

Supporting Information

The Samholides, Swinholide Related Metabolites from a Marine Cyanobacterium cf. *Phormidium* sp.

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Table of Contents

Tables

Table S1 ¹³C NMR data comparison of samholide A (1), swinholide A and ankaraholide A

Table S2 ¹H NMR data comparison of samholide A (1), swinholide A and ankaraholide A

Table S3 NMR data for samholide B (2)

Table S4 NMR data for samholide C (3)

Table S5 NMR data for samholide D (4)

Table S6 NMR data for samholide E (5)

Table S7 NMR data for samholide F (6)

Table S8 NMR data for samholide G (7)

Table S9 NMR data for samholide H (8)

Table S10 NMR data for samholide I (9)

Figures

Figure S1 The ESI MS spectrum of samholide A (1)

Figure S2 The ESI MS² spectrum of samholide A (1)

Figure S3 The positive HRESIMS spectrum of samholide A (1)

Figure S4 ¹H NMR (600 MHz, DMSO) spectrum of samholide A (1)

- Figure S5 Amplified ^1H NMR (600 MHz, DMSO) spectrum of samholide A (1)
- Figure S6 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide A (1)
- Figure S7 Amplified ^{13}C NMR (150 MHz, DMSO) spectrum of samholide A (1)
- Figure S8 DEPT spectrum of samholide A (1)
- Figure S9 ^1H - ^1H COSY spectrum of samholide A (1)
- Figure S10 HMBC spectrum of samholide A (1)
- Figure S11 Amplified HMBC spectrum of samholide A (1)
- Figure S12 HMQC spectrum of samholide A (1)
- Figure S13 HSQC-TOCSY spectrum of samholide A (1)
- Figure S14 ROESY spectrum of samholide A (1)
- Figure S15 Amplified ROESY spectrum of samholide A (1)
- Figure S16 The ESI MS spectrum of samholide B (2)
- Figure S17 The ESI MS² spectrum of samholide B (2)
- Figure S18 The positive HRESIMS spectrum of samholide B (2)
- Figure S19 ^1H NMR (600 MHz, DMSO) spectrum of samholide B (2)
- Figure S20 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide B (2)
- Figure S21 DEPT spectrum of samholide B (2)
- Figure S22 ^1H - ^1H COSY spectrum of samholide B (2)
- Figure S23 HMBC spectrum of samholide B (2)
- Figure S24 HMQC spectrum of samholide B (2)
- Figure S25 HSQC-TOCSY spectrum of samholide B (2)
- Figure S26 ROESY spectrum of samholide B (2)
- Figure S27 The ESI MS spectrum of samholide C (3)
- Figure S28 The ESI MS² spectrum of samholide C (3)
- Figure S29 The positive HRESIMS spectrum of samholide C (3)
- Figure S30 ^1H NMR (600 MHz, DMSO) spectrum of samholide C (3)
- Figure S31 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide C (3)
- Figure S32 DEPT spectrum of samholide C (3)
- Figure S33 ^1H - ^1H COSY spectrum of samholide C (3)
- Figure S34 HMBC spectrum of samholide C (3)
- Figure S35 HMQC spectrum of samholide C (3)
- Figure S36 HSQC-TOCSY spectrum of samholide C (3)
- Figure S37 ROESY spectrum of samholide C (3)
- Figure S38 The ESI MS spectrum of samholide D (4)
- Figure S39 The ESI MS² spectrum of samholide D (4)
- Figure S40 The positive HRESIMS spectrum of samholide D (4)
- Figure S41 ^1H NMR (600 MHz, DMSO) spectrum of samholide D (4)
- Figure S42 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide D (4)
- Figure S43 ^1H - ^1H COSY spectrum of samholide D (4)
- Figure S44 HMBC spectrum of samholide D (4)
- Figure S45 HMQC spectrum of samholide D (4)
- Figure S46 HSQC-TOCSY spectrum of samholide D (4)
- Figure S47 ROESY spectrum of samholide D (4)
- Figure S48 The ESI MS spectrum of samholide E (5)

- Figure S49 The ESI MS² spectrum of samholide E (5)
- Figure S50 The positive HRESIMS spectrum of samholide E (5)
- Figure S51 ¹H NMR (600 MHz, DMSO) spectrum of samholide E (5)
- Figure S52 ¹³C NMR (150 MHz, DMSO) spectrum of samholide E (5)
- Figure S53 DEPT spectrum of samholide E (5)
- Figure S54 ¹H-¹H COSY spectrum of samholide E (5)
- Figure S55 HMBC spectrum of samholide E (5)
- Figure S56 HMQC spectrum of samholide E (5)
- Figure S57 ROESY spectrum of samholide E (5)
- Figure S58 The ESI MS spectrum of samholide F (6)
- Figure S59 The ESI MS² spectrum of samholide F (6)
- Figure S60 The positive HRESIMS spectrum of samholide F (6)
- Figure S61 ¹H NMR (600 MHz, DMSO) spectrum of samholide F (6)
- Figure S62 ¹³C NMR (150 MHz, DMSO) spectrum of samholide F (6)
- Figure S63 ¹H-¹H COSY spectrum of samholide F (6)
- Figure S64 Amplified ¹H-¹H COSY spectrum of samholide F (6)
- Figure S65 HMBC spectrum of samholide F (6)
- Figure S66 Amplified HMBC spectrum of samholide F (6)
- Figure S67 HMQC spectrum of samholide F (6)
- Figure S68 HSQC-TOCSY spectrum of samholide F (6)
- Figure S69 ROESY spectrum of samholide F (6)
- Figure S70 Amplified ROESY spectrum of samholide F (6)
- Figure S71 The ESI MS spectrum of samholide G (7)
- Figure S72 The ESI MS² spectrum of samholide G (7)
- Figure S73 The positive HRESIMS spectrum of samholide G (7)
- Figure S74 ¹H NMR (600 MHz, DMSO) spectrum of samholide G (7)
- Figure S75 ¹³C NMR (150 MHz, DMSO) spectrum of samholide G (7)
- Figure S76 ¹H-¹H COSY spectrum of samholide G (7)
- Figure S77 HMBC spectrum of samholide G (7)
- Figure S78 HMQC spectrum of samholide G (7)
- Figure S79 HSQC-TOCSY spectrum of samholide G (7)
- Figure S80 ROESY spectrum of samholide G (7)
- Figure S81 The ESI MS spectrum of samholide H (8)
- Figure S82 The ESI MS² spectrum of samholide H (8)
- Figure S83 The positive HRESIMS spectrum of samholide H (8)
- Figure S84 ¹H NMR (600 MHz, DMSO) spectrum of samholide H (8)
- Figure S85 ¹³C NMR (150 MHz, DMSO) spectrum of samholide H (8)
- Figure S86 ¹H-¹H COSY spectrum of samholide H (8)
- Figure S87 Amplified ¹H-¹H COSY spectrum of samholide H (8)
- Figure S88 HMBC spectrum of samholide H (8)
- Figure S89 Amplified HMBC spectrum of samholide H (8)
- Figure S90 HMQC spectrum of samholide H (8)
- Figure S91 HSQC-TOCSY spectrum of samholide H (8)
- Figure S92 Amplified HSQC-TOCSY spectrum of samholide H (8)

- Figure S93 ROESY spectrum of samholide H (8)
- Figure S94 The ESI MS spectrum of samholide I (9)
- Figure S95 The ESI MS² spectrum of samholide I (9)
- Figure S96 The positive HRESIMS spectrum of samholide I (9)
- Figure S97 ¹H NMR (600 MHz, DMSO) spectrum of samholide I (9)
- Figure S98 ¹³C NMR (150 MHz, DMSO) spectrum of samholide I (9)
- Figure S99 ¹H-¹H COSY spectrum of samholide I (9)
- Figure S100 HMBC spectrum of samholide I (9)
- Figure S101 HMQC spectrum of samholide I (9)
- Figure S102 HSQC-TOCSY spectrum of samholide I (9)
- Figure S103 ROESY spectrum of samholide I (9)
- Figure S104 MS²-based molecular networking of fractions D-I of cf. *Phormidium* sp.

Table S1 ¹³C NMR data comparison of samholide A (**1**), swinholide A and ankaraholide A^a

No. in 1	Compound 1 (CDCl ₃) 20-demethyl	Swinholide A (CDCl ₃) 16,20-dimethyl	Δ	Ankaraholide A ((CDCl ₃) 16-demethyl	Δ
1	170.64	170.1	0.54	170.1	0.54
2	113.54	113.3	0.24	115	-1.46
3	153.07	153.3	-0.23	151.9	1.17
4	133.91	134.3	-0.39	134.6	-0.69
5	142.86	142.3	0.56	139.8	3.06
6	33.53	33.9	-0.37	33.6	-0.07
7	78.98	76	2.98	76.7	2.28
8	39.86	38.5	1.36	39.7	0.16
9	68.7	65.9	2.8	69.4	-0.7
10	123.27	123.3	-0.03	123.6	-0.33
11	129.67	129.9	-0.23	129.6	0.07
12	31.47	30	1.47	31.9	-0.43
13	63.36	64.6	-1.24	64.4	-1.04
14	36.41	37.4	-0.99	37.2	-0.79
15	75.02	74.4	0.62	74.8	0.22
16	41.19	40.9	0.29	40.7	0.49
17	73.48	73.9	-0.42	74.7	-1.22
18	41.39	41.1	0.29	41.7	-0.31
19	69.62	66.7	2.92	69.9	-0.28
20	42.1	41.1	1	43.6	-1.5
21	70.34	71.4	-1.06	71.4	-1.06
22	40.49	38.7	1.79	40.1	0.39
23	75.81	75.1	0.71	76.6	-0.79
24	33.43	33.3	0.13	33.5	-0.07
25	23.22	24	-0.78	24	-0.78
26	29.29	29.4	-0.11	29.7	-0.41
27	71.53	71.4	0.13	71.6	-0.07
28	35.05	34.9	0.15	35.4	-0.35
29	73.45	73.3	0.15	73.7	-0.25
30	38.88	37.7	1.18	39	-0.12
31	64.7	65.8	-1.1	65	-0.3
32	102.11	—	—	103	-0.89
33	73.16	—	—	73	0.16
34	82.43	—	—	84	-1.57
35	79.26	—	—	79.6	-0.34
36	62.32	—	—	62.8	-0.48
37	170.7	—	—	—	—
38	72.37	—	—	—	—
39	64.66	—	—	—	—
4-Me	12.06	12.3	-0.24	12.7	-0.64
16-Me	9.32	9.1	0.22	N	—
20-Me	N	9.4	—	9.7	—
22-Me	9.69	9.2	0.49	9.8	-0.11
24-Me	17.22	17.8	-0.58	17.9	-0.68
31-Me	21.87	21.8	0.07	22.3	-0.43

^a Andrianasolo, E. H.; Gross, H.; Goeger, D.; Musafija-Girt, M.; McPhail, K.; Leal, R. M.; Mooberry, S. L.; Gerwick, W. H., Isolation of Swinholide A and Related Glycosylated Derivatives from Two Field Collections of Marine Cyanobacteria. *Organic Letters* 2005, 7 (7), 1375-1378.

Table S2 ¹H NMR data comparison of samholide A (**1**), swinholide A and ankaraholide A^a

No. in 1	Compound 1 (CDCl ₃) 20-demethyl	Swinholide A (CDCl ₃) 16,20-dimethyl	Ankaraholide A (CDCl ₃) 16-demethyl
2	5.78 (overlapped)	5.79 d (15.8)	5.84 d (15.6)
3	7.6 (d, 15.5)	7.58 d (15.8)	7.51 d (15.6)
5	6.34 (dd, 9.44, 3.17)	6.08 dd (9.0, 5.1)	6.25 dd (6.4, 6.3)
6	2.50 (d, 12.76)	2.46 ddd (19.9, 9.7, 9.7)	2.69 m
	2.37 (m)	2.17 br d (14.9)	2.45 m
7	4.10 (m)	4.16 dd (7.2, 7.2)	4.07 m
8	2.33 (m), 1.53 (m)	1.60 m	1.60 m, 1.35 m
9	4.21 (d, 11.81)	4.52 br d (9.2)	4.38 m
10	5.68 (d, 10.26)	5.69 d (10.2)	5.74 d (10.0)
11	5.77 (m)	5.78 m	5.83 m
12	2.08 (d, 17.58), 1.96 (m)	2.28 br d (17.2), 1.89 m	2.00 m, 1.98 m
13	3.69 (m)	3.90 m	3.7 m
14	1.86 (m), 1.64 (m)	1.45 m, 2.15 m	2.22 m, 1.63 m
15	4.07 (m)	4.01 m	3.75 m
16	1.59 (m)	1.68 m	1.65 m, 1.37 m
17	3.84 (t, 9.5)	3.84 dd (9.5, 9.5)	4.11 m
18	1.80 (m), 1.62 (m)	1.63 m, 1.58 m	1.76 m
19	3.95 (m)	4.01 m	3.90 m
20	1.94 (m), 1.52 (m)	1.75 dq (9.7, 7.2)	1.69 m
21	5.84 (d, 11.37)	5.35 d (10.8)	5.38 d (10.1)
22	1.65 (m)	1.93 m	1.92 m
23	3.18 (d, 9.01)	3.13 d (9.7)	3.12 d (8.5)
24	1.65 (m)	1.66 m	1.69 m
25	1.22 (m)	1.38 m, 1.26 m	1.39 m, 1.27 m
26	1.80 (m), 1.22 (m)	1.87 m, 1.25 m	1.90 m, 1.27 m
27	3.94 (m)	4.01 m	4.02 m
28	1.76 (m), 1.55 (m)	1.82 m, 1.59 m	1.84 m, 1.62 m
29	3.50 (m)	3.54 m	3.56 m
30	1.94 (m), 1.15 (m)	1.97 m, 1.17 m	2.01 m, 1.19 m
31	3.64 (m)	3.70 m	3.66 m
32	4.78 (d, 6.09)	—	4.58 d (5.5)
33	4.76 (dd, 8.21, 6.29)	—	3.30 m
34	3.25 (t, 7.50)	—	3.26 m
35	3.33 (m)	—	3.38 m
36	4.00 (dd, 14.79, 7.83), 3.30 (m)	—	4.03 m, 3.29 m
38	4.06 (m)	—	—
39	3.70 (m), 3.50 (m)	—	—
4-Me	1.74 (s)	1.81 s	1.84 s
16-Me	0.83 (d, 6.85)	0.81 d (6.9)	—
20-Me	—	0.98 d (6.9)	0.88 d (7.0)
22-Me	0.90 (d, 6.85)	0.83 d (6.9)	0.94 d (6.7)
24-Me	0.95 (d, 6.67)	0.99 d (7.2)	1.01 d (6.3)
31-Me	1.16 (d, 6.19)	1.20 d (5.9)	1.22 d (6.3)

^a Andrianasolo, E. H.; Gross, H.; Goeger, D.; Musafija-Girt, M.; McPhail, K.; Leal, R. M.; Mooberry, S. L.; Gerwick, W. H., Isolation of Swinholide A and Related Glycosylated Derivatives from Two Field Collections of Marine Cyanobacteria. *Organic Letters* 2005, 7 (7), 1375-1378.

Table S3 NMR data for samholide B (2)

	δ_C	$\delta_{C'}$	δ_H	$\delta_{H'}$	COSY	HMBC(H→C)	HSQC-TOCSY	ROESY
1,1'	167.9	170.1						
2,2'	116.3	114.3	5.67 m	5.79 m	3/3'	1, 1', 4, 4', 21, 21'	3/3', 2/2'	4'-Me
3,3'	148.6	152.2	6.51 d (12.6)	7.50 d (15.6)	2/2'	1, 1', 2', 4', 4-Me, 4'-Me, 5, 5'	2/2', 3/3',	5/5'
4,4'	134.1							
4,4'-Me	15.7	12.4	1.86 s	1.77 s	5/5'	3/3', 4/4', 5/5'	4/4'-Me, 5/5'	2/2', 8/8'
5,5'	135.0	140.6	5.84 dd (7.06, 6.27)	6.14 dd (6.47)	6/6', 4/4'-Me	3/3', 4/4'-Me, 6/6', 7/7'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	3/7, 3'/7'
6,6'	33.0	33.1	2.55 dd (14.73, 5.62)	2.62 br d (13.34)	5/5', 7/7'	4/4', 5/5', 7/7', 8/8'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	9/9',
			2.38 m	2.28 m				
7,7'	77.4 ^b	77.7 ^b	4.06 m	4.10 m	6/6', 8/8'	32/32'	6/6', 8/8', 9/9', 7/7', 5/5'	32'
8,8'	39.5	39.6	2.15 m, 1.52 m	2.28 m, 1.54 m	7/7', 9/9'	6/6', 7/7', 8/8', 9/9'	5/5', 7/7', 9/9', 8/8', 6/6'	
9,9'	69.5		4.30 m		8/8', 10/10'	8/8', 10/10', 11/11', 13/13'	6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a'
10,10'	129.7 ^a	129.6 ^a	5.70 m		9/9', 11/11', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	123.8 ^a	123.7 ^a	5.80 m		10/10', 12/12'	9/9', 12/12', 13/13'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.5 ^a	31.4 ^a	2.01 m		11/11', 13/13'	10/10', 11/11', 13/13', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	64.1	63.8	3.67 m		12/12', 14/14'a		12/12', 14/14', 15/15', 13/13'	
14,14'	36.2	35.9	1.87 m, 1.62 m		13/13', 15/15'		12/12', 14/14', 13/13', 15/15'	
15,15'	77.2 ^b		4.06 m		14/14'		12/12', 14/14', 13/13', 15/15',	
16,16'	41.5		1.54 m		16/16'-Me, 15/15'		13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	9.9 ^a	9.6 ^a	0.81 d (6.0)	0.82 d (6.0)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	73.9	73.6	3.85 m		18/18'		16/16'-Me, 18/18', 17/17', 19/19'	
18,18'	40.9	41.2	1.76 m, 1.63 m				17/17', 18/18', 19/19', 20/20'	
19,19'	69.3	68.8	3.93 m	3.88, m			20/20', 21/21', 19/19', 18/18'	
20,20'	41.1	41.5	1.94 m, 1.53 m		20/20'		20/20', 21/21', 19/19'	
21,21'	71.1	71.4	5.63 d (9.82)	5.71 m		1', 1,19, 19', 20', 22-Me, 22'-Me, 23, 23'	20/20', 19/19'	
22,22'	41.1	40.9	1.64 m		22/22'		22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
22,22'-Me	10.0	10.2	0.87 d (6.81)	0.89 d (6.86)	22/22', 24/24'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	
23,23'	76.6	76.1	3.17 d (9.69)	3.12 d (9.59)		21/21', 22/22', 24/24'-Me, 25/25'	22/22'-Me, 22/22', 23/23'	22/22'-Me, 24/24'-Me
24,24'	33.5		1.67 m		24/24'		24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
24,24'-Me	17.6 ^a	17.5 ^a	0.97 d (7.15)	0.95 d (7.07)		23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	24.0 ^a	23.8 ^a	1.25 m				24,24'-Me, 26/26', 25/25', 24/24', 27/27'	

26,26'	29.4	29.3		1.88 m, 1.25 m			24/24'-Me, 25/25', 26/26', 27/27'
27,27'	71.6	71.5		3.99 m			24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'
28,28'		35.1		1.82 m, 1.59 m			31/31', 30/30', 28/28', 29/29', 27/27'
29,29'		73.4		3.53 m			28/28', 29/29', 30/30', 31/31', 31/31'-Me,
30,30'		38.9		1.99 m, 1.18 m			31/31'-Me, 28/28', 30/30', 31/31', 29/29'
31,31'		64.8		3.67 m			31/31'-Me, 28/28', 30/30', 31/31', 29/29'
31,31'-Me	22.0 ^a	21.9 ^a	1.18 d (6.36)	1.17 d (6.14)	31/31'	30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'
32,32'	100.7	101.2	4.67 d (6.91)	4.74 d (6.80)		7/7', 33/33', 36/36'	32/32', 33/33', 34/34', 35/35', 36/36'
33,33'		73.4		4.82 dd (8.33, 7.02)	34/34'	32/32', 34/34', 37/37'	32/32', 33/33', 34/34', 35/35', 36/36'
34,34'	82.1	82.4		3.34 m	33/33'		32/32', 33/33', 34/34', 35/35', 36/36'
35,35'	79.0	79.3		3.34 m			32/32', 33/33', 34/34', 35/35', 36/36'
36,36'		62.7		4.05 m, 3.28 m	35/35'	32/32', 34/34', 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'
37,37'	171.4	170.9					
38,38'	72.5	72.4	4.28 m	4.20 brs	39/39'	37/37', 39/39'	38/38', 39/39'
39,39'	64.4	64.5		3.88 m, 3.66 m	38/38'	38/38'	38/38', 39/39'
15,15'-OMe	57.1 ^a	57.2 ^a		3.34 s		15,15'-OMe	
29,29'-OMe		55.4		3.32 s		29,29'-OMe	
34,34'-OMe	60.2 ^a	60.1 ^a		3.48 s		34,34'-OMe	
35,35'-OMe	58.6 ^a	58.7 ^a		3.44 s		35,35'-OMe	

^a Can be exchanged.

^b Overlapped with CDCl₃, assigned using HMBC, HSQC and HSQC-TOCSY.

Table S4 NMR data for samholide C (3)

	δ_C/δ_C'	δ_H/δ_H'	COSY	HMBC	HSQC-TOCSY	ROESY
1,1'	170.3					
2,2'	114.2	5.79 d (15.59)	3/3'	3/3', 1/1'	3/3', 2/2'	4/4'-Me
3,3'	152.4	7.53 d (15.56)	2/2'	1/1', 2/2', 4/4', 4/4'-Me, 5/5'	2/2', 3/3'	5/5'
4,4'	134.6					
4,4'-Me	12.4	1.82 s	5/5'	3/3', 4/4', 5/5'	4/4'-Me, 5/5'	2/2', 6/6'
5,5'	140.8	6.31 dd (7.55, 7.37)	6/6', 4/4'-Me	4/4'-Me, 3/3', 6/6', 7/7'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	7/7', 3/3'
6,6'	33.2	2.59 ddd (2.85, 6.14, 14.47) 2.37 dt (8.86, 14.34)	5/5', 7/7'	4/4', 5/5', 7/7', 8/8'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	4/4'-Me, 9/9'
7,7'	76.6 ^a	4.04 m	6/6', 8/8'	5/5', 6/6', 8/8', 9/9', 32/32'	6/6', 8/8', 9/9', 7/7', 5/5'	5/5', 32/32'
8,8'	39.8	2.25 ddd (5.02, 9.81, 15.0) 1.63 m	7/7', 9/9'	6/6', 7/7', 9/9', 10/10'	5/5', 7/7', 9/9', 8/8', 6/6'	4/4'-Me, 13/13'
9,9'	69.6	4.30 m	8/8', 10/10'	7/7', 8/8', 10/10', 11/11', 13/13',	6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a', 14/14'
10,10'	129.8	5.74 m	9/9', 11/11', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	123.5	5.74 m	10/10', 12/12'	9/9', 12/12', 13/13'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.6	1.97 m	11/11', 13/13'	10/10', 11/11', 13/13', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	63.6	3.63 m	12/12', 14/14' ^a		12/12', 14/14', 15/15', 13/13'	5/5', 7/7', 8a/8a'
14,14'	36.9	1.78 m, 1.64 m	13/13', 15/15'	9/9', 14/14', 15/15'	12/12', 14/14', 13/13', 15/15'	
15,15'	76	4.01 m	14/14'	14/14', 15/15'-OMe, 16/16'-Me, 16/16', 17/17'	12/12', 14/14', 13/13', 15/15',	13/13'
16,16'	41.5	1.51 m	16/16'-Me, 15/15'	16/16'-Me, 15/15'	13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	9.3	0.78 d (6.98)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	74	3.84 t (9.70)	18/18'	15/15', 16/16'-Me, 16/16', 18/18', 19/19'	16/16'-Me, 18/18', 17/17', 19/19'	16/16'-Me
18,18'	40.8	1.70 m, 1.41 m		17/17', 19/19'	17/17', 18/18', 19/19', 20/20'	
19,19'	69.9	3.88 t (10.55)		17/17', 18/18', 21/21'	20/20', 21/21', 19/19', 18/18'	
20,20'	42.2	1.87 m	20/20'	21/21',	20/20', 21/21', 19/19'	
21,21'	70.6	5.56 d (11.09)		1/1', 19/19', 23/23', 20/20', 22/22', 22/22'-Me	20/20', 19/19'	22-Me, 19/19'
22,22'	40.8	1.65 m	22/22'		22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
22,22'-Me	10.1	0.90 d (6.89)	22/22', 24/24'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	
23,23'	76.3	3.19 m		21/21', 22/22', 24/24', 24/24'-Me, 25/25'	22/22'-Me, 22/22', 23/23'	22/22'-Me, 24/24'-Me, 21/21'
24,24'	33.2	1.68 m	24/24'	23/23', 24/24'-Me	24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	

24,24'-Me	17.4	0.93 d (6.73)		23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	23.9	1.34 m, 1.17 m		24/24', 24/24'-Me, 26/26'	24,24'-Me, 26/26', 25/25', 24/24', 27/27'	
26,26'	29.4	1.83 m, 1.26 m		25/25', 27/27'	24/24'-Me, 25/25', 26/26', 27/27'	
27,27'	71	3.98 m			24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'	
28,28'	35	1.79 m, 1.59 m		29/29'	31/31', 30/30', 28/28', 29/29', 27/27'	
29,29'	73.4	3.52 ddd (4.4, 9.83, 14.17)		27/27', 28/28', 31/31', 29/29'-OMe	28/28', 29/29', 30/30', 31/31', 31/31'-Me,	
30,30'	38.7	1.95 m, 1.18 m			31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'	64.9	3.69 dddd (2.88, 6.13, 12.0, 15.0)		27/27', 29/29', 31/31'-Me	31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'-Me	22	1.20 d (6.18)	31/31'	30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'	
32,32'	103.3	4.43 d (6.64)		7/7', 34/34', 36/36'	32/32', 33/33', 34/34', 35/35', 36/36'	6/6', 7/7', 34/34', 5/5'
33,33'	73.4	3.28 t (7.15)	34/34'	32/32', 34/34'	32/32', 33/33', 34/34', 35/35', 36/36'	
34,34'	83.5	3.24 m	33/33'	34/34'-OMe	32/32', 33/33', 34/34', 35/35', 36/36'	
35,35'	79.4	3.24 m		34/34'	32/32', 33/33', 34/34', 35/35', 36/36'	
36,36'	62.5	3.98 m, 3.16 m	35/35'	32/32', 34/34', 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'	
15,15'-OMe	57.5	3.35 s		15/15'		
29,29'-OMe	55.4	3.32 s		29/29'		
34,34'-OMe	60.2	3.56 s		34/34'		
35,35'-OMe	58.6	3.45 s		35/35'		

^a Overlapped with CDCl₃, assigned using HMBC, HSQC and HSQC-TOCSY.

Table S5 NMR data for samholide D (4)

	δ_C	$\delta_{C'}$	δ_H	$\delta_{H'}$	COSY	HMBC	HSQC-TOCSY	ROESY
1,1'	167.4	170.9						
2,2'	116.7	115.8	5.69 m	5.82 m	3/3'	4/4', 1/1'	3/3', 2/2'	3, 4'-Me
3,3'	148.5	150.5	6.46 d (12.41)	7.39 d (15.56)	2/2'	1, 2, 4, 4'-Me, 5	1', 4', 4'-Me	2/2', 3/3',
4,4'		133.6						5/5'
4,4'-Me	16.2	12.7	1.84 s	1.82 s	5/5'	3/3', 4/4', 5/5'	4/4'-Me, 5/5'	6, 6', 2'
5,5'	134.8	137.9	5.98 t (6.33)	6.09 t (6.23)	6/6', 4/4'-Me	4/4'-Me, 3/3', 6/6'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	7/7', 3/3'
6,6'	33.3	33.4	2.56 m	2.64 m	5/5', 7/7'	4/4', 5/5', 7/7', 8/8'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	9/9',
			2.34 m	2.36 m				
7,7'	76.7 ^b	75.7 ^b	4.01 m	4.00 m	6/6', 8/8'		6/6', 8/8', 9/9', 7/7', 5/5'	
8,8'		39.1	2.10 m, 1.64 m		7/7', 9/9'	6/6', 7/7', 9/9'	5/5', 7/7', 9/9', 8/8', 6/6'	13/13'
9,9'	69.2	68.6	4.36 m		8/8', 10/10'		6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a'
10,10'	129.6 ^a	129.5 ^a	5.74 m		9/9', 11/11', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	124.0	123.2	5.80 m		10/10', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.4	31.3	1.96 m		11/11', 13/13'	10/10', 11/11', 13/13', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	64.4	64.3	3.64 m		12/12', 14/14' ^a		12/12', 14/14', 15/15', 13/13'	
14,14'	36.1	35.7	1.87 m, 1.55 m		13/13', 15/15'		12/12', 14/14', 13/13', 15/15'	
15,15'		78.0 ^b	3.78 m		14/14'	15/15'-OMe	12/12', 14/14', 13/13', 15/15',	16/16'-Me, 15/15'-OMe
16,16'	41.0	41.2	1.55 m		16/16'-Me, 15/15'		13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	10.0	10.2	0.83 d (6.54)	0.84 d (6.32)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	73.8	74.2	3.80 m		18/18'		16/16'-Me, 18/18', 17/17', 19/19'	16/16'-Me
18,18'		41.7	1.79 m, 1.41 m				17/17', 18/18', 19/19', 20/20'	
19,19'		69.5	3.85 m	3.79 m			20/20', 21/21', 19/19', 18/18'	
20,20'	41.9	42.1	1.87 m, 1.53 m		20/20'		20/20', 21/21', 19/19'	
21,21'	71.1	70.7	5.64 m	5.66 m		1'/1', 22/22'-Me, 19/19'	20/20', 19/19'	19/19', 23/23'
22,22'		40.5	1.64 m		22/22'		22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
22,22'-Me	10.3	10.5	0.87 d (8.45)	0.89 d (7.47)	22/22', 24/24'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	
23,23'		76.5	3.09 m			21/21', 24/24'-Me, 25/25'	22/22'-Me, 22/22', 23/23'	22/22'-Me, 24/24'-Me, 21/21'
24,24'	33.0	32.8	1.69 m		24/24'		24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
24,24'-Me	17.7	17.6	0.97 d (6.10)			23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	24.2	23.9	1.37 m, 1.25 m				24,24'-Me, 26/26', 25/25', 24/24', 27/27'	
26,26'	29.8	29.3	1.86 m, 1.25 m				24/24'-Me, 25/25', 26/26', 27/27'	

27,27'	71.7			3.98 m				24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'
28,28'	35			1.82 m, 1.56 m				31/31', 30/30', 28/28', 29/29', 27/27'
29,29'	73.4			3.52 m			OMe, 31/31'	28/28', 29/29', 30/30', 31/31', 31/31'-Me,
30,30'	38.9			1.97 m, 1.16 m				31/31'-Me, 28/28', 30/30', 31/31', 29/29'
31,31'	64.7			3.68 m			31/31'-Me	31/31'-Me, 28/28', 30/30', 31/31', 29/29'
31,31'-Me	22			1.20 d (5.9)	31/31'		30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'
32,32'	101.9	102.6		4.46 d (6.6)	4.39 m		7/7', 36/36'	32/32', 33/33', 34/34', 35/35', 36/36'
33,33'	73.4			3.29 m		34/34'	32/32', 34/34'	32/32', 33/33', 34/34', 35/35', 36/36'
34,34'	83.4	83.5		3.20 m		33/33'	33/33', 35/35', OMe,	32/32', 33/33', 34/34', 35/35', 36/36'
35,35'	79.0	79.3		3.25 m			34/34', 36/36', OMe	32/32', 33/33', 34/34', 35/35', 36/36'
36,36'	62.6			3.99 m, 3.21 m		35/35'	32/32'	32/32', 33/33', 34/34', 35/35', 36/36'
15,15'-OMe	57.1			3.35 s				15,15'-OMe
29,29'-OMe	55.4			3.34 s				29,29'-OMe
34,34'-OMe	60.3	60.2		3.59 s				34,34'-OMe
35,35'-OMe	58.5			3.45 s	3.44 s			35,35'-OMe

^a Can be exchanged.

^b Overlapped with CDCl₃, assigned using HMBC, HSQC and HSQC-TOCSY.

Table S6 NMR data for samholide E (5)

	δ_C	$\delta_{C'}$	δ_H	$\delta_{H'}$	COSY	HMBC	ROESY
1,1'	170.5	169.9					
2,2'	113.5	114.4		5.79 d (15.48)	3/3'	1/1', 4/5'	4/4'-Me, 22/22'-Me
3,3'	153.1	152.1	7.57 d (15.55)	7.52 d (15.56)	2/2'	1/1', 2/2', 4/4', 4/4'-Me, 5/5'	5/5', 38
4,4'	133.7	134.5					
4,4'-Me	12.1	12.4	1.75 s	1.82 s	5/5'	3/3', 4/4', 5/5'	2/2', 6/6'
5,5'	142.7	140.3	6.32 m	6.33 m	6/6', 4/4'-Me	4/4'-Me, 3/3', 6/6', 7/7'	7/7', 3/3'
6,6'	33.6	33.2	2.50 d (13.39)	2.67 d (12.99)	5/5', 7/7'(weak)	4/4', 5/5', 7/7',	7/7', 9/9'
			2.35 m	2.35 m			
7,7'	78.6	76.6	4.15 m	4.07 m	6/6', 8/8'		5/5', 32
8,8'	39.8	39.7		2.29 m, 1.67 m	7/7', 9/9'	6/6', 7/7', 9/9', 10/10'	13/13'
9,9'	68.9	69.2	4.21 d (11.37)	4.31 brs	8/8', 10	8/8', 10, 13/13'	6a/6a'
10,10'	129.7	129.8	5.72 m	5.78 m	9/9', 11/11', 12/12'	9/9', 12/12'	
11,11'	123.4	123.7	5.80 m	5.71 m	10/10', 12/12'	9/9', 12/12', 13/13'	
12,12'		31.5		2.08 d (17.61), 1.98 m	11/11', 13/13'	10/10', 11/11', 13/13', 14/14'	
13,13'	63.5	64.1		3.69 m	12/12', 14/14'a		8/8', 7/7'
14,14'	36.2	36.7		1.84 m, 1.63 m	13/13', 15/15'		15/15'-OMe
15,15'	75.7	75.4		4.05 m	14/14'	14/14', 15/15'-OMe, 16/16'-Me, 16/16'	16/16'-Me
16,16'		41.6		1.59 m	16/16'-Me, 15/15'		
16,16'-Me	9.2	9.0	0.80 d (7.14)	0.78 d (7.02)	16/16'	15/15', 16/16', 17/17'	17/17'
17,17'	73.6	73.8		3.88 m	18/18'	15/15', 16/16', 18/18', 19/19'	16/16'-Me
18,18'	40.9	40.6		1.74 m, 1.55 m			
19,19'	70.0	69.4	3.99 m	3.88 m			
20,20'		42.4		1.90 m, 1.55 m	20/20'		
21,21'	70.3	70.5		5.71 m		1/1'	
22,22'	41.2	40.9		1.69 m	22/22'	22/22'-Me, 23/23'	
22,22'-Me	9.9	10.1	0.91 d (6.92)	0.89 d (7.13)	22/22', 24/24'	21/21', 22/22', 23/23'	
23,23'	76.1	76.5		3.20 m		21/21', 22/22', 24/24'-Me, 25/25'	22/22'-Me, 24/24'-Me, 21/21'
24,24'	33.4	33.0		1.69 m	24/24'	23/23', 24/24'-Me	
24,24'-Me		17.5	0.96 d (7.17)	0.95 d (7.23)		23/23', 24/24', 25/25'	
25,25'	23.6	24.0		1.35 m, 1.20 m			
26,26'		29.8		1.86 m, 1.27 m			

27,27'	71.4	71.3		3.98 m		
28,28'	35.1	35.0		1.81 m, 1.59 m		29/29', 30/30'
29,29'		73.4		3.52 m		29/29'-OMe
30,30'		38.8		1.98 m, 1.19 m		,
31,31'	64.8	64.9		3.69 m		29/29', 31/31'-Me
31,31'-Me	21.9	22.0	1.17 d (5.90)	1.19 d (6.44)	31/31'	30/30', 31/31'
32,32'	101.4	102.9	4.81 d (4.98)	4.46 d (5.45)		7/7', 33, 36/36'
33,33'	73.1	73.3	4.74 t (6.11)	3.27 m	34/34'	32/32', 34/34', 35, 37
34,34'	82.1	83.3	3.32 m	3.25 m	33/33'	33', 34/34'-OMe, 35/35'
35,35'		79.2		3.31 m		32/32'
36,36'	62.2	62.5	4.01 m, 3.25 m	4.00 m, 3.23 m	35/35'	34/34'
37,37'	170.5	/N				32/32', 34/34'
38,38'	72.6	/N	4.13 m	N	39/39'	37, 39
39,39'	64.6	/N	3.77 m, 3.63 m	N	38/38'	3/3'
15,15'-OMe	57.6	57.5	3.35 s	3.33 s		37
29,29'-OMe		55.4		3.32 s		
34,34'-OMe		60.1	3.47 s	3.56 s		
35,35'-OMe		58.5	3.43 s	3.45 s		

Table S7 NMR data for samholide F (6)

	δ_C	$\delta_{C'}$	δ_H	$\delta_{H'}$	COSY	HMBC	HSQC-TOCSY	ROESY
1,1'	167.6	169.5						
2,2'	116.5	115.3	5.68 d (12.47)	5.81 d (15.68)	3/3'	1'/1,4/4'	3/3', 2/2'	4/4'-Me,
3,3'	148.7	151.1	6.52 d (12.62)	7.44 d (15.54)	2/2'	1'/1, 2/2', 4/4', 4/4'-Me, 5/5'	2/2', 3/3',	5/5'
4,4'		134.7						
4,4'-Me	15.8	12.6	1.86 s	1.81 s	5/5' (weak)	3/3', 4/4', 5/5'	4/4'-Me, 5/5'	2/2', 6/6'
5,5'	134.1	138.5	5.86 t (7.00)	6.14 t (6.87)	6/6', 4/4'-Me	4/4'-Me, 3/3', 6/6', 7/7'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	7/7', 3/3', 8/8'
6,6'		33	2.57 ddd (4.06, 6.48, 13.87)	2.69 ddd (4.38, 6.03, 11.73)	5/5', 7/7'	4/4', 5/5', 7/7', 8/8'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	9/9', 4/4'-Me
			2.40 dt (7.02, 15.36)	2.28 dt (7.45, 15.12)				
7,7'	77.0	75.7	4.00 m	3.97 m	6/6', 8/8'	5/5', 32/32'	6/6', 8/8', 9/9', 7/7', 5/5'	5/5', 32/32'
8,8'	39.6	39.3	2.10 m	2.10 m	7/7', 9/9'	6/6', 7/7', 9/9', 10/10'	5/5', 7/7', 9/9', 8/8', 6/6'	13/13'
			1.55 m	1.67 m				
9,9'	69.0	69.6	4.29 m	4.39 m	8/8', 10/10' (weak)	8/8', 10/10', 11/11', 13/13',	6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a', 7/7'
10,10'		129.6	5.69 m	5.78 m	9/9', 11/11'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	124.0	123.8	5.80 m	5.69 m	10/10', 12/12'	9/9', 12/12', 13/13'(weak)	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.3	31.2		1.97 m	11/11', 13/13'	11/11', 13/13', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	64.4	64.3		3.68 m	12/12', 14/14'a		12/12', 14/14', 15/15', 13/13'	8/8'
14,14'	35.7	35.6		1.88 m, 1.56 m	13/13', 15/15'	12/12', 13/13', 15/15', 16/16'	12/12', 14/14', 13/13', 15/15'	
15,15'		77.0 ^a	3.78 ma	3.82 ma	14/14'	15/15'-OMe, 16/16'-Me, 16/16'	12/12', 14/14', 13/13', 15/15',	
16,16'	40.9	40.5		1.65 m	16/16'-Me, 15/15'	16/16'-Me, 17/17'	13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	10.2	9.9	0.82 d (6.91)	0.81 d (7.13)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	74.3	74.2	3.76 m	3.86 m	18/18'	15/15', 16/16'-Me, 18/18', 19/19'	16/16'-Me, 18/18', 17/17', 19/19'	16/16'-Me
18,18'	41.7	41.4		1.70 m, 1.55 m	17/17', 19/19'	17/17', 19/19'	17/17', 18/18', 19/19', 20/20'	
19,19'		69		3.88 m	18/18', 20/20'	17/17', 18/18'	20/20', 21/21', 19/19', 18/18'	
20,20'		41.8		1.87 m, 1.53 m	19/19', 21/21'	21/21'	20/20', 21/21', 19/19'	

21,21'	71.3	70.8	5.60 d (10.39)	5.63 d (10.00)	20/20', 22/22'	1/1', 19/19', 23/23', 20/20', 22/22', 22/22'-Me	20/20', 19/19'	19/19', 23/23'
22,22'	41.1	40.9		1.76 m	22/22'-Me, 21/21', 23/23'	22/22'-Me, 23/23'	22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
22,22'-Me	10.3		0.89 d (6.78)	0.88 d (6.78)	22/22'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	
23,23'	76.7		3.15 d (9.39)	3.12 d (9.83)	22/22', 24/24'	21/21', 22/22', 22/2'-Me, 24/24'-Me, 24/24', 25/25'	22/22'-Me, 22/22', 23/23'	22/22'-Me, 24/24'-Me, 21/21'
24,24'	33.4			1.68 m	24/24'-Me,	22/22'-Me, 24/24'-Me	24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
24,24'-Me	17.6		0.98 d (6.80)	0.96 d (6.80)	24/24'	23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	24			1.39 m, 1.24 m	26/26',		24,24'-Me, 26/26', 25/25', 24/24', 27/27'	
26,26'	29.3			1.87 m, 1.25 m	25/25', 27/27',		24/24'-Me, 25/25', 26/26', 27/27'	
27,27'	71.5			3.99 m	26/26', 28/28'	29/29', 31/31'	24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'	29/29'-OMe, 31/31'
28,28'	35			1.82 m, 1.58 m	29/29', 30/30'		31/31', 30/30', 28/28', 29/29', 27/27'	
29,29'	73.4			3.52 m	28/28', 31/31'	27/27', 28/28', 31/31'	28/28', 29/29', 30/30', 31/31', 31/31'-Me,	31/31'
30,30'	38.9			1.99 m, 1.18 m	29/29',		31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'	64.7			3.69 m	31/31'-Me	29/29', 31/31'-Me	31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'-Me	22			1.19 d (6.25)	31/31'	30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'	
32,32'	100.4	102.1	4.65 d (6.77)	4.39 d (6.72)		7/7', 34/34', 36/36'	32/32', 33/33', 34/34', 35/35', 36/36'	7/7', 34/34', 5/5', 6/6'
33,33'	73.4		4.83 dd (6.85, 8.39)	3.52 m	34/34'	32/32', 34/34', 37/37', 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'	34-OMe, 36
34,34'	82.0	83.5	3.35 m	3.21 m	33/33'		32/32', 33/33', 34/34', 35/35', 36/36'	
35,35'	79.1			3.30 m		34/34', 36/36', 35/35'-OMe	32/32', 33/33', 34/34', 35/35', 36/36'	

36,36'	62.6		3.99 m, 3.25 m		35/35'	32/32', 34/34', 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'
37,37'	171.5	N					
38,38'	72.4	N	4.27 m	N	39/39'	37/37', 39/39'	38/38', 39/39'
39,39'	64.3	N	3.80 m	N	38/38'	37/37'	38/38', 39/39'
15,15'-OMe	57.2	57.1	3.34 s	3.32 s		15,15'	
29,29'-OMe	55.4			3.32 s		29,29'	
34,34'-OMe	60.2	60.3		3.48 s		34	
35,35'-OMe	58.7	58.5 ^a		3.44 s		35	

^a Overlapped with CDCl₃, assigned using HMBC, HSQC and HSQC-TOCSY.

