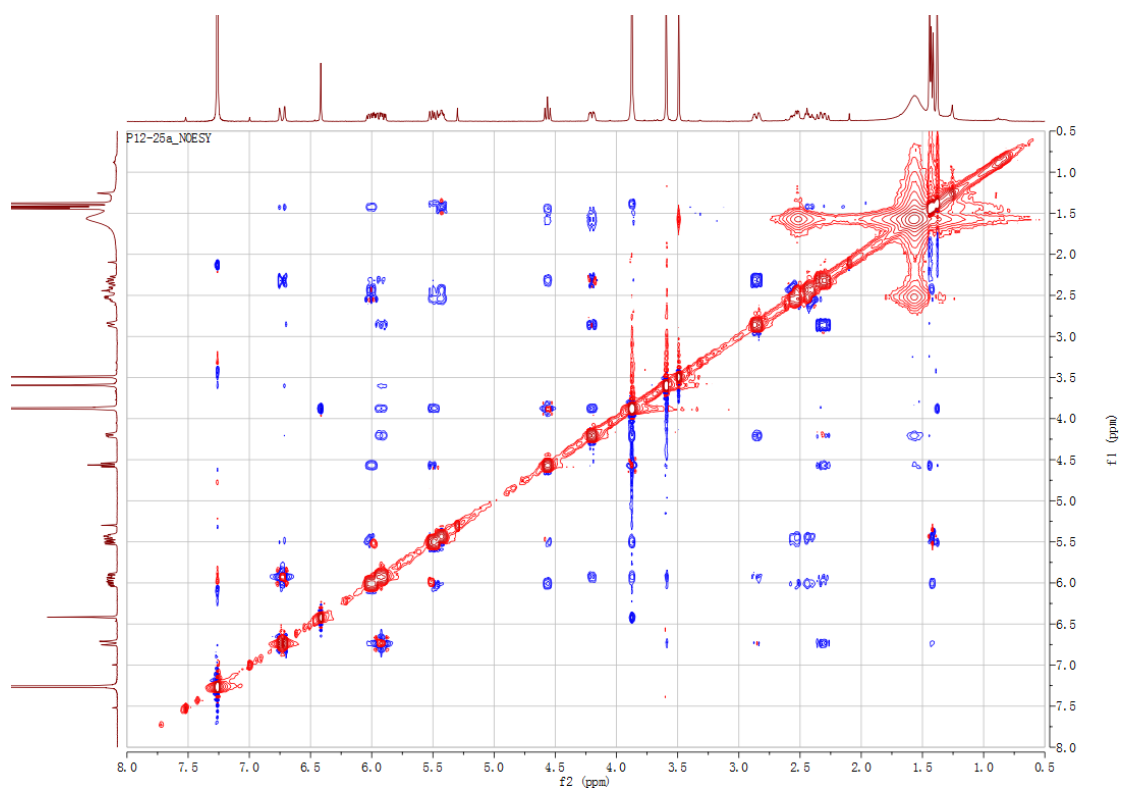


Figure S20. NOESY spectrum of **1a** ( $\text{CDCl}_3$ )

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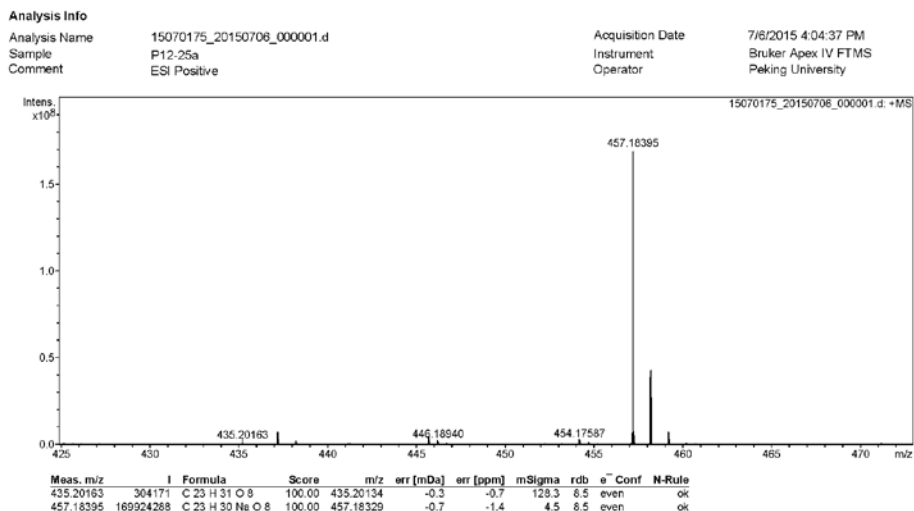


Figure S21. HRESIMS spectrum of **1a**

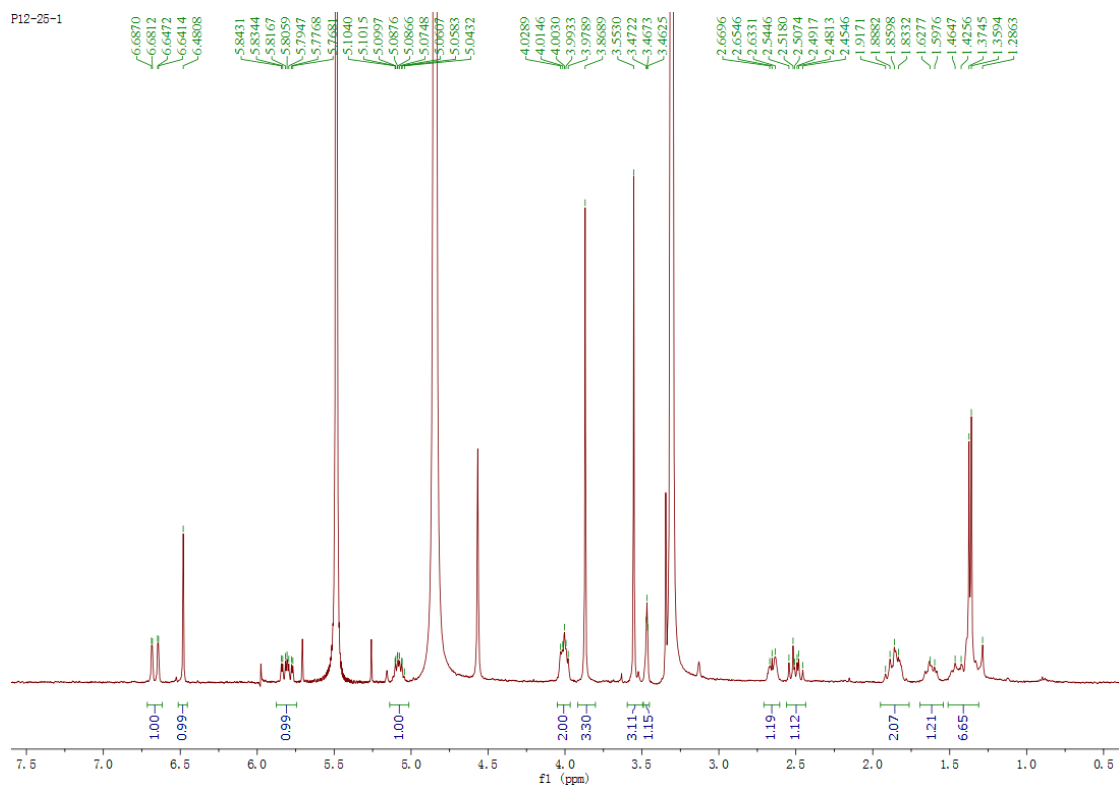
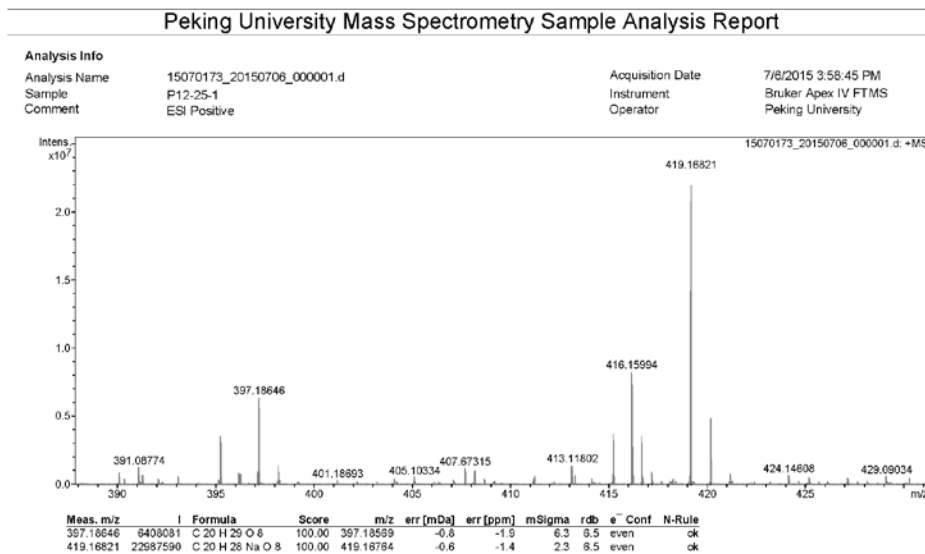
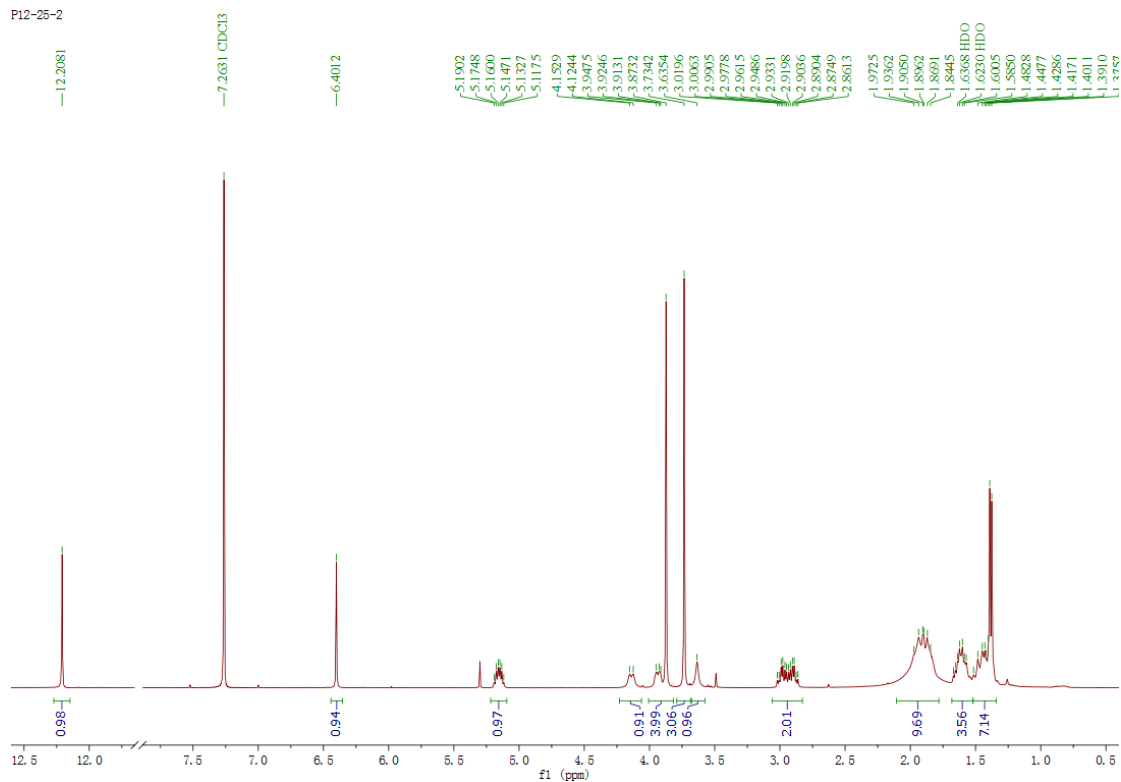


Figure S22. <sup>1</sup>H NMR spectrum of **1b** (CD<sub>3</sub>OD, 400MHz)





**Figure S23.** HRESIMS spectrum of **1b**



**Figure S24.** <sup>1</sup>H NMR spectrum of **1c** (CDCl<sub>3</sub>, 400MHz)

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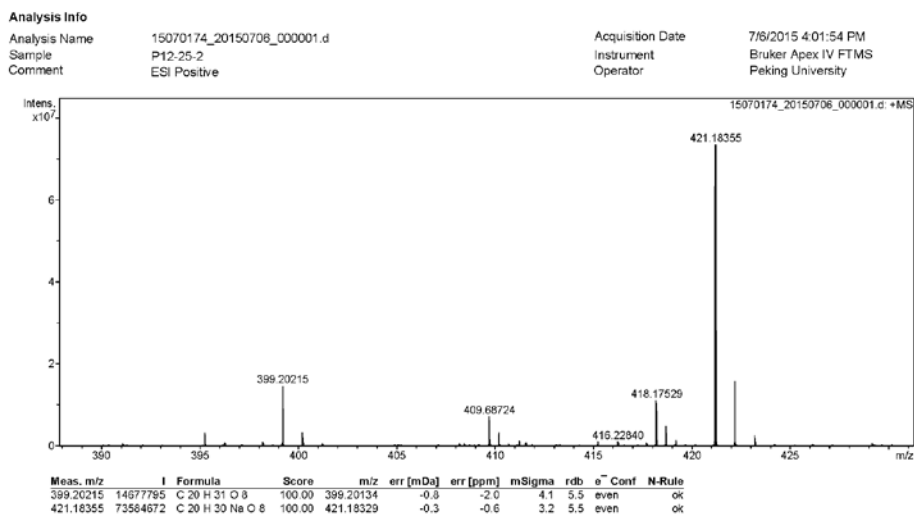


Figure S25. HRESIMS spectrum of 1c

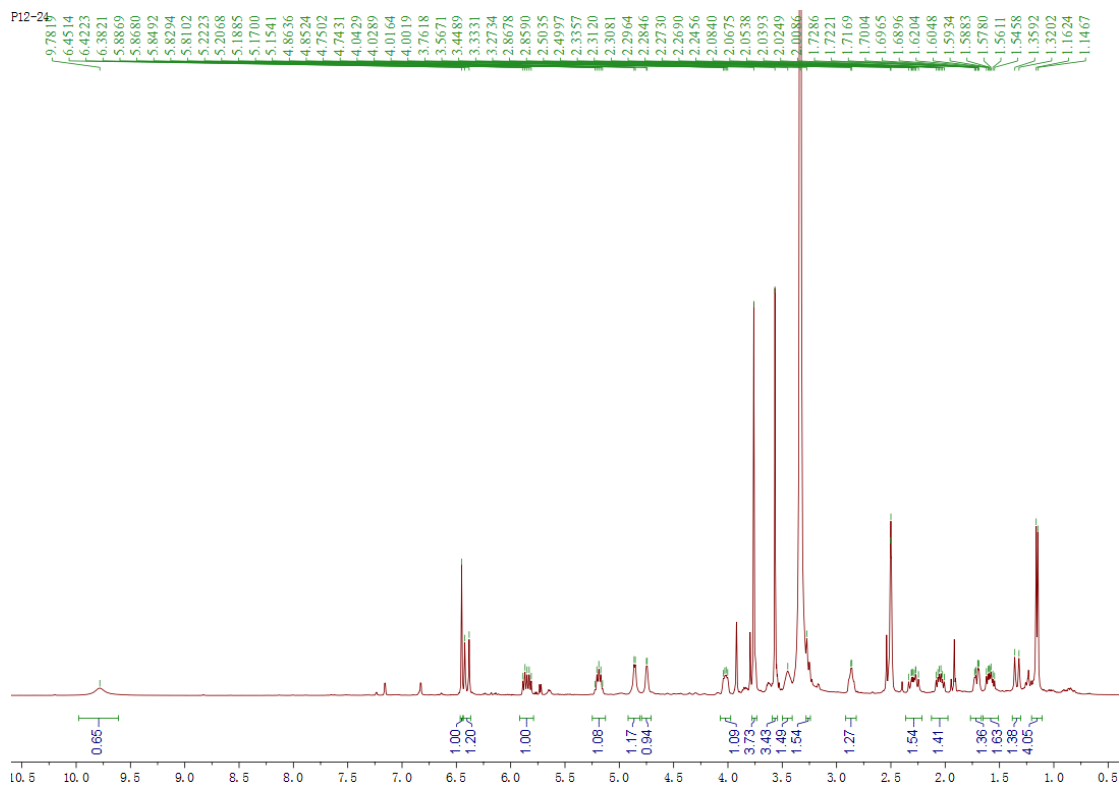


Figure S26. <sup>1</sup>H NMR spectrum of 2 (DMSO-*d*<sub>6</sub>, 400MHz)

