

Supporting Information

Heterocornols from the Sponge-Derived Fungus *Pestalotiopsis heterocornis* with Anti-Inflammatory Activity

Hui Lei ^a, Xiaoxu Bi ^b, Xiuping Lin ^c, Jianglian She ^c, Xiaowei Luo ^d, Hong Niu ^a, Dan Zhang ^a and Bin Yang ^{c,*}

^a School of Pharmacy, Southwest Medical University, Luzhou 646000, China; huilei@swmu.edu.cn; dawn123454@swmu.edu.cn; zhangdan@swmu.edu.cn

^b College of Agriculture and Life Sciences, Kunming University, Kunming 50241, China; bxx2797@163.com

^c CAS Key Laboratory of Tropical Marine Bio-resources and Ecology, Guangdong Key Laboratory of Marine Materia Medica, South China Sea Institute of Oceanology, Chinese Academy of Sciences, Guangzhou 510301, China

^d Institute of Marine Drugs, Guangxi University of Chinese Medicine, Nanning 530200, China

*Correspondence: yangbin@scsio.ac.cn (B. Yang); Tel: +86-020-89023174 (B.Y.)

Figure S1. HRESI-MS spectrum of the new compound **1**

Figure S2. ¹H NMR (500 MHz, CD₃OD) spectrum of the new compound **1**

Figure S3. ¹³C NMR (125 MHz, CD₃OD) spectrum of the new compound **1**

Figure S4. HSQC spectrum of the new compound **1**

Figure S5. HMBC spectrum of the new compound **1**

Figure S6. COSY spectrum of the new compound **1**

Figure S7. NOESY spectrum of the new compound **1**

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Figure S45. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **6**

Figure S46. HSQC spectrum of compound **6**

Figure S47. HMBC spectrum of compound **6**

Figure S48. HRESI-MS spectrum of the new compound **7**

Figure S49. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **7**

Figure S50. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **7**

Figure S51. HSQC spectrum of the new compound **7**

Figure S52. HMBC spectrum of the new compound **7**

Figure S53. HRESI-MS spectrum of the new compound **8**

Figure S54. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **8**

Figure S55. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **8**

Figure S56. HSQC spectrum of the new compound **8**

Figure S57. HMBC spectrum of the new compound **8**

Figure S58. HRESI-MS spectrum of the new compound **9**

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Figure S60. ^1H NMR (500 MHz, CDCl_3) spectrum of the new compound **9**

Figure S61. ^{13}C NMR (125 MHz, CDCl_3) spectrum of the new compound **9**

Figure S62. HSQC spectrum of the new compound **9**

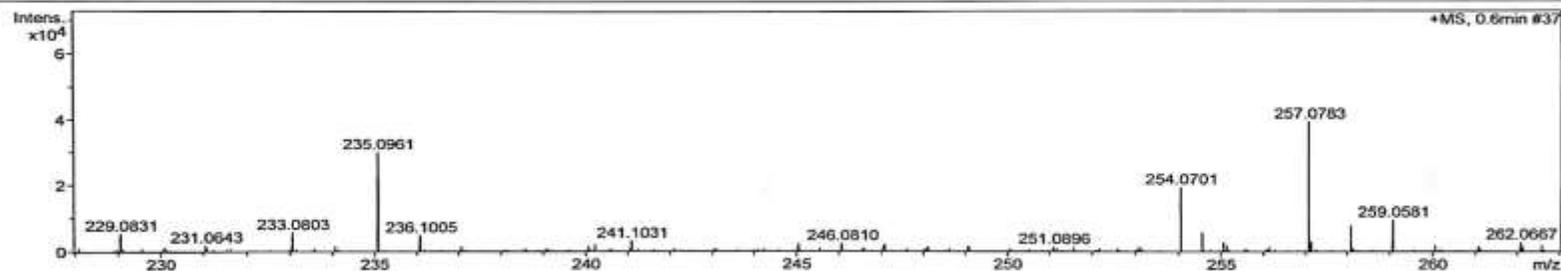
Figure S63. HMBC spectrum of the new compound **9**

Figure S64. HPLC chromatograms of EtOAc extracts monitored

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/5/2018 4:00:09 PM
Analysis Name	D:\Data\MS\data\201812\yangbin_L32_neg_21_01_5869.d	Operator	SCSIO
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis
Sample Name	yangbin_L32_neg		255552.00029
Comment			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
235.0961	1	C13H15O4	100.00	235.0965	-1.5	-0.4	14.2	6.5	even	ok
257.0783	1	C13H14NaO4	100.00	257.0784	0.7	0.2	33.1	6.5	even	ok

