

## Supporting Information

### **Antimicrobial polyketides and sesquiterpene lactones from the deep-sea cold-seep-derived fungus *Talaromyces minioluteus* CS-113 triggered by histone deacetylase inhibitor SAHA**

Sui-Qun Yang,<sup>\*a,†</sup> Qi Song,<sup>a,b,†</sup> Xiao-Ming Li,<sup>a</sup> Xin Li,<sup>a</sup> Hong-Lei Li,<sup>a</sup> Ling-Hong Meng<sup>a</sup> and Bin-Gui Wang<sup>\*a,b,c</sup>

<sup>a</sup>*CAS and Shandong Province Key Laboratory of Experimental Marine Biology, Institute of Oceanology, Chinese Academy of Sciences, and Laboratory of Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Nanhai Road 7, Qingdao 266071, People's Republic of China*

<sup>b</sup>*College of Marine Science, University of Chinese Academy of Sciences, Yuquan Road 19A, Beijing 100049, People's Republic of China*

<sup>c</sup>*Center for Ocean Mega-Science, Chinese Academy of Sciences, Nanhai Road 7, Qingdao 266071, People's Republic of China*

<sup>†</sup>These authors contributed equally to this work.

\*Phone (S.-Q. Yang): +86-532-82898890. E-mail: yangsuiqun@qdio.ac.cn.

\*Phone (B.-G. Wang): +86-532-82898553. E-mail: wangbg@ms.qdio.ac.cn.

## Content

- Figure S1.** HPLC analysis of *Talaromyces minioluteus* CS-113 triggered by SAHA compared with negative control cultured in a single conical flask;
- Figure S2.** HPLC analysis of isolated compounds **1-18** of *T. minioluteus* CS-113 within the combined EtOAc extracts of all flasks;
- Figure S3.** HRESI mass spectrum of compound **1**;
- Figure S4.** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **1**;
- Figure S5.** <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) and DEPT spectra of compound **1**;
- Figure S6.** COSY spectrum of compound **1**;
- Figure S7.** HSQC spectrum of compound **1**;
- Figure S8.** HMBC spectrum of compound **1**;
- Figure S9.** NOESY spectrum of compound **1**;
- Figure S10.** ECD spectrum of compound **1**;
- Figure S11.** HRESI mass spectrum of compound **2**;
- Figure S12.** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **2**;
- Figure S13.** <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) and DEPT spectra of compound **2**;
- Figure S14.** COSY spectrum of compound **2**;
- Figure S15.** HSQC spectrum of compound **2**;
- Figure S16.** HMBC spectrum of compound **2**;
- Figure S17.** NOESY spectrum of compound **2**;
- Figure S18.** ECD spectrum of compound **2**;
- Figure S19.** HRESI mass spectrum of compound **3**;
- Figure S20.** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **3**;
- Figure S21.** <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) and DEPT spectra of compound **3**;
- Figure S22.** COSY spectrum of compound **3**;
- Figure S23.** HSQC spectrum of compound **3**;
- Figure S24.** HMBC spectrum of compound **3**;
- Figure S25.** NOESY spectrum of compound **3**;
- Figure S26.** ECD spectrum of compound **3**;
- Figure S27.** HRESI mass spectrum of compound **4**;
- Figure S28.** <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **4**;
- Figure S29.** <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) and DEPT spectra of compound **4**;
- Figure S30.** COSY spectrum of compound **4**;

**Figure S31.** HSQC spectrum of compound **4**;  
**Figure S32.** HMBC spectrum of compound **4**;  
**Figure S33.** ECD spectra of compounds **4a** and **4b**;  
**Figure S34.** HRESI mass spectrum of compound **5**;  
**Figure S35.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **5**;  
**Figure S36.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **5**;  
**Figure S37.** COSY spectrum of compound **5**;  
**Figure S38.** HSQC spectrum of compound **5**;  
**Figure S39.** HMBC spectrum of compound **5**;  
**Figure S40.** HRESI mass spectrum of compound **6**;  
**Figure S41.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6**;  
**Figure S42.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **6**;  
**Figure S43.** COSY spectrum of compound **6**;  
**Figure S44.** HSQC spectrum of compound **6**;  
**Figure S45.** HMBC spectrum of compound **6**;  
**Figure S46.** NOESY spectrum of compound **6**;  
**Figure S47.** ECD spectrum of compound **6**;  
**Figure S48.** Scanning electron microscope analysis of compounds **6** and **10**;  
**Figure S49.** HRESI mass spectrum of compound **7**;  
**Figure S50.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **7**;  
**Figure S51.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **7**;  
**Figure S52.** COSY spectrum of compound **7**;  
**Figure S53.** HSQC spectrum of compound **7**;  
**Figure S54.** HMBC spectrum of compound **7**;  
**Figure S55.** NOESY spectrum of compound **7**;  
**Figure S56.** ECD spectrum of compound **7**;  
**Figure S57.** HRESI mass spectrum of compound **8**;  
**Figure S58.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **8**;  
**Figure S59.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **8**;  
**Figure S60.** COSY spectrum of compound **8**;  
**Figure S61.** HSQC spectrum of compound **8**;  
**Figure S62.** HMBC spectrum of compound **8**;  
**Figure S63.** NOESY spectrum of compound **8**;

**Figure S64.** ECD spectrum of compound **8**;

**Figure S65.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **10**;

**Figure S66.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **10**;

**Figure S67.** Structure and population of the low-energy (weighting factors) conformers for **4a** and **4b** at the B3LYP/6-31+g(d) level above 1% population;

**Figure S68.** Structure and population of the low-energy (weighting factors) conformers of (7*R*,8*aS*)-**7** at the B3LYP/6-31+g(d) level above 1% population;

**Figure S69.** Structure and population of the low-energy (weighting factors) conformers of (7*S*,8*aS*)-**7** at the B3LYP/6-31+g(d) level above 1% population;

**Figure S70.** DP4+ probability analysis data of compound **7**;

**Figure S71.** Structure and population of the low-energy (weighting factors) conformers of (7*S*,8*S*,8*aS*)-**10** at the B3LYP/6-31+g(d) level above 1% population;

**Figure S72.** Structure and population of the low-energy (weighting factors) conformers of (7*R*,8*S*,8*aS*)-**10** at the B3LYP/6-31+g(d) level above 1% population;

**Figure S73.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **9**;

**Figure S74.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **9**;

**Figure S75.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **11**;

**Figure S76.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **11**;

**Figure S77.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **12**;

**Figure S78.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **12**;

**Figure S79.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **13**;

**Figure S80.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **13**;

**Figure S81.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **14**;

**Figure S82.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **14**;

**Figure S83.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **15**;

**Figure S84.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **15**;

**Figure S85.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **16**;

**Figure S86.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **16**;

**Figure S87.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **17**;

**Figure S88.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **17**;

**Figure S89.**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **18**;

**Figure S90.**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) and DEPT spectra of compound **18**;

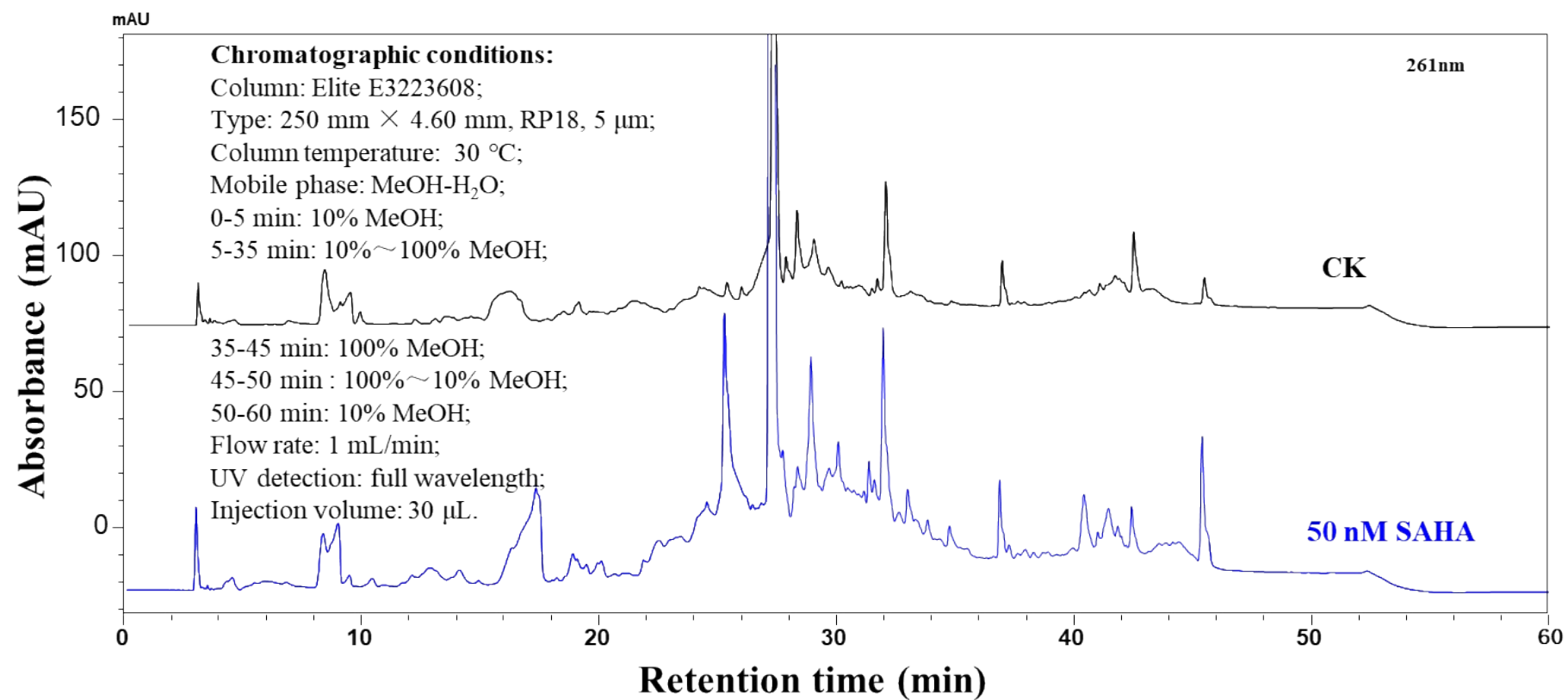
**Figure S91.** LCMS analysis of *T. minioluteus* CS-113 with and without SAHA cultured in a

single conical flask;

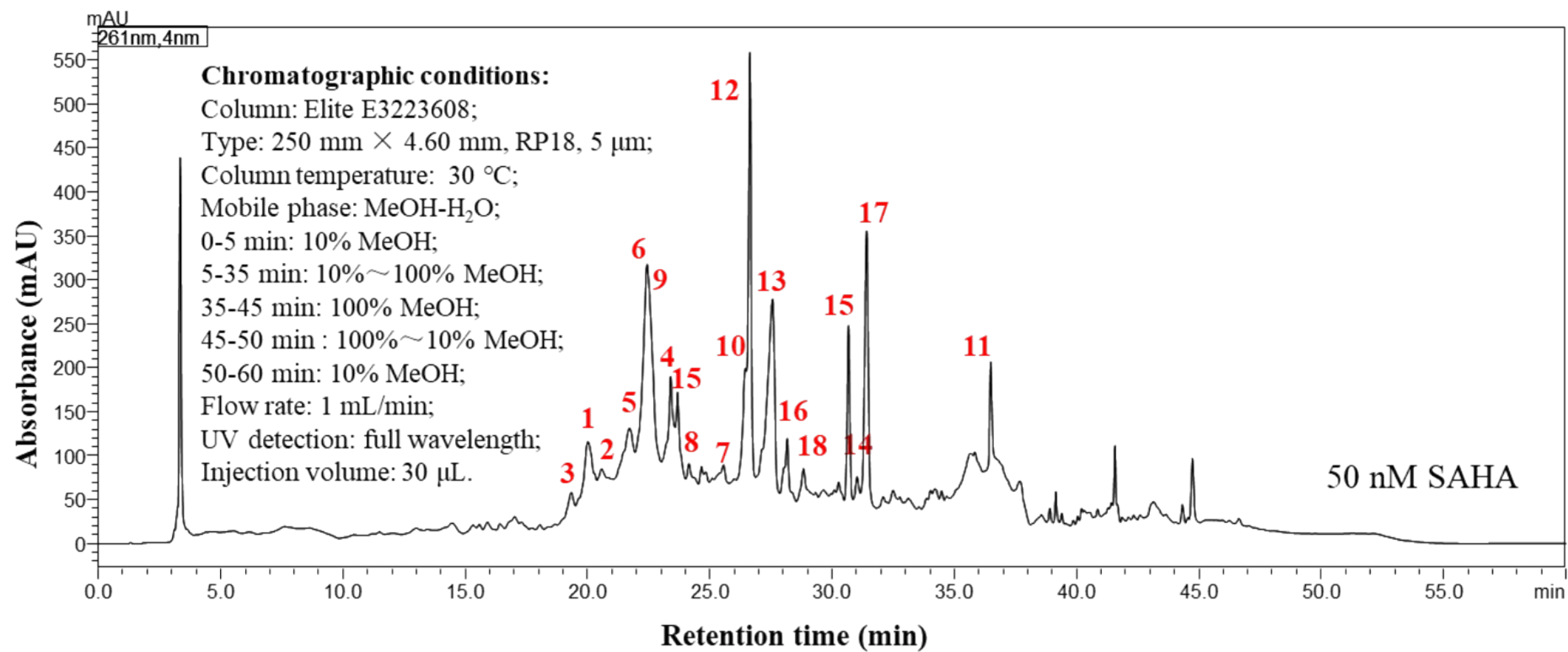
**Figure S92.** Identification of compound **3** by LCMS analysis of *T. minioluteus* CS-113 triggered by SAHA compared with negative control;

**Figure S93.** Identification of compound **4** by LCMS analysis of *T. minioluteus* CS-113 triggered by SAHA compared with negative control.

**Figure S1.** HPLC analysis of *Talaromyces minioluteus* CS-113 triggered by SAHA compared with negative control cultured in a single conical flask;

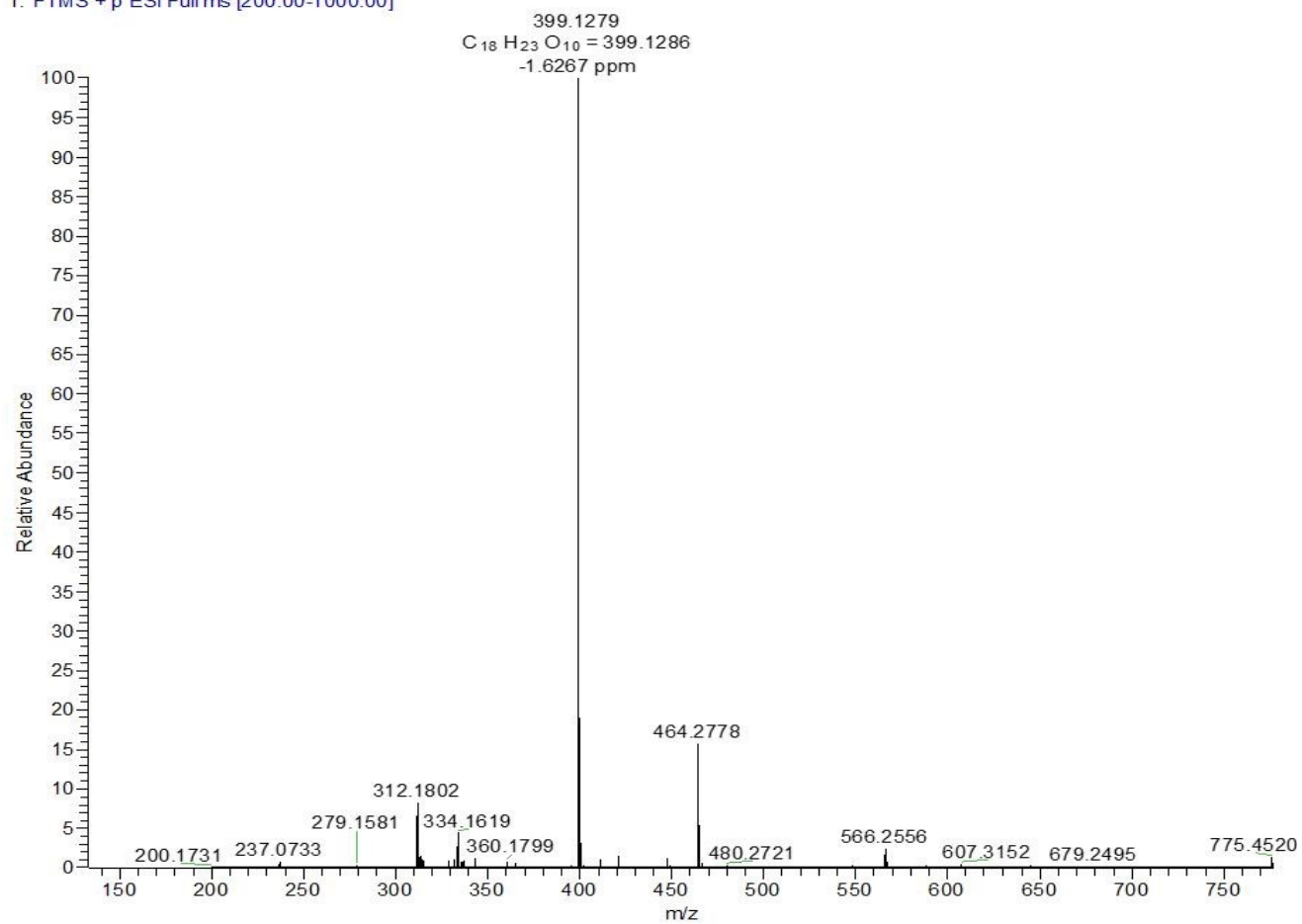


**Figure S2.** HPLC analysis of isolated compounds **1–18** of *T. minioluteus* CS-113 within the combined EtOAc extracts of all flasks;



**Figure S3.** HRESI mass spectrum of compound **1**;

20201015-CS113-50\_201015153826 #74 RT: 0.68 AV: 1 SB: 22 0.01-0.19 NL: 3.46E7  
T: FTMS + p ESI Full ms [200.00-1000.00]





**Figure S4.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **1**;

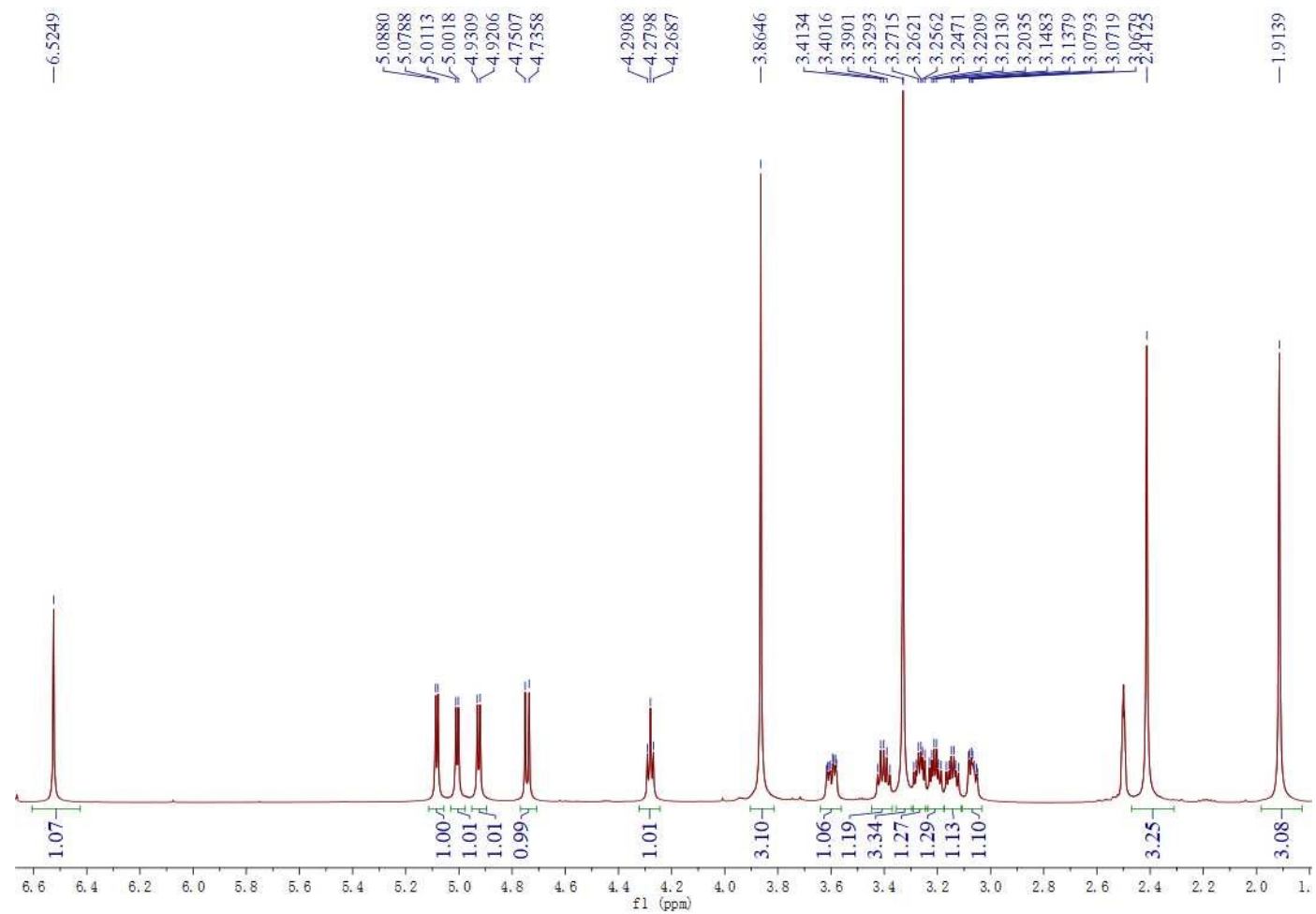


Figure S5.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **1**;

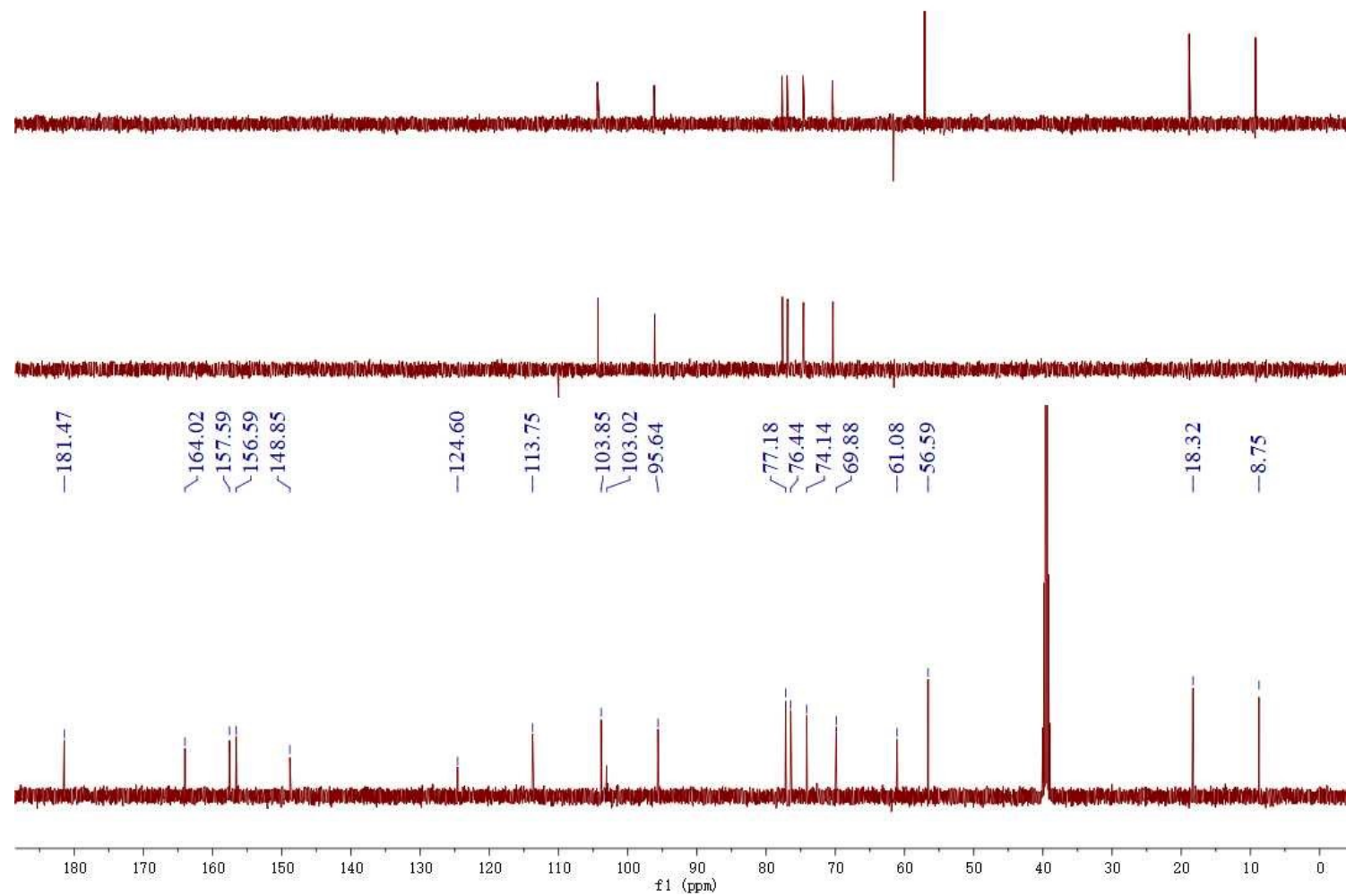


Figure S6. COSY spectrum of compound 1;

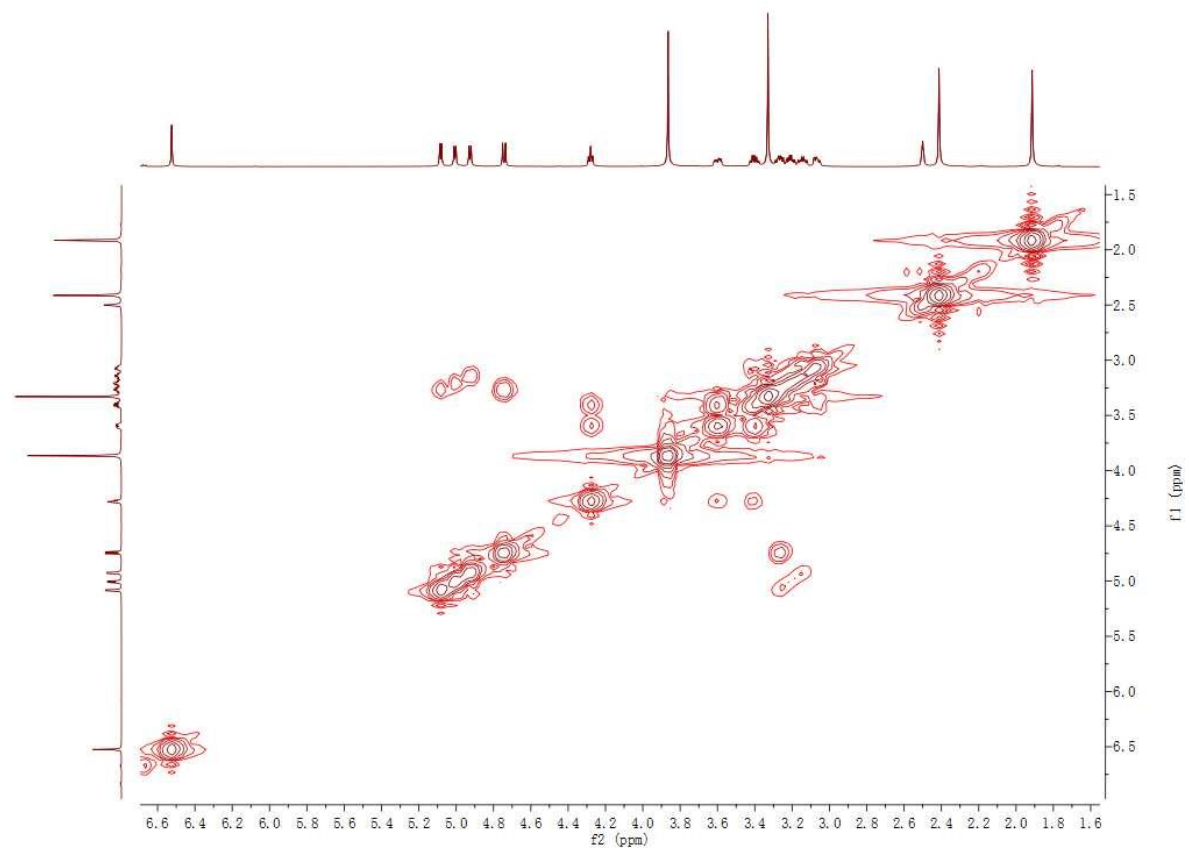


Figure S7. HSQC spectrum of compound 1;

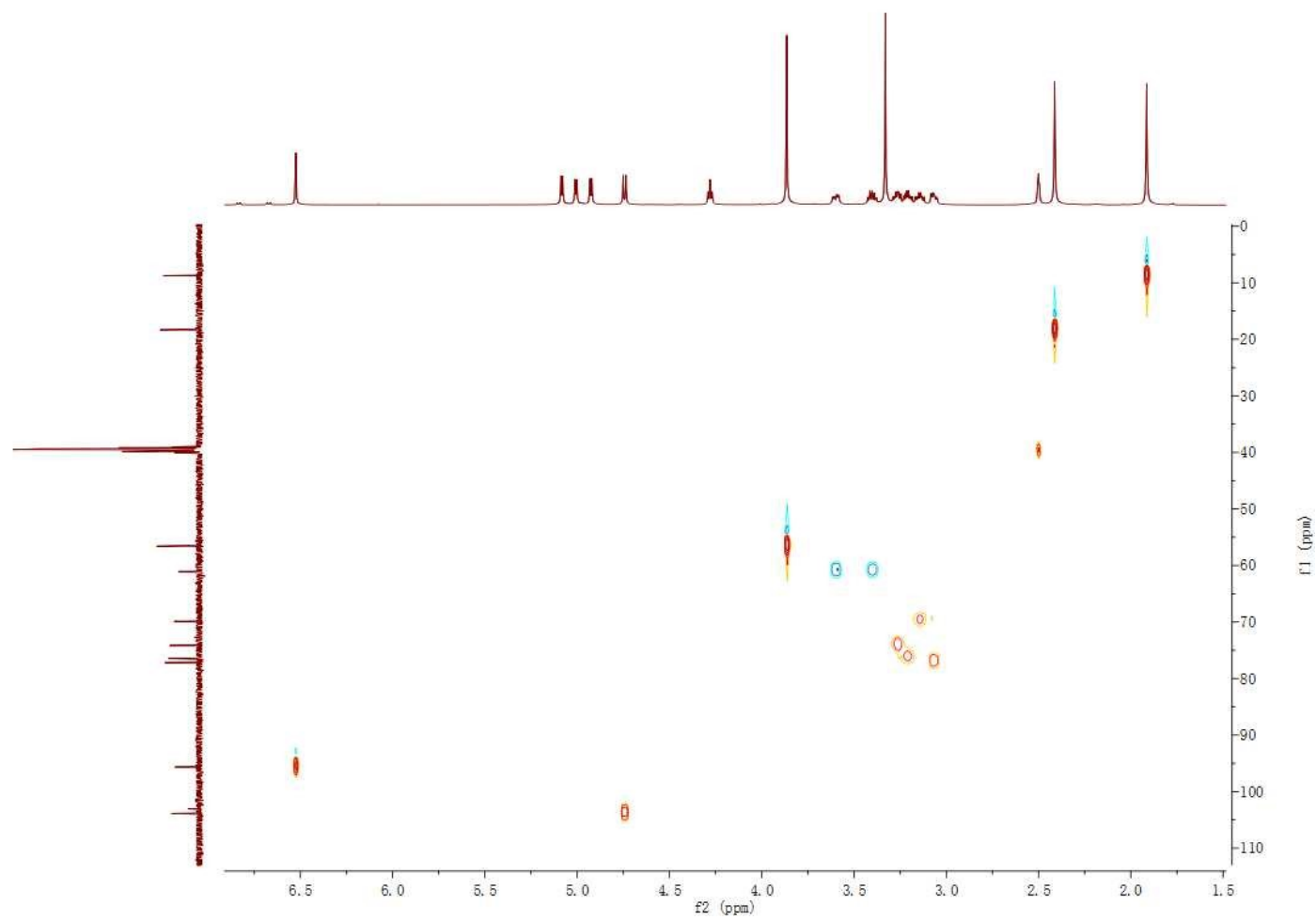
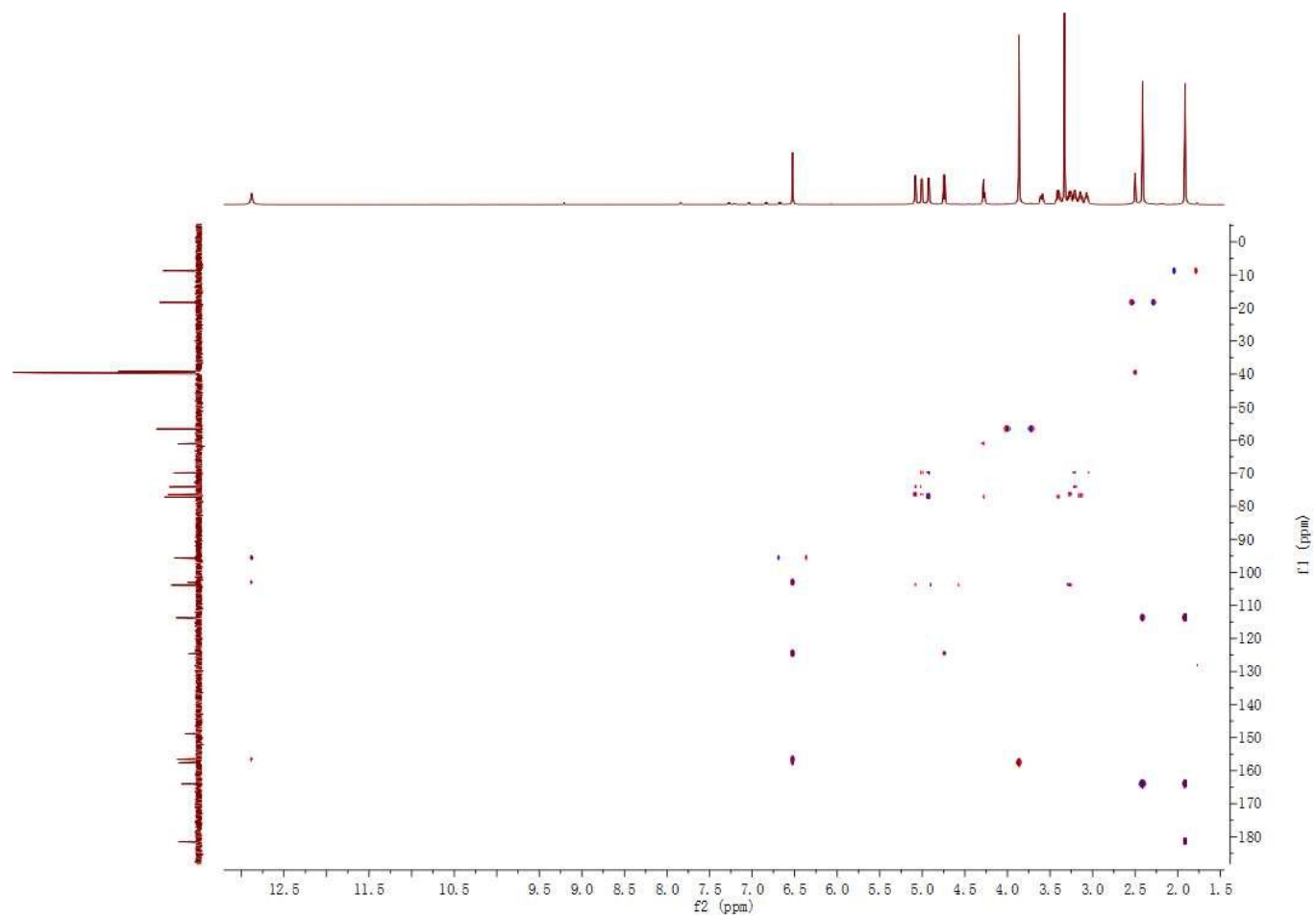


Figure S8. HMBC spectrum of compound 1;



**Figure S9.** NOESY spectrum of compound **1**;

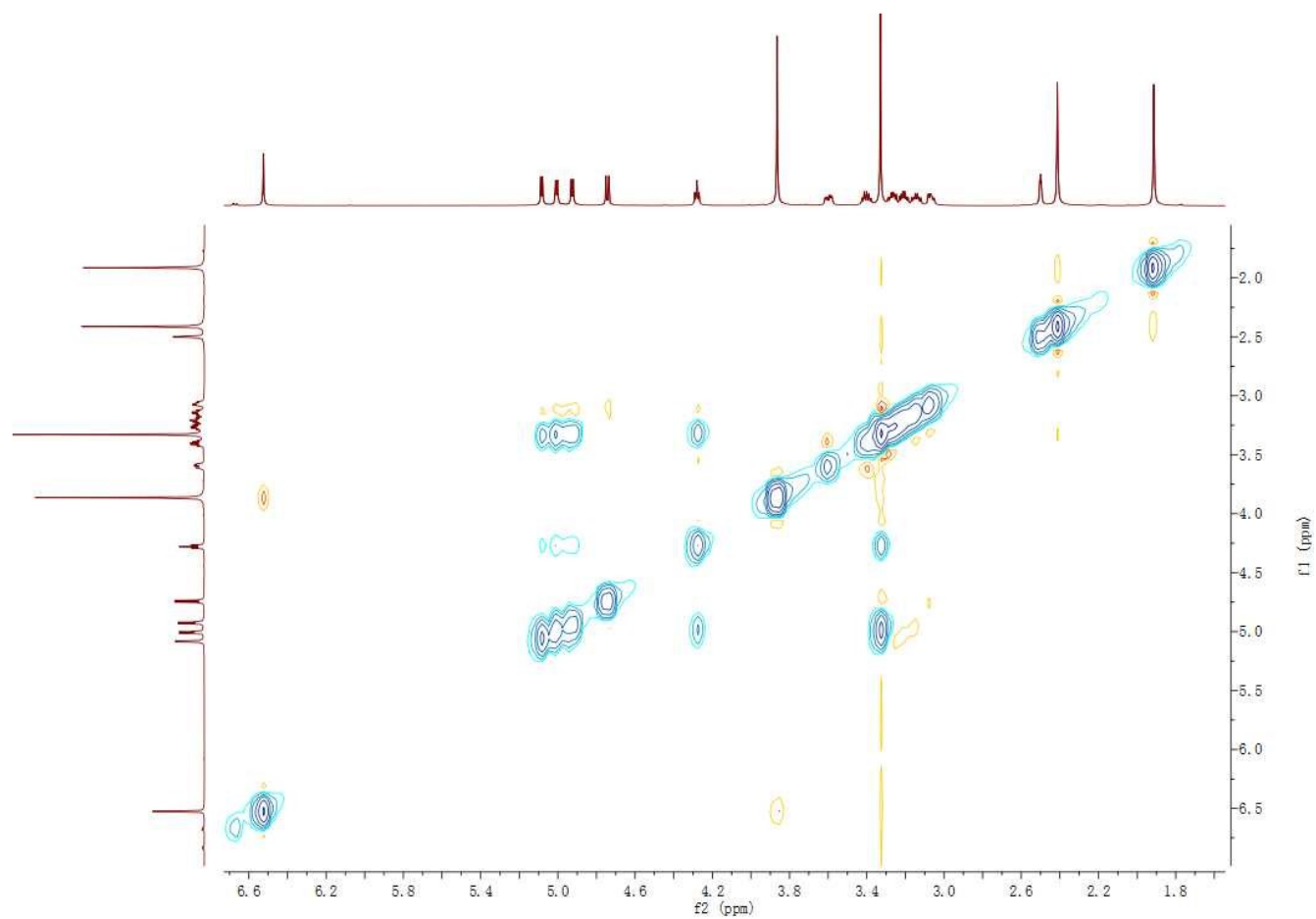
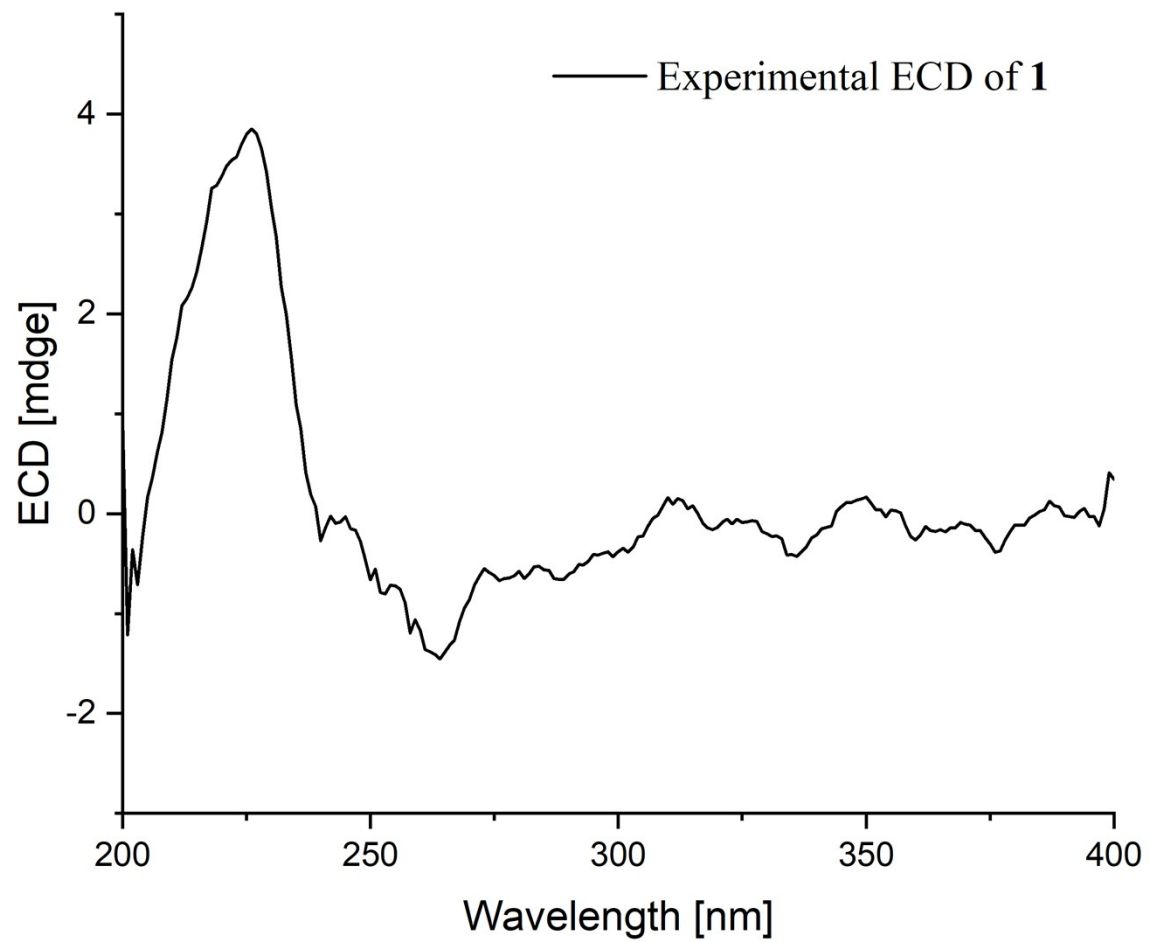
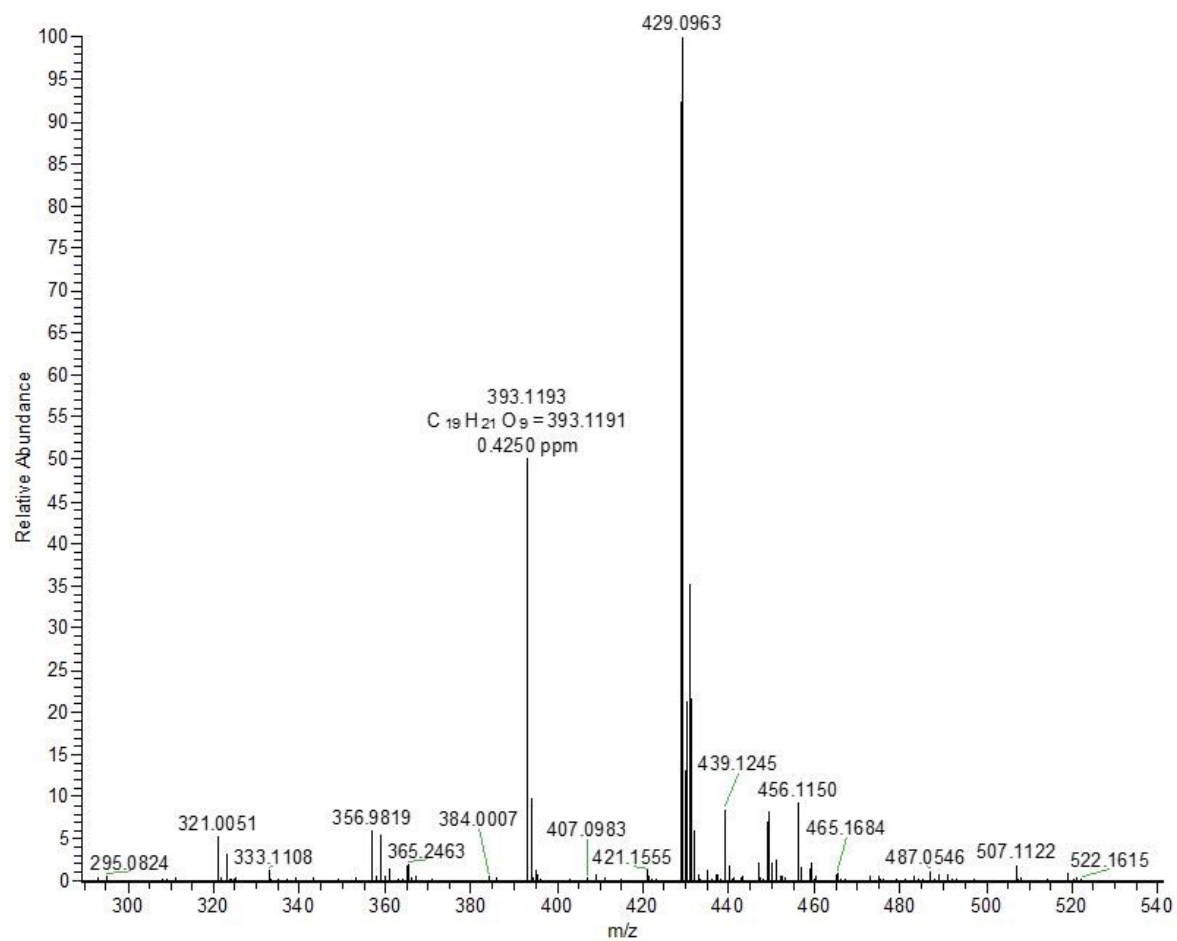


