

Supporting Information

for

Deletion of the side chain assembly reveals diverse post-PKS modifications in the biosynthesis of ansatrienins

Xiaomei Li,^a Jing Zhu,^b Guoyin Shi,^b Mingwei Sun,^a Zhixing Guo,^a Haoxin Wang,^b Chunhua Lu,^{*,a}
and Yuemao Shen^{*,a,b}

^aKey Laboratory of Chemical Biology (Ministry of Education), School of Pharmaceutical Sciences, Shandong University, No. 44 West Wenhua Road, Jinan, Shandong 250012, P. R. China.

^bState Key Laboratory of Microbial Technology, School of Life Sciences, Shandong University, Jinan, Shandong 250100, P. R. China

*Correspondence:

Chunhua Lu

[Tel: +86-531-88382108](tel:+86-531-88382108), E-mail: ahua0966@sdu.edu.cn

Yuemao Shen

[Tel: +86-531-88382108](tel:+86-531-88382108), E-mail: yshen@sdu.edu.cn

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Table S1: NMR spectroscopy data (CD₃OD) for compound **1**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		172.6s		
2 α	2.93 (dd, 17.5, 7.9)		C-4, C-3, C-1	H-2 β , H-3
2 β	2.62 (dd, 17.5, 4.9)	38.8t	C-4, C-3, C-1	H-2 α , H-3
3	4.03 (m)	77.0d	MeO-3, C-5, C-1	H-2 α , H-2 β , H-4
4	3.63 (dd, 6.1, 4.2)	66.2d	C-3, C-6, C-20, C-1	H-3, H-5
5	4.63 (dd, 8.5, 6.3)	78.5d	C-4, C-3, C-6, C-19, C-7	H-4, H-6
6	6.07 (dd, 15.8, 6.2)	126.1d	C-4, C-5, C-8	H-7, H-5
7	6.69 (dd, 15.8, 10.5)	140.3d	C-5, C-6, C-8, C-9	H-8, H-6
8	6.29 (dd, 15.1, 10.7)	132.1d	C-10, C-6, C-7	H-9, H-7
9	5.64 (ddd, 15.4, 10.7, 4.9)	135.1d	C-10, C-11, C-19	H-10 α , H-10 β , H-8
10 α	2.52 (m)		C-12, C-11, C-8, C-9	H-10 β , H-11, H-9
10 β	2.39 (m)	38.2t	C-12, C-11, C-8, C-9	H-10 α , H-11, H-9
11	3.60 (m)	72.2d	C-24, C-13, C-9	H-12, H-10 α , H-10 β
12	2.00 (m)	44.3d	C-24, C-10, C-13, C-11	H-11, H-13, H-24
13	4.38 (d, 9.4)	70.7d	C-24, C-25, C-12, C-15, C-14	H-12
14		138.0s		
15	5.44 (dd, 10.2, 4.1)	130.6d	C-25, C-13	H-16 α , H-16 β
16 α	3.02(m)		C-17, C-15, C-14	H-16 β , H-17 α , H-17 β , H-15
16 β	1.81 (m)	29.6t	C-17, C-15, C-14	H-16 α , H-17 α , H-17 β , H-15
17 α	2.87 (m)		C-16, C-23, C-18, C-19	H-16 α , H-16 β , H-17 β
17 β	2.22 (m)	34.0t	C-16, C-23, C-18, C-19	H-16 α , H-16 β , H-17 α
18		132.6s		
19		140.0s		
20		125.5s		
21	7.22 (d, 2.8)	107.2d	C-23, C-20, C-19, C-22	H-23
22		151.3s		
23	6.45 (d, 2.8)	115.5d	C-17, C-21, C-19, C-22	H-21
24	1.10 (d, 6.9)	10.6q	C-12, C-13, C-11	H-12
25	1.77 (s)	19.3q	C-13, C-15, C-14	
MeO-3	3.35 (s)	57.6q	C-3	

Table S2: NMR spectroscopy data [(CD₃)₂CO] for compound **2**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		171.7s		
2 α	2.79 (dd, 17.3, 5.3)	38.4t	C-1	H-2 β , H-3
2 β	2.59 (d, 17.5)		C-4, C-3, C-1	H-2 α
3	4.20 (t, 4.9)	75.0d	MeO-3, C-1	H-2 α , H-4
4	3.97 (dd, 7.5, 4.9)	63.4d	C-3, C-6	H-3, H-5
5	4.94 (t, 7.0)	75.1d	C-4, C-3, C-6, C-19	H-4, H-6
6	5.95 (dd, 15.7, 6.3)	126.9d	C-4, C-5, C-8	H-7, H-5
7	6.65 (dd, 15.6, 10.3)	138.5d	C-9, C-5	H-8, H-6
8	6.23 (dd, 15.1, 10.3)	131.6d	C-10, C-6, C-7	H-9, H-7
9	5.81 (dt, 15.2, 7.6)	134.8d	C-10, C-11, C-7	H-10 α , H-10 β , H-8
10 α	2.45 (m)		C-12, C-11, C-8, C-9	H-10 β , H-11, H-9
10 β	2.38 (m)	37.8t	C-12, C-11, C-8, C-9	H-10 α , H-11, H-9
11	3.68 (m)	72.8d	C-24, C-13, C-9	H-12, H-10 α , H-10 β
12	1.93 (m)	42.9d	C-24, C-10, C-13, C-11	H-11, H-13, H-24
13	4.44 (d, 3.1)	70.2d		H-12
14		138.9s		
15	5.23 (t, 5.6)	129.1d	C-17, C-13	H-16 α , H-16 β
16 α	2.06(m)			H-16 β , H-17 α , H-17 β , H-15
16 β	2.47 (m)	28.5t	C-17	H-16 α , H-17 α , H-17 β , H-15
17 α	2.82 (dt, 12.6, 5.5)		C-16, C-23, C-15, C-18, C-19	H-16 α , H-16 β , H-17 β
17 β	2.28 (dt, 12.5, 4.6)	33.0t	C-16, C-23, C-15, C-18, C-19	H-16 α , H-16 β , H-17 α
18		131.9s		
19		138.4s		
20		127.5s		
21	7.56 (d, 2.4)	105.3d	C-23, C-20, C-19, C-22	H-23
22		151.6s		
23	6.42 (d, 2.7)	113.5d	C-17, C-21, C-19, C-22	H-21
24	1.00 (d, 6.9)	11.3q	C-11, C-12, C-13	H-12
25	1.76 (s)	20.1q	C-13, C-14, C-15	
MeO-3	3.35 (s)	57.0q	C-3	

Table S3: NMR spectroscopy data (CD₃OD) for compound **3**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		172.5s		
2 α	2.78 (m)	45.5t	C-4, C-3, C-1	H-2 β , H-3
2 β	2.73 (dd, 11.4, 5.6)		C-4, C-3, C-1	H-2 α , H-3
3	4.00 (dt, 9.7, 5.6)	82.1d	C-2, MeO-3, C-5	H-2 α , H-2 β , H-4
4	5.57 (dd, 15.6, 8.8)	130.6d	C-2, C-6	H-3, H-5
5	6.04 (dd, 15.6, 9.8)	135.5d	C-3, C-6, C-7	H-4, H-6
6	5.86 (dd, 14.8, 9.8)	128.3d	C-8, C-9, C-7	H-7, H-5
7	5.98 (dd, 14.8, 10.3)	137.0d	C-6, C-9	H-8, H-6
8	5.90 (dd, 14.6, 10.5)	131.7d	C-10, C-6	H-9, H-7
9	5.52 (ddd, 14.7, 9.1, 6.7)	136.0d	C-10, C-11, C-7	H-10 α , H-10 β , H-8
10 α	2.27 (dd, 13.3, 6.6)		C-12, C-11, C-8, C-9	H-10 β , H-9
10 β	1.85 (dt, 13.3, 9.5)	37.6t	C-12, C-8, C-9	H-10 α , H-11, H-9
11	3.28 (t, 10.2)	84.2d	C-24, C-12, C-9	H-12, H-10 β
12	1.67 (m)	43.5d	C-24, C-10, C-13, C-11	H-11, H-13, H-24
13	3.82 (d, 10.0)	84.0d	C-24, C-25, C-12, C-15, C-14	H-12
14		85.2s		
15	3.38 (t, 2.9)	48.9d	C-16, C-17, C-23	H-16 α , H-16 β
16 α	1.72 (dt, 14.2, 3.9)		C-17, C-15, C-14	H-16 β , H-17 α , H-17 β , H-15
16 β	2.50 (ddd, 14.2, 6.4, 3.6)	22.8t	C-18	H-16 α , H-15
17 α	2.44 (ddd, 18.4, 13.8, 4.7)		C-16, C-18, C-23	H-16 α , H-17 β
17 β	2.77 (m)	19.6t	C-15, C-18, C-23	H-16 α , H-17 α
18		134.5s		
19		179.0s		
20		140.5s		
21	7.15 (s)	114.0d	C-20, C-23, C-19	
22		186.3s		
23		147.9s		
24	1.03 (d, 6.4)	13.0q	C-11, C-12, C-13	H-12
25	1.14 (s)	20.5q	C-13, C-14, C-15	
MeO-3	3.32 (s)	56.7q	C-3	

Table S4: NMR spectroscopy data (CD₃OD) for compound **4**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		172.0s		
2 α	2.88 (dd, 12.7, 4.4)	44.1t	C-4, C-3, C-1	H-2 β , H-3
2 β	2.71 (dd, 12.5, 10.2)		C-4, C-3, C-1	H-2 α , H-3
3	4.15 (dt, 9.5, 4.4)	81.3d	C-2, MeO-3, C-5, C-1	H-2 α , H-2 β , H-4
4	5.58 (dd, 15.3, 8.0)	131.1d	C-2, C-3, C-6	H-3, H-5
5	6.27 (m)	136.1d	C-3, C-6, C-7	H-4, H-6
6	6.11 (m)	130.2d	C-8	H-7, H-5
7	6.10 (m)	135.8d	C-5, C-6	H-8, H-6
8	6.07 (m)	133.7d	C-10, C-6, C-7	H-9, H-7
9	5.74 (ddd, 14.7, 8.9, 6.1)	132.1d	C-10, C-11, C-7	H-10 α , H-10 β , H-8
10 α	2.41 (m)		C-12, C-11, C-8, C-9	H-10 β , H-11, H-9
10 β	2.31 (m)	37.5t	C-12, C-11, C-8, C-9	H-10 α , H-11, H-9
11	3.65 (dt, 6.7, 3.2)	72.8d	C-24, C-9	H-12, H-10 α , H-10 β
12	1.81 (m)	41.8d	C-24, C-10, C-13, C-11	H-11, H-13, H-24
13	4.69 (d, 4.8)	70.5d	C-24, C-25, C-12	H-12
14		140.2s		
15	5.19 (t, 8.0)	125.9d	C-25, C-17, C-13	H-16 α , H-16 β
16 α	2.39(m)		C-17, C-18, C-15, C-14	H-16 β , H-17 α , H-17 β , H-15
16 β	2.18 (m)	27.6t		H-16 α , H-17 α , H-17 β , H-15
17 α	2.97 (m)		C-16, C-18, C-15, C-23, C-19	H-16 α , H-16 β , H-17 β
17 β	2.84 (m)	33.0t	C-16, C-18, C-15, C-23, C-19	H-16 α , H-16 β , H-17 α
18		123.7s		
19		146.3s		
20		128.5s		
21	8.14 (s)	114.4d	C-20, C-23, C-19	
22		147.0s		
23		133.5s		
24	0.87 (d, 6.9)	10.5q	C-12, C-13, C-11	H-12
25	1.74 (s)	20.6q	C-13, C-15, C-14	
26	9.02 (s)	154.5d	C-23, C-22	
MeO-3	3.36 (s)	56.8q	C-3	

Table S5: NMR spectroscopy data (CD₃OD) for compound **5**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		172.0s		
2 α	2.76 (m)	45.9t	C-4, C-3, C-1	H-2 β , H-3
2 β	2.66 (dd, 12.7, 9.6)		C-4, C-3, C-1	H-2 α , H-3
3	4.56 (m)	71.6d		H-2 α , H-2 β , H-4
4	5.64 (dd, 15.3, 7.3)	133.0d	C-2, C-3, C-5, C-6	H-3, H-5
5	6.21 (dd, 15.2, 10.0)	133.6d	C-3, C-6, C-7	H-4, H-6
6	6.10 (m)	130.4d	C-8	H-7, H-5
7	6.13 (dd, 14.7, 9.8)	135.5d	C-5, C-9	H-8, H-6
8	6.06 (m)	133.8d	C-6, C-7, C-10	H-9, H-7
9	5.73 (m)	131.8d	C-7, C-10, C-11	H-10 α , H-10 β , H-8
10 α	2.45 (m)		C-12, C-11, C-8, C-9	H-10 β , H-11, H-9
10 β	2.32 (m)	37.6t	C-8, C-9	H-10 α , H-11, H-9
11	3.65 (m)	72.9d		H-12, H-10 α , H-10 β
12	1.81 (m)	42.0d	C-24, C-10, C-13, C-11	H-11, H-13, H-24
13	4.67 (d, 4.9)	70.6d	C-24, C-25, C-12, C-14, C-15	H-12
14		139.6s		
15	5.20 (d, 8.0)	126.5d	C-25, C-17, C-13	H-16 α , H-16 β
16 α	2.31 (m)		C-17, C-15, C-14	H-16 β , H-17 α , H-17 β , H-15
16 β	2.03 (m)	27.9t		H-16 α , H-17 α , H-17 β , H-15
17 α	2.81 (m)		C-16, C-18, C-15, C-23, C-19	H-16 α , H-16 β , H-17 β
17 β	2.76 (m)	29.9t	C-16, C-18, C-15, C-23, C-19	H-16 α , H-16 β , H-17 α
18		130.1s		
19		144.3s		
20		126.4s		
21	7.10 (s)	110.4d	C-20, C-23, C-19, C-22	
22		131.1s		
23		119.1s		
24	0.89 (d, 6.8)	10.5q	C-12, C-13, C-11	H-12
25	1.75 (s)	20.5q	C-13, C-15, C-14	
26	3.35 (m)		C-23, C-27	
	3.33 (m)	30.7t	C-23, C-27	
27		168.3s		

Table S6: NMR spectroscopy data (CD₃OD) for compound **6**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		171.2s		
2 α	2.68 (dd, 12.0, 4.3)	46.9t	C-4, C-3, C-1	H-2 β , H-3
2 β	2.51 (m)		C-4, C-3, C-1	H-2 α , H-3
3	4.51 (m)	72.0d		H-2 α , H-2 β , H-4
4	5.69 (dd, 14.4, 7.7)	134.3d	C-6	H-3, H-5
5	6.11 (m)	132.7d	C-3	H-4, H-6
6	6.16 (m)	130.9d	C-8	H-7, H-5
7	6.06 (m)	135.0d	C-5	H-8, H-6
8	6.09 (m)	133.8d	C-6	H-9, H-7
9	5.70 (m)	131.7d	C-7	H-10 α , H-10 β , H-8
10 α	2.41 (m)		C-12, C-11, C-8, C-9	H-10 β , H-11, H-9
10 β	2.31 (m)	37.7t	C-12, C-11, C-8, C-9	H-10 α , H-11, H-9
11	3.66 (m)	73.0d		H-12, H-10 α , H-10 β
12	1.85 (m)	42.5d	C-24, C-10, C-11	H-11, H-13, H-24
13	4.63 (d, 6.1)	70.7d	C-24, C-25, C-12, C-14, C-15	H-12
14		139.1s		
15	5.25 (dd, 8.2, 4.9)	127.1d		H-16 α , H-16 β
16 α	2.29(m)		C-17, C-15, C-14	H-16 β , H-17 α , H-17 β , H-15
16 β	2.01 (m)	30.6t		H-16 α , H-17 α , H-17 β , H-15
17 α	2.48 (m)		C-16, C-18, C-23	H-16 α , H-16 β , H-17 β
17 β	2.44 (m)	37.5t	C-16, C-18, C-23	H-16 α , H-16 β , H-17 α
18		145.1s		
19	6.42 (t, 1.7)	113.1d	C-20, C-23, C-17, C-21	H-21, H-23
20		140.1s		
21	7.02 (t, 2.0)	107.1d	C-20, C-19, C-22	H-19, H-23
22		158.6s		
23	6.38 (t, 1.7)	112.8d	C-19, C-22, C-17, C-21	H-19, H-21
24	0.95 (d, 6.9)	10.5q	C-12, C-13, C-11	H-12
25	1.76 (s)	20.3q	C-13, C-15, C-14	

Table S7: NMR spectroscopy data (CD₃OD) for compound **7**

position	δ_{H} (mult, J in Hz)	δ_{C} mult.	HMBC	^1H - ^1H COSY
1		171.1s		
2 α	2.72 (dd, 12.1, 4.4)	47.0t	C-4, C-3, C-1	H-2 β , H-3
2 β	2.46 (m)		C-4, C-3, C-1	H-2 α , H-3
3	4.52 (m)	72.1d	C-5	H-2 α , H-2 β , H-4
4	5.65 (dd, 14.9, 7.8)	134.7d	C-6	H-3, H-5
5	6.16 (m)	132.8d	C-4, C-3, C-7	H-4, H-6
6	6.18 (m)	131.3d	C-9	H-7, H-5
7	6.17 (m)	134.6d	C-5	H-8, H-6
8	6.10 (m)	133.3d	C-10, C-6, C-7	H-9, H-7
9	6.02 (m)	132.2d	C-8	H-10 α , H-10 β , H-8
10 α	2.68 (m)		C-8	H-10 β , H-11, H-9
10 β	2.33 (dd, 14.6, 10.1)	41.8t	C-8, C-11, C-12	H-10 α , H-11, H-9
11	3.88 (d, 5.9)	77.0d	C-24, C-12, C-13, C-9	H-12, H-10 α , H-10 β
12	1.72 (m)	39.2d	C-24, C-10, C-11	H-11, H-13, H-24
13	3.97 (d, 10.1)	74.7d	C-24, C-14, C-15, C-11	H-12, H-14
14	1.76 (m)	43.9d	C-25, C-16, C-15	H-25, H-15, H-13
15	3.74 (m)	72.4d	C-25, C-17	H-16 α , H-16 β
16 α	1.59 (m)		C-17,	H-16 β , H-17 α , H-17 β , H-15
16 β	1.46 (m)	33.3t	C-15	H-16 α , H-17 α , H-17 β , H-15
17 α	2.82 (m)		C-16, C-18	H-16 α , H-16 β , H-17 β
17 β	2.45 (m)	33.4t	C-16, C-18	H-16 α , H-16 β , H-17 α
18		145.7s		
19	6.58 (s)	112.7d	C-17, C-21, C-23, C-20	H-21, H-23
20		140.0s		
21	6.86 (s)	107.0d	C-19, C-20, C-22	H-19, H-23
22		158.6s		
23	6.42 (s)	113.4d	C-17, C-21, C-19, C-22	H-19, H-21
24	1.05 (d, 7.0)	12.1q	C-12, C-13, C-11	H-12
25	0.69 (d, 6.8)	10.6q	C-13, C-15, C-14	H-14