Figure S1. HRESI-MS spectrum of the new compound **1**

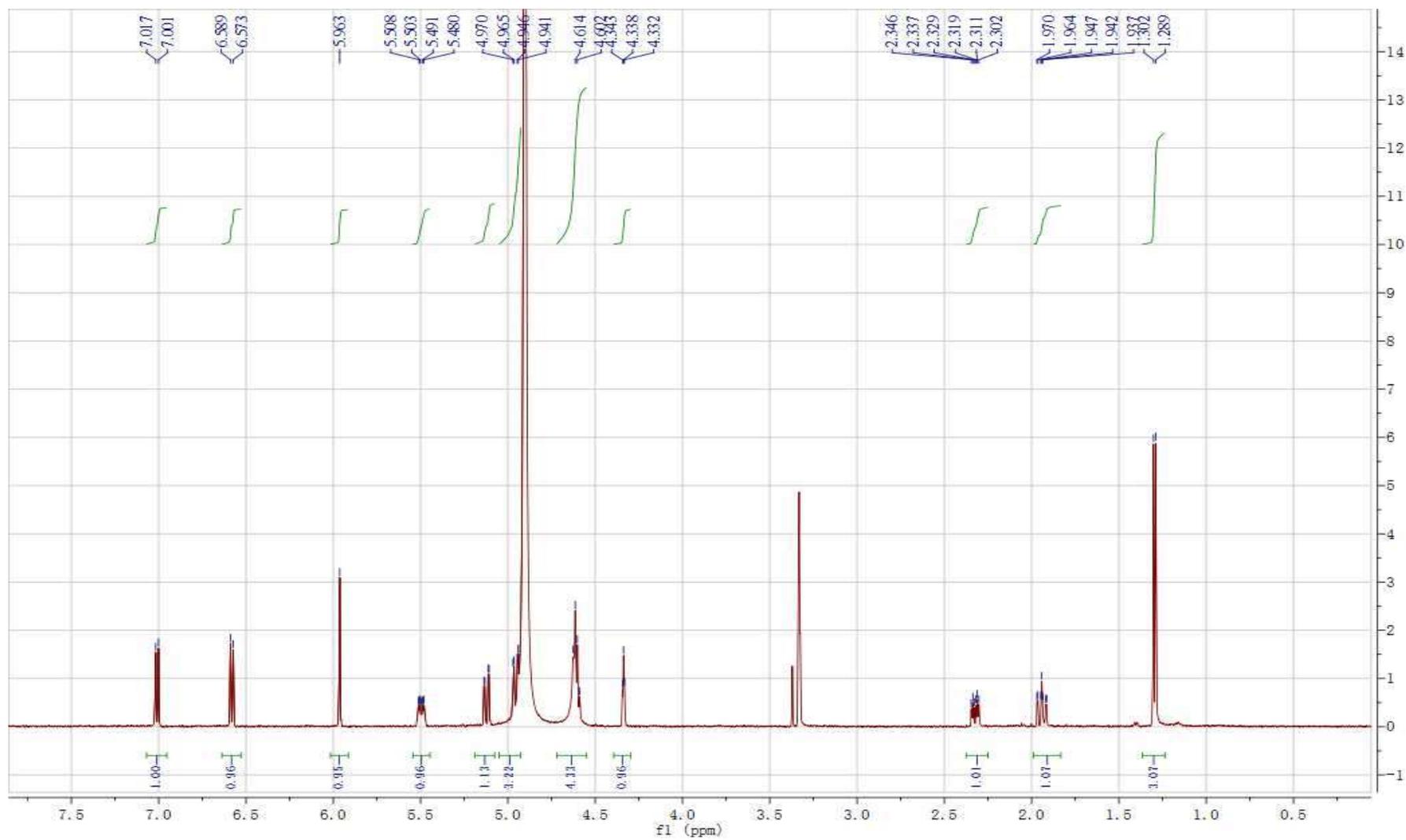


Figure S2. ¹H NMR (500 MHz, CD₃OD) spectrum of the new compound **1**

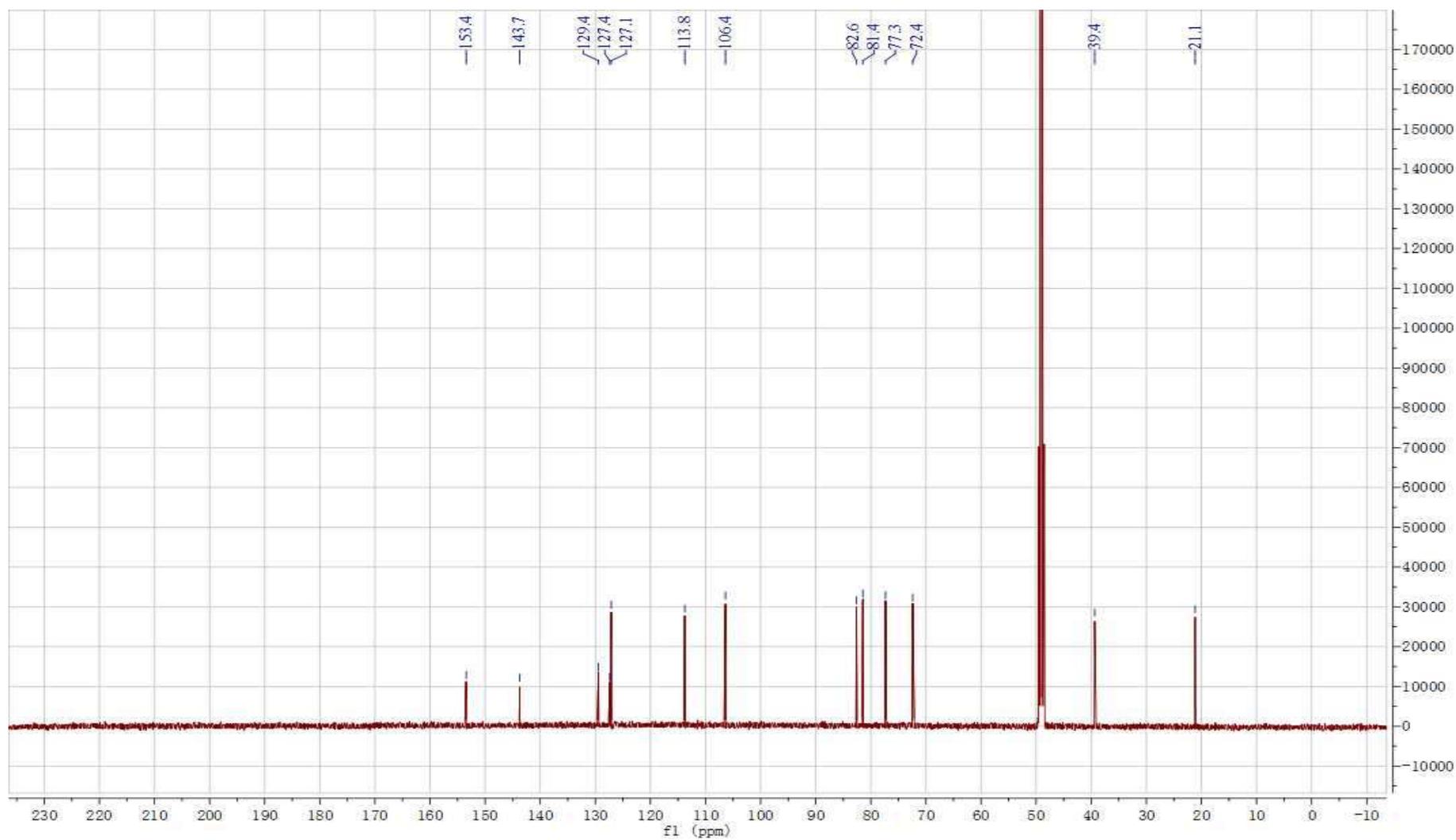


Figure S3. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **1**

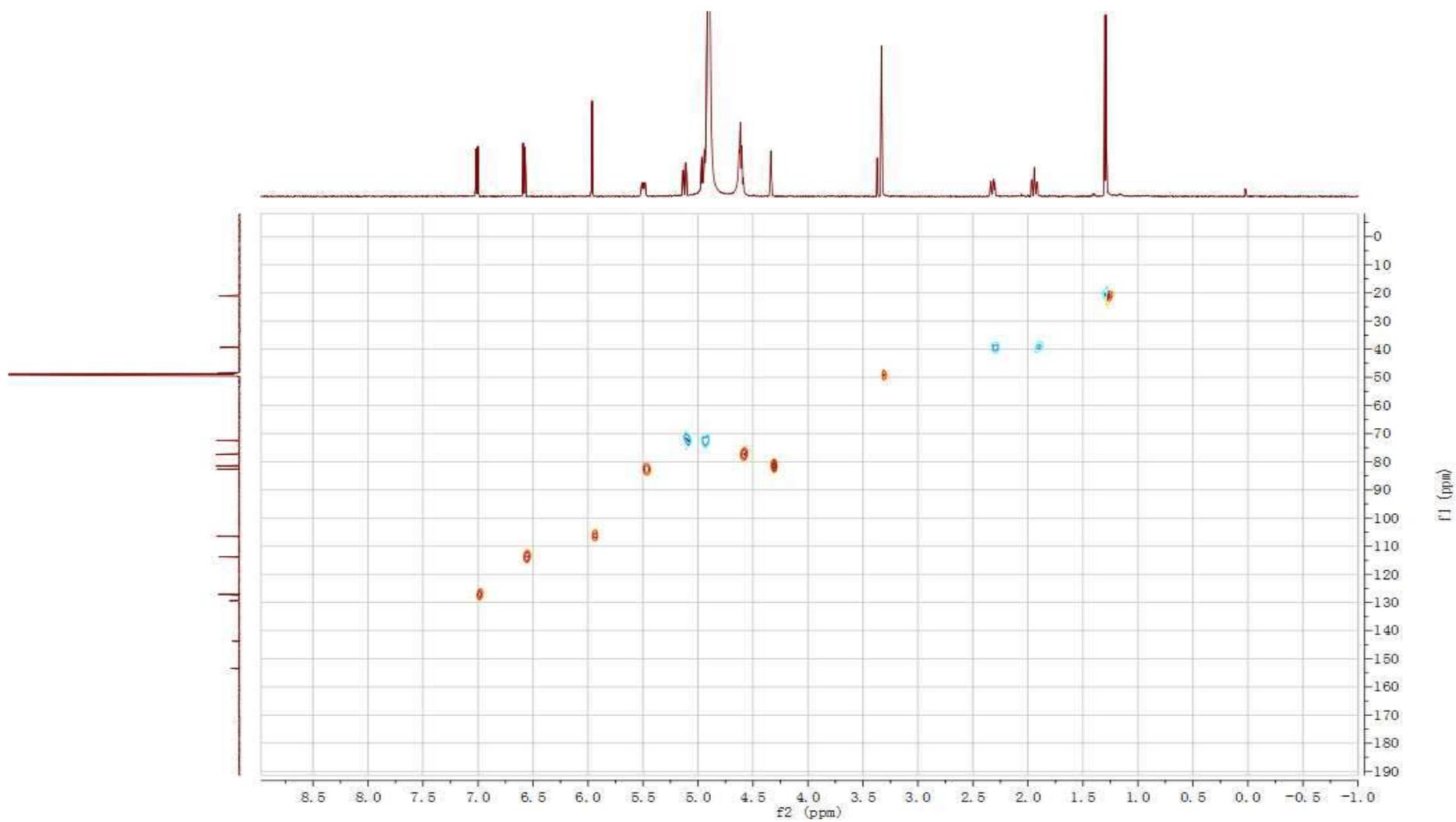


Figure S4. HSQC spectrum of the new compound **1**

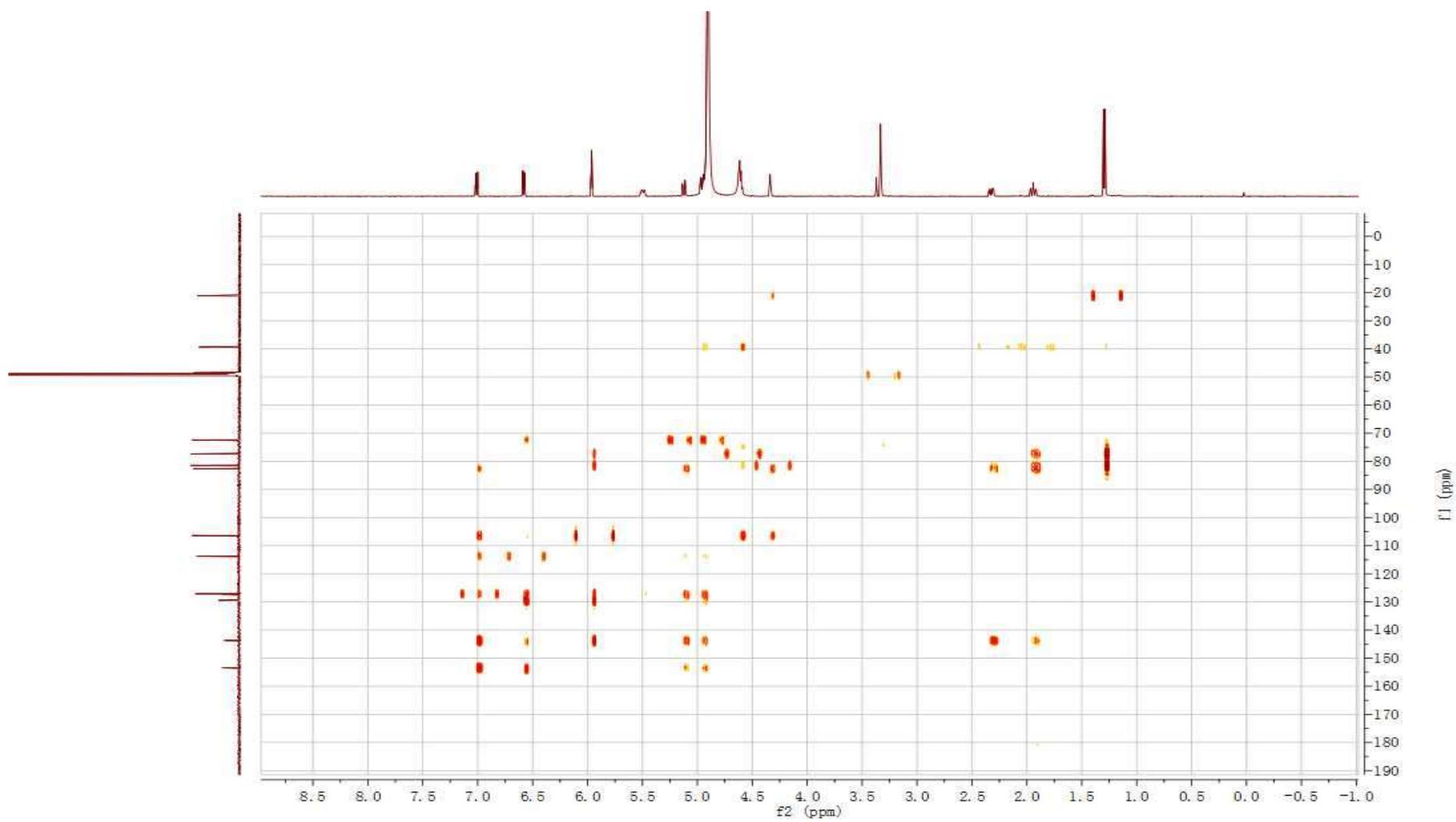


Figure S5. HMBC spectrum of the new compound **1**

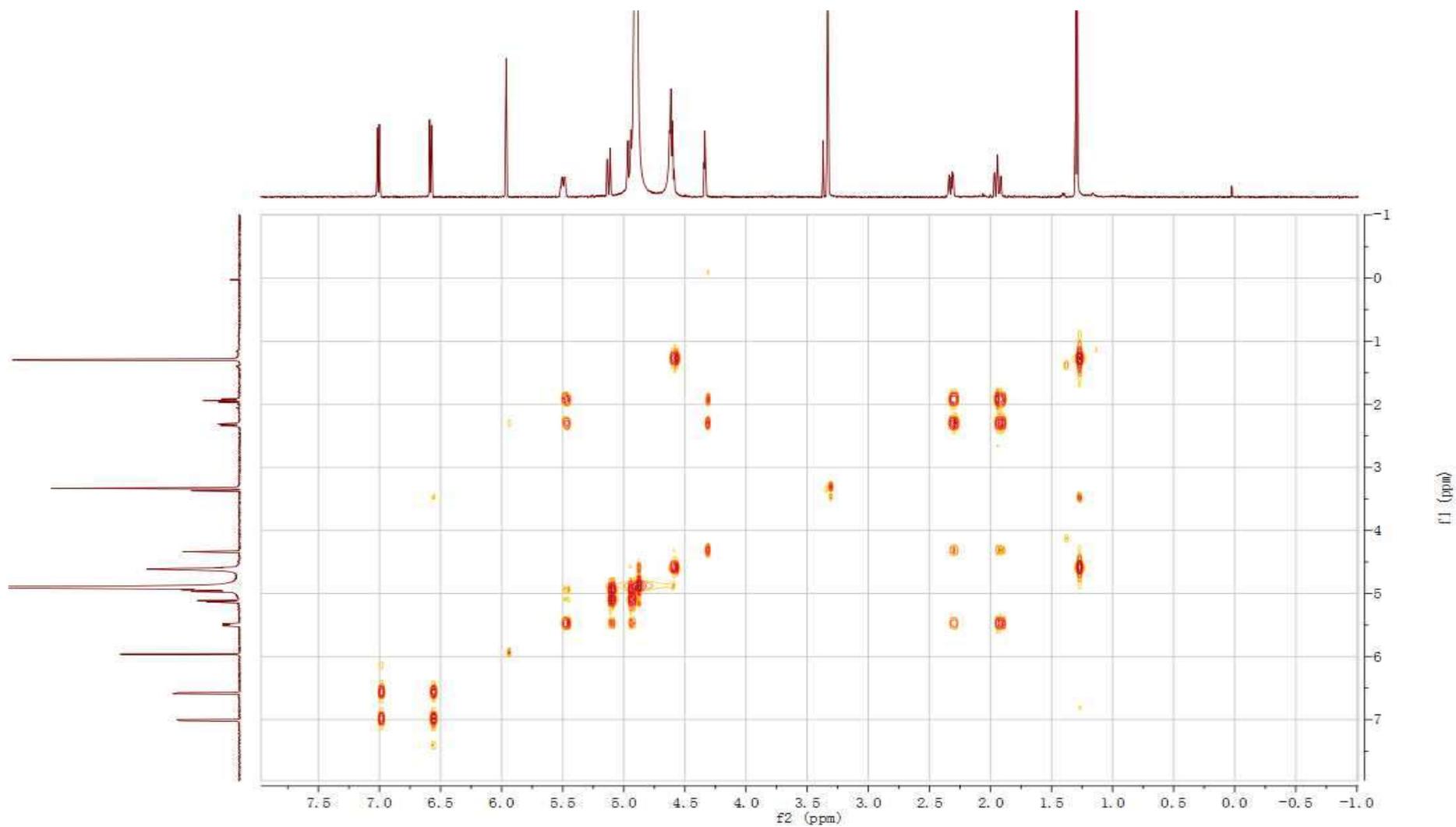


Figure S6. COSY spectrum of the new compound **1**

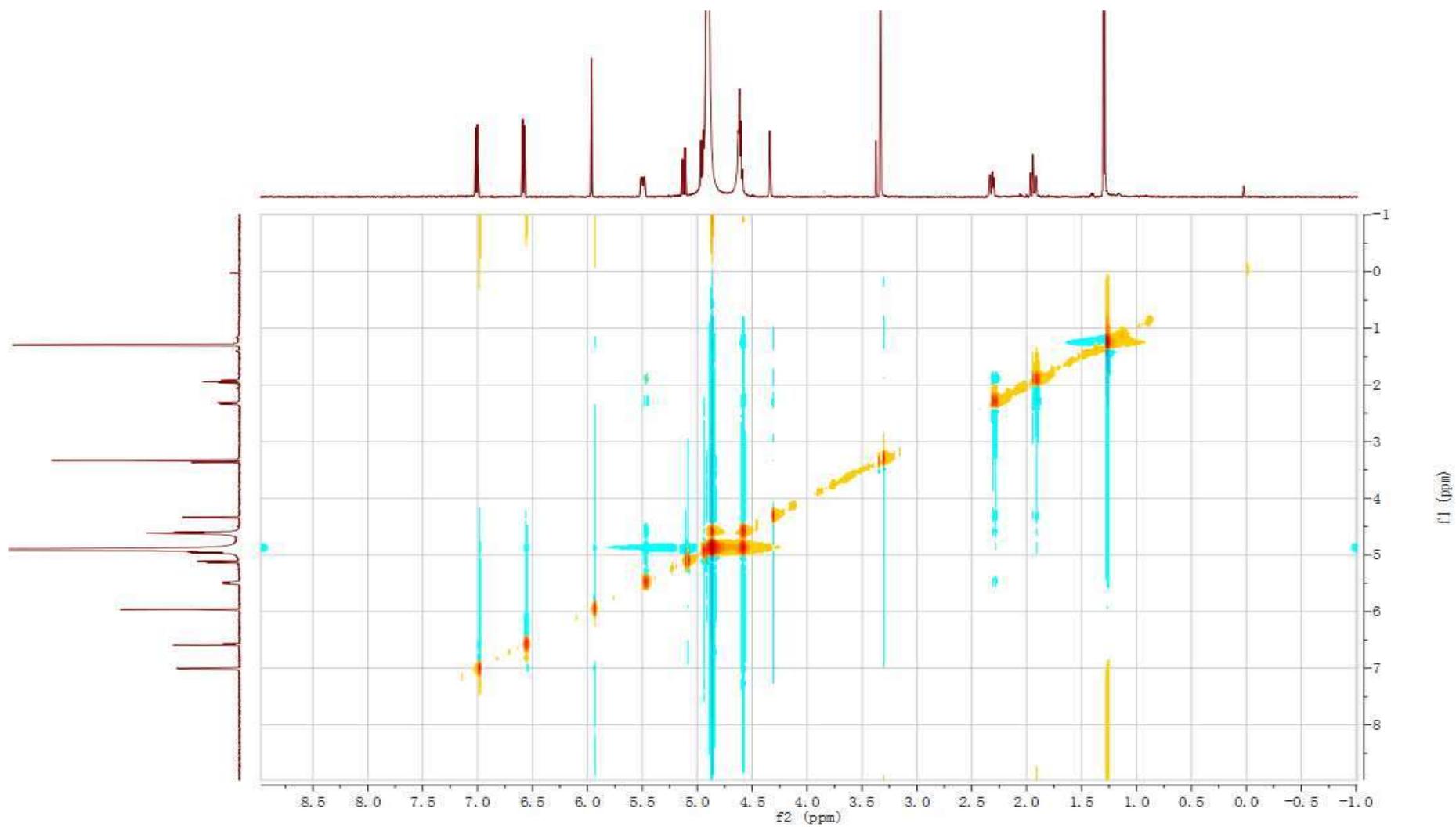


Figure S7. NOESY spectrum of the new compound **1**

HR-ESI-MS-NEG

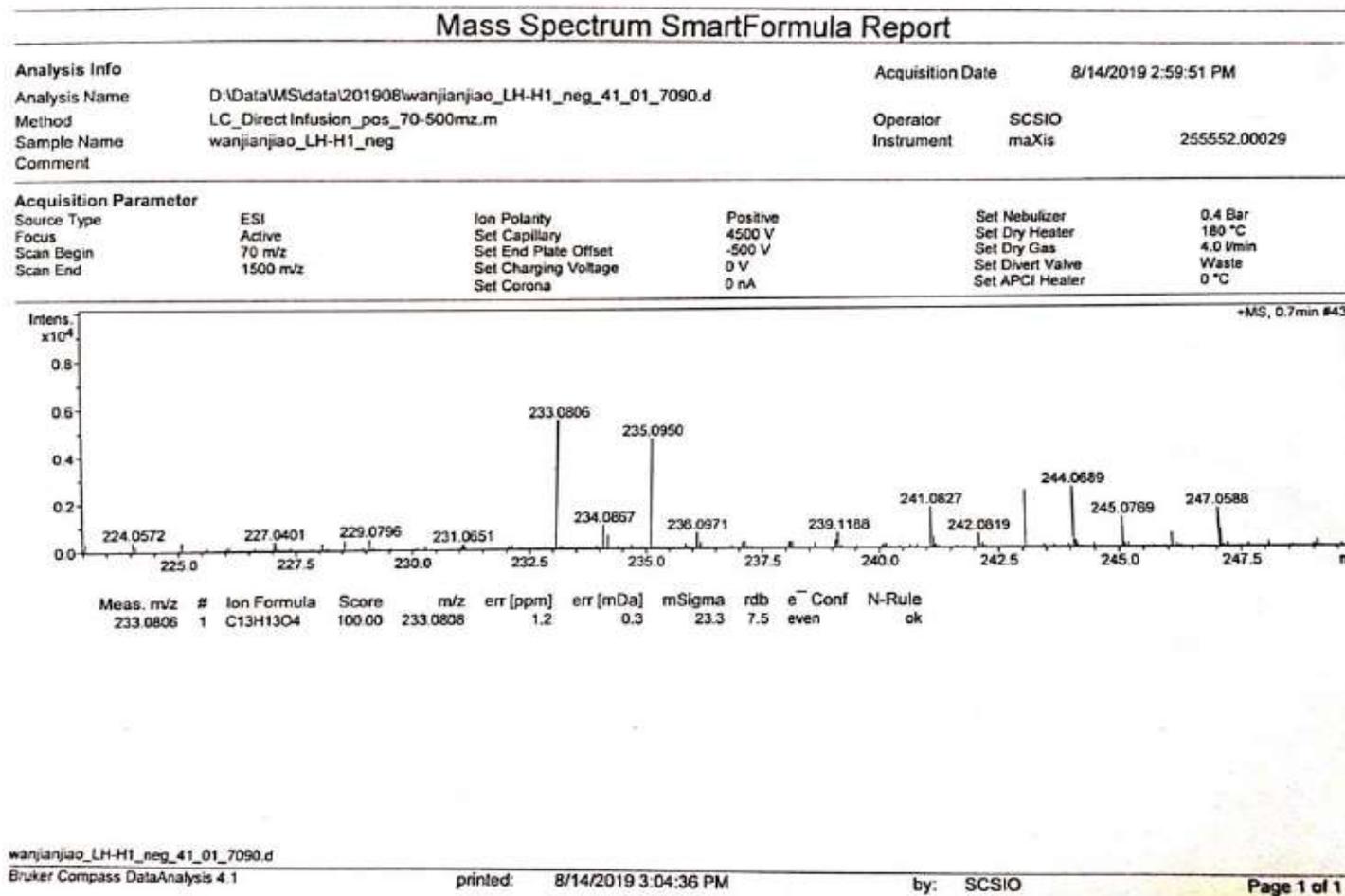


Figure S8. HRESI-MS spectrum of the new compound 2

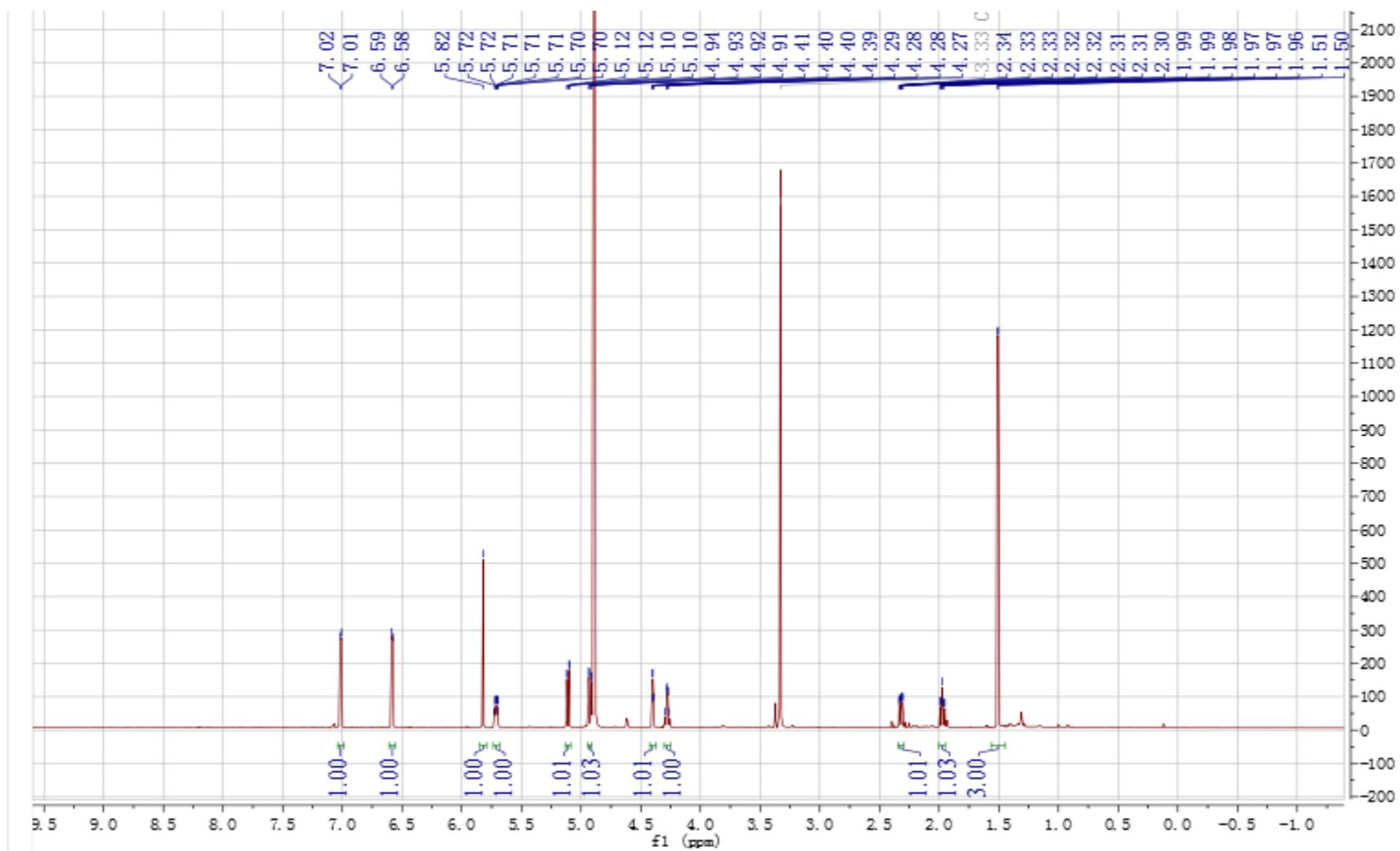


Figure S9. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **2**

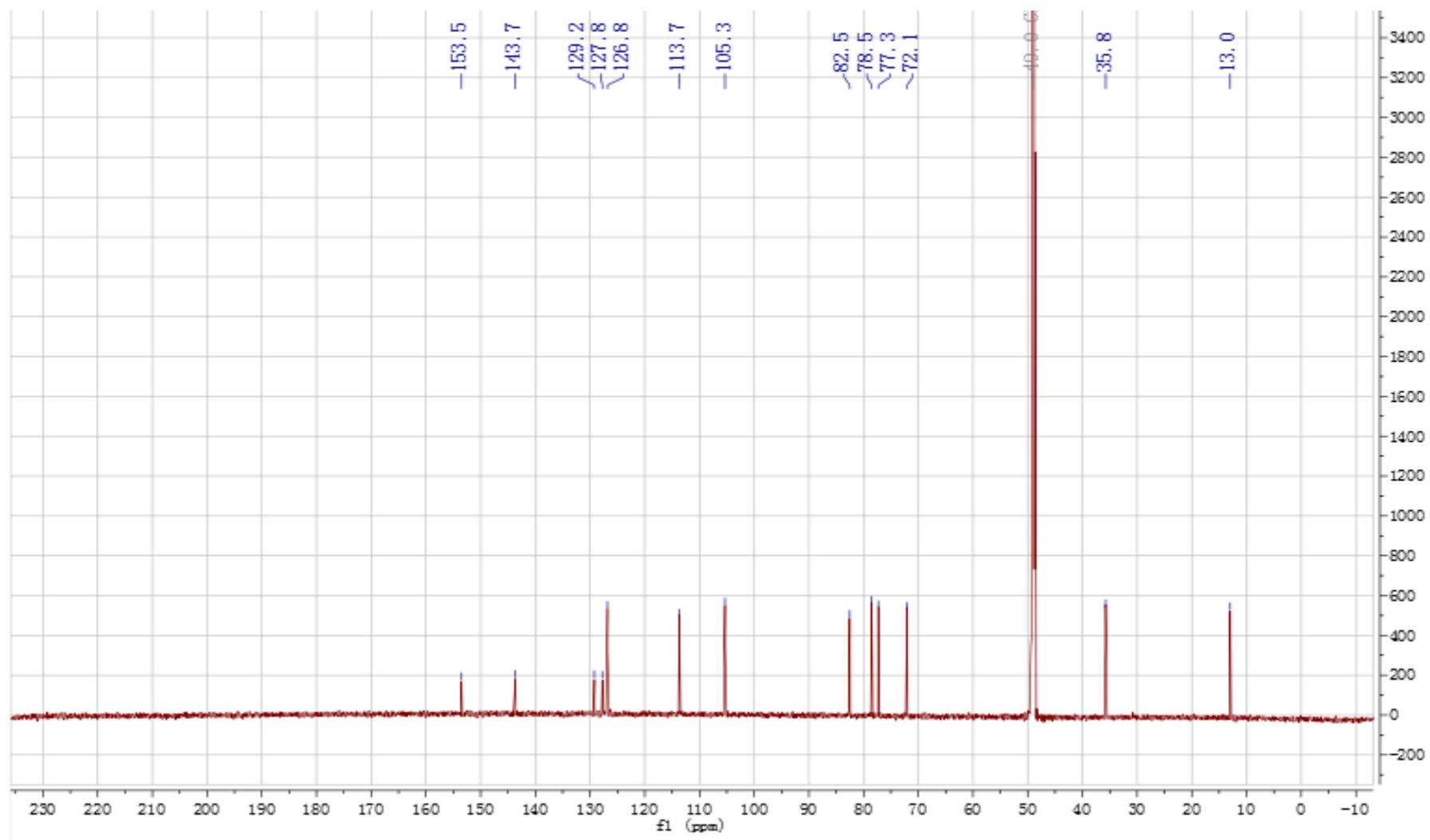


Figure S10. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the newcompound **2**

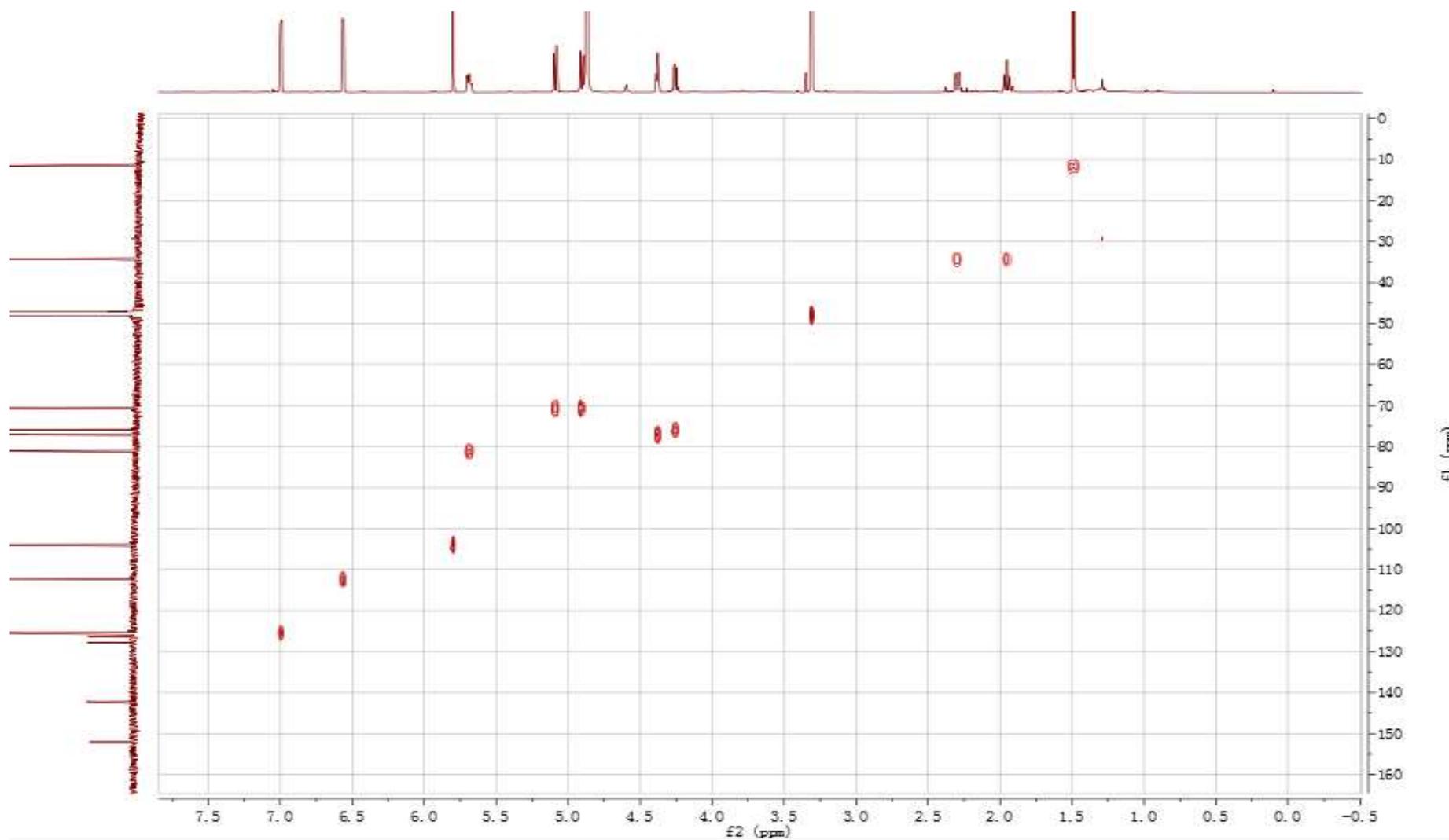


Figure S11. HSQC spectrum of the new compound **2**

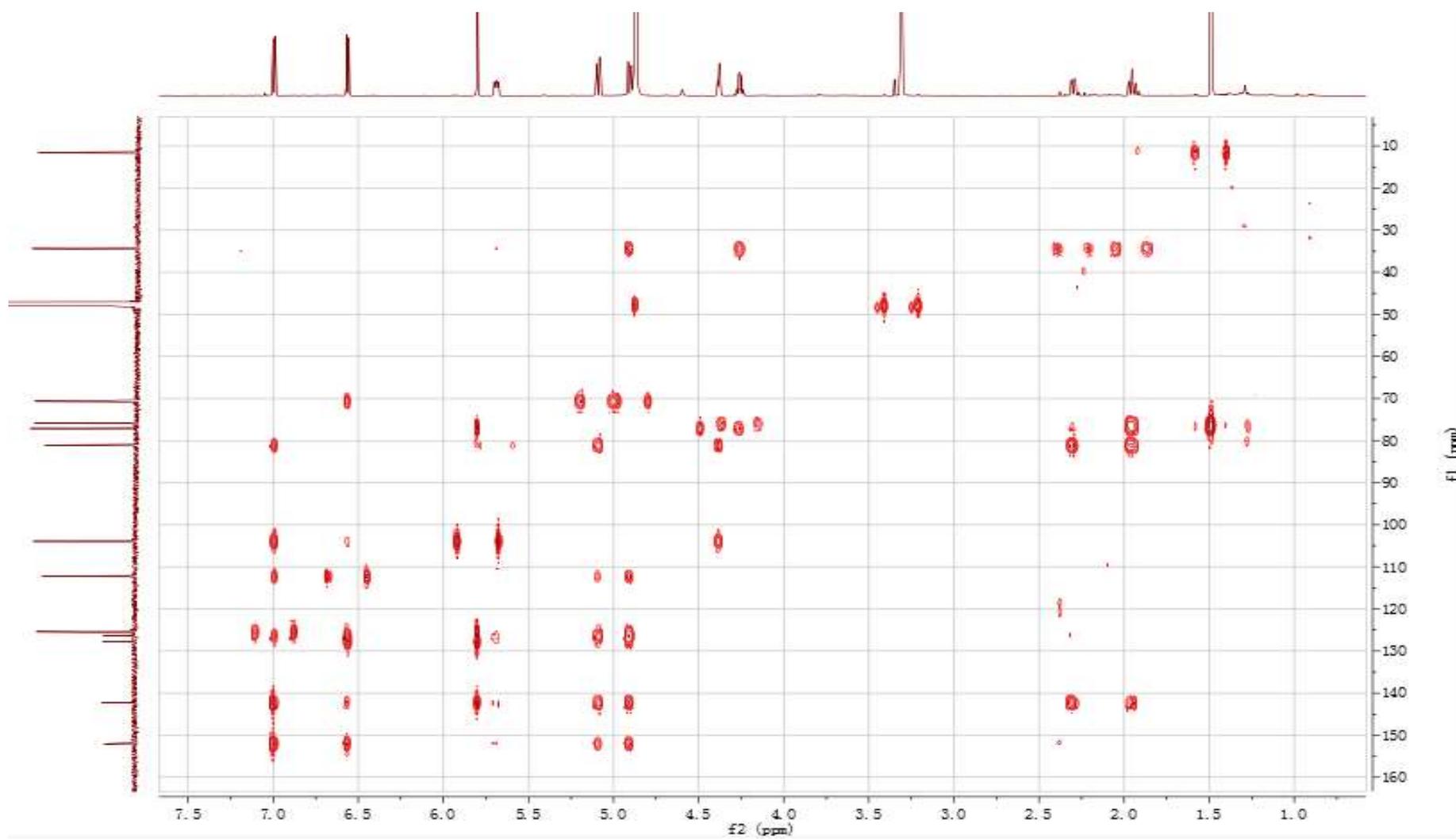


Figure S12. HMBC spectrum of the new compound **2**

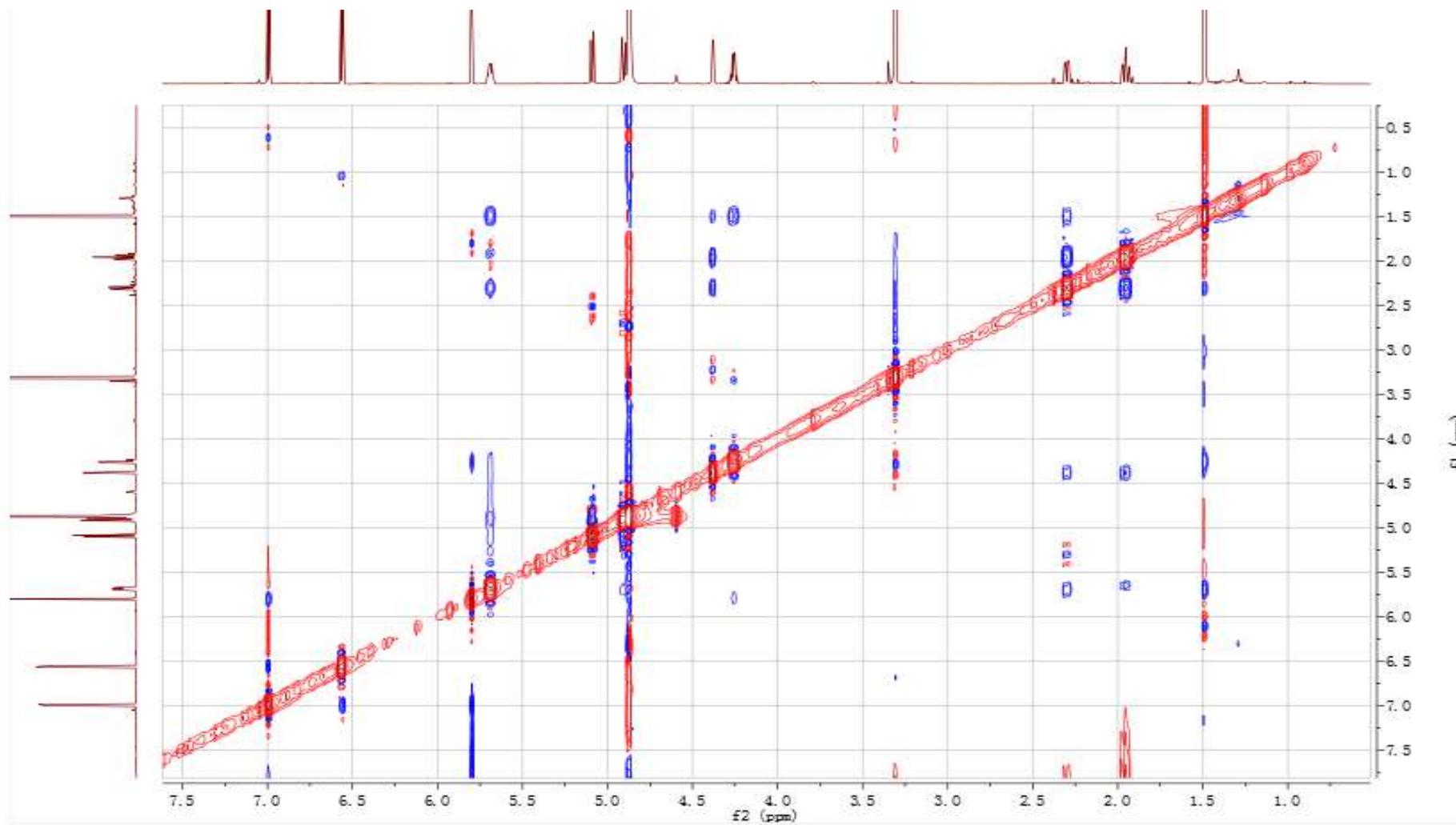
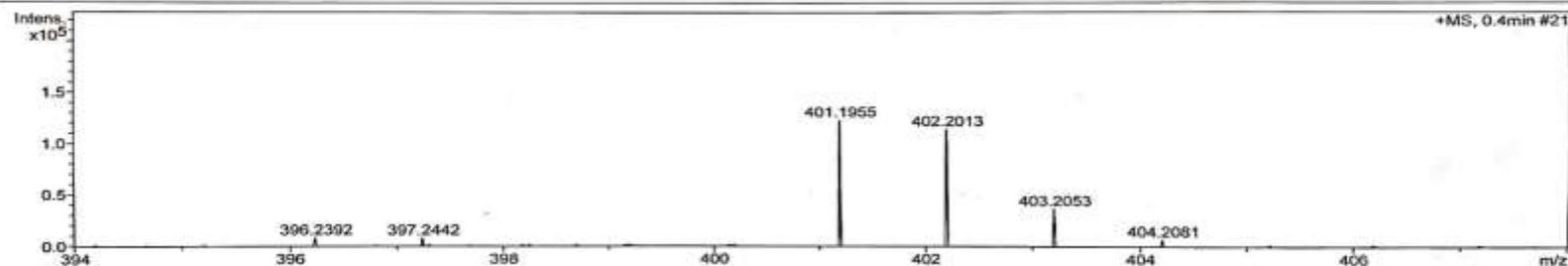


Figure S14. NOESY spectrum of the new compound **2**

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/5/2018 3:53:15 PM	
Analysis Name	D:\Data\MS\data\201812\yangbin_L37_pos_22_01_5867.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis	
Sample Name	yangbin_L37_pos		255552.00029	
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
379.2100	1	C21H31O6	100.00	379.2115	-4.0	-1.5	291.1	6.5	even	ok
401.1955	1	C21H30NaO6	100.00	401.1935	5.2	2.1	372.7	6.5	even	ok
779.4017	1	C42H60NaO12	100.00	779.3977	5.2	4.0	483.3	12.5	even	ok

