

# Supplementary Materials: Dichotocejpins A–C: New Diketopiperazines from a Deep-Sea-Derived Fungus *Dichotomomyces cepii* FS110

Zhen Fan, Zhang-Hua Sun, Zhong Liu, Yu-Chan Chen, Hong-Xin Liu, Hao-Hua Li and Wei-Min Zhang

## List of Supporting Information

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

**Figure S2.**  $^{13}\text{C}$  NMR and DEPT135 spectra of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .

**Figure S3.** HSQC spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .

**Figure S4.**  $^1\text{H}$ – $^1\text{H}$  COSY spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .

**Figure S5.** HMBC spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .

**Figure S6.** HRESIMS spectrum of dichotocejpin A (**1**).

**Figure S7.** IR spectrum of dichotocejpin A (**1**).

**Figure S8.** UV spectrum of dichotocejpin A (**1**).

**Figure S9.**  $^1\text{H}$  NMR spectrum of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .

**Figure S10.**  $^{13}\text{C}$  NMR and DEPT135 spectra of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .

**Figure S11.** HSQC spectrum of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .

**Figure S12.**  $^1\text{H}$ – $^1\text{H}$  COSY spectrum of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .

**Figure S13.** HMBC spectrum of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .

**Figure S14.** NOESY spectrum of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .

**Figure S15.** HRESIMS spectrum of dichotocejpin B (**2**).

**Figure S16.** IR spectrum of dichotocejpin A (**2**).

**Figure S17.** UV spectrum of dichotocejpin A (**2**).

**Figure S18.**  $^1\text{H}$  NMR spectrum of dichotocejpin C (**3**) in  $\text{DMSO}-d_6$ .

**Figure S19.**  $^{13}\text{C}$  NMR spectrum of dichotocejpin C (**3**) in  $\text{DMSO}-d_6$ .

**Figure S20.** HSQC spectrum of dichotocejpin C (**3**) in  $\text{DMSO}-d_6$ .

**Figure S21.**  $^1\text{H}$ – $^1\text{H}$  COSY spectrum of dichotocejpin C (**3**) in  $\text{DMSO}-d_6$ .

**Figure S22.** HMBC spectrum of dichotocejpin C (**3**) in  $\text{DMSO}-d_6$ .

**Figure S23.** HRESIMS spectrum of dichotocejpin C (**3**) in  $\text{DMSO}-d_6$ .

**Figure S24.** IR spectrum of dichotocejpin A (**3**).

**Figure S25.** UV spectrum of dichotocejpin A (**3**).

**Figure S26.**  $^1\text{H}$  NMR spectrum of compound **4** in  $\text{CD}_3\text{OD}$ .

**Figure S27.** ESI-MS spectrum of compound **4**.

**Figure S28.**  $^1\text{H}$  NMR spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S29.**  $^{13}\text{C}$  NMR spectrum of compound **5** in  $\text{CD}_3\text{OD}$ .

**Figure S30.**  $^1\text{H}$  NMR spectrum of compound **6** in  $\text{CDCl}_3$ .

**Figure S31.**  $^{13}\text{C}$  NMR spectrum of compound **6** in  $\text{CDCl}_3$ .

**Figure S32.** ESI-MS spectrum of compound **6**.

**Figure S33.**  $^1\text{H}$  NMR spectrum of compound **7** in  $\text{DMSO}-d_6$ .

**Figure S34.**  $^{13}\text{C}$  NMR spectrum of compound **7** in  $\text{DMSO}-d_6$ .

**Figure S35.** ESI-MS spectrum of compound **7**.

**Figure S36.**  $^1\text{H}$  NMR spectrum of compound **8** in  $\text{DMSO}-d_6$ .

**Figure S37.**  $^{13}\text{C}$  NMR spectrum of compound **8** in  $\text{DMSO}-d_6$ .

**Figure S38.** ESI-MS spectrum of compound **8**.

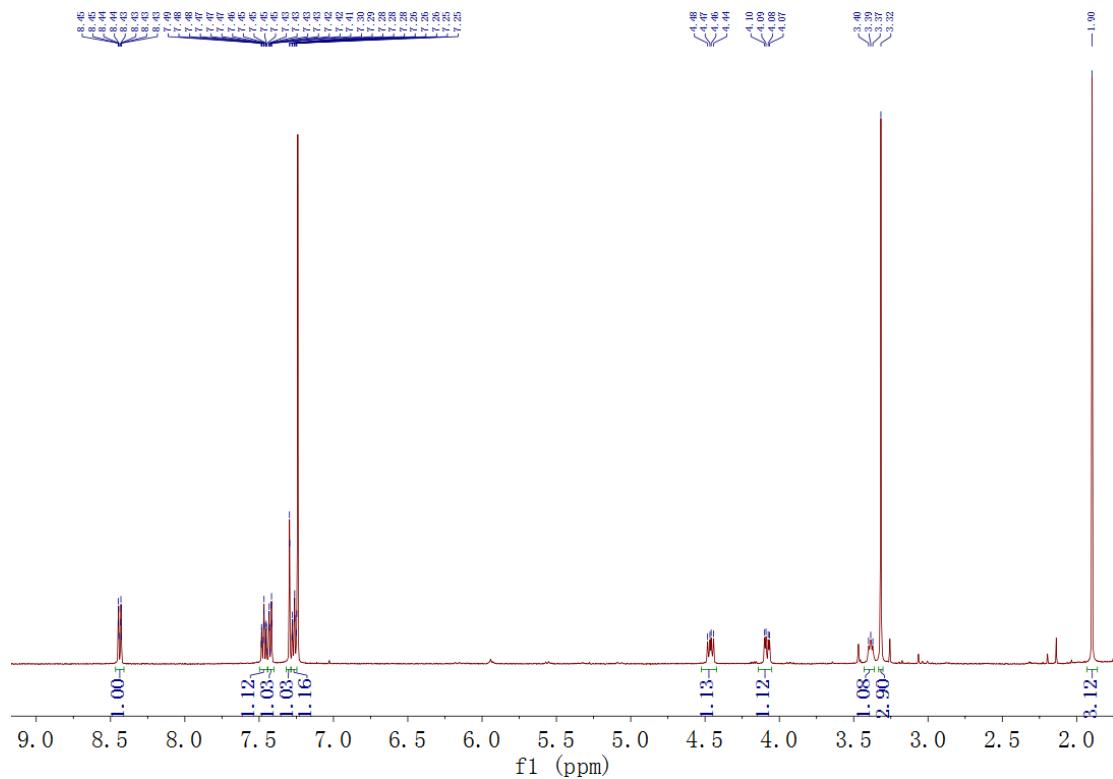
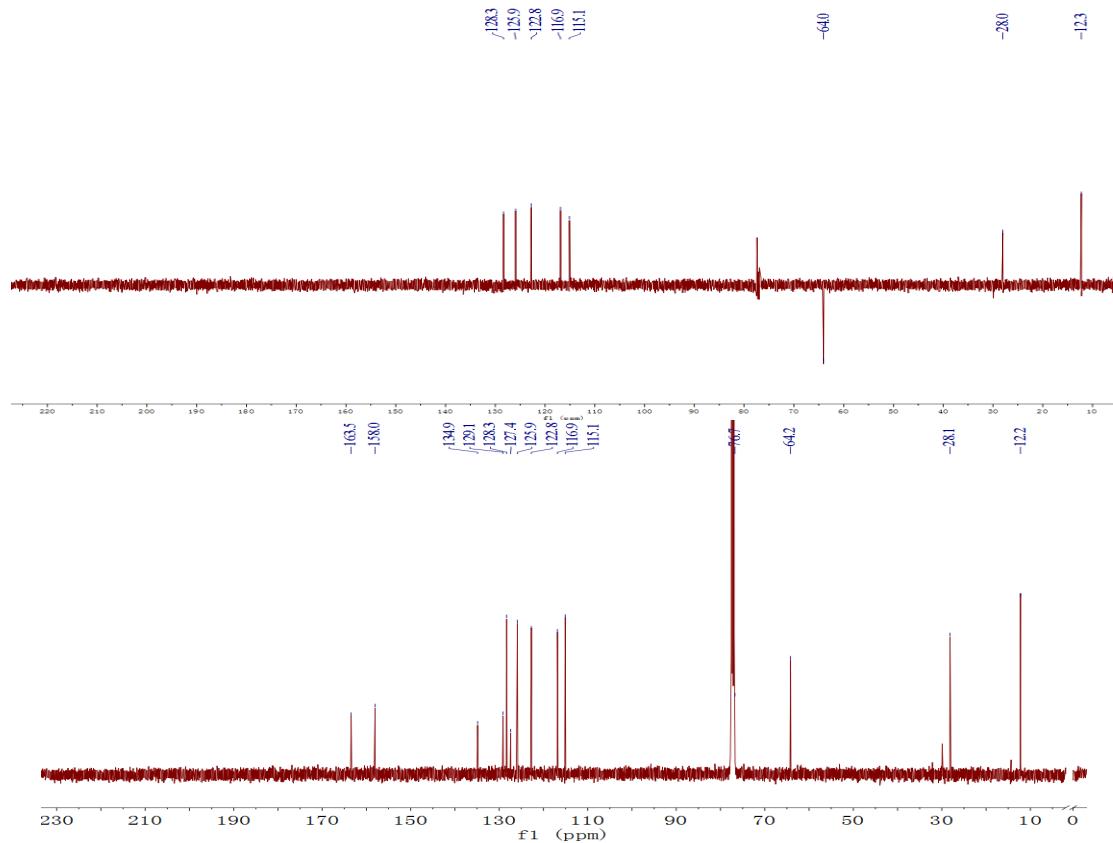
**Figure S39.**  $^1\text{H}$  NMR spectrum of compound **9** in  $\text{CD}_3\text{OD}$ .

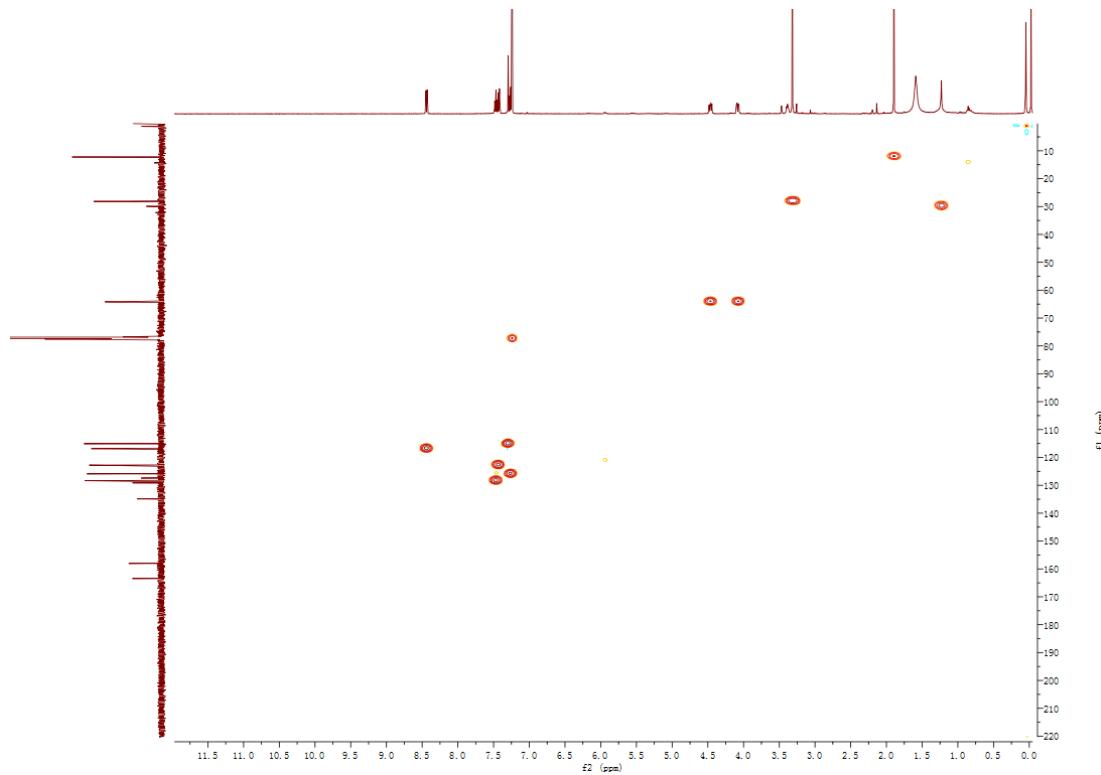
**Figure S40.**  $^{13}\text{C}$  NMR spectrum of compound **9** in  $\text{CD}_3\text{OD}$ .

**Figure S41.** ESI-MS spectrum of compound **9**.

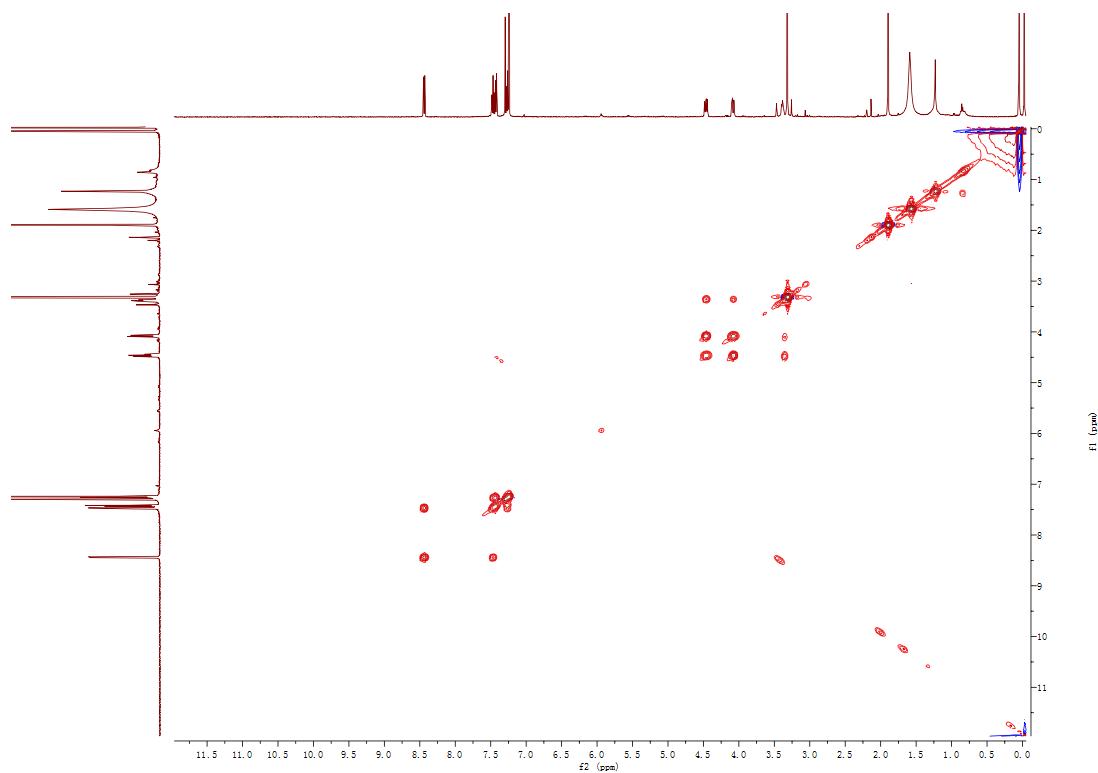
**Figure S42.**  $^1\text{H}$  NMR spectrum of compound **10** in  $\text{CD}_3\text{OD}$ .

