

## Electronic Supporting Information

Fig. S1. The structures of compounds 6-18.

Fig. S2.  $^1\text{H}$  NMR spectrum of 1 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S3.  $^{13}\text{C}$  NMR spectrum of 1 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S4. H-H COSY spectrum of 1 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S5. HSQC spectrum of 1 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S6. HMBC spectrum of 1 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S7. HR-ESI-MS spectrum of 1

Fig. S8.  $^1\text{H}$  NMR spectrum of 2 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S9.  $^{13}\text{C}$  NMR spectrum of 2 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S10.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 2 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S11. HSQC spectrum of 2 in  $\text{CD}_3\text{COCD}_3$

Fig. S12. HMBC spectrum of 2 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S13. HR-ESI-MS spectrum of 2.

Fig. S14.  $^1\text{H}$  NMR spectrum of 3 in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6$  5:1.

Fig. S15.  $^{13}\text{C}$  NMR spectrum of 3 in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6$  5:1.

Fig. S16.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 3 in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6$  5:1.

Fig. S17. HMQC spectrum of 3 in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6$  5:1.

Fig. S18. HMBC spectrum of 3 in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6$  5:1.

Fig. S19. HR-ESI-MS spectrum of 3.

Fig. S20.  $^1\text{H}$  NMR spectrum of 4 in  $\text{CD}_3\text{OD}$ .

Fig. S21.  $^{13}\text{C}$  NMR spectrum of 4 in  $\text{CD}_3\text{OD}$ .

Fig. S22.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 3 in  $\text{CD}_3\text{OD}$ .

Fig. S23. HMQC spectrum of 4 in  $\text{CD}_3\text{OD}$ .

Fig. S24. HMBC spectrum of 4 in  $\text{CD}_3\text{OD}$ .

Fig. S25. HR-ESI-MS spectrum of 4

Fig. S26.  $^1\text{H}$  NMR spectrum of 5 in  $\text{CD}_3\text{COCD}_3$ .

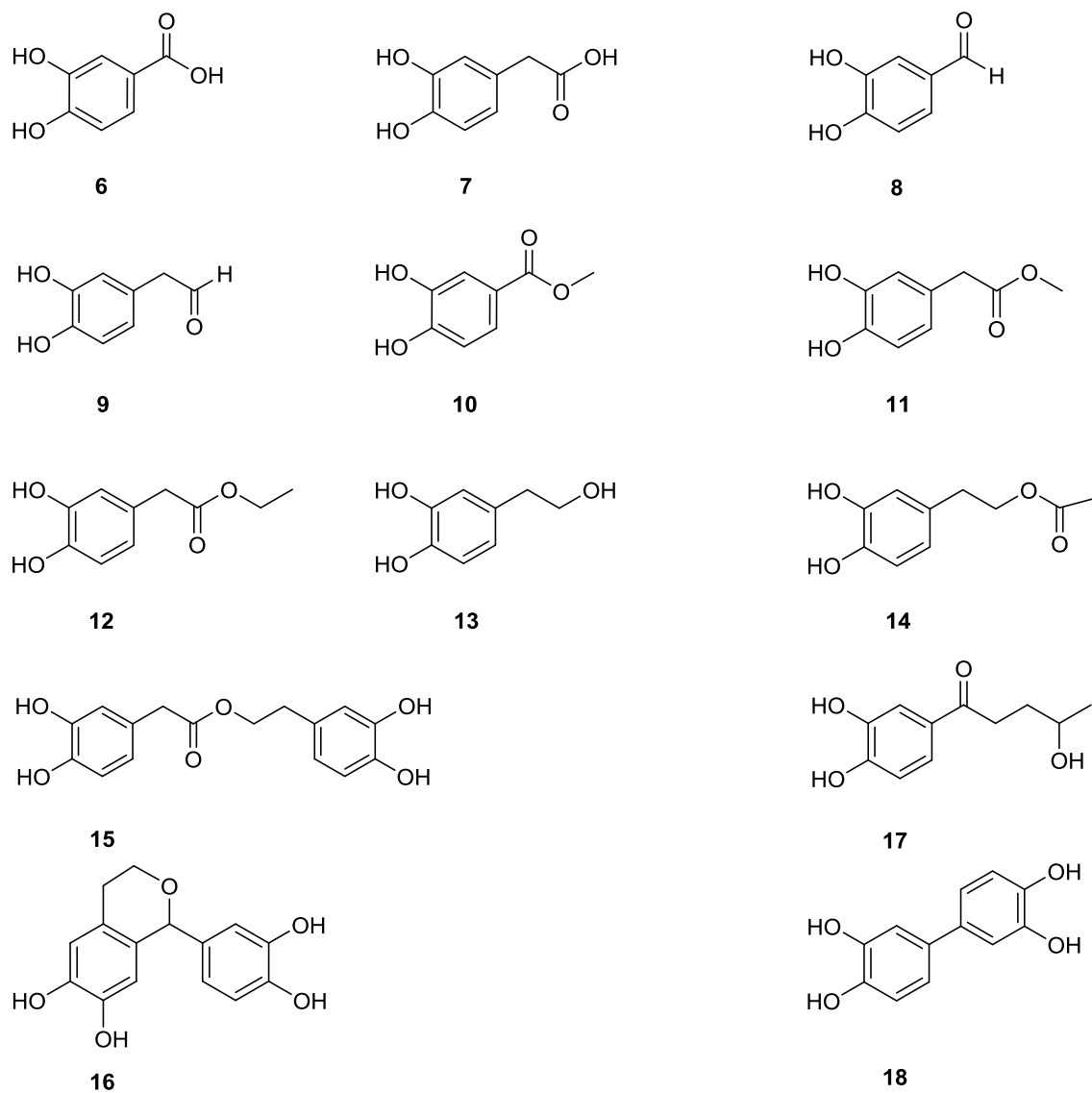
Fig. S27.  $^{13}\text{C}$  NMR spectrum of 5 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S28.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 5 in  $\text{CD}_3\text{COCD}_3$ .

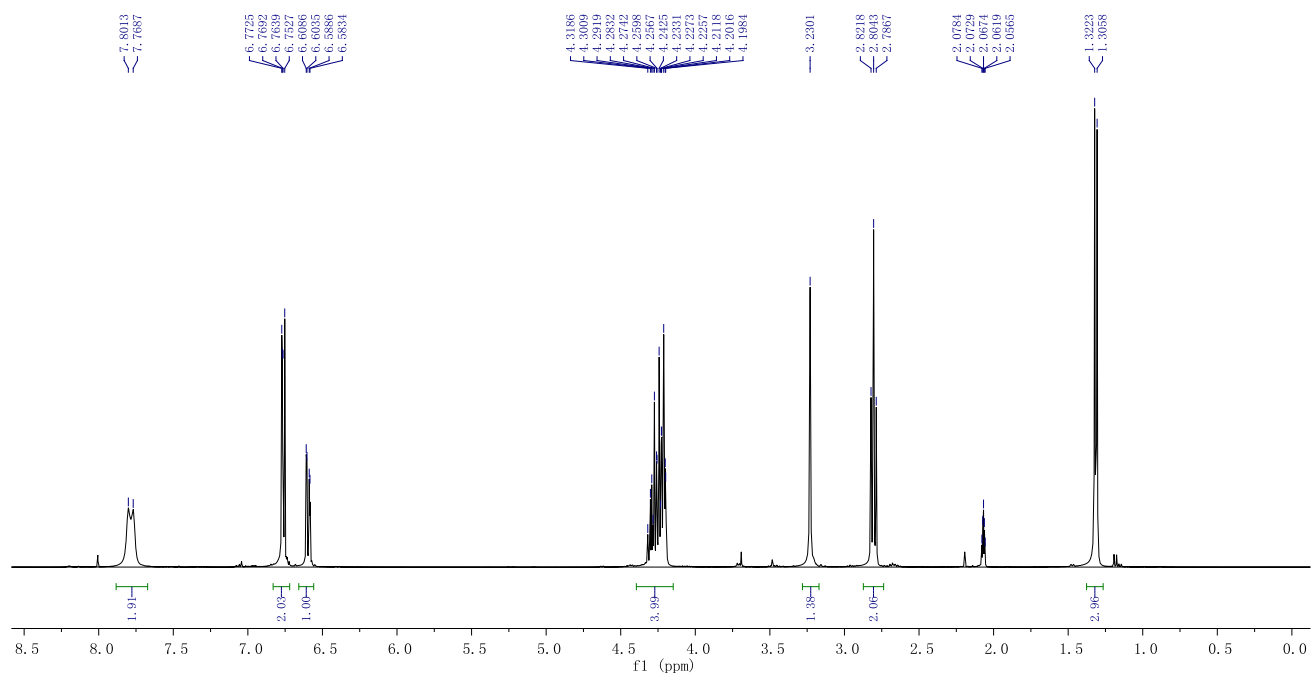
Fig. S29. HMQC spectrum of 5 in  $\text{CD}_3\text{COCD}_3$ .

Fig. S30. HMBC spectrum of 5 in  $\text{CD}_3\text{COCD}_3$ .

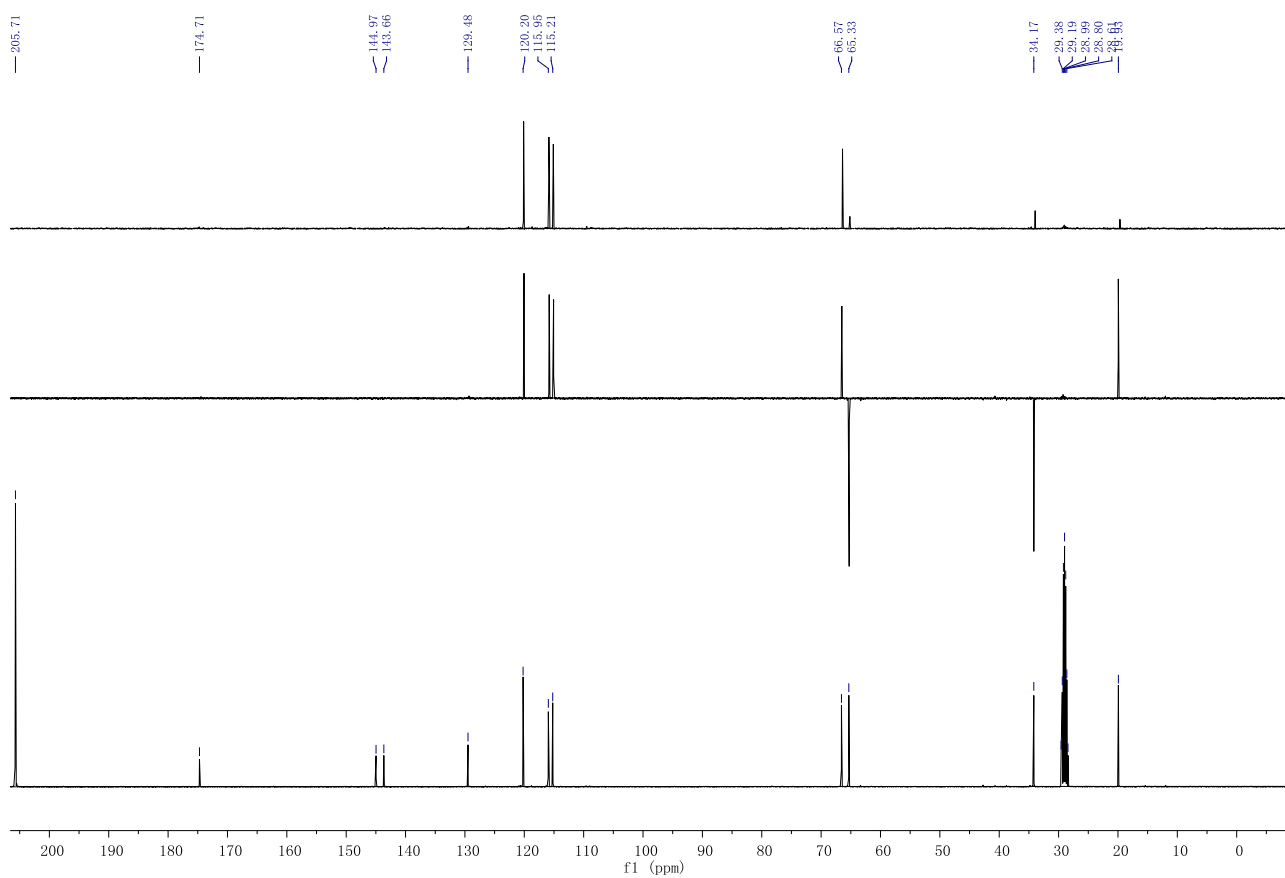
Fig. S31. HR-ESI-MS spectrum of 5.