P12-24\_13C

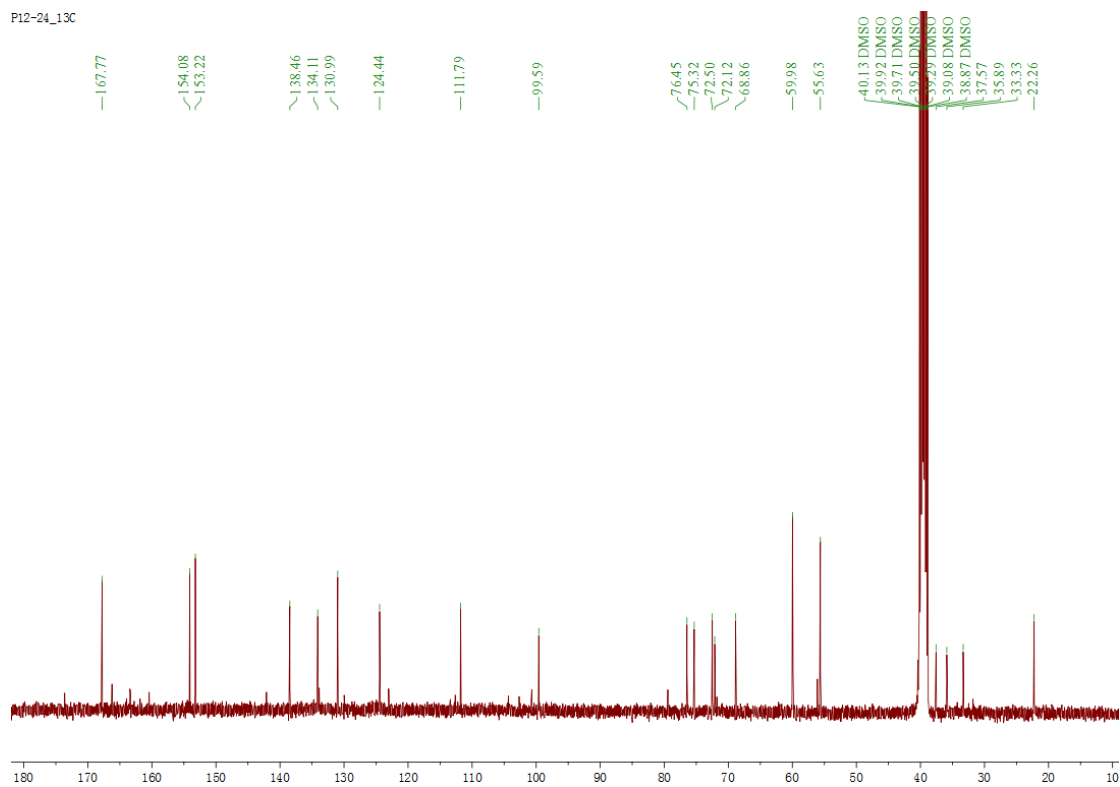
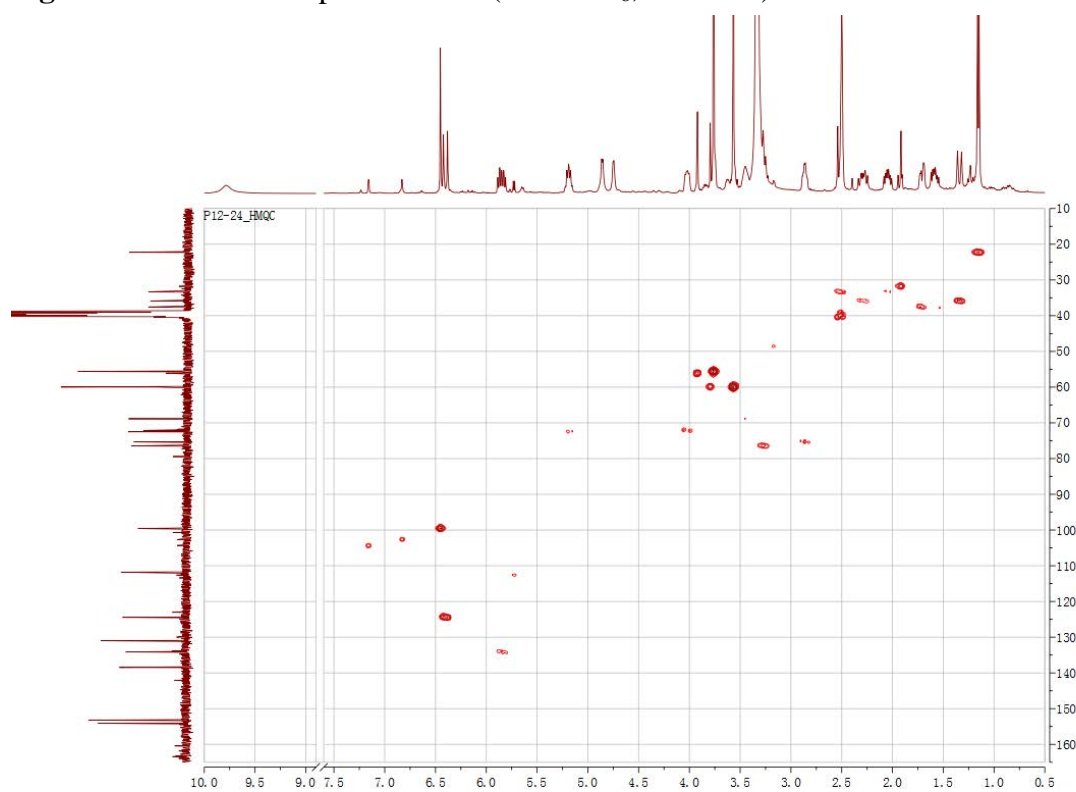
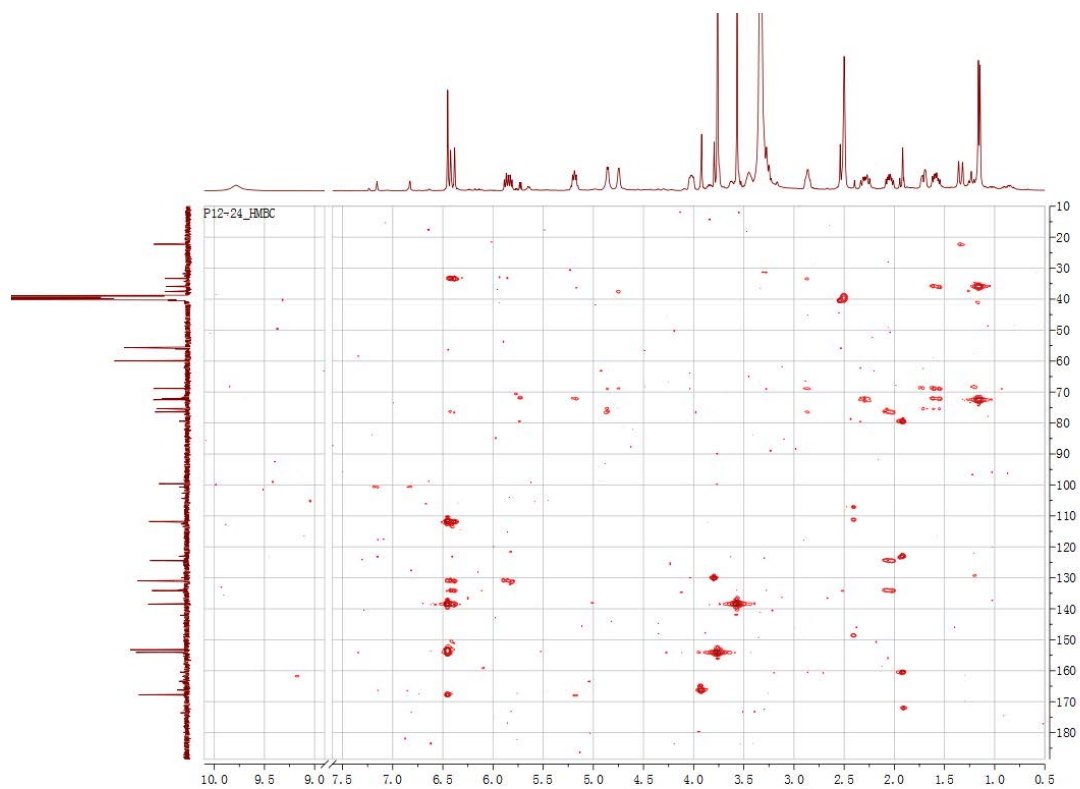
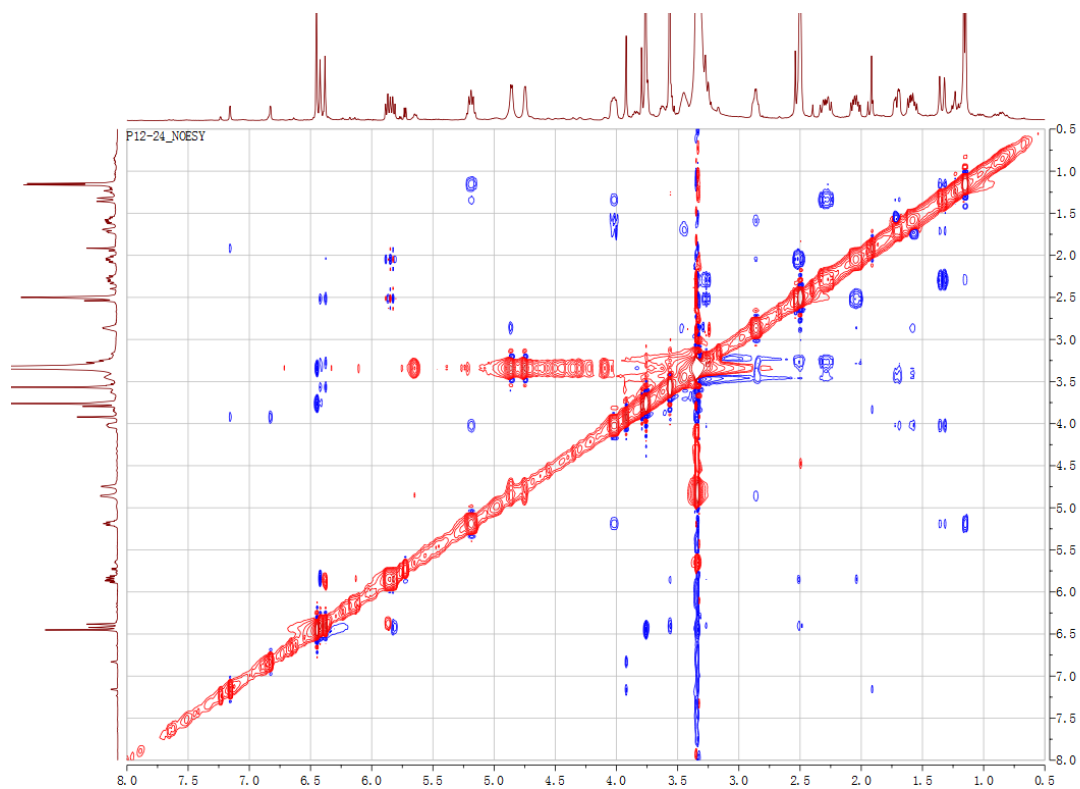


Figure S27.  $^{13}\text{C}$  NMR spectrum of **2** (DMSO- $d_6$ , 100MHz)