Figure S15. HRESI-MS spectrum of the new compound **3**

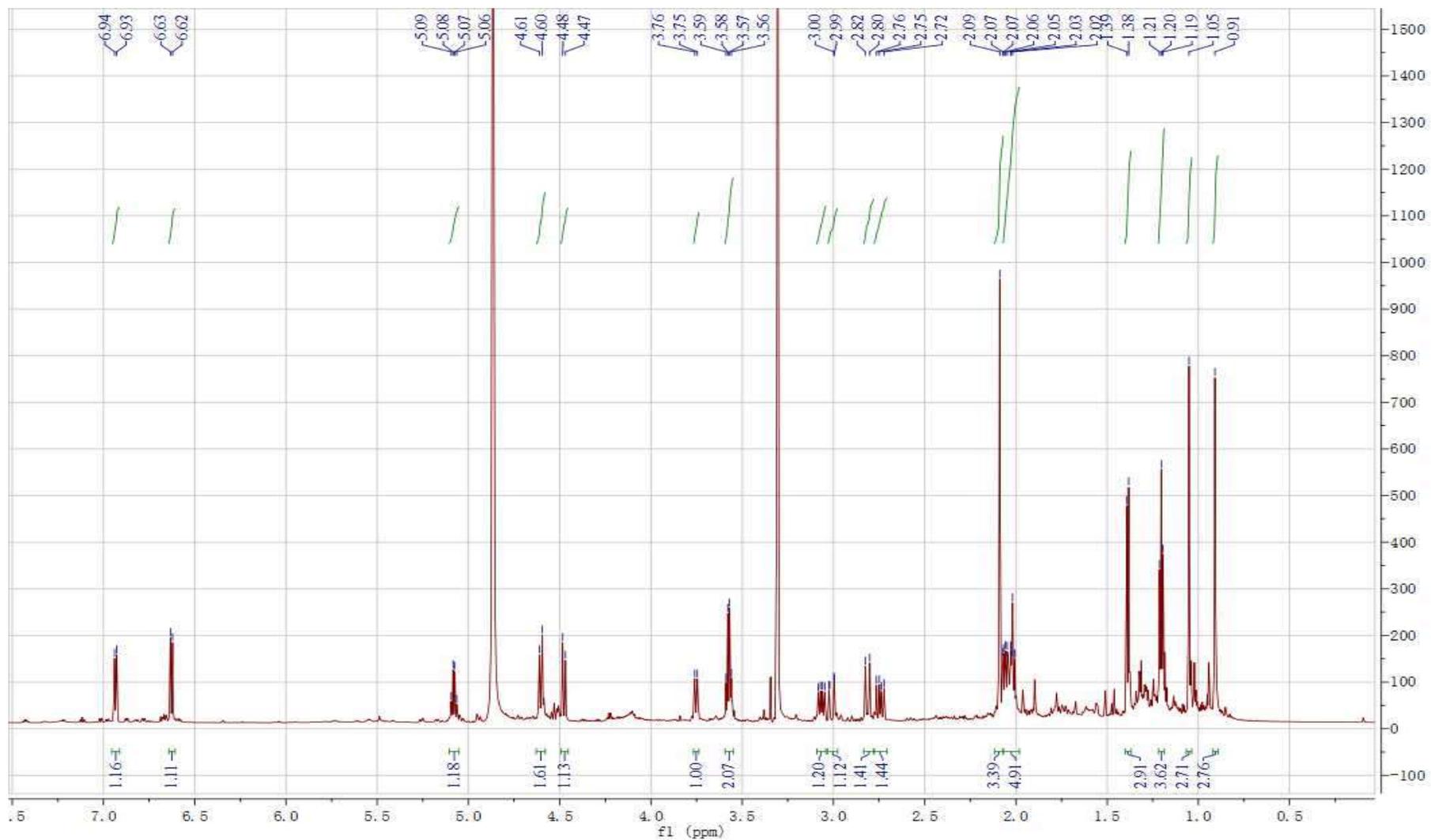


Figure S16. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **3**

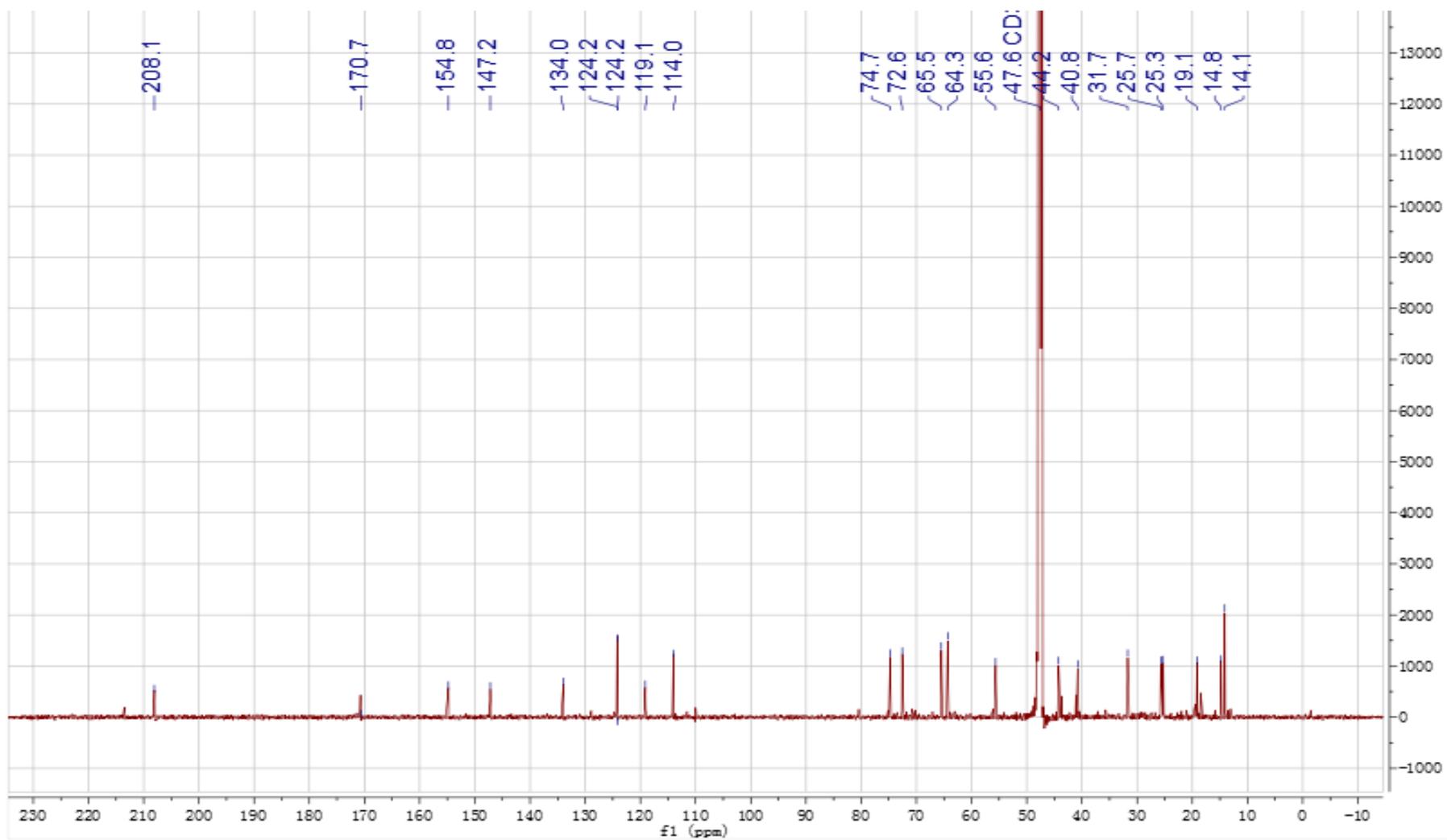


Figure S17. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **3**

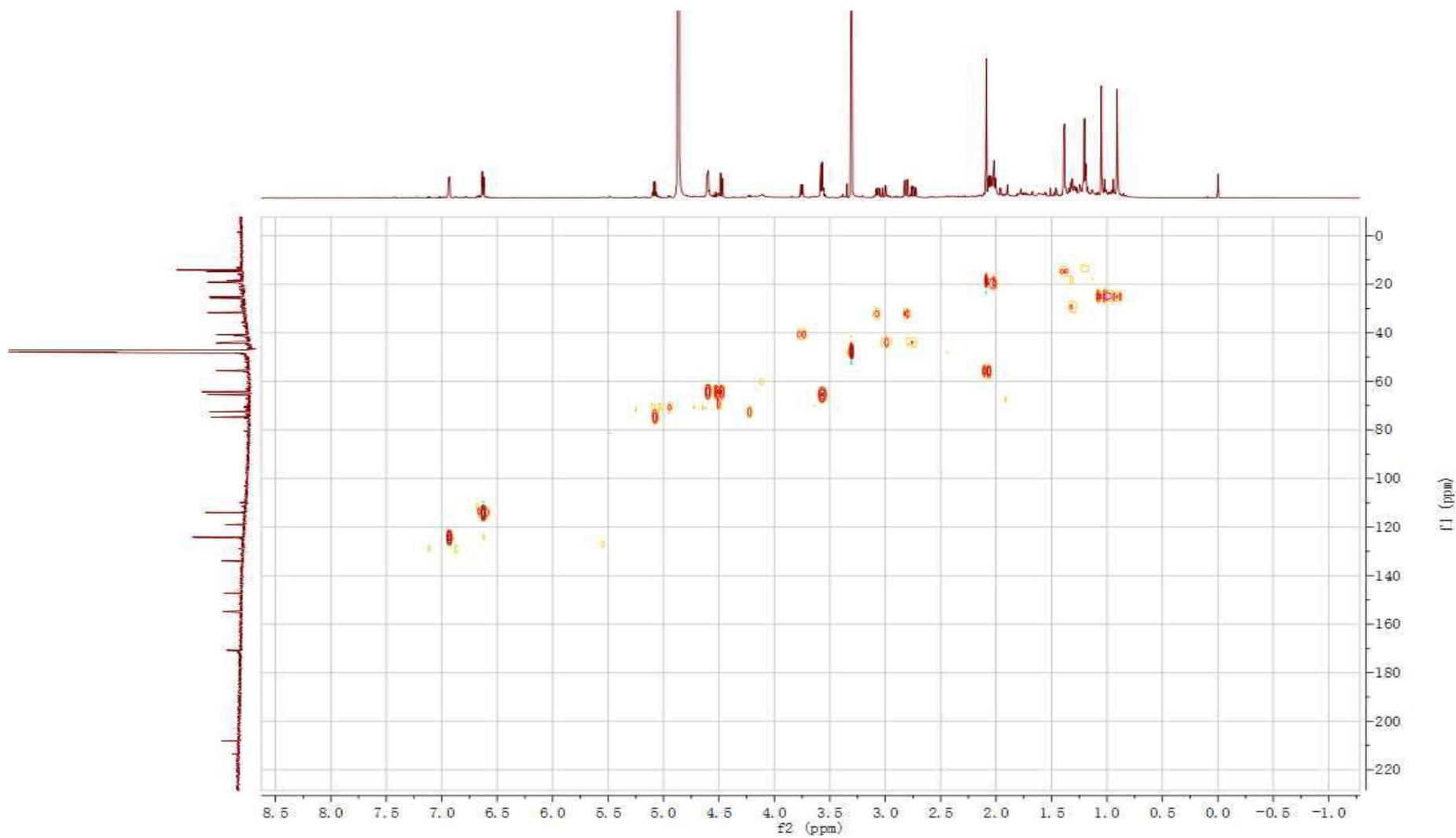


Figure S18. HSQC spectrum of the new compound **3**

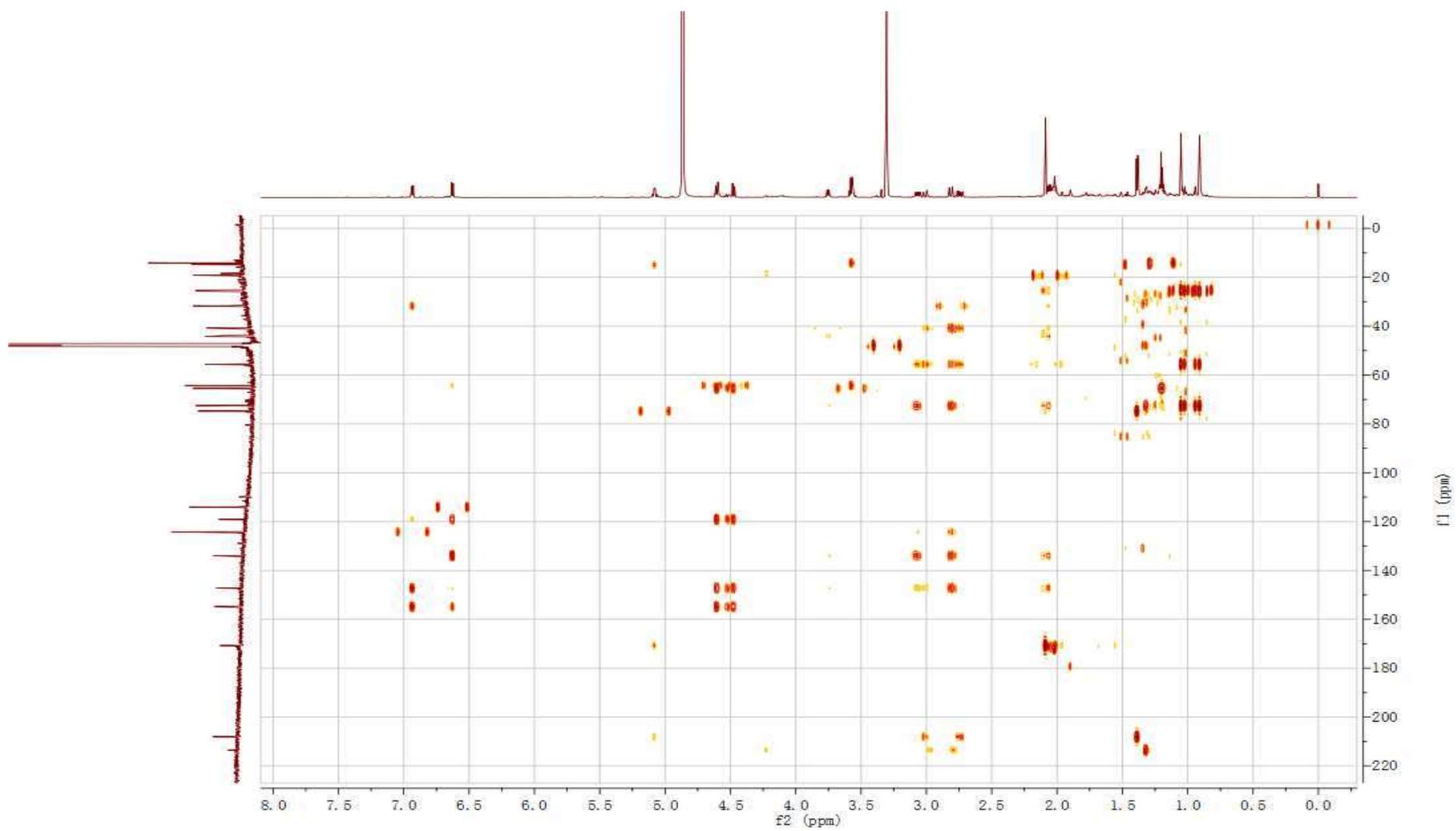


Figure S19. HMBC spectrum of the new compound **3**

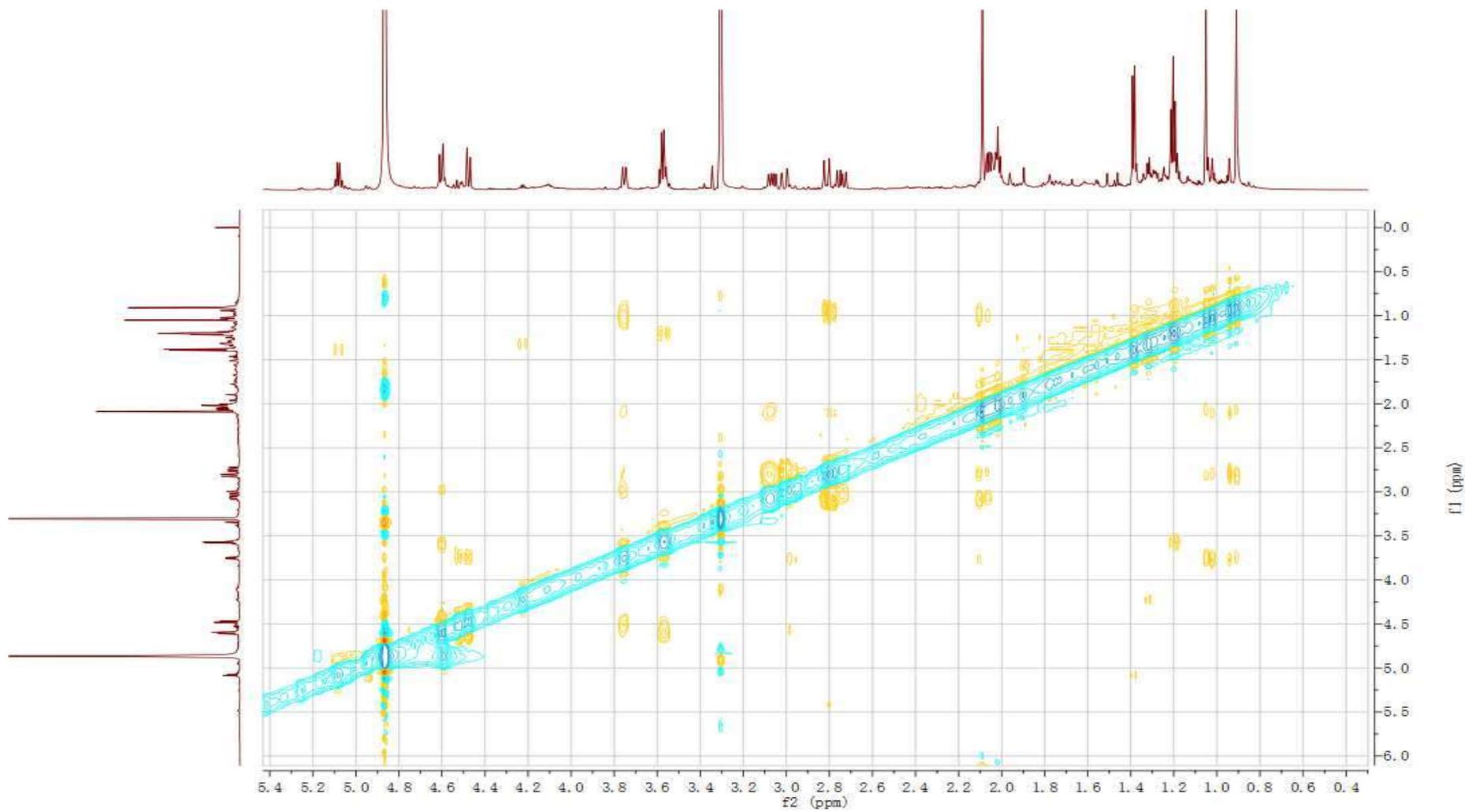
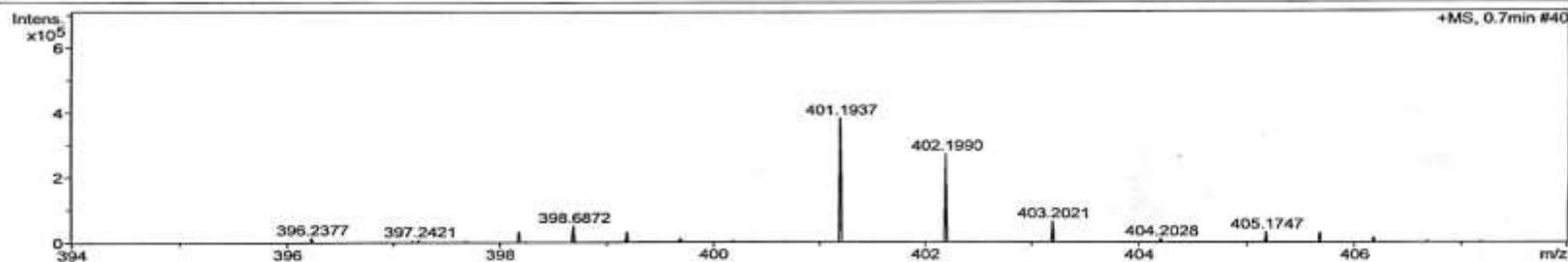


Figure S20. NOESY spectrum of the new compound **3**

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/5/2018 3:56:42 PM	
Analysis Name	D:\Data\MS\data\201812\yangbin_L38_pos_23_01_5868.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis	
Sample Name	yangbin_L38_pos		255552.00029	
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
401.1937	1	C21H30NaO6	100.00	401.1935	0.7	0.3	249.3	6.5	even	ok
779.3962	1	C42H60NaO12	100.00	779.3977	-1.9	-1.5	370.1	12.5	even	ok

yangbin_L38_pos_23_01_5868.d
Bruker Compass DataAnalysis 4.1

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Figure S21. HRESI-MS spectrum of the new compound **4**