Figure S1. ^1H NMR (600 MHz, CD_3OD) spectrum for compound **1**

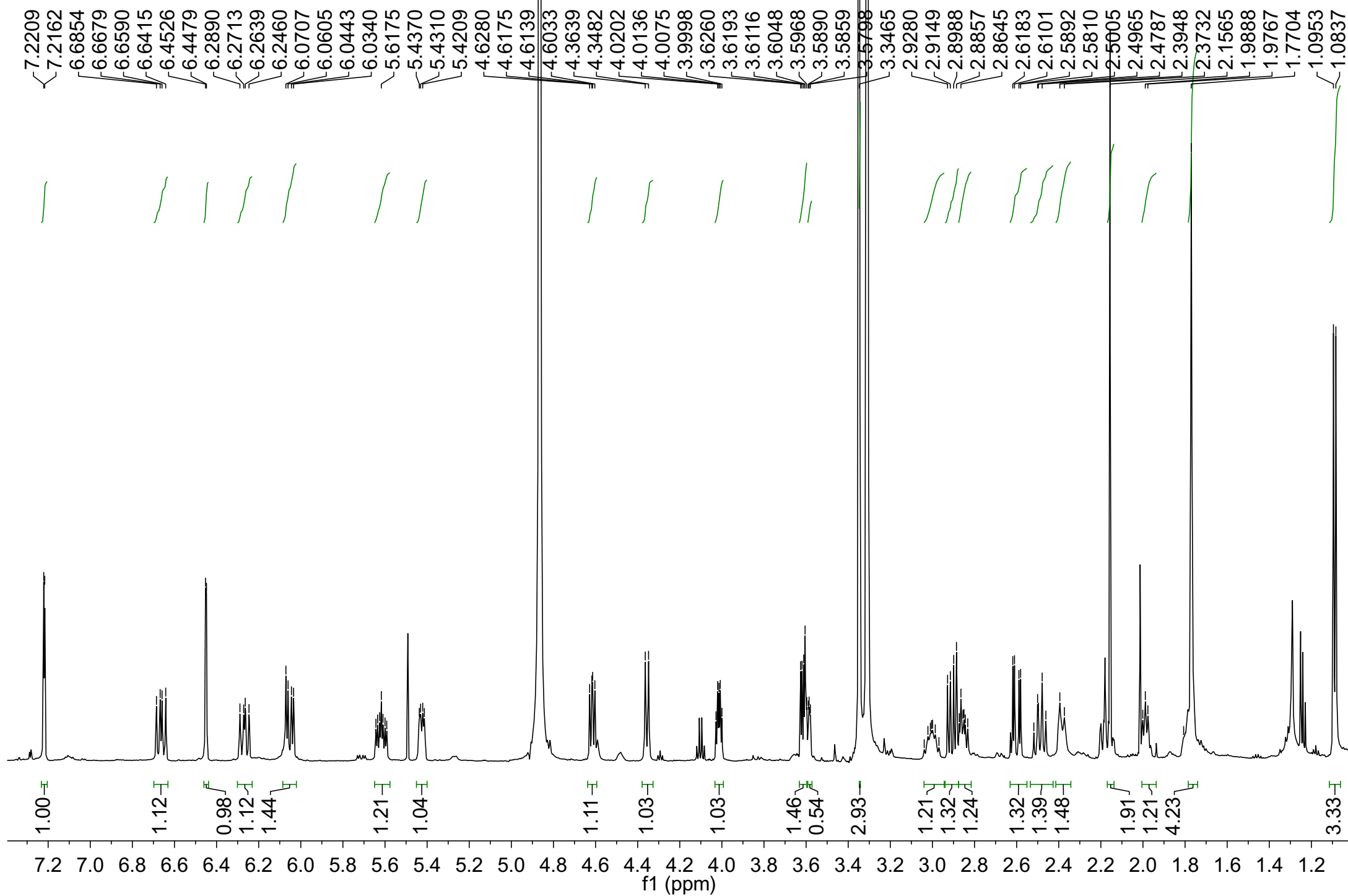


Figure S2. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **1**

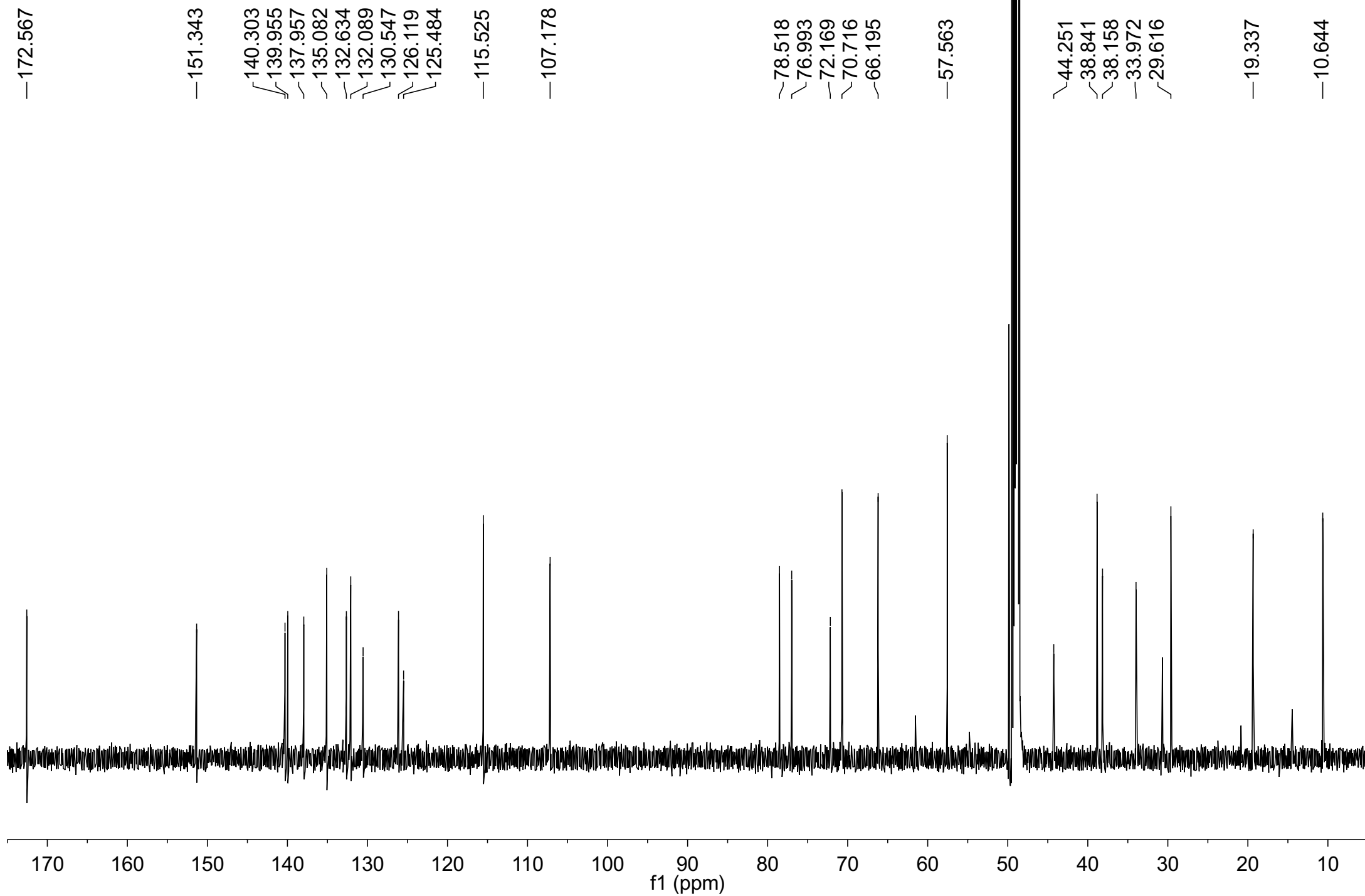


Figure S3. HSQC spectrum for compound **1**

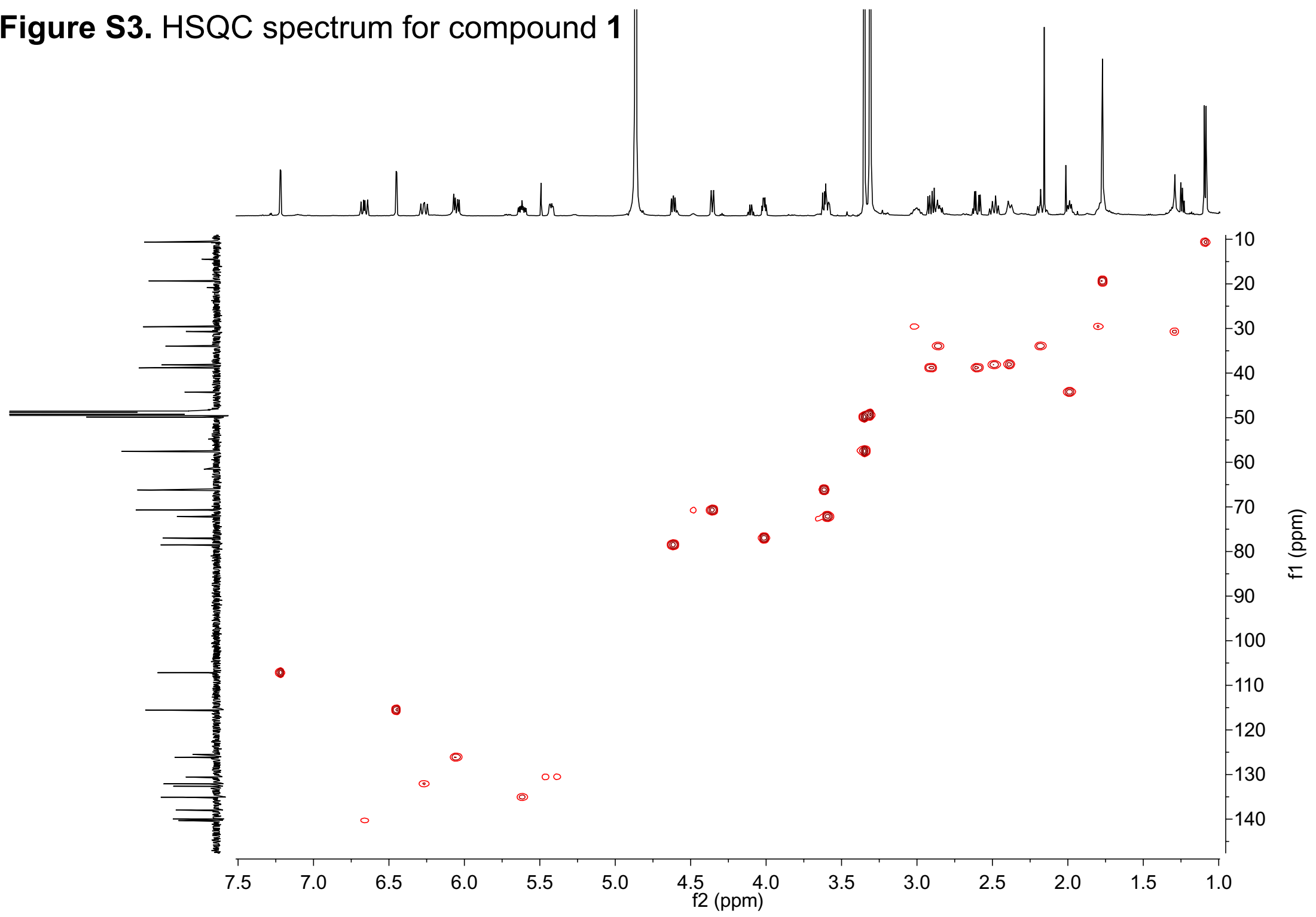


Figure S4. HMBC spectrum for compound **1**

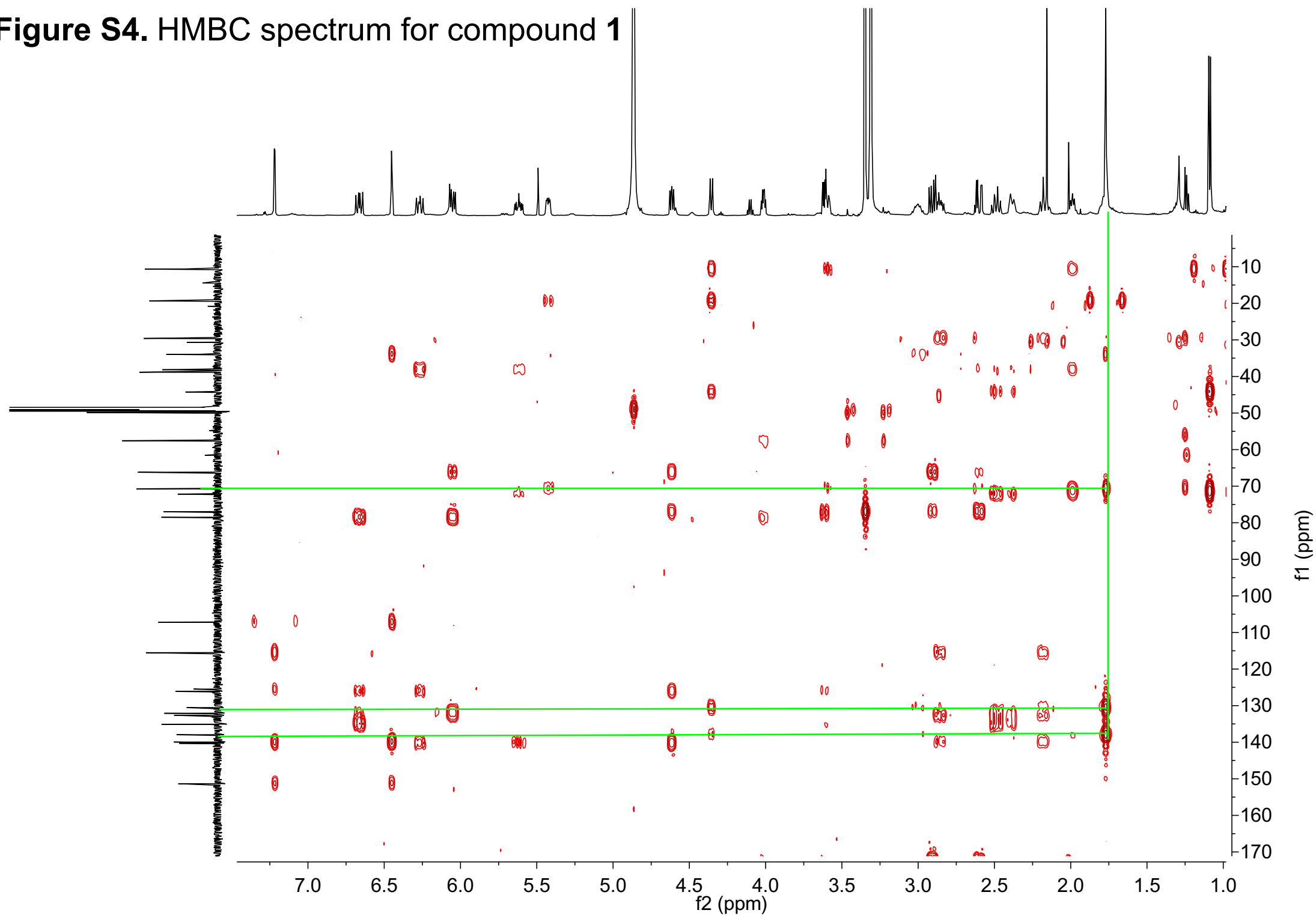


Figure S5. Enlarged HMBC spectrum 1 for compound **1**

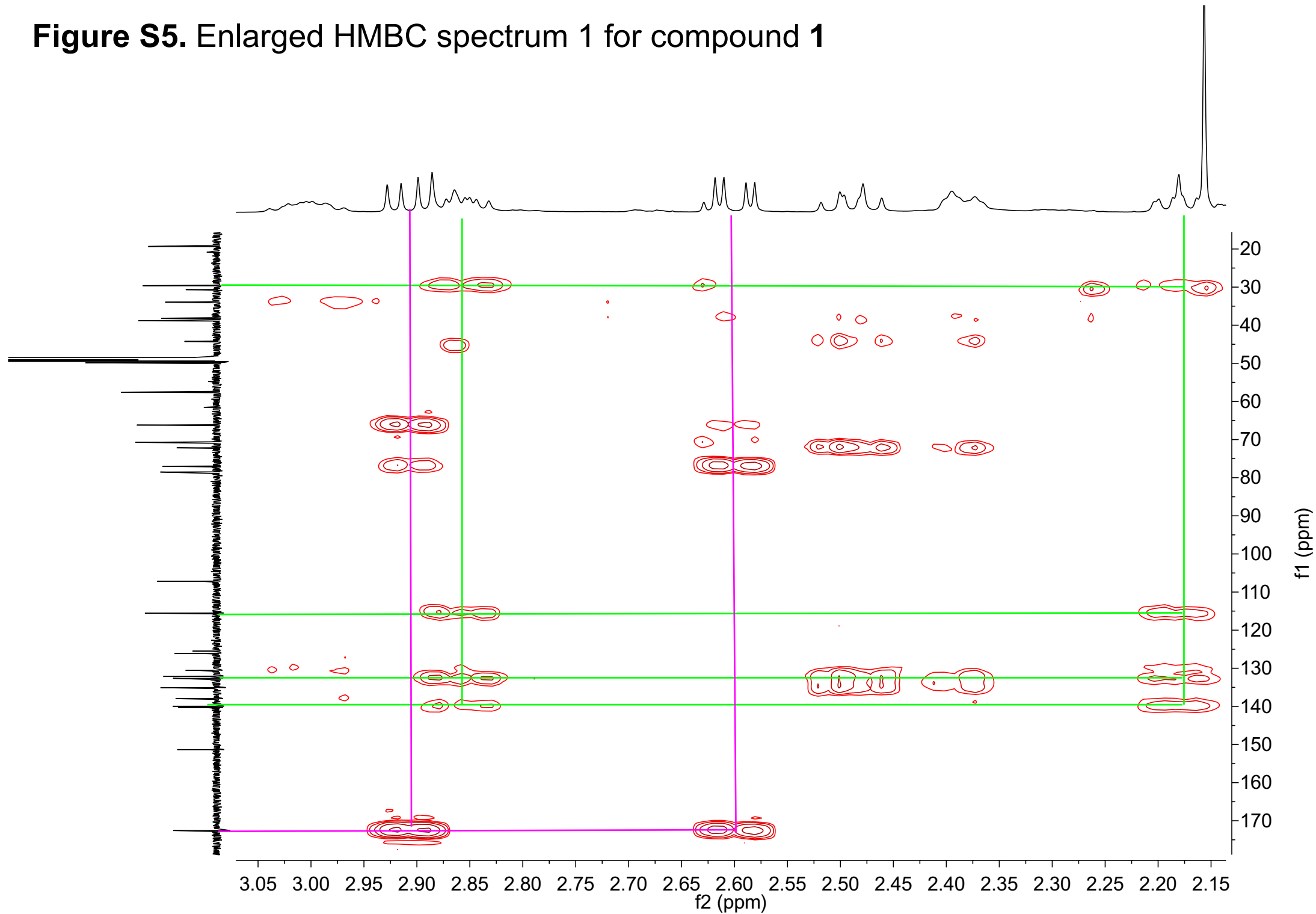


Figure S6. Enlarged HMBC spectrum 2 for compound **1**

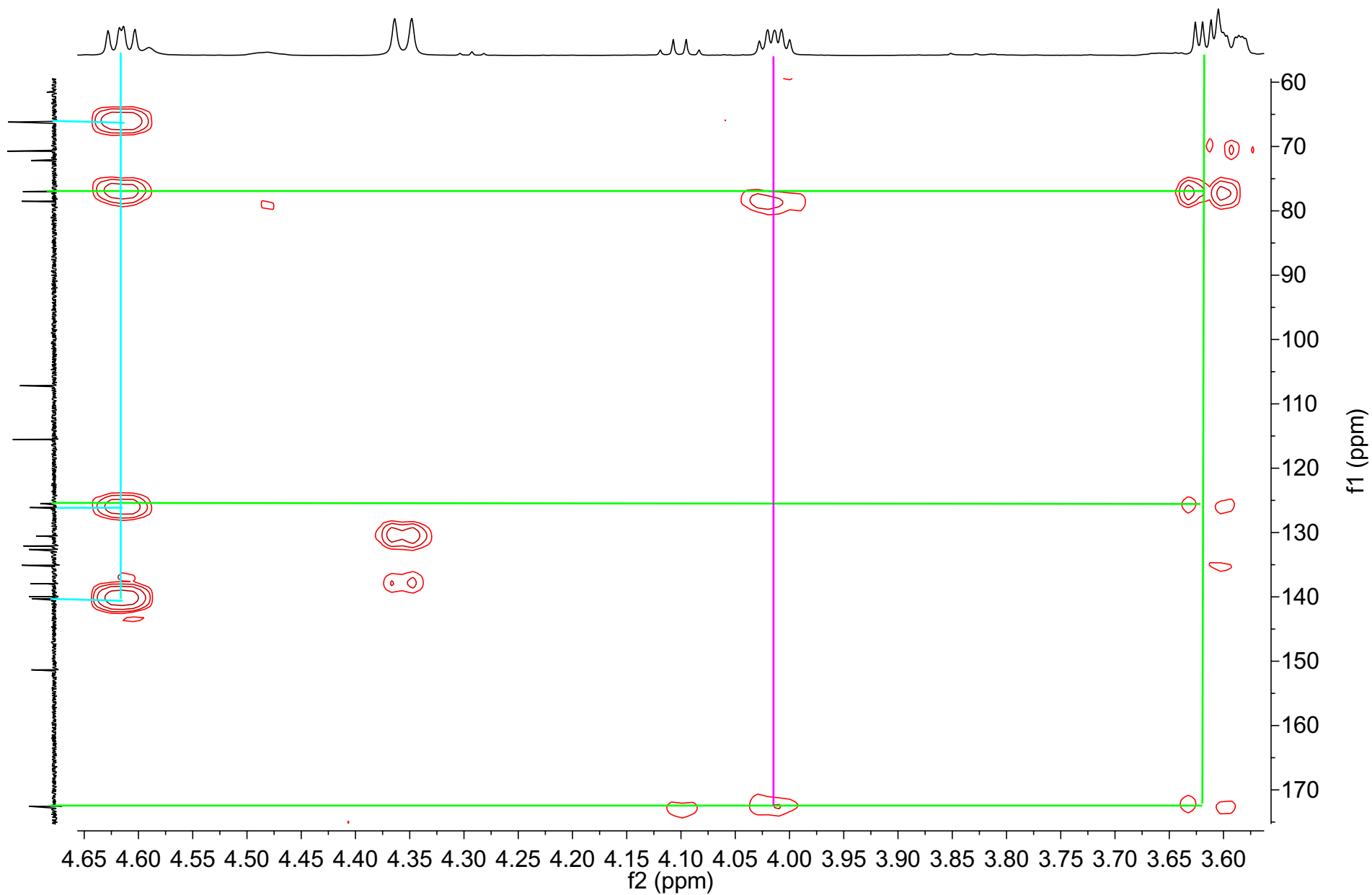


Figure S7. Enlarged HMBC spectrum 3 for compound **1**

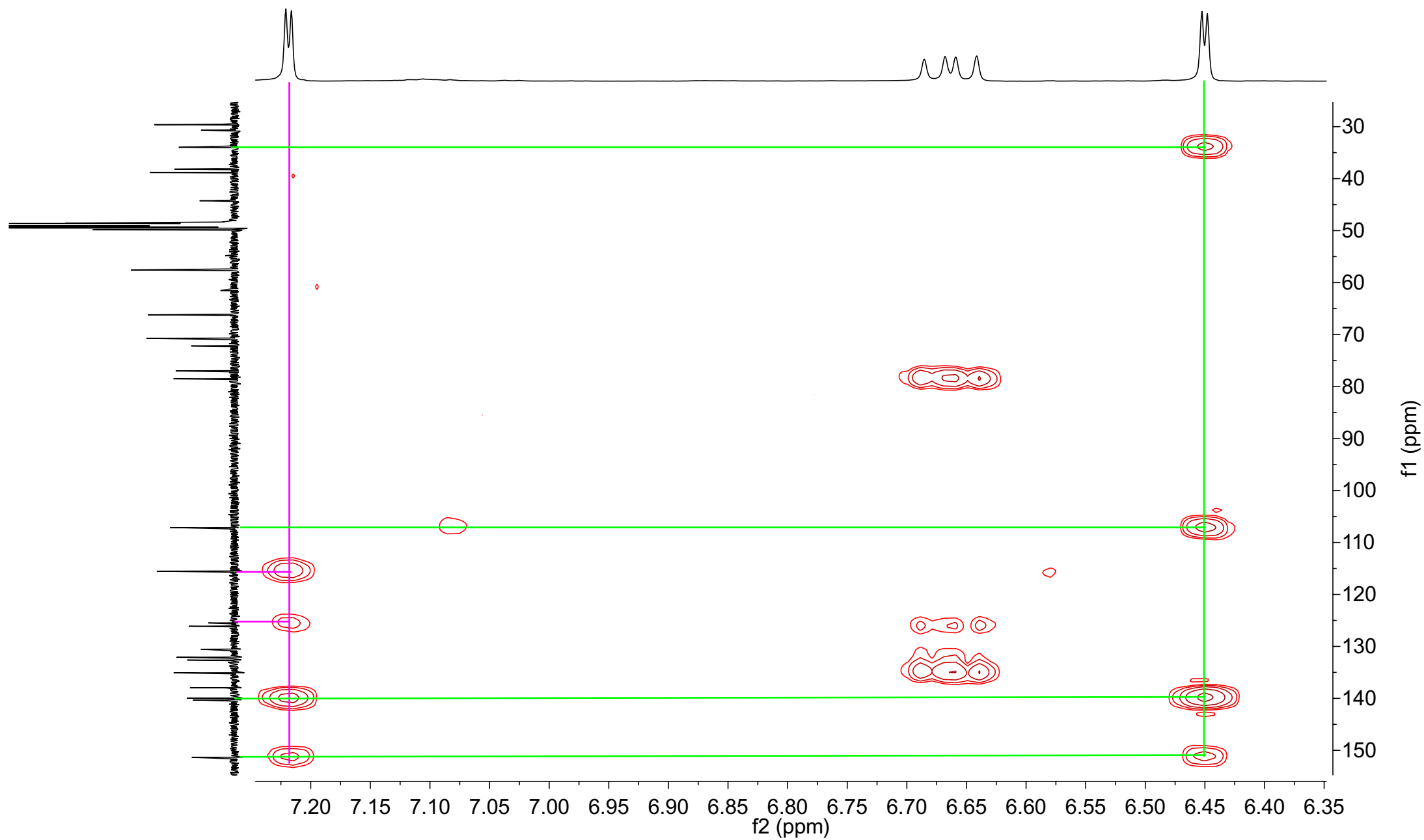


Figure S8. ^1H - ^1H COSY spectrum for compound **1**

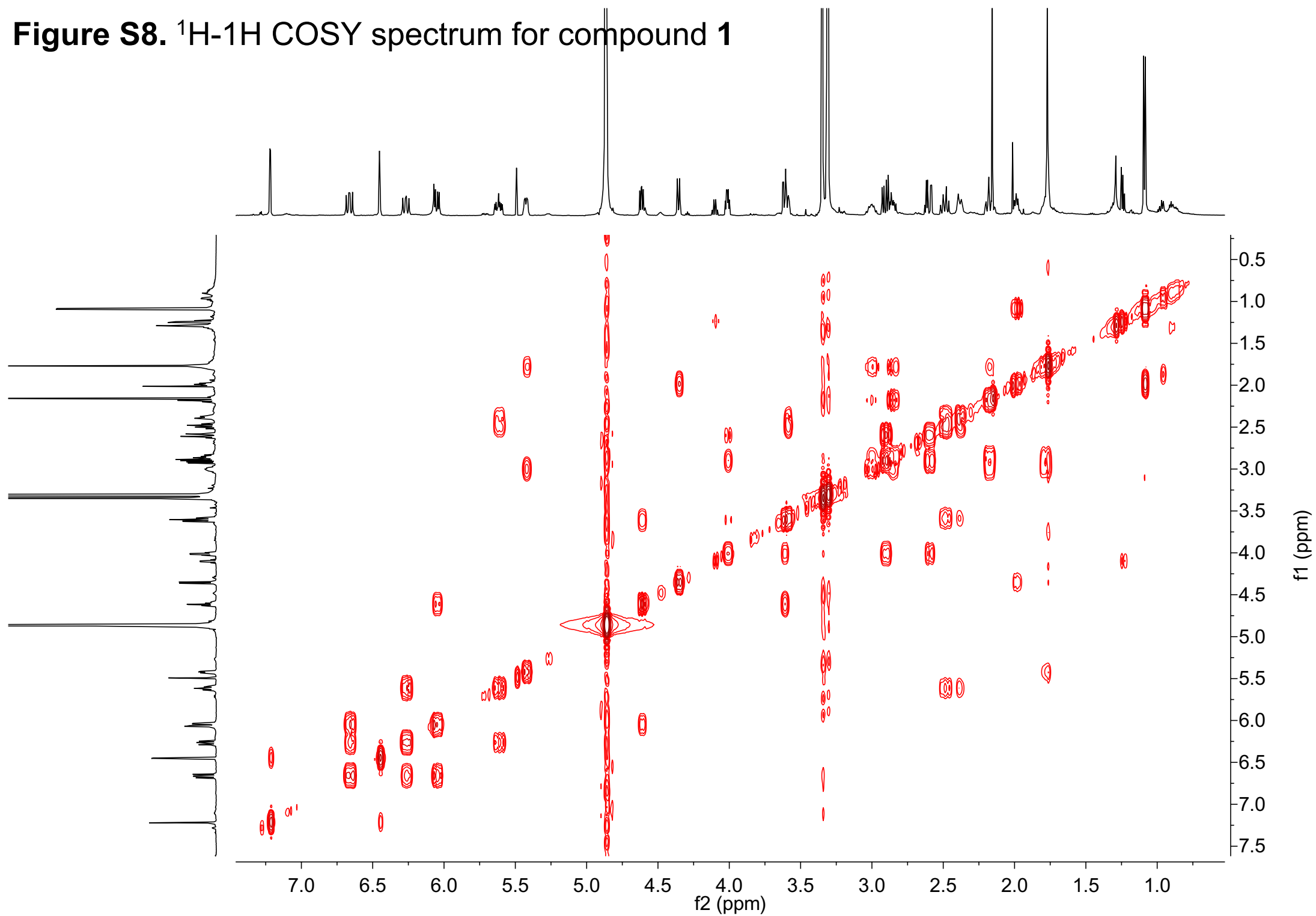


Figure S9. NOESY spectrum for compound 1

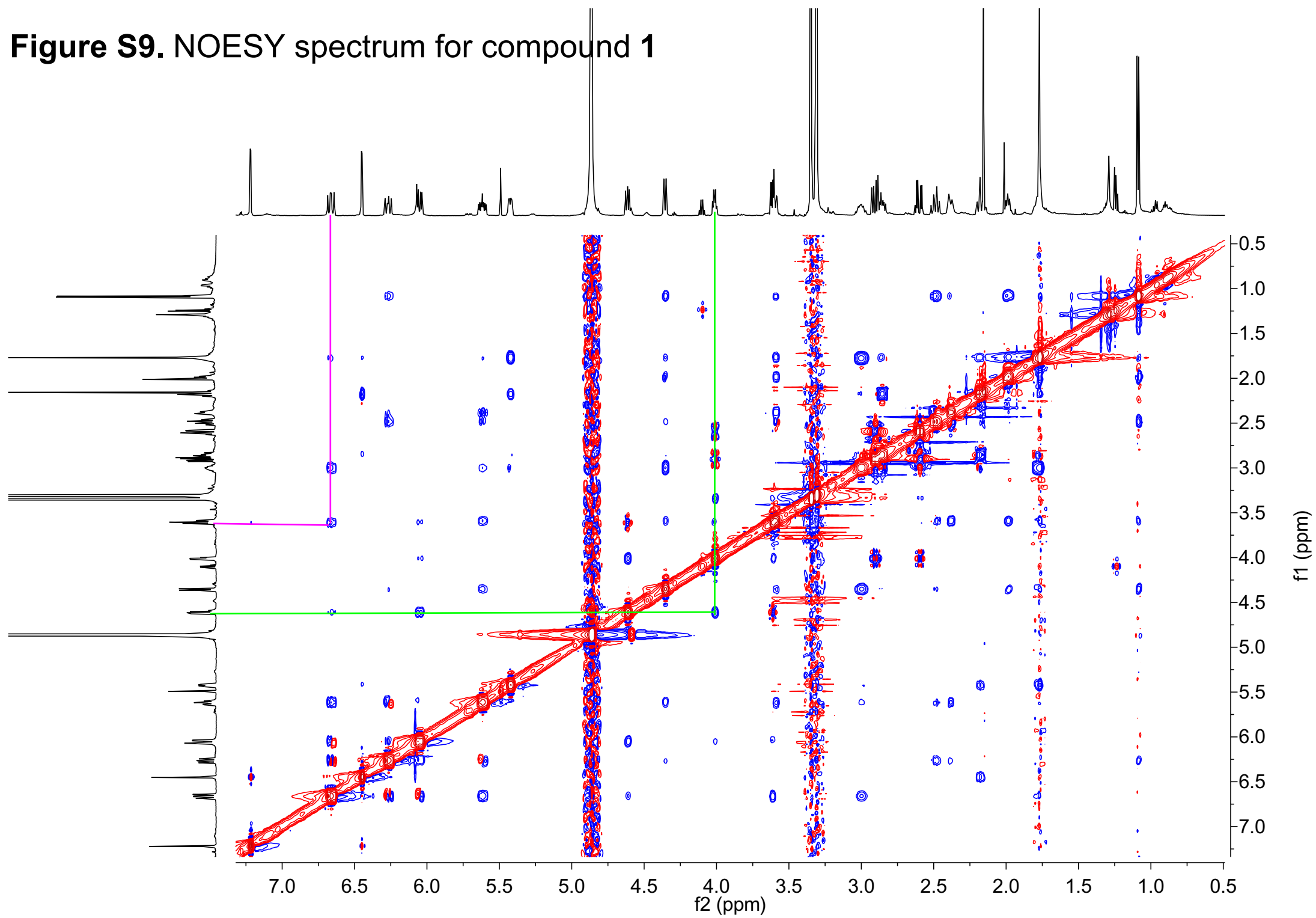


Figure S10. ^1H NMR [600 MHz, $(\text{CD}_3)_2\text{CO}$] spectrum for compound **2**

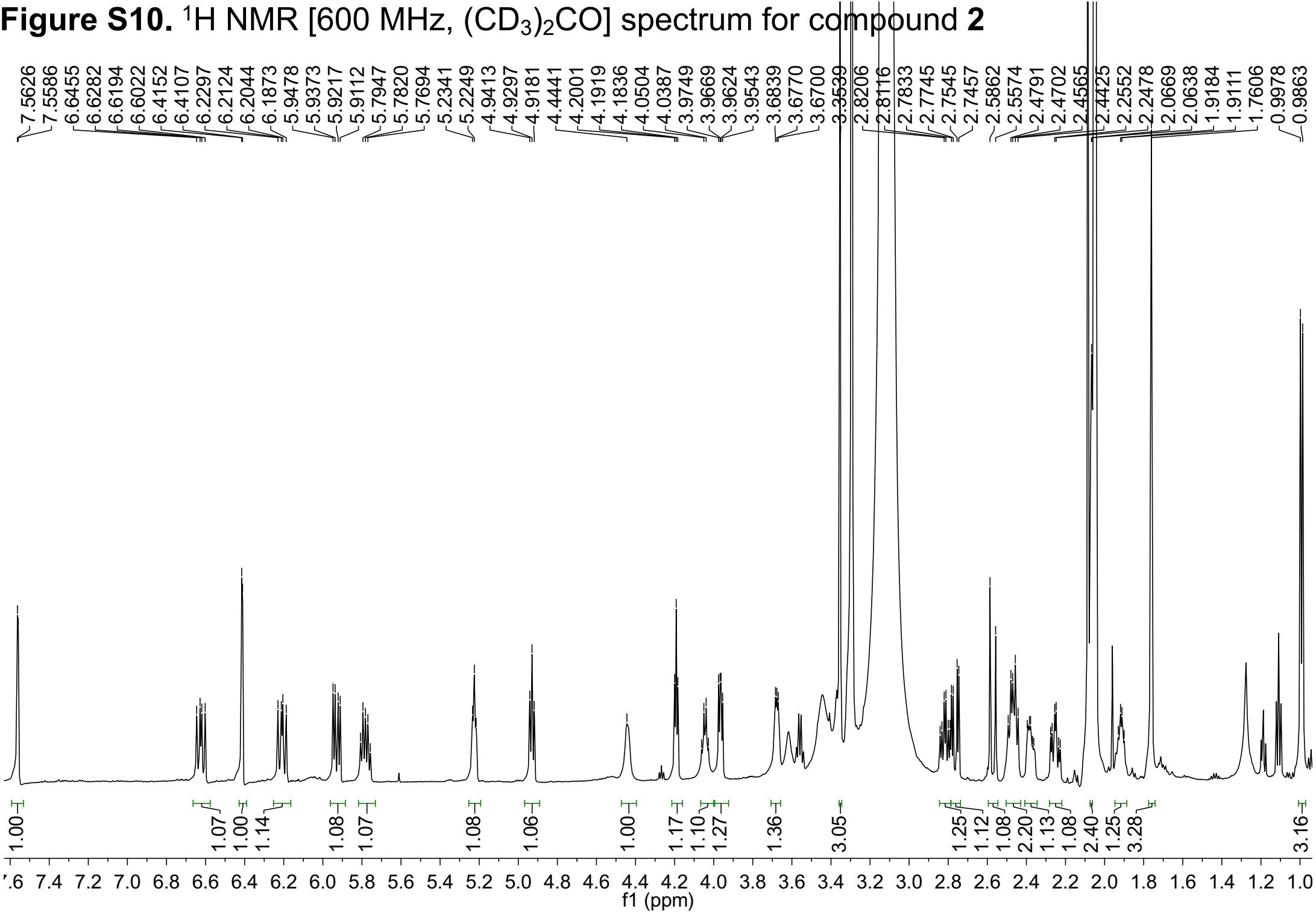


Figure S11. ^{13}C NMR [151 MHz, $(\text{CD}_3)_2\text{CO}$] spectrum for compound **2**