**Figure S43.**  $^{13}\text{C}$  NMR spectrum of compound **10** in  $\text{CD}_3\text{OD}$ .

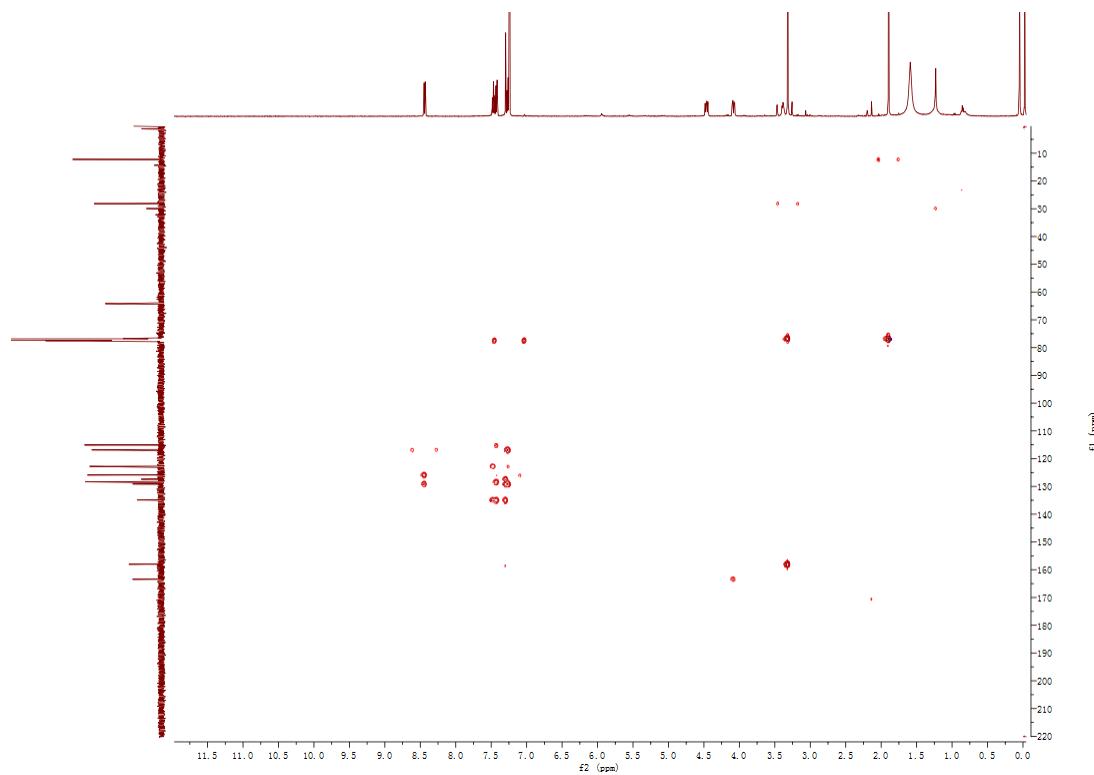
**Figure S44.** ESI-MS spectrum of compound **10**.**Figure S45.**  $^1\text{H}$  NMR spectrum of compound **11** in  $\text{DMSO}-d_6$ .**Figure S46.**  $^{13}\text{C}$  NMR spectrum of compound **11** in  $\text{CDCl}_3$ .**Figure S47.** ESI-MS spectrum of compound **11**.**Figure S1.**  $^1\text{H}$  NMR spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .**Figure S2.**  $^{13}\text{C}$  NMR and DEPT135 spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .



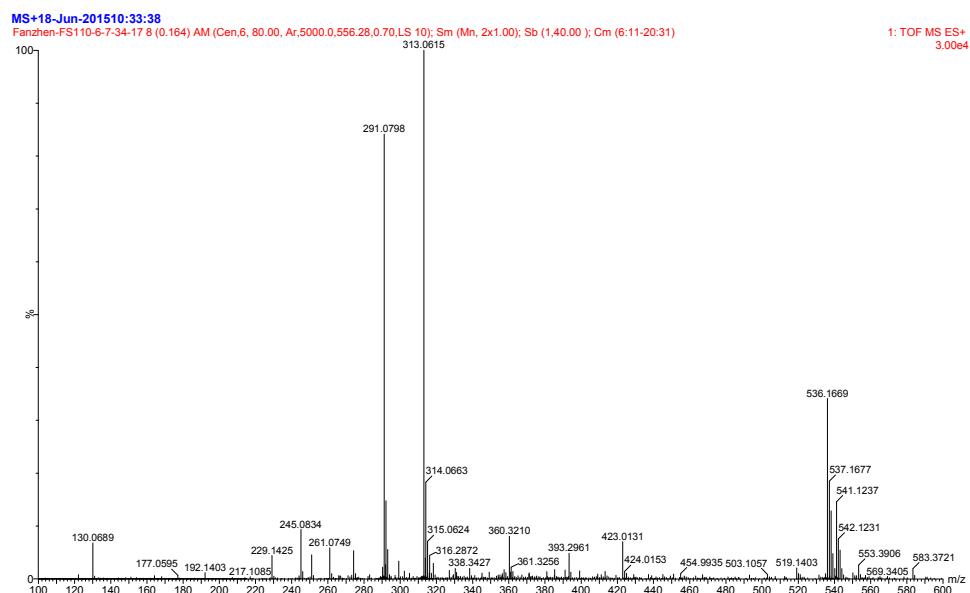
**Figure S3.** HSQC spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .



**Figure S4.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of dichotocejpin A (**1**) in  $\text{CDCl}_3$ .



**Figure S5.** HMBC spectrum of dichotocejpin A (1) in  $\text{CDCl}_3$ .



**Figure S6.** HRESIMS spectrum of dichotocejpin A (1).

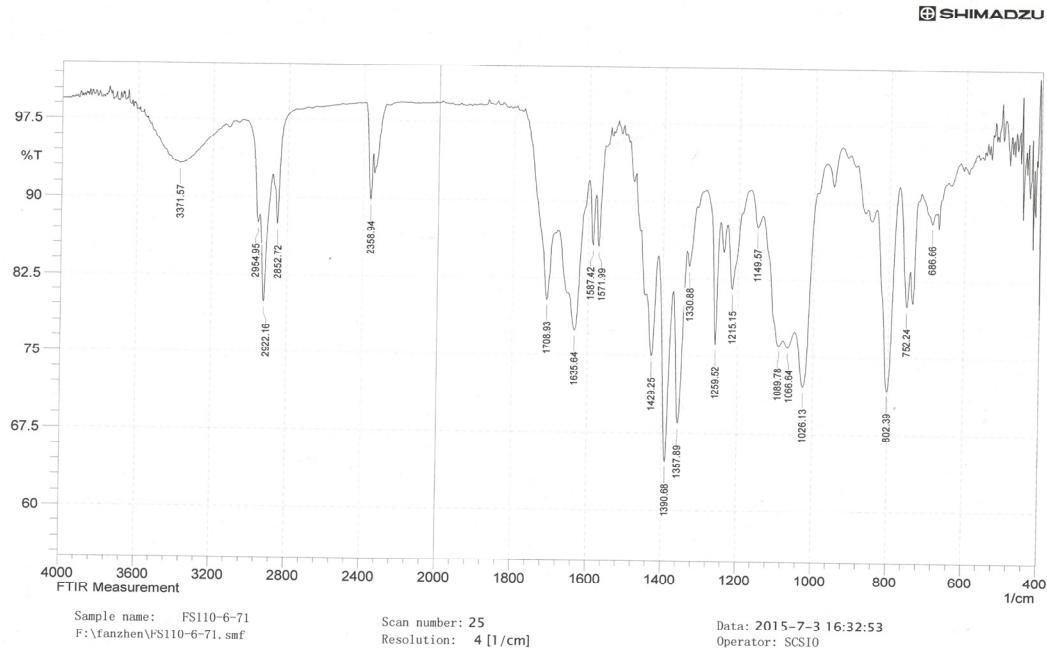
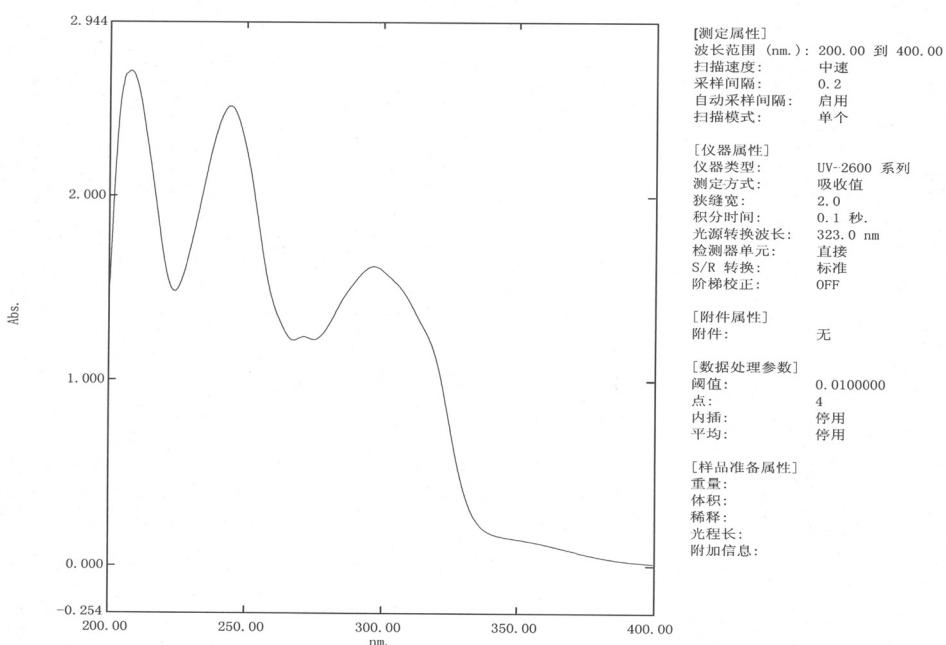


Figure S7. IR spectrum of dichotocejpin A (1).

## 光谱峰值检测报告

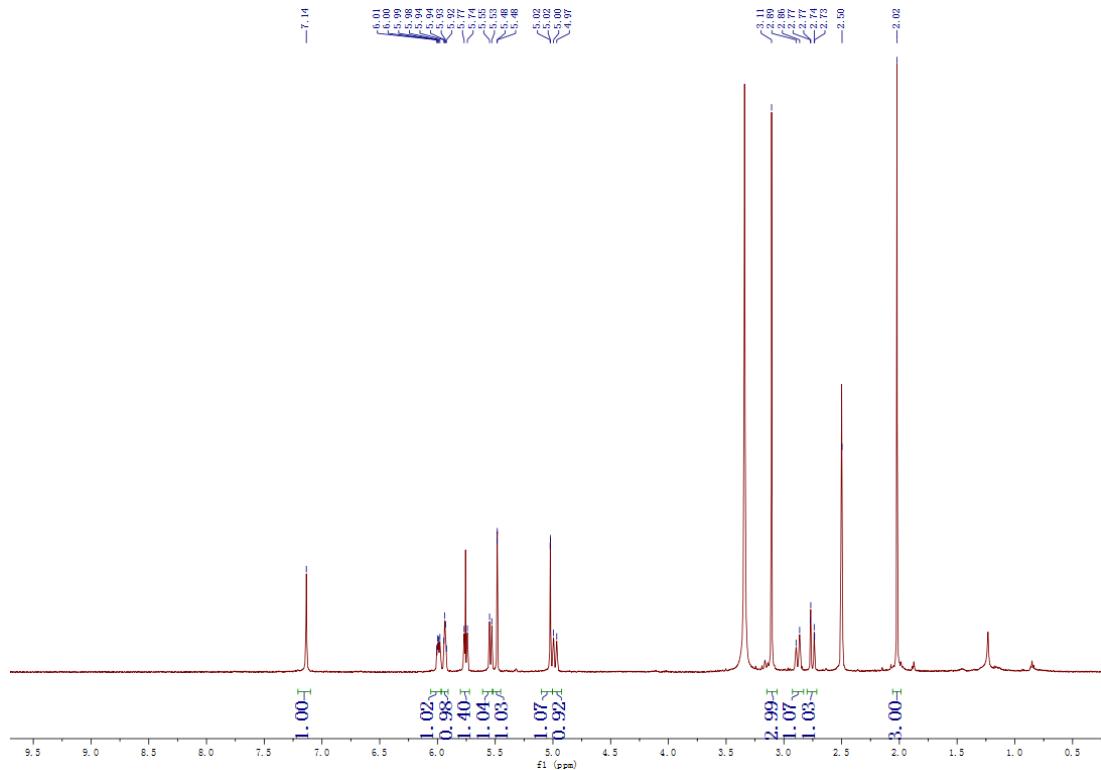
2015-07-03 14:56:30

数据集: FS110-6-7-2 - RawData

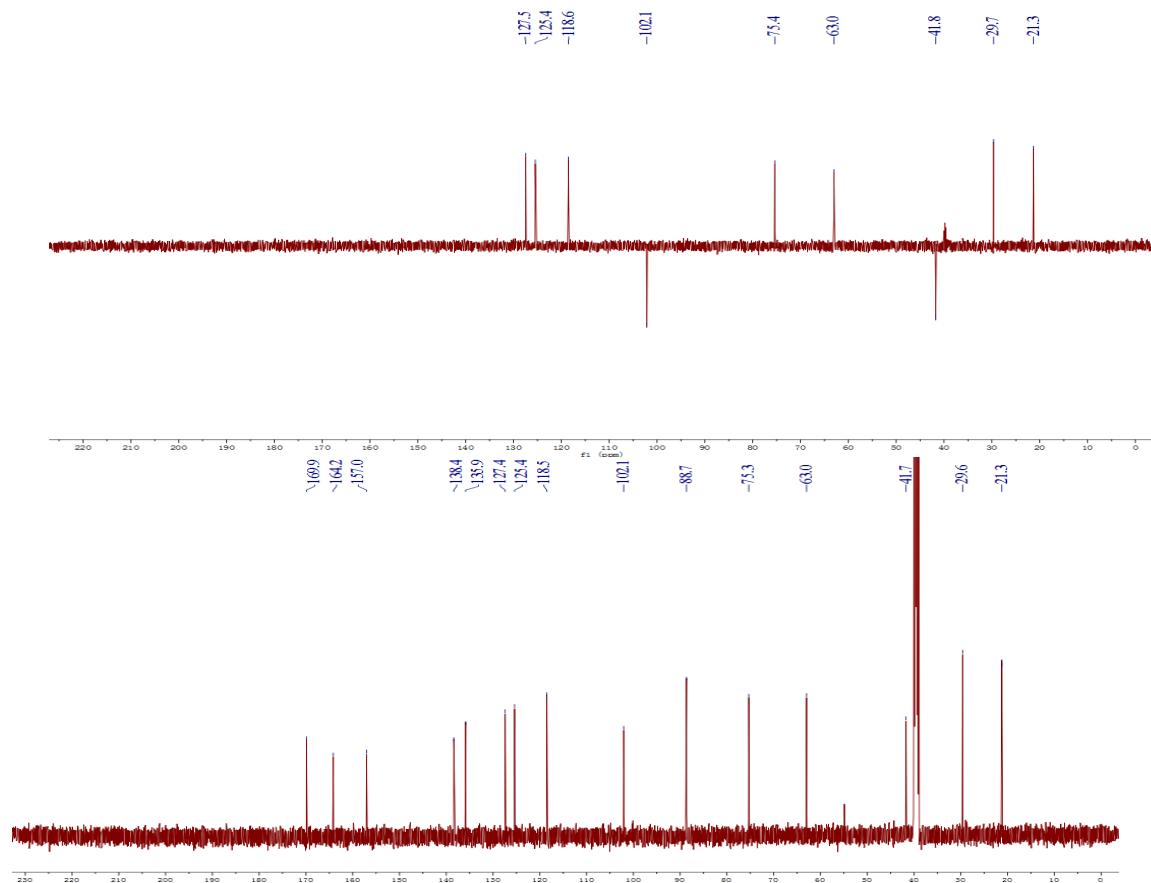


No.	P/V	波长(nm)	吸收值	描述
1	●	296.60	1.620	
2	●	271.40	1.237	
3	●	244.40	2.488	
4	●	207.80	2.677	
5	●	275.00	1.222	
6	●	267.60	1.219	
7	●	224.20	1.484	