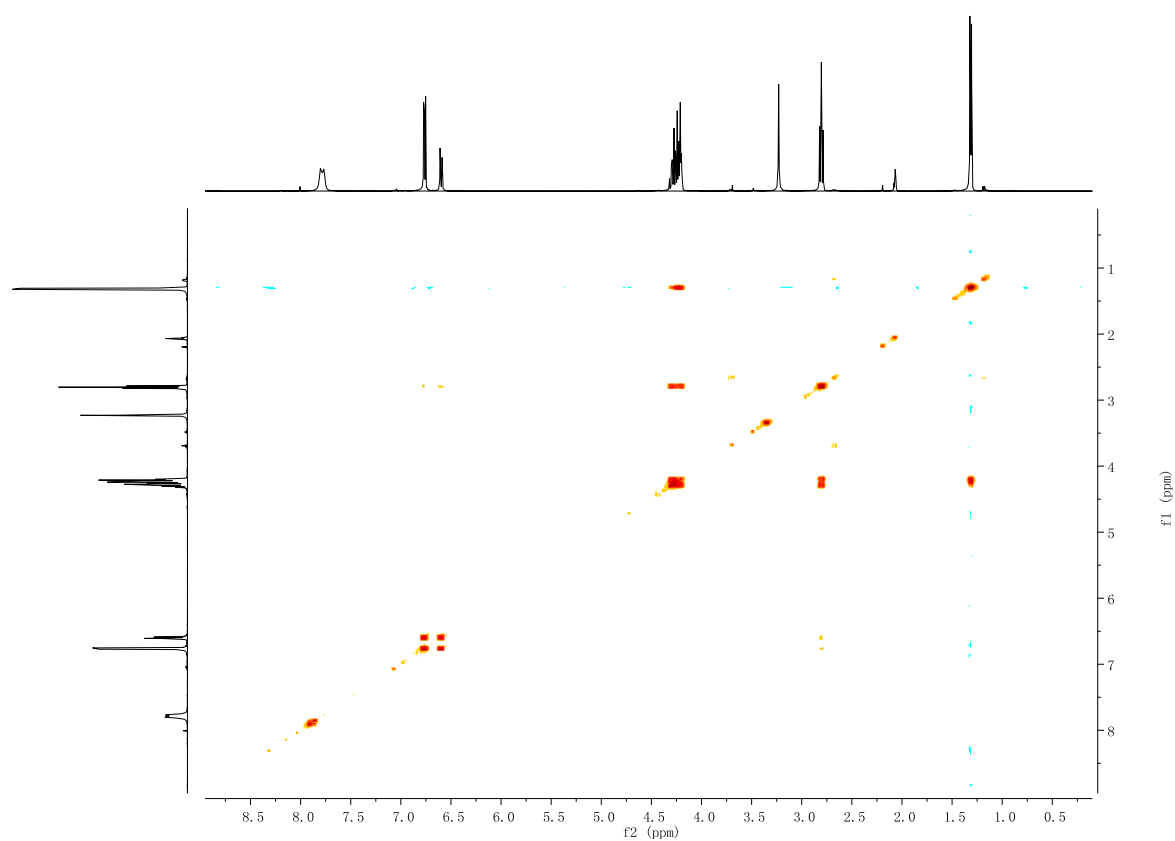
**Fig. S1. The structures of compounds 6-18.**



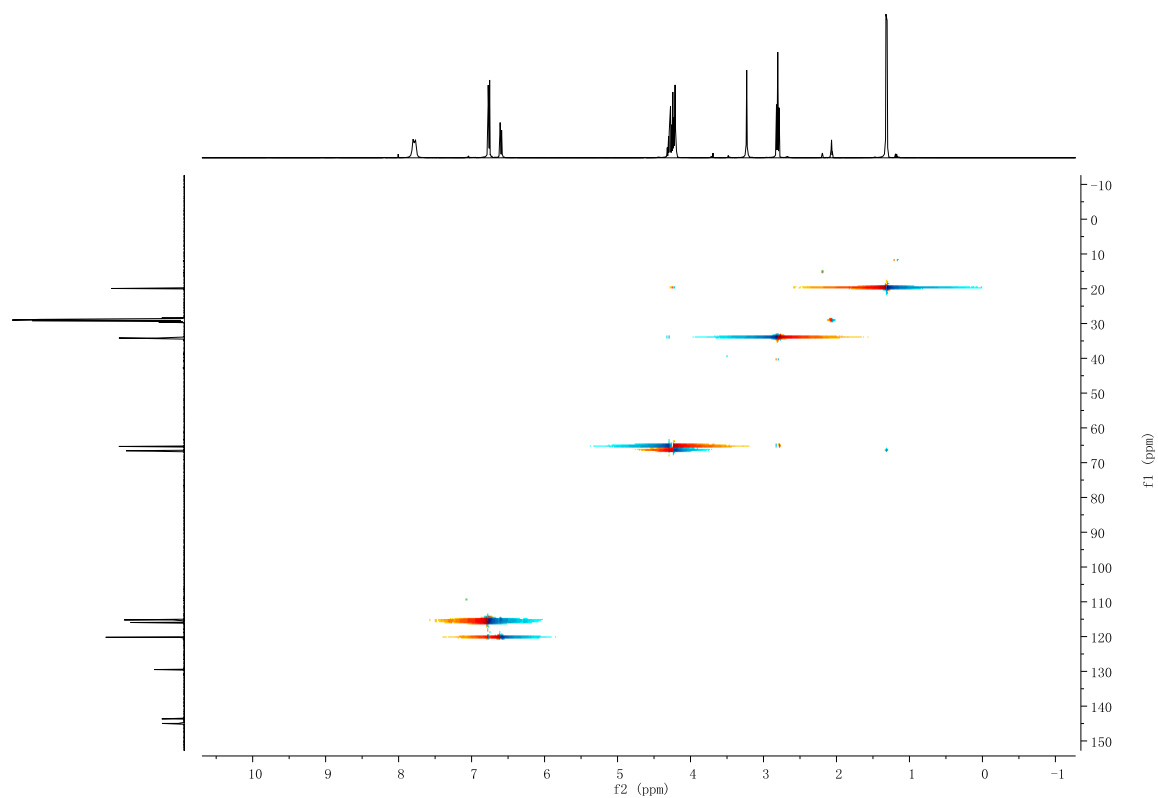
**Fig. S2. <sup>1</sup>H NMR spectrum of 1 in CD<sub>3</sub>COCD<sub>3</sub>**



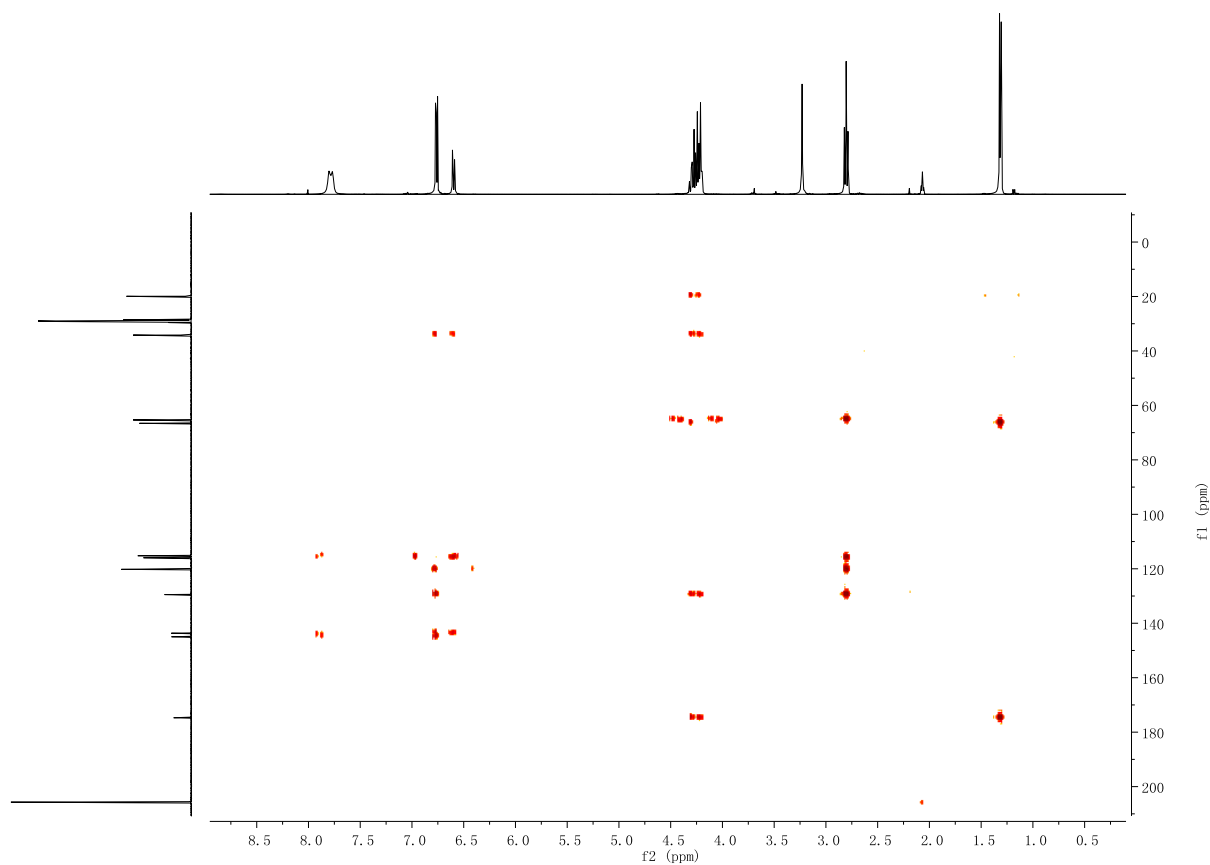
**Fig. S3. <sup>13</sup>C NMR spectrum of 1 in CD<sub>3</sub>COCD<sub>3</sub>**