**Figure S29.** HMBC spectrum of **2** (DMSO- $d_6$ )



**Figure S30.** NOESY spectrum of **2** (DMSO- $d_6$ )

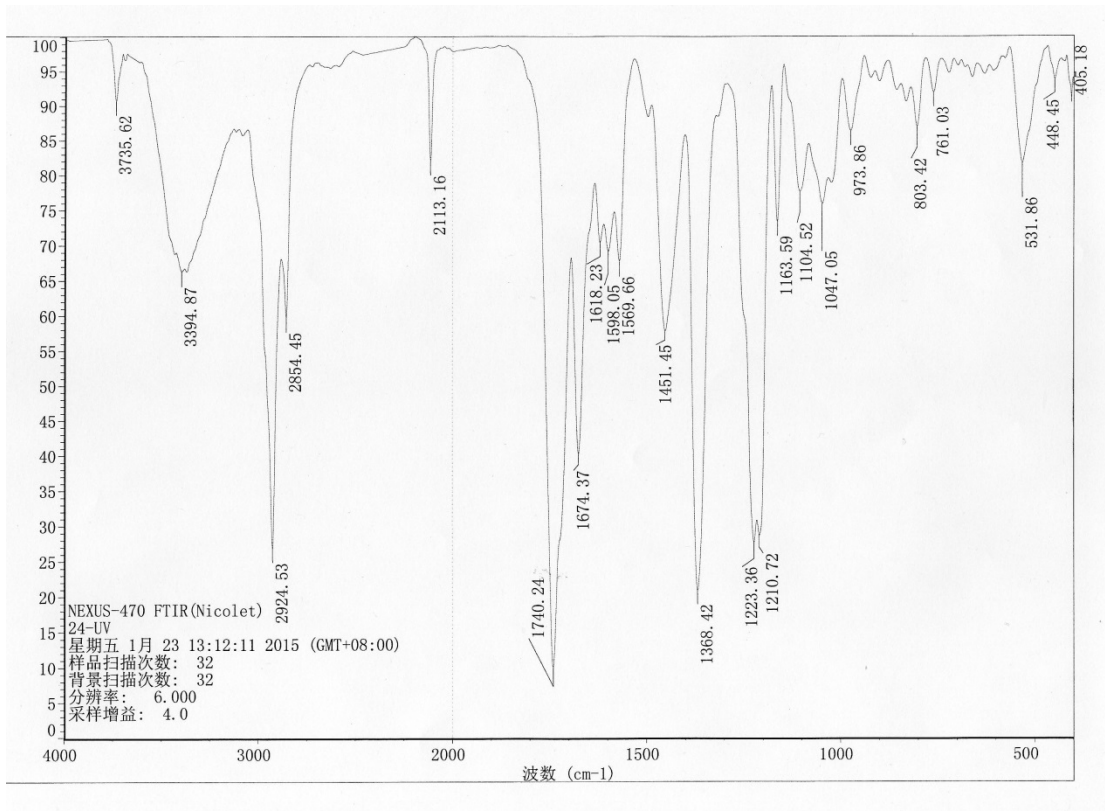


Figure S31. IR spectrum of 2

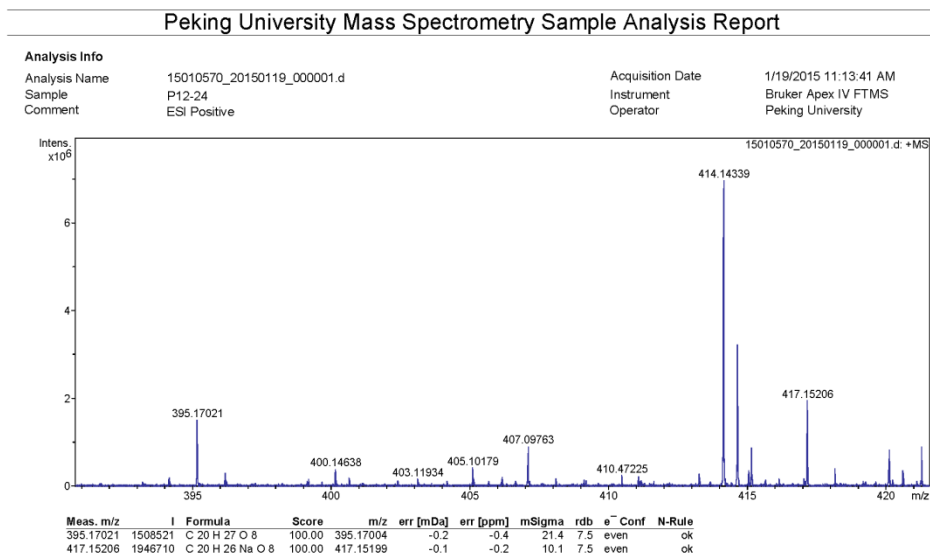


Figure S32. HRESIMS spectrum of 2

P12-21

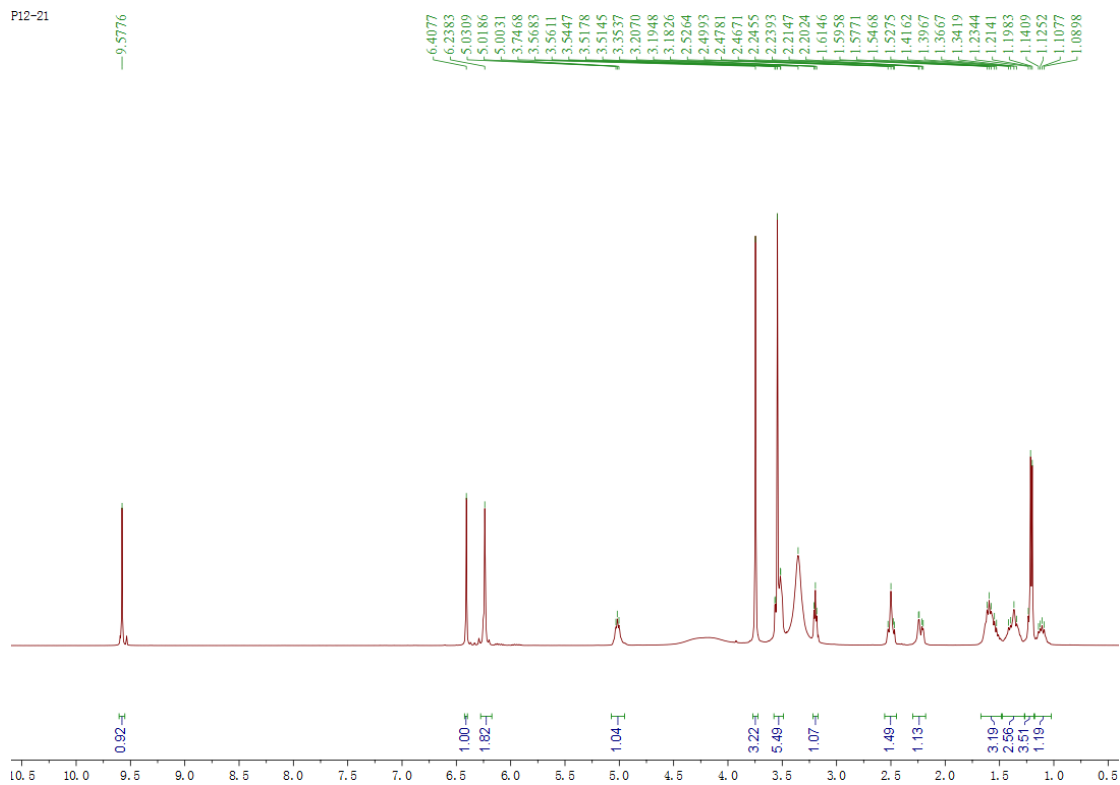


Figure S33.  $^1\text{H}$  NMR spectrum of **3** (DMSO- $d_6$ , 400MHz)

P12-21\_13C

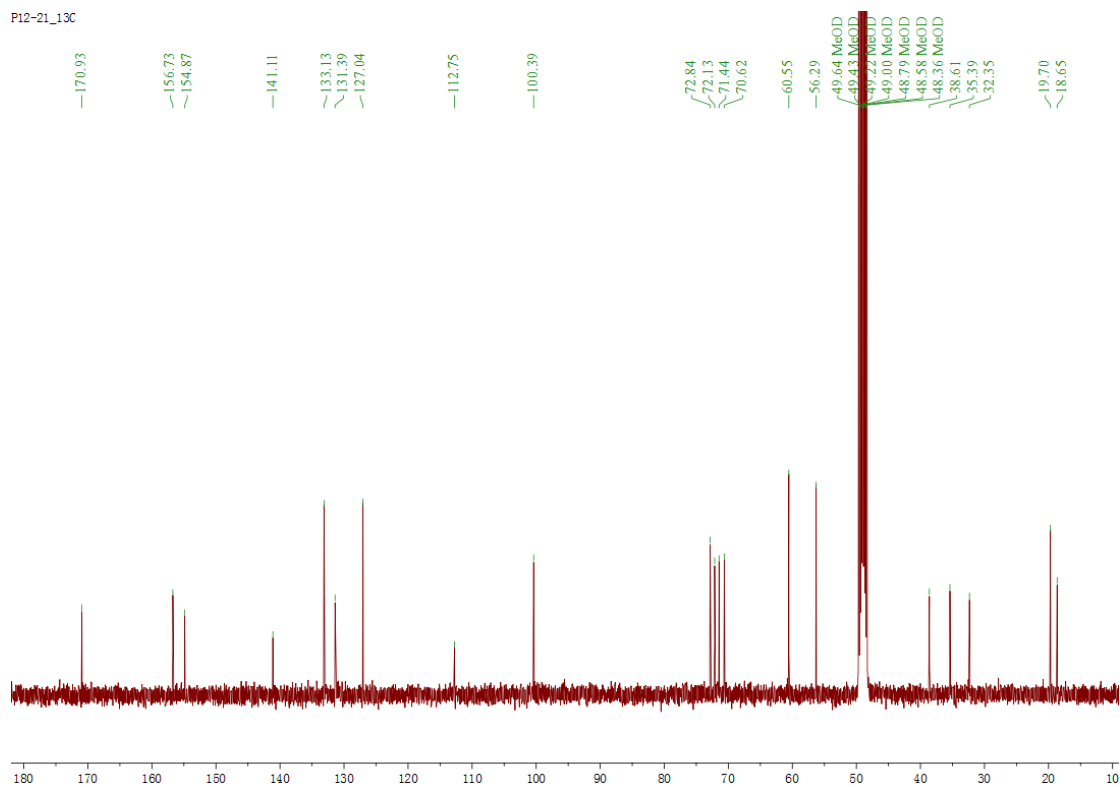


Figure S34.  $^{13}\text{C}$  NMR spectrum of **3** (DMSO- $d_6$ , 100MHz)

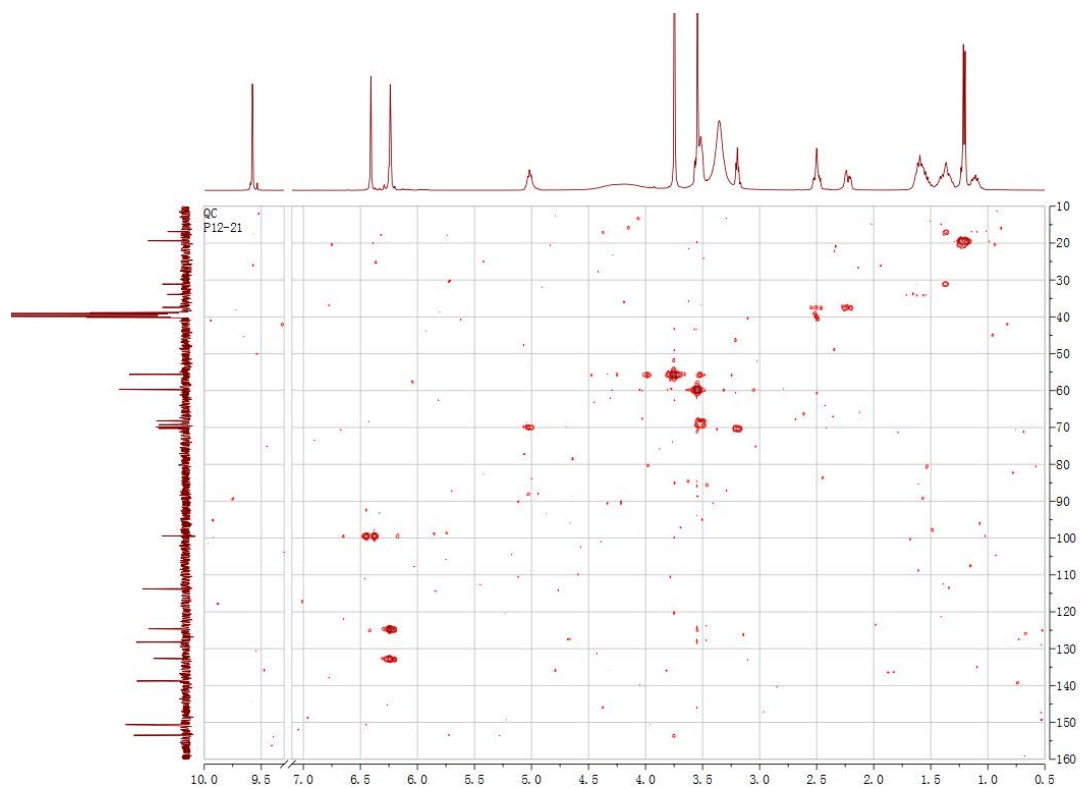


Figure S35. HMQC spectrum of **3** (DMSO- $d_6$ )

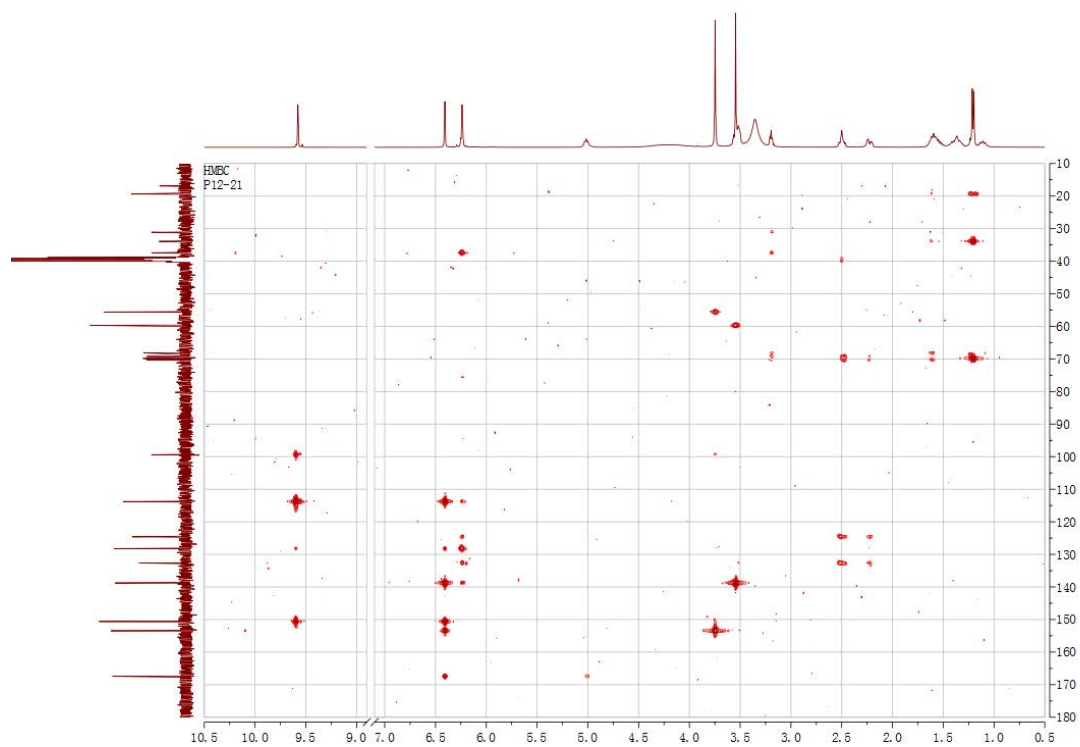
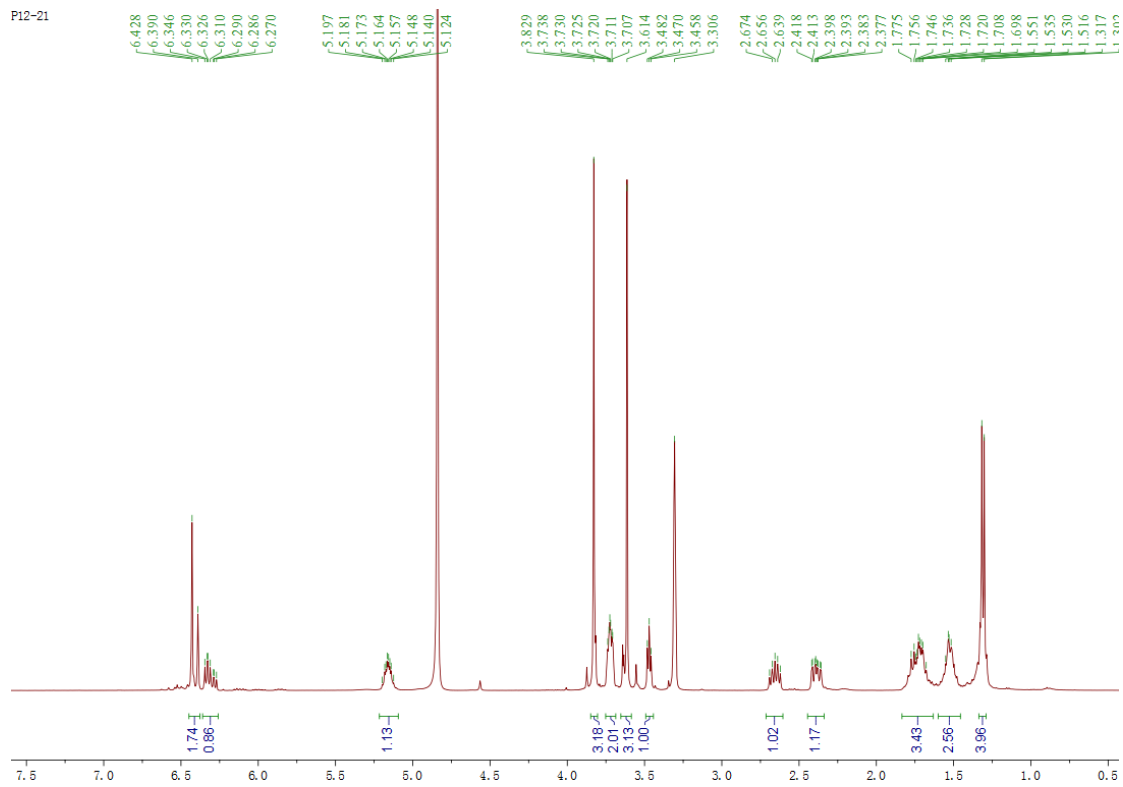
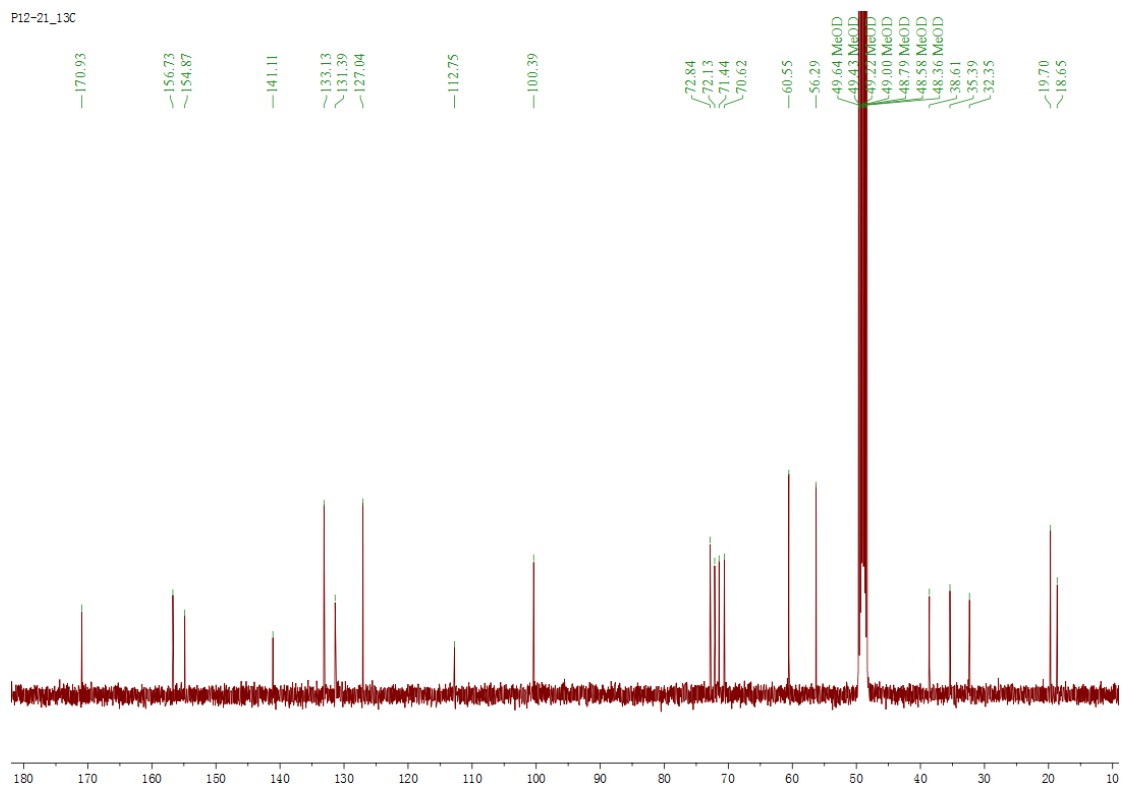


