

Supporting information for

Neoansamycins from *Streptomyces* sp. LZ35

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NMR data

Table S1: NMR spectroscopy data for neoansamycin D (in CD₃OD).

Pos.	δ_C , type	δ_H , Mult (J, Hz)	¹ H- ¹ H COSY	HMBC	NOESY
1	194.2, C				
2	70.0, C				
3	49.9, CH ₂	2.46, d (9.4) 2.72, d (10.9)	H-19	C-1, C-2, C-4, C-5, C-18	
4	89.9, C				
5	157.1, C				
6	119.0, C				
7	129.3, CH	7.75, d (8.4)	H-8	C-1, C-4, C-5, C-6, C-9	
8	119.3, CH	6.96, d (8.4)	H-7	C-6, C-9, C-11	
9	159.1 C				
10	118.6, C				
11	150.3, C				
12	118.7, C				
13	30.0, CH ₂	2.12, m 2.91, m	H-14	C-11, C-12, C-14	
14	25.14, CH ₂	1.68, m 1.98, m	H-13, H-15		
15	32.4, CH ₂	1.43, m 2.04, m	H-14, H-16		
16	88.7, CH	5.02, d (6.0)	H-15	C-14, C-15, C-16a	
17	215.9, C				
18	61.9, C				
19	60.6, CH	2.25, d (9.8)	H-20	C-1, C-2, C-3, C-4, C-18, C-20, C-20a	H-18a, H-20a
20	46.8, CH	2.66, m	H-19, H-20a	C-20a, C-20b, C-21	
21	180.4, C				
12a	25.08, CH ₂	2.49, m 2.86, m	H-12b	C-11, C-12, C-12b, C-13	
12b	15.3, CH ₃	1.12, t (7.3)	H-12a	C-12, C-12a	
16a	58.8, CH ₃	3.37, s		C-16	
18a	31.2, CH ₃	1.08, s		C-4, C-18	H-19
20a	31.8, CH ₂	1.91, m	H-20, H-20b	C-20b, C-20c	
20b	27.2, CH ₂	1.55, m	H-20a, H-20c		
20c	30.7, CH ₂	1.32, m		C-20e	
20d	23.7, CH ₂	1.29, m		C-20c	
20e	32.9, CH ₂	1.33, m	H-20f	C-20f	
20f	14.4, CH ₃	0.91, t (6.7)	H-20e	C-20d, C-20e	

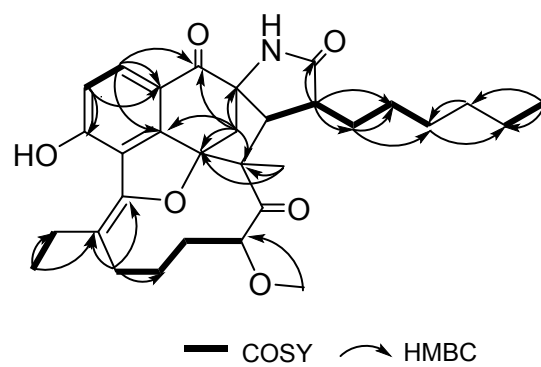


Fig S1: Selected ^1H - ^1H COSY and HMBC correlations for neoansamycin D.

Table S2: NMR spectroscopy data for neoansmycin E (in CD₃OD).

Pos.	δ_C , type	δ_H , Mult (J, Hz)	¹ H- ¹ H COSY	HMBC
1	195.3, C			
2	70.1, C			
3	51.3, CH ₂	2.29, d (9.6) 3.05, d (10.8)		C-1, C-2, C-4, C-5, C-18
4	95.2, C			
5	156.9, C			
6	119.2, C			
7	131.8, CH	7.86, d (8.4)	H-8	C-1, C-4, C-5, C-6, C-9, C-10
8	119.0, CH	6.96, d (8.4)	H-7	C-6, C-10
9	161.4, C			
10	121.6, C			
11	209.5, C			
12	49.6, CH	2.21, t (6.9)	H-12a, H-13	C-10, C-11, C-12a, C-12b
13	29.8, CH ₂	2.01, m	H-12, H-14	C-12
14	26.0, CH ₂	1.62, m	H-13	
15	30.0, CH ₂	1.95, m	H-16	C-16
16	92.5, CH	4.26, br s	H-15	
17	214.2, C			
18	60.1, C			
19	61.2, CH	2.27, d (8.4)	H-20	C-1, C-2, C-3, C-18, C-18a, C-20, C-20a
20	45.6, CH	2.75, m	H-19, H-20a	C-18, C-20b, C-21
21	180.7, C			
12a	24.6, CH ₂	2.52, m	H-12, H-12b	C-10, C-12, C-12b, C-13
12b	13.2, CH ₃	0.93, t (7.8)	H-12a	C-12, C-12a
16a	58.4, CH ₃	3.37, s		C-16
18a	25.4, CH ₃	1.41, s		C-4, C-17, C-19
20a	31.5, CH ₂	1.70, m	H-20, H-20b	C-20b, C-21
20b	26.8, CH ₂	1.27, m	H-20a	C-20d
20c	23.5, CH ₂	1.45, m	H-20b	
20d	33.3, CH ₂	1.29, m		C-20b
20e	23.6, CH ₂	1.30, m	H-20f	C-20f
20f	14.4, CH ₃	0.91, t (6.0)	H-20e	C-20d, C-20e

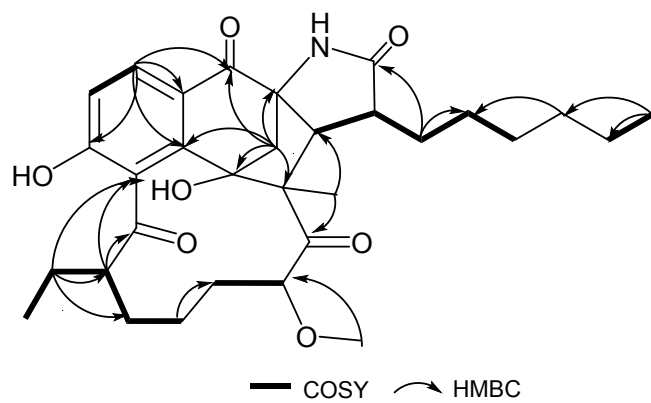


Fig S2: Selected ^1H - ^1H COSY and HMBC correlations for neoansamycin E.

Table S3: NMR spectroscopy data for neoansamycin F (in DMSO-*d*₆).

Pos.	δ_c , type	δ_H , Mult (J, Hz)	¹ H- ¹ H COSY	HMBC	NOESY
1	190.3, C				
2	73.9, C				
3	91.2, C				
4	94.9, C				
5	153.0, C				
6	116.3, C				
7	128.2, CH	7.64, d (8.4)	H-8	C-5, C-9	
8	109.0, CH	7.01, d (8.2)	H-7	C-10	
9	158.7, C				
10	117.9, C				
11	149.5, C				
12	115.7, C				
13	28.4, CH ₂	2.00, m 2.80, m	H-14	C-11, C-12, C-15	
14	24.5, CH ₂	1.59, m 1.80, m	H-13		
15	30.4, CH ₂	1.19, m 1.93, t (13.9)	H-16		
16	85.4, CH	4.81, d (8.0)	H-15	C-14, C-15, C-16a	
17	211.1, C				
18	57.7, C				
19	56.5, CH	2.04, d (9.6)	H-20		H-18a
20	44.6, CH	2.64, m	H-19, H-20a		
21	178.7, C				
12a	23.3, CH ₂	2.48, m 2.75, m	H-12b	C-11, C-12, C-12b	
12b	14.9, CH ₃	1.06, t (7.3)	H-12a	C-12, C-12a	
16a	56.7, CH ₃	3.11, s		C-16	
18a	31.1, CH ₃	0.95, s		C-4, C-17, C-19	H-19, H-20a
20a	30.9, CH ₂	1.19, m 1.72, m	H-20		
20b	25.3, CH ₂	1.19, m 1.51, m	H-20a, H-20c		
20c	29.1, CH ₂	1.23, m	H-20b		
20d	31.7, CH ₂	1.22, m			
20e	22.1, CH ₂	1.28, m	H-20f		
20f	14.0, CH ₃	0.86, t (7.1)	H-20e	C-20d, C-20e	
N-H		8.63, s		C-2, C-19, C-20	

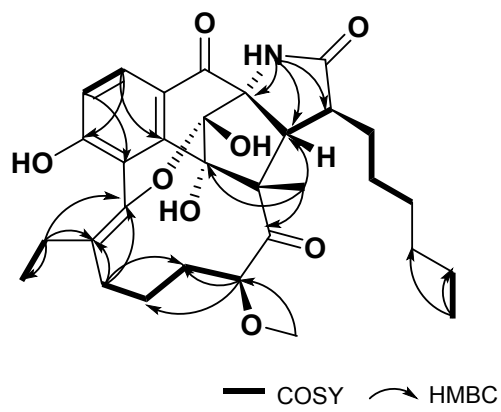


Fig S3: Selected ^1H - ^1H COSY and HMBC correlations for neoansamycin F.

Table S4: NMR spectroscopy data for neoansamycin G (in CD₃OD).

Pos.	δ_C , type	δ_H , Mult (J, Hz)	¹ H- ¹ H COSY	HMBC
1	194.4, C			
2	70.2, C			
3	50.1, CH ₂	2.46, d (10.9) 2.76, d (10.9)		C-1, C-2, C-4, C-5, C-18
4	90.1, C			
5	156.71, C			
6	121.4, C			
7	129.6, CH	7.89, d (8.6)	H-8	C-1, C-5, C-9
8	117.2, CH	7.33, d (8.7)	H-7	C-9, C-10, C-11
9	156.72, C			
10	121.8, C			
11	149.8, C			
12	120.9, C			
13	30.5, CH ₂	2.16, m		
14	25.1, CH ₂	2.01, m	H-15	
15	32.4, CH ₂	1.47, m	H-14	C-13, C-16
16	88.7, CH	5.00, d (7.4)	H-15	C-14, C-16a, C-18a
17	215.9, C			
18	61.9, C			
19	60.7, CH	2.28, d (10.0)	H-20	C-1, C-2, C-16, C-18, C-20, C-20a
20	46.9, CH	2.68, m	H-19, H-20a	C-18, C-21
21	180.4, C			
12a	25.6, CH ₂	2.61, m 2.72, m	H-12b	C-11, C-12, C-12b, C-13
12b	15.0, CH ₃	1.19, t (7.4)	H-12a	C-12, C-12a
16a	58.9, CH ₃	3.38, s		C-16
18a	31.2, CH ₃	1.09, s		C-4, C-19
20a	31.9, CH ₂	1.89, m	H-20, H-20b	
20b	27.0, CH ₂	1.29, m		C-20d
20c	33.4, CH ₂	1.37, m		
20d	23.7, CH ₂	1.32, m	H-20e	C-20c
20e	14.4, CH ₃	0.92, t (7.1)	H-20d	C-20c, C-20d
1'	101.0, CH	5.42, d (7.6)	H-2'	C-9
2'	74.3, CH	3.63, m	H-1', H-3'	C-1', C-3'
3'	77.8, CH	3.55, m	H-2', H-4'	C-2', C-4'
4'	72.7, CH	3.67, m	H-5'	C-5', C-6'
5'	76.9, CH	4.18, d (9.6)	H-4'	C-1', C-3', C-4', C-6'
6'	170.7, C			
7'	53.0, CH ₃	3.77, s		C-6'

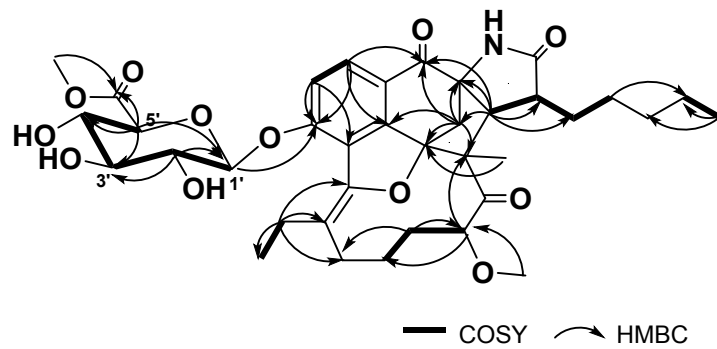


Fig S4: Selected ^1H - ^1H COSY and HMBC correlations for neoansamycin G.

Table S5: NMR spectroscopy data for neoansamycin H (in CD₃OD).

Pos.	δ_C , type	δ_H , Mult (J, Hz)	¹ H- ¹ H COSY	HMBC	NOESY
1	194.2, C				
2	69.7, C				
3	52.2, CH ₂	2.83, d (10.2) 3.10, d (11.7)	H-19	C-1, C-2, C-4, C-5, C-10	
4	84.6, C				
5	150.7, C				
6	121.3, C				
7	138.0, CH	8.29, d (8.6)	H-8	C-1, C-5, C-9	
8	119.9, CH	7.15, d (8.7)	H-7	C-6, C-10	
9	166.7, C				
10	114.3, C				
11	203.8, C				
12	85.8, C				
13	26.5, CH ₂	1.49, m		C-12	
14	19.8, CH ₂	1.83, m 2.00, m	H-15, H-16		
15	35.1, CH ₂	2.05, m	H-14		
16	87.1, CH	4.79, d (9.0)	H-15	C-15, C-16a	
17	214.8, C				
18	63.0, C				
19	61.1, CH	2.10, m	H-20	C-1, C-2, C-3, C-4, C-18, C-18a, C-20, C-20a	H-18a
20	45.9, CH	2.82, m	H-20a	C-18, C-19, C-20a, C- 20b, C-21	
21	180.2, C				
12a	35.0, CH ₂	1.76, m 1.94, m	H-12b	C-11, C-12, C-12b	H-18a
12b	8.6, CH ₃	0.80, t (7.3)	H-12a	C-12, C-12a	
16a	57.5, CH ₃	3.39, s		C-16	
18a	27.5, CH ₃	0.96, s		C-4, C-18, C-19	H-19
20a	31.2, CH ₂	1.53, m	H-20		H-19
20b	26.6, CH ₂	1.27, m	H-20a		
20c	33.2, CH ₂	1.24, m			
20d	23.6, CH ₂	1.30, m	H-20e	C-20c, C-20e	
20e	14.5, CH ₃	0.89, t (6.7)	H-20d	C-20c, C-20d	

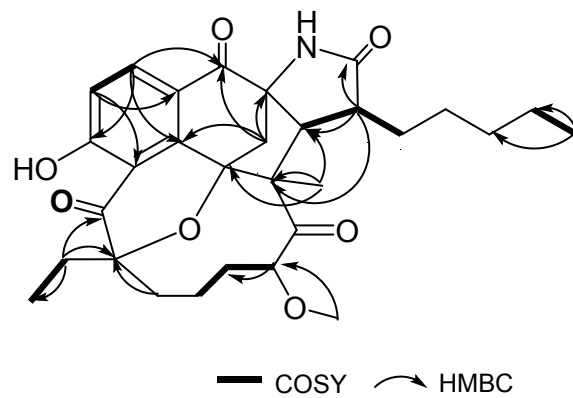


Fig S5: Selected ^1H - ^1H COSY and HMBC correlations for neoansamycin H.

Table S6: NMR spectroscopy data for neoansamycin I (in DMSO).

position	δ_C , type	δ_H , Mult (J, Hz)	1H - 1H COSY	HMBC
1	195.3, C			
2	71.2, C			
3	70.2, CH	3.11, s		C-1, C-2, C-4, C-17, C-18
4	195.1, C			
5	134.5, C			
6	129.3, C			
7	129.9, CH	7.85, d (8.6)	H-8	C-1, C-5
8	122.4, CH	7.22, d (8.6)	H-7	C-6, C-10
9	160.8, C			
10	124.5, C			
11	207.9, C			
12	53.5, CH	2.35, m	H-13	
13	29.6, CH ₂	1.51, m 1.78, m	H-12	
14	25.4, CH ₂	1.45, m	H-13	
15	30.5, CH ₂	1.21, m	H-16	
16	82.6, CH	3.24, d (8.3)	H-15	C-14, C-16a, C-17, C-18
17	88.8, C			
18	40.6, CH	2.16, m	H-18a	C-18a, C-19, C-20
19	56.6, CH	2.33, m	H-18, H-20	C-17
20	42.3, CH	2.68, m	H-19, H-20a	
21	178.2, C			
12a	27.1, CH ₂	1.46, m 2.00, m	H-12b	
12b	11.3, CH ₃	0.89, t (7.4)	H-12a	C-12, C-12a
16a	61.9, CH ₃	3.40, s		C-16
18a	10.2, CH ₃	0.92, d (6.8)	H-18	C-17, C-18, C-19
20a	32.6, CH ₂	1.49, m	H-20	
20b	24.4, CH ₂	1.19, m 1.26, m	H-20a, H-20c	
20c	31.4, CH ₂	1.22, m		
20d	22.0, CH ₂	1.25, m 1.28, m	H-20e	C-20c
20e	14.0, CH ₃	0.86, t (7.2)	H-20d	C-20c, C-20d
N-H		7.41, s		C-2, C-19, C-20

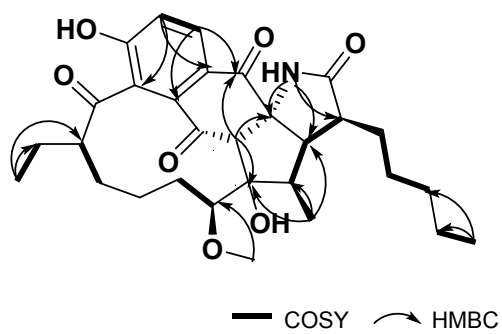


Fig S6: Selected ^1H - ^1H COSY and HMBC correlations for neoansamycin I.