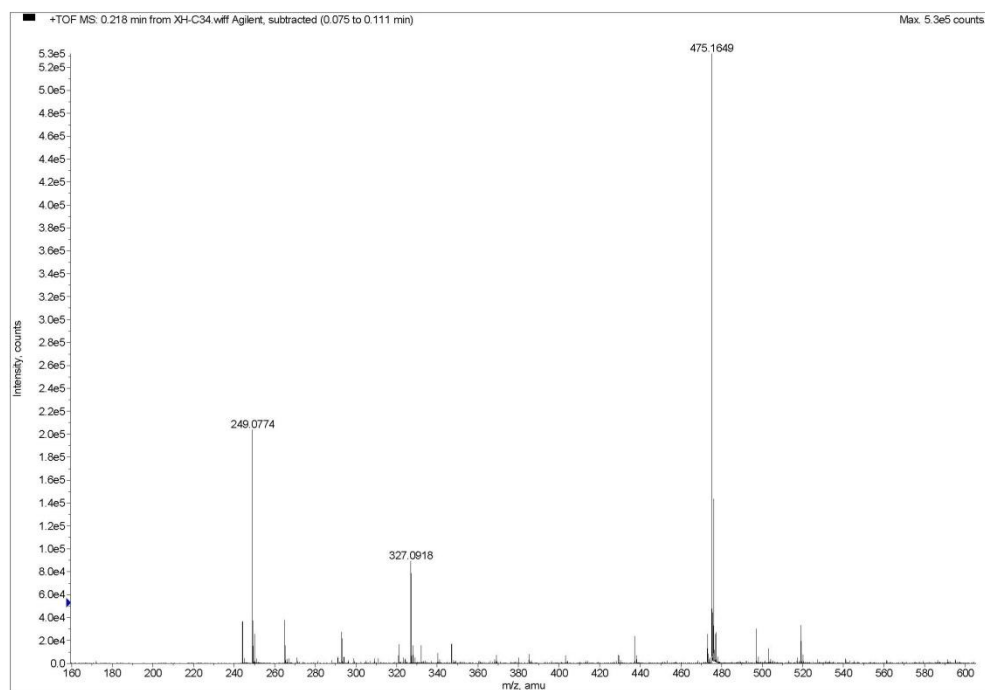
**Fig. S4.** H-H COSY spectrum of **1** in  $\text{CD}_3\text{COCD}_3$



**Fig. S5.** HSQC spectrum of **1** in  $\text{CD}_3\text{COCD}_3$



**Fig. S6.** HMBC spectrum of **1** in  $\text{CD}_3\text{COCD}_3$



**Fig. S7.** HR-ESI-MS spectrum of **1**.

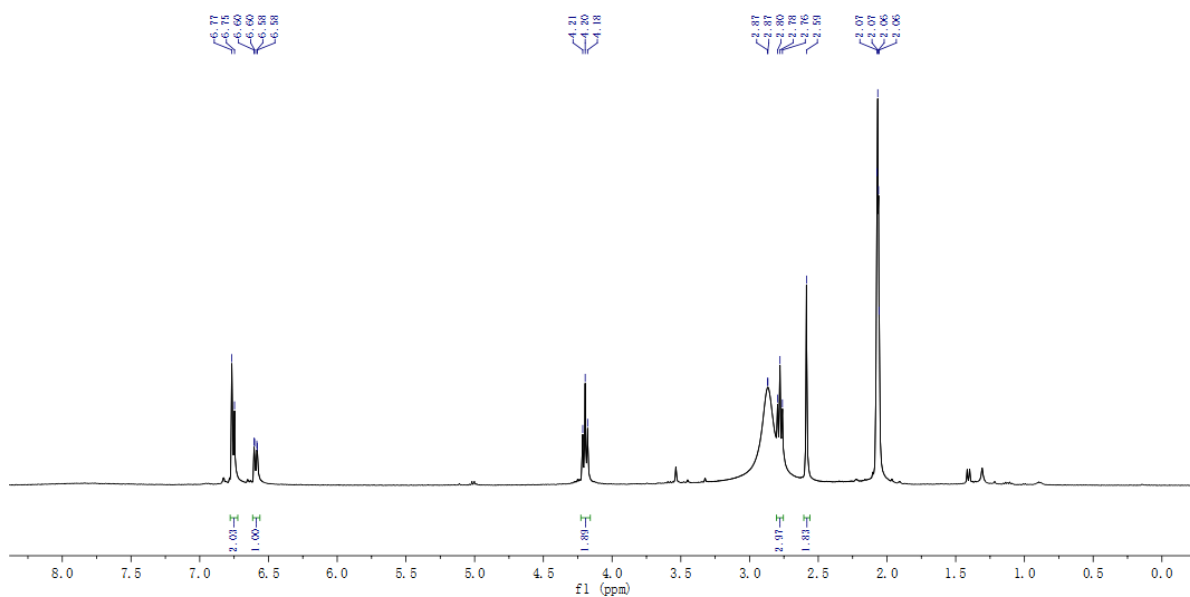


Fig. S8. <sup>1</sup>H NMR spectrum of 2 in CD<sub>3</sub>COCD<sub>3</sub>

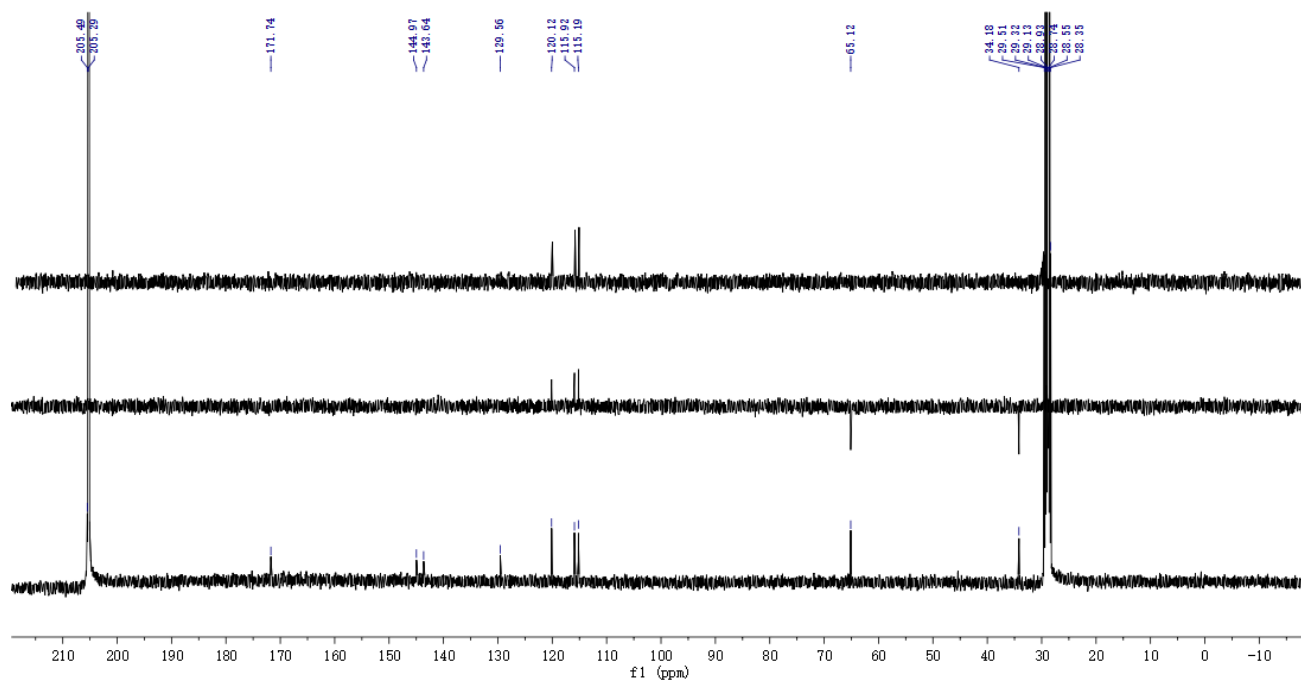
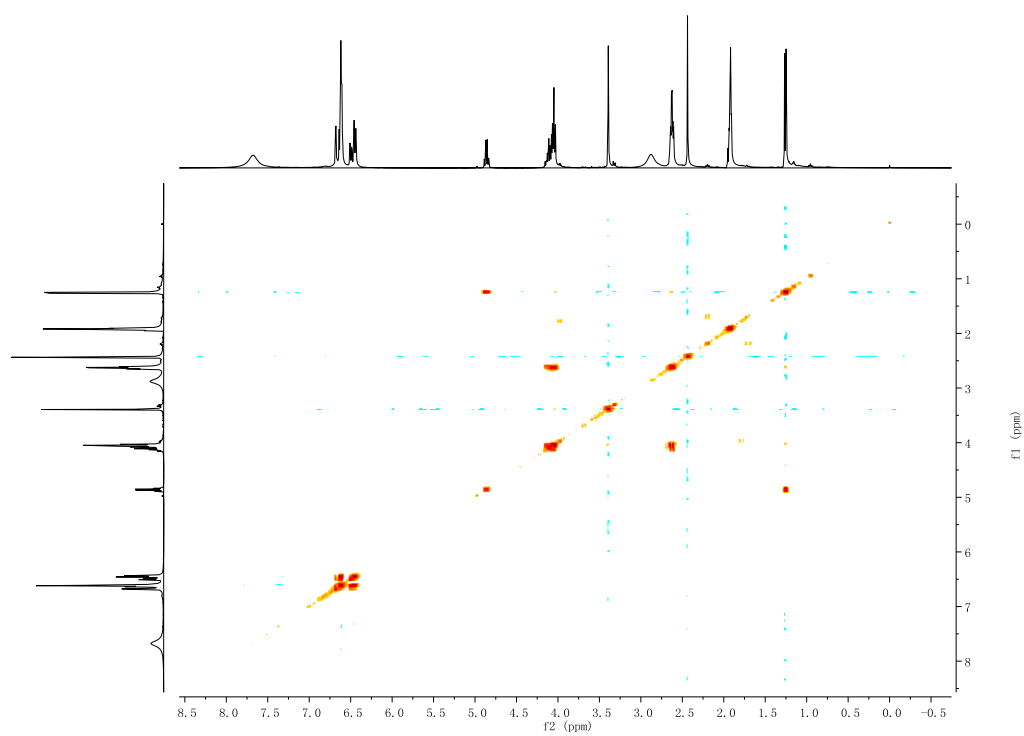
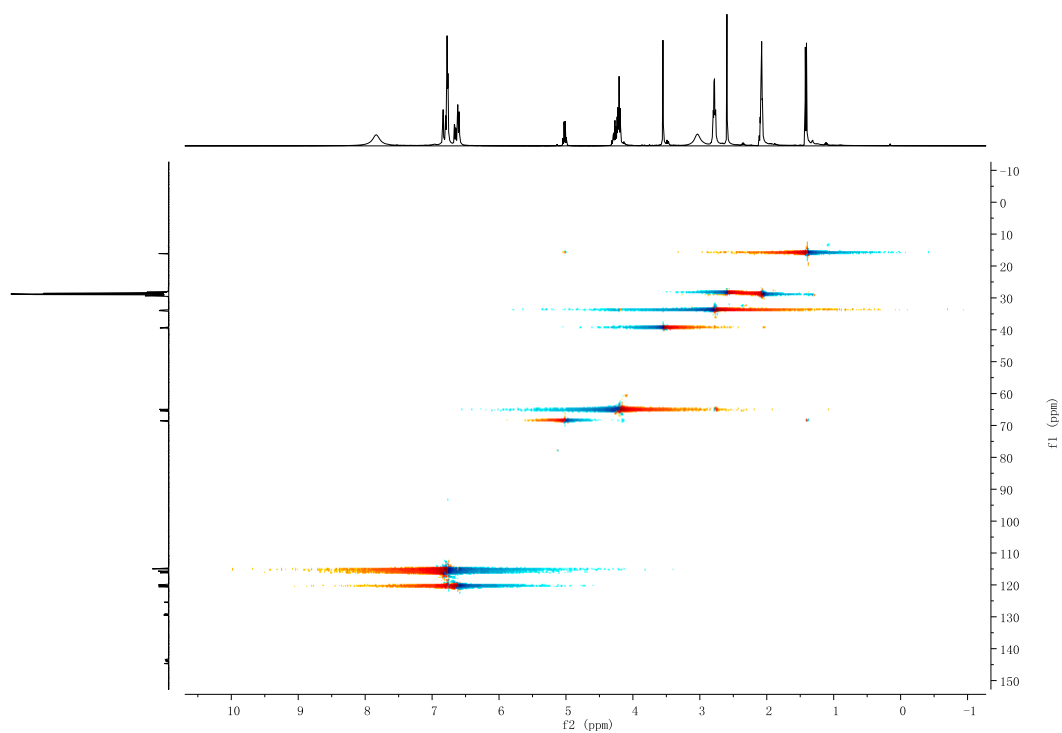