Figure S36. HMBC spectrum of **3** (DMSO- $d_6$ )



**Figure S37.**  $^1\text{H}$  NMR spectrum of **3** ( $\text{CD}_3\text{OD}$ , 400MHz)



**Figure S38.**  $^{13}\text{C}$  NMR spectrum of **3** ( $\text{CD}_3\text{OD}$ , 100MHz)



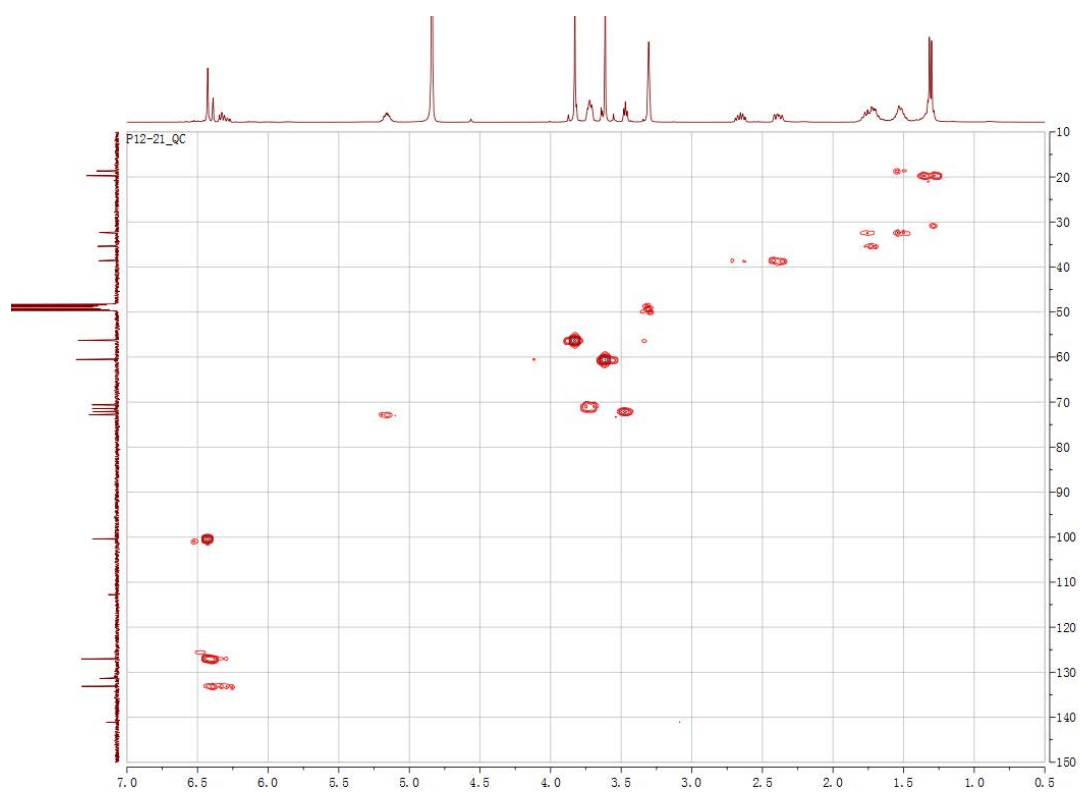


Figure S39. HMQC spectrum of **3** (CD<sub>3</sub>OD)

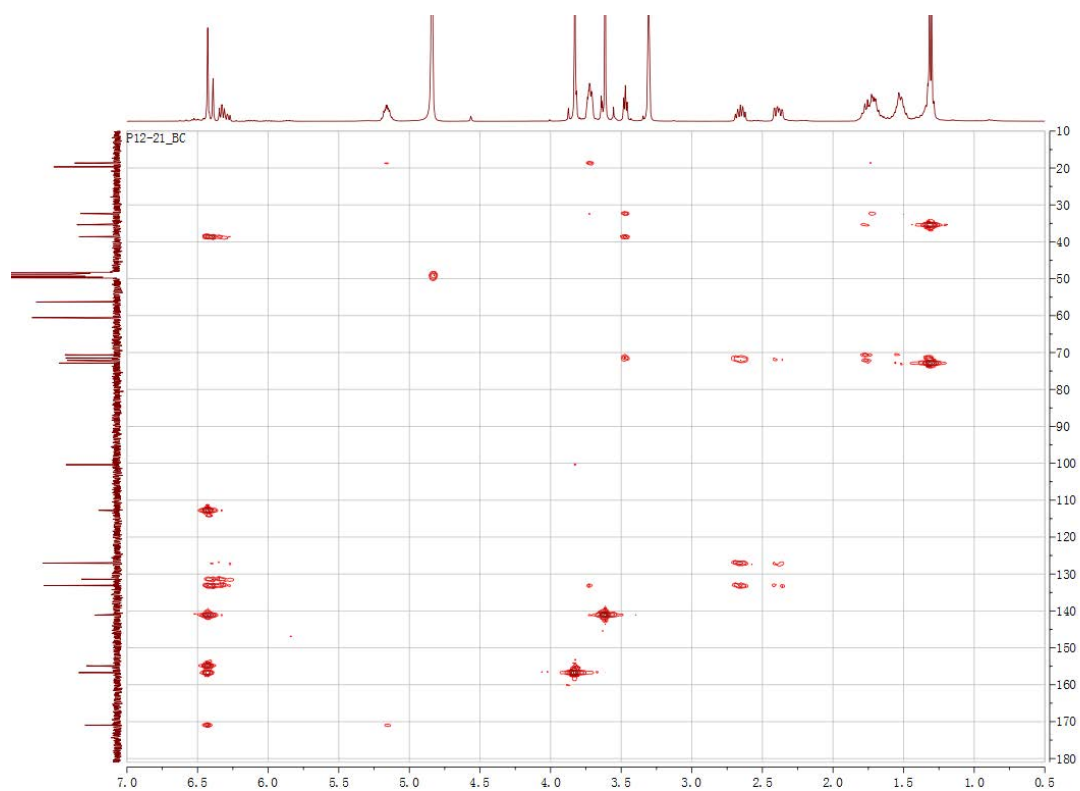


Figure S40. HMBC spectrum of **3** (CD<sub>3</sub>OD)

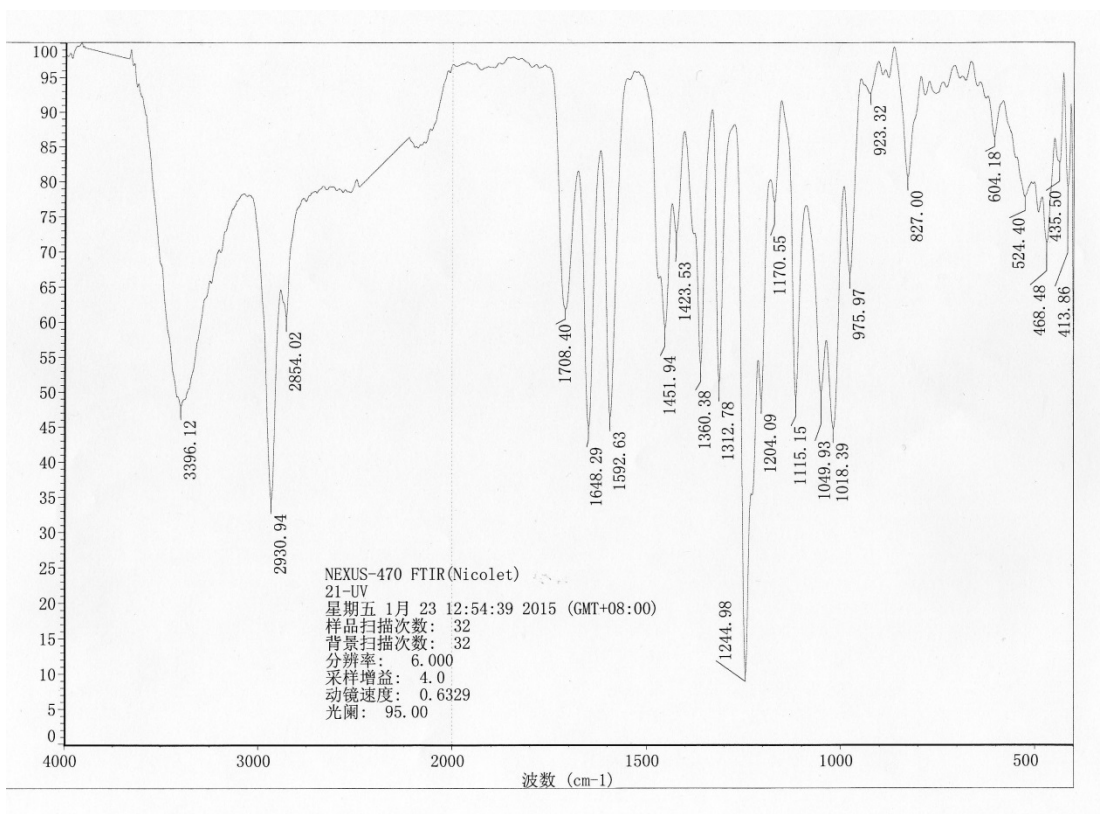


Figure S41. IR spectrum of 3

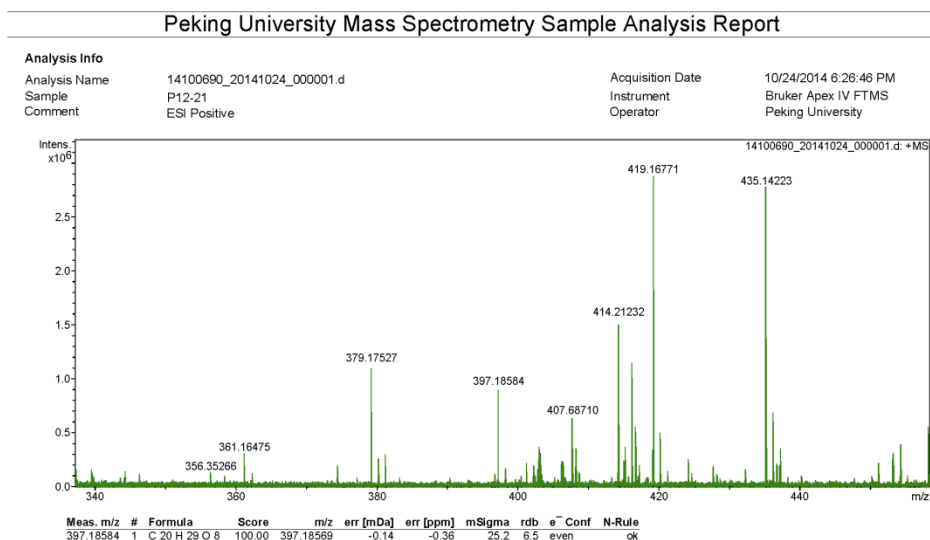


Figure S42. HRESIMS spectrum of 3

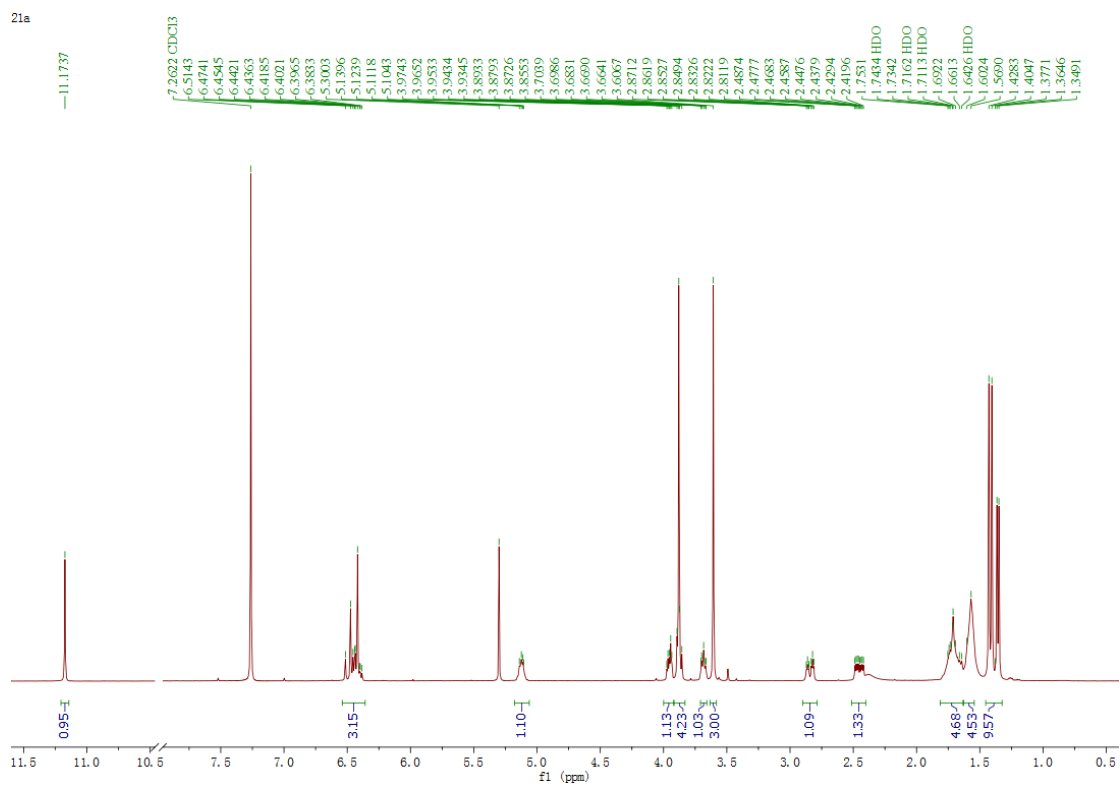


Figure S43.  $^1\text{H}$  NMR spectrum of **3a** ( $\text{CDCl}_3$ , 400MHz)