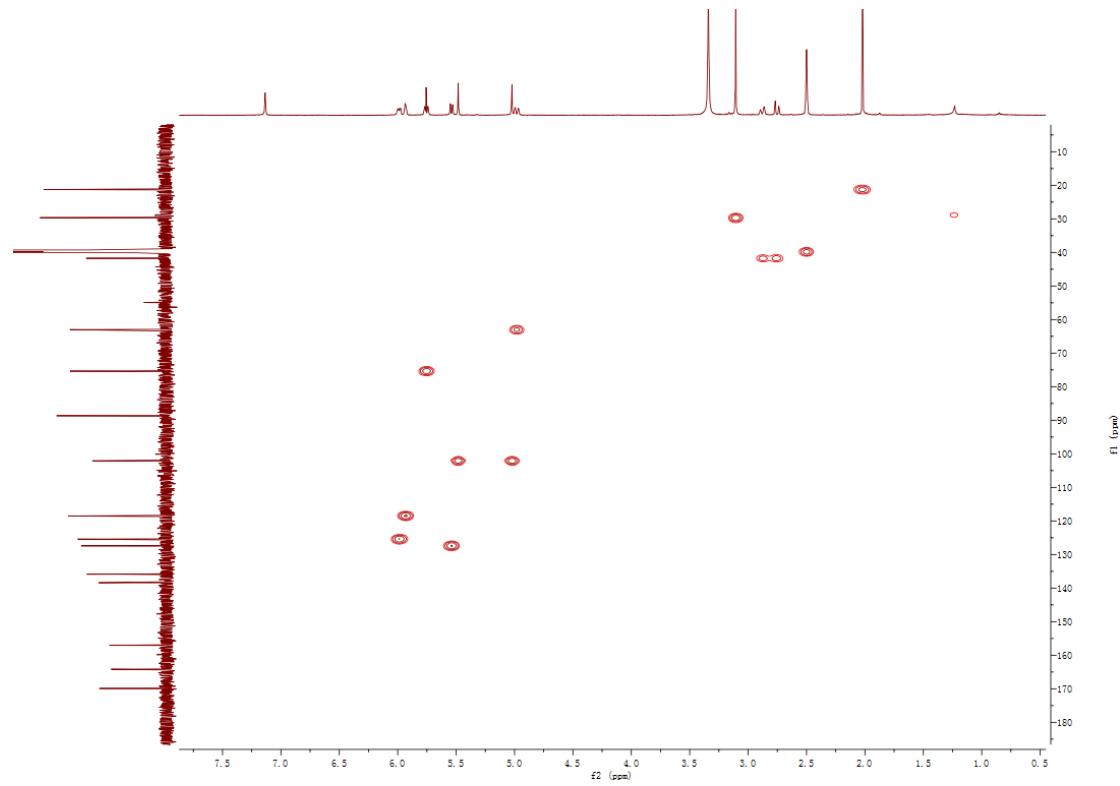
Figure S8. UV spectrum of dichotocejpin A (1).



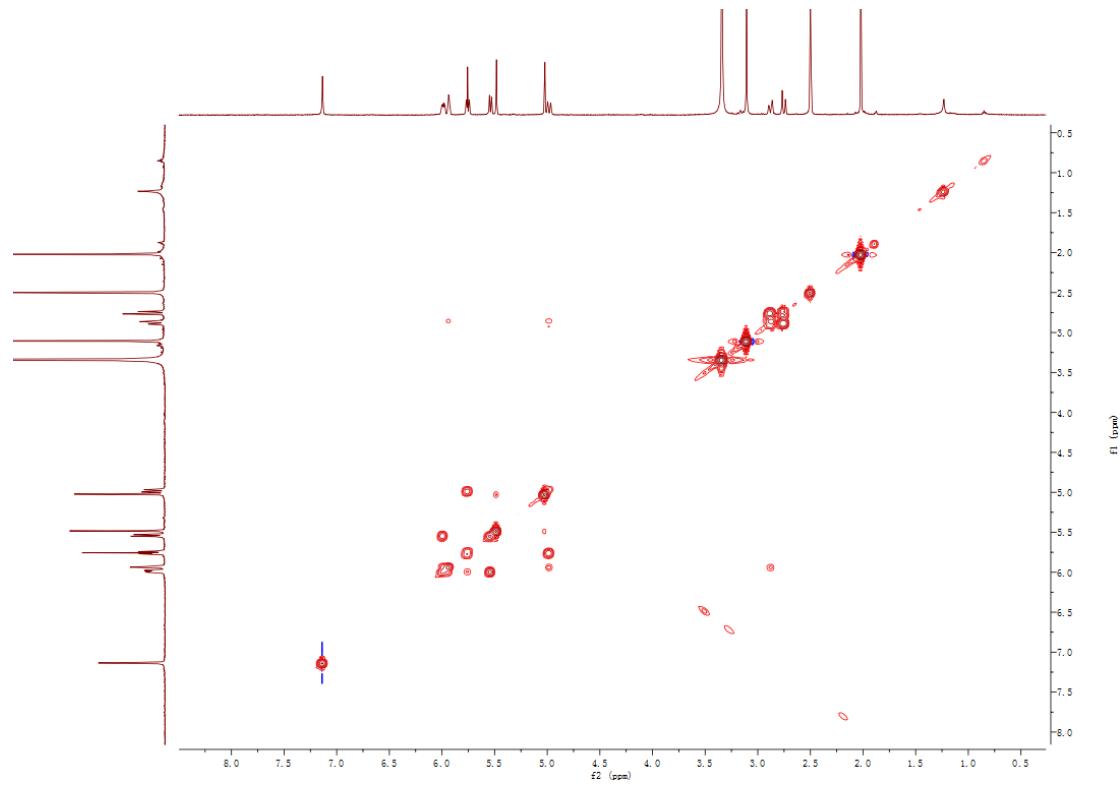
**Figure S9.**  $^1\text{H}$  NMR spectrum of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .



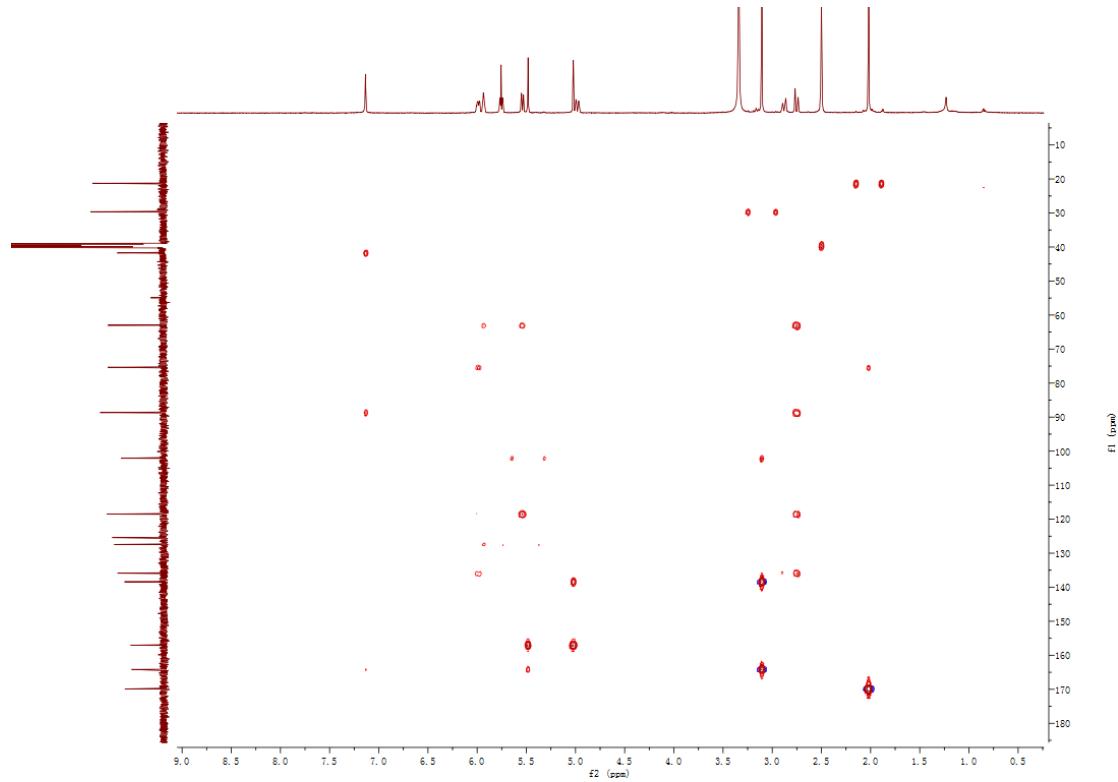
**Figure S10.**  $^{13}\text{C}$  NMR and DEPT135 spectra of dichotocejpin B (**2**) in  $\text{DMSO}-d_6$ .



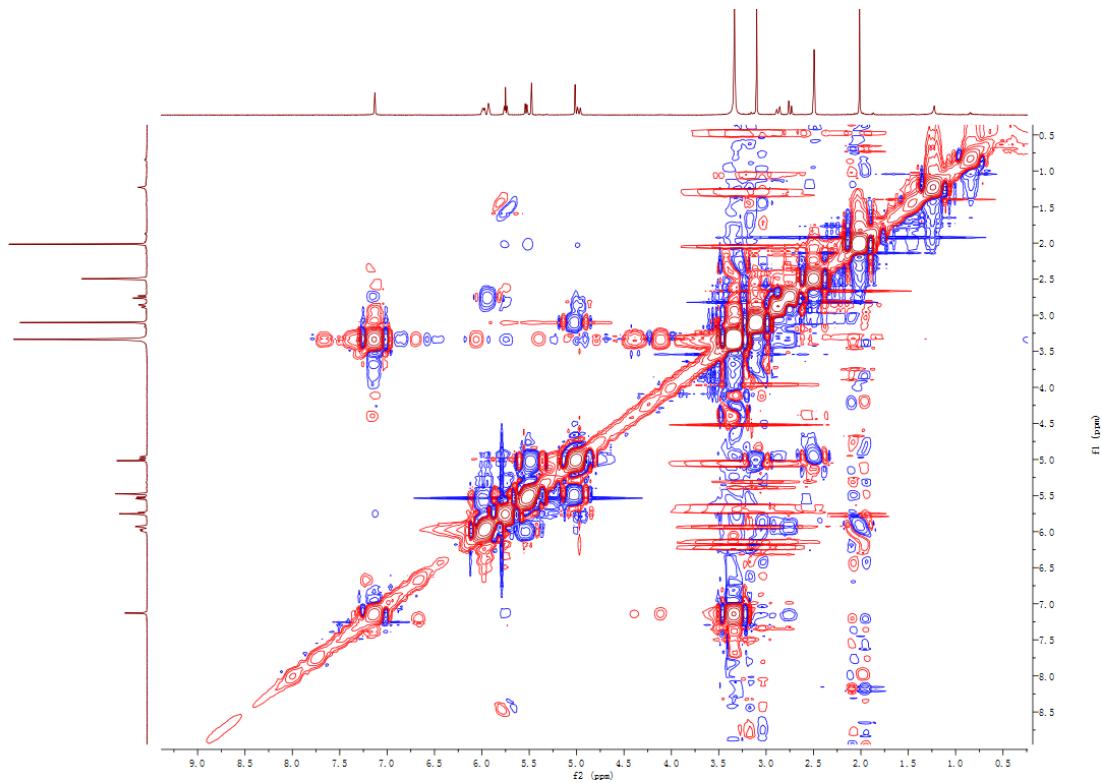
**Figure S11.** HSQC spectrum of dichotocejpin B (2) in  $\text{DMSO}-d_6$ .



**Figure S12.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of dichotocejpin B (2) in  $\text{DMSO}-d_6$ .



**Figure S13.** HMBC spectrum of dichotocejpin B (2) in  $\text{DMSO}-d_6$ .



**Figure S14.** NOESY spectrum of dichotocejpin B (2) in  $\text{DMSO}-d_6$ .

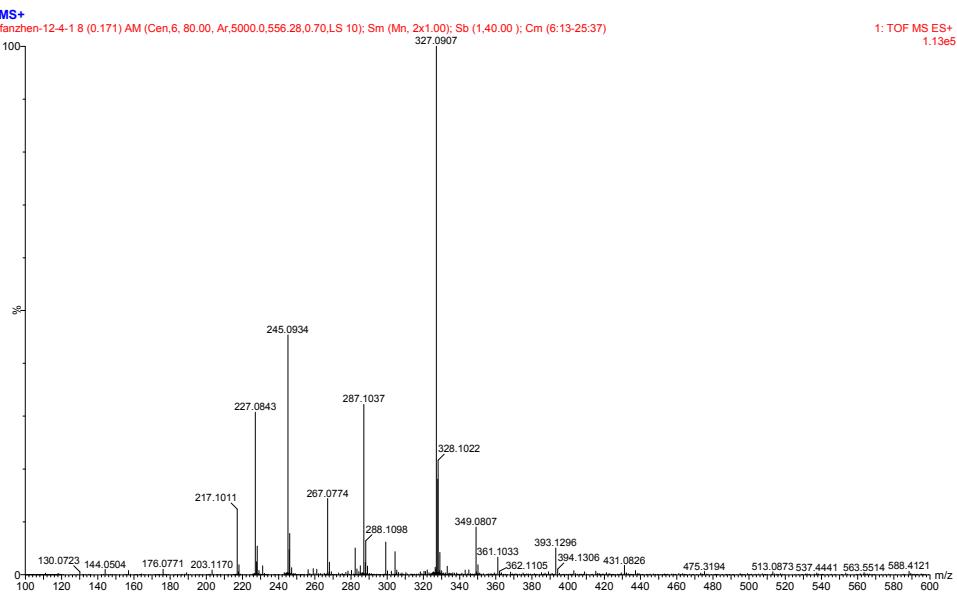


Figure S15. HRESIMS spectrum of dichotocejpin B (2).

SHIMADZU

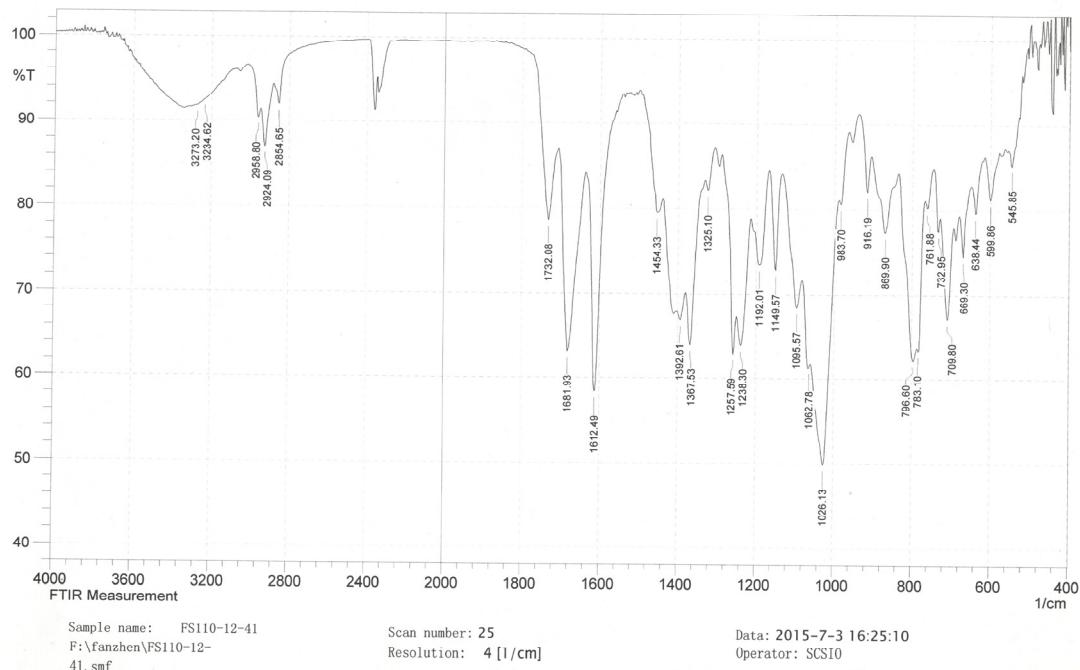


Figure S16. IR spectrum of dichotocejpin A (2).

