

Isolation and Identification of Secondary Metabolites from *Streptomyces* sp. SP301

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NMR data

Table S1: NMR spectroscopy data for compound **1** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC
1		131.9 s		
2	7.01 (d, 8.5)	130.9 d	H-3	C-3, C-4, C-6, C-7
3	6.68 (d, 8.5)	116.0 d	H-2	C-1, C-4, C-5
4		156.7 s		
5	6.68 (d, 8.5)	116.0 d	H-6	C-1, C-3, C-4
6	7.01 (d, 8.5)	130.9 d	H-5	C-2, C-4, C-7
7	2.62 (m) 2.78 (m)	39.1 t	H-8	C-1, C-8, C-9, C-8a
8	2.43 (m)	51.9 d	H-7, H-8a	C-7, C-9, C-8a, C-8b
9		181.1 s		
8a	1.66 (m)	26.6 t	H-8, H-8b	C-7, C-8, C-9, C-8b
8b	0.94 (t, 7.4)	12.3 q	H-8a	C-8, C-8a

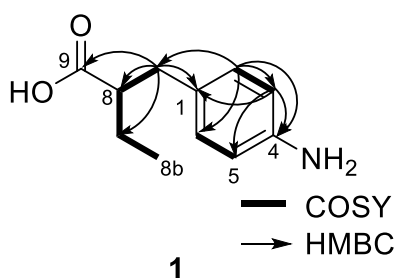
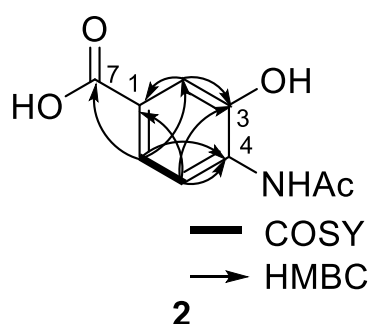


Fig S1: Selected ^1H - ^1H COSY and HMBC correlations for compound **1**.

The structural identification of compound 1 : The molecular formula of compound **1** was assigned as $\text{C}_{11}\text{H}_{15}\text{NO}_2$ on the basis of high resolution ESIMS data (m/z 194.1178 for $[\text{M} + \text{H}]^+$). Interpretation of the NMR data (Tables 1 and 2) revealed that **1** contained one methyl, two methylenes, five methenyls and three quaternary carbons. The ^1H -NMR data (Tables 1 and 2) of compound **1** revealed that it contained four aromatic protons δ_H 7.01 (d, $J = 8.5$ Hz, 2 H) and 6.68 (dd, $J = 8.5$ Hz, 2 H). Combined with ^{13}C -NMR, HSQC and HMBC related signals, it can be determined that the carbon signals δ_C 130.9 d and 116.0 d connected with above-mentioned aromatic protons. These two evidences proved the existence of *para*-disubstituted benzene ring in compound **1**. By the analysis of ^1H - ^1H COSY signals, it can be observed that the existence of fragment [a : $-\text{CH}_3$ (8b)- CH_2 (8a)- CH (8)- CH_2 (7)]. The existence of *para*-disubstituted benzene ring, fragment [a] and HMBC correlations from H-7 to C-1, C-8, C-9, C-8a, H-2 to C-3, C-4, C-6, C-7, H-3 to C-1, C-4, C-5 revealed the whole structure of **1**. According to literatures search and database comparison, we found compound **1** was known compound (*p*-amino- α -ethyl-hydrocinnamic acid).

Table S2: NMR spectroscopy data for compound **2** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC
1		127.9 s		
2	7.50 (m)	117.4 d		C-1, C-3, C-6
3		148.4 s		
4		131.9 s		
5	7.98 (d, 8.8)	122.0 d	H-6	C-1, C-3, C-4
6	7.49 (m)	122.5 d	H-5	C-2, C-4, C-7
7		169.8 s		
1-AcNH-4		172.2 s		
2-AcNH-4	2.20 (s)	23.9 q		C-1-Ac

**Fig S2:** Selected ^1H - ^1H COSY and HMBC correlations for compound **2**.

The structural identification of compound 2 : Compound **2** was determined to have molecular formula $\text{C}_9\text{H}_9\text{NO}_4$ on the basis of HRESIMS (m/z 196.0605 $[\text{M} + \text{H}]^+$). According to ^1H -NMR data, it revealed that **2** contained three aromatic protons ($\delta_H = 7.98$ (d, $J = 8.8$ Hz), 7.50 m, 7.49 m), and the latter two protons overlapped. Combined with ^1H - ^1H COSY and HMBC related signals, it can be further determined that the existence of trisubstituted benzene ring in compound **2**. According to NMR data and molecular weight, it can be confirmed the complete structure of compound **2**. By analyzing literatures and database comparison, we found compound **2** was known compound (4-acetamido-3-hydroxybenzoic acid).

Table S3: NMR spectroscopy data for compound **3** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC	NOESY
1		140.8 s			
2	6.71 (d, 1.7)	118.1 d		C-4, C-6, C-7	
3		149.8 s			
4		124.8 s			
5	7.44 (d, 8.1)	124.0 d	H-6	C-1, C-3, C-4	
6	6.67 (dd, 8.2, 1.8)	121.4 d	H-5	C-2, C-4	
7	2.47 (m)	35.6 t	H-8	C-1, C-2, C-6, C-8, C-9, C-8a	
	2.71 (dd, 13.8, 5.6)				
8	1.65 (m)	48.7 d	H-7, H-9		
9	3.75 (m)	72.0 d	H-8, H-10		H-8a, H-8b
10	2.40 (m)	37.9 t	H-9, H-11	C-9, C-11, C-12	
11	7.04 (m)	148.4 d	H-10, H-12	C-10, C-13	
12	5.90 (d, 15.7)	124.4 d	H-11	C-10, C-13	
13		169.8 s			
1-AcNH-4		172.2 s			
2-AcNH-4	2.16 (s)	23.3 q		C-1-Ac	
8a	1.29 (m)	23.0 t	H-8b	C-7, C-8, C-9, C-8b	
	1.51 (m)				
8b	0.91 (t, 7.4)	11.9 q	H-8a	C-8, C-8a	

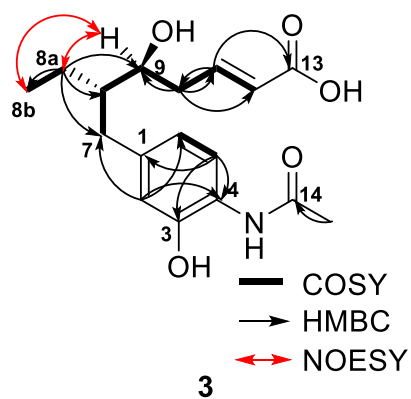
**Fig S3:** Selected ^1H - ^1H COSY, HMBC correlations for compound **3**.

Table S4: NMR spectroscopy data for compound **4** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC	NOESY
1		117.8 s			
2	7.71 (dd, 8.4, 1.6)	132.7 d	H-3	C-4, C-6, C-7	
3	6.30 (d, 8.5)	104.1 d	H-2	C-1, C-5	
4		157.5 s			
5		128.7 s			
6	7.57 (d, 1.4)	126.7 d	H-8	C-2, C-4, C-7	
7		170.6 s			
8	3.13 (m)	29.3 t	H-6, H-9	C-4, C-5, C-9, C-10	
9	4.17 (dd, 8.4, 5.6)	67.6 d	H-8	C-4, C-5, C-10, C-17	H-11 α , H-15, H-16
10		71.7 s			
11 α	2.05 (m)	38.1 t		C-13	H-9
11 β	1.61 (m)				H-17
12	1.80 (m) 2.13 (m)	22.2 t	H-11, H-13	C-14	
13	3.47 (d, 6.9)	58.6 d	H-12	C-4, C-9, C-11, C-12, C-14	
14		76.8 s			
15	1.25 (s)	27.9 q		C-13, C-14, C-16	
16	1.30 (s)	28.4 q		C-13, C-14, C-15	
17	0.98 (s)	19.4 q		C-9, C-10, C-11	

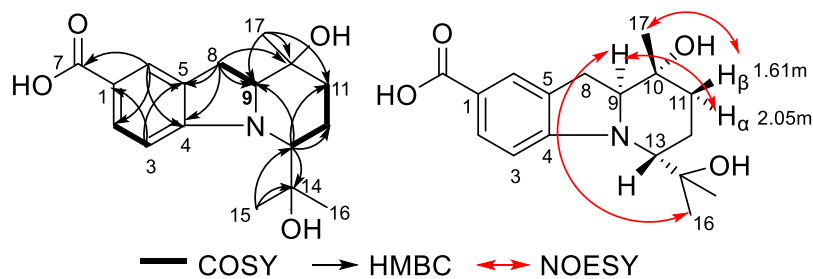
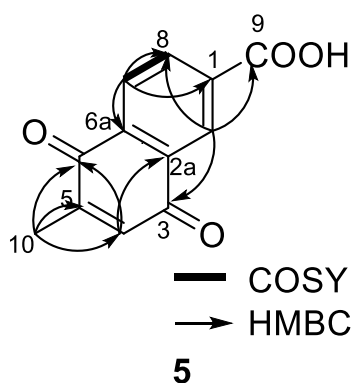
**4****Fig S4:** Selected ^1H - ^1H COSY, HMBC and NOESY correlations for compound **4**.

Table S5: NMR spectroscopy data for compound **5** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC
1		136.0 s		
2	8.60 (d, 1.5)	128.1 d	H-8	C-3, C-8, C-9
3		185.6 s		
4	6.94 (m)	136.8 d	H-10	C-6, C-10, C-2a
5		150.1 s		
6		186.1 s		
7	8.17 (d, 8.0)	127.7 d	H-8	C-1, C-6, C-8, C-6a
8	8.38 (dd, 8.0, 1.7)	135.2 d	H-7	C-1, C-9
9		168.3 s		
10	2.19 (d, 1.6)	16.4 q	H-4	C-4, C-5, C-6
2a		133.7 s		
6a		136.8 s		

**Fig S5:** Selected ^1H - ^1H COSY and HMBC correlations for compound **5**.

The structural identification of compound **5 :** The molecular formula of compound **5** was assigned as $\text{C}_{12}\text{H}_8\text{O}_4$ on the basis of high resolution ESIMS data (m/z 217.0491 for $[\text{M} + \text{H}]^+$). Interpretation of the ^1H -NMR data (Tables 1 and 2) revealed that **5** contained three aromatic protons ($\delta_H = 8.17$ (d, $J = 8.0$ Hz), 8.38 (dd, $J = 8.0$ Hz, 1.7 Hz), 8.60 (d, $J = 1.5$ Hz)). Combined with ^{13}C -NMR, HSQC, and HMBC related signals, it can be determined that the carbon signals ($\delta_C = 127.7$ d, 135.2 d, 128.1 d) connected with above-mentioned aromatic protons. These two evidences proved the existence of trisubstituted benzene ring in **5**. The fragment [$-\text{CH}$ (7)- CH (8)-] can be observed from ^1H - ^1H COSY signals of **5**. The HMBC correlations from H-2 to C-3, C-8, C-9, H-4 to C-6, C-2a, H-7 to C-1, C-6, C-8, C-6a, and H-10 to C-4, C-5, C-6 revealed the connection of each fragments. Finally, it can be confirmed the complete structure of **5** on the basis of NMR data and molecular weight. By the comparison of database, we found that compound **5** was an known compound (3,6-dihydro-5-methyl-3,6-dioxo-1-naphthalenecarboxylic acid).

Table S6: NMR spectroscopy data for compound **6** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC	NOESY
1		120.4 s			
2	8.88 (d, 1.4)	126.9 d	H-8	C-3, C-8, C-9, C-6a	
3		152.5 s			
4	6.70 (s)	112.3 d	H-10	C-3, C-6, C-10, C-2a	
5		133.2 s			
6		143.7 s			
7	8.45 (d, 8.9)	123.9 d	H-8	C-6, C-8, C-2a	
8	7.97 (dd, 8.9, 1.7)	126.4 d	H-7	C-2, C-6a	
9		170.4 s			
10	2.47 (s)	17.9 q		C-4, C-5, C-6	
2a		124.9 s			
6a		132.3 s			
1'	4.77 (d, 7.8)	106.6 d	H-2'	C-6, C-2'	H-3', H-5'
2'	3.71 (m)	75.5 d	H-1', H-3'	C-1', C-3'	
3'	3.50 (t, 9.0)	77.5 d	H-2', H-4'	C-4'	
4'	3.64 (m)	73.3 d	H-3'	C-5', C-6'	
5'	3.59 (d, 9.7)	76.9 d		C-1', C-4', C-6'	
6'		173.0 s			

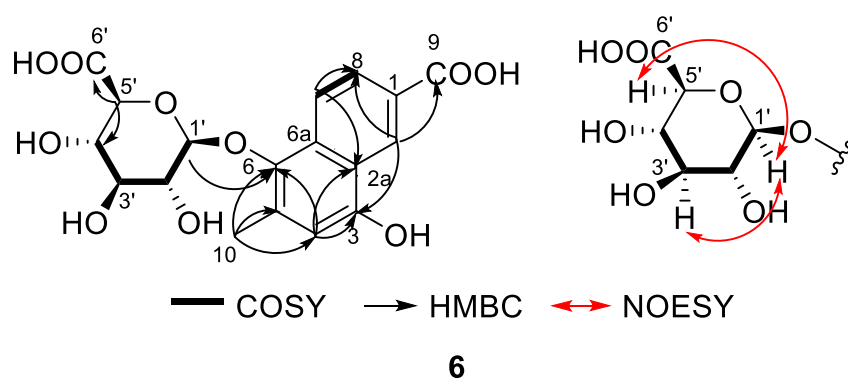
**Fig S6:** Selected ^1H - ^1H COSY, HMBC and NOESY correlations for compound **6**.

Table S7: NMR spectroscopy data for compound **7** (400 and 100 MHz, respectively, δ in ppm, J in Hz).

Pos.	δ_H	δ_C	COSY	HMBC	NOESY
2		167.8 s			
3		110.1 s			
4		166.2 s			
5	6.37 (s)	97.7 d		C-3, C-4, C-6, C-9	
6		169.1 s			
7	2.51 (m)	17.7 t	H-8	C-2, C-3, C-4, C-8	
8	1.08 (t, 7.4)	12.8 q	H-7	C-3, C-7	
9	2.60 (m)	41.4 d	H-10, H-12	C-5, C-10, C-12	
10	1.62 (m)	28.5 t	H-9, H-11	C-6, C-9, C-11, C-12	
	1.74 (m)				
11	0.92 (t, 7.4)	11.9 q	H-10	C-9, C-10	
12	1.24 (d, 6.9)	18.4 q	H-9	C-6, C-9, C-10	
1'	5.15 (m)	100.8 d	H-2'	C-4	H-3', H-5'
2'	3.52 (m)	74.4 d	H-1'	C-3'	
3'	3.51 (m)	77.4 d		C-2'	H-9
4'	3.63 (m)	72.8 d	H-5'	C-3'	
5'	4.01 (d, 9.6)	76.6 d	H-4'	C-4', C-6'	
6'		173.1 s			

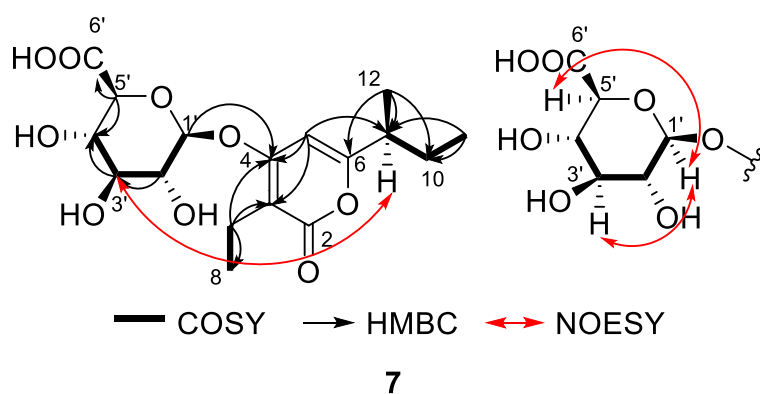


Fig S7: Selected ^1H - ^1H COSY, HMBC and NOESY correlations for compound **7**.