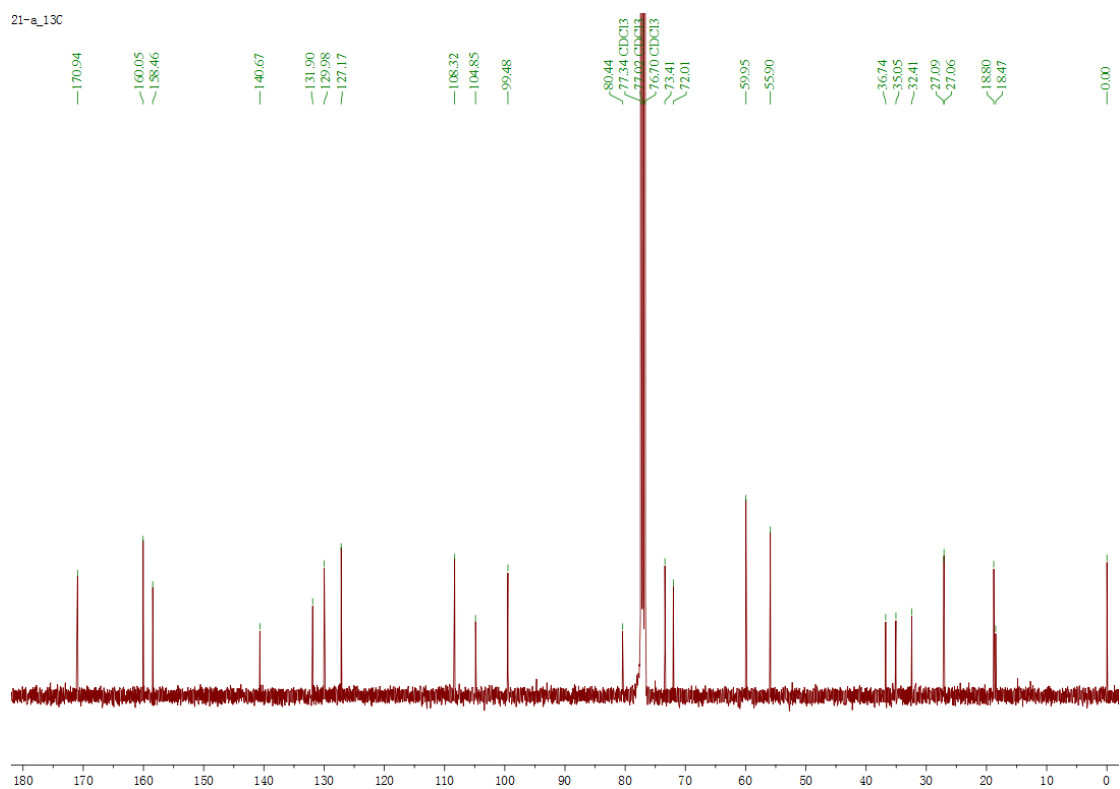
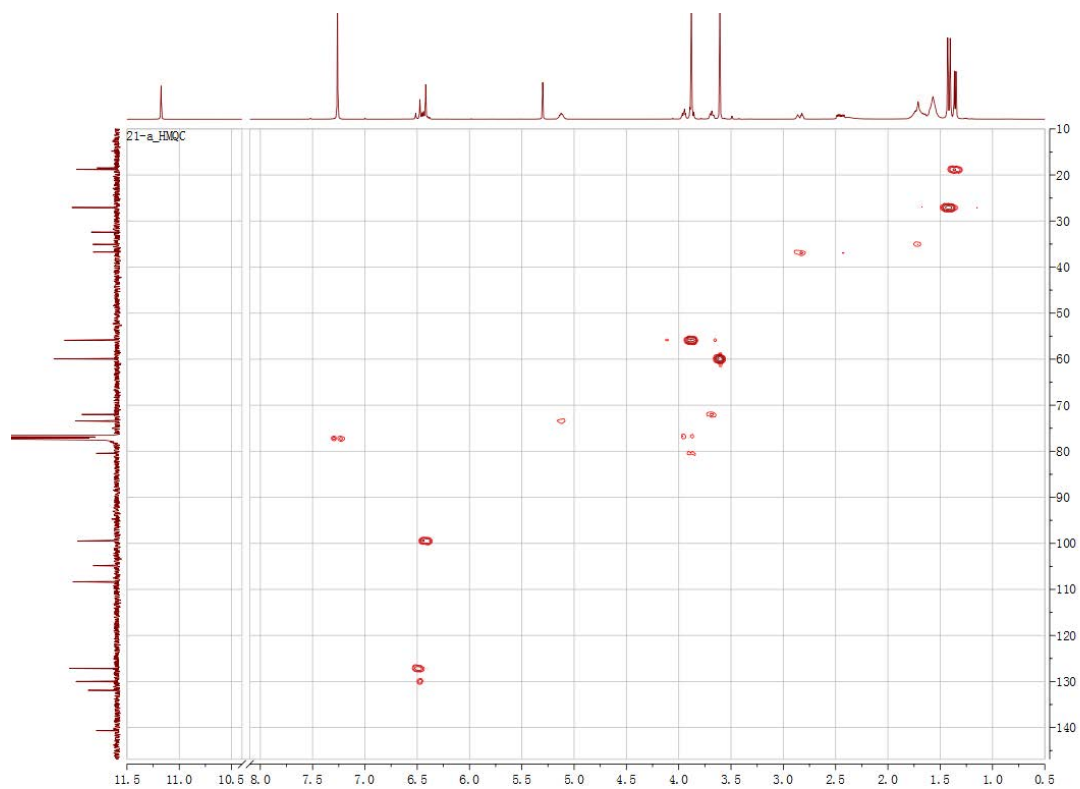
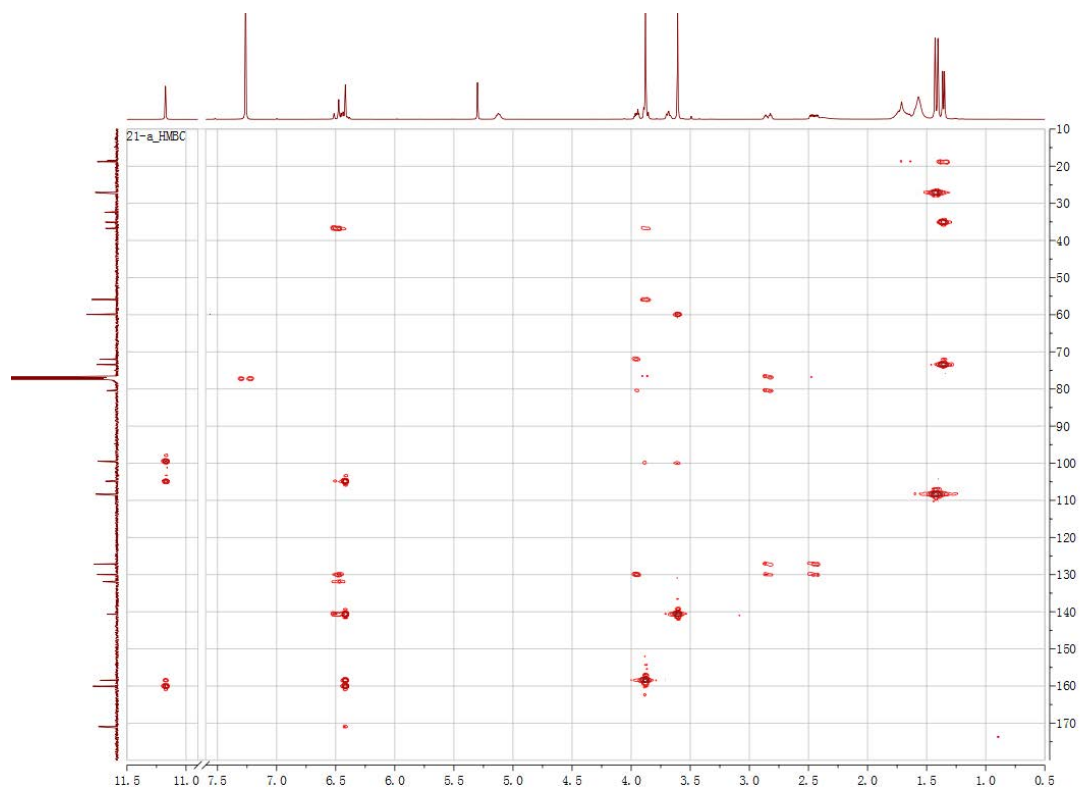


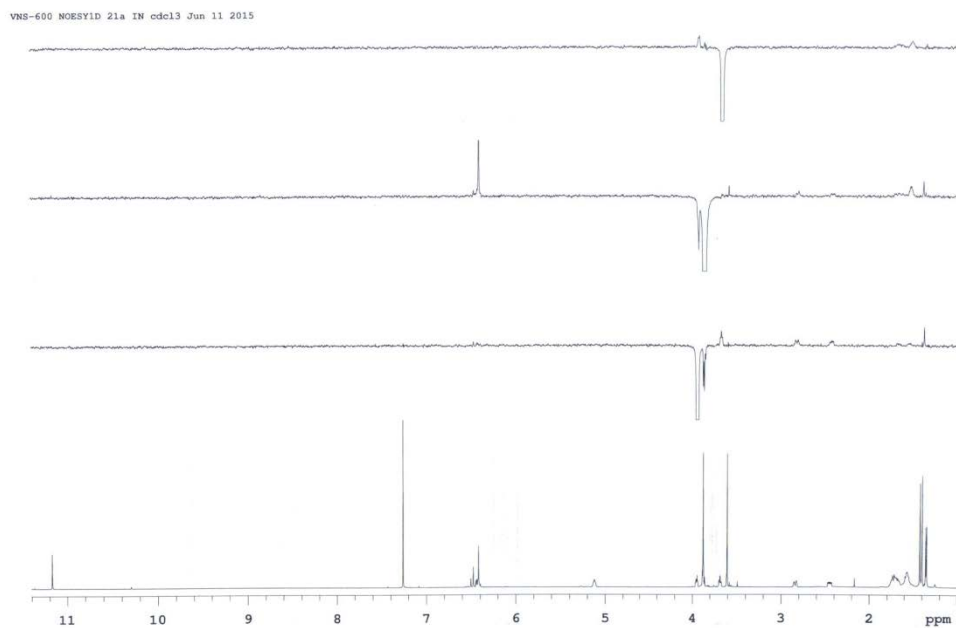
Figure S44.  $^{13}\text{C}$  NMR spectrum of **3a** ( $\text{CDCl}_3$ , 100MHz)



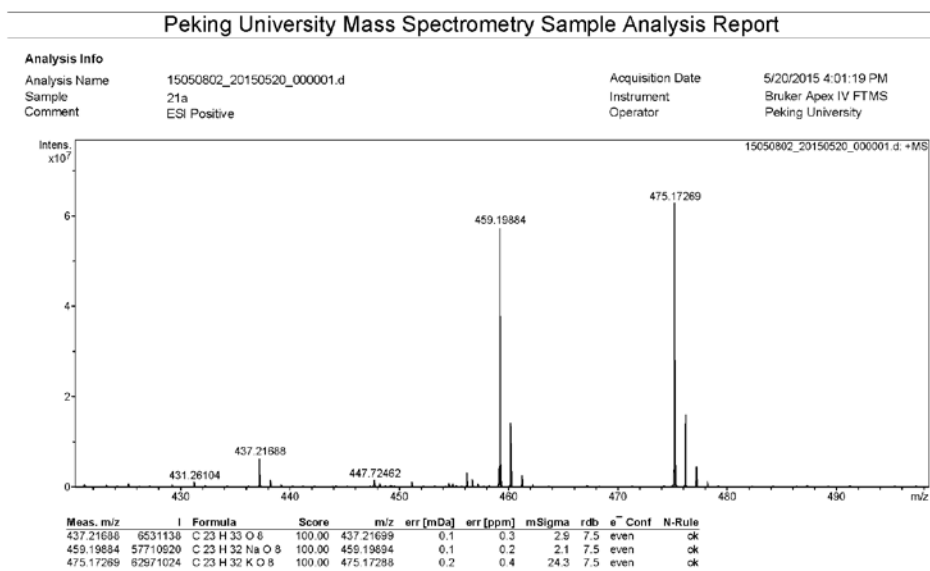
**Figure S45.** HMQC spectrum of **3a** (CDCl<sub>3</sub>)



**Figure S46.** HMBC spectrum of **3a** (CDCl<sub>3</sub>)



**Figure S47.** 1D NOE spectrum of **3a** ( $\text{CDCl}_3$ , 600MHz)



**Figure S48.** HRESIMS spectrum of **3a**

P12-21-1

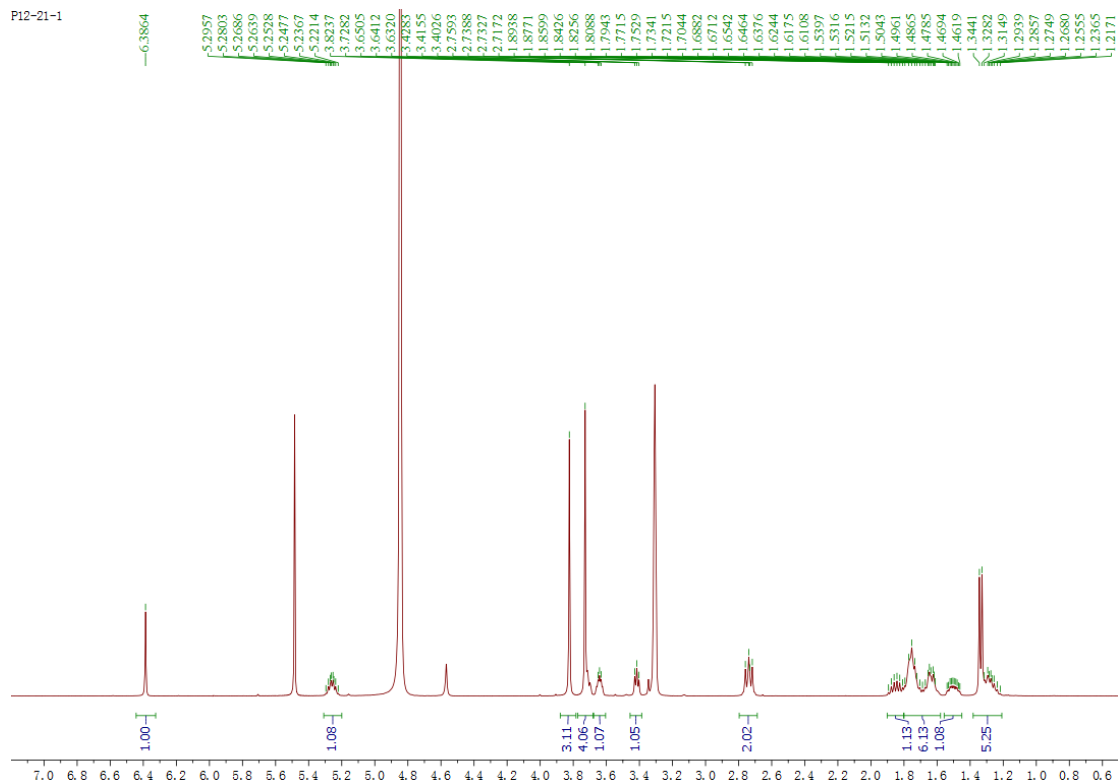


Figure S49. <sup>1</sup>H NMR spectrum of **3b** (CD<sub>3</sub>OD, 400MHz)

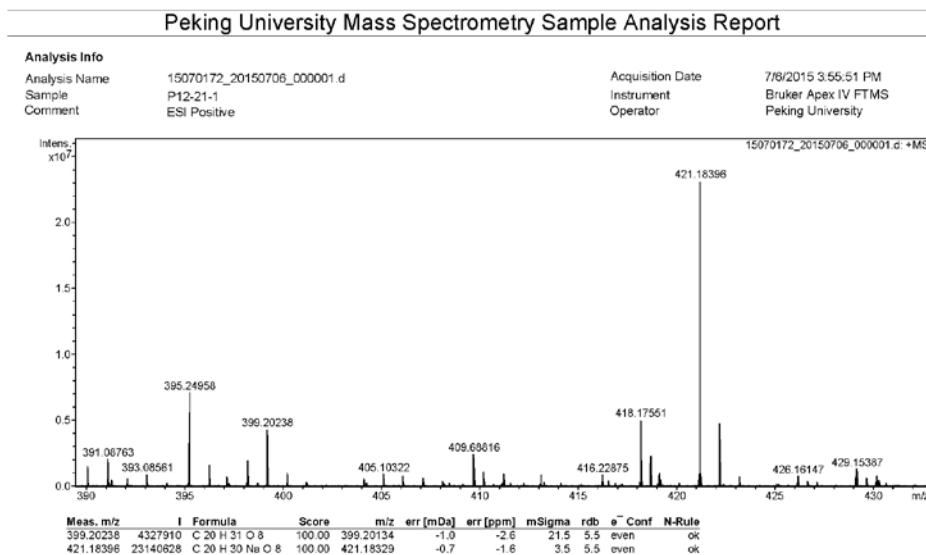


Figure S50. HRESIMS spectrum of **3b**

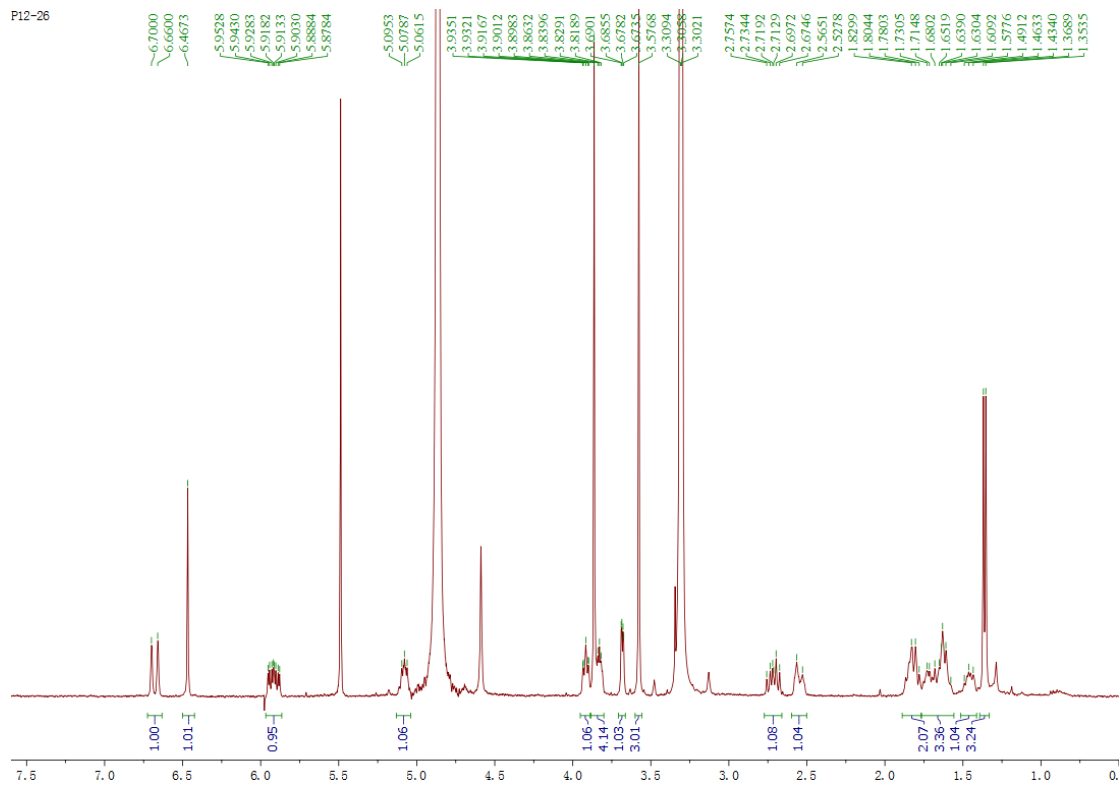


Figure S51.  $^1\text{H}$  NMR spectrum of **4** ( $\text{CD}_3\text{OD}$ , 400MHz)