## 光谱峰值检测报告

2015-07-03 15:12:08

数据集: FS110-12-4 - RawData

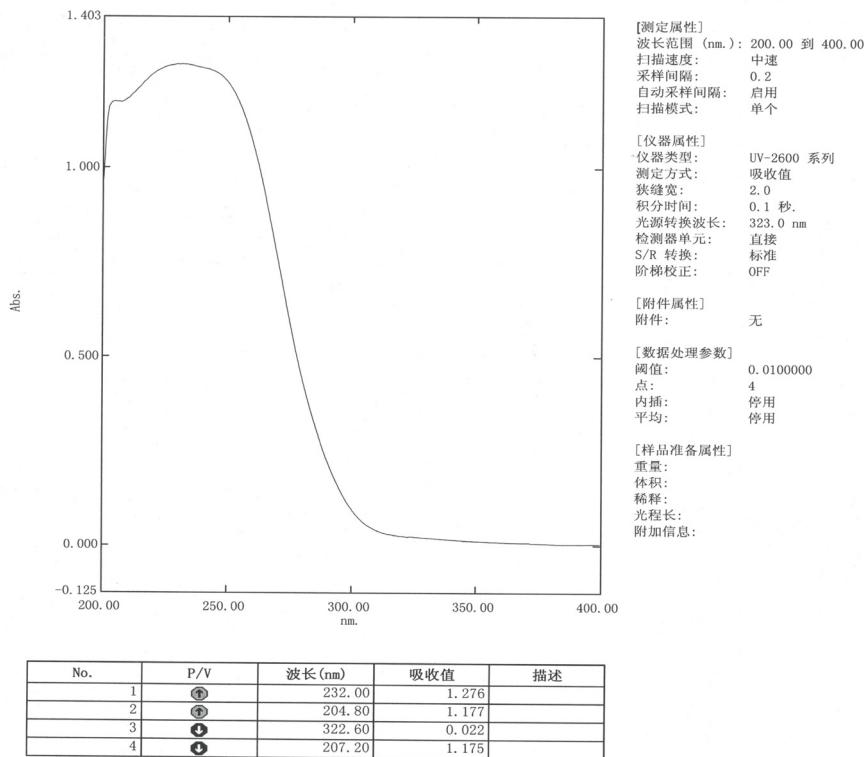
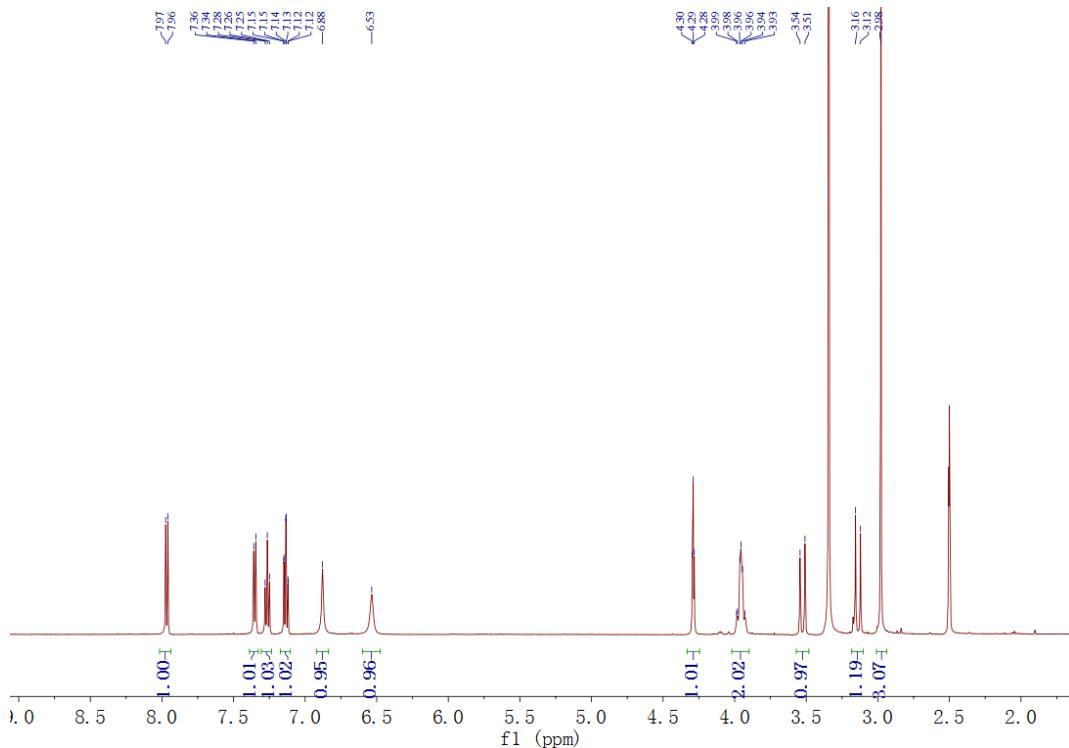
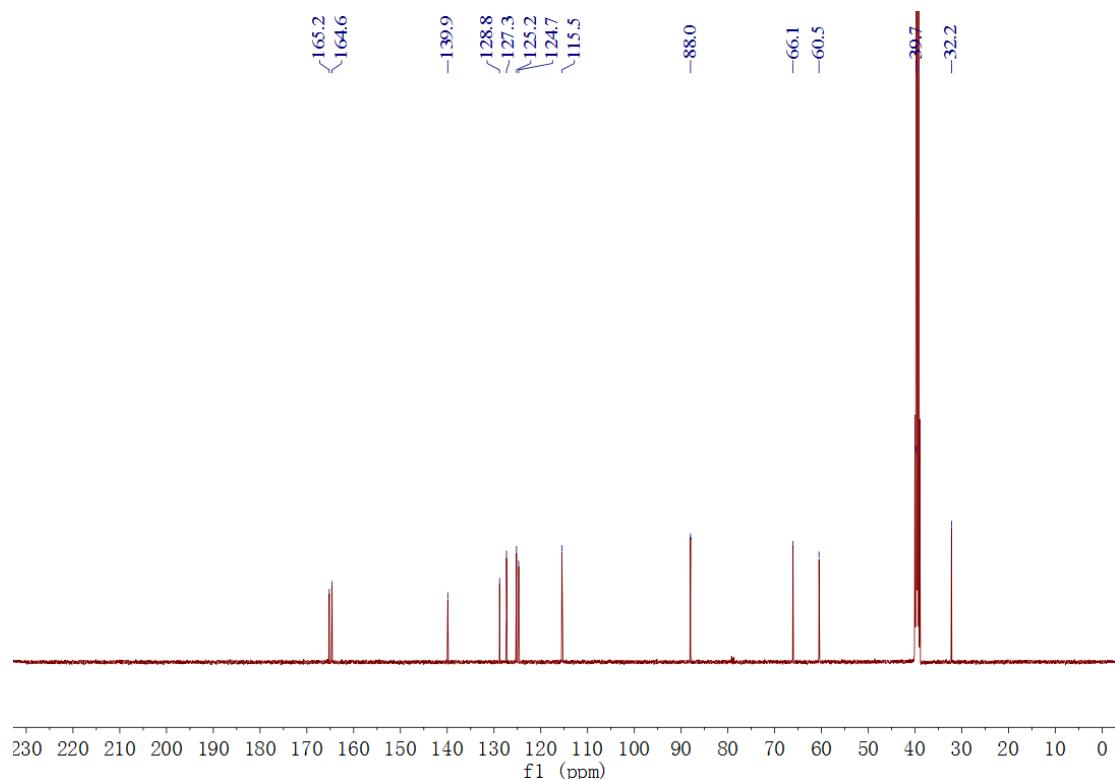
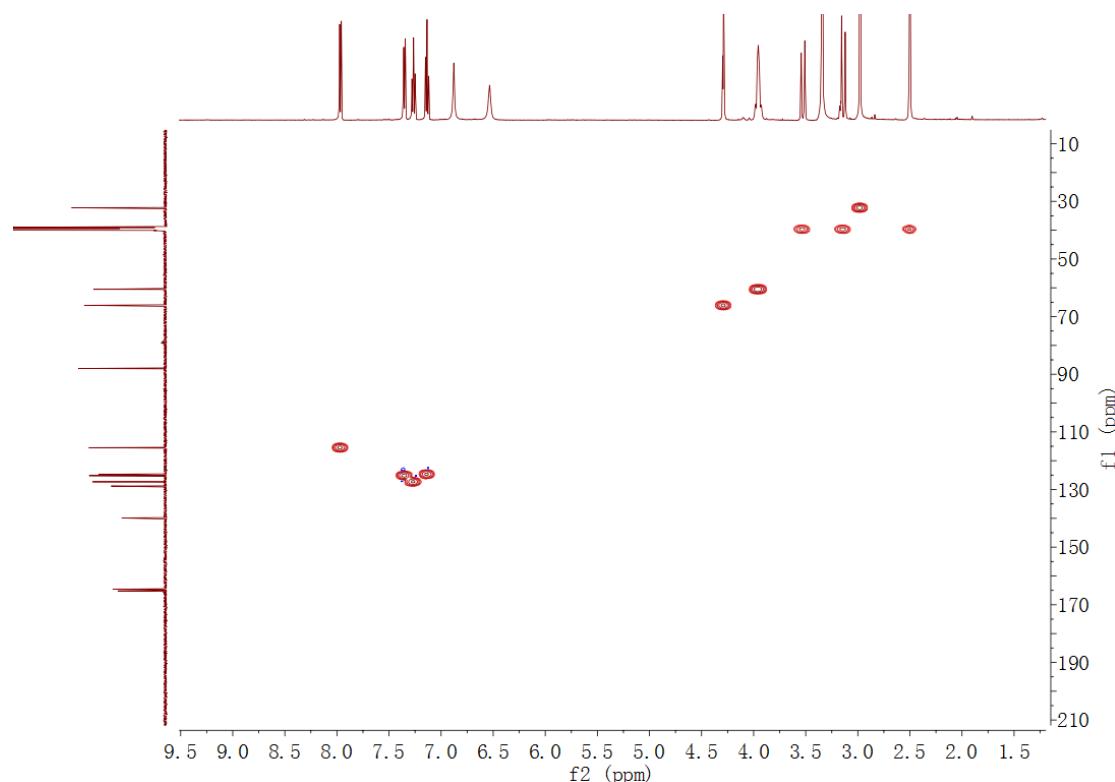


Figure S17. UV spectrum of dichotocejpin A (2).

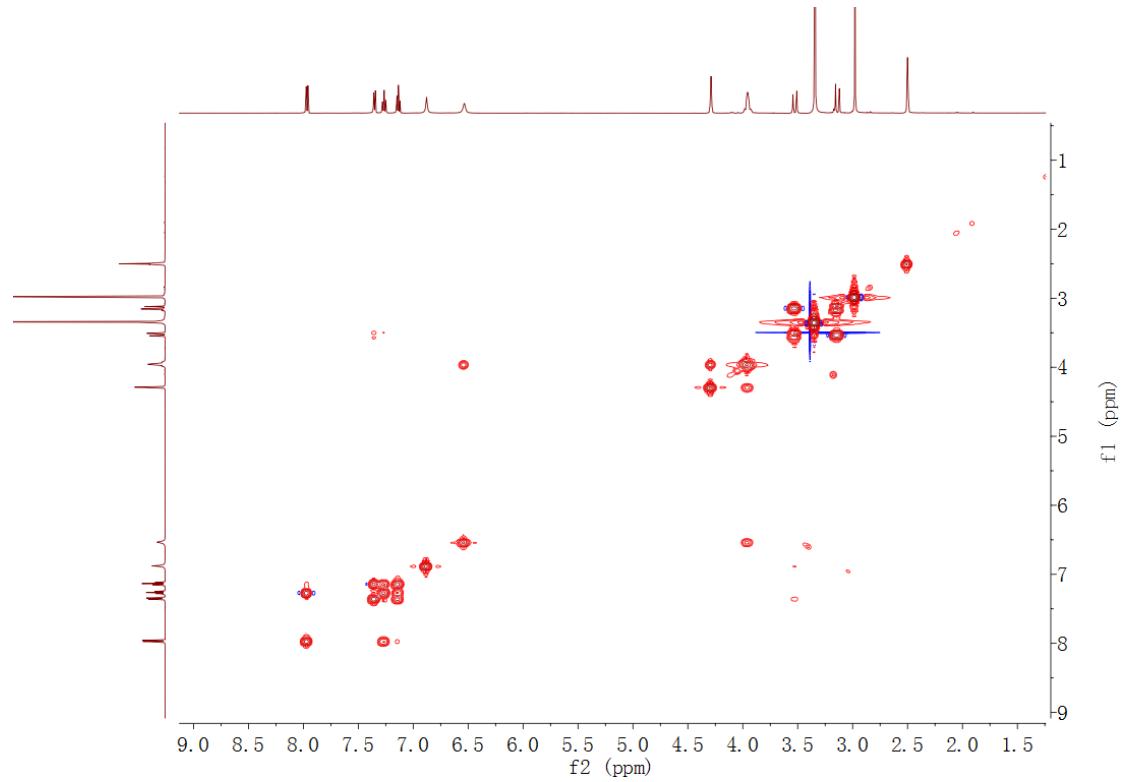




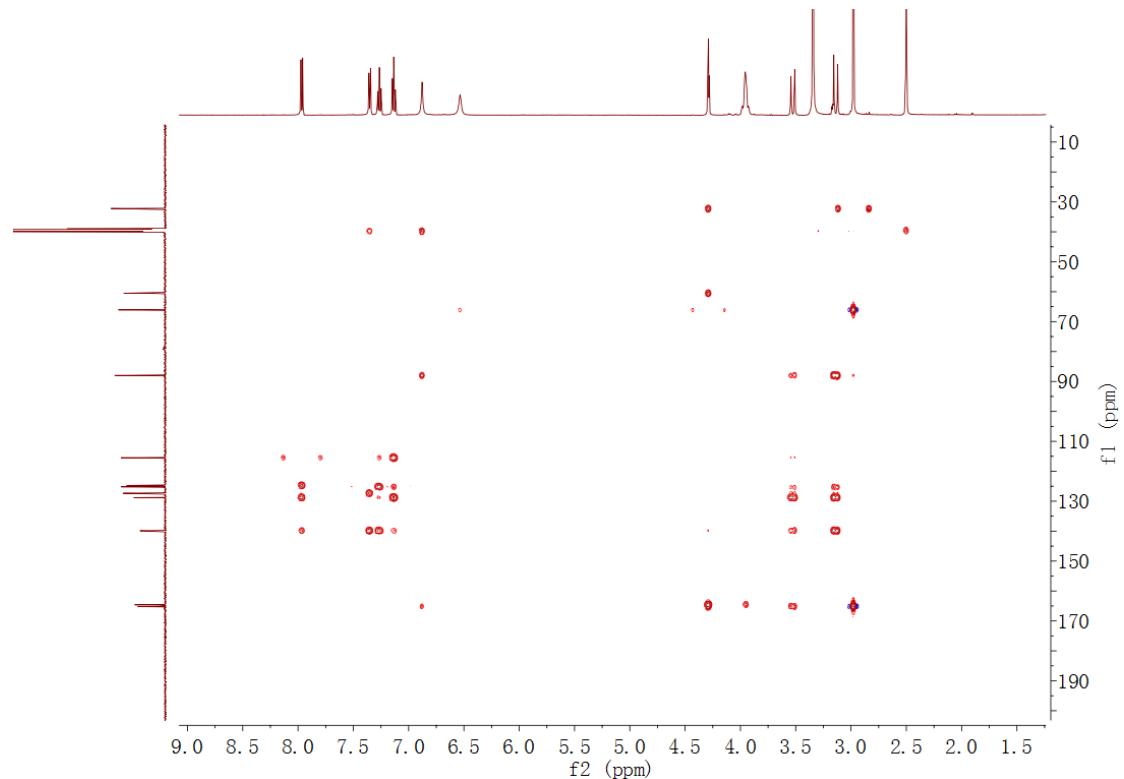
**Figure S19.**  $^{13}\text{C}$  NMR spectra of dichotocejpin C (3) in  $\text{DMSO}-d_6$ .