Figure S10. ECD spectrum of compound 1;



**Figure S11.** HRESI mass spectrum of compound **2**;

20210906-CS113-102 210906110302#106-107 RT: 1.48-1.49 AV: 2 NL: 7.81E6  
T: FTMS - p ESI Full ms [150.00-2000.00]





**Figure S12.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2**;

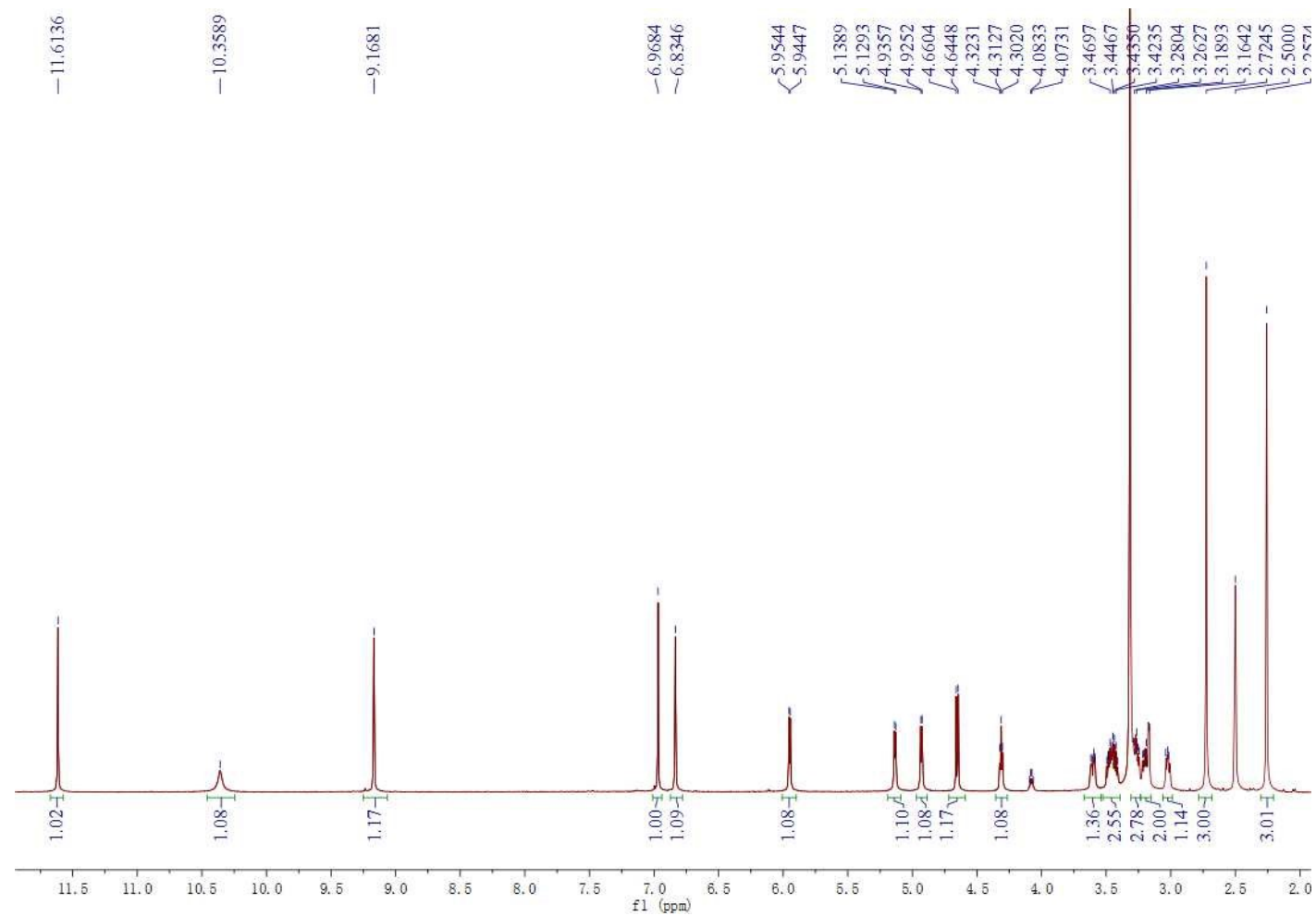


Figure S13.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **2**;

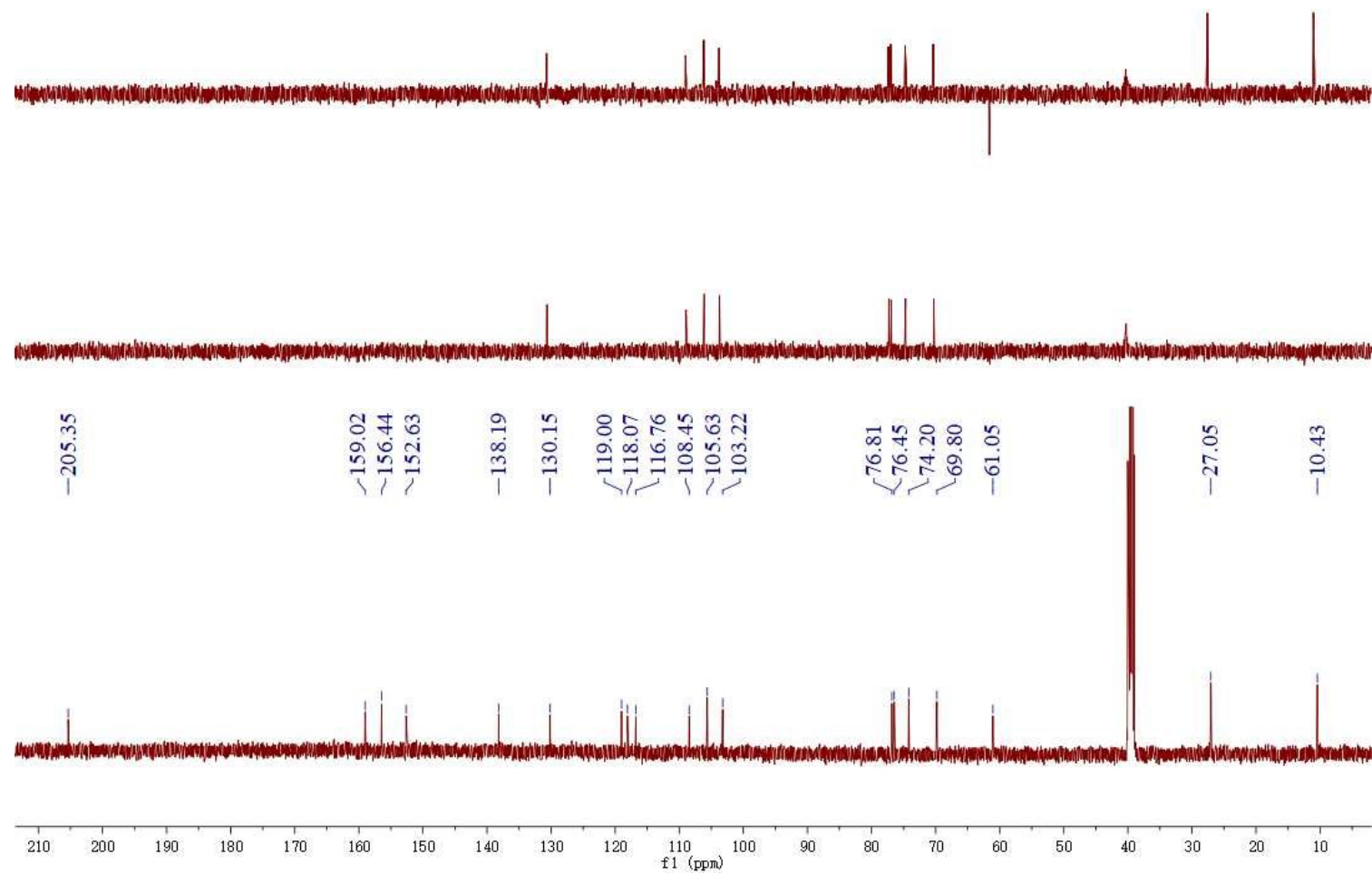


Figure S14. COSY spectrum of compound 2;

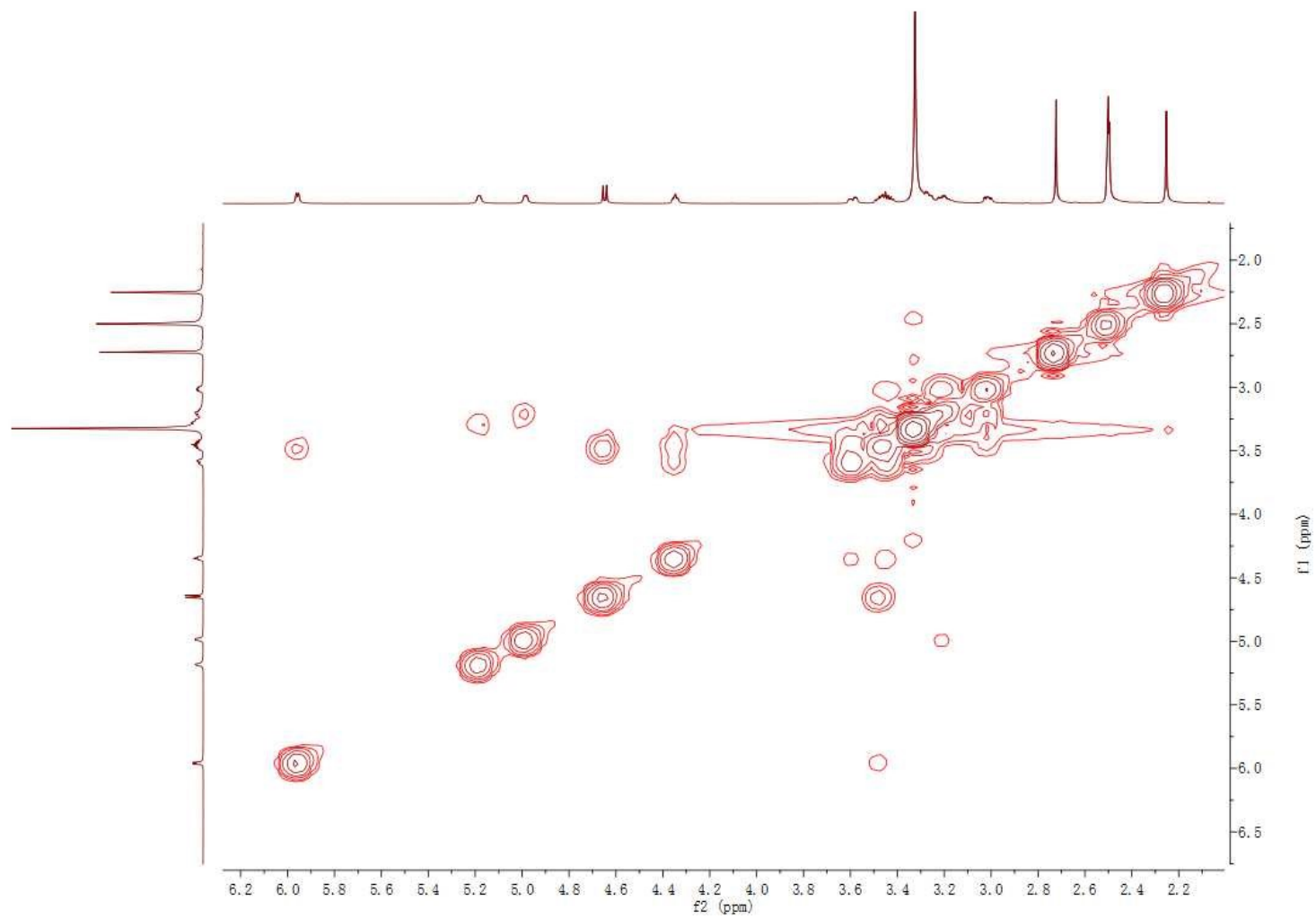


Figure S15. HSQC spectrum of compound 2;

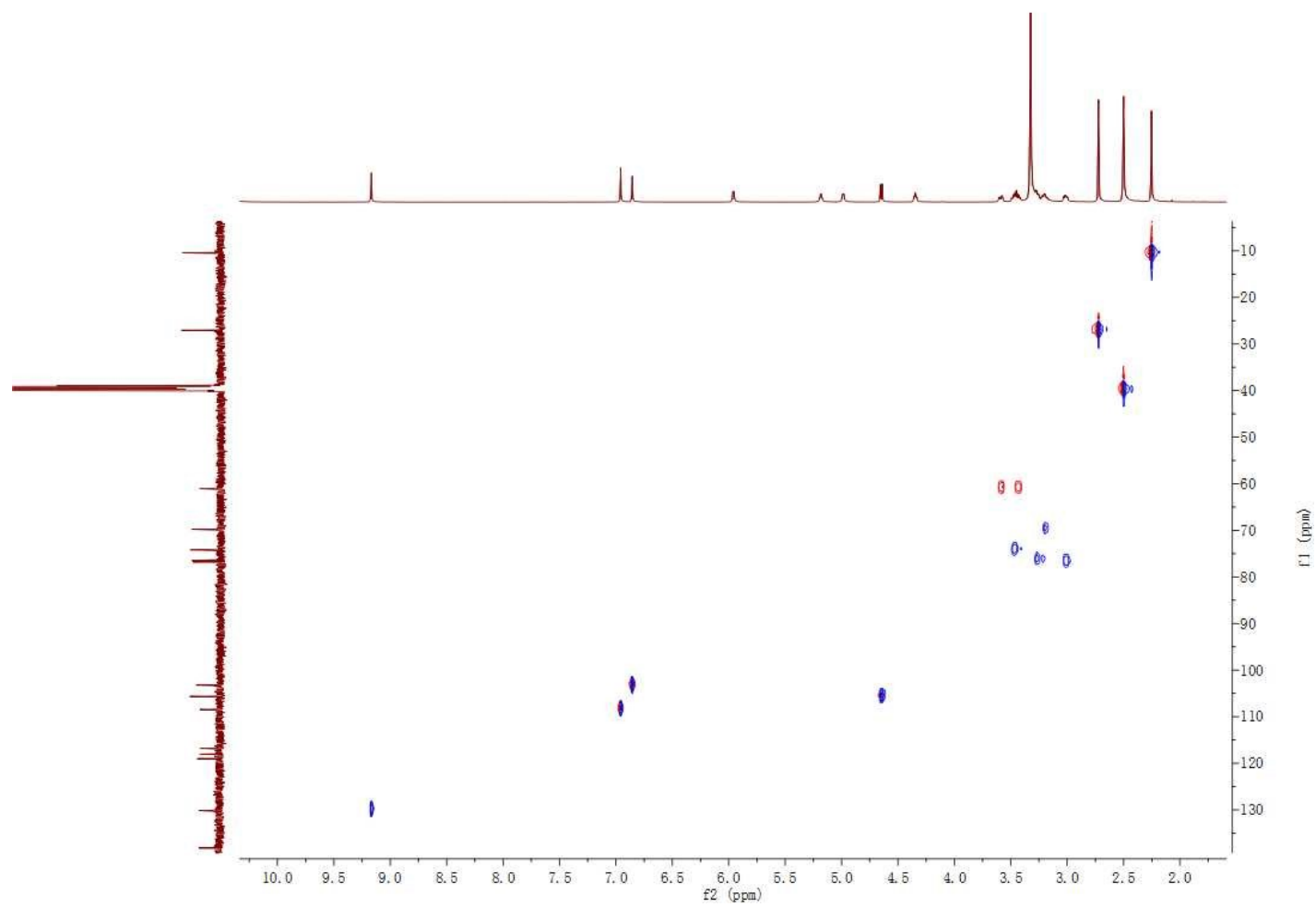


Figure S16. HMBC spectrum of compound 2;

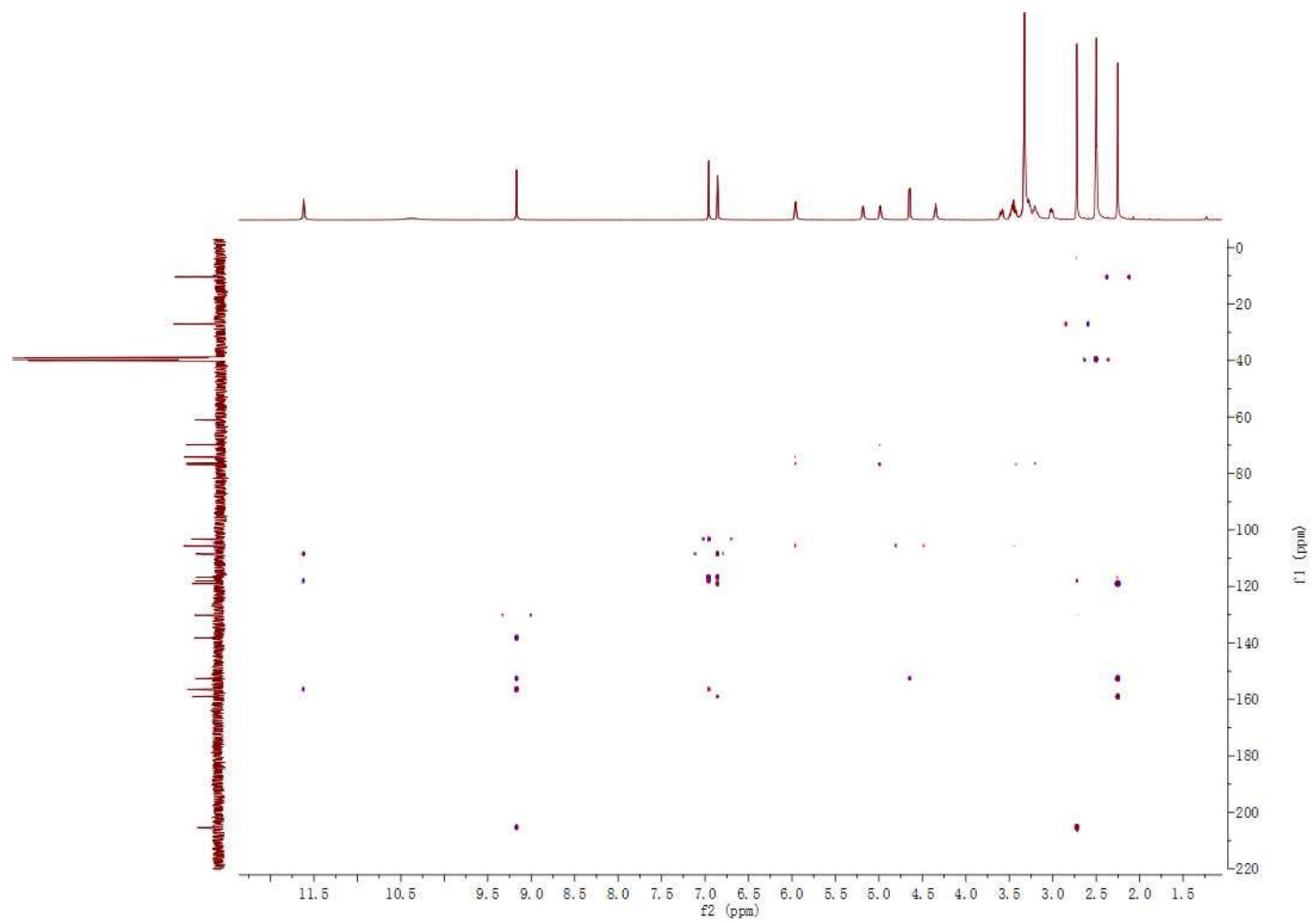
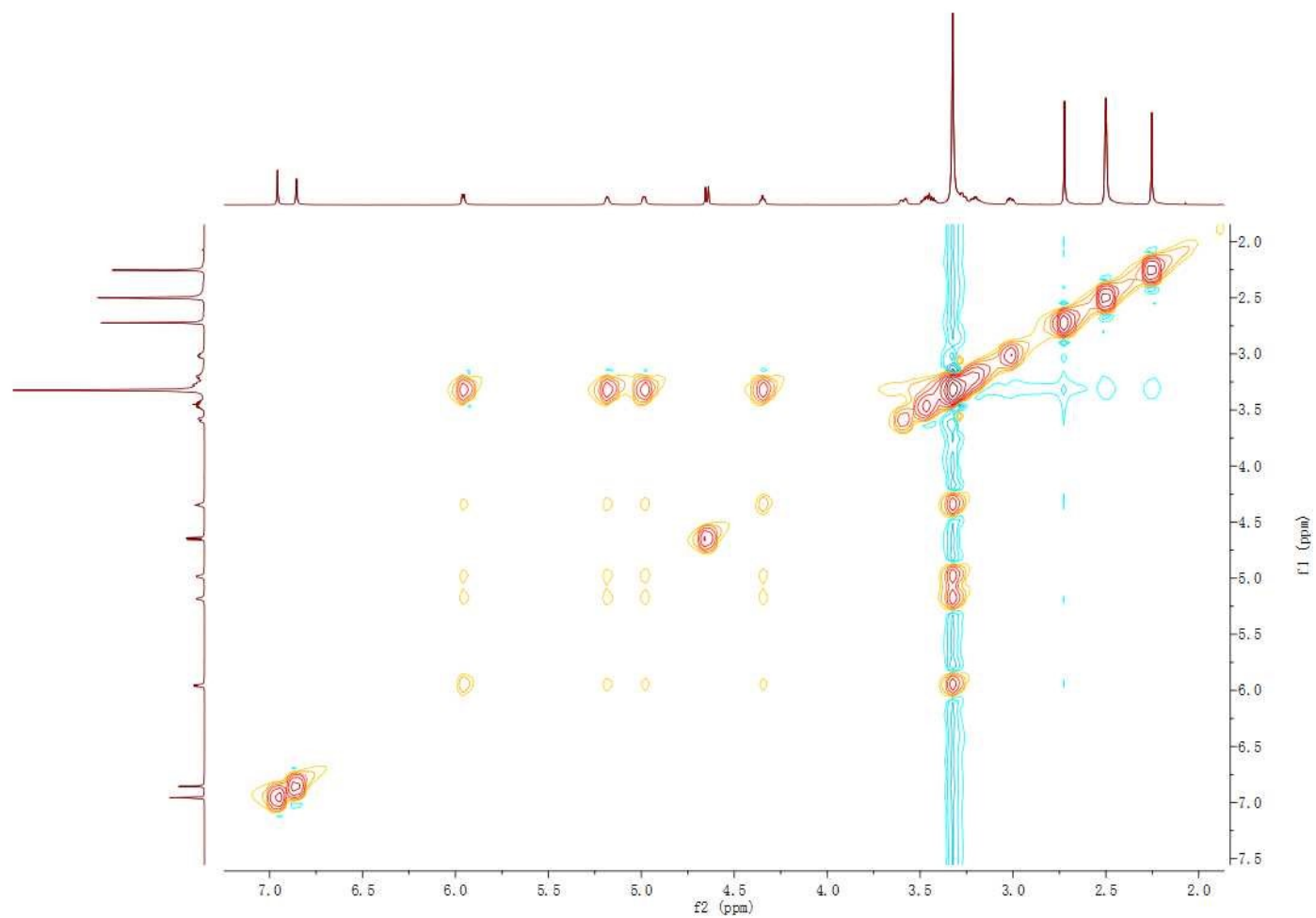
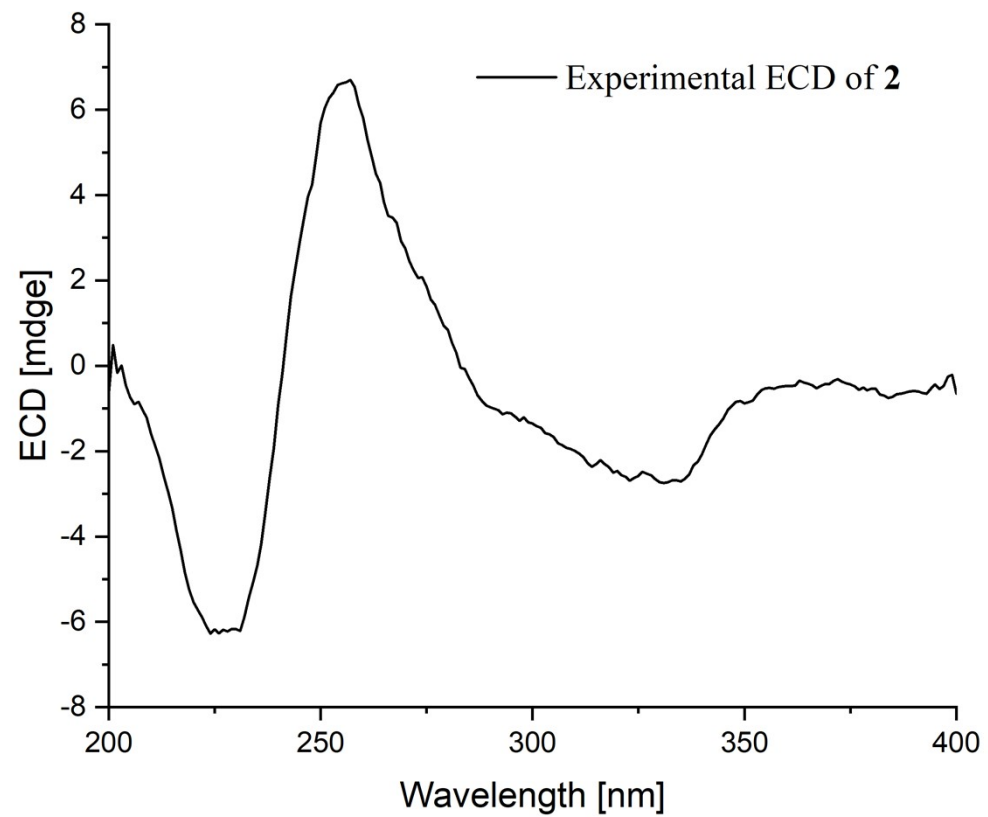


Figure S17. NOESY spectrum of compound 2;

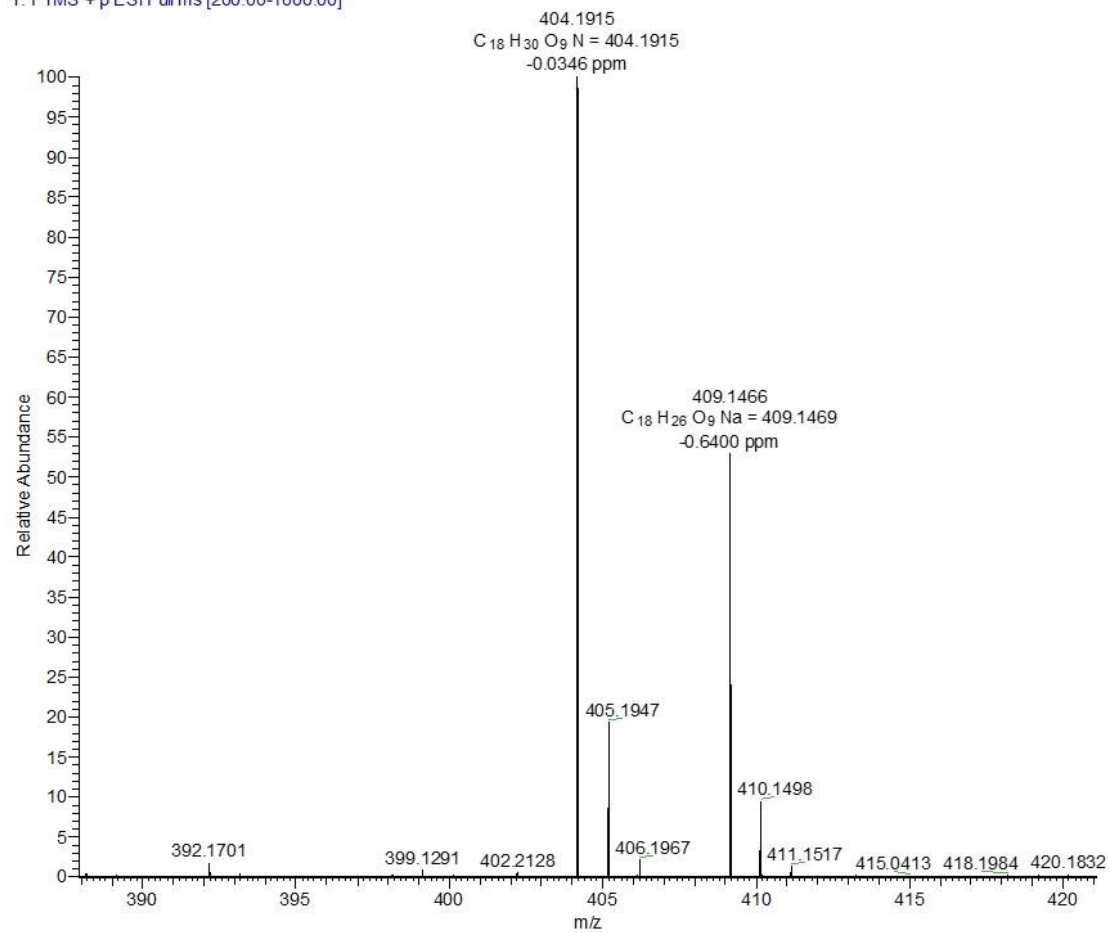


**Figure S18.** ECD spectrum of compound **2**;



**Figure S19.** HRESI mass spectrum of compound **3**;

20201015-CS113-56\_201015153826 #83 RT: 0.70 AV: 1 SB: 10 0.00-0.08 NL: 7.04E6  
T: FTMS + p ESI Full ms [200.00-1000.00]





**Figure S20.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **3**;

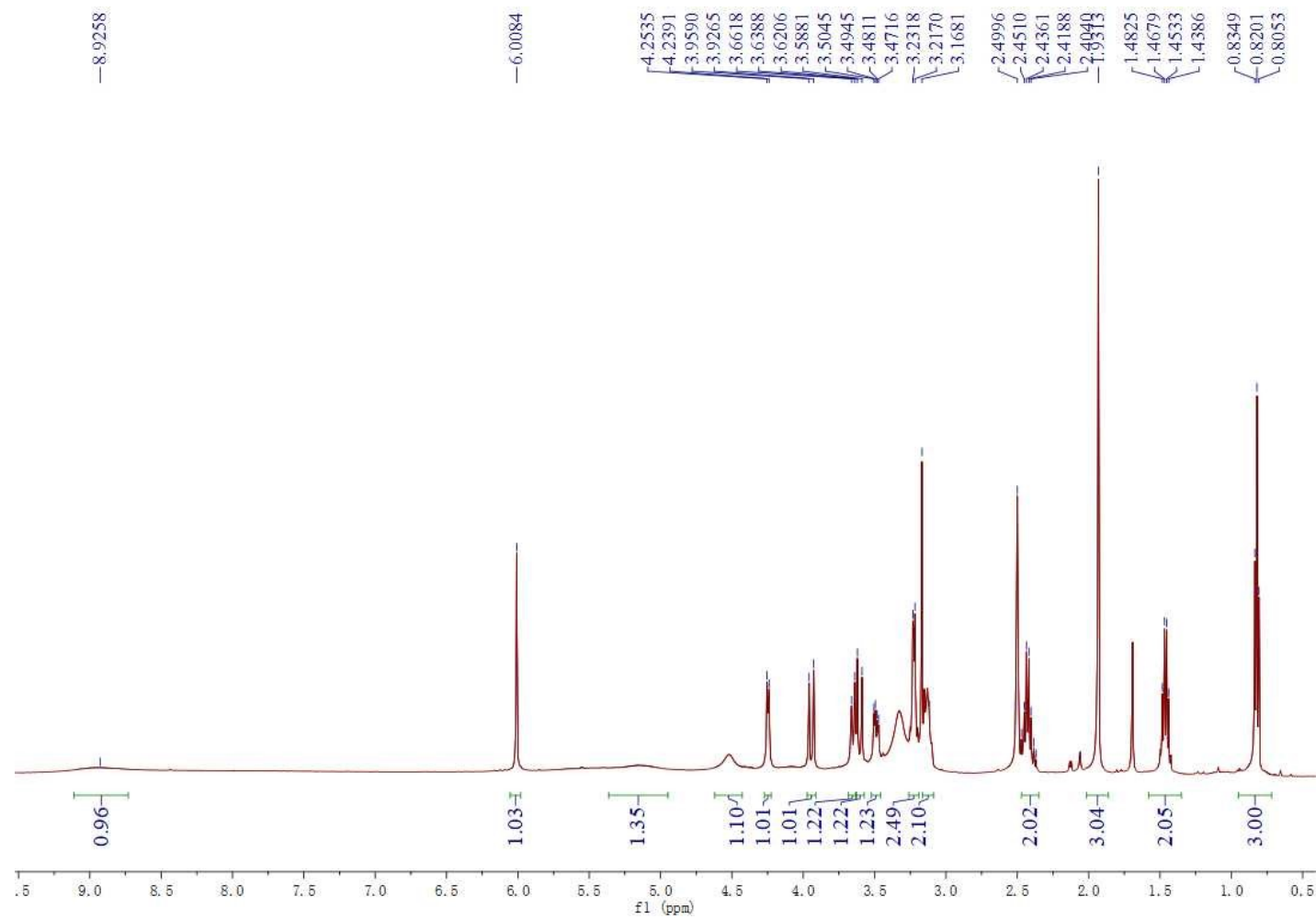
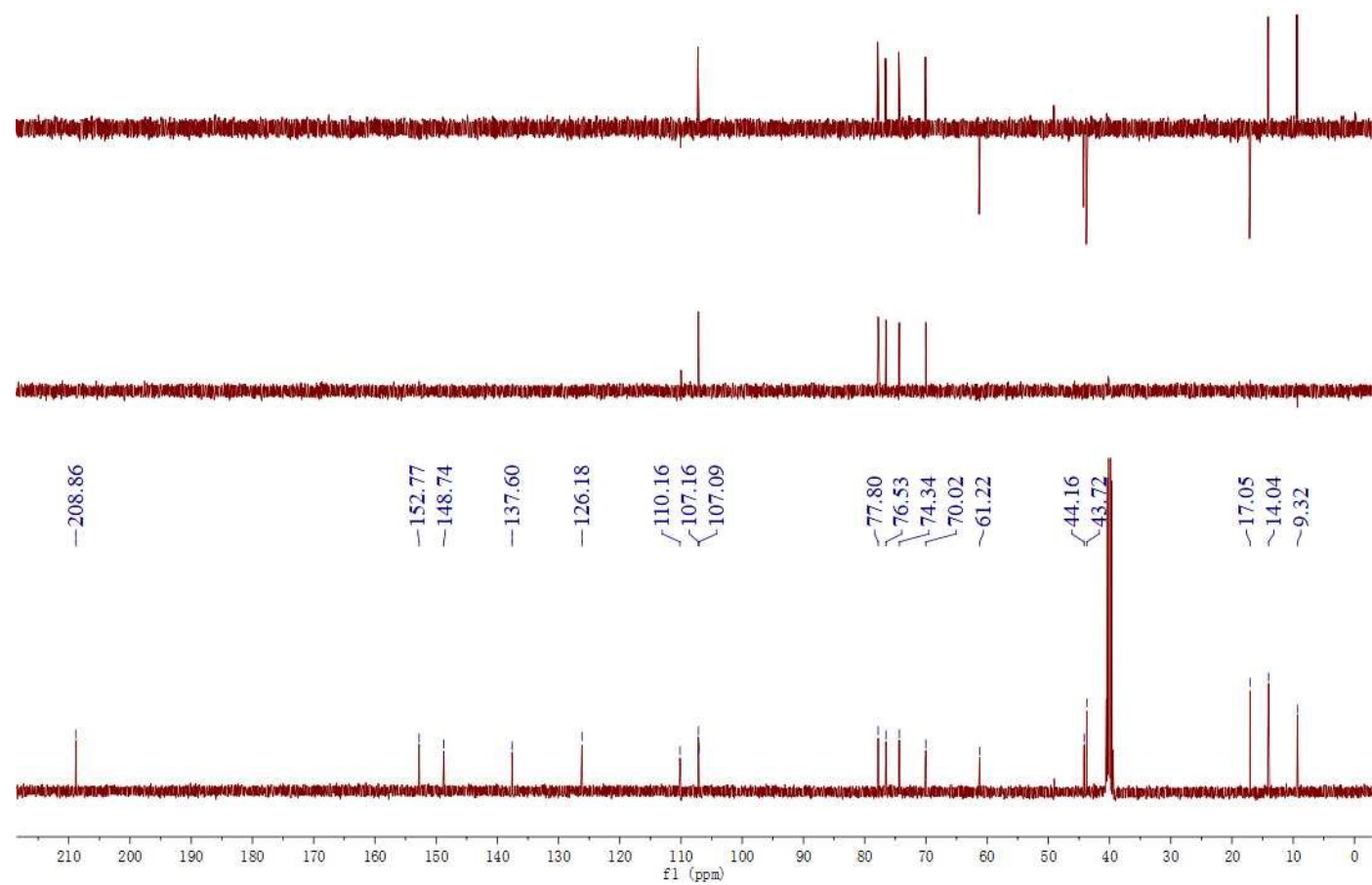


Figure S21.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **3**;