Spectroscopic data informations

Figure S8. ^1H NMR (400 MHz, CD_3OD) spectrum for compound **1**

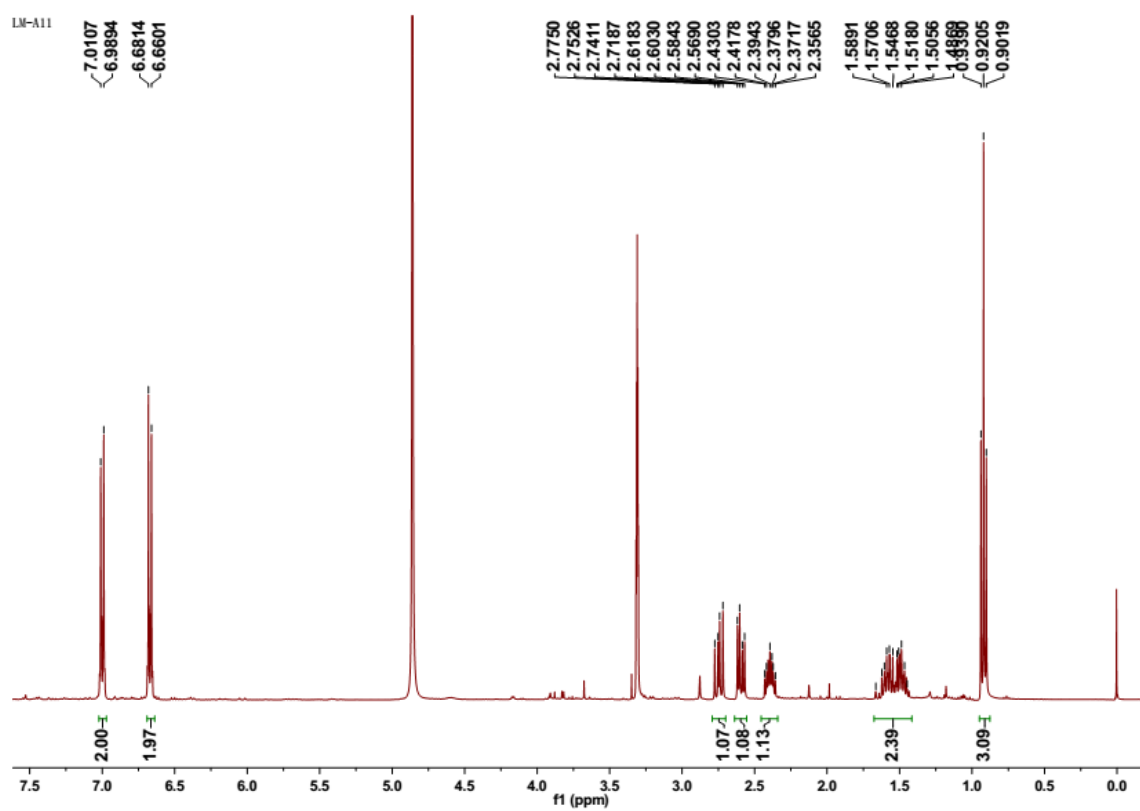


Figure S9. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound **1**

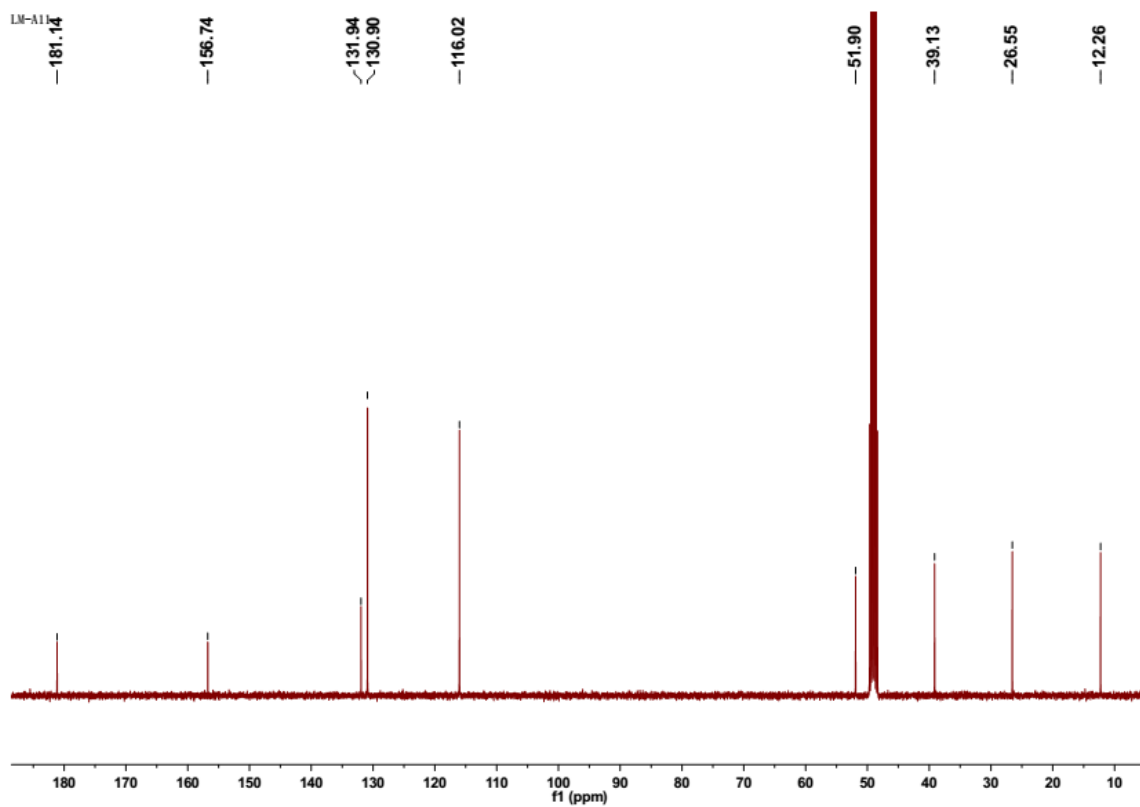


Figure S10. The HSQC spectrum for compound **1**

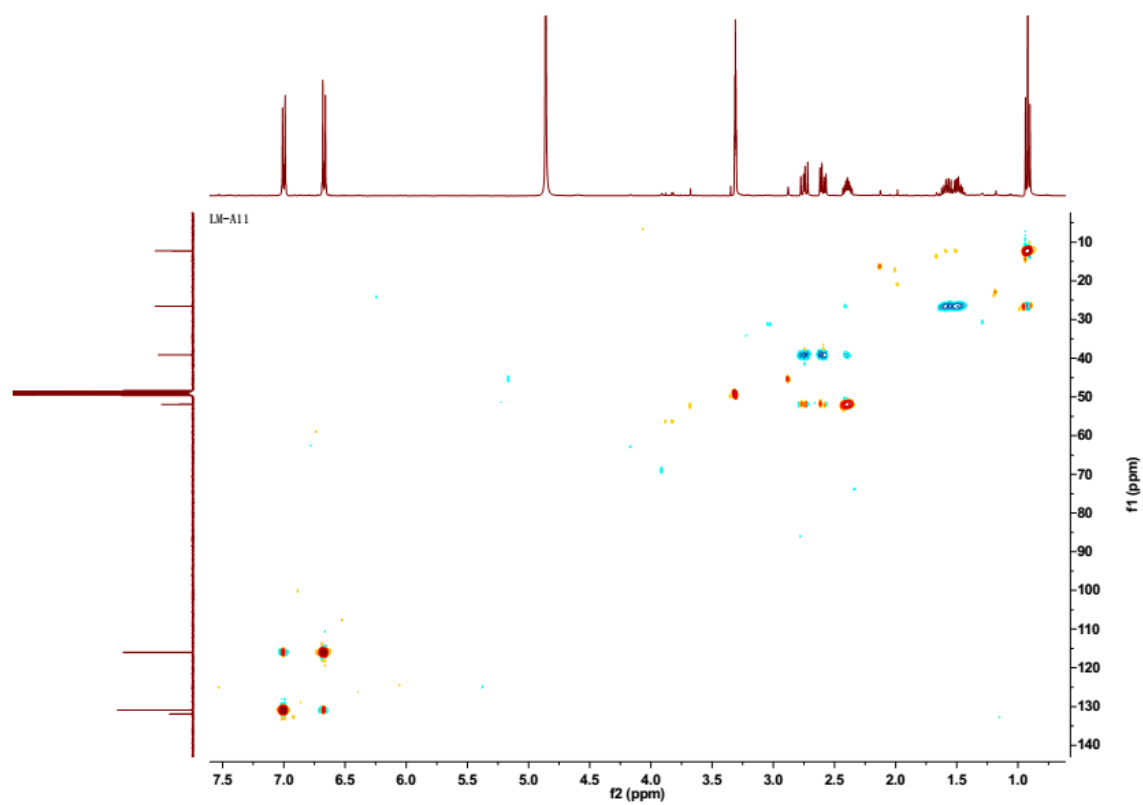


Figure S11. The HMBC spectrum for compound **1**

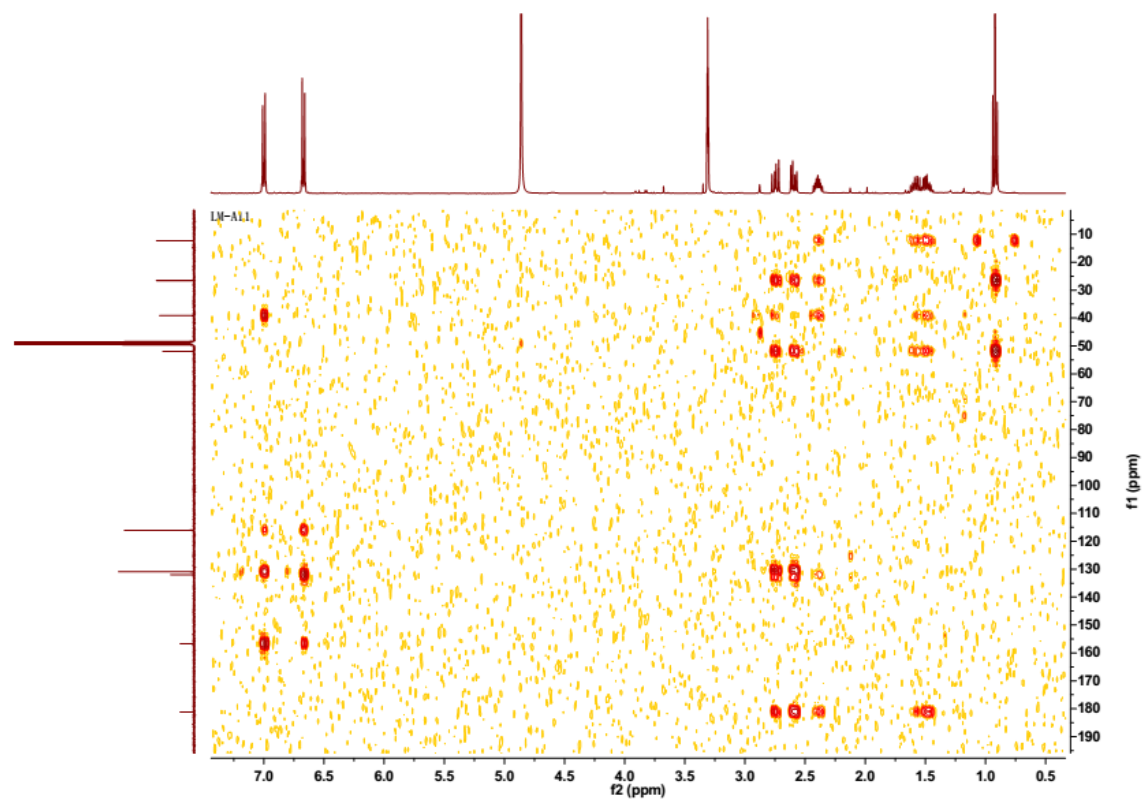


Figure S12. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 1

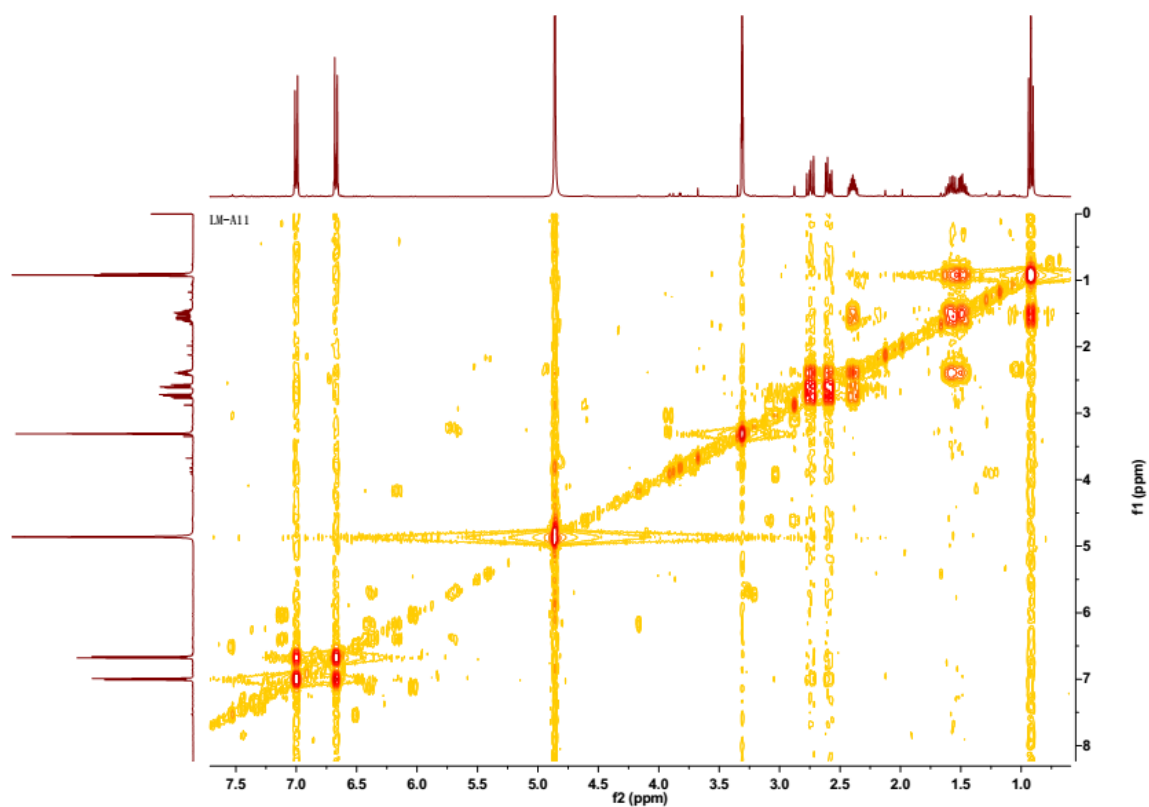


Figure S13. The HRMS-ESI spectrum for compound 1

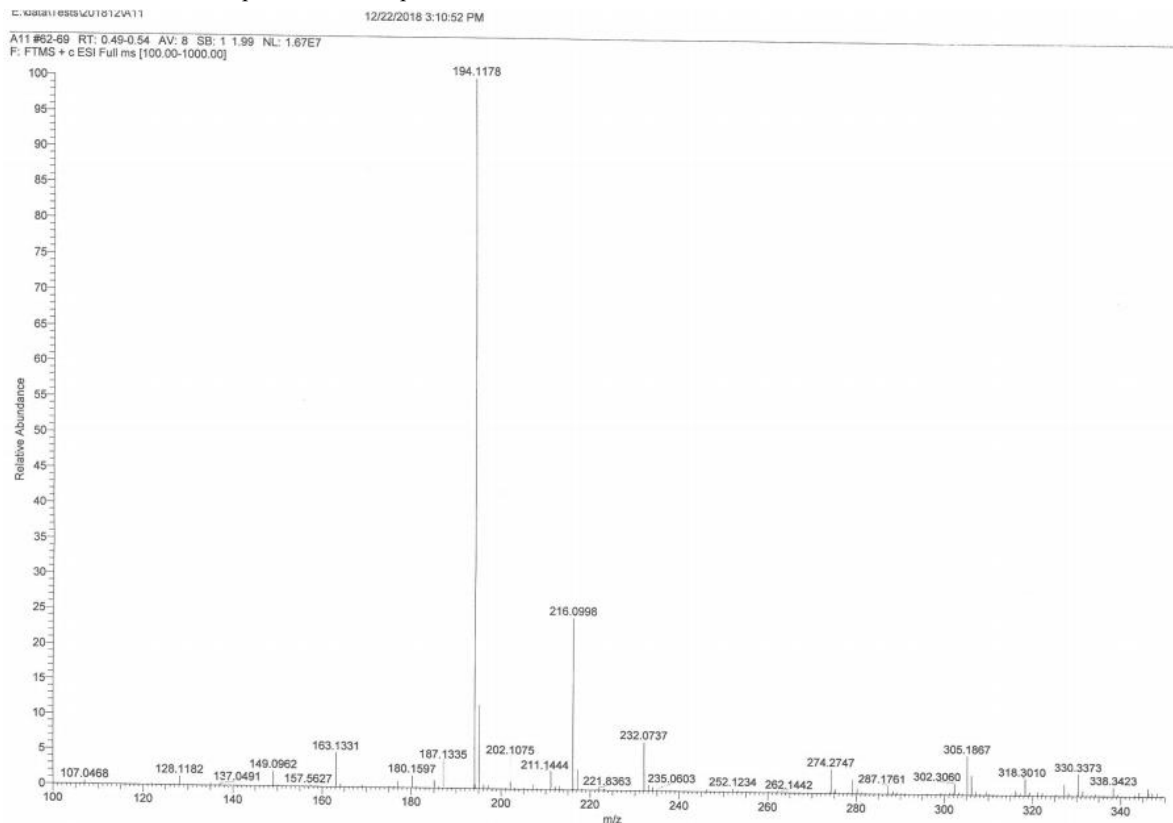