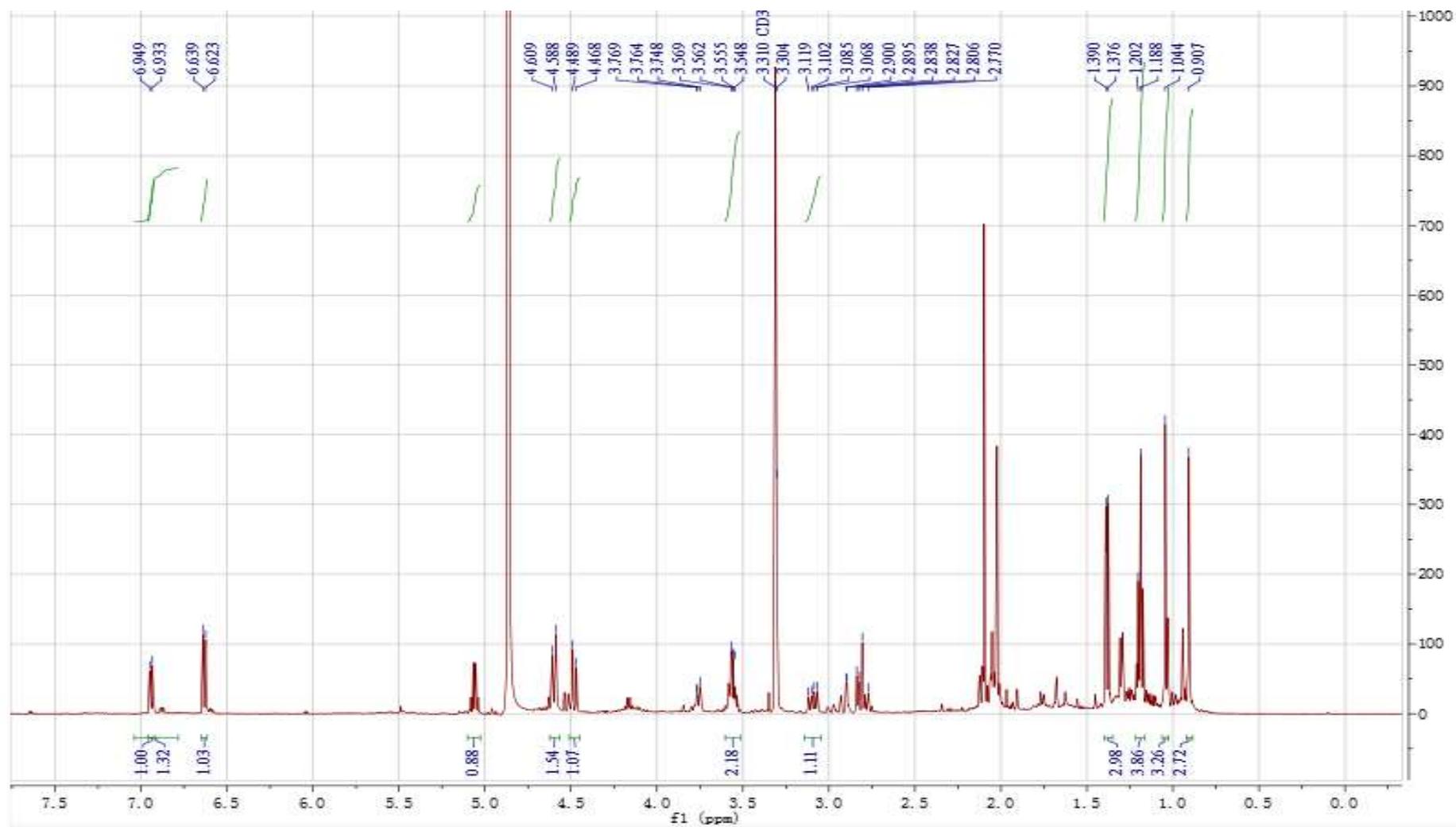


Figure S22. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound 4

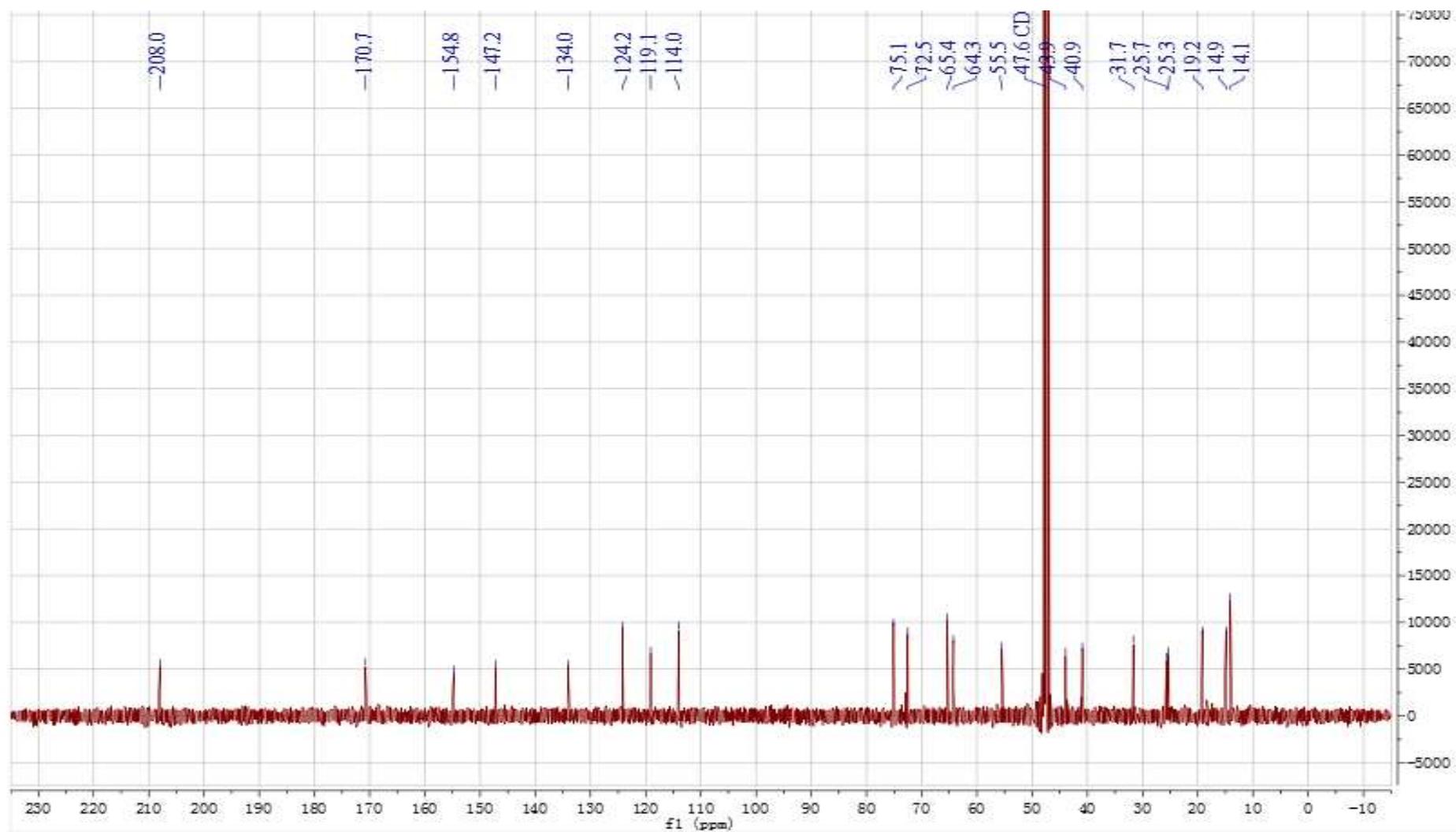


Figure S23. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound 4

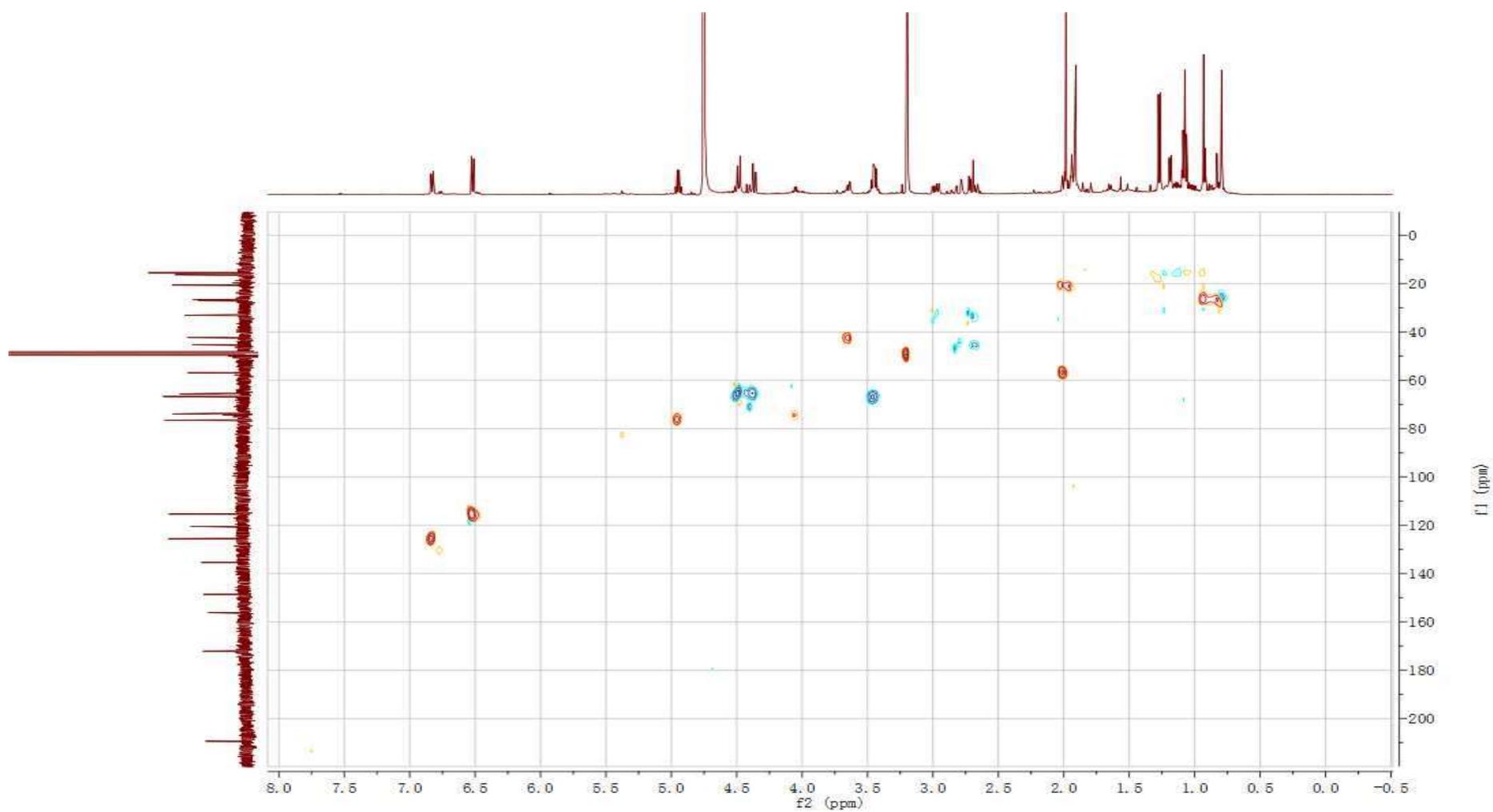


Figure S24. HSQC spectrum of the new compound **4**

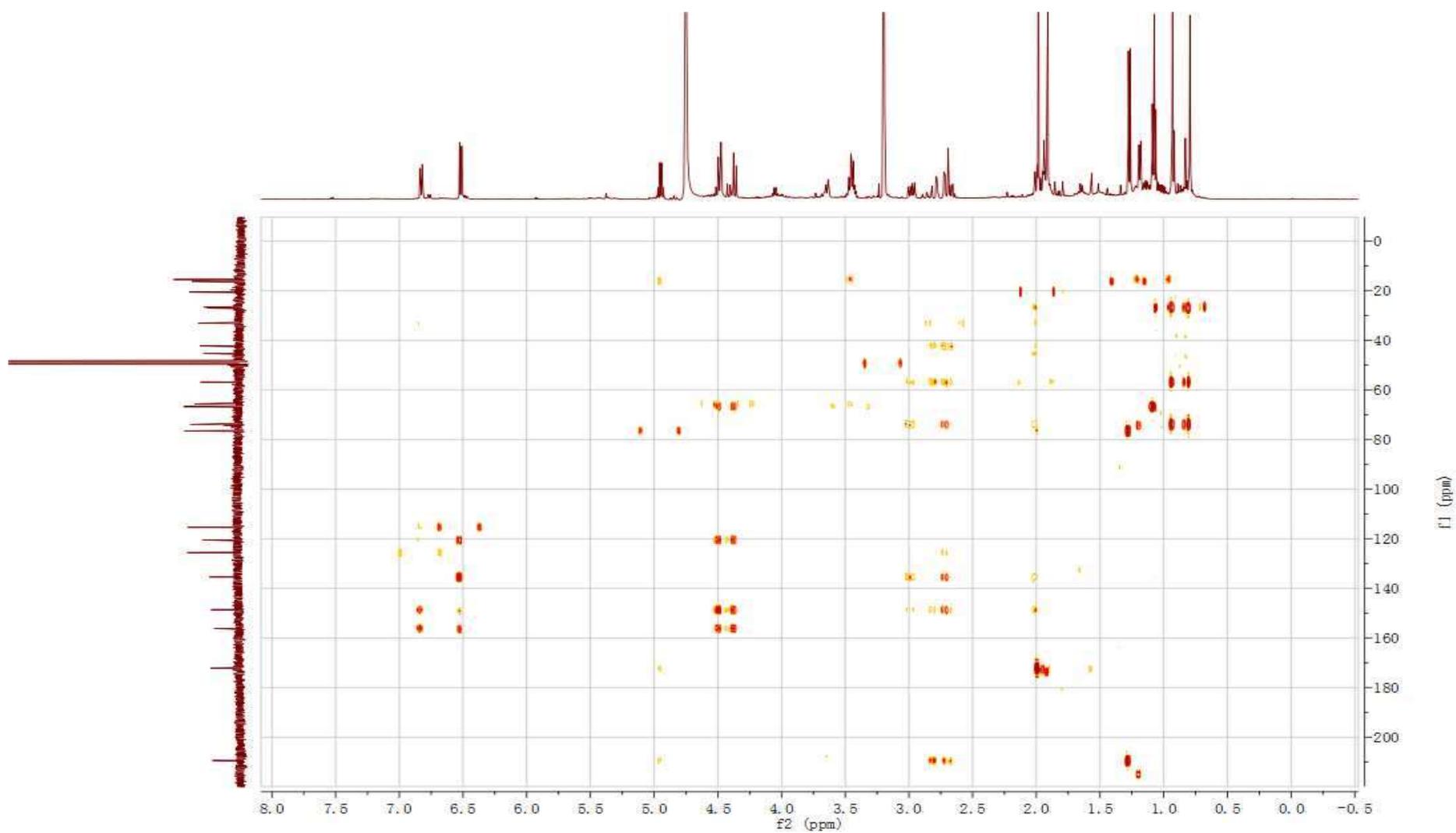


Figure S25. HMBC spectrum of the new compound 4

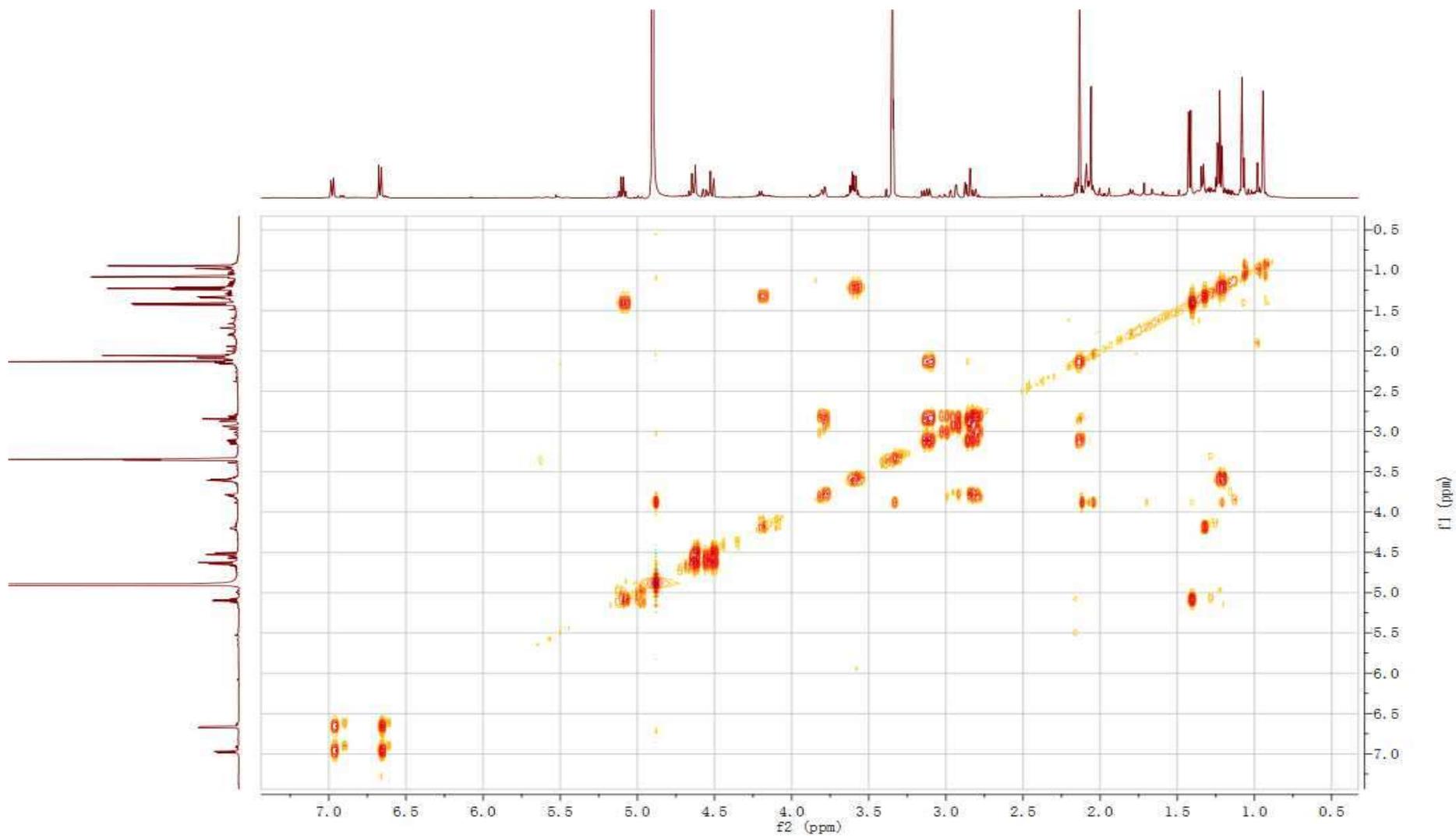


Figure S26. COSY spectrum of the new compound **4**

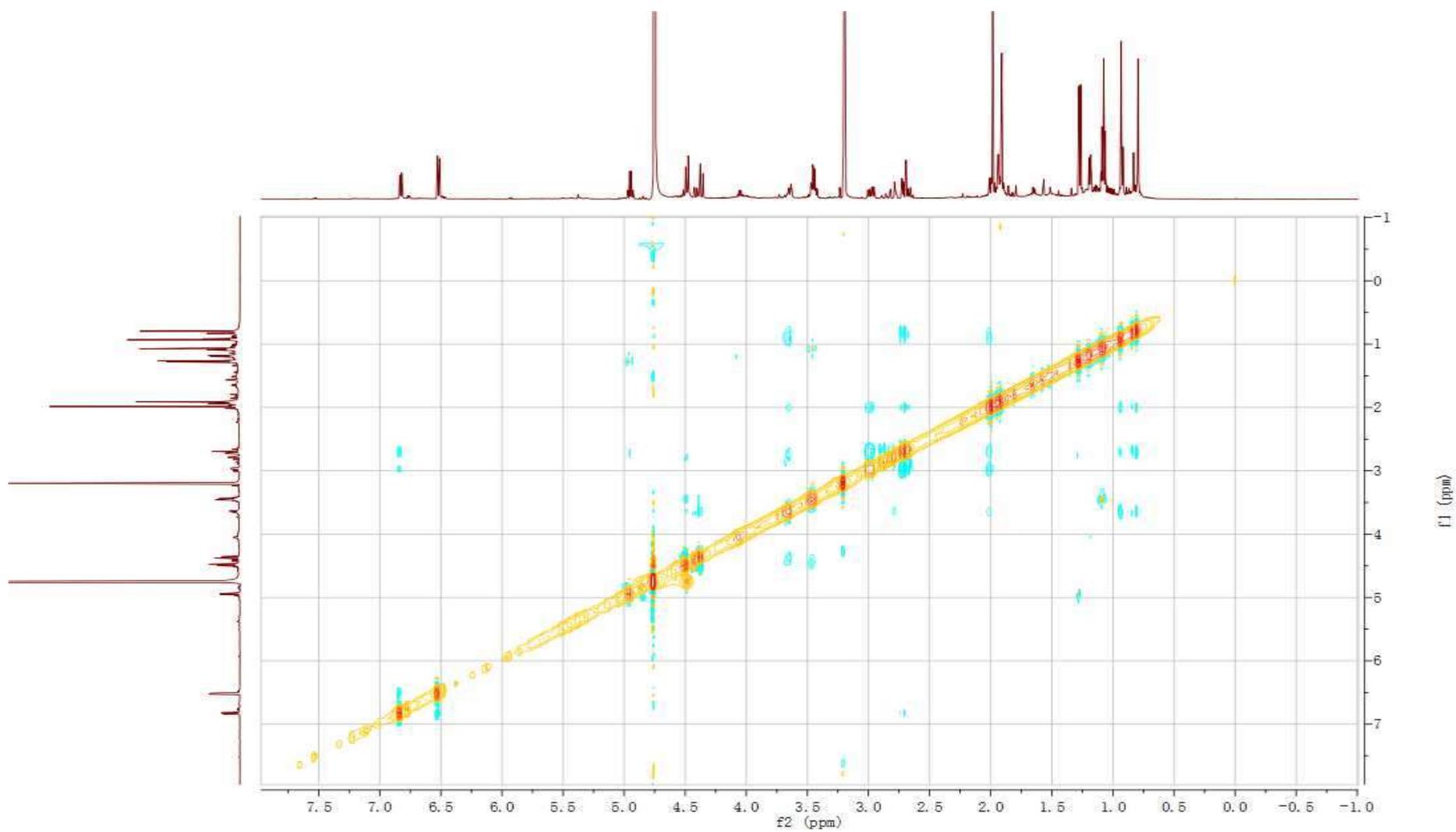


Figure S27. NOESY spectrum of the new compound **4**

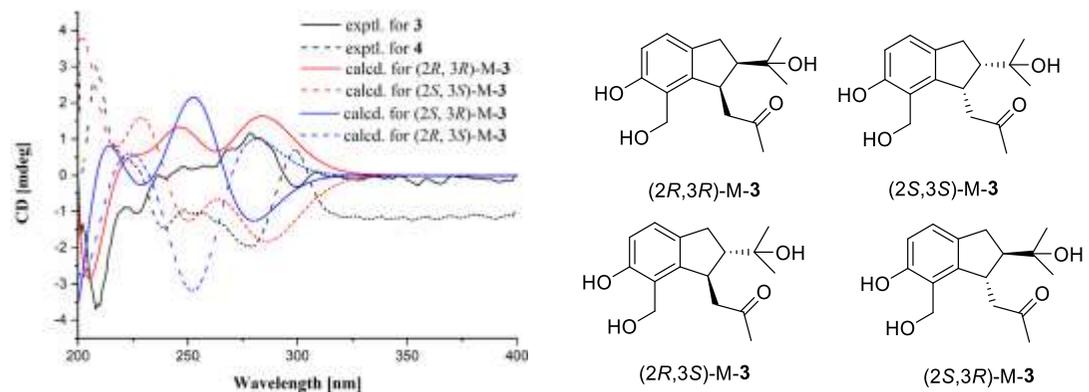


Figure S28. calculated and experimental ECD spectra of **3** and **4** using a truncated model.

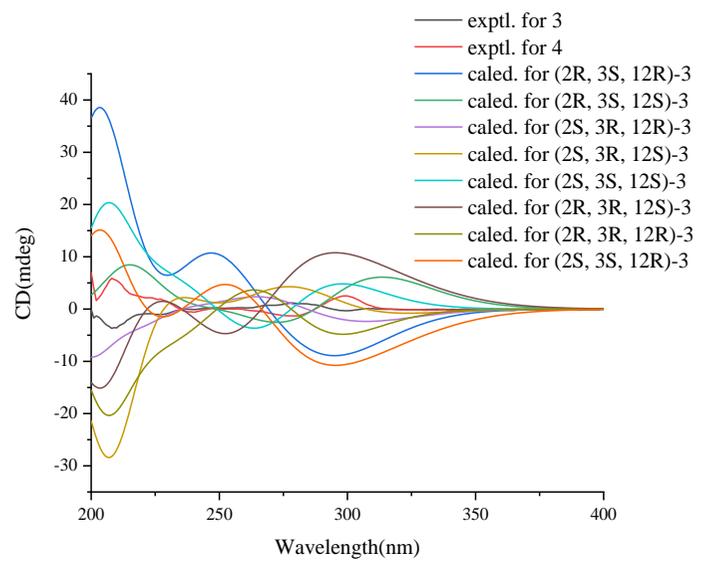


Figure S29. calculated and experimental ECD spectras of **3** and **4**.

1	Functional	Solvent?	Basis Set	Type of Data								
2	mPW1P91	PC1	6-31G(d)	Shielding Tensors								
3												
12		DP4+	0.00%	0.00%	0.00%	0.00%	50.08%	25.45%	4.38%	20.08%		
14	Nuclei	sp2?	experimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9
15	C	x	114	85.2	84.9	85.1	85.2	84.5	84.3	84.2	84.5	
16	C	x	154.8	44.4	44.4	44.4	44.4	45.1	44.6	44.6	45.2	
17	C	x	119.1	83.1	82.8	83.1	83.0	81.9	82.4	82.6	82.2	
18	C	x	147.4	50.7	50.7	50.5	50.7	52.8	52.9	53.0	52.8	
19	C	x	134	66.8	67.2	67.1	66.8	65.2	65.2	65.0	65.2	
20	C	x	124.2	73.8	73.9	73.9	73.8	73.9	73.7	73.7	74.0	
21	C		40.8	153.6	153.2	154.0	153.6	151.4	151.8	151.8	151.3	
22	C		55.6	141.8	142.2	142.2	141.9	141.9	140.3	140.3	141.7	
23	C		31.7	162.2	162.2	162.2	162.3	159.6	159.1	159.1	159.5	
24	C		64.3	128.3	127.7	127.9	128.1	126.2	127.3	127.5	128.3	
25	C		65.5	132.9	132.5	132.7	132.9	132.9	131.9	132.0	132.6	
26	C		14.1	179.19	178.88	179.16	179.17	178.9	178.5	178.5	179.0	
27	C		72.8	126.16	125.57	125.68	126.21	125.3	124.8	124.7	125.3	
28	C		25.3	162.93	163.07	163.08	163.00	171.7	170.8	170.8	171.8	
29	C		25.7	166.48	165.59	165.74	166.62	165.8	166.2	166.4	165.7	
30	C		44.2	152.79	154.80	154.57	152.79	148.9	148.2	147.6	148.9	
31	C	x	208.1	-4.73	-13.05	-10.65	-4.73	-6.8	-9.9	-9.8	-6.7	
32	C		74.7	117.68	120.33	119.12	117.78	119.4	118.5	118.7	119.4	
33	C	x	170.7	28.16	28.39	28.10	28.15	27.3	26.2	26.0	27.3	
34	C		14.8	178.44	176.35	176.40	178.34	176.0	177.8	177.7	177.9	
35	C		19.1	172.97	172.68	172.74	173.03	173.0	172.3	172.0	173.0	

Figure S30. The data of DP4plus method of compound 3

1	Functional	Solvent?	Basis Set	Type of Data								
2	mPW1P91	PC1	6-31G(d)	Shielding Tensors								
3												
4		Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9		
5	sDP4+ (H data)	-	-	-	-	-	-	-	-	-		
6	sDP4+ (C data)	0.42%	0.00%	0.00%	0.54%	58.90%	1.40%	0.61%	38.12%	-		
7	sDP4+ (all data)	0.42%	0.00%	0.00%	0.54%	58.90%	1.40%	0.61%	38.12%	-		
8	uDP4+ (H data)	-	-	-	-	-	-	-	-	-		
9	uDP4+ (C data)	0.01%	0.00%	0.01%	0.02%	3.17%	68.04%	26.79%	1.97%	-		
10	uDP4+ (all data)	0.01%	0.00%	0.01%	0.02%	3.17%	68.04%	26.79%	1.97%	-		
11	DP4+ (H data)	-	-	-	-	-	-	-	-	-		
12	DP4+ (C data)	0.00%	0.00%	0.00%	0.00%	50.08%	25.45%	4.38%	20.08%	-		
13	DP4+ (all data)	0.00%	0.00%	0.00%	0.00%	50.08%	25.45%	4.38%	20.08%	-		

Figure S31. Comparison of the experimental ¹³C NMR data and mean absolute error of compound 3

configuration	R_2	RMSE	DP4+(%)
a (2 <i>R</i> ,3 <i>R</i> ,12 <i>R</i>)	0.9982	2.52	0.00
b (2 <i>R</i> ,3 <i>R</i> ,12 <i>S</i>)	0.9973	3.16	0.00
c (2 <i>S</i> ,3 <i>S</i> ,12 <i>R</i>)	0.9977	2.91	0.00
d (2 <i>S</i> ,3 <i>S</i> ,12 <i>S</i>)	0.9982	2.51	0.00
e (2 <i>R</i> ,3 <i>S</i> ,12 <i>R</i>)	0.9987	2.20	50.08
f (2 <i>S</i> ,3 <i>R</i> ,12 <i>R</i>)	0.9985	2.65	25.45
g (2 <i>R</i> ,3 <i>S</i> ,12 <i>S</i>)	0.9984	2.70	4.38
h (2 <i>S</i> ,3 <i>R</i> ,12 <i>S</i>)	0.9987	2.22	20.08

Figure S32. DP4⁺ probability of ¹³C NMR chemical shifts (compound **3**) .