Table S8 NMR data for samholide G (7)

	δ_C	$\delta_{C'}$	δ_H	$\delta_{H'}$	COSY	HMBC	HSQC-TOCSY	ROESY
1,1'	169.5	167.4						
2,2'	114.5	116.2	5.80 m	5.66 d (12.72)	3/3'	1/1', 3/3', 4/4'	3/3', 2/2'	4-Me
3,3'	153.9	148.3	7.47 d (15.63)	6.46 d (12.69)	2/2'	1.1', 2/2', 4, 4/4'-Me, 5/5'	2/2', 3/3',	5/5', 38, 4'-Me
4,4'	134.1							
4,4'-Me	12.5	16.1	1.78 s	1.86 s	5/5'	3/3', 4/4', 5/5'	4/4'-Me, 5/5'	2/2', 6/6'
5,5'	140	134	6.11 t (6.88)	5.97 brs	6/6', 4/4'-Me	4/4'-Me, 3, 6, 7	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	7/7', 3/3'
6,6'	33.6	33.2	2.59 m	2.57 m	5/5', 7/7'	4/4', 5/5', 7/7', 8/8'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	9/9'
			2.34 m	2.41 dt (7.38, 14.56)				
7,7'	77.2	76.7 ^b	4.03 m	3.97 m	6/6', 8/8'	32/32'	6/6', 8/8', 9/9', 7/7', 5/5'	5/5', 32/32'
8,8'	39.5	39.1	2.19 m	2.05 m	7/7', 9/9'	7/7'	5/5', 7/7', 9/9', 8/8', 6/6'	13/13'
			1.54 m	1.64 m				
9,9'	69.4	69.7	4.28 m	4.38 m	8/8', 10/10'		6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a'
10,10'	129.5	129.6		5.71 m	9/9', 11/11', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	123.9	123.6		5.74 m	10/10', 12/12'	9/9', 12/12', 13/13'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.4			1.95 m	11/11', 13/13'	10/10', 11/11', 13/13', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	64.5			3.79 m	12/12', 14/14'a		12/12', 14/14', 15/15', 13/13'	
14,14'	36.1	35.9	1.84 m, 1.58 m		13/13', 15/15'	16/16'	12/12', 14/14', 13/13', 15/15'	
15,15'	77.0 ^b			3.82 m	14/14'		12/12', 14/14', 13/13', 15/15',	16/16'-Me
16,16'	40.8	40.6		1.63 m	16/16'-Me, 15/15'		13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	9.9		0.83 d (7.13)	0.84 d (7.75)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	74.3	74.1		3.79 m	18/18'		16/16'-Me, 18/18', 17/17', 19/19'	16/16'-Me,
18,18'	41.7	41.5		1.85 m, 1.50 m			17/17', 18/18', 19/19', 20/20'	
19,19'	69.8	68.3	3.87 m	3.85 m		17/17'	20/20', 21/21', 19/19', 18/18'	
20,20'	42.1			1.87 m, 1.57 m	20/20'		20/20', 21/21', 19/19'	
21,21'	70.9	71.3	5.65 m	5.69 m		1/1', 19/19', 23/23', 20/20', 22/22', 22/22'-Me	20/20', 19/19'	19/19', 23/23'
22,22'	41.3	40.9		1.73 m	22/22'	22/22'-Me, 23/23'	22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	

22,22'-Me	10.3	10.2	0.86 d (7.03)	0.90 d (6.95)	22/22', 24/24'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	
23,23'	76.3			3.12 m		21/21', 22/22', 24/24', 24/24'-Me, 25/25'	22/22'-Me, 22/22', 23/23'	22/22'-Me, 24/24'-Me, 21/21',
24,24'	33			1.66 m	24/24'		24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
24,24'-Me	17.6		0.97 d (6.18)	0.96 d (6.3)		23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	24.2	23.6		1.35 m, 1.24 m		24/24'-Me, 26/26',	24,24'-Me, 26/26', 25/25', 24/24', 27/27'	
26,26'	29.3	29.2		1.86 m, 1.22 m		25/25', 27/27'	24/24'-Me, 25/25', 26/26', 27/27'	
27,27'	71.5	71.7		3.97 m		29/29', 31/31'	24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'	29/29'-OMe
28,28'	35			1.80 m, 1.57 m		29/29', 30/30'	31/31', 30/30', 28/28', 29/29', 27/27'	
29,29'	73.4			3.52 m		27/27', 28/28', 31/31', 29/29'-OMe	28/28', 29/29', 30/30', 31/31', 31/31'-Me,	
30,30'	38.9			1.94 m, 1.17 m		29/29'	31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'	64.7			3.67 m		29/29'	31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'-Me	21.9		1.18 d (6.24)	1.20 d (6.3)	31/31'	30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'	
32,32'	100.8	102.5	4.71 m	4.43 d (6.29)			32/32', 33/33', 34/34', 35/35', 36/36'	7/7', 34/34', 5/5'
33,33'	73.4	72.9	4.83 dd (7.18, 8.13)	3.37 m	34/34'	32/32', 34/34', 37	32/32', 33/33', 34/34', 35/35', 36/36'	35, 35-OMe
34,34'	82.4	83.6	3.31 m	3.21 m	33/33'	32/32', 34/34'-OMe, 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'	32/32'
35,35'	79.3		3.31 m	3.26 m		33/33', 35/35'-OMe	32/32', 33/33', 34/34', 35/35', 36/36'	
36,36'	62.7			3.99 m, 3.23 m	35/35'	32/32', 34/34'	32/32', 33/33', 34/34', 35/35', 36/36'	
37,37'	170.8	N						
38,38'	72.4	N	4.21 m	N	39/39'		38/38', 39/39'	3
39,39'	64.5	N	3.81 m	N	38/38'		38/38', 39/39'	
15,15'-OMe	57.3	56.9	3.34 s	3.32 s		15/15'		
29,29'-OMe	55.4			3.34 s		29/29'		
34,34'-OMe	60.2	60.1	3.48 s	3.58 s		34		
35,35'-OMe	58.6	58.5 ^a	3.44 s	3.45s		35		

Table S9 NMR data for samholide H (8)

	δ_C	$\delta_{C'}$	δ_H	$\delta_{H'}$	COSY	HMBC	HSQC-TOCSY	ROESY
1,1'	170.3							
2,2'	114.3	113.9	5.80 d (15.6)		3/3'	1/1',4/4'	3/3', 2/2'	4/4'-Me
3,3'	152.2	152.1	7.55 d (15.6)		2/2'	1/1', 2/2', 4/4', 4/4'-Me, 5/5'	2/2', 3/3',	5/5'
4,4'	134.4							
4,4'-Me	12.5	12.4	1.83 s		5/5'	3/3', 4/4', 5/5'	4/4'-Me, 5/5'	2/2', 6/6'
5,5'	141	134	6.35 m		6/6', 4/4'-Me	4/4'-Me, 3/3'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	7/7', 3/3'
6,6'	33.6	33.3	2.60 m, 2.38 m		5/5', 7/7'	4/4', 5/5', 7/7'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	5/5', 9/9'
7,7'	76.0	76.3	4.08 m		6/6', 8/8'		6/6', 8/8', 9/9', 7/7', 5/5'	5/5', 32/32'
8,8'	39.8	39.7	2.26 m, 1.62 m		7/7', 9/9'	6/6', 7/7', 9/9'	5/5', 7/7', 9/9', 8/8', 6/6'	13/13'
9,9'	69.6		4.29 m		8/8', 10/10'		6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a', 10/10', 14/14'
10,10'	129.8		5.74 m		9/9', 11/11', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	123.6		5.77 m		10/10', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.4	31.6	1.97 m		11/11', 13/13'	10/10', 11/11', 13/13', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	63.7	63.5	3.64 m		12/12', 14/14'a		12/12', 14/14', 15/15', 13/13'	
14,14'	36.9	36.8	1.77 m, 1.64 m		13/13', 15/15'	15/15'	12/12', 14/14', 13/13', 15/15'	
15,15'	75.8	76.0	4.08 m		14/14'		12/12', 14/14', 13/13', 15/15',	6a/6a', 5/5', 14/14', 8/8'
16,16'	41.5	41.4	1.66 m		16/16'-Me, 15/15'	16/16'-Me	13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	9.4	9.3	0.79 d (6.36)	0.78 d (6.35)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	74.0	74.1	3.85 m		18/18'		16/16'-Me, 18/18', 17/17', 19/19'	16/16'-Me,
18,18'	40.8		1.72 m, 1.41 m			17/17'	17/17', 18/18', 19/19', 20/20'	
19,19'	69.8		3.90 m				20/20', 21/21', 19/19', 18/18'	
20,20'	42.1	42.0	1.85 m, 1.53 m		20/20'		20/20', 21/21', 19/19'	
21,21'	70.7	70.6	5.55 d (11.17)			1/1', 19/19', 22/22', 22/22'-Me	20/20', 19/19'	19/19'
22,22'	40.8	40.7	1.76 m		22/22'		22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
22,22'-Me	10.3	10.2	0.91 m		22/22', 24/24'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	
23,23'	76.8 ^a		3.20 m				22/22'-Me, 22/22', 23/23'	22/22'-Me, 24/24'-Me
24,24'	33.2	33.3	1.68 m		24/24'	23/23', 24/24'-Me	24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
24,24'-Me	17.5	17.4	0.93 m			23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	24		1.36 m, 1.21 m			24/24'-Me	24,24'-Me, 26/26', 25/25', 24/24', 27/27'	
26,26'	29.4	29.5	1.84 m, 1.26 m			27/27'	24/24'-Me, 25/25', 26/26', 27/27'	
27,27'	71.1	71.0	3.97 m				24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'	29/29'-OMe

28,28'	35		1.79 m, 1.58 m				31/31', 30/30', 28/28', 29/29', 27/27'
29,29'	73.4		3.52 m			29/29'-OMe	28/28', 29/29', 30/30', 31/31', 31/31'-Me,
30,30'	38.7		1.97 m, 1.17 m			29/29', 31/31'	31/31'-Me, 28/28', 30/30', 31/31', 29/29'
31,31'	64.9		3.70 m				31/31'-Me, 28/28', 30/30', 31/31', 29/29'
31,31'-Me	21.9		1.21 d (6.6)	31/31'		30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'
32,32'	103.2	102.9	4.47 d (6.69)	4.53 d (5.45)		7/7', 36/36'	32/32', 33/33', 34/34', 35/35', 36/36'
33,33'	73.1	72.1	3.36 m	3.29 m	34/34'	32/32', 34/34'	32/32', 33/33', 34/34', 35/35', 36/36'
34,34'	83.2	83.3	3.20 m	3.26 m	33/33'	33/33', 34/34'-OMe, 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'
35,35'	79.3	68.9	3.29 m	3.36 m			32/32', 33/33', 34/34', 35/35', 36/36'
36,36'	62.5	64.2	3.99 m	3.96 m	35/35'	32/32', 34/34', 35/35'	32/32', 33/33', 34/34', 35/35', 36/36'
			3.18 m	3.31 m			
15,15'-OMe	57.5		3.35 s	3.36 s		15,15'	
29,29'-OMe	55.5			3.34 s		29,29'	
34,34'-OMe	60.1	59.8		3.55 s		34,34'	
35,35'-OMe	58.5	N	3.45	N		35	

^a Overlapped with CDCl₃, assigned using HMBC, HSQC and HSQC-TOCSY.

Table S10 NMR data for samholide I (9)

	δ_C/δ_C'	δ_H/δ_H'	COSY	HMBC	HSQC-TOCSY	ROESY
1,1'	169.6					
2,2'	114.5	5.80 d (15.62)	3/3'	1/1', 4/4'	3/3', 2/2'	4/4'-Me
3,3'	152	7.47 d (15.62)	2/2'	1/1', 2/2', 4/4', 4/4'-Me, 5/5'	2/2', 3/3',	5/5'
4,4'	134.2					
4,4'-Me	12.5	1.80 s		3/4', 4/4', 5/5'	4/4'-Me, 5/5'	2/2'
5,5'	140.3	6.19 t (7.03)	6/6'	4/4'-Me, 3/3', 6/6', 7/7'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	7/7', 3/3'
6,6'	36.7	2.47 ddd (3.24, 7.14, 14.94) 2.31 dt (7.56, 15.19)	5/5', 7/7'	4/4', 5/5', 7/7', 8/8'	4/4'-Me, 6/6', 8/8', 9/9', 7/7', 5/5'	8/8', 9/9'
7,7'	69.8	4.04 m	6/6', 8/8'		6/6', 8/8', 9/9', 7/7', 5/5'	9/9'
8,8'	40.7 ^a	1.89 m, 1.52 m	7/7'	7/7', 9/9'	5/5', 7/7', 9/9', 8/8', 6/6'	7/7'
9,9'	72.6	4.34 d (10.74)	8/8', 10/10'	10/10', 13/13'	6/6', 12/12', 8/8', 9/9', 7/7', 10/10', 11/11', 5/5'	6a/6a', 7/7'
10,10'	129.4	5.65 m	9/9', 11/11', 12/12'	9/9', 12/12'	12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
11,11'	124.2	5.81 m	10/10', 12/12'		12/12', 14/14', 8/8', 13/13', 9/9', 10/10', 11/11'	
12,12'	31.3	1.98 m	11/11', 13/13'	10/10', 11/11', 14/14'	12/12', 14/14', 13/13', 7/7', 10/10', 11/11'	
13,13'	64.5	3.68 m	12/12', 14/14'		12/12', 14/14', 15/15', 13/13'	
14,14'	35.9	1.86 m, 1.59 m	13/13', 15/15'	13/13', 16/16'	12/12', 14/14', 13/13', 15/15'	
15,15'	77.6	3.83 m	14/14'	15/15'-OMe, 16/16'-Me, 16/16', 17/17'	12/12', 14/14', 13/13', 15/15',	16/16'-Me
16,16'	40.5 ^a	1.68 m	16/16'-Me, 15/15'	16/16'-Me, 18/18', 17/17'	13/13', 15/15', 16/16', 14/14', 16,16'-Me	
16,16'-Me	9.8	0.83 d (7.02)	16/16'	15/15', 16/16', 17/17'	16,16'-Me, 16/16', 19/19', 17/17', 18/18'	
17,17'	75	3.84 m	18/18'	15/15', 16/16', 17/17'	16/16'-Me, 18/18', 17/17', 19/19'	16/16'-Me
18,18'	40.8 ^a	1.87 m, 1.50 m		17/17', 19/19'	17/17', 18/18', 19/19', 20/20'	
19,19'	69.2	3.84 m	18/18', 20/20'		20/20', 21/21', 19/19', 18/18'	21/21'
20,20'	41.7	1.89 m, 1.55 m		21/21'	20/20', 21/21', 19/19'	
21,21'	70.4	5.65 m	20/20'	1/1', 22/22'-Me	20/20', 19/19'	19/19', 23/23', 22/22'-Me
22,22'	40.9 ^a	1.74 m		22/22'-Me, 23/23'	22,22'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
22,22'-Me	10.2	0.91 d (6.93)	22/22'	21/21', 22/22', 23/23'	22,22'-Me, 22/22', 23/23'	21/21'
23,23'	76.6 ^b	3.14 dd (1.52, 9.66)		24/24', 24/24'-Me, 25/25'	22/22'-Me, 22/22', 23/23'	24/24'-Me, 21/21'
24,24'	33.3	1.66 m			24/24'-Me, 25/25', 26/26', 24/24', 22/22', 23/23'	
24,24'-Me	17.7	0.98 d (6.74)	24/24'	23/23', 24/24', 25/25'	24,24'-Me, 26/26', 24/24', 27/27', 25/25'	
25,25'	24.2	1.37 m, 1.23 m		24/24'-Me	24,24'-Me, 26/26', 25/25', 24/24', 27/27'	
26,26'	29.4	1.87 m, 1.24 m		27/27', 28/28'	24/24'-Me, 25/25', 26/26', 27/27'	

27,27'	71.6	3.98 m	26/26', 28/28'	31/31'	24/24'-Me, 25/25', 26/26', 28/28', 30/30', 29/29'	31/31'-Me, 29/29'-OMe
28,28'	35	1.81 m, 1.58 m		29/29', 30/30'	31/31', 30/30', 28/28', 29/29', 27/27'	
29,29'	73.4	3.52 m	28/28', 30/30'	31/31', 29/29'-OMe	28/28', 29/29', 30/30', 31/31', 31/31'-Me,	26/26'
30,30'	38.8	1.98 m, 1.16 m		29/29',	31/31'-Me, 28/28', 30/30', 31/31', 29/29'	
31,31'	64.8	3.69 m	31/31'-Me	29/29'	31/31'-Me, 28/28', 30/30', 31/31', 29/29'	26/26'
31,31'-Me	22	1.20 d (6.18)	31/31'	30/30', 31/31'	31,31'-Me, 30/30', 31/31', 28/28', 29/29'	27/27'
15,15'-OMe	57.2	3.35 s		15,15'		
29,29'-OMe	55.5	3.34 s		29,29'		

^a Can be exchanged.

^b Overlapped with CDCl₃, assigned using HMBC, HSQC and HSQC-TOCSY.

F4-a #12-18 RT: 0.29-0.44 AV: 7 SB: 1 0.17 NL: 2.81E7
T: + c Full ms [300.00-2000.00]

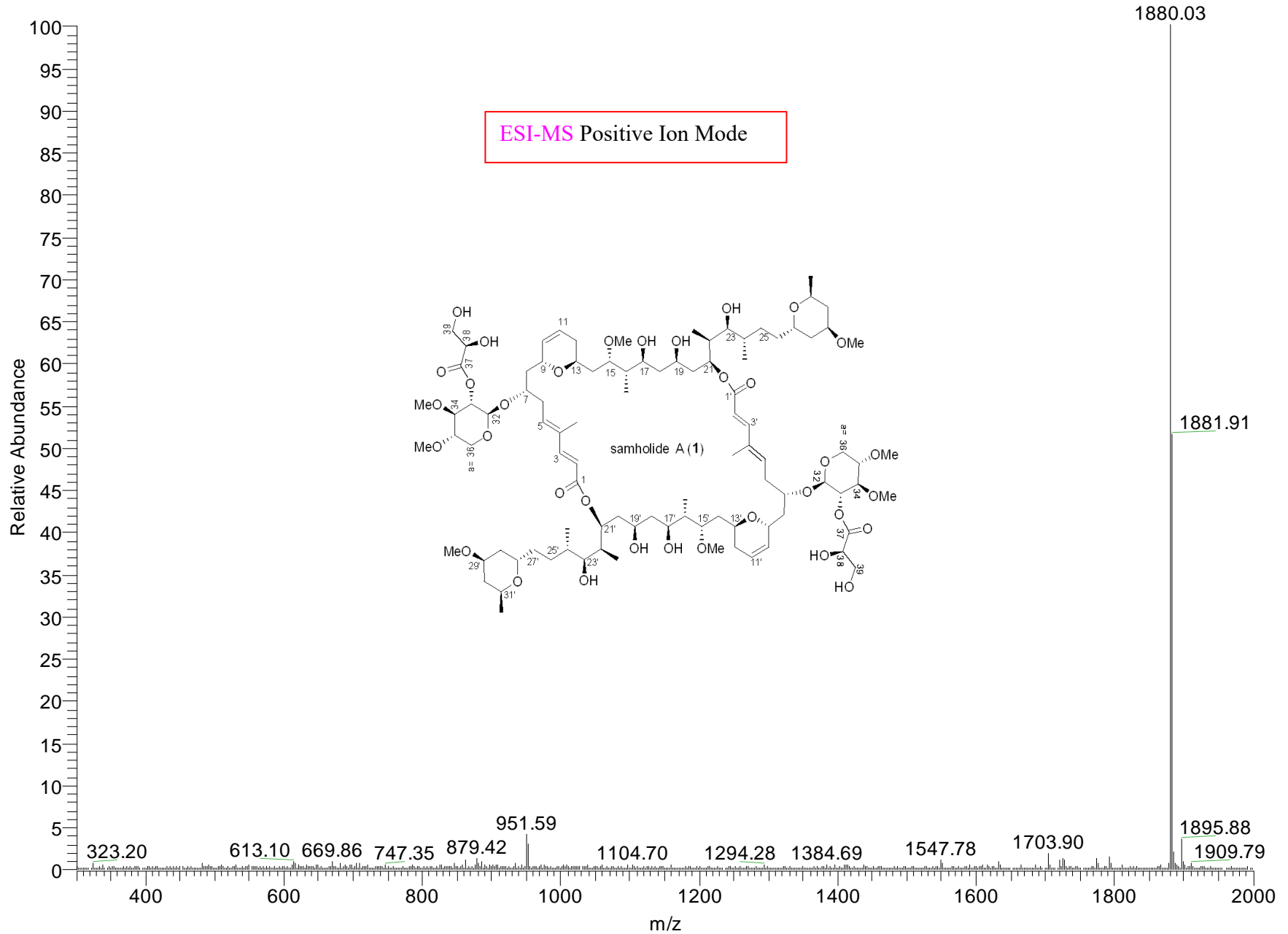


Figure S1 The ESI MS spectrum of samholide A (1)

F4-a #29-34 RT: 0.66-0.74 AV: 6 SB: 3 0.80-0.84 NL: 2.67E6
T: + c Full ms2 1880.00@35.00 [515.00-2000.00]

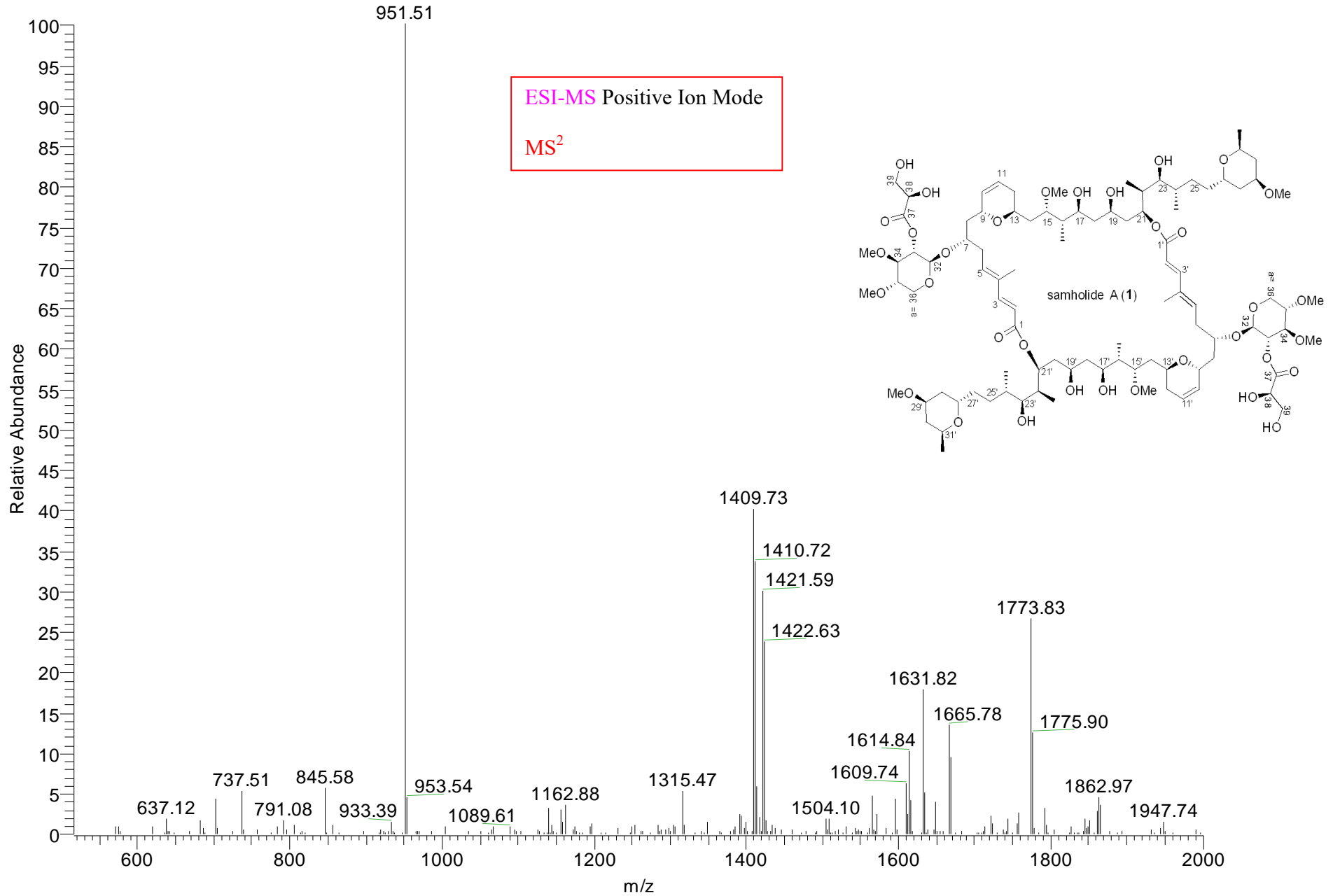


Figure S2 The ESI MS² spectrum of samholide A (1)

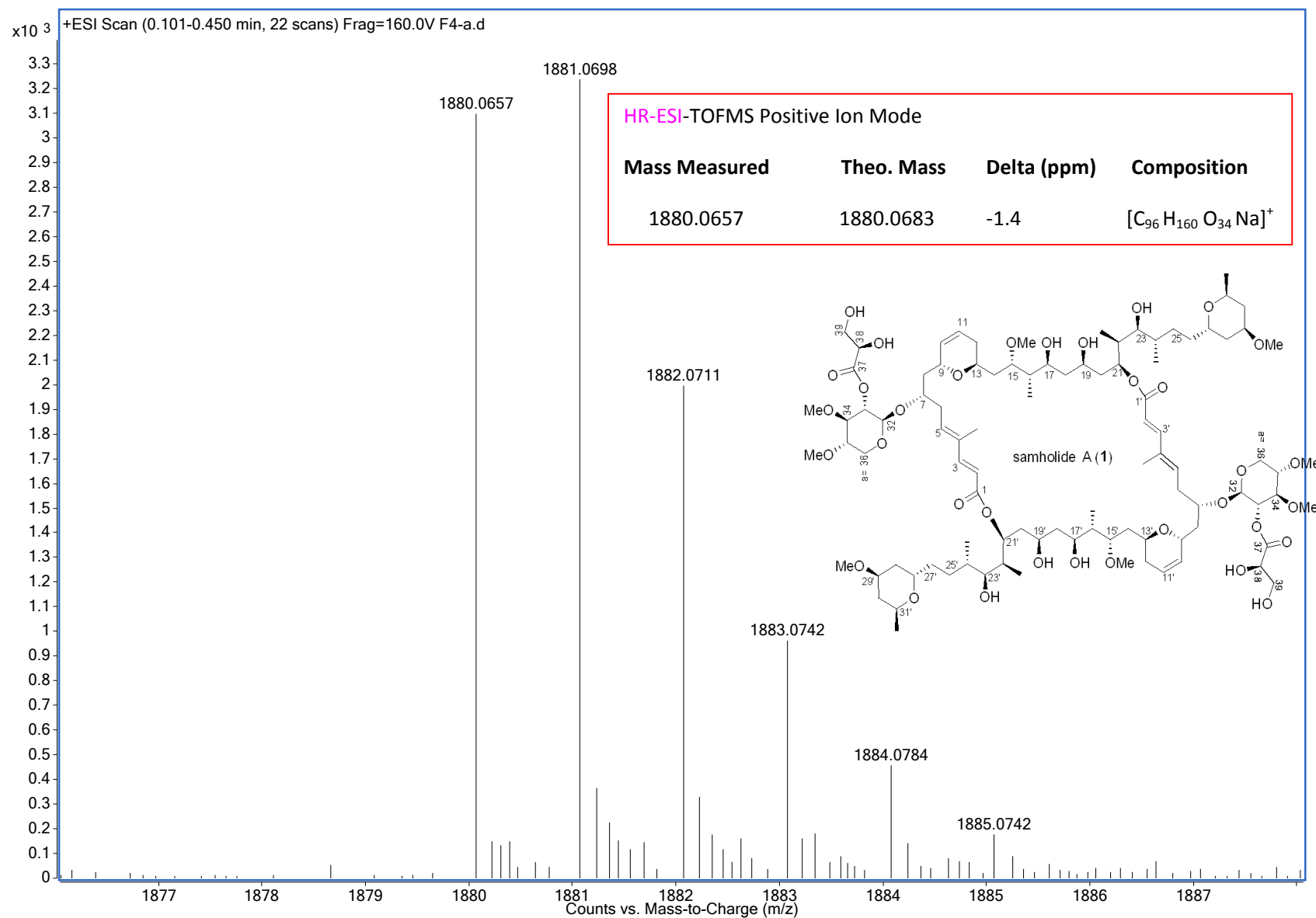
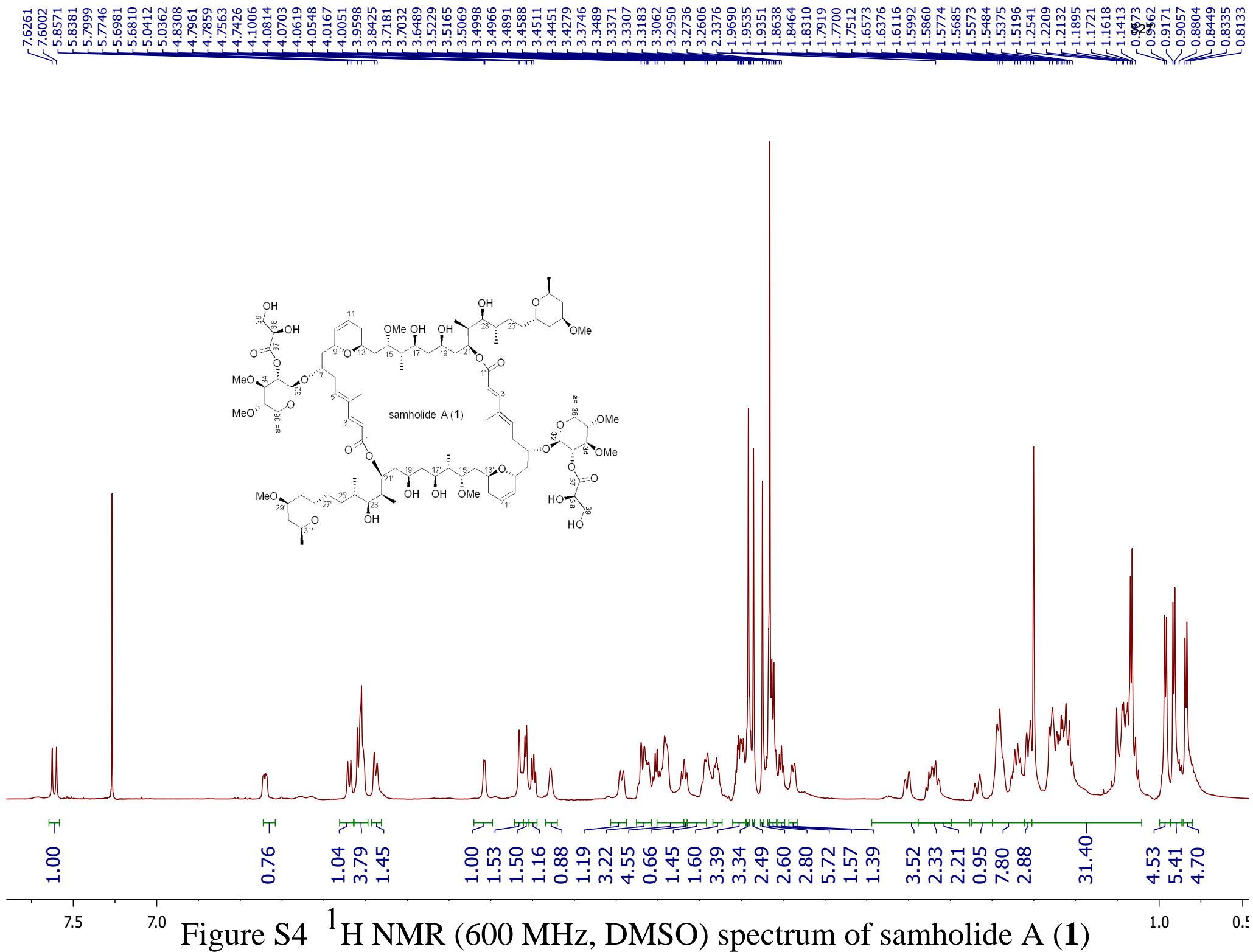


Figure S3 The positive HRESIMS spectrum of samholide A (1)