Figure S14. ^1H NMR (400 MHz, CD_3OD) spectrum for compound 2

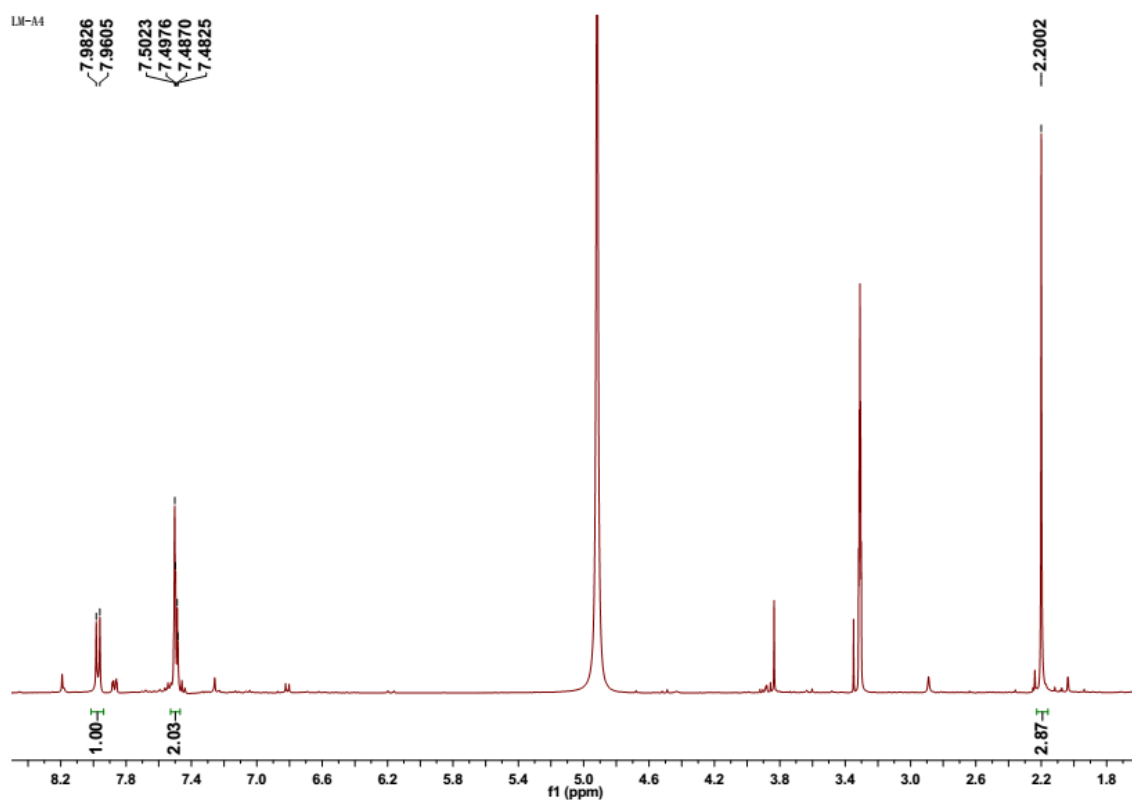


Figure S15. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound 2

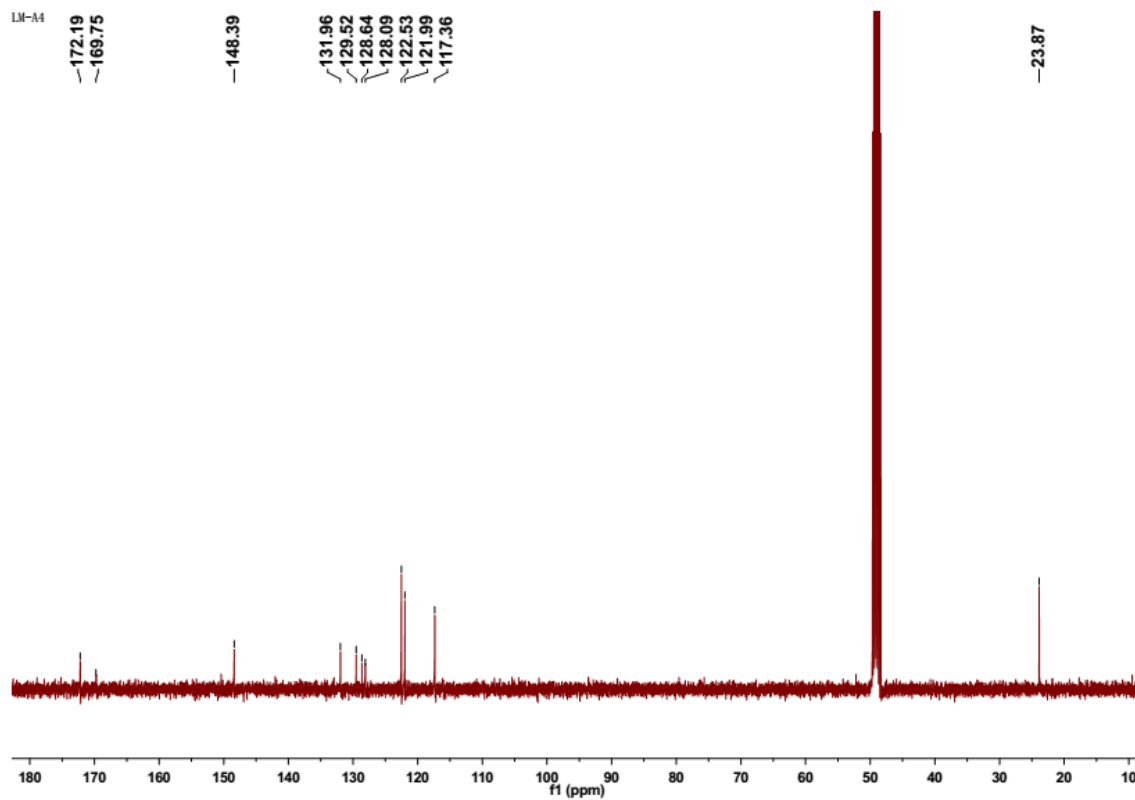


Figure S16. The HSQC spectrum for compound 2

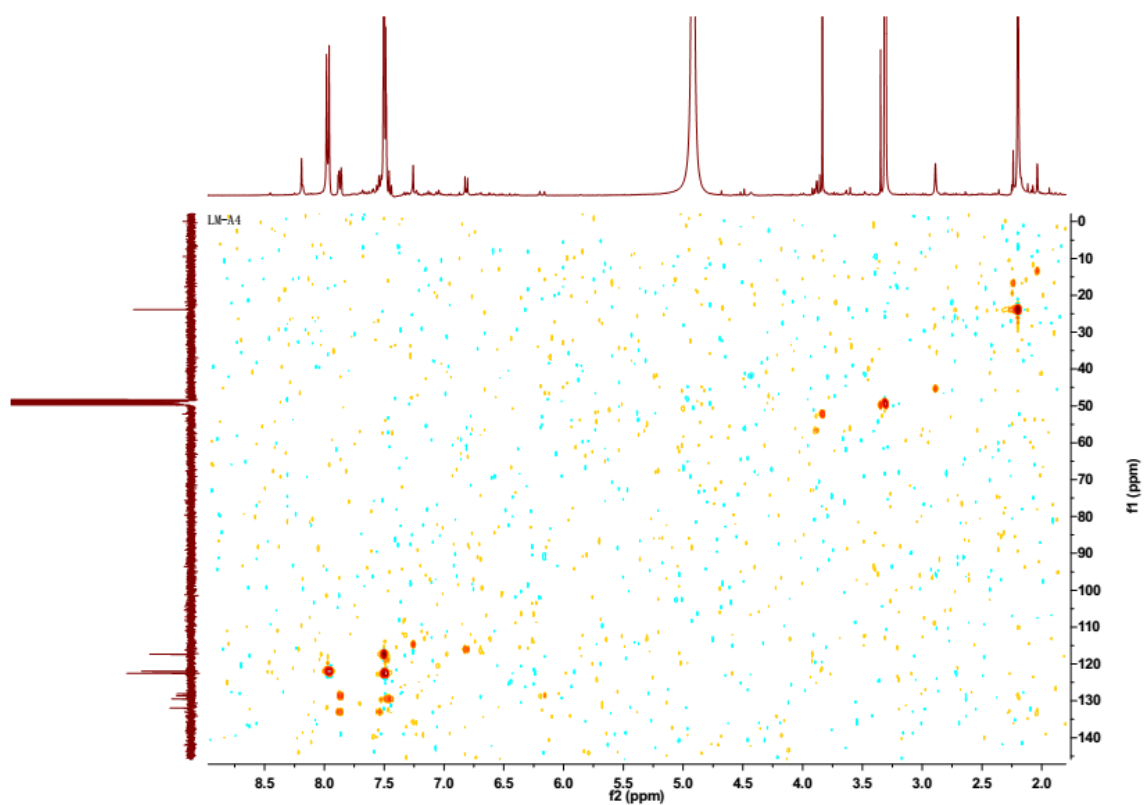


Figure S17. The HMBC spectrum for compound 2

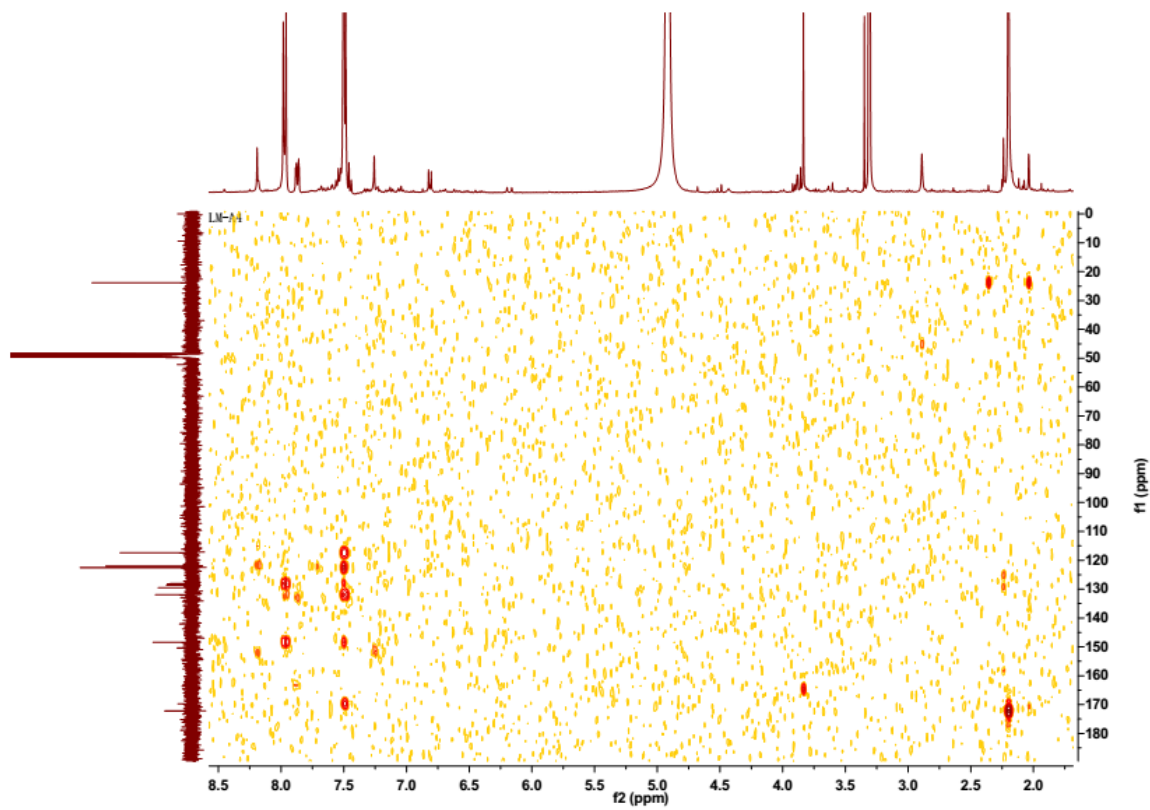


Figure S18. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 2

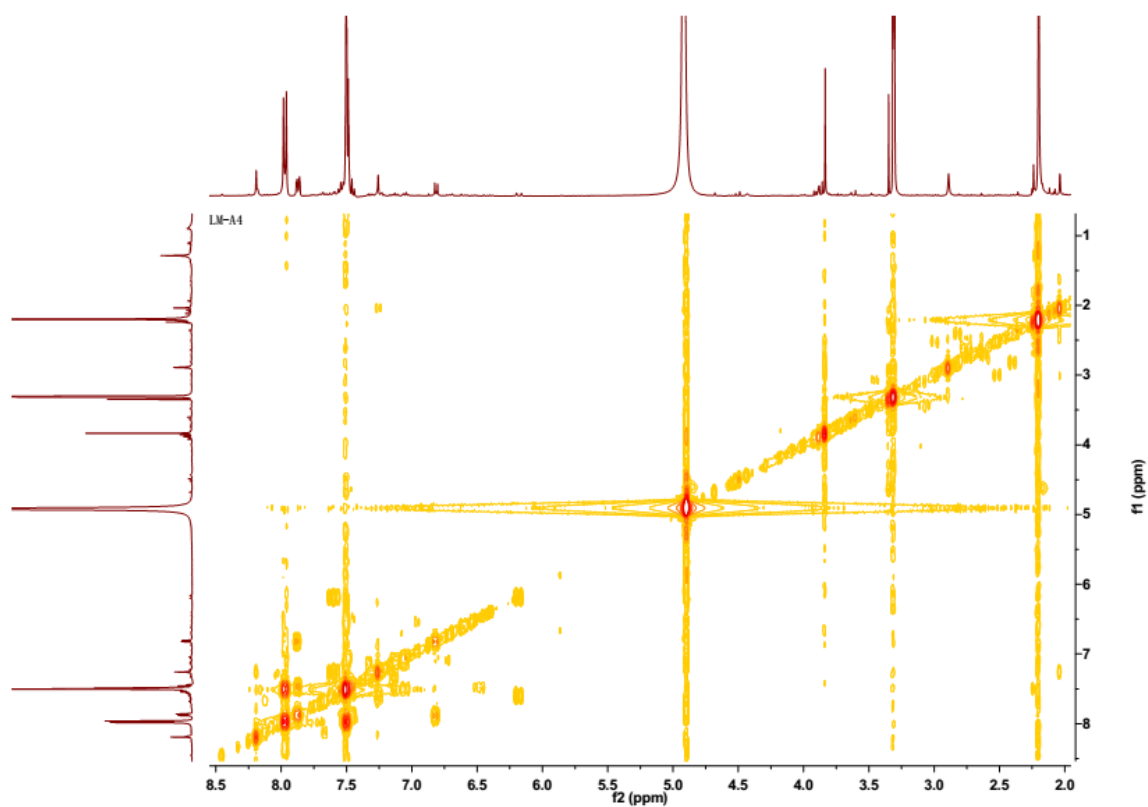


Figure S19. The HRMS-ESI spectrum for compound 2

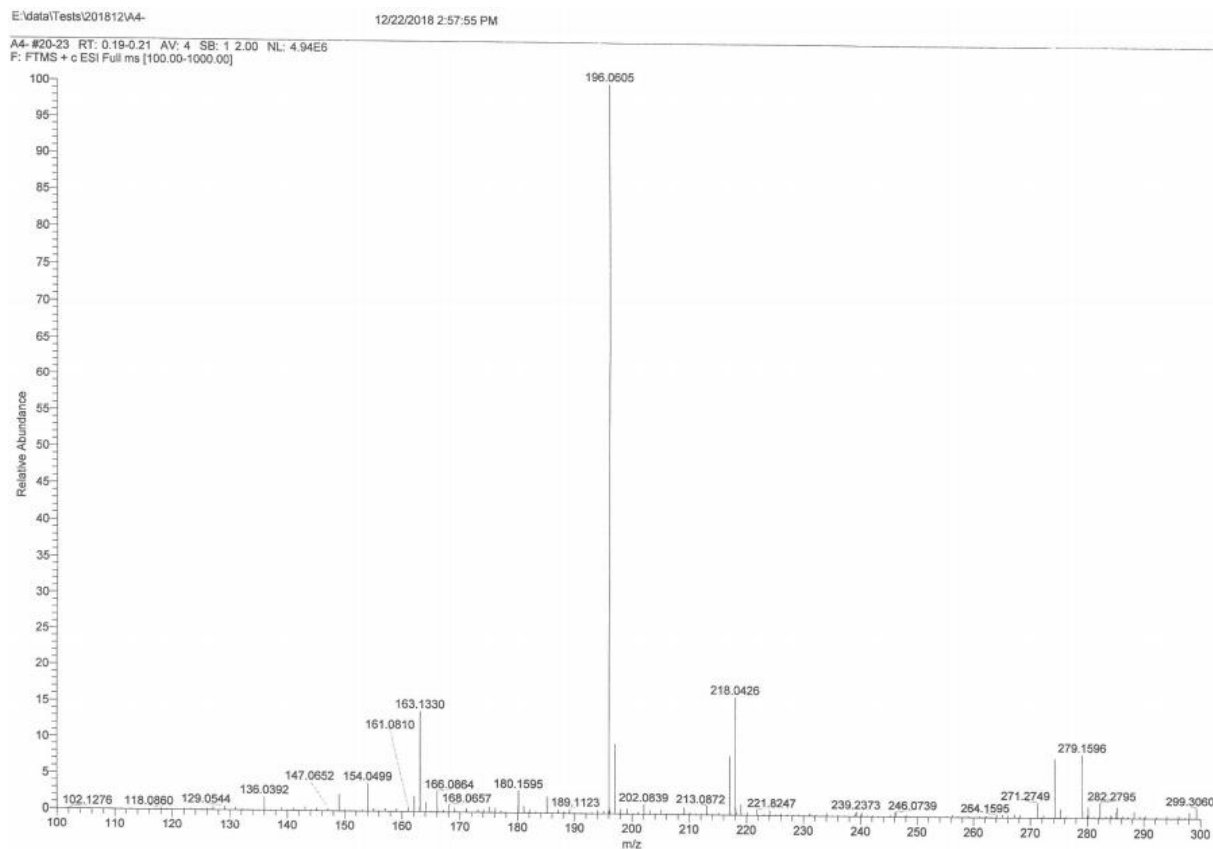


Figure S20. ^1H NMR (400 MHz, CD_3OD) spectrum for compound 3