Spectroscopic data informations

Figure S7. ^1H NMR (600 MHz, CD_3OD) spectrum for compound **1**

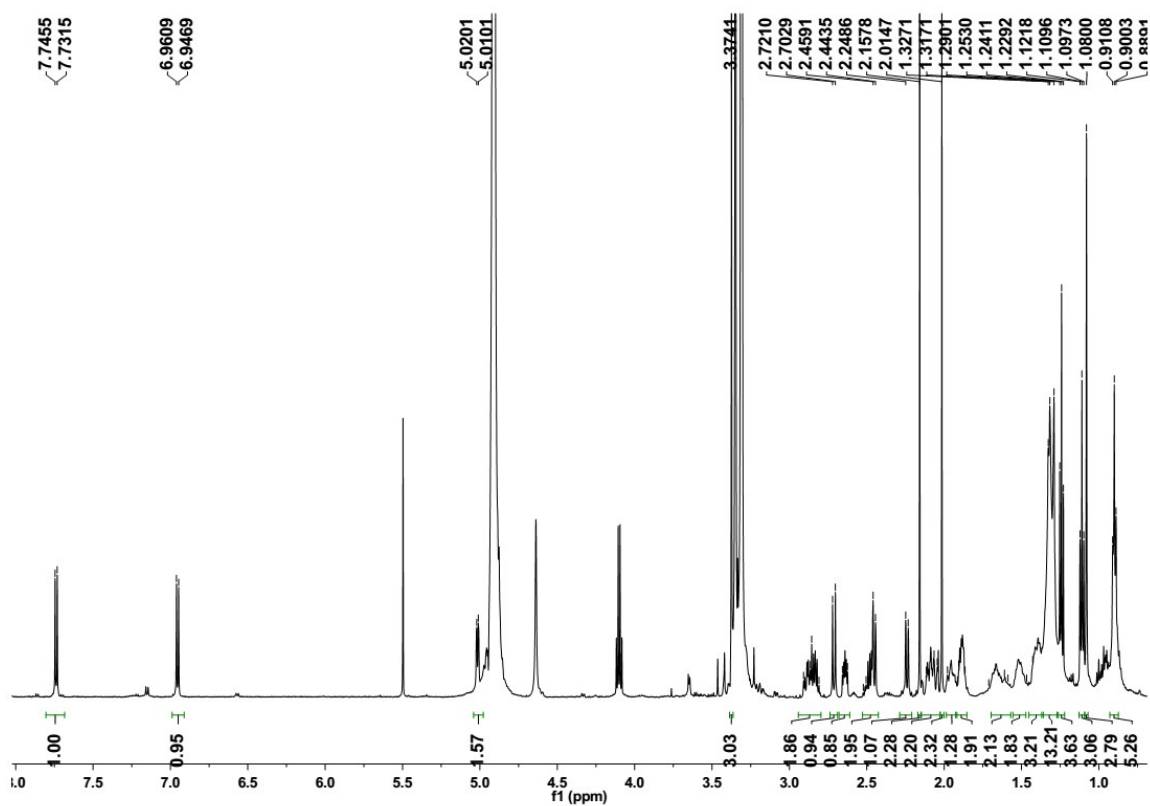


Figure S8. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **1**

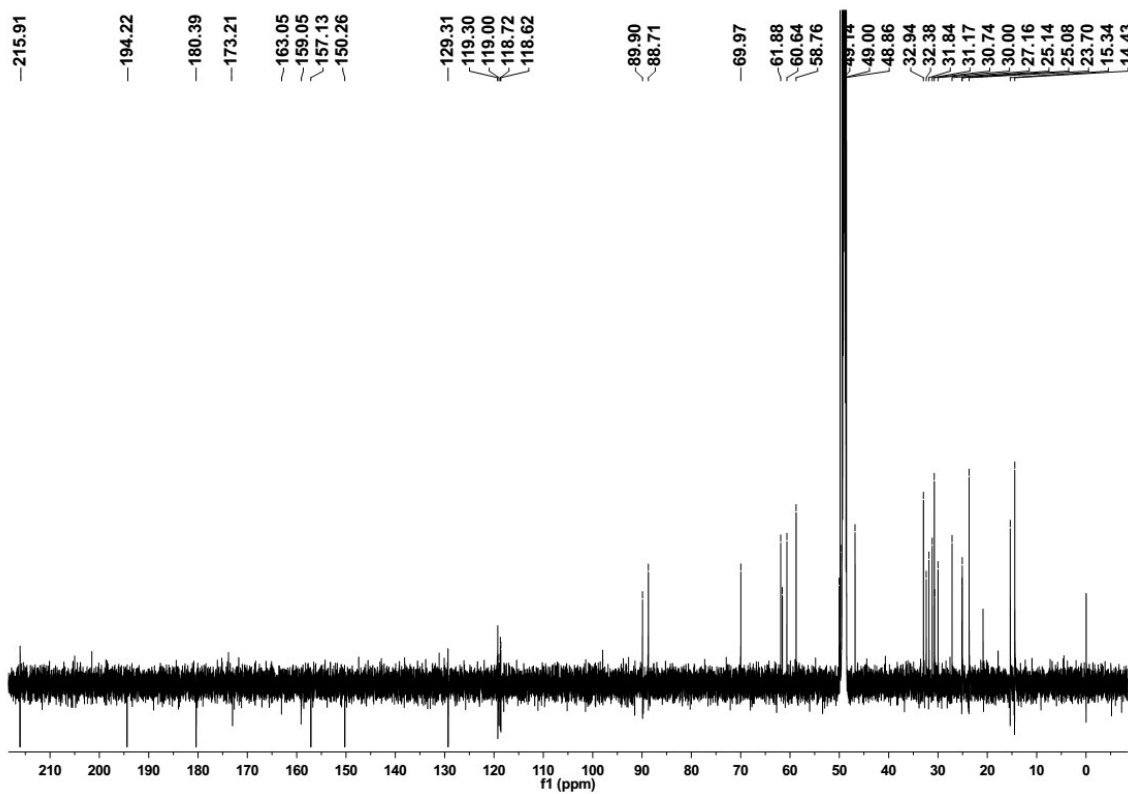


Figure S9. The HSQC spectrum for compound 1

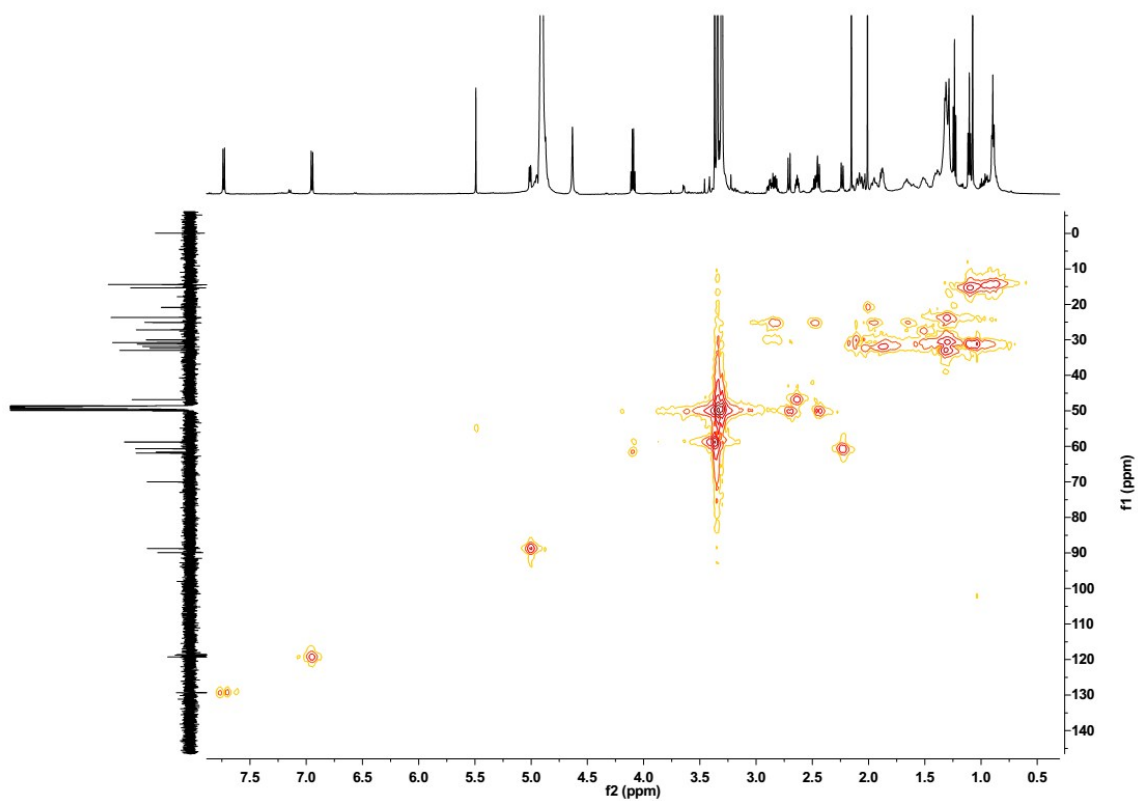


Figure S10. The HMBC spectrum for compound 1

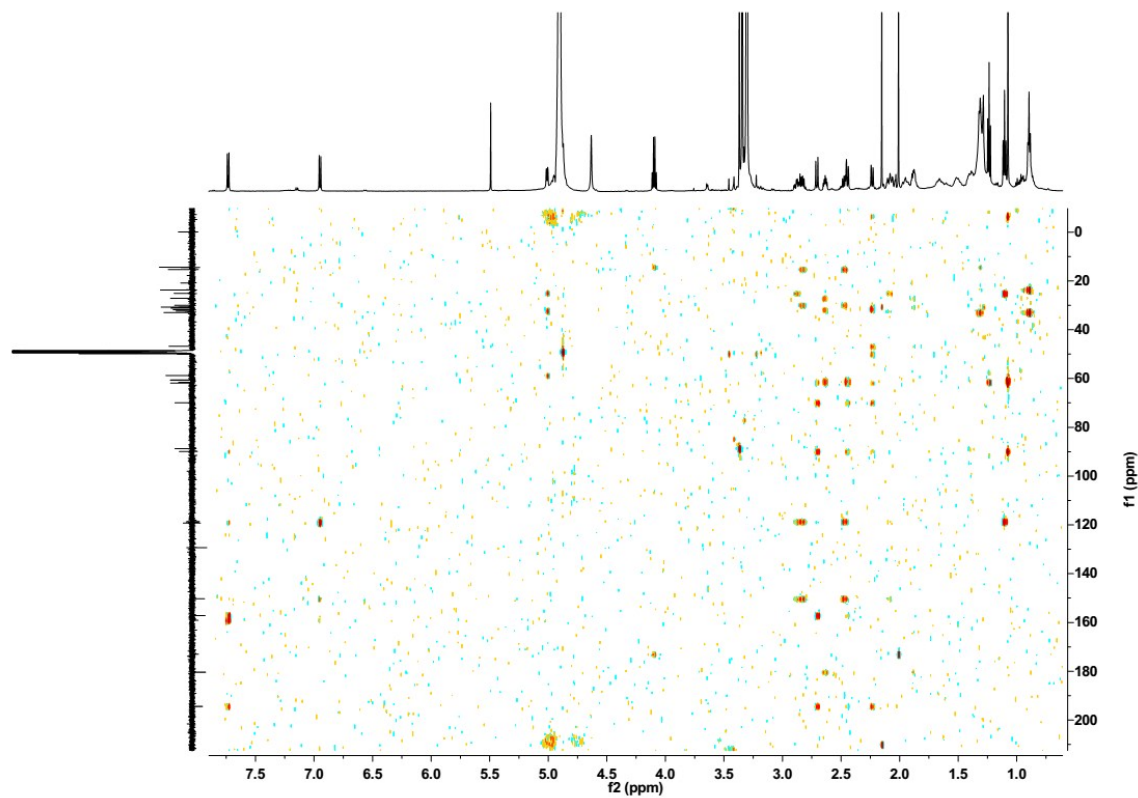


Figure S11. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 1

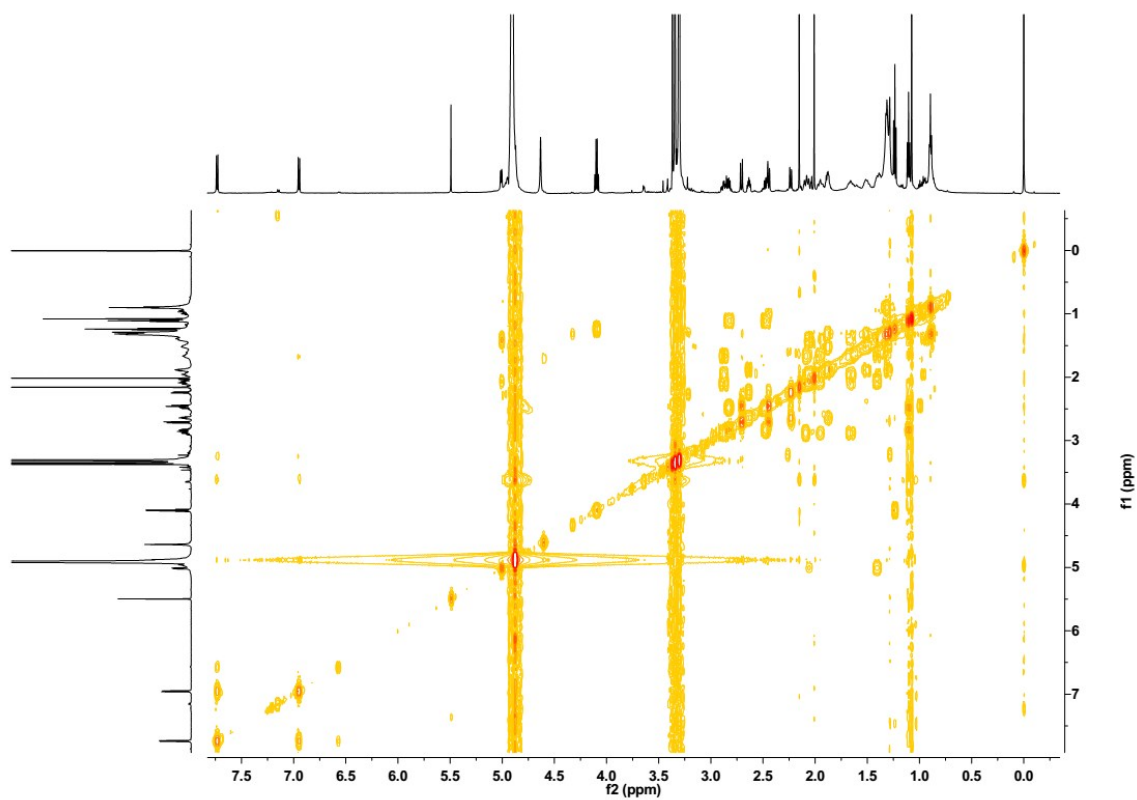


Figure S12. The NOESY spectrum for compound 1

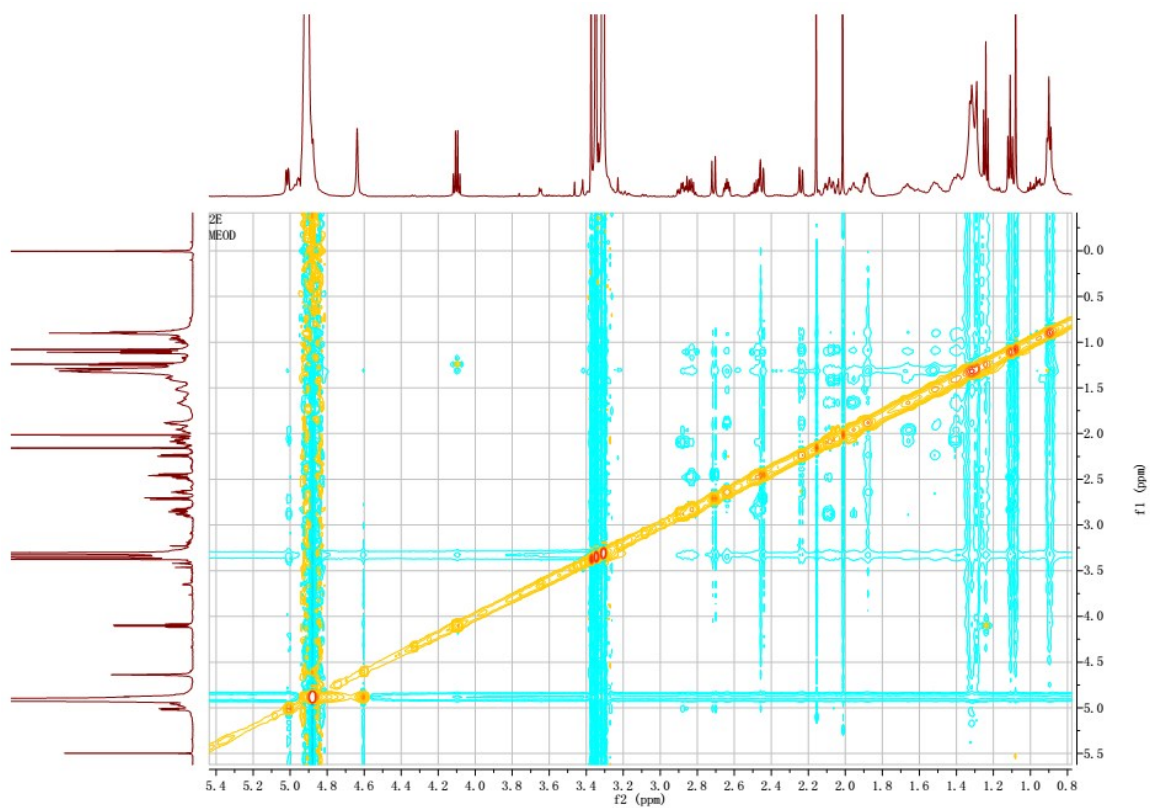


Figure S13. The HRMS-ESI spectrum for compound 1

2e #8-12 RT: 0.23-0.34 AV: 5 NL: 1.03E6
T: FTMS + c ESI Full ms [300.00-1000.00]