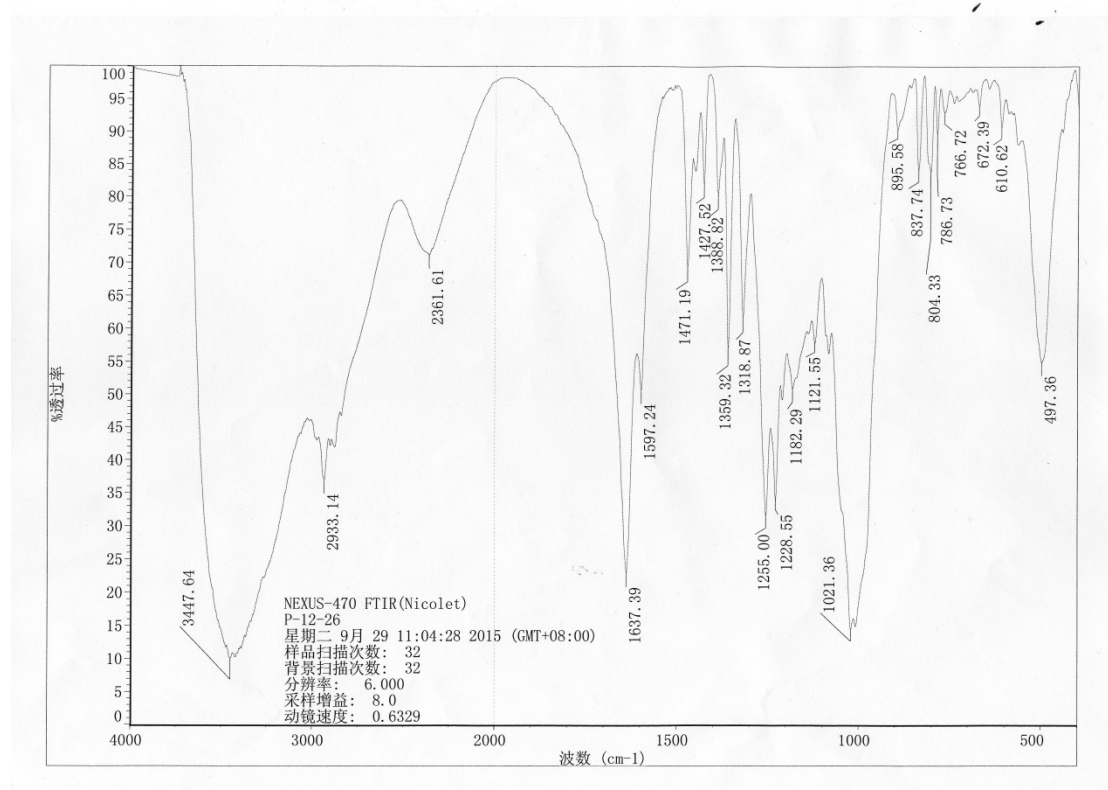
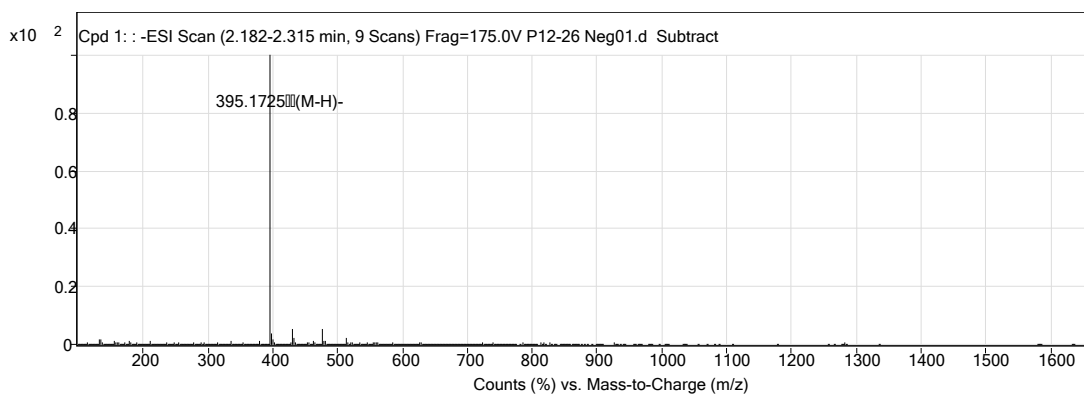


Figure S52. IR spectrum of **4**



### MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
395.1725	395.1711	3.43	- 1	129127.	C <sub>20</sub> H <sub>27</sub> O <sub>8</sub>	(M-H) -

Figure S53. HRESIMS spectrum of **4**

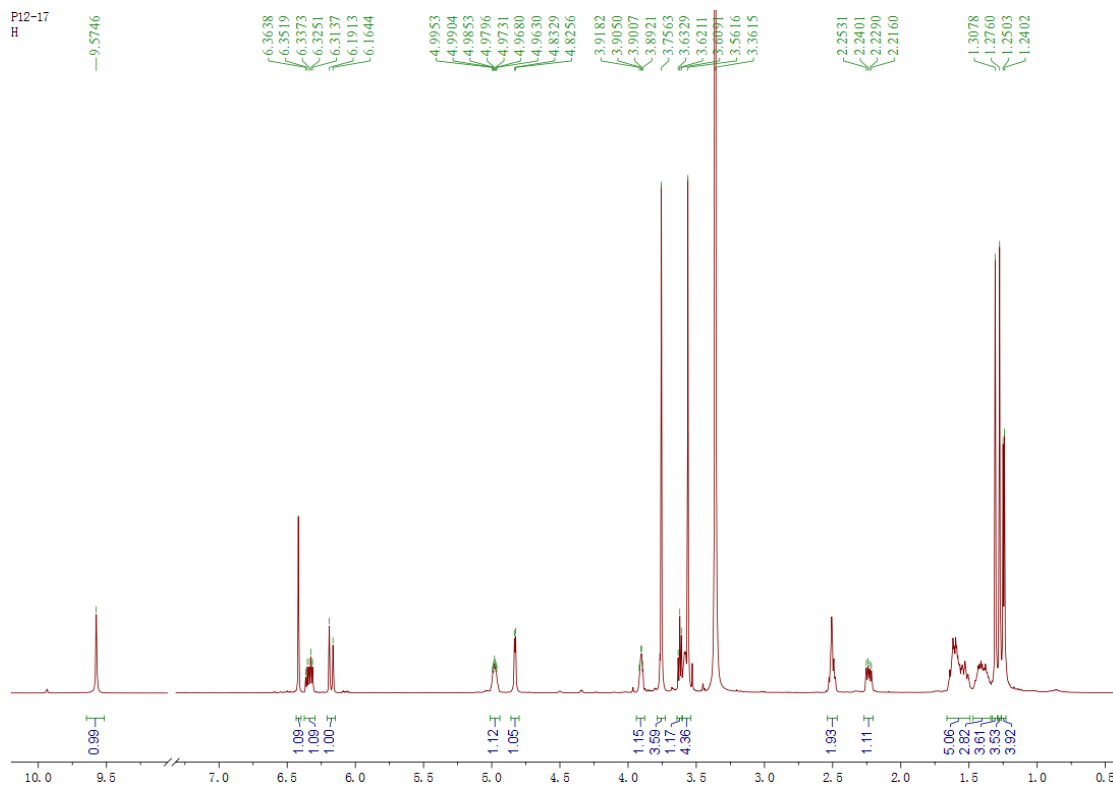


Figure S54. <sup>1</sup>H NMR spectrum of **5** (DMSO-*d*<sub>6</sub>, 600MHz)



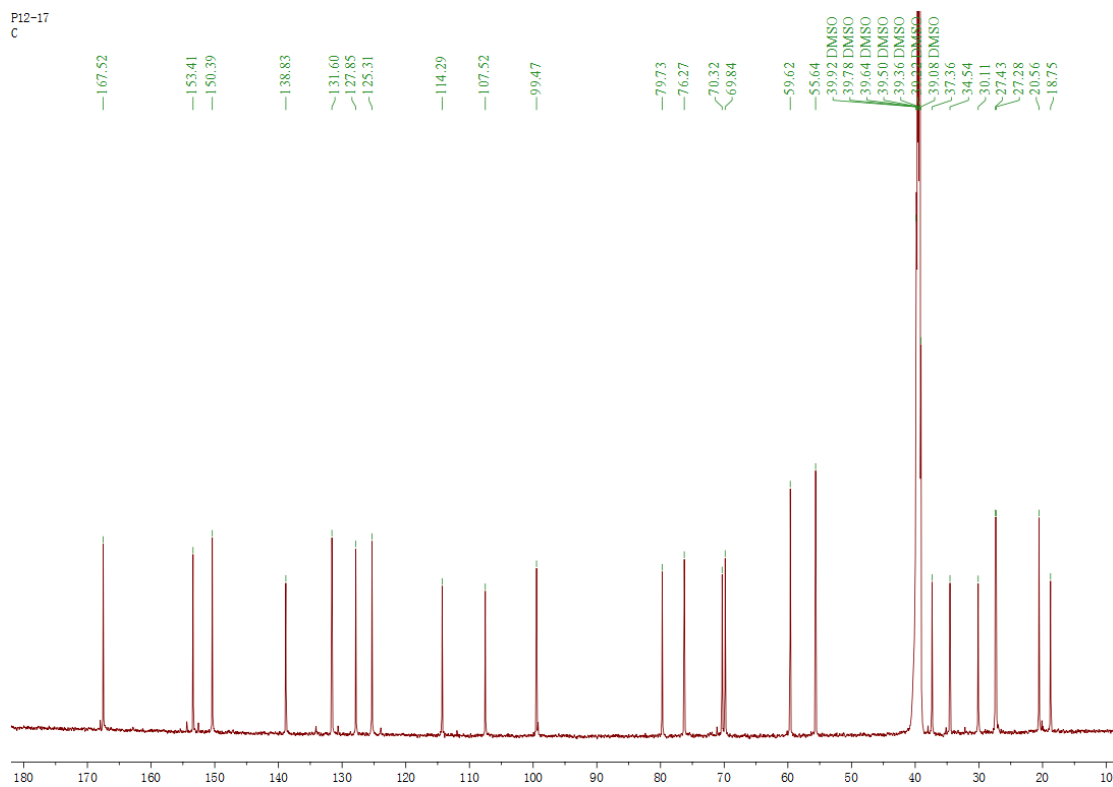


Figure S55.  $^{13}\text{C}$  NMR spectrum of **5** (DMSO- $d_6$ , 150MHz)

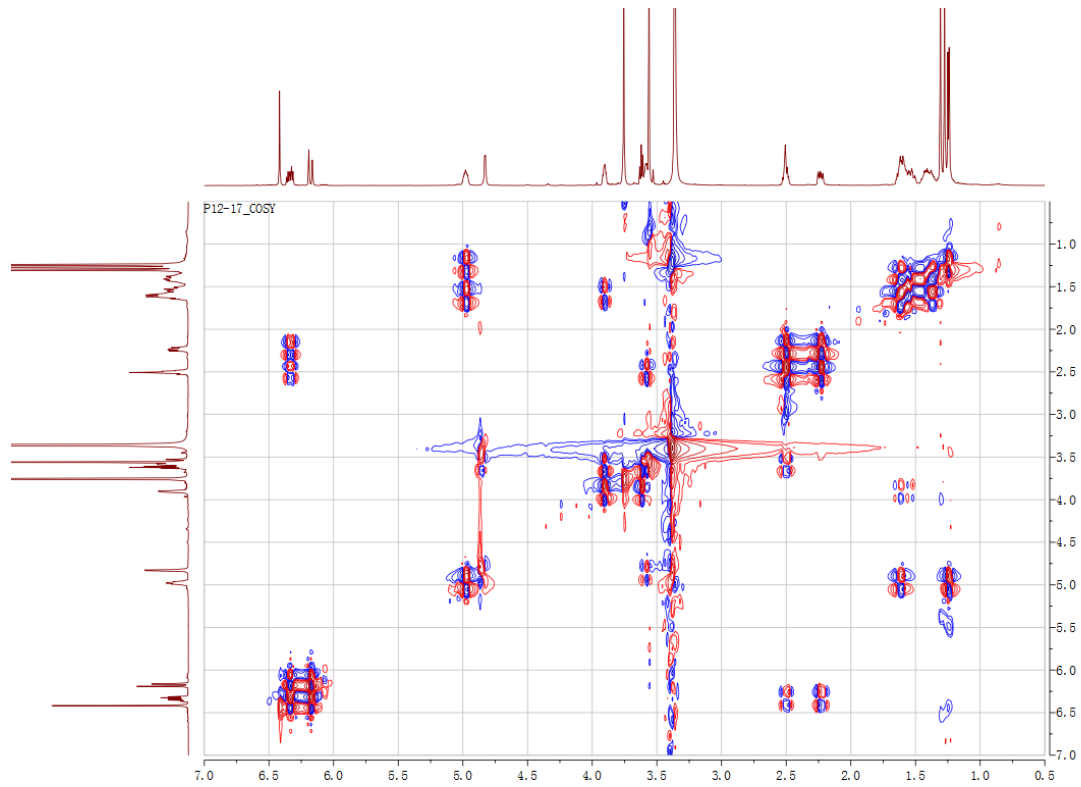


Figure S56.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **5** (DMSO- $d_6$ )

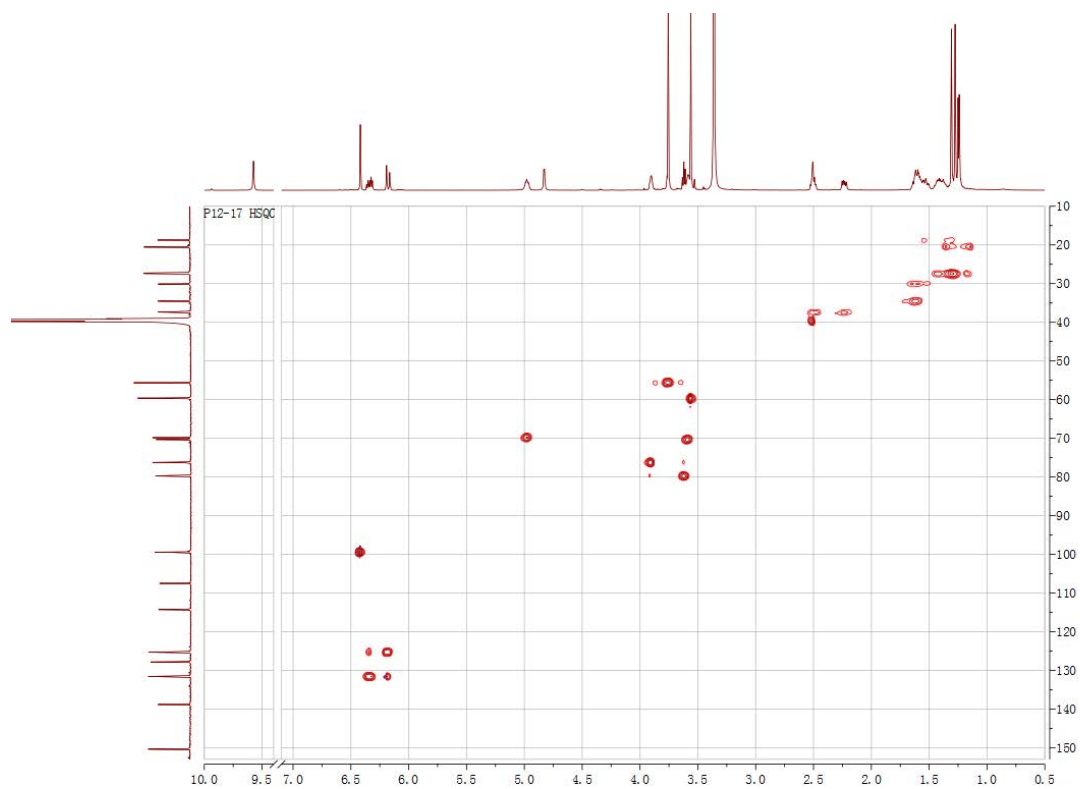


Figure S57. HSQC spectrum of **5** (DMSO- $d_6$ )