	A	B	C	D	E	F	G	H	I	J	K	L
2	sp ² 11991		PCM	G-31C(d)			Shielding Tensors					
3												
13			DP4+	0.00%	0.00%	0.00%	0.00%	51.62%	23.50%	4.23%	####	-
14	Nuclei	sp2?	experimts	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9
15	C	x	114	85.2	84.9	85.1	85.2	84.5	84.3	84.2	84.5	
16	C	x	194.8	44.4	44.4	44.4	44.4	45.1	44.6	44.6	45.2	
17	C	x	118.1	83.1	82.8	83.1	83.0	81.9	82.4	82.6	82.2	
18	C	x	147.2	50.7	50.7	50.5	50.7	52.8	52.9	53.0	52.8	
19	C	x	134	66.8	67.2	67.1	66.8	65.2	65.2	65.0	65.2	
20	C	x	124.2	73.8	73.9	73.9	73.8	73.9	73.7	73.7	74.0	
21	C		40.9	153.6	153.2	154.0	153.6	151.4	151.8	151.8	151.3	
22	C		93.5	141.8	142.2	142.2	141.9	141.9	140.3	140.3	141.7	
23	C		11.7	162.2	162.2	162.2	162.3	159.6	159.1	159.1	159.5	
24	C		64.3	128.3	127.7	127.9	128.1	128.2	127.3	127.5	128.3	
25	C		65.4	132.9	132.5	132.7	132.9	132.3	131.9	132.0	132.6	
26	C		14.1	179.19	178.85	179.16	179.17	178.9	178.5	178.5	179.0	
27	C		72.5	126.16	125.57	125.68	126.21	125.3	124.8	124.7	125.3	
28	C		25.3	162.93	163.07	163.08	163.00	171.7	170.8	170.8	171.8	
29	C		25.7	166.48	165.59	165.74	166.62	165.8	166.2	166.4	165.7	
30	C		43.9	152.79	154.80	154.57	152.79	148.9	148.2	147.6	148.8	
31	C	x	708	-4.73	-13.05	-10.65	-4.73	-6.8	-9.9	-9.8	-6.7	
32	C		75.1	117.68	120.33	119.12	117.78	119.4	118.5	118.7	119.4	
33	C	x	170.7	28.16	28.39	28.10	28.15	27.3	26.2	26.0	27.3	
34	C		14.9	178.44	176.95	176.40	178.34	178.0	177.8	177.7	177.9	
35	C		18.7	172.97	172.68	172.74	173.03	173.0	172.3	172.0	173.0	
36												

Figure S33. The data of DP4plus method of compound 4

	A	B	C	D	E	F	G	H	I	J	K	
1	Functional	Solvent?	Basis Set	Type of Data								
2	mPW91	PCM	6-31G(d)	Shielding Tensors								
3												
4				Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	Isomer 7	Isomer 8	Isomer 9
5	sDP4+ (H data)	-	-	-	-	-	-	-	-	-	-	-
6	sDP4+ (C data)	0.46%	0.00%	0.00%	0.59%	59.06%	1.22%	0.58%	38.09%	-	-	-
7	sDP4+ (all data)	0.46%	0.00%	0.00%	0.59%	59.06%	1.22%	0.58%	38.09%	-	-	-
8	uDP4+ (H data)	-	-	-	-	-	-	-	-	-	-	-
9	uDP4+ (C data)	0.02%	0.00%	0.01%	0.03%	3.12%	58.93%	25.97%	1.92%	-	-	-
10	uDP4+ (all data)	0.02%	0.00%	0.01%	0.03%	3.12%	58.93%	25.97%	1.92%	-	-	-
11	DP4+ (H data)	-	-	-	-	-	-	-	-	-	-	-
12	DP4+ (C data)	0.00%	0.00%	0.00%	0.00%	51.62%	23.60%	4.23%	20.53%	-	-	-
13	DP4+ (all data)	0.00%	0.00%	0.00%	0.00%	51.62%	23.60%	4.23%	20.53%	-	-	-

Figure S34. Comparison of the experimental ^{13}C NMR data and mean absolute error of compound **4**

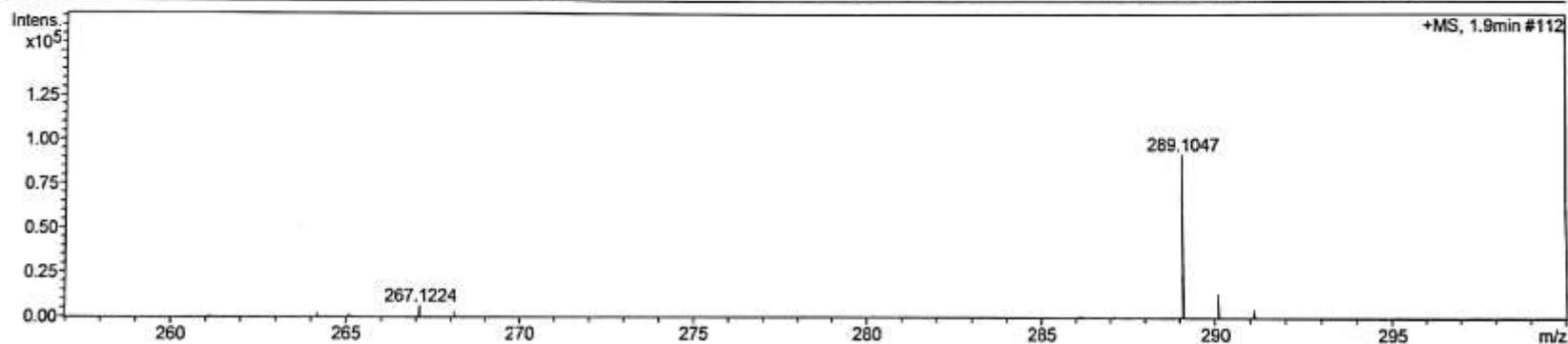
configuration	R_2	RMSE	DP4+(%)
a (2 <i>R</i> ,3 <i>R</i> ,12 <i>R</i>)	0.9983	2.47	0.00
b (2 <i>R</i> ,3 <i>R</i> ,12 <i>S</i>)	0.9974	3.13	0.00
c (2 <i>S</i> ,3 <i>S</i> ,12 <i>R</i>)	0.9977	2.87	0.00
d (2 <i>S</i> ,3 <i>S</i> ,12 <i>S</i>)	0.9983	2.45	0.00
e (2 <i>R</i> ,3 <i>S</i> ,12 <i>R</i>)	0.9988	2.17	51.62
f (2 <i>S</i> ,3 <i>R</i> ,12 <i>R</i>)	0.9985	2.64	23.60
g (2 <i>R</i> ,3 <i>S</i> ,12 <i>S</i>)	0.9985	2.69	4.23
h (2 <i>S</i> ,3 <i>R</i> ,12 <i>S</i>)	0.9987	2.20	20.53

Figure S35. DP4⁺ probability of ^{13}C NMR chemical shifts.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	7/16/2019 3:12:22 PM	
Analysis Name	D:\Data\MS\data\201907>wangjianjiao_LH-C1_pos_65_01_6940.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis	255552.00029
Sample Name	wangjianjiao_LH-C1_pos			
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
267.1224	1	C14H19O5	100.00	267.1227	1.3	0.3	15.4	5.5	even	ok
289.1047	1	C14H18NaO5	100.00	289.1046	-0.3	-0.1	10.1	5.5	even	ok
555.2195	1	C28H36NaO10	100.00	555.2201	1.0	0.6	28.8	10.5	even	ok