**Figure S22.** COSY spectrum of compound **3**;

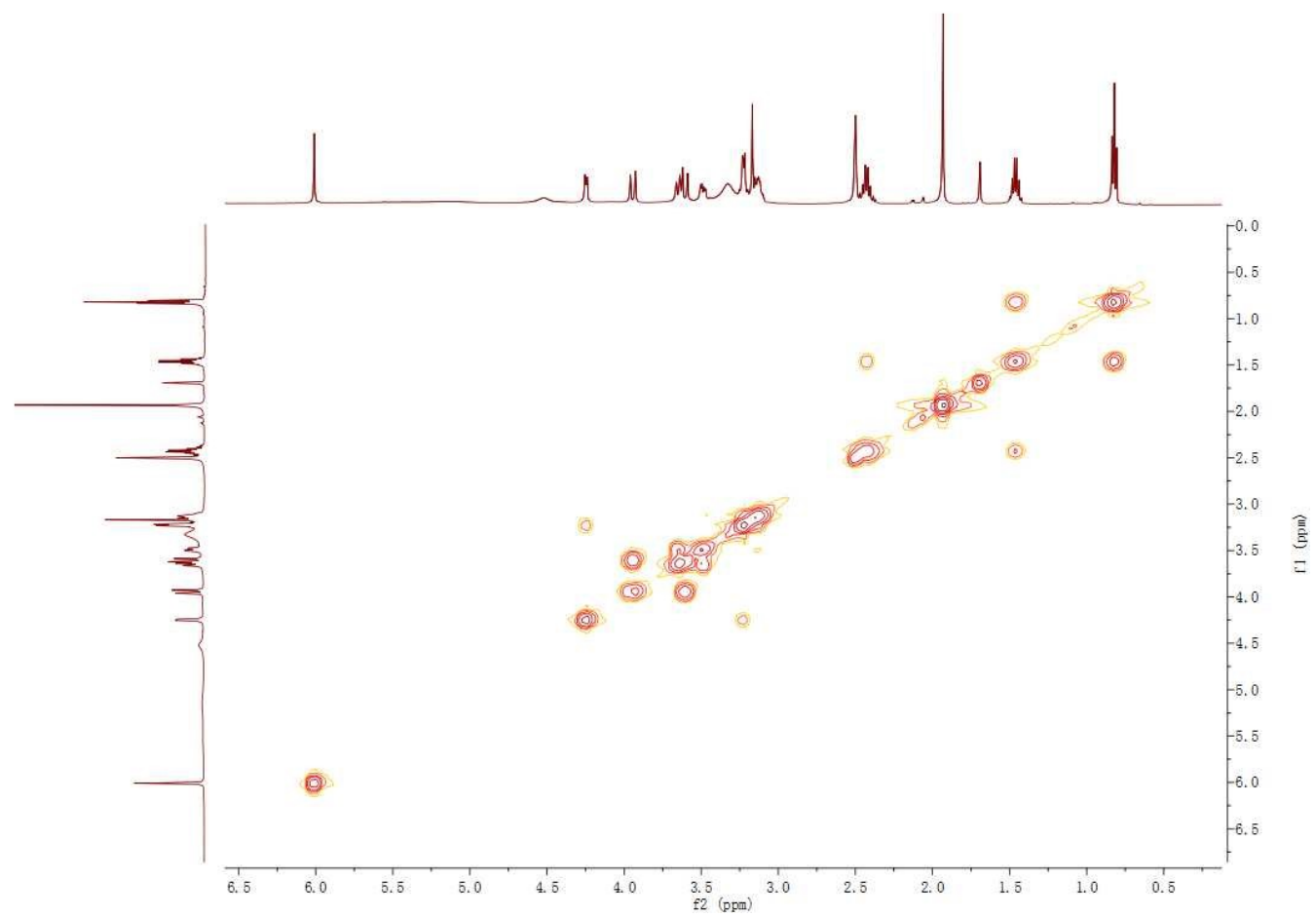


Figure S23. HSQC spectrum of compound **3**;

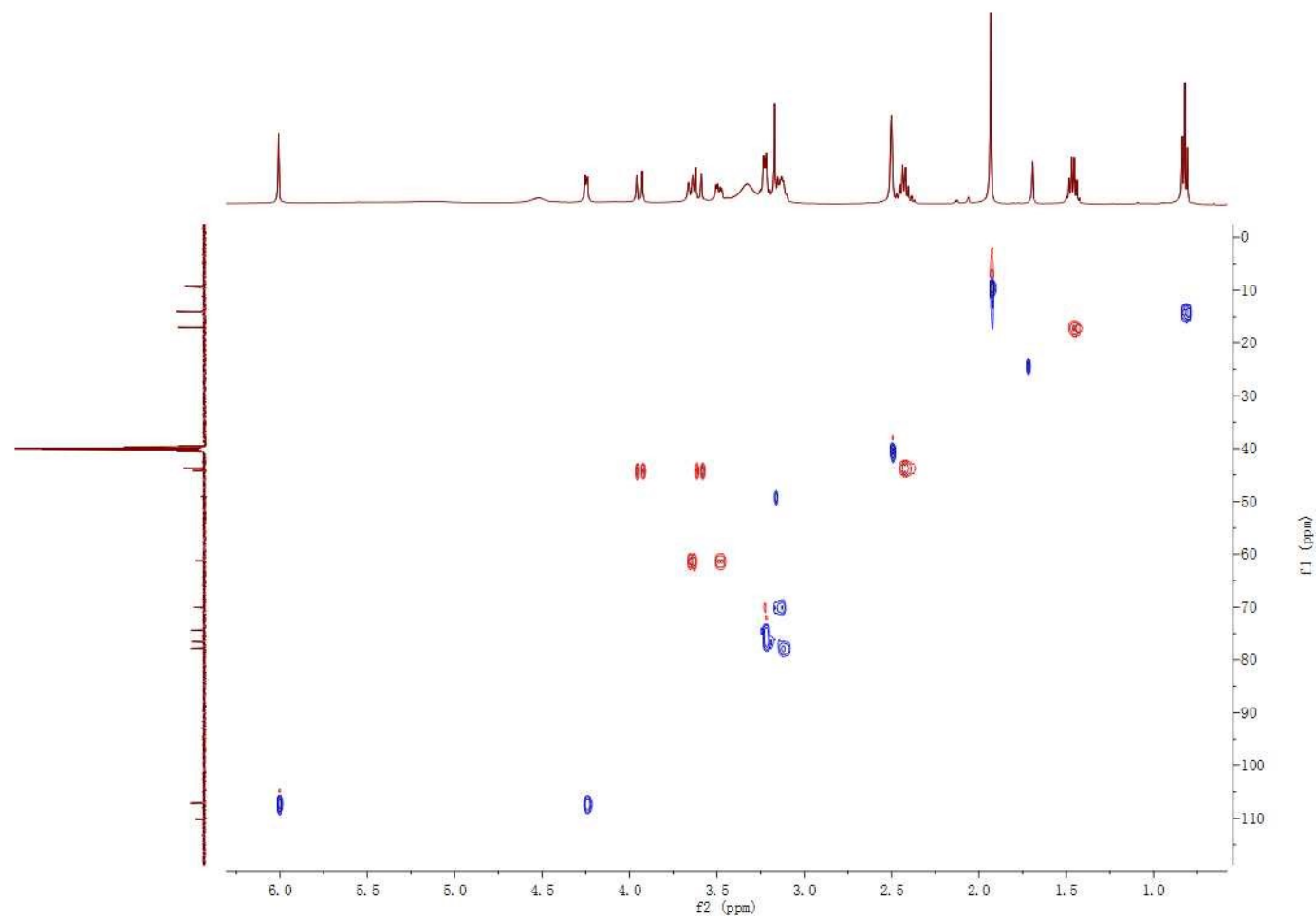


Figure S24. HMBC spectrum of compound 3;

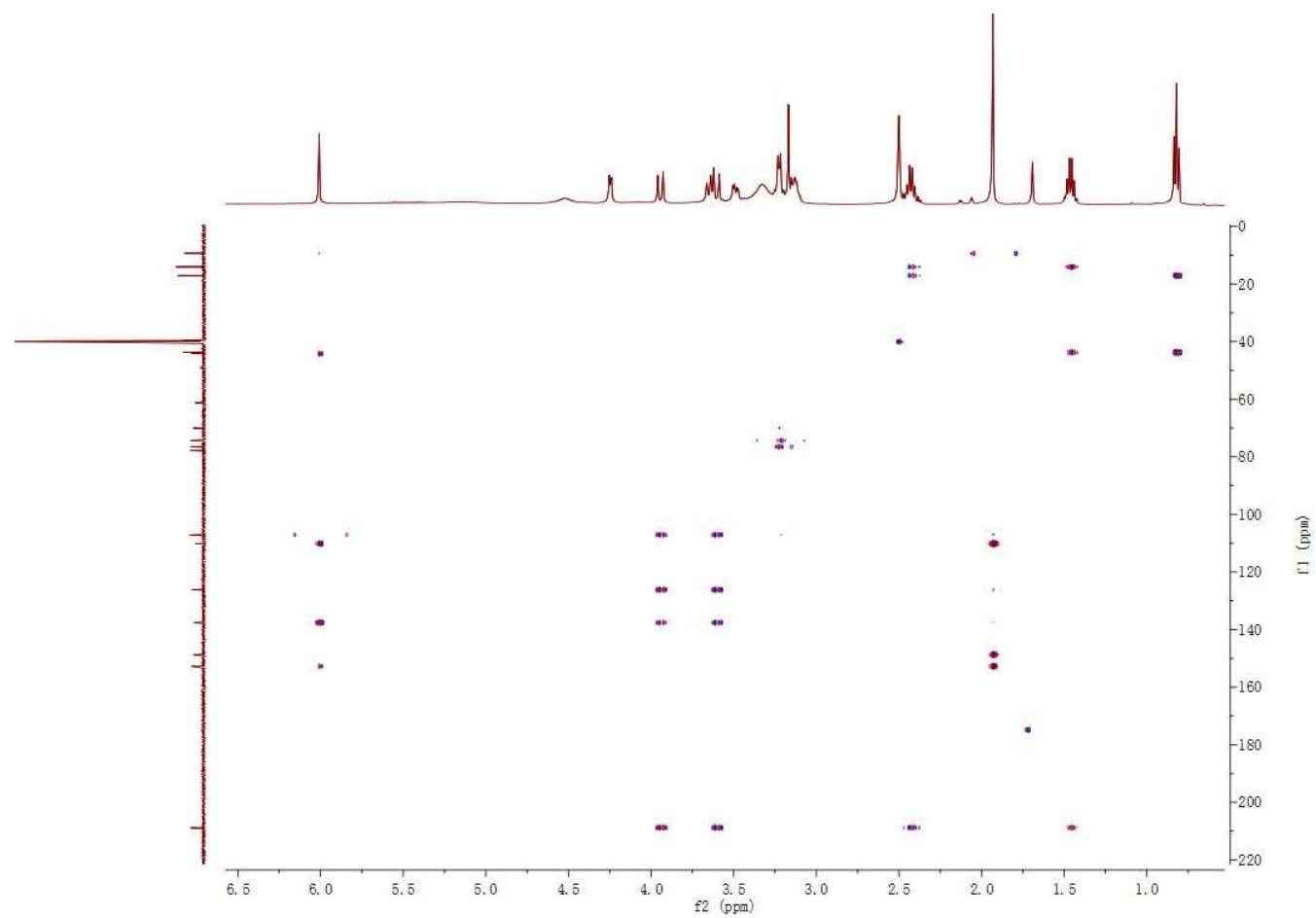
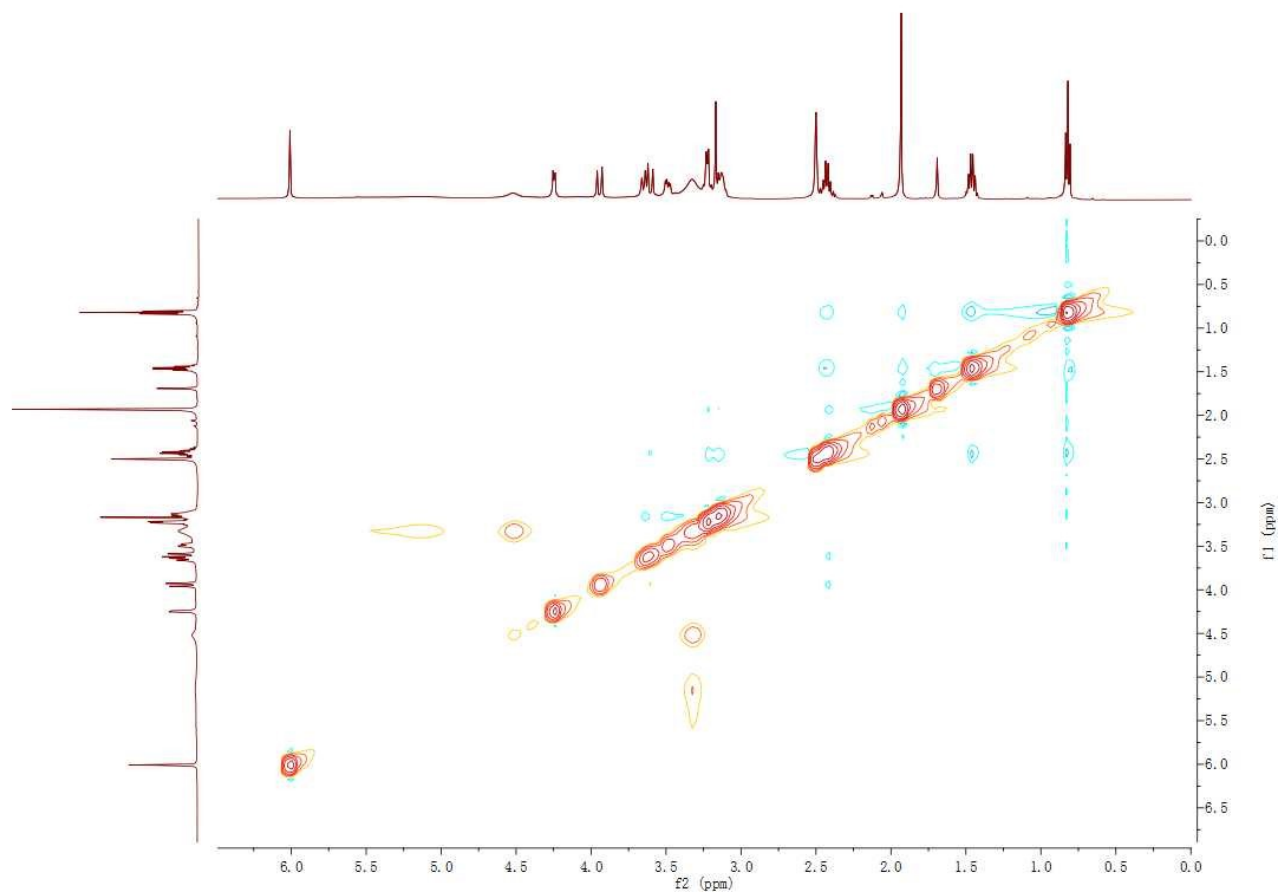
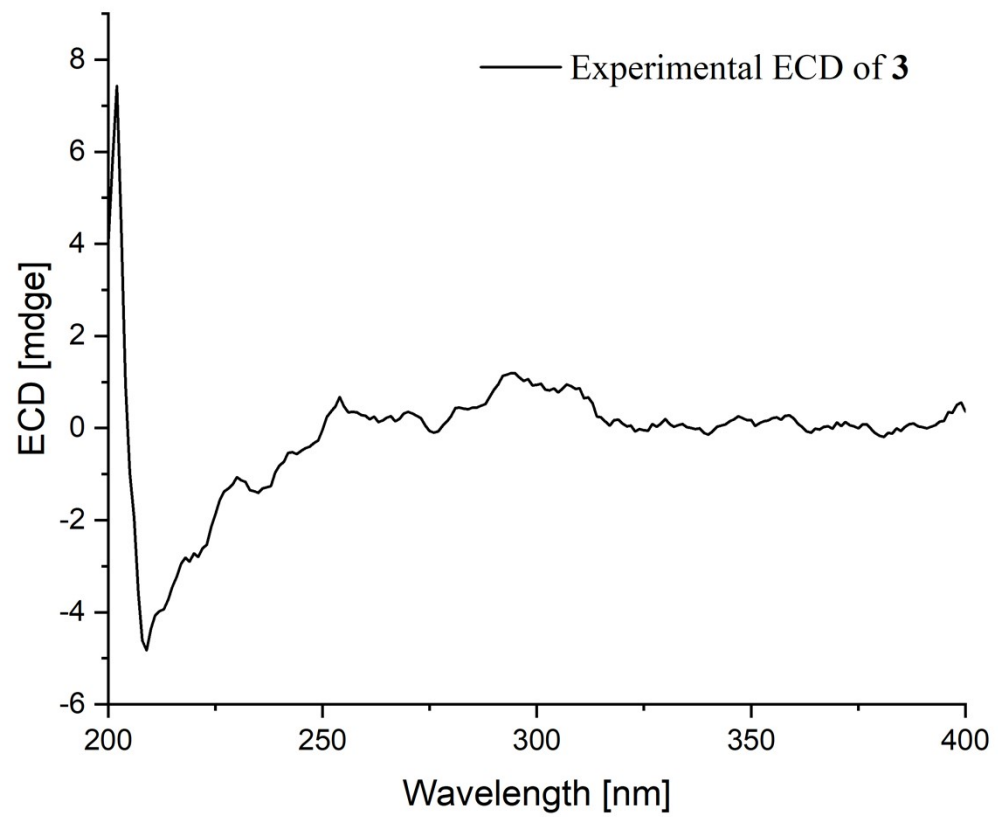


Figure S25. NOESY spectrum of compound 3;

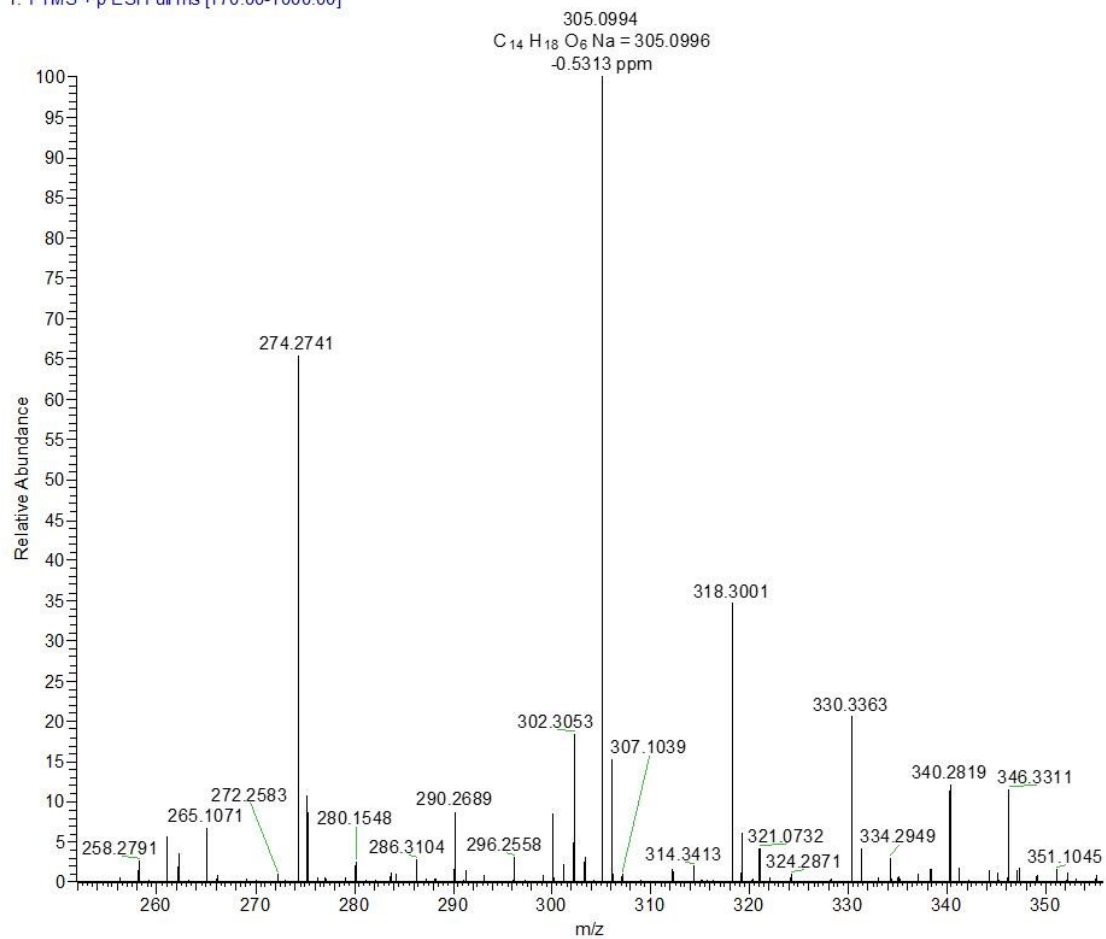


**Figure S26.** ECD spectrum of compound **3**;



**Figure S27.** HRESI mass spectrum of compound **4**;

20200901-CS113-36\_200901075917 #76-77 RT: 0.74-0.74 AV: 2 NL: 8.51E6  
T: FTMS + p ESI Full ms [170.00-1000.00]





**Figure S28.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **4**;

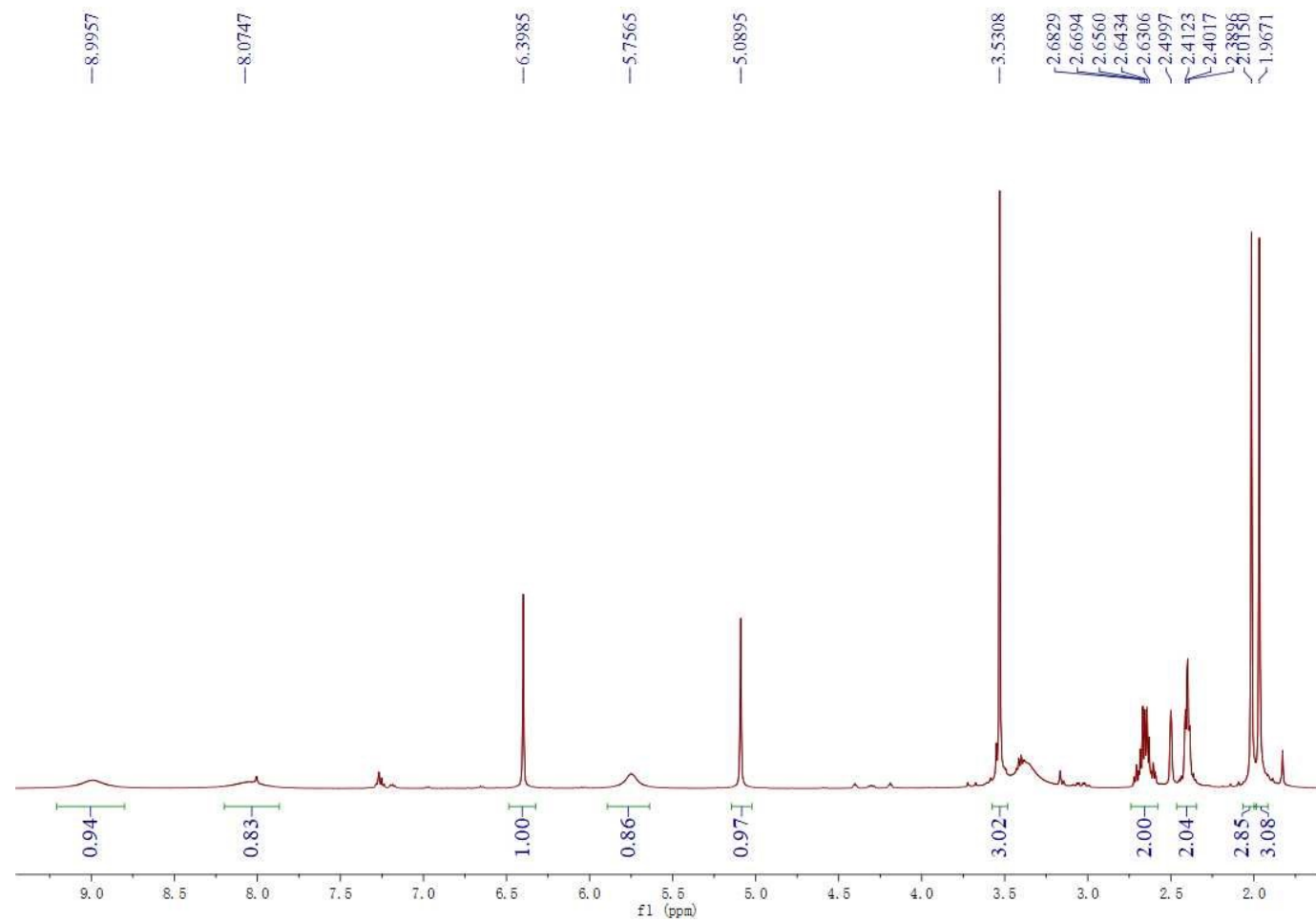


Figure S29.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound 4;

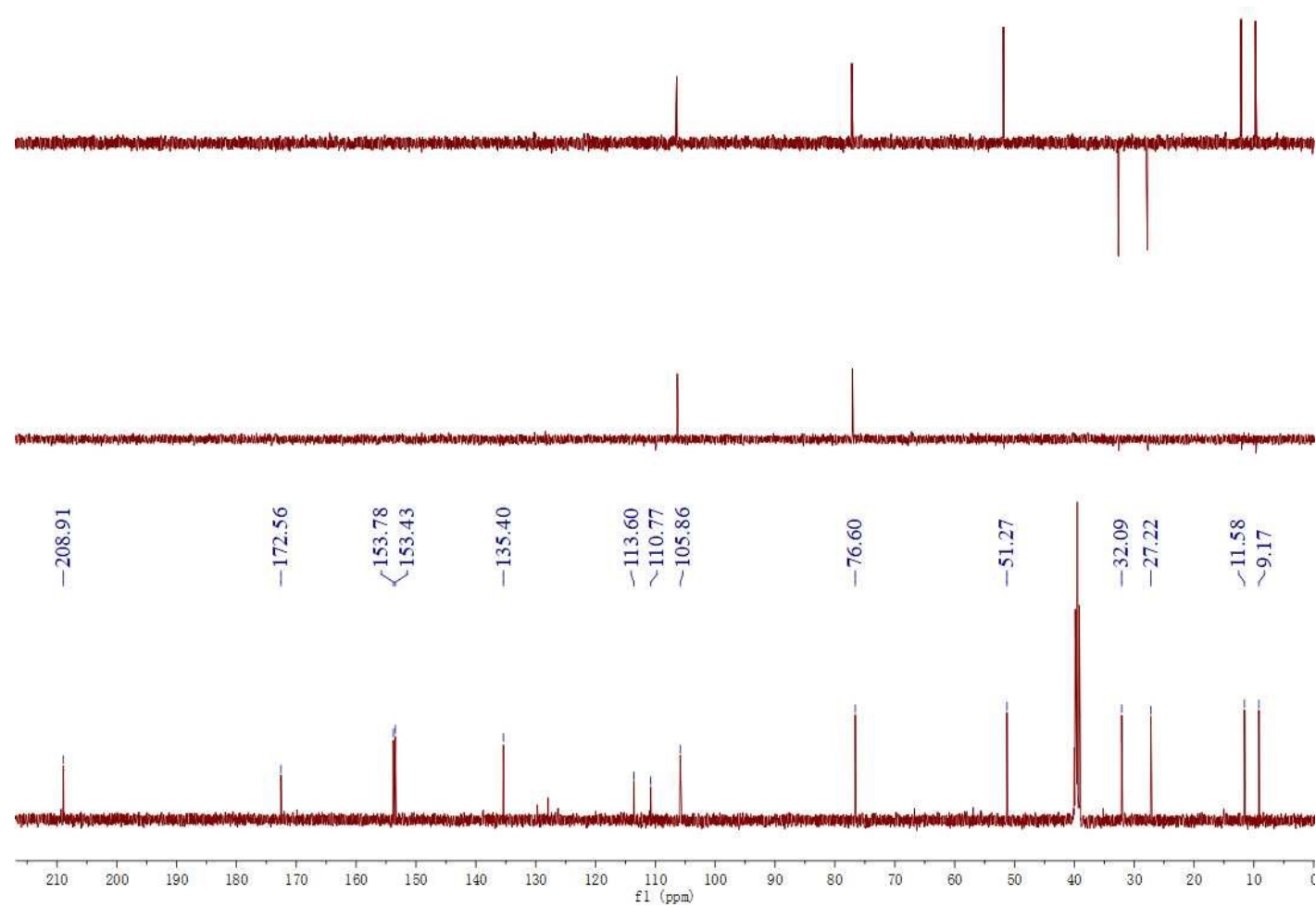


Figure S30. COSY spectrum of compound 4;

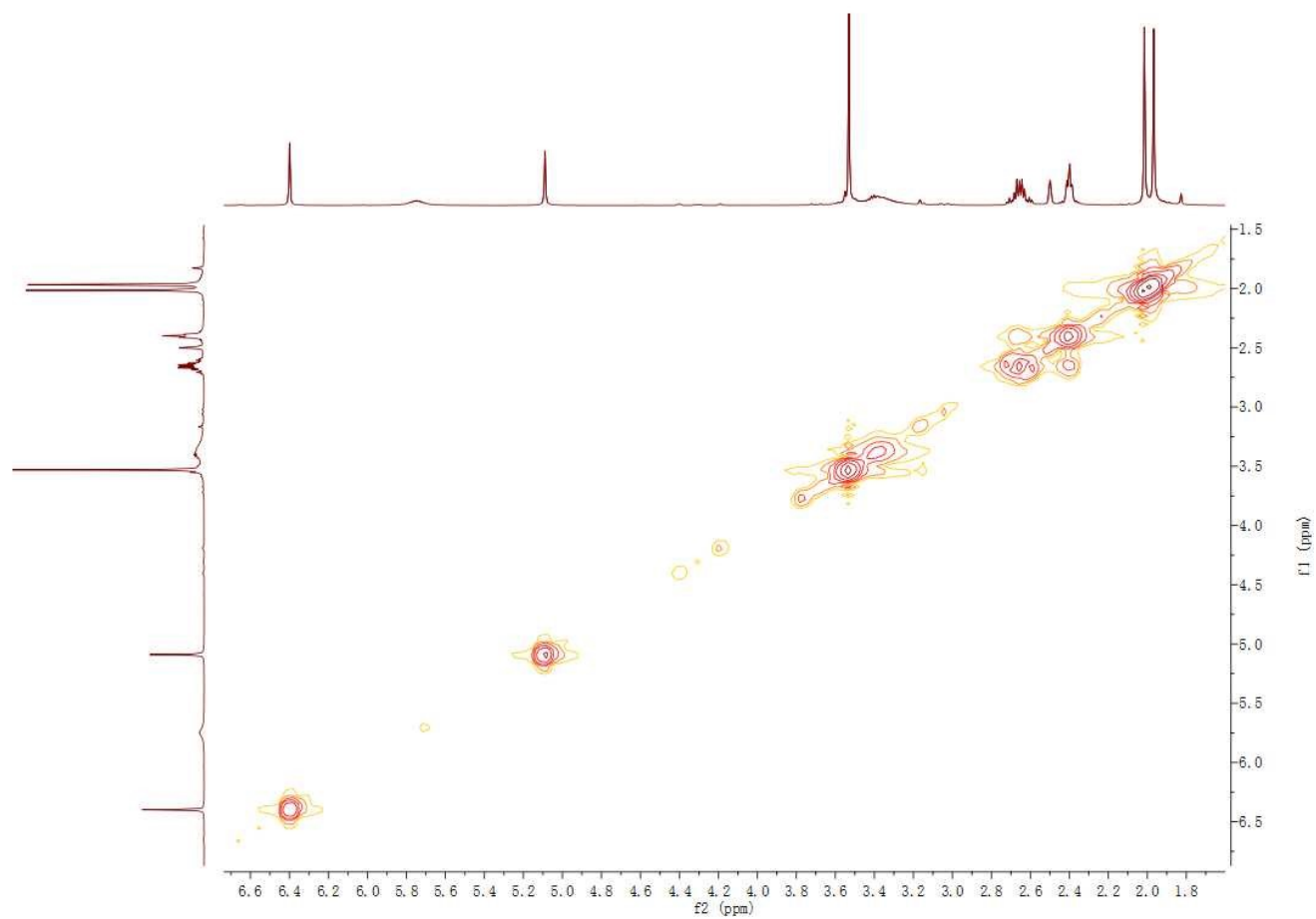


Figure S31. HSQC spectrum of compound 4;

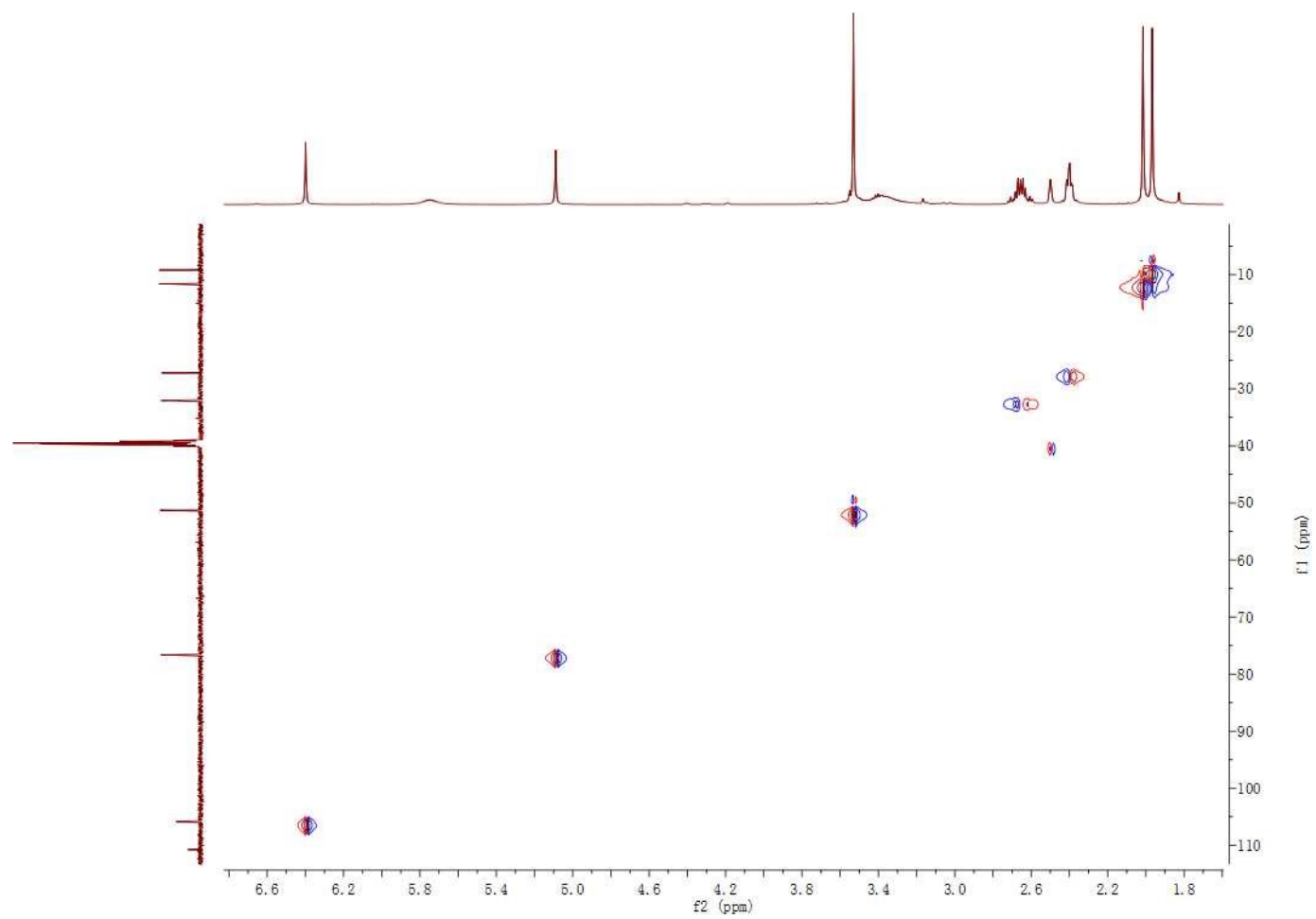


Figure S32. HMBC spectrum of compound 4;

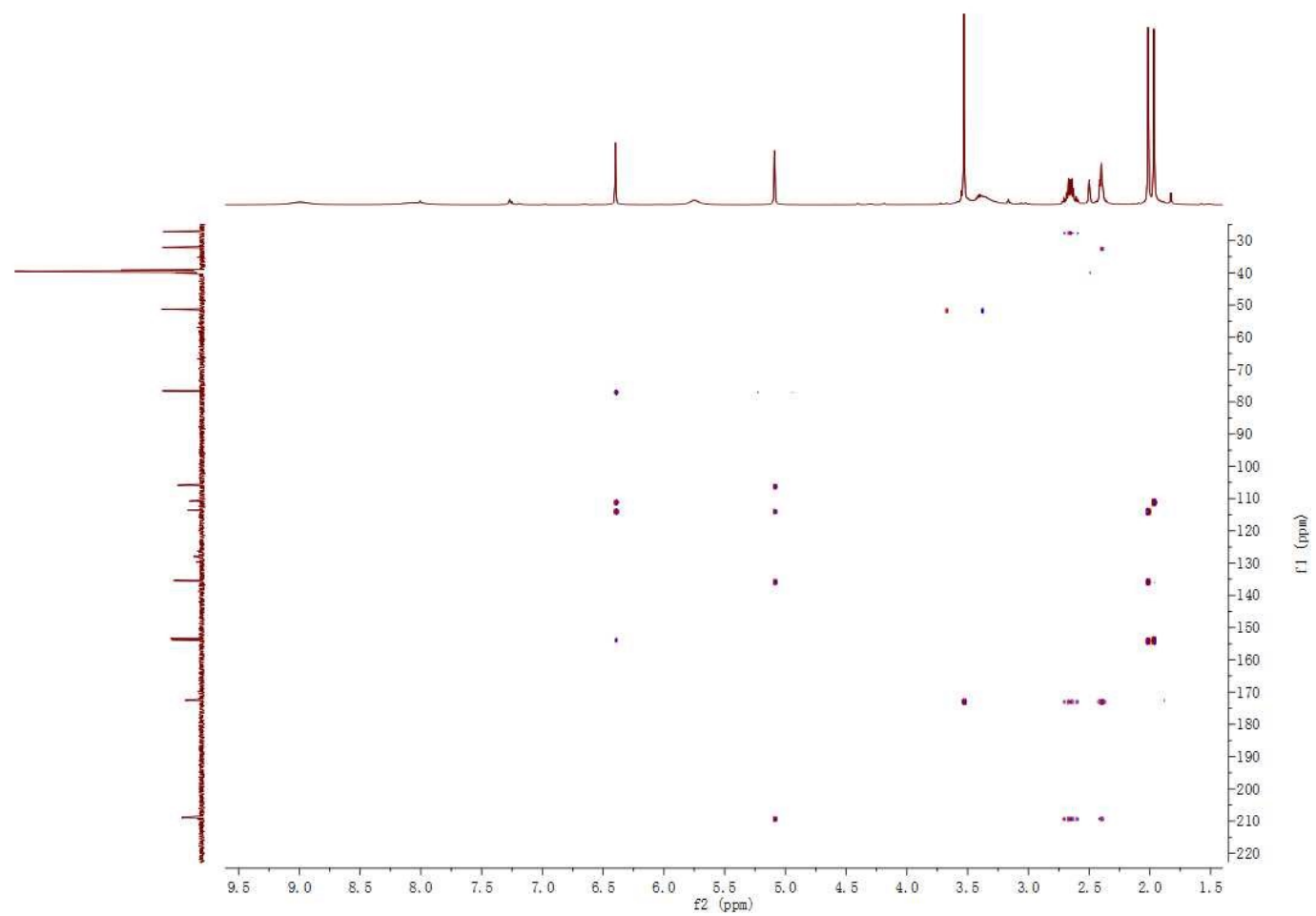
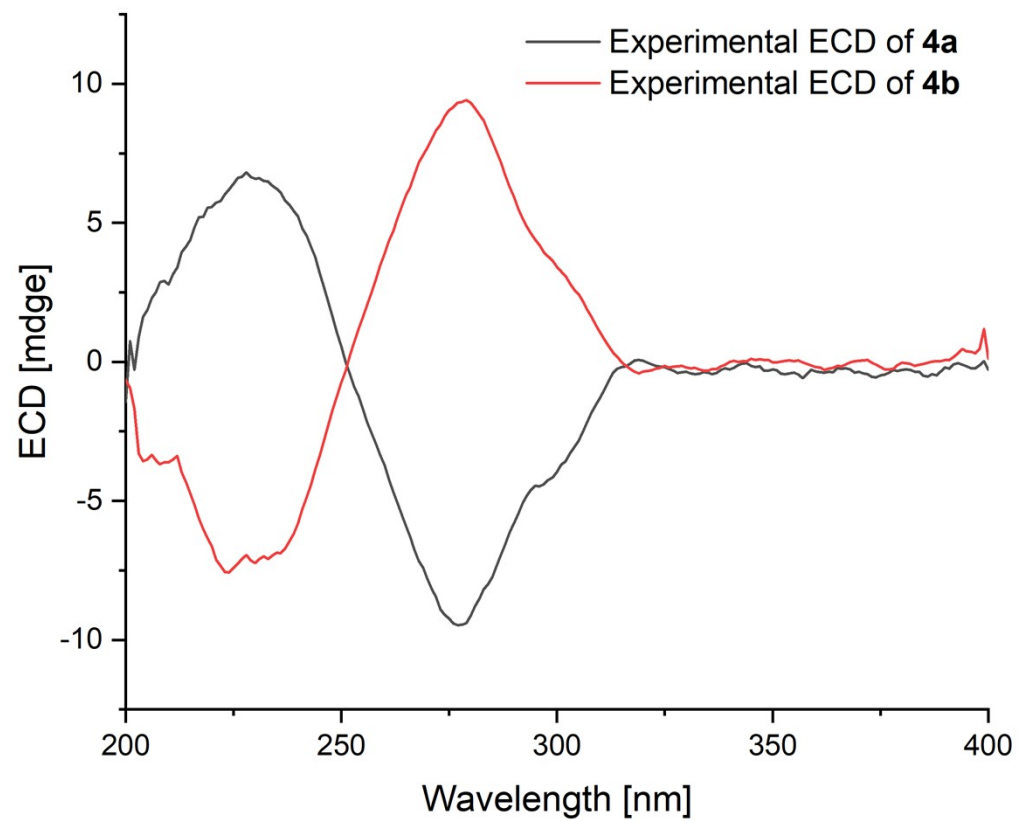
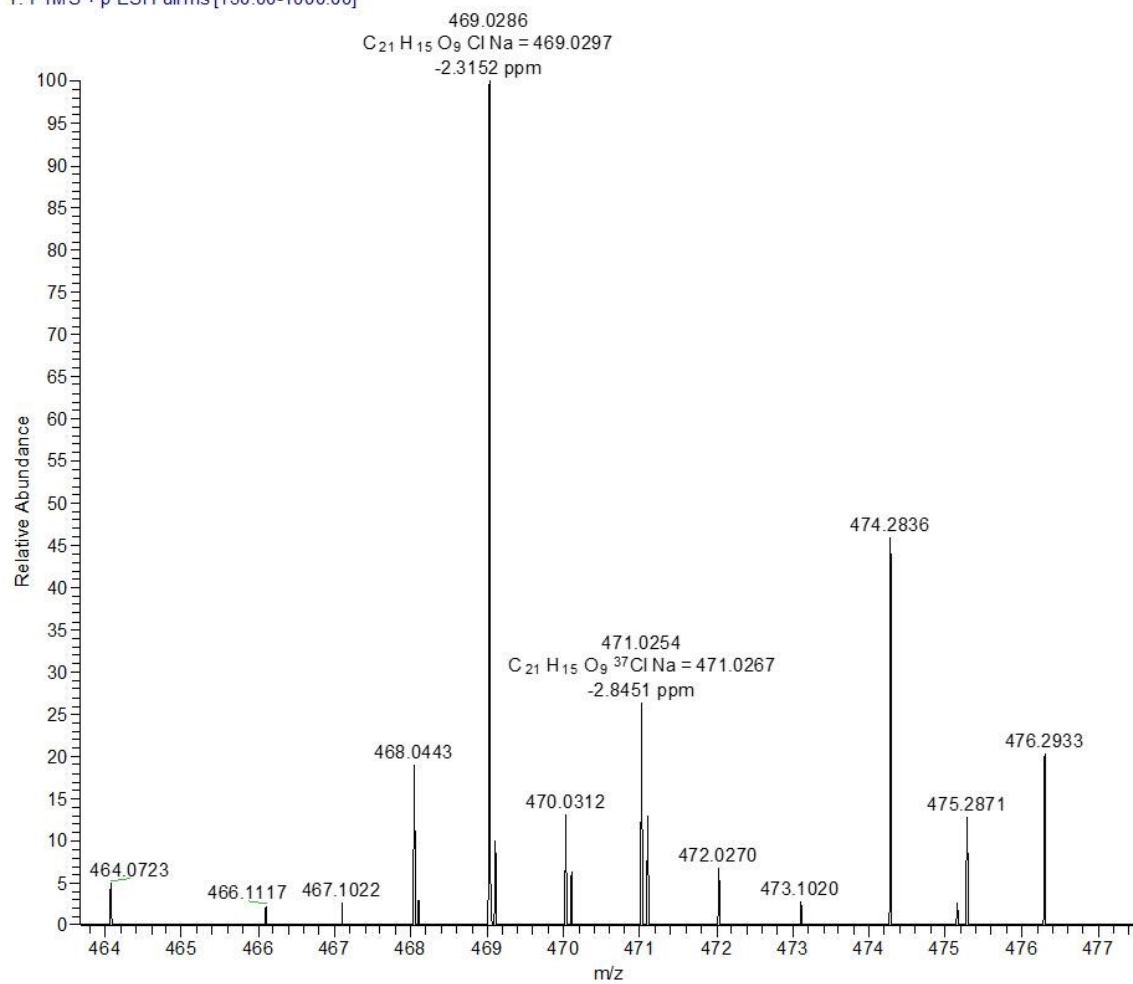