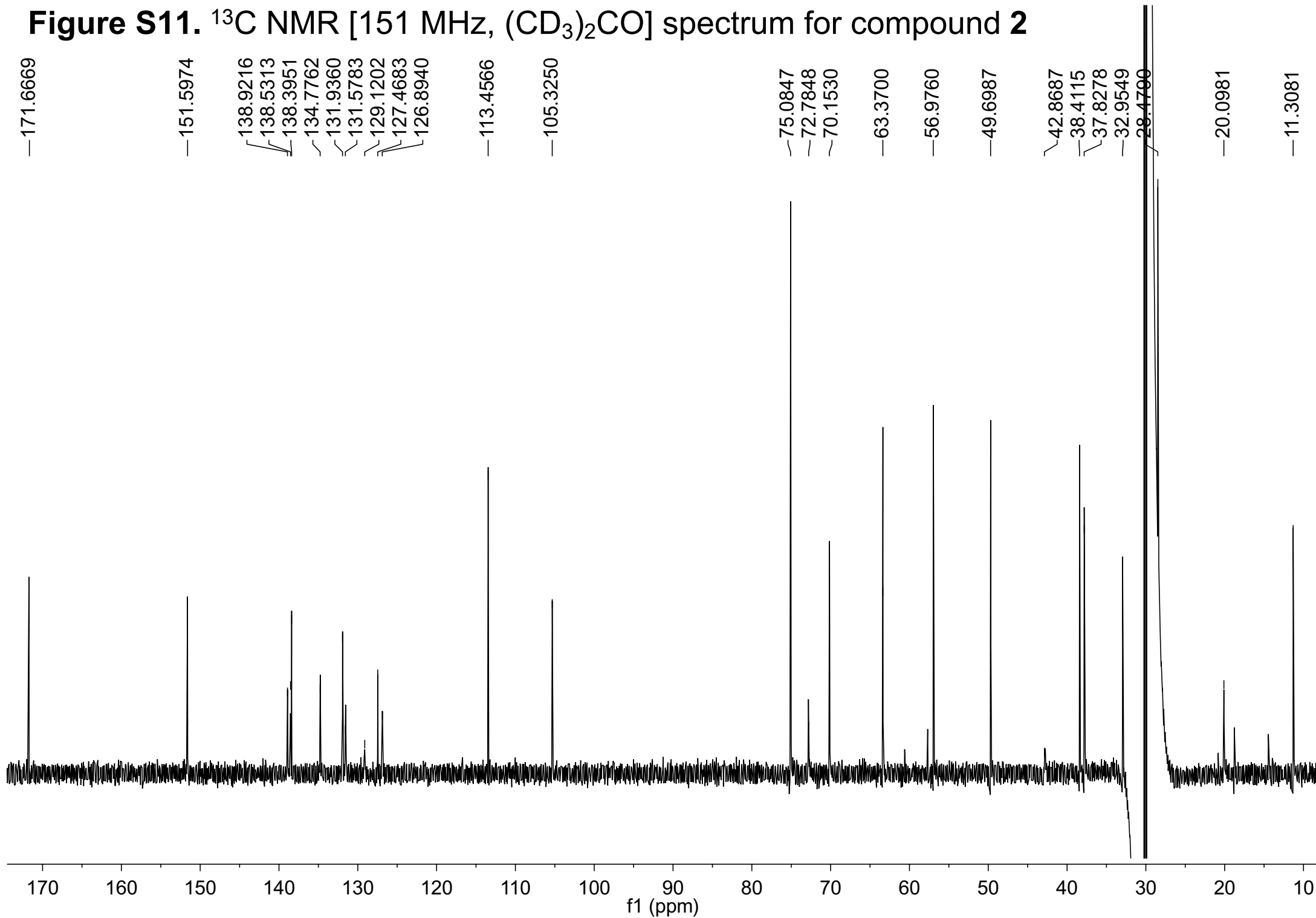


Figure S12. HSQC spectrum for compound **2**

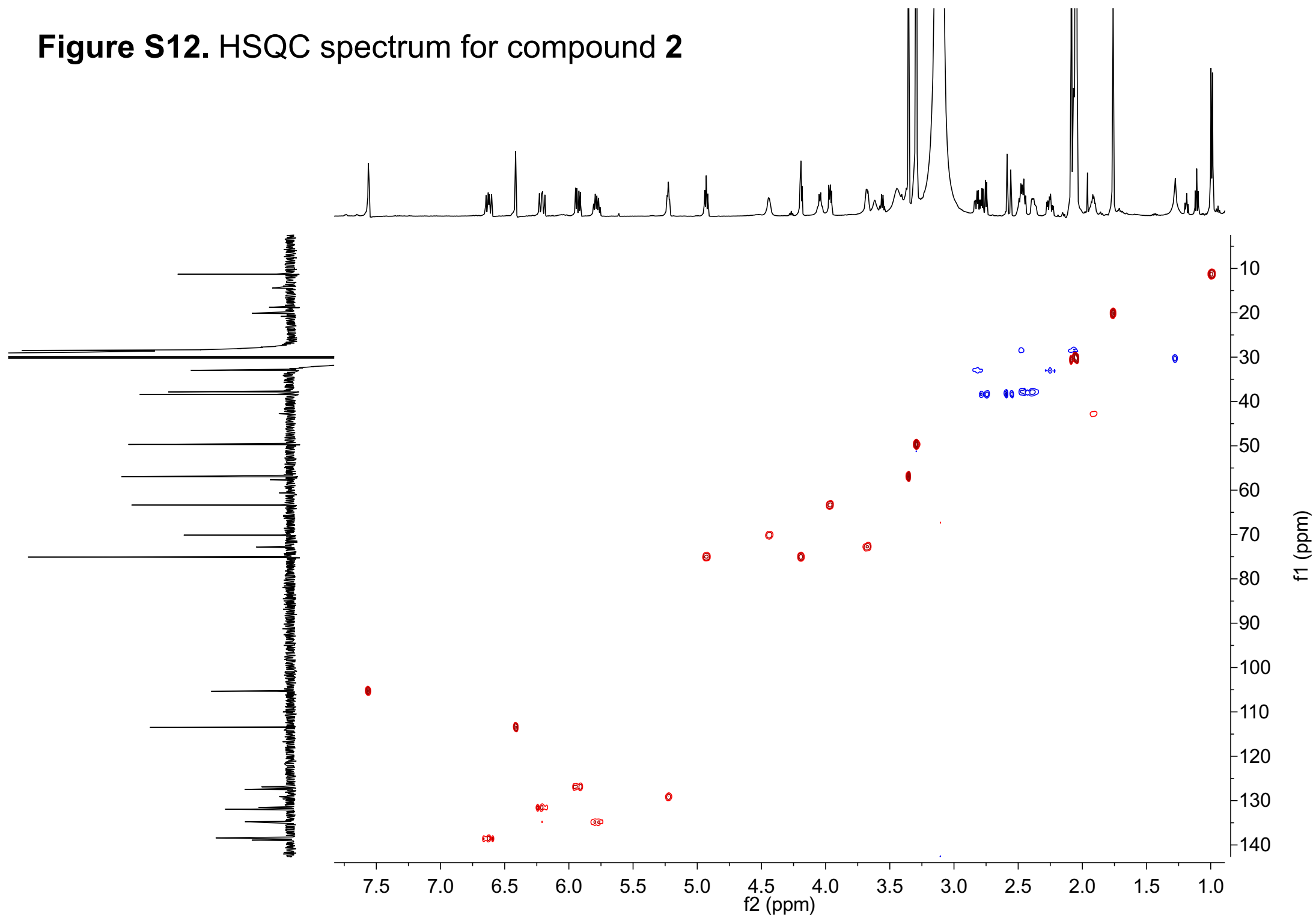


Figure S13. HMBC spectrum for compound **2**

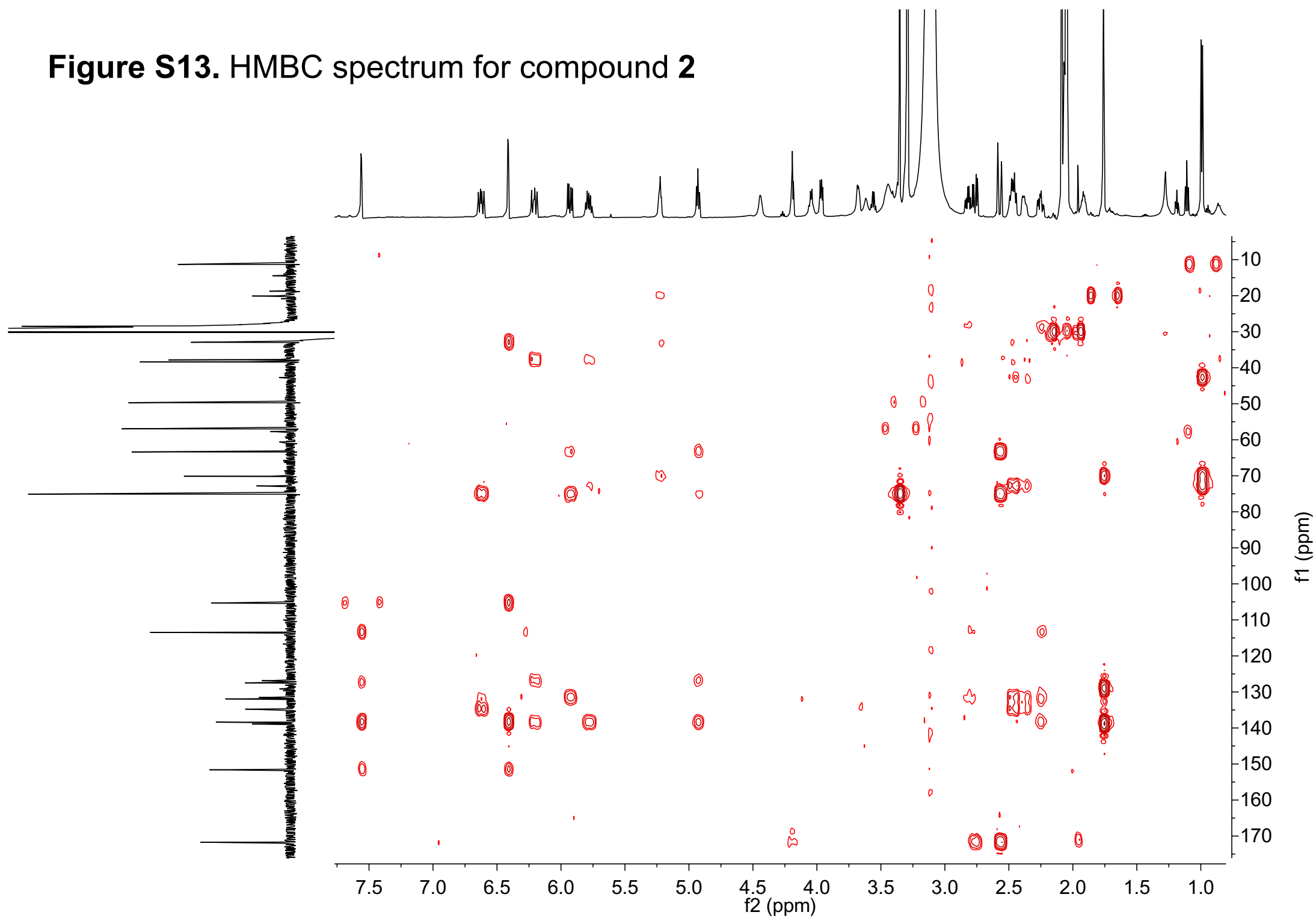


Figure S14. ^1H - ^1H COSY spectrum for compound **2**

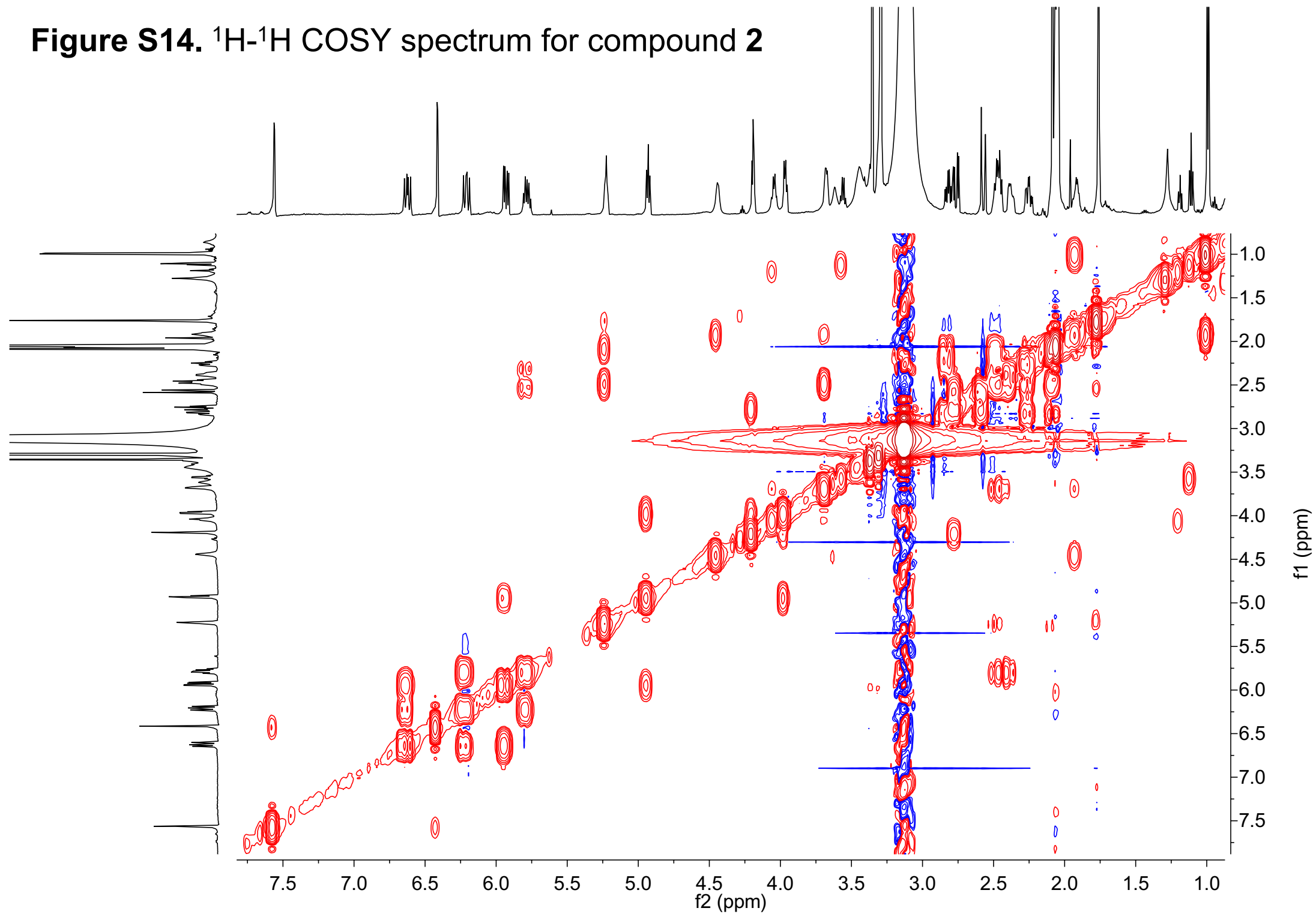


Figure S15. NOESY spectrum for compound 2

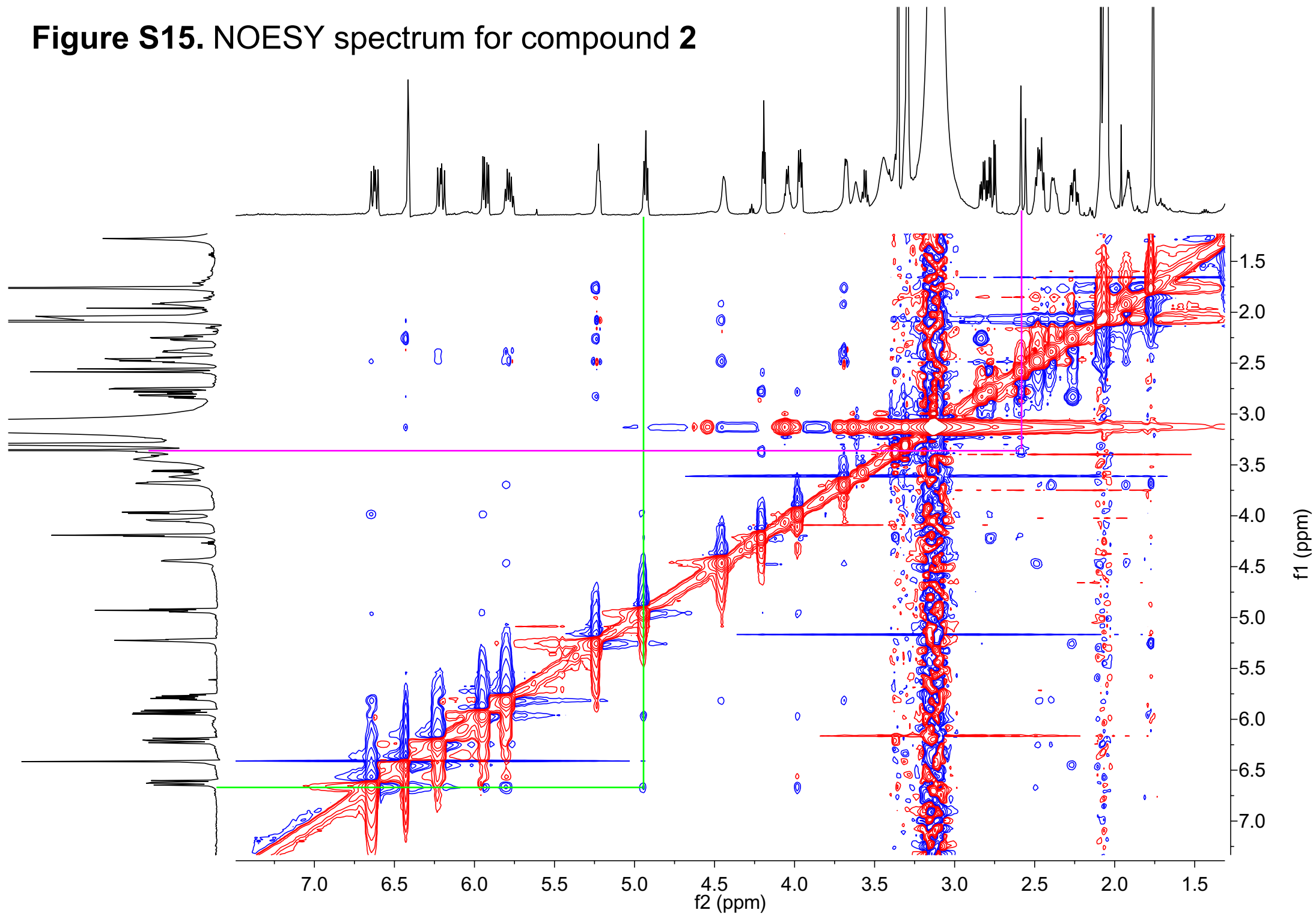


Figure S16. Enlarged NOESY spectrum for compound **2**

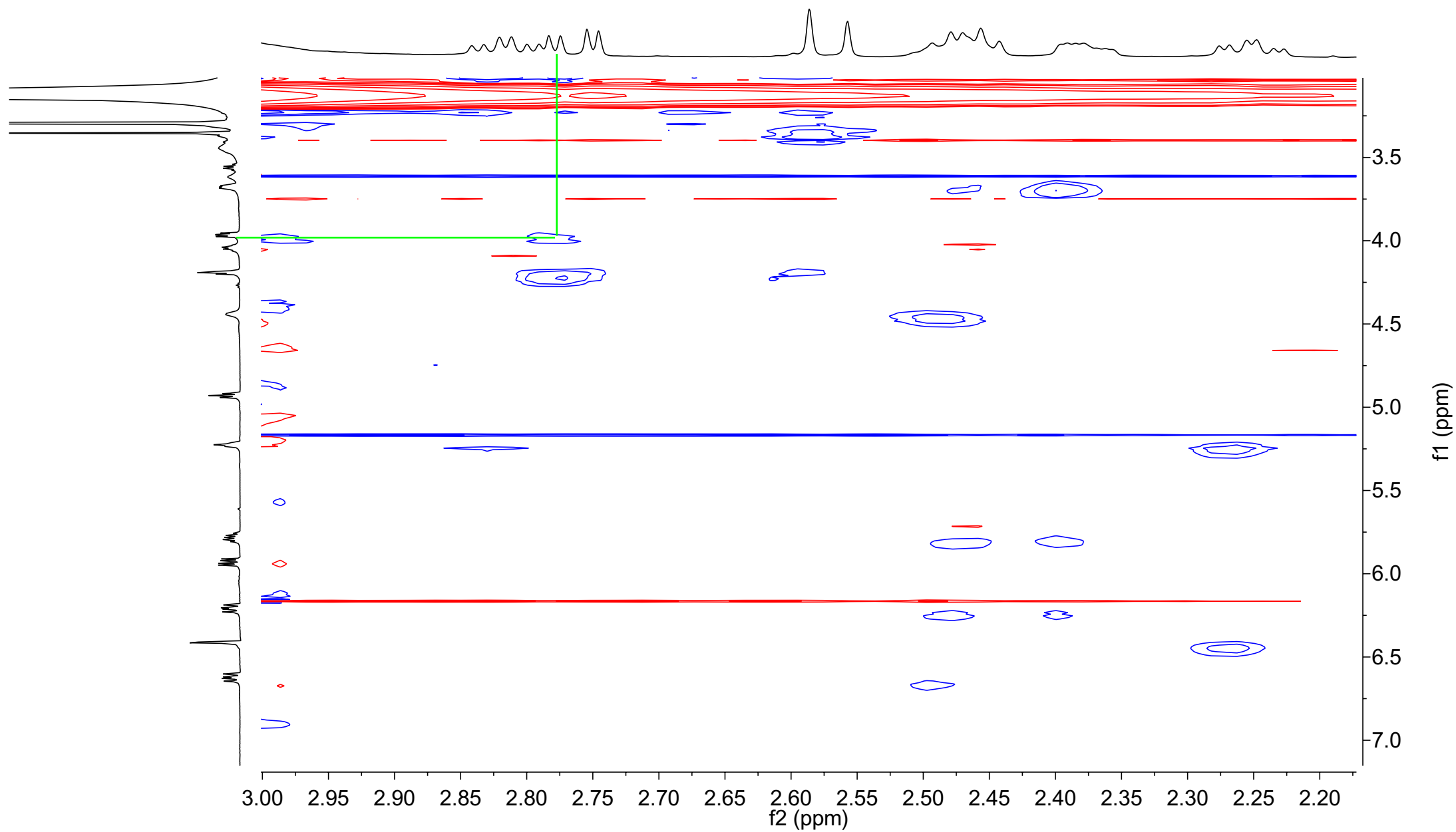


Figure S17. ^1H NMR (600 MHz, CD_3OD) spectrum for compound **3**

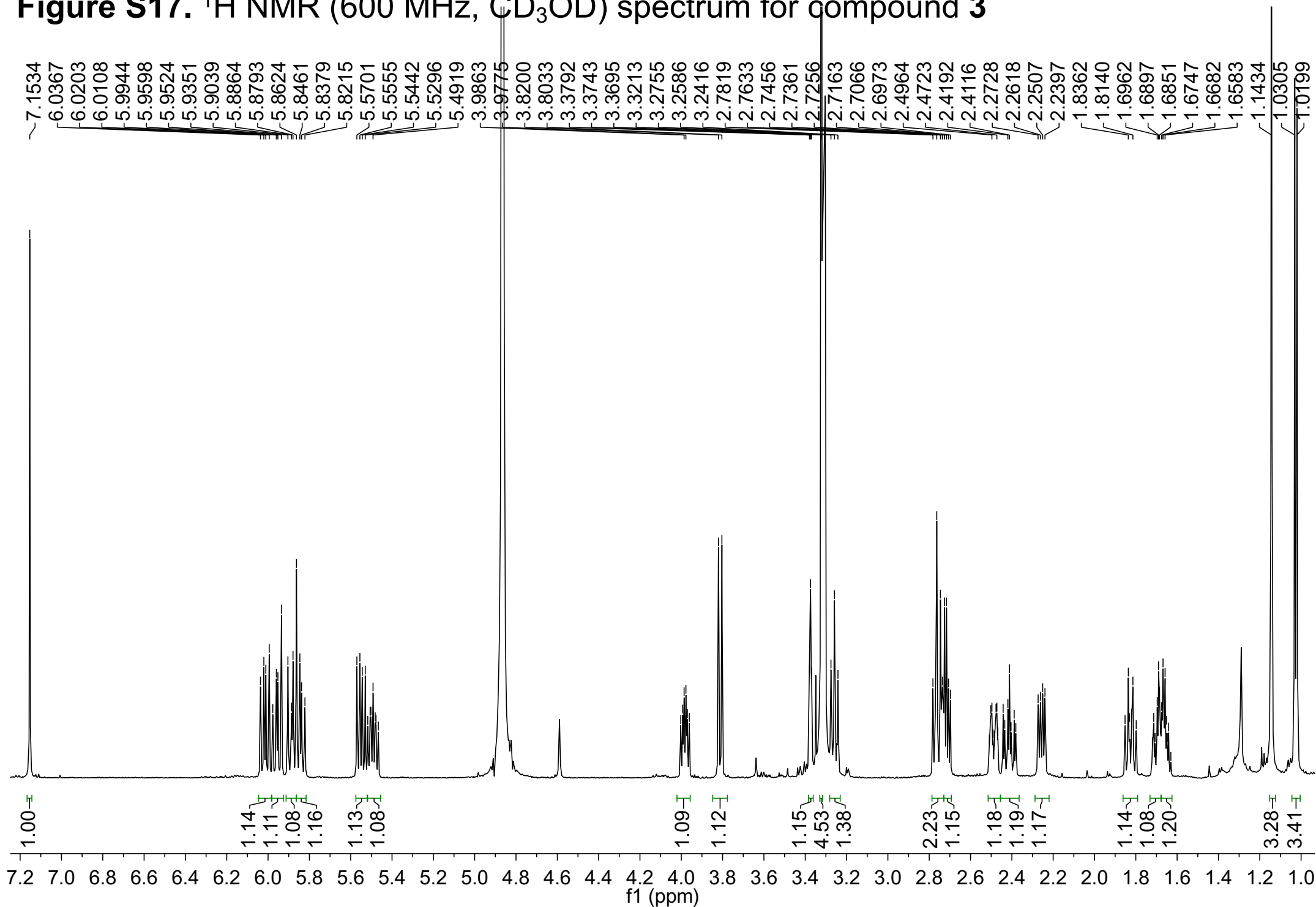


Figure S18. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **3**

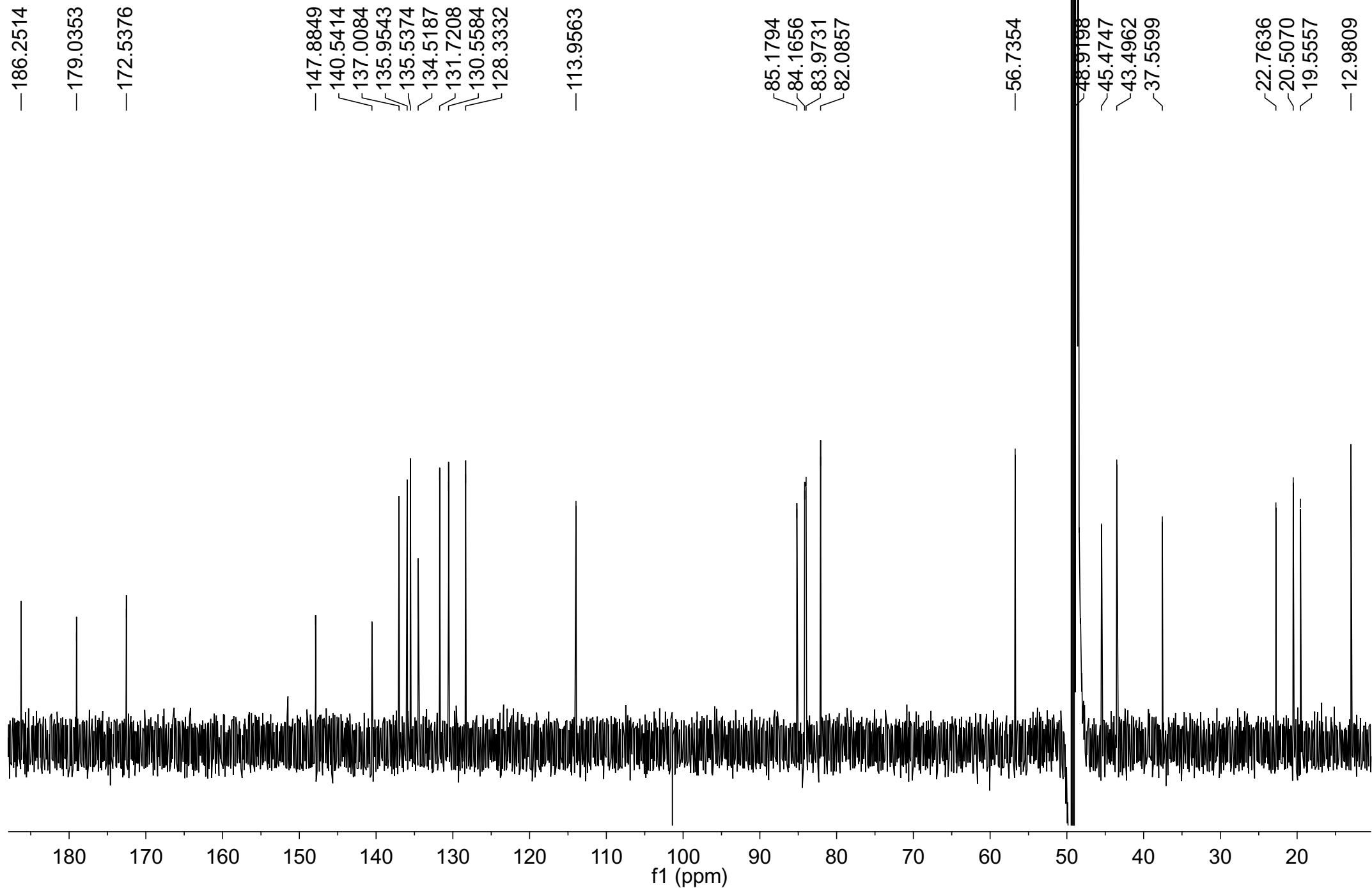


Figure S19. HSQC spectrum for compound **3**

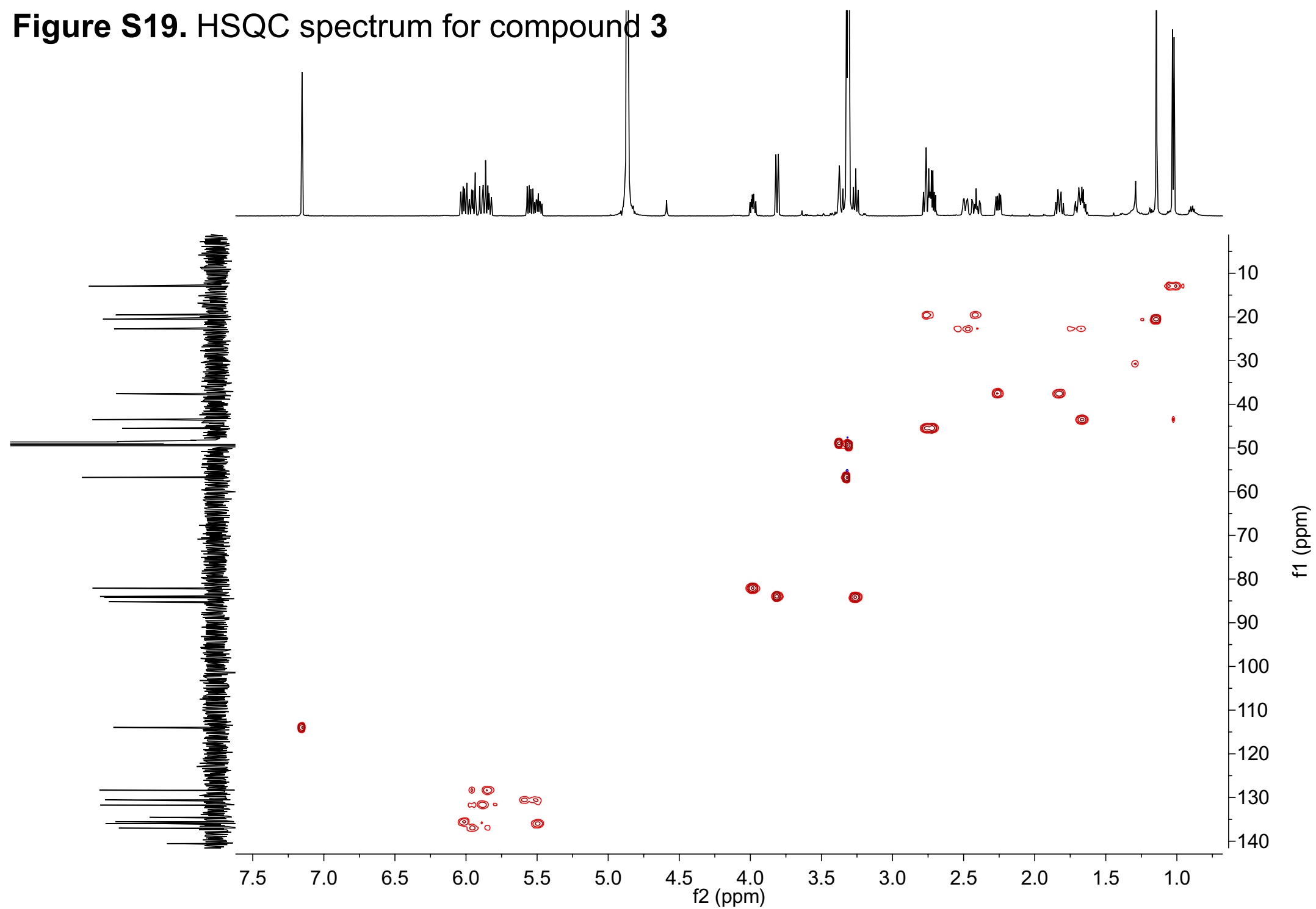


Figure S20. HMBC spectrum for compound **3**