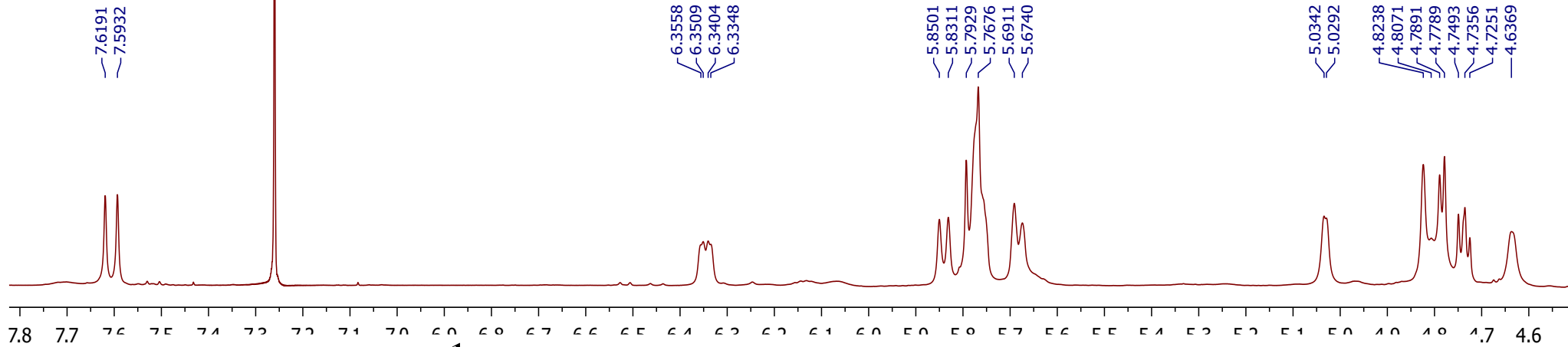
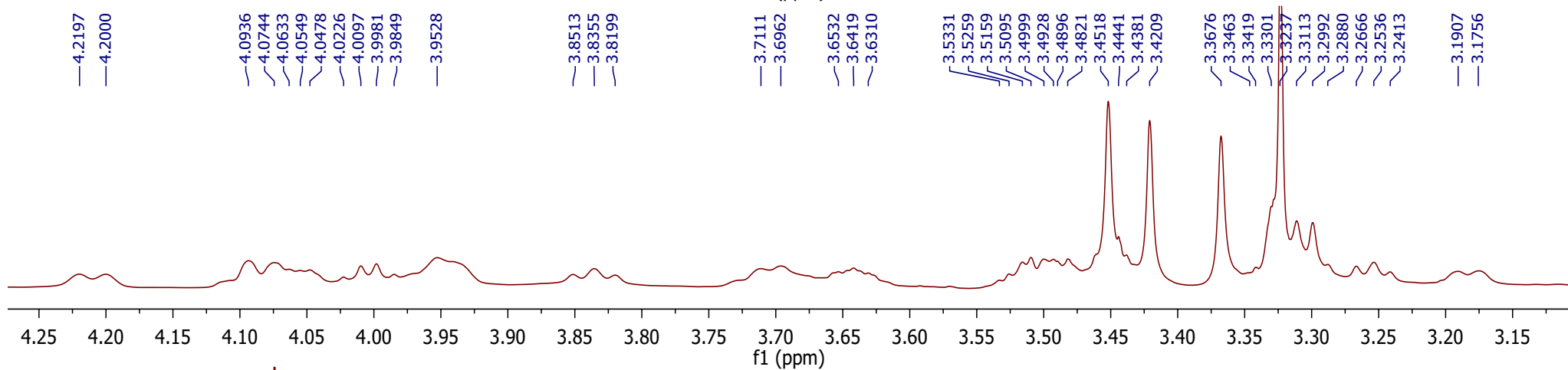
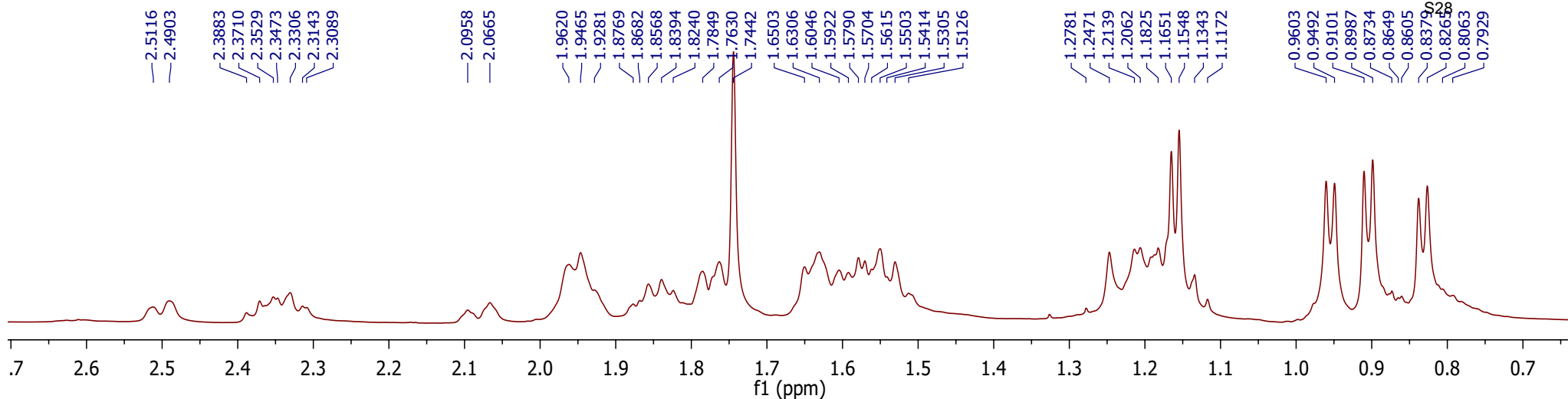
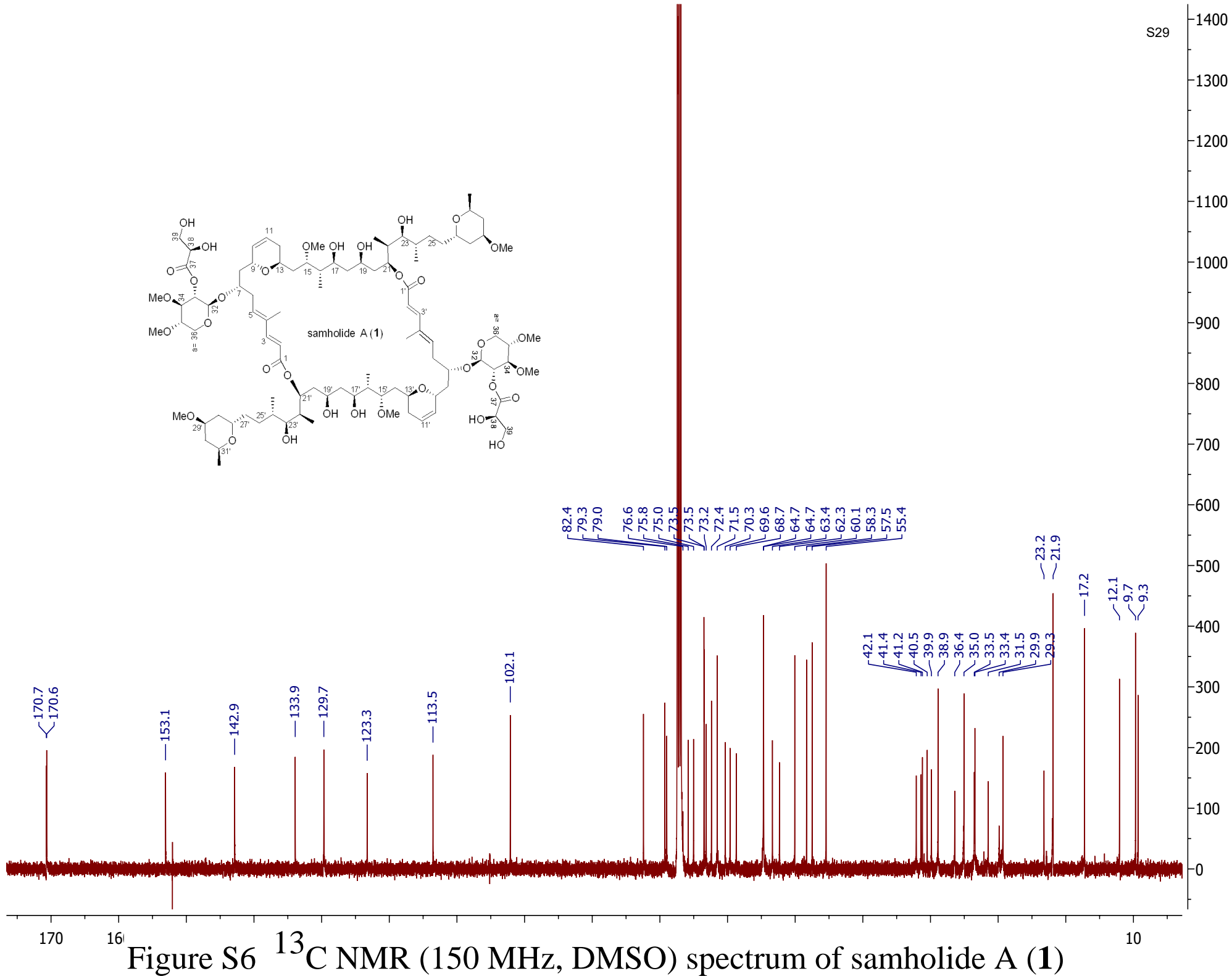
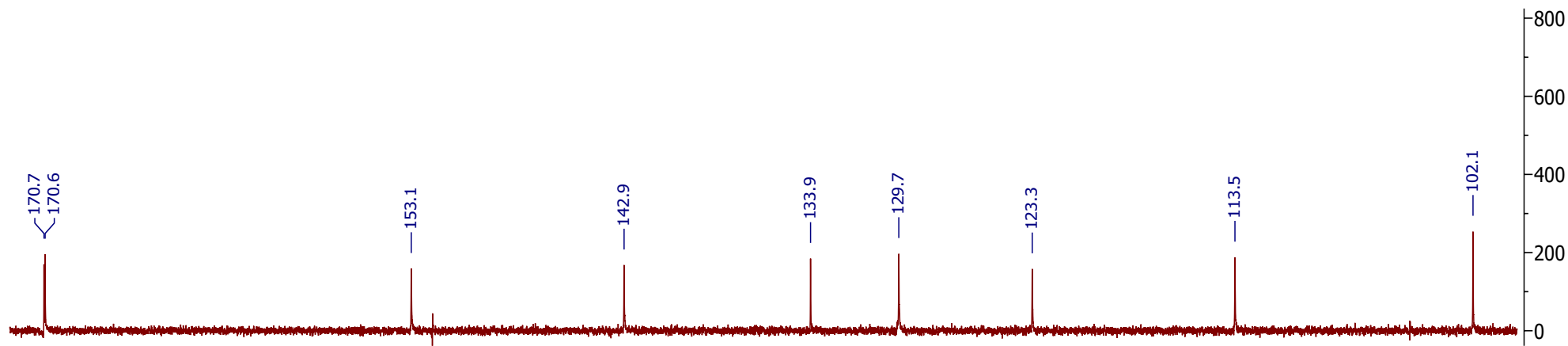
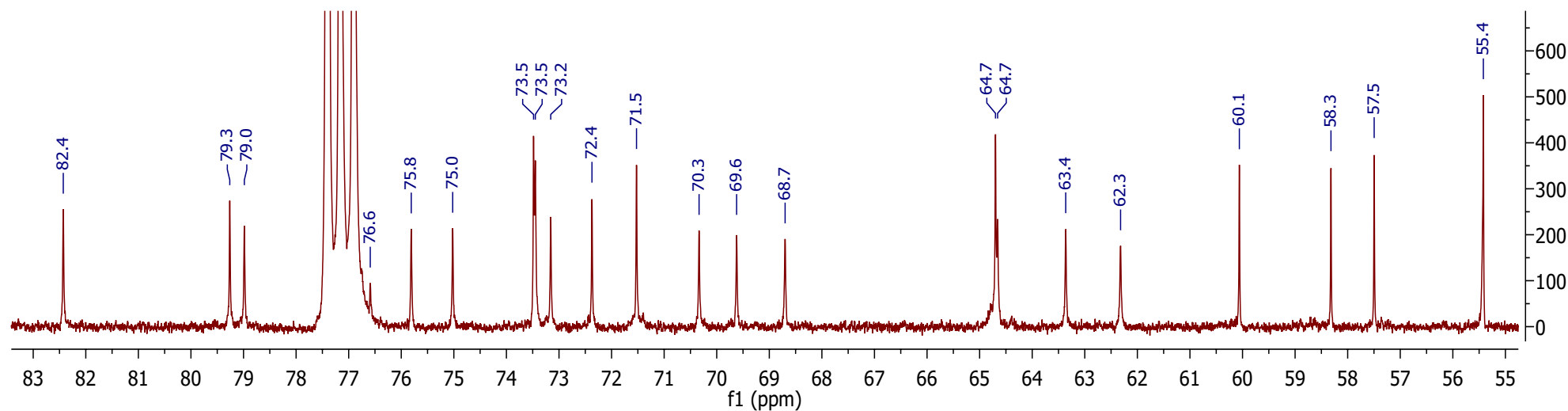
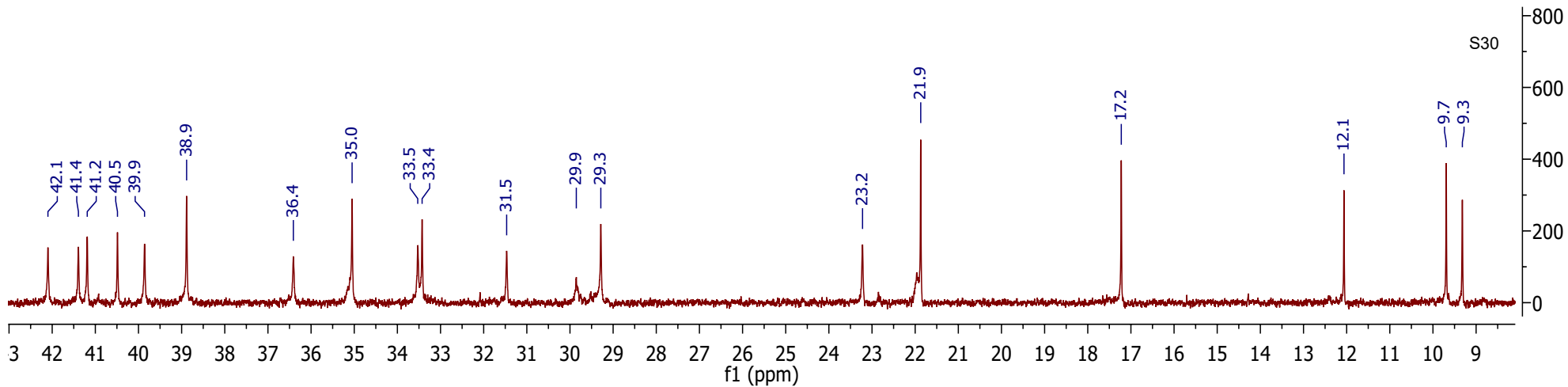


Figure S5 Amplified ^1H NMR (600 MHz, DMSO) spectrum of samholide A (**1**)





^{13}C Figure S7 Amplified ^{13}C NMR (150 MHz, DMSO) spectrum of samholide A (1)

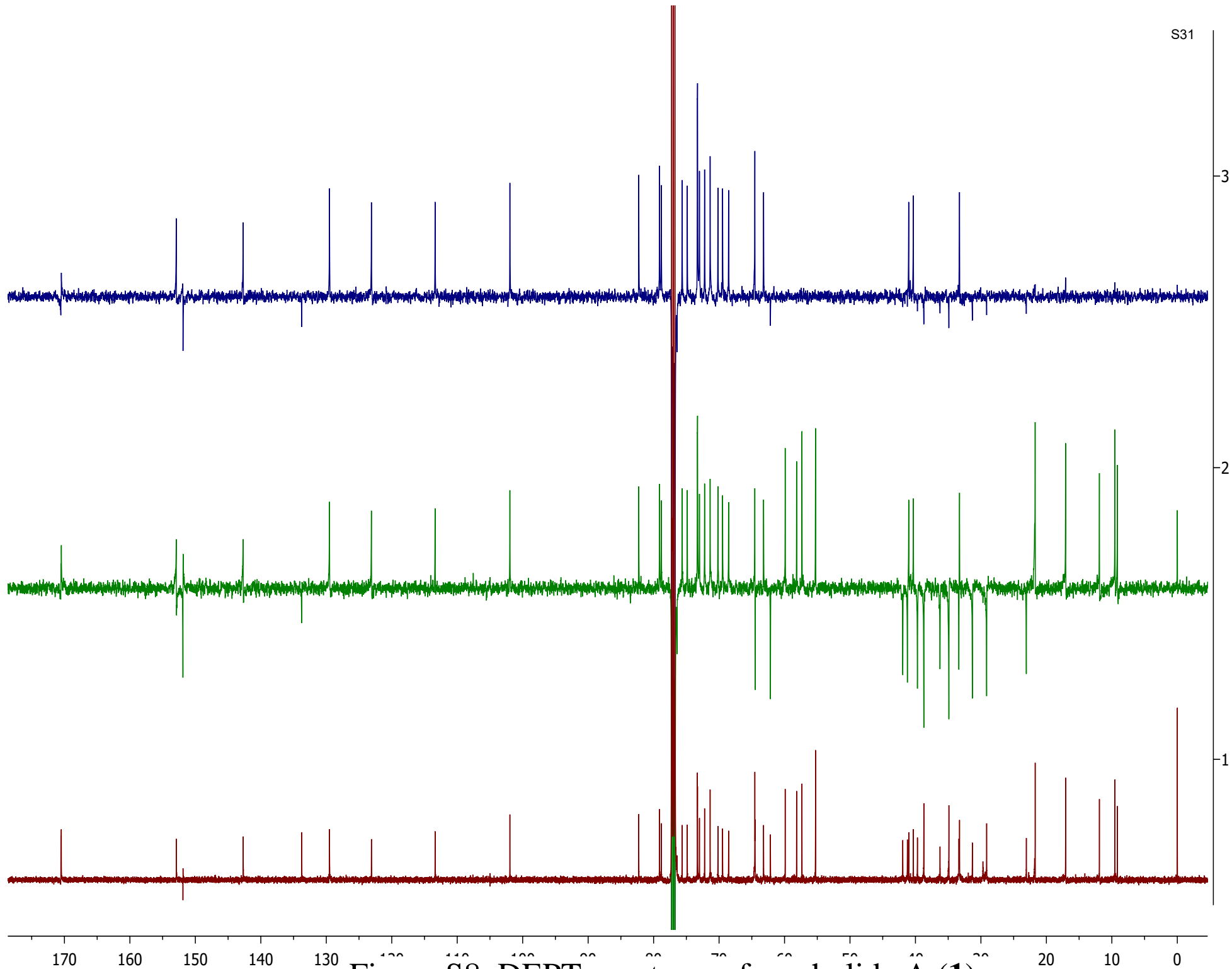


Figure S8 DEPT spectrum of samholide A (1)

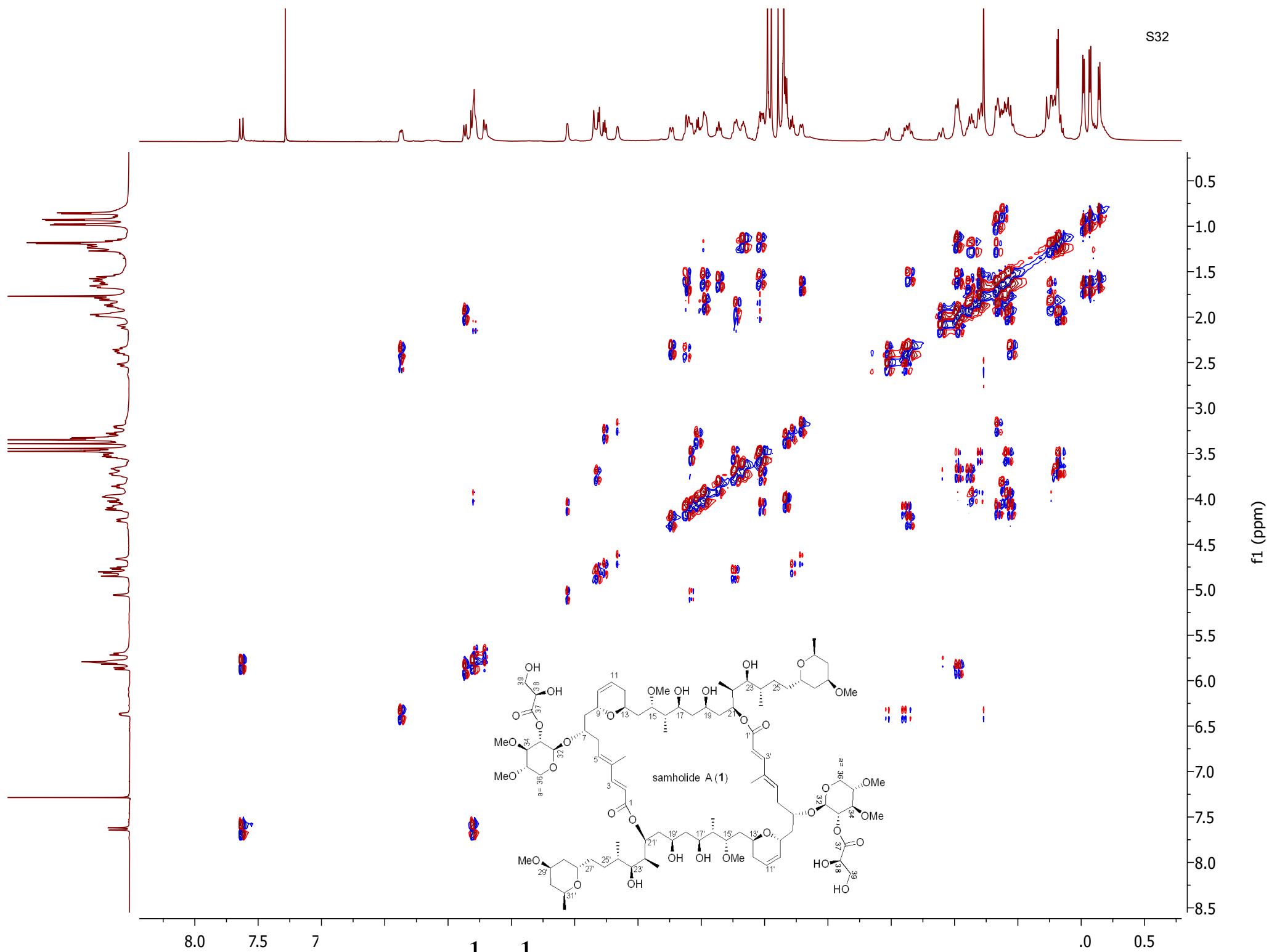


Figure S9 ^1H - ^1H COSY spectrum of samholide A (1)

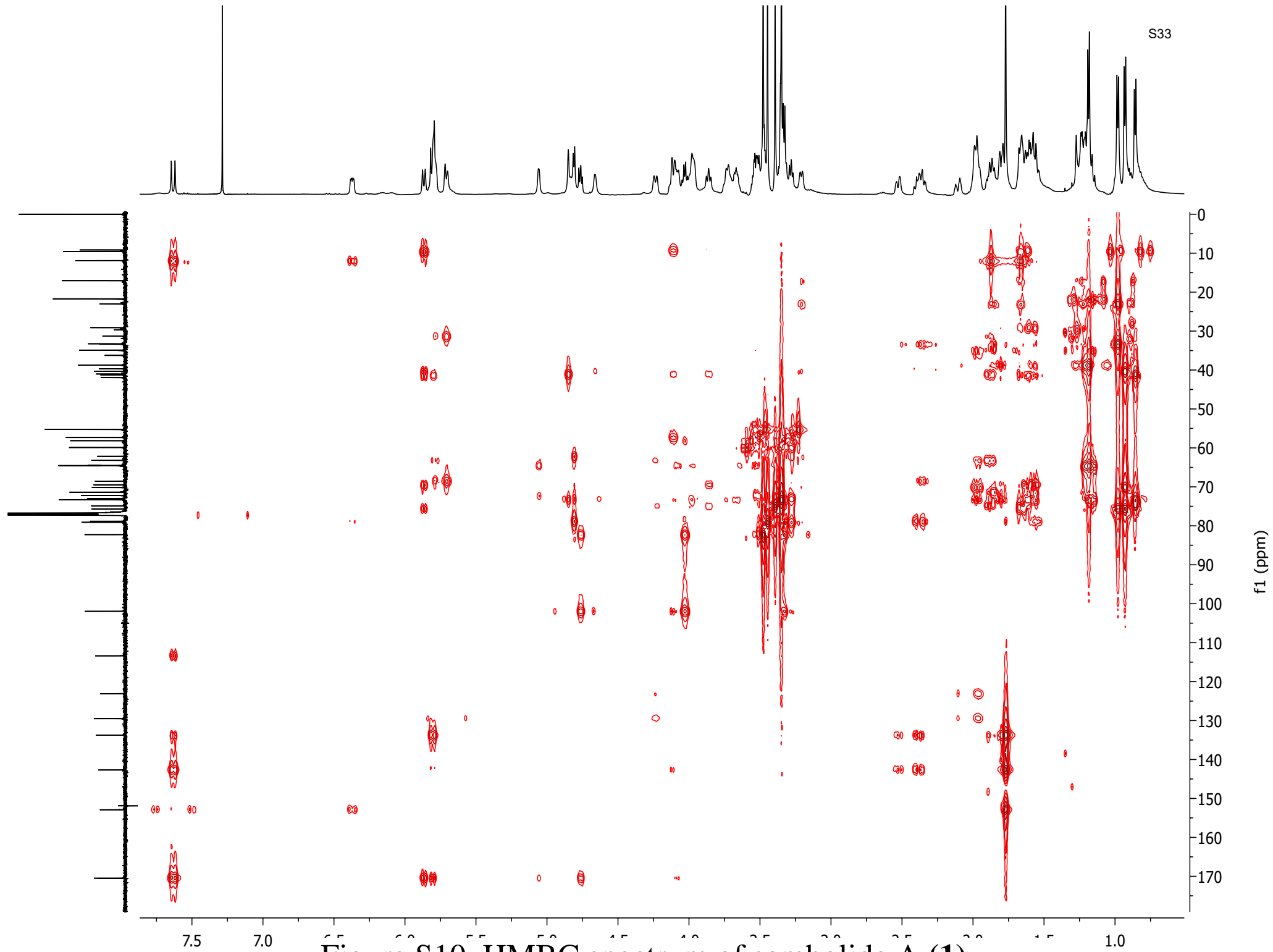


Figure S10 HMBC spectrum of samholide A (**1**)

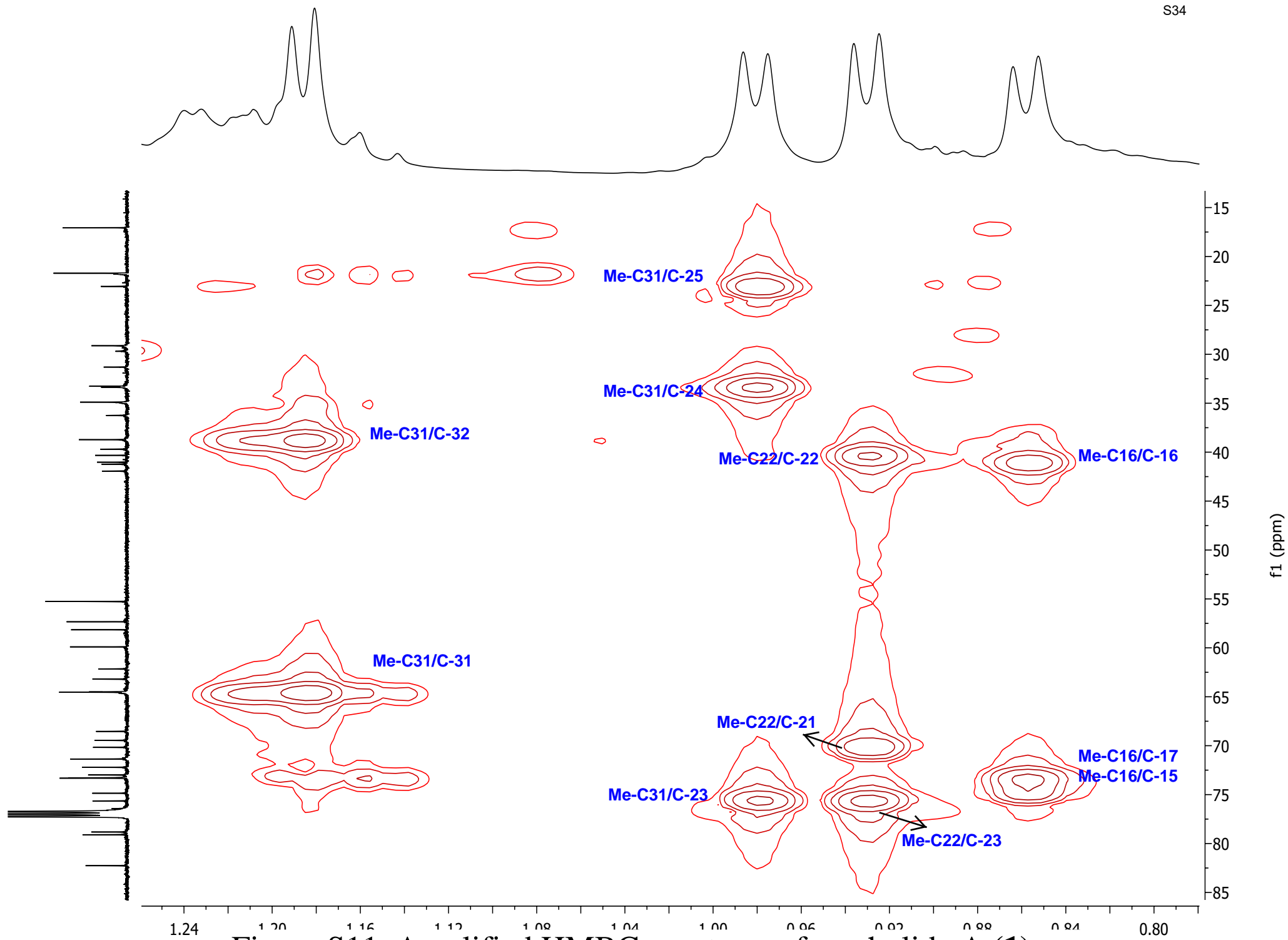


Figure S11 Amplified HMBC spectrum of samholide A (1)

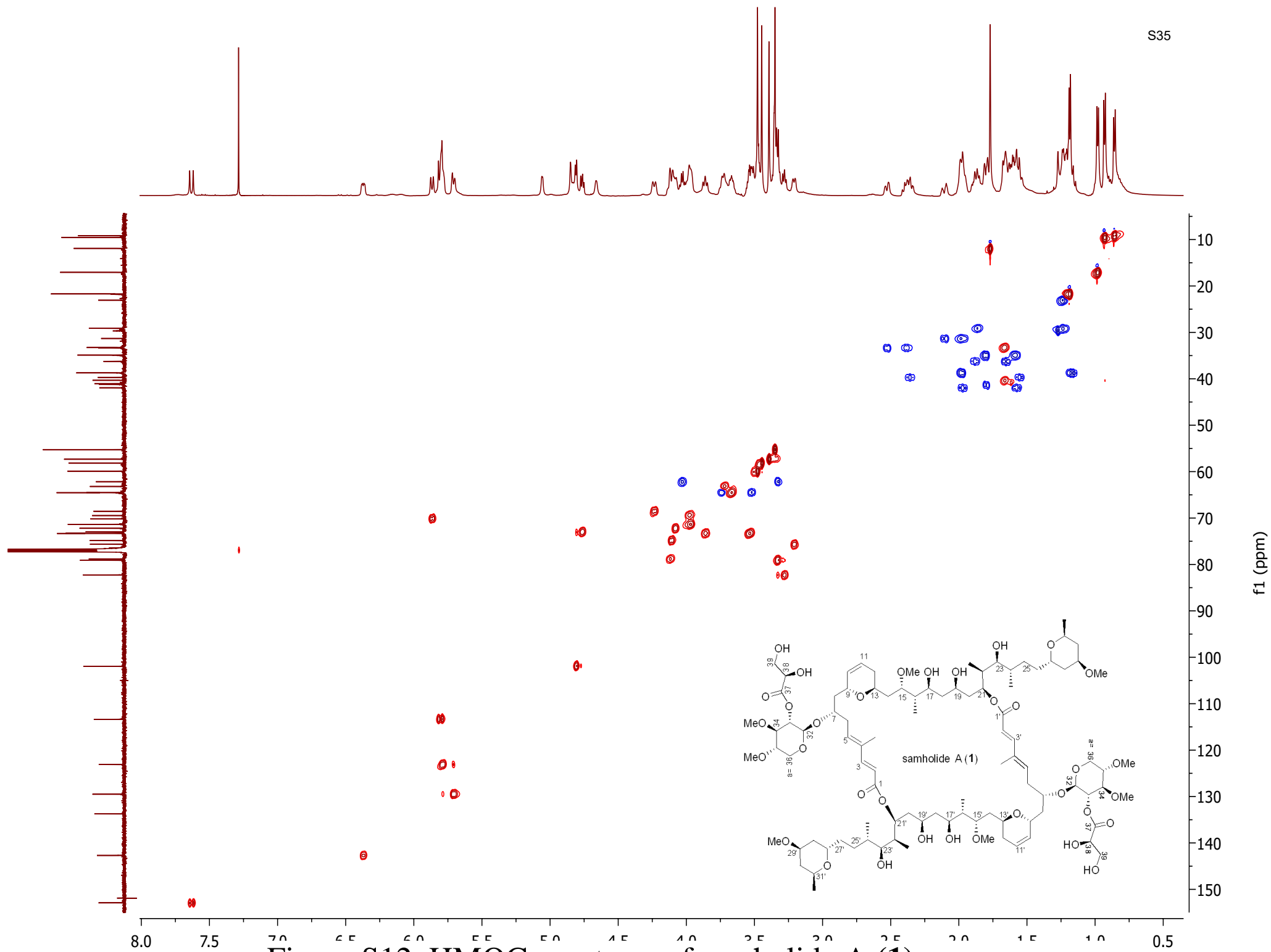


Figure S12 HMBC spectrum of samholide A (1)

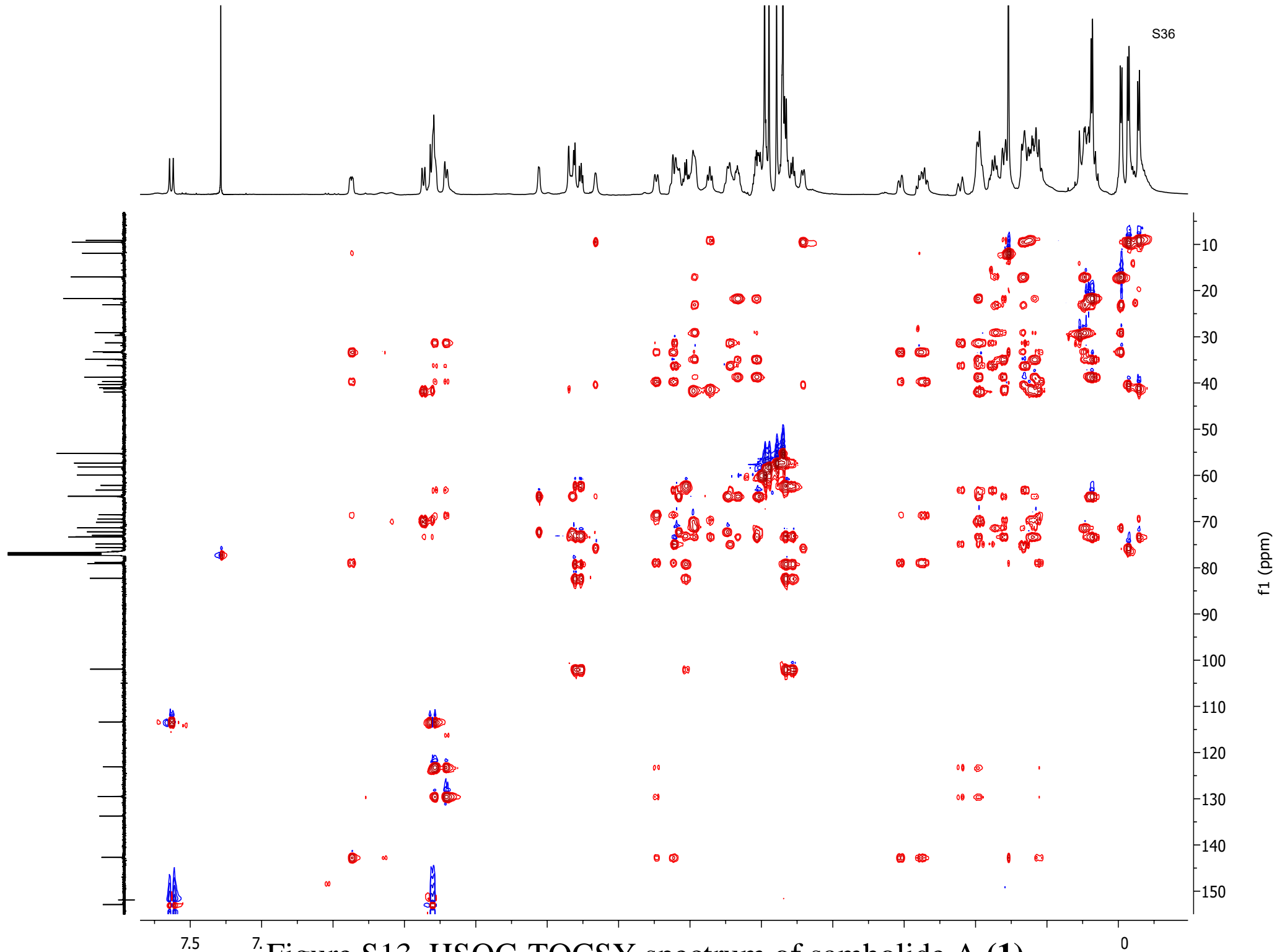


Figure S13 HSQC-TOCSY spectrum of samholide A (1)

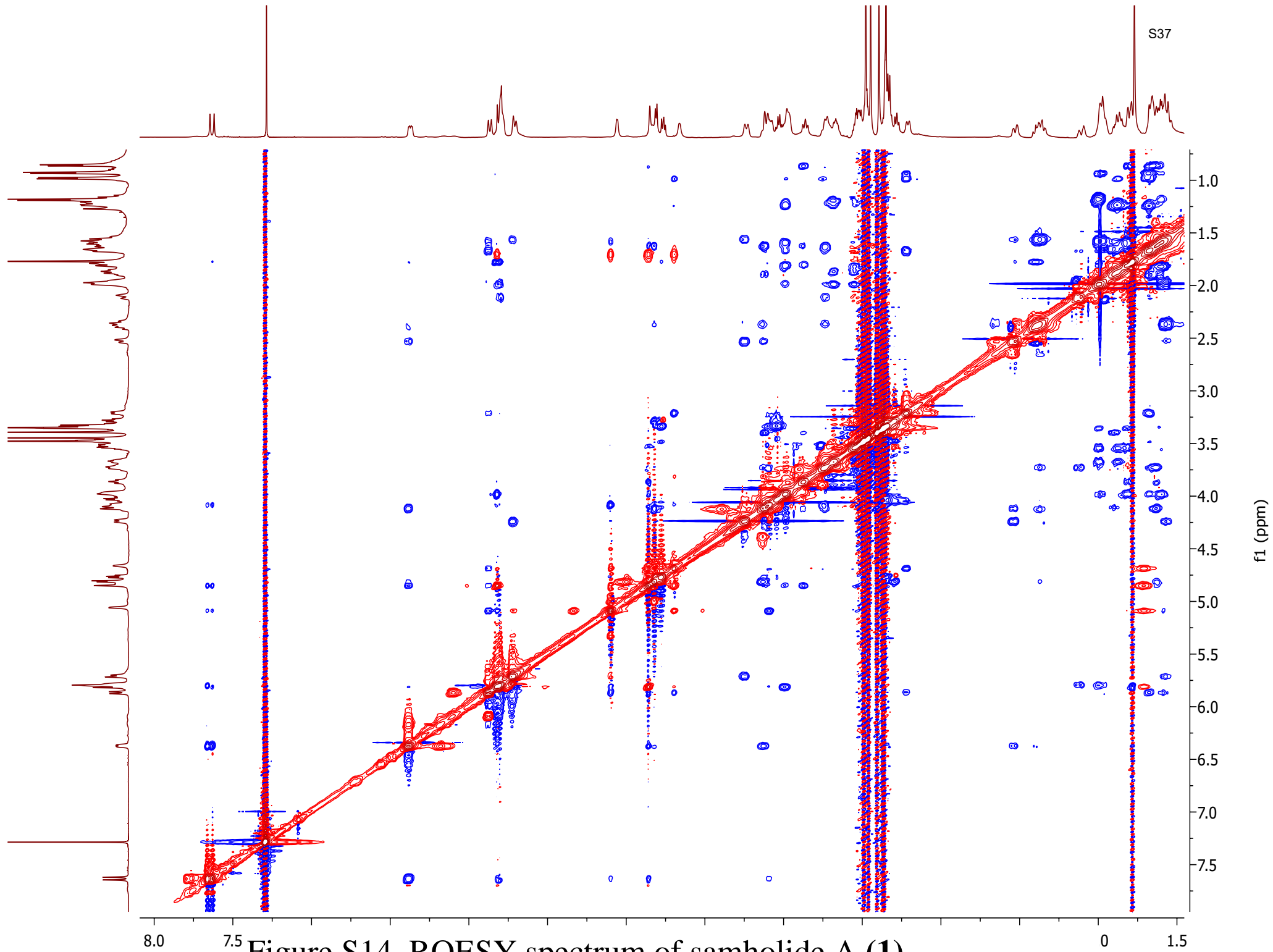


Figure S14 ROESY spectrum of samholide A (1)

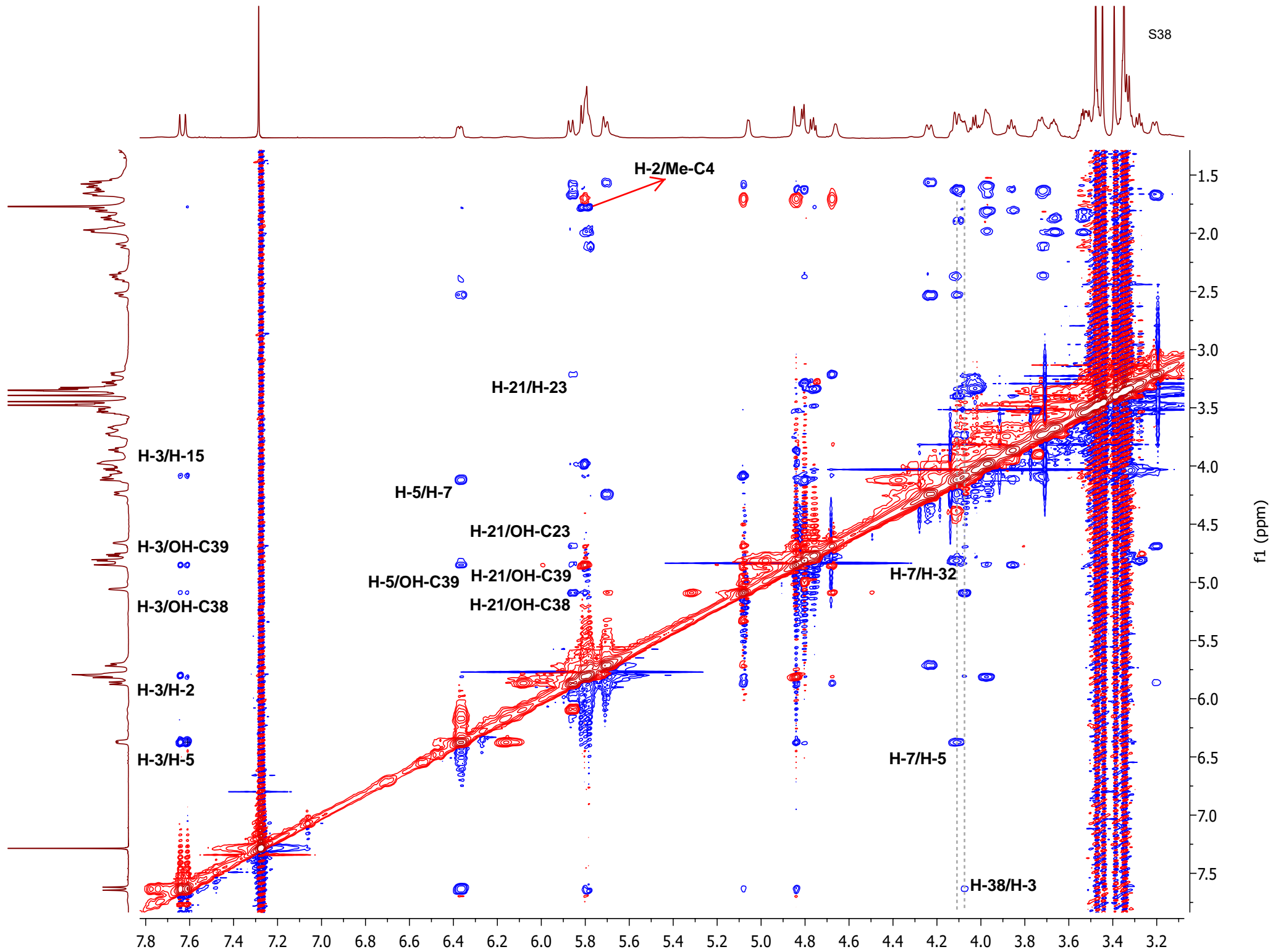


Figure S15 Amplified ROESY spectrum of samholide A (1)