Fig. S9. <sup>13</sup>C NMR spectrum of 2 in CD<sub>3</sub>COCD<sub>3</sub>

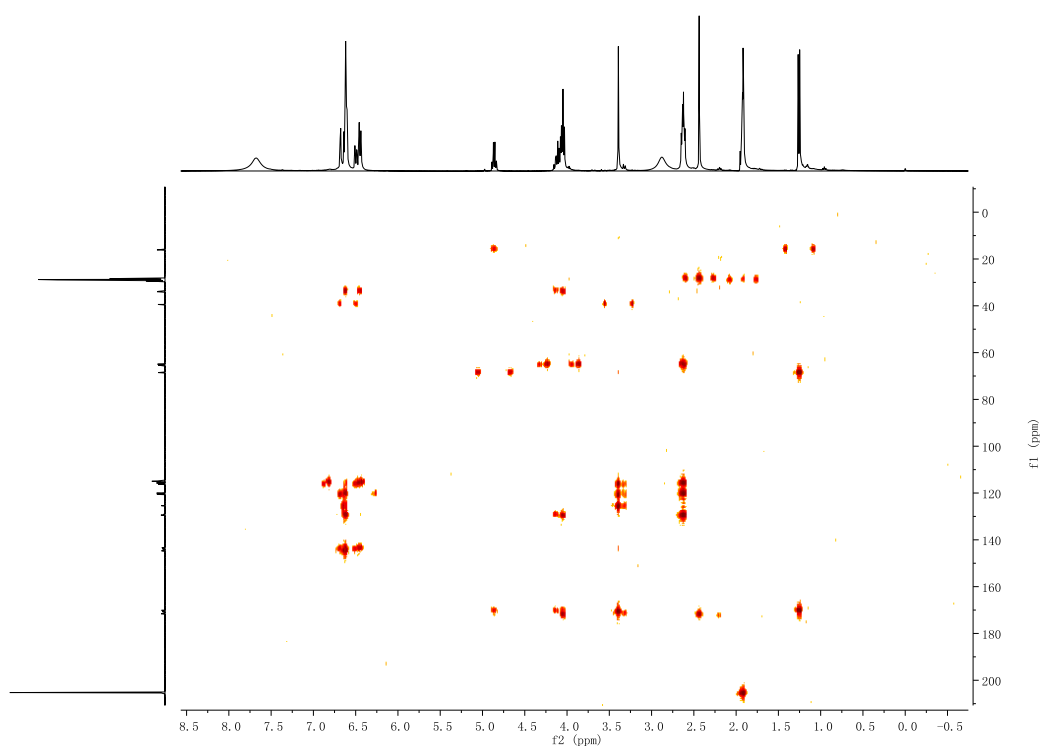


**Fig. S10.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{CD}_3\text{COCD}_3$

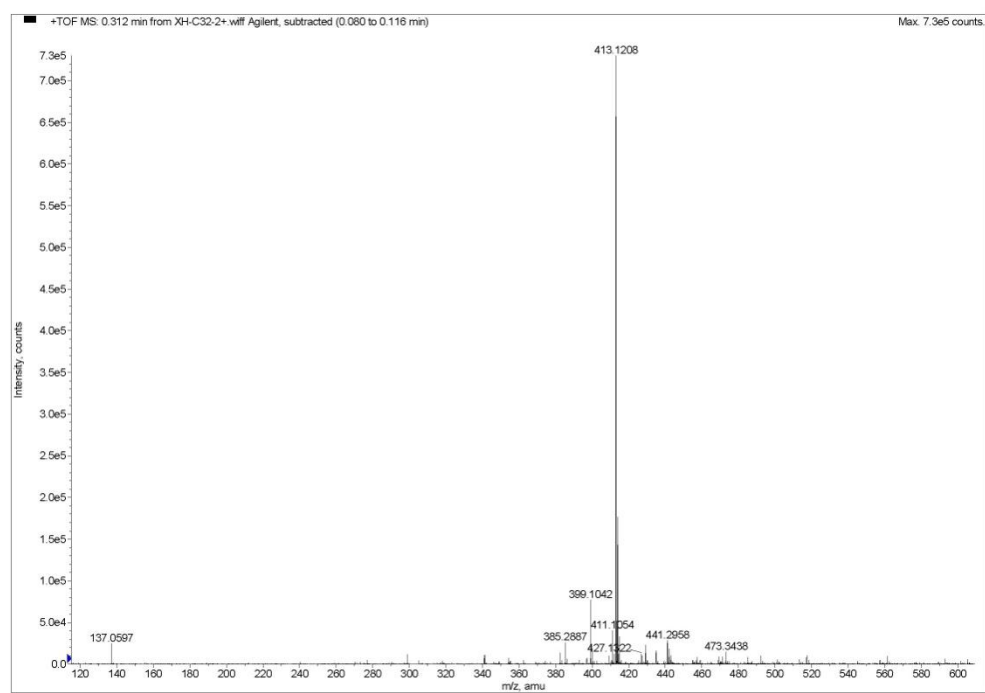


**Fig. S11.** HSQC spectrum of **2** in  $\text{CD}_3\text{COCD}_3$





**Fig. S12.** HMBC spectrum of **2** in  $\text{CD}_3\text{COCD}_3$



**Fig. S13.** HR-ESI-MS spectrum of **2**.

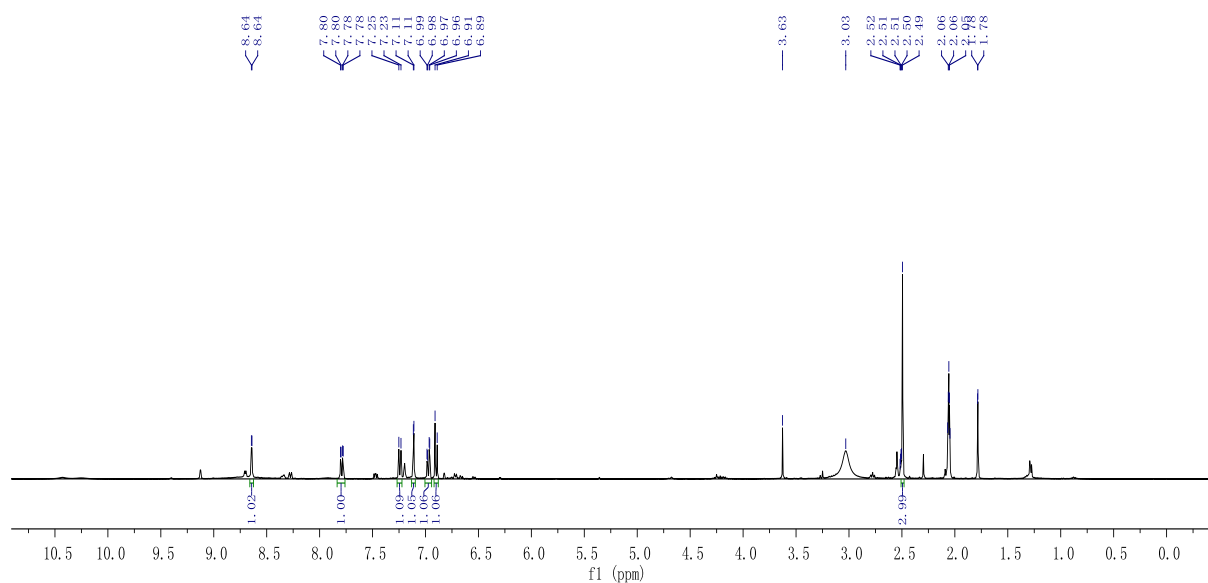


Fig. S14. <sup>1</sup>H NMR spectrum of 3 in CD<sub>3</sub>COCD<sub>3</sub>: DMSO-*d*<sub>6</sub> = 5:1