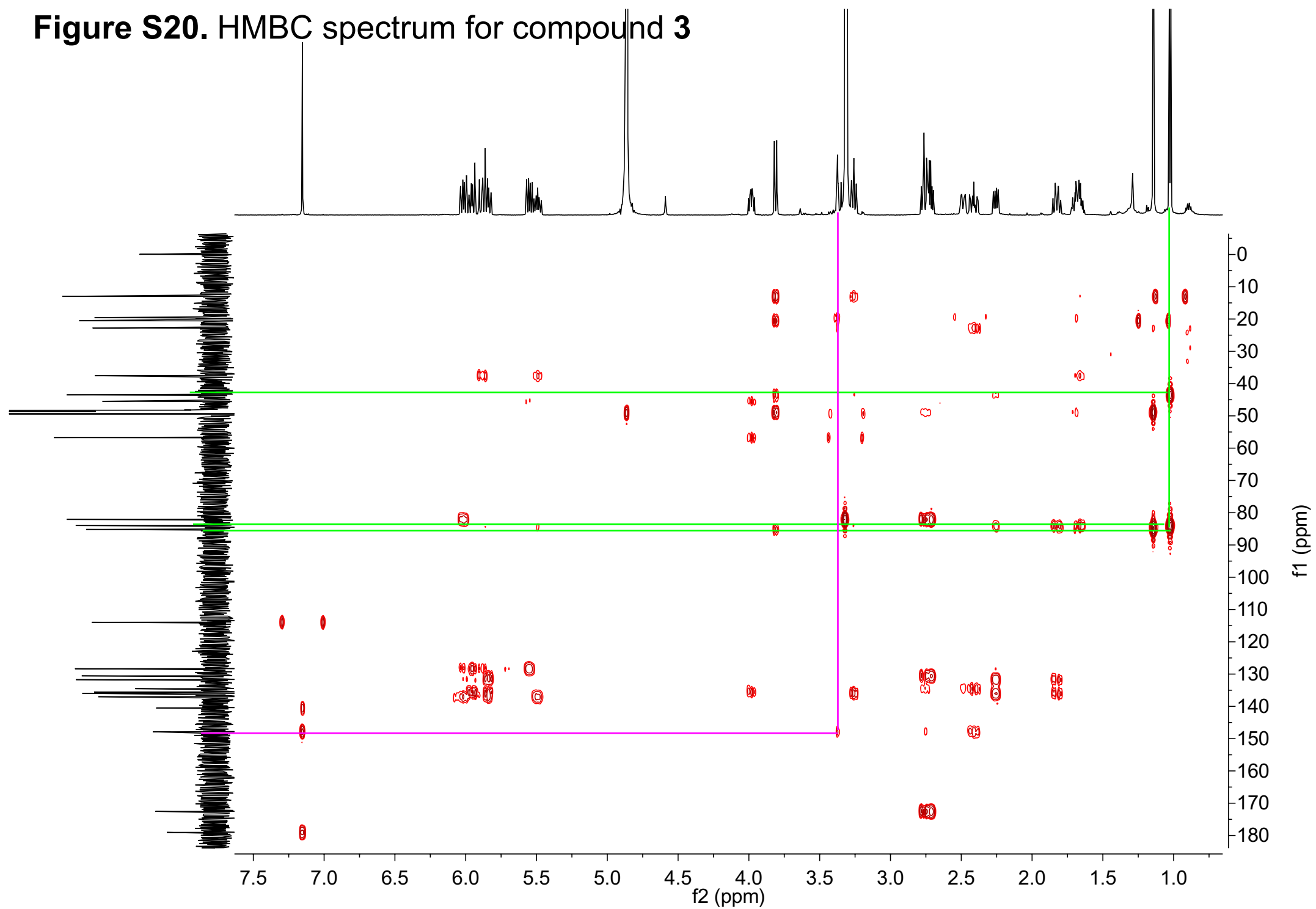


Figure S21. ^1H - ^1H COSY spectrum for compound **3**

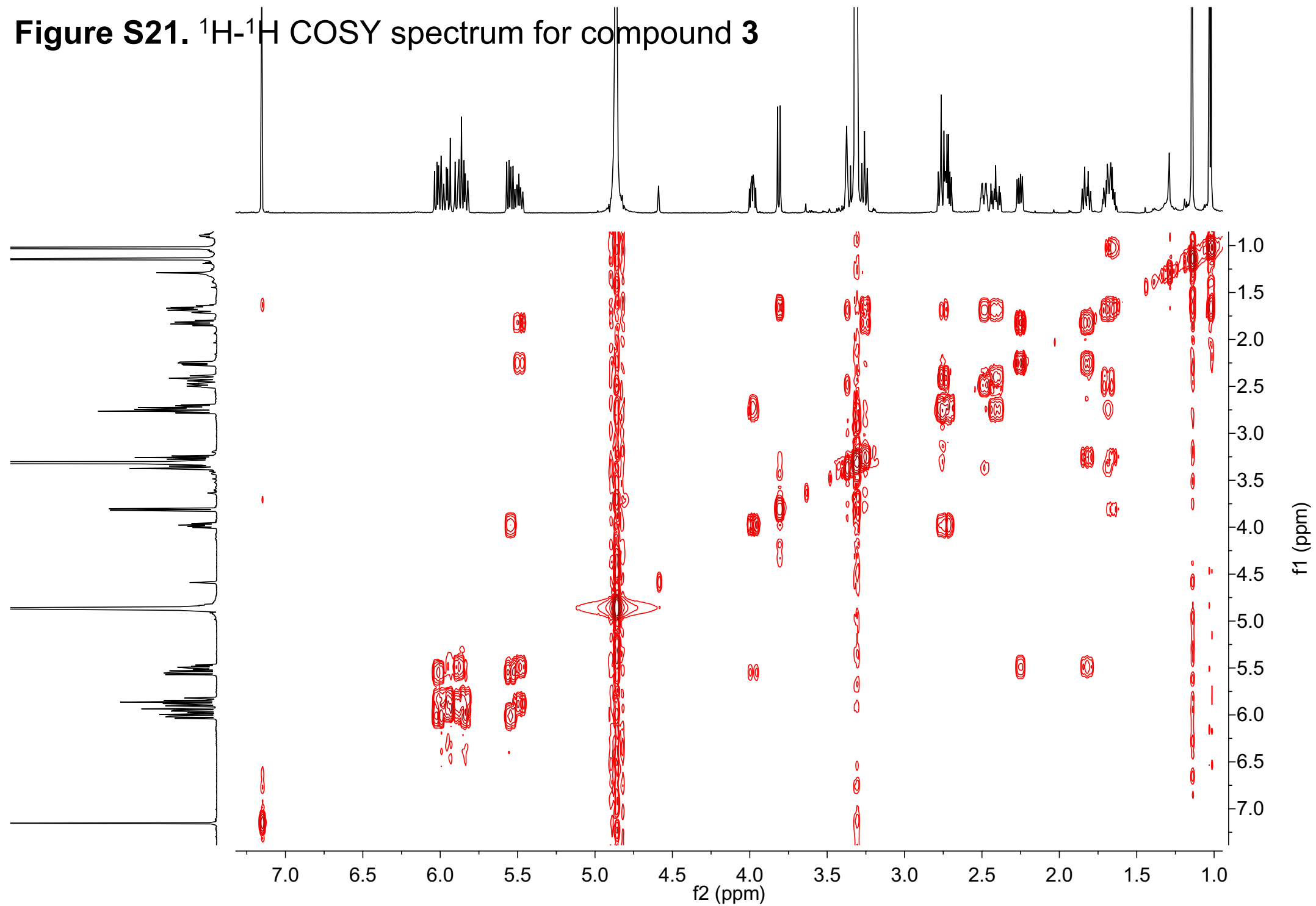


Figure S22. NOESY spectrum for compound **3**

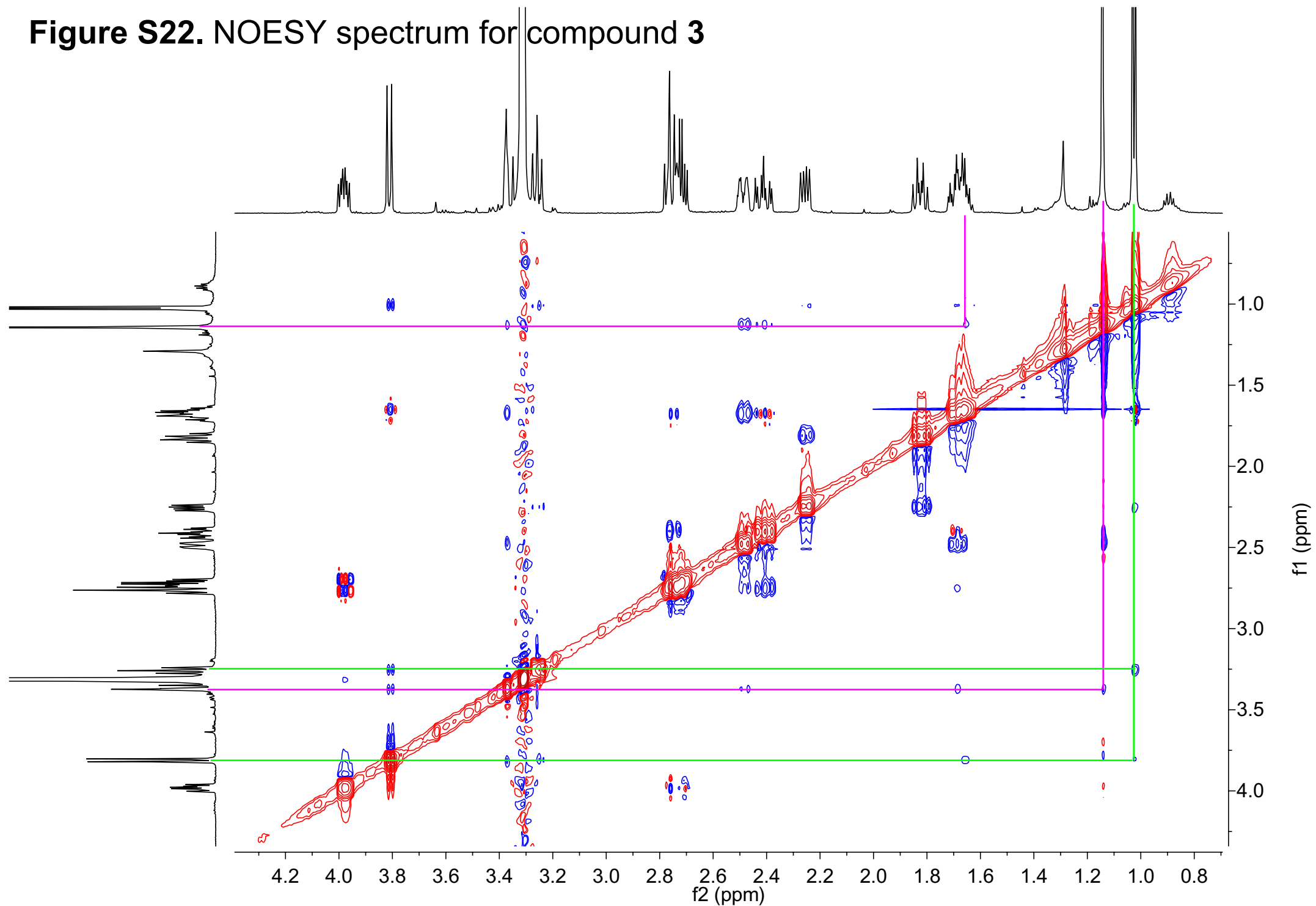


Figure S23. ^1H NMR (600 MHz, CD_3OD) spectrum for compound **4**

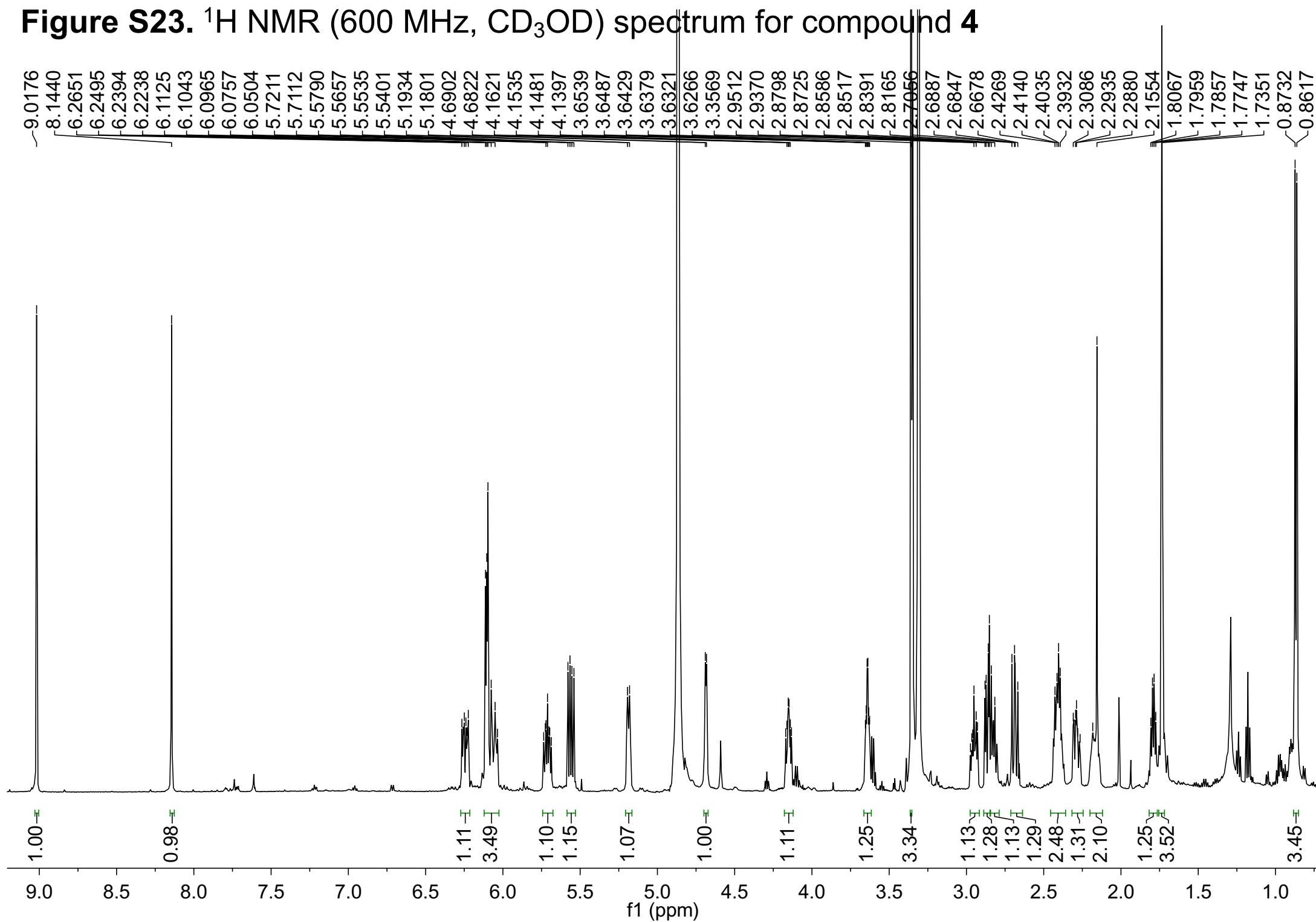


Figure S24. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **4**

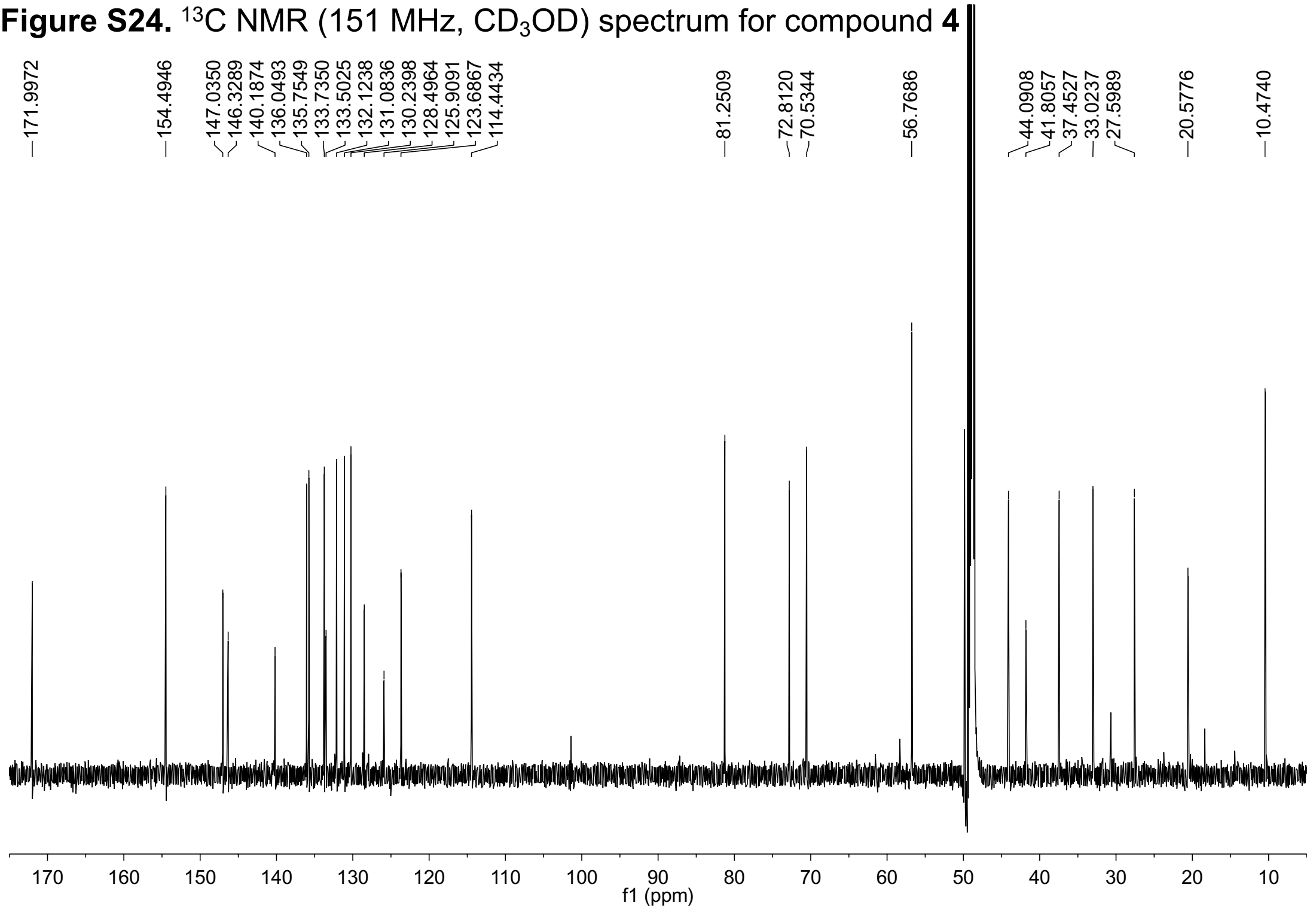


Figure S25. HSQC spectrum for compound **4**

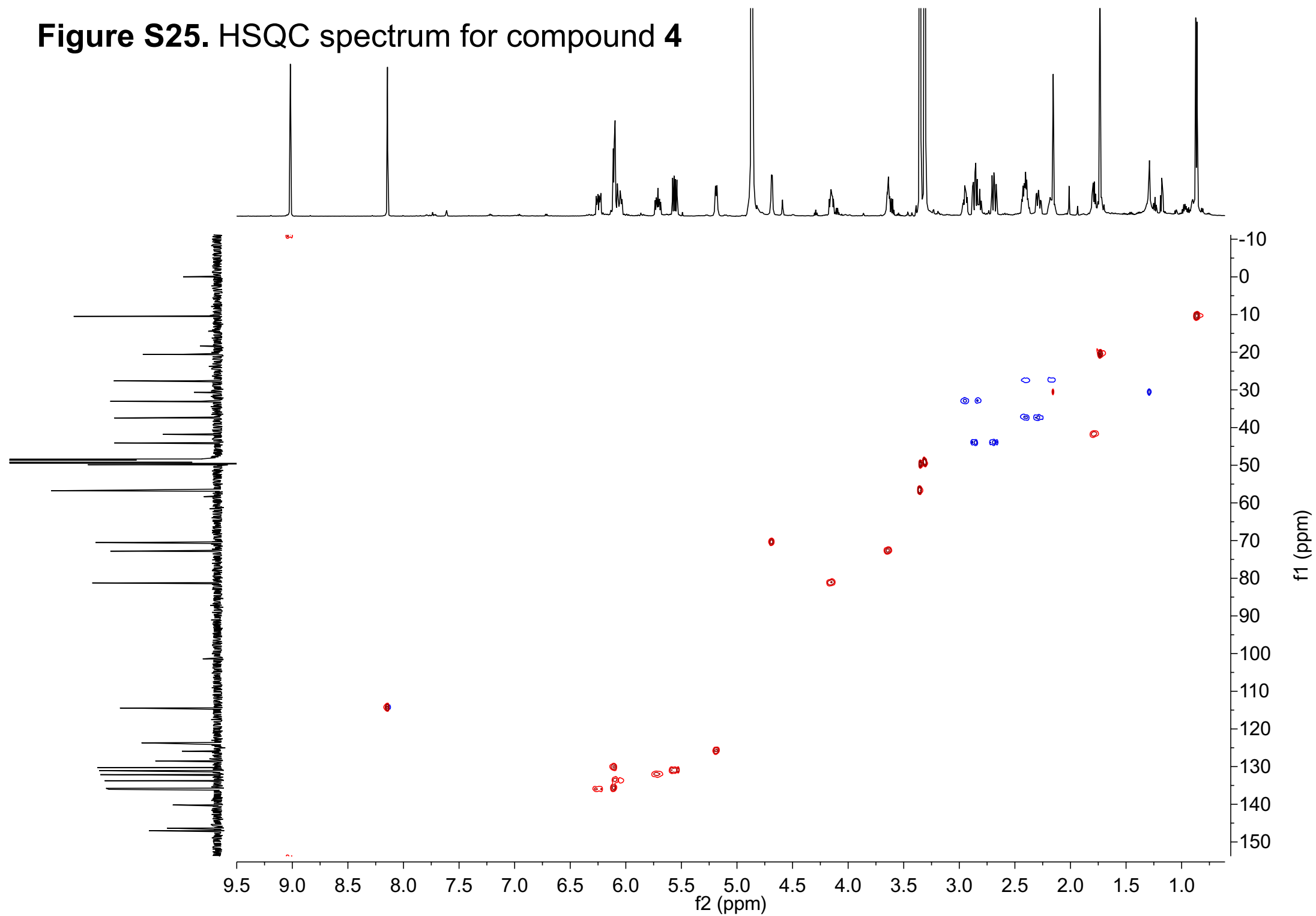


Figure S26. HMBC spectrum for compound **4**

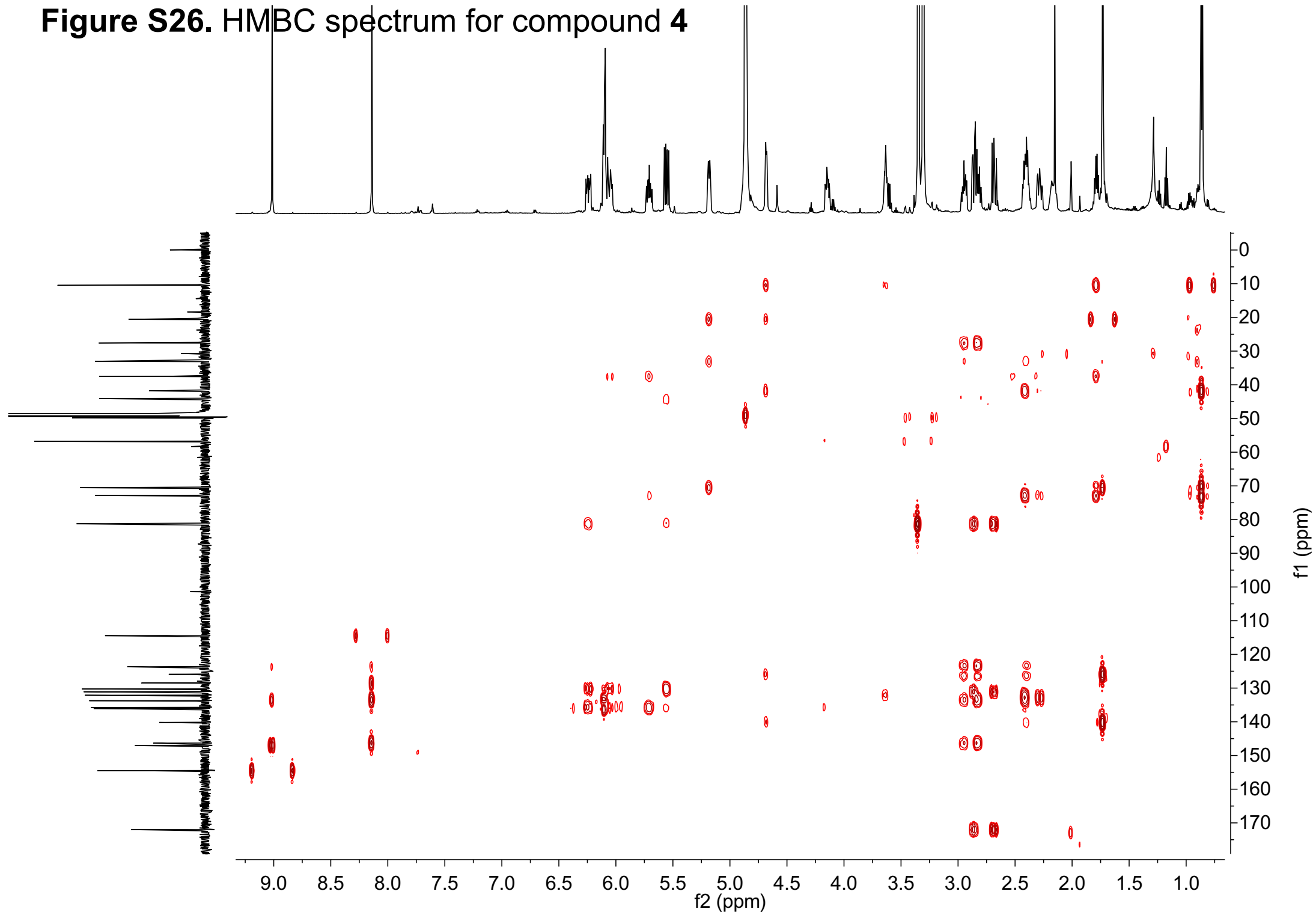


Figure S27. Enlarged HMBC spectrum for compound **4**

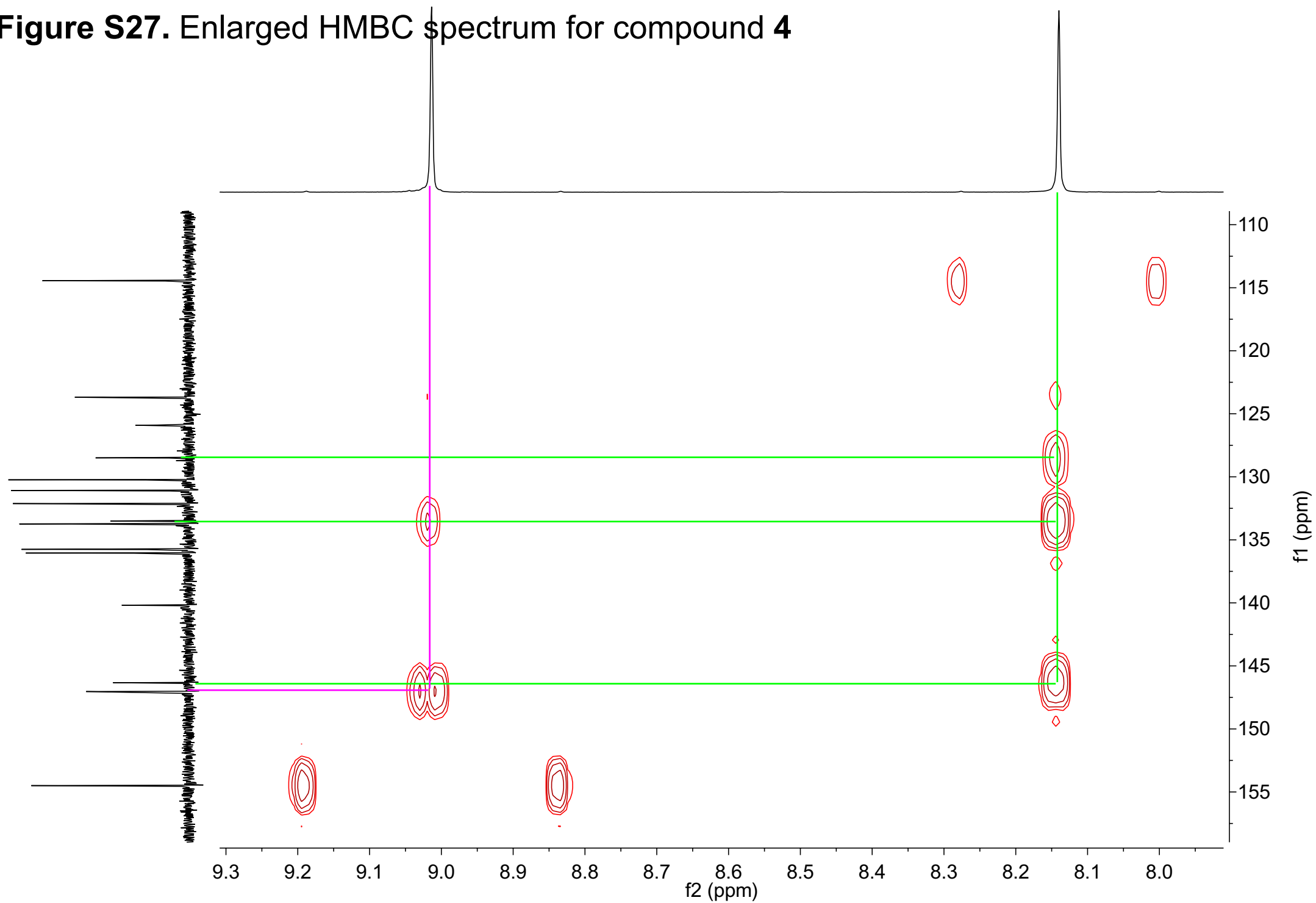


Figure S28. ^1H - ^1H COSY spectrum for compound **4**

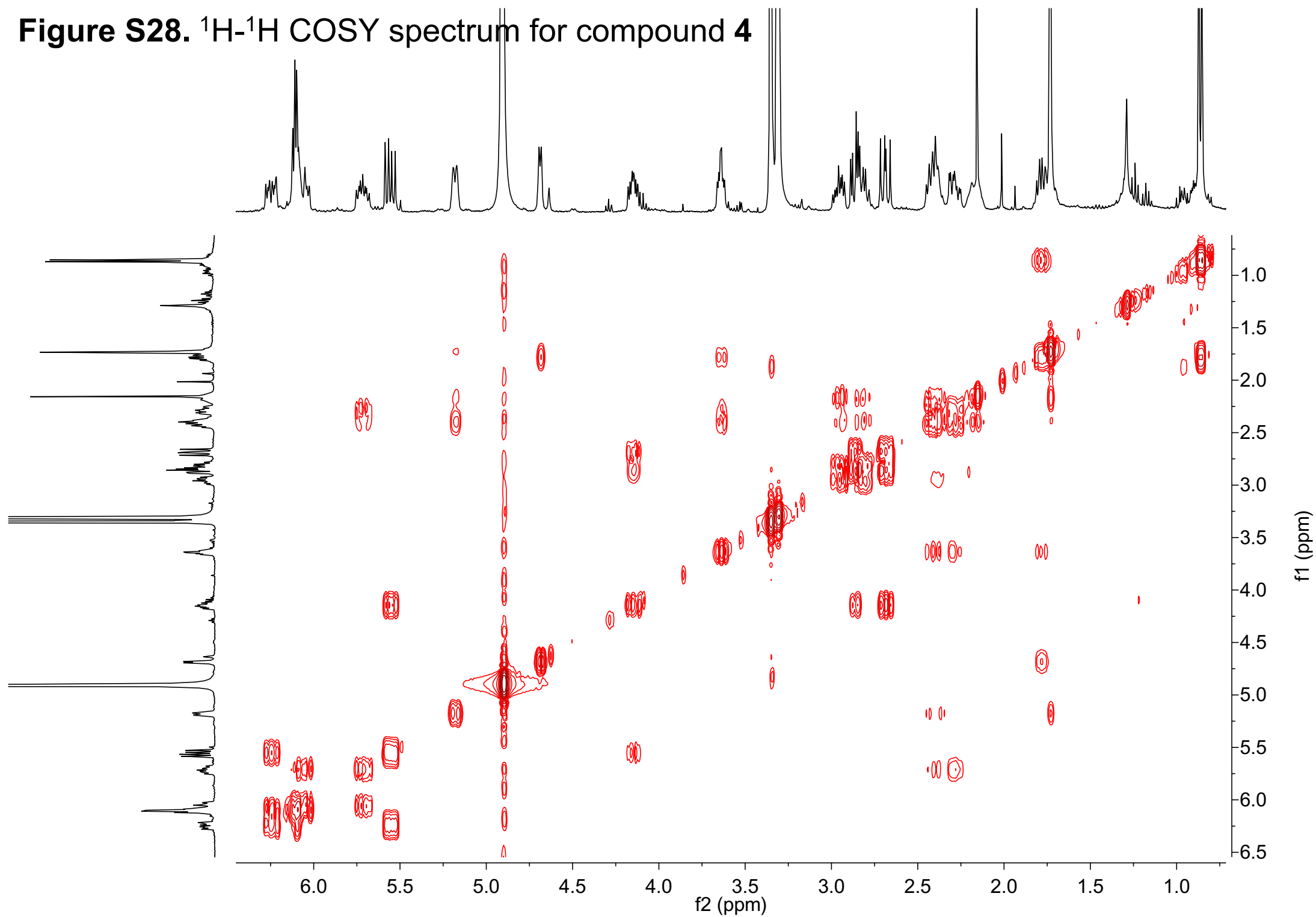


Figure S29. NOESY spectrum for compound **4**