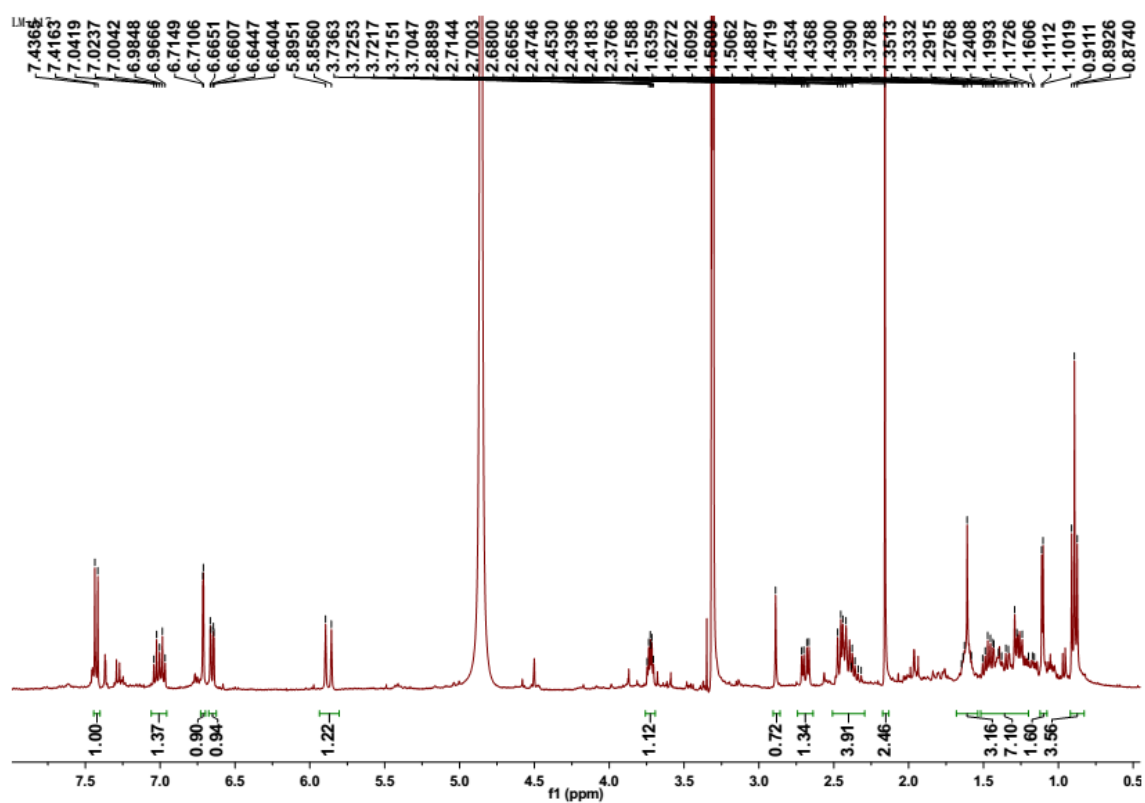


Figure S21. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound 3

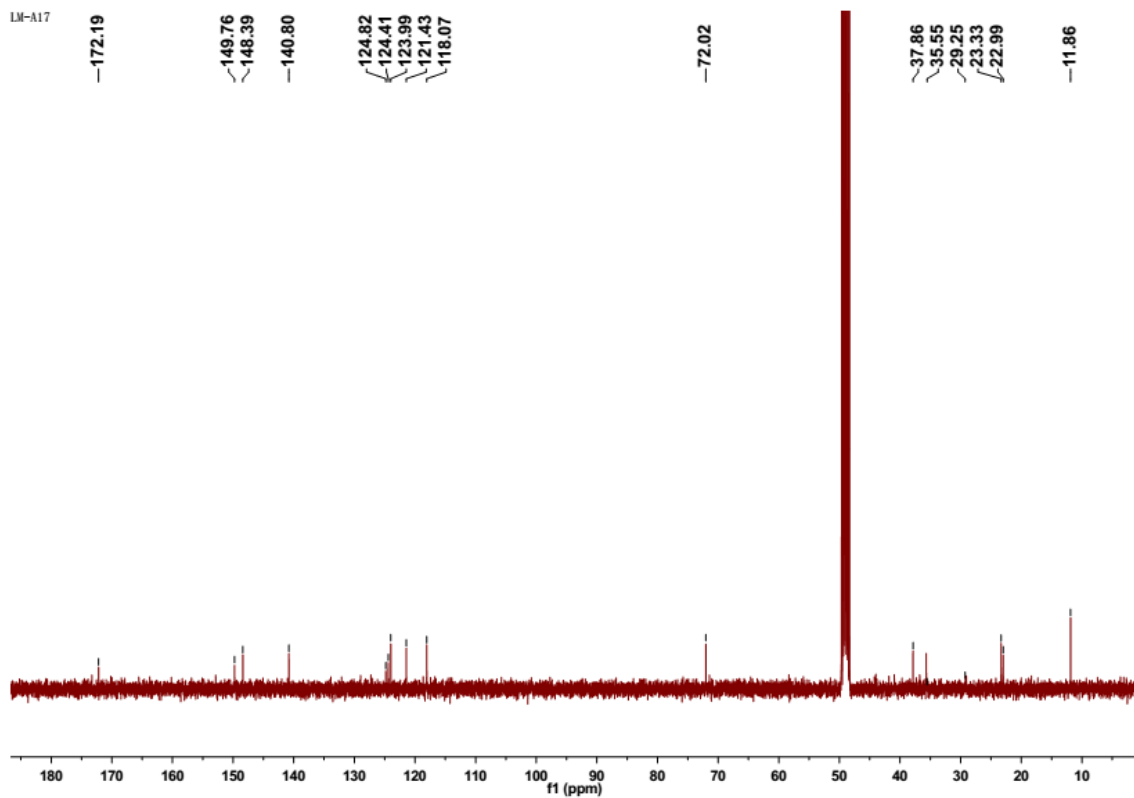


Figure S22. The HSQC spectrum for compound 3

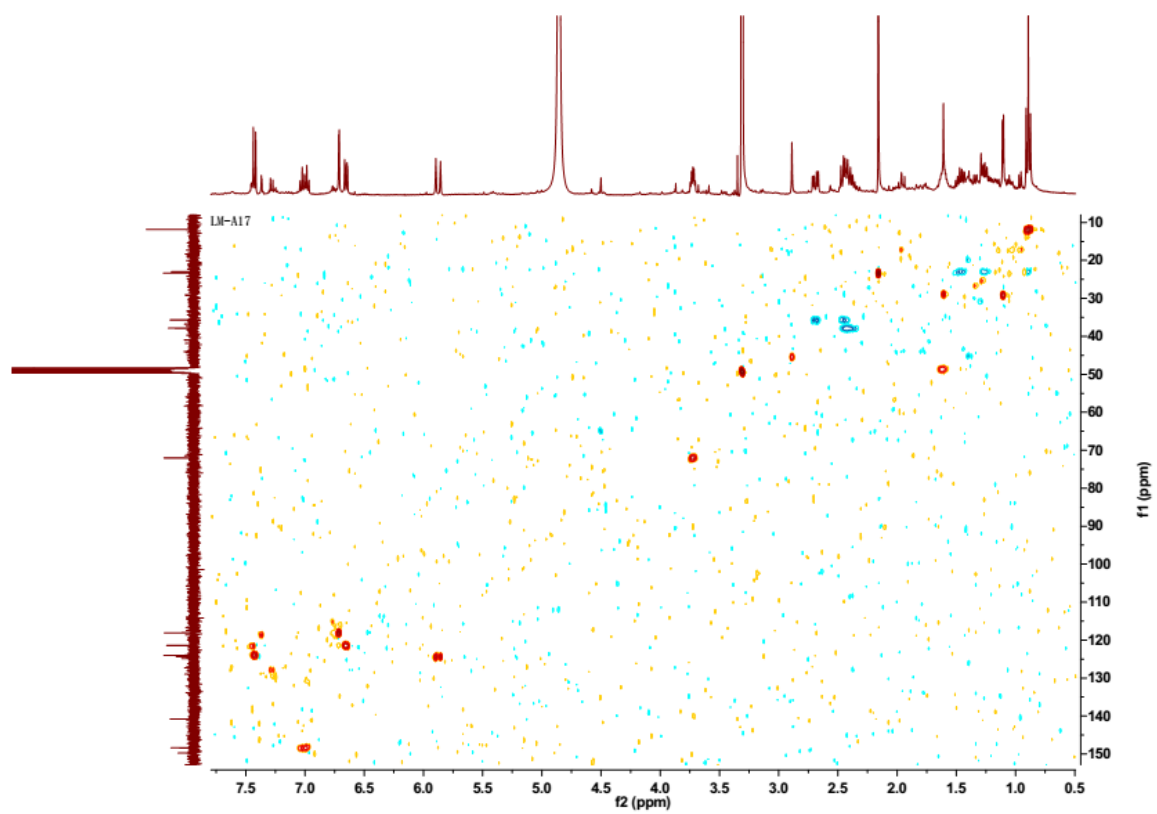


Figure S23. The HMBC spectrum for compound 3

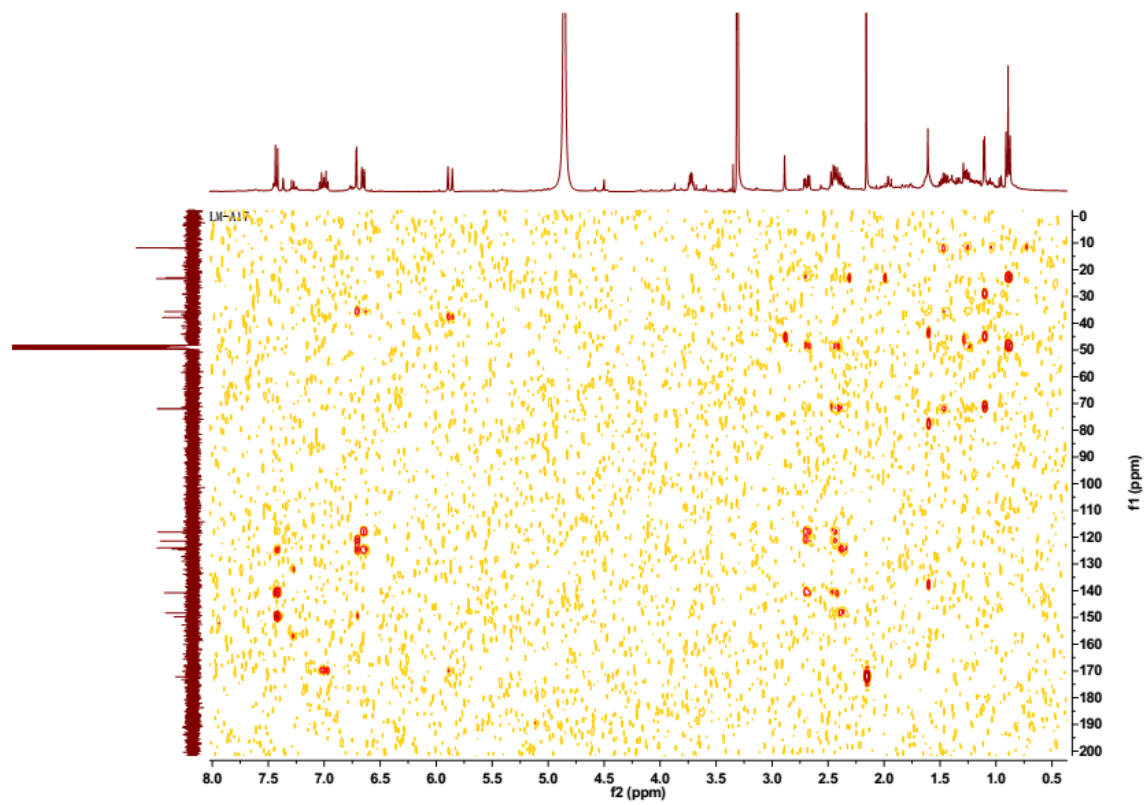


Figure S24. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 3

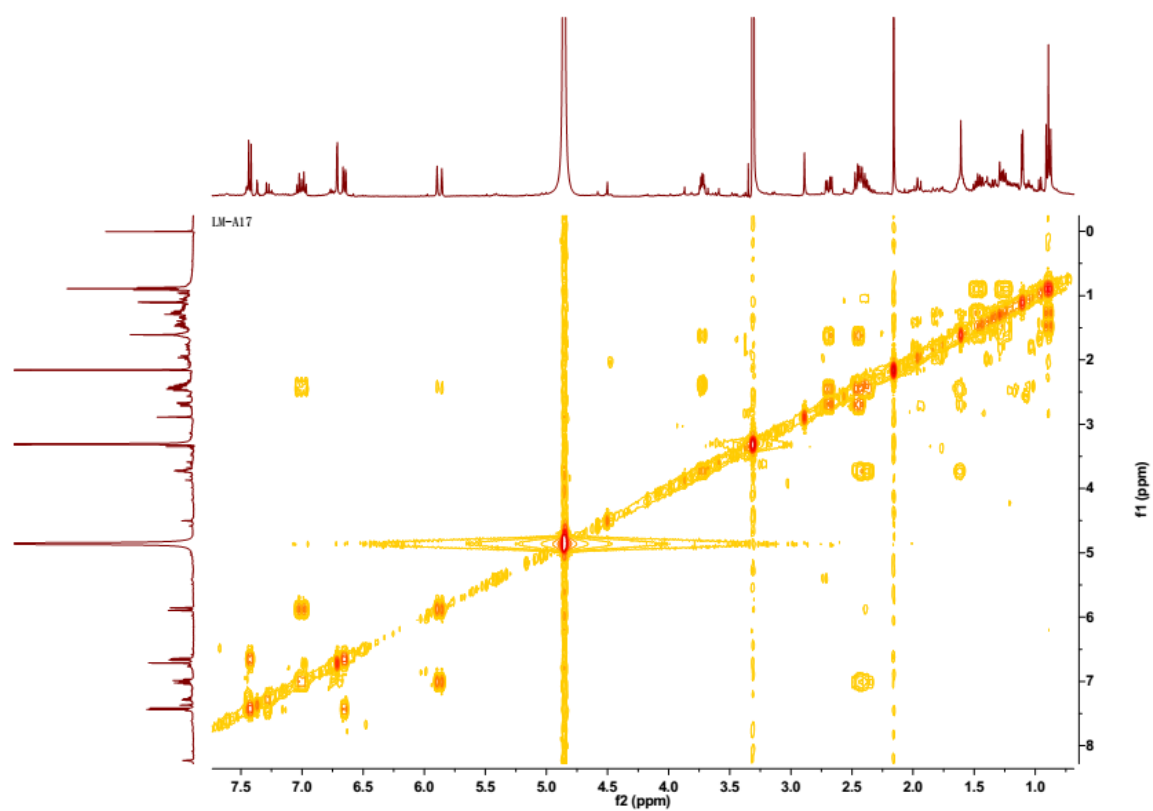


Figure S25. NOESY spectrum for compound 3

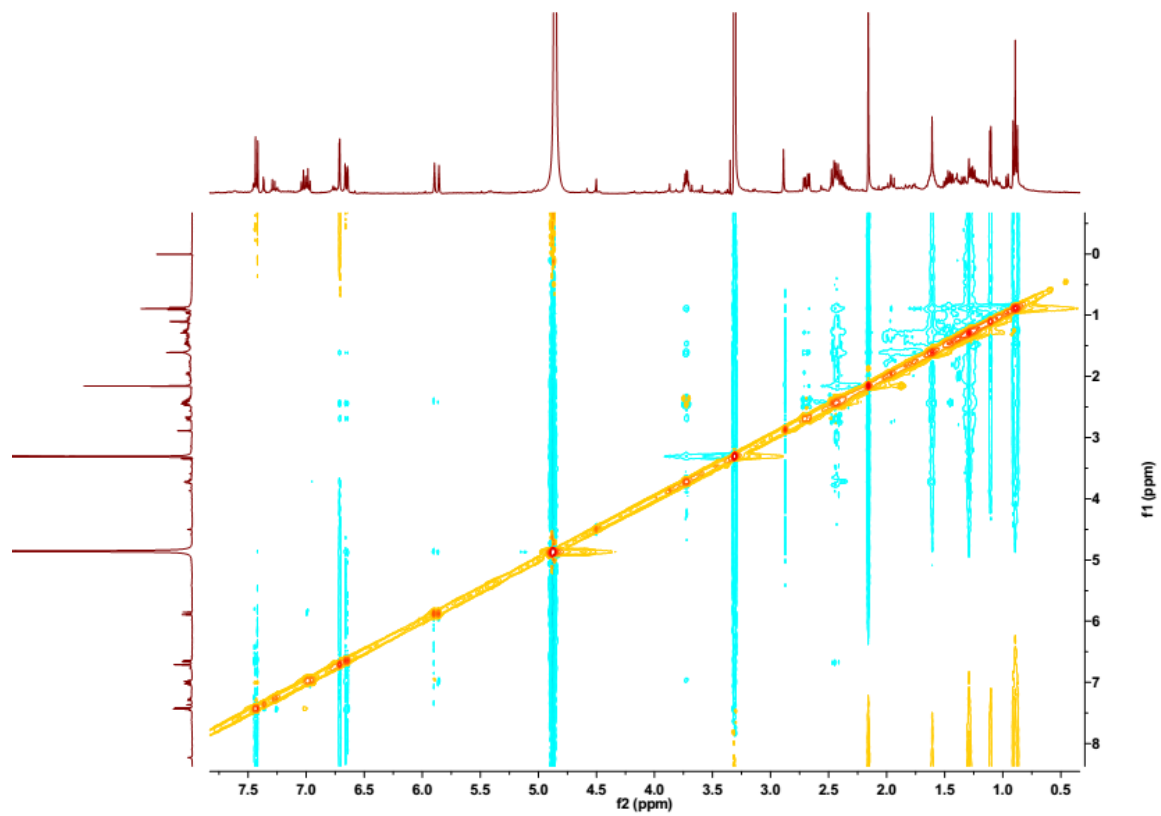


Figure S26. The HRM S-ESI spectrum for compound **3**

20161228_lm_A17 #11-14 RT: 0.27-0.35 AV: 4 NL: 1.52E7
T: FTMS + p ESI Full ms [160.00-600.00]