Figure S33. ECD spectra of compounds **4a** and **4b**;



**Figure S34.** HRESI mass spectrum of compound **5**;

20200707-CS113-28\_200706102148 #80 RT: 0.62 AV: 1 NL: 1.07E6  
T: FTMS +p ESI Full ms [150.00-1000.00]



**Figure S35.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **5**;

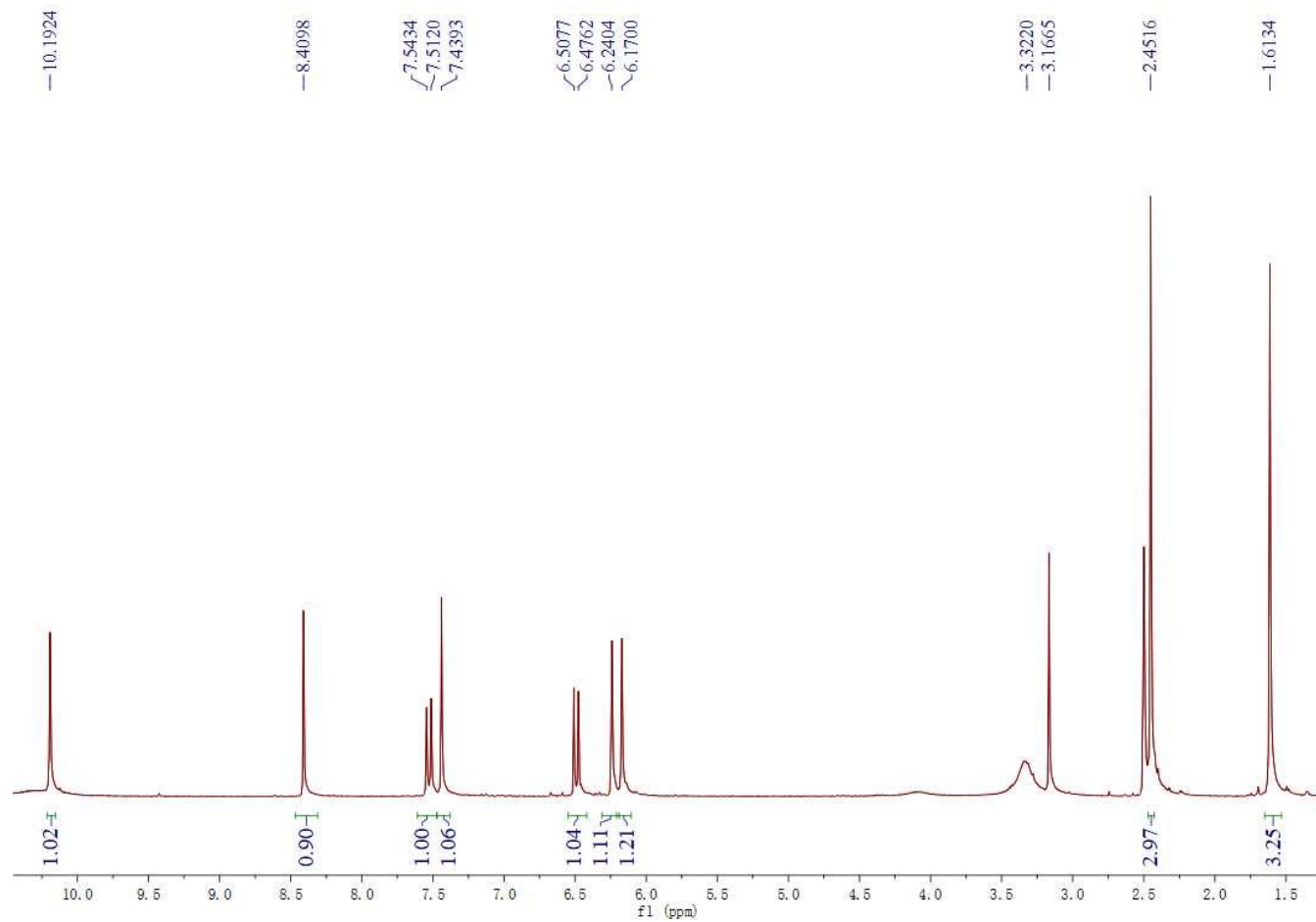
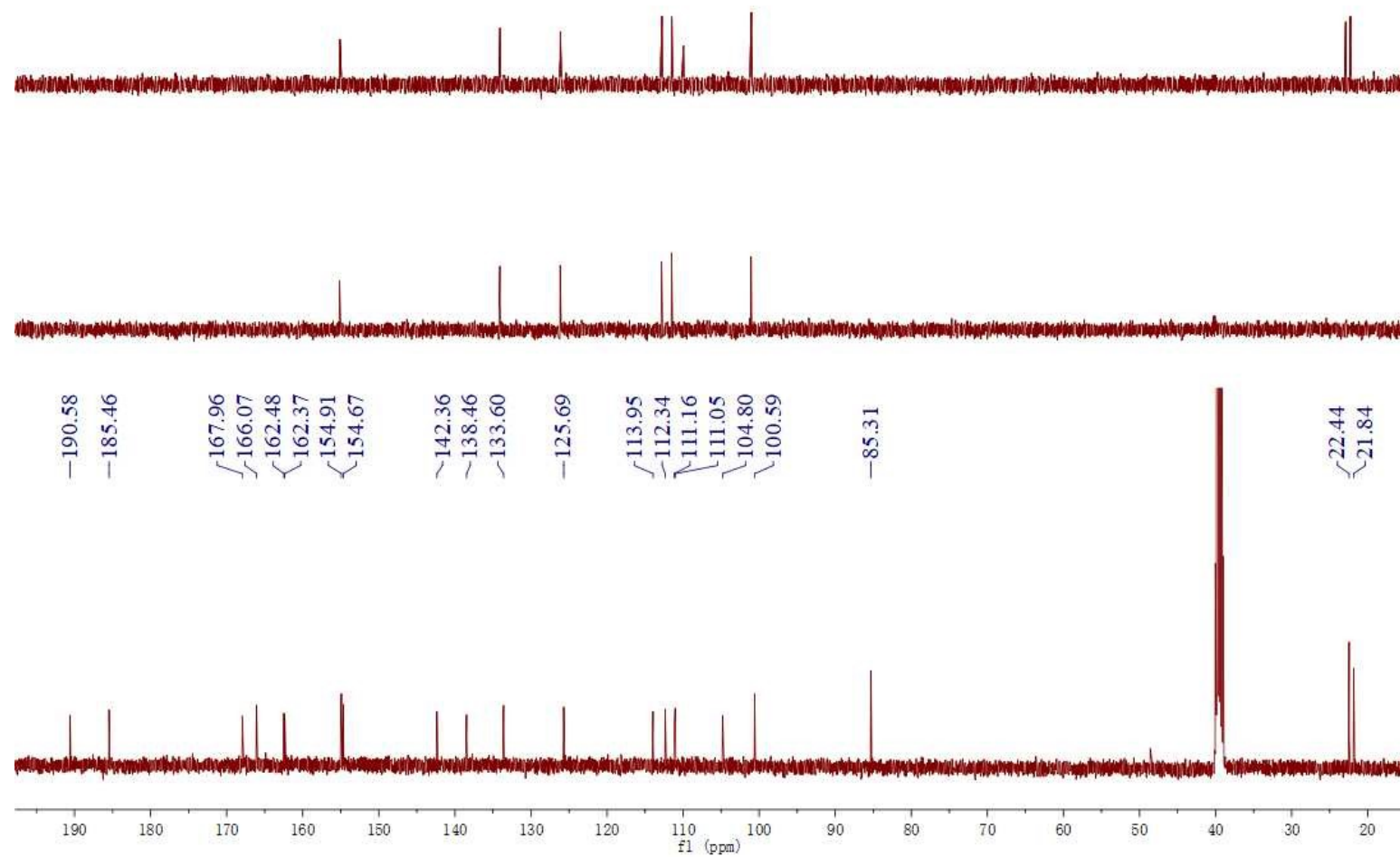




Figure S36.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **5**;



**Figure S37.** COSY spectrum of compound **5**;

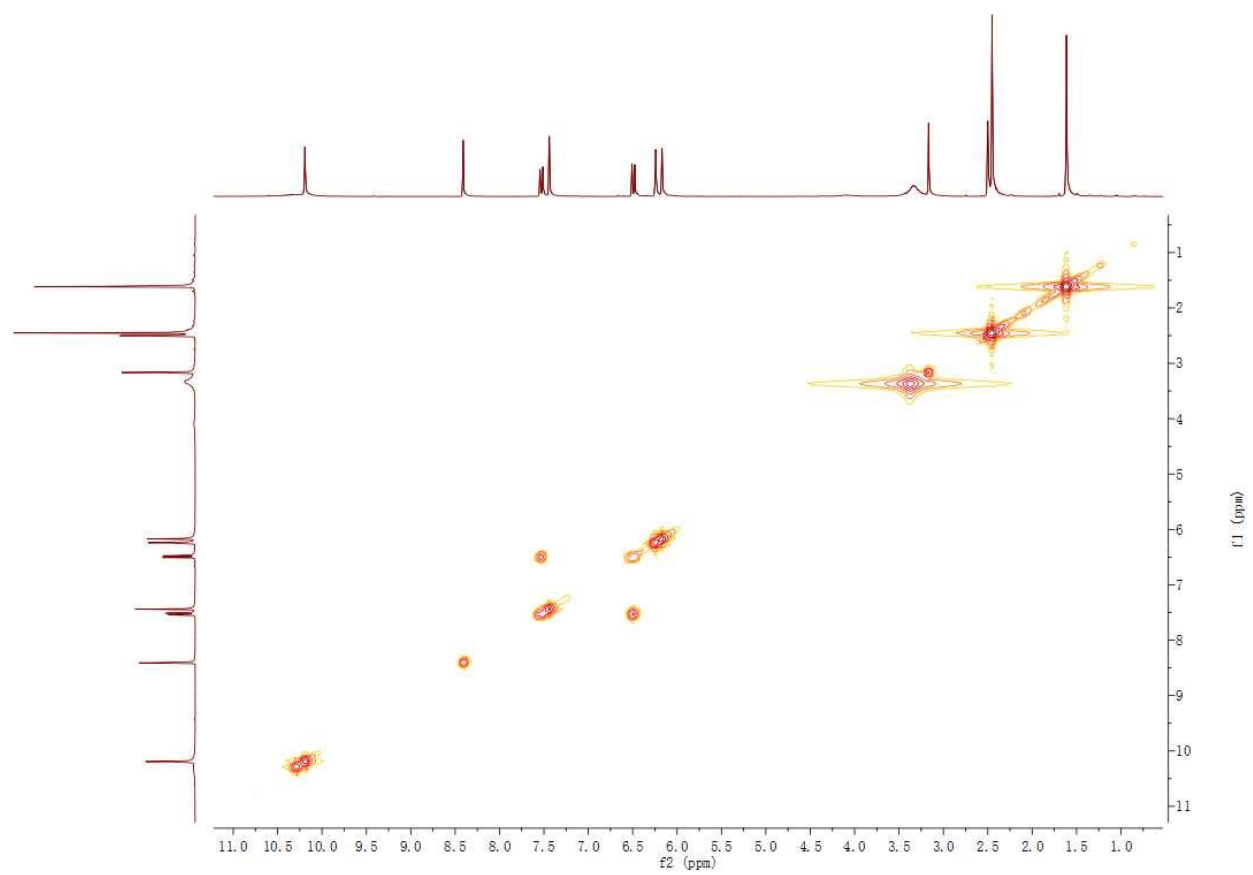


Figure S38. HSQC spectrum of compound 5;

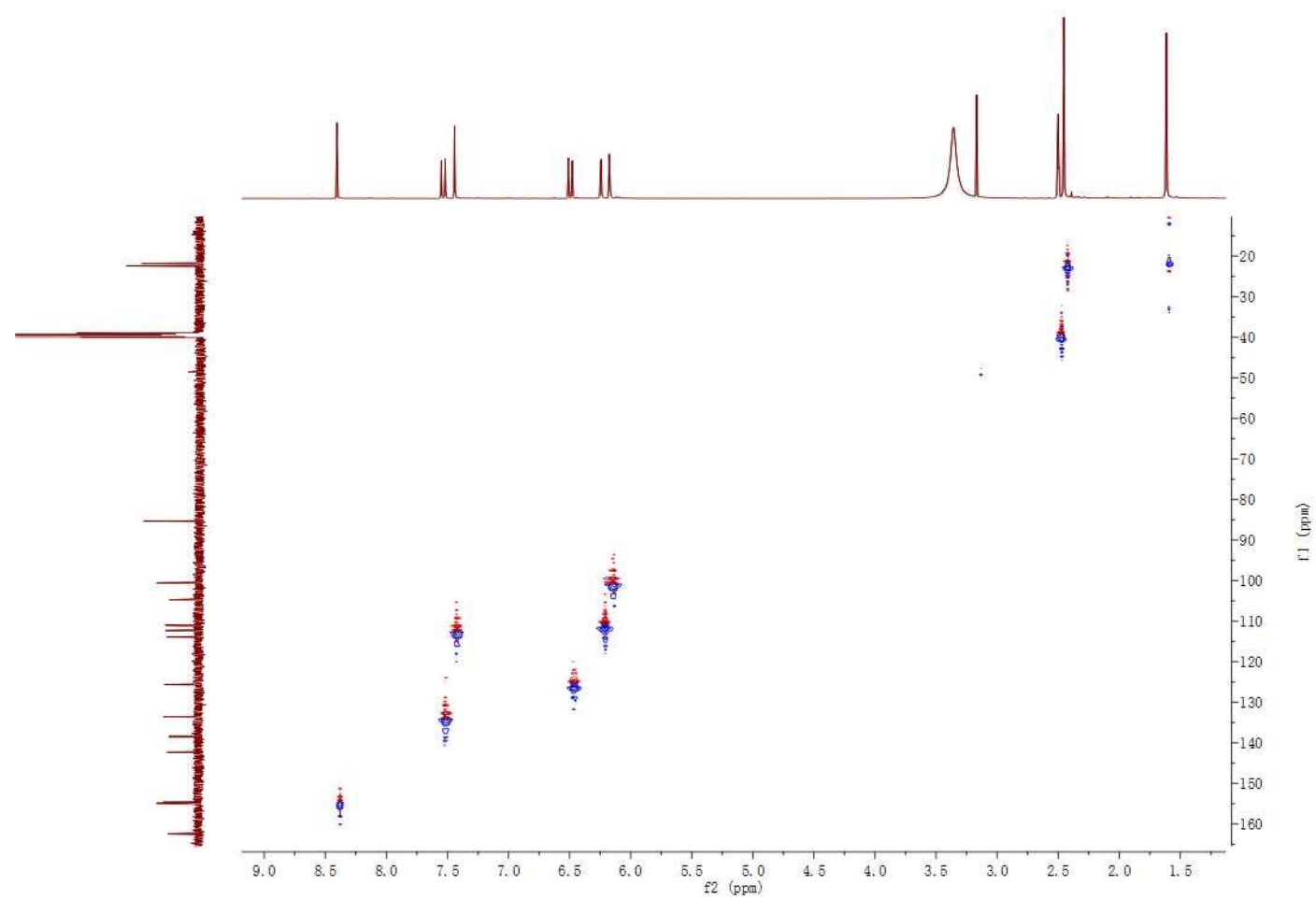
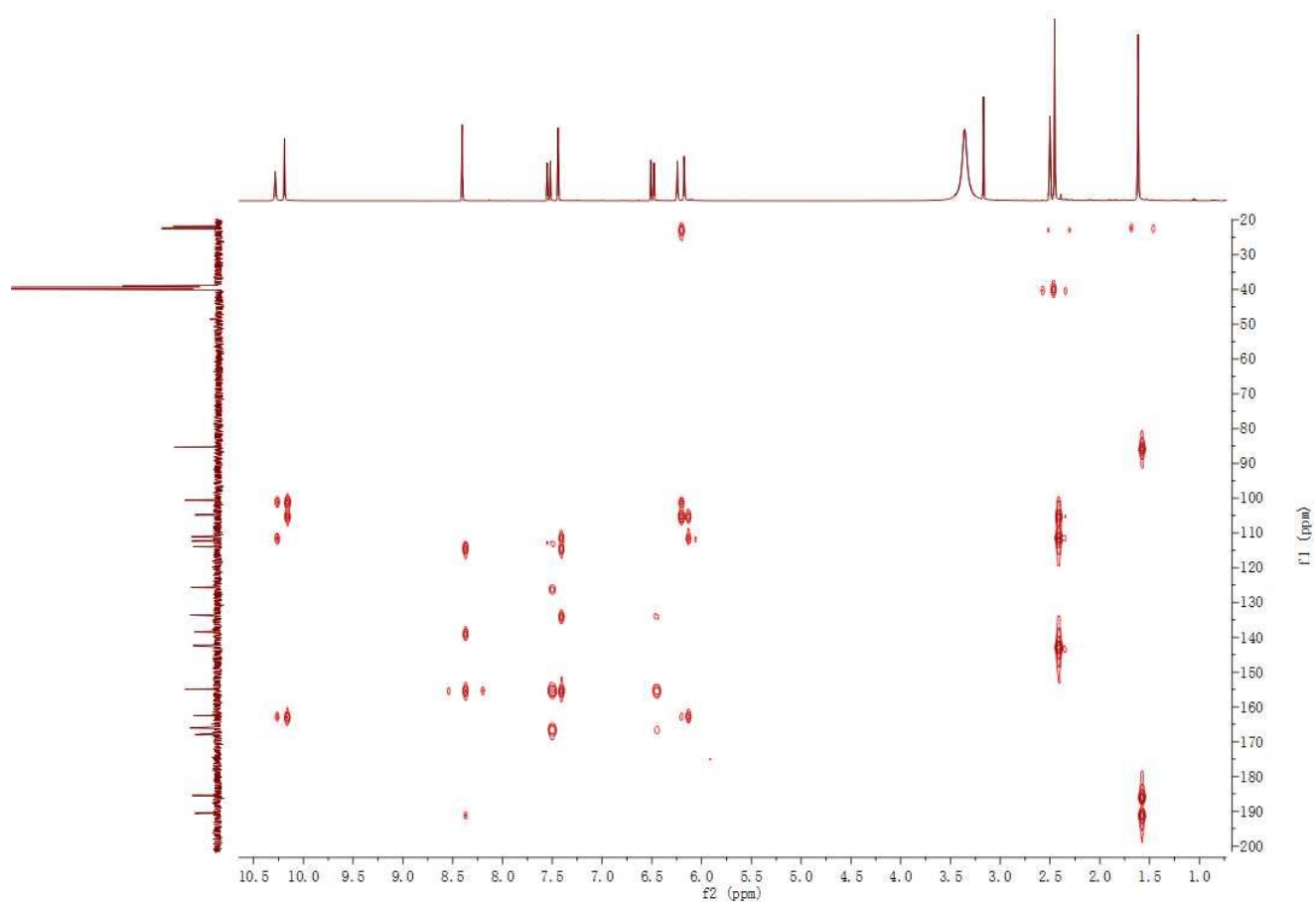
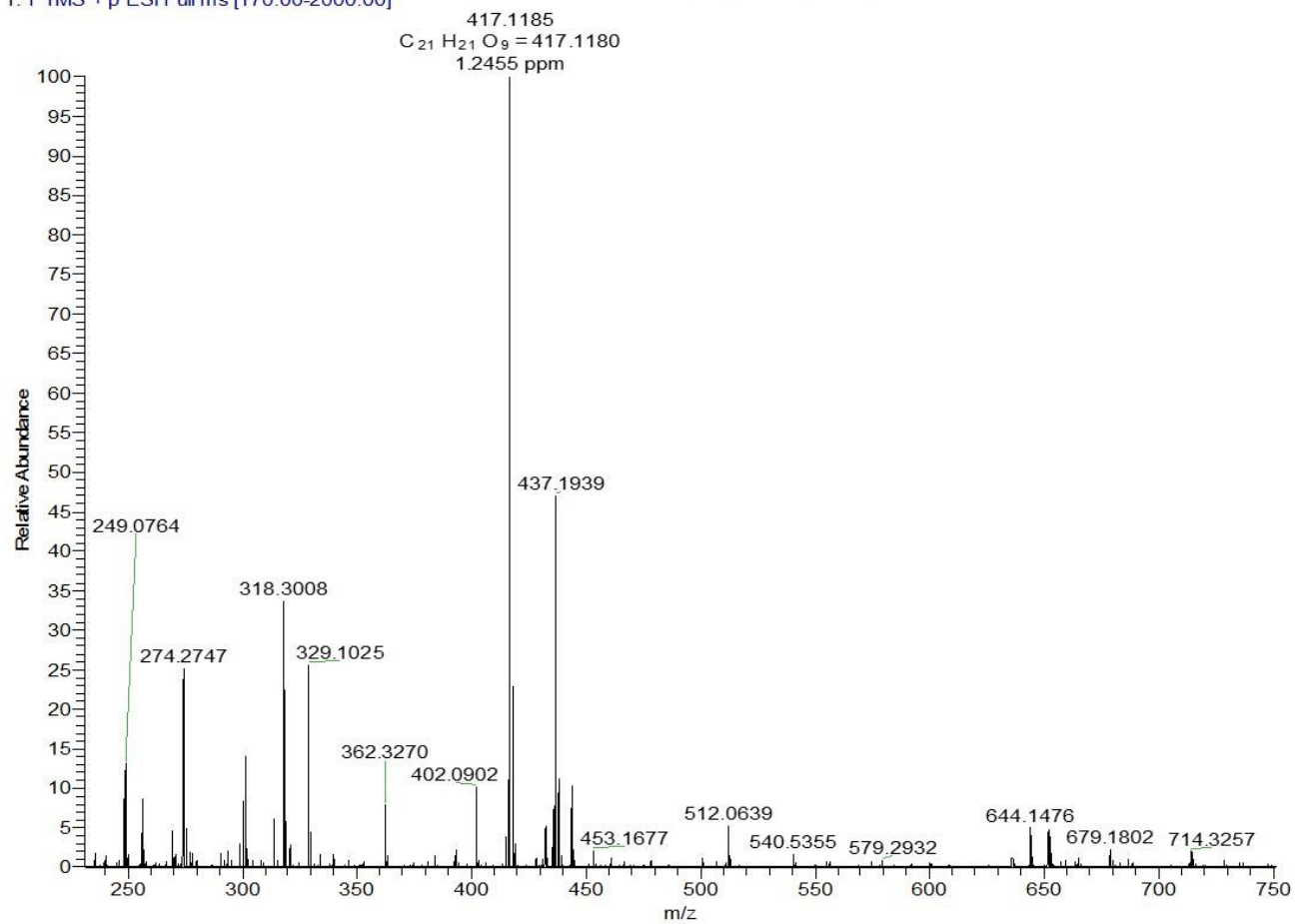


Figure S39. HMBC spectrum of compound 5;



**Figure S40.** HRESI mass spectrum of compound **6**;

20200901-CS113-14\_200831152624 #121-122 RT: 1.01-1.02 AV: 2 SB: 15 0.12-0.24 NL: 6.07E6  
T: FTMS + p ESI Full ms [170.00-2000.00]



**Figure S41.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **6**;

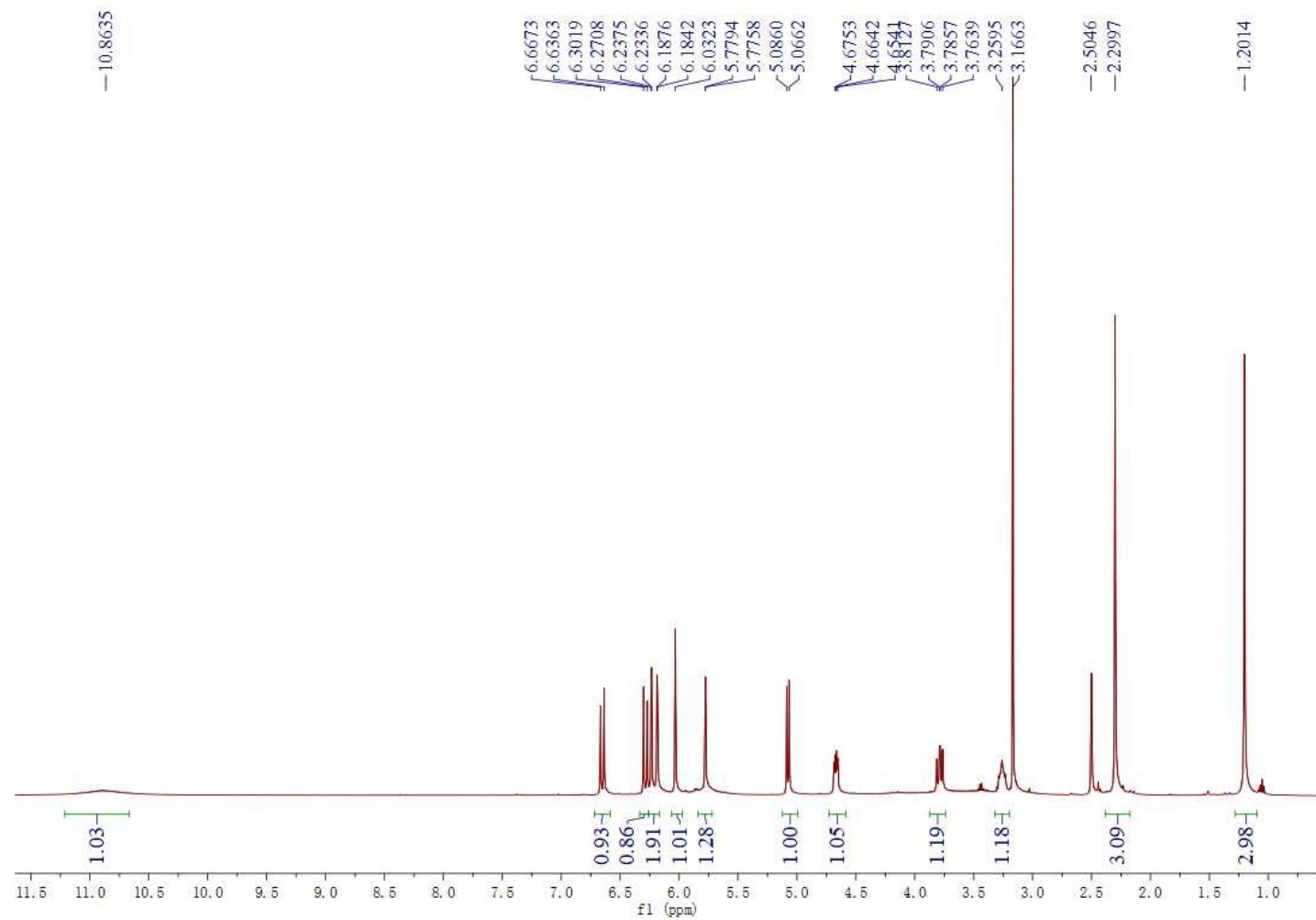


Figure S42.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound 6;

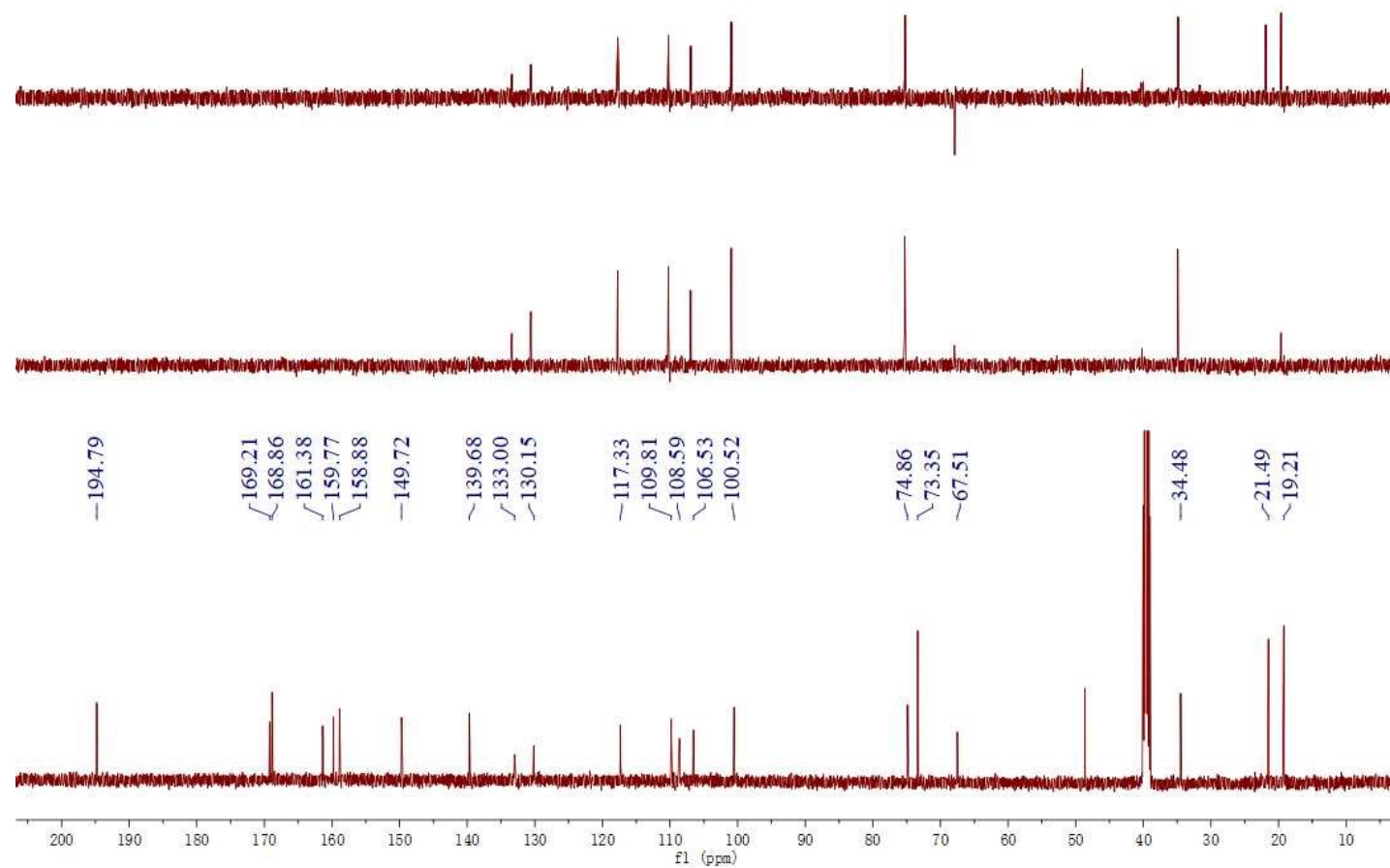


Figure S43. COSY spectrum of compound 6;

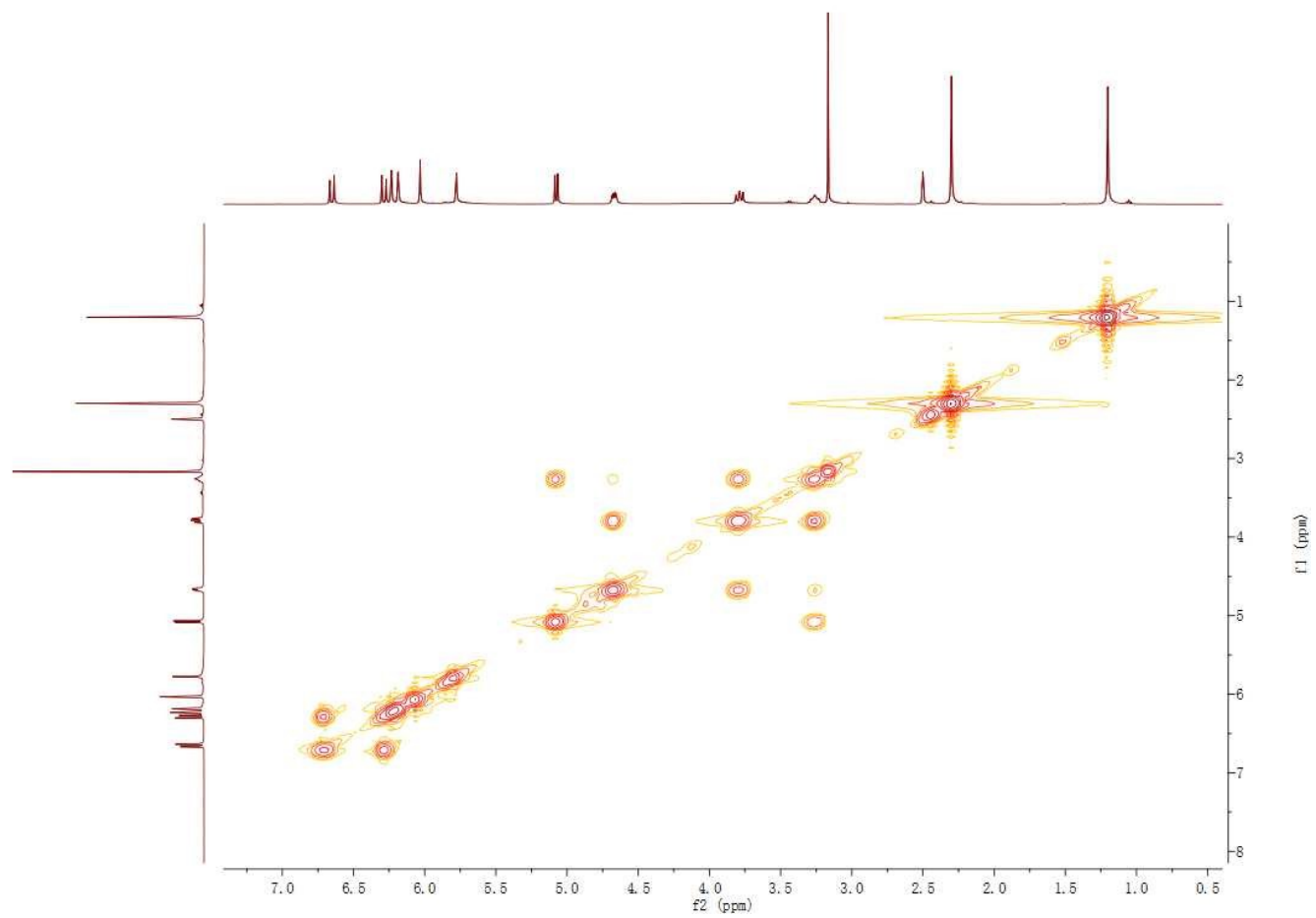




Figure S44. HSQC spectrum of compound 6;

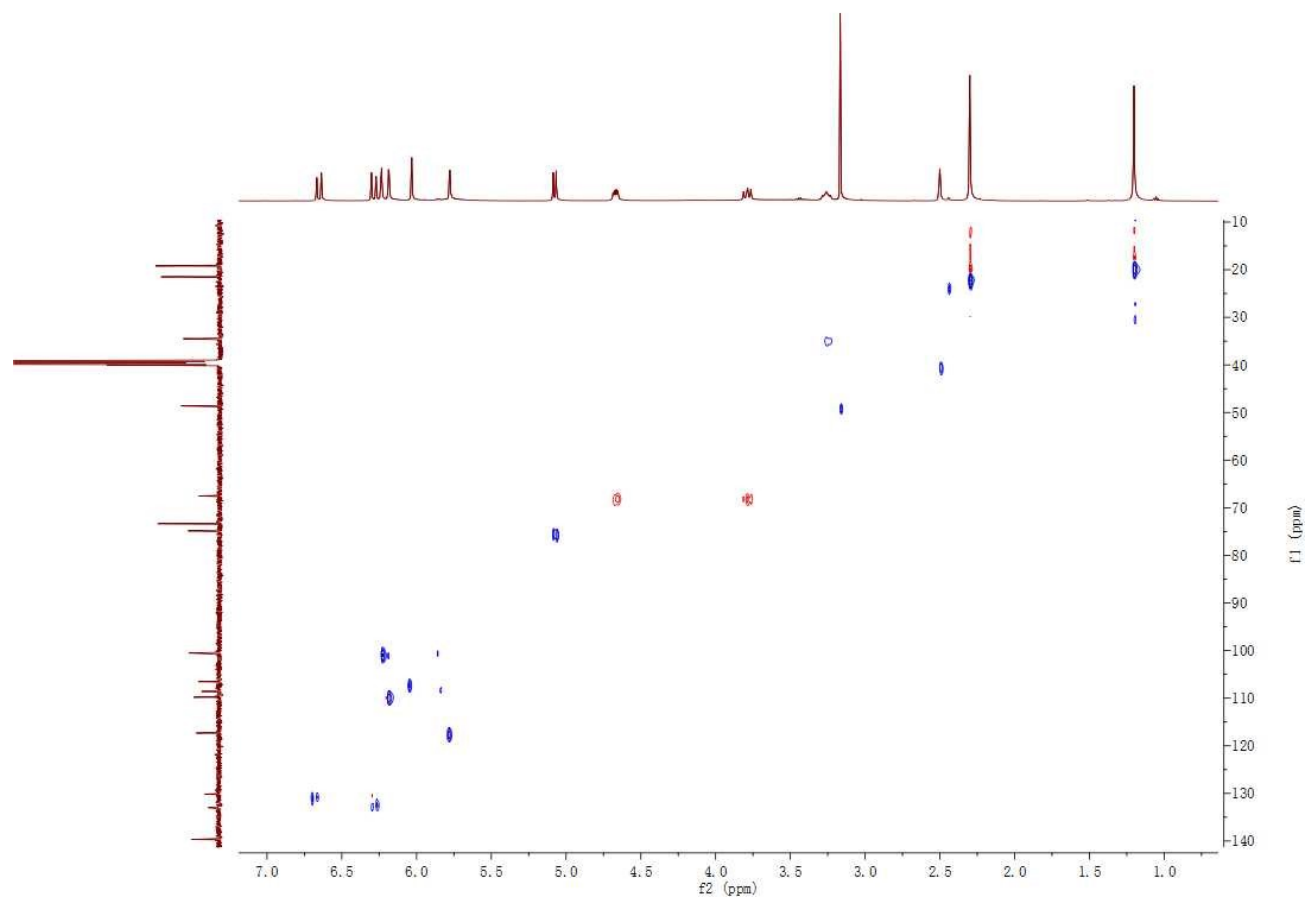


Figure S45. HMBC spectrum of compound 6;