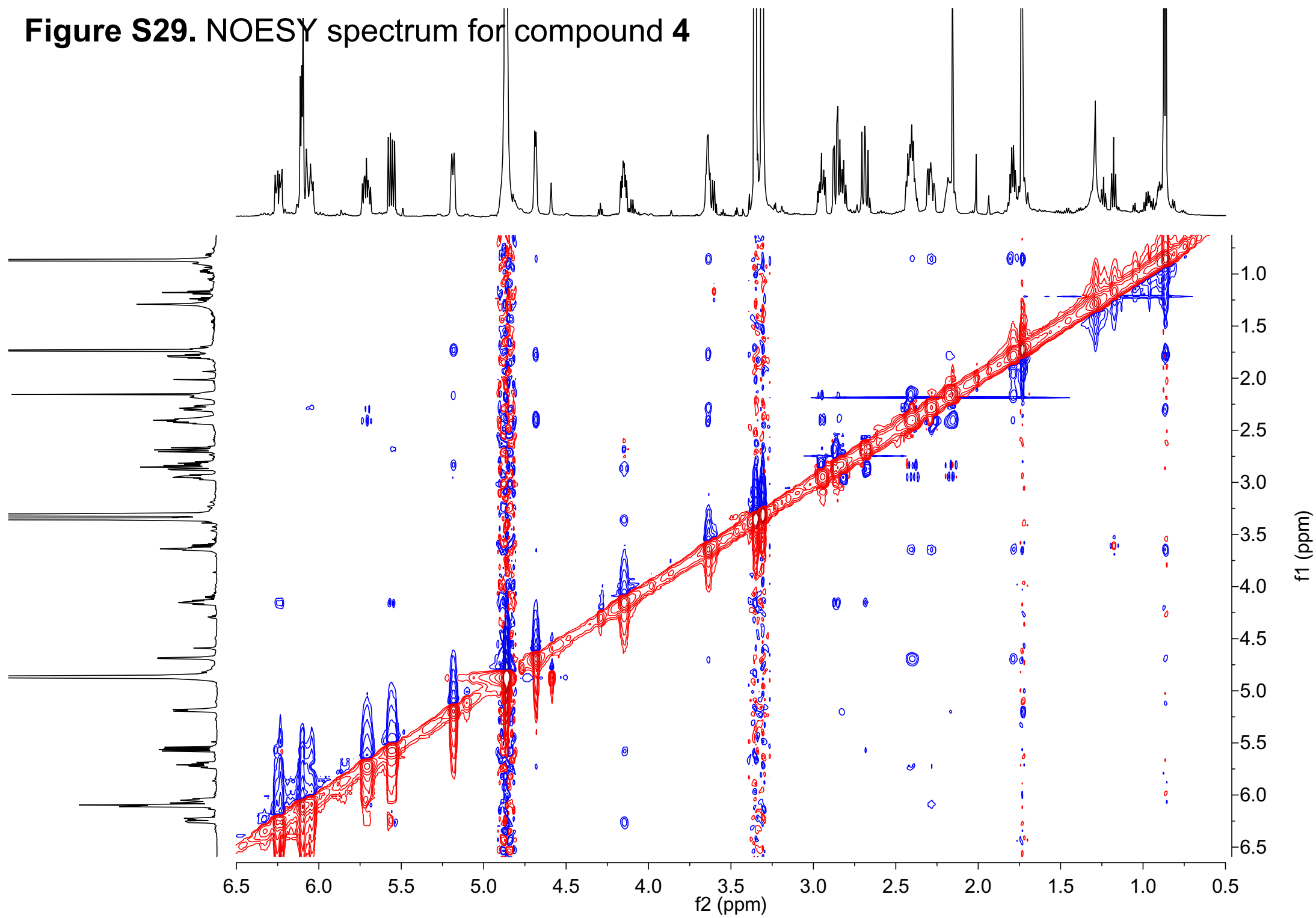


Figure S30. ^1H NMR (600 MHz, CD_3OD) spectrum for compound **5**

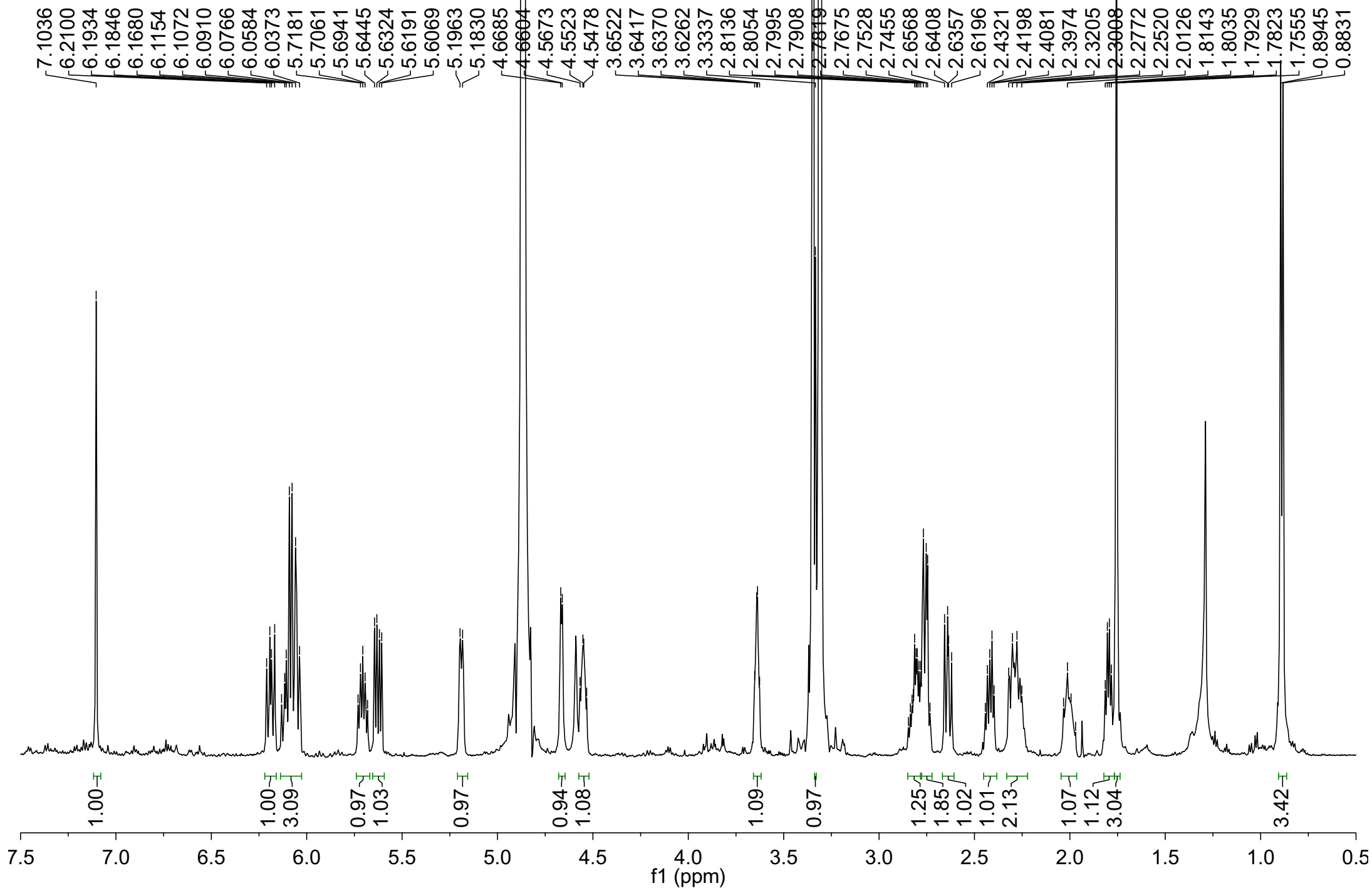


Figure S31. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **5**

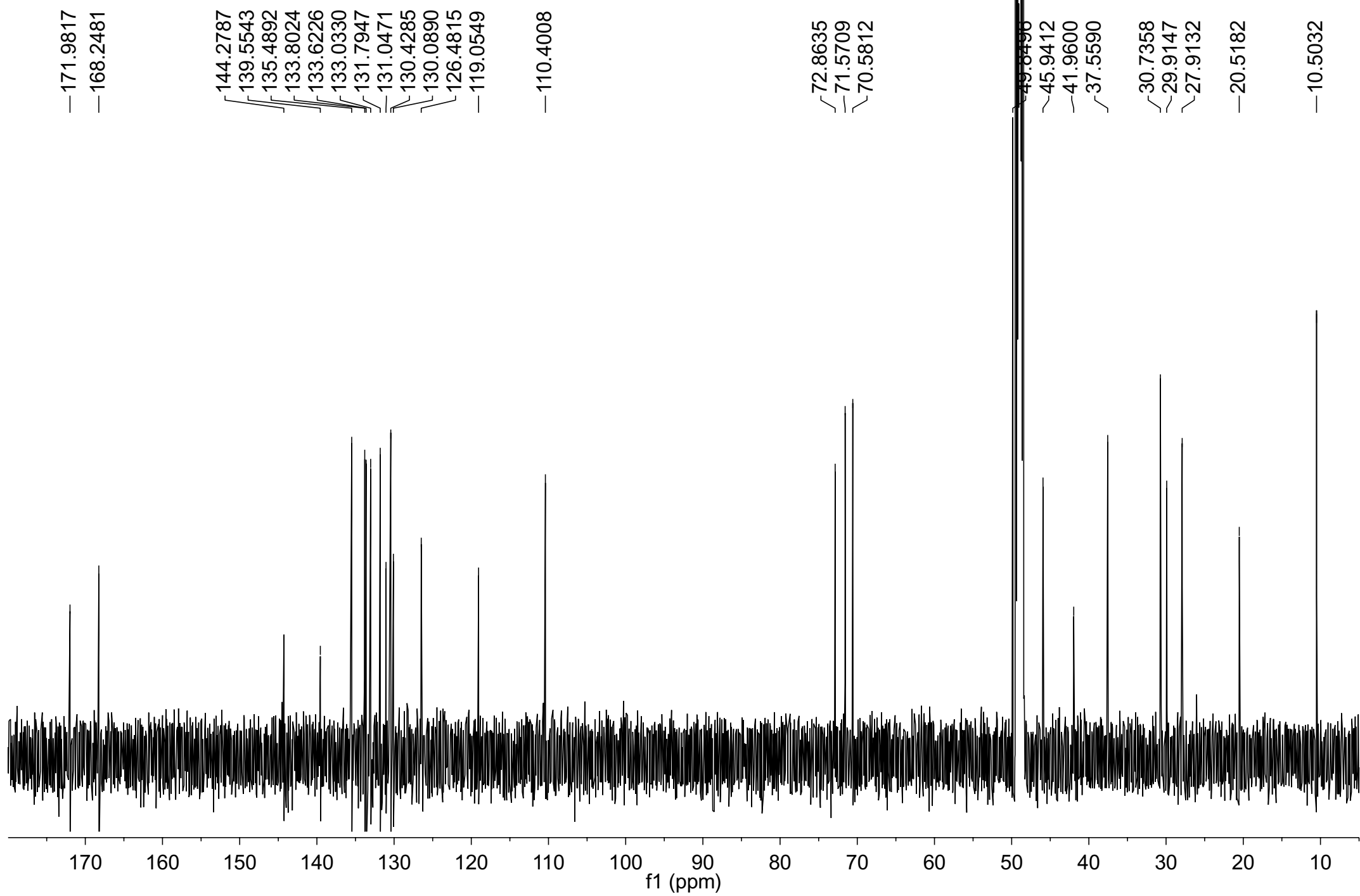


Figure S32. HSQC spectrum for compound **5**

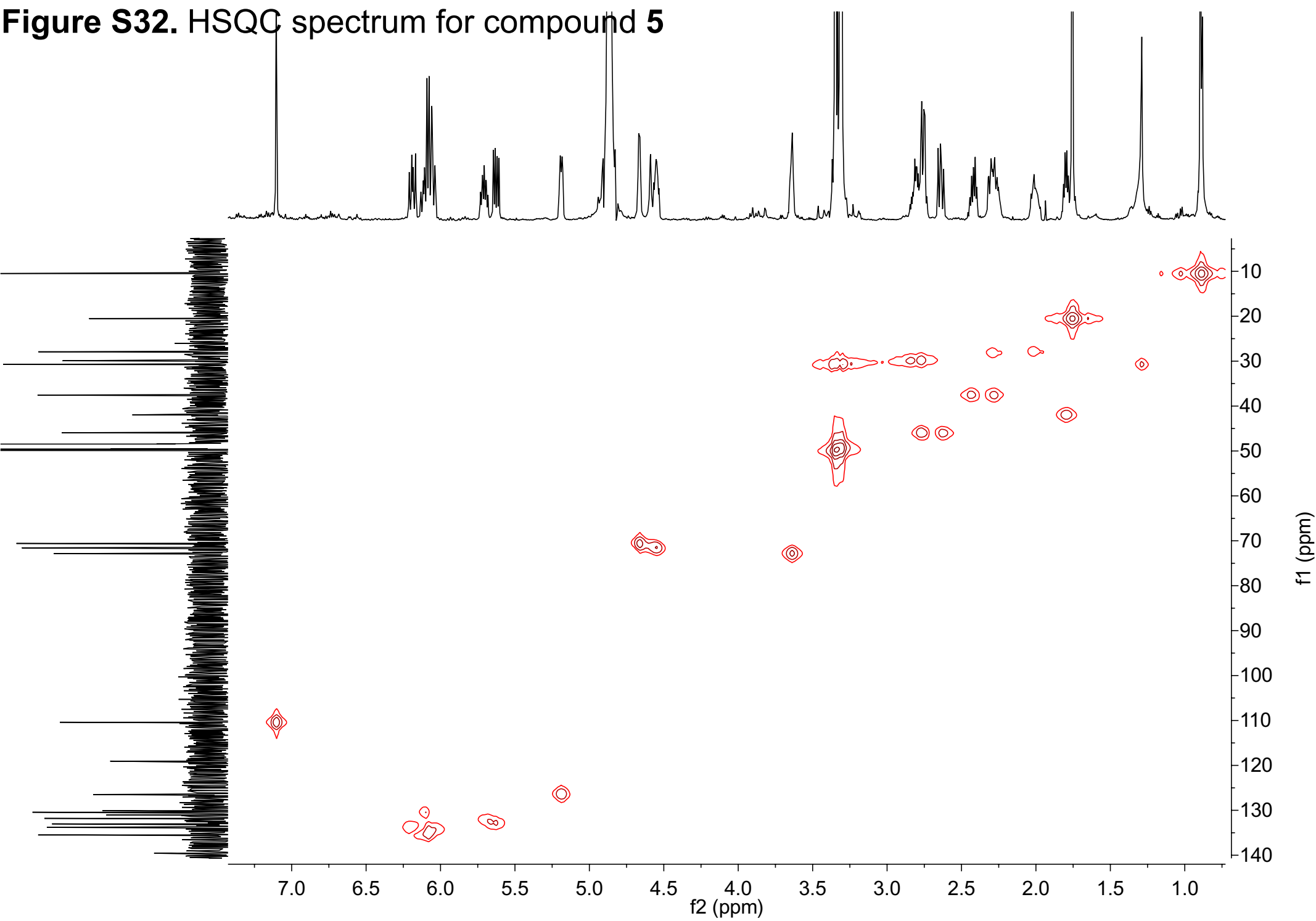


Figure S33. HMBC spectrum for compound **5**

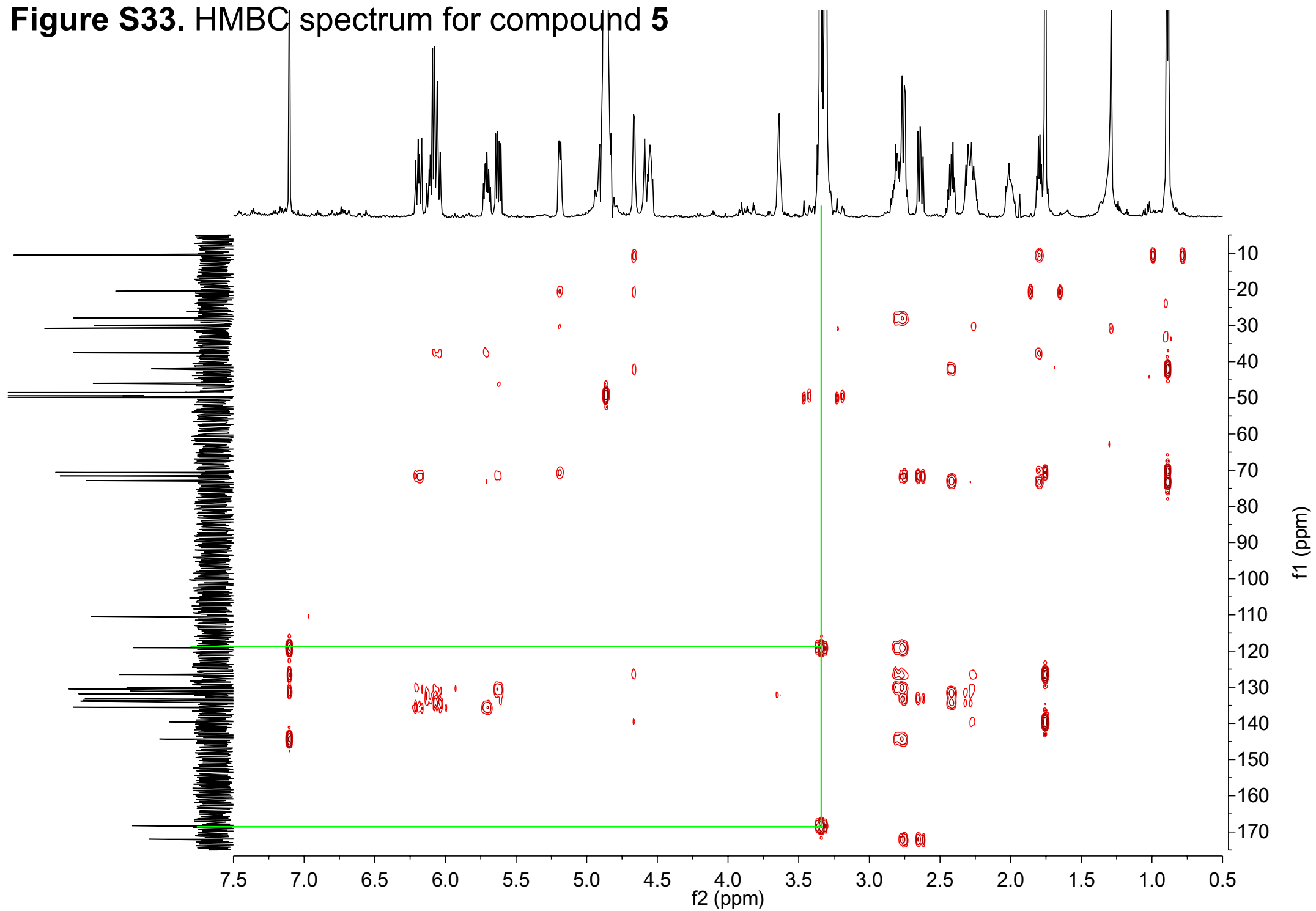


Figure S34. ^1H - ^1H COSY spectrum for compound **5**

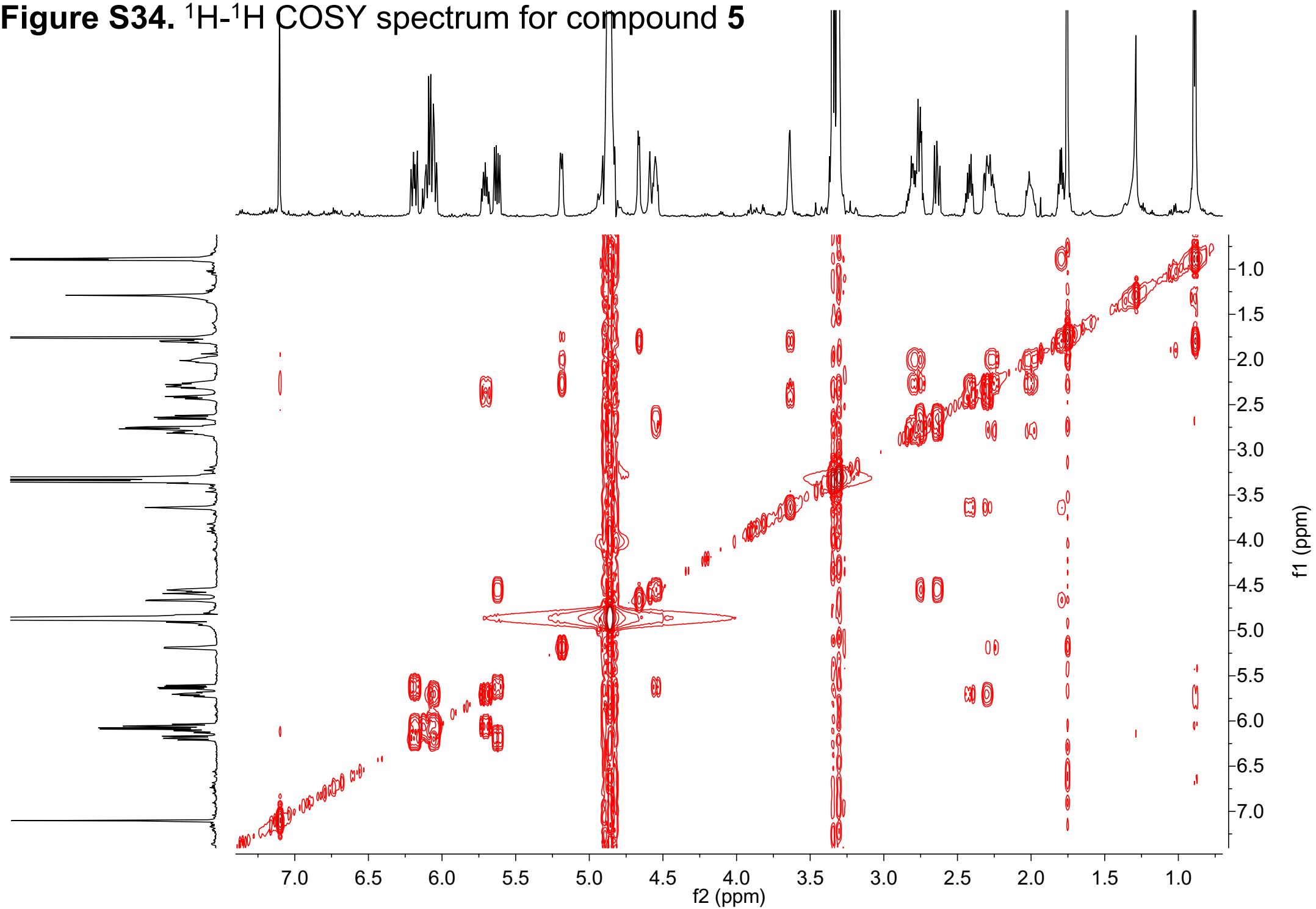


Figure S35. NOESY spectrum for compound **5**

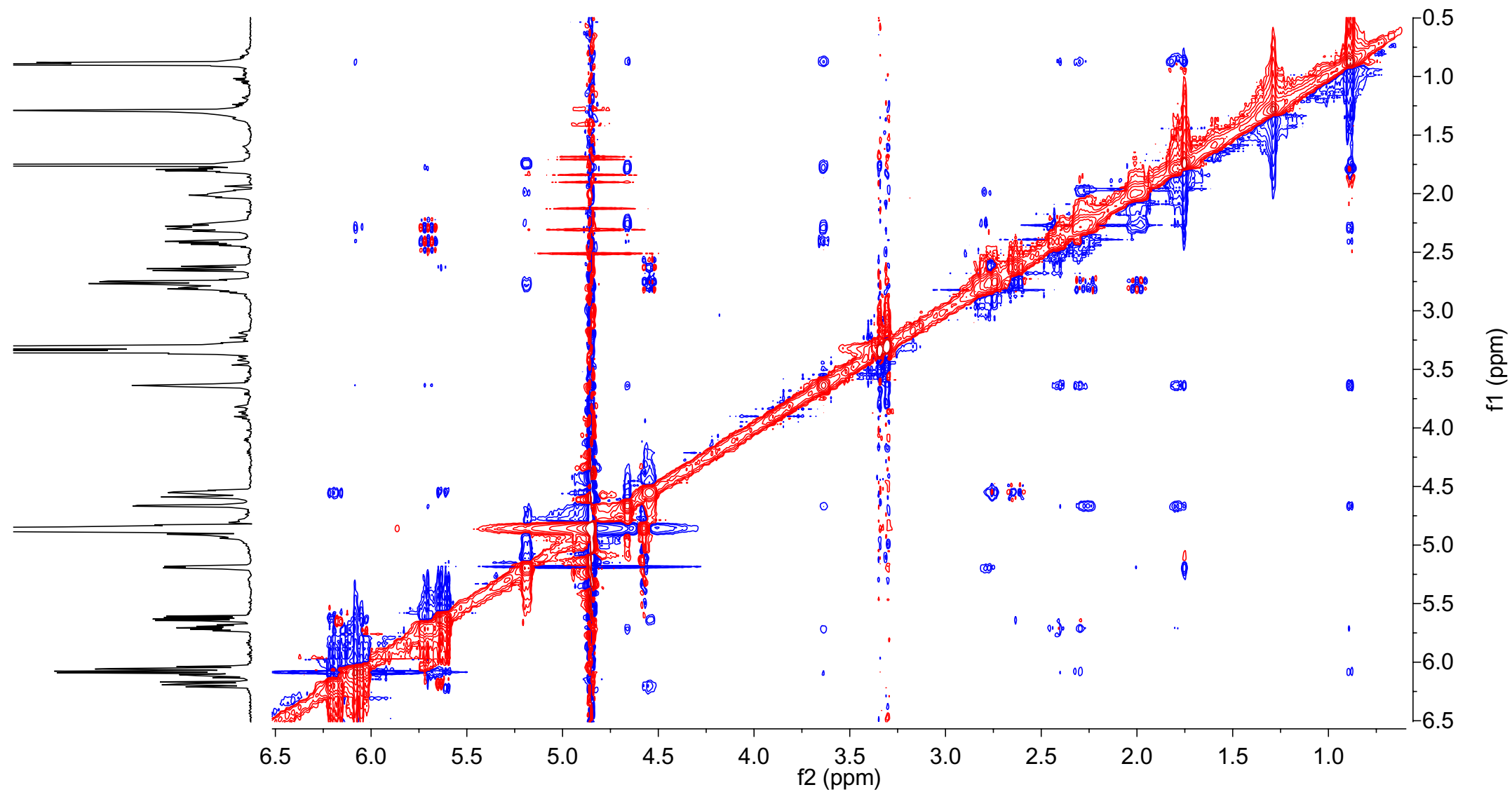


Figure S36. ^1H NMR (400 MHz, CD_3OD) spectrum for compound **6**

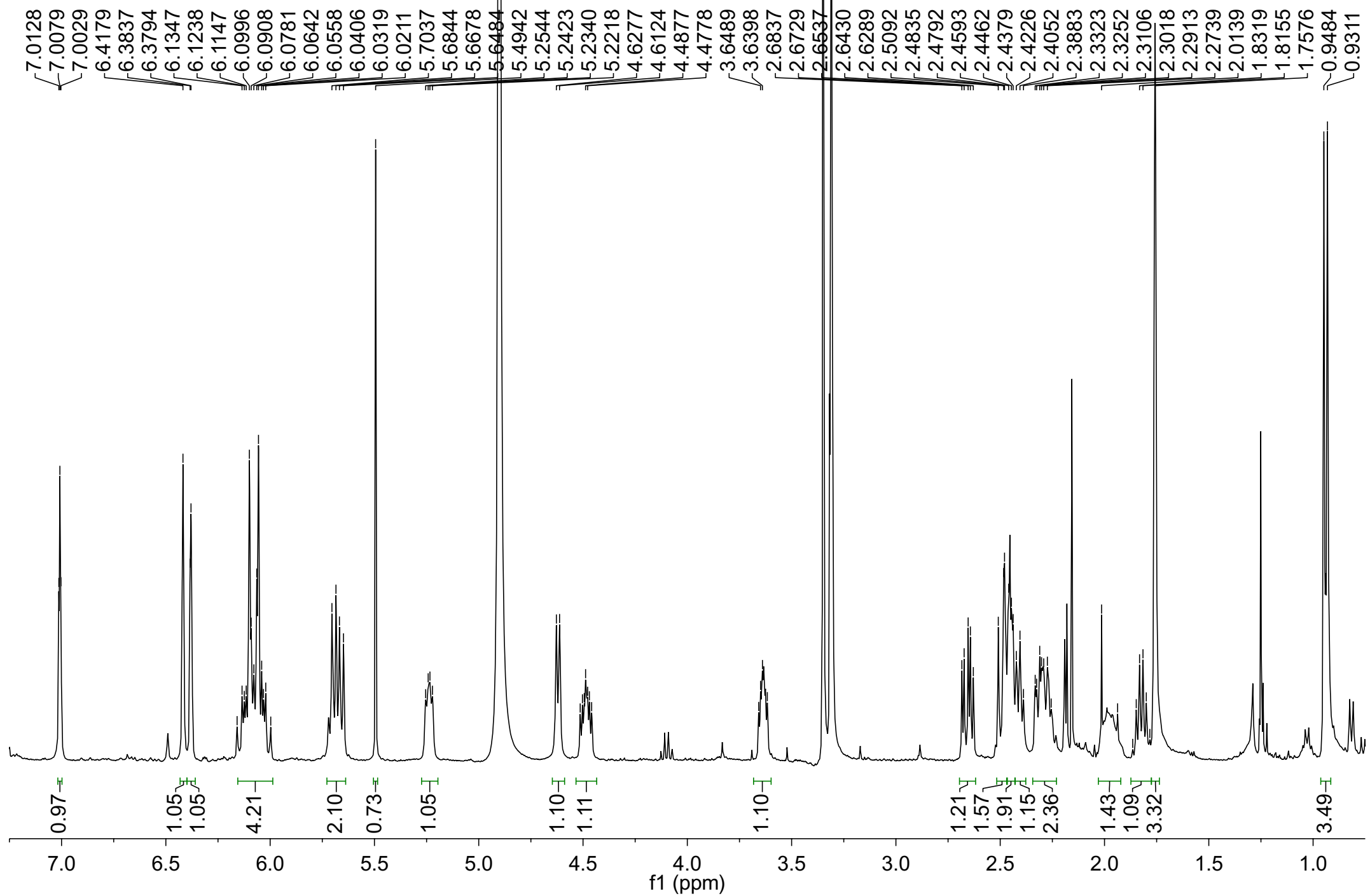


Figure S37. ^{13}C NMR (101 MHz, CD_3OD) spectrum for compound **6**

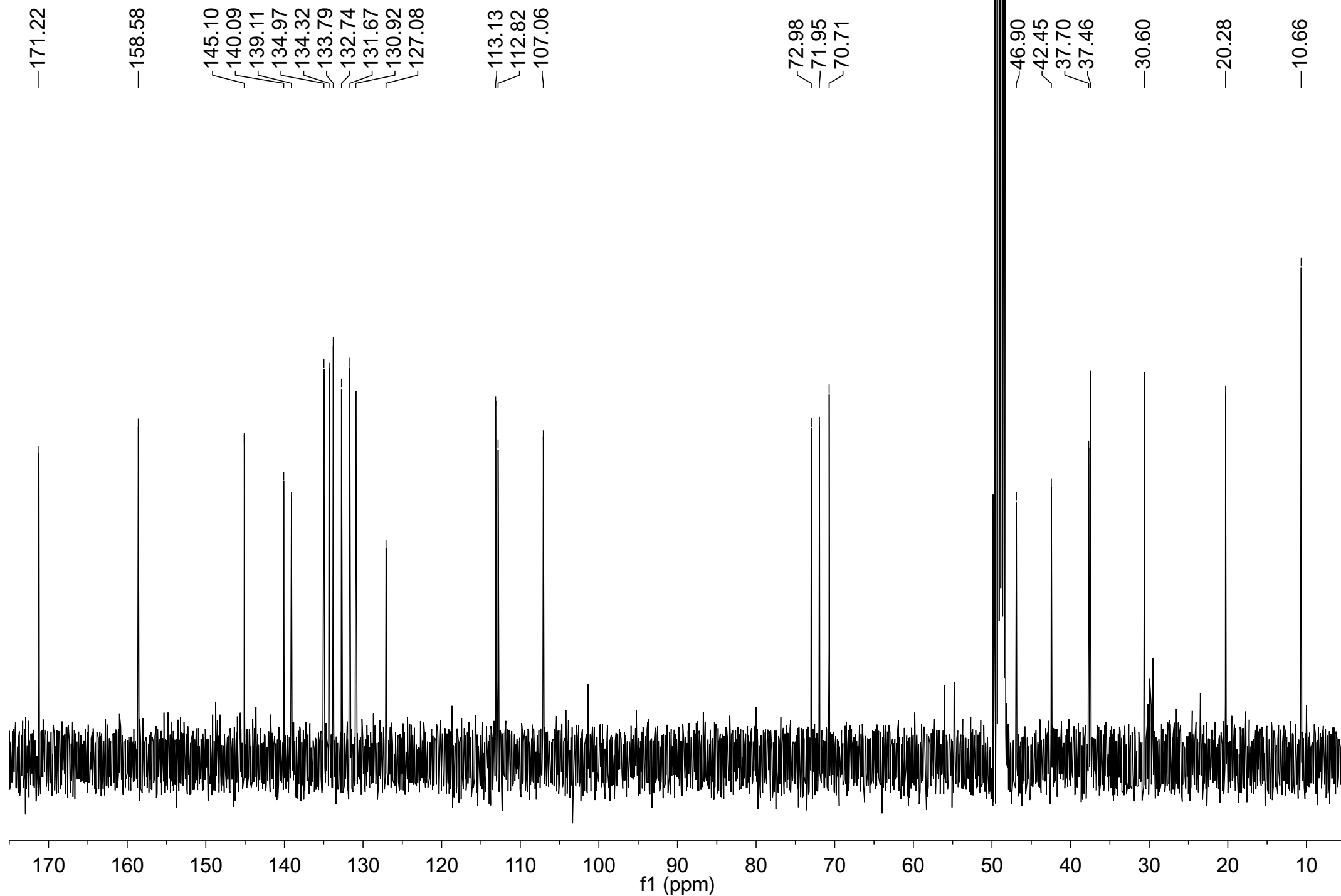


Figure S38. HSQC spectrum for compound **6**