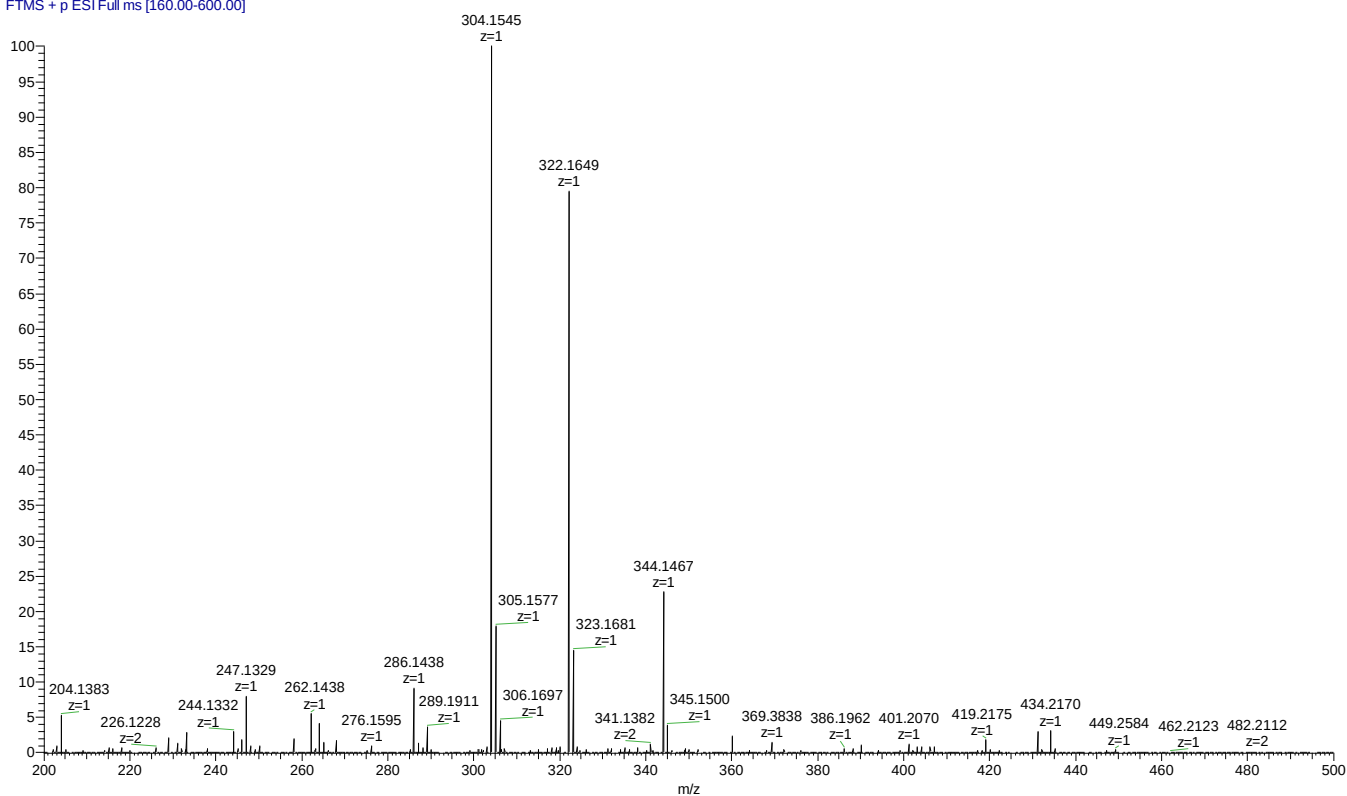


Figure S27. ^1H NMR (400 MHz, CD_3OD) spectrum for compound **4**

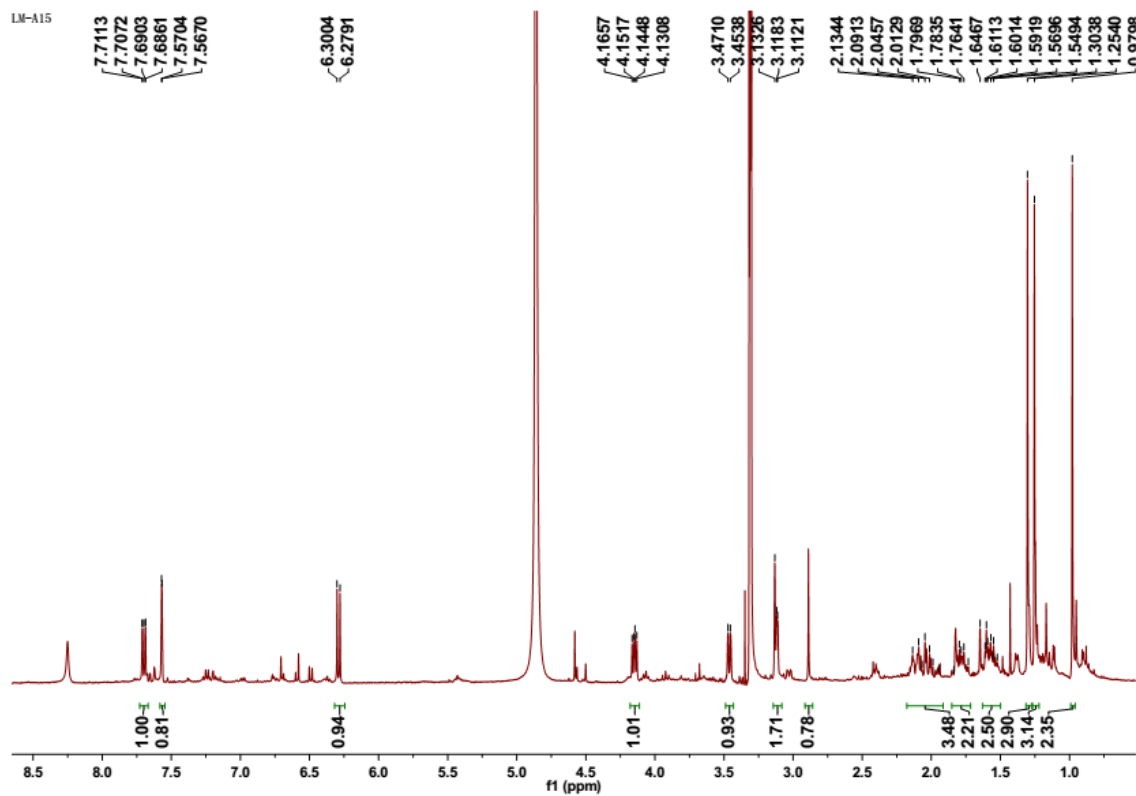


Figure S28. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound **4**

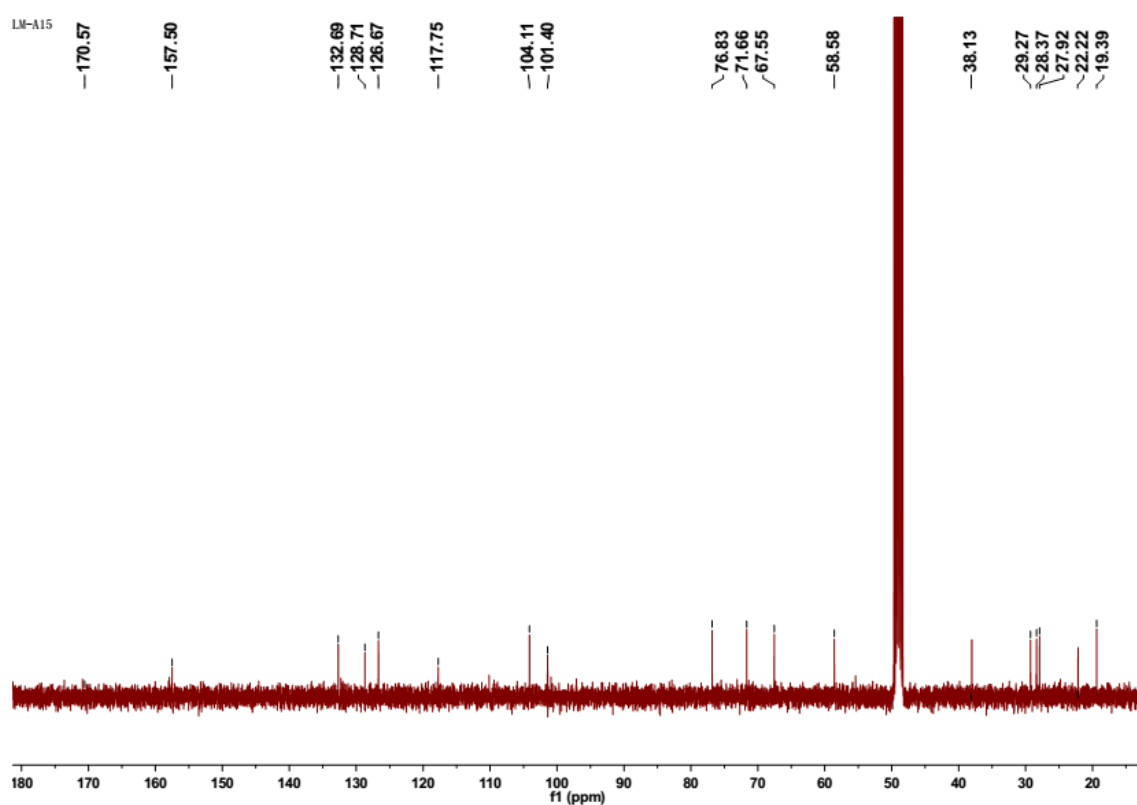


Figure S29. The HSQC spectrum for compound **4**

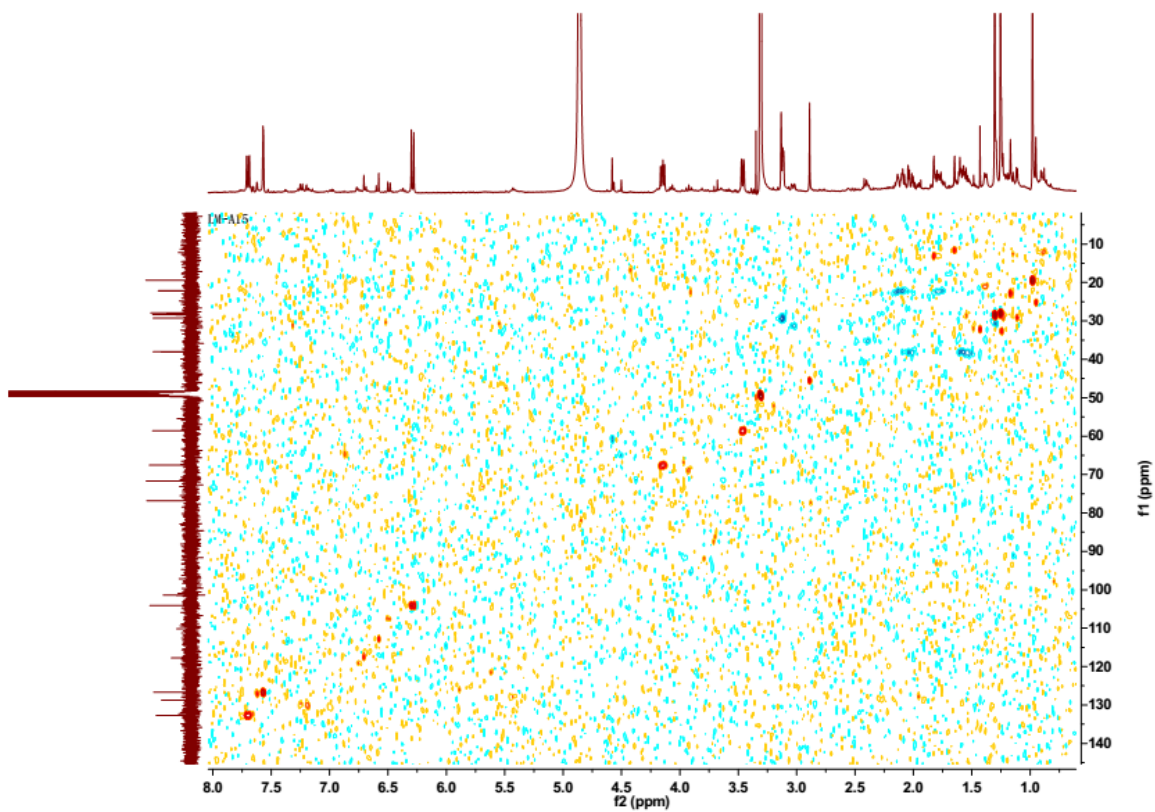


Figure S30. The HMBC spectrum for compound 4

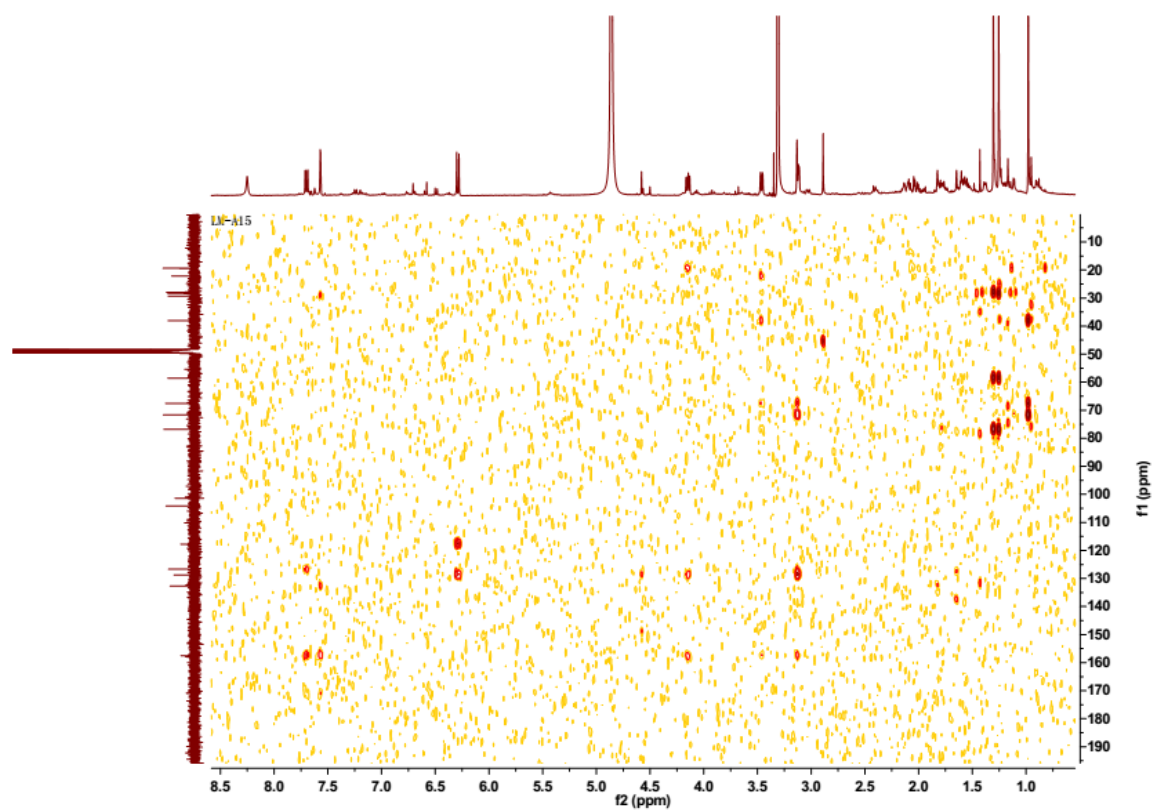


Figure S31. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 4

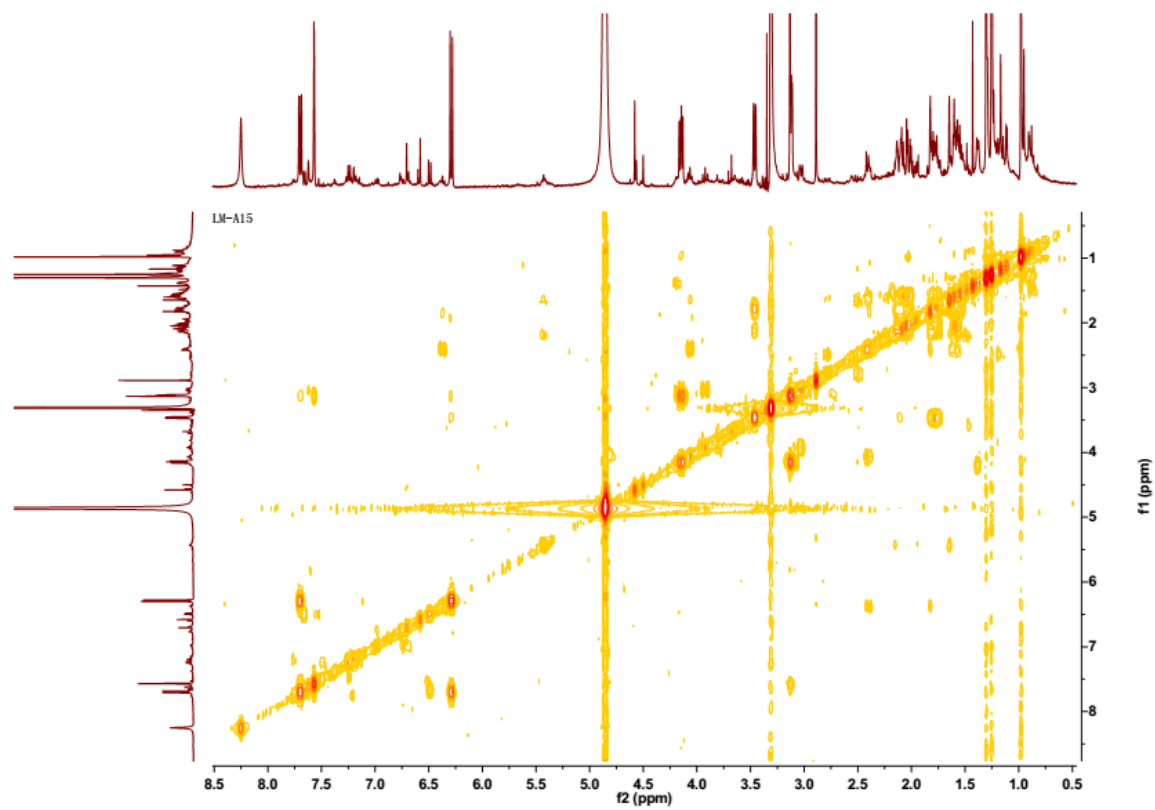


Figure S32. NOESY spectrum for compound **4**

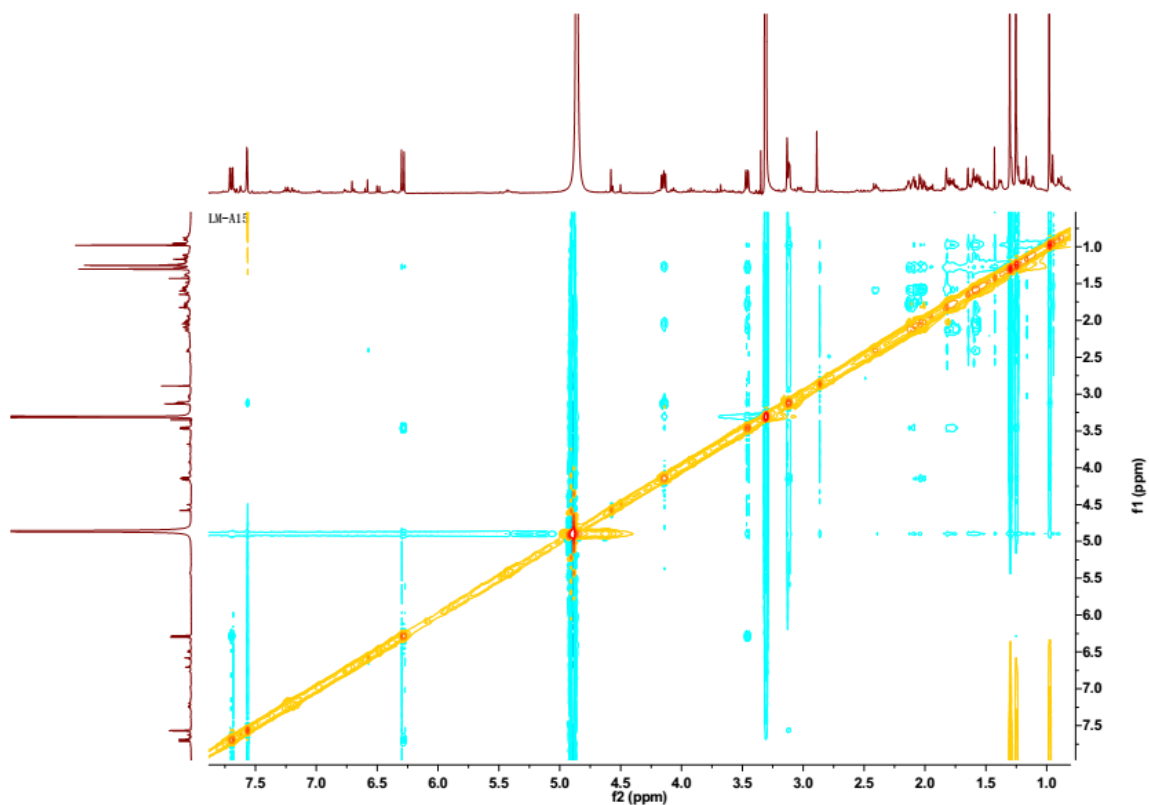


Figure S33. The HRMS-ESI spectrum for compound **4**

20161228 Im A15 #11-17 RT: 0.27-0.43 AV: 7 NL: 1.47E7