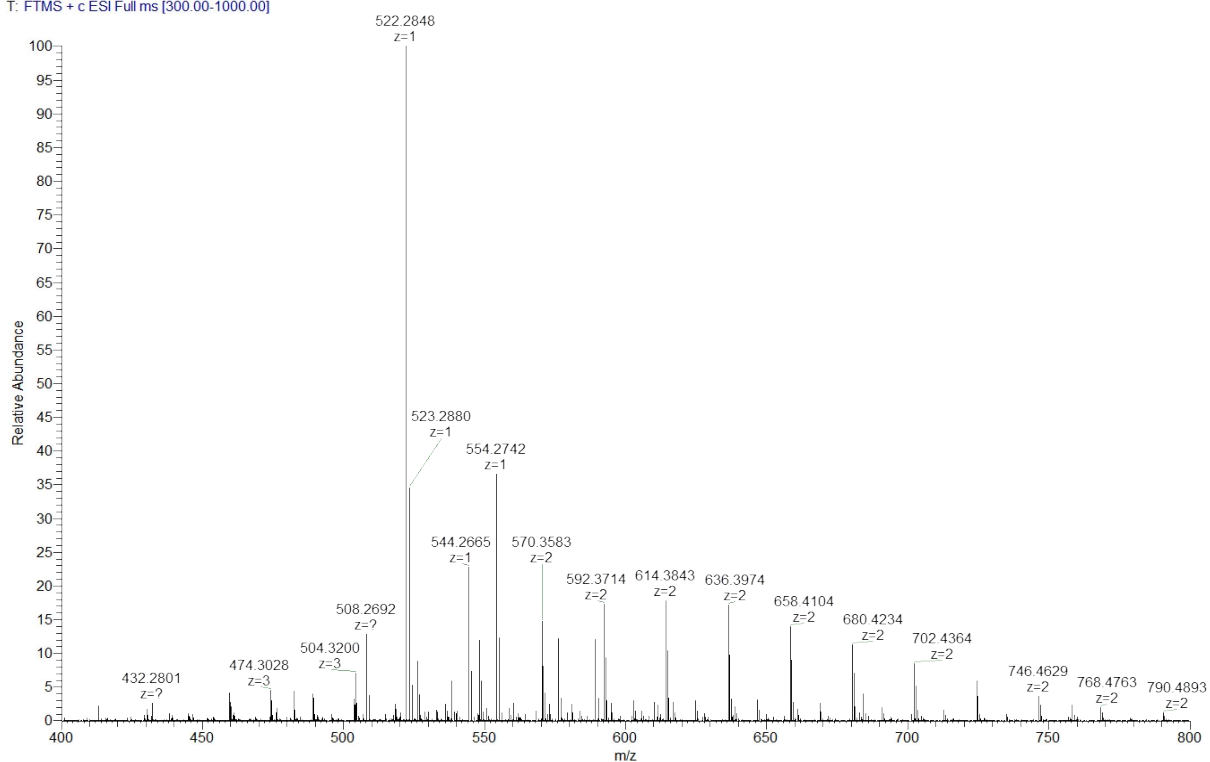


Figure S14. ¹H NMR (600 MHz, CD₃OD) spectrum for compound 2

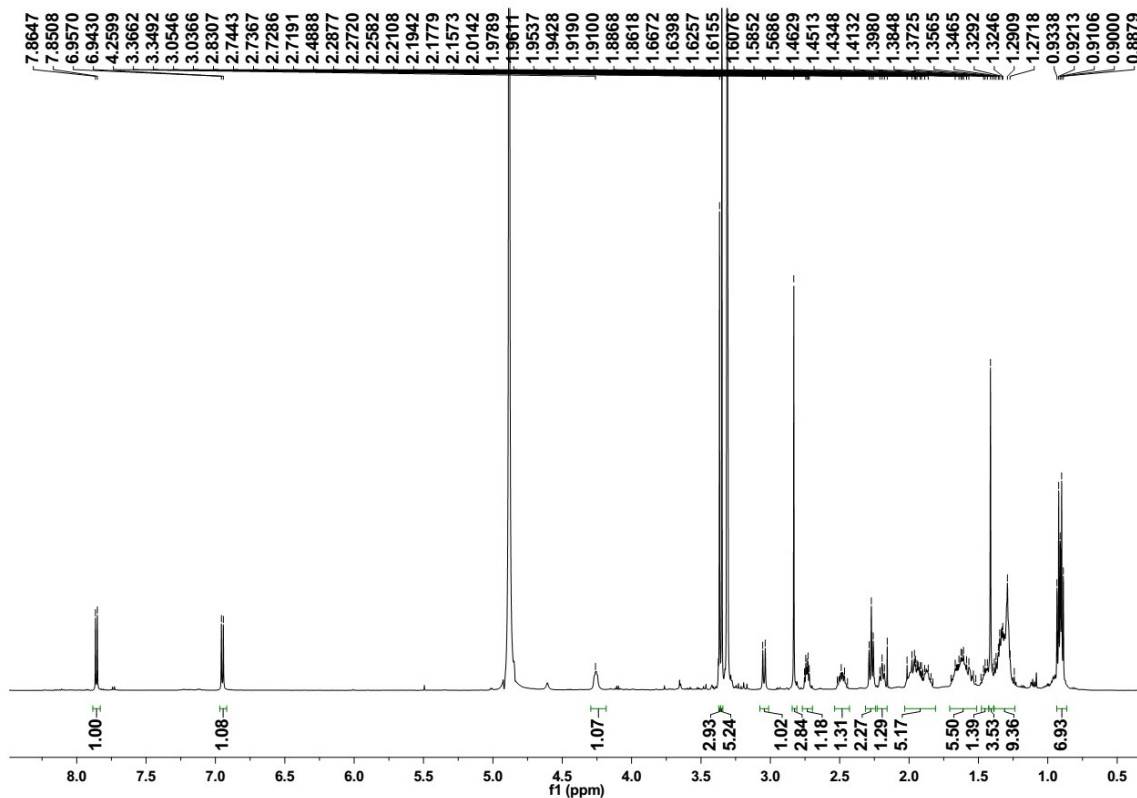


Figure S15. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound 2

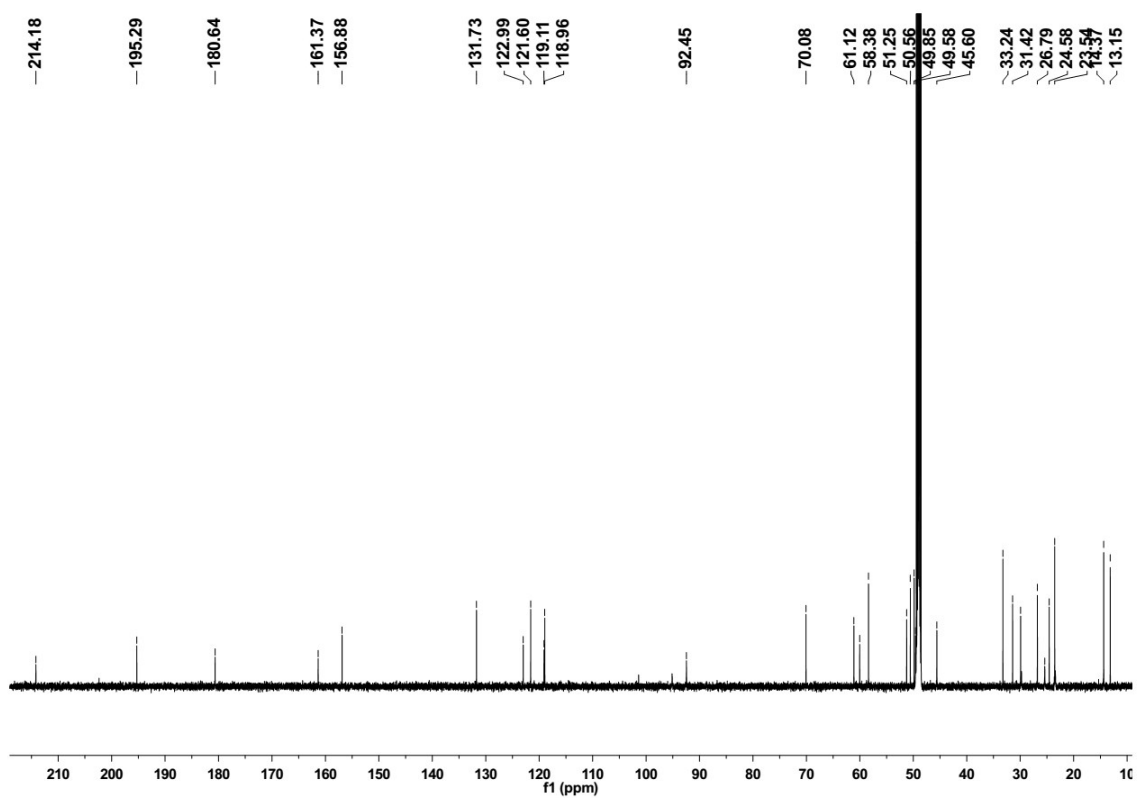


Figure S16. The HSQC spectrum for compound 2

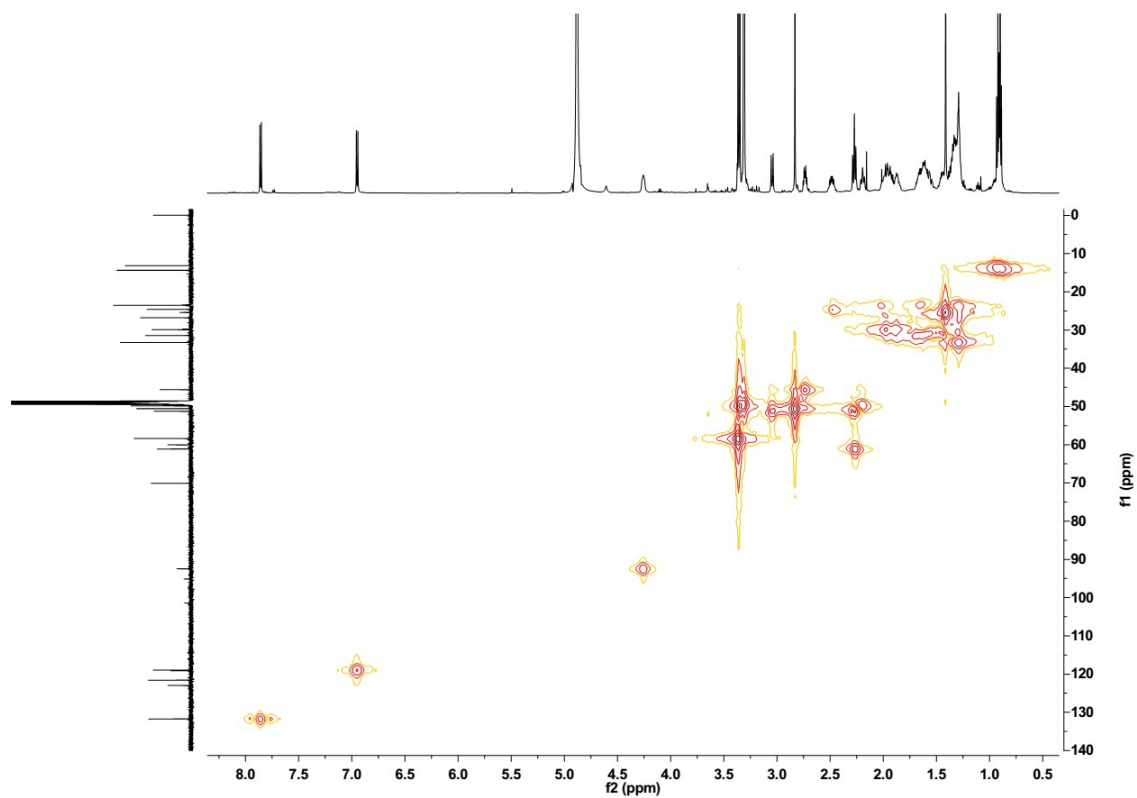


Figure S17. The HMBC spectrum for compound 2

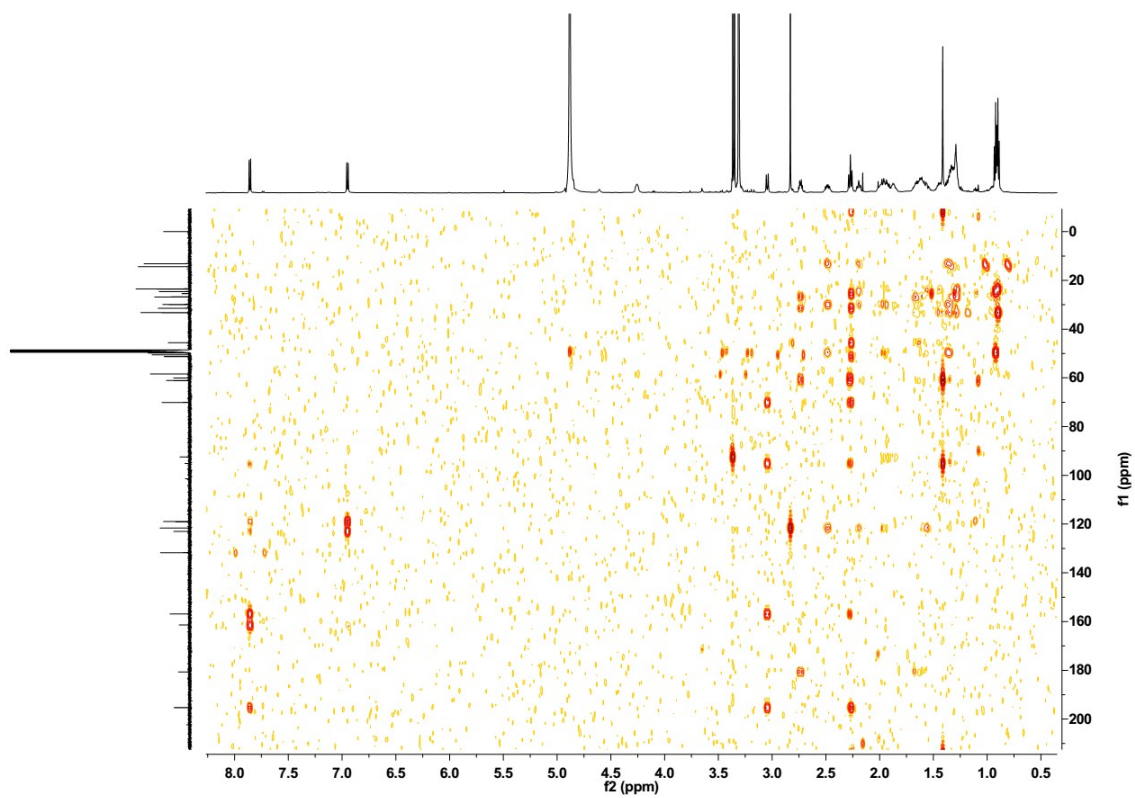


Figure S18. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 2

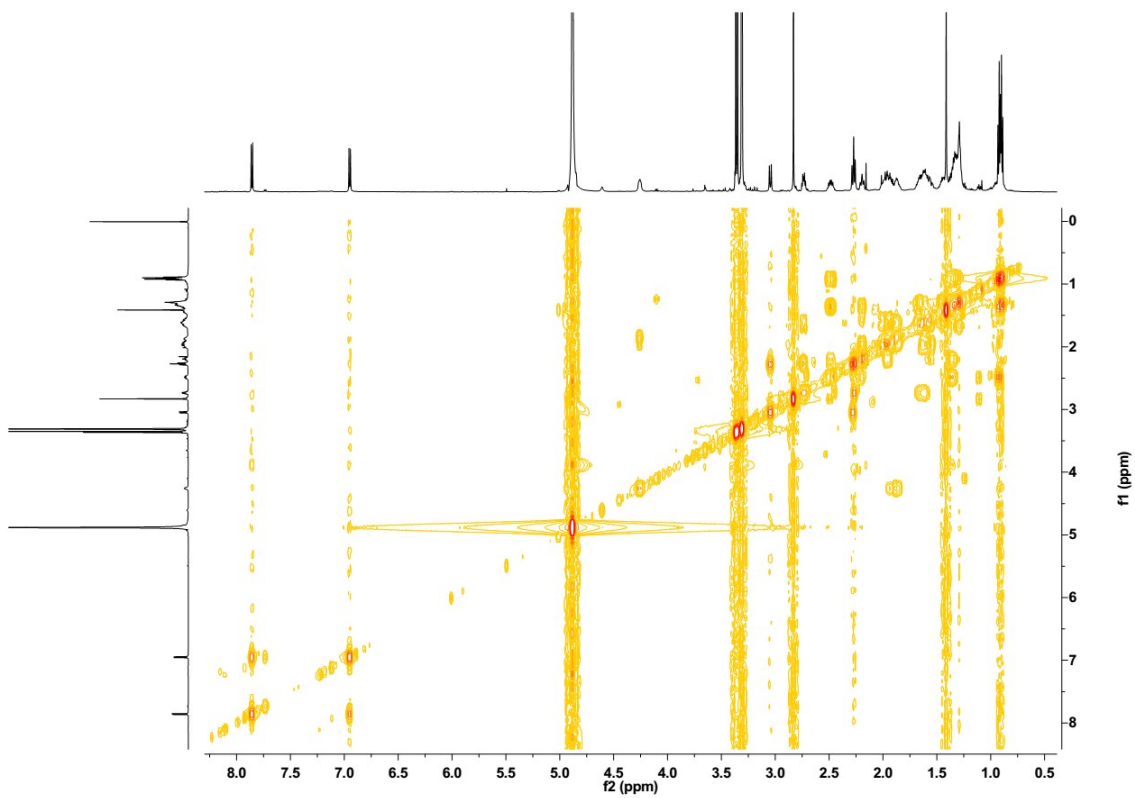


Figure S19. The HRMS-ESI spectrum for compound 2

2d-a #20 RT: 0.58 AV: 1 NL: 1.40E5
T: FTMS + c ESI Full ms [300.00-1000.00]