C7-a #44-52 RT: 1.06-1.25 AV: 9 SB: 7 0.74-0.89 NL: 2.70E7
T: + c Full ms [300.00-2000.00]

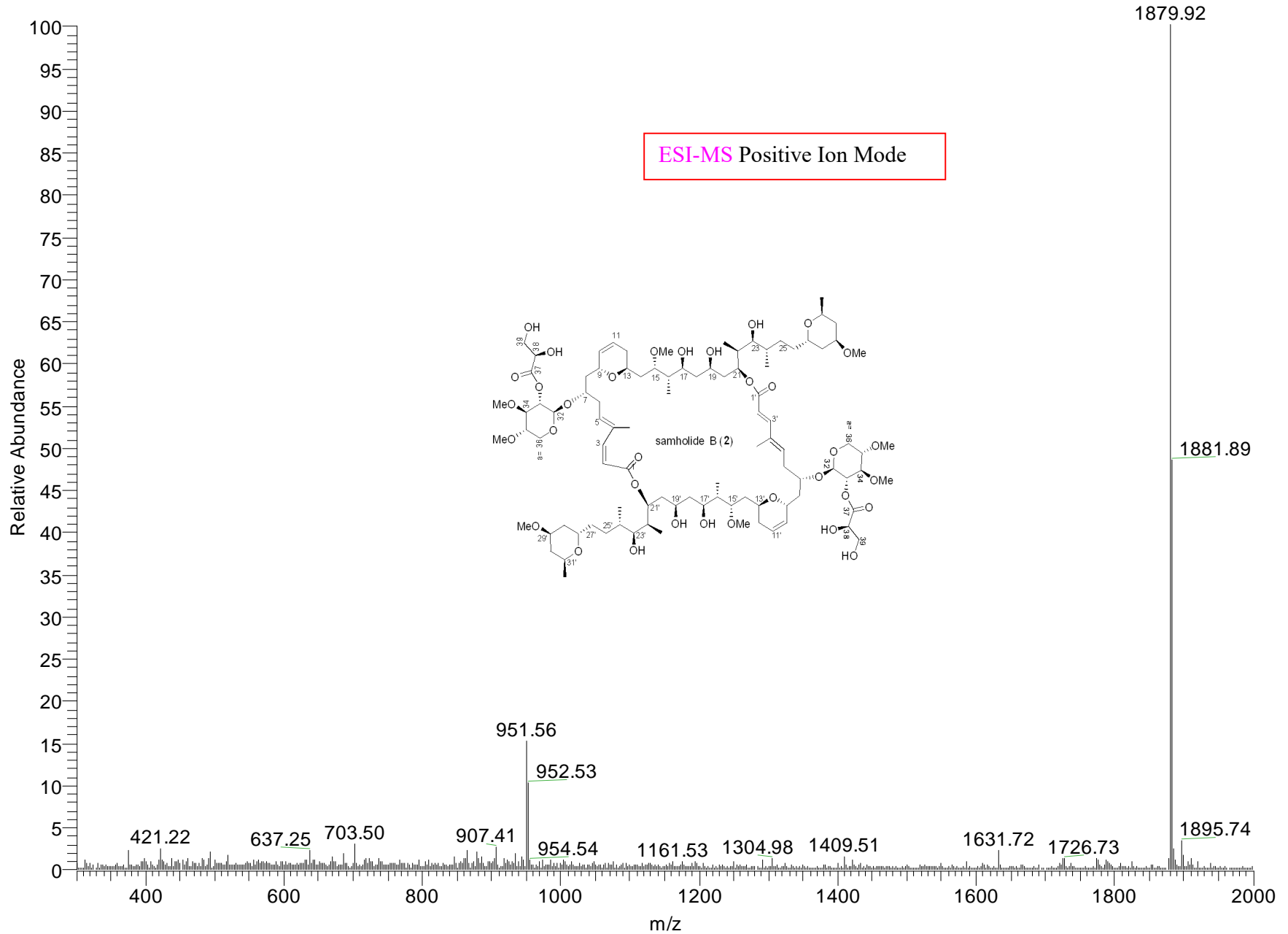


Figure S16 The ESI MS spectrum of samholide B (2)

C7-a #162-172 RT: 3.96-4.13 AV: 11 SB: 7 3.62-3.79 NL: 1.10E7
T: +c Full ms2 1880.00@35.00 [515.00-2000.00]

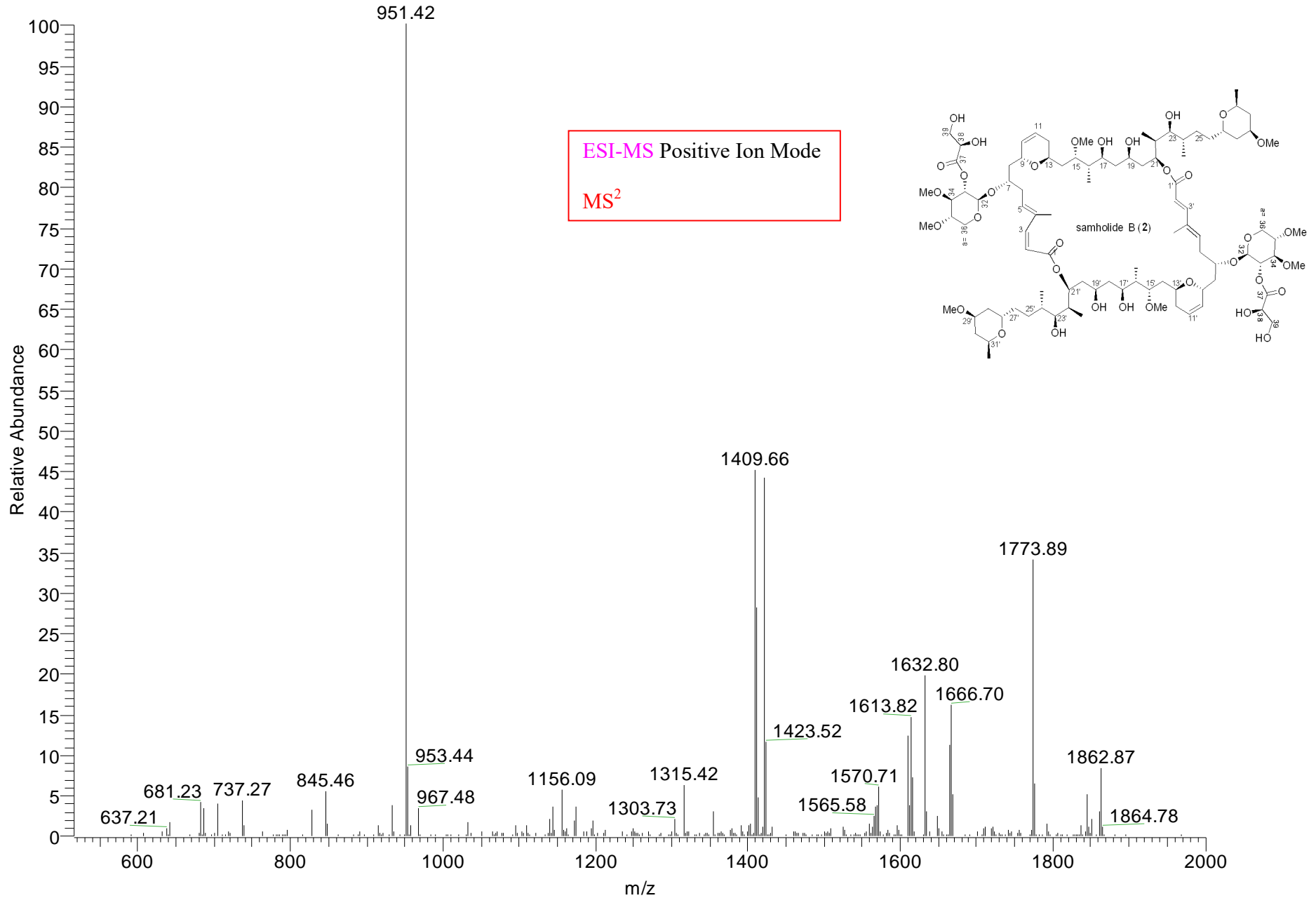


Figure S17 The ESI MS² spectrum of samholide B (2)

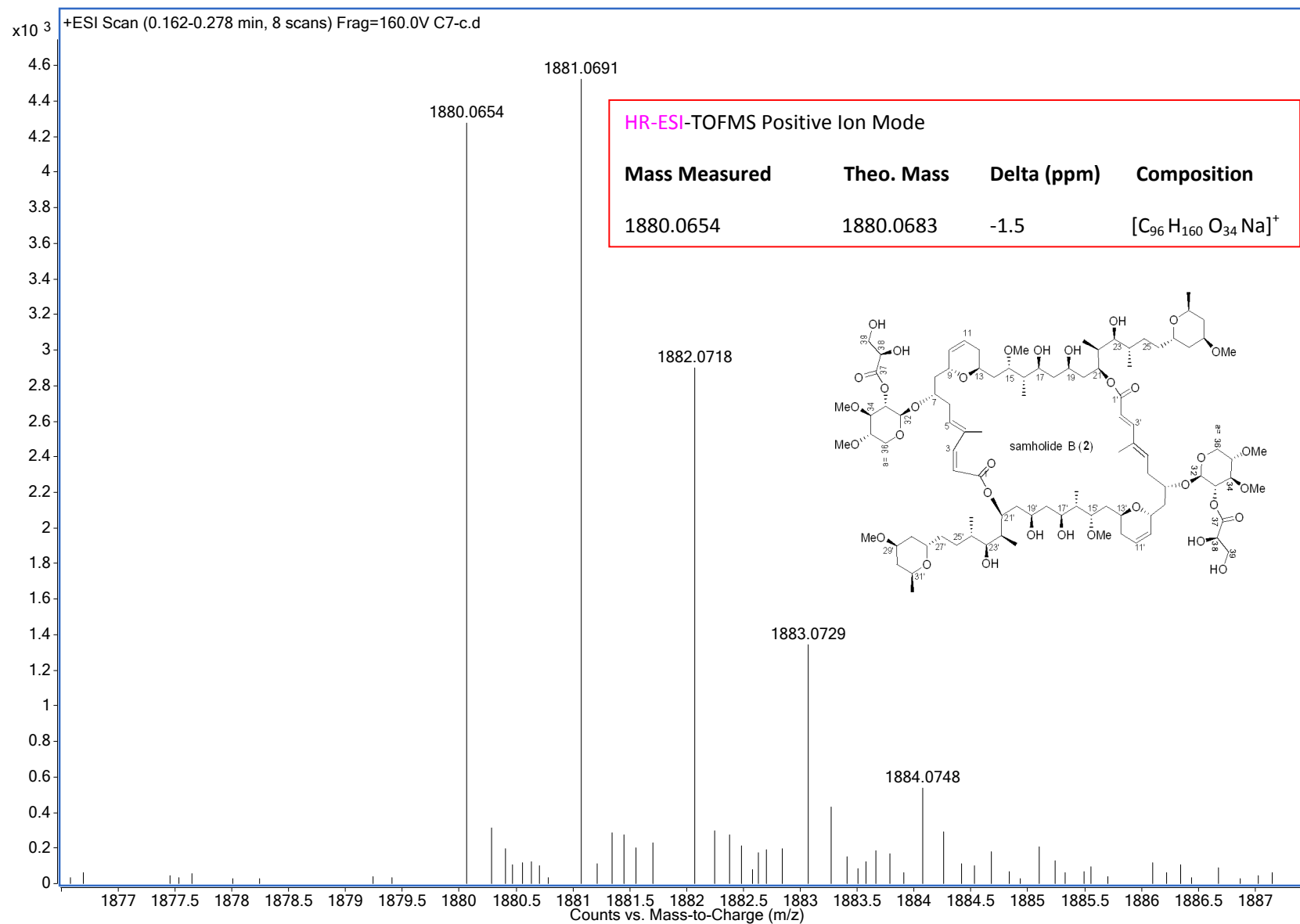
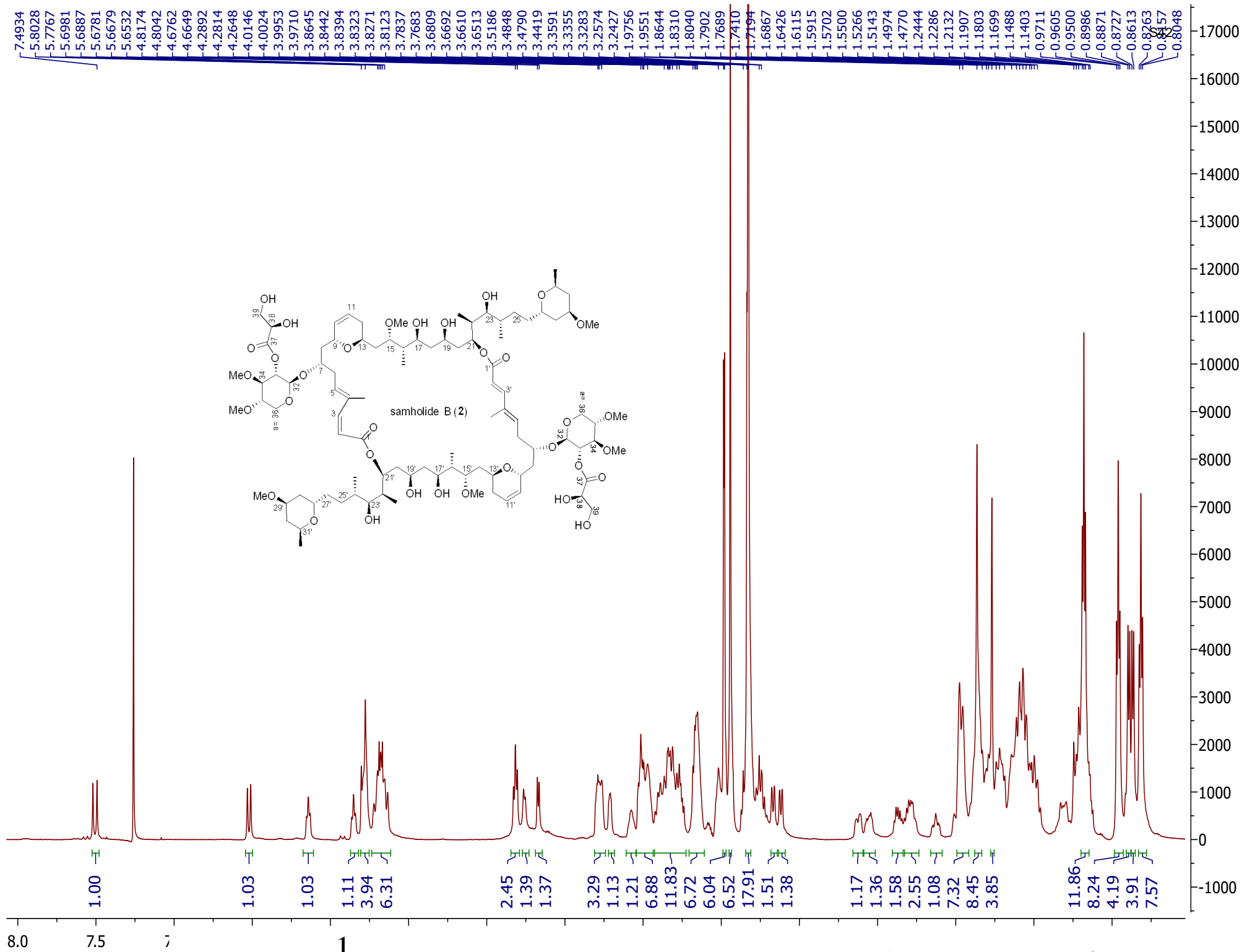
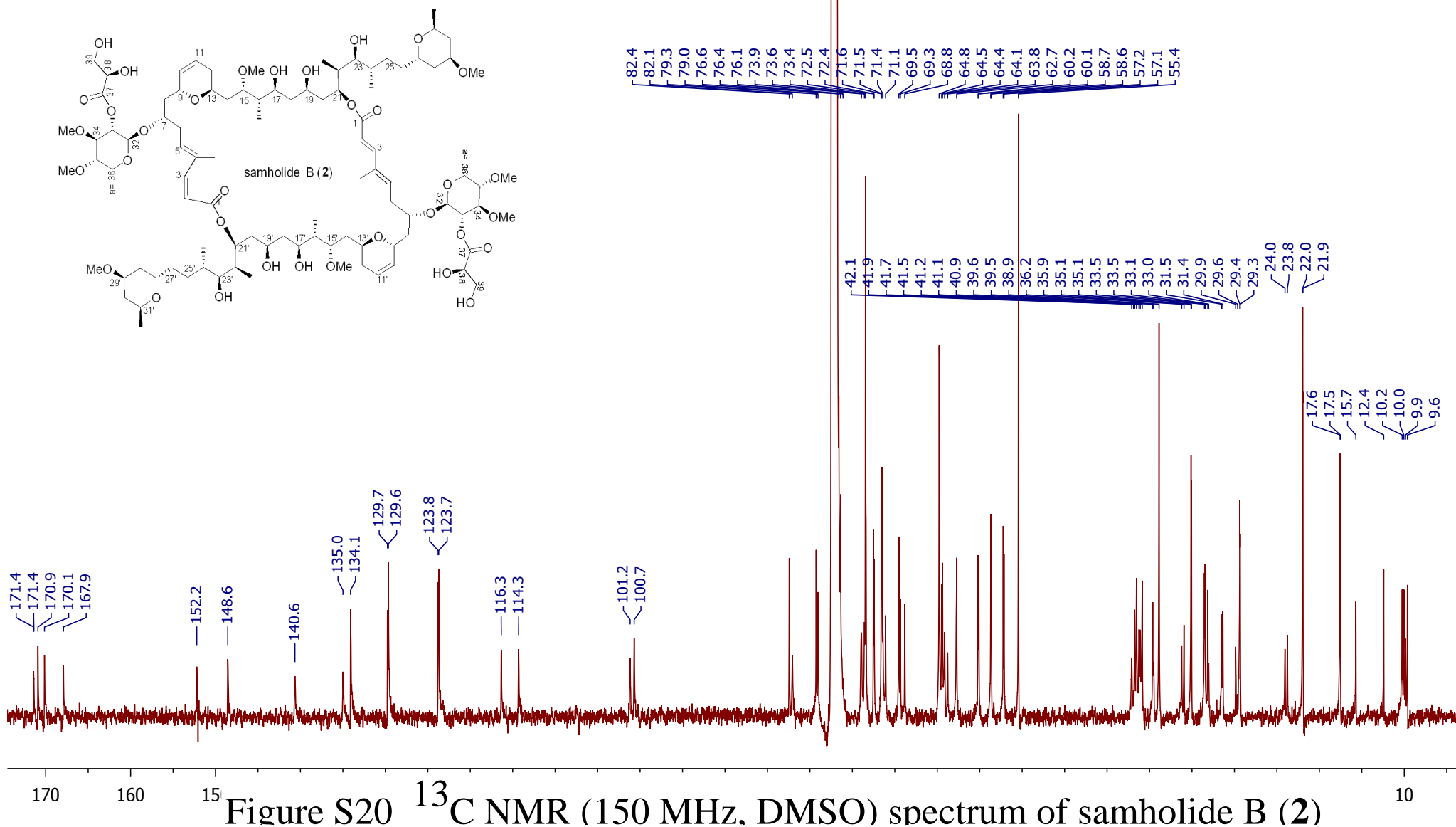
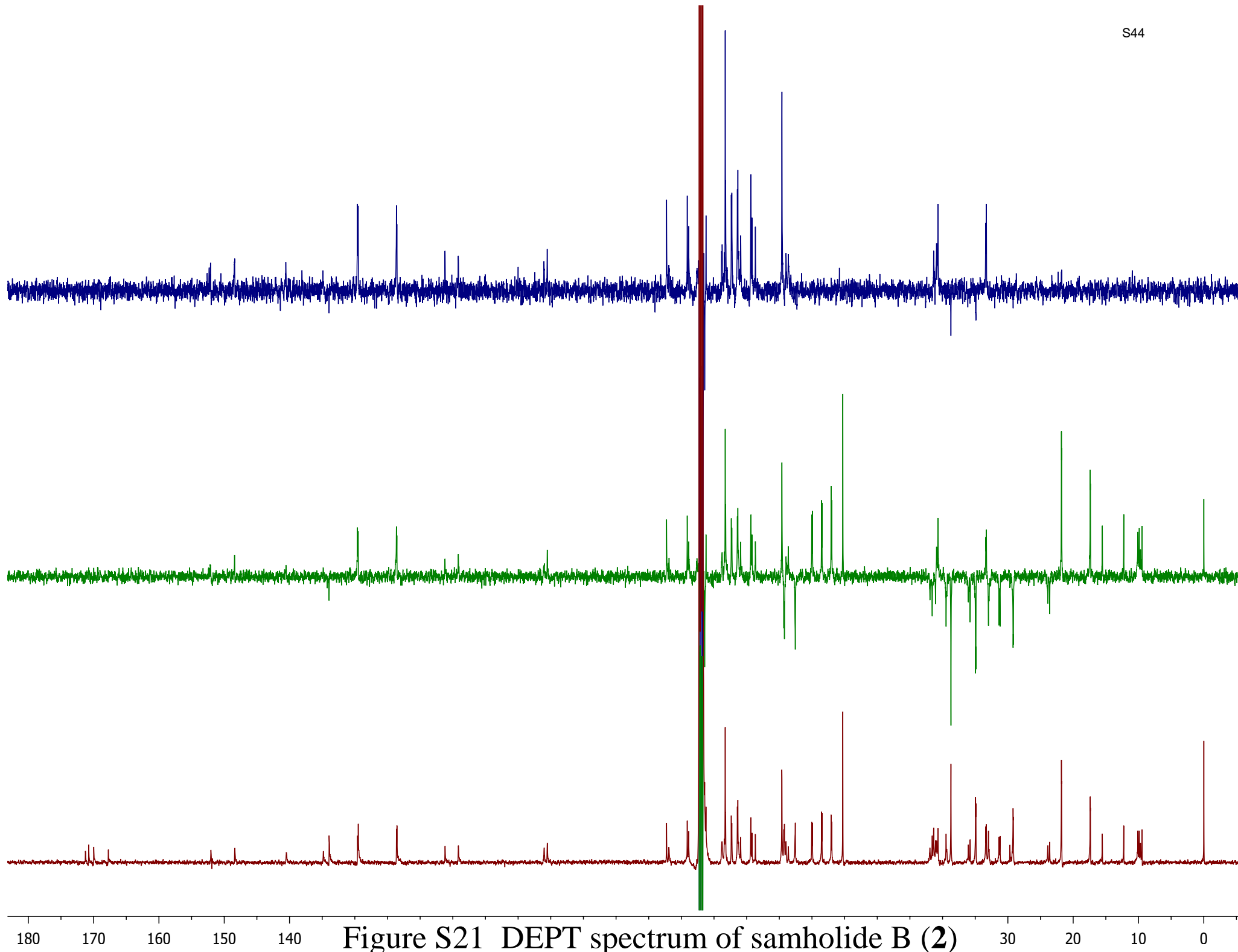


Figure S18 The positive HRESIMS spectrum of samholide B (2)







S45

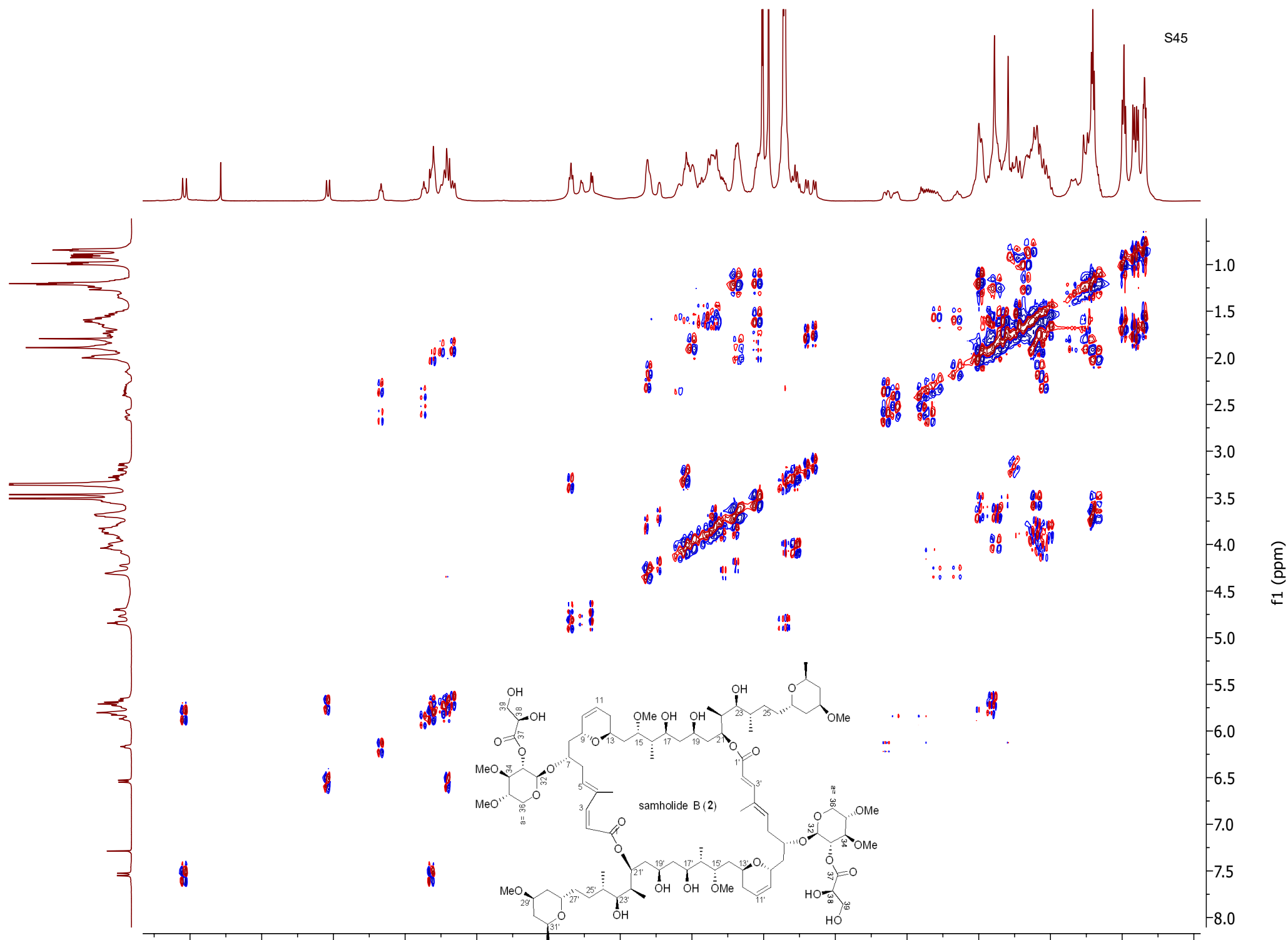


Figure S22 ^1H - ^1H COSY spectrum of samholide B (2)

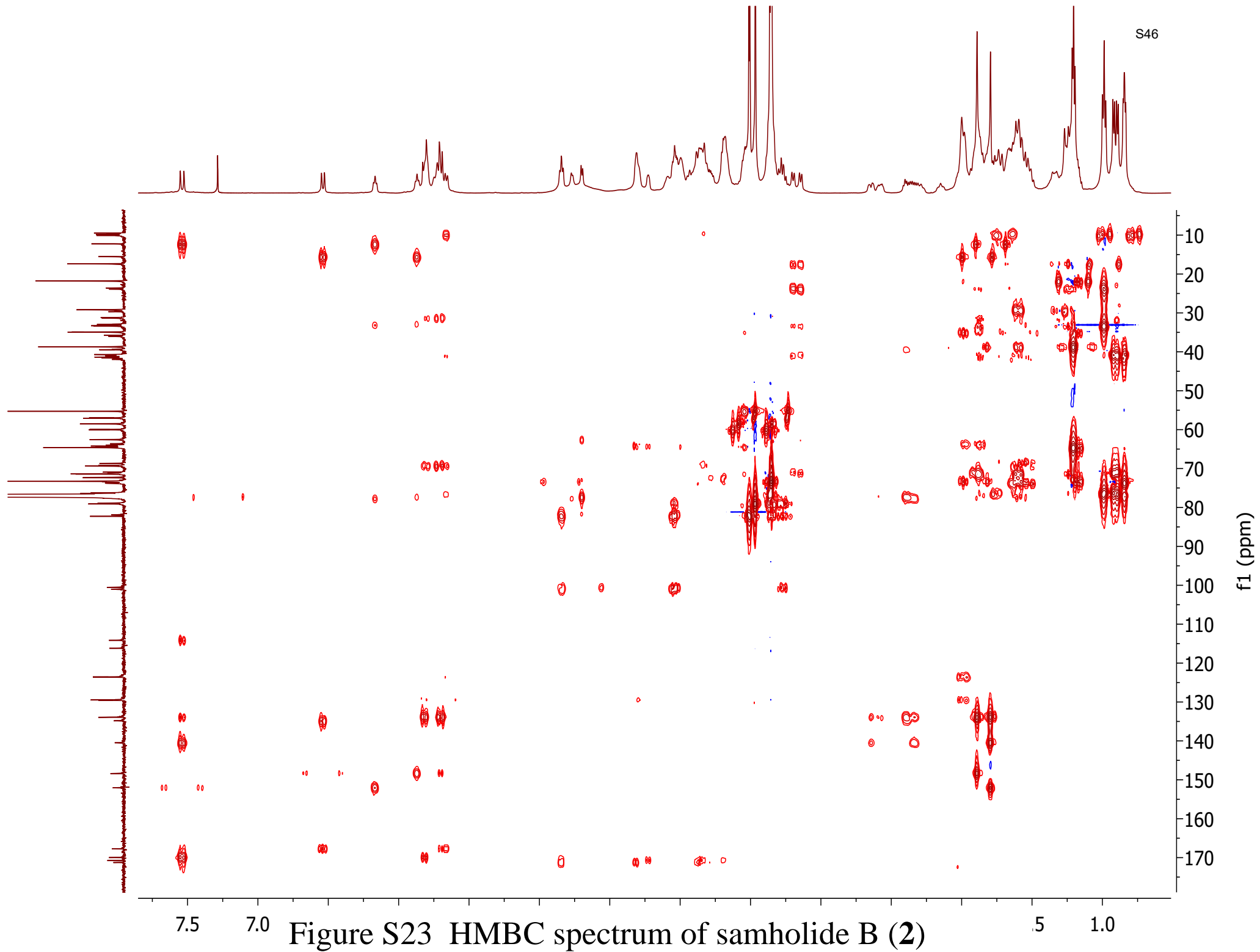


Figure S23 HMBC spectrum of samholide B (2)

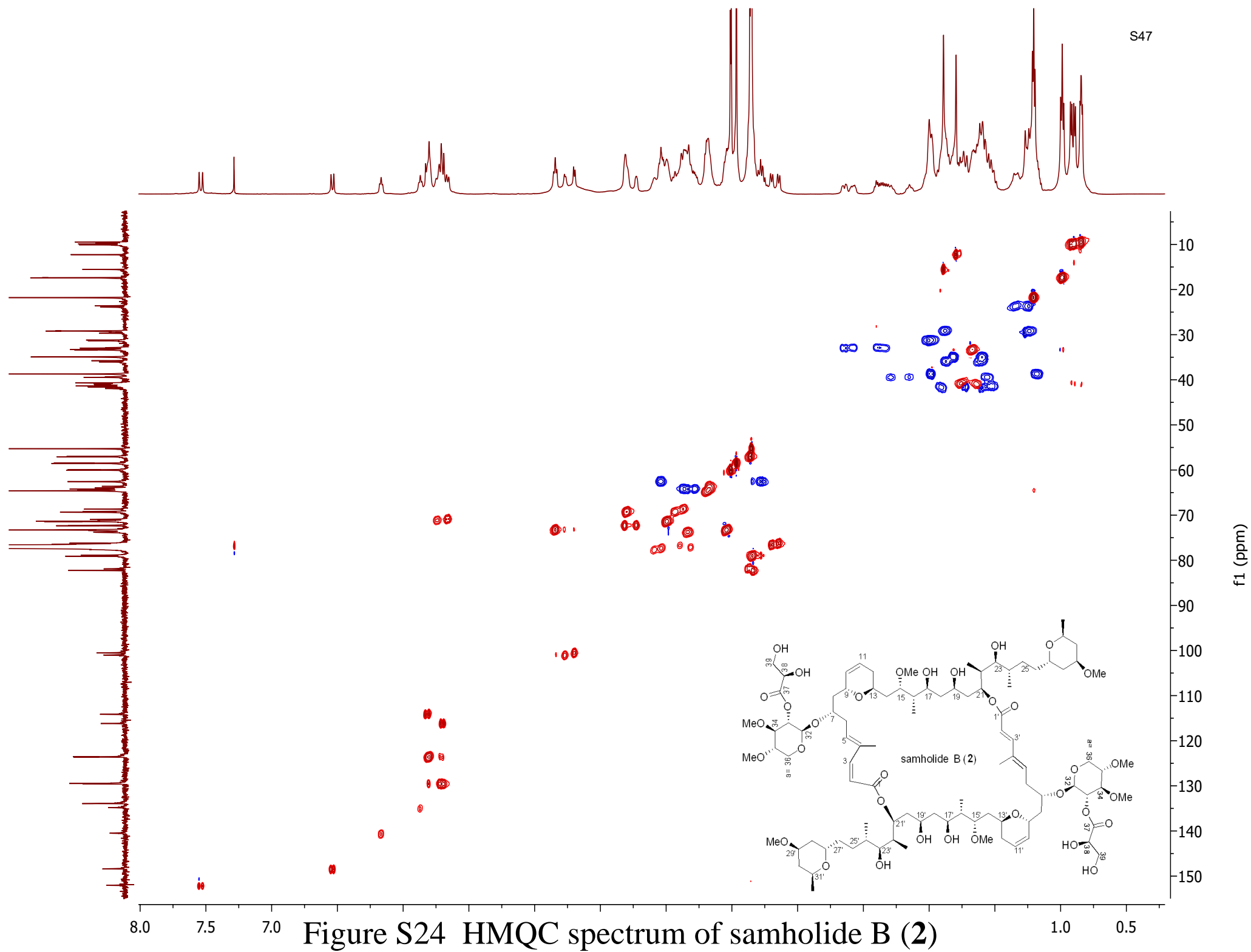
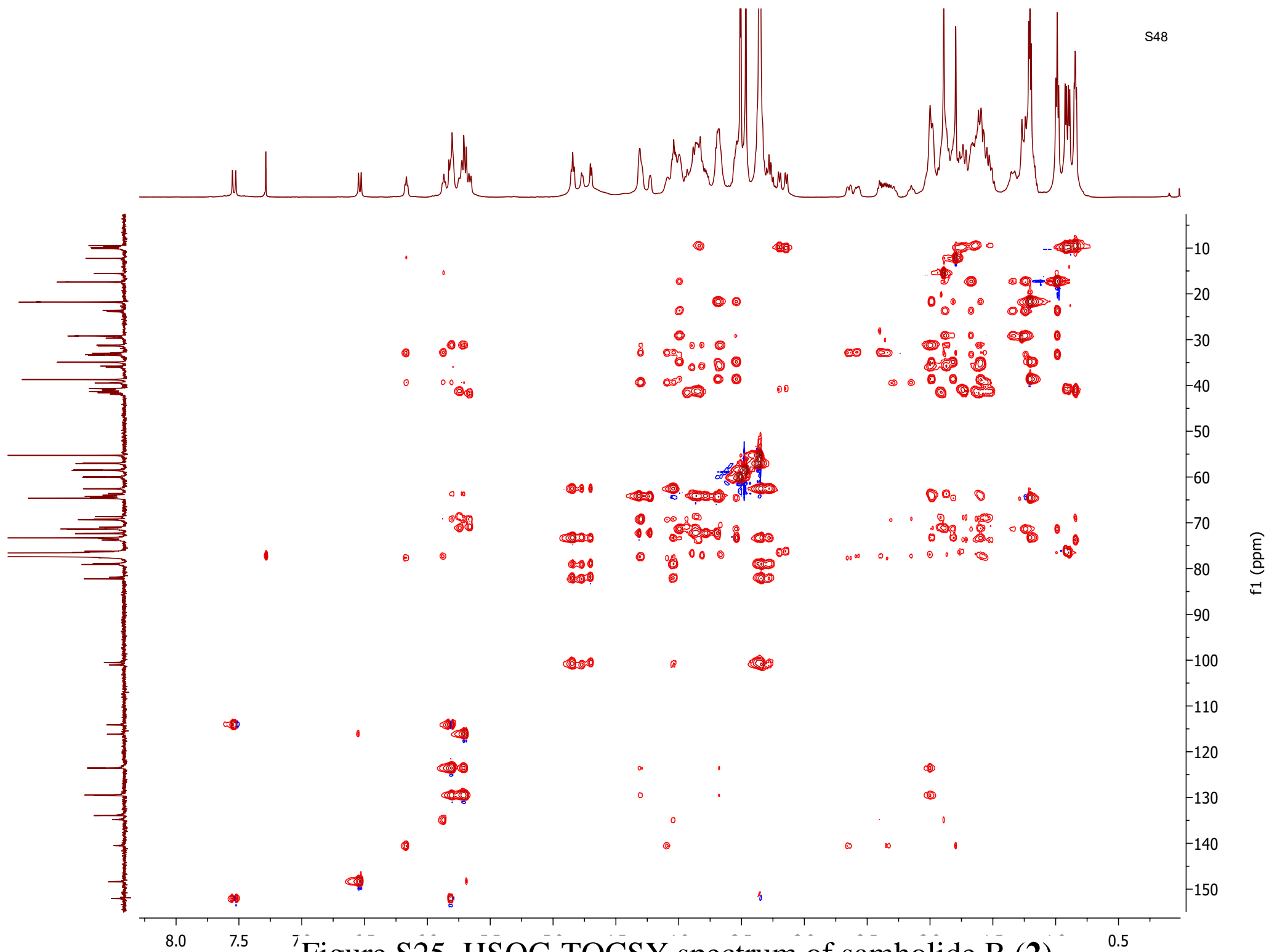


Figure S24 HMQC spectrum of samholide B (2)