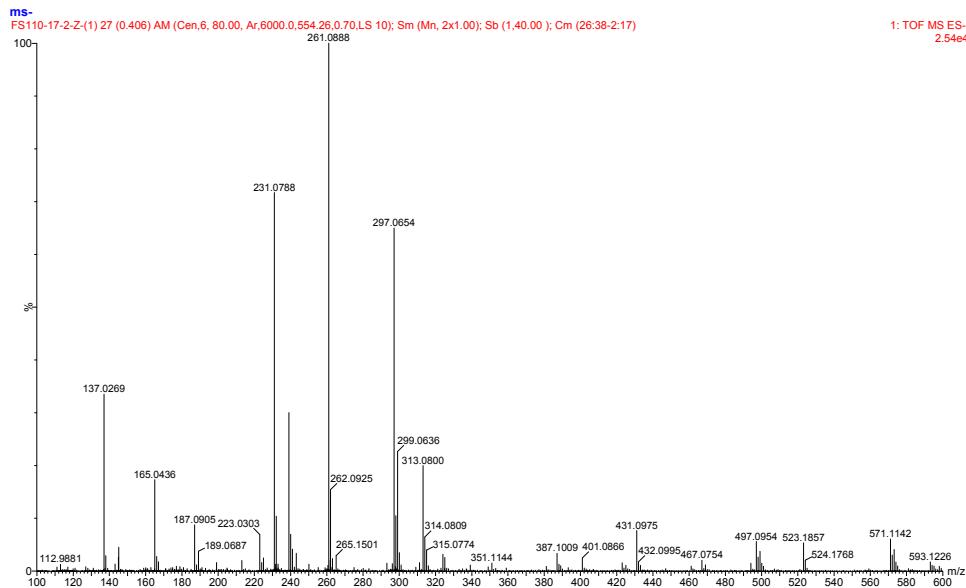
**Figure S20.** HSQC spectrum of dichotocejpin C (3) in  $\text{DMSO}-d_6$ .



**Figure S21.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of dichotocejpin C (3) in  $\text{DMSO}-d_6$ .

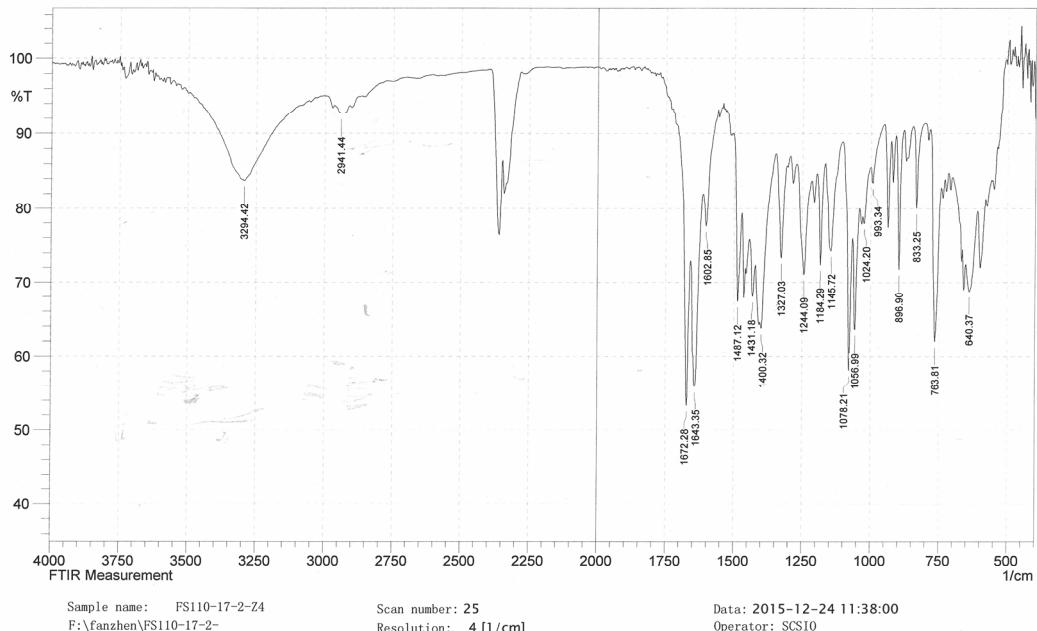


**Figure S22.** HMBC spectrum of dichotocejpin C (3) in  $\text{DMSO}-d_6$ .



**Figure S23.** HRESIMS spectrum of dichotocejpin C (3).

SHIMADZU



**Figure S24.** IR spectrum of dichotocejpin A (3).

## 光谱峰值检测报告

2015-12-24 09:56:58

数据集: FS110-17-2-Z 25ug - RawData

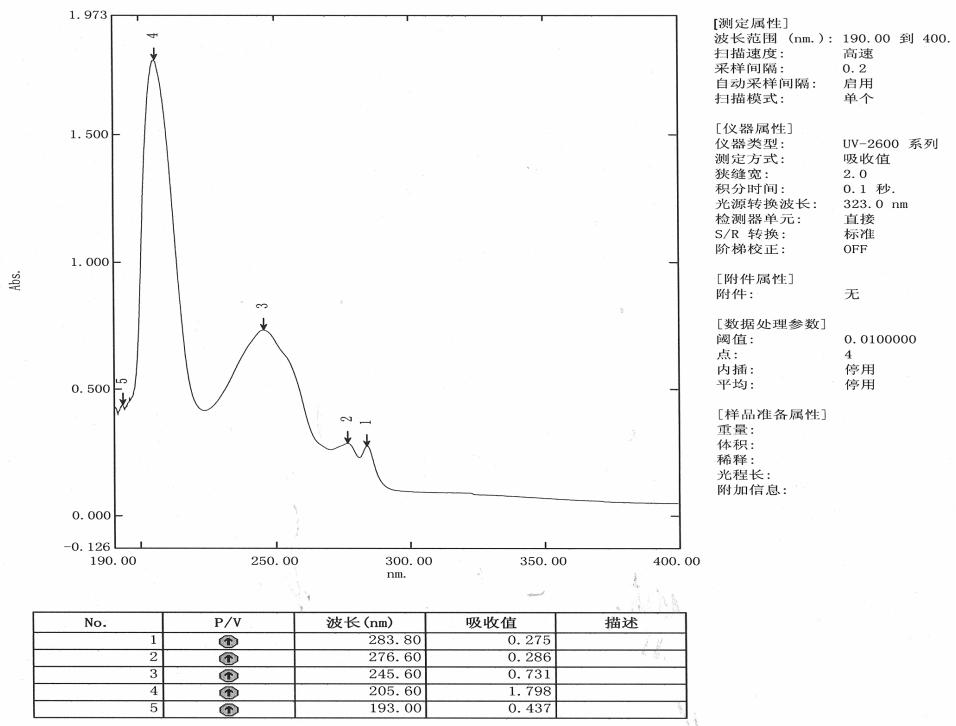
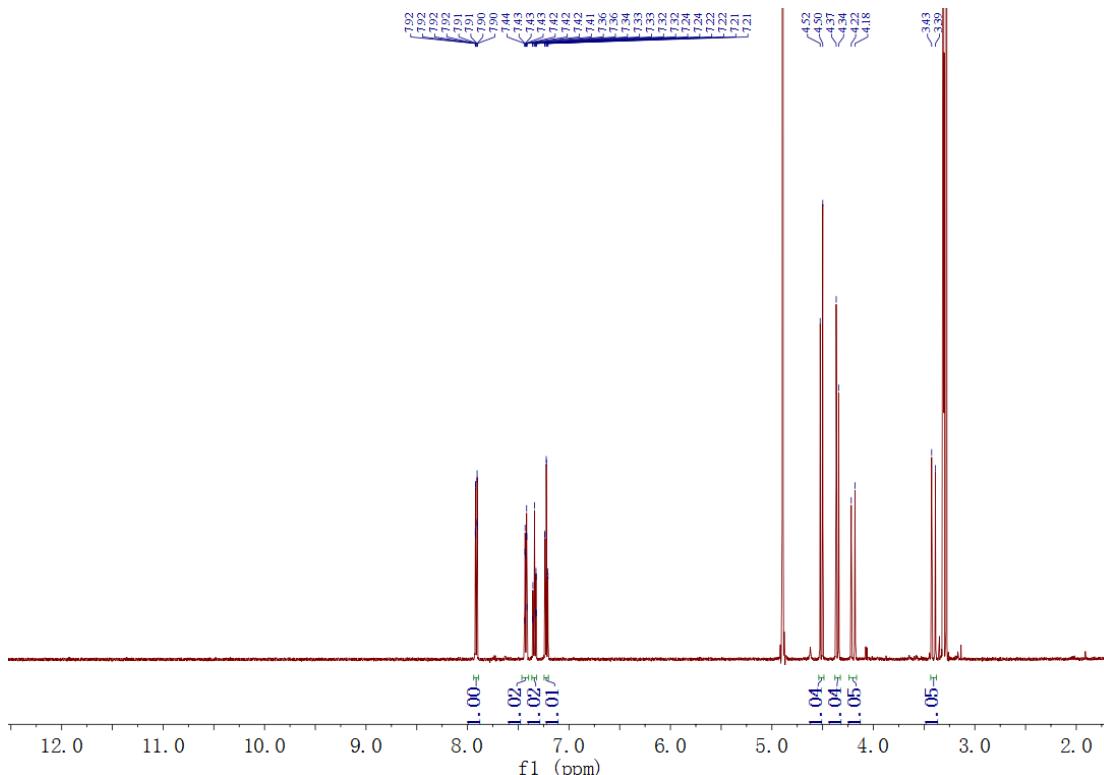


Figure S25. UV spectrum of dichotocejpin A (3).

Figure S26.  $^1\text{H}$  NMR spectrum of compound 4 in  $\text{CD}_3\text{OD}$ .