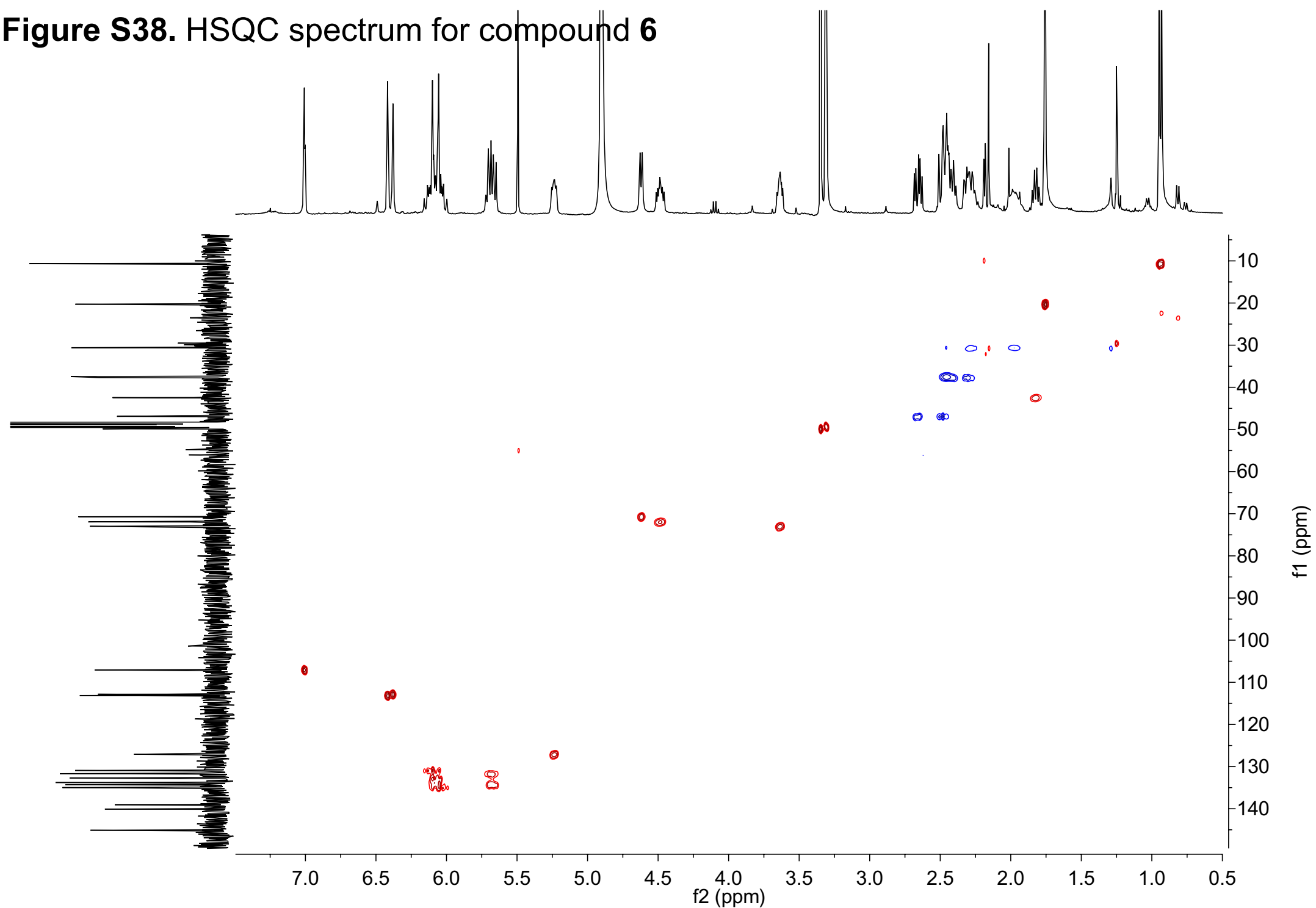


Figure S39. HMBC spectrum for compound **6**

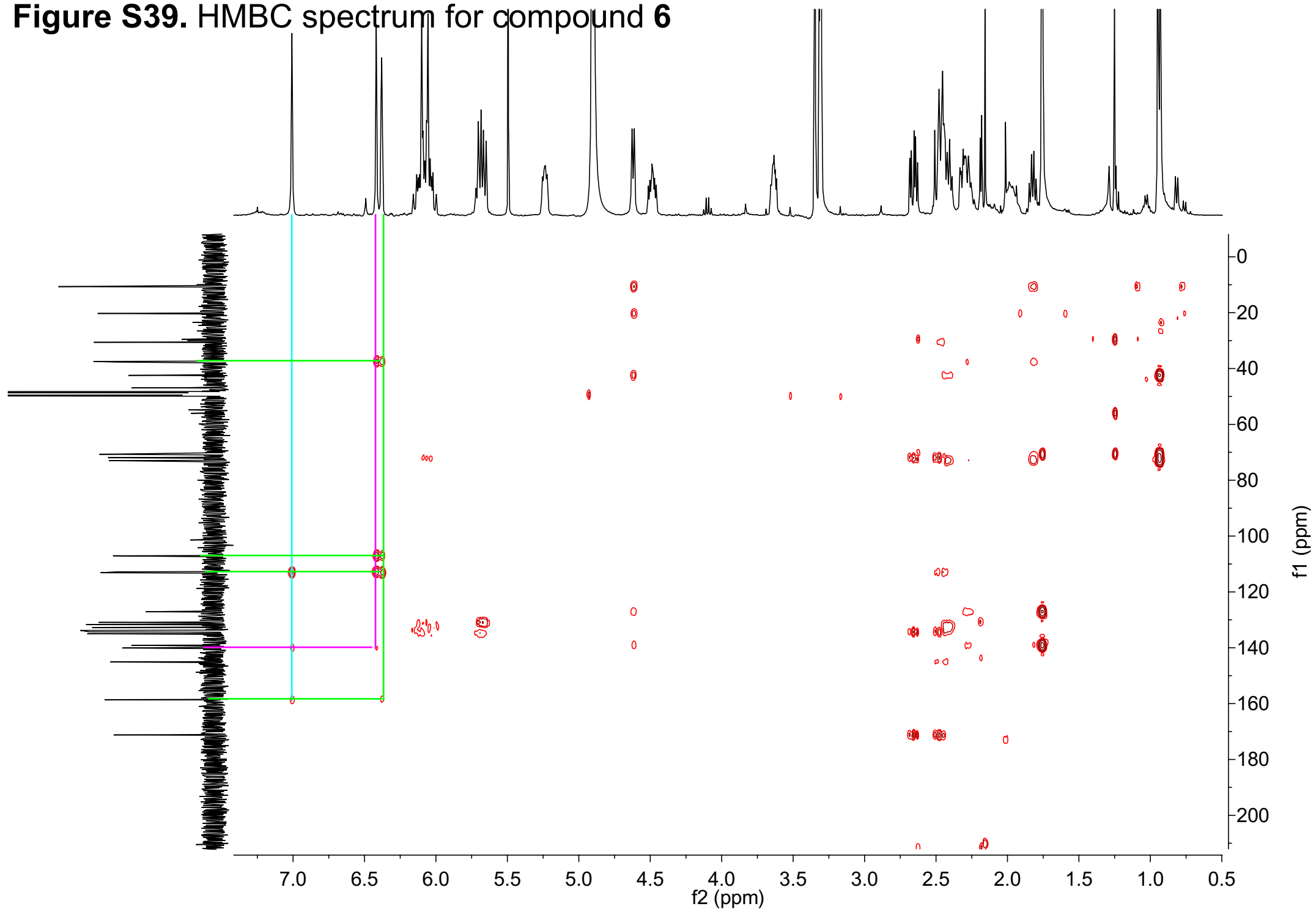


Figure S40. ^1H - ^1H COSY spectrum for compound **6**

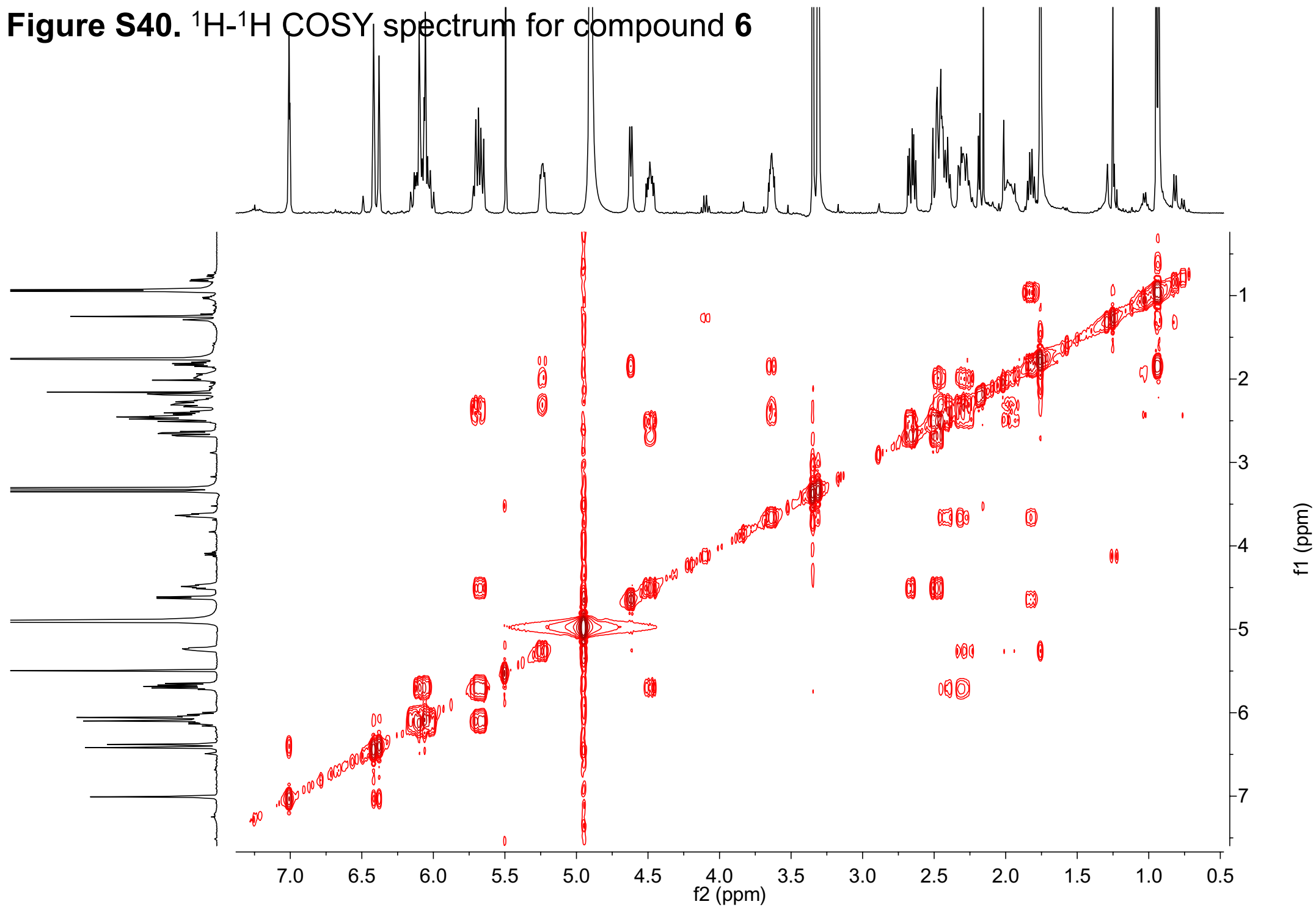


Figure S41. NOESY spectrum for compound **6**

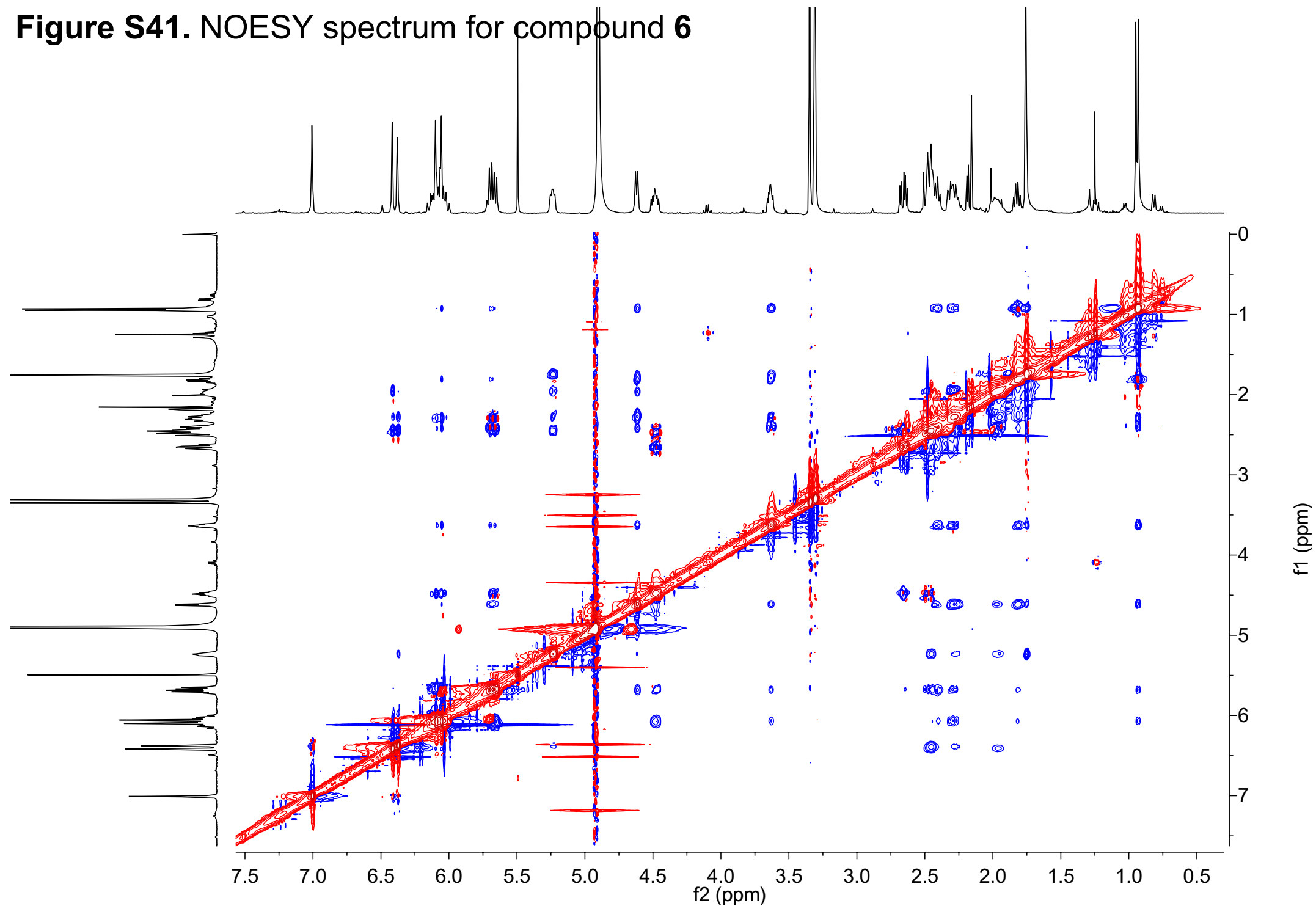


Figure S42. ^1H NMR (600 MHz, CD_3OD) spectrum for compound 7

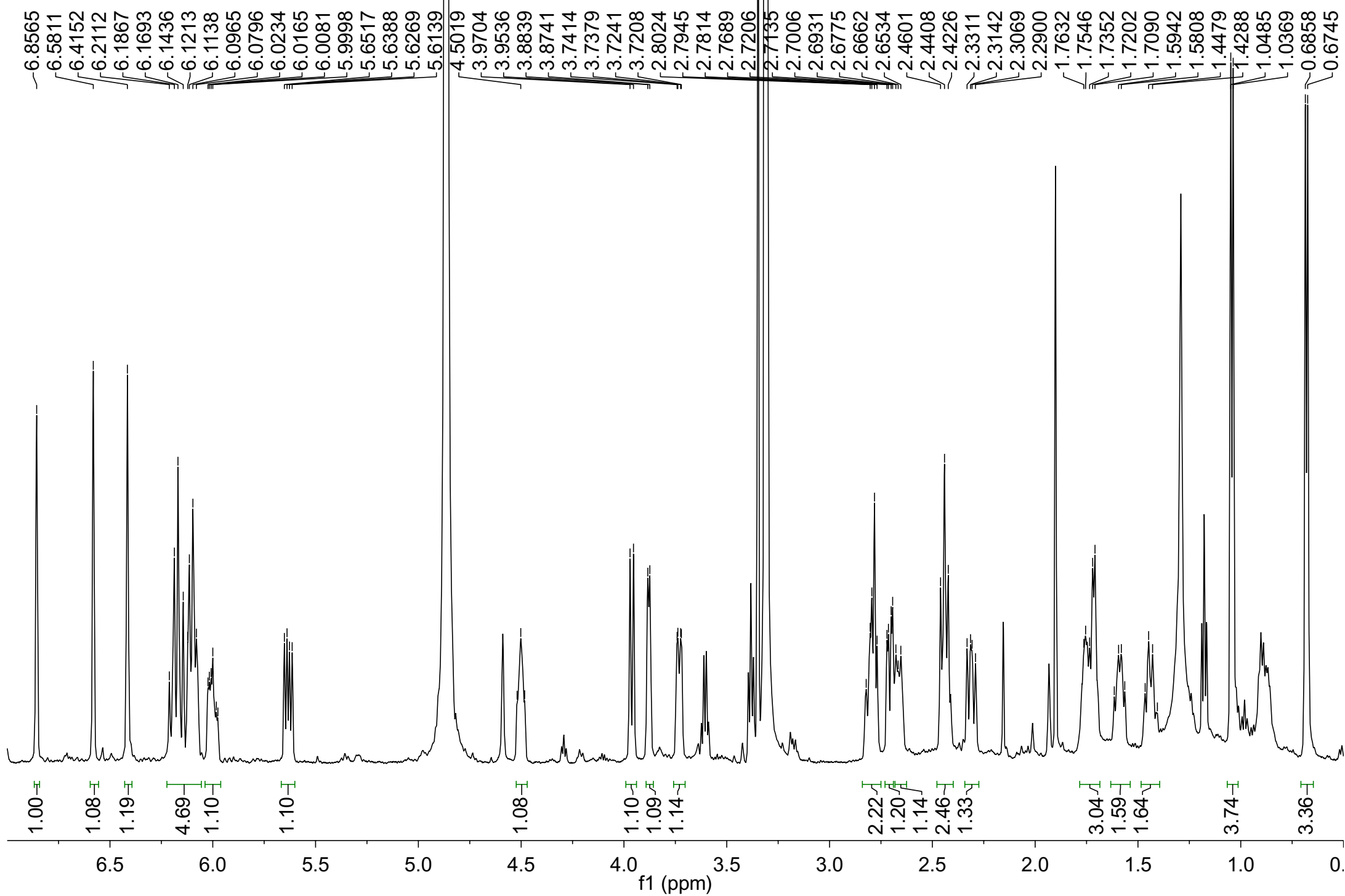


Figure S43. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **7**

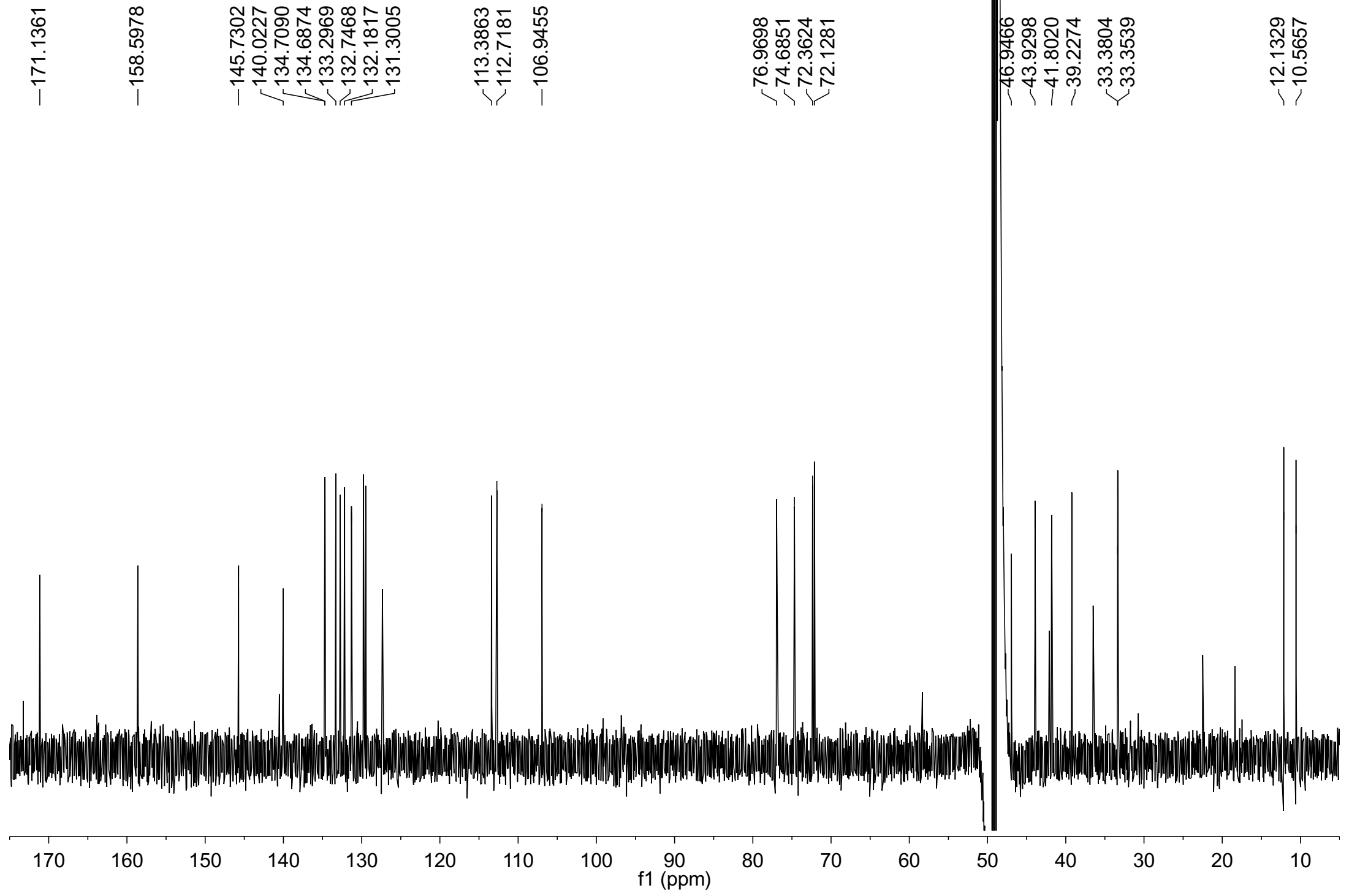


Figure S44. HSQC spectrum for compound **7**

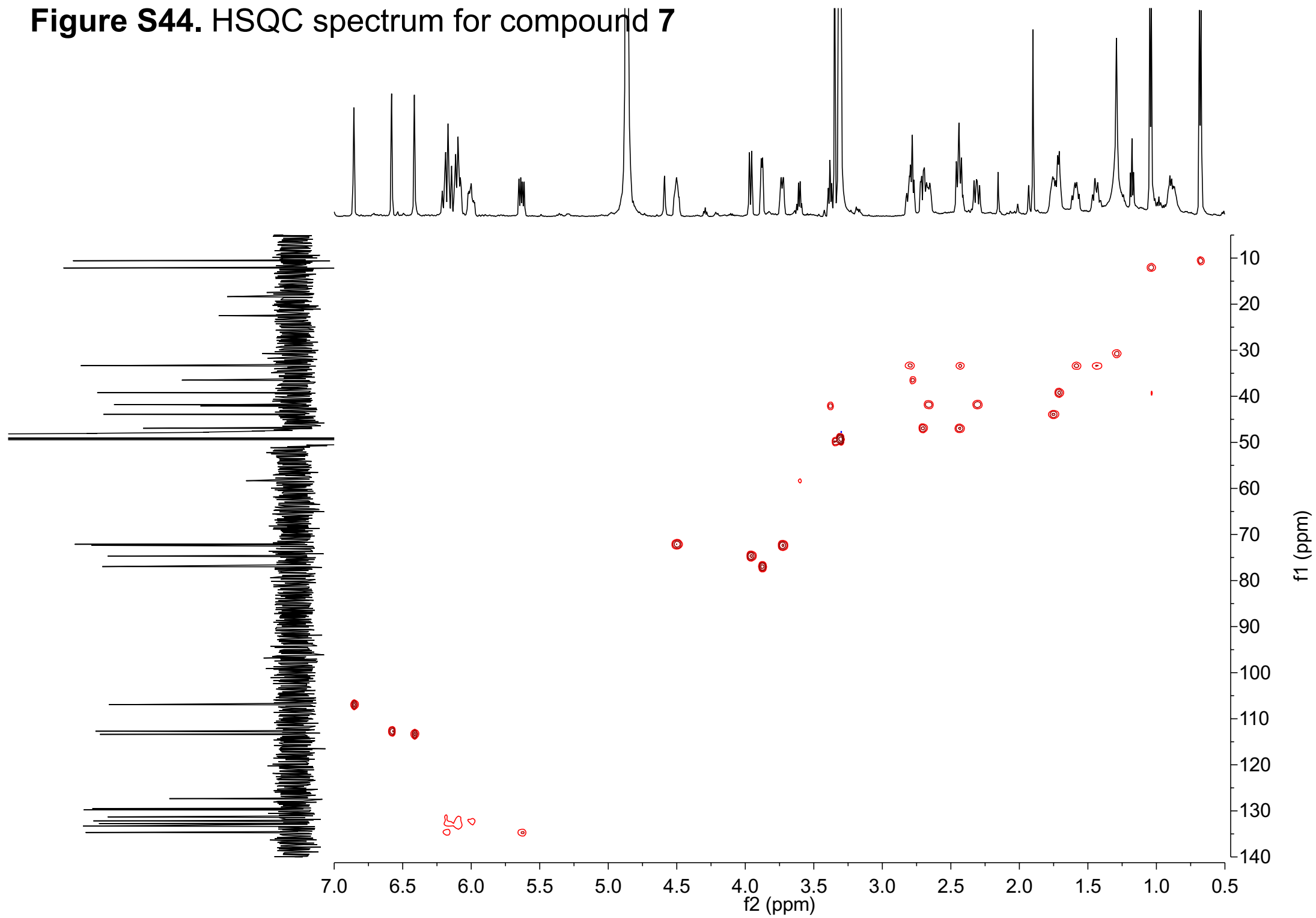


Figure S45. HMBC spectrum for compound **7**

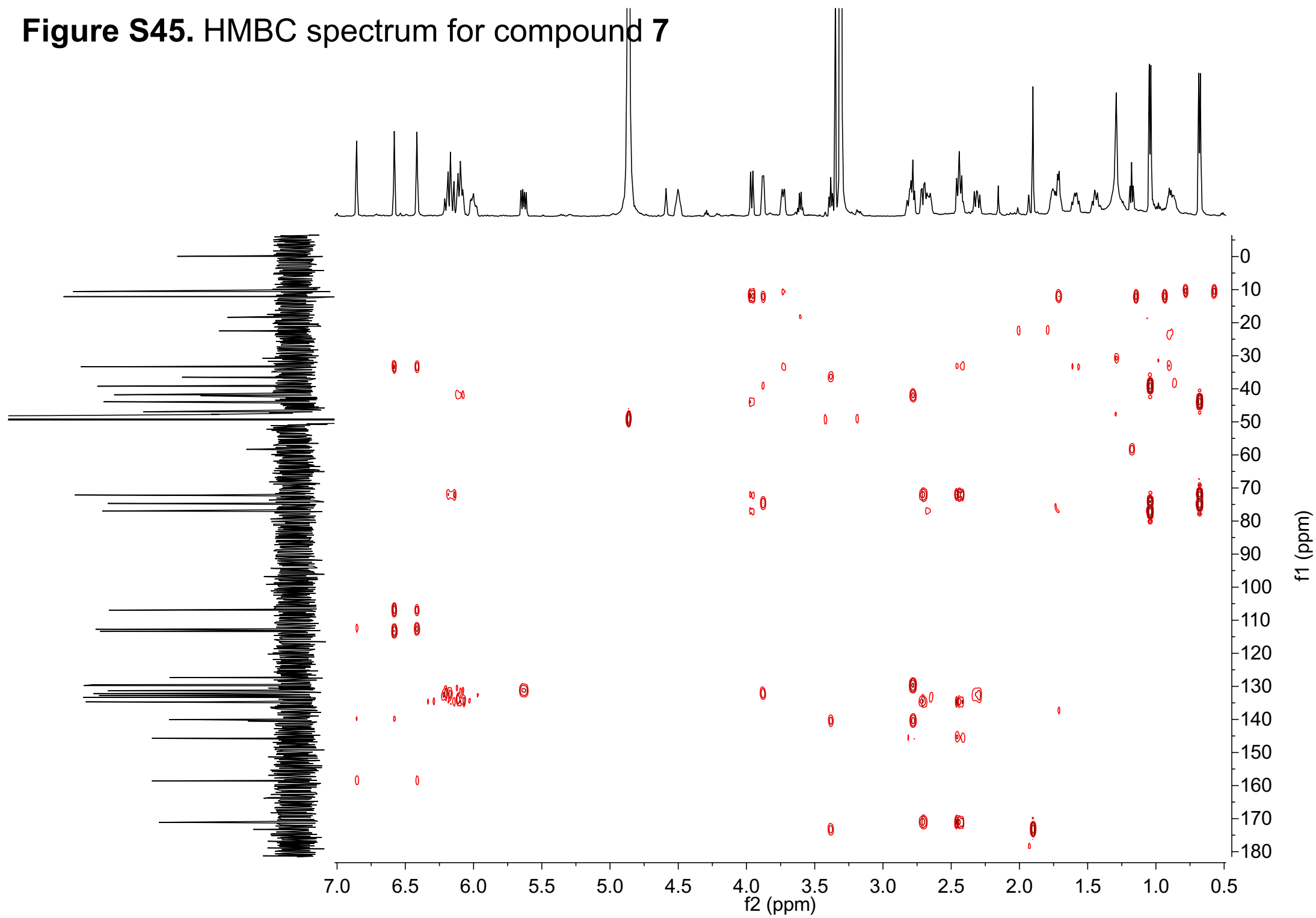


Figure S46. ^1H - ^1H COSY spectrum for compound **7**

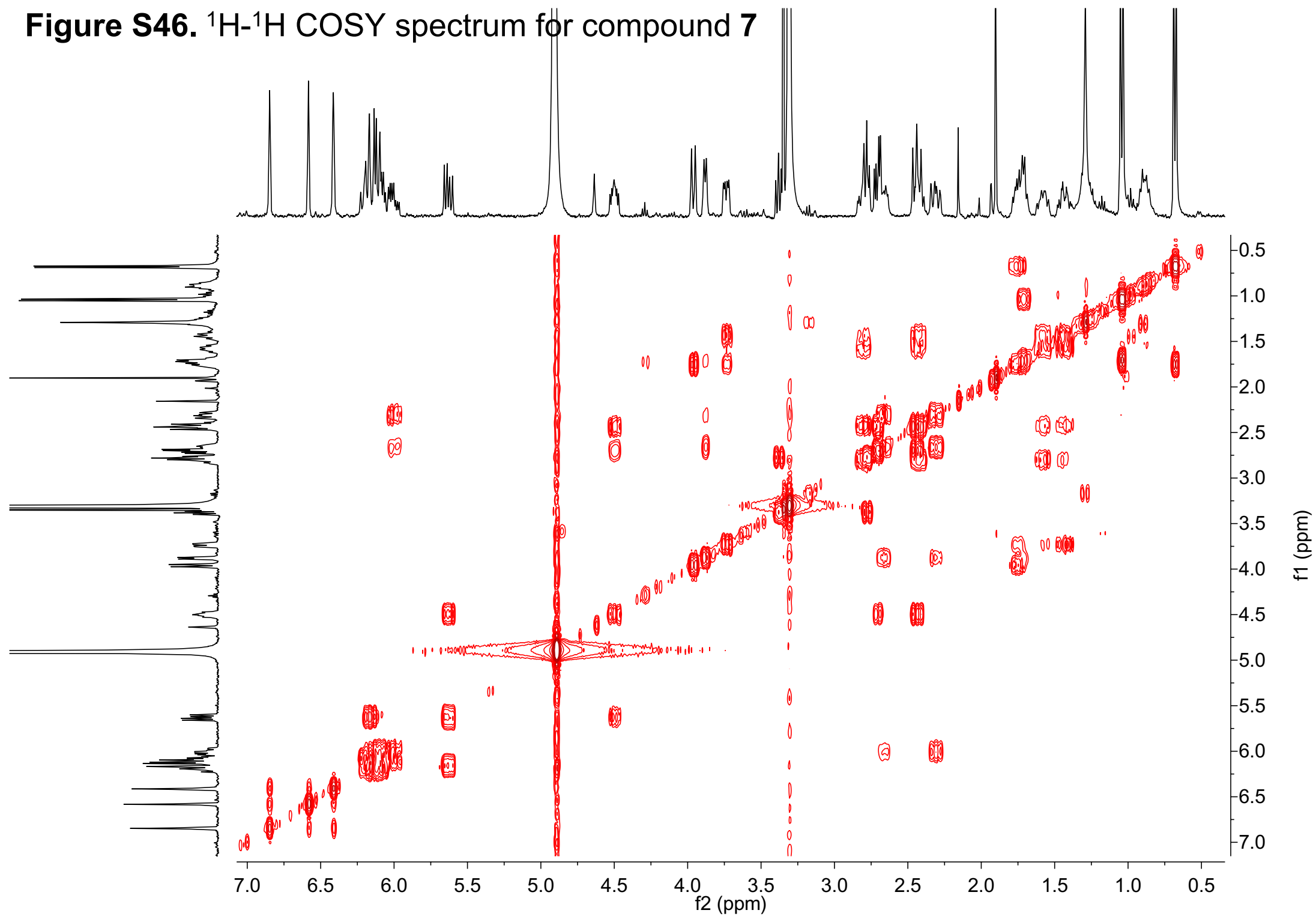


Figure S47. NOESY spectrum for compound 7