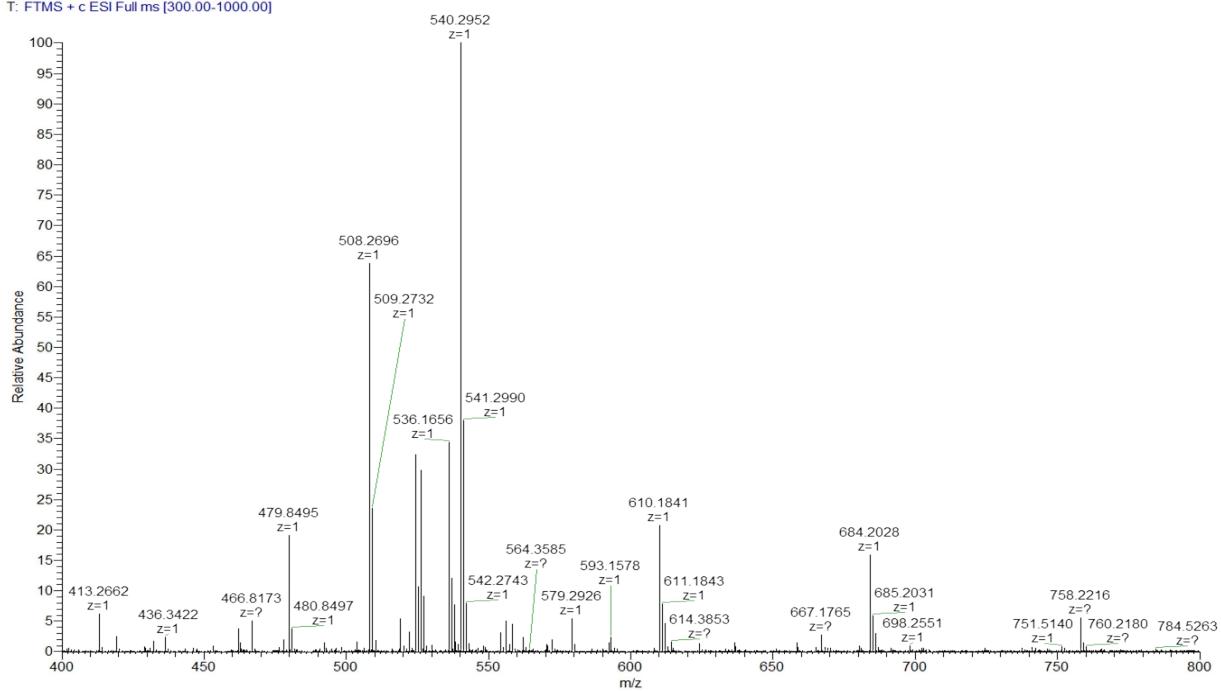


Figure S20. ¹H NMR (600 MHz, DMSO) spectrum for compound 3

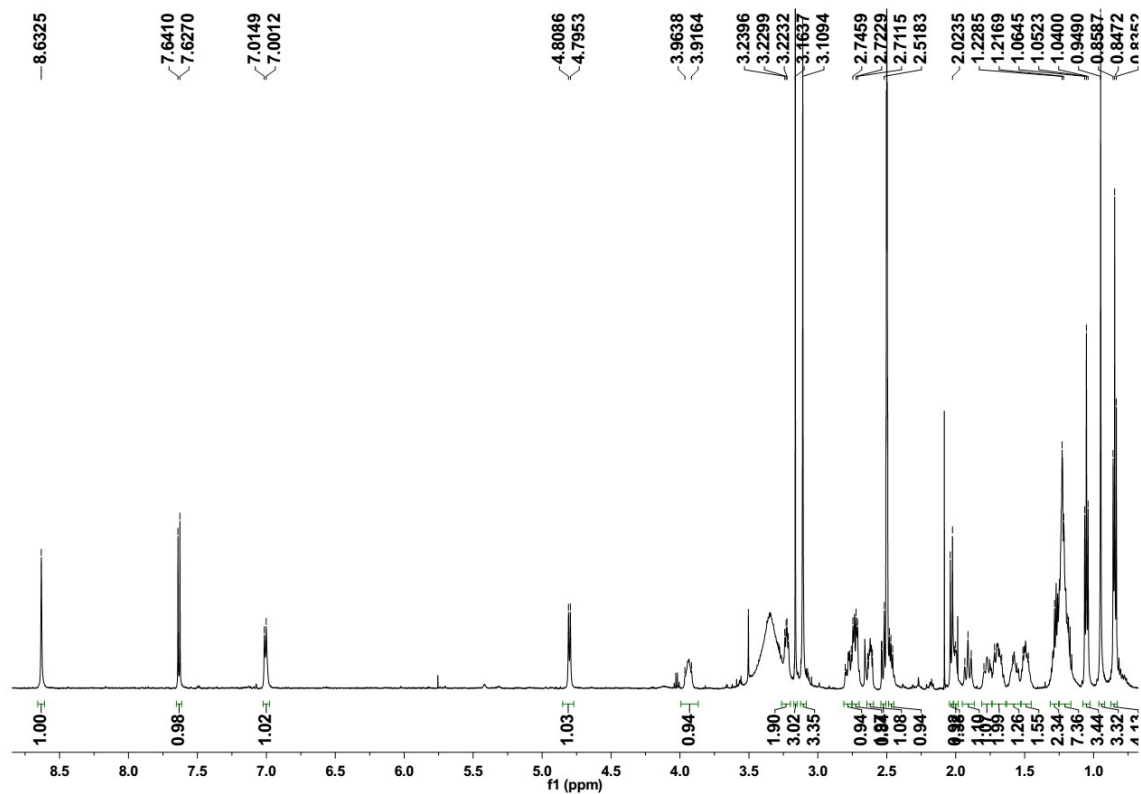


Figure S21. ^{13}C NMR (151 MHz, DMSO) spectrum for compound **3**

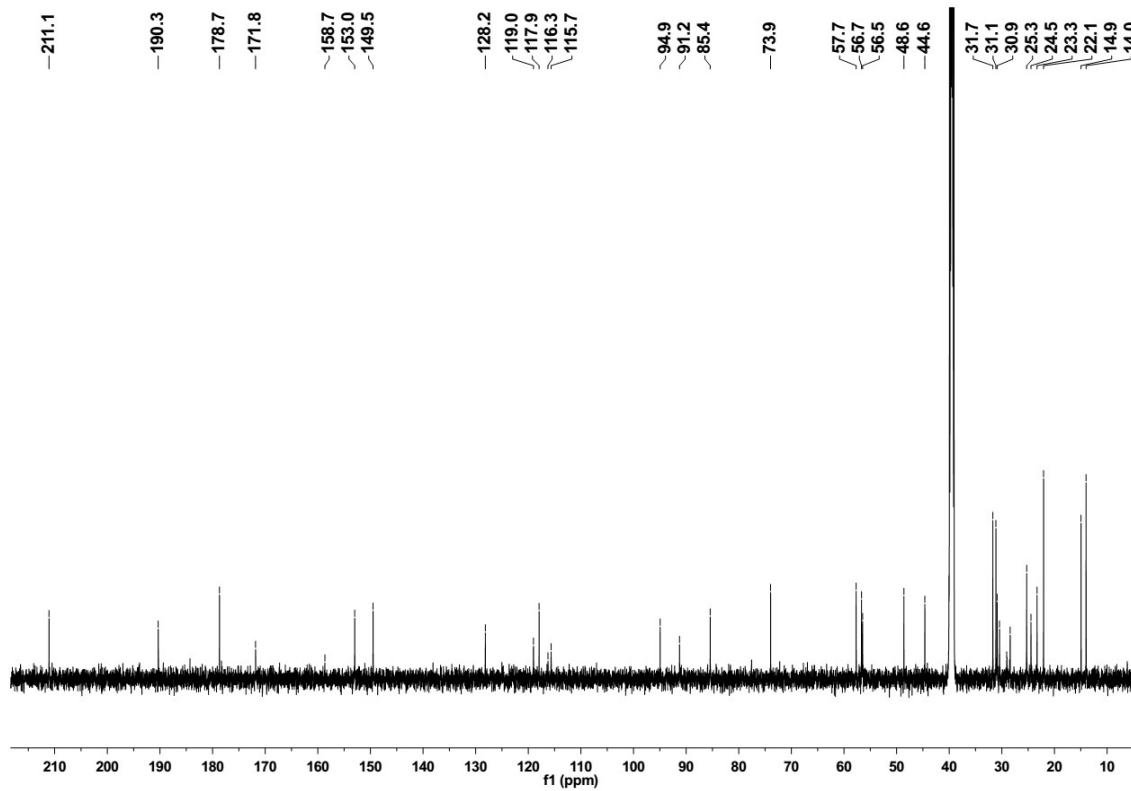


Figure S22. The HSQC spectrum for compound **3**

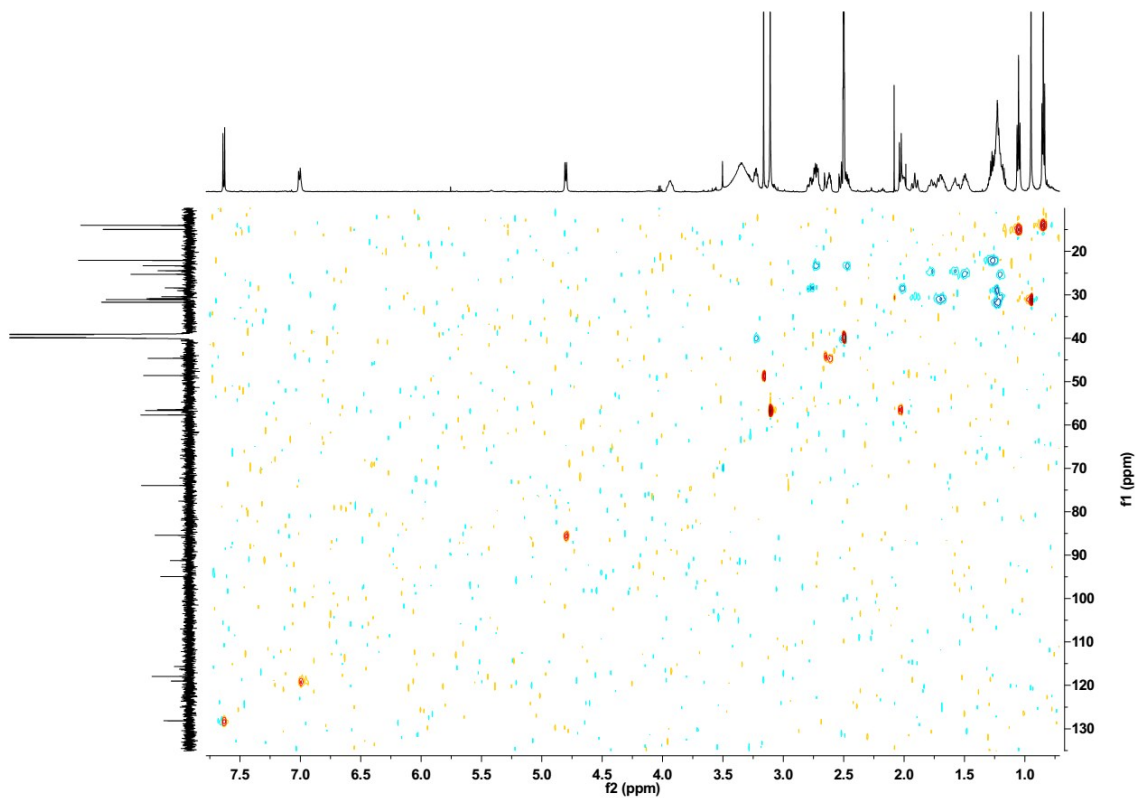


Figure S23. The HMBC spectrum for compound 3

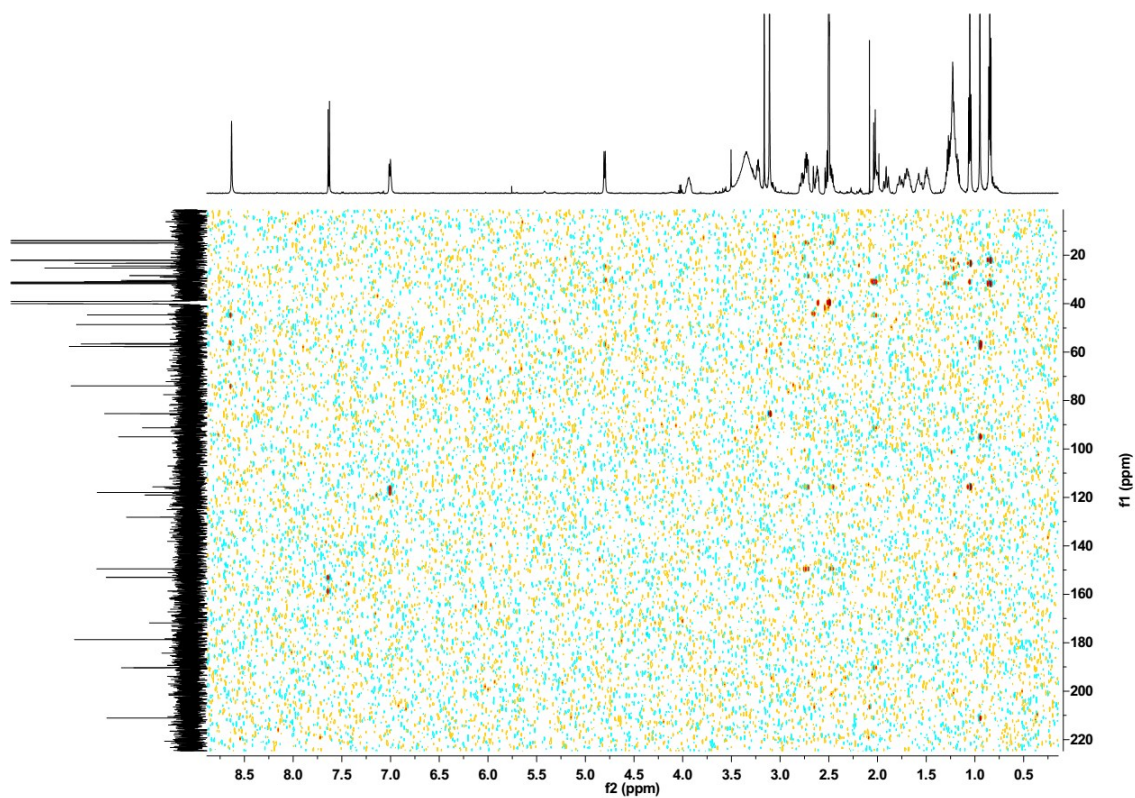


Figure S24. ¹H/¹H COSY spectrum for compound 3

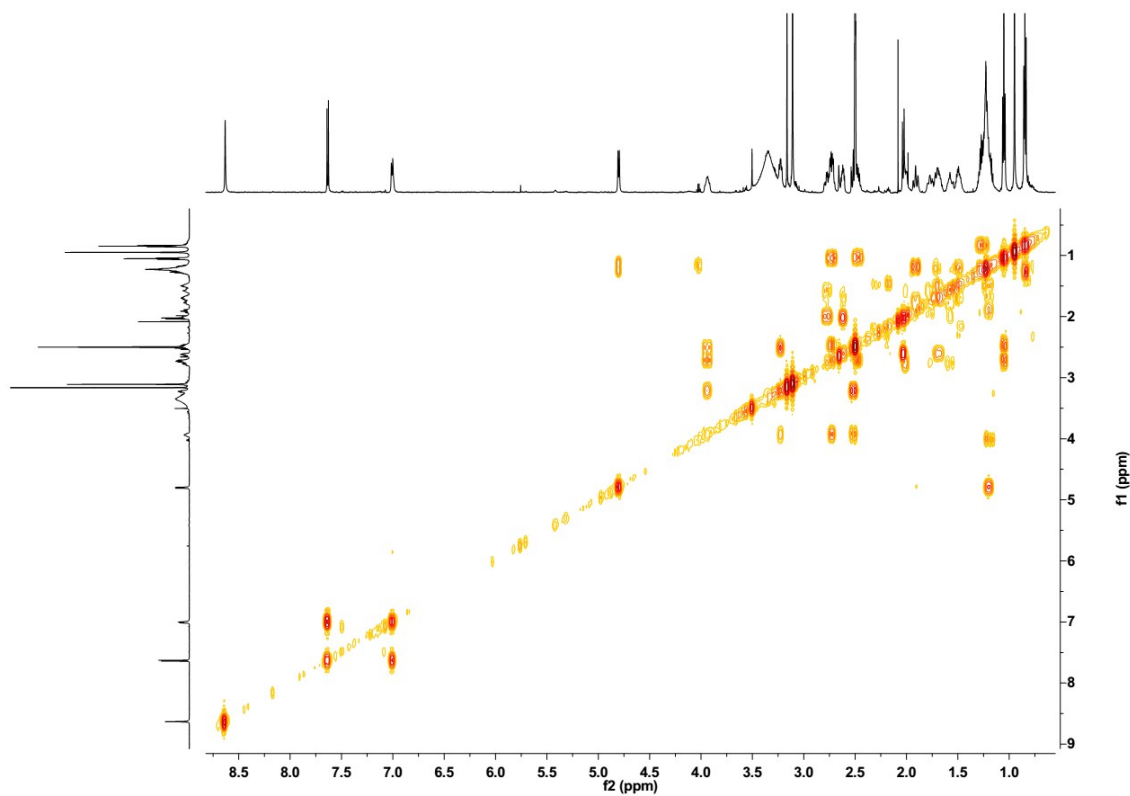


Figure S25. The NOESY spectrum for compound **3**

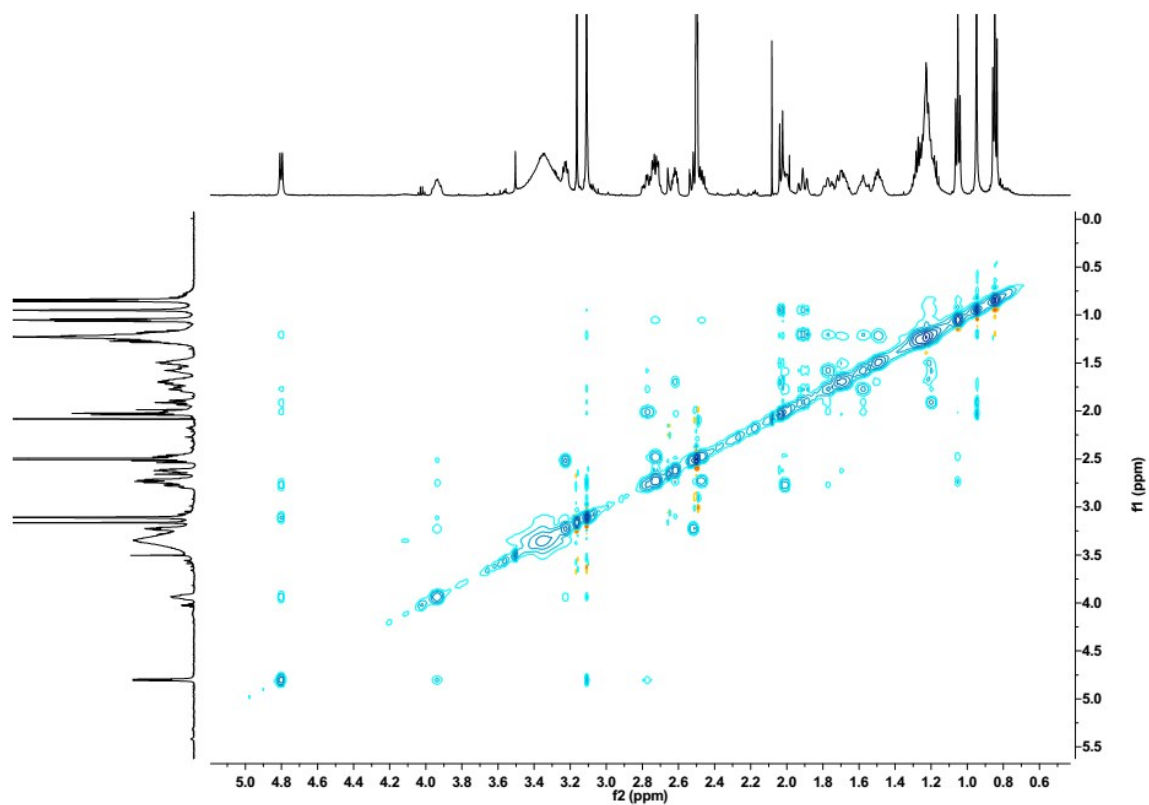


Figure S26. The HRMS-ESI spectrum for compound **3**

y4 #11 RT: 0.31 AV: 1 NL: 6.33E5
T: FTMS + c ESI Full ms [300.00-1000.00]