T: FTMS + p ESI Full ms [160.00-600.00]

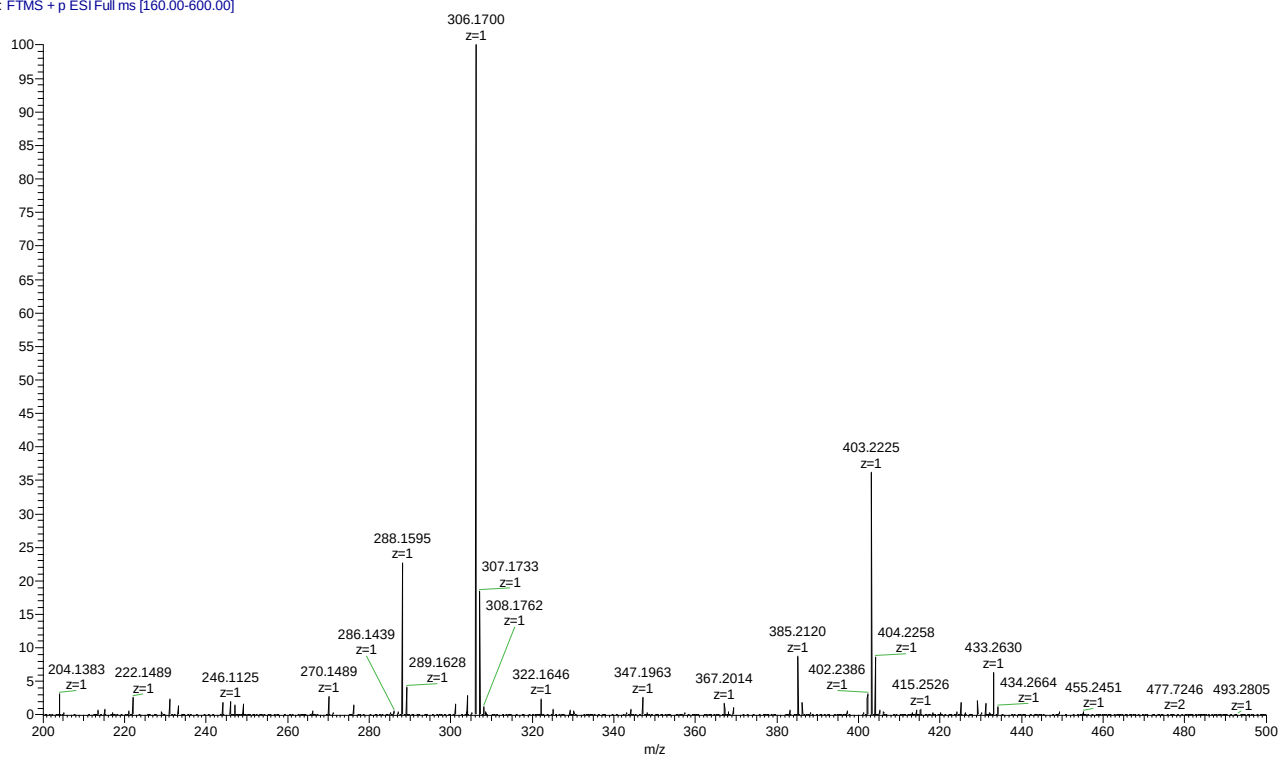


Figure S34. ^1H NMR (400 MHz, CD_3OD) spectrum for compound **5**

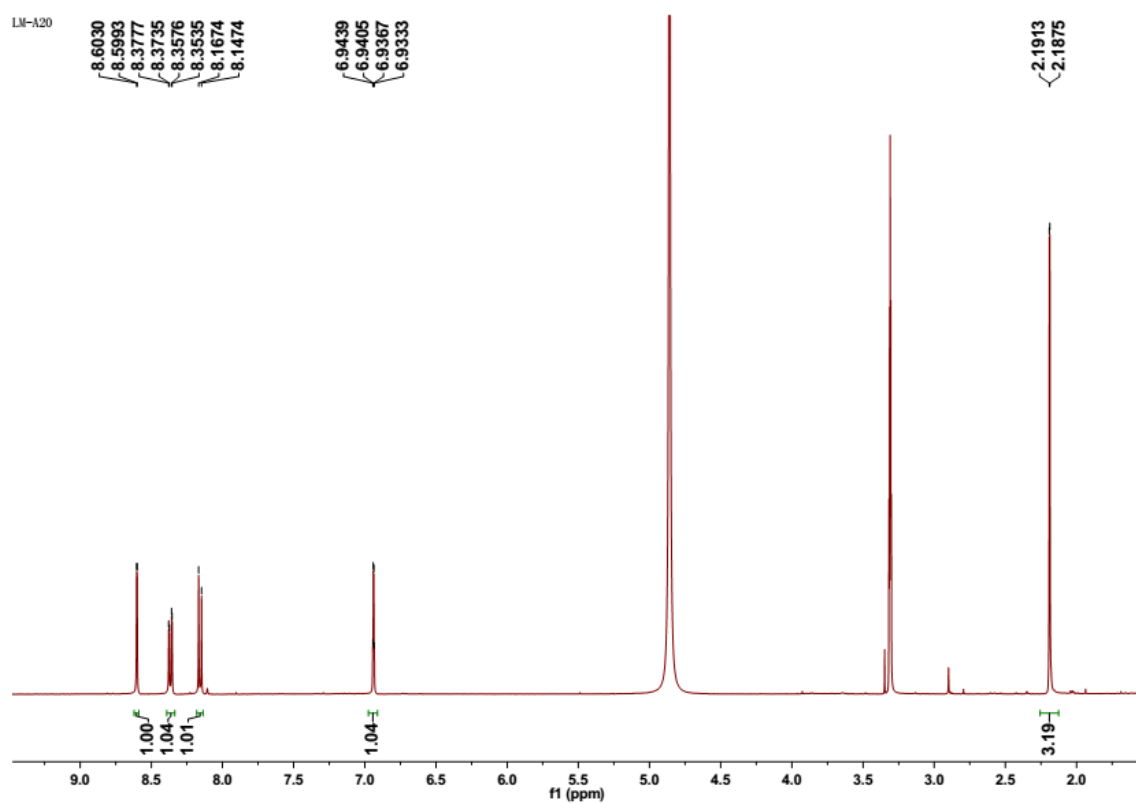


Figure S35. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound **5**

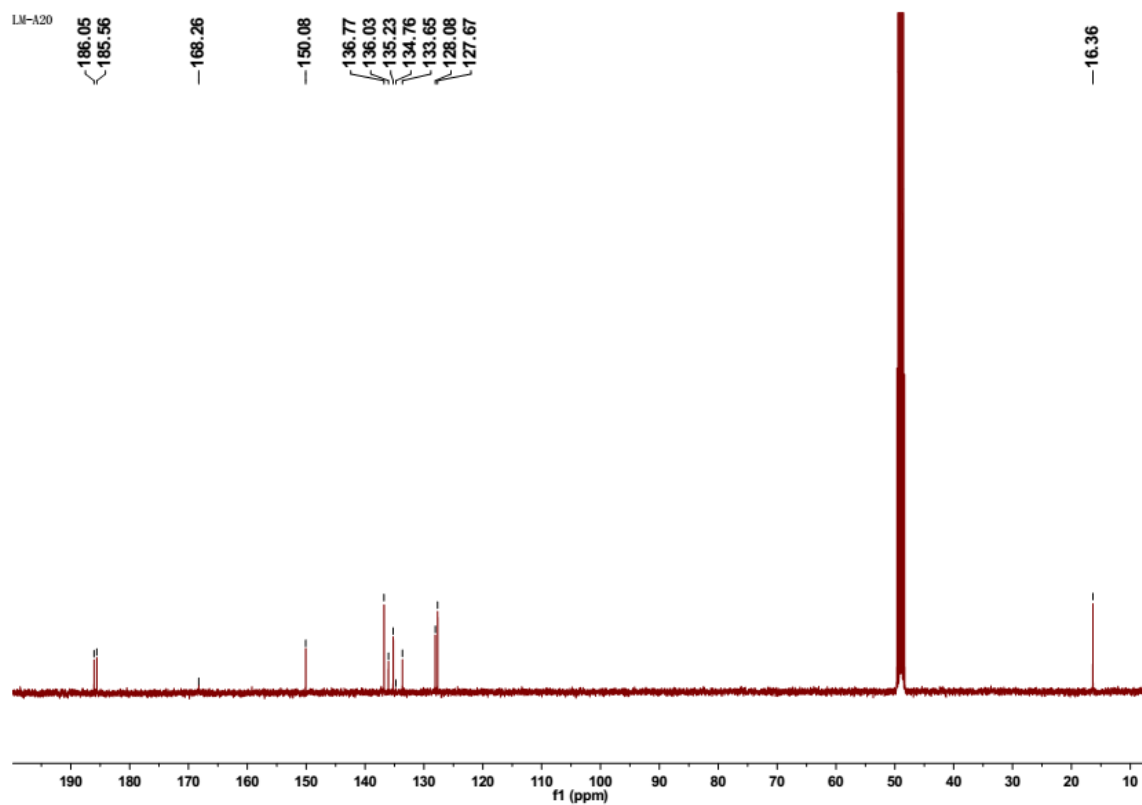


Figure S36. The HSQC spectrum for compound **5**

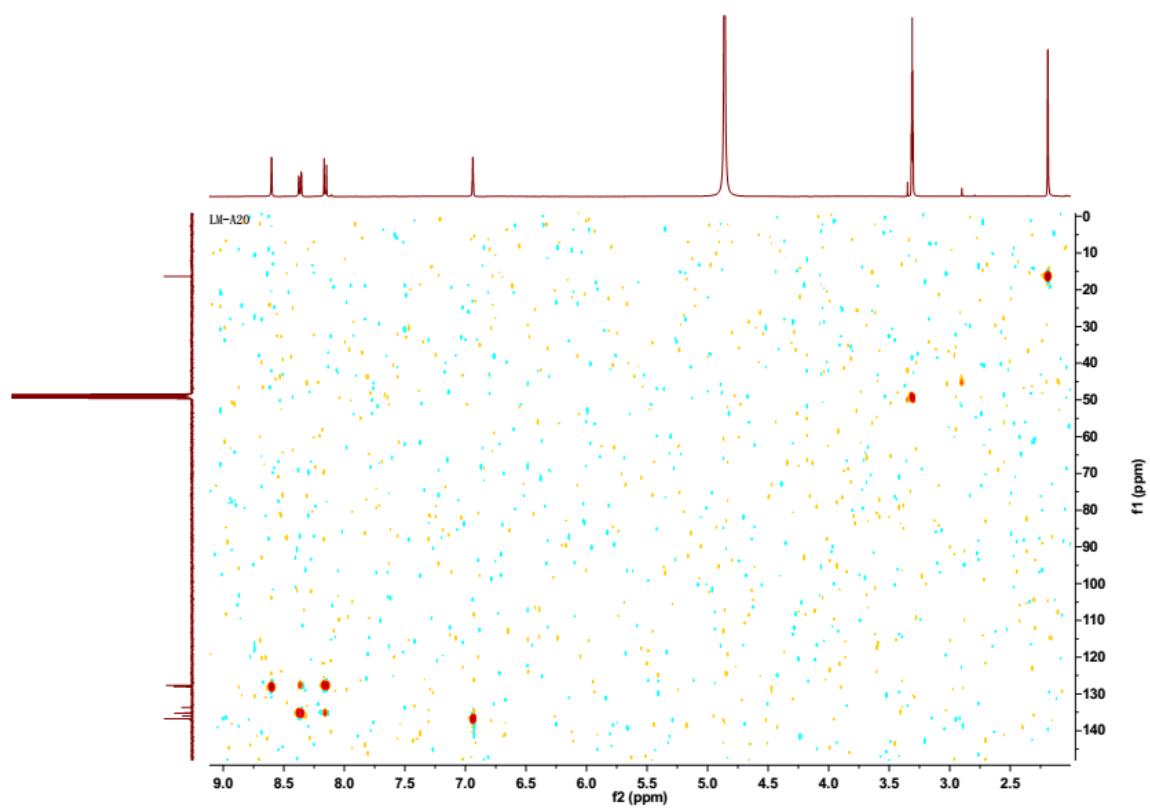


Figure S37 The HMBC spectrum for compound **5**

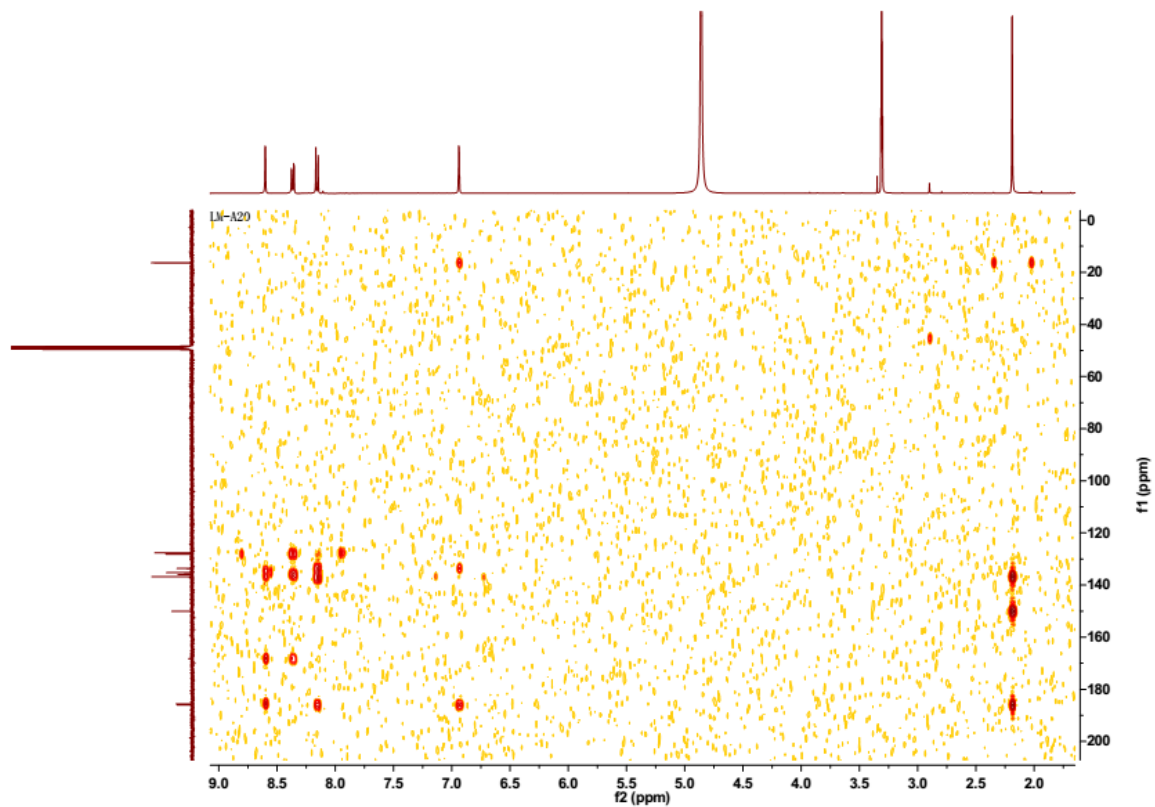


Figure S38. $^1\text{H}/^1\text{H}$ COSY spectrum for compound **5**

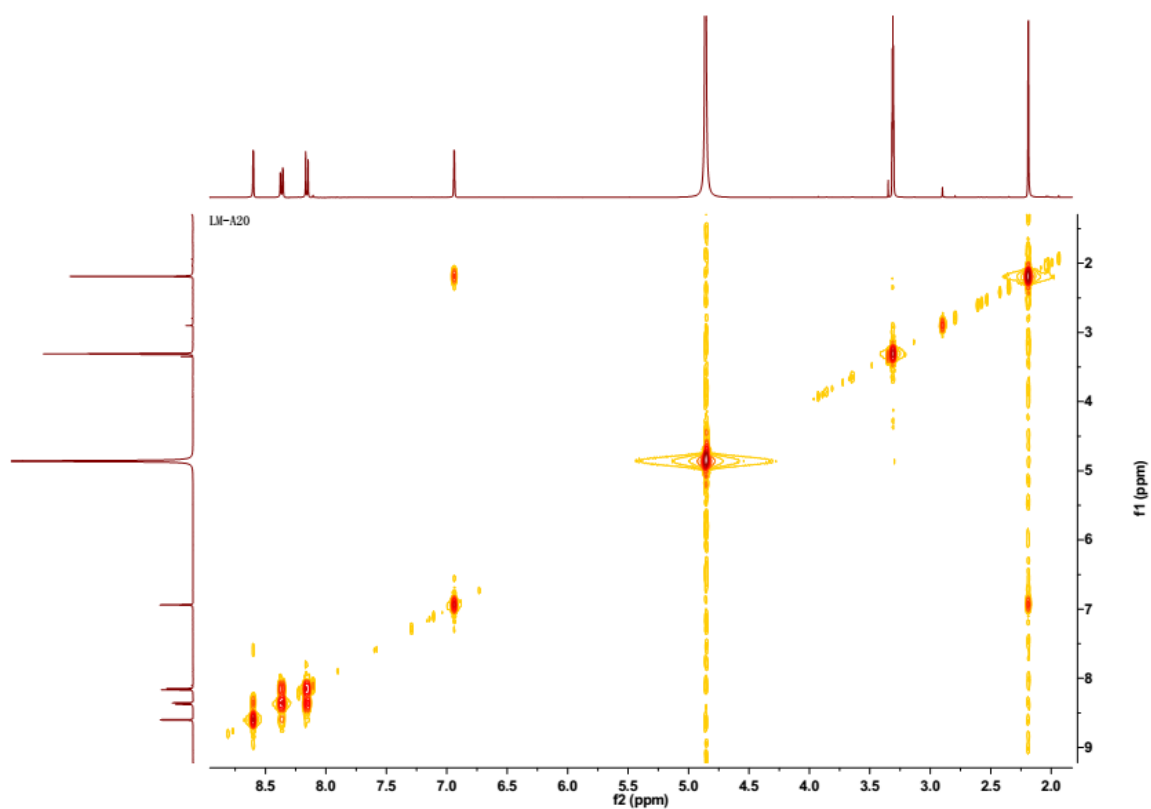


Figure S39. The HRMS-ESI spectrum for compound **5**

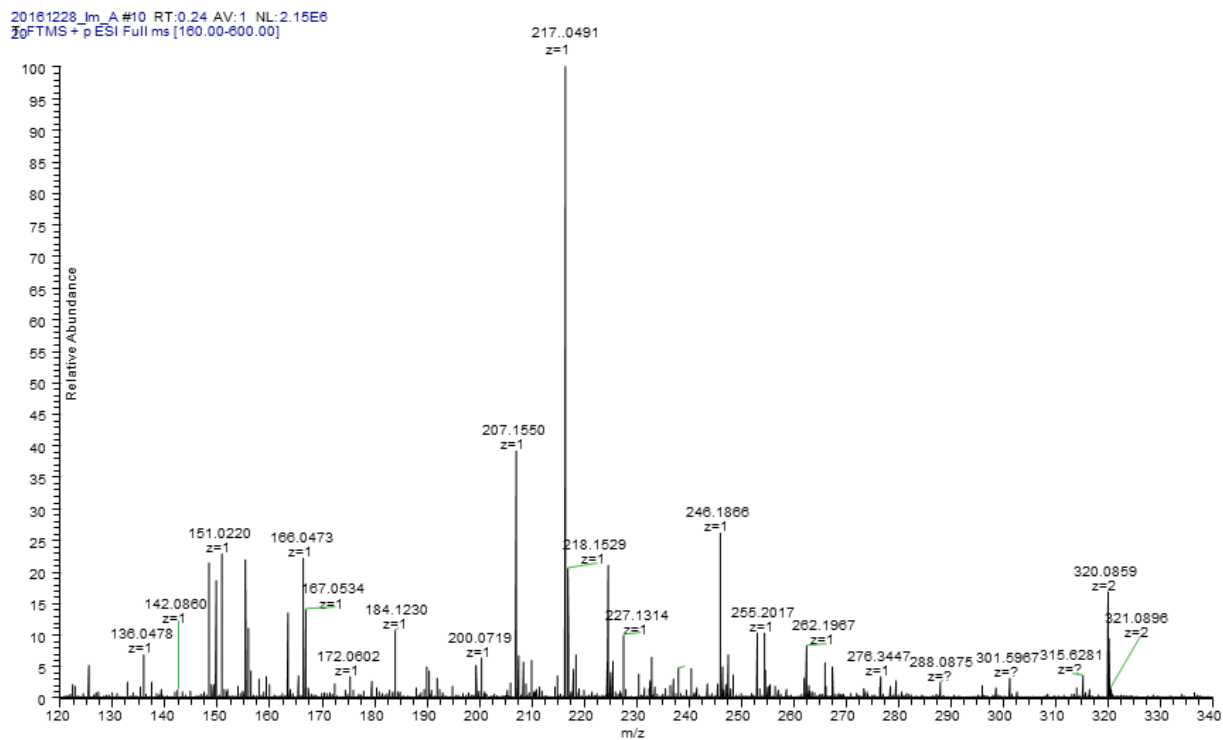