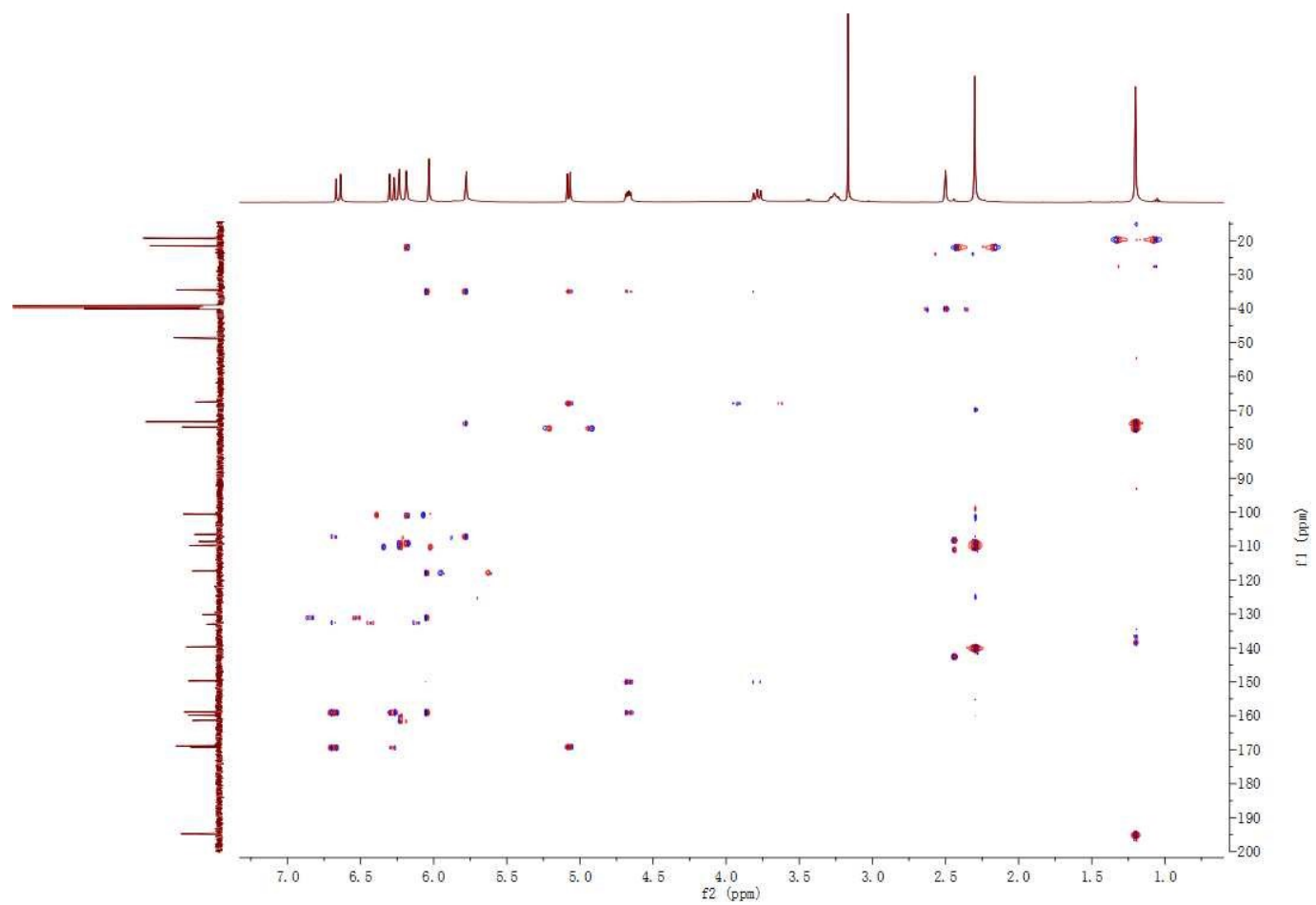
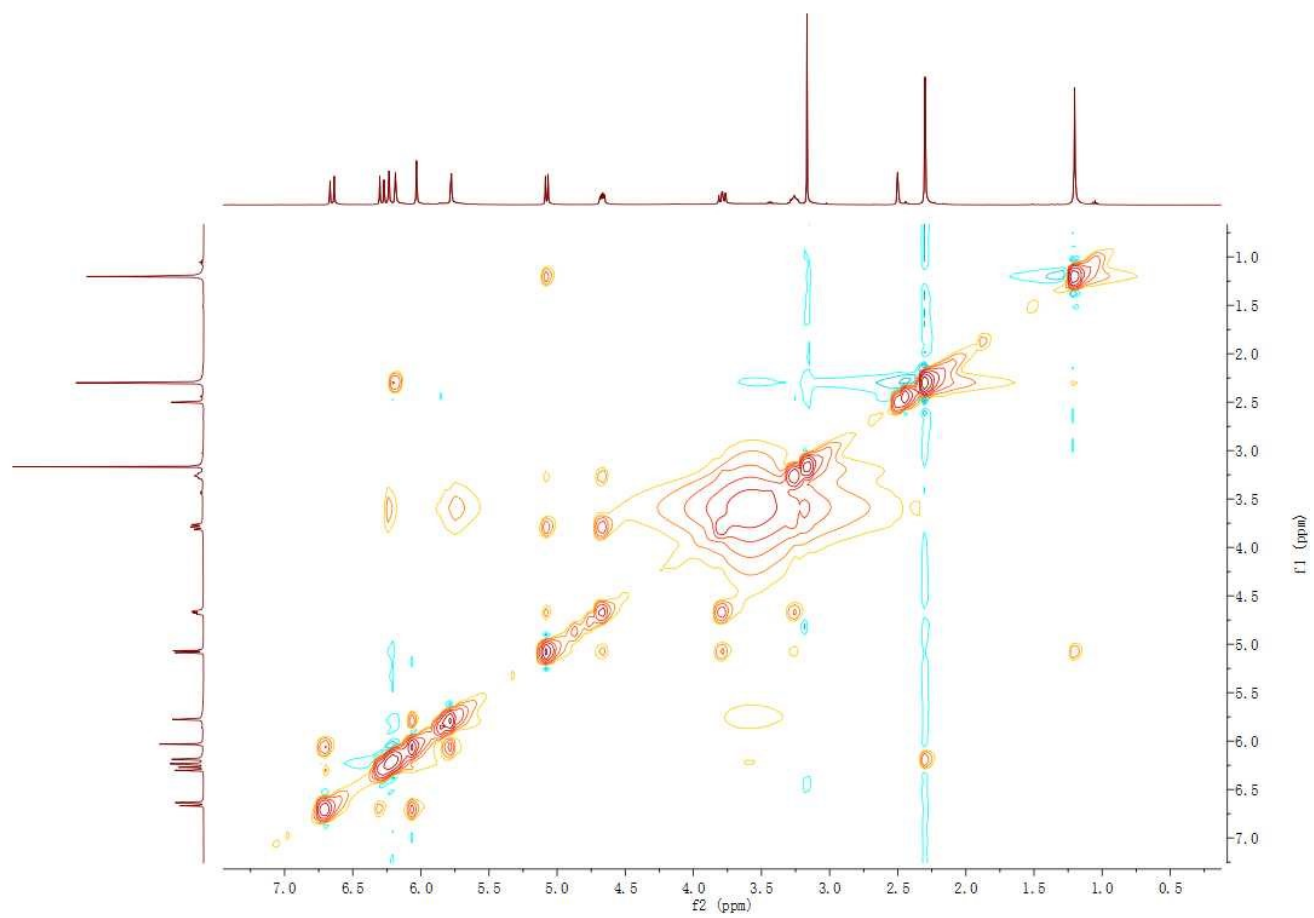
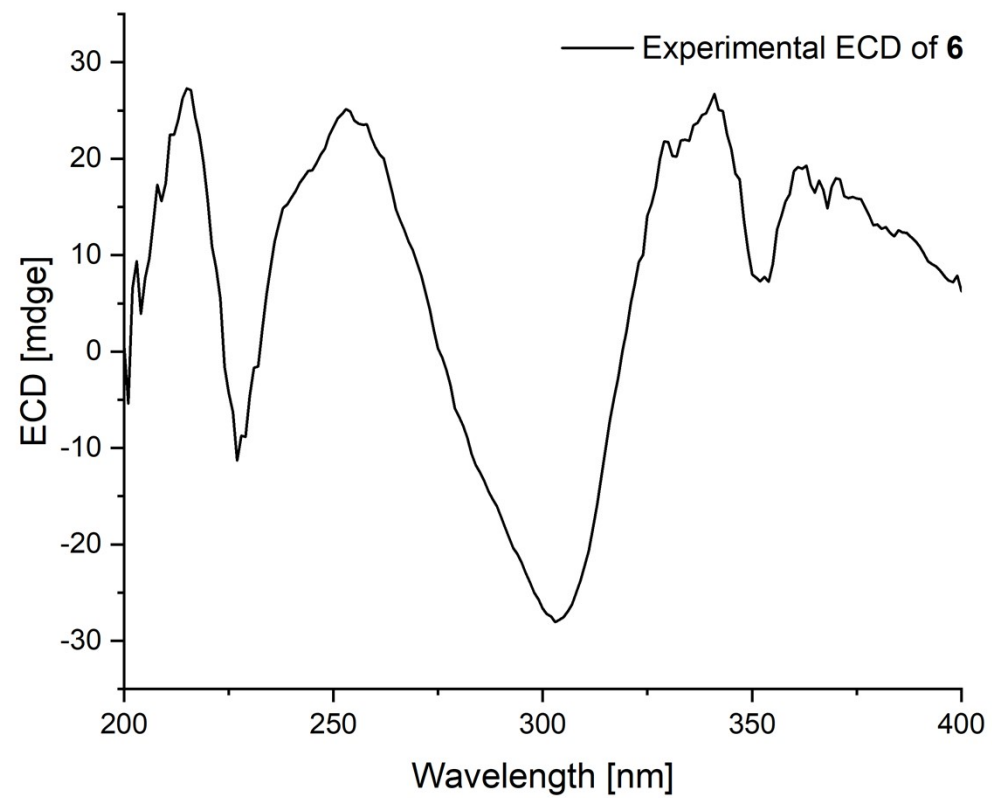


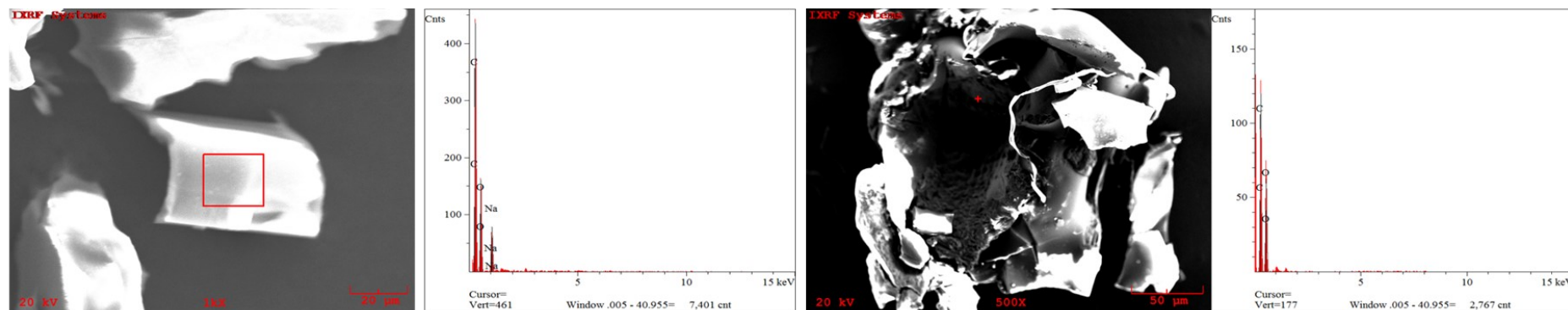
Figure S46. NOESY spectrum of compound 6;



**Figure S47.** ECD spectrum of compound **6**;



**Figure S48.** Scanning electron microscope analysis of compounds **6** and **10**;



Elt.	Line	Intensity (c/s)	Atomic %	Atomic Ratio	Conc	Units	Error 2-sig	MDL 3-sig	
C	Ka	183.62	59.899	1.000	51.911	wt. %	.835	.379	
O	Ka	71.97	36.542	.610	42.185	wt. %	1.104	.448	
Na	Ka	37.82	3.559	.059	5.903	wt. %	.229	.181	
			100.000		100.000	wt. %			Total

Elt.	Line	Intensity (c/s)	Atomic %	Atomic Ratio	Conc	Units	Error 2-sig	MDL 3-sig	
C	Ka	53.01	48.432	1.000	41.351	wt. %	1.234	.453	
O	Ka	29.66	51.568	1.065	58.649	wt. %	2.303	.000	
			100.000		100.000	wt. %			Total

**Figure S49.** ESI mass spectrum of compound 7;

CS113-100 #24 RT: 0.26 AV: 1 NL: 4.19E7

T: FTMS - p ESI Full ms [100.00-2000.00]

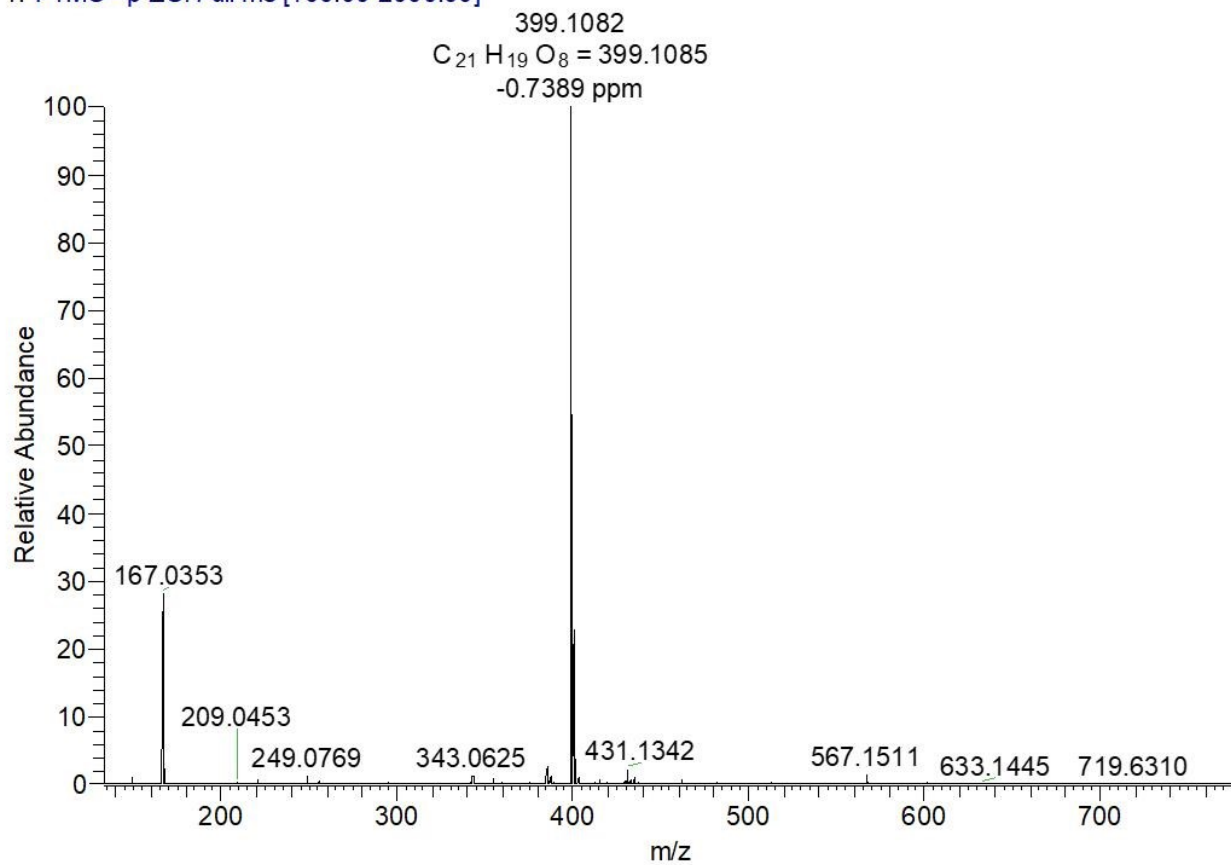


Figure S50.  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 7;

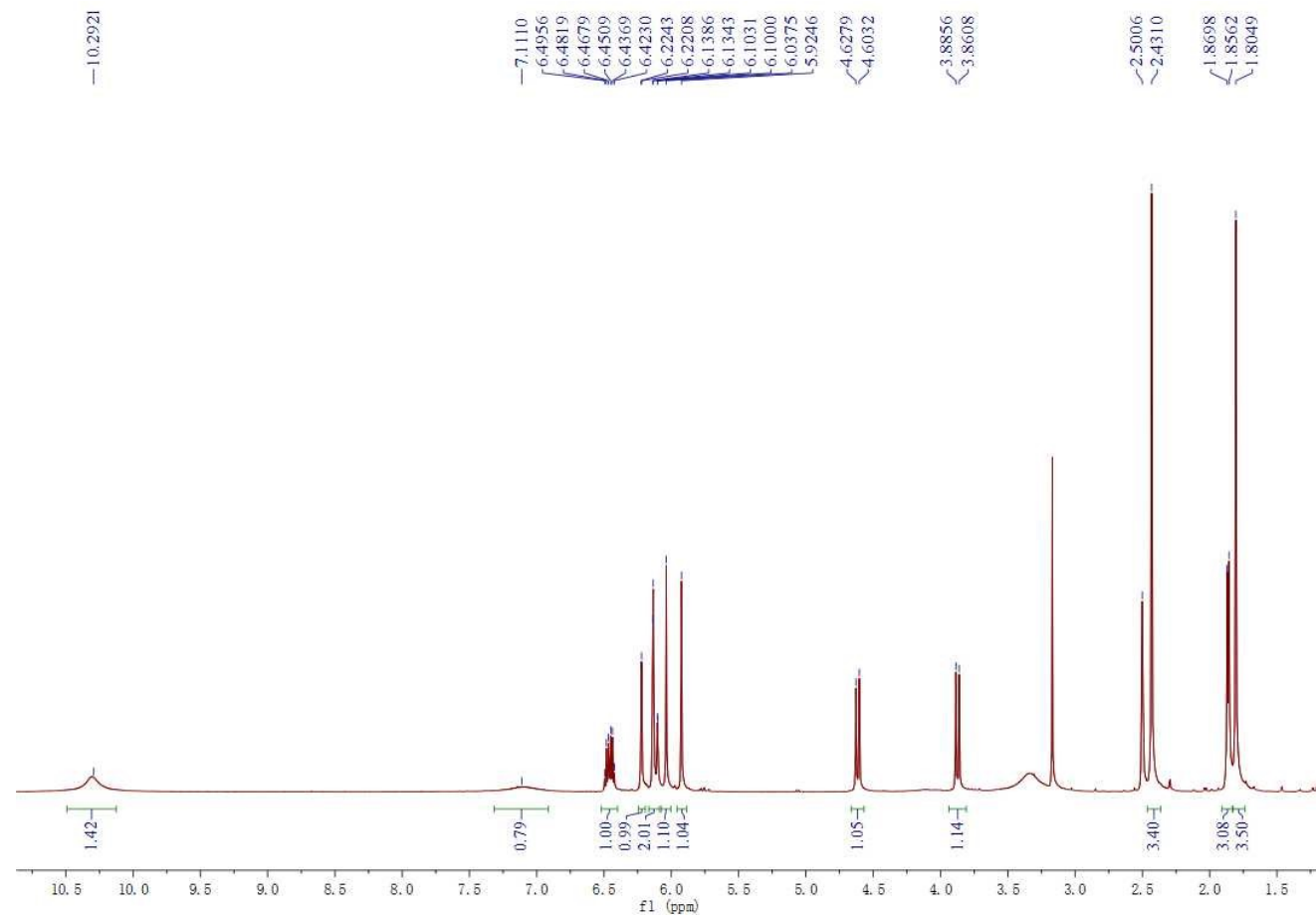


Figure S51.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound 7;

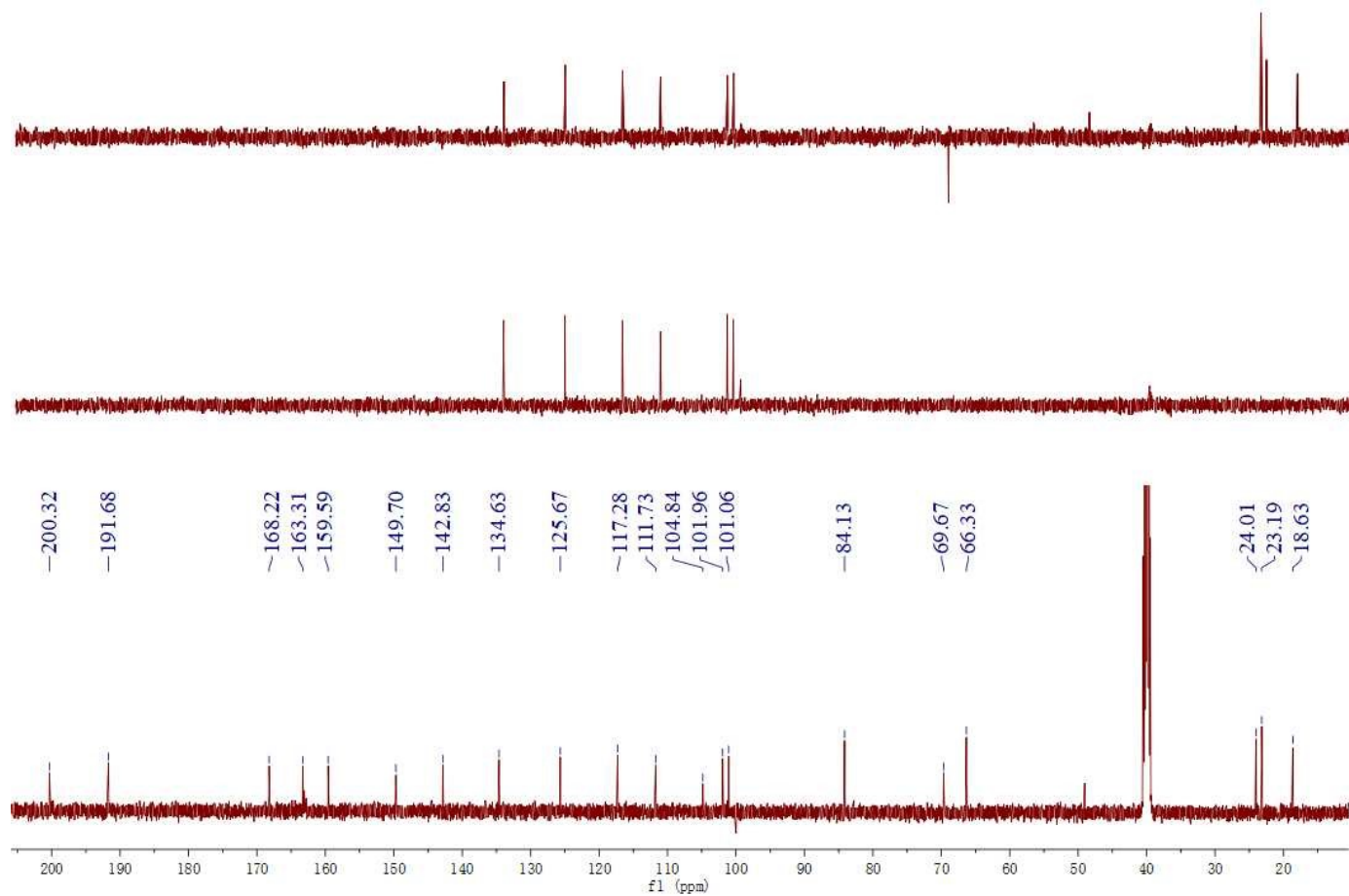




Figure S52. COSY spectrum of compound 7;

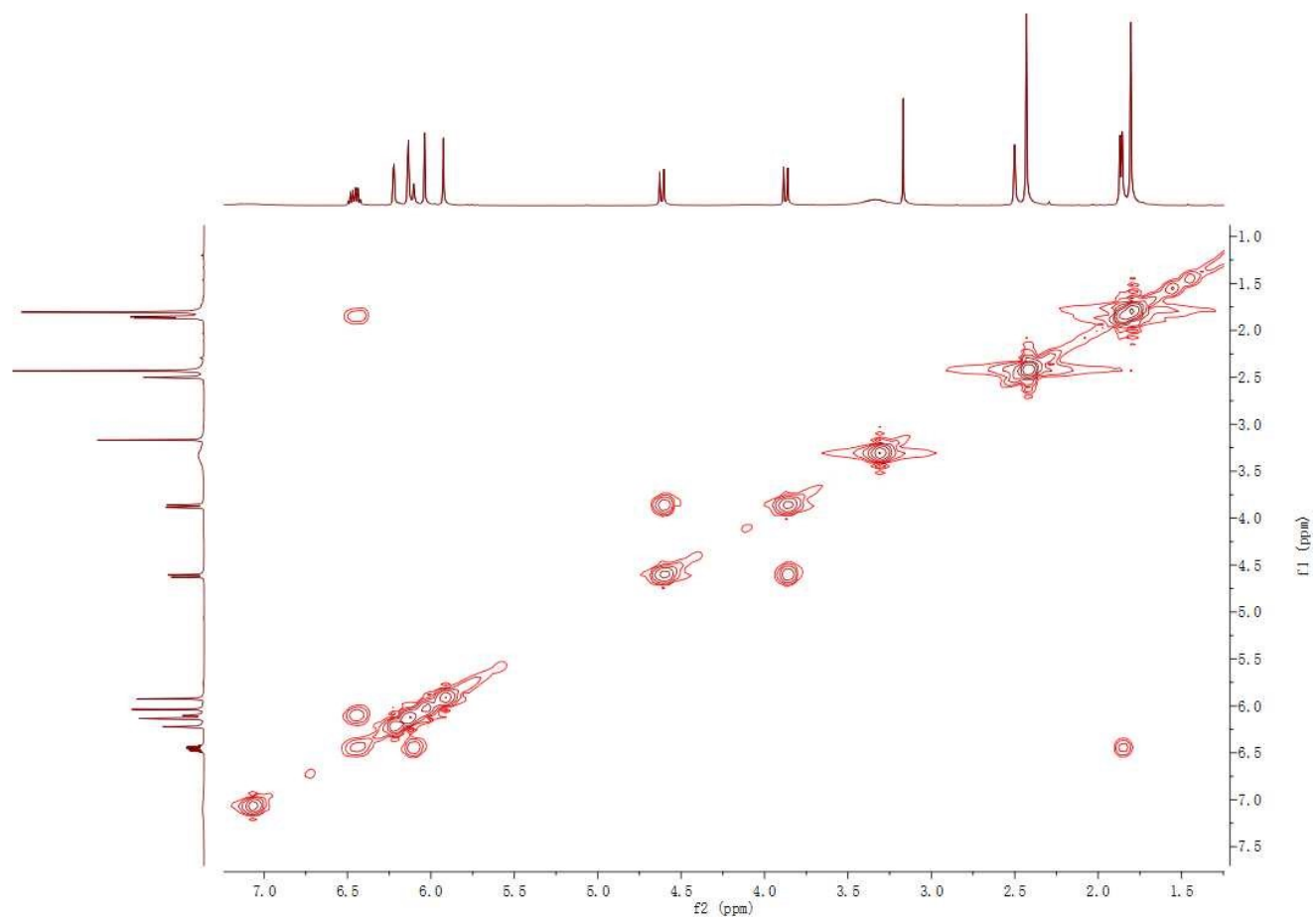


Figure S53. HSQC spectrum of compound 7;

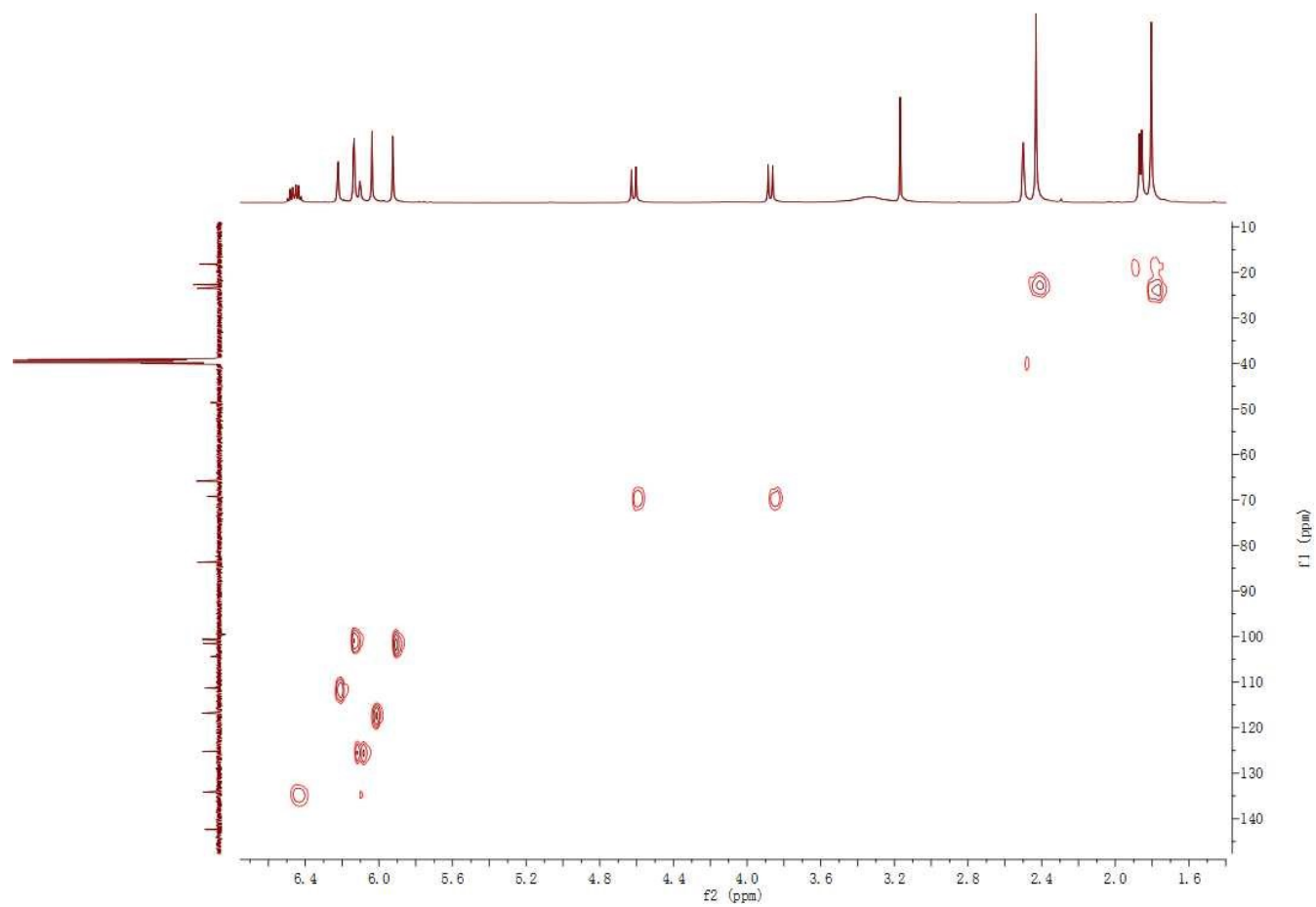


Figure S54. HMBC spectrum of compound 7;

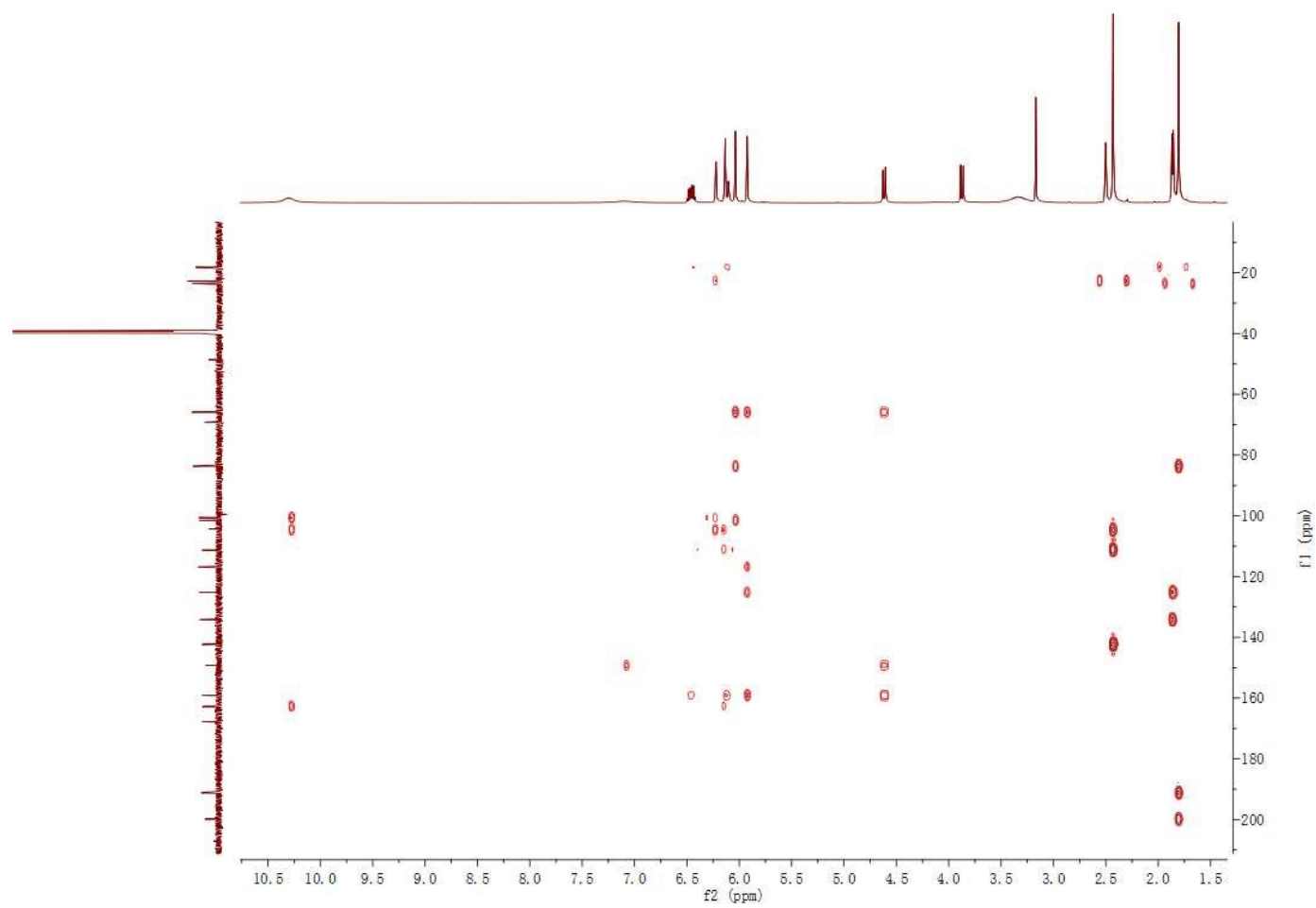


Figure S55. NOESY spectrum of compound 7;

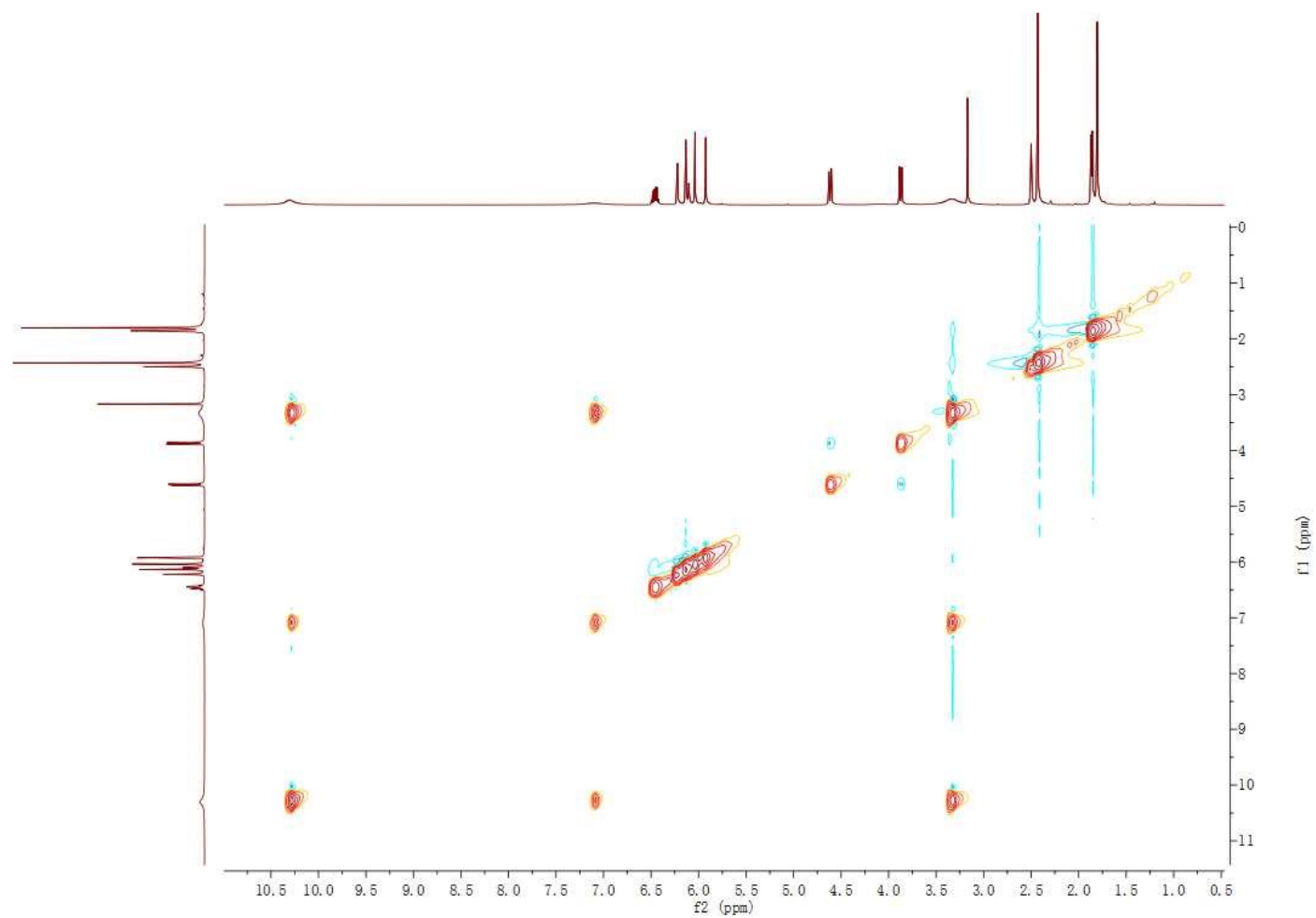
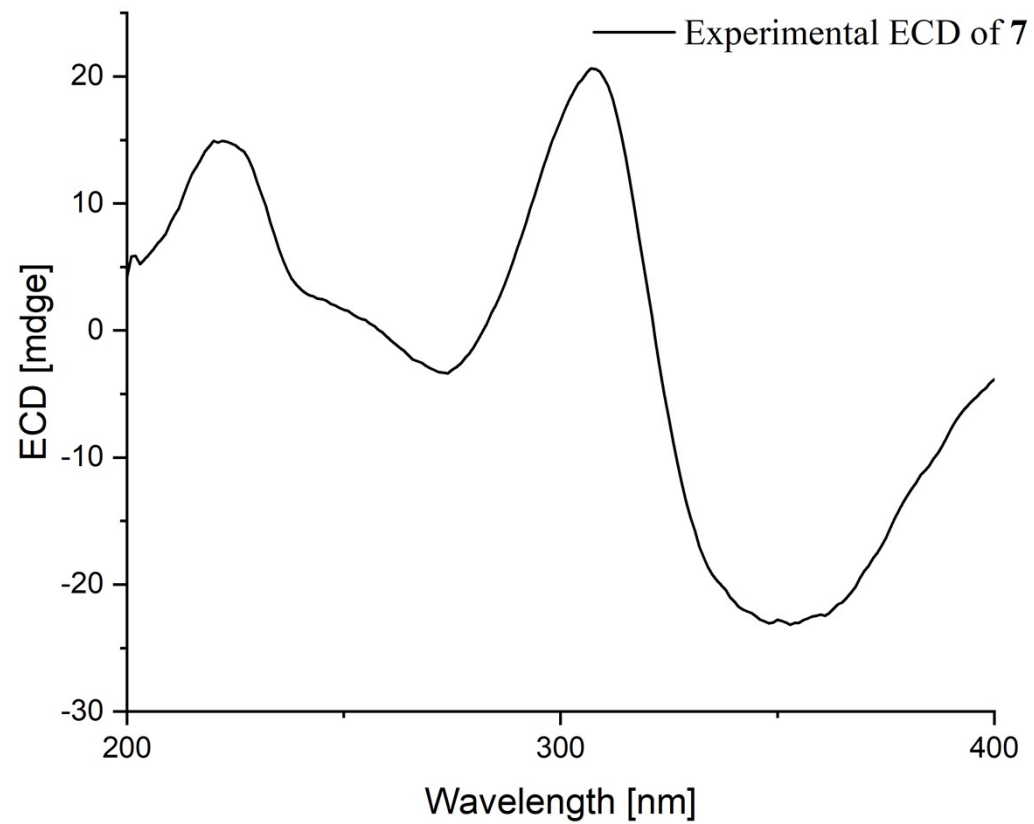
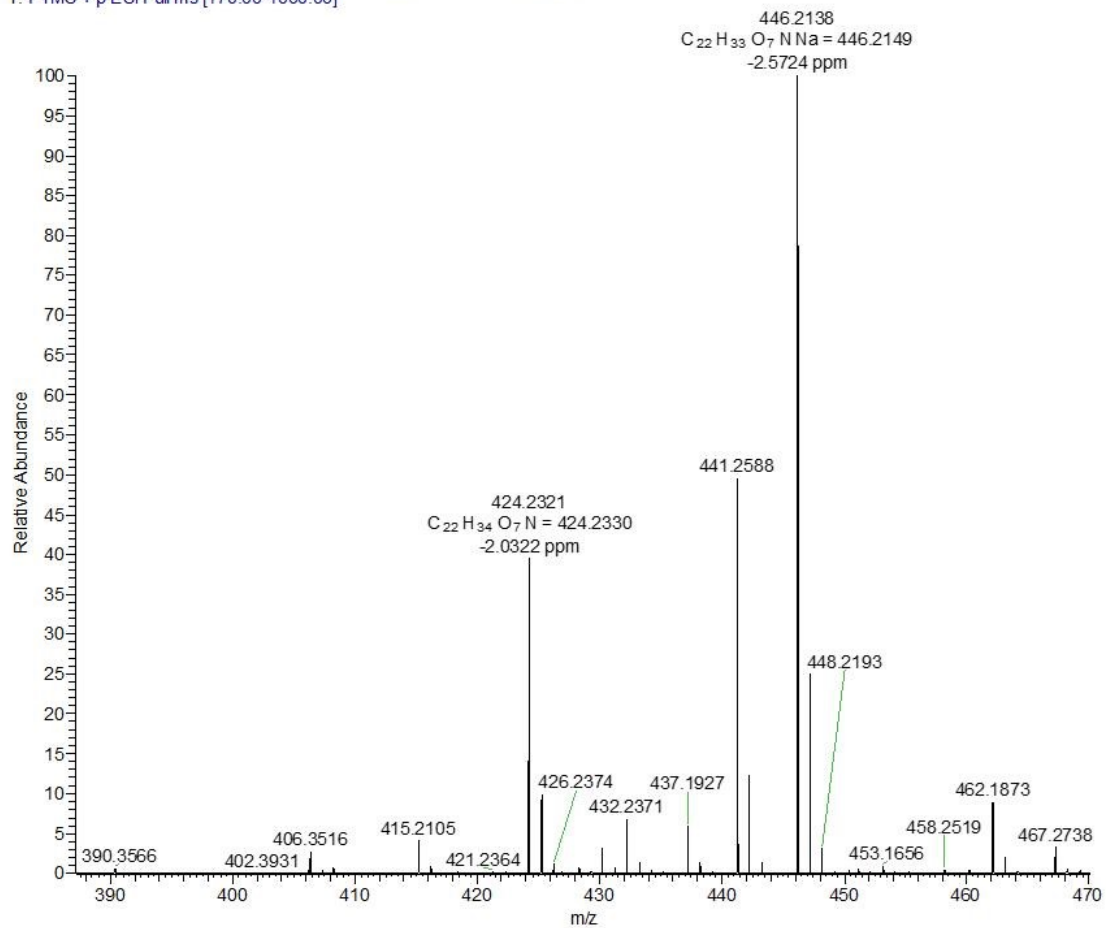