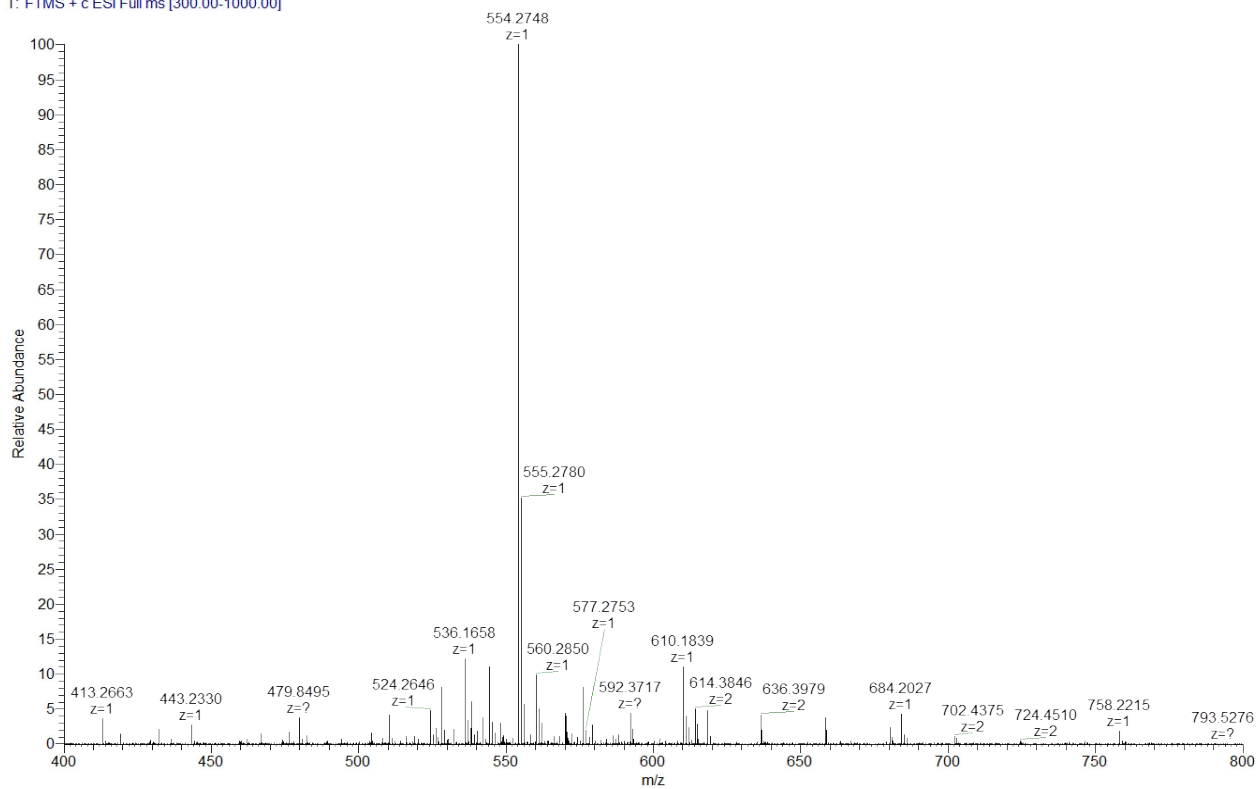


Figure S27. ¹H NMR (600 MHz, CD₃OD) spectrum for compound 4

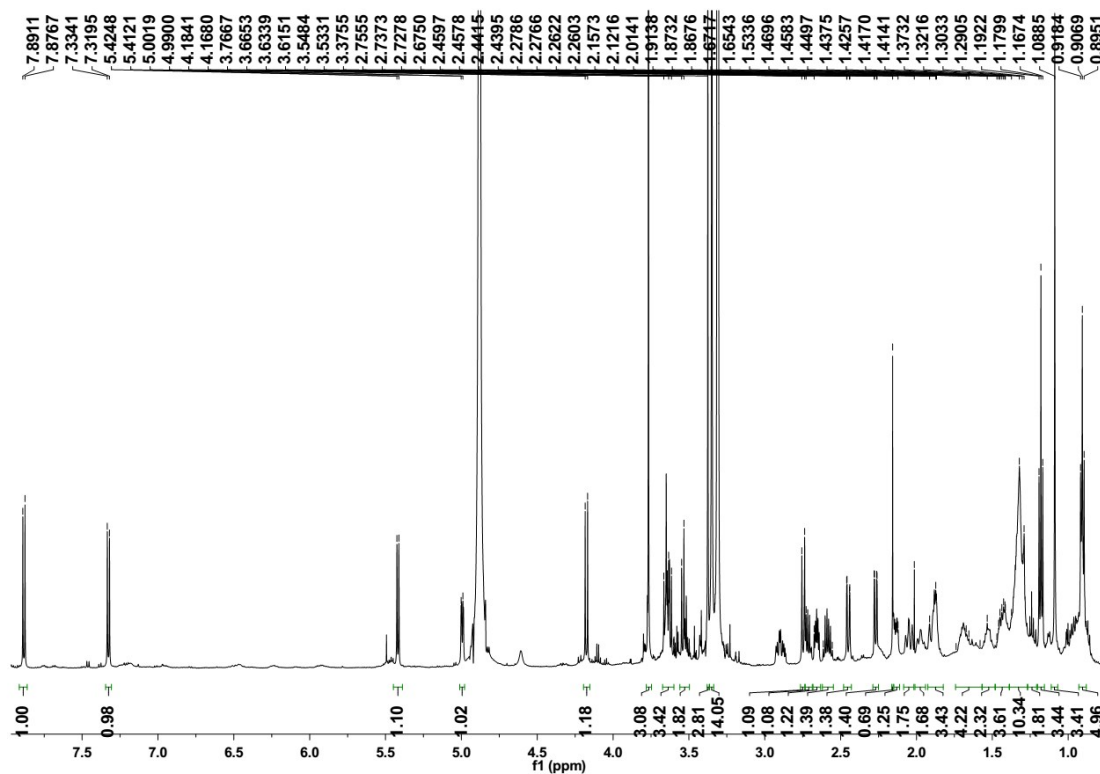


Figure S28. ¹³C NMR (151 MHz, CD₃OD) spectrum for compound 4

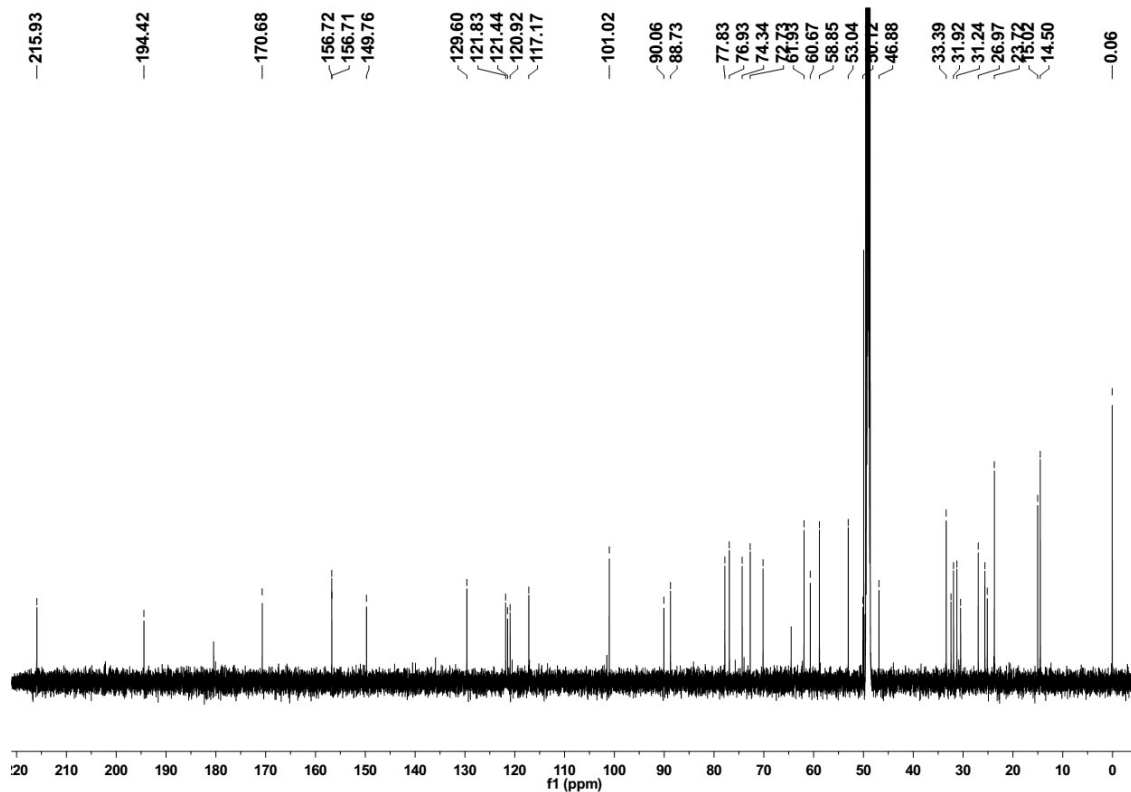


Figure S29. The HSQC spectrum for compound 4

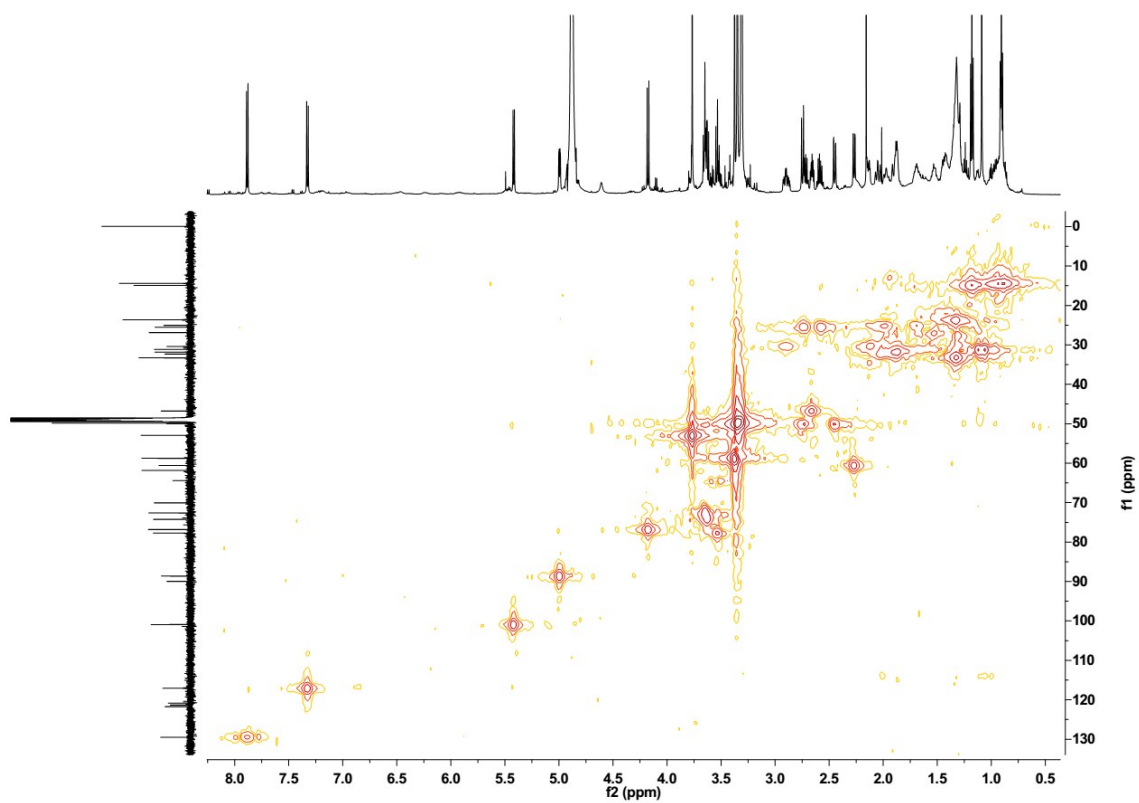


Figure S30. The HMBC spectrum for compound 4

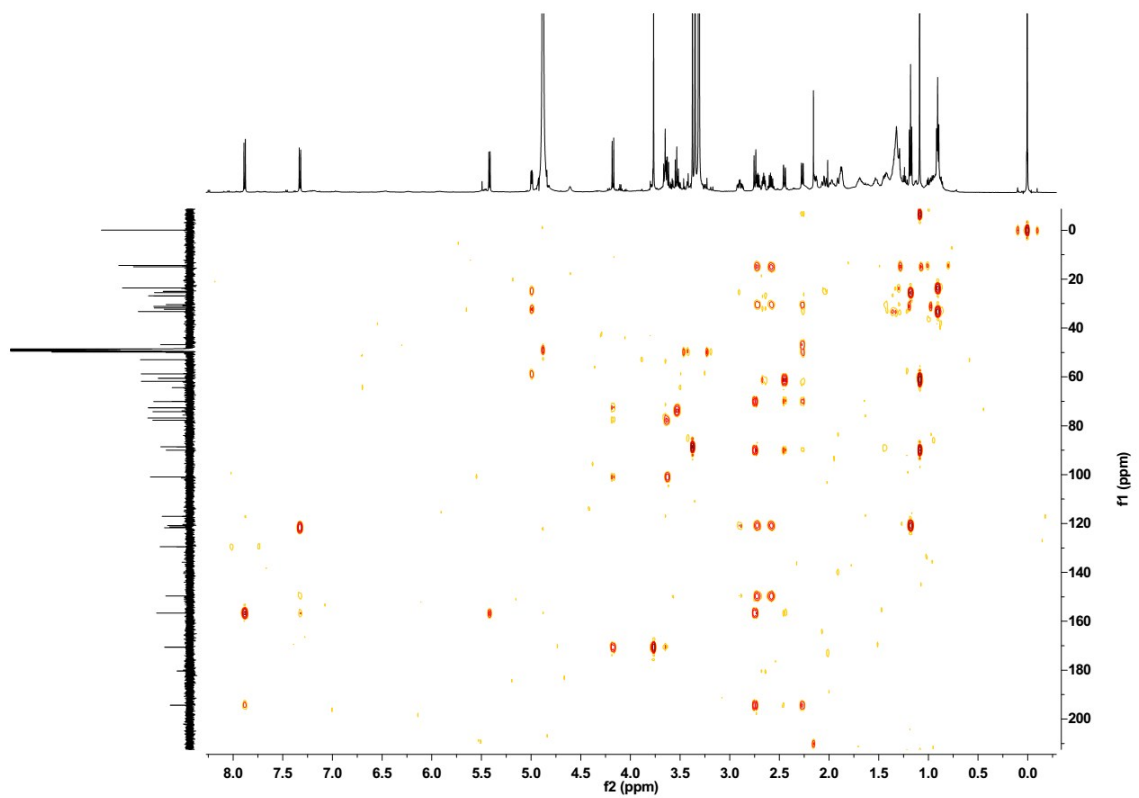


Figure S31. $^1\text{H}/^1\text{H}$ COSY spectrum for compound 4

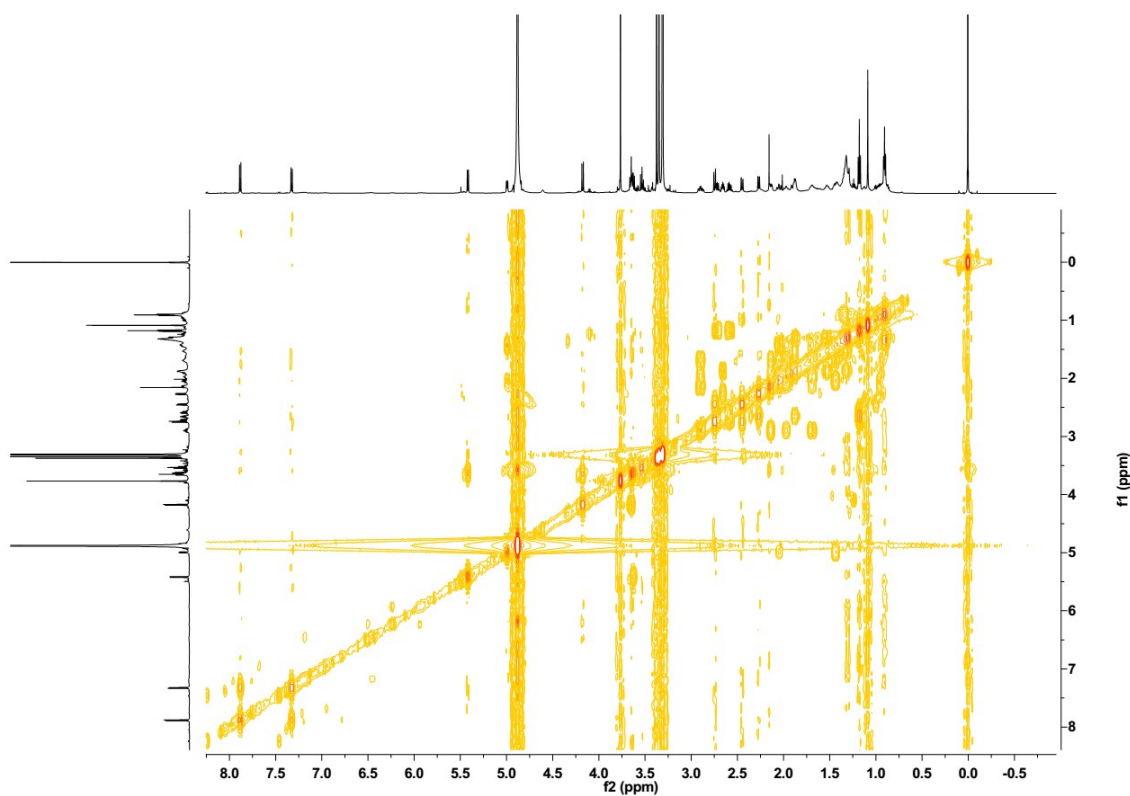


Figure S32. The HRMS-ESI spectrum for compound 4

3F #7-16 RT: 0.19-0.43 AV: 10 NL: 2.67E6
T: FTMS + c ESI Full ms [300.00-1000.00]