Figure S40. ^1H NMR (400 MHz, CD_3OD) spectrum for compound 6

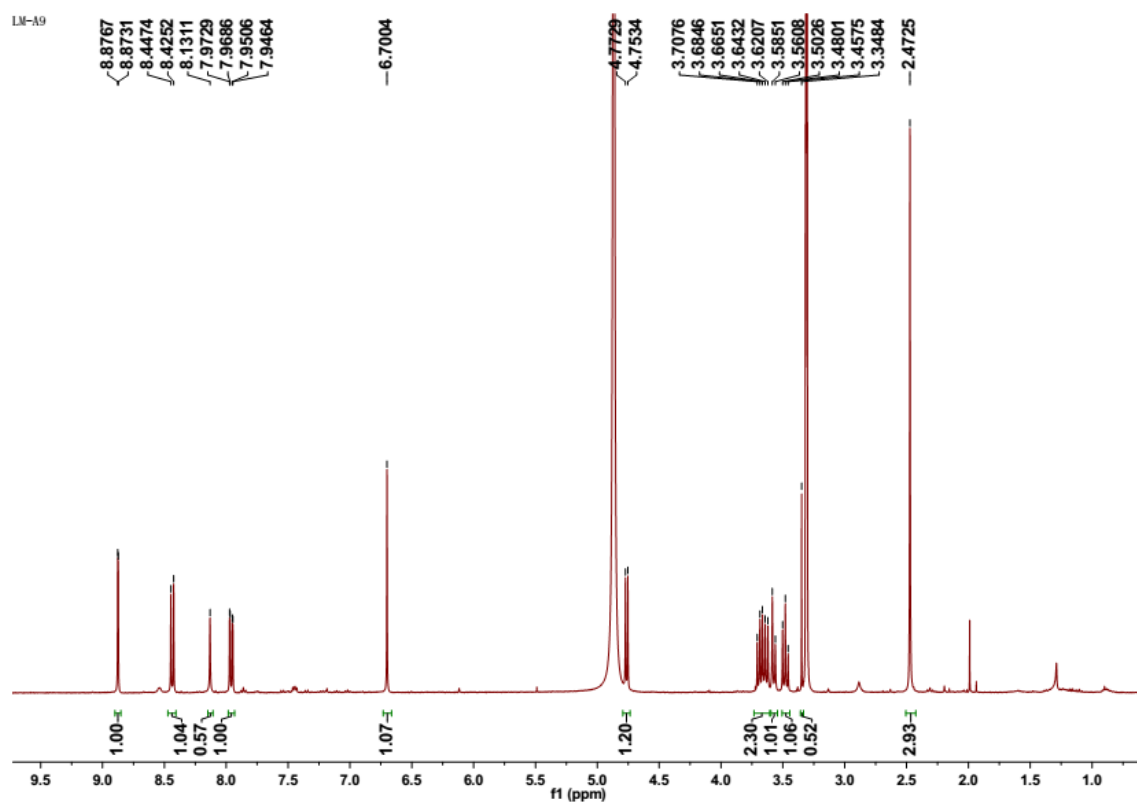


Figure S41. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound 6

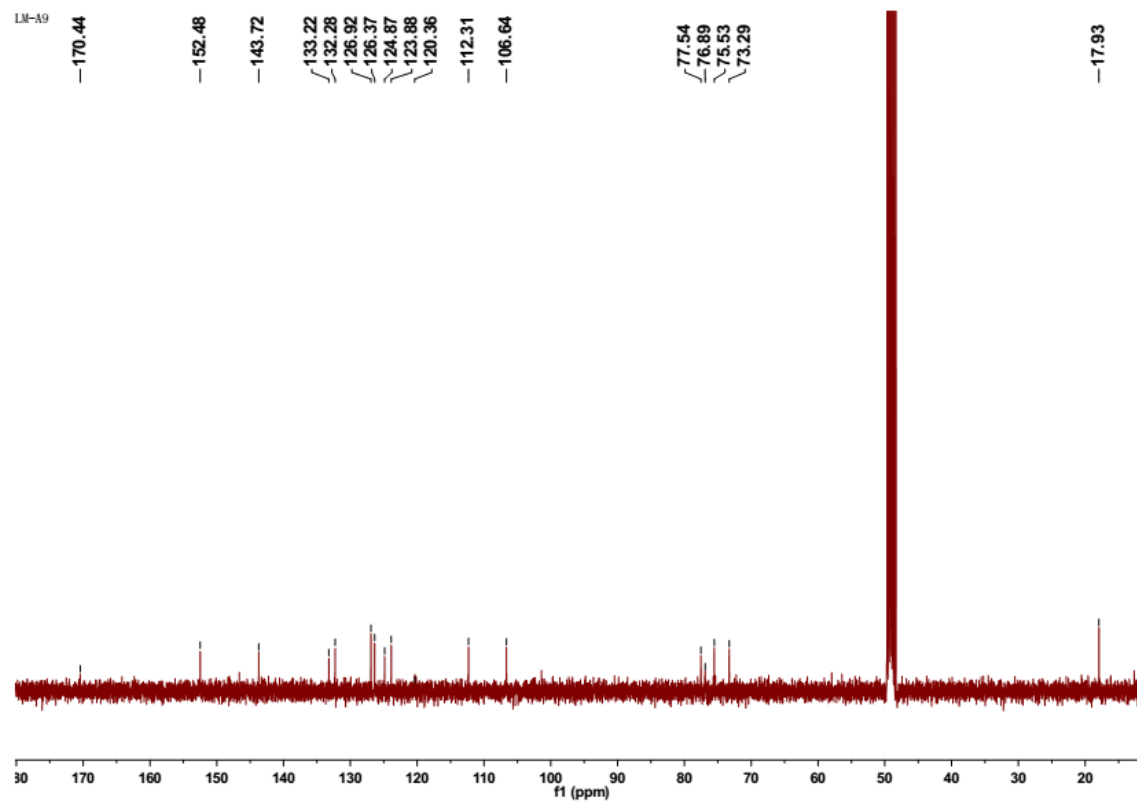


Figure S42. The HSQC spectrum for compound 6

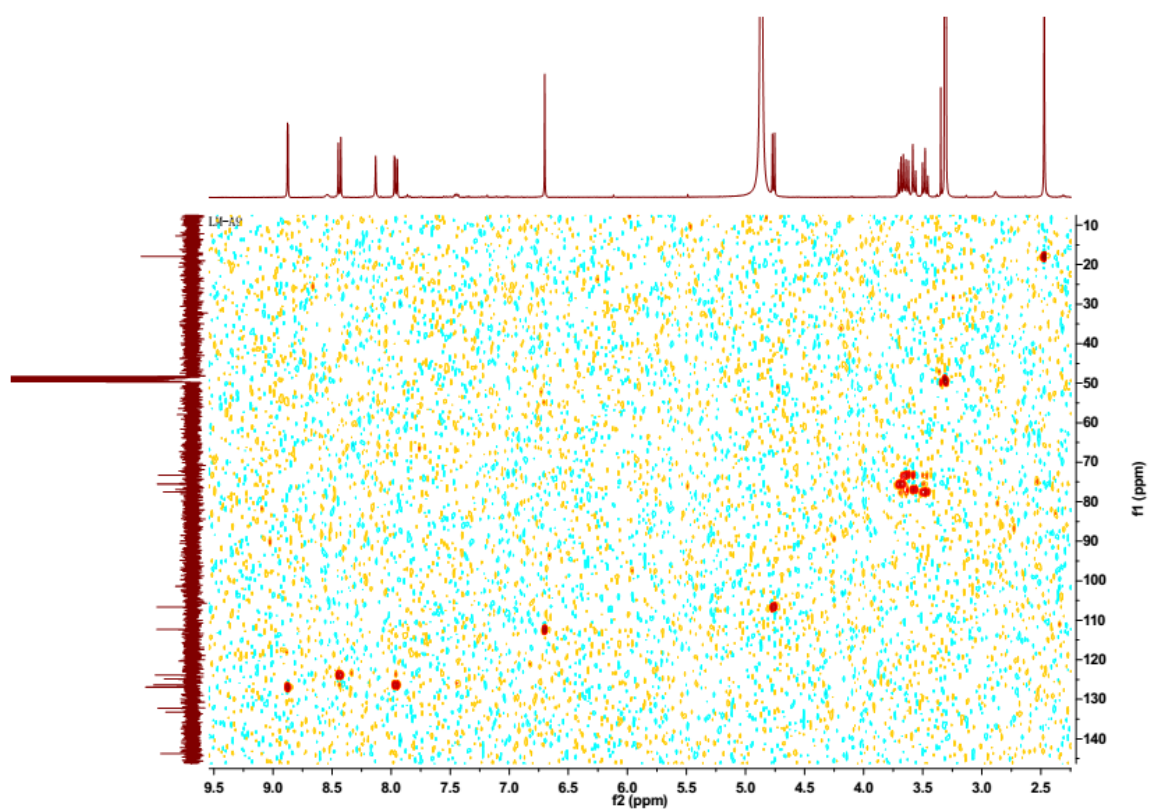


Figure S43. The HMBC spectrum for compound 6

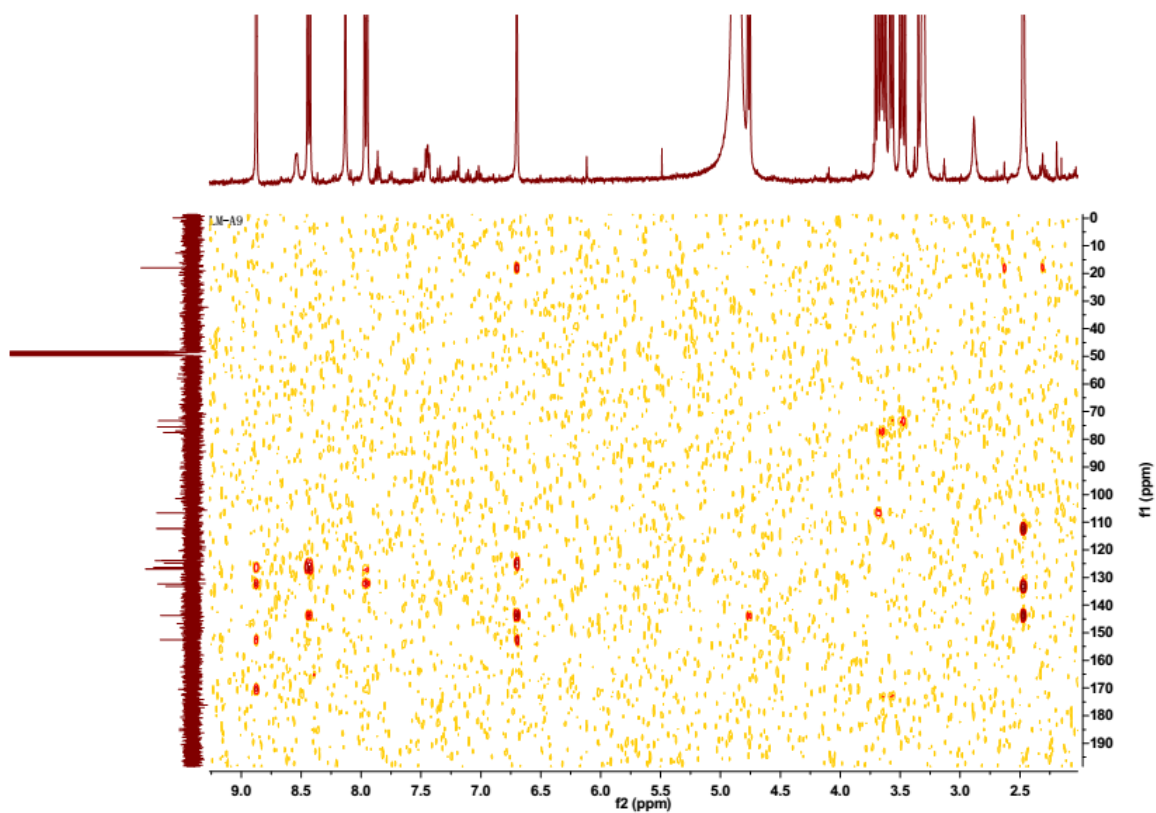


Figure S44. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 6

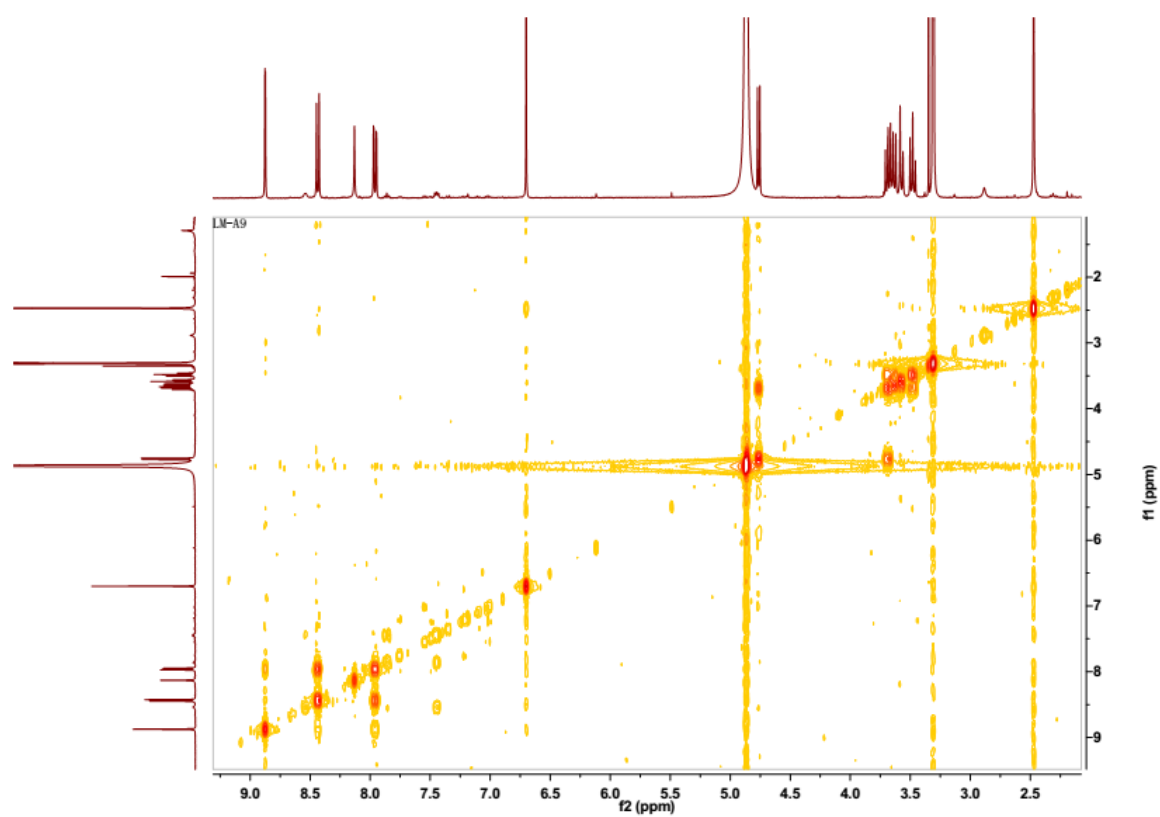


Figure S45. NOESY spectrum for compound 6

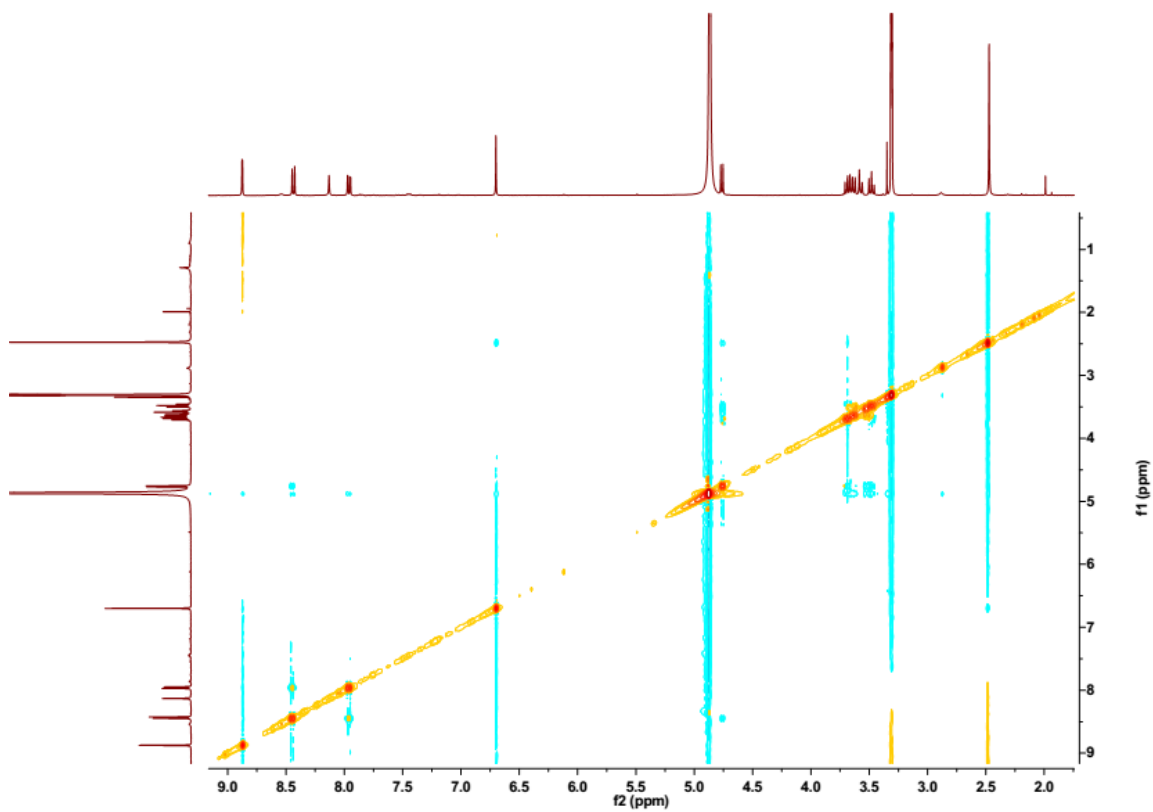


Figure S46. The HRMS-ESI spectrum for compound **6**

20161228_lm_A9_161228145300 #10 RT: 0.24 AV: 1 NL: 1.82E6
T: FTMS + p ESI Full ms [160.00-600.00]