Figure S36. HRESI-MS spectrum of the new compound 5

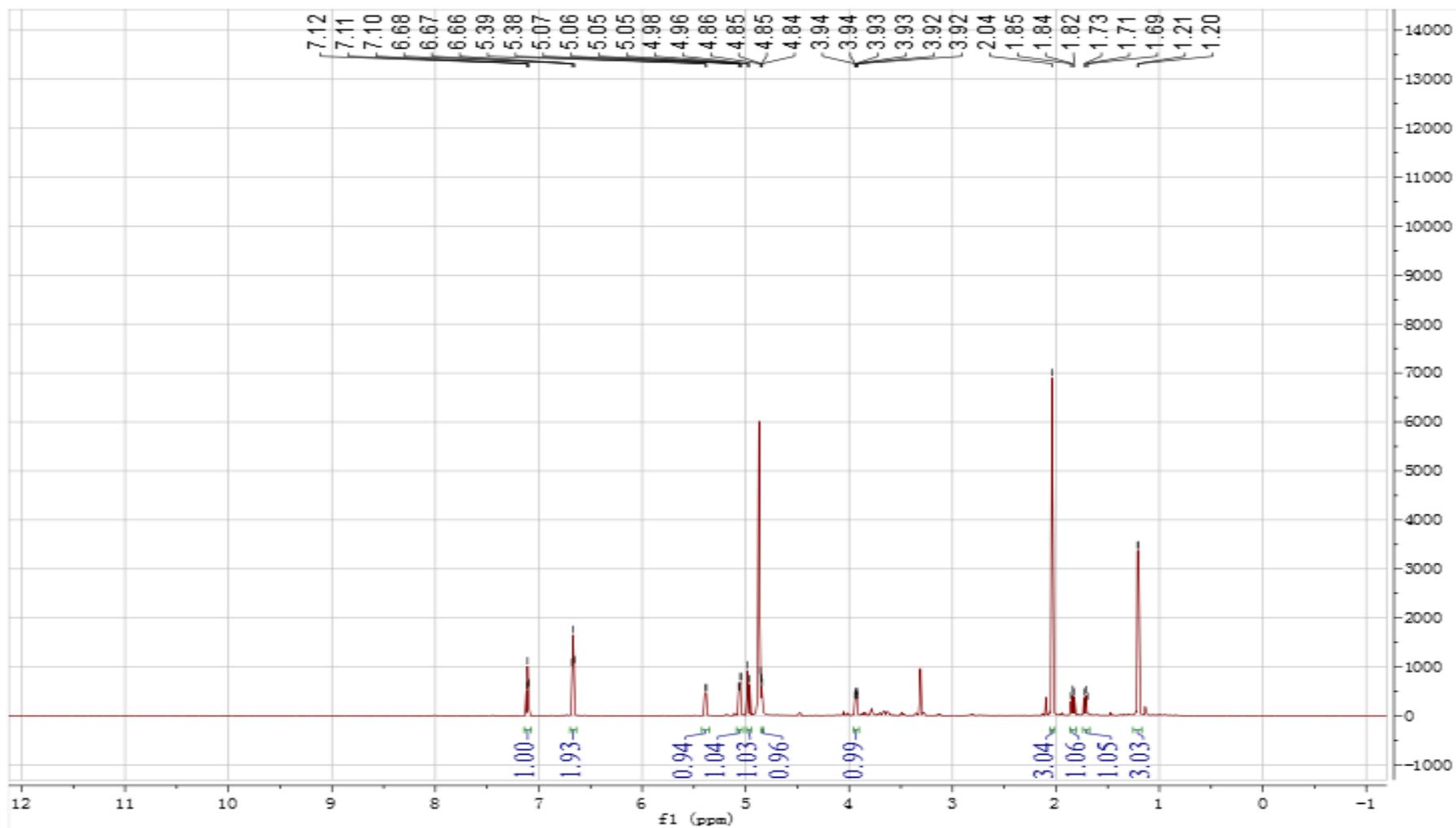


Figure S37. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **5**

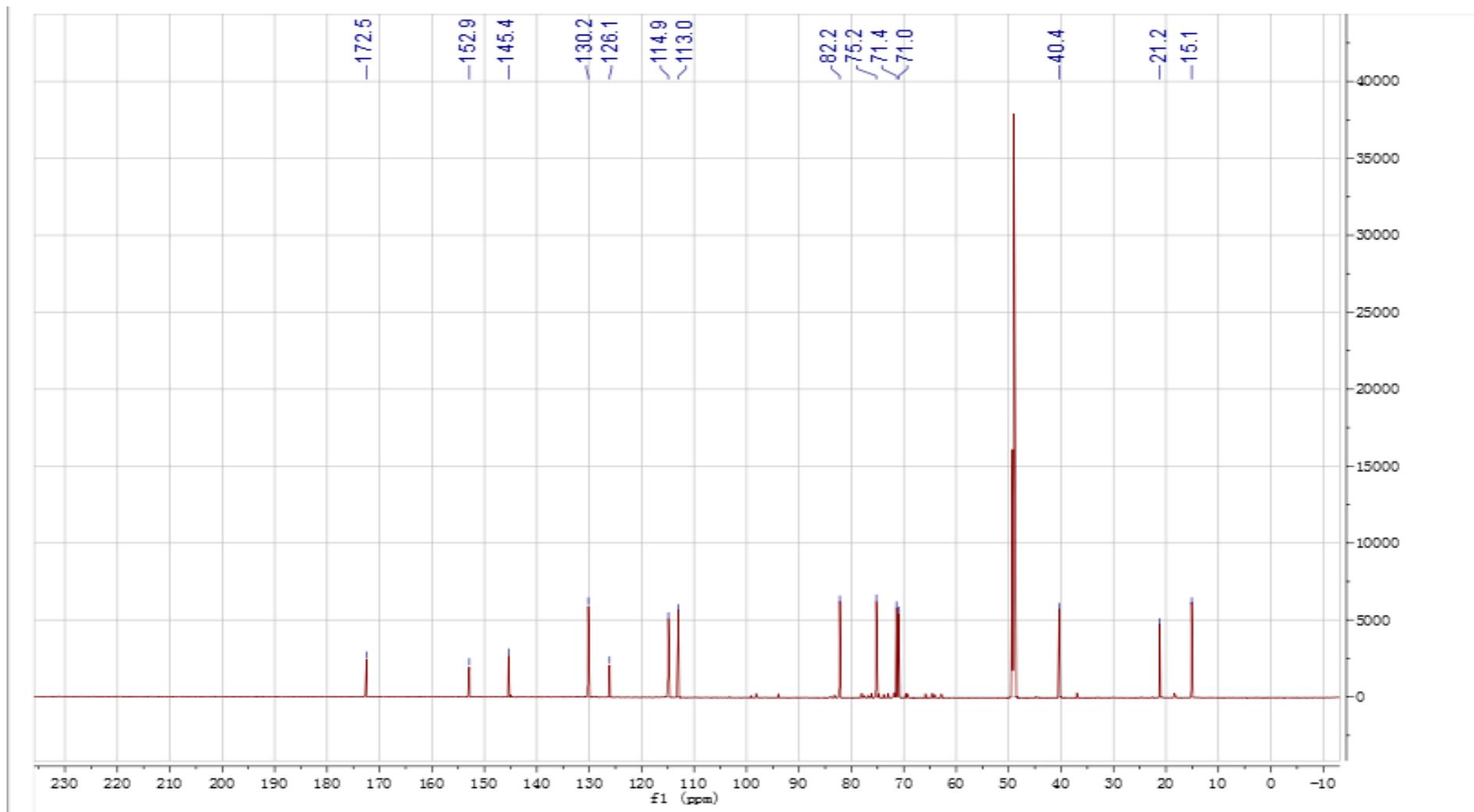


Figure S38. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **5**

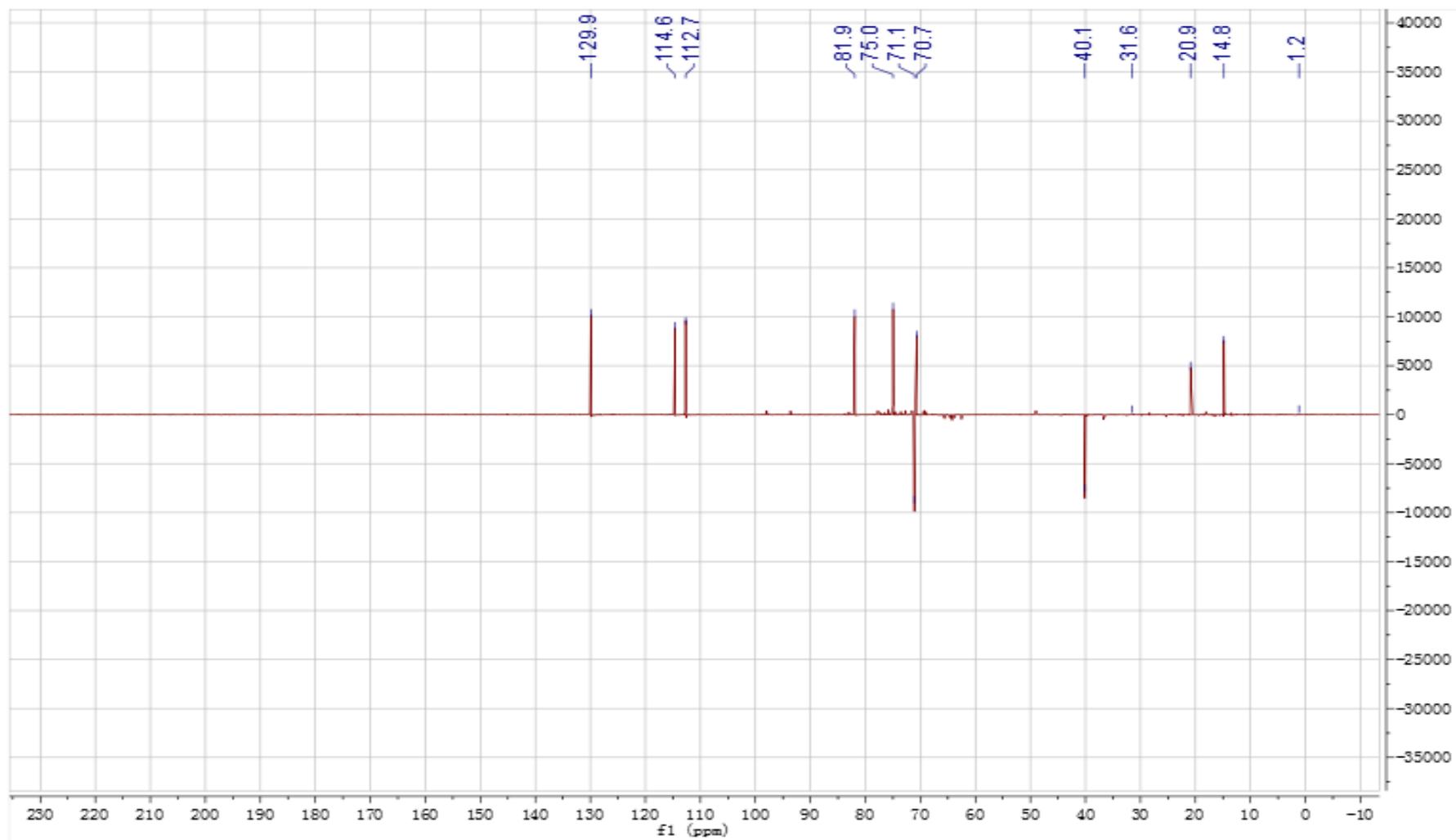


Figure S39. 135 DEPT (125 MHz, CD_3OD) spectrum of the new compound **5**

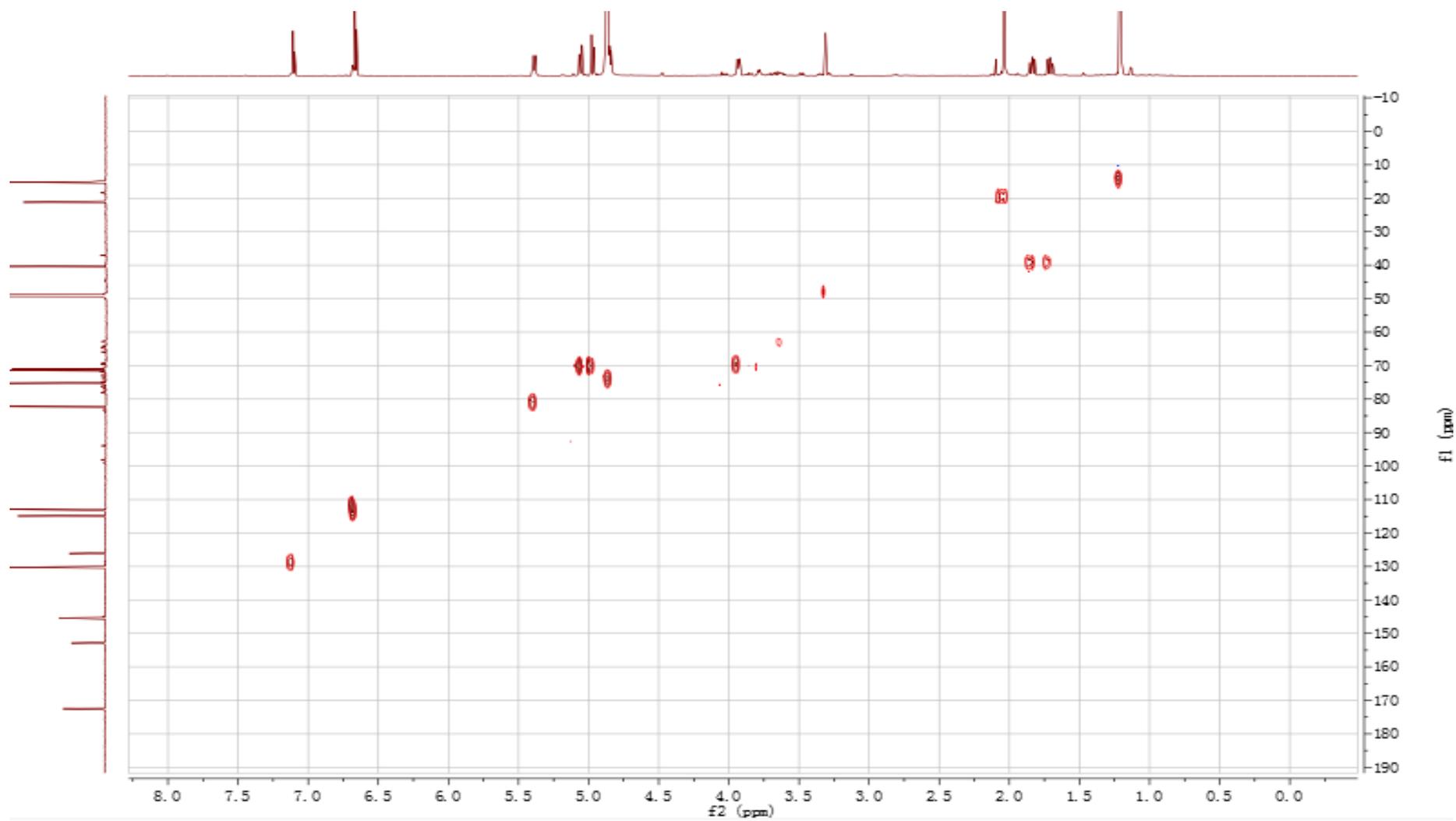


Figure S40. HSQC spectrum of the new compound **5**

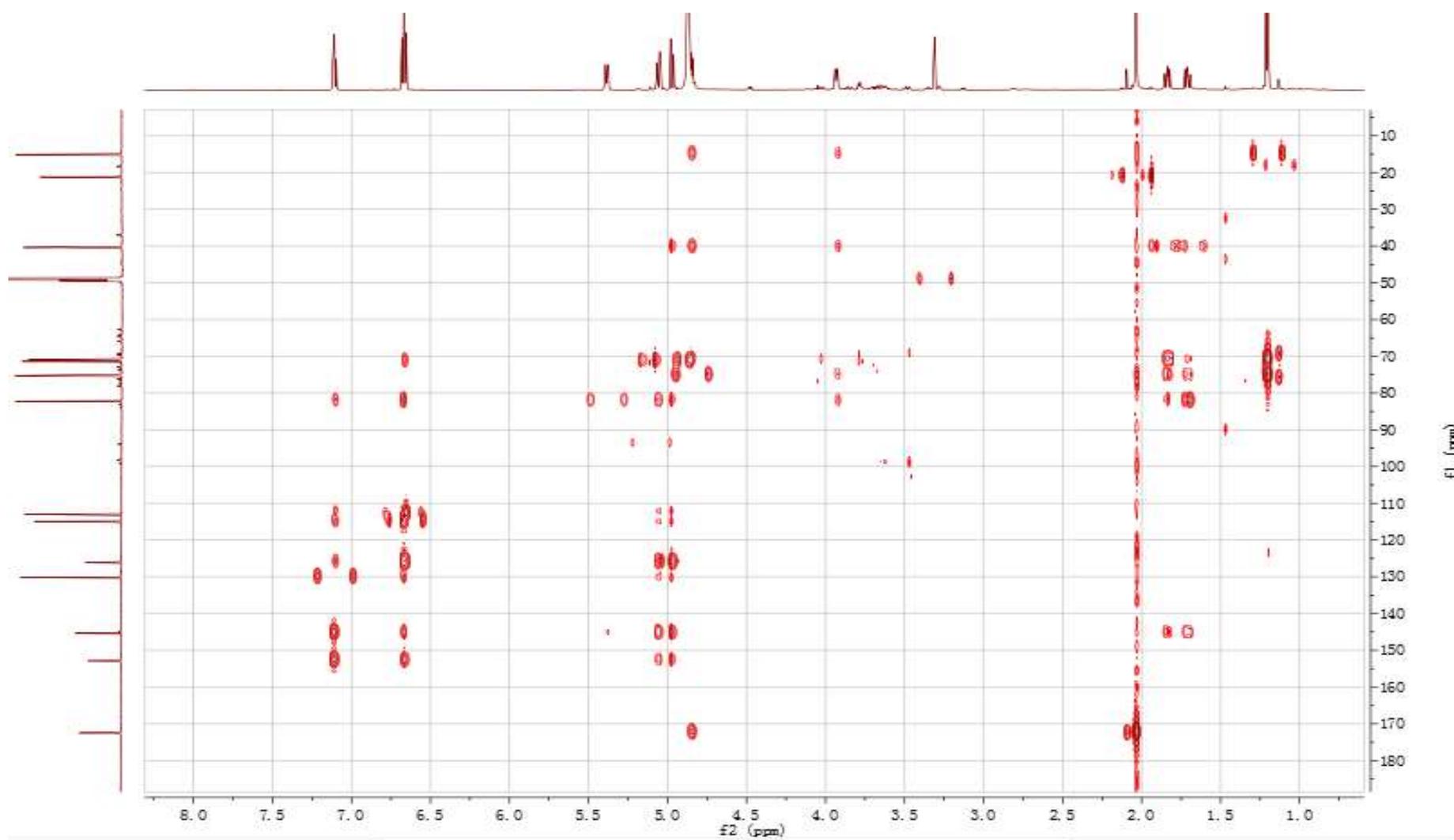


Figure S41. HMBC spectrum of the new compound **5**

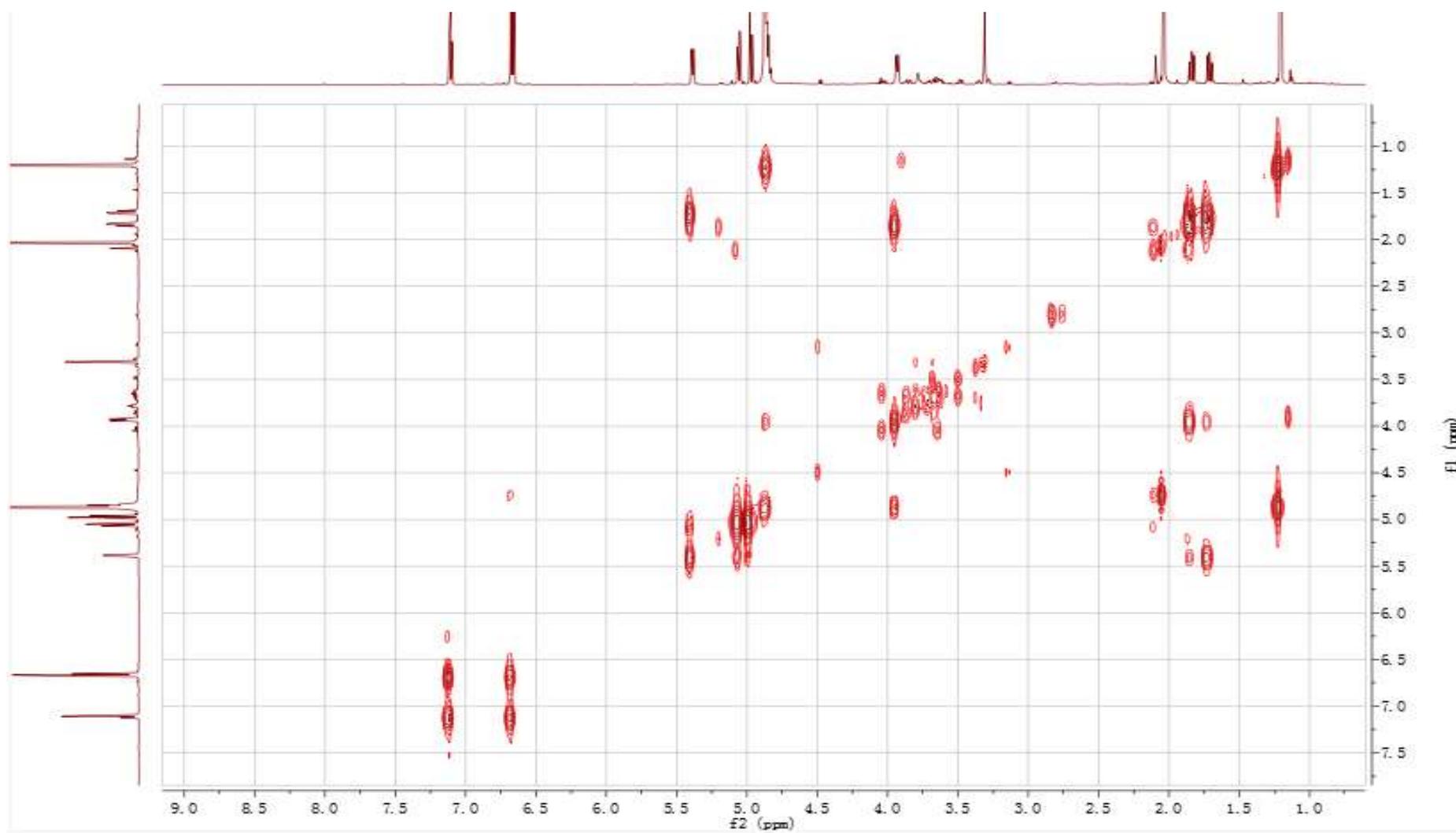
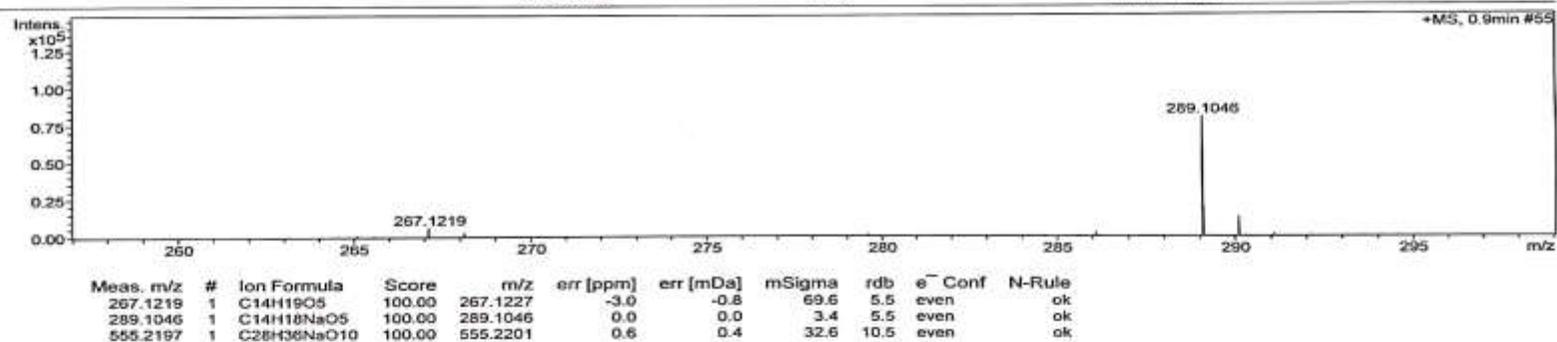


Figure S42. COSY spectrum of the new compound **5**

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	1/17/2019 4:13:43 PM	
Analysis Name	D:\Data\MS\data\201901\yangbin_L-41_pos_26_01_6106.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis	
Sample Name	yangbin_L-41_pos		255552.00029	
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



yangbin_L-41_pos_26_01_6106.d
Bruker Compass DataAnalysis 4.1

printed: 1/17/2019 4:18:54 PM

by: SCSIO

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Figure S43. HRESI-MS spectrum of compound 6

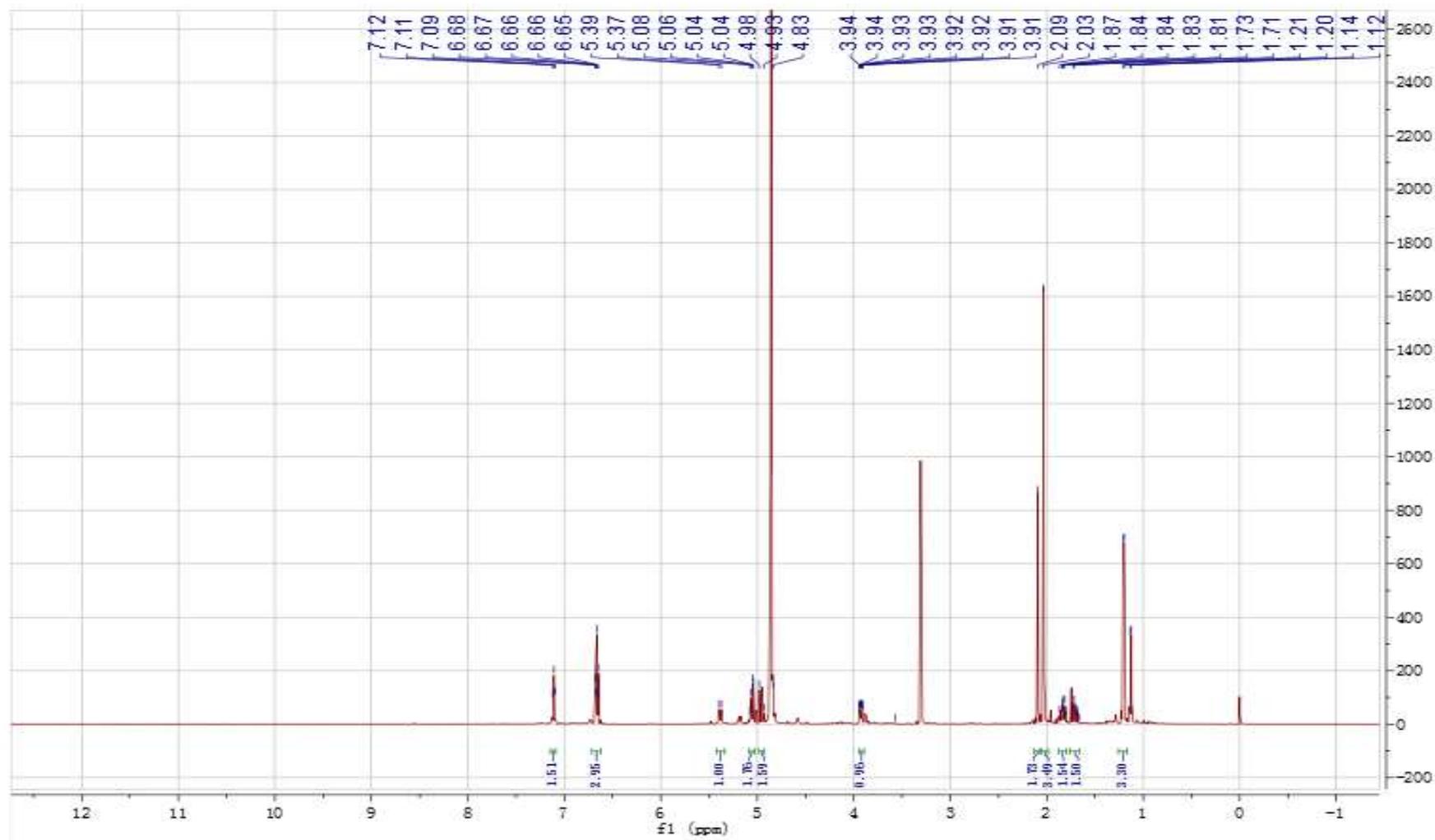


Figure S44. ^1H NMR (500 MHz, CD_3OD) spectrum of compound **6**

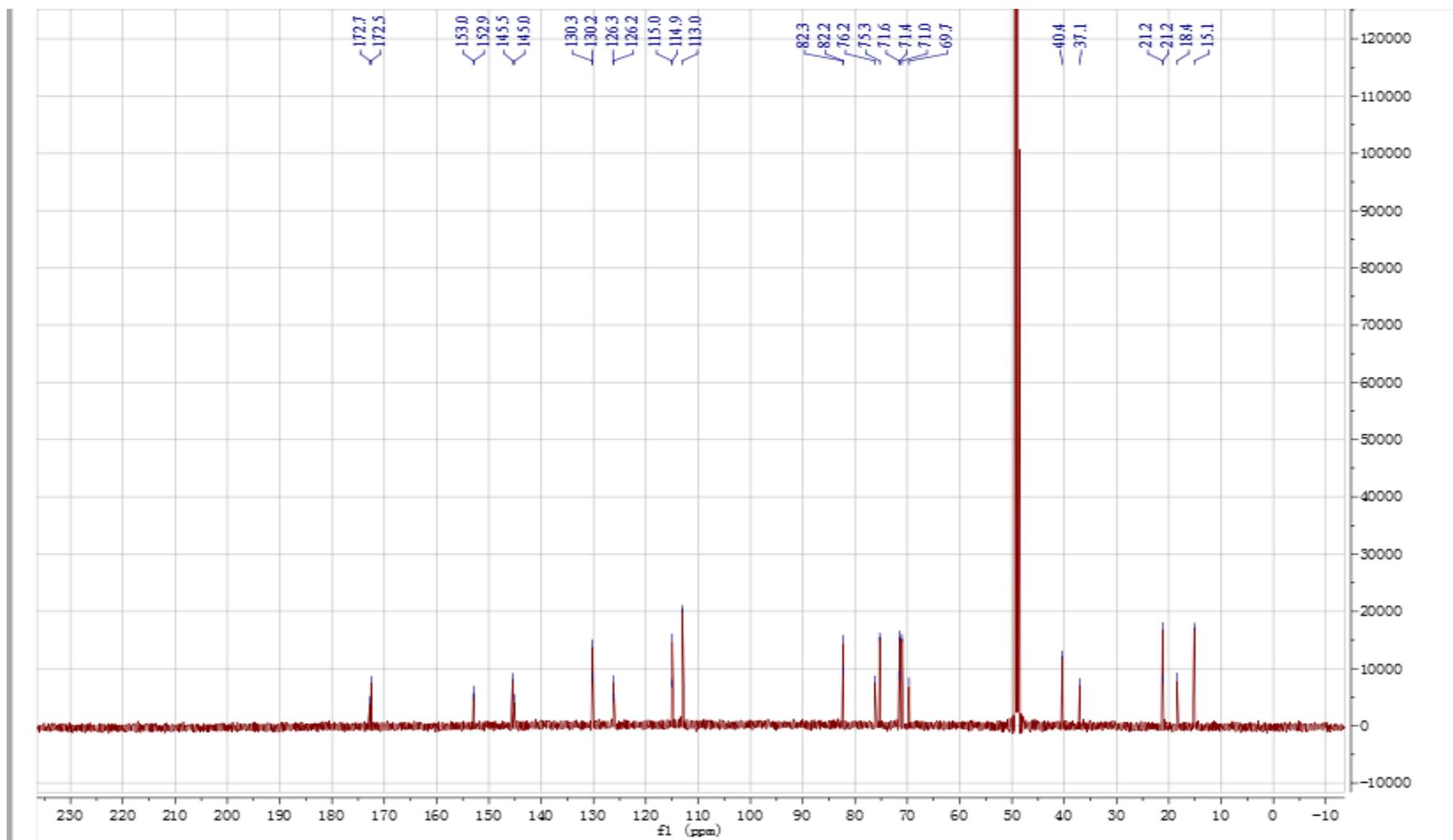


Figure S45. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **6**

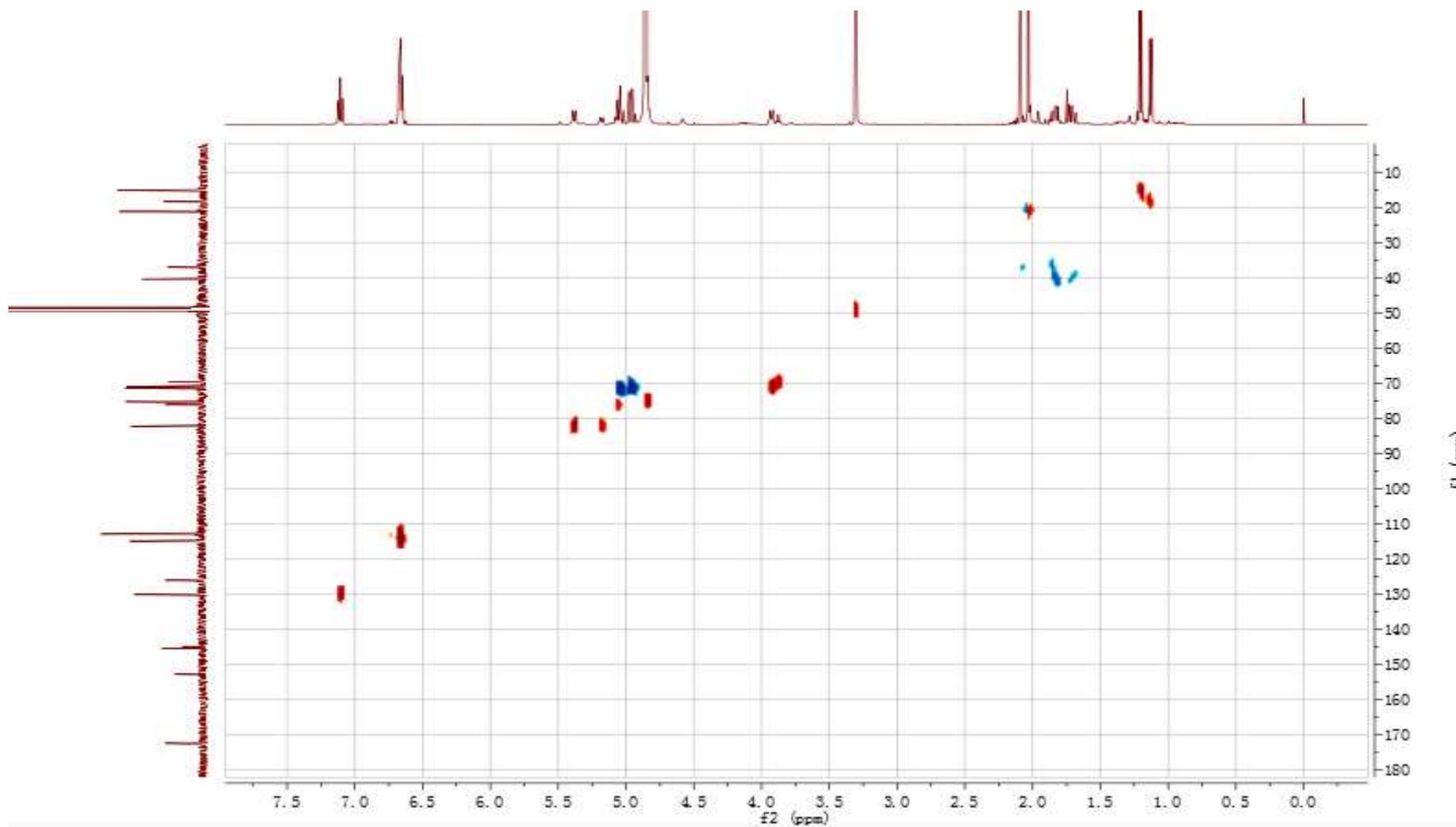


Figure S46. HSQC spectrum of compound **6**

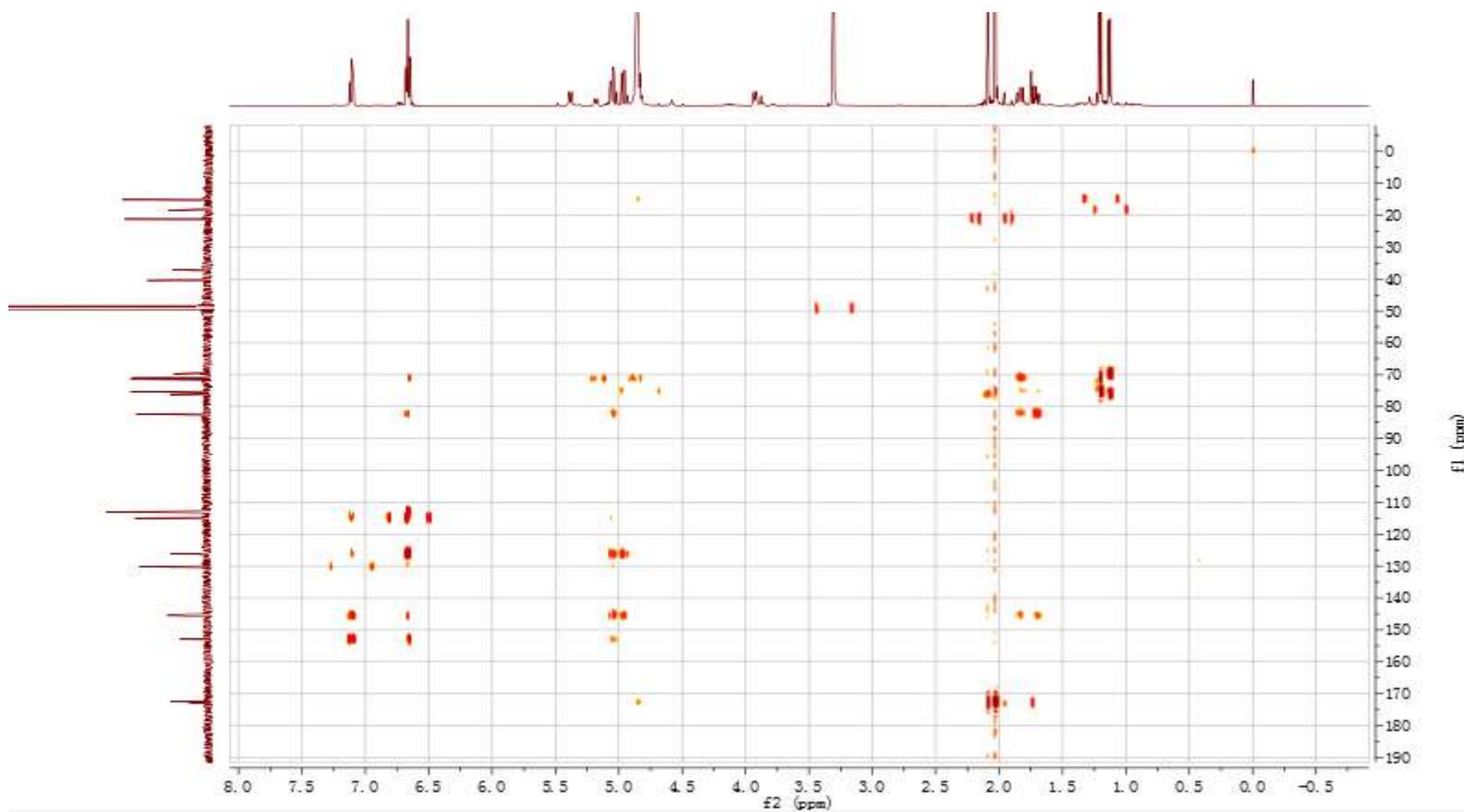
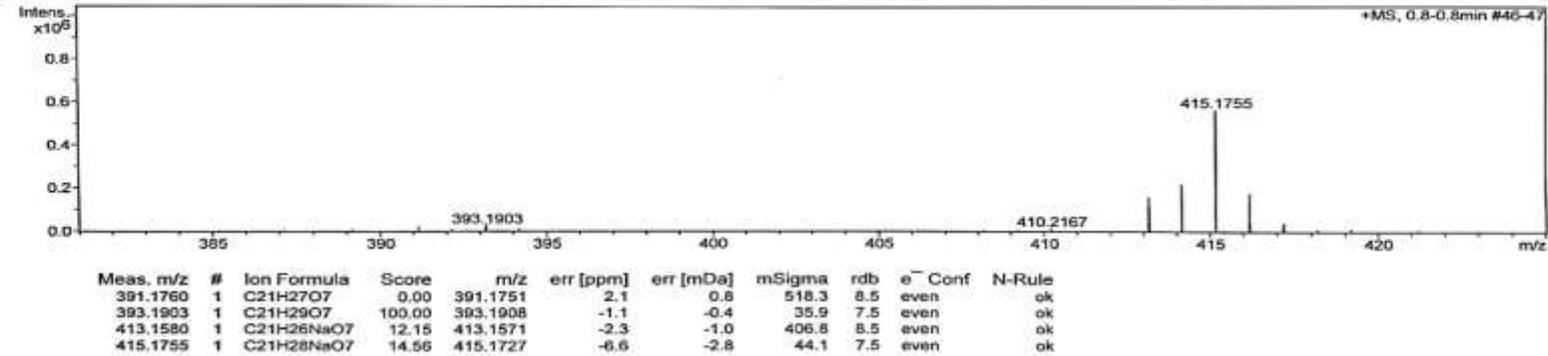


Figure S47. HMBC spectrum of compound **6**

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	1/17/2019 4:06:47 PM	
Analysis Name	D:\Data\MS\data\201901\yangbin_L-39_pos_24_01_6104.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis	
Sample Name	yangbin_L-39_pos		255552.00029	
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



yangbin_L-39_pos_24_01_6104.d
Bruker Compass DataAnalysis 4.1

printed: 1/17/2019 4:13:21 PM

by: SCSIO

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Figure S48. HRESI-MS spectrum of the new compound **7**