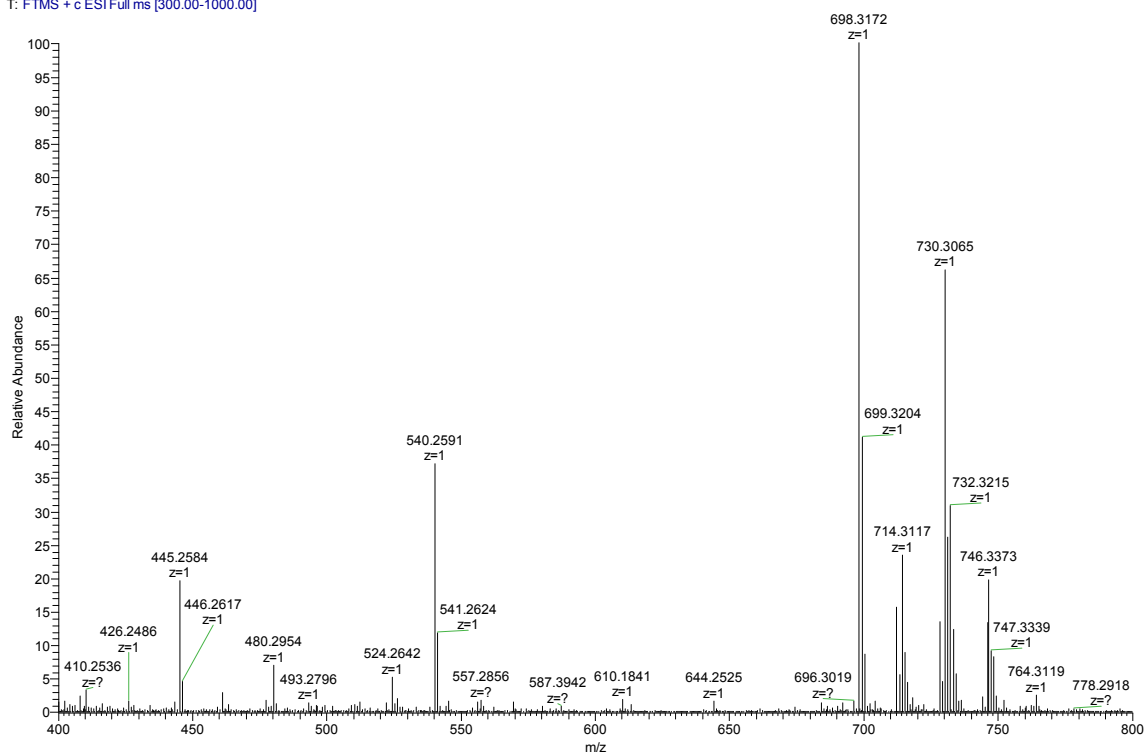


Figure S33. ¹H NMR (600 MHz, CD₃OD) spectrum for compound 5

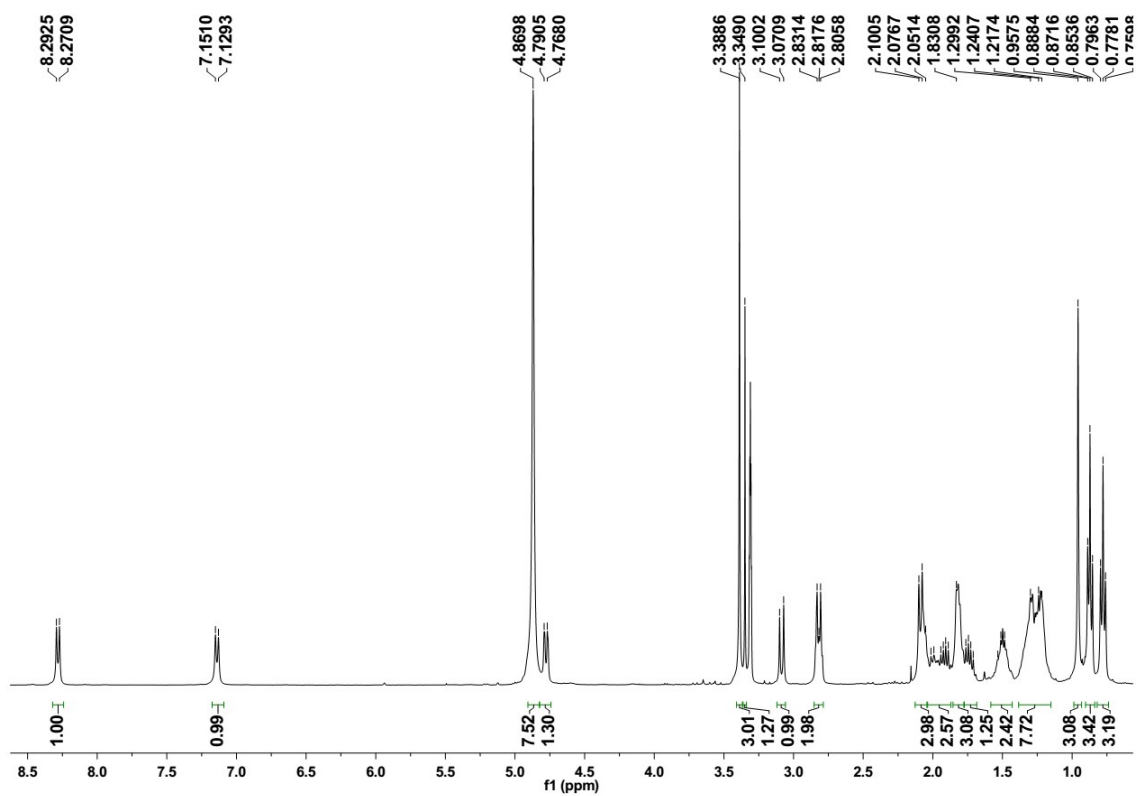


Figure S34. ¹³C NMR (151 MHz, CD₃OD) spectrum for compound 5

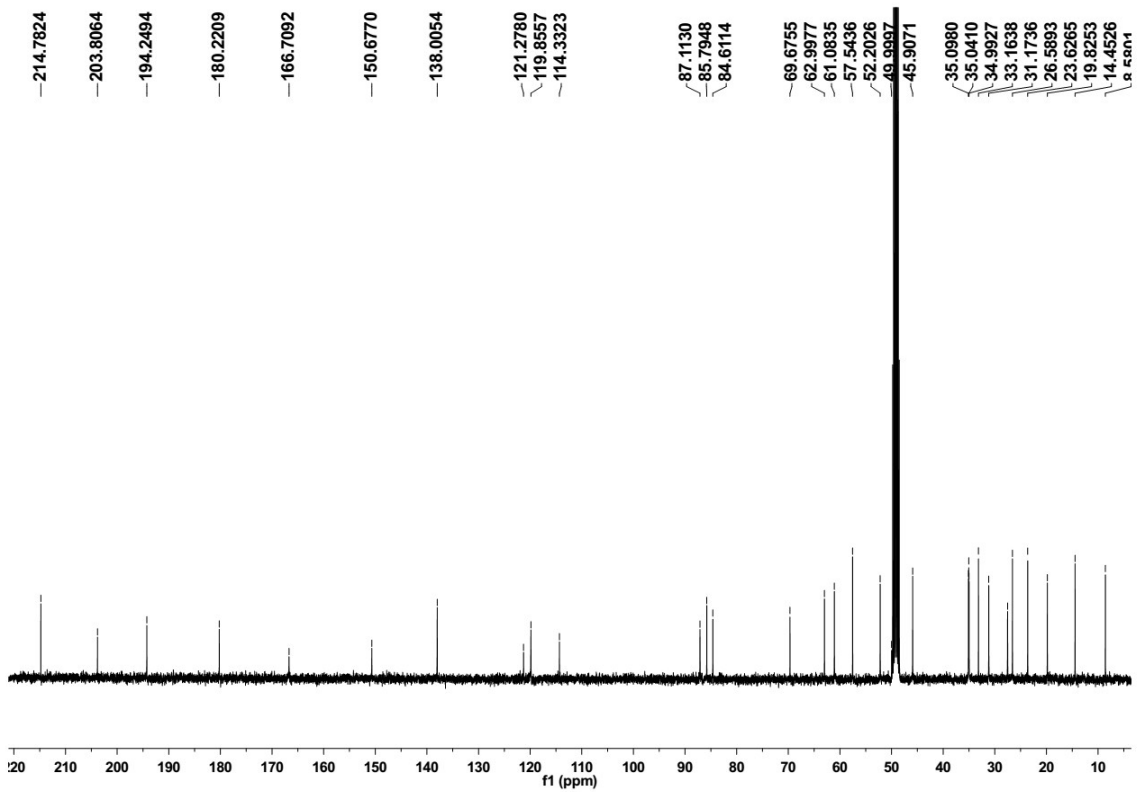


Figure S35. The HSQC spectrum for compound 5

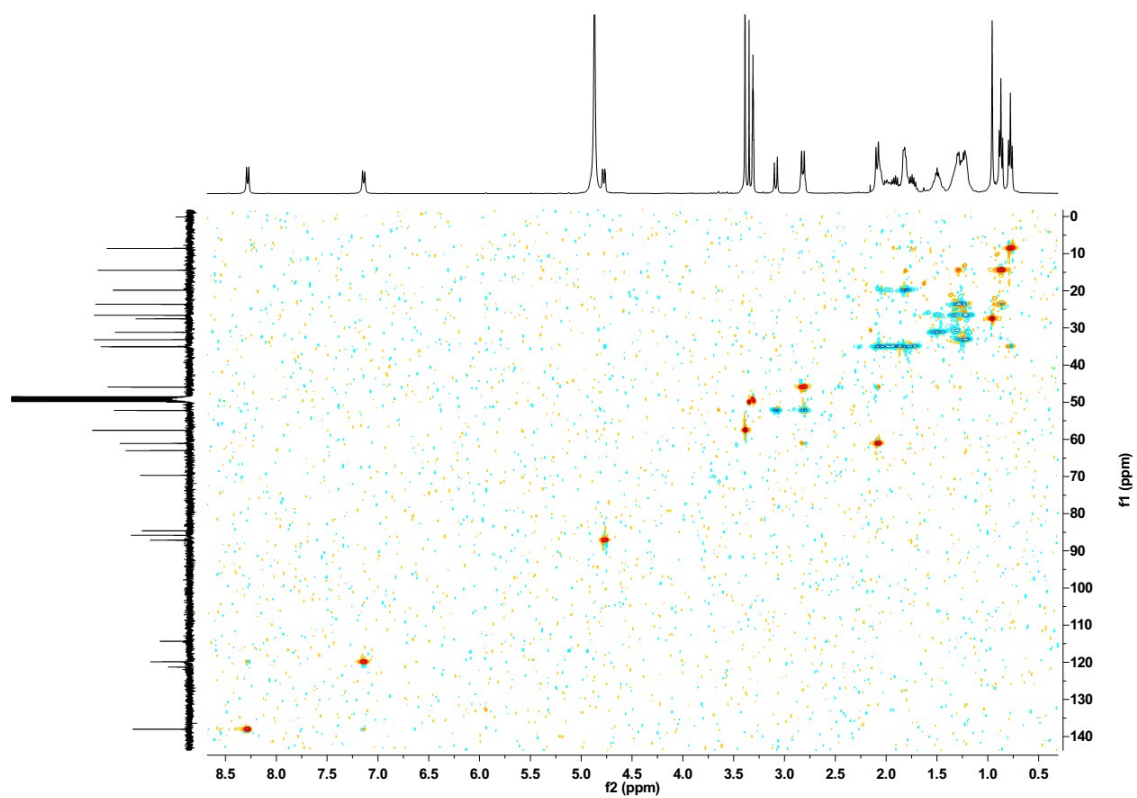


Figure S36. The HMBC spectrum for compound 5

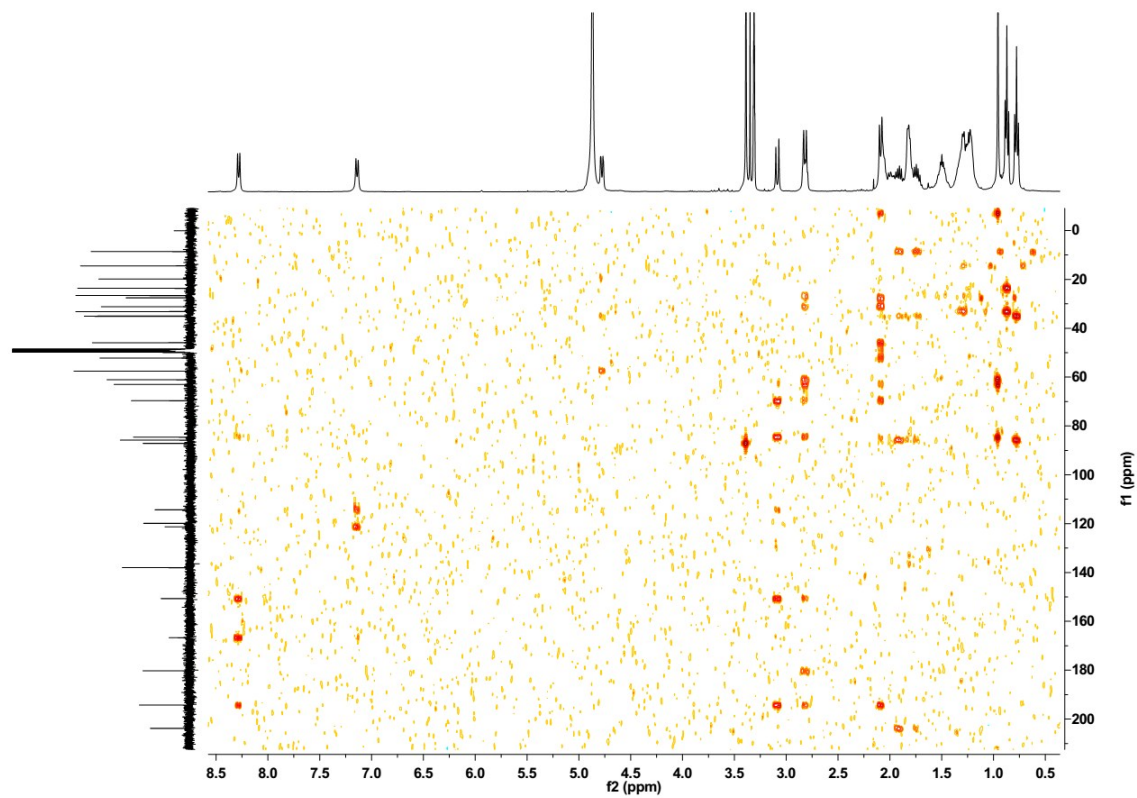