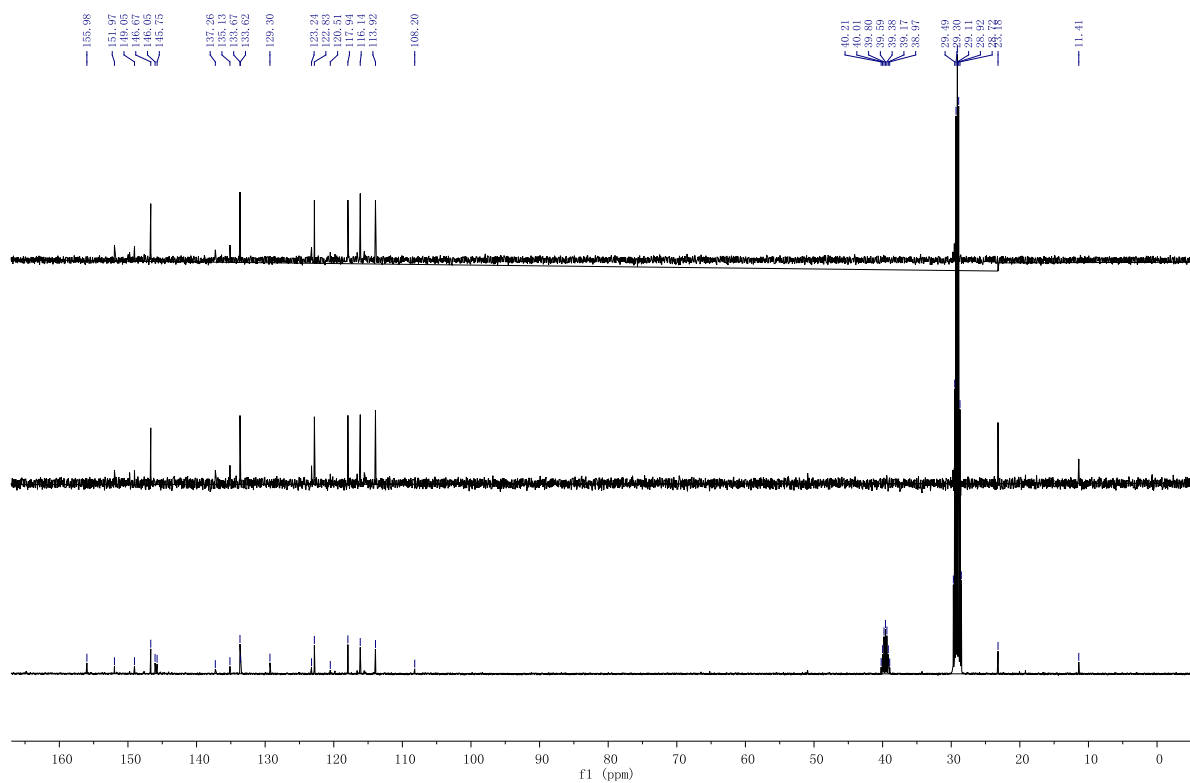
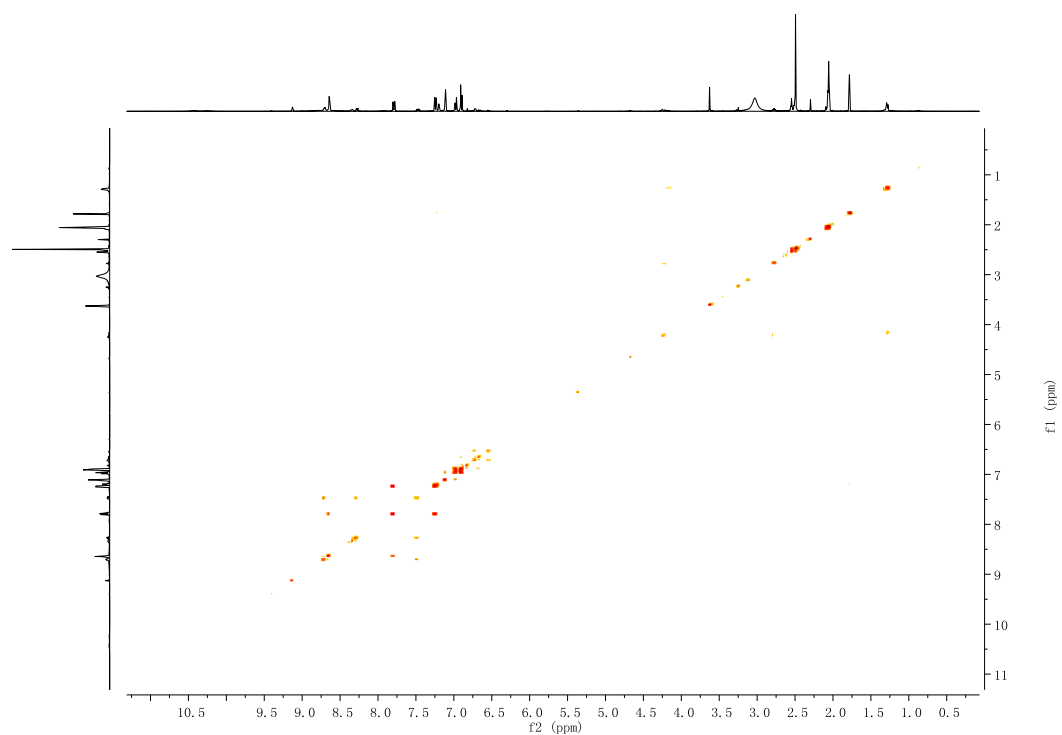
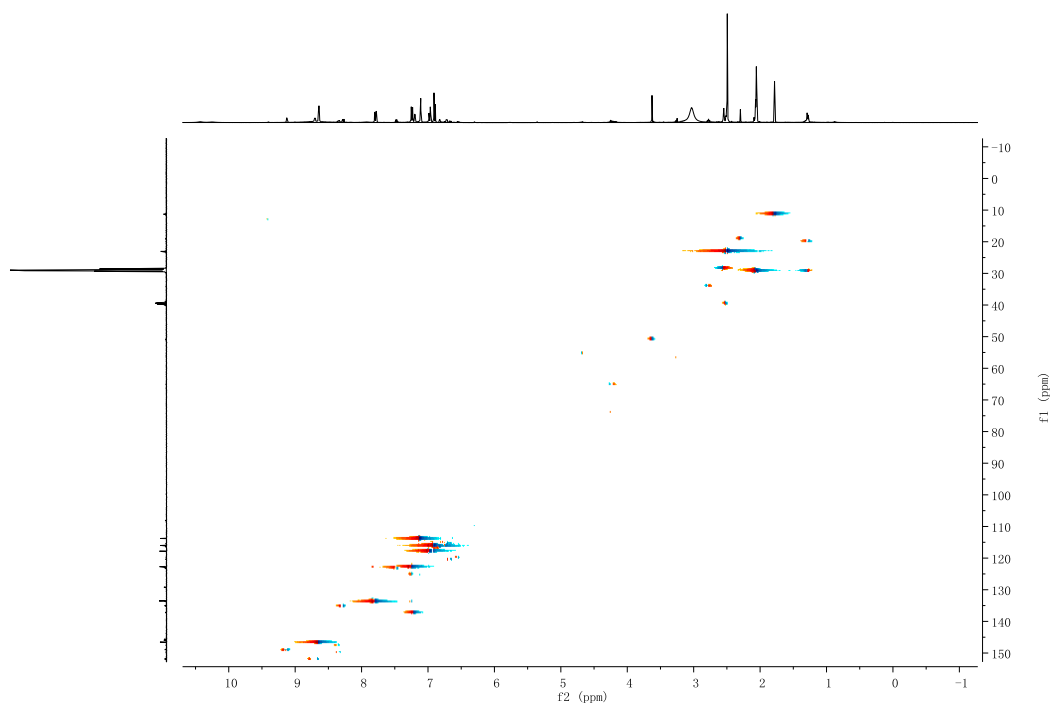


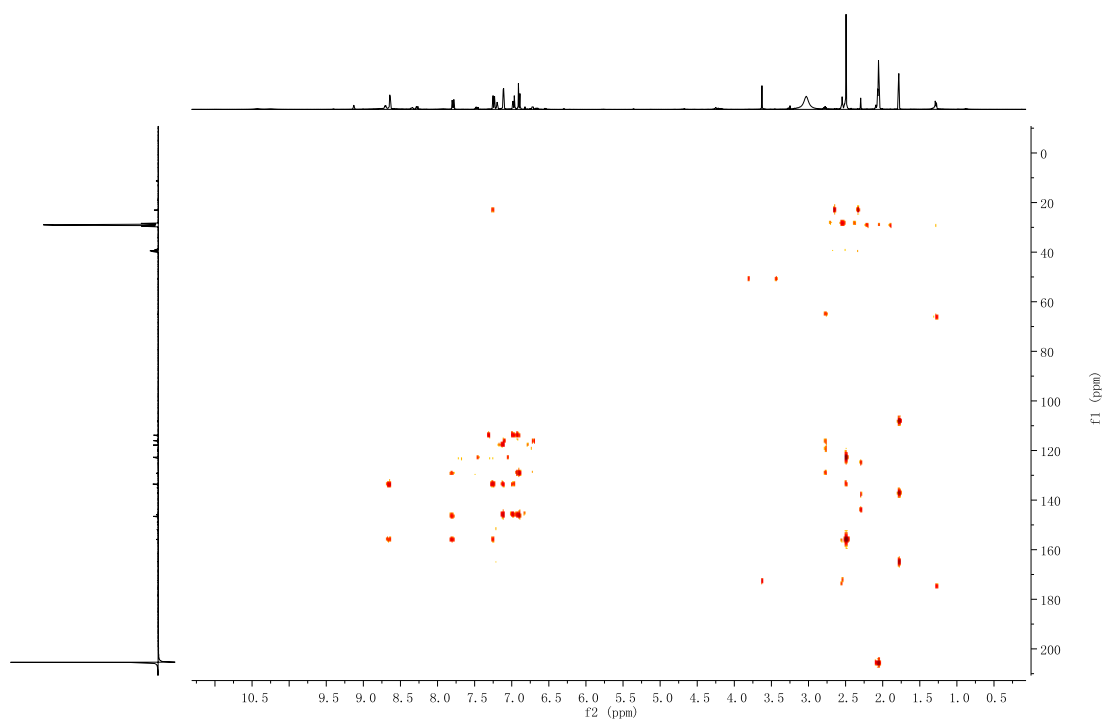
Fig. S15. <sup>13</sup>C NMR spectrum of 3 in CD<sub>3</sub>COCD<sub>3</sub>: DMSO-*d*<sub>6</sub> = 5:1



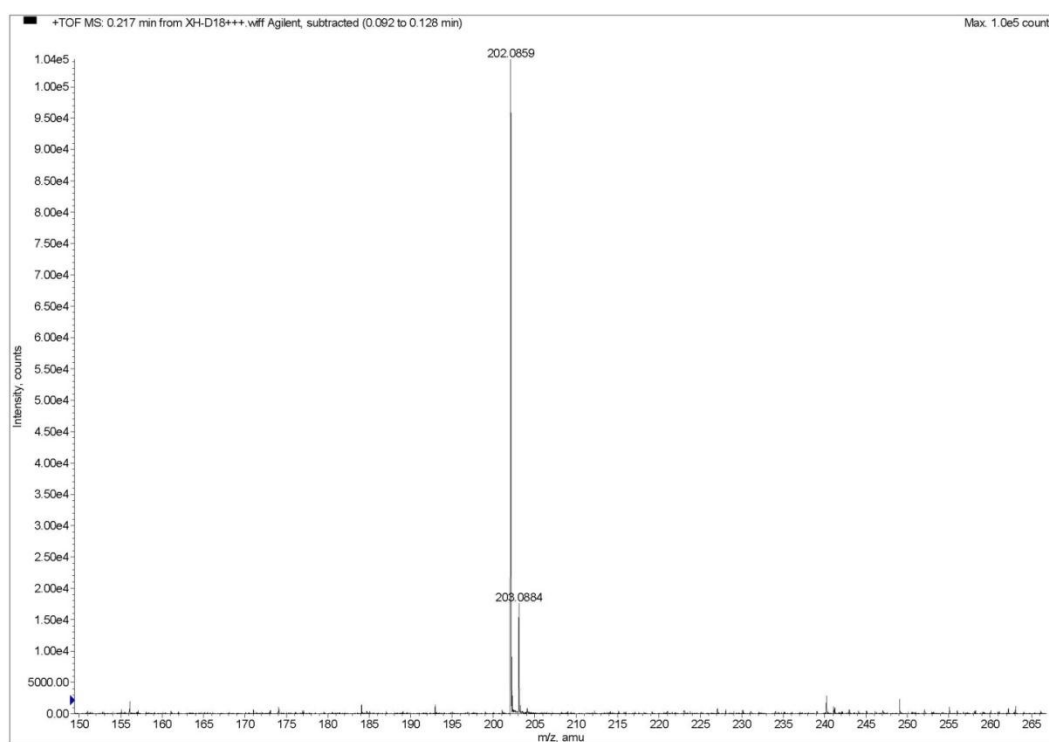
**Fig. S16.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6 = 5:1$