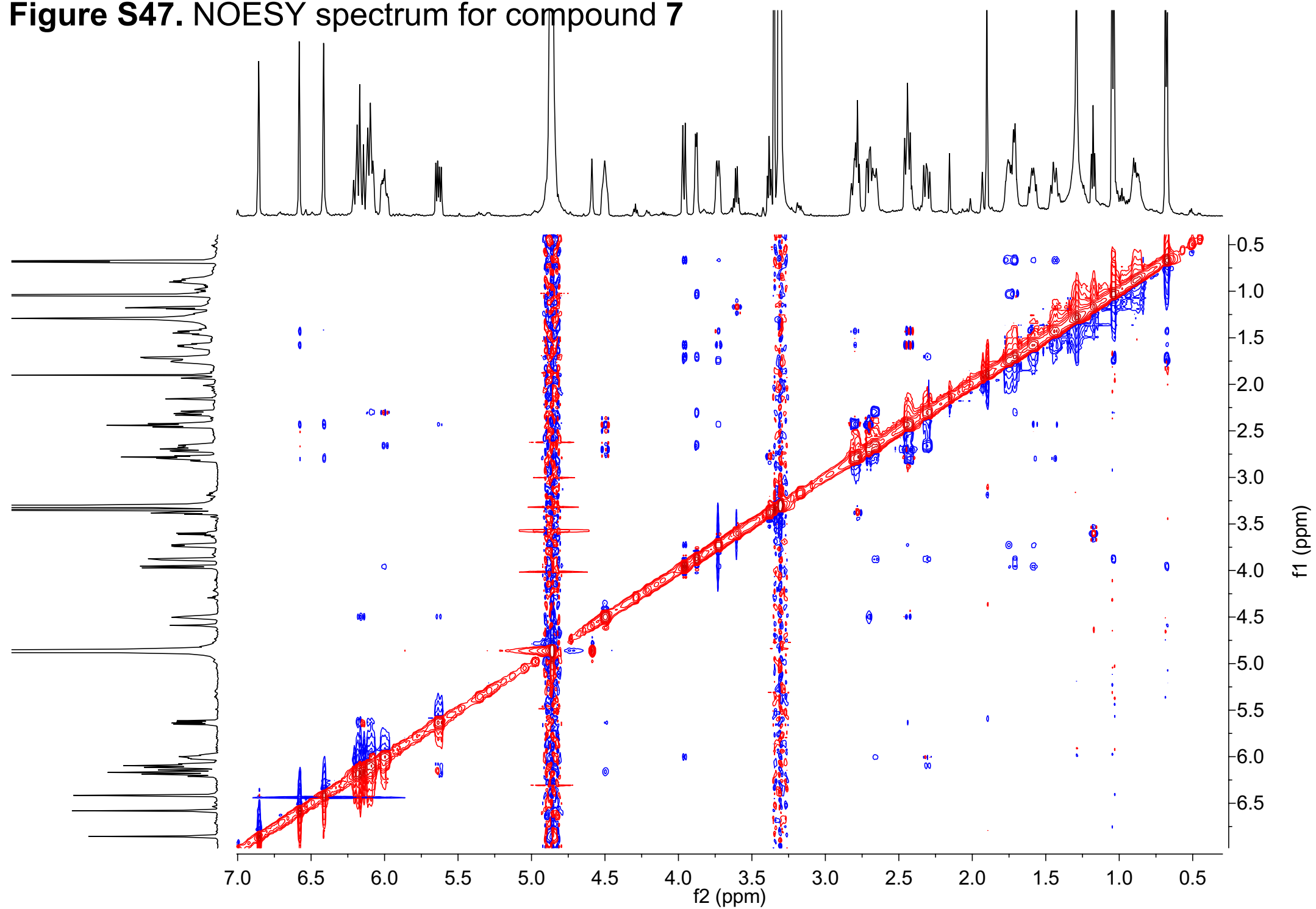


Figure S48. High-resolution ESIMS spectrum for compound **1**

1_N18_160718170135 #8-16 RT: 0.22-0.44 AV: 9 SB: 2 1.49 , 1.49 NL: 2.31E6
T: FTMS + p ESI Full ms [200.00-800.00]

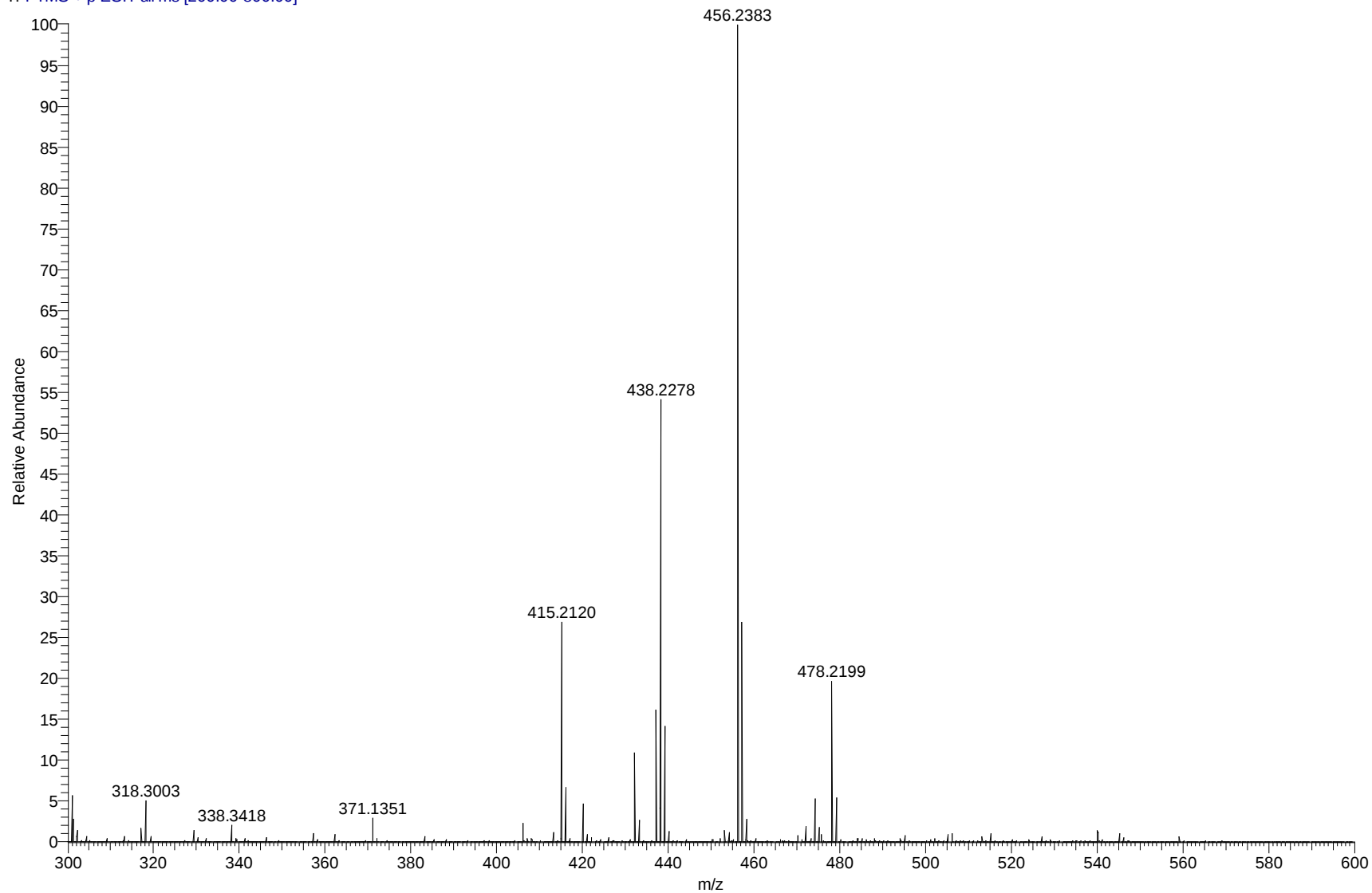


Figure S49. High-resolution ESIMS spectrum for compound **2**

2_N20_160718170335 #7-14 RT: 0.20-0.39 AV: 8 SB: 2 0.62 , 0.62 NL: 3.15E6
T: FTMS + p ESI Full ms [200.00-800.00]

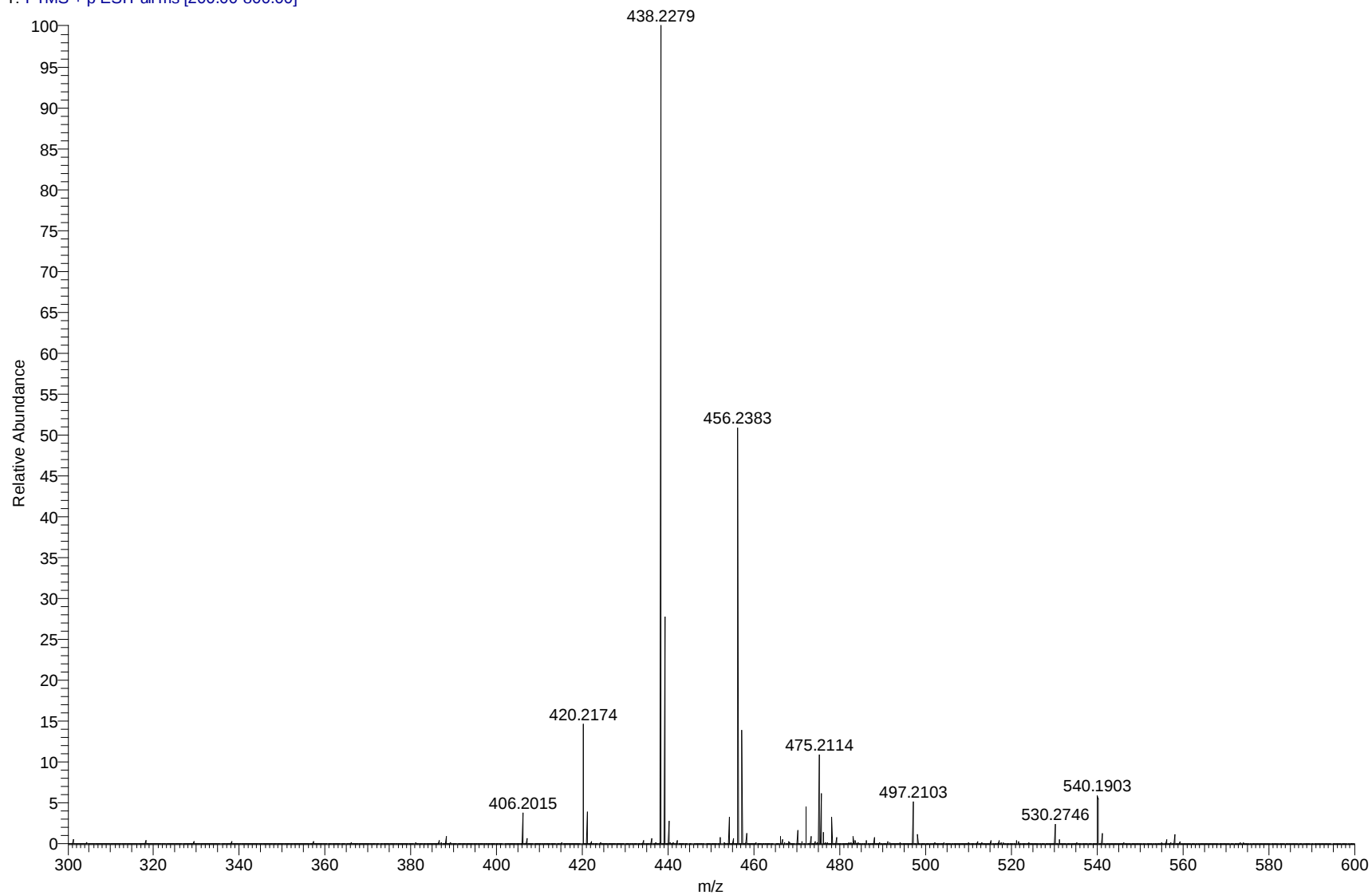


Figure S50. High-resolution ESIMS spectrum for compound **3**

3_N42_160718171045 #7-12 RT: 0.20-0.34 AV: 6 SB: 2 0.47, 0.47 NL: 8.82E5
T: FTMS + p ESI Full ms [200.00-800.00]

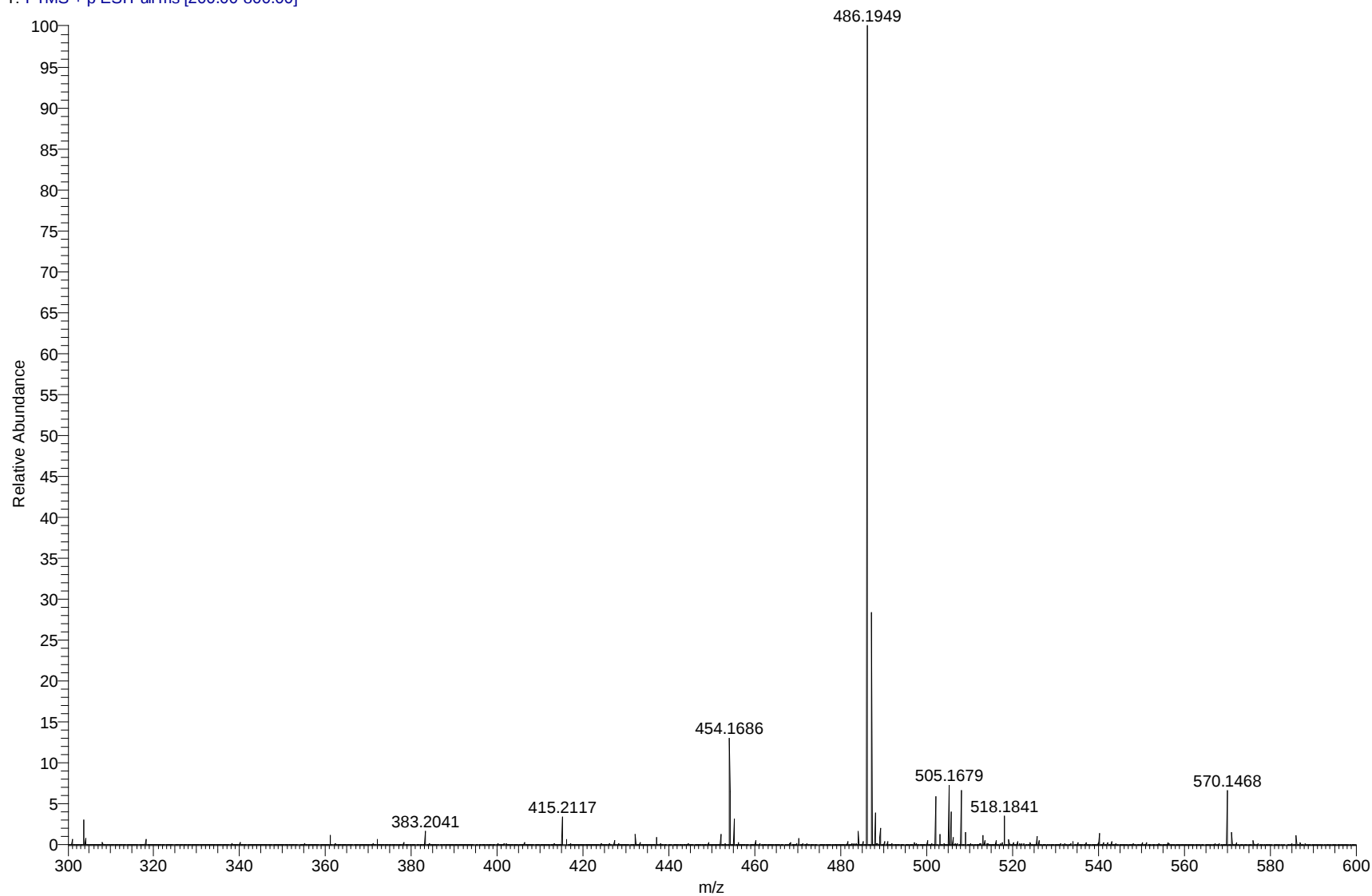


Figure S51. High-resolution ESIMS spectrum for compound **4**

4_N23_160718171246 #7-12 RT: 0.20-0.34 AV: 6 SB: 2 1.49 , 1.49 NL: 3.50E6
T: FTMS + p ESI Full ms [200.00-800.00]