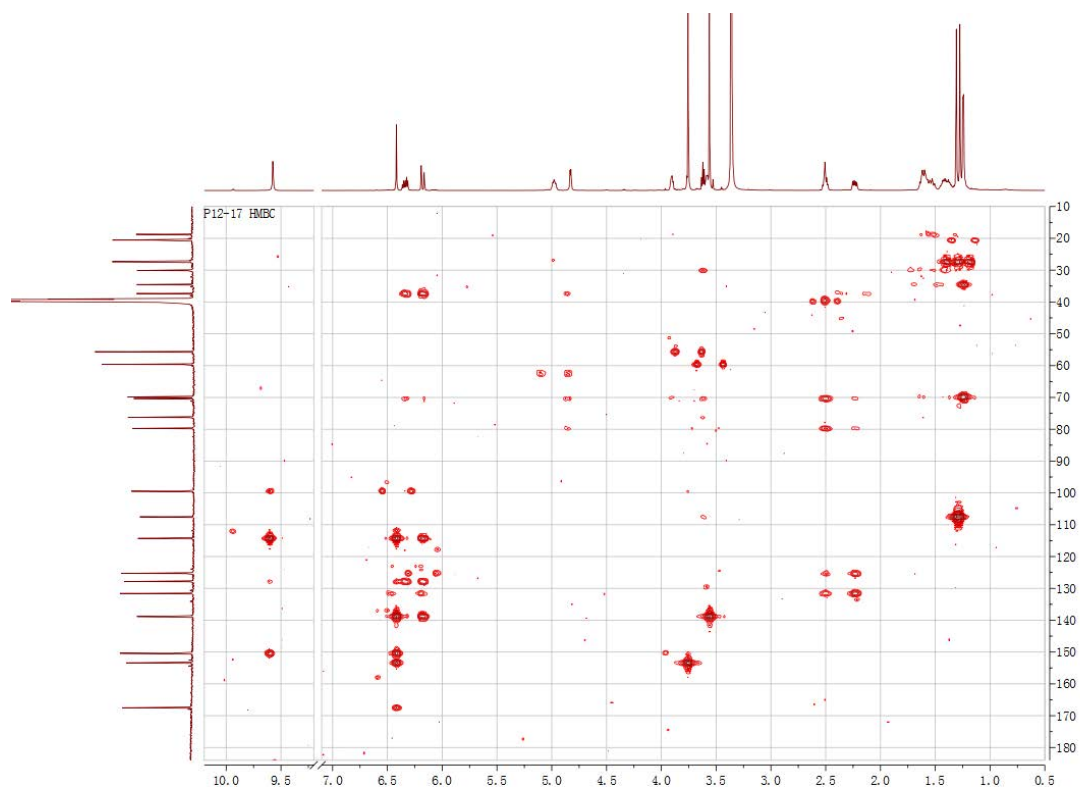


Figure S58. HMBC spectrum of **5** (DMSO- $d_6$ )

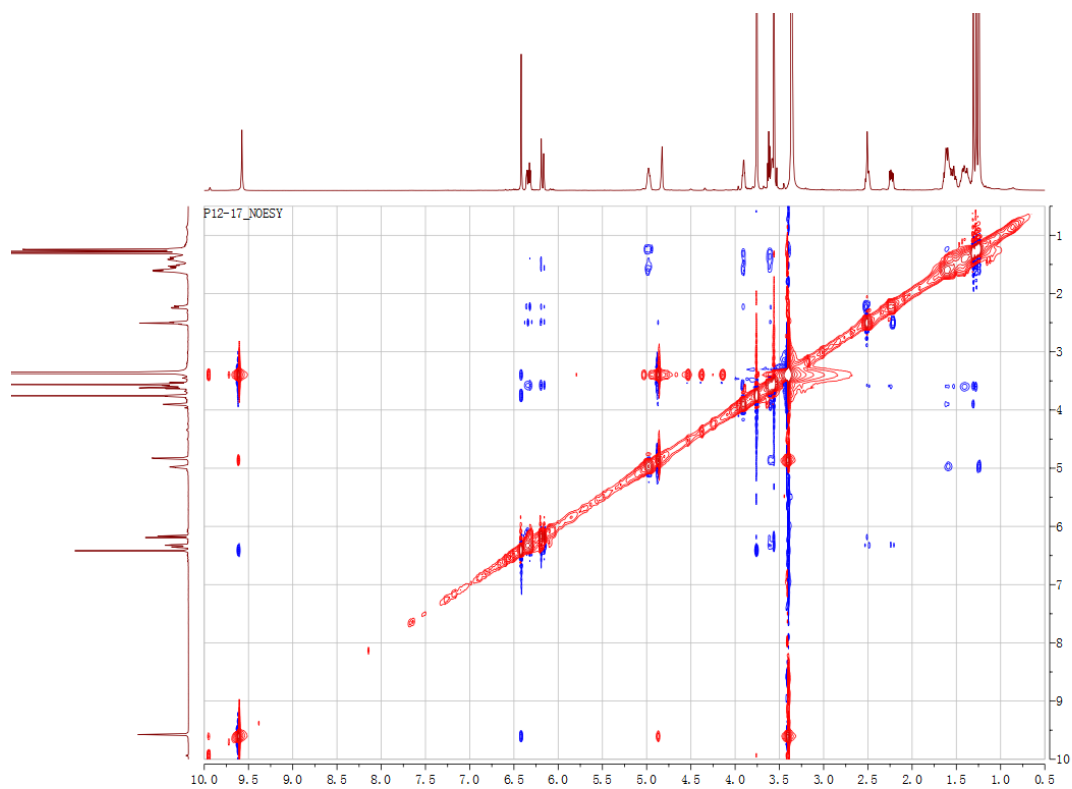


Figure S59. NOESY spectrum of **5** (DMSO- $d_6$ )

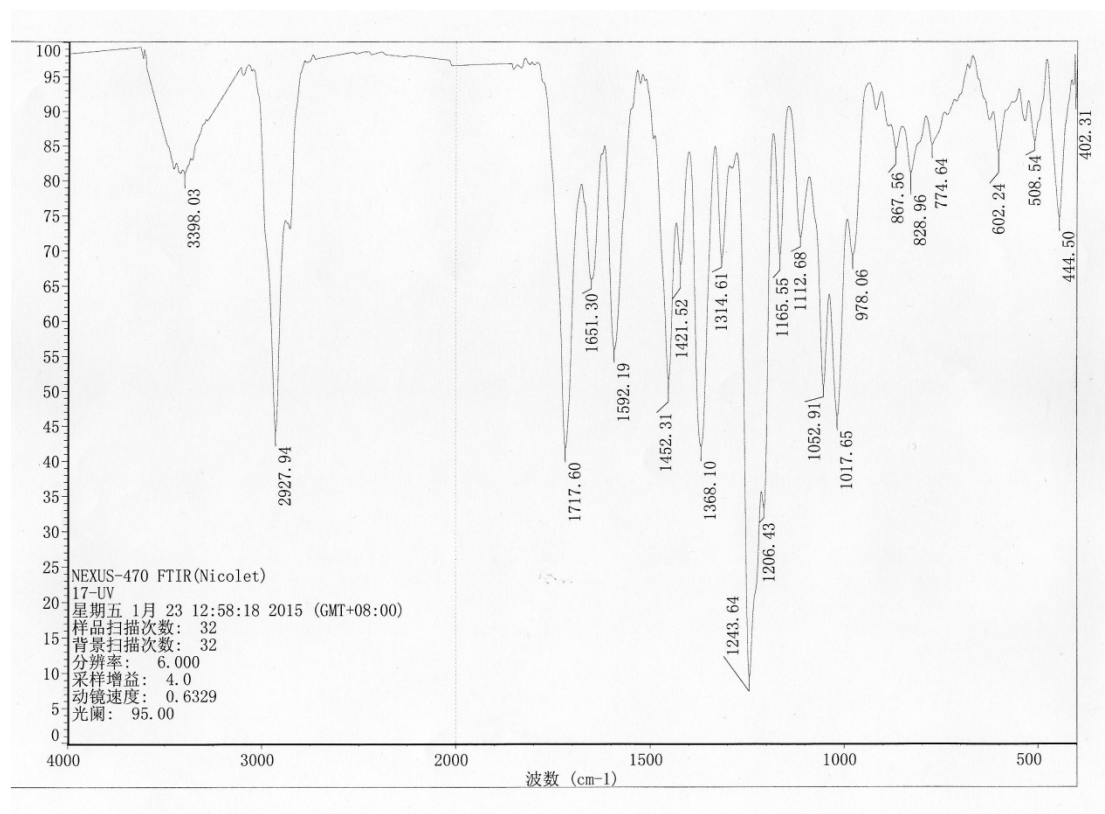


Figure S60. IR spectrum of **5**

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Analysis Info

Analysis Name 14100684\_20141024\_000001.d  
 Sample P12-17  
 Comment ESI Positive

Acquisition Date 10/24/2014 6:19:48 PM  
 Instrument Bruker Apex IV FTMS  
 Operator Peking University

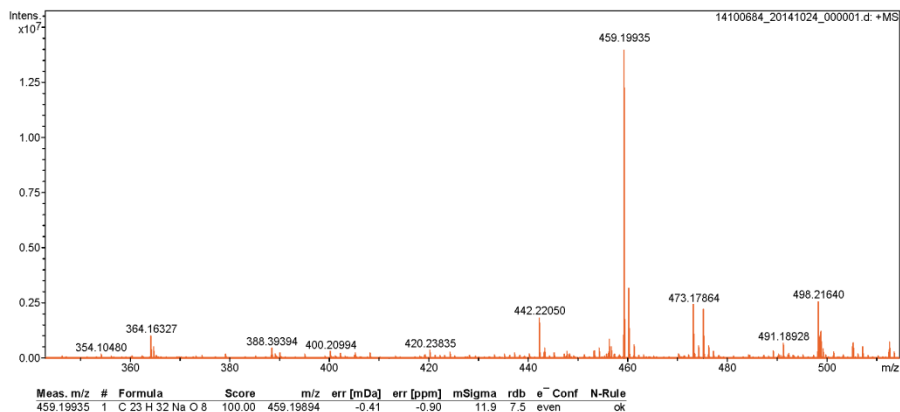


Figure S61. HRESIMS spectrum of 5

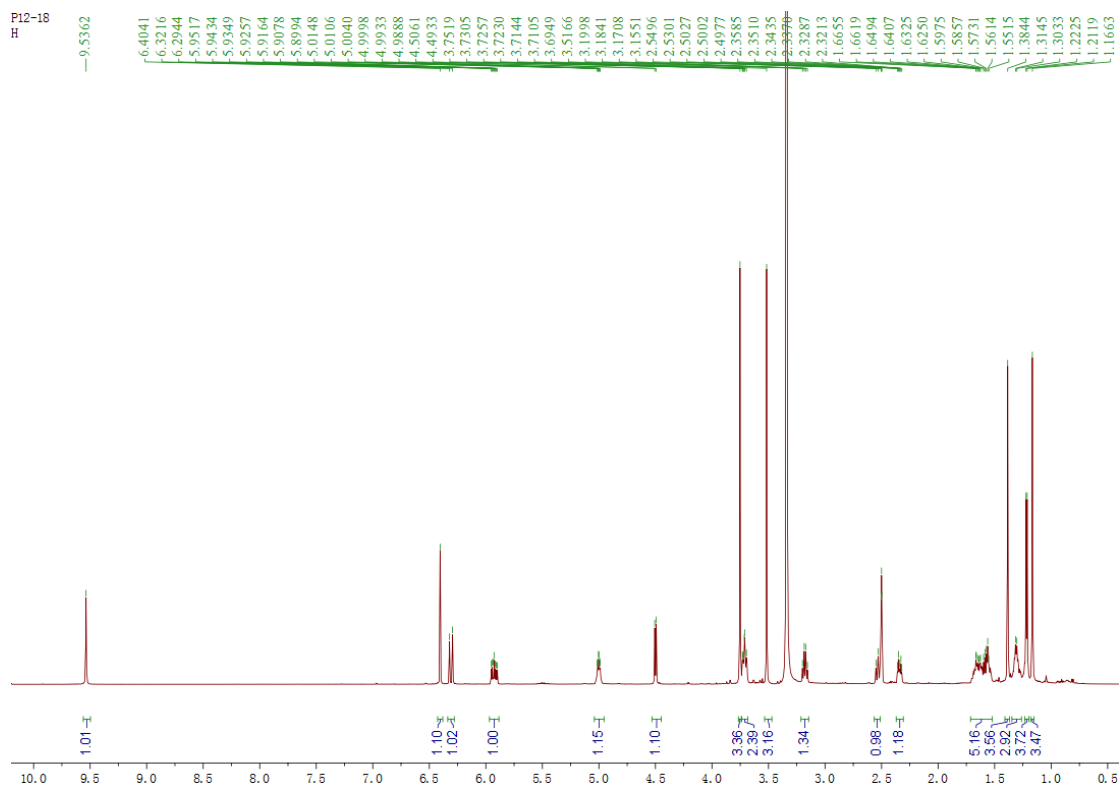


Figure S62. <sup>1</sup>H NMR spectrum of 6 (DMSO-*d*<sub>6</sub>, 600MHz)

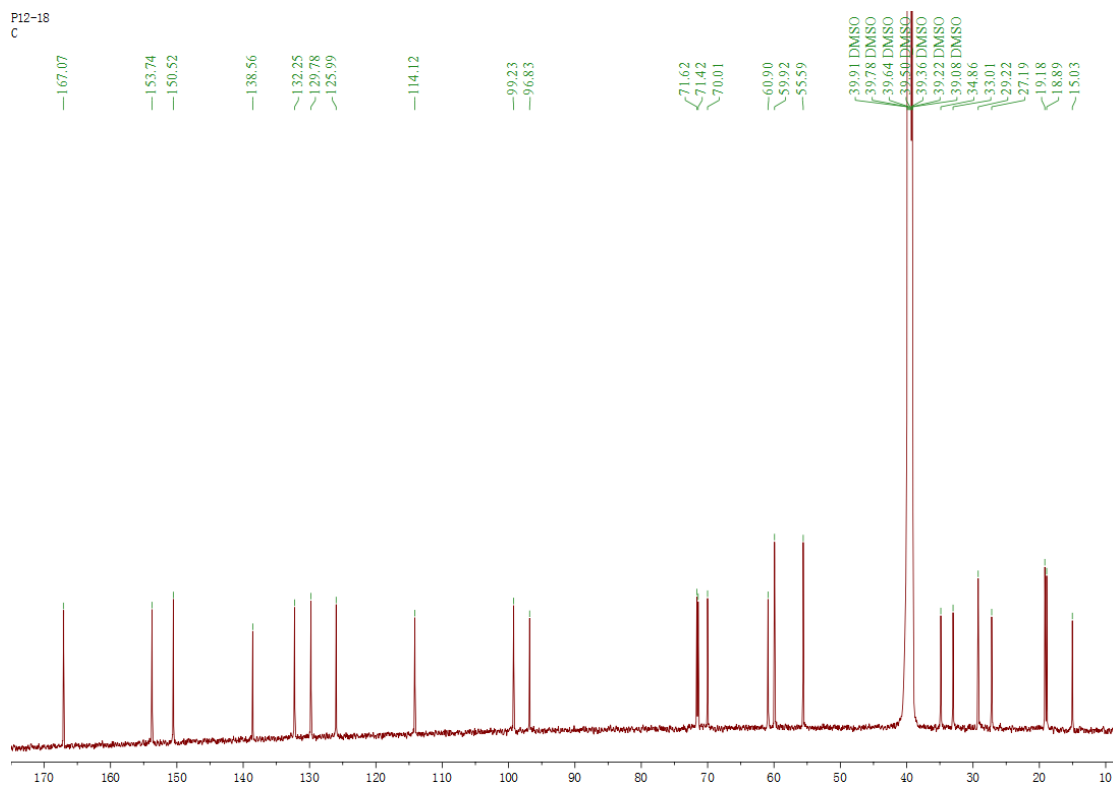


Figure S63.  $^{13}\text{C}$  NMR spectrum of **6** (DMSO- $d_6$ , 150MHz)