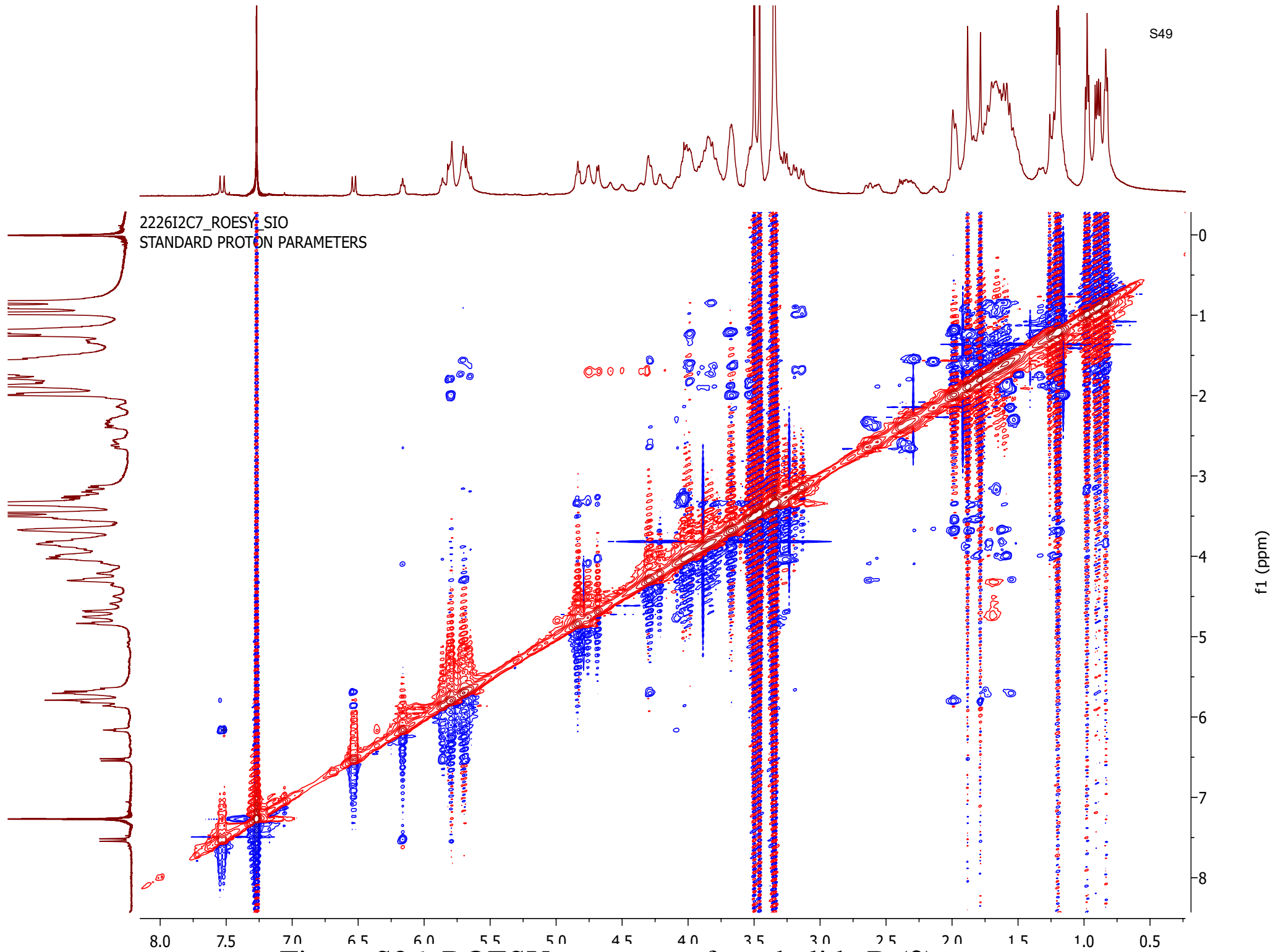


Figure S26 ROESY spectrum of samholide B (2)

F5-a #13-18 RT: 0.30-0.42 AV: 6 SB: 3 0.06-0.11 NL: 4.11E7
T: + c Full ms [300.00-2000.00]

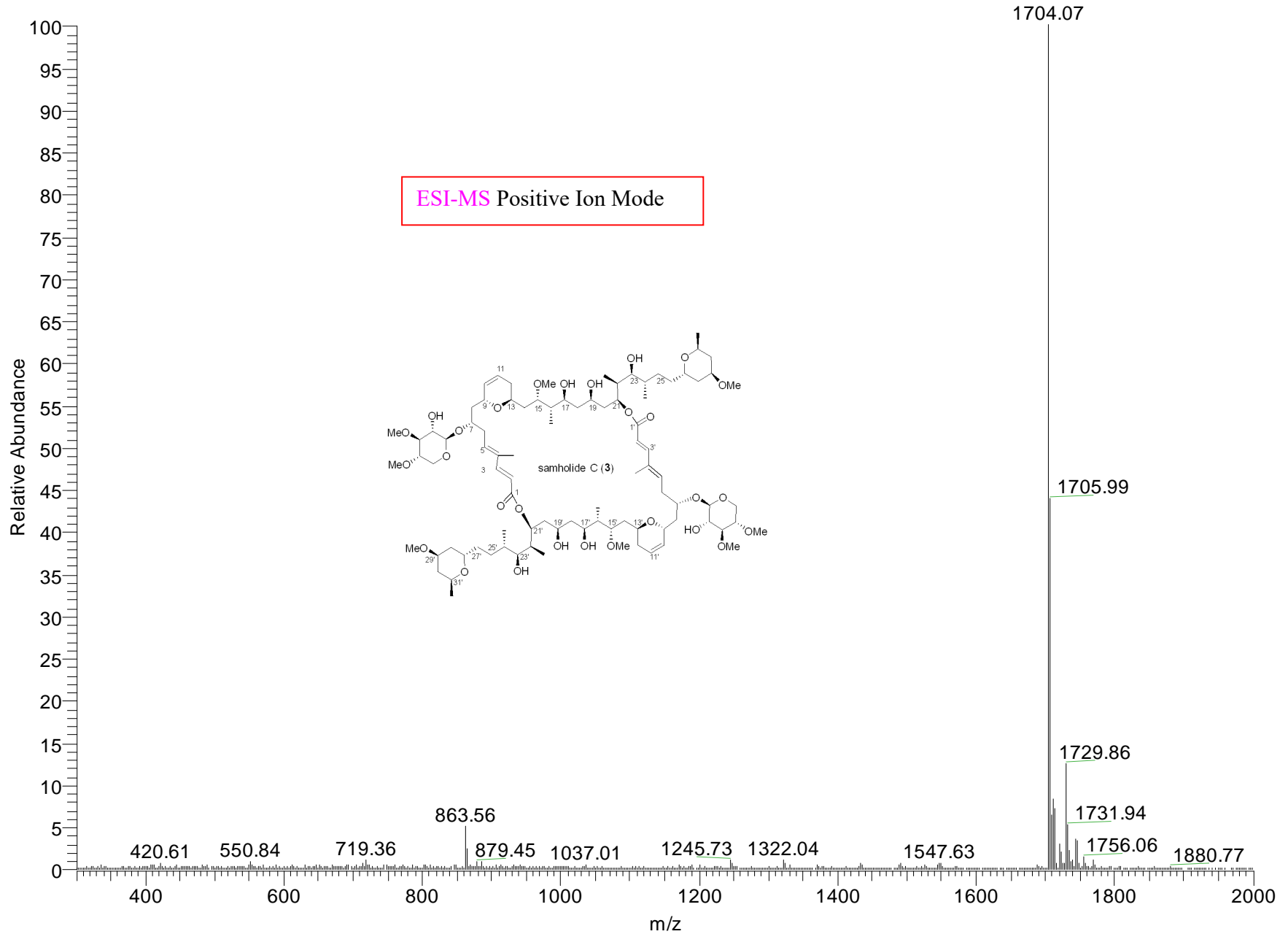


Figure S27 The ESI MS spectrum of samholide C (3)

F5-a #51-56 RT: 1.10-1.18 AV: 6 SB: 5 0.93-1.01 NL: 3.45E7
T: + c Full ms2 1704.00@35.00 [465.00-2000.00]

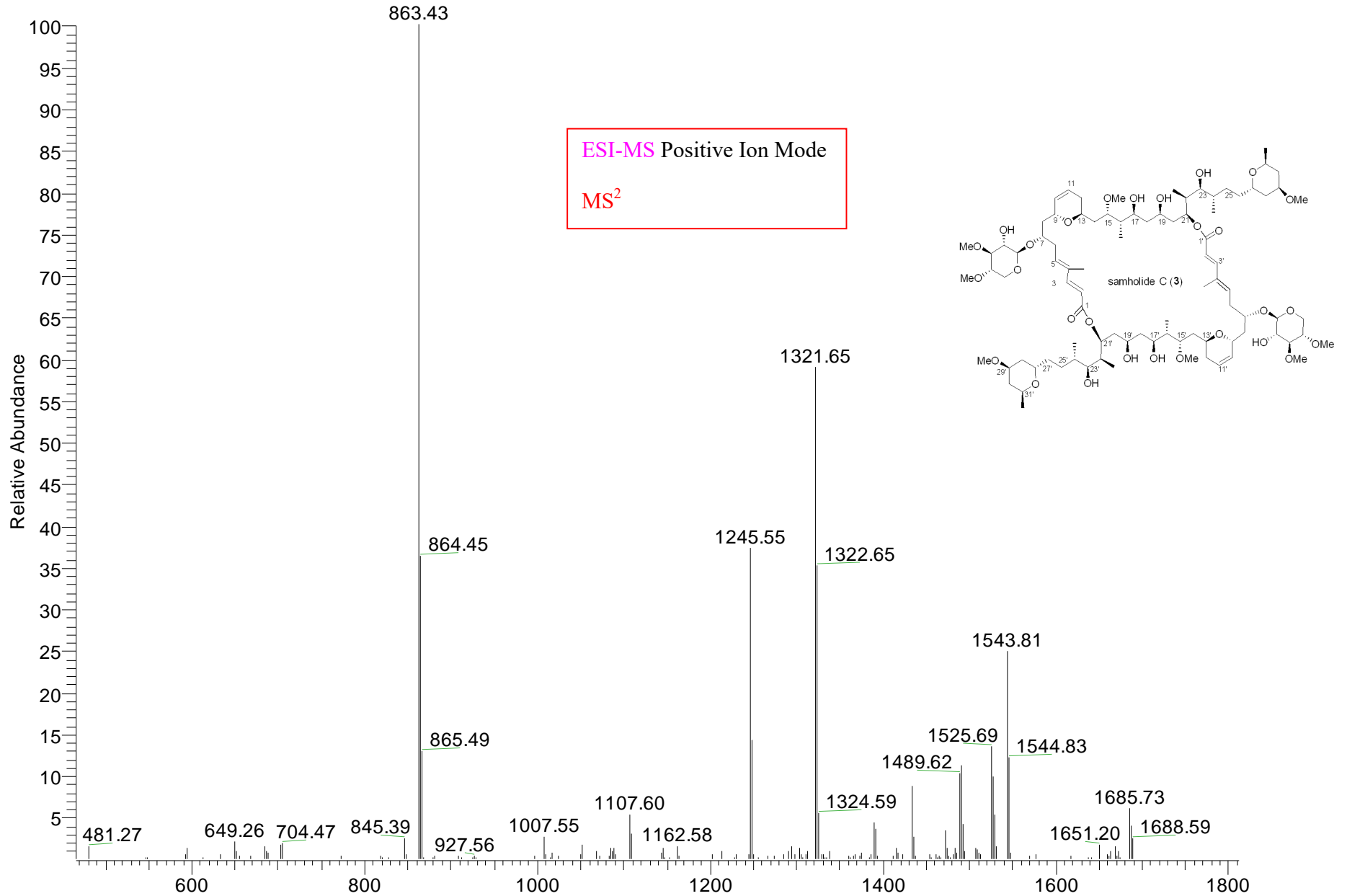


Figure S28 The ESI MS² spectrum of samholide C (3)

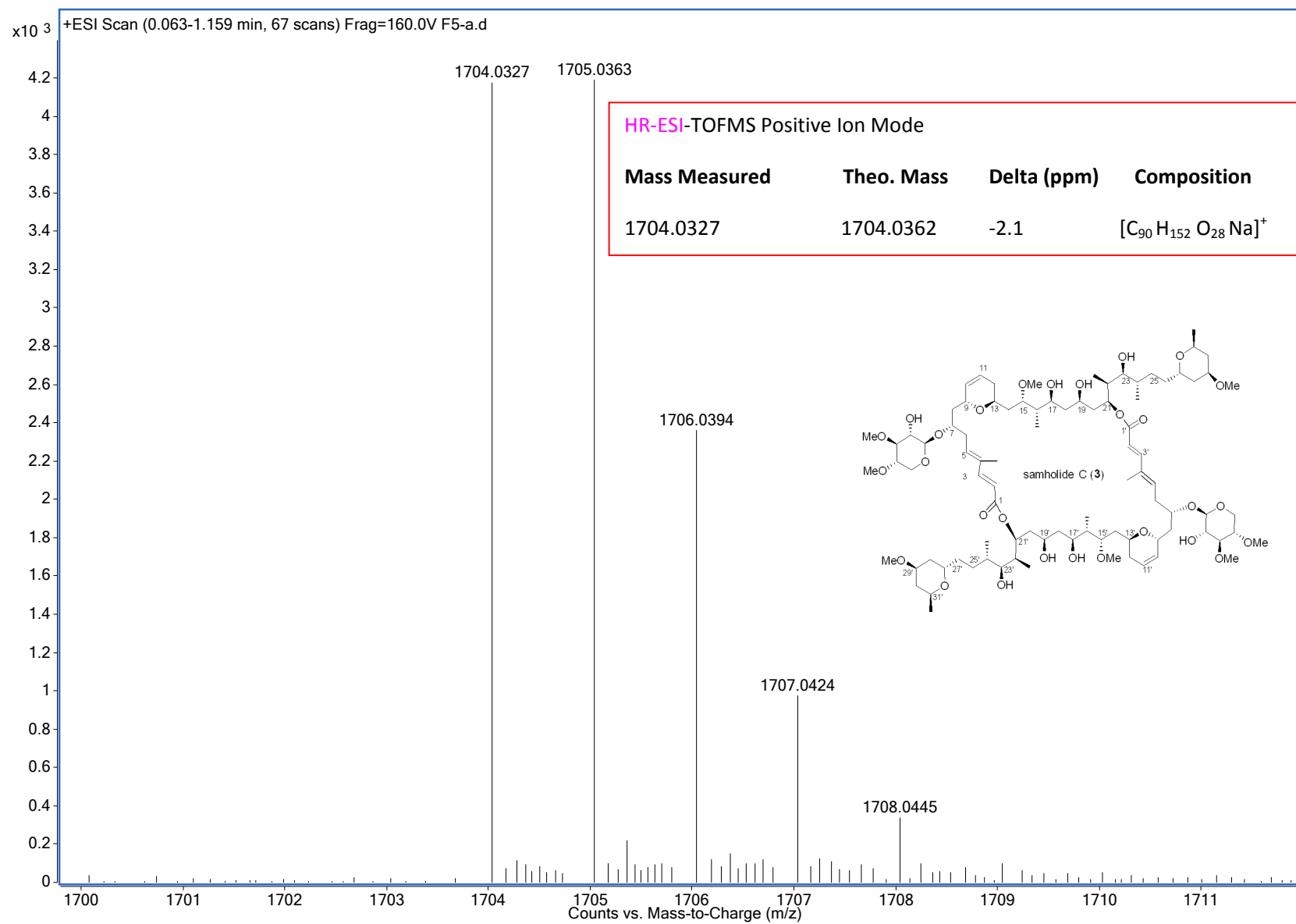
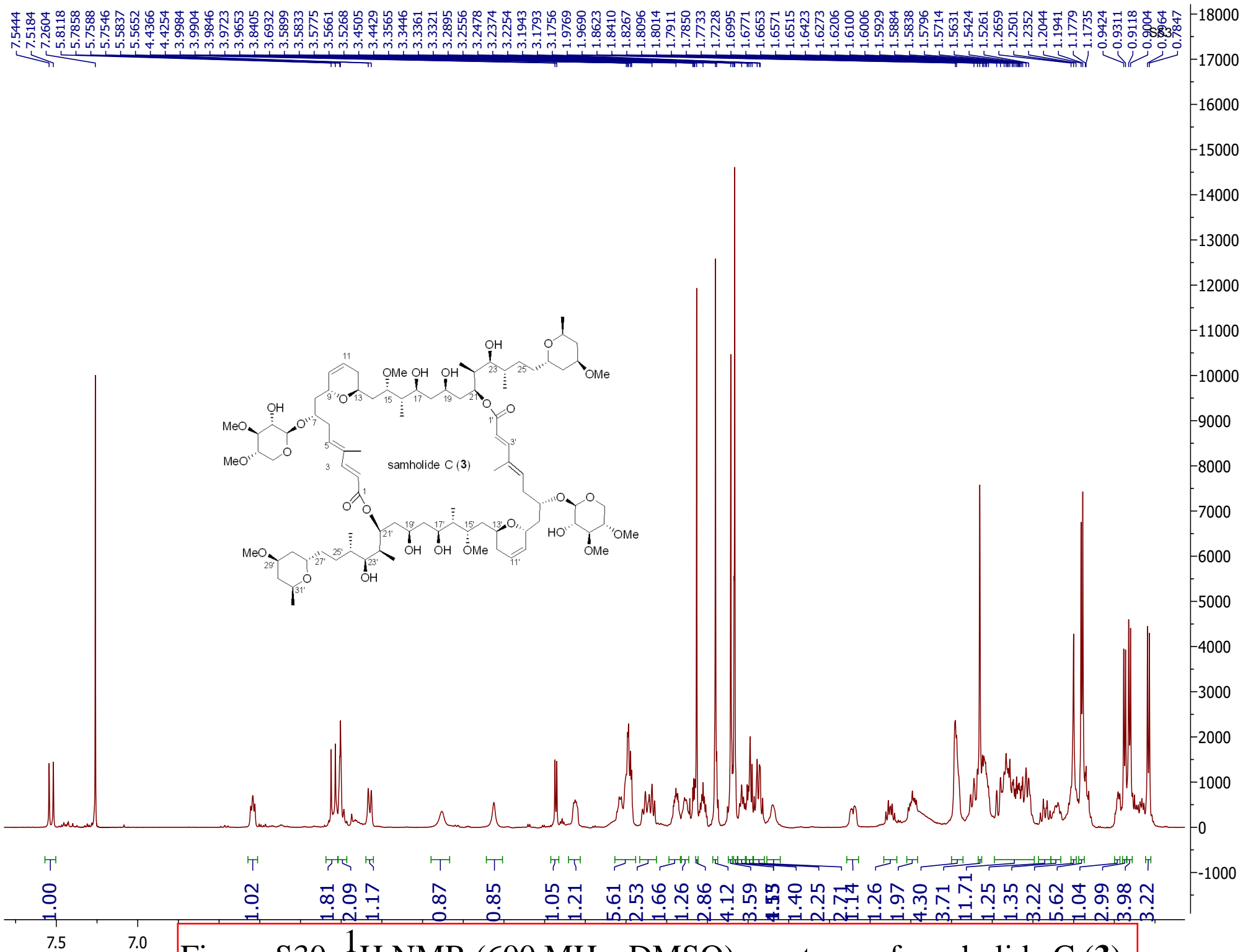


Figure S29 The positive HRESIMS spectrum of samholide C (3)



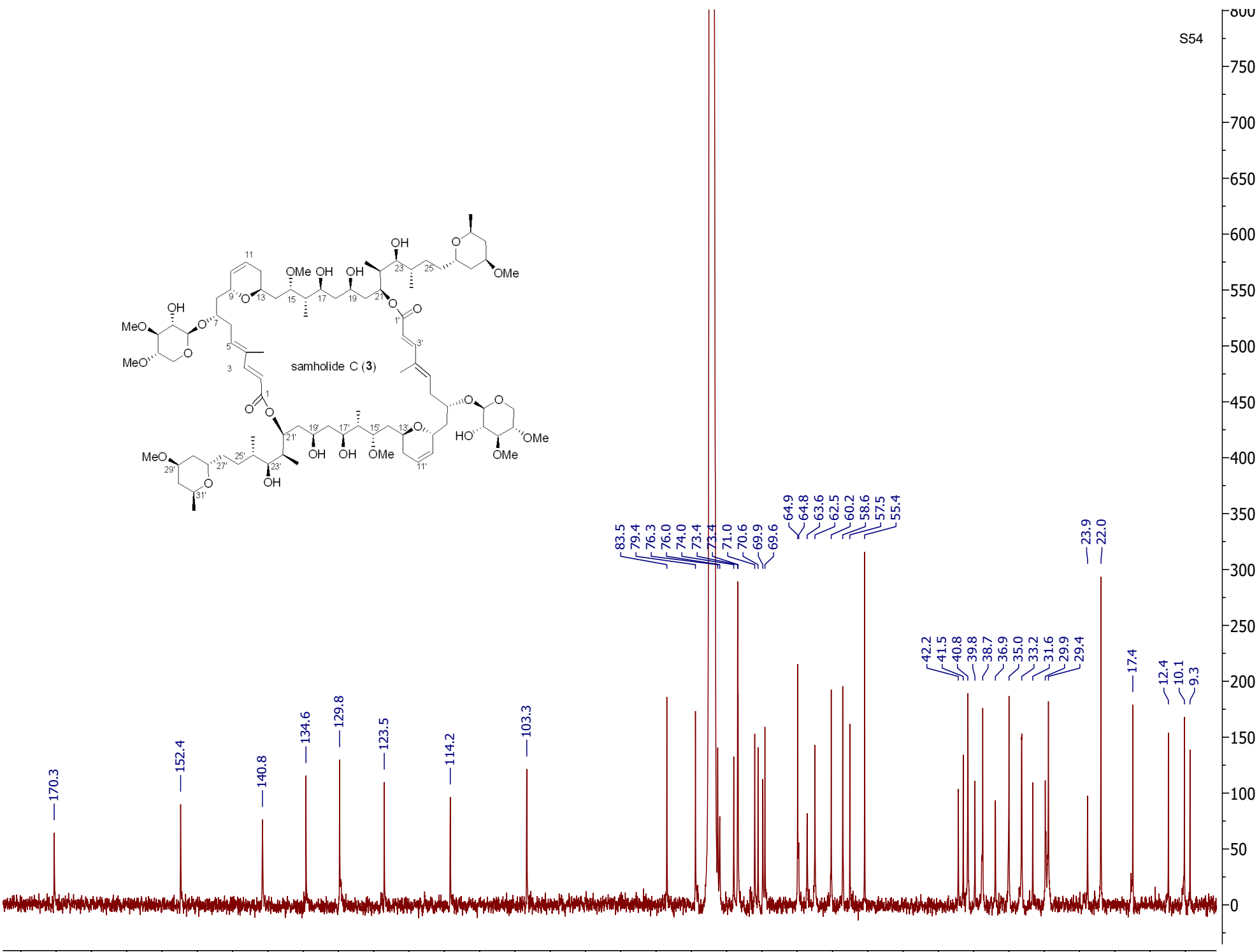
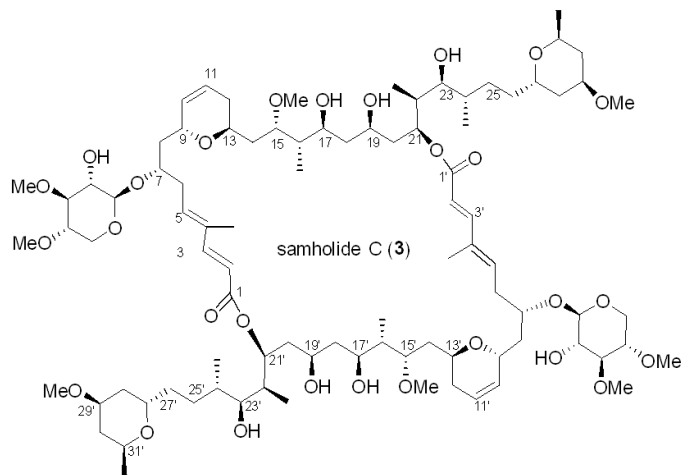


Figure S31 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide C (3)

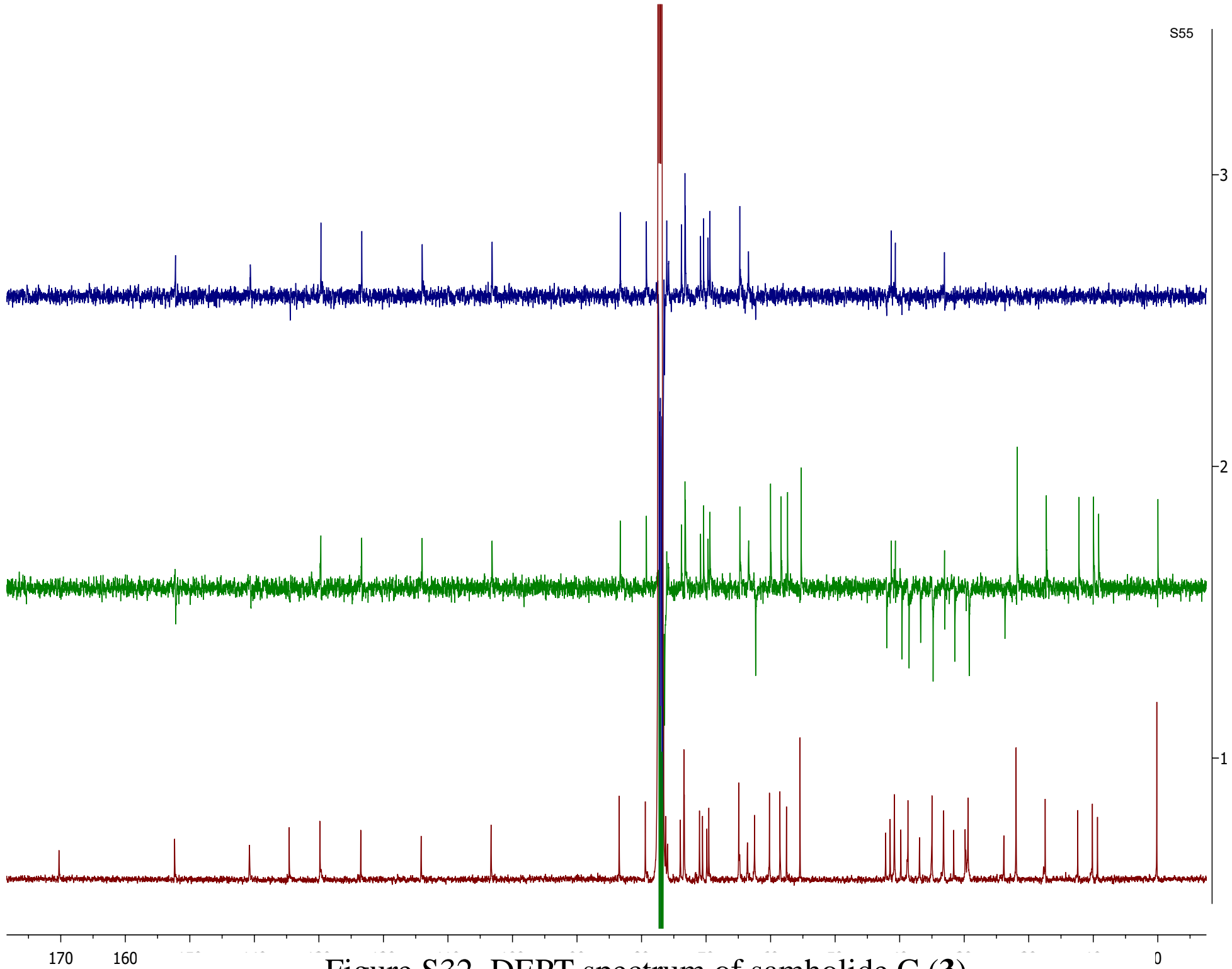
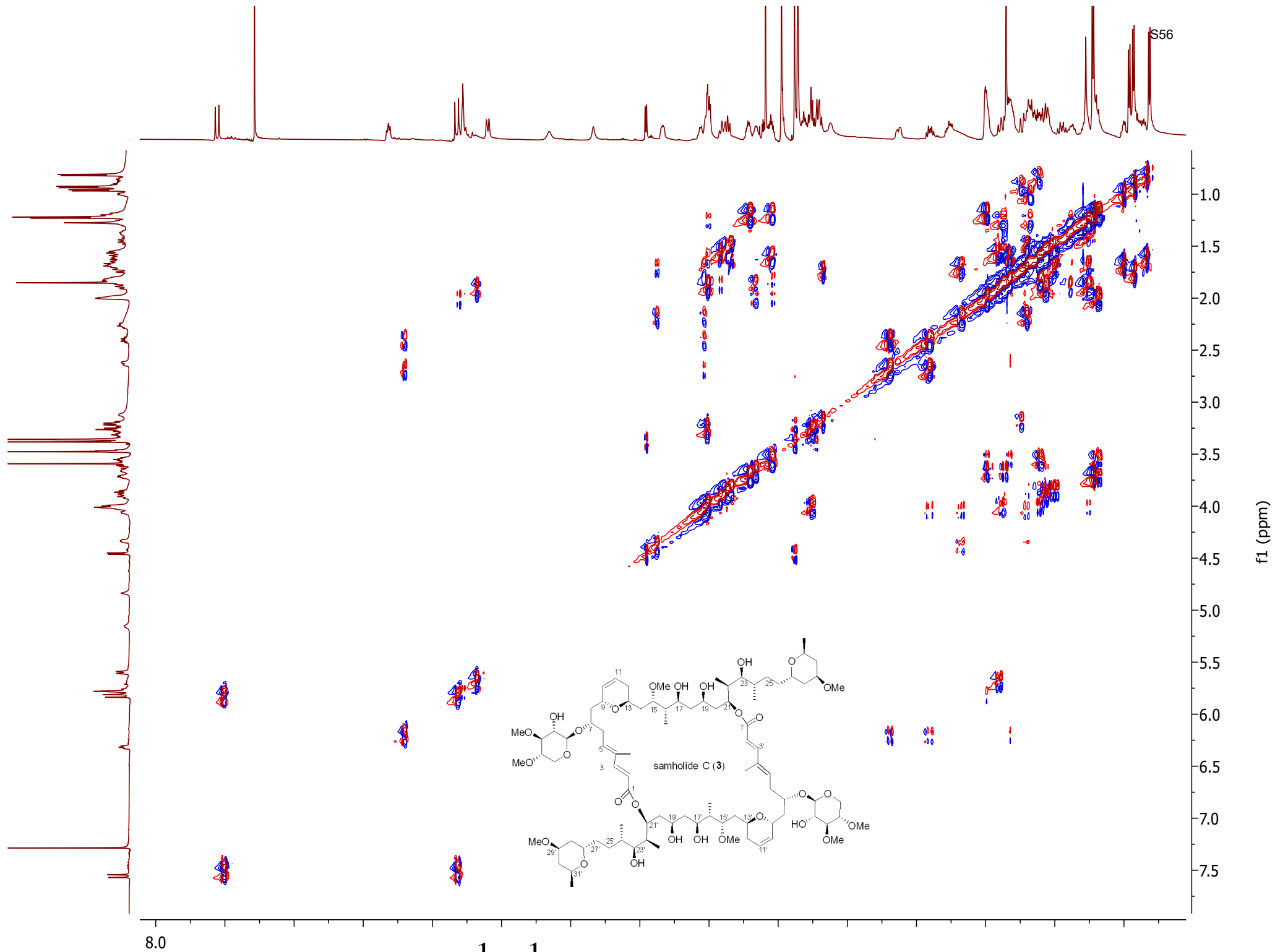


Figure S32 DEPT spectrum of samholide C (**3**)



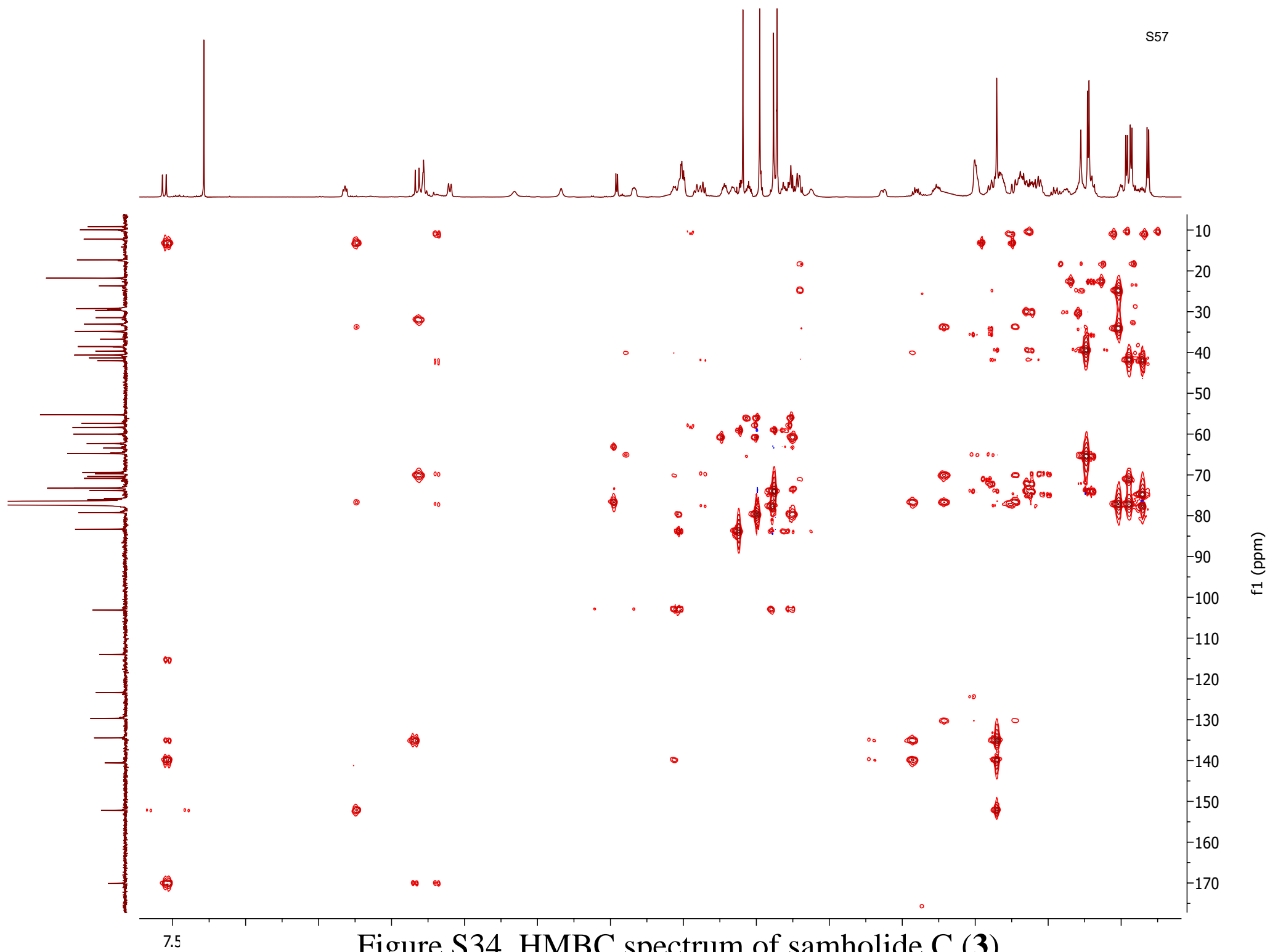
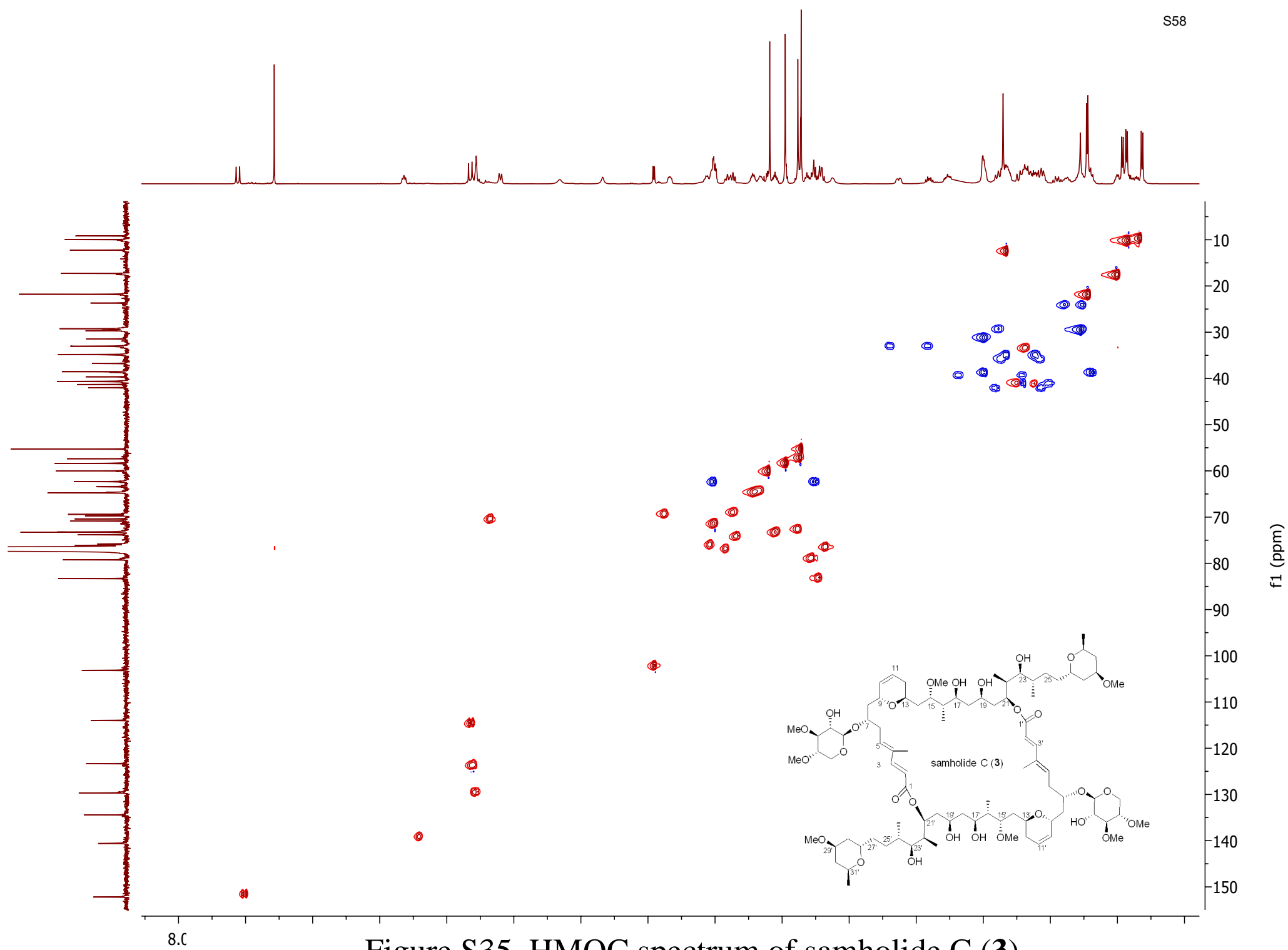


Figure S34 HMBC spectrum of samholide C (3)



8.0

Figure S35 HMBC spectrum of samholide C (3)