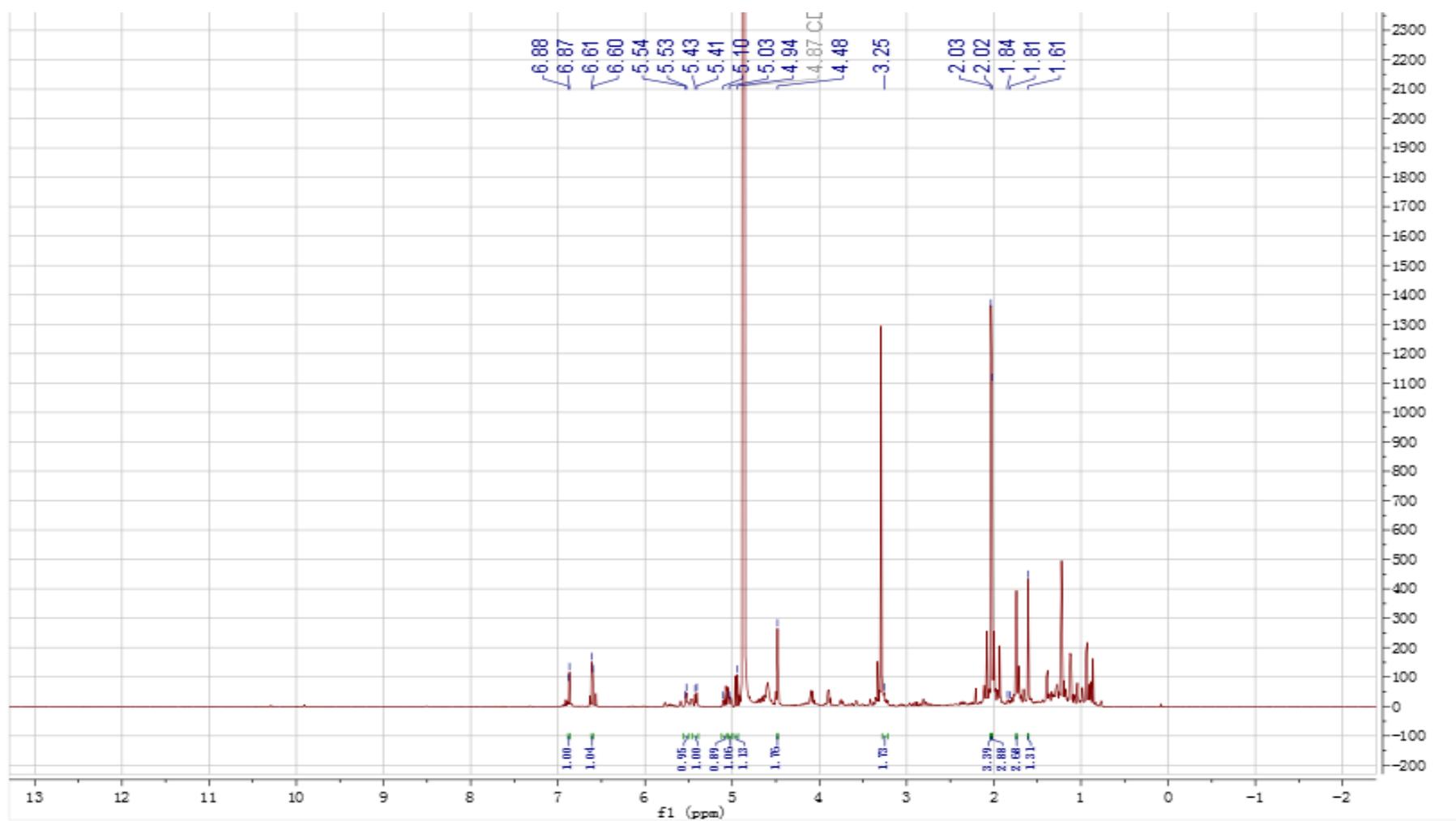


Figure S49. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **7**

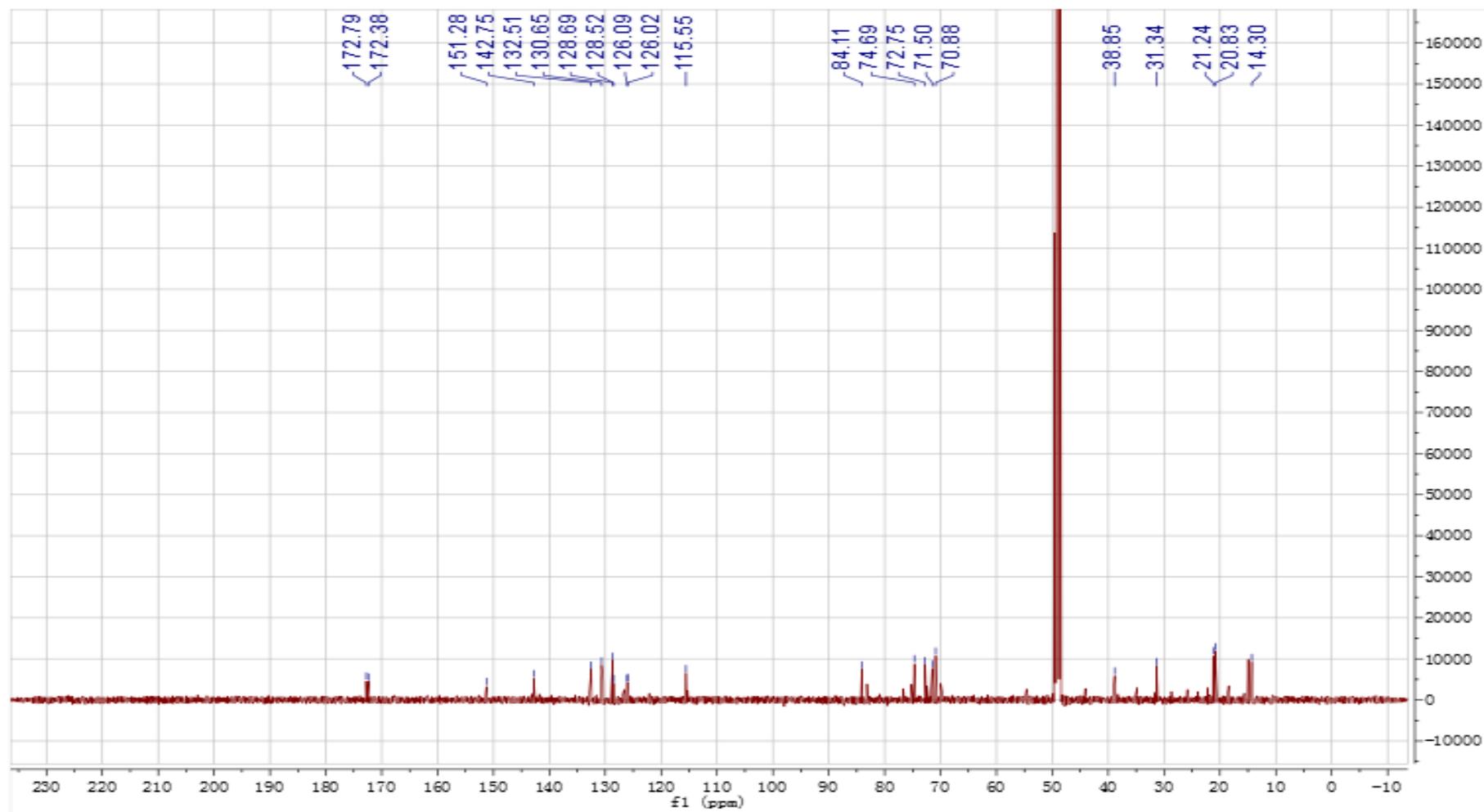


Figure S50. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **7**

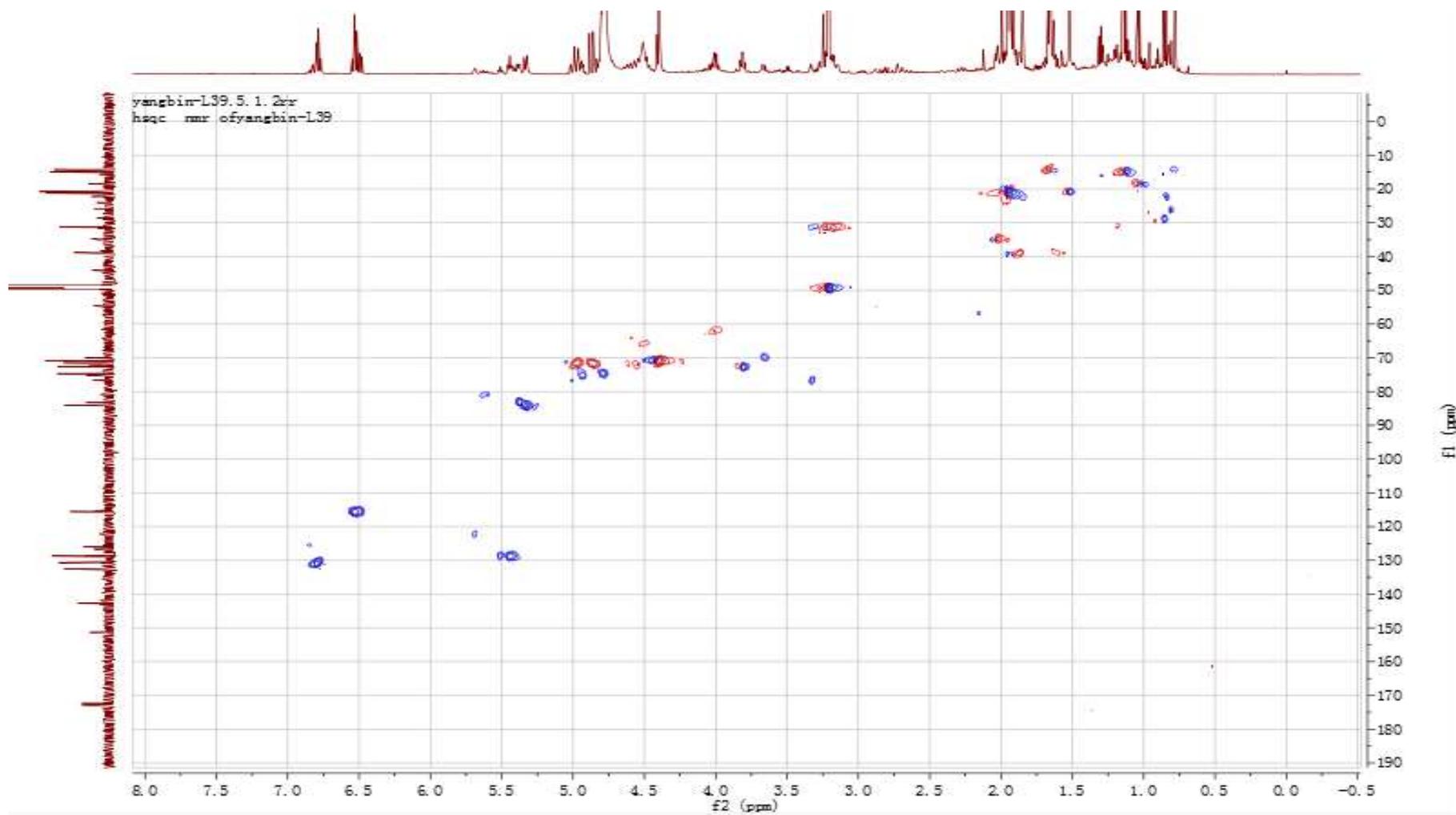


Figure S51. HSQC spectrum of the new compound **7**

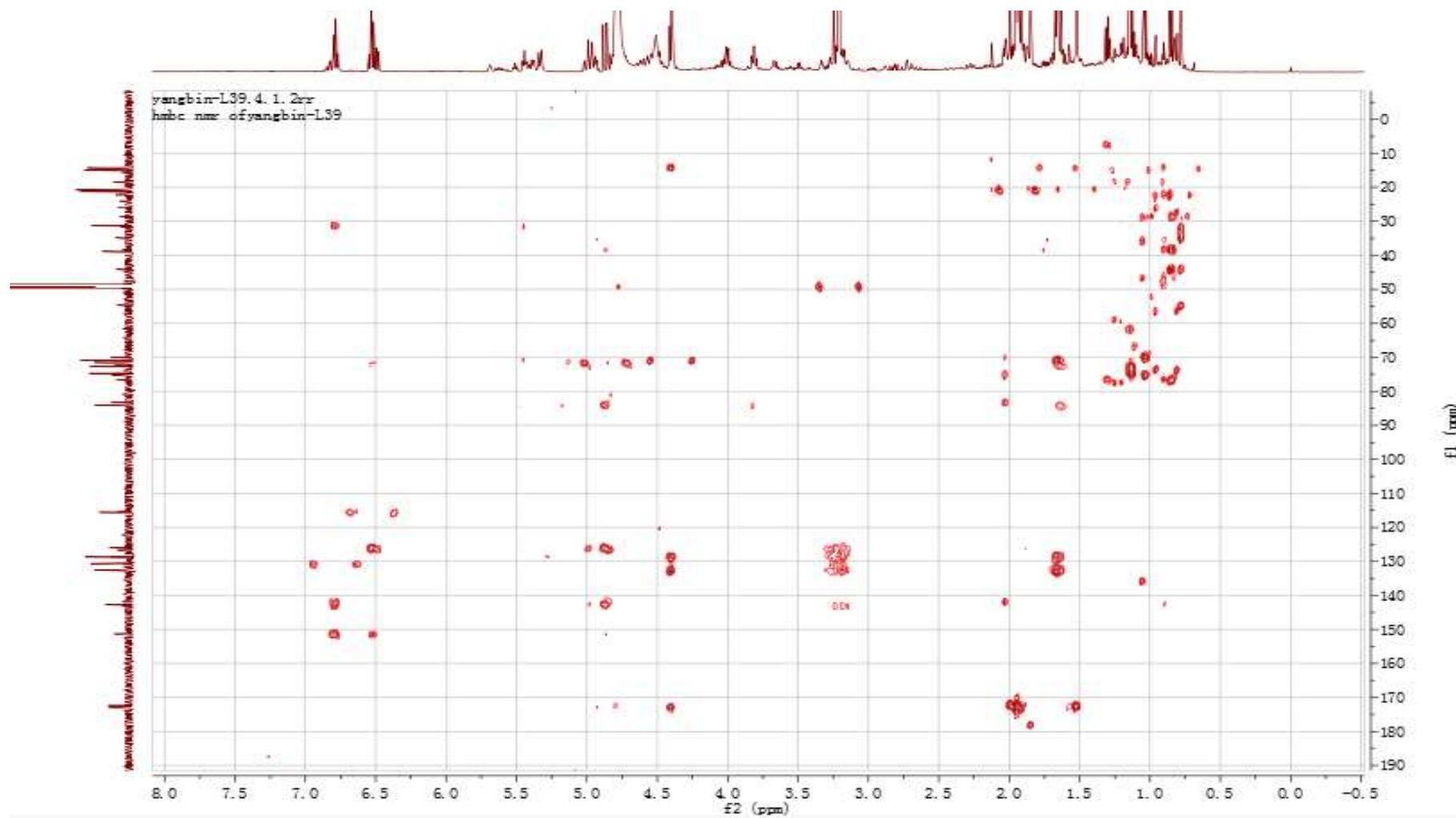
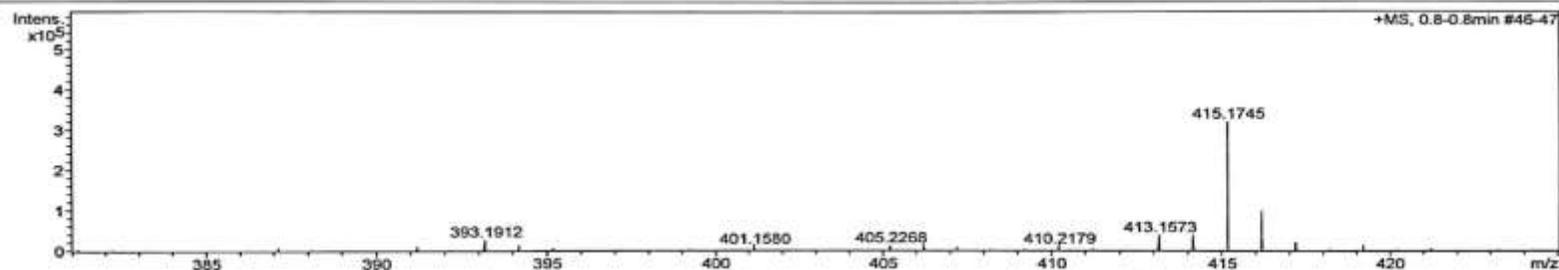


Figure S52. HMBC spectrum of the new compound **7**

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	1/17/2019 4:10:16 PM	
Analysis Name	D:\Data\MS\data\201901\yangbin_L-40_pos_25_01_6105.d	Operator	SCSIO	
Method	LC_Direct Infusion_pos_70-500mz.m	Instrument	maXis	
Sample Name	yangbin_L-40_pos		255552.00029	
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdB	e ⁻ Conf	N-Rule
393.1912	1	C21H29O7	100.00	393.1908	-1.0	-0.4	65.3	7.5	even	ok
415.1745	1	C21H28NaO7	35.20	415.1727	-4.3	-1.8	37.3	7.5	even	ok
805.3423	1	C42H54NaO14	100.00	805.3406	-2.2	-1.8	602.9	15.5	even	ok
807.3575	1	C42H56NaO14	100.00	807.3562	-1.5	-1.2	27.9	14.5	even	ok

Figure S53. HRESI-MS spectrum of the new compound **8**

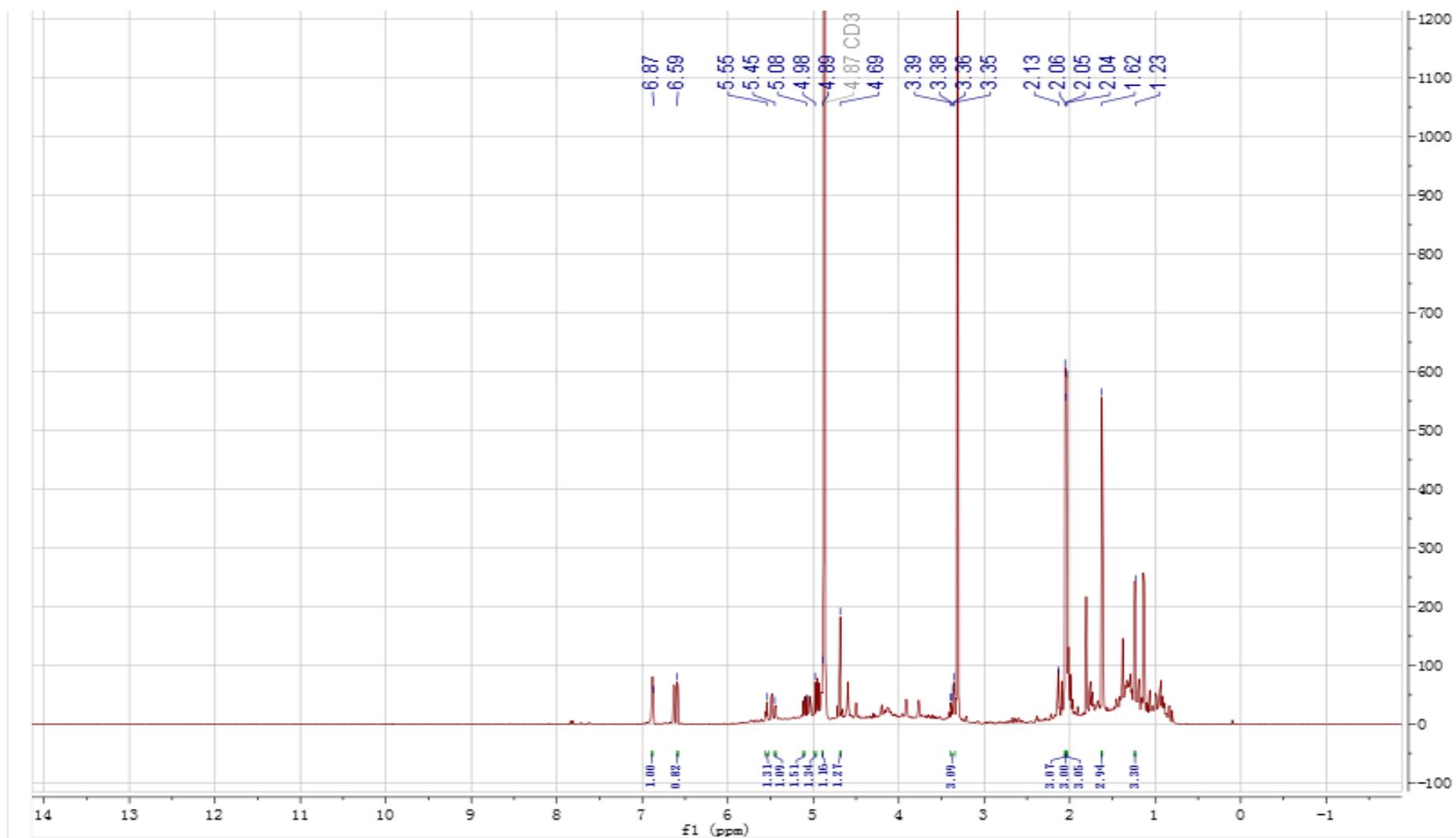


Figure S54. ^1H NMR (500 MHz, CD_3OD) spectrum of the new compound **8**

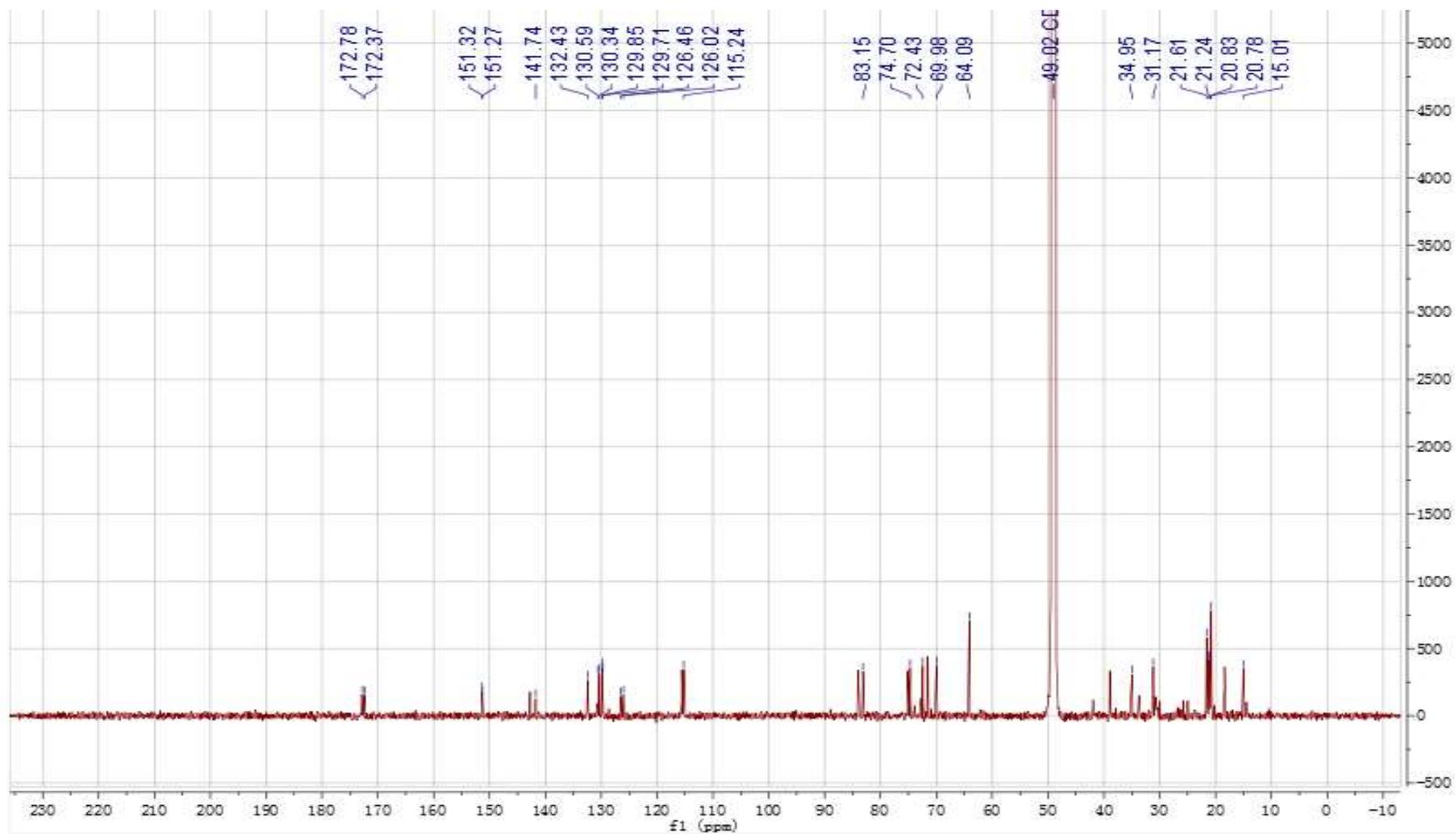


Figure S55. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the new compound **8**