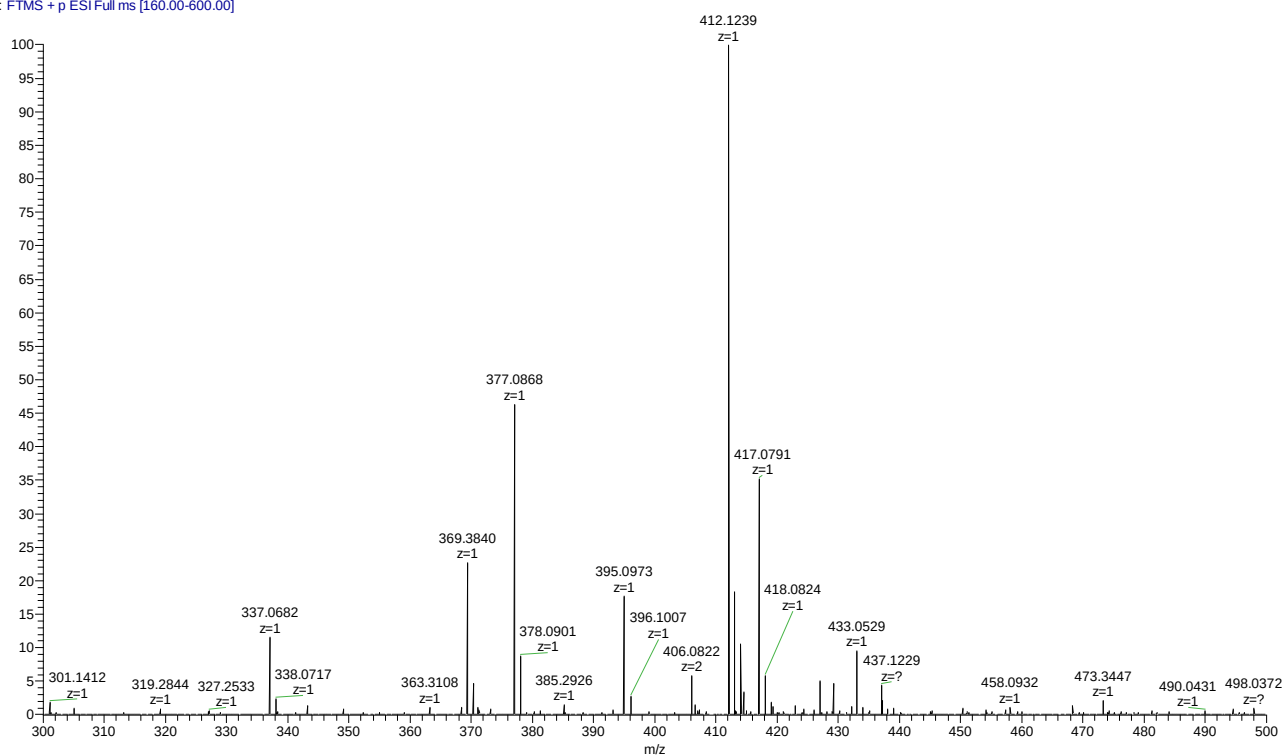


Figure S47. ^1H NMR (400 MHz, CD_3OD) spectrum for compound **7**

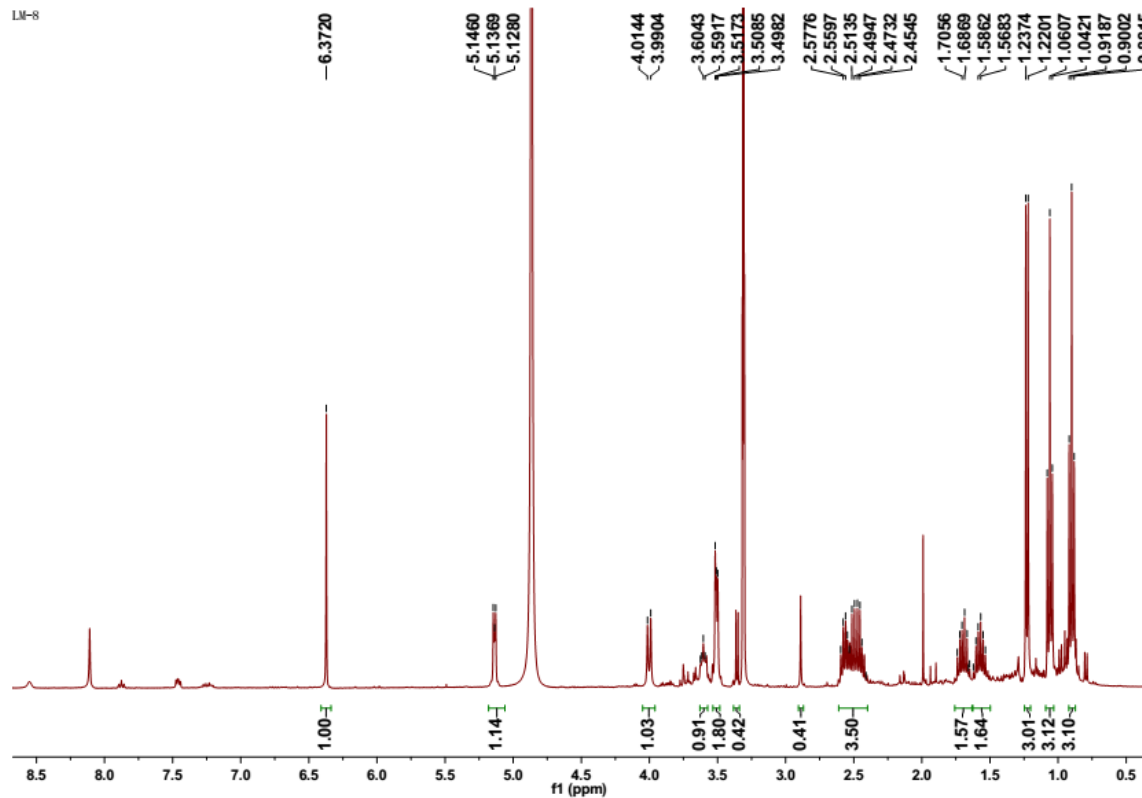


Figure S48. ^{13}C NMR (100 MHz, CD_3OD) spectrum for compound 7

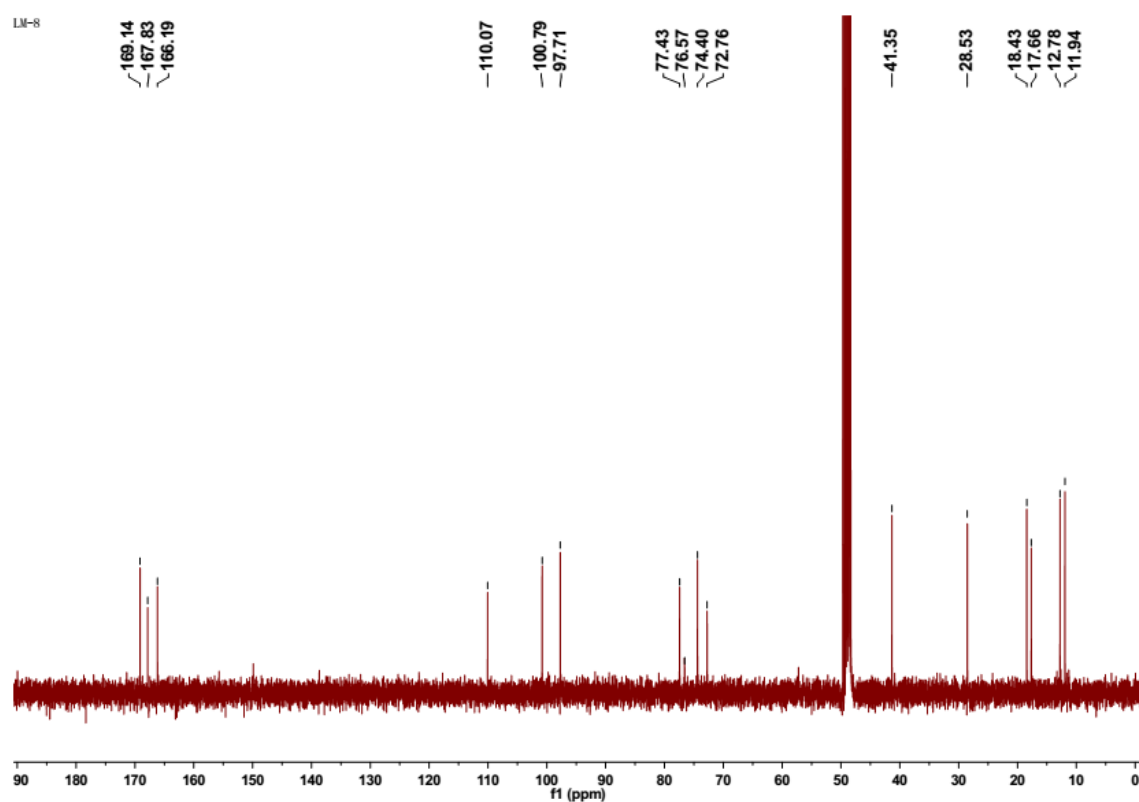


Figure S49 The HSQC spectrum for compound 7

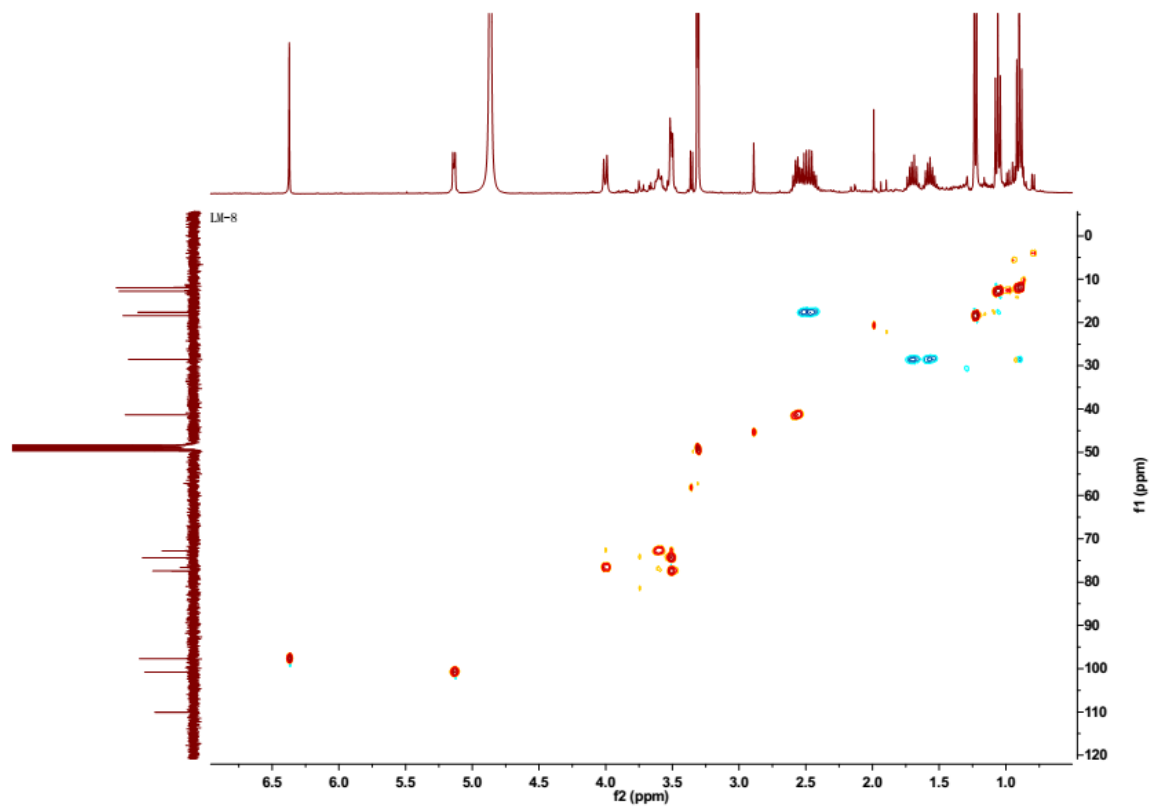


Figure S50. The HMBC spectrum for compound 7

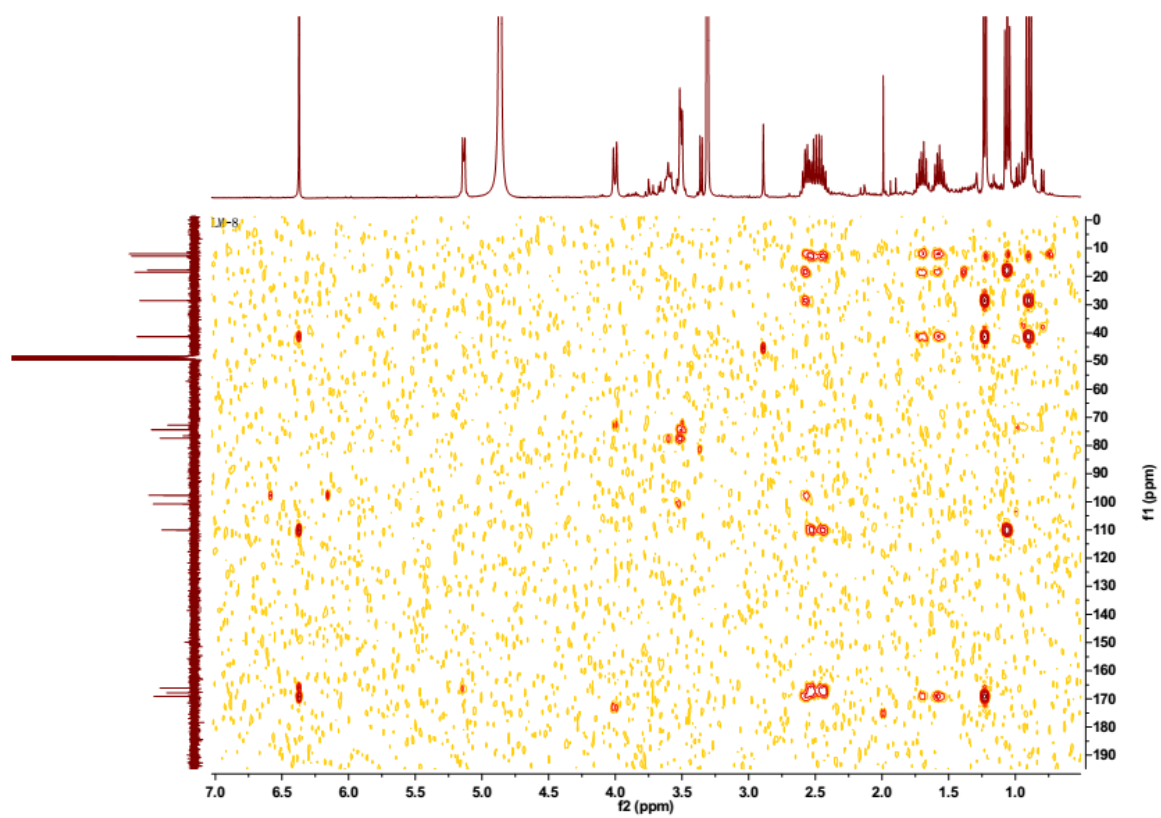


Figure S51. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 7

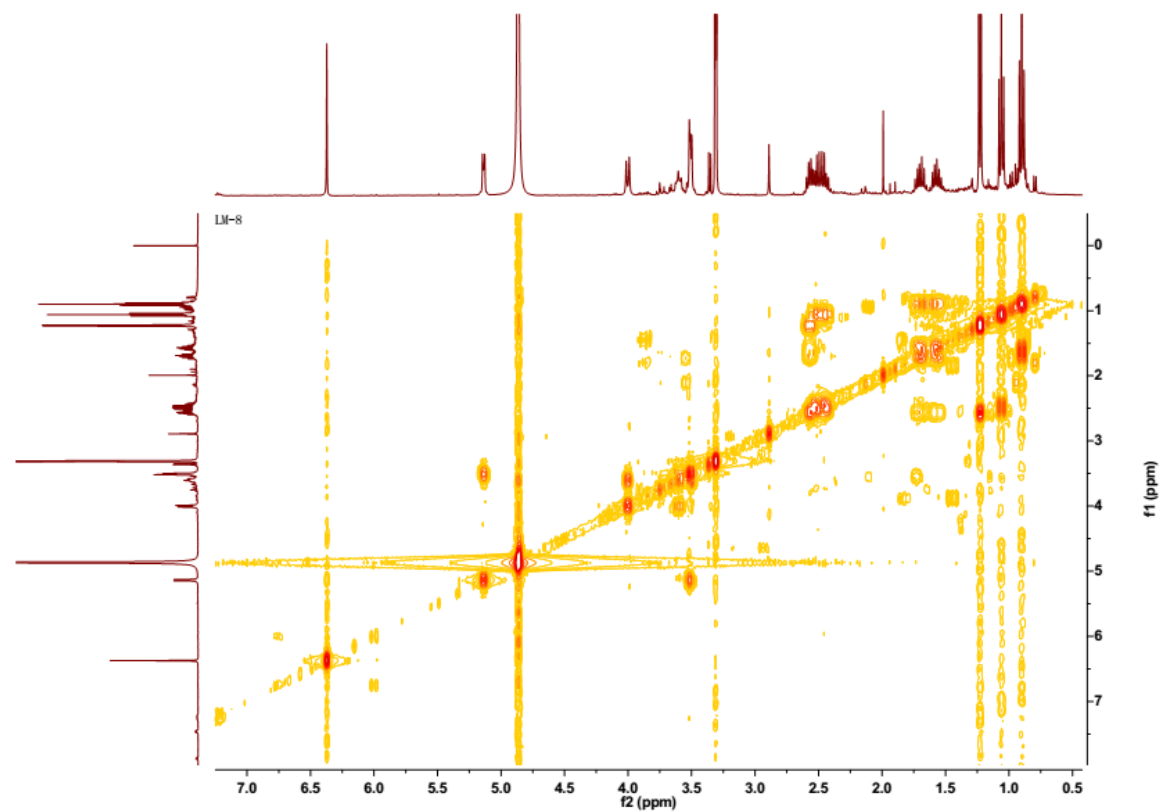


Figure S52. NOESY spectrum for compound **7**

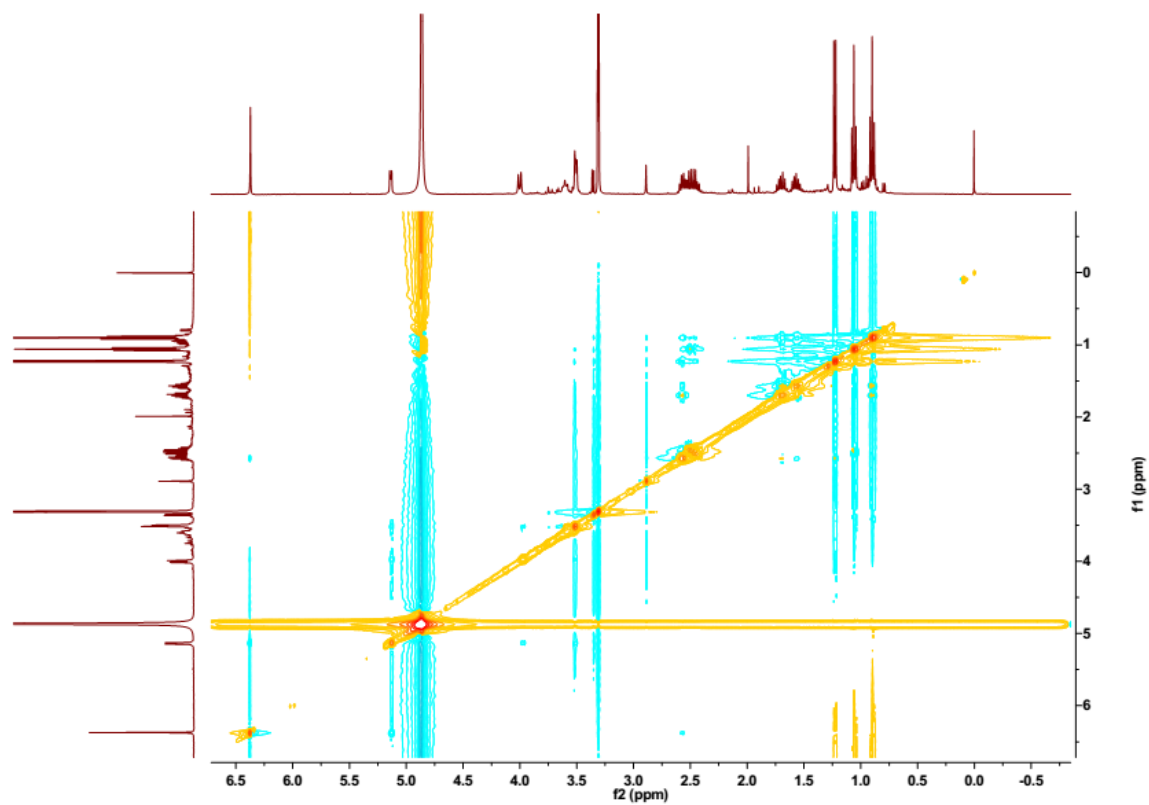


Figure S53. The HRMS-ESI spectrum for compound **7**