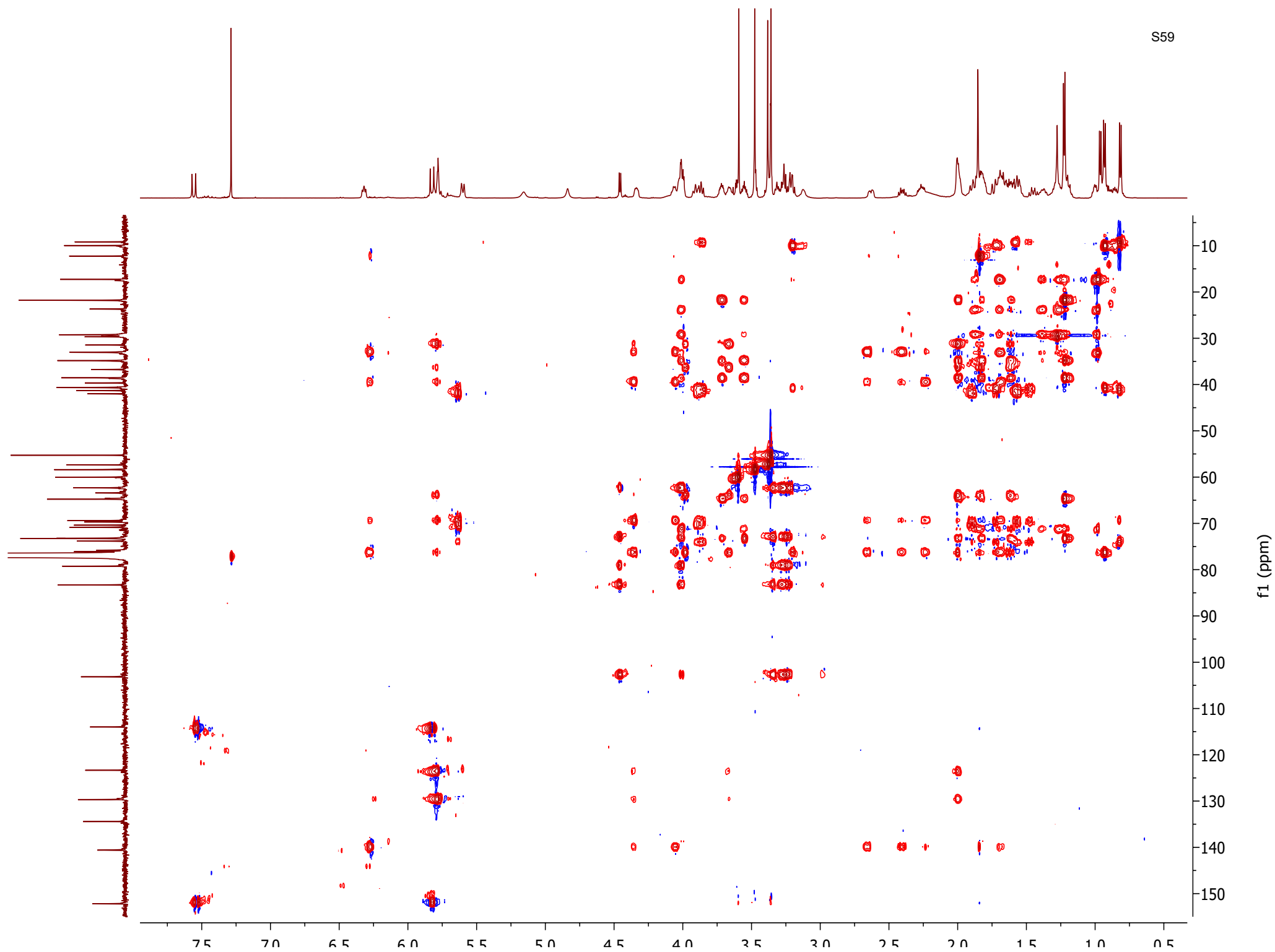


Figure S36 HSQC-TOCSY spectrum of samholide C (3)

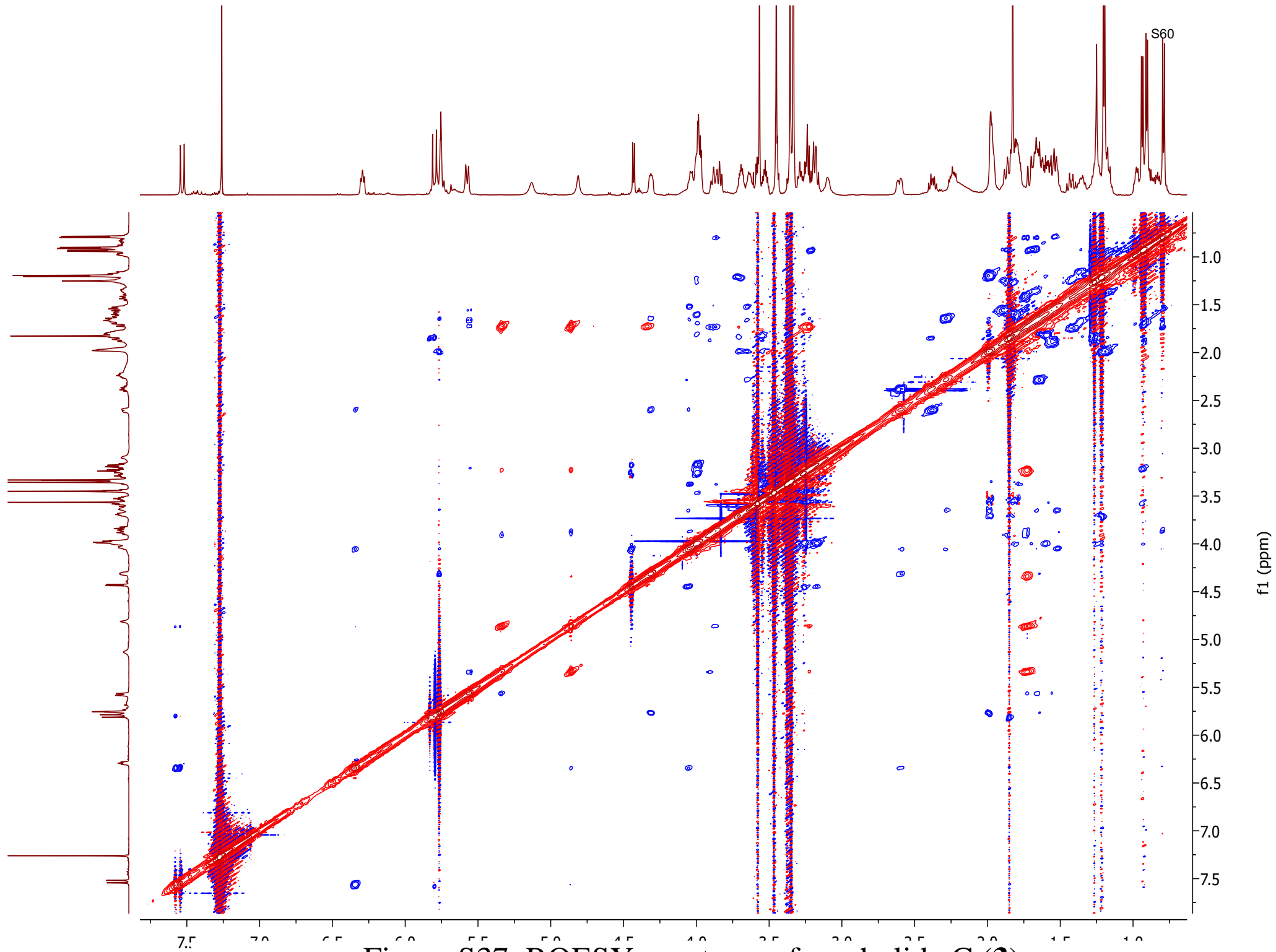


Figure S37 ROESY spectrum of samholide C (3)

2226H3D2B-a #20-22 RT: 0.48-0.53 AV: 3 SB: 6 0.07-0.19 NL: 2.71E8
T: + c Full ms [200.00-2000.00]

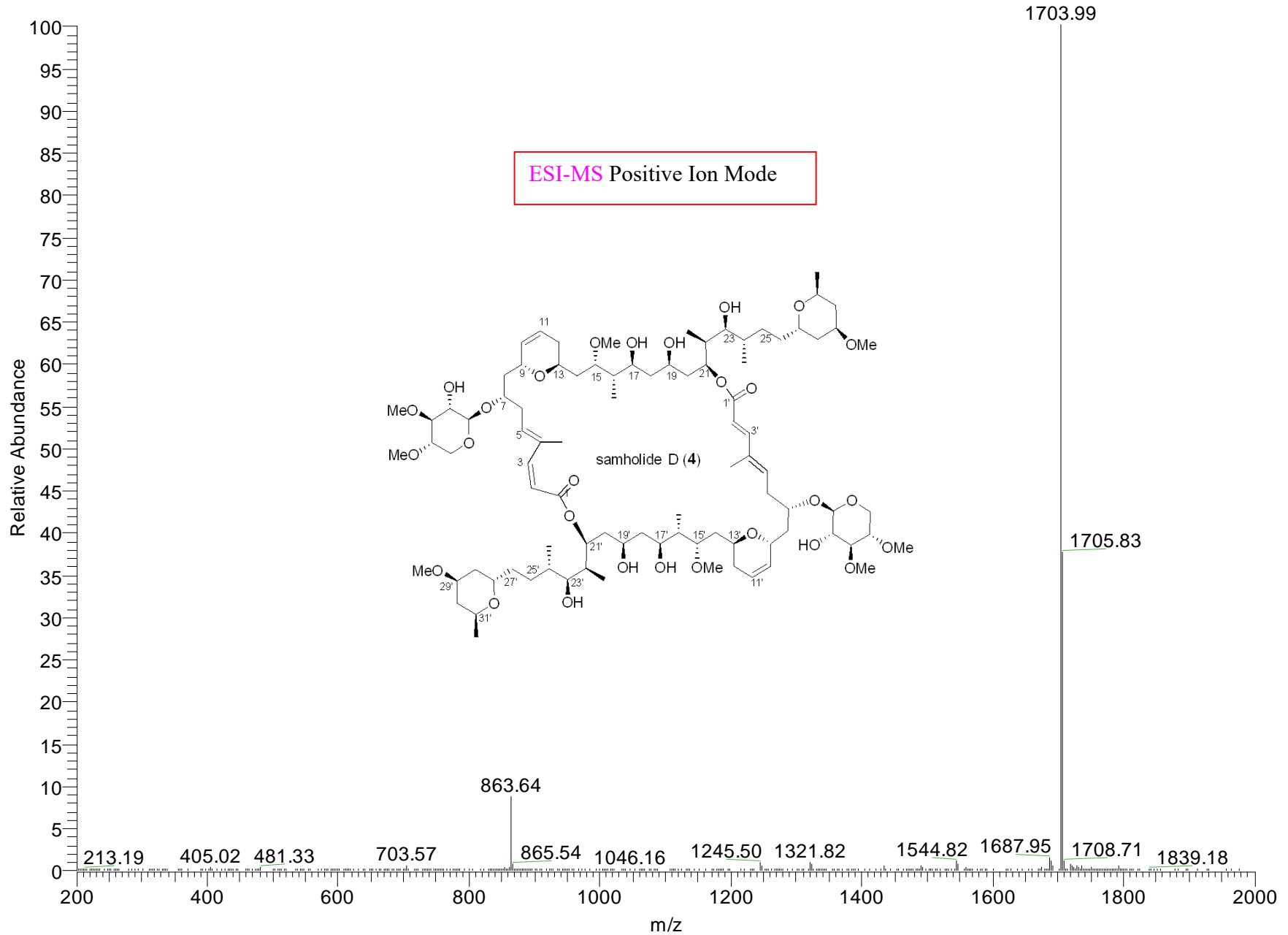


Figure S38 The ESI MS spectrum of samholide D (4)

2226H3D2B-a #24-33 RT: 0.58-0.72 AV: 10 NL: 3.76E7
F: + c Full ms2 1704.00@35.00 [490.00-2000.00]

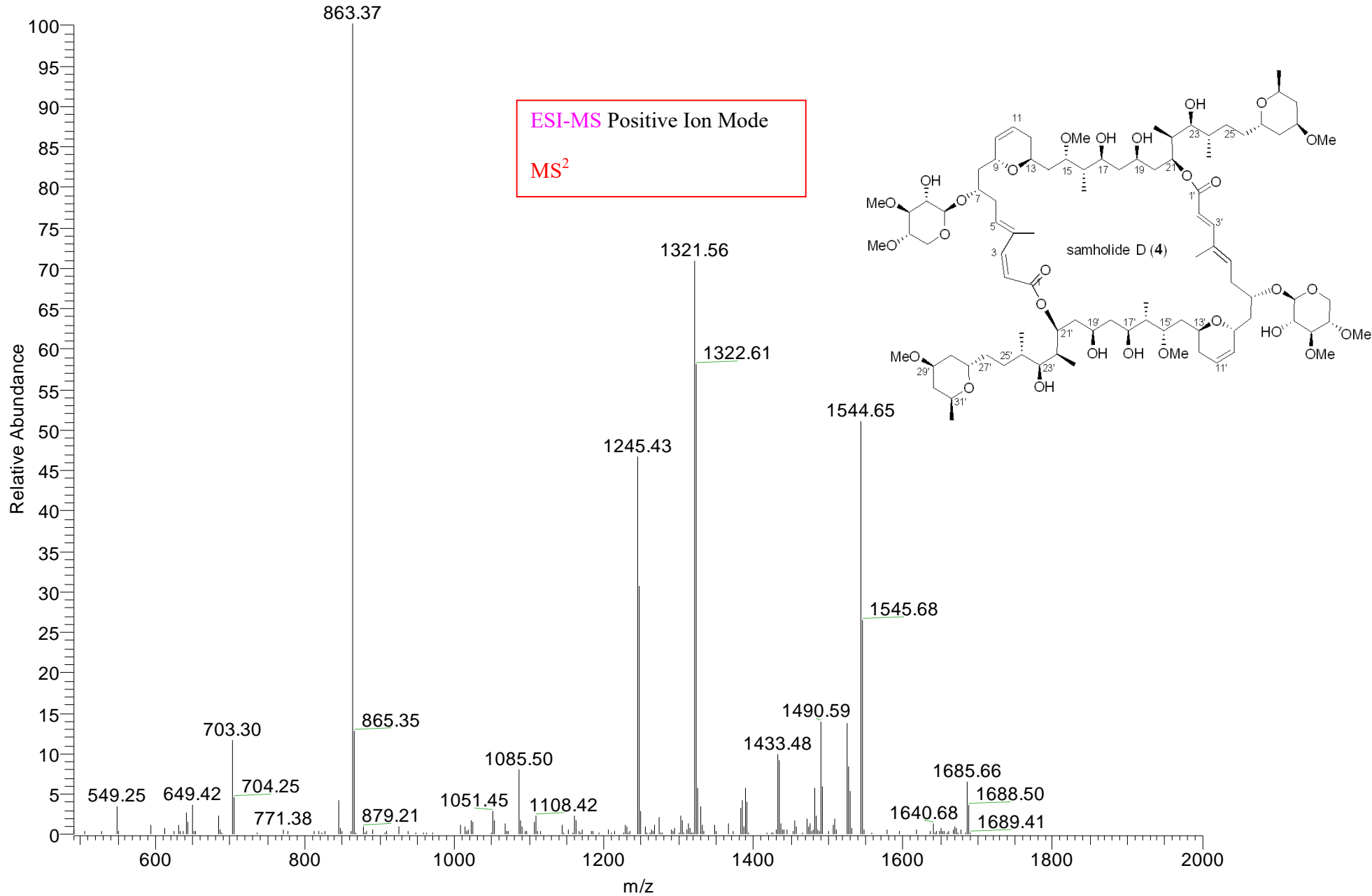


Figure S39 The ESI MS² spectrum of samholide D (4)

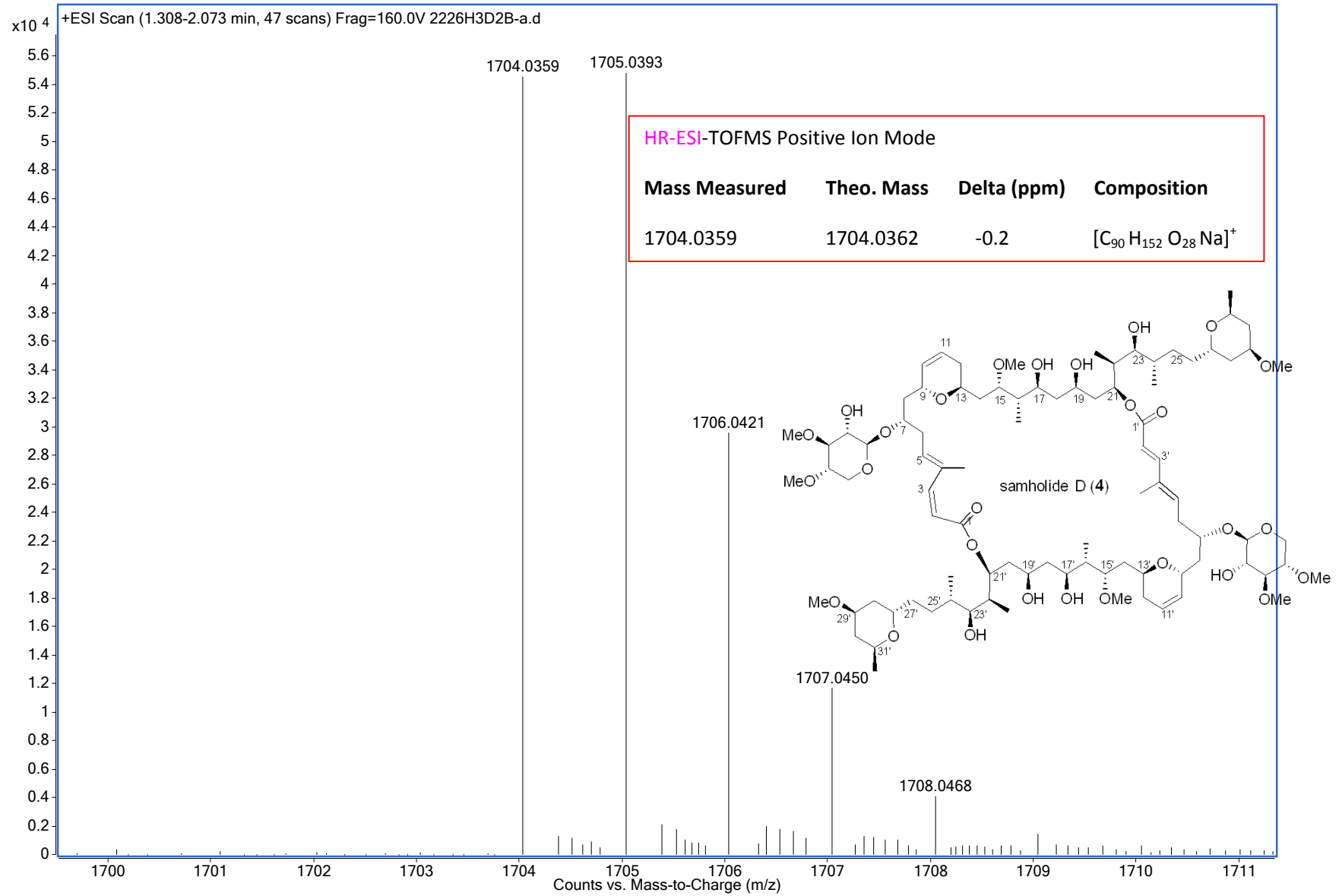
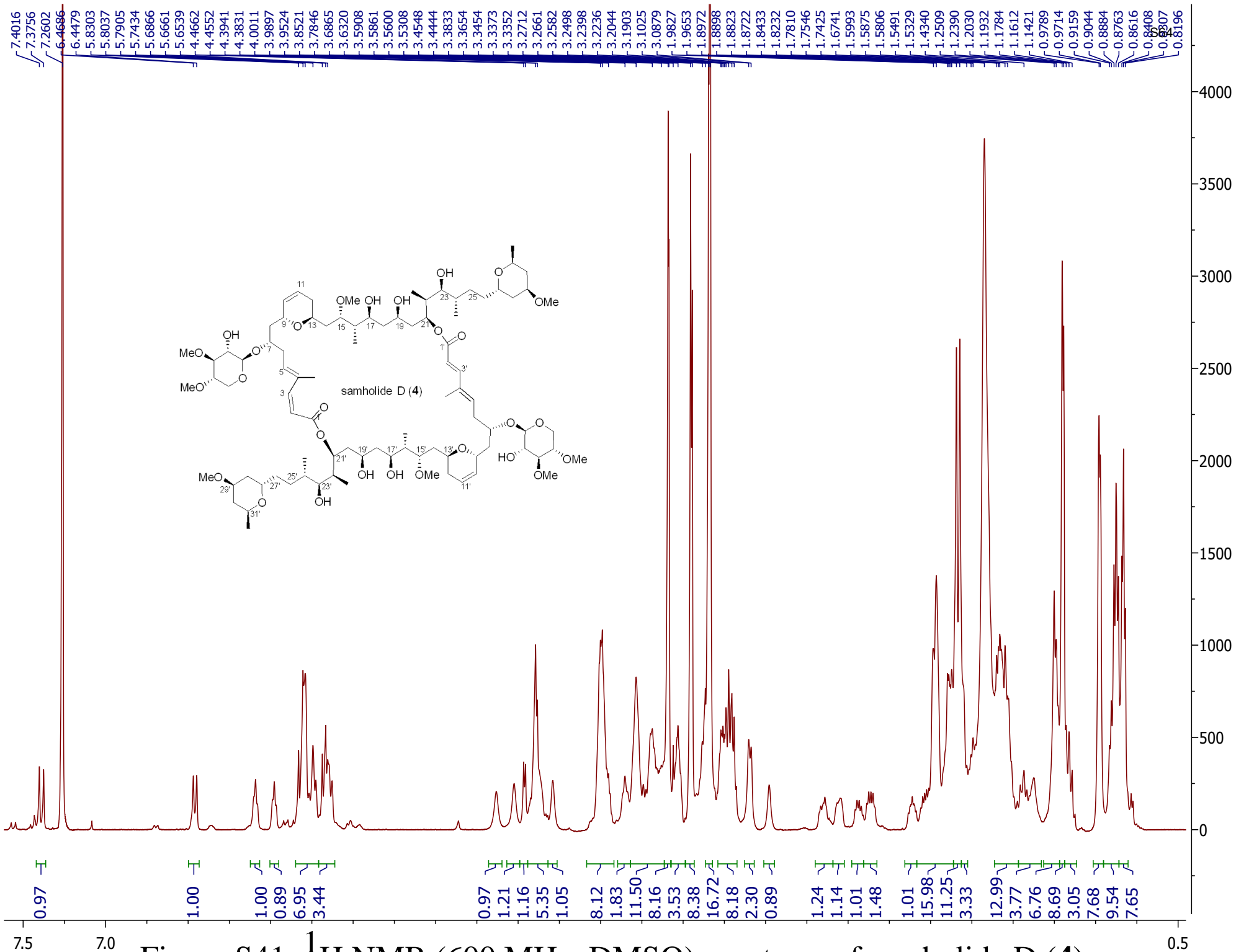


Figure S40 The positive HRESIMS spectrum of samholide D (4)



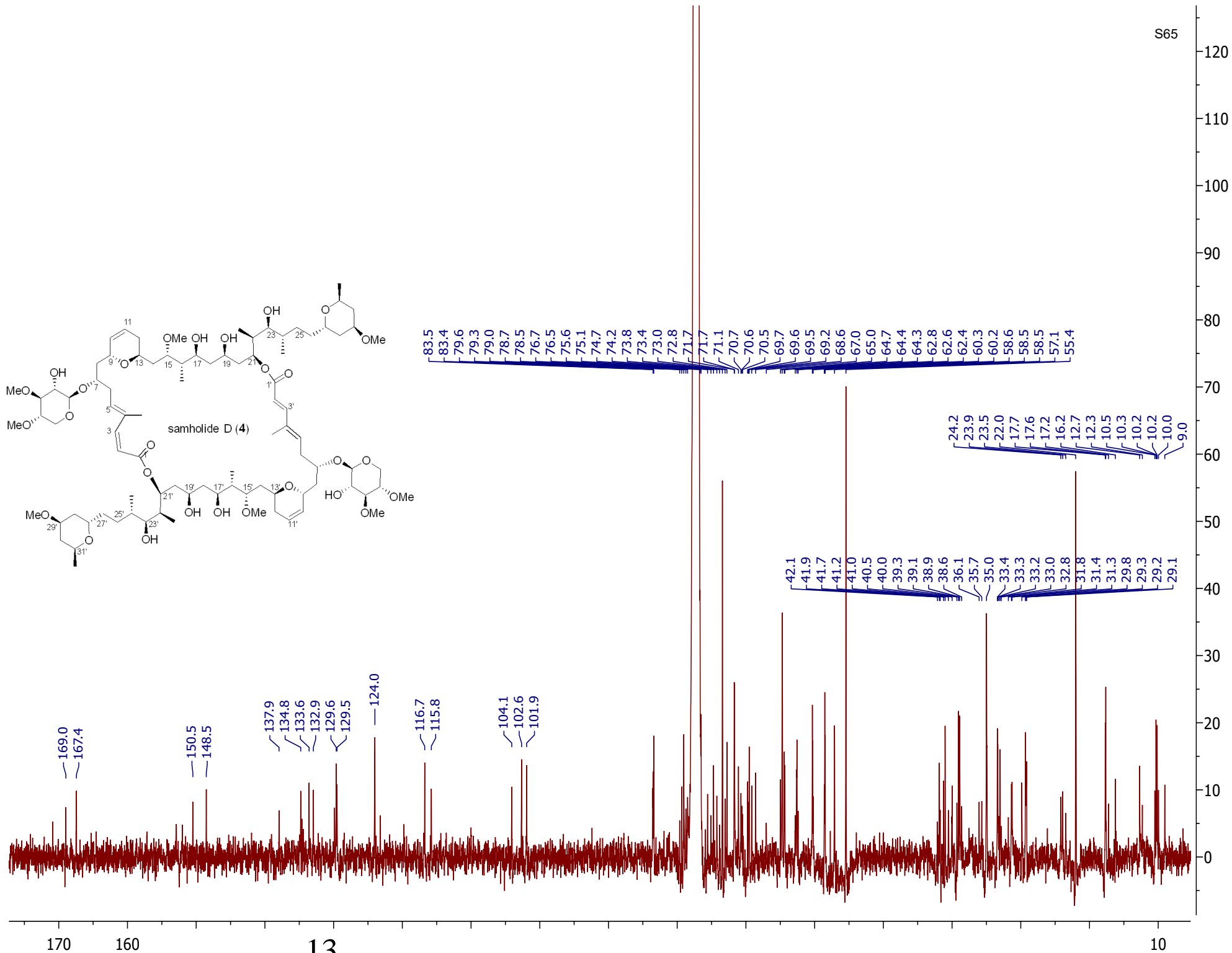


Figure S42 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide D (4)

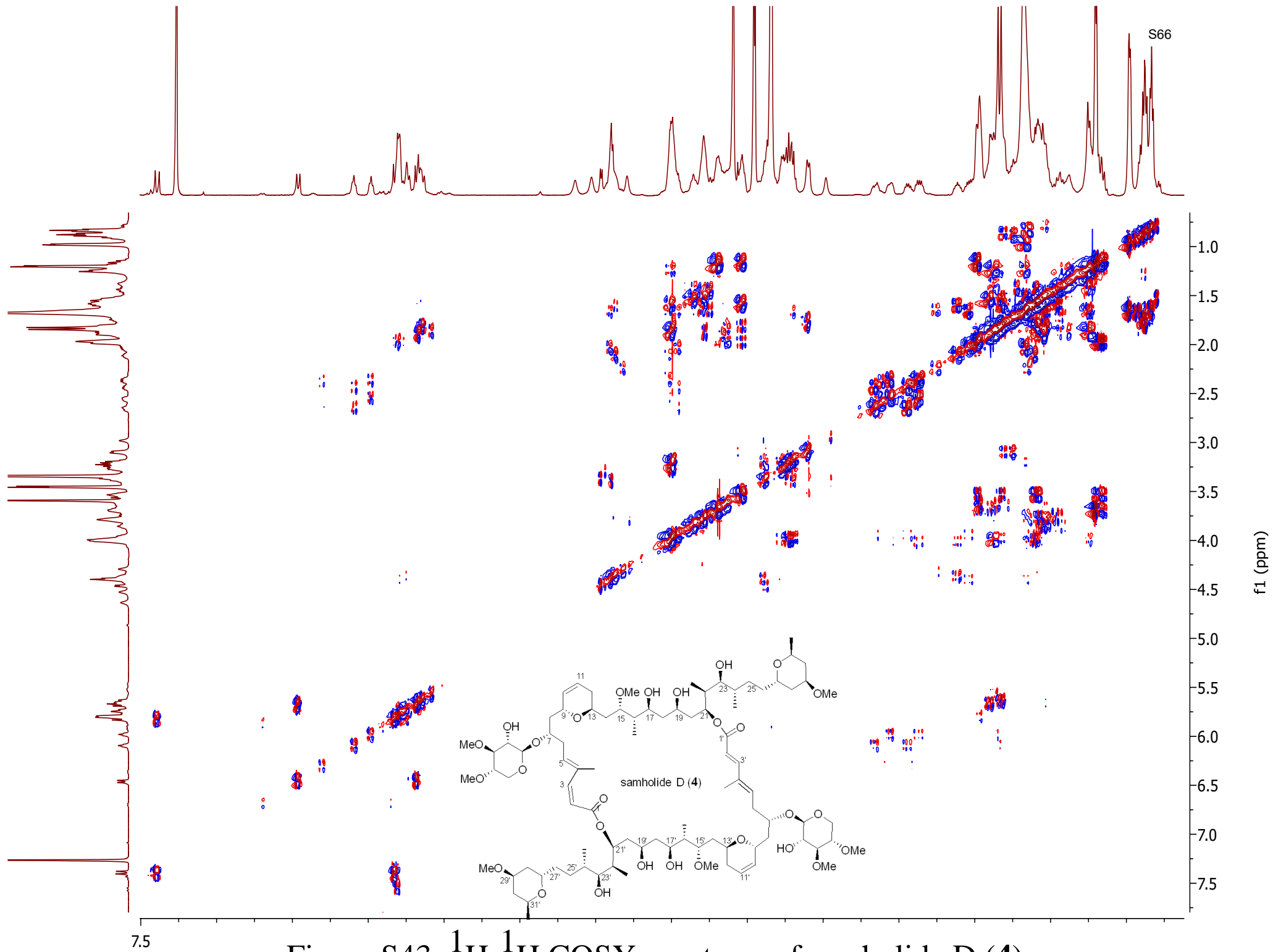


Figure S43 ^1H - ^1H COSY spectrum of samholide D (**4**)

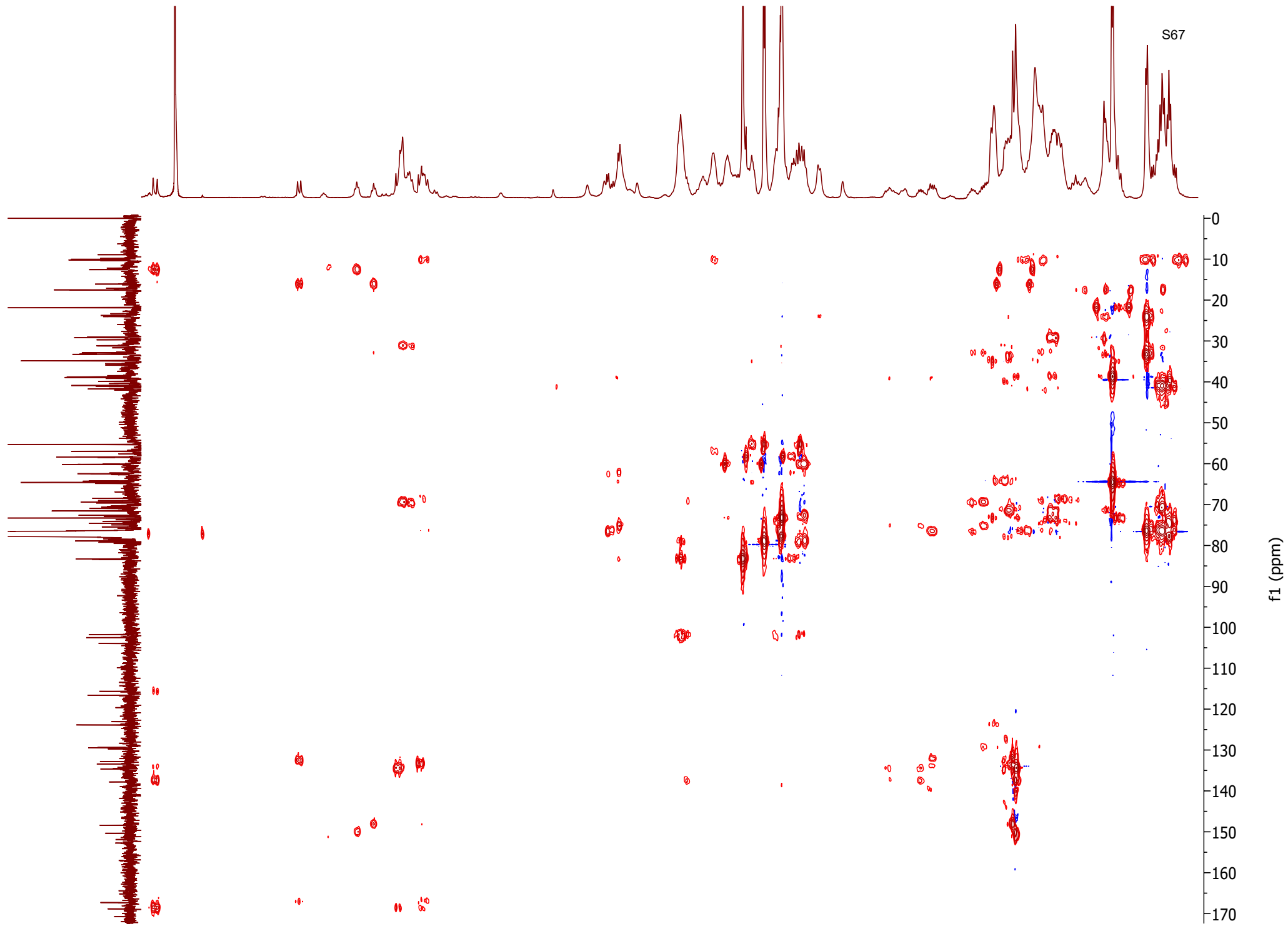


Figure S44 HMBC spectrum of samholide D (4)

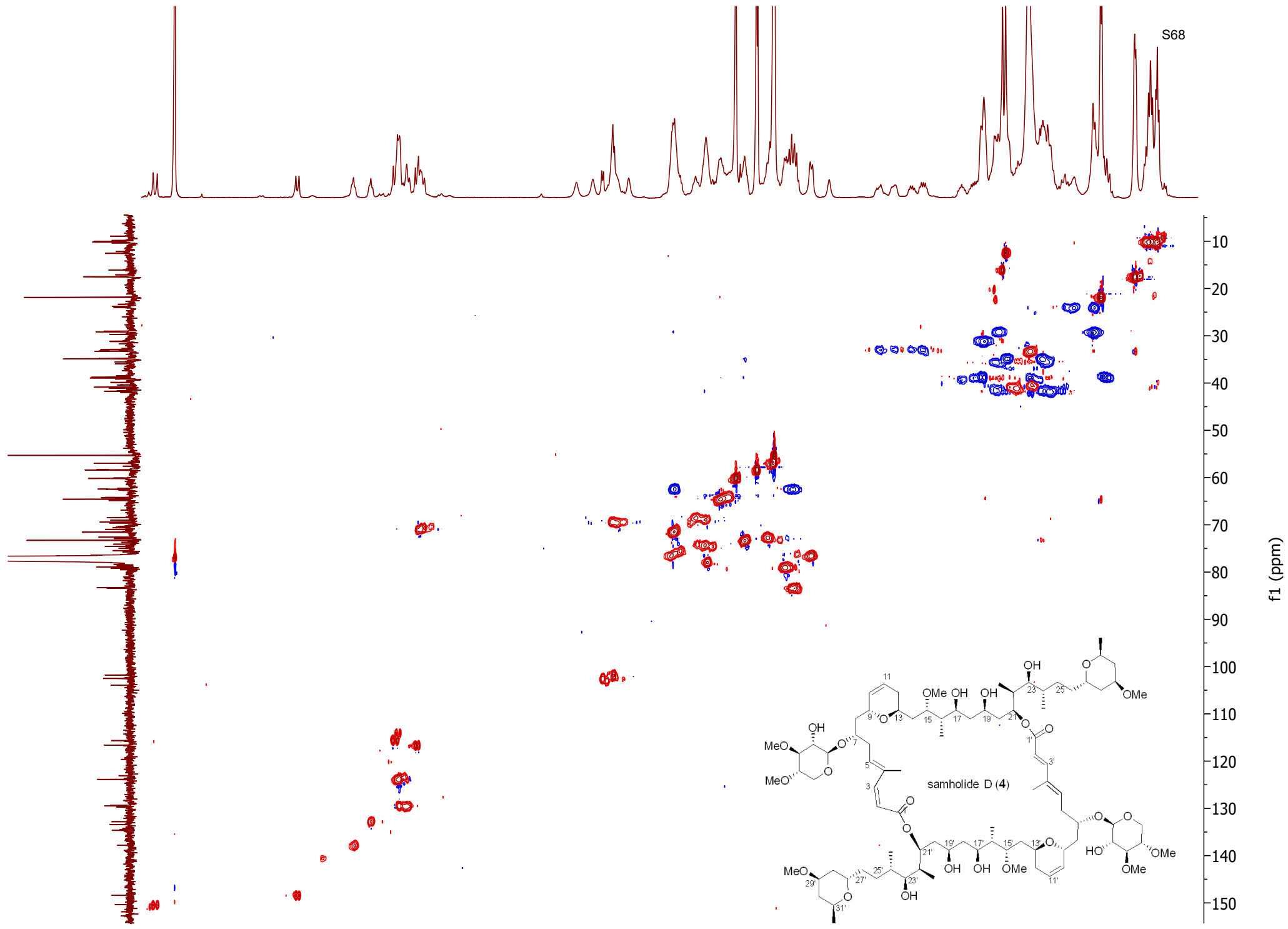
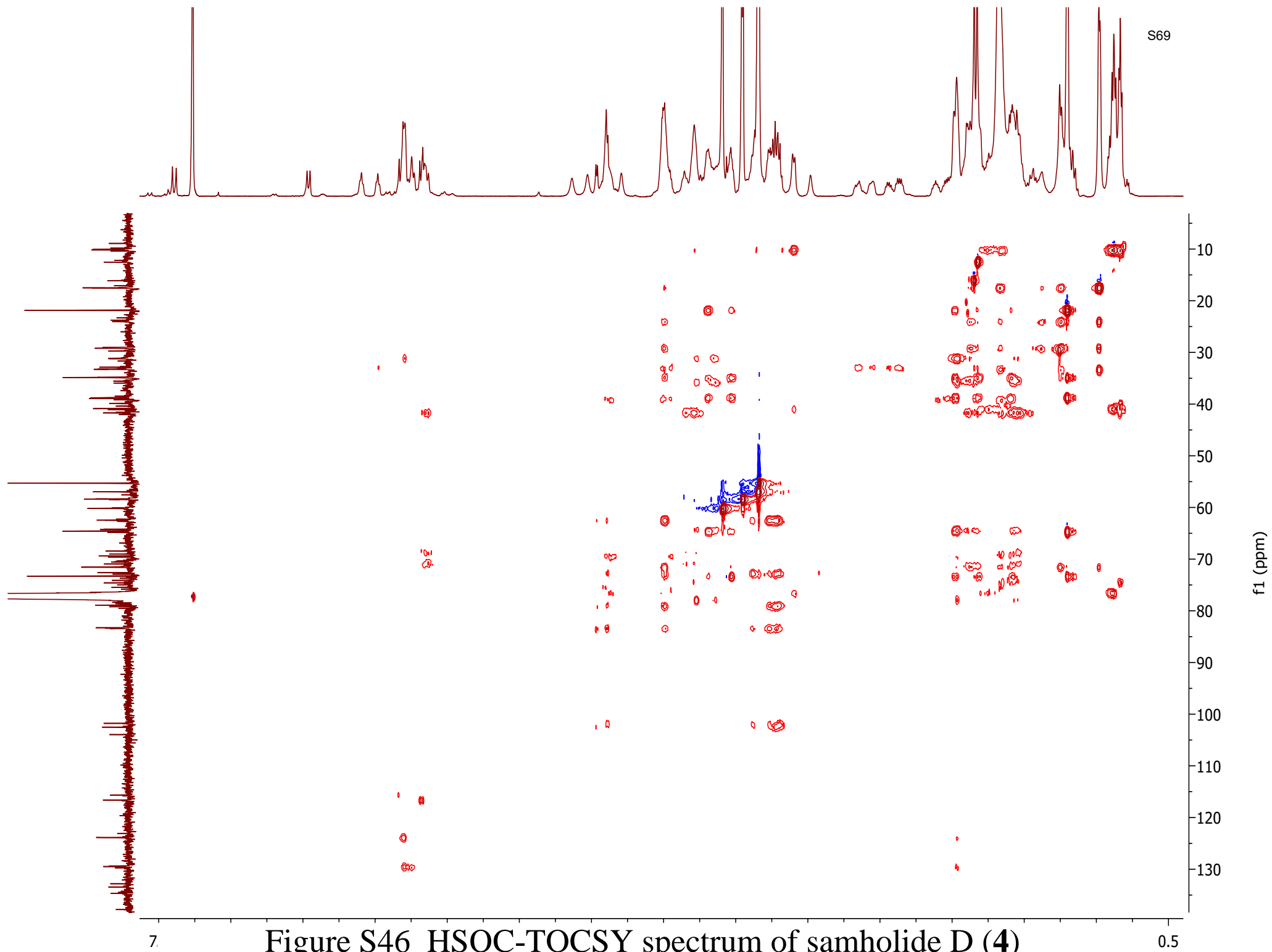


Figure S45 HMQC spectrum of samholide D (4)