Figure S37. $^1\text{H}/^1\text{H}$ COSY spectrum for compound **5**

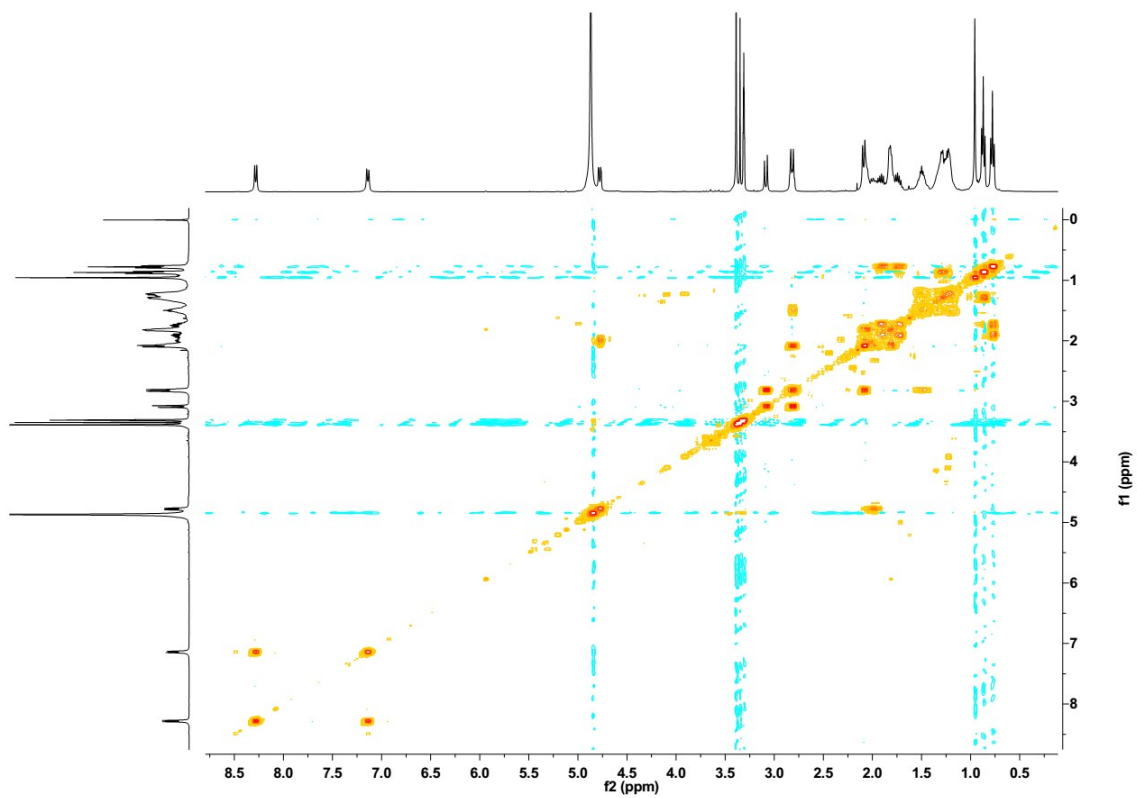


Figure S38. The NOESY spectrum for compound **5**

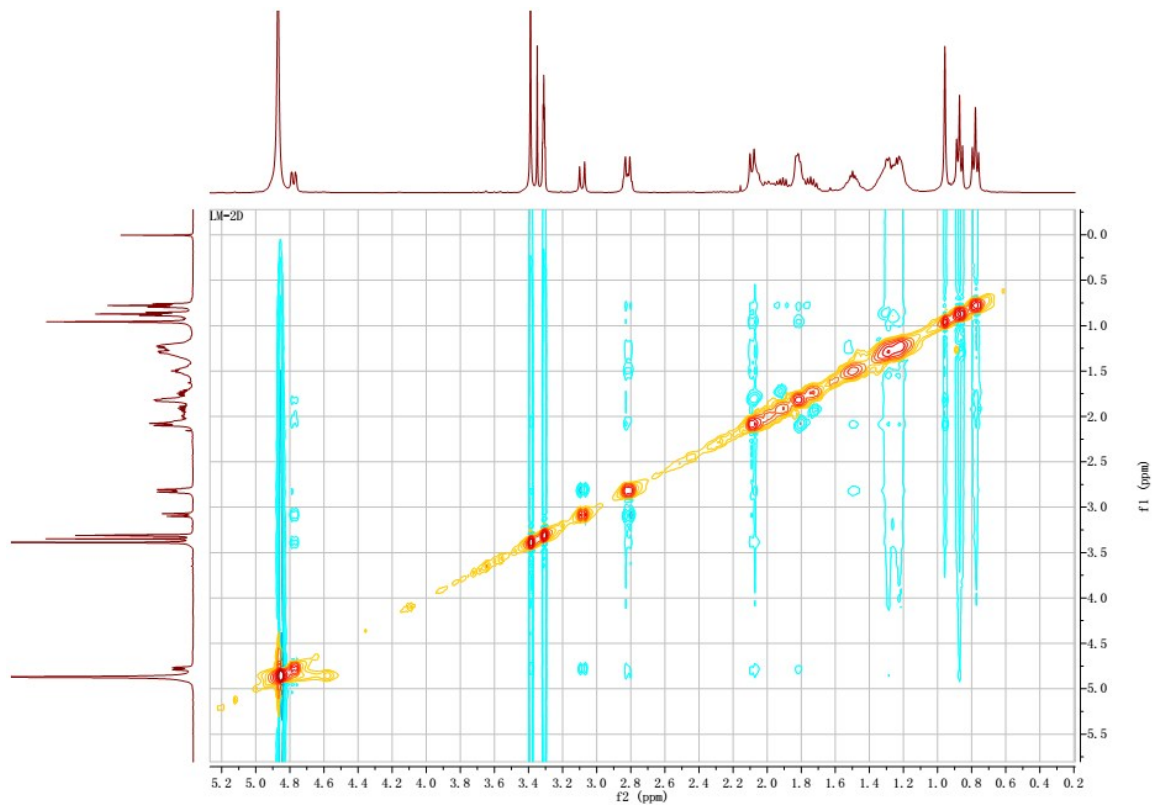


Figure S39. The HRMS-ESI spectrum for compound 5

2g #12 RT: 0.33 AV: 1 NL: 2.65E7
T: FTMS + c ESI Full ms [300.00-1000.00]

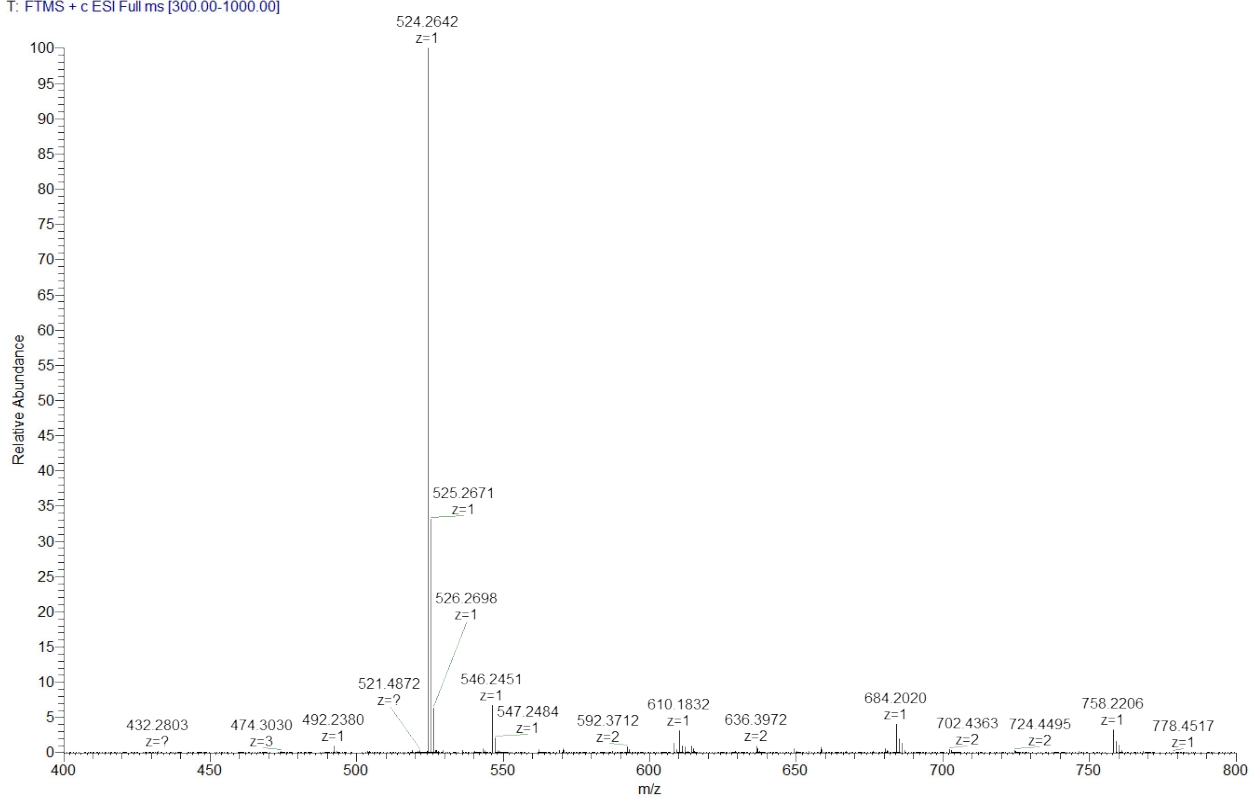


Figure S40. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum for compound 6