**Fig. S17.** HSQC spectrum of **3** in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO-}d_6 = 5:1$



**Fig. S18.** HMBC spectrum of **3** in  $\text{CD}_3\text{COCD}_3$ :  $\text{DMSO}-d_6$  = 5:1



**Fig. S19.** HR-ESI-MS spectrum of **3**

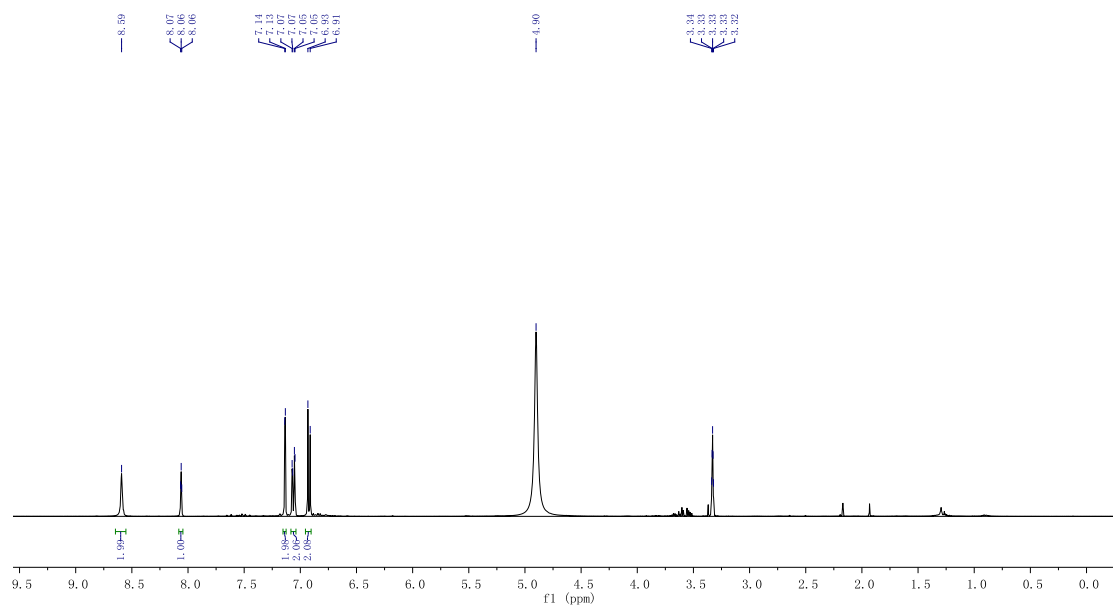


Fig. S20. <sup>1</sup>H-NMR spectrum of 4 in CD<sub>3</sub>OD

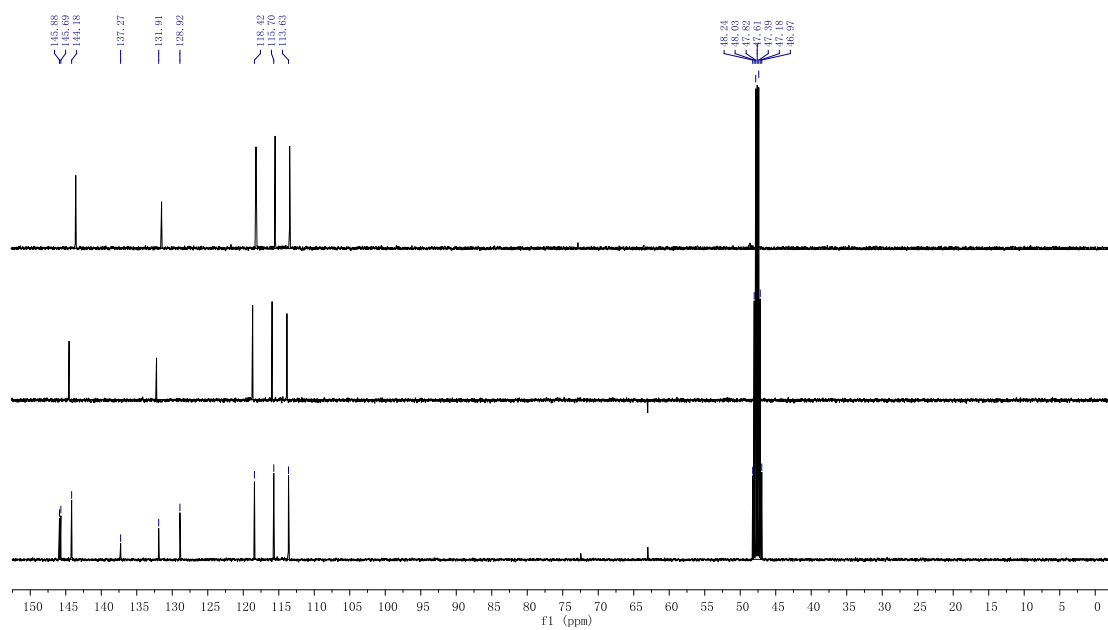
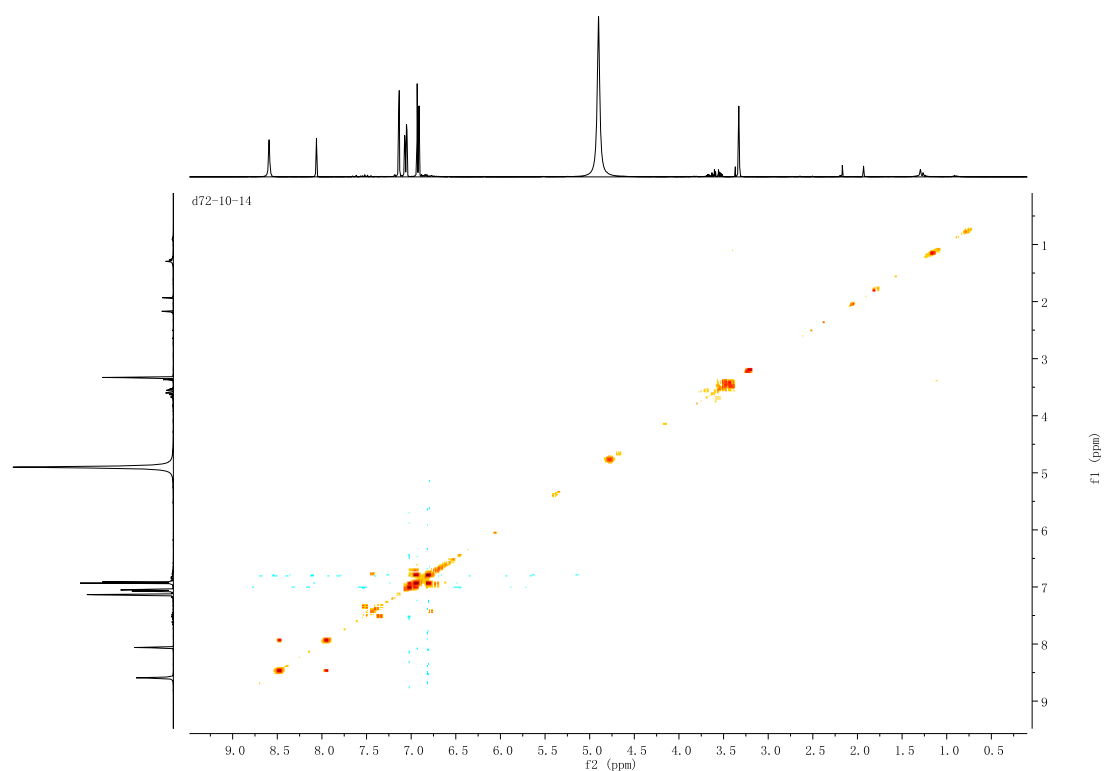
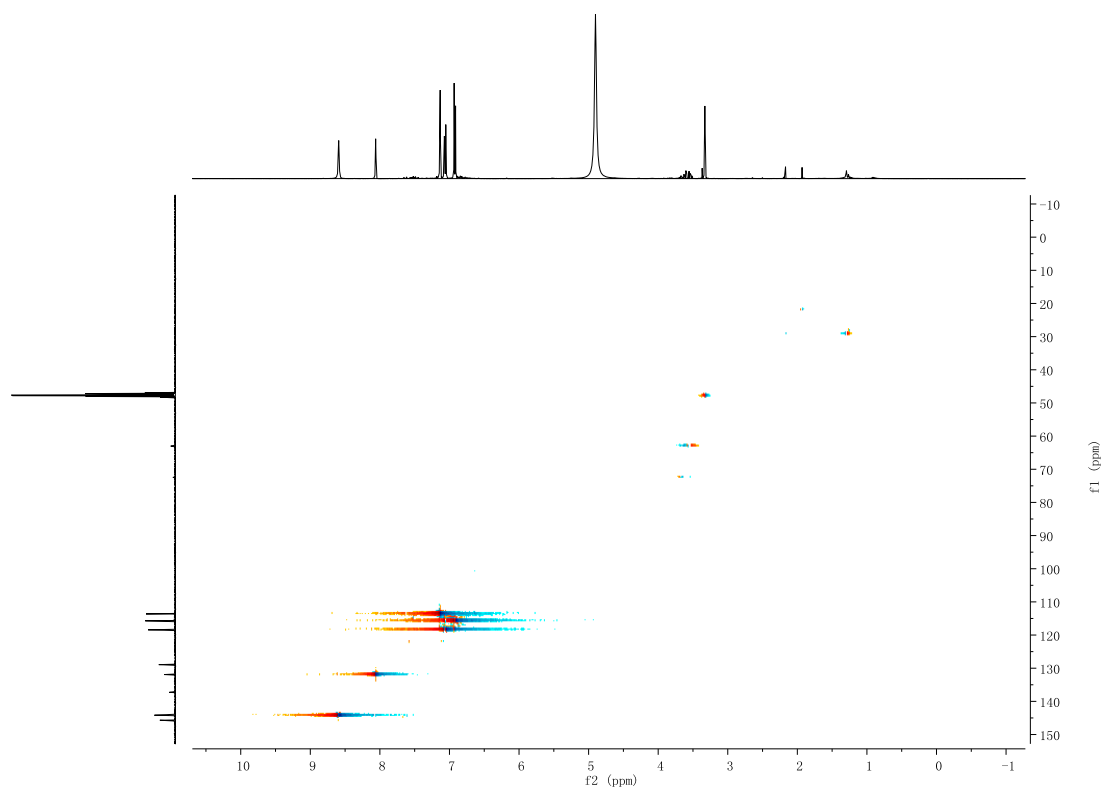