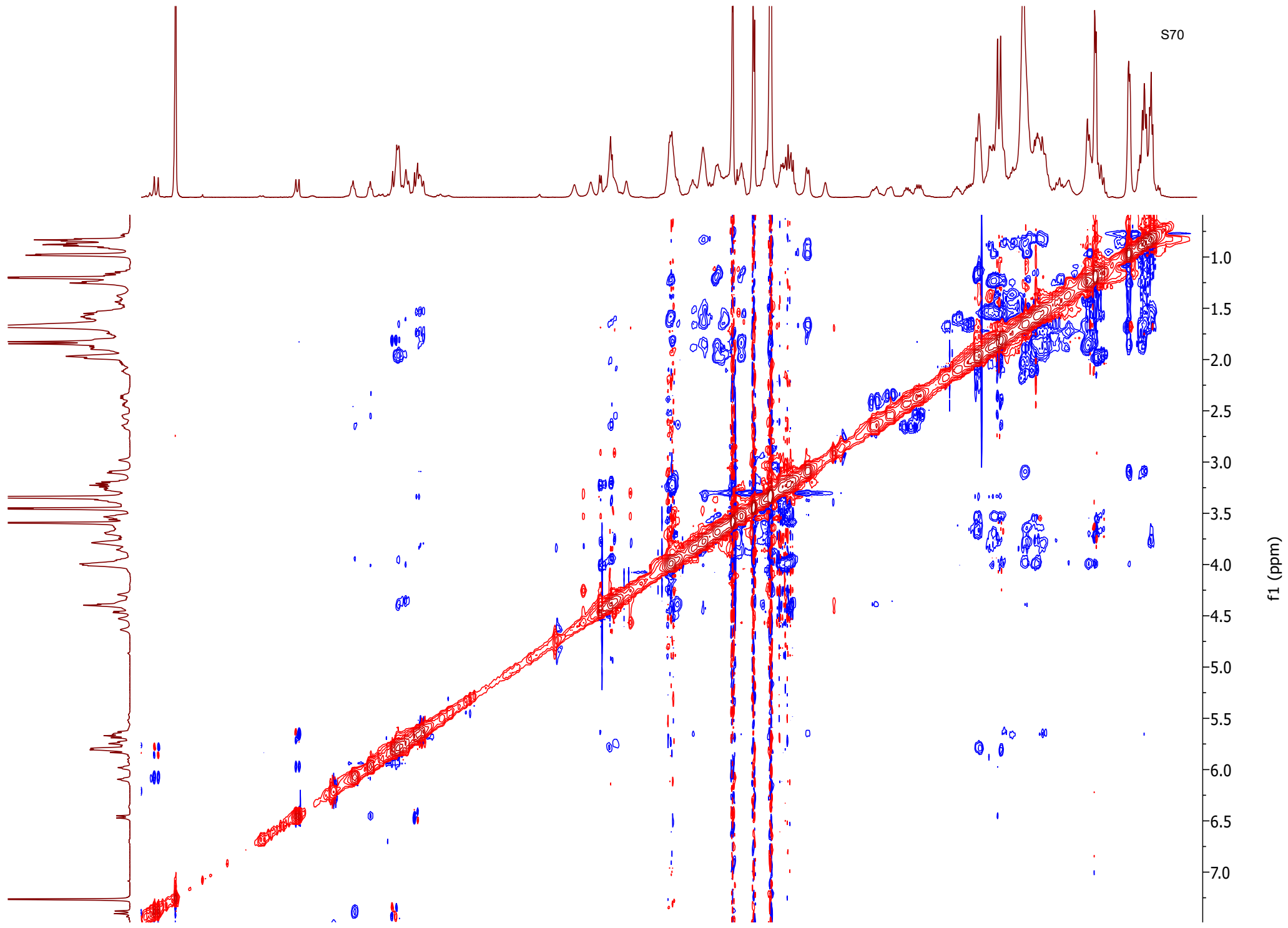


Figure S47 ROESY spectrum of samholide D (4)

E4-a #68-77 RT: 1.79-2.01 AV: 10 SB: 4 1.41-1.49 NL: 7.68E6
T: + c Full ms [300.00-2000.00]

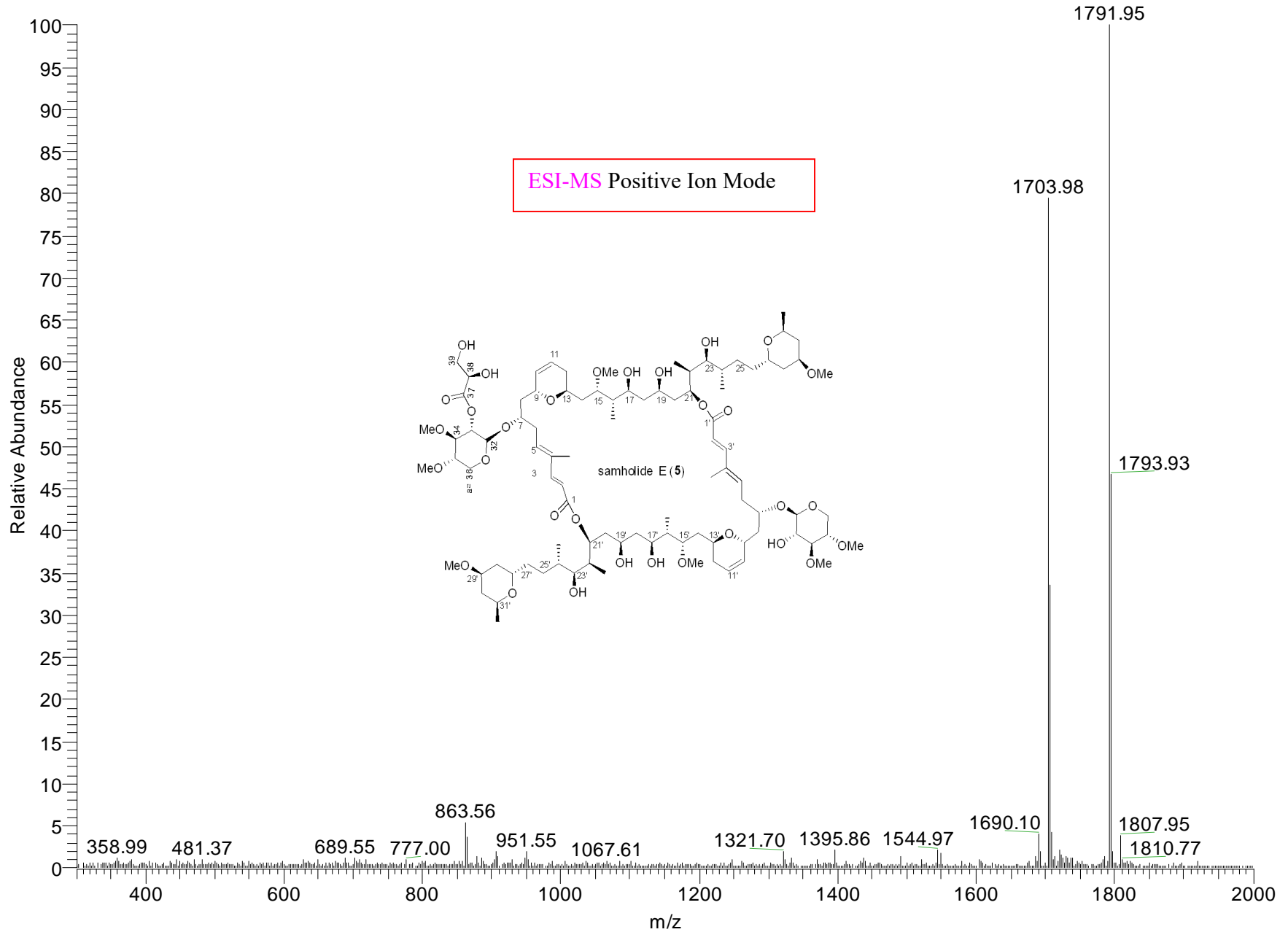


Figure S48 The ESI MS spectrum of samholide E (5)

E4-a #89-97 RT: 2.27-2.40 AV: 9 SB: 6 2.13-2.23 NL: 3.31E6
T: +c Full ms2 1792.00@35.00 [490.00-2000.00]

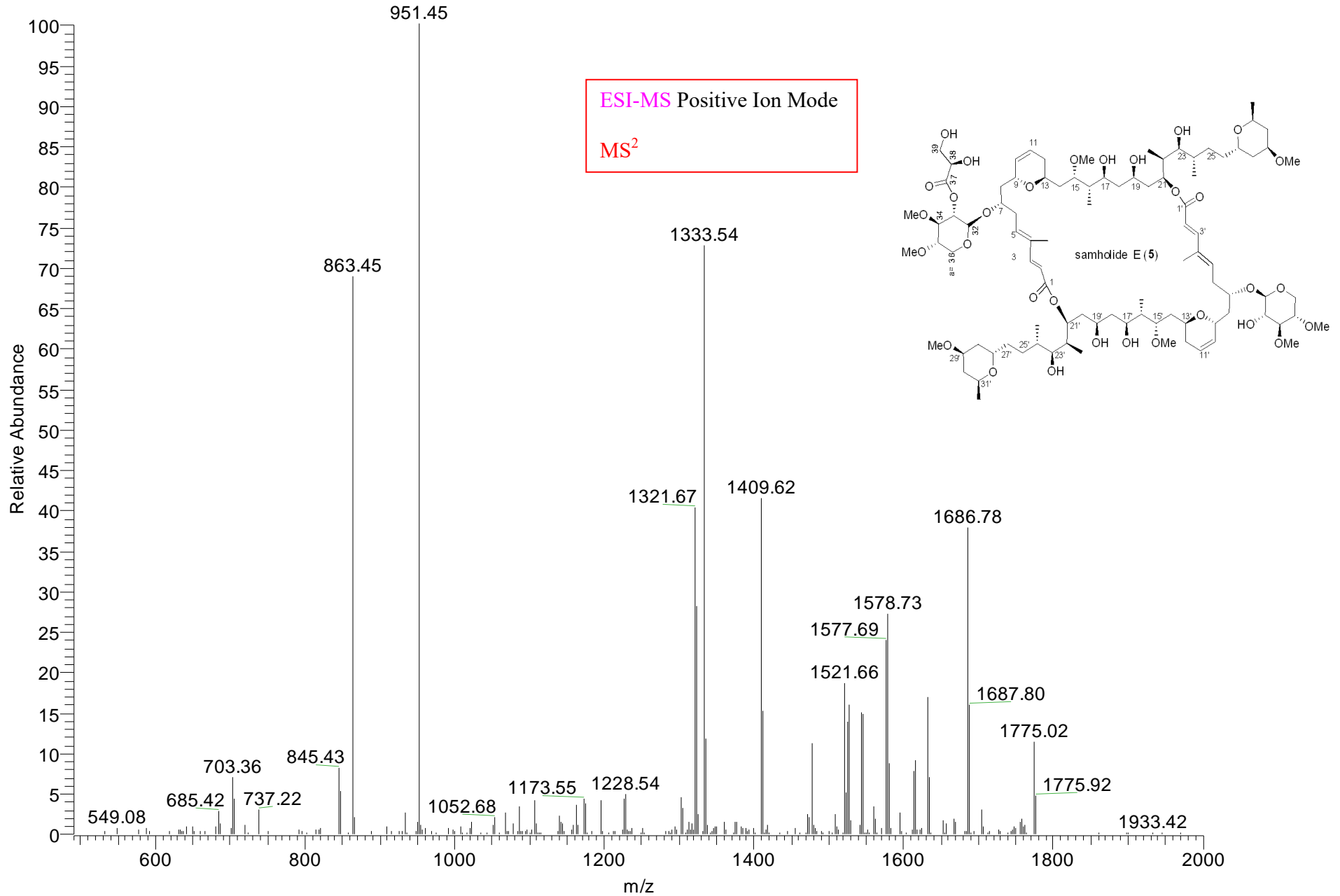


Figure S49 The ESI MS² spectrum of samholide E (5)

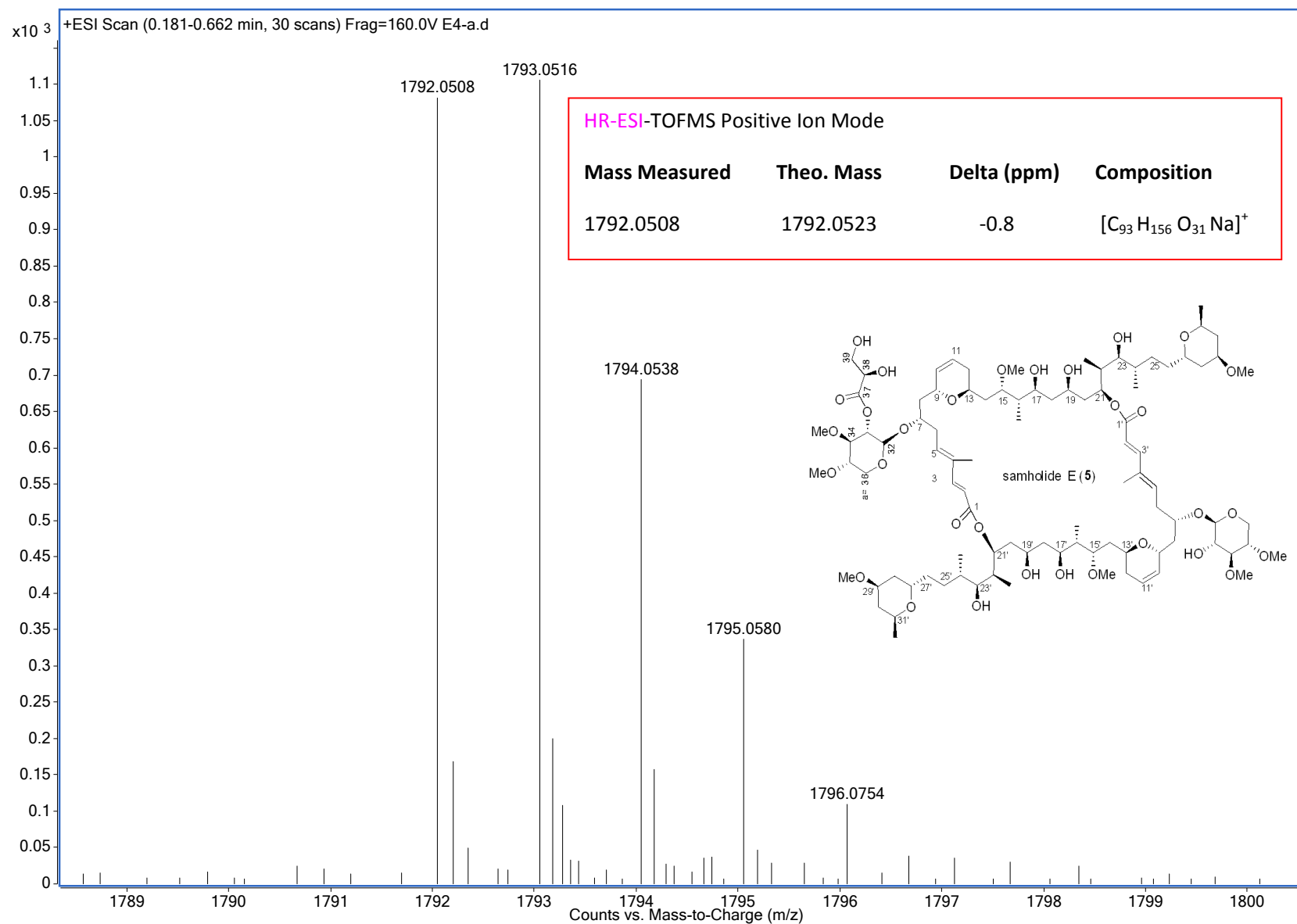
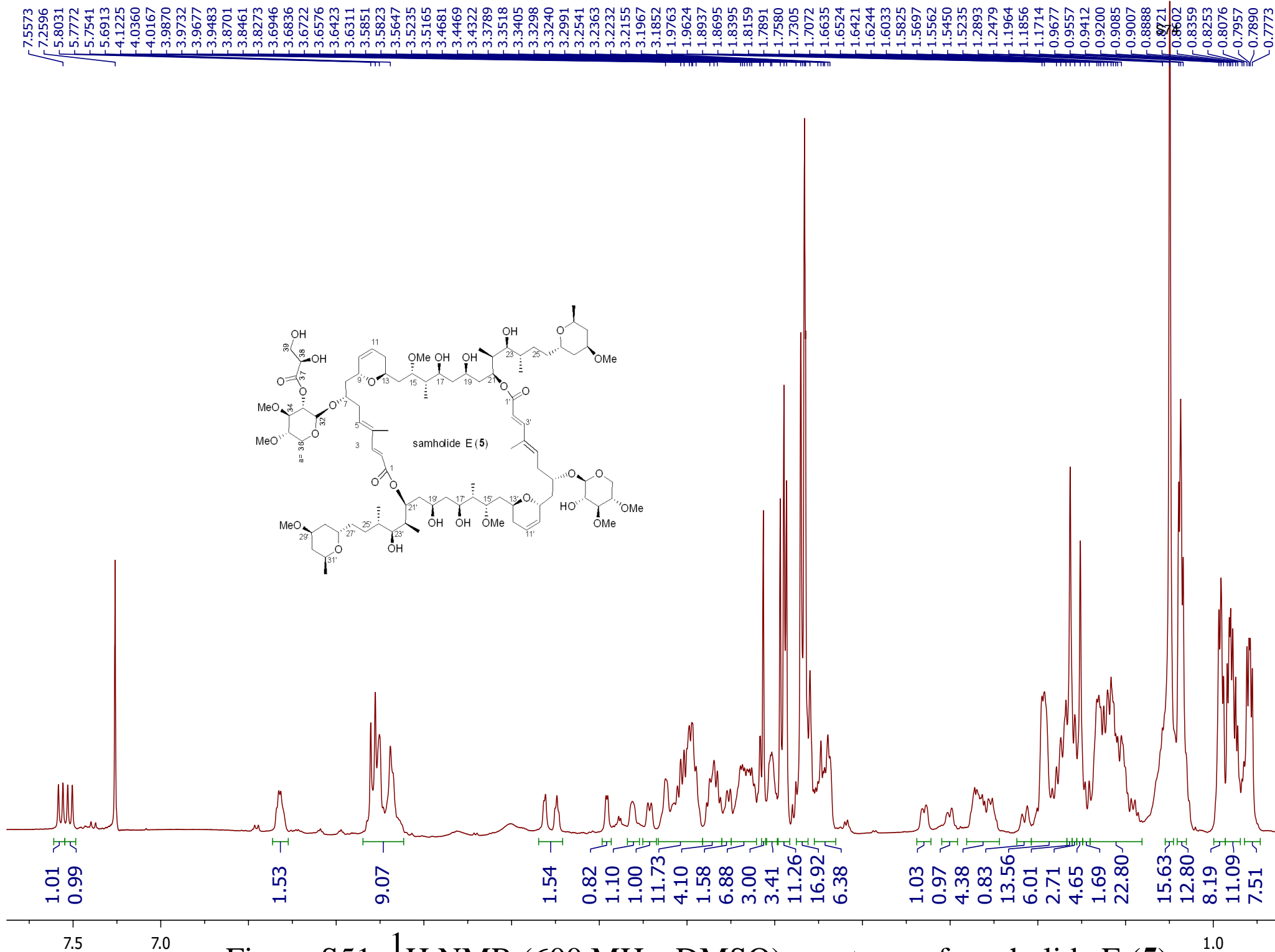
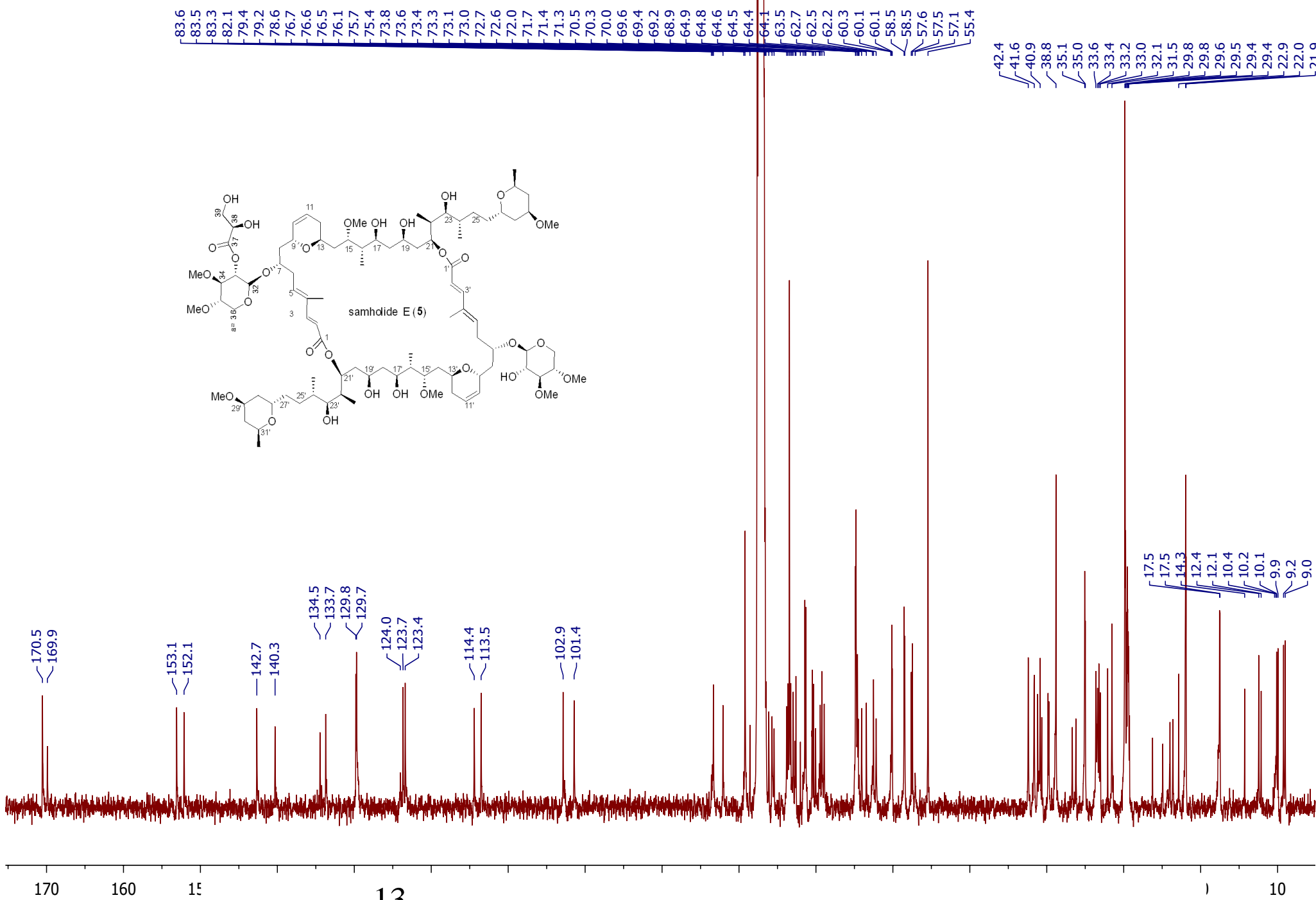


Figure S50 The positive HRESIMS spectrum of samholide E (5)





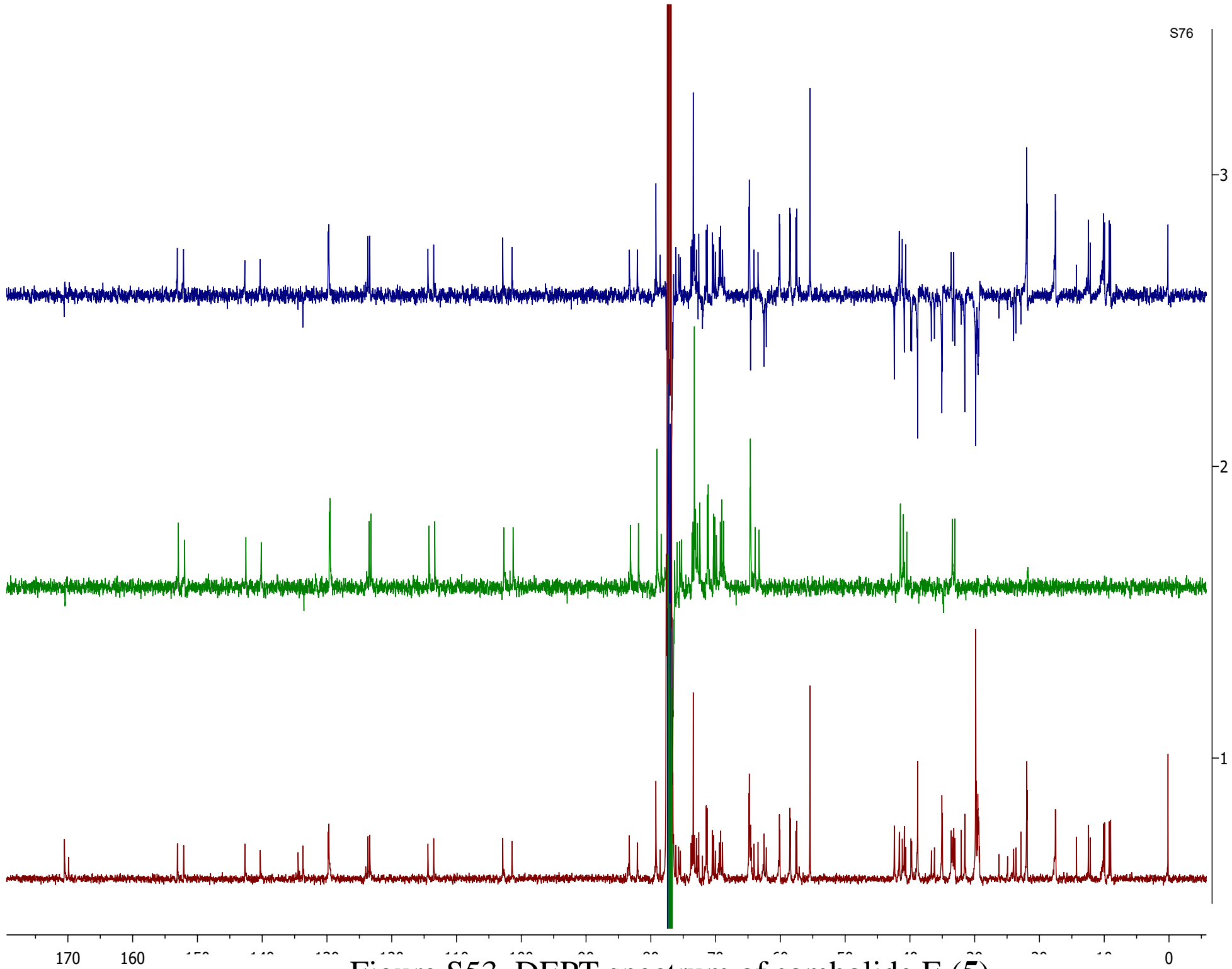


Figure S53 DEPT spectrum of samholide E (5)

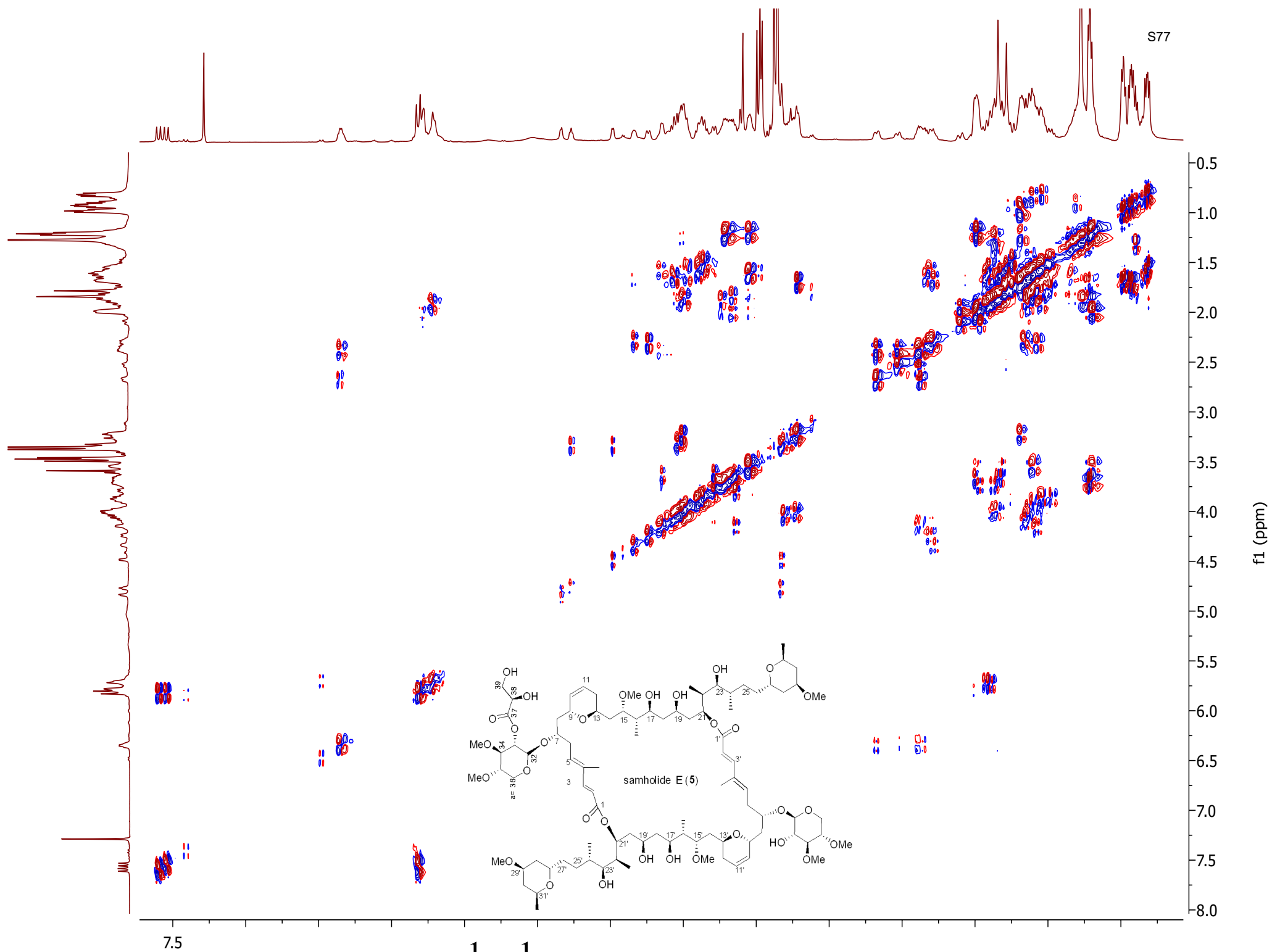


Figure S54 ^1H - ^1H COSY spectrum of samholide E (5)

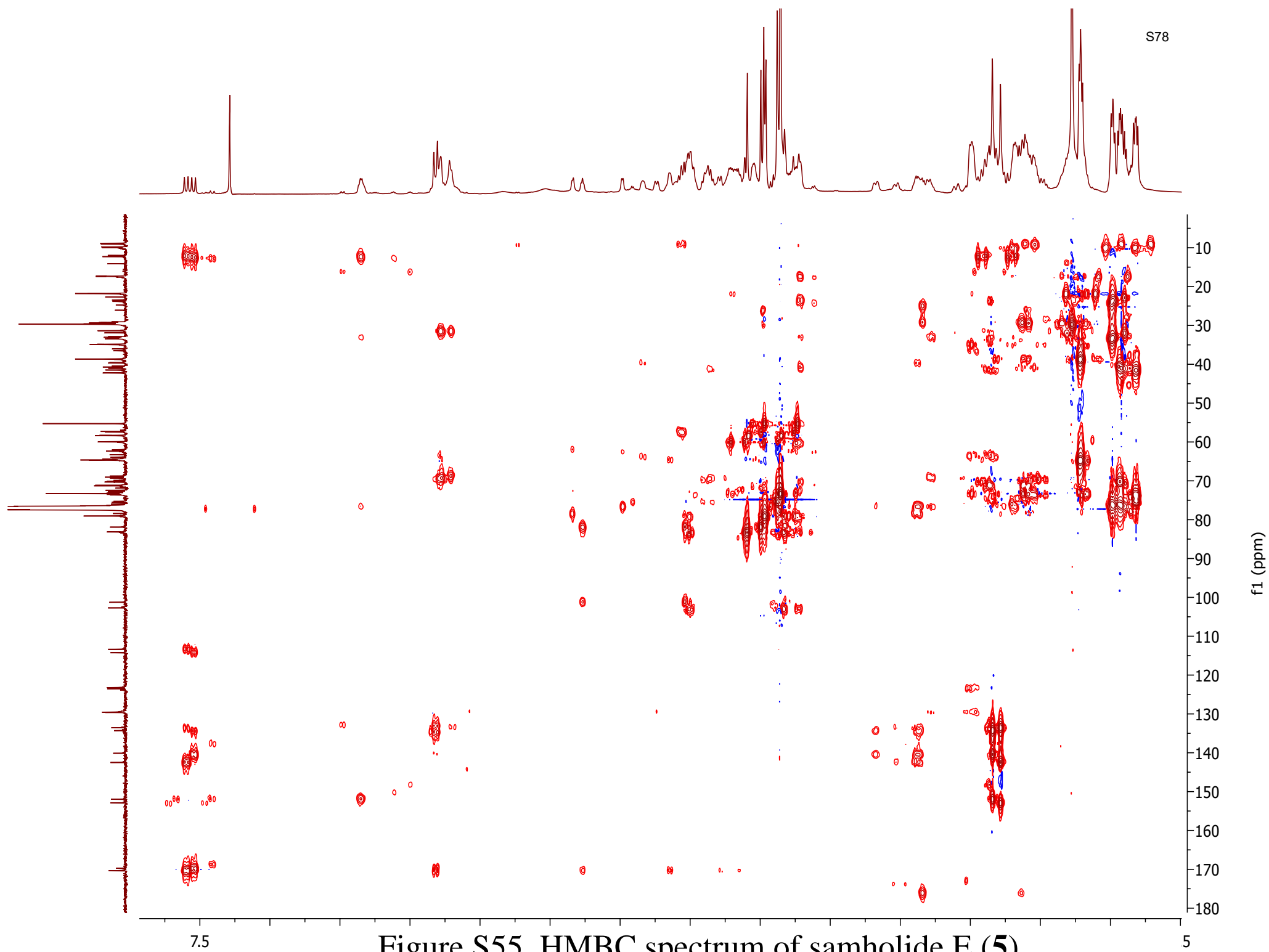


Figure S55 HMBC spectrum of samholide E (5)

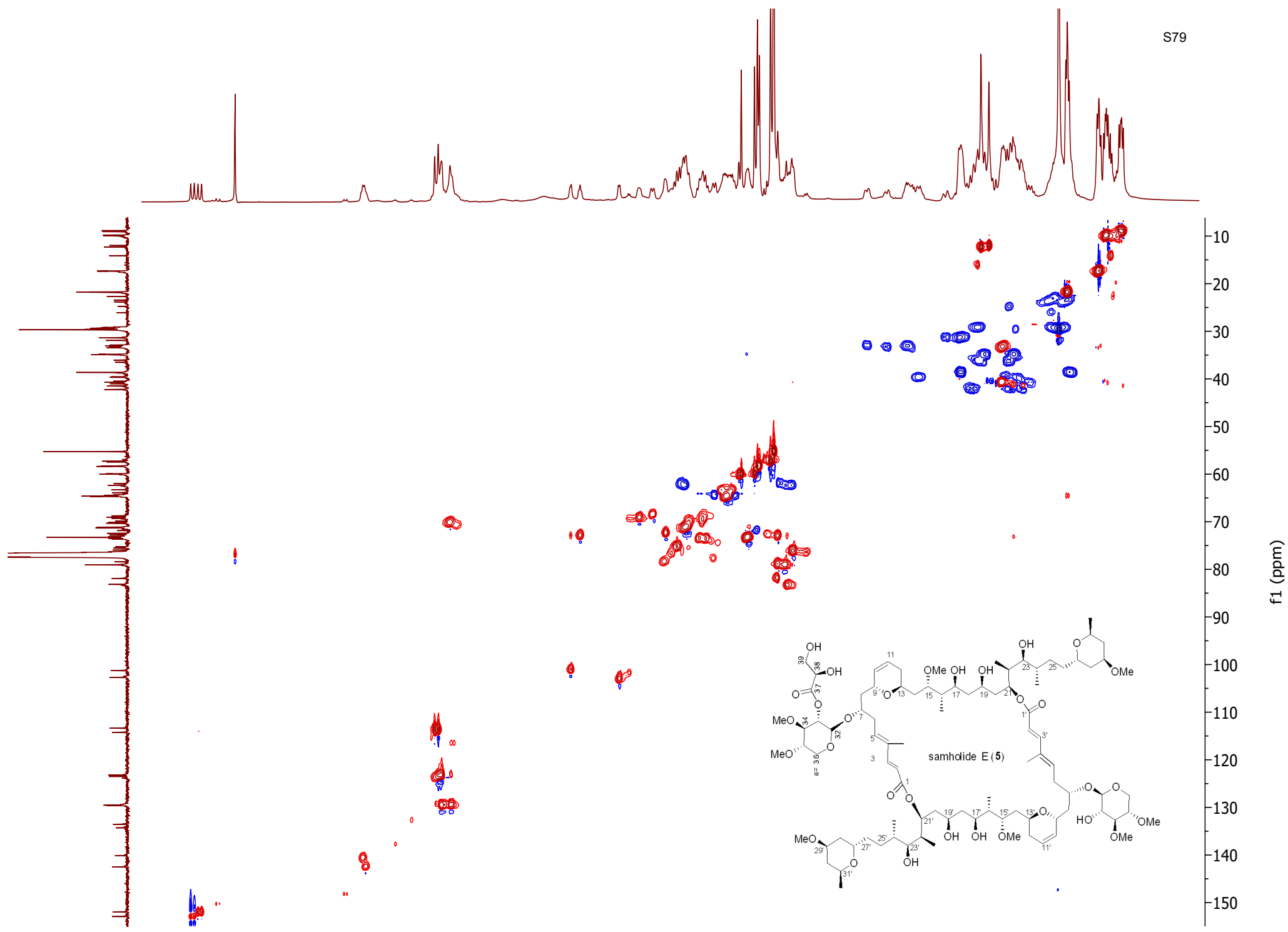


Figure S56 HMBC spectrum of samholide E (5)