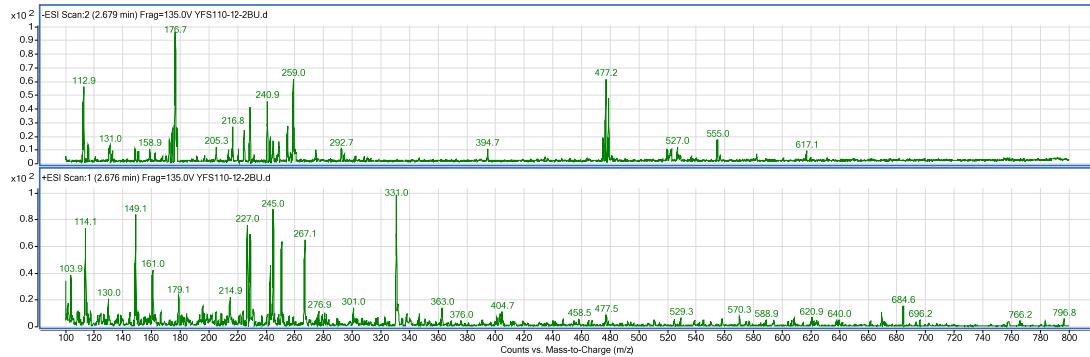
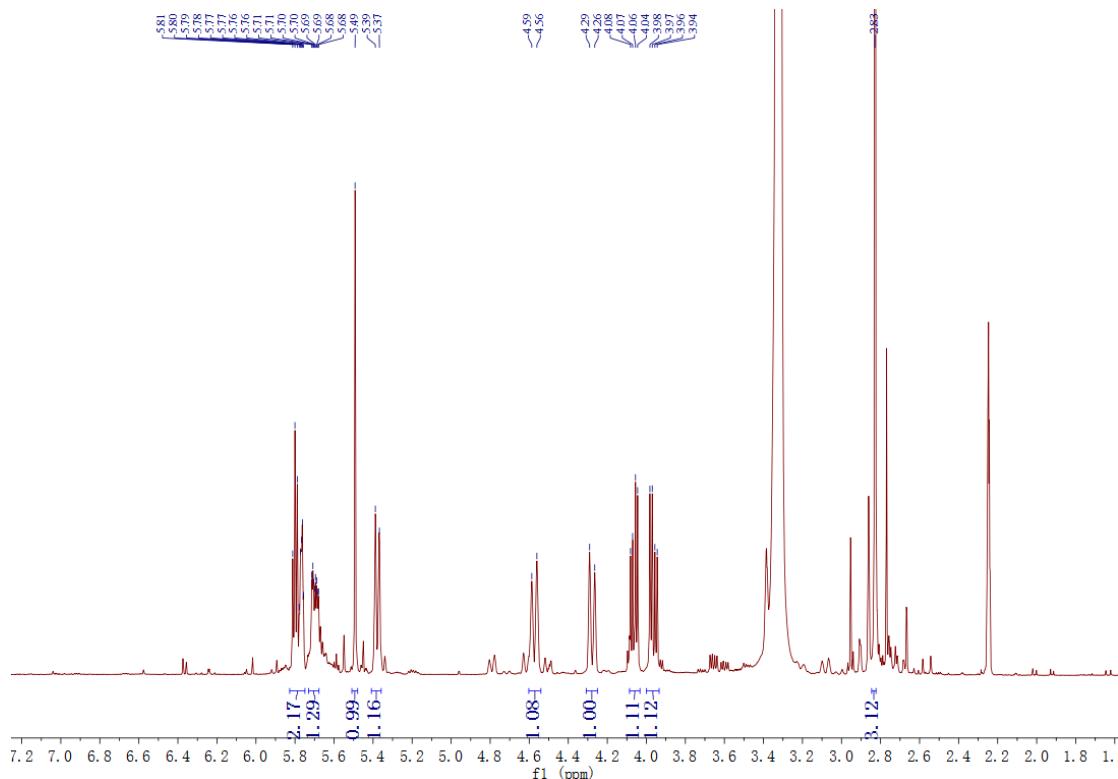
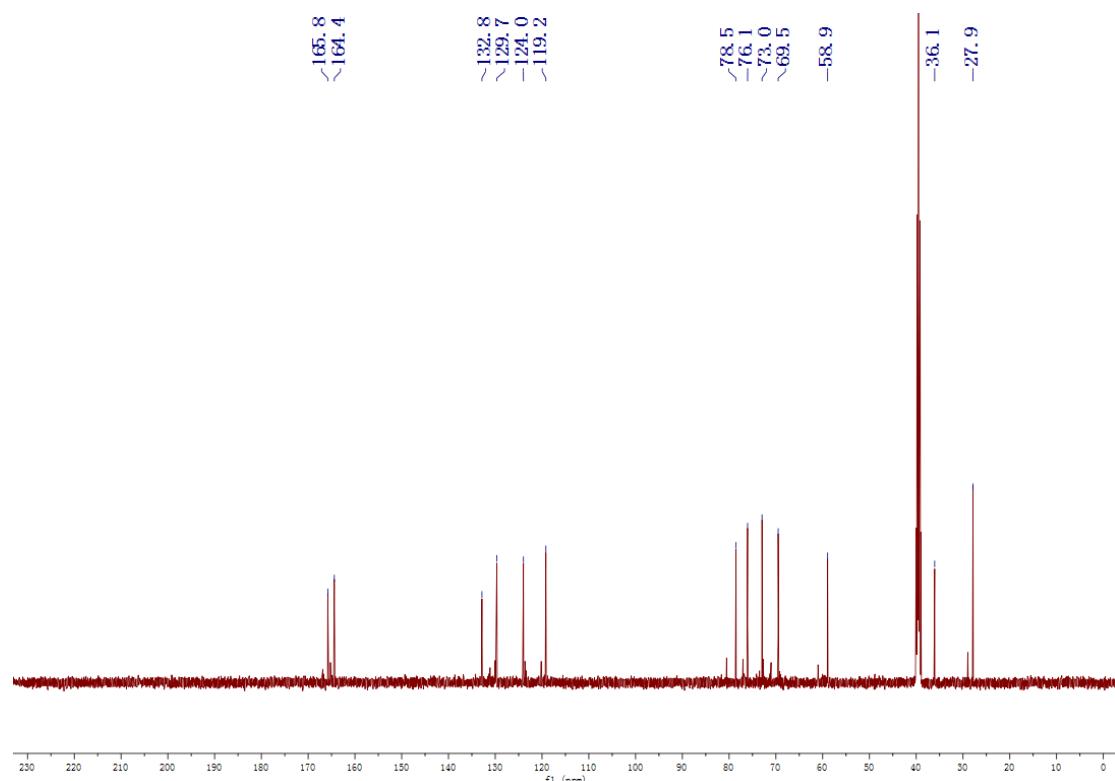
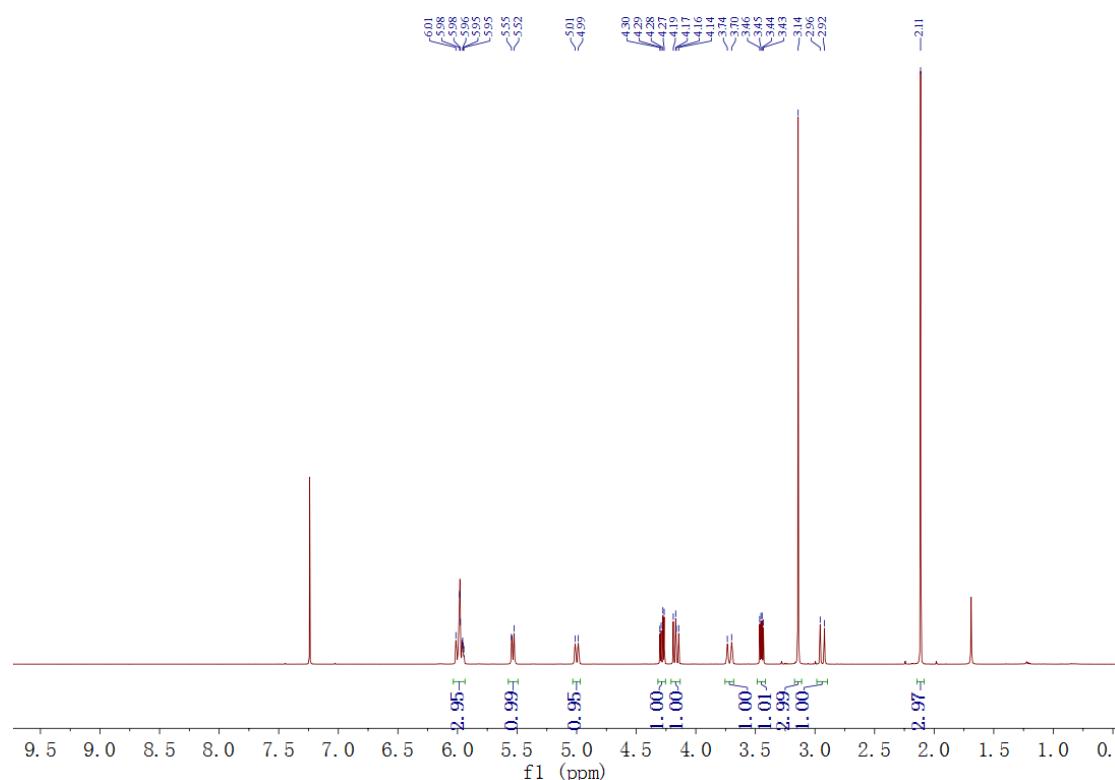
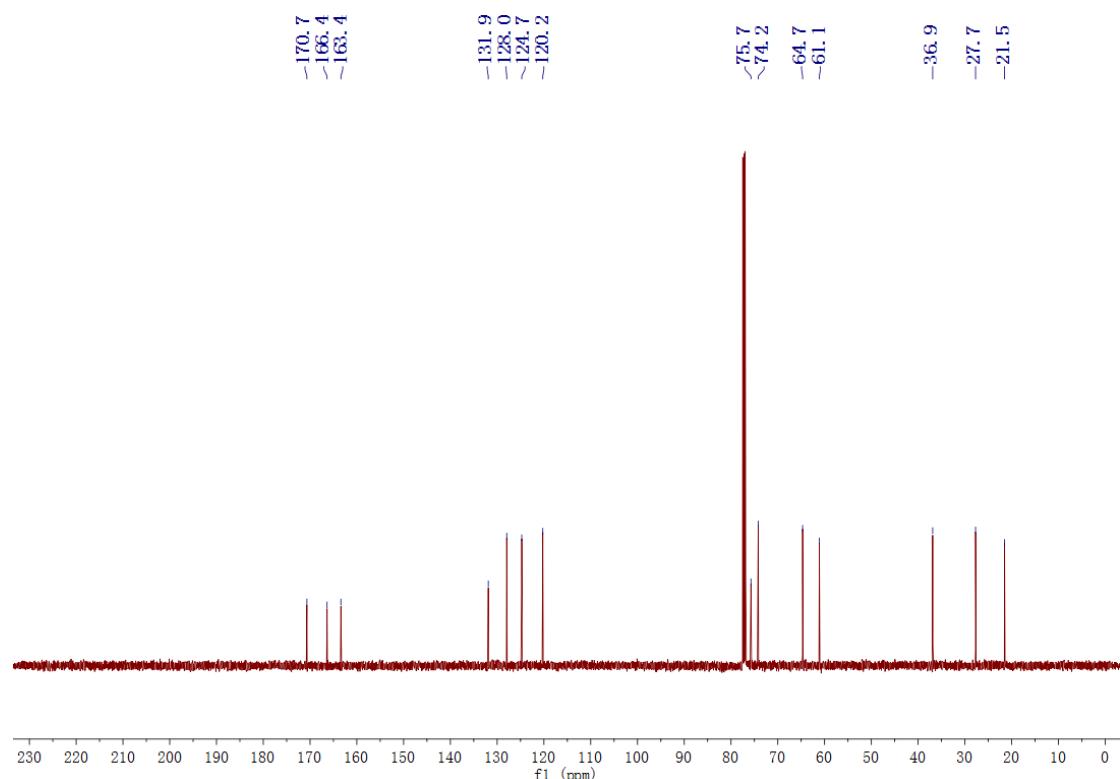


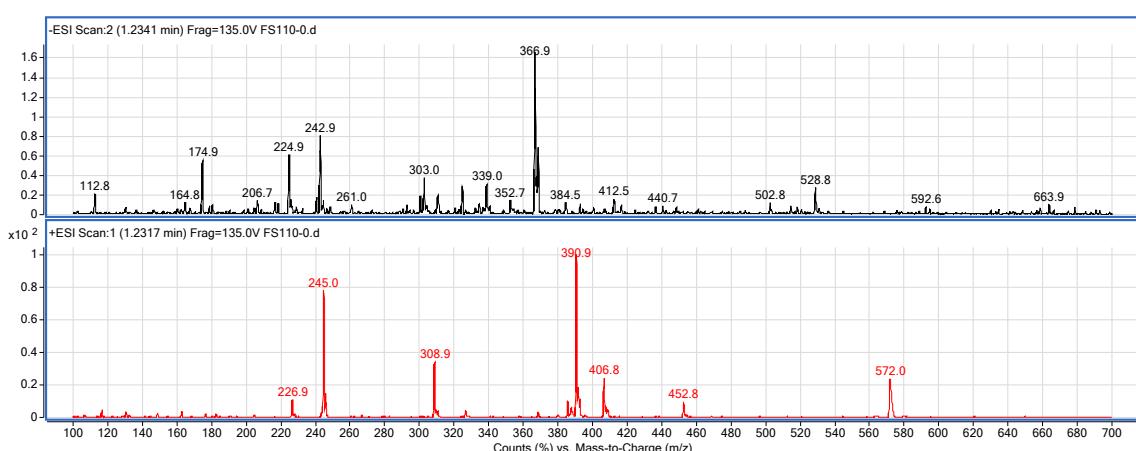
Figure S27. ESI-MS spectrum of compound 4.

Figure S28. <sup>1</sup>H NMR spectrum of compound 5 in CD<sub>3</sub>OD.

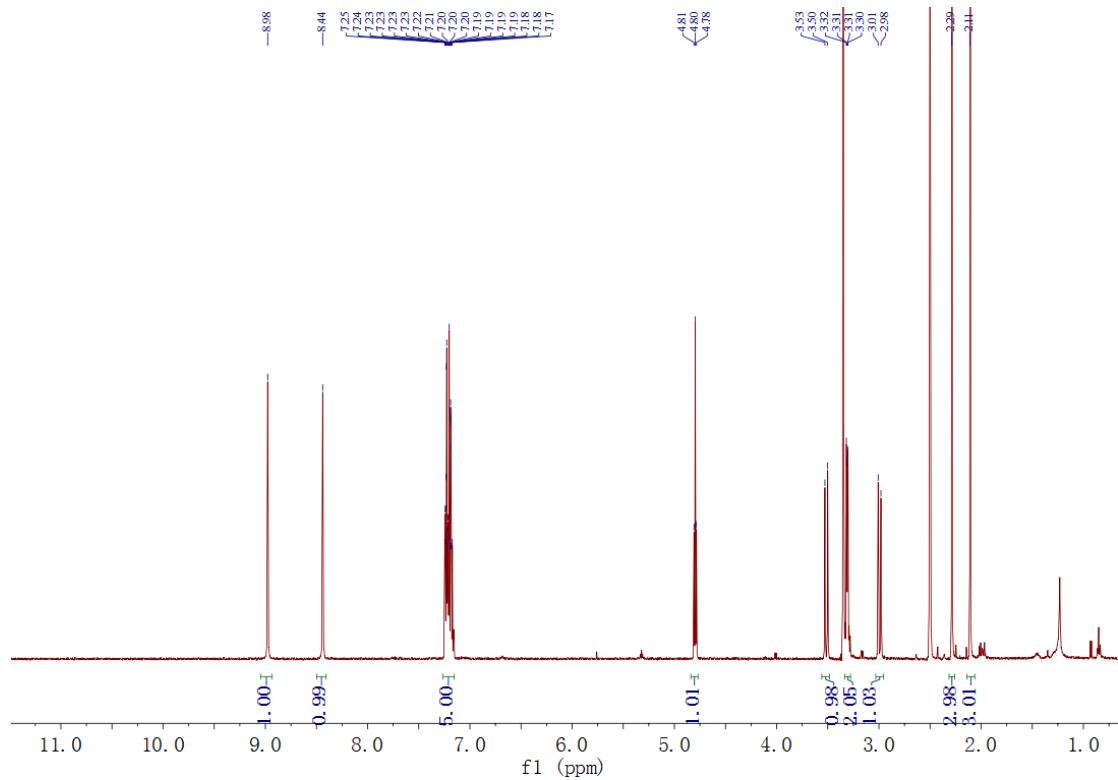
**Figure S29.**  $^{13}\text{C}$  NMR spectrum of compound 5 in  $\text{CD}_3\text{OD}$ .**Figure S30.**  $^1\text{H}$  NMR spectrum of compound 6 in  $\text{CDCl}_3$ .



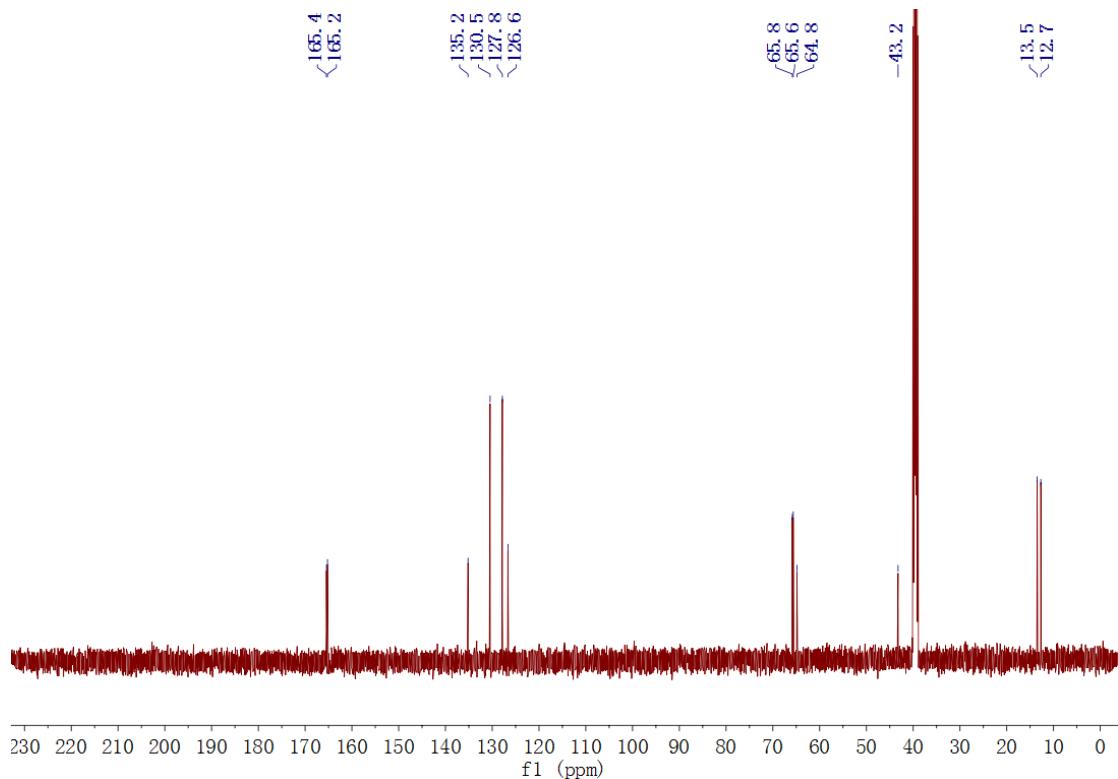
**Figure S31.** <sup>13</sup>C NMR spectrum of compound 6 in CDCl<sub>3</sub>.