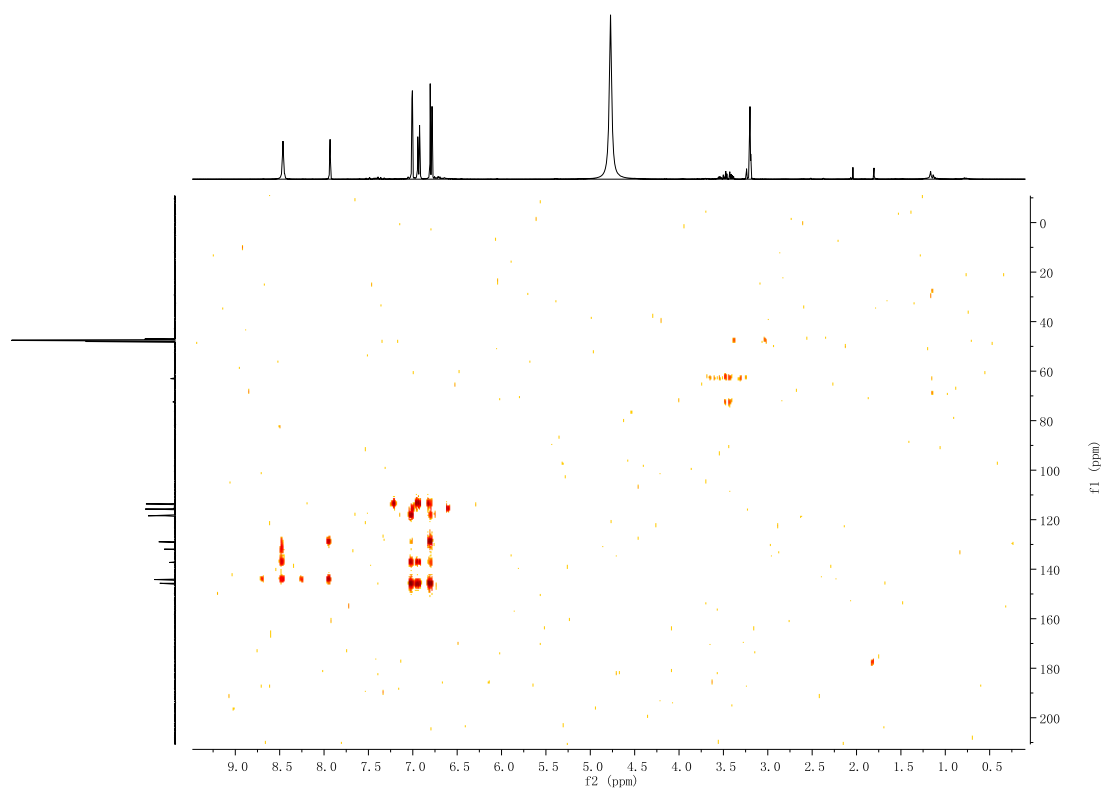
Fig. S21. <sup>13</sup>C NMR spectrum of 4 in CD<sub>3</sub>OD



**Fig. S22.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in  $\text{CD}_3\text{OD}$



**Fig. S23.** HSQC spectrum of **4** in  $\text{CD}_3\text{OD}$



**Fig. S24.** HMBC spectrum of **4** in CD<sub>3</sub>OD

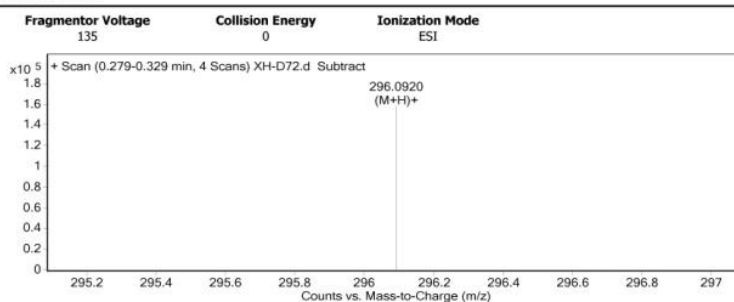
## Qualitative Analysis Report

|                               |              |                      |                     |
|-------------------------------|--------------|----------------------|---------------------|
| <b>Data Filename</b>          | XH-D72.d     | <b>Sample Name</b>   | XH-D72              |
| <b>Sample Type</b>            | Sample       | <b>Position</b>      | P1-D3               |
| <b>Instrument Name</b>        | Instrument 1 | <b>User Name</b>     |                     |
| <b>Acq Method</b>             | SIBU.m       | <b>Acquired Time</b> | 1/6/2015 1:49:26 PM |
| <b>IRM Calibration Status</b> | Success      | <b>DA Method</b>     | Default.m           |
| <b>Comment</b>                |              |                      |                     |

|                       |                             |              |  |
|-----------------------|-----------------------------|--------------|--|
| <b>Sample Group</b>   |                             | <b>Info.</b> |  |
| <b>Acquisition SW</b> | 6200 series TOF/6500 series |              |  |
| <b>Version</b>        | Q-TOF B.05.01 (B5125.2)     |              |  |

### User Spectra



### Peak List

| m/z      | z | Abund     | Formula      | Ion    |
|----------|---|-----------|--------------|--------|
| 296.092  | 1 | 158063.61 | C17 H13 N O4 | (M+H)+ |
| 297.0952 | 1 | 31812.14  | C17 H13 N O4 | (M+H)+ |
| 297.2396 | 1 | 3672.2    |              |        |
| 298.0969 | 1 | 3902.19   | C17 H13 N O4 | (M+H)+ |
| 301.1419 | 1 | 7029.75   |              |        |
| 301.2852 | 1 | 8580.91   |              |        |
| 310.1078 | 1 | 5058.93   |              |        |
| 341.2665 | 1 | 6015.52   |              |        |
| 385.2931 | 1 | 7487.52   |              |        |
| 429.3182 | 1 | 4323.08   |              |        |

### Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C       | 3   | 60  |
| H       | 0   | 120 |
| O       | 0   | 10  |
| N       | 0   | 5   |

### Formula Calculator Results

| Formula      | CalculatedMass | CalculatedMz | Mz       | Diff. (mDa) | Diff. (ppm) | DBE     |
|--------------|----------------|--------------|----------|-------------|-------------|---------|
| C17 H13 N O4 | 295.0845       | 296.0917     | 296.0920 | -0.3        | -1.0        | 12.0000 |