Figure S56. ECD spectrum of compound 7;



**Figure S57.** HRESI mass spectrum of compound **8**;

20210112-CS113-87 210112143837 #81 RT: 0.64 AV: 1 NL: 2.93E7  
T: FTMS + p ESI Full ms [170.00-1000.00]



**Figure S58.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **8**;

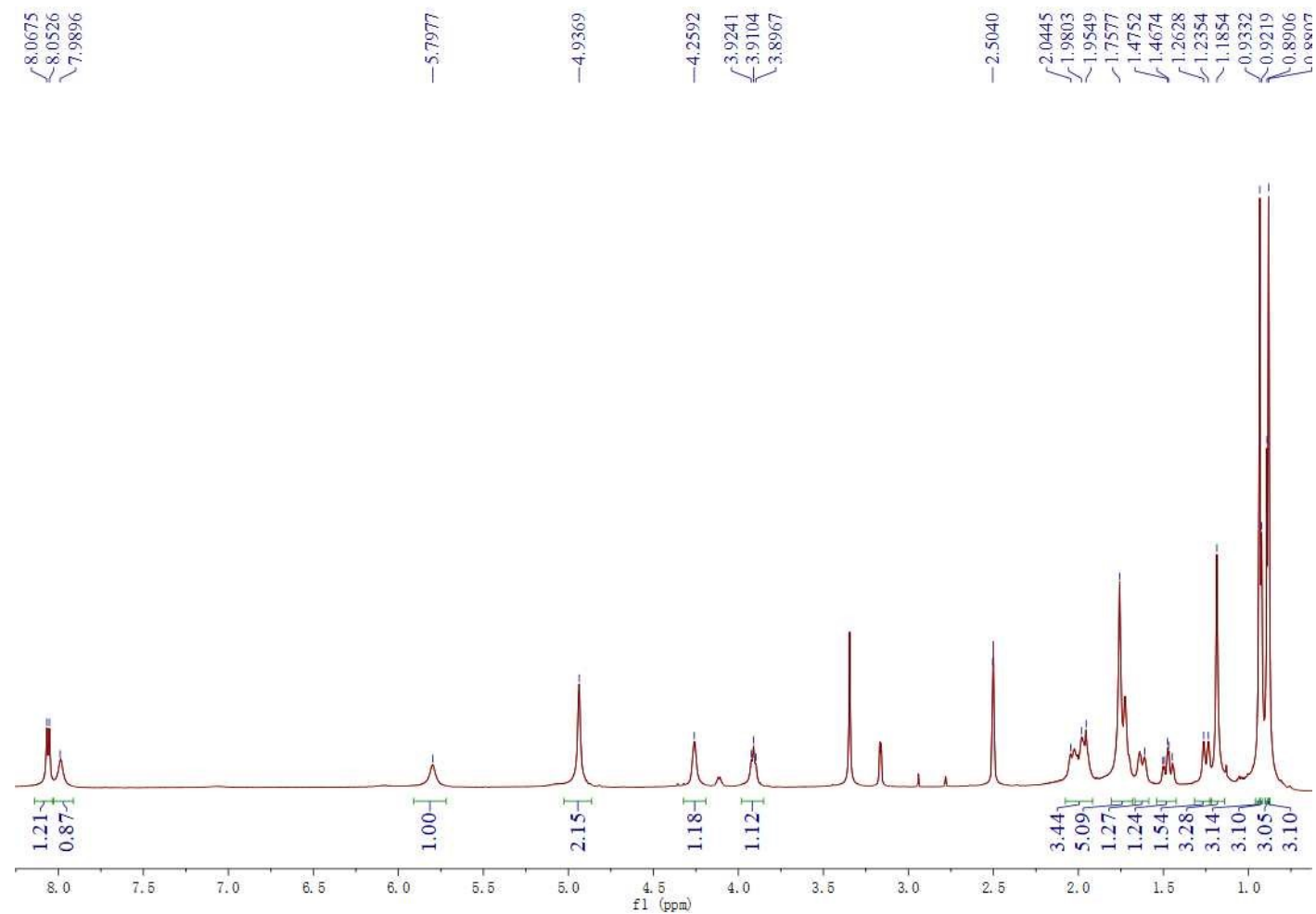


Figure S59.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **8**;

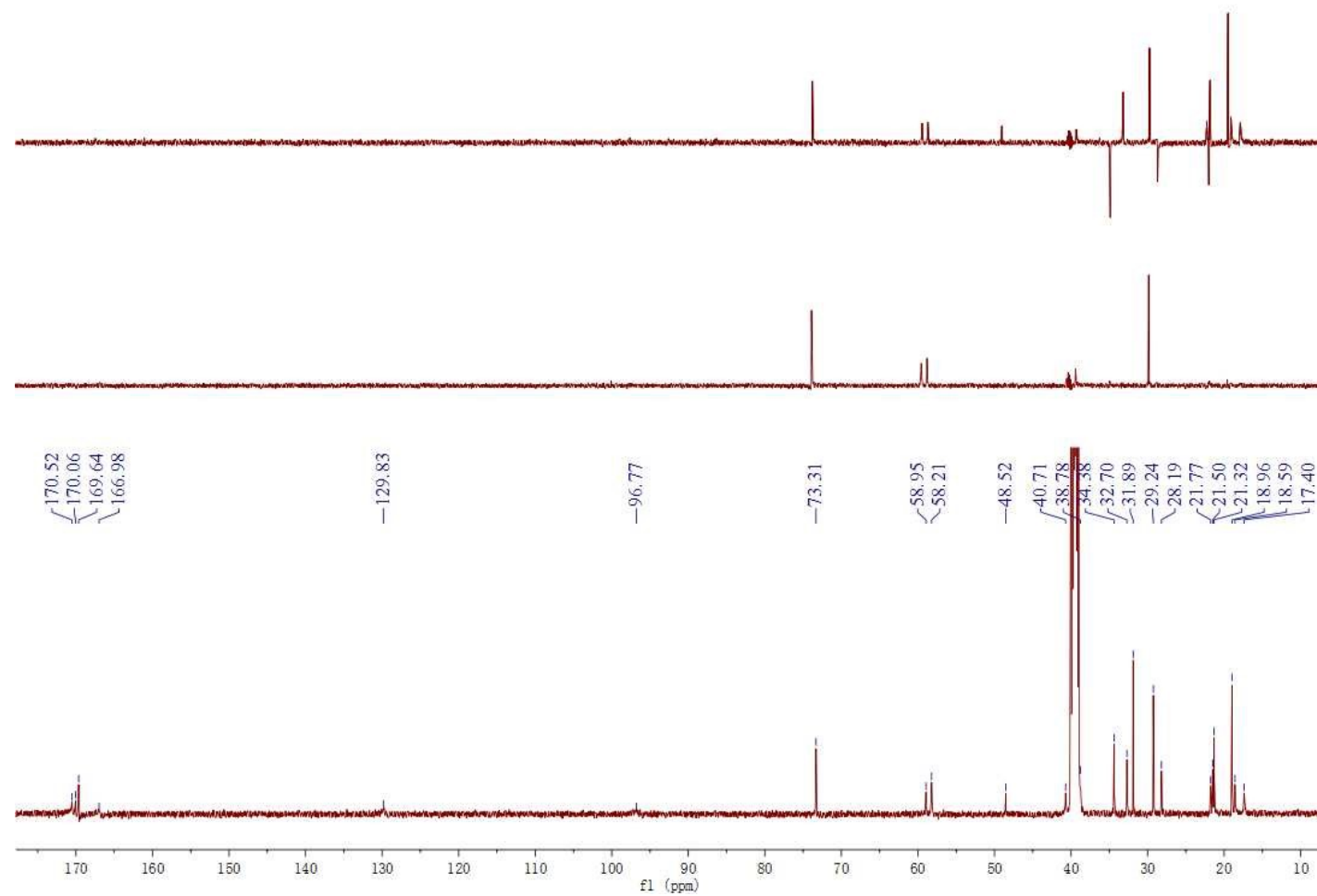




Figure S60. COSY spectrum of compound **8**;

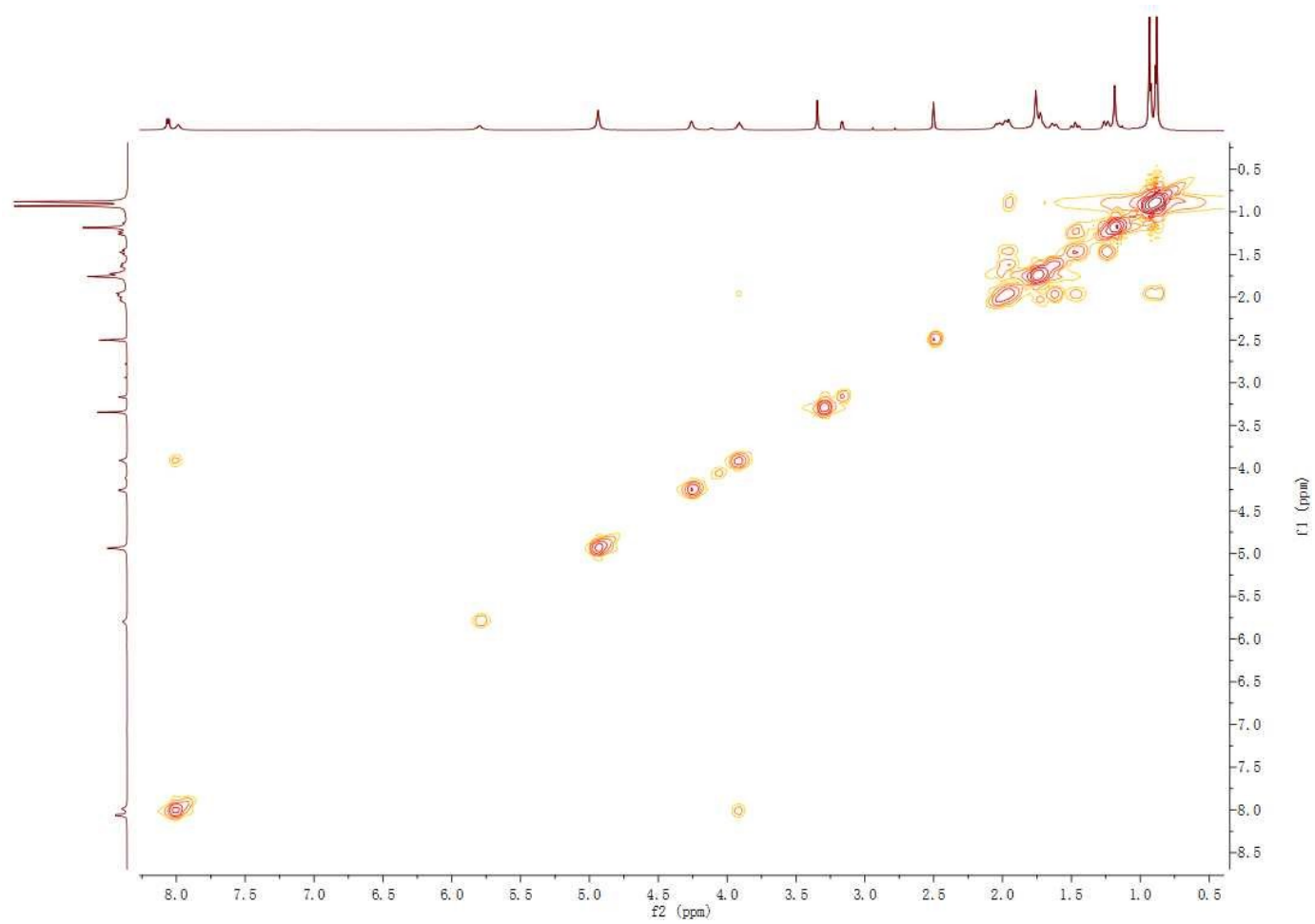


Figure S61. HSQC spectrum of compound **8**;

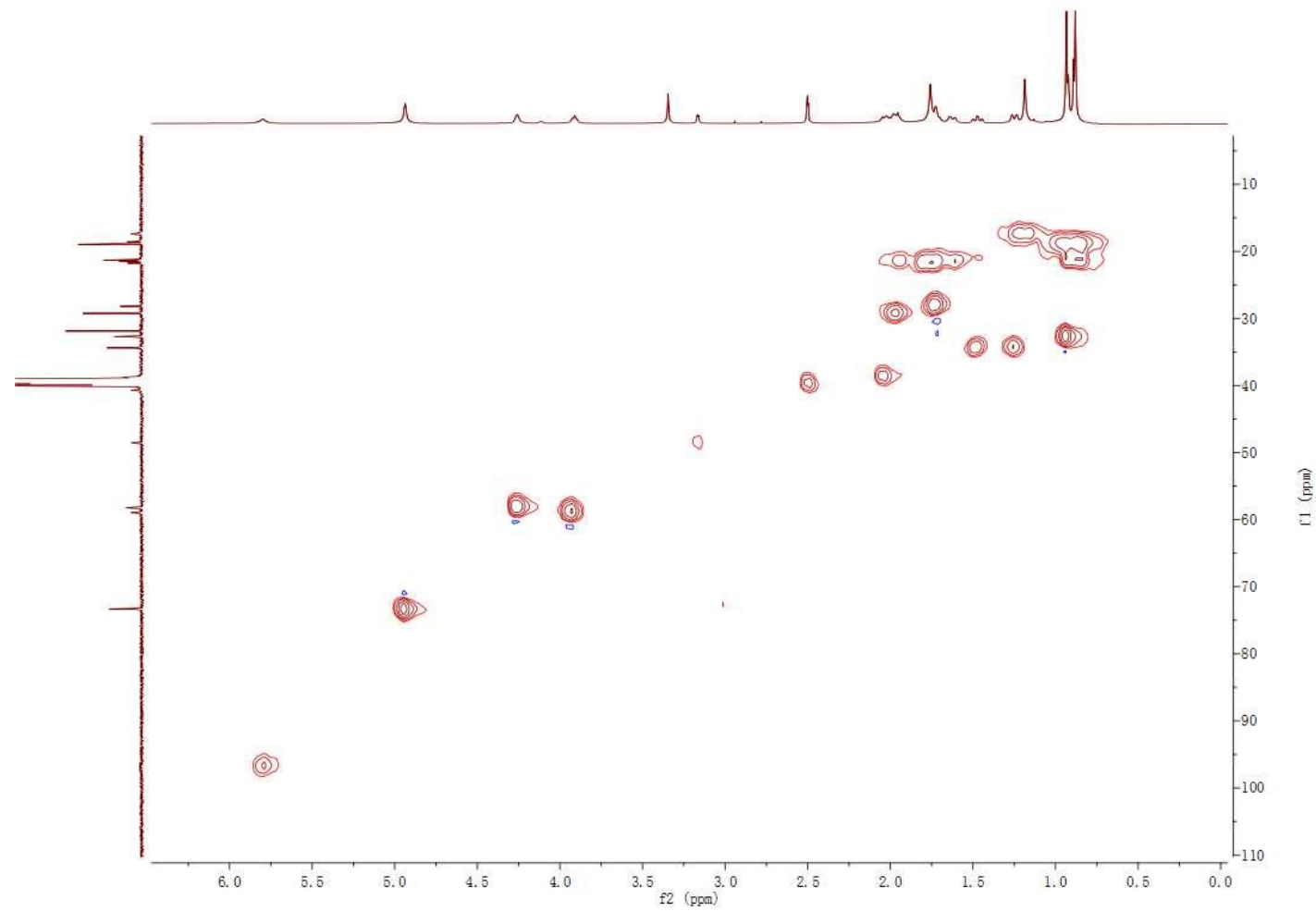
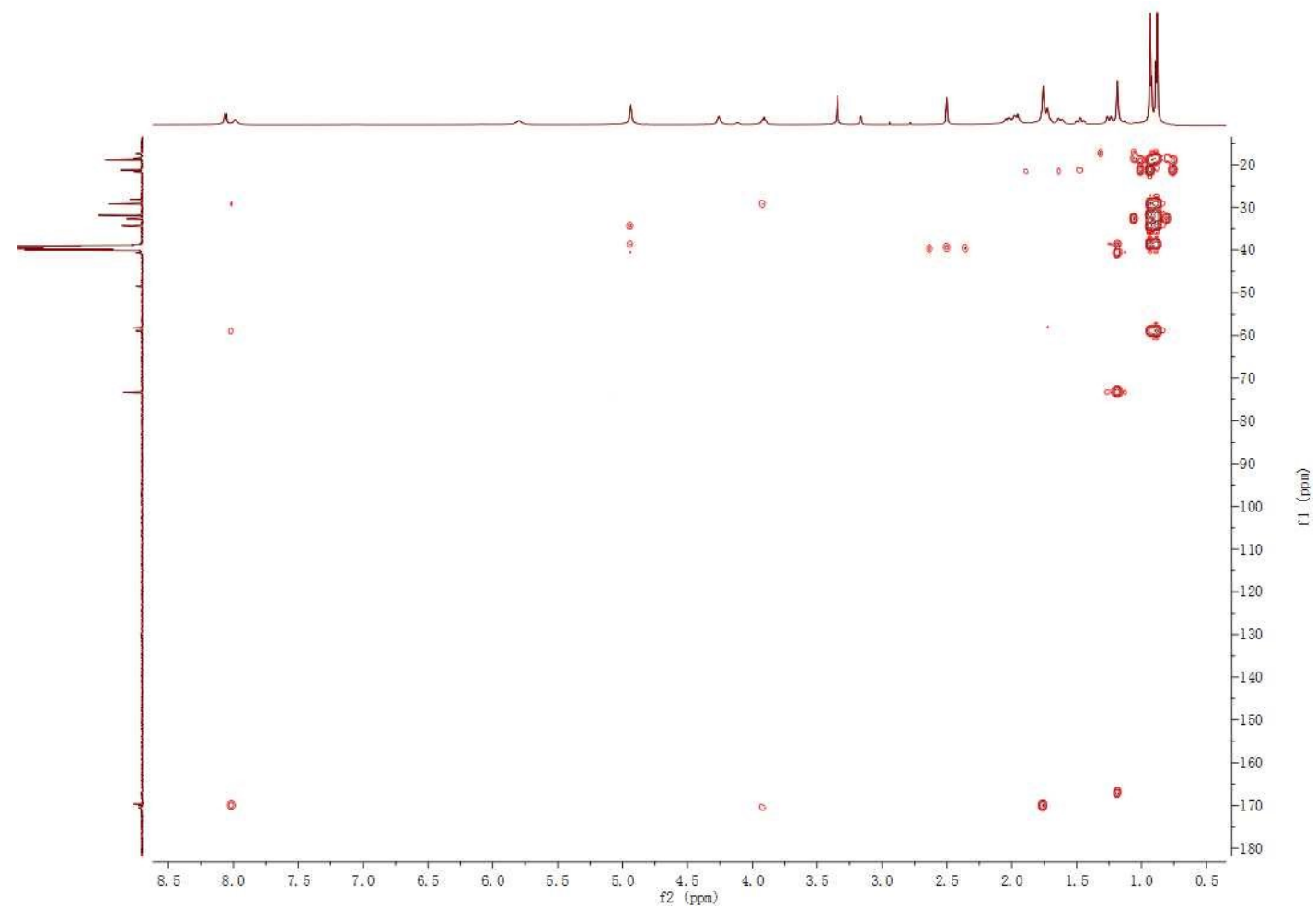


Figure S62. HMBC spectrum of compound 8;



**Figure S63.** NOESY spectrum of compound **8**;

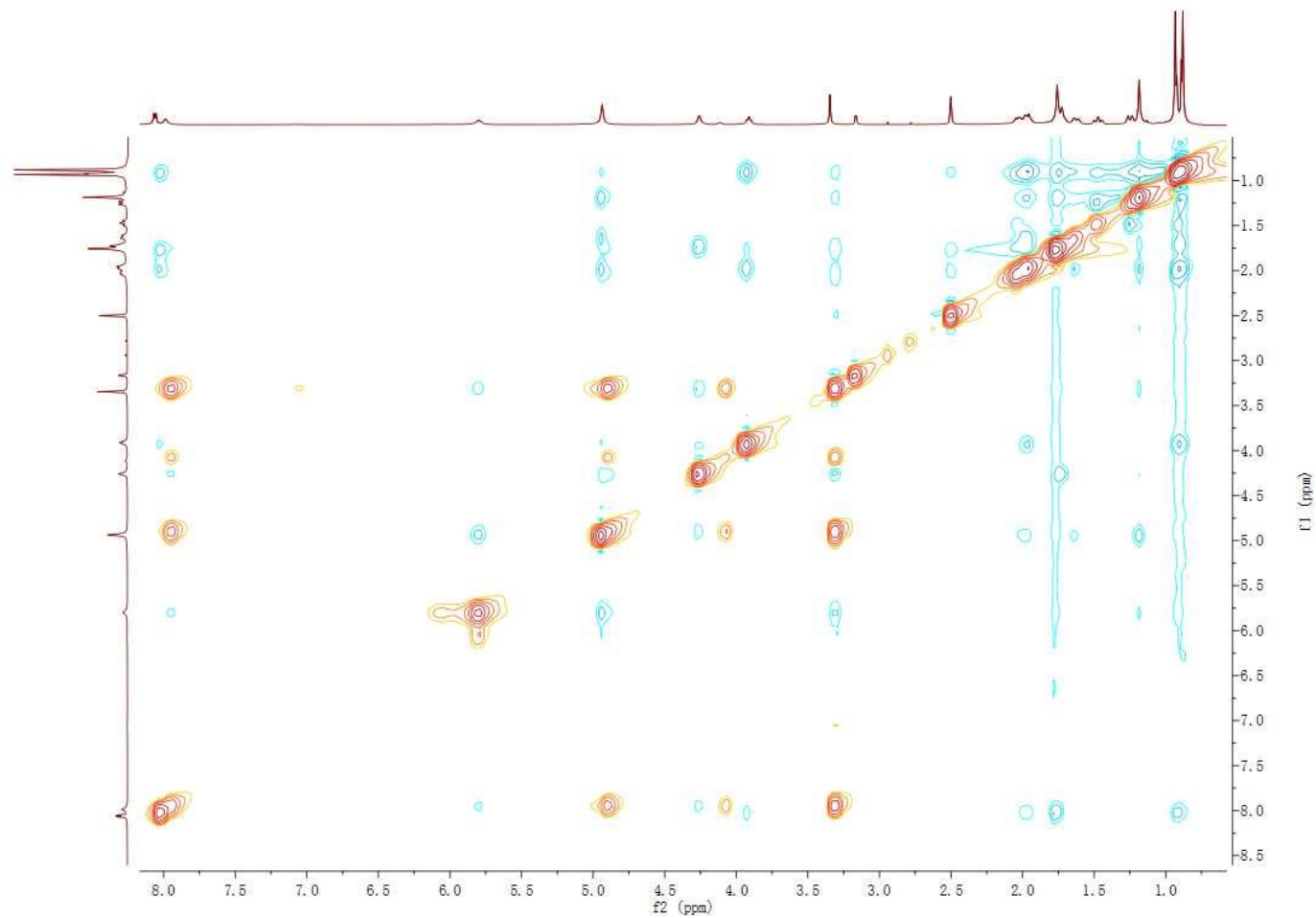
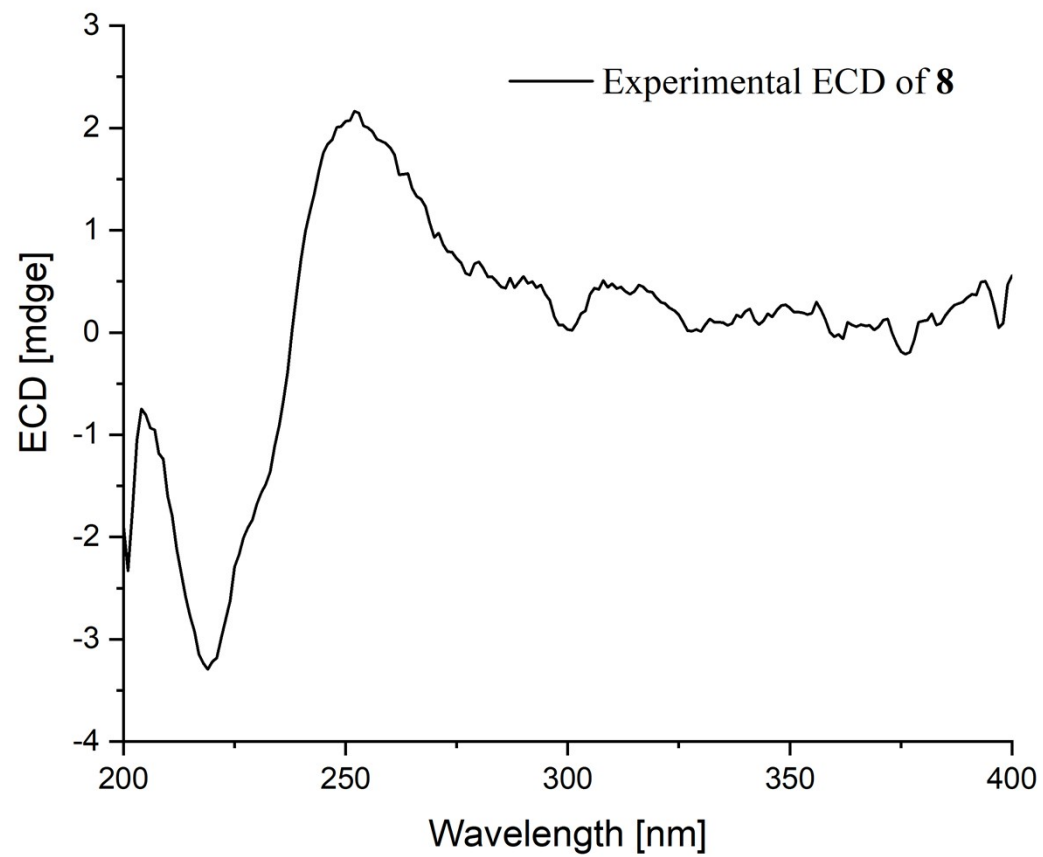


Figure S64. ECD spectrum of compound **8**;



**Figure S65.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **10**;

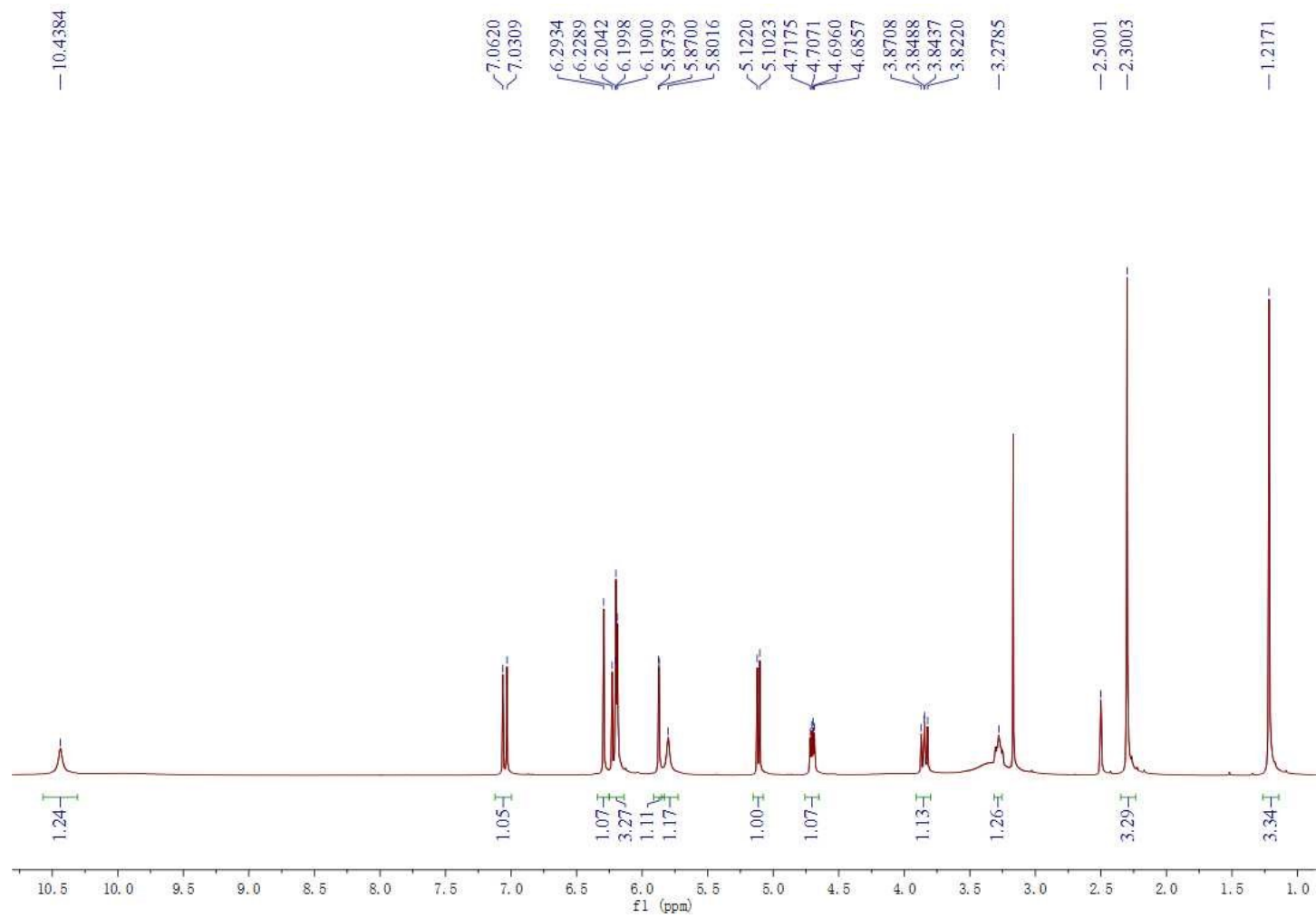
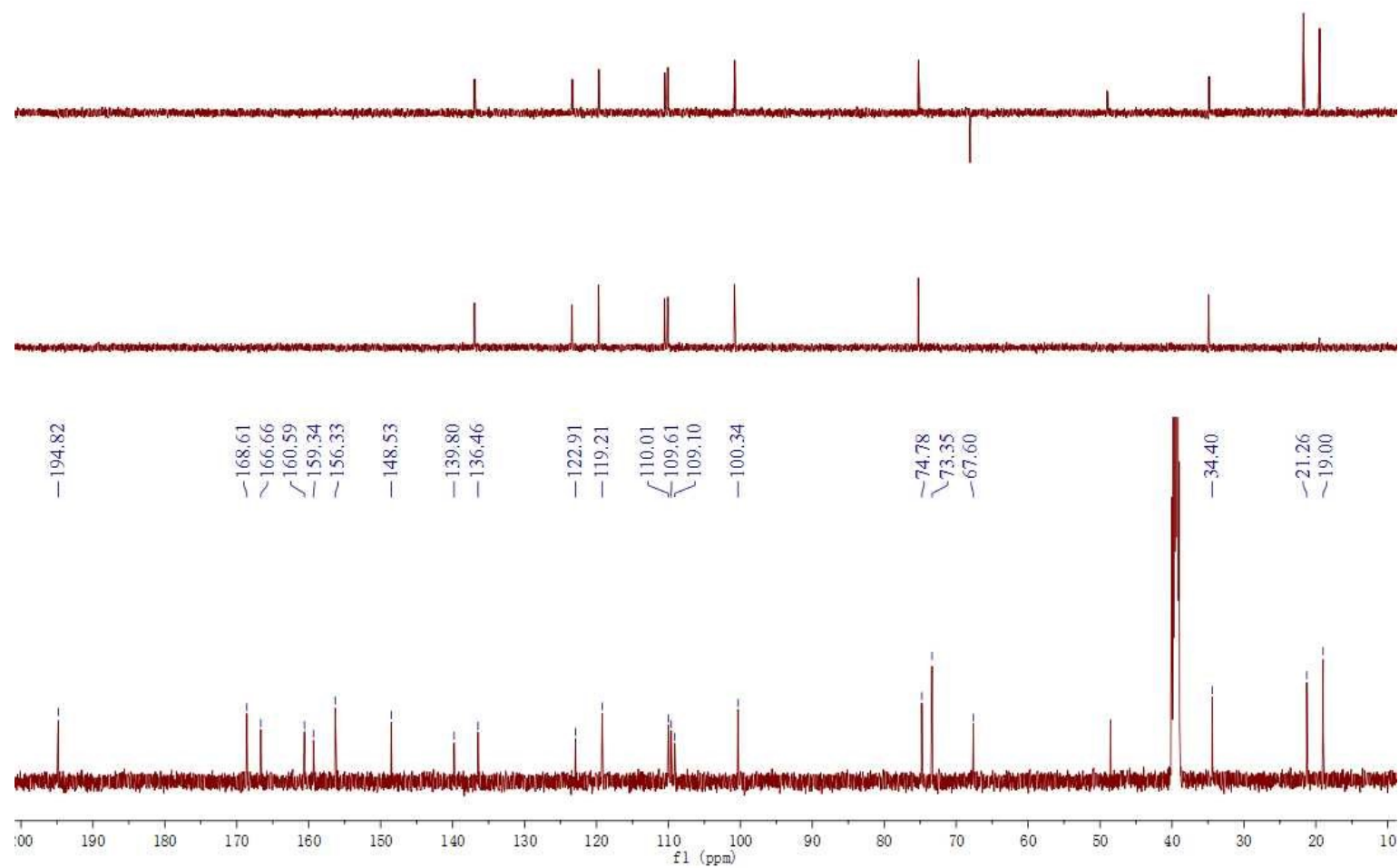
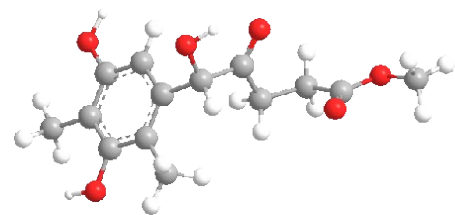


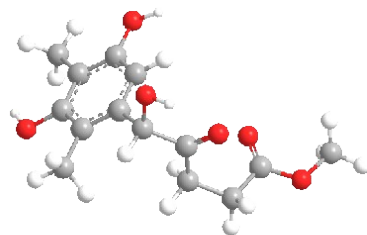
Figure S66.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **10**;



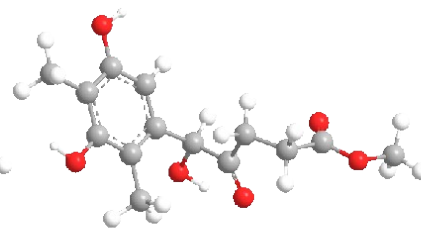
**Figure S67.** Structure and population of the low-energy (weighting factors) conformers for **4a** and **4b** at the B3LYP/6-31g(d) level above 1% population;



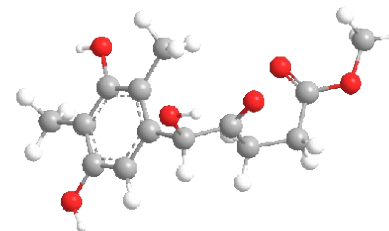
Conf. **4a-1**, 83.0%



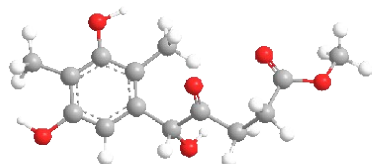
Conf. **4a-2**, 8.3%



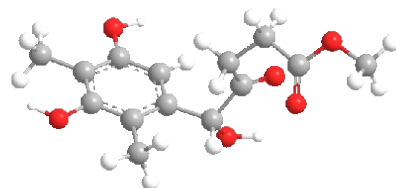
Conf. **4a-3**, 6.3%



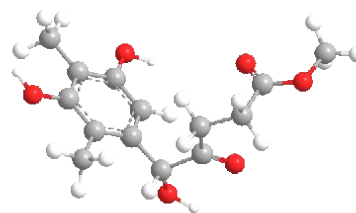
Conf. **4a-4**, 1.6%



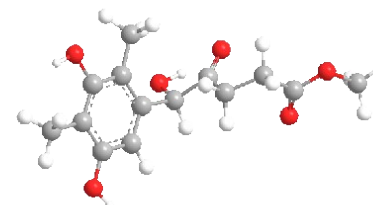
Conf. **4b-1**, 83.5%



Conf. **4b-2**, 8.0%



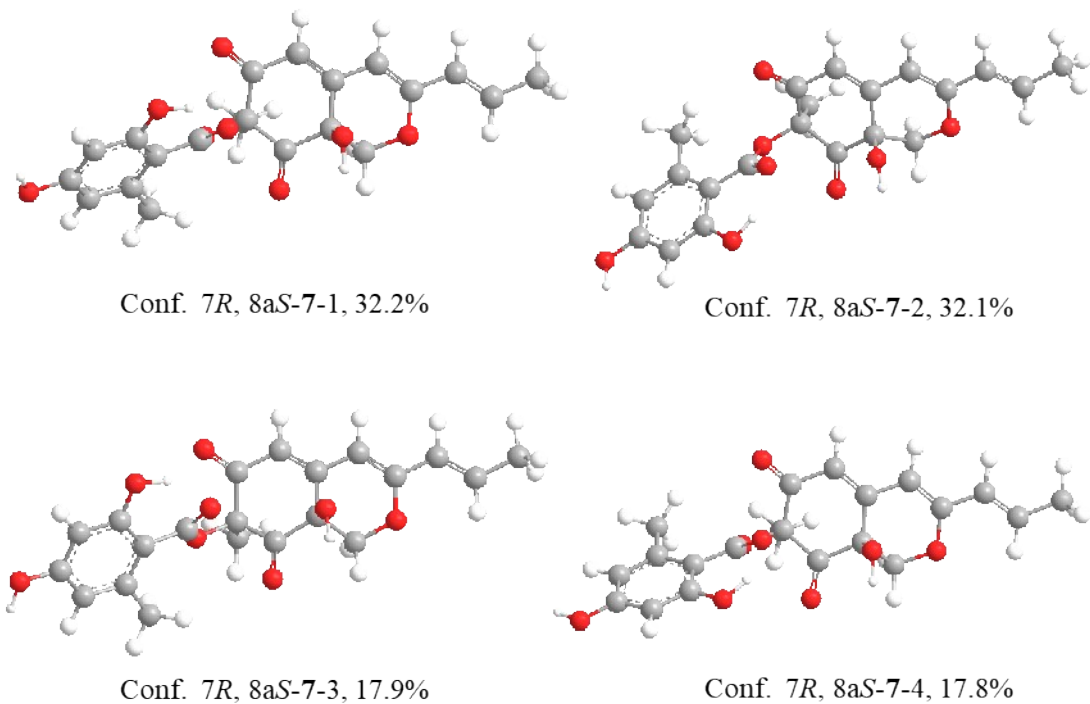
Conf. **4b-3**, 6.1%



Conf. **4b-4**, 1.6%



**Figure S68.** Structure and population of the low-energy (weighting factors) conformers of (7*R*,8*aS*)-7 at the B3LYP/6-31g(d) level above 1% population;



**Figure S69.** Structure and population of the low-energy (weighting factors) conformers of (7*S*,8*aS*)-7 at the B3LYP/6-31g(d) level above 1% population;