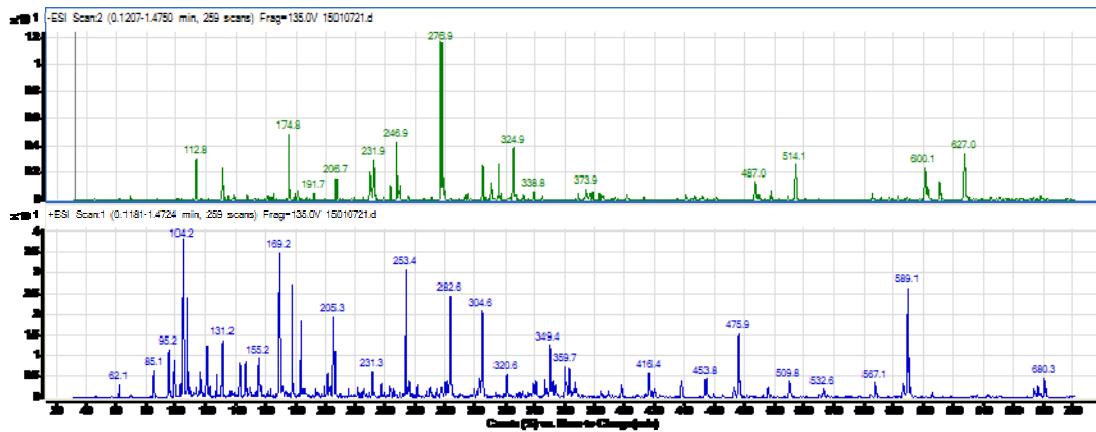
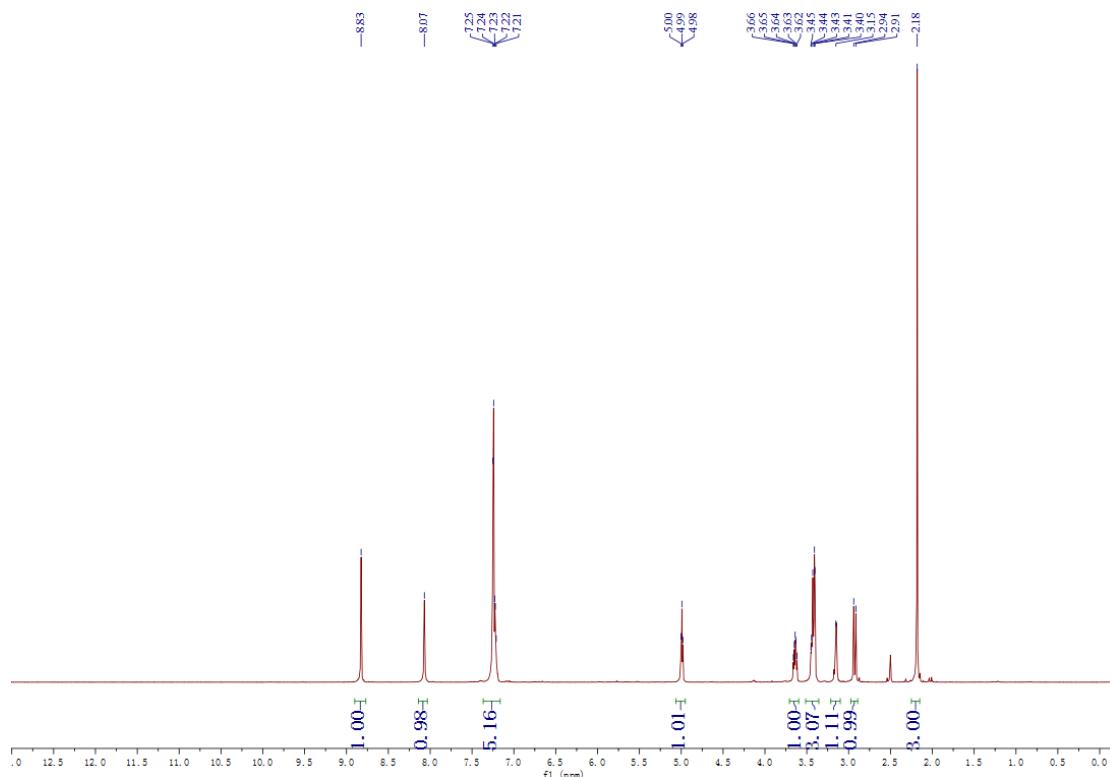
**Figure S32.** ESI-MS spectrum of compound 6.

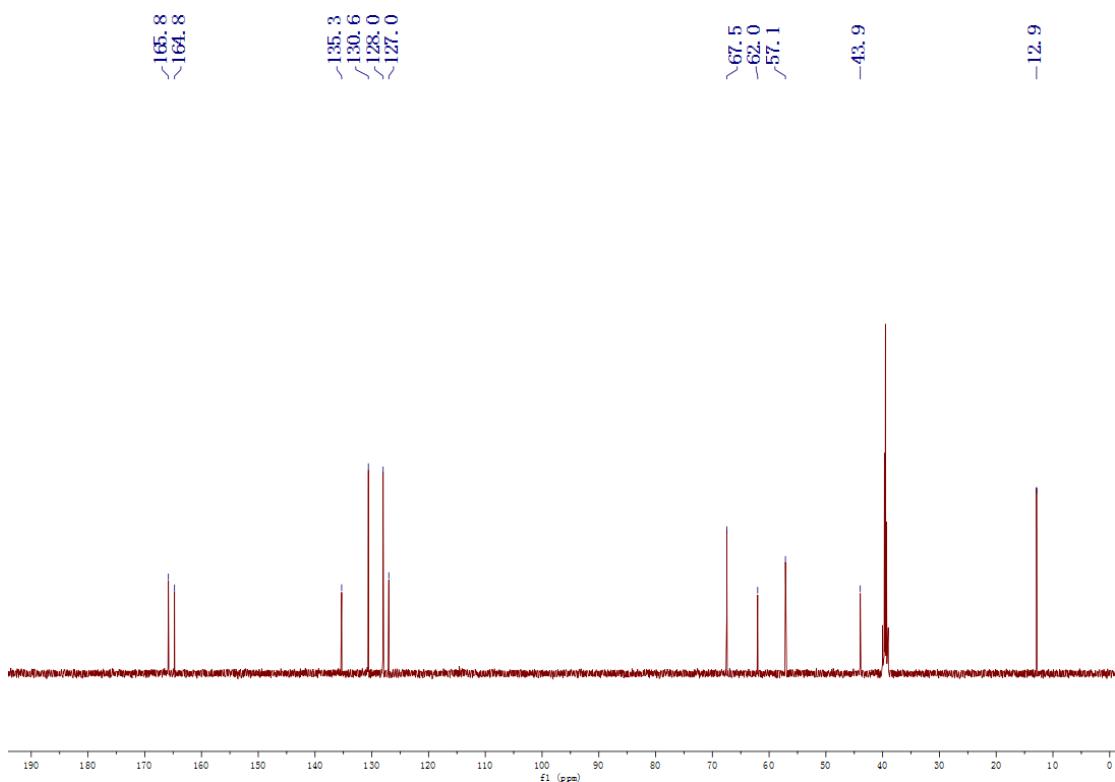


**Figure S33.**  $^1\text{H}$  NMR spectrum of compound 7 in  $\text{DMSO}-d_6$ .

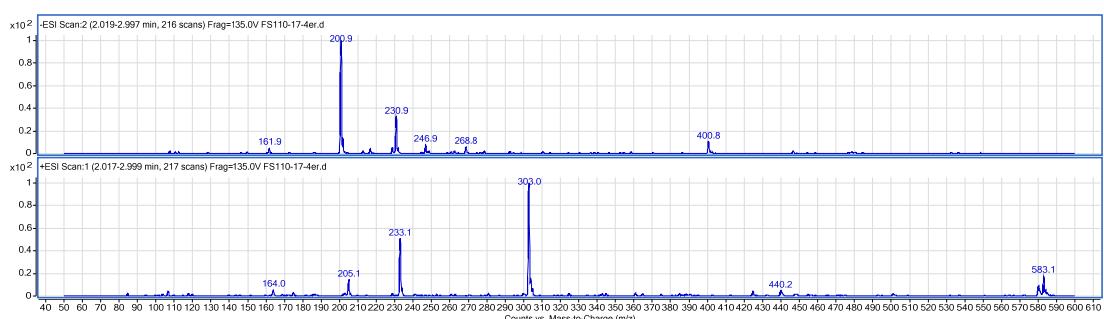


**Figure S34.**  $^{13}\text{C}$  NMR spectrum of compound 7 in  $\text{DMSO}-d_6$ .

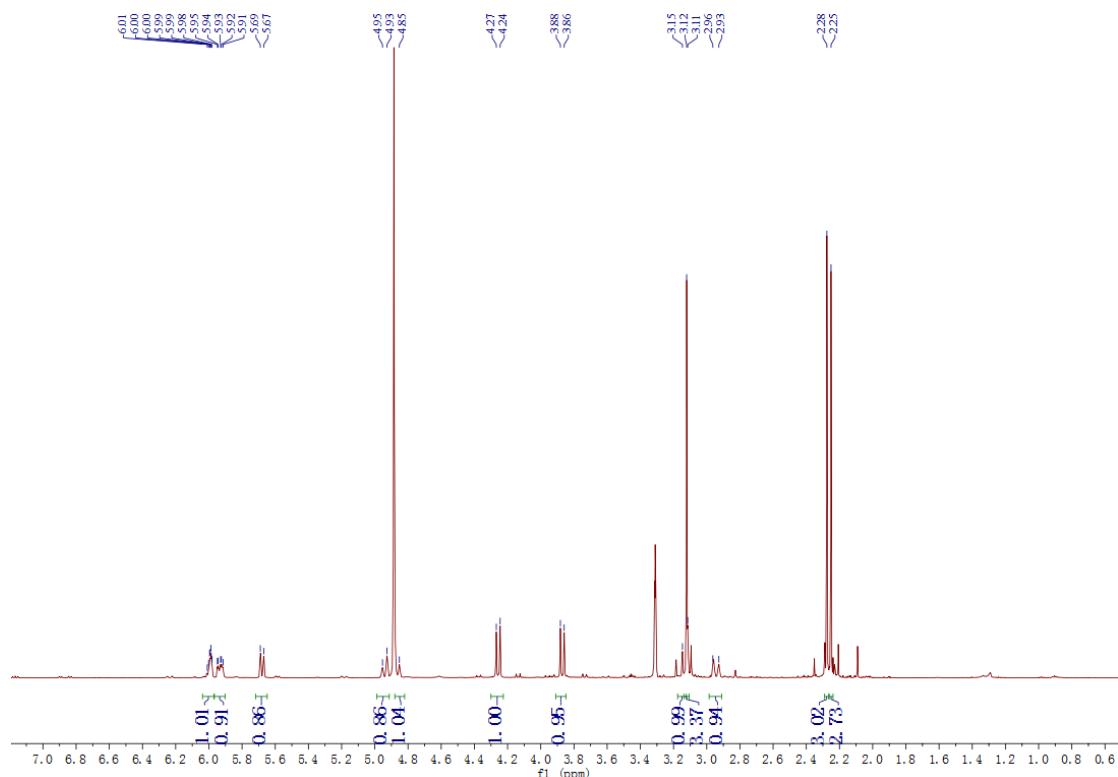
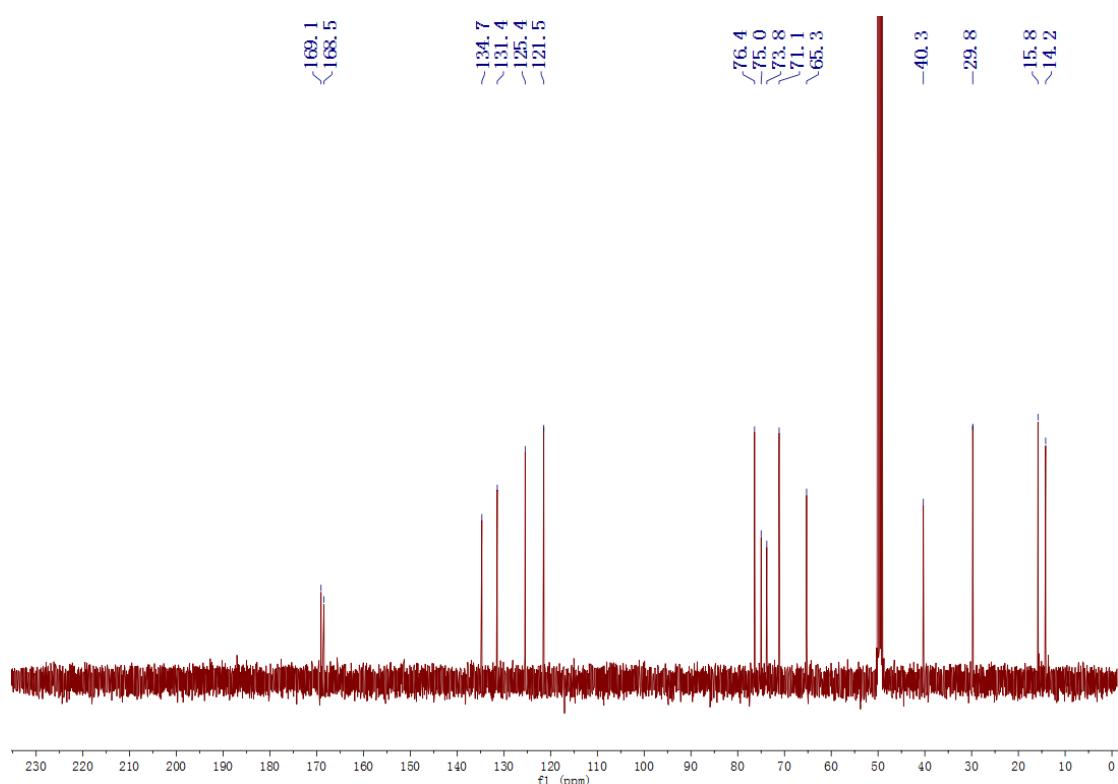
**Figure S35.** ESI-MS spectrum of compound 7.**Figure S36.** <sup>1</sup>H NMR spectrum of compound 8 in DMSO-*d*<sub>6</sub>.