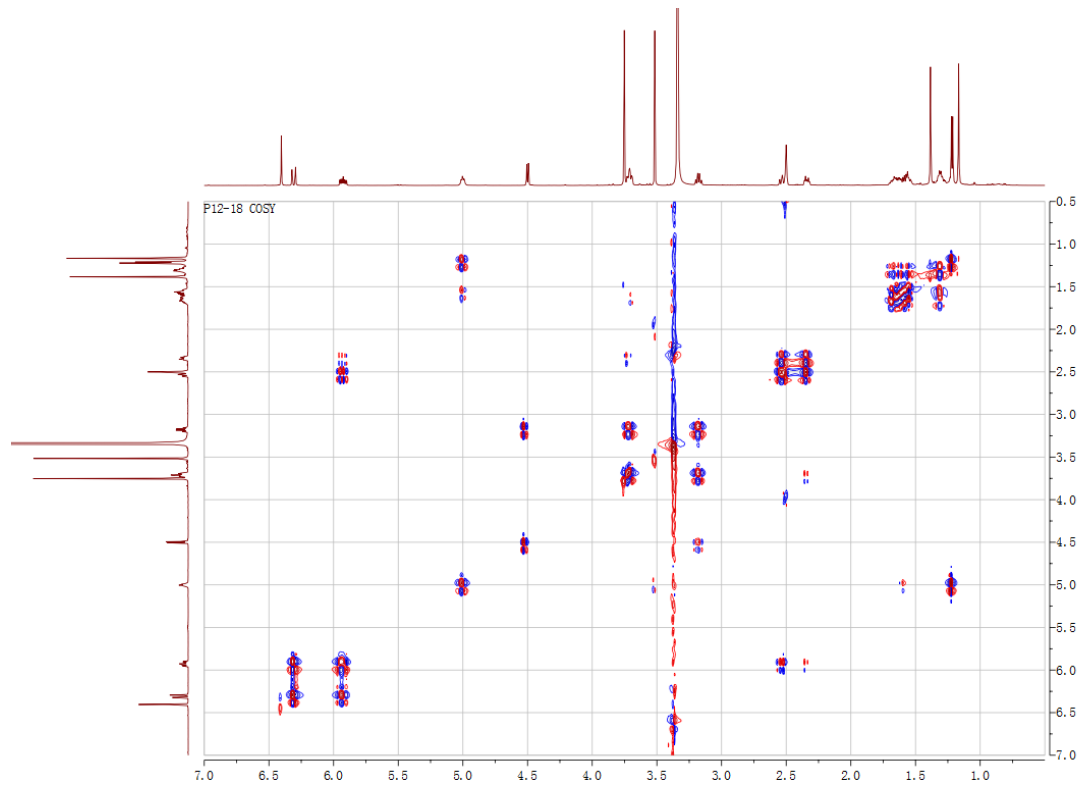


Figure S64.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **6** (DMSO- $d_6$ )

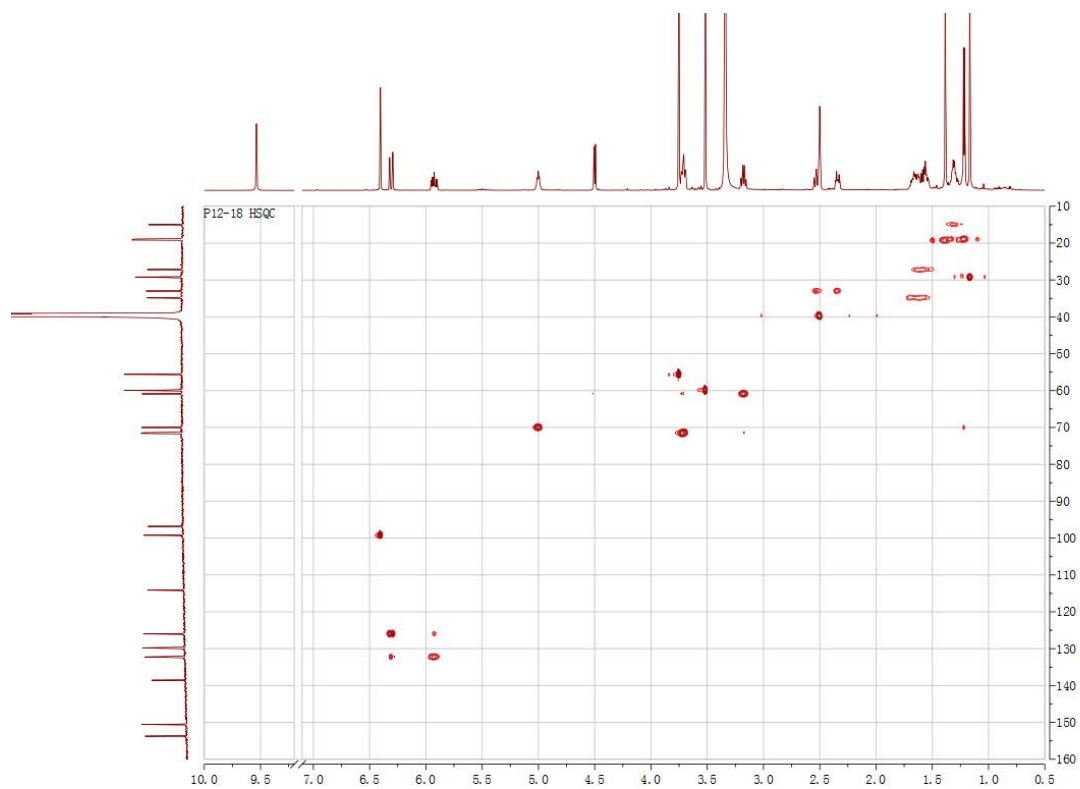


Figure S65. HSQC spectrum of **6** (DMSO- $d_6$ )

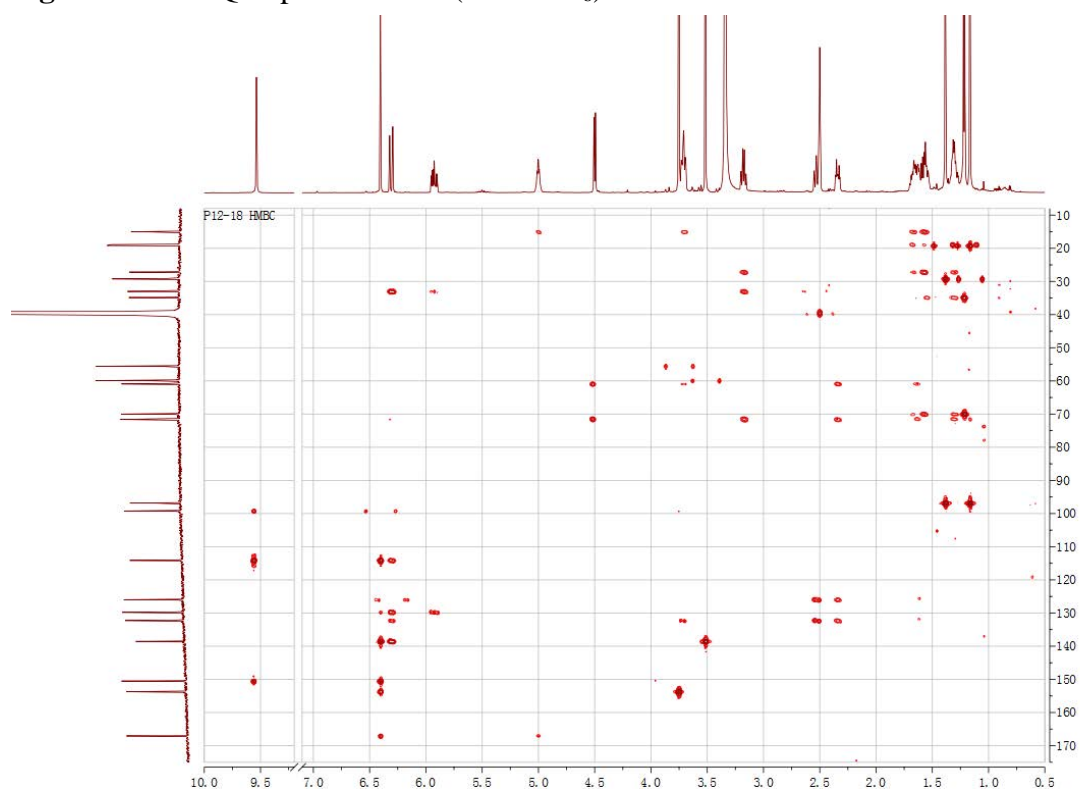


Figure S66. HMBC spectrum of **6** (DMSO- $d_6$ )

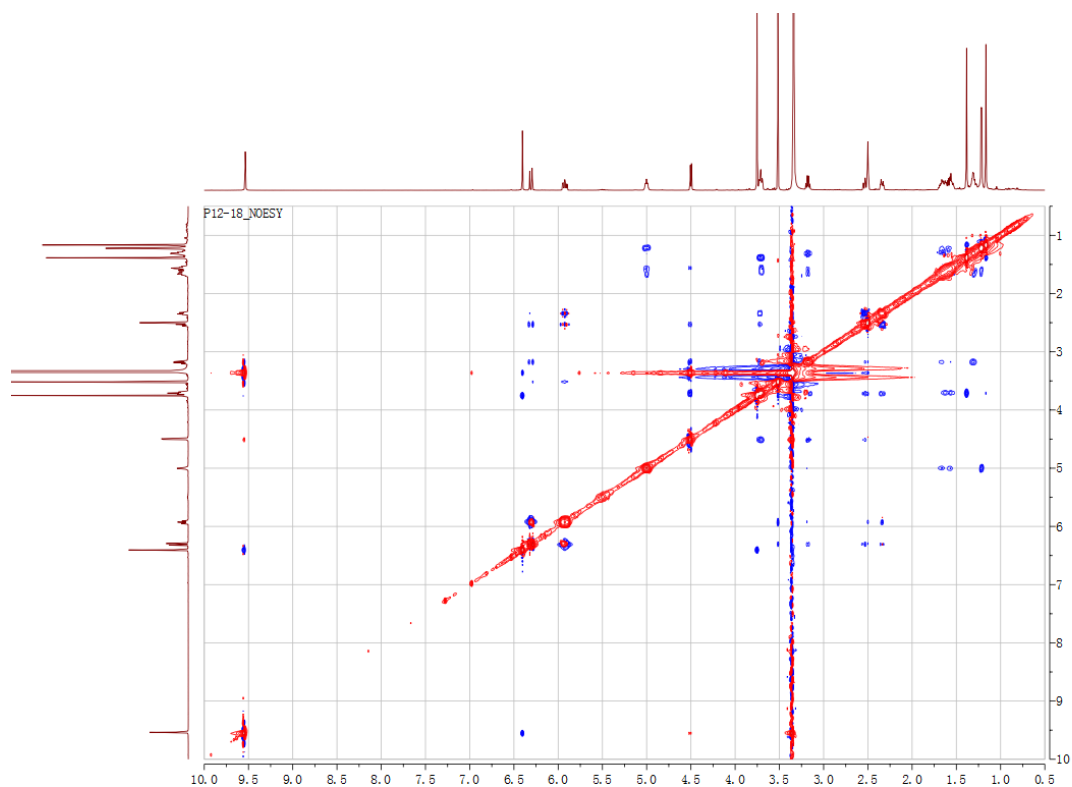


Figure S67. NOESY spectrum of **6** (DMSO- $d_6$ )

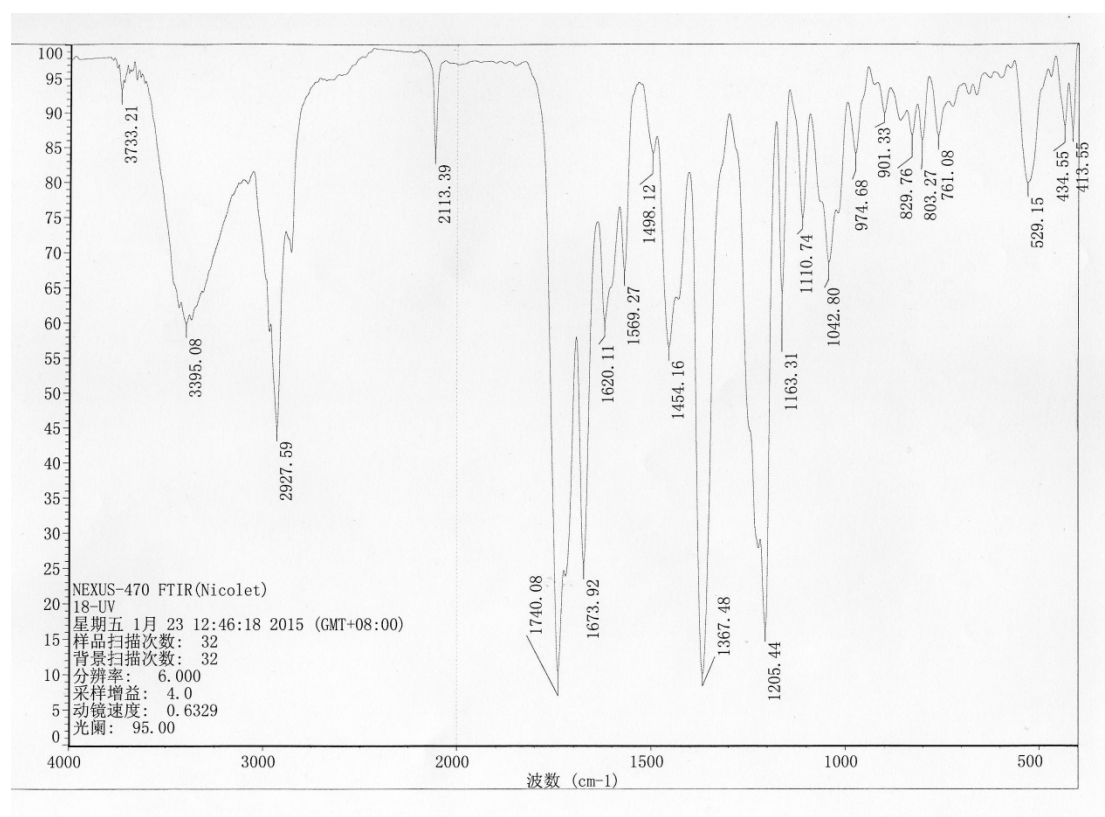


Figure S68. IR spectrum of **6**

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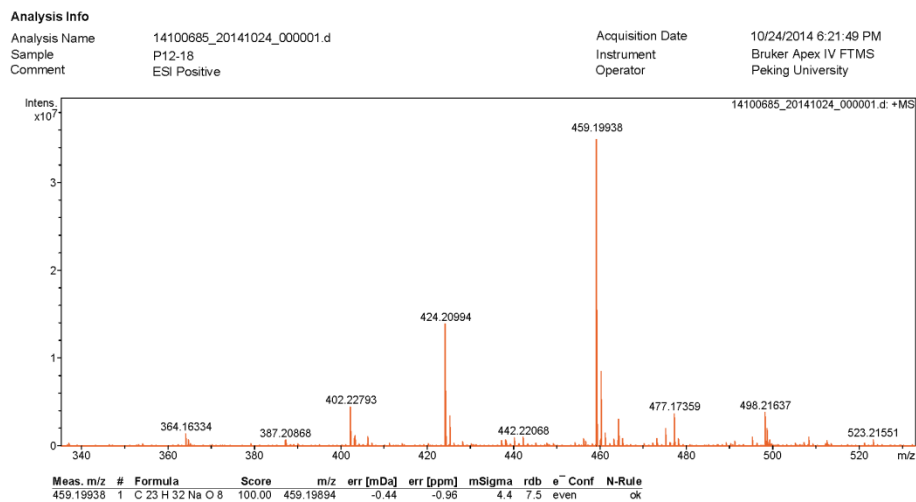


Figure S69. HRESIMS spectrum of 6