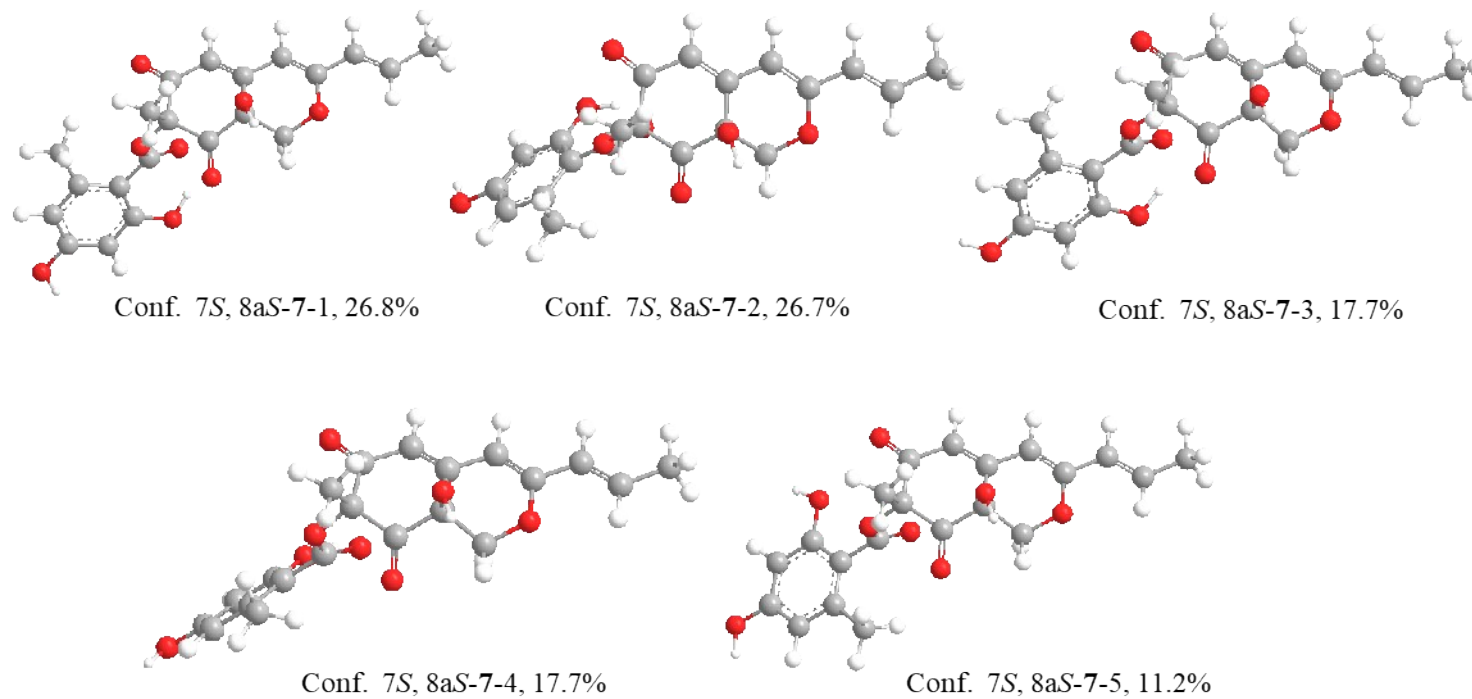
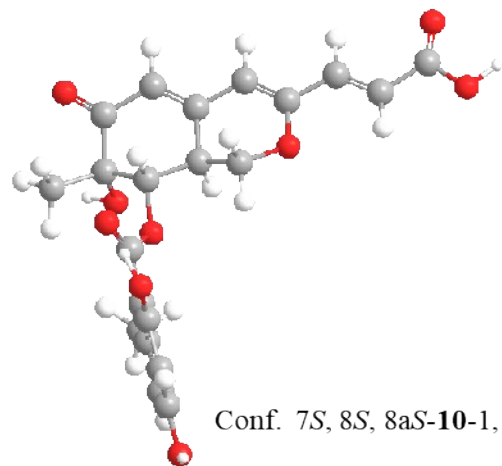


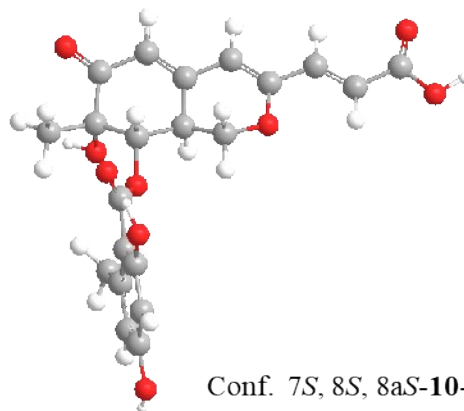
Figure S70. DP4+ probability analysis data of compound 7;

A	B	C	D	E	F	G	H
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-31+G (d,p)		Shielding Tensors	
		DP4+	100.00%	0.00%	-	-	-
Nuclei	sp2?	xperimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	191.7	2.8572563	2.572421			
C		84.1	105.110673	106.455114			
C	x	200.3	-15.179795	-14.330022			
C		66.3	119.886621	123.127484			
C	x	149.7	48.3481189	49.1790788			
C	x	117.3	73.8302239	70.5610806			
C		69.7	119.05237	119.22238			
C	x	159.6	38.8890641	37.5066775			
C	x	102.1	89.860018	89.3887834			
C		24.1	166.472671	163.25933			
C	x	125.7	70.320706	70.1792023			
C	x	134.6	55.2485646	54.4849032			
C		18.6	168.04992	167.939384			
C	x	168.2	27.9513186	27.0762416			
C	x	104.4	84.4081093	84.3629929			
C	x	142.8	50.7340759	51.337518			
C	x	111.7	84.3563698	84.4265838			
C	x	163.3	38.5321875	38.8977008			
C	x	101.1	95.0861326	94.8614751			
C	x	163.3	39.0898603	39.7122008			
C		23.2	167.057631	166.909088			
H	x	6.04	24.09	24.0514996			
H		4.62	25.89	25.8287068			
H		3.87	26.30	26.2372563			
H	x	5.92	24.6153946	24.5387133			
H		1.8	28.7449057	28.5260664			
H	x	6.12	24.2235893	24.1863612			
H	x	6.46	23.6007972	23.6102607			
H		1.86	28.5163334	28.527305			
H	x	6.22	24.0178127	24.2691679			
H	x	6.13	24.2743256	24.3423312			
H		2.43	28.0217929	27.0880522			

**Figure S71.** Structure and population of the low-energy (weighting factors) conformers of (7*S*,8*S*,8a*S*)-**10** at the B3LYP/6-31g(d) level above 1% population;

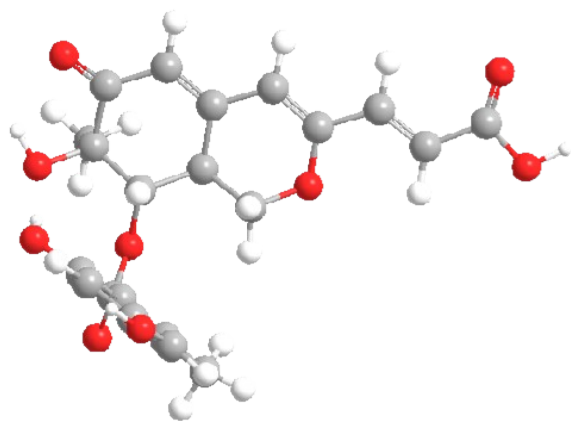


Conf. 7*S*, 8*S*, 8a*S*-**10**-1, 63.6%

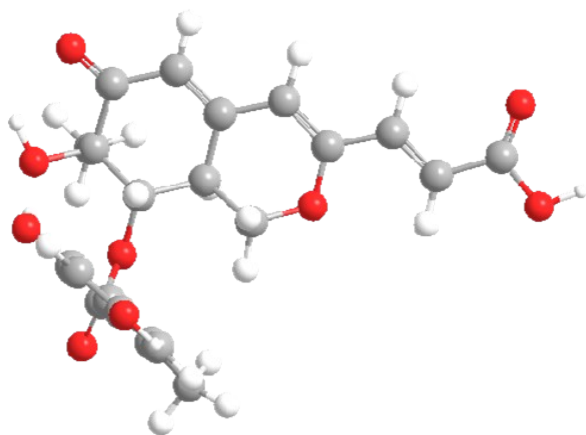


Conf. 7*S*, 8*S*, 8a*S*-**10**-2, 36.4%

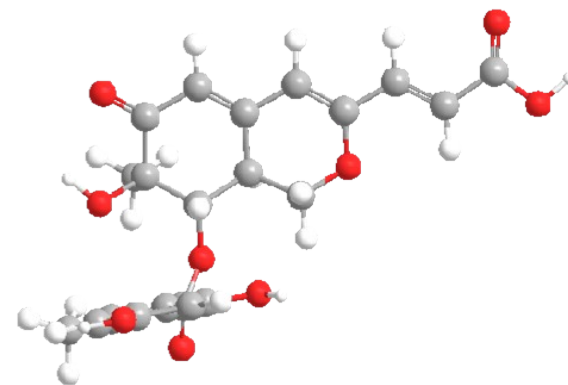
**Figure S72.** Structure and population of the low-energy (weighting factors) conformers of (7*R*,8*S*,8*aS*)-**10** at the B3LYP/6-31g(d) level above 1% population;



Conf. 7*R*, 8*S*, 8*aS*-**10**-1, 64.1%



Conf. 7*R*, 8*S*, 8*aS*-**10**-2, 29.8%



Conf. 7*R*, 8*S*, 8*aS*-**10**-3, 3.6%

**Figure S73.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **9**;

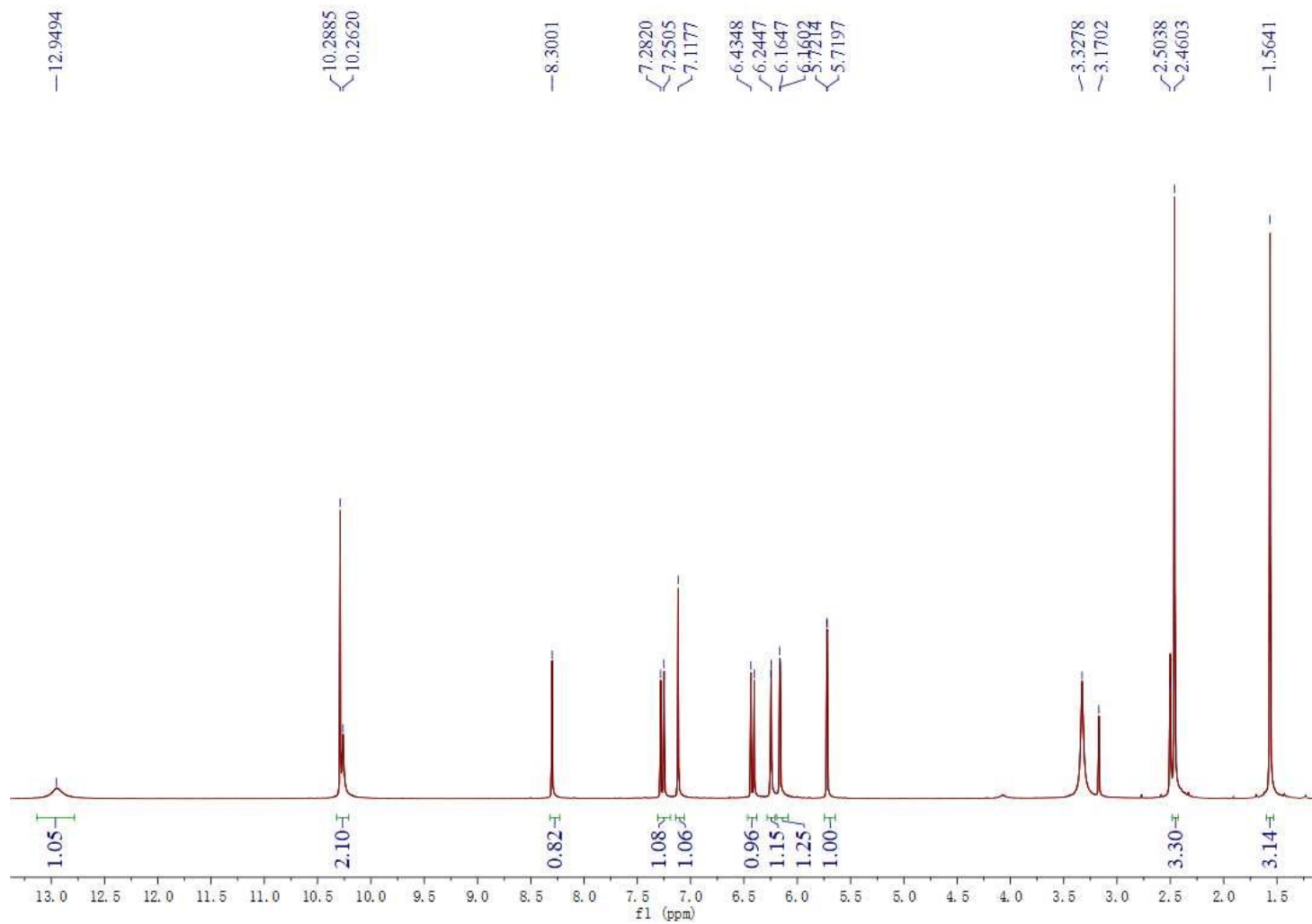


Figure S74.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound 9;

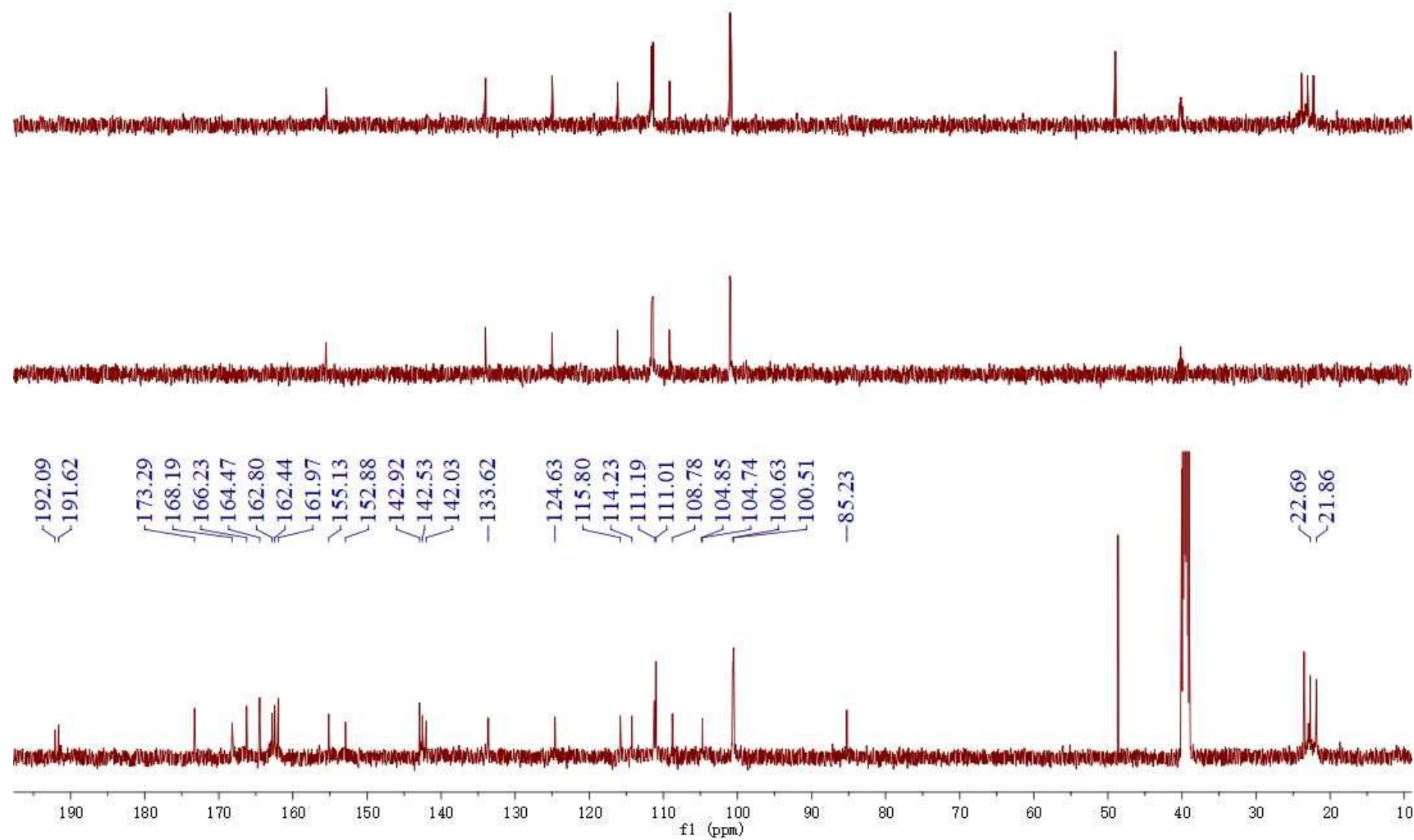


Figure S75.  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 11;

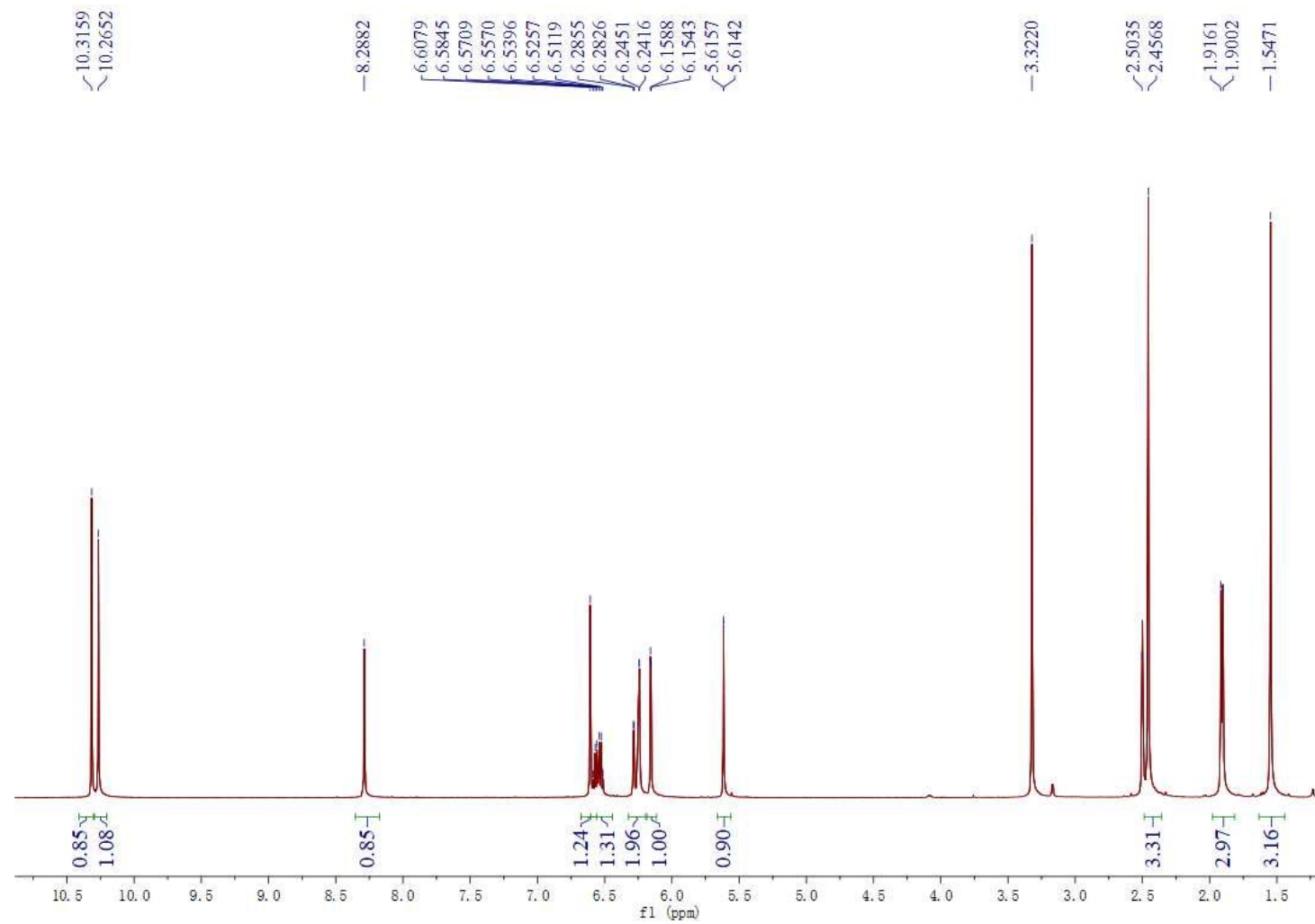
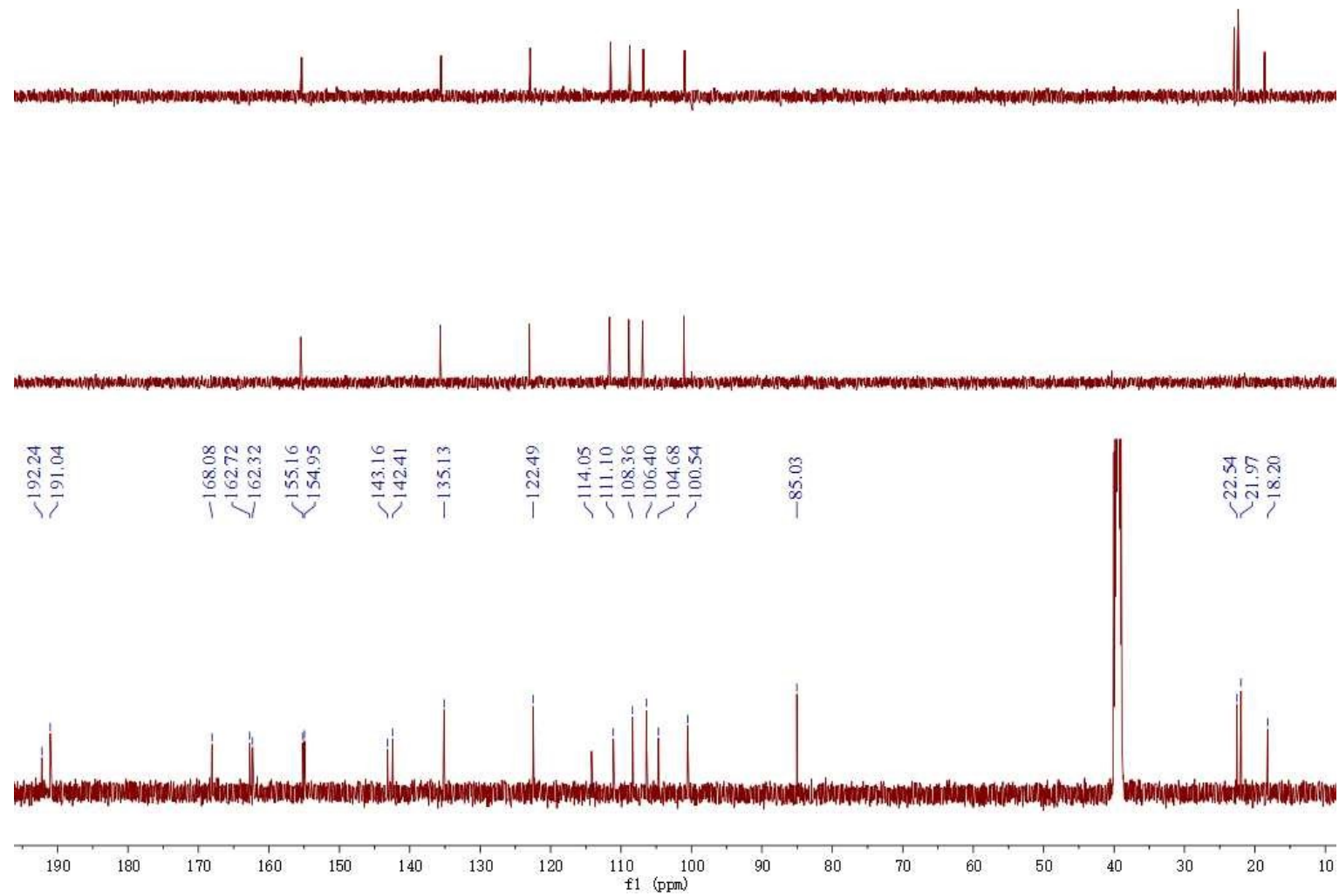




Figure S76.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **11**;



**Figure S77.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **12**;

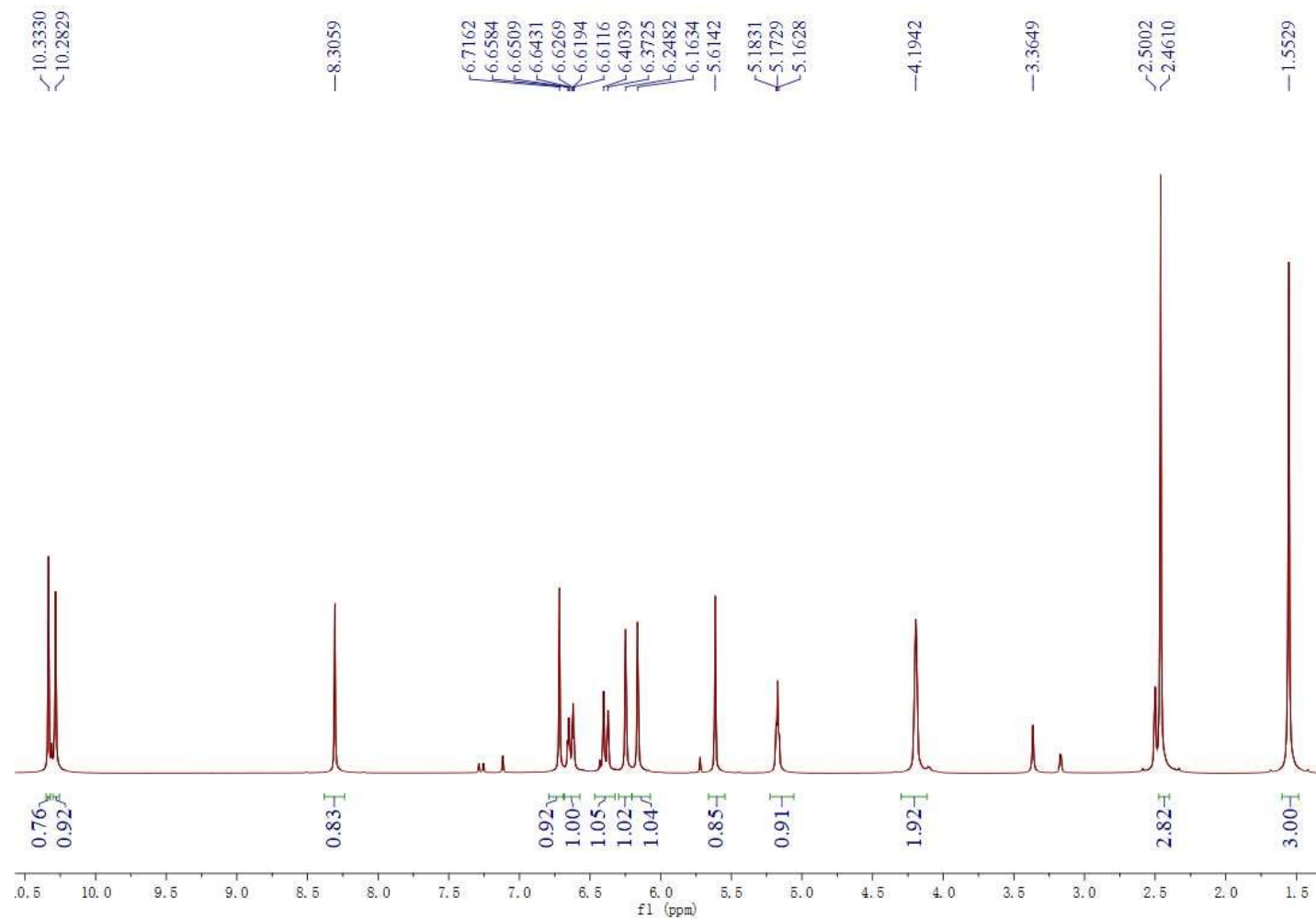
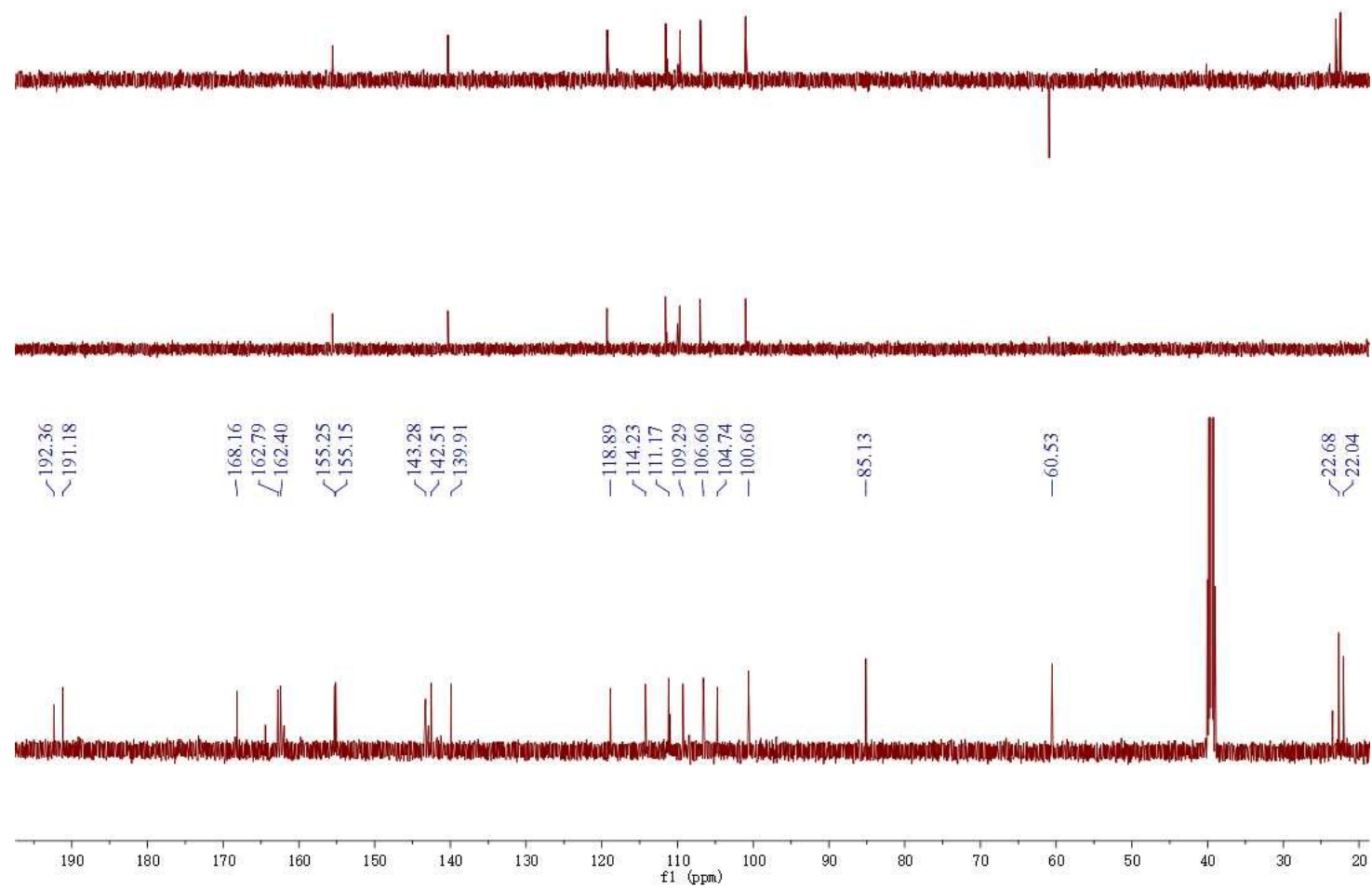


Figure S78.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **12**;



**Figure S79.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **13**;

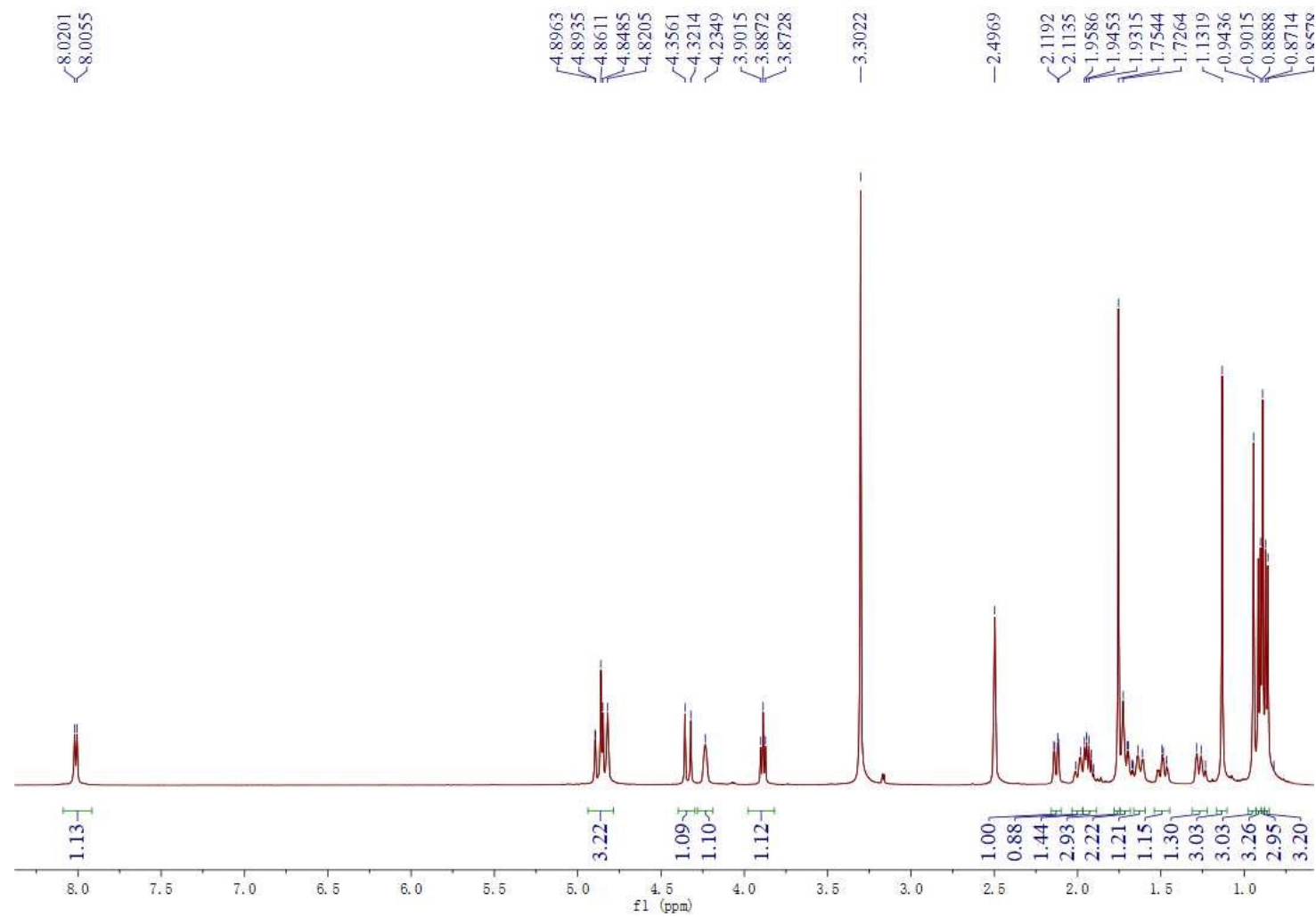
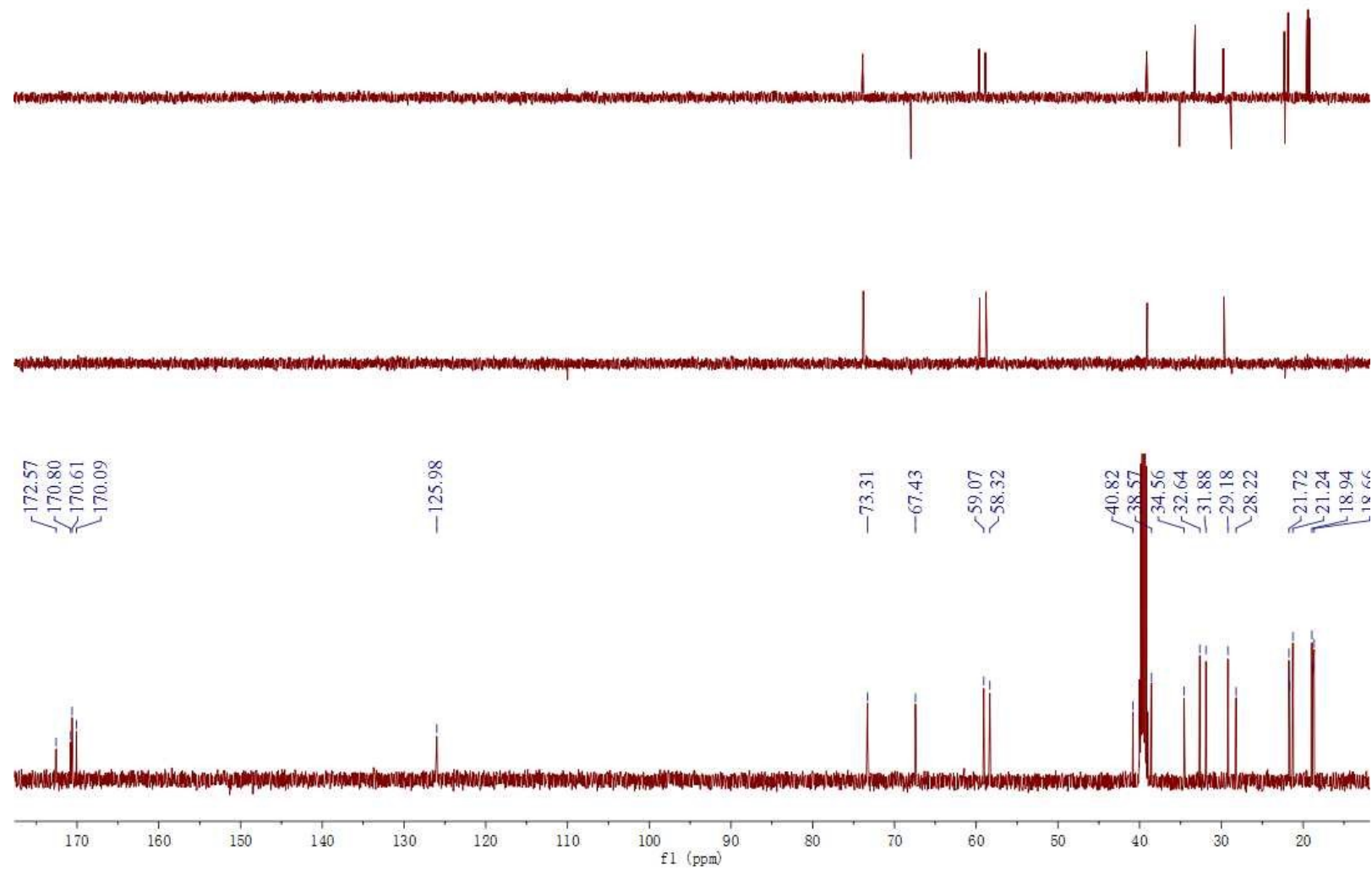


Figure S80.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **13**;