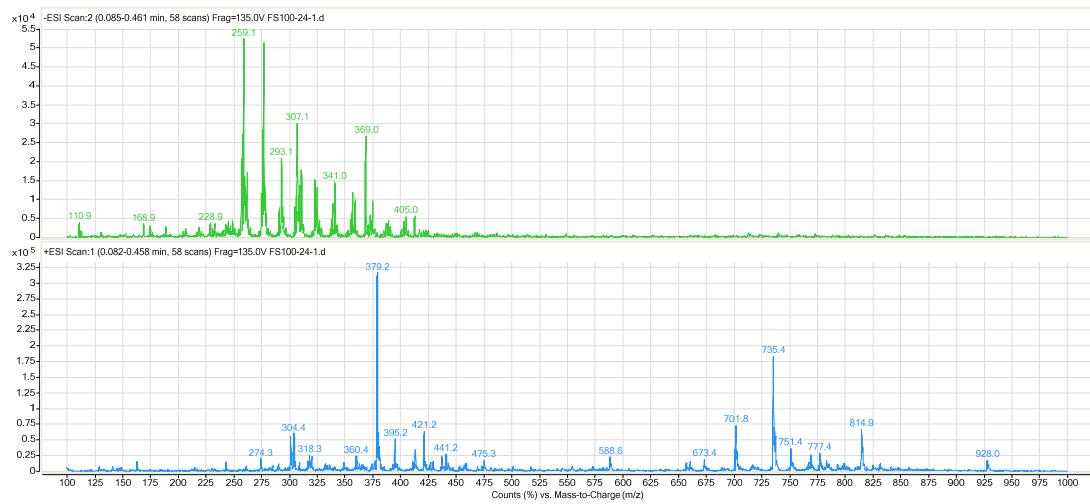
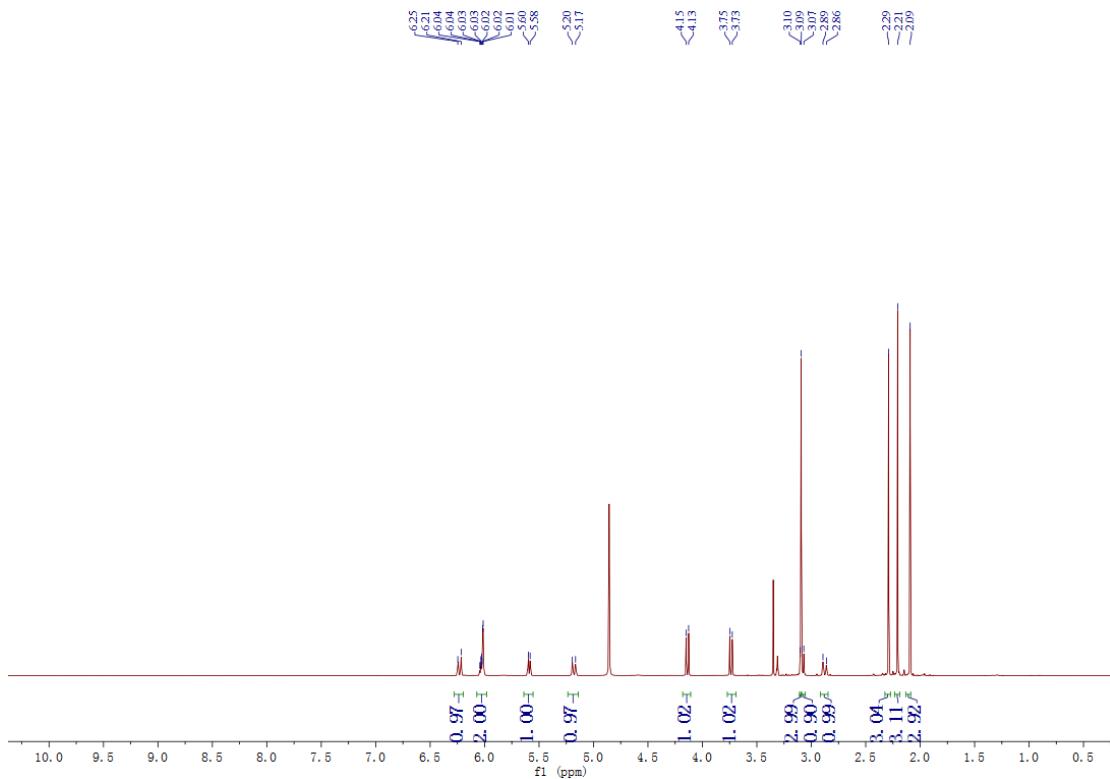


**Figure S37.**  $^{13}\text{C}$  NMR spectrum of compound 8 in  $\text{DMSO}-d_6$ .



**Figure S38.** ESI-MS spectrum of compound 8.

**Figure S39.**  $^1\text{H}$  NMR spectrum of compound 9 in  $\text{CD}_3\text{OD}$ .**Figure S40.**  $^{13}\text{C}$  NMR spectrum of compound 9 in  $\text{CD}_3\text{OD}$ .

**Figure S41.** ESI-MS spectrum of compound 9.**Figure S42.**  $^1\text{H}$  NMR spectrum of compound 10 in  $\text{CD}_3\text{OD}$ .

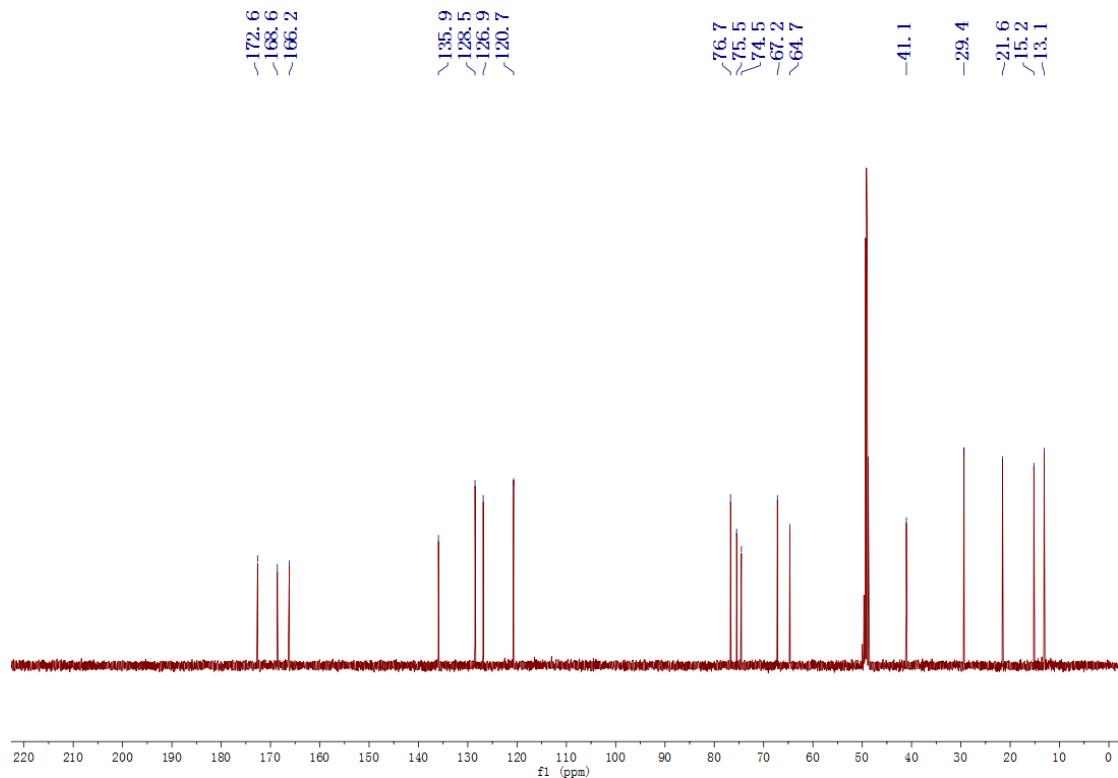
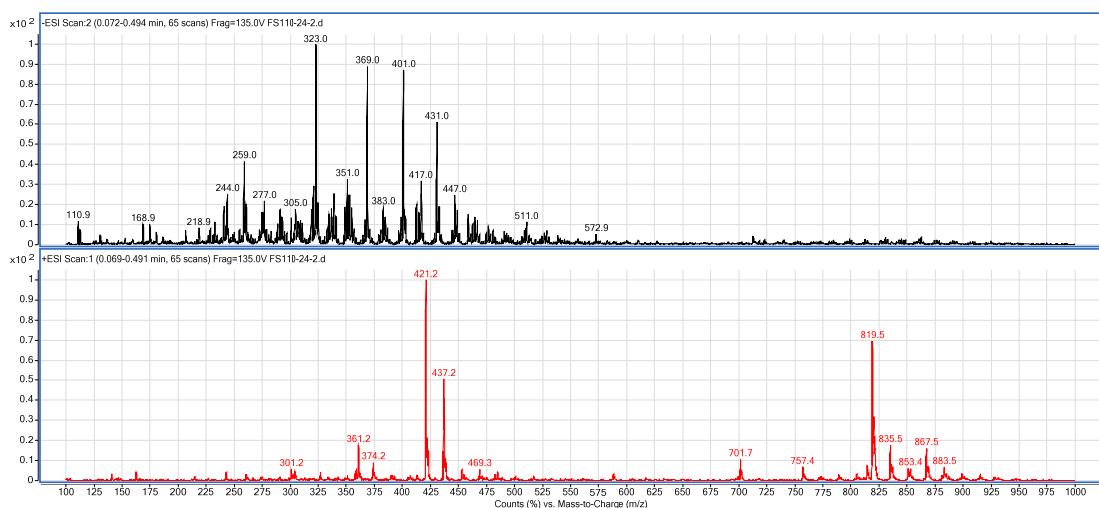
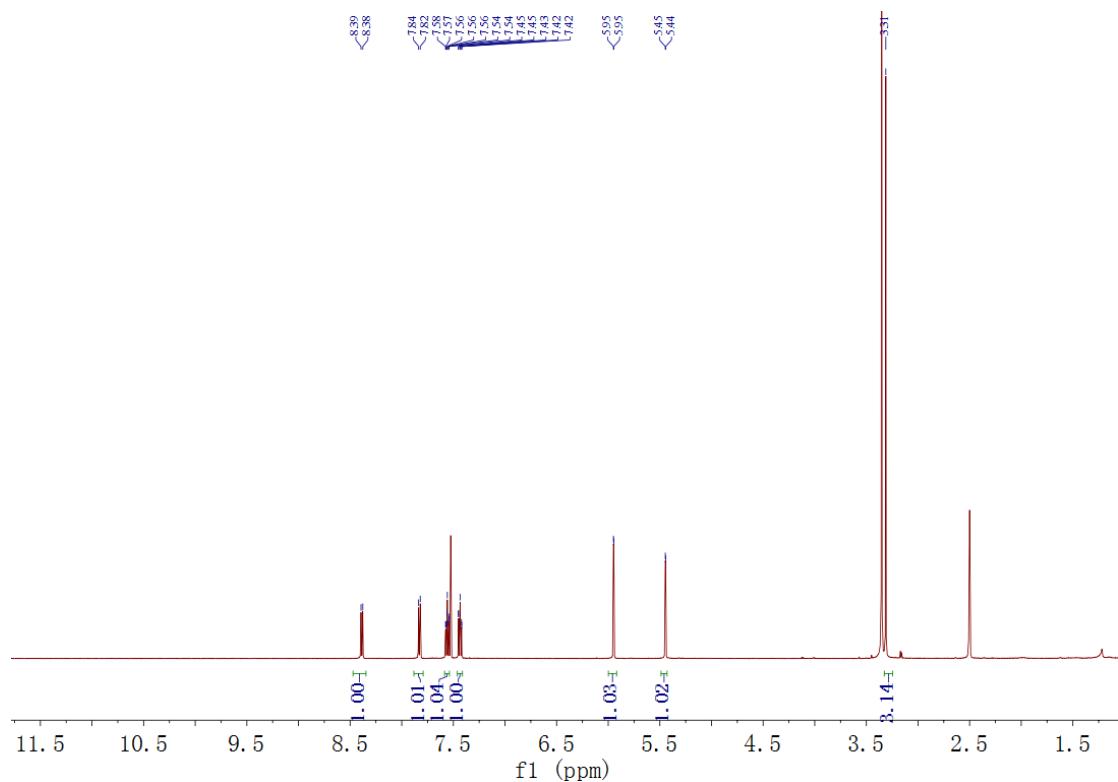
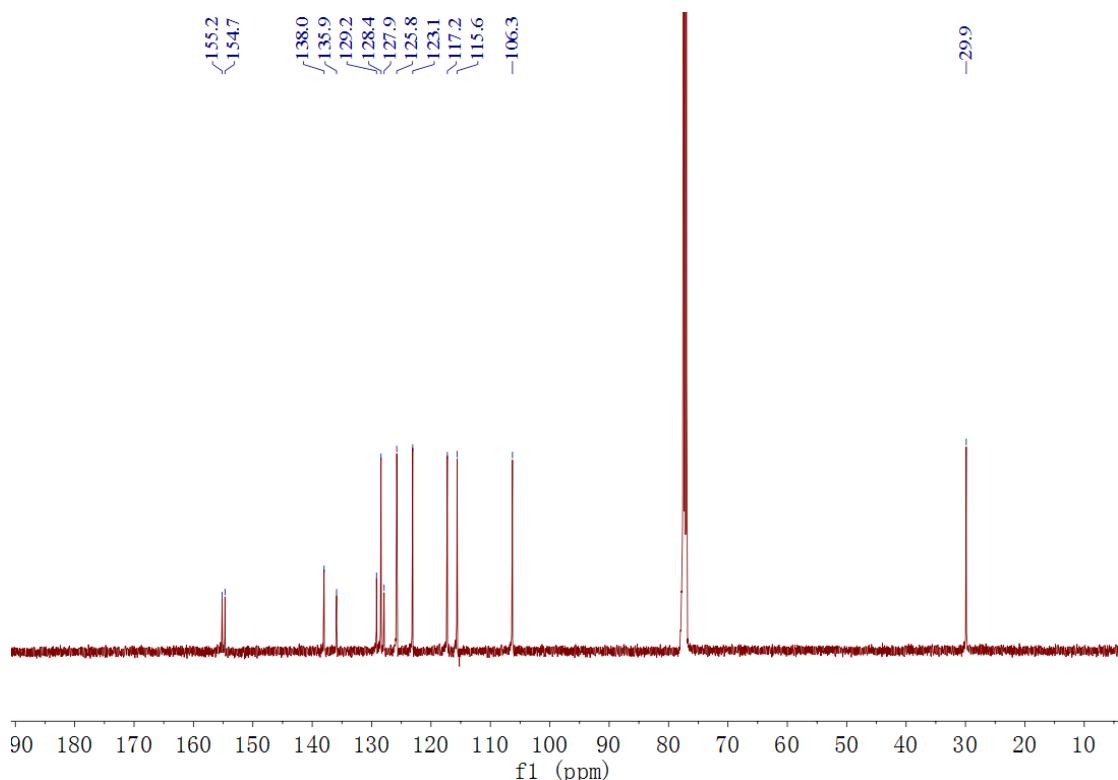
Figure S43.  $^{13}\text{C}$  NMR spectrum of compound 10 in  $\text{CD}_3\text{OD}$ .

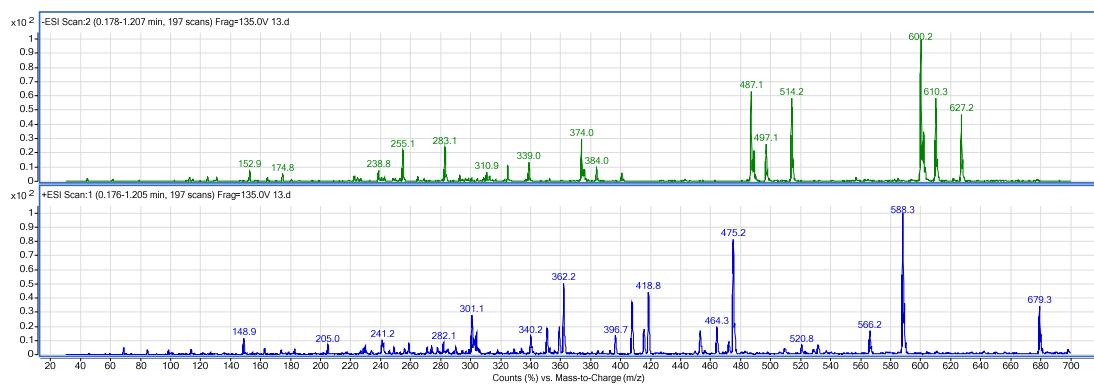
Figure S44. ESI-MS spectrum of compound 10.



**Figure S45.** <sup>1</sup>H NMR spectrum of compound 11 in DMSO-*d*<sub>6</sub>.



**Figure S46.** <sup>13</sup>C NMR spectrum of compound 11 in CDCl<sub>3</sub>.



**Figure S47.** ESI-MS spectrum of compound 11.