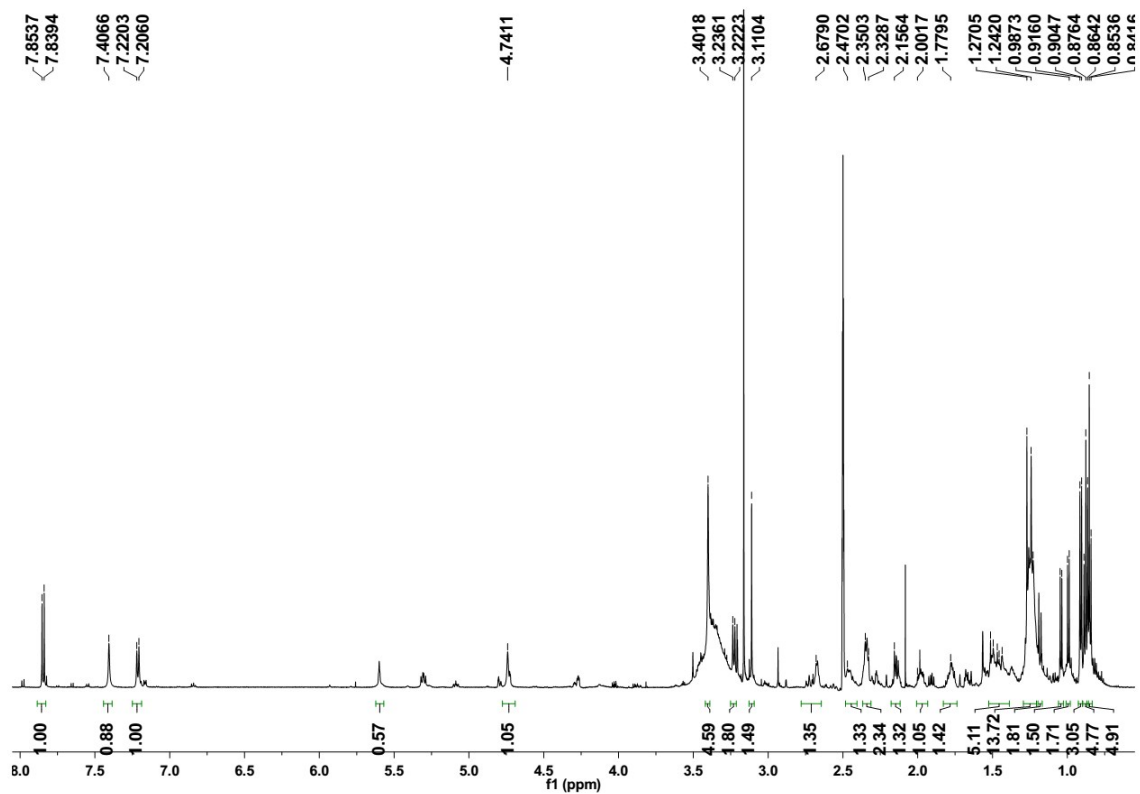


Figure S41. ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) spectrum for compound 6

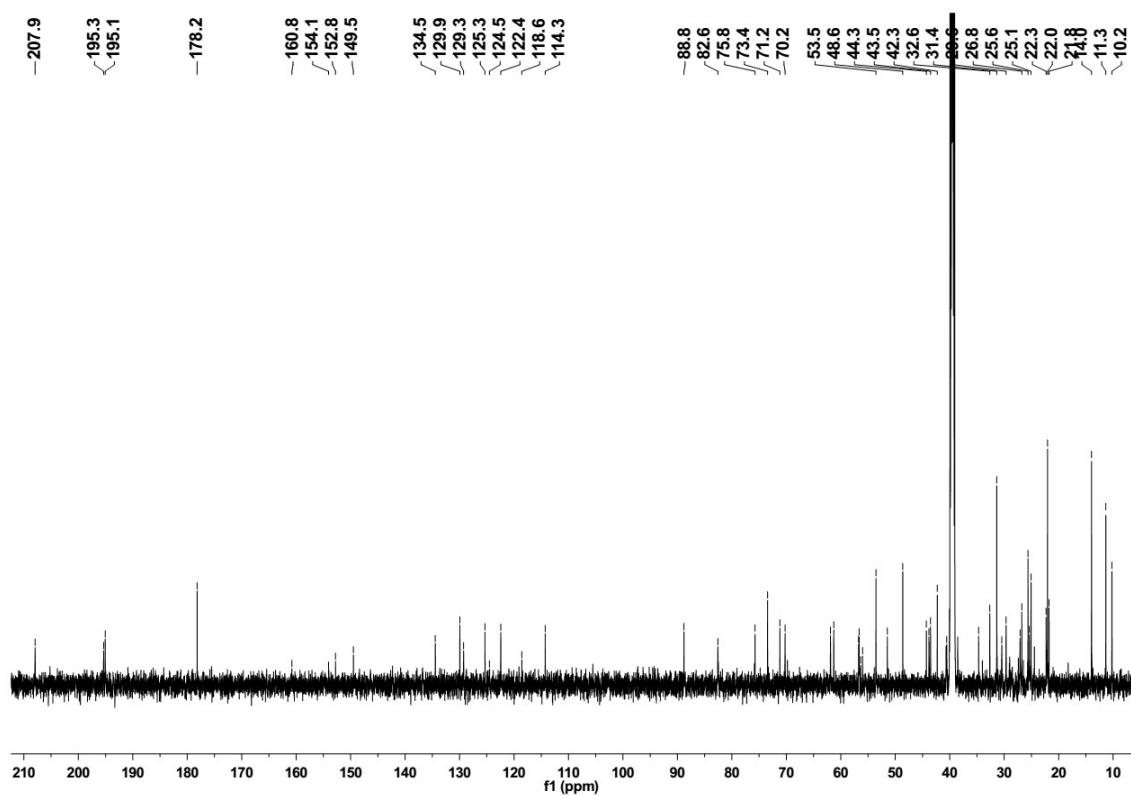


Figure S42. The HSQC spectrum for compound 6

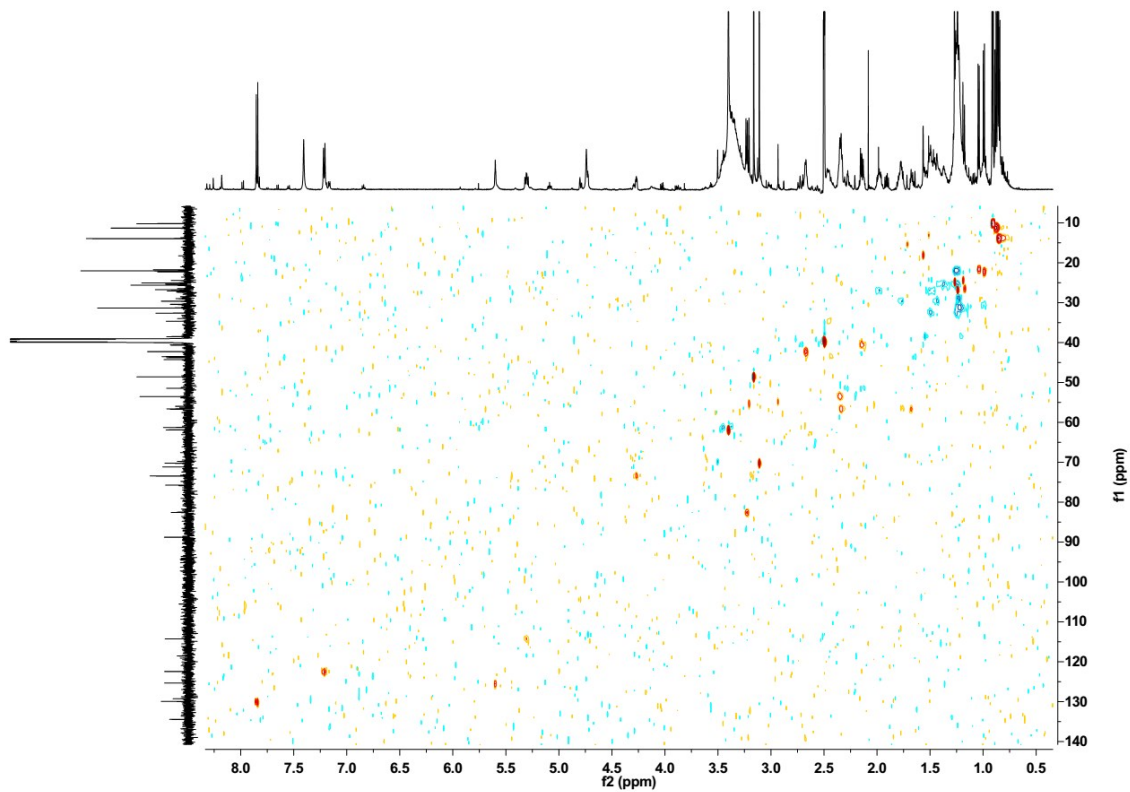


Figure S43. The HMBC spectrum for compound **6**

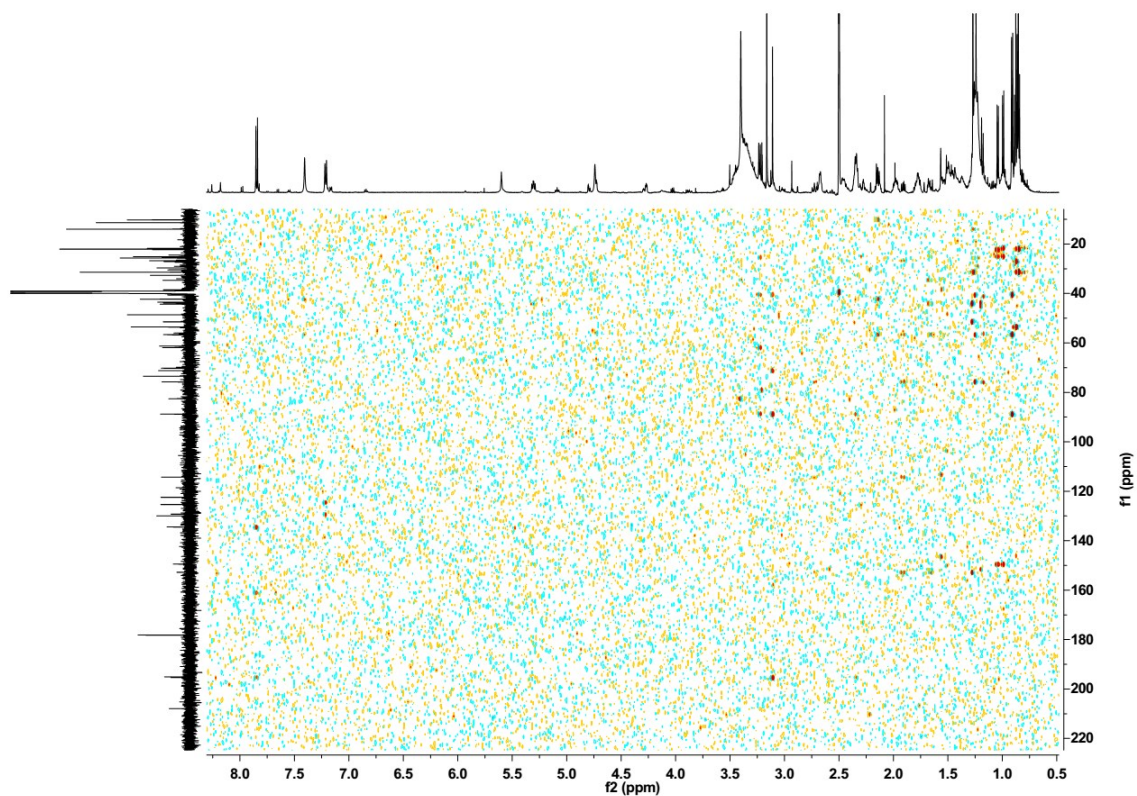


Figure S44. $^1\text{H}/^1\text{H}$ COSY spectrum for compound **6**

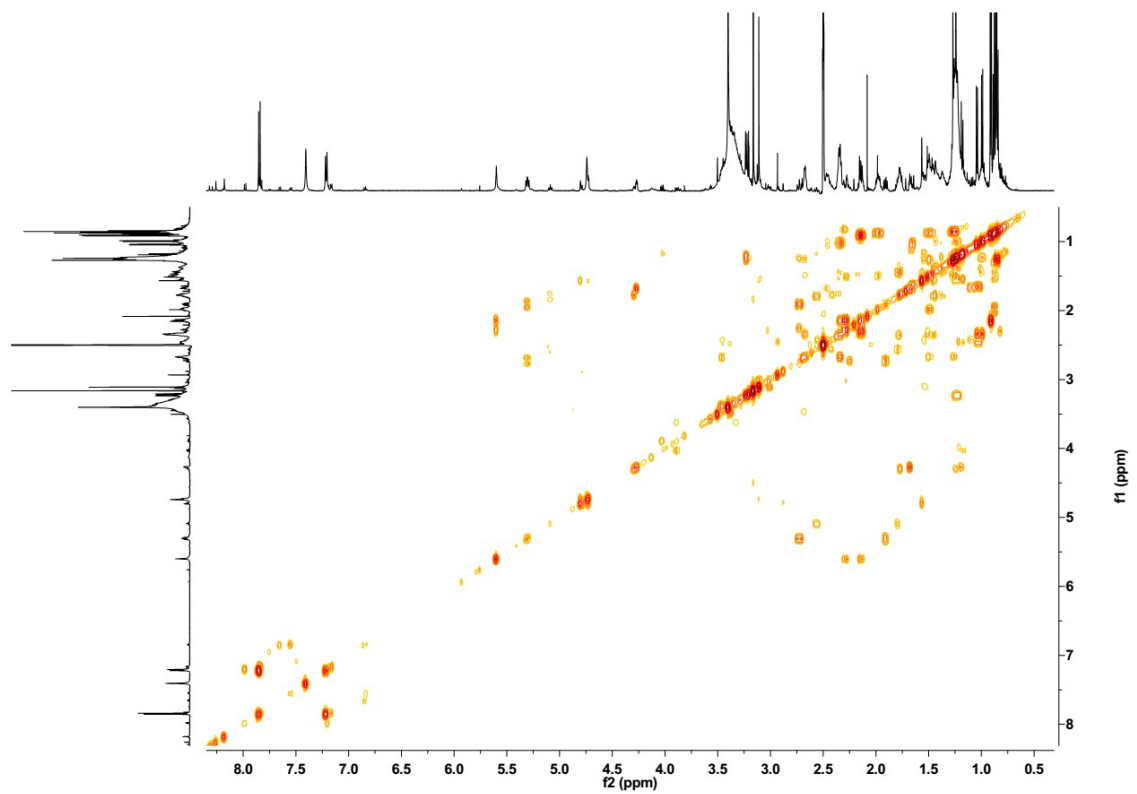


Figure S45. The HRMS-ESI spectrum for compound **6**

ya #10 RT: 0.29 AV: 1 NL: 4.17E6
T: FTMS + c ESI Full ms [300.00-1000.00]