**Figure S81.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **14**;

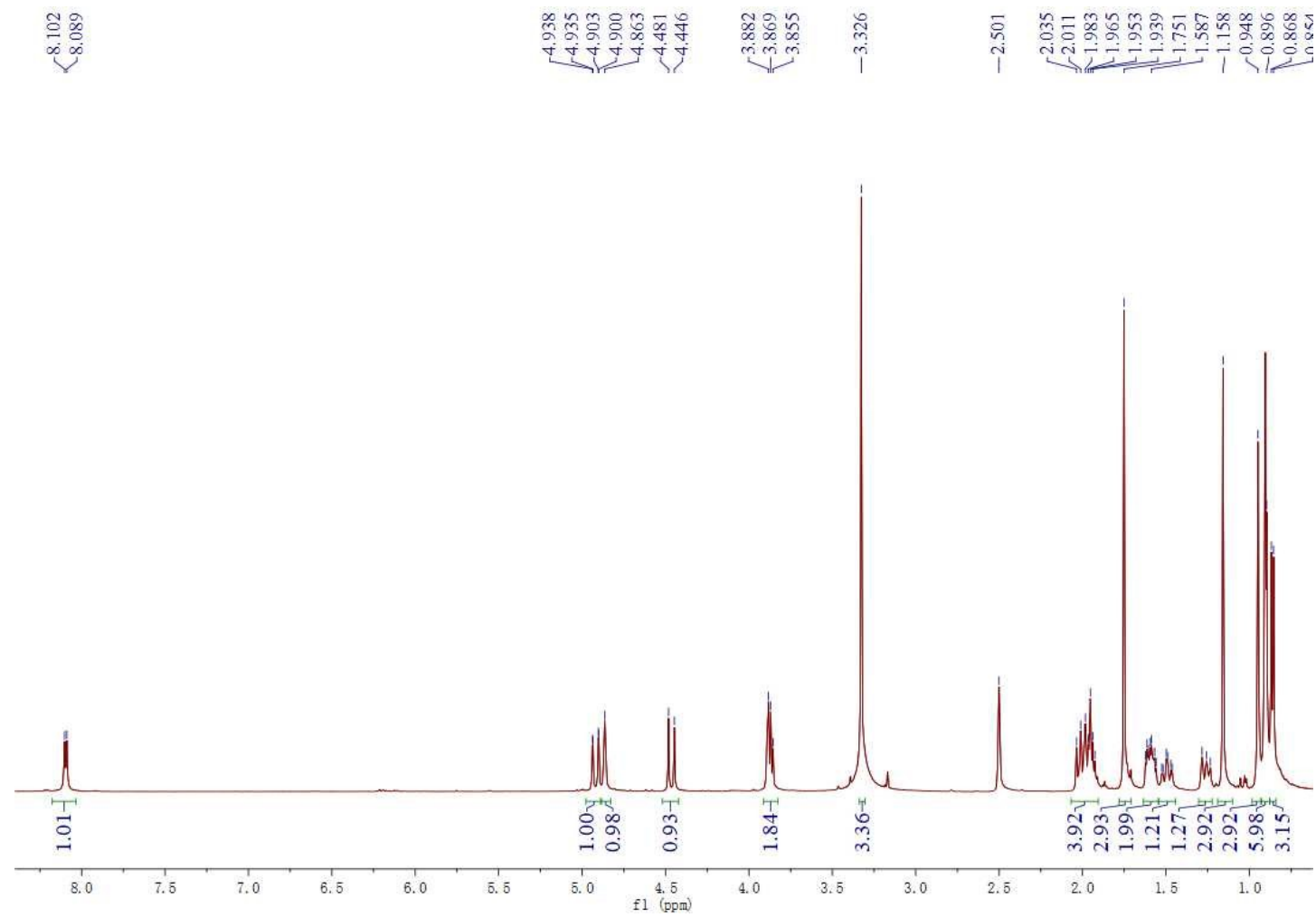
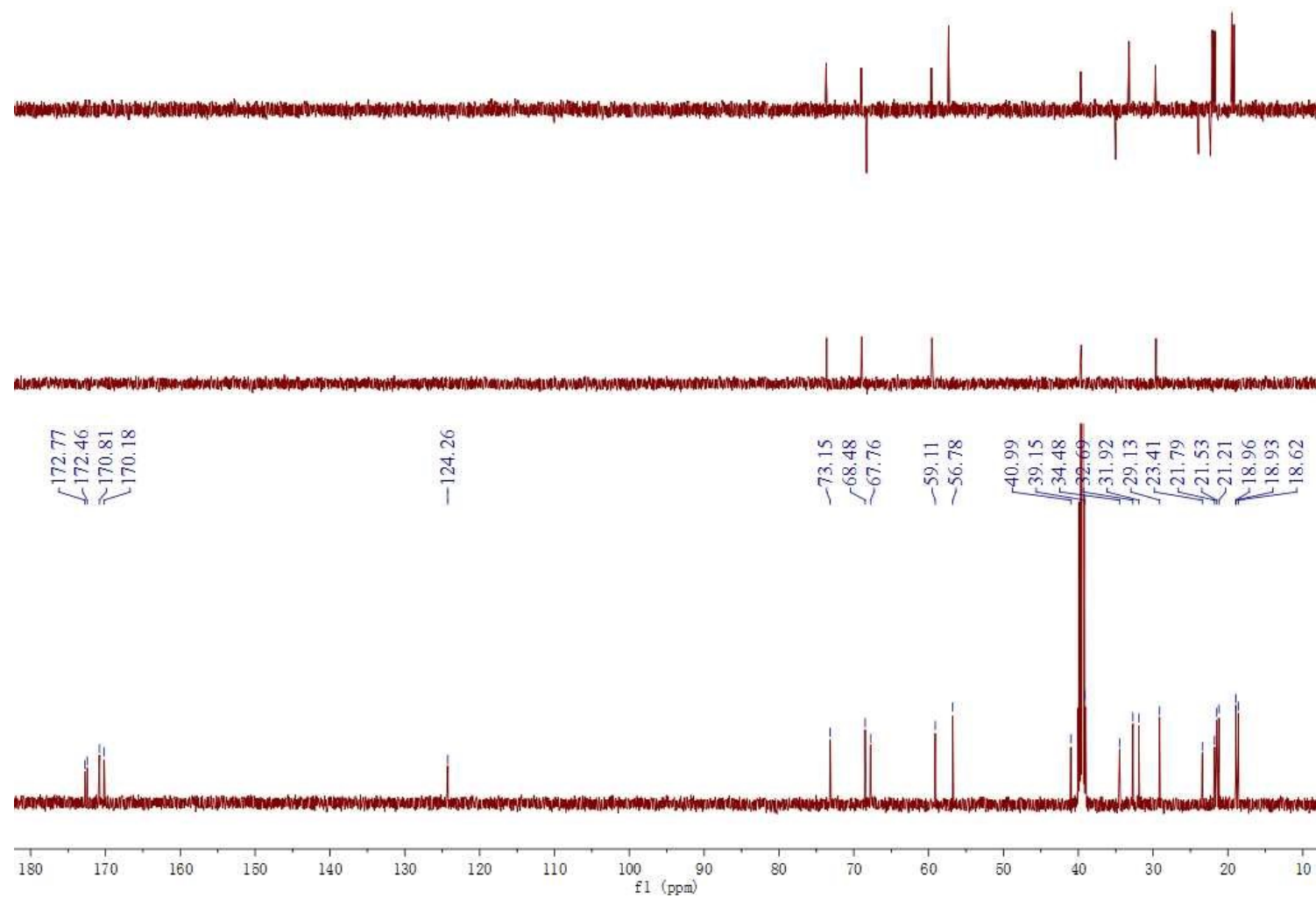


Figure S82.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **14**;



**Figure S83.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **15**;

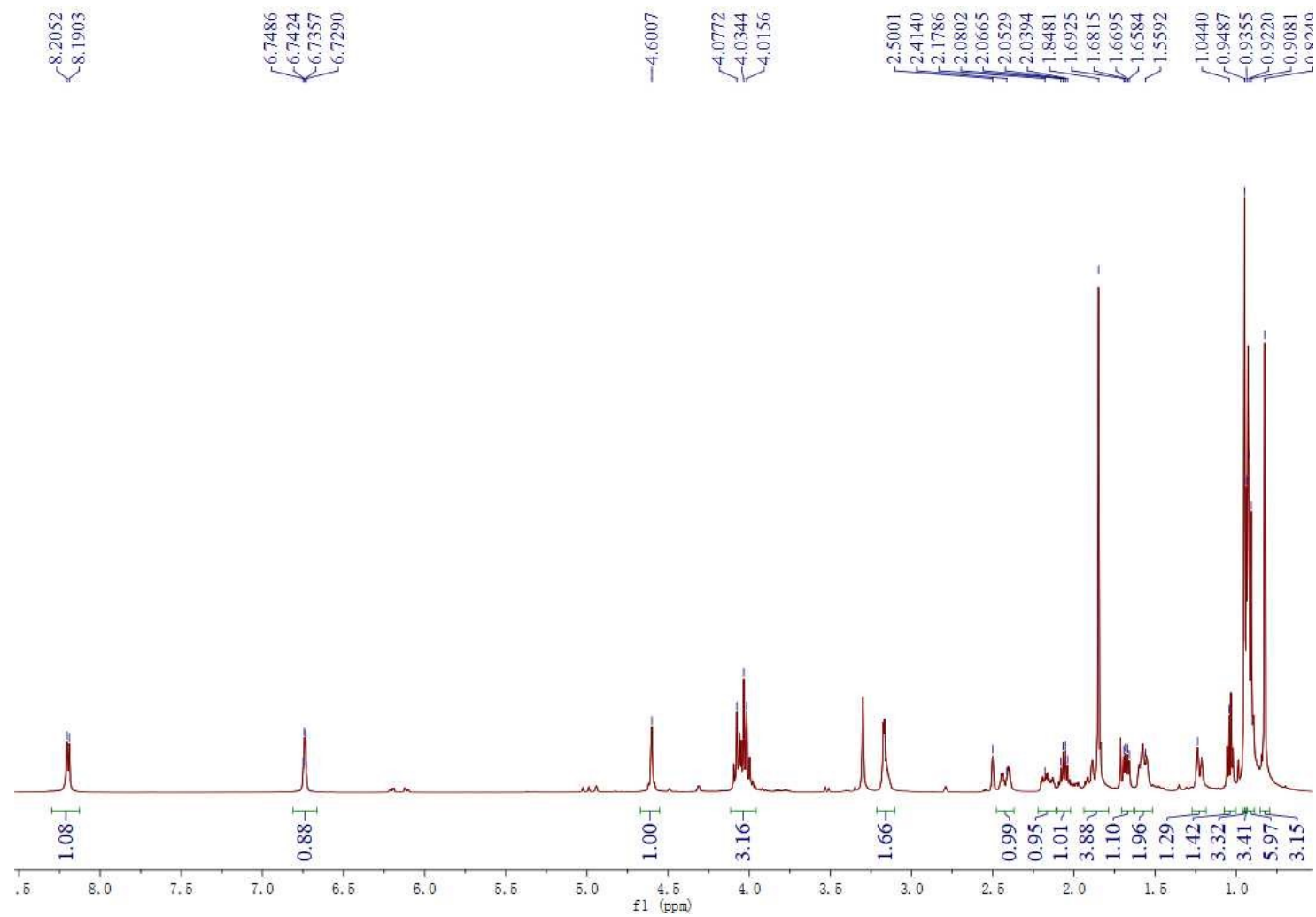
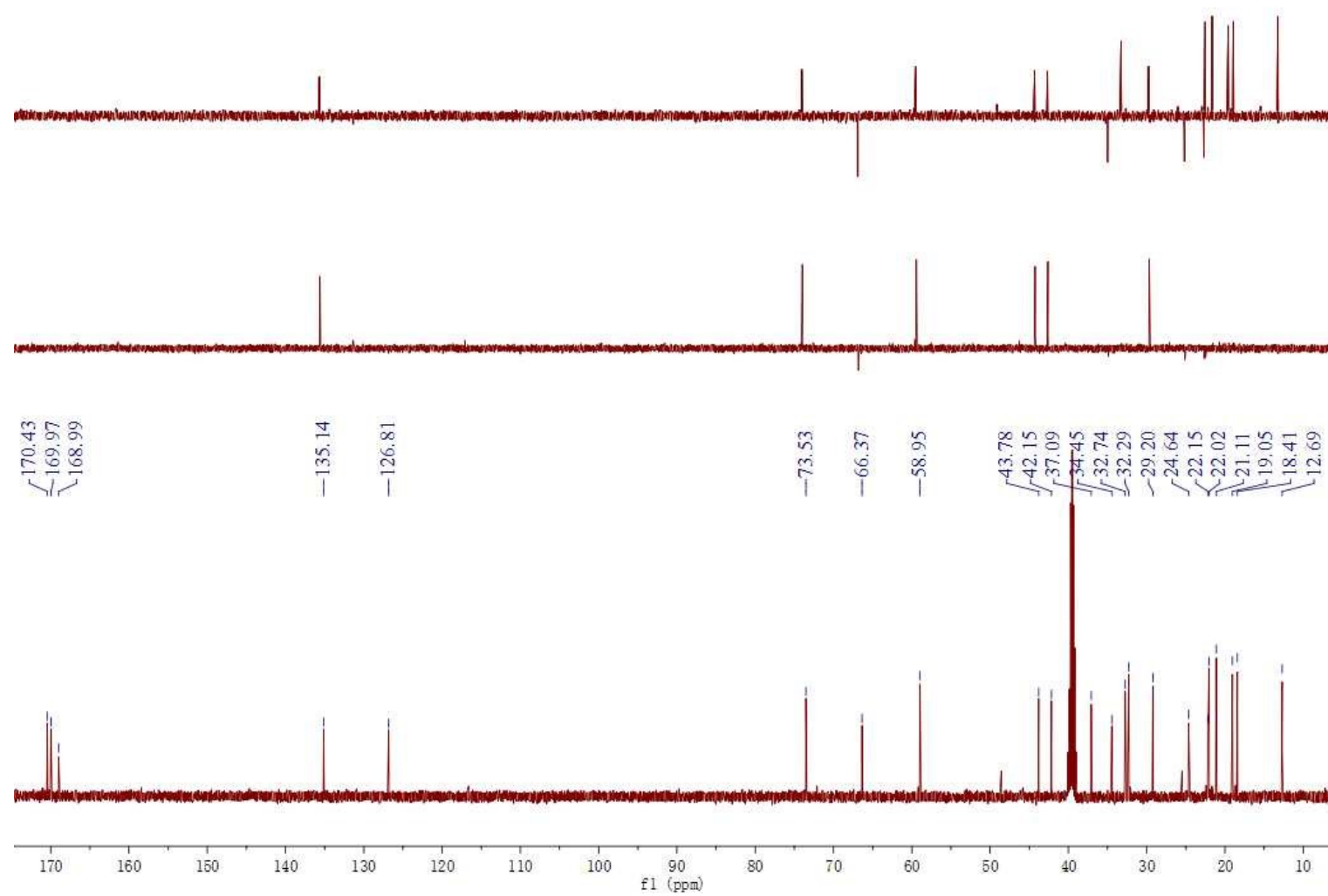




Figure S84.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **15**;



**Figure S85.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **16**;

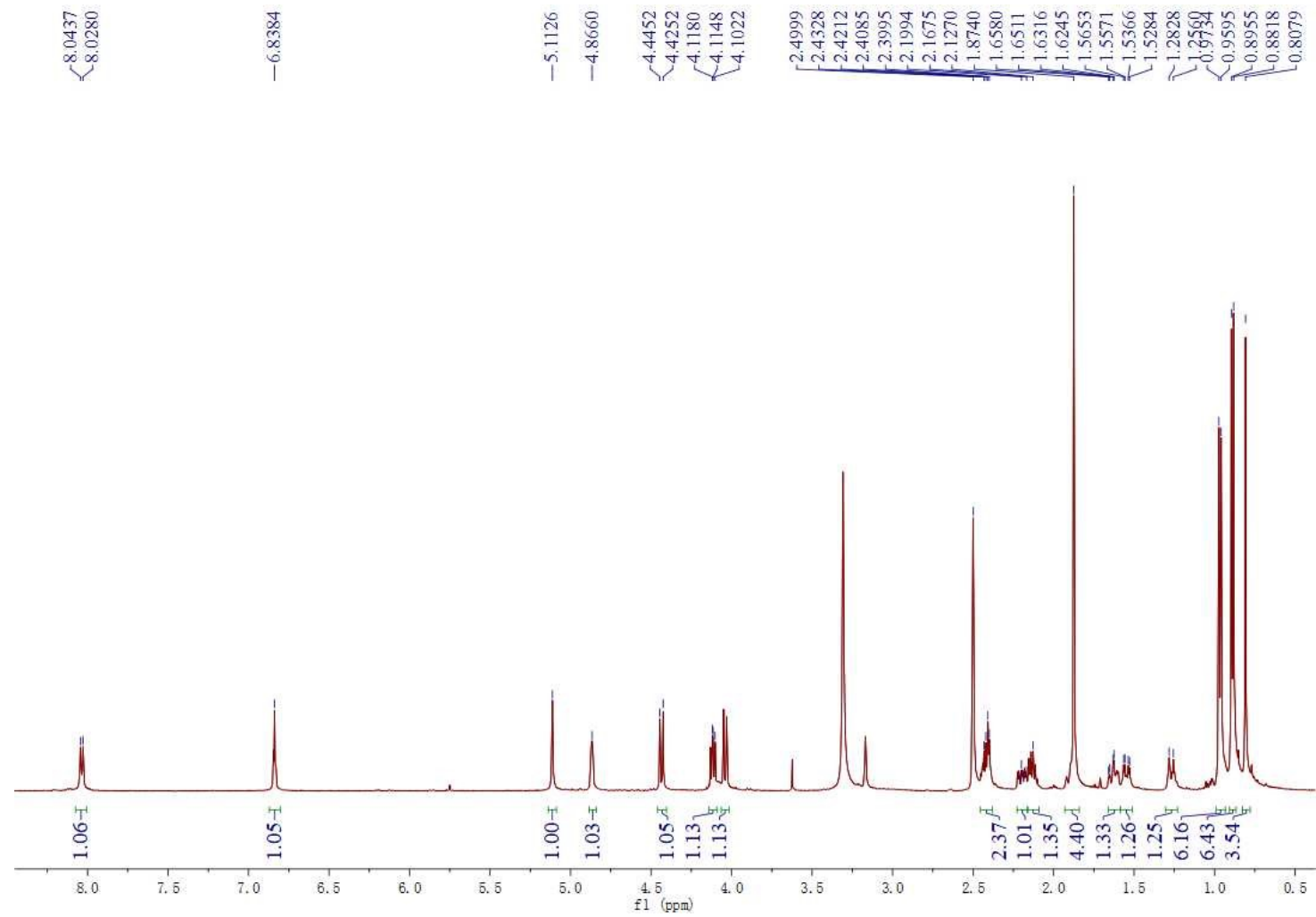


Figure S86.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **16**;

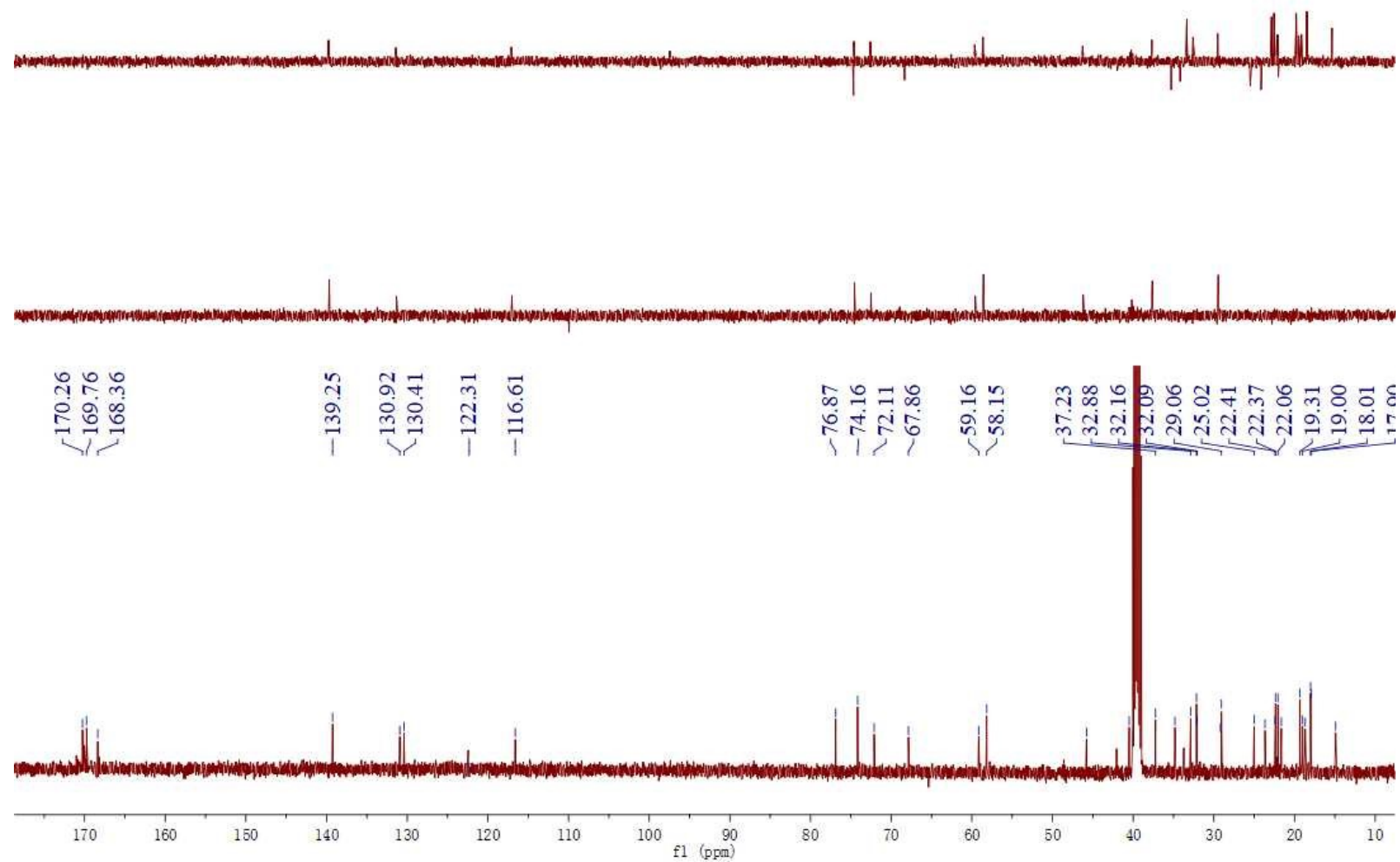


Figure S87.  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 17;

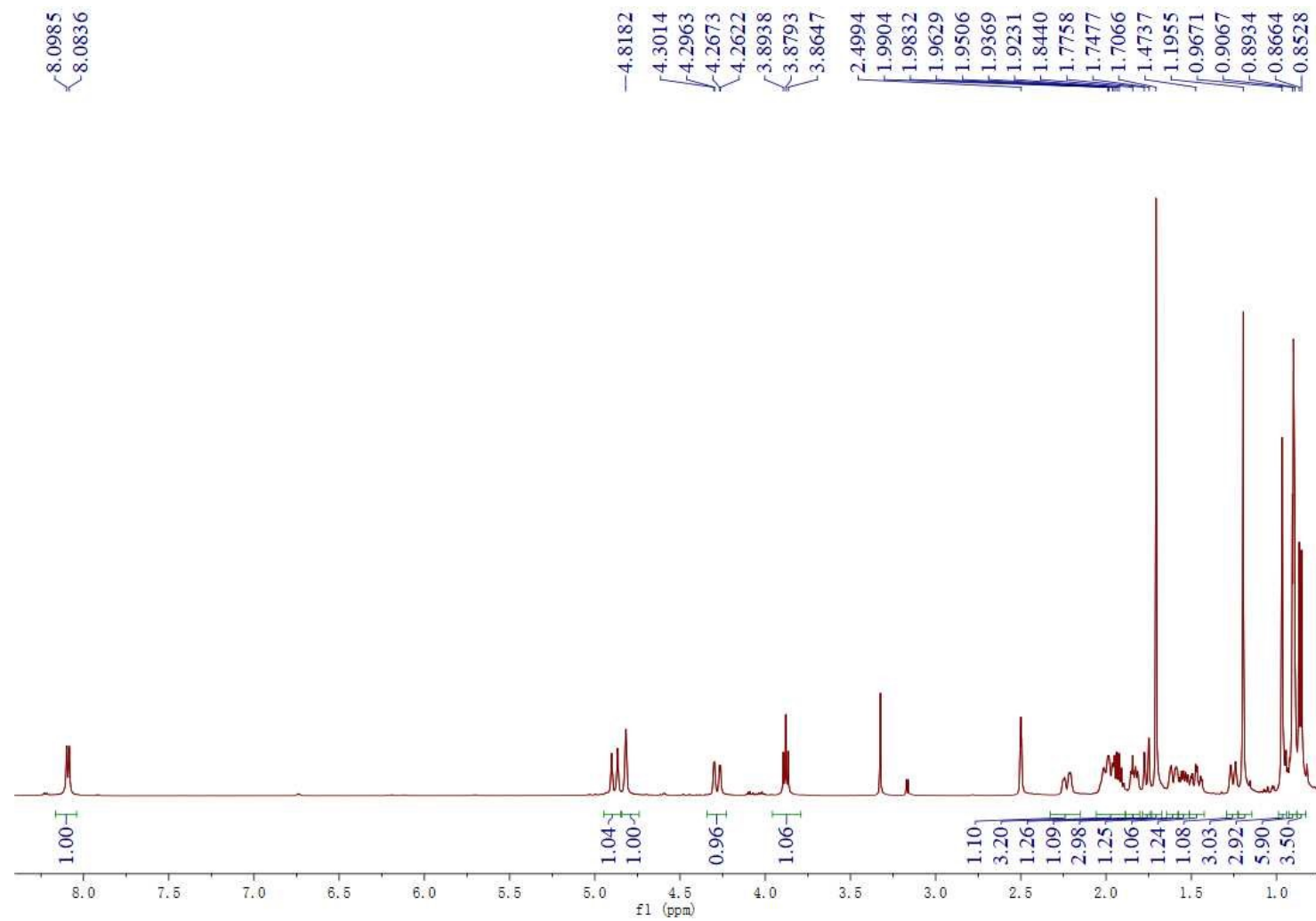
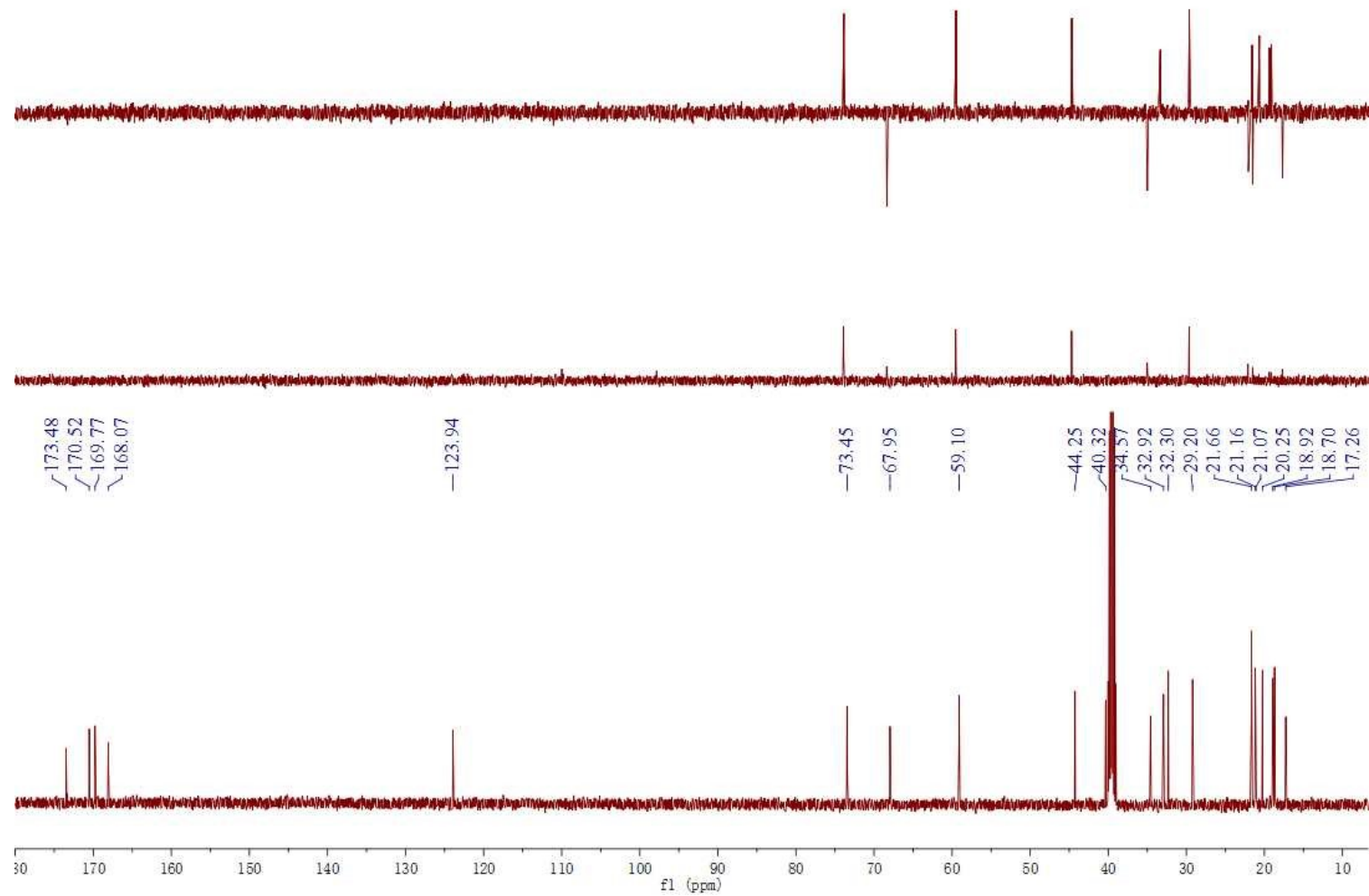


Figure S88.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **17**;



**Figure S89.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **18**;

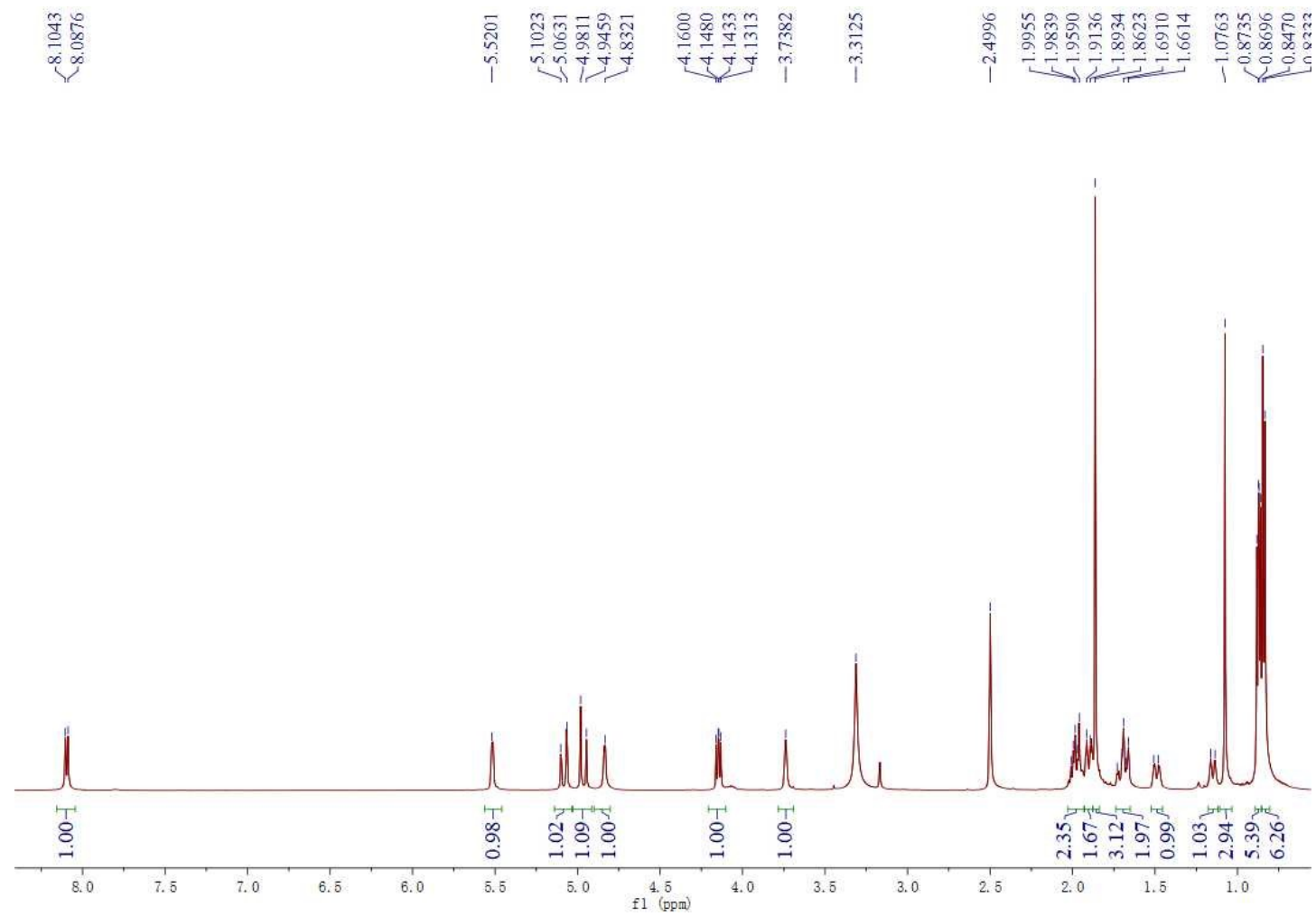
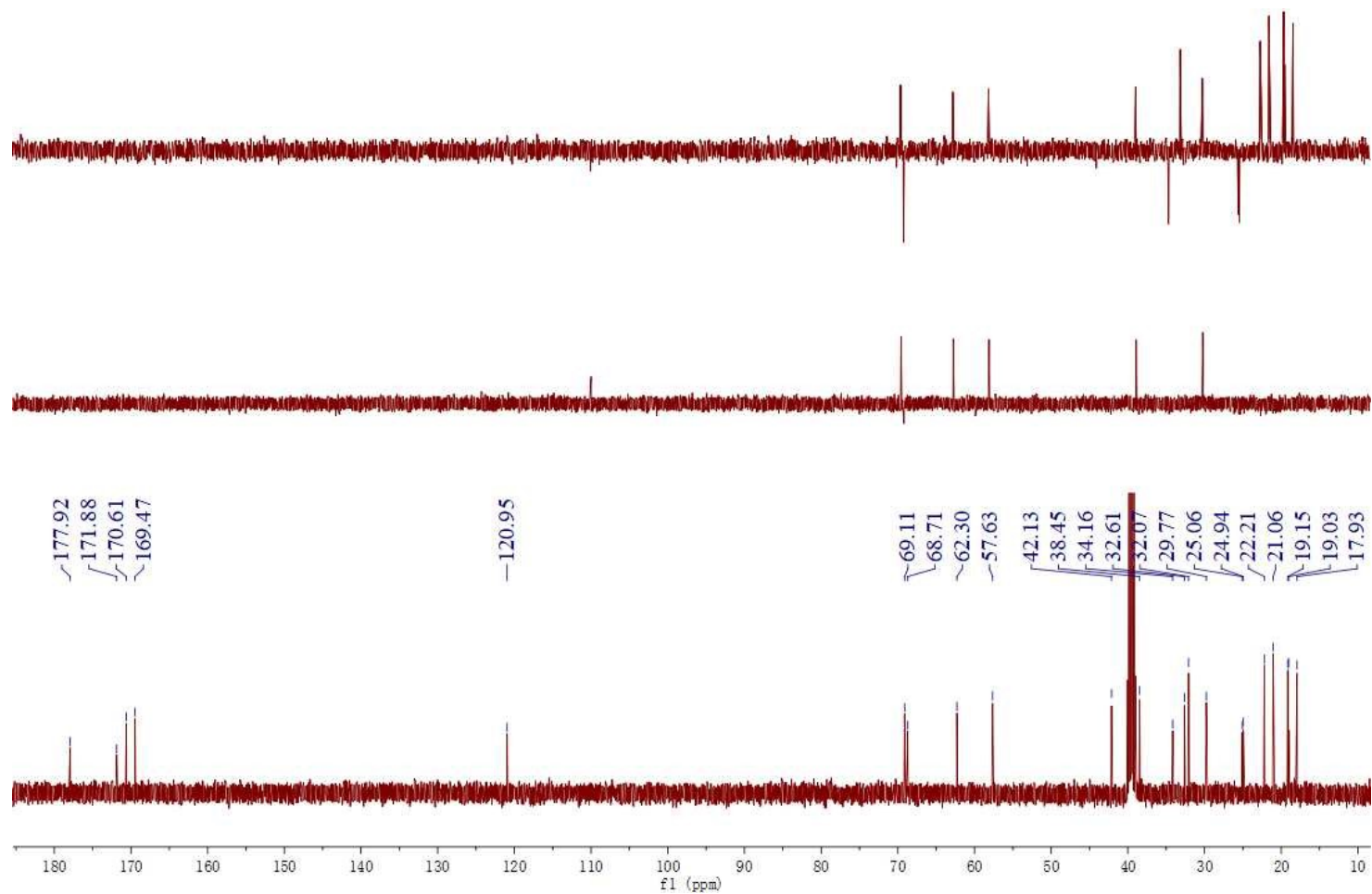
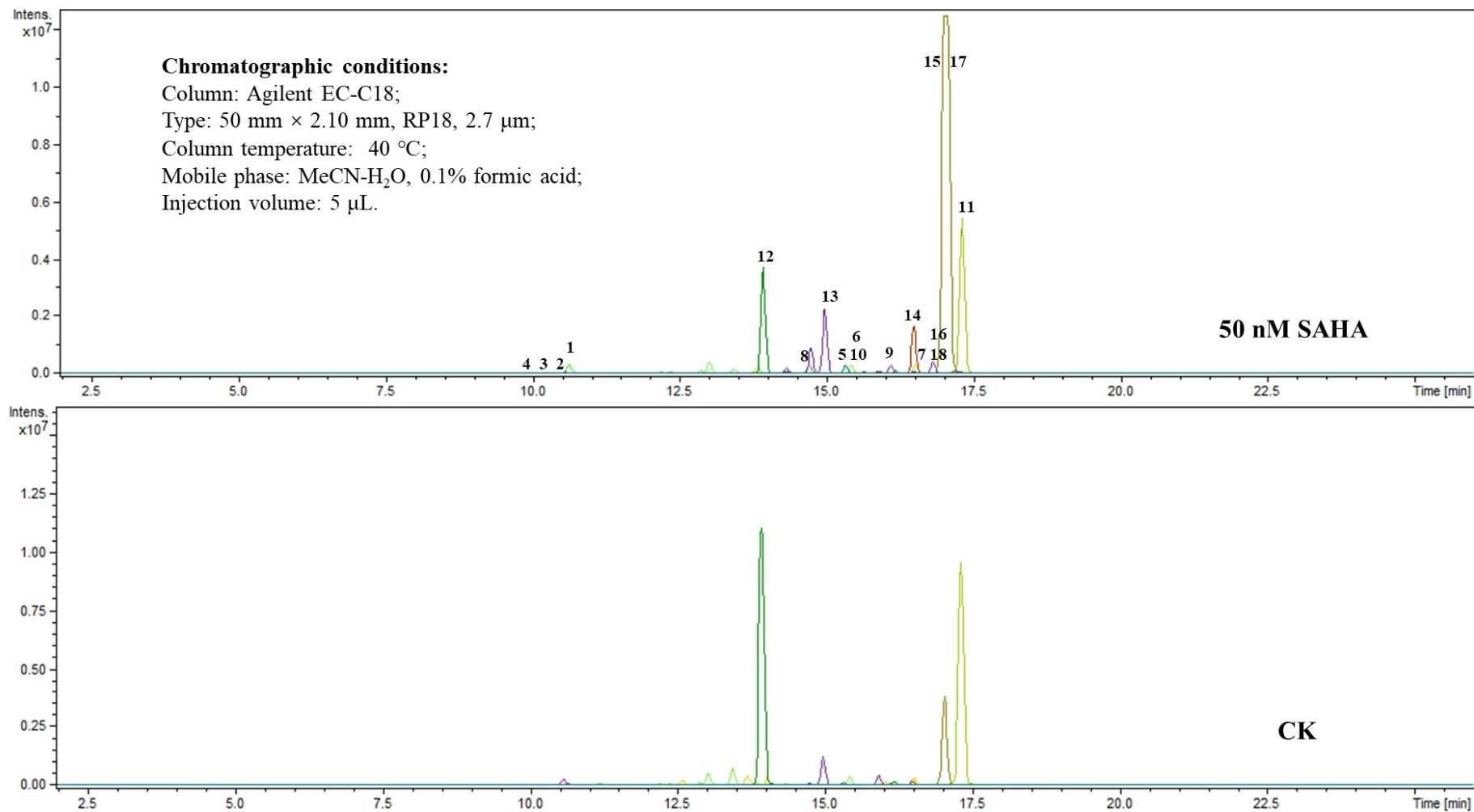


Figure S90.  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **18**.

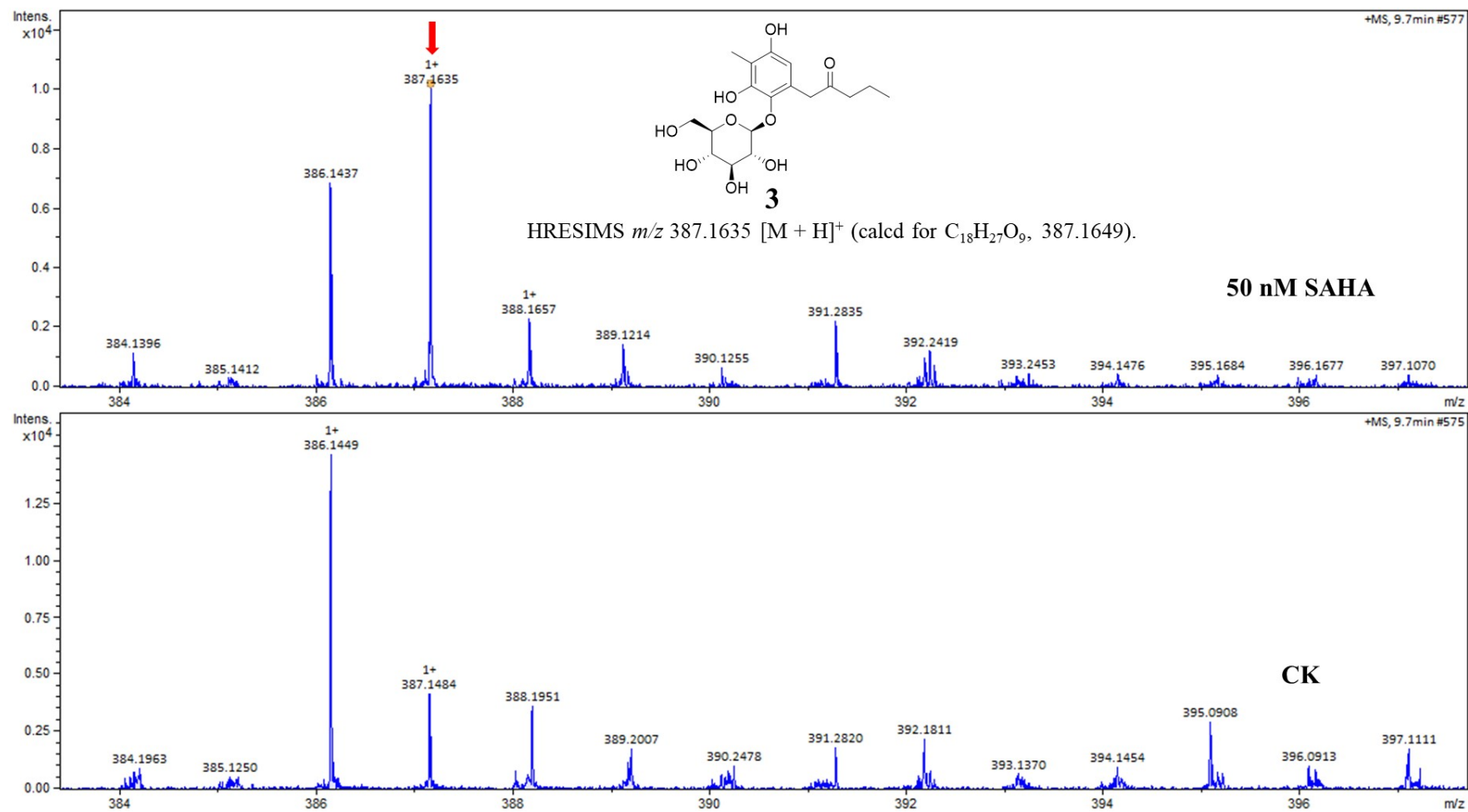


**Figure S91.** LCMS analysis of *T. minioluteus* CS-113 with and without SAHA cultured in a single conical flask;





**Figure S92.** Identification of compound **3** by LCMS analysis of *T. minioluteus* CS-113 triggered by SAHA compared with negative control;



**Figure S93.** Identification of compound **4** by LCMS analysis of *T. minioluteus* CS-113 triggered by SAHA compared with negative control.