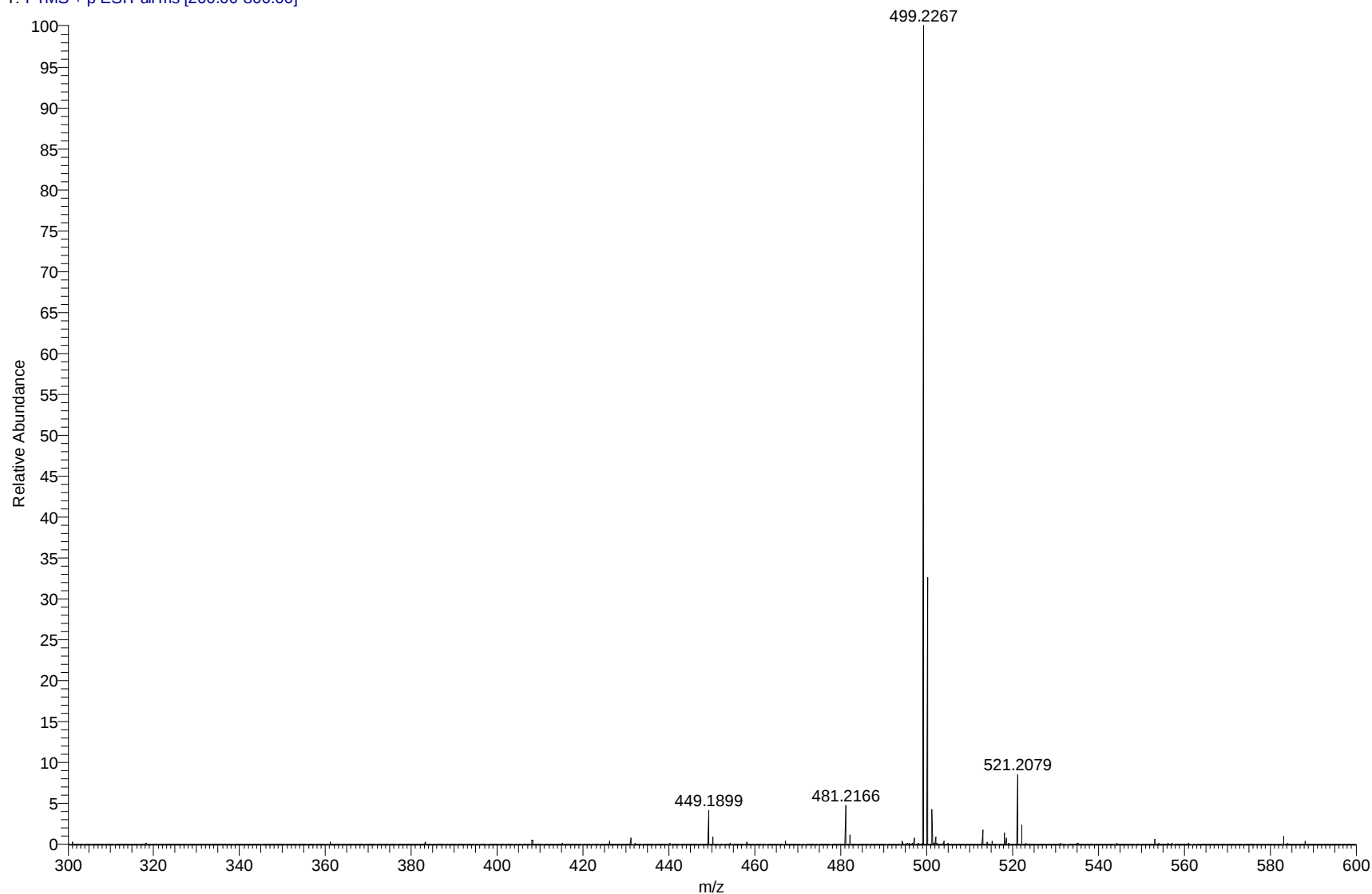


Figure S52. High-resolution ESIMS spectrum for compound **5**

5_N33_160718171445 #6-12 RT: 0.17-0.34 AV: 7 SB: 2 1.50, 1.50 NL: 7.77E5
T: FTMS + p ESI Full ms [200.00-800.00]

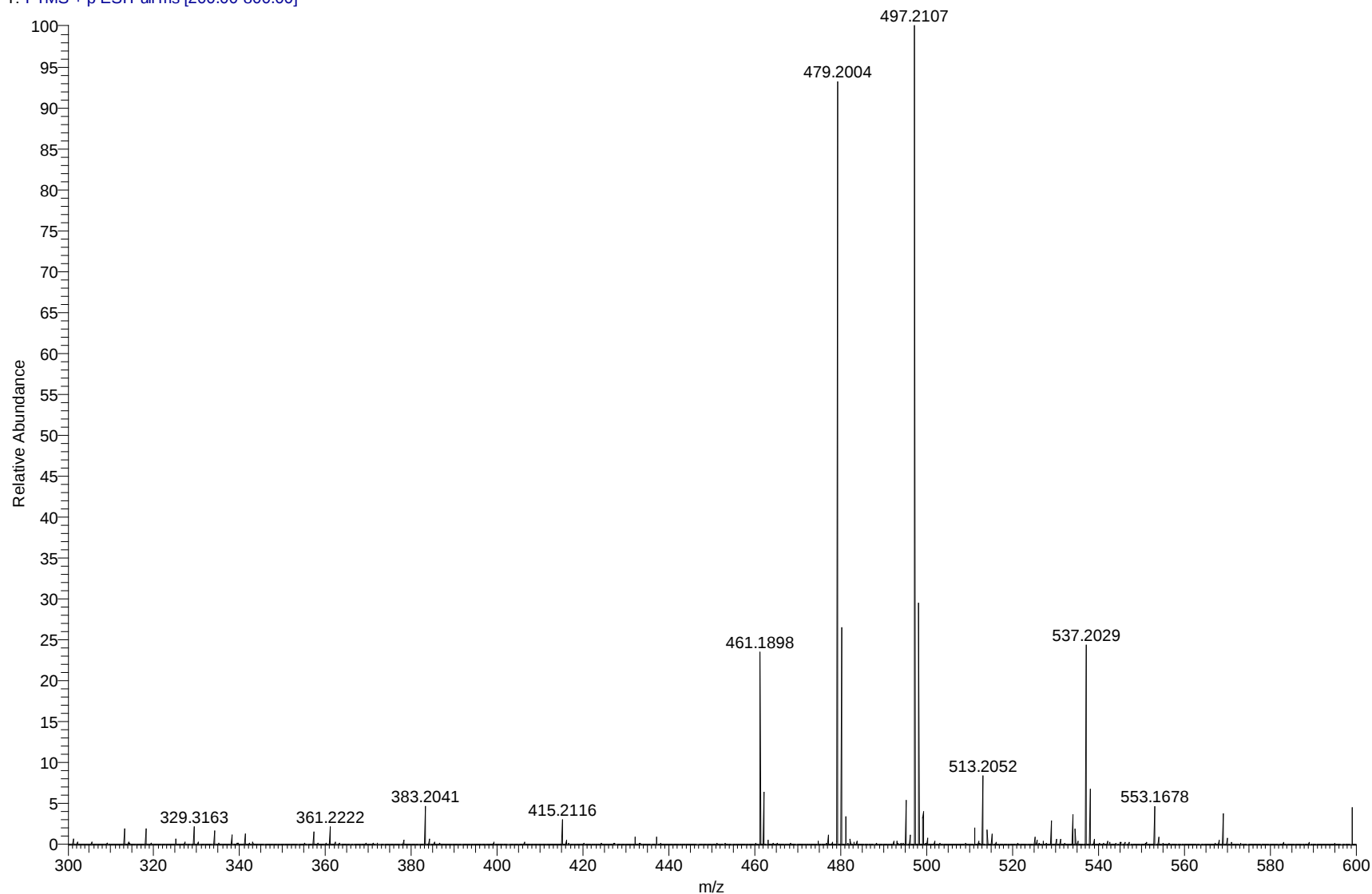


Figure S53. High-resolution ESIMS spectrum for compound **6**

6_N5_160718171847 #6-13 RT:0.17-0.37 AV: 8 SB: 2 1.50, 1.50 NL: 6.74E5
T: FTMS + p ESI Full ms [200.00-800.00]

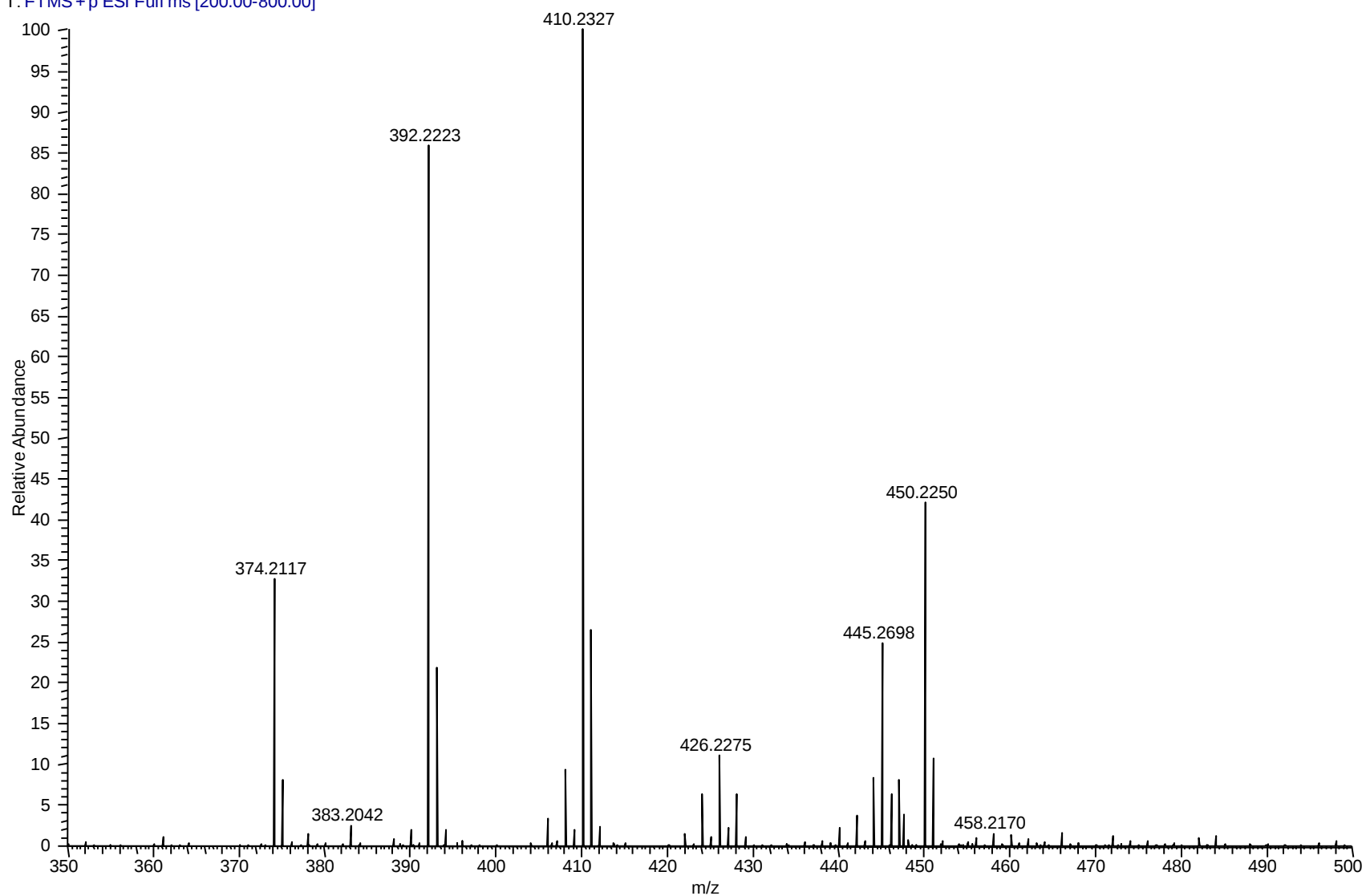


Figure S54. High-resolution ESI/MS spectrum for compound **7**

7_N24_160718171647-13 RT:0.20-0.37 AV: 7 SB: 2 1.49, 1.49 NL: 1.46E6
T: FTMS +p ESI Full ms [200.00-800.00]

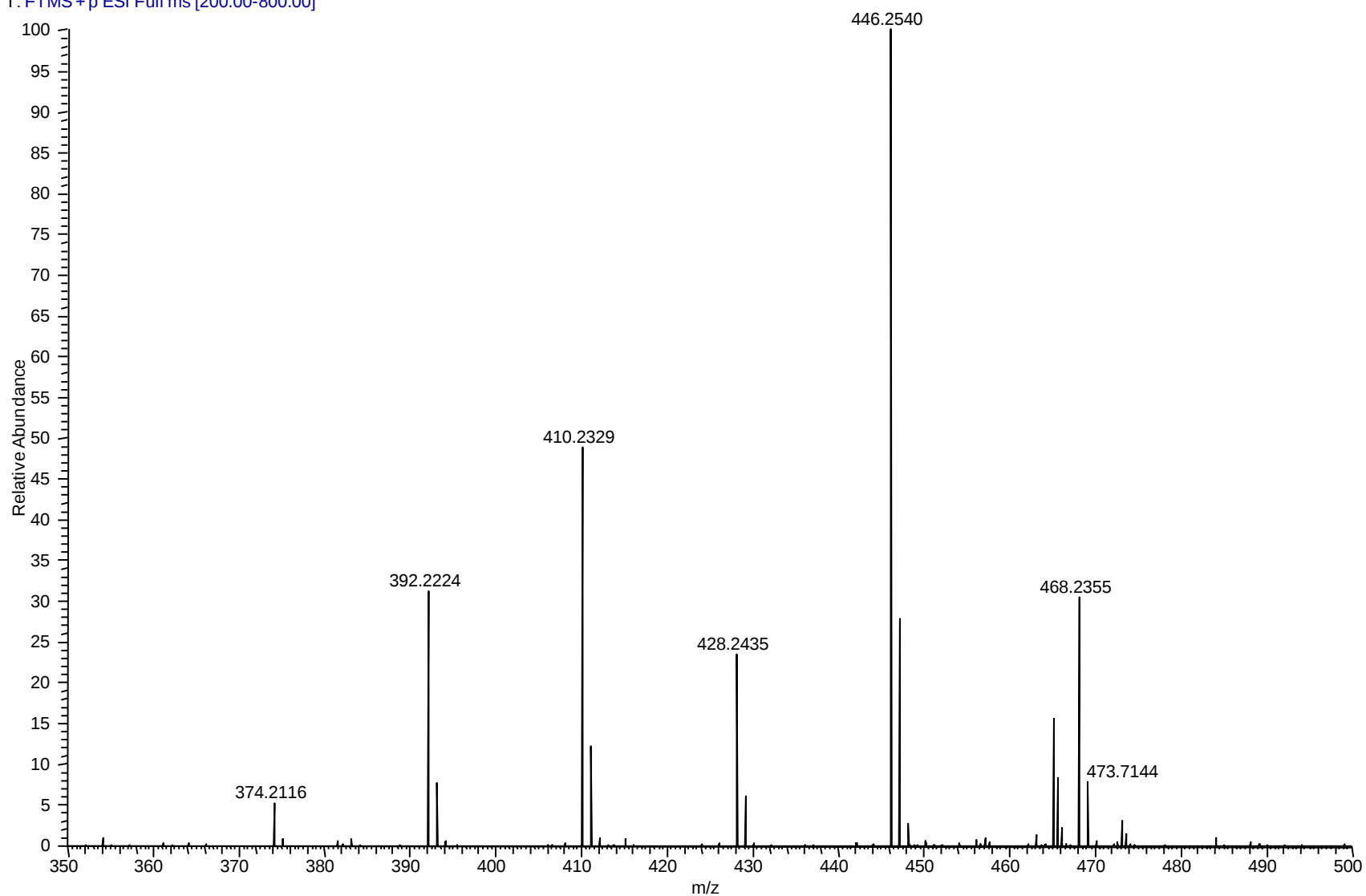


Figure S55. Cell viability was quantified by SRB assay at 72 h after treatment with 40 μ M of indicated compounds.

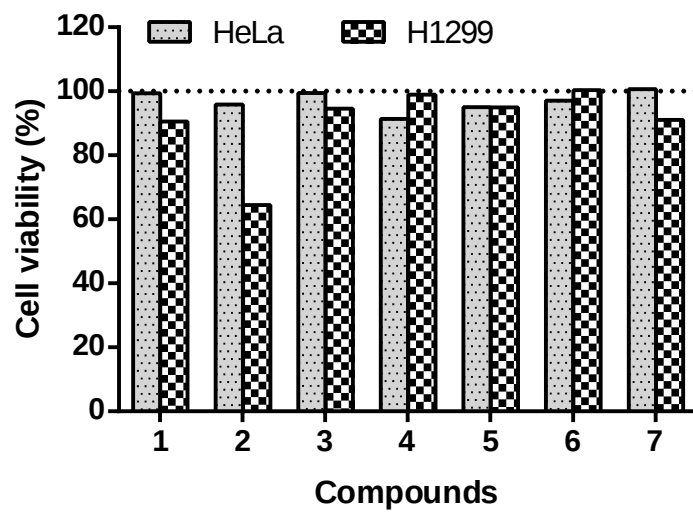
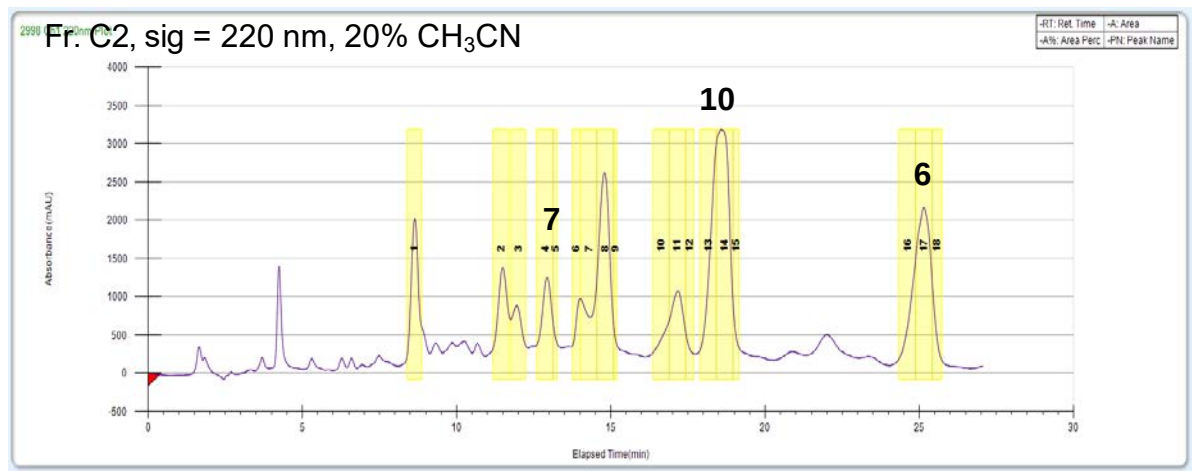
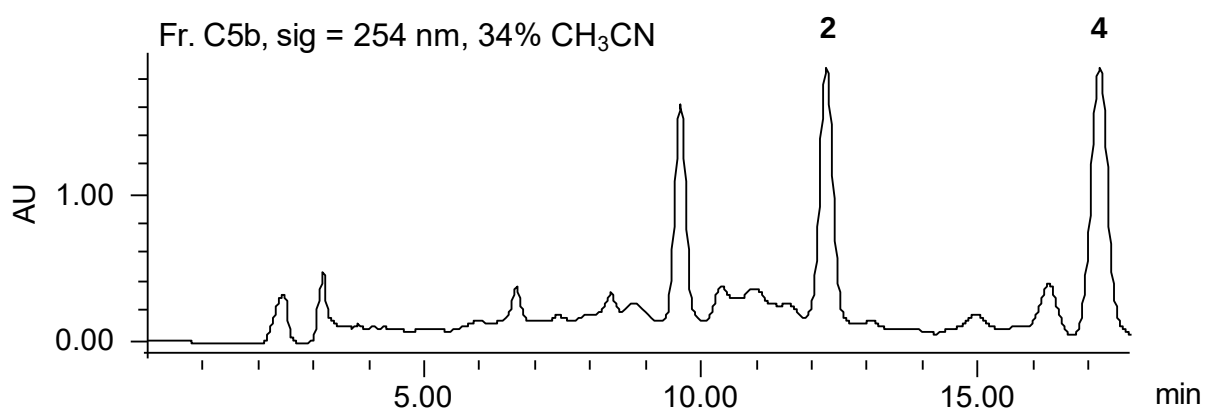
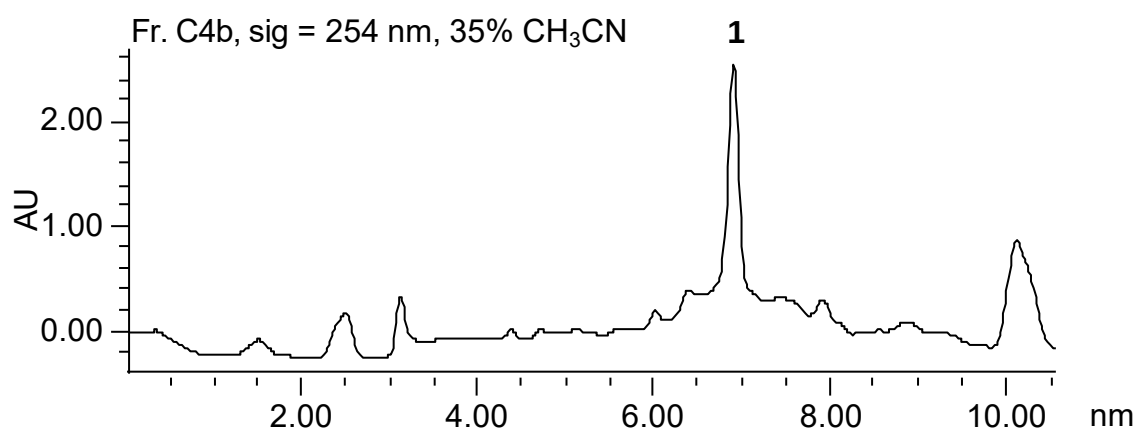
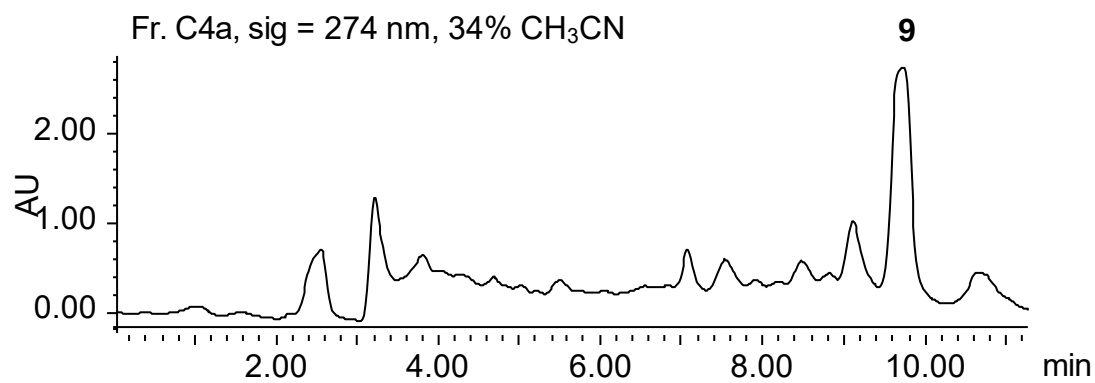
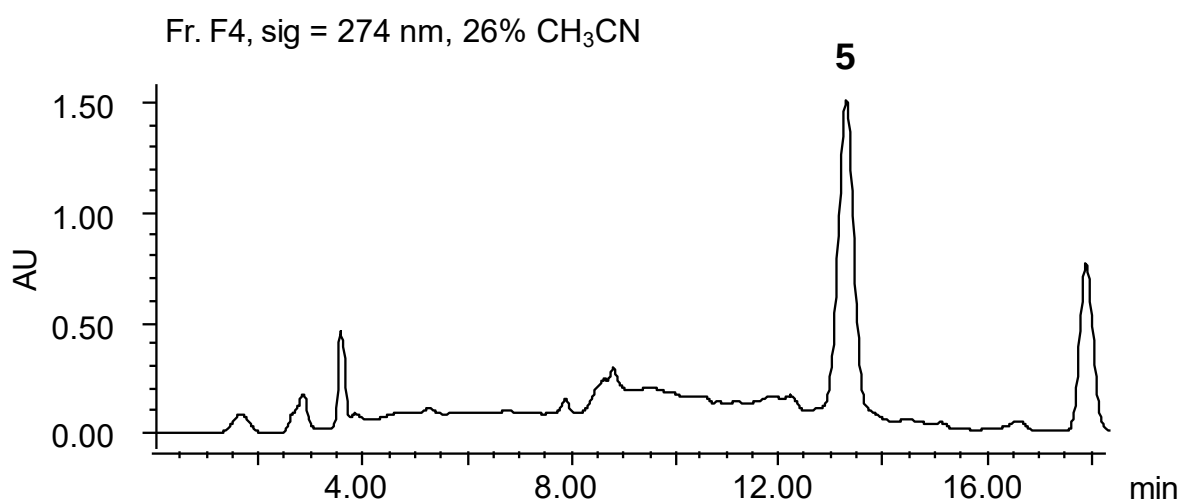
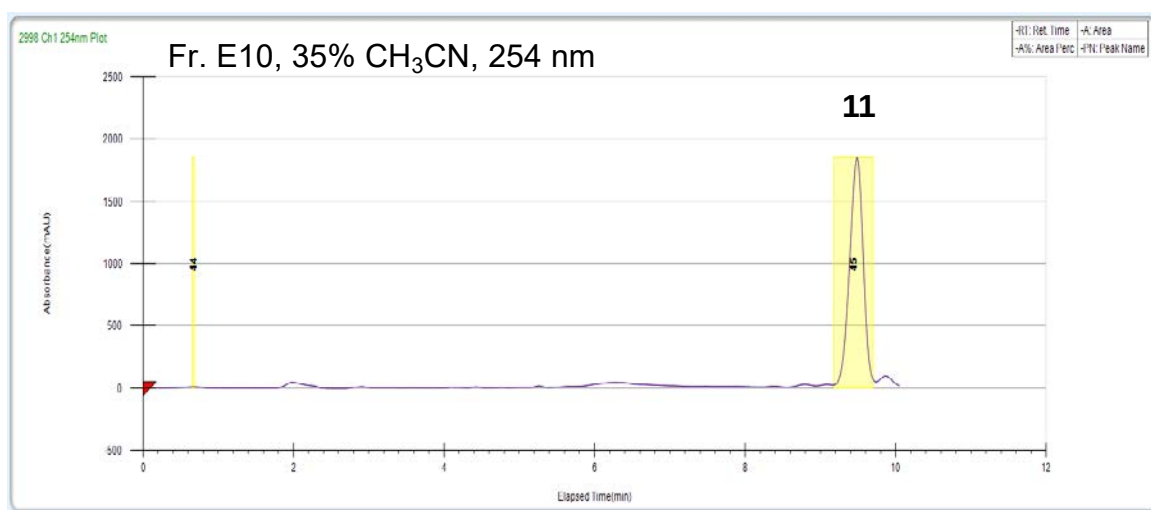
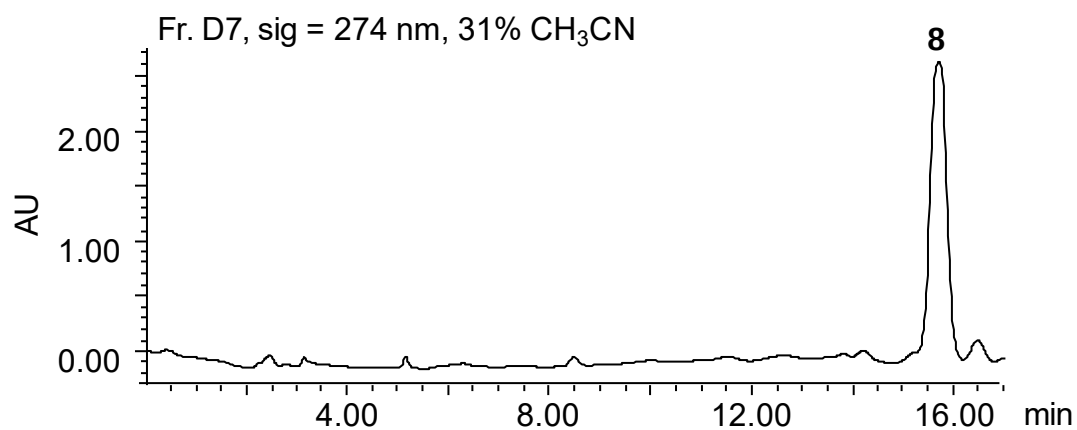


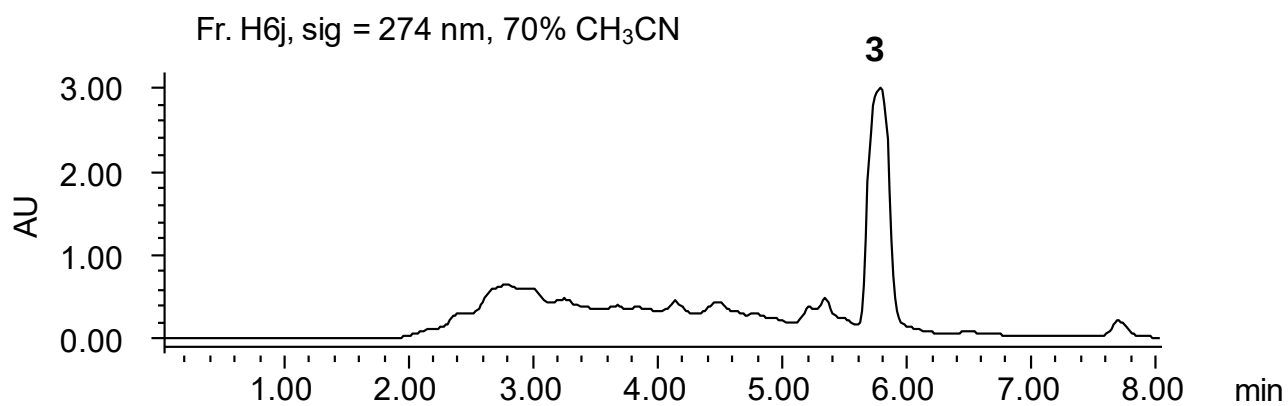
Figure S56. A. HPLC preparation of compounds **1–11**. B. Ultraviolet absorption curve of compounds **1–11**.

A.









B.