--- End Of Report ---

Fig. S25. HR-ESI-MS spectrum of 4



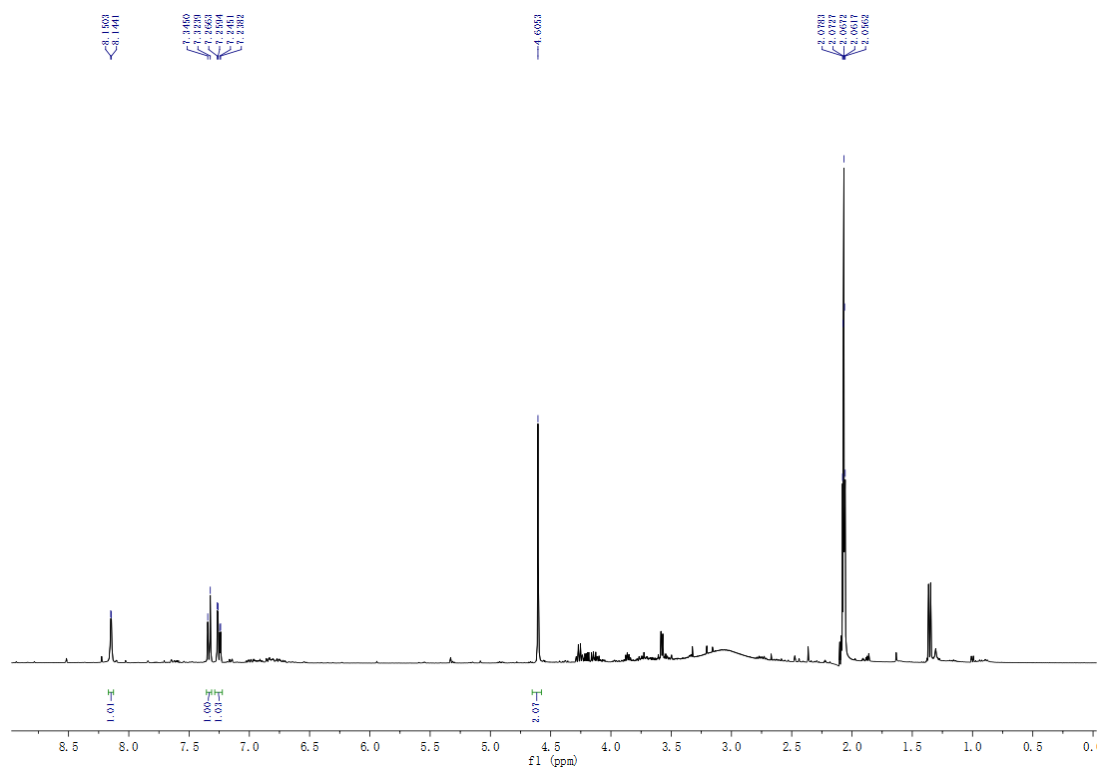


Fig. S26  $^1\text{H}$ -NMR spectrum of 5 in  $\text{CD}_3\text{COCD}_3$

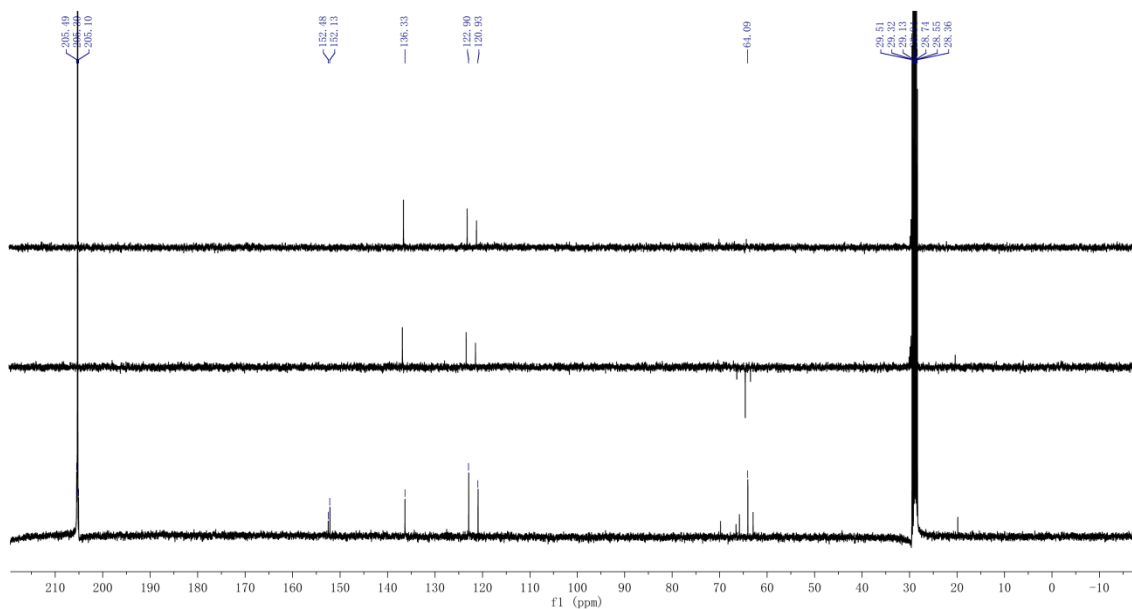
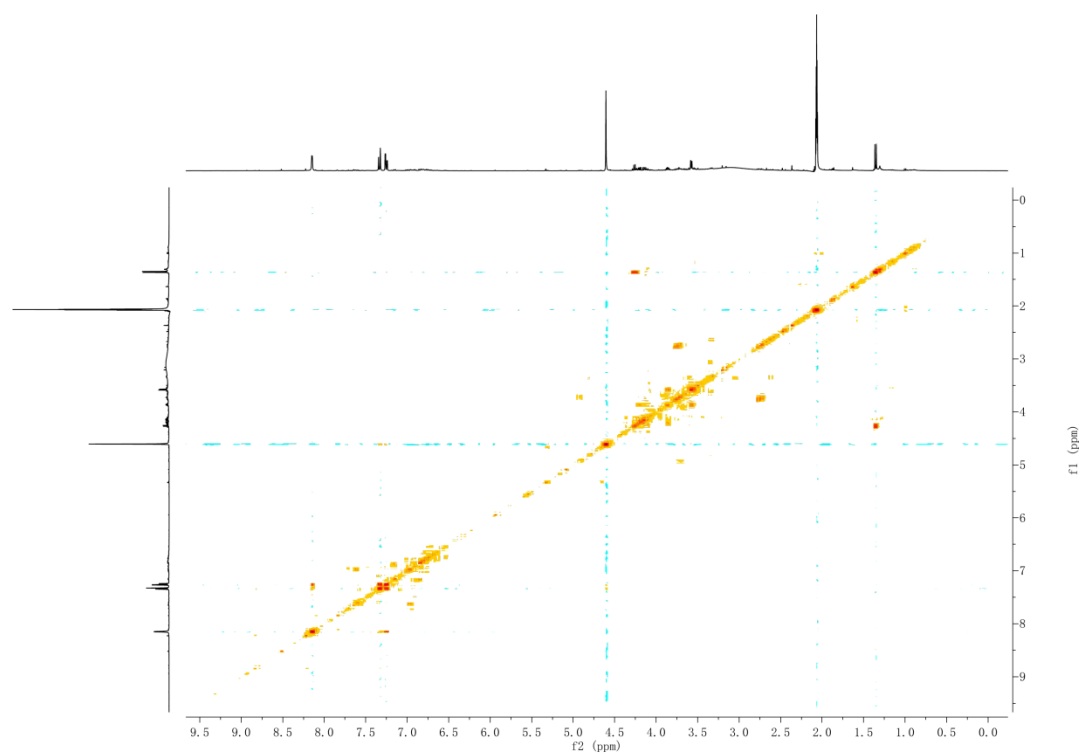
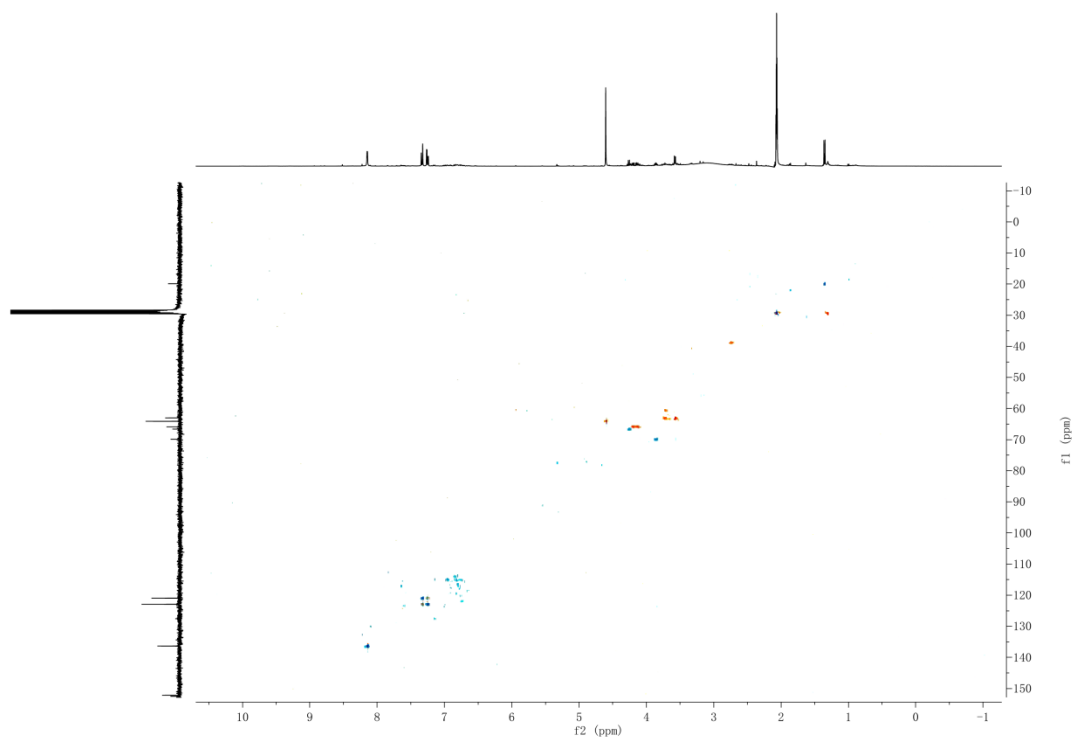


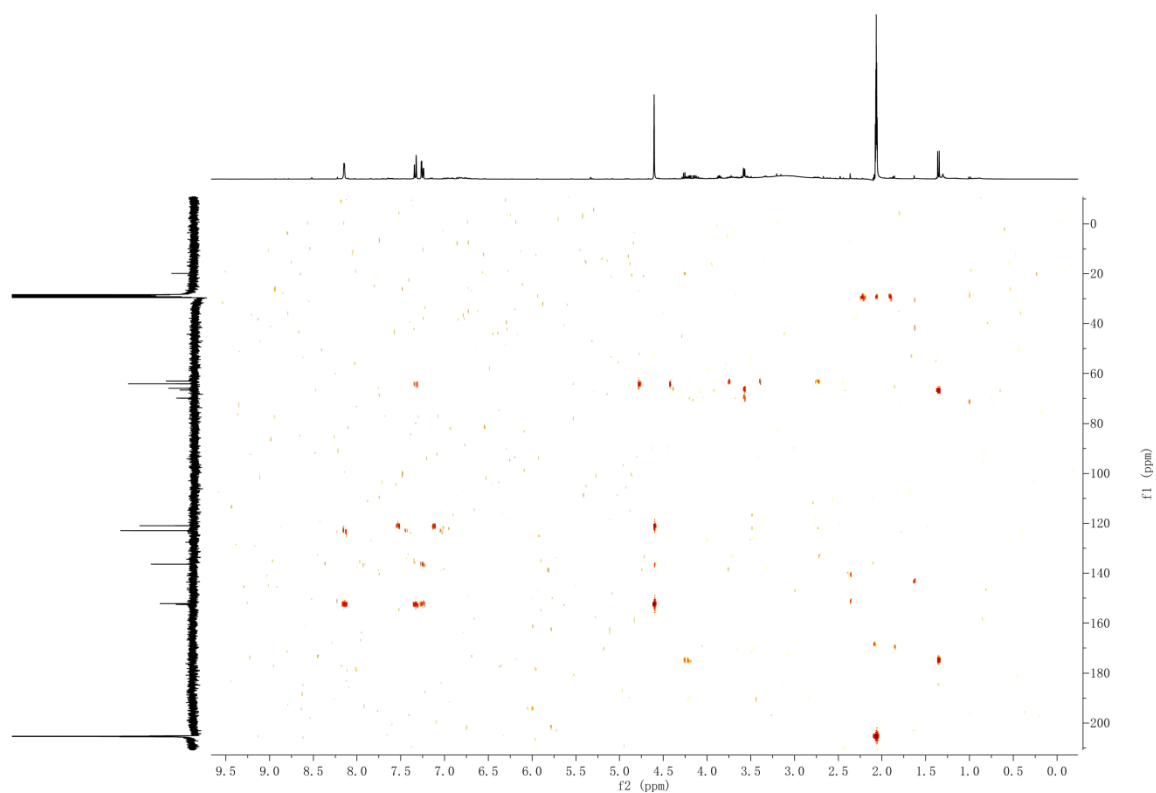
Fig. S27.  $^{13}\text{C}$ -NMR spectrum of 5 in  $\text{CD}_3\text{COCD}_3$



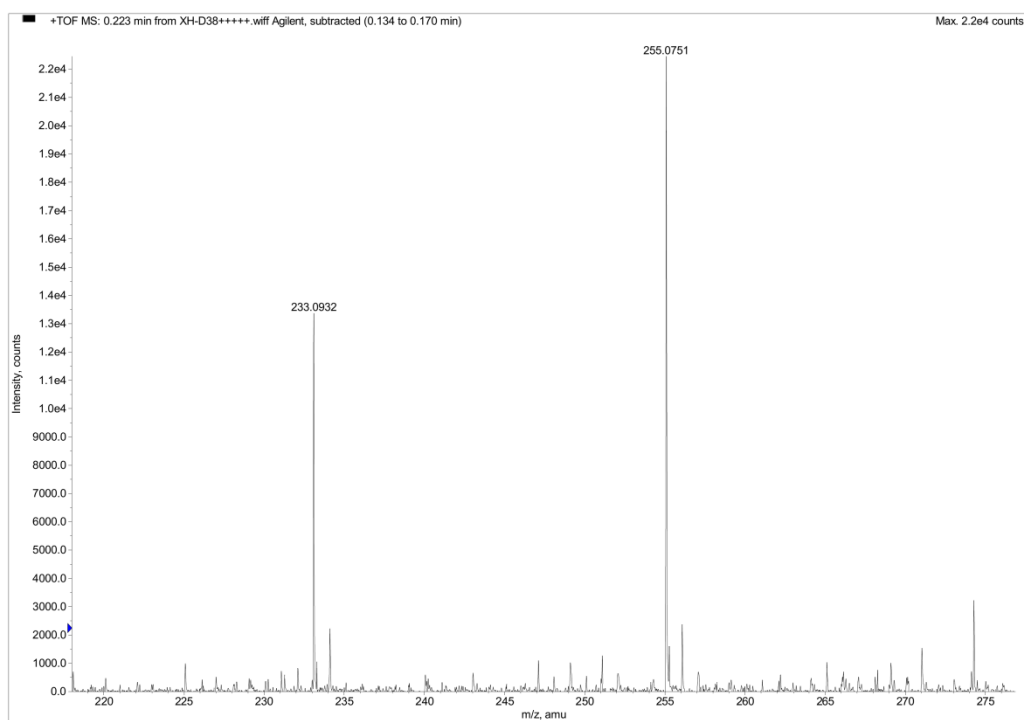
**Fig. S28.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 5 in  $\text{CD}_3\text{COCD}_3$



**Fig. S29.** HSQC spectrum of 5 in  $\text{CD}_3\text{COCD}_3$



**Fig. S30.** HMBC spectrum of **5** in  $\text{CD}_3\text{COCD}_3$



**Fig. S31. HR-ESI-MS spectrum of 5**