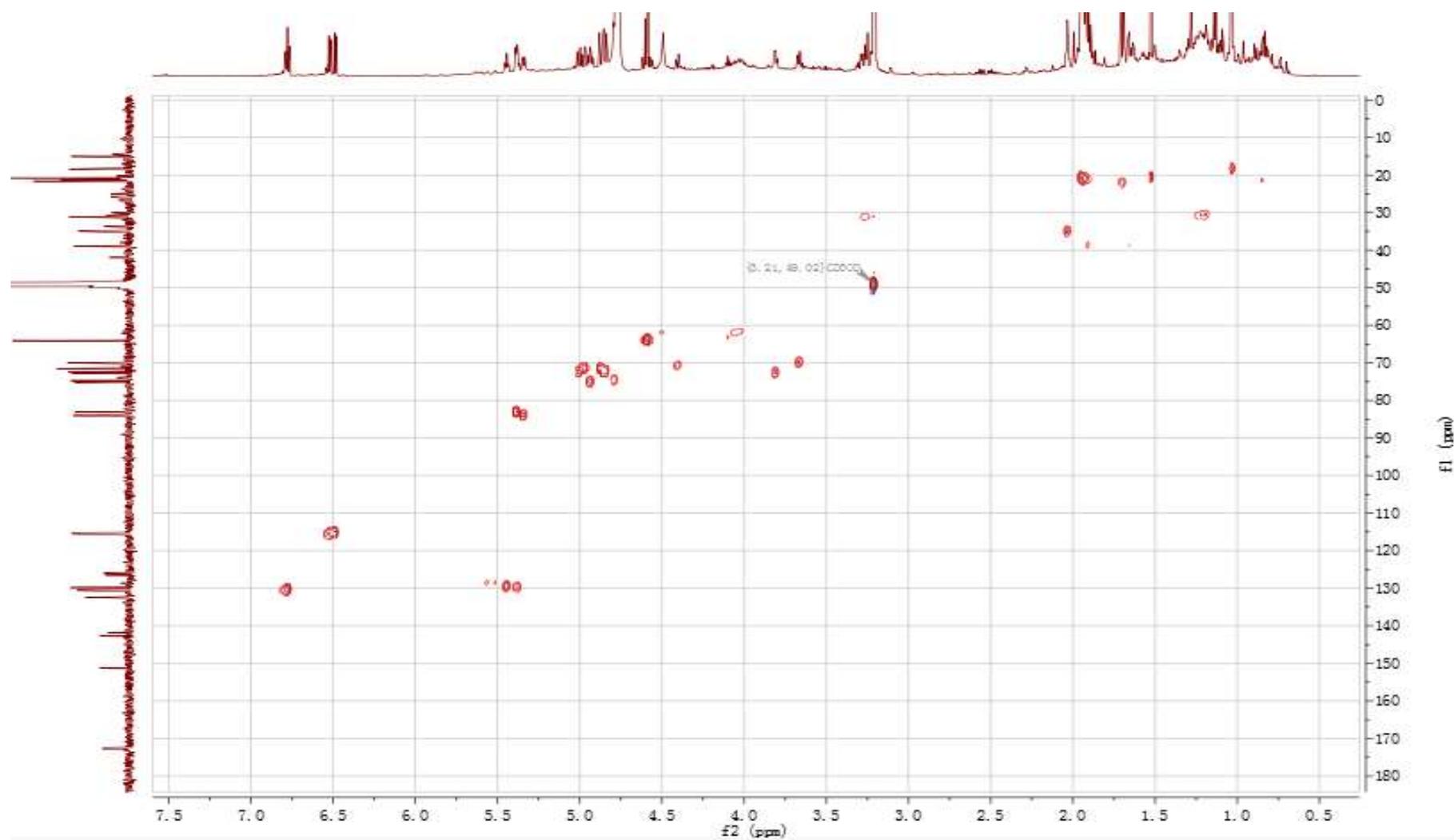


Figure S56. HSQC spectrum of the new compound **8**

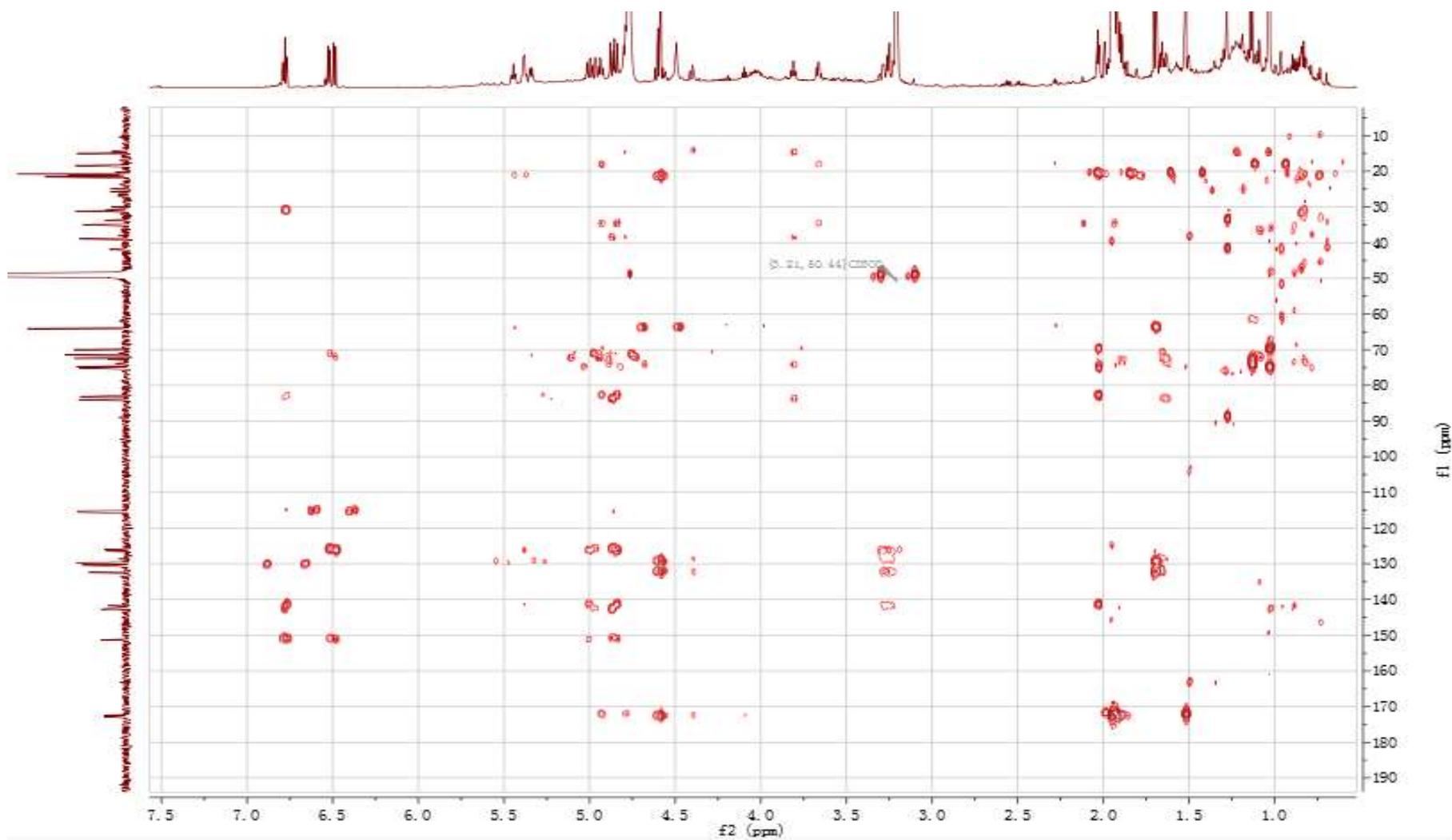
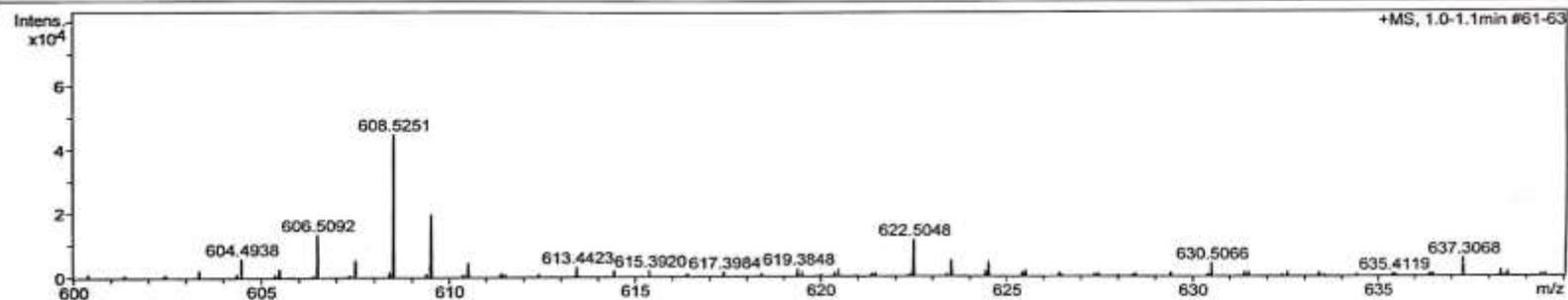


Figure S57. HMBC spectrum of the new compound **8**

Mass Spectrum SmartFormula Report

Analysis Info	Acquisition Date	12/27/2018 5:21:48 PM		
Analysis Name	D:\Data\MS\data\201812\yangbin_L28_pos_31_01_6015.d			
Method	LC_Direct Infusion_pos_70-500mz.m	Operator		
Sample Name	yangbin_L28_pos	Instrument	maXis	255552.00029
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
608.5251	1	C37H70NO5	100.00	608.5249	-0.4	-0.3	13.9	3.5	even	ok
630.5066	1	C37H69NNaO5	100.00	630.5068	0.3	0.2	51.9	3.5	even	ok
1216.0430	1	C74H139N2O10	100.00	1216.0424	0.4	0.5	20.3	6.5	even	ok

Figure S58. HRESI-MS spectrum of the new compound **9**

Instrument: DSQ (Thermo)
Ionization Method: EI
D:\DSQ\DATA-LR\19\010901
010901 #97 RT: 2.50 AV: 1 NL: 1.15E7
T: + c Full ms [45.00-800.00]

1/9/2019 10:10:40 AM

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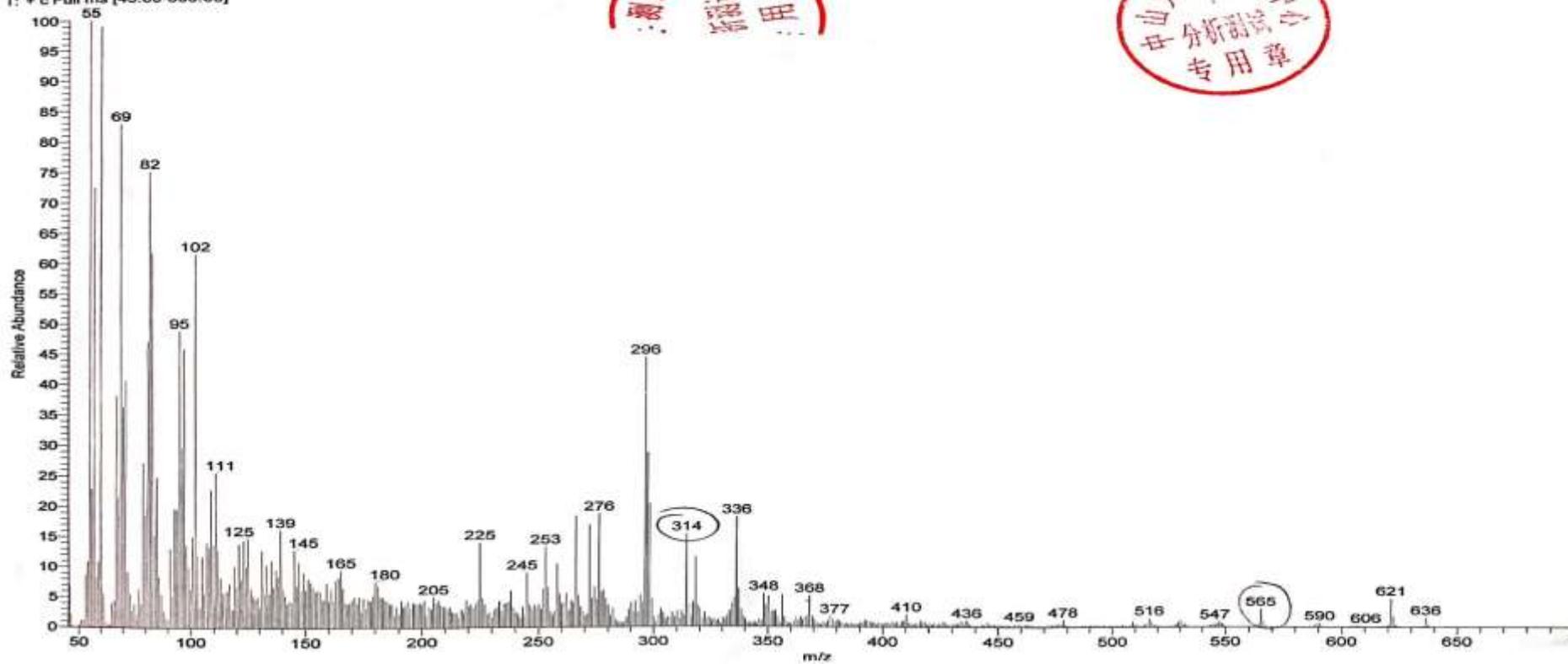


Figure S59. EI-MS spectrum of the new compound 9

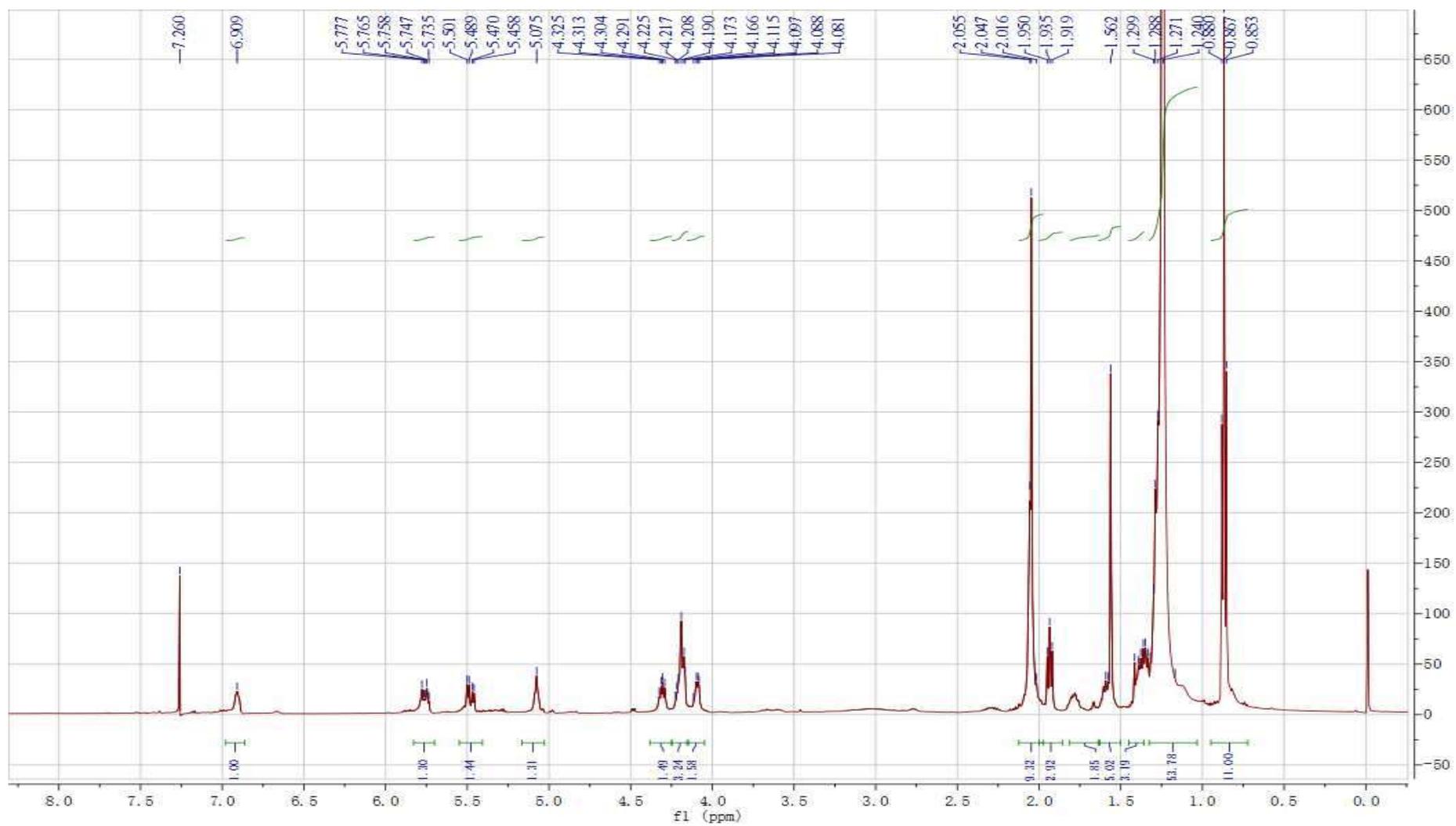


Figure S60. ^1H NMR (500 MHz, CDCl_3) spectrum of the new compound **9**

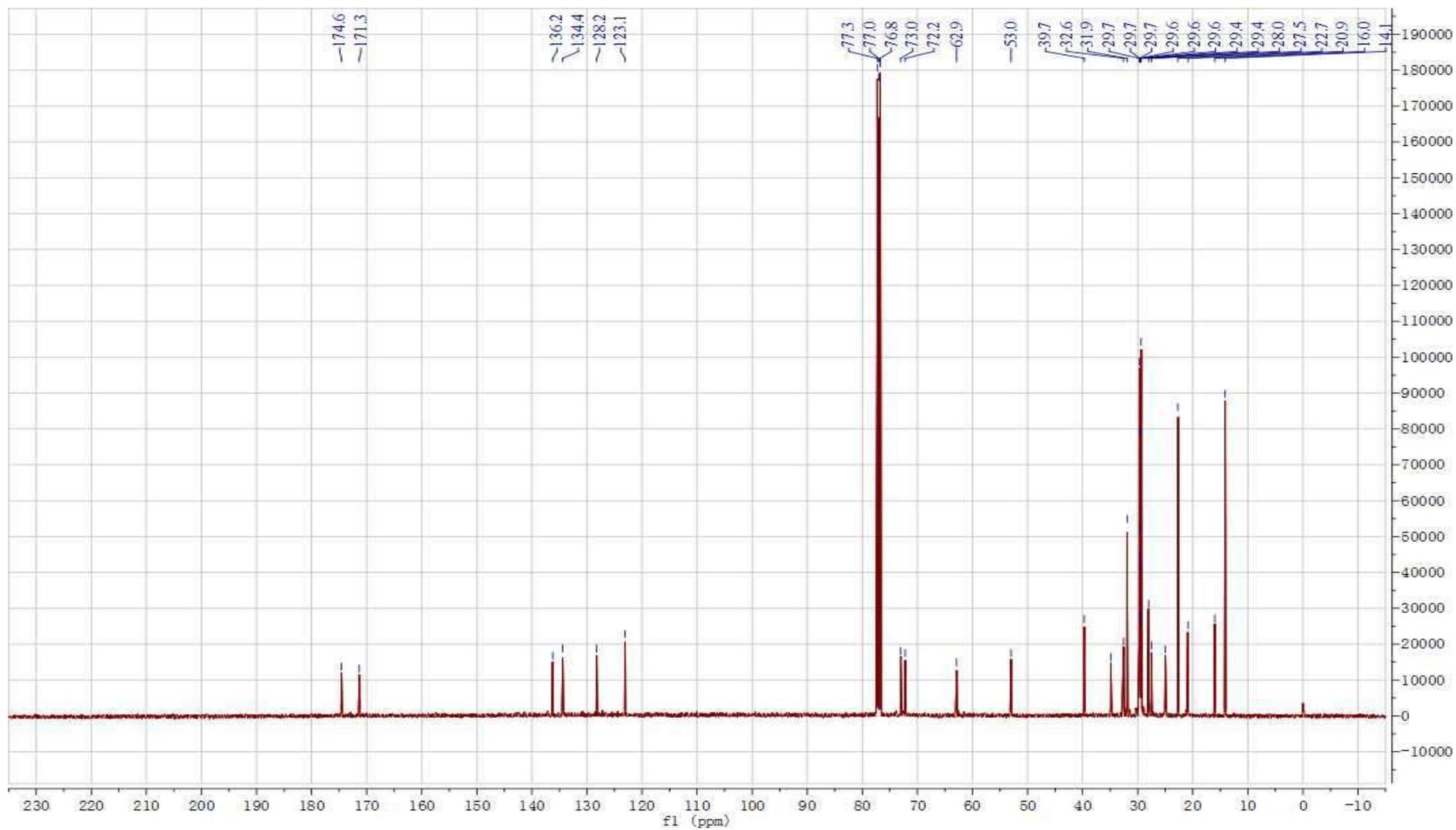


Figure S61. ^{13}C NMR (125 MHz, CDCl_3) spectrum of the new compound **9**

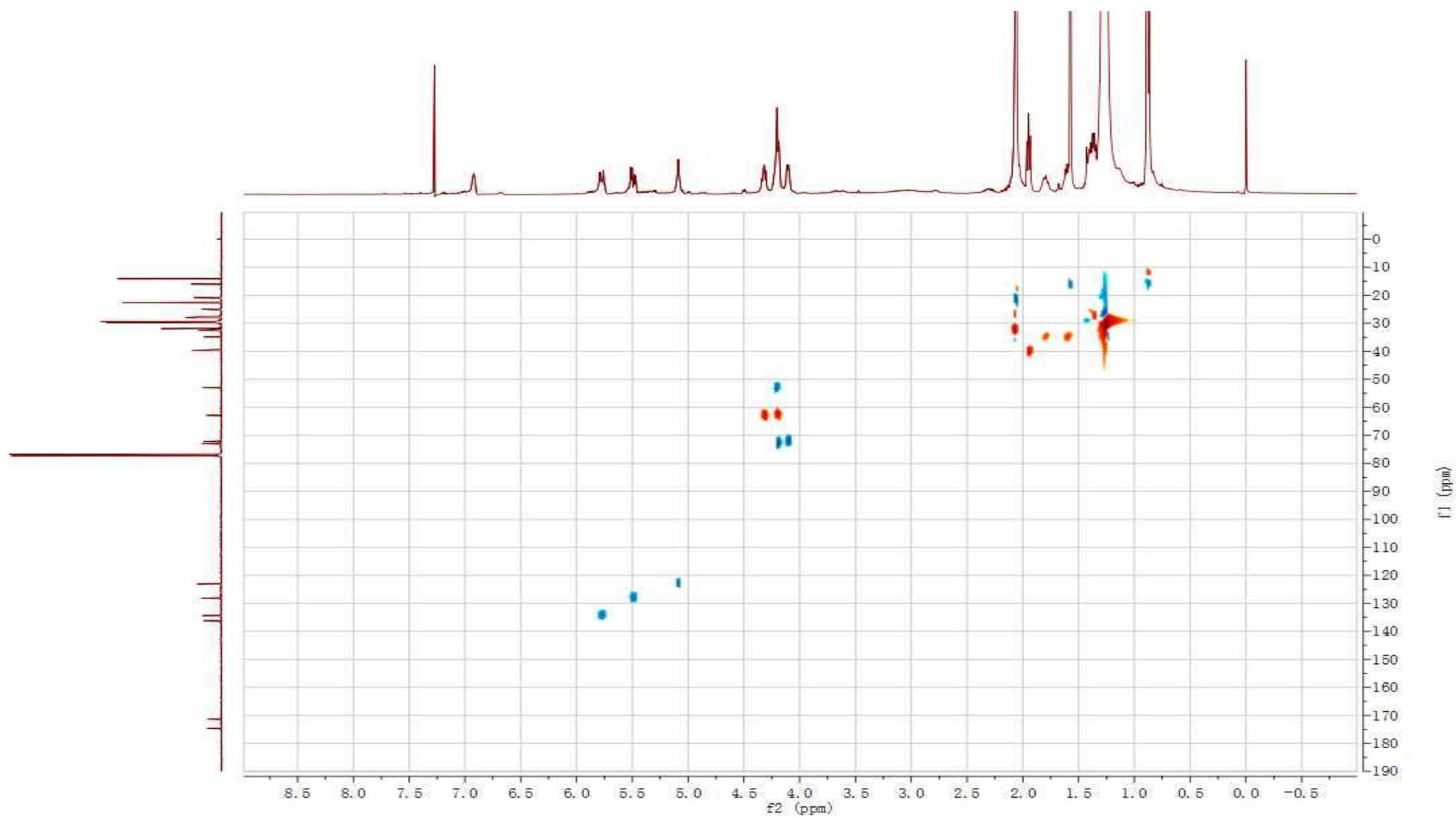


Figure S62. HSQC spectrum of the new compound **9**

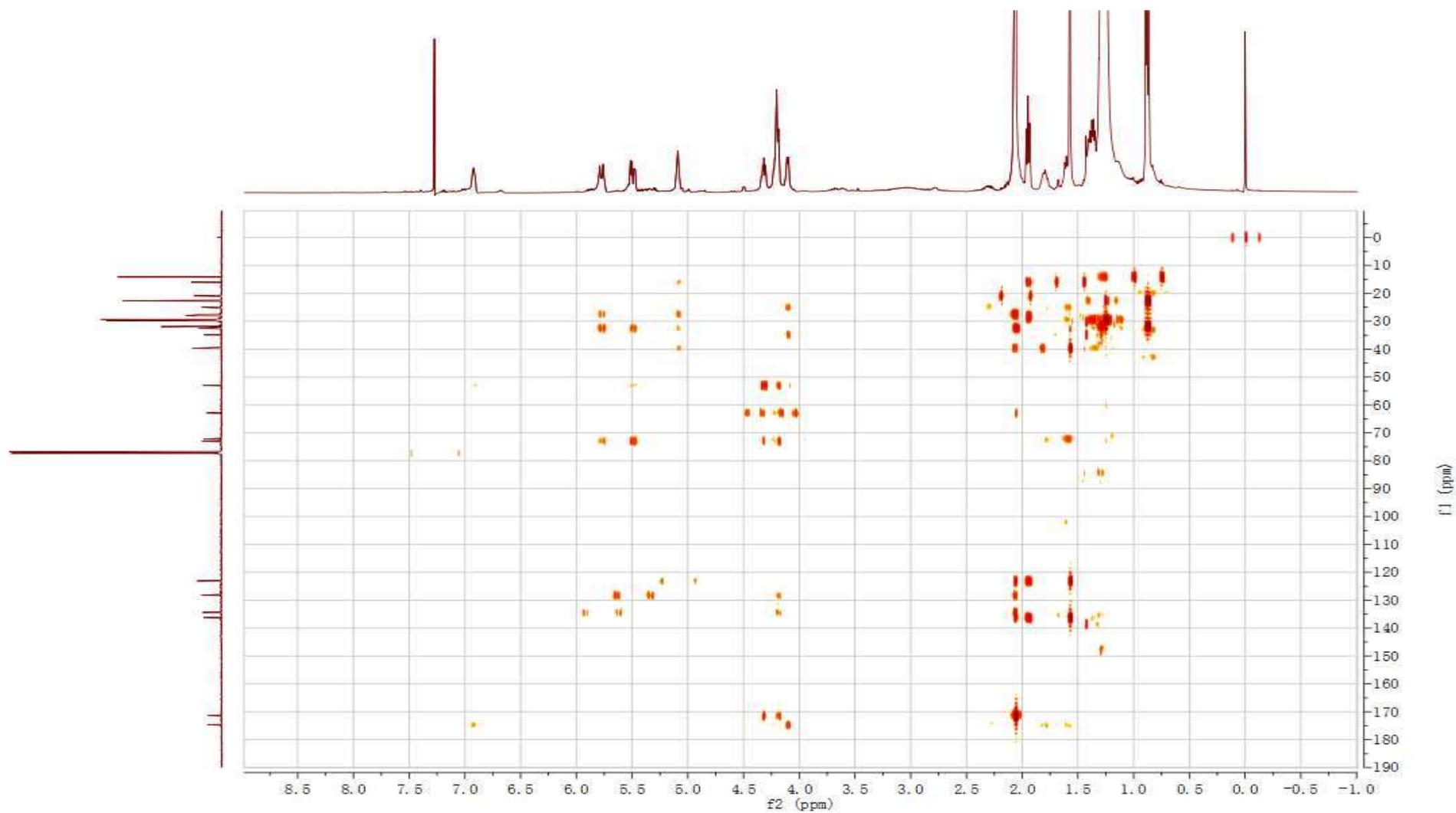


Figure S63. HMBC spectrum of the new compound **9**

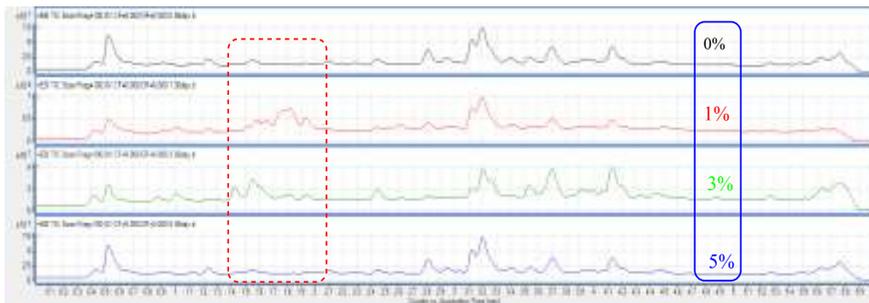


Figure S64. HPLC chromatograms of EtOAc extracts monitored (black line: 0% NaCl rice medium, red line: 1% NaCl rice medium, green line: 3% NaCl rice medium, blue line: 5% NaCl rice medium).