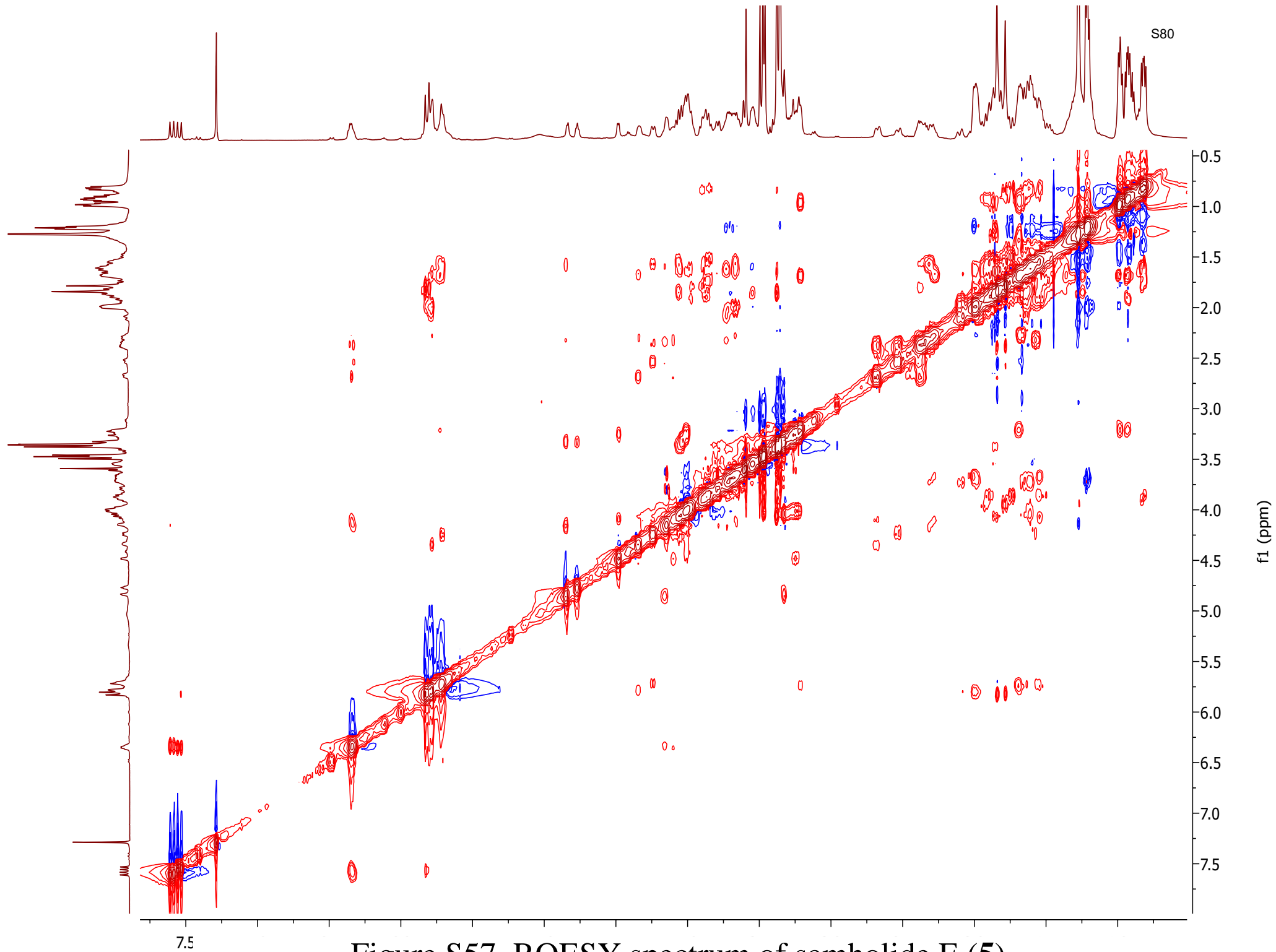


Figure S57 ROESY spectrum of samholide E (5)

2226H3C7A1-a #9-13 RT: 0.23-0.33 AV: 5 SB: 3 0.08-0.13 NL: 2.09E6
T: + c Full ms [200.00-2000.00]

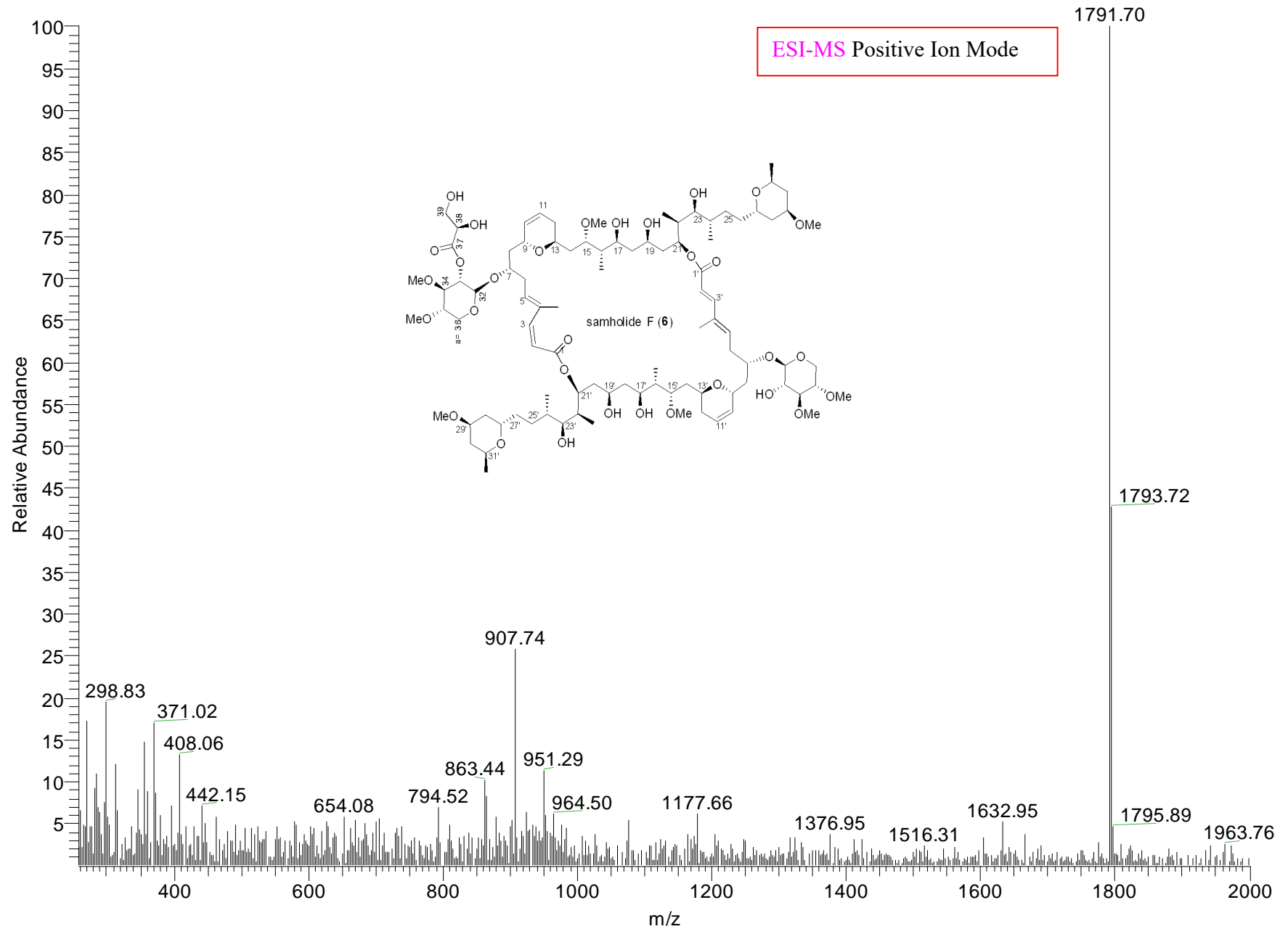


Figure S58 The ESI MS spectrum of samholide F (6)

2226H3C7A1-a #25-28 RT: 0.61-0.66 AV: 4 NL: 1.93E6
F: + c Full ms2 1792.00@35.00 [490.00-2000.00]

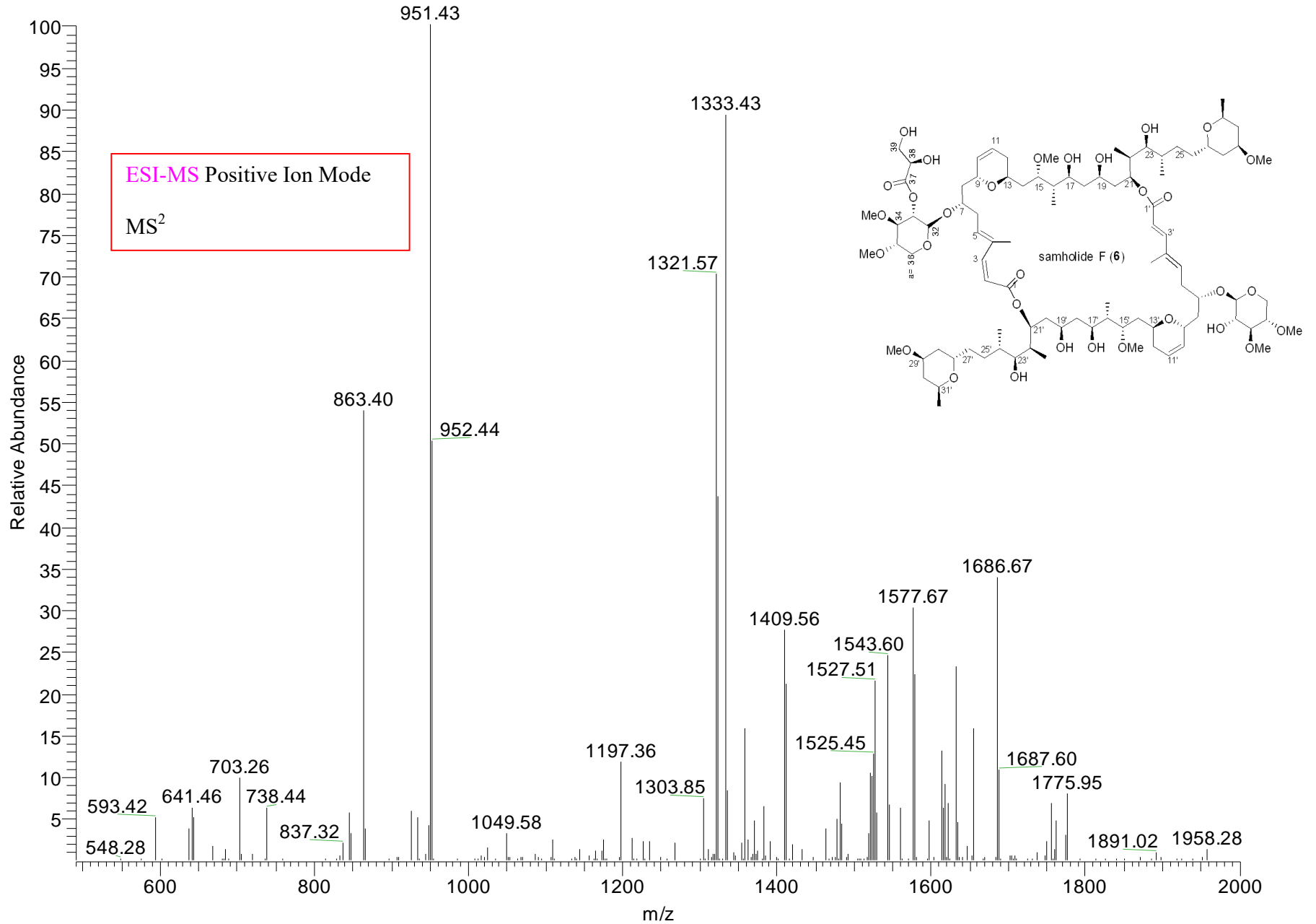


Figure S59 The ESI MS² spectrum of samholide F (6)

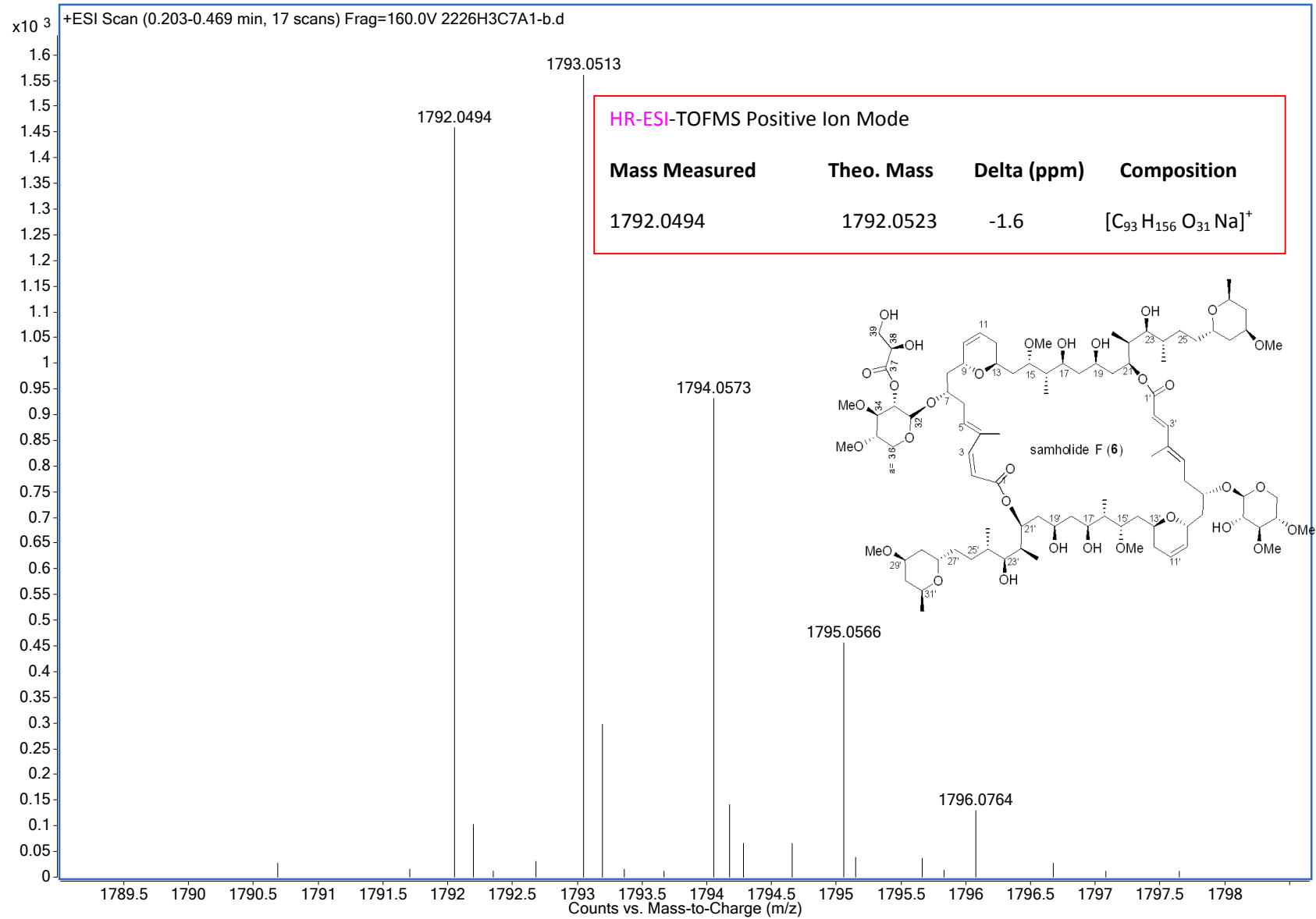
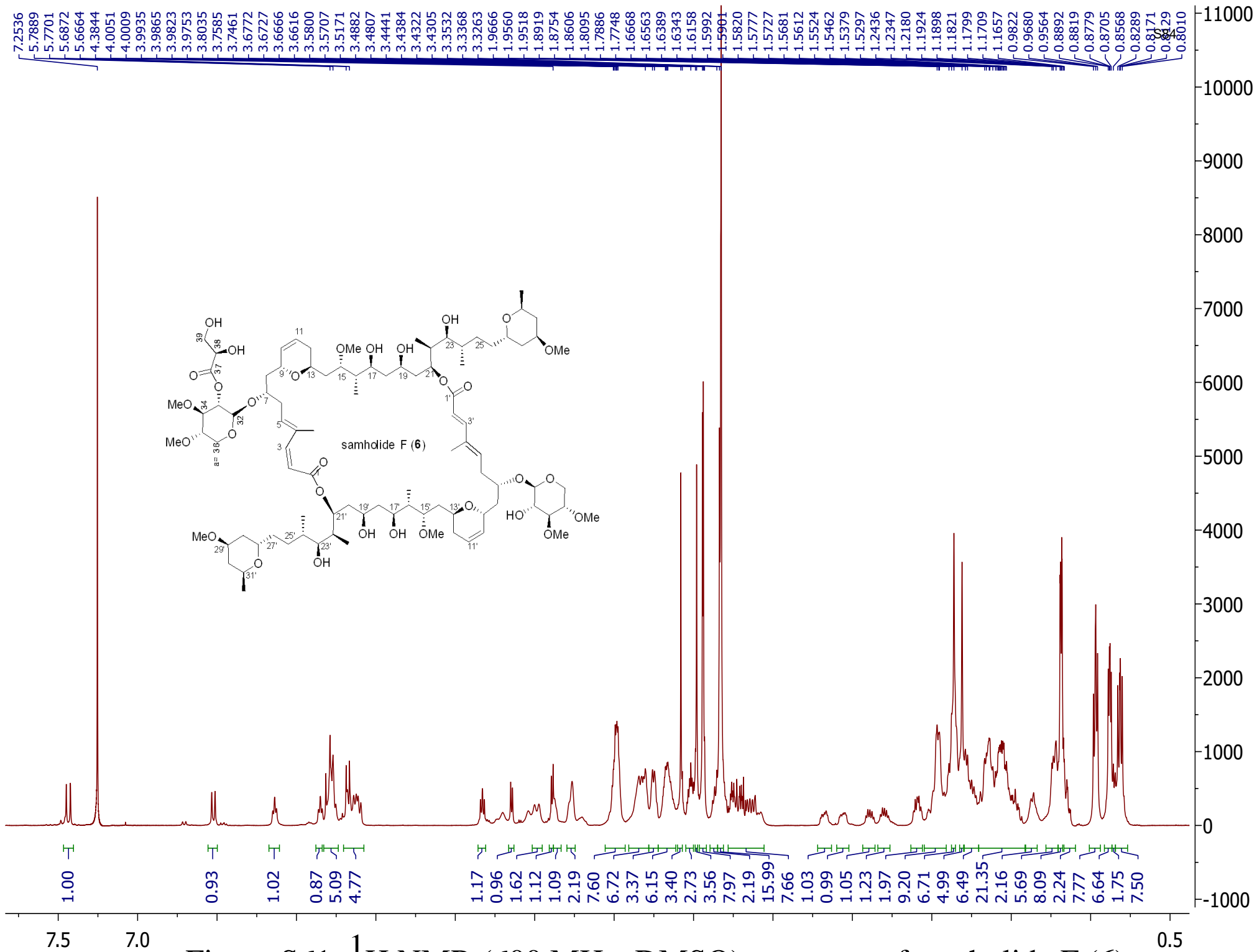
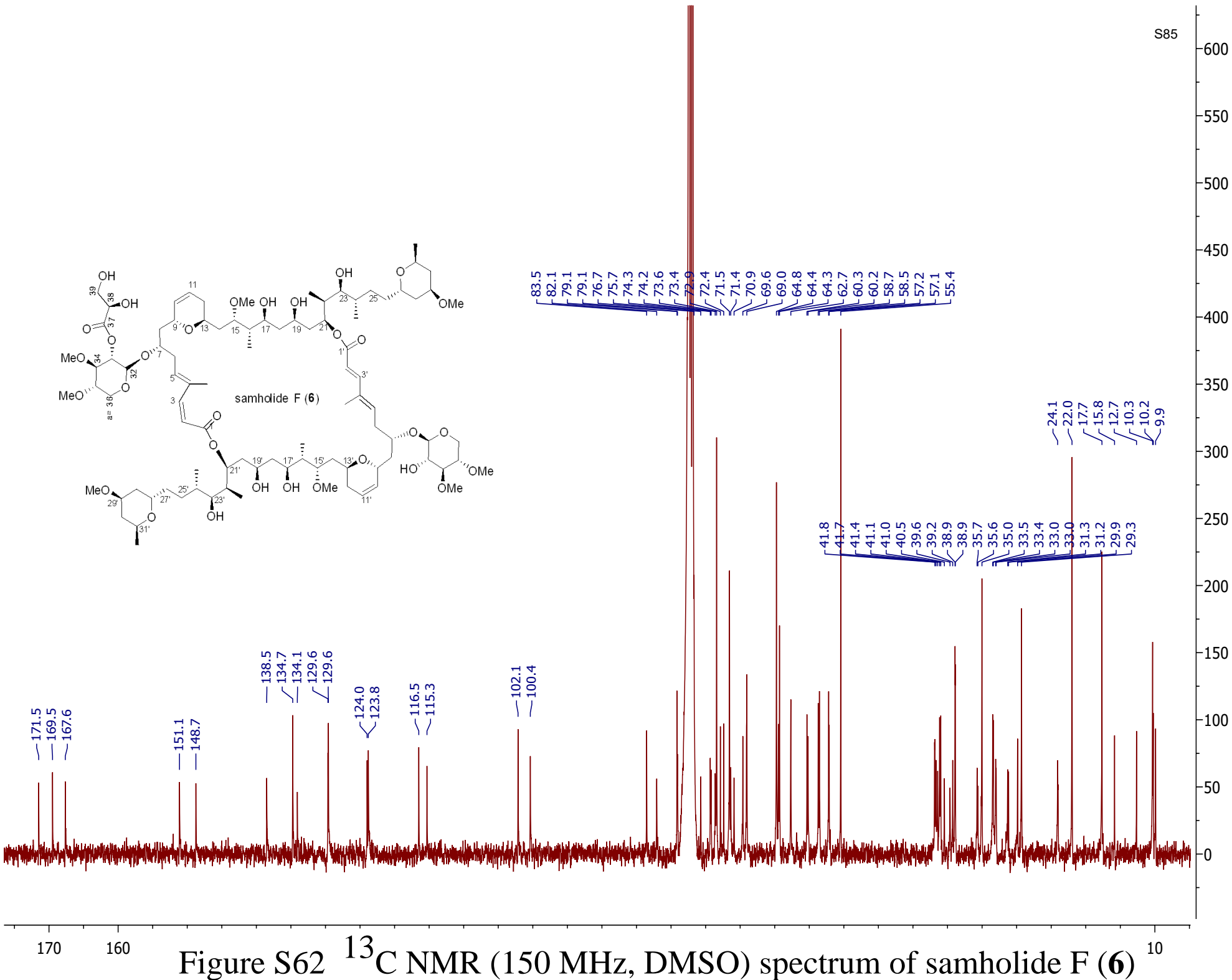


Figure S60 The positive HRESIMS spectrum of samholide F (6)





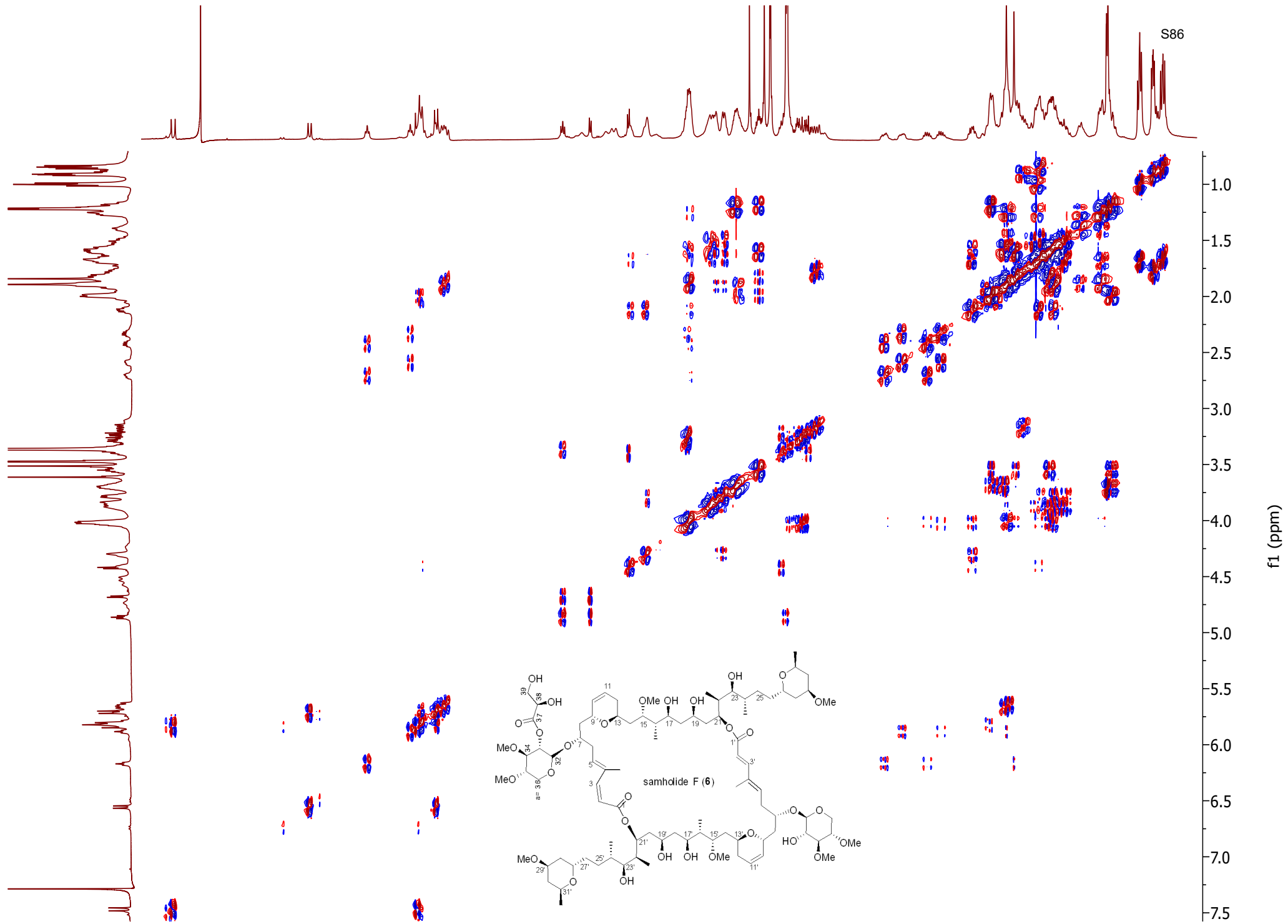
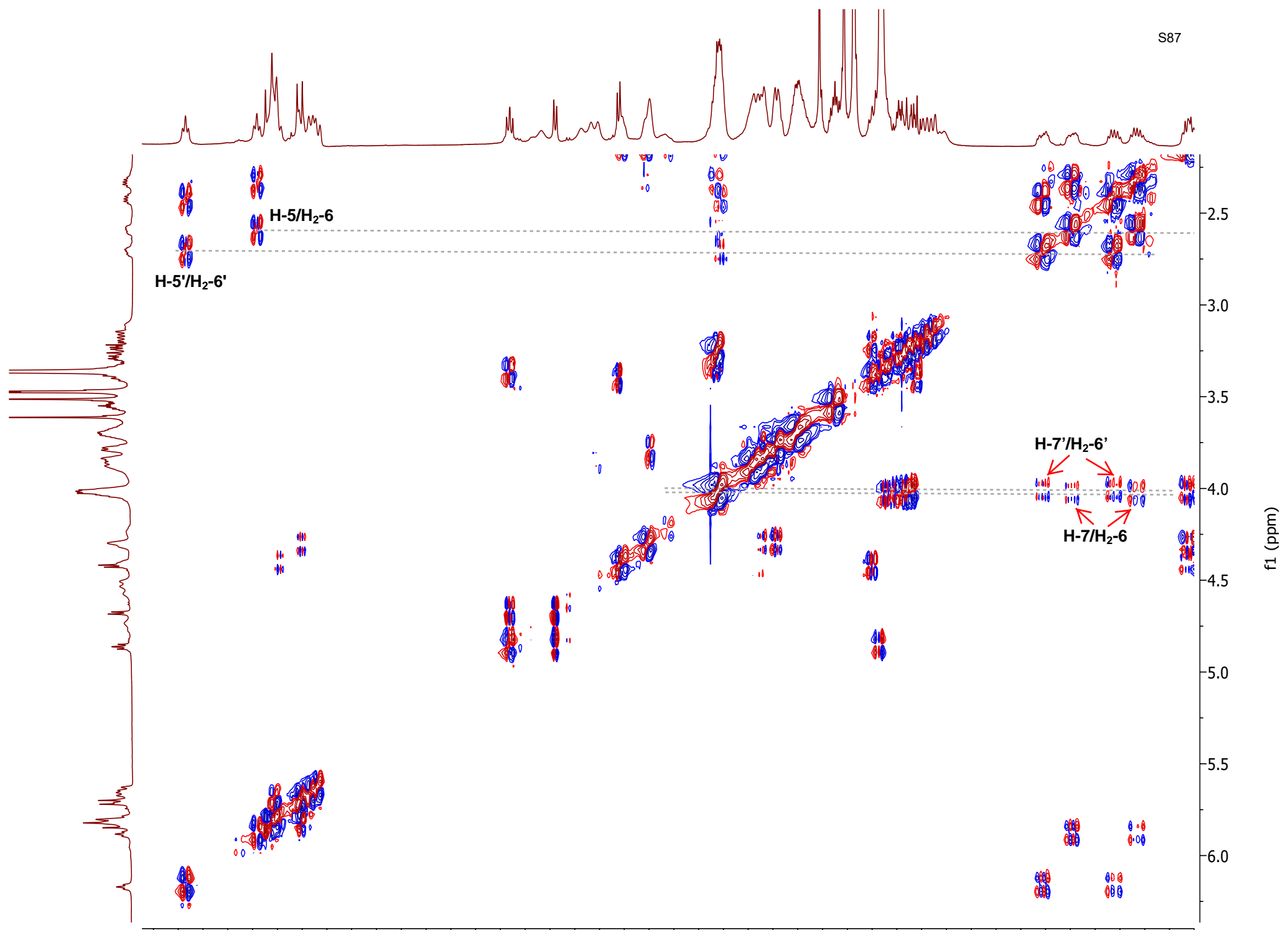


Figure S63 ^1H - ^1H COSY spectrum of samholide F (6)



6.2 6.1

Figure S64 Amplified ^1H - ^1H COSY spectrum of samholide F (**6**)

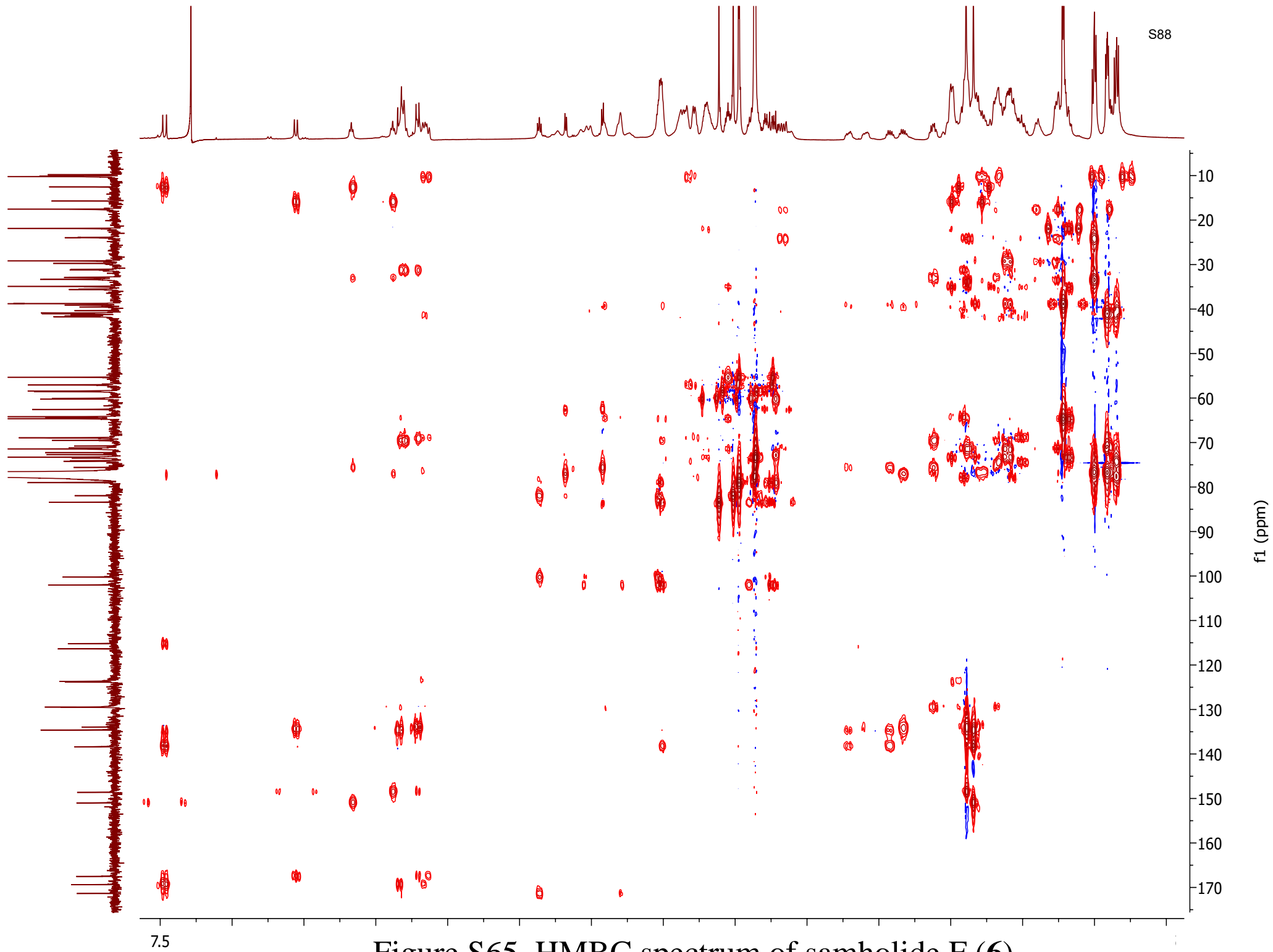
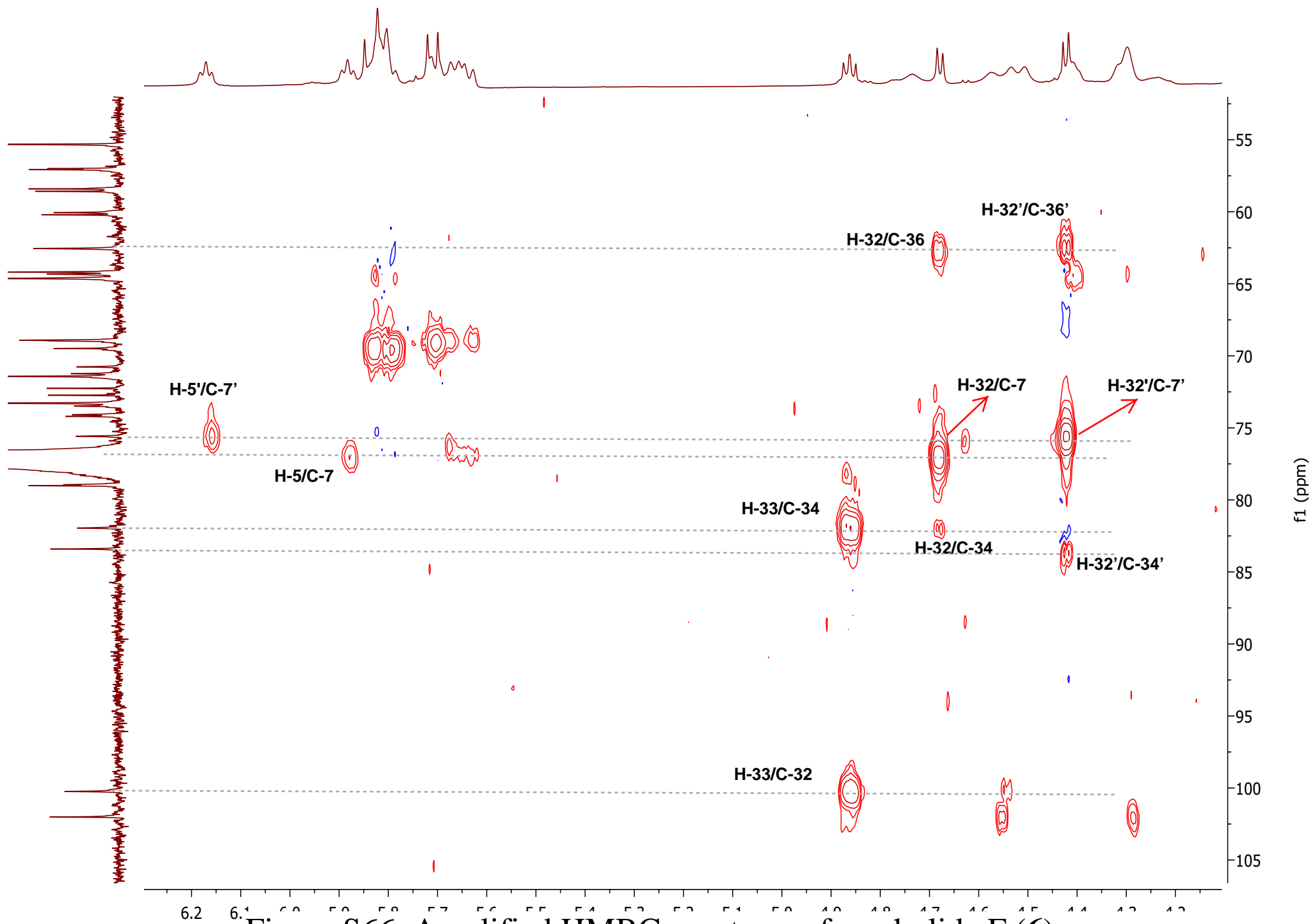


Figure S65 HMBC spectrum of samholide F (6)

Figure S66 Amplified HMBC spectrum of samholide F (**6**)

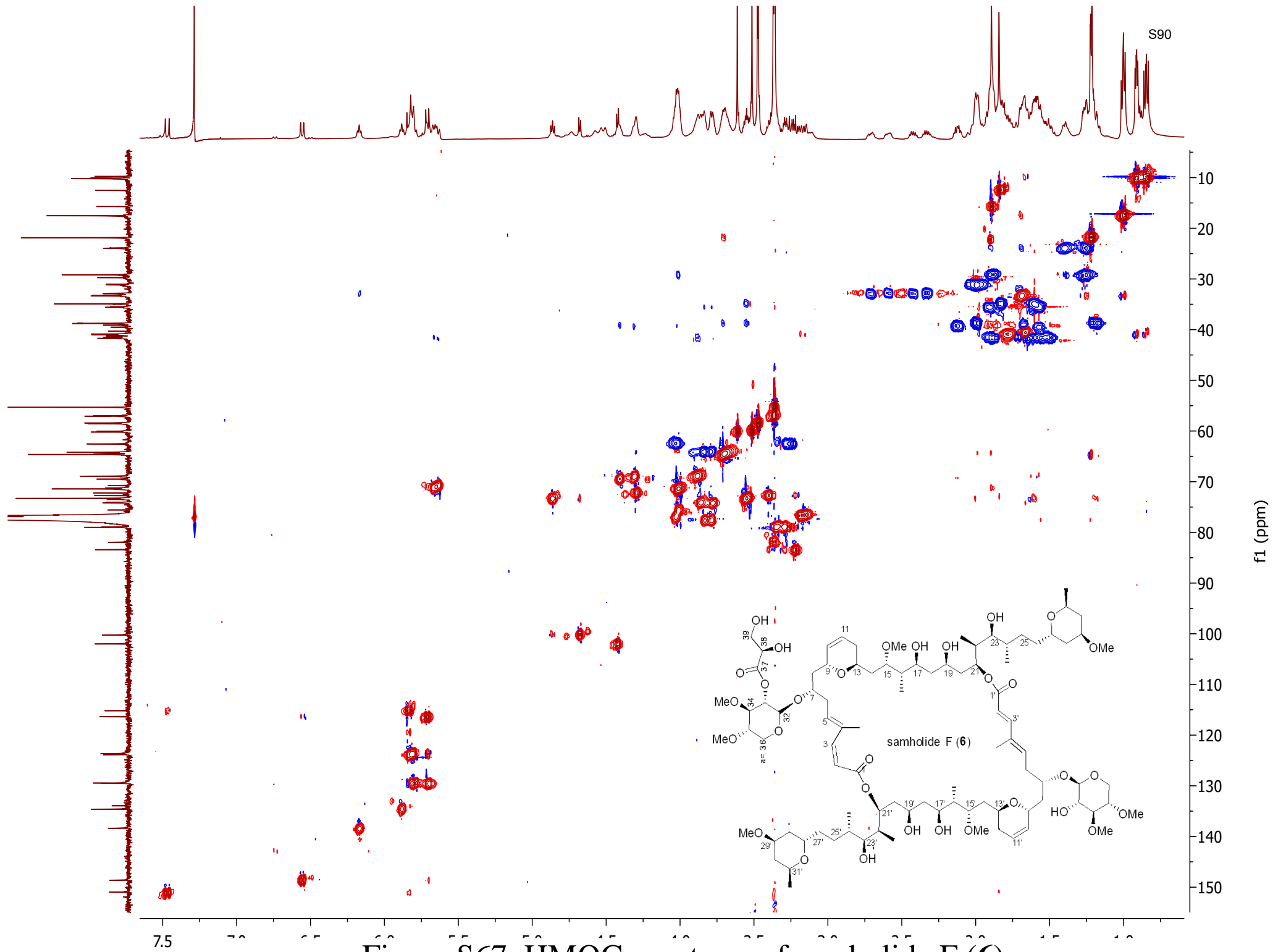


Figure S67 HMQC spectrum of samholide F (6)



Figure S68 HSQC-TOCSY spectrum of samholide F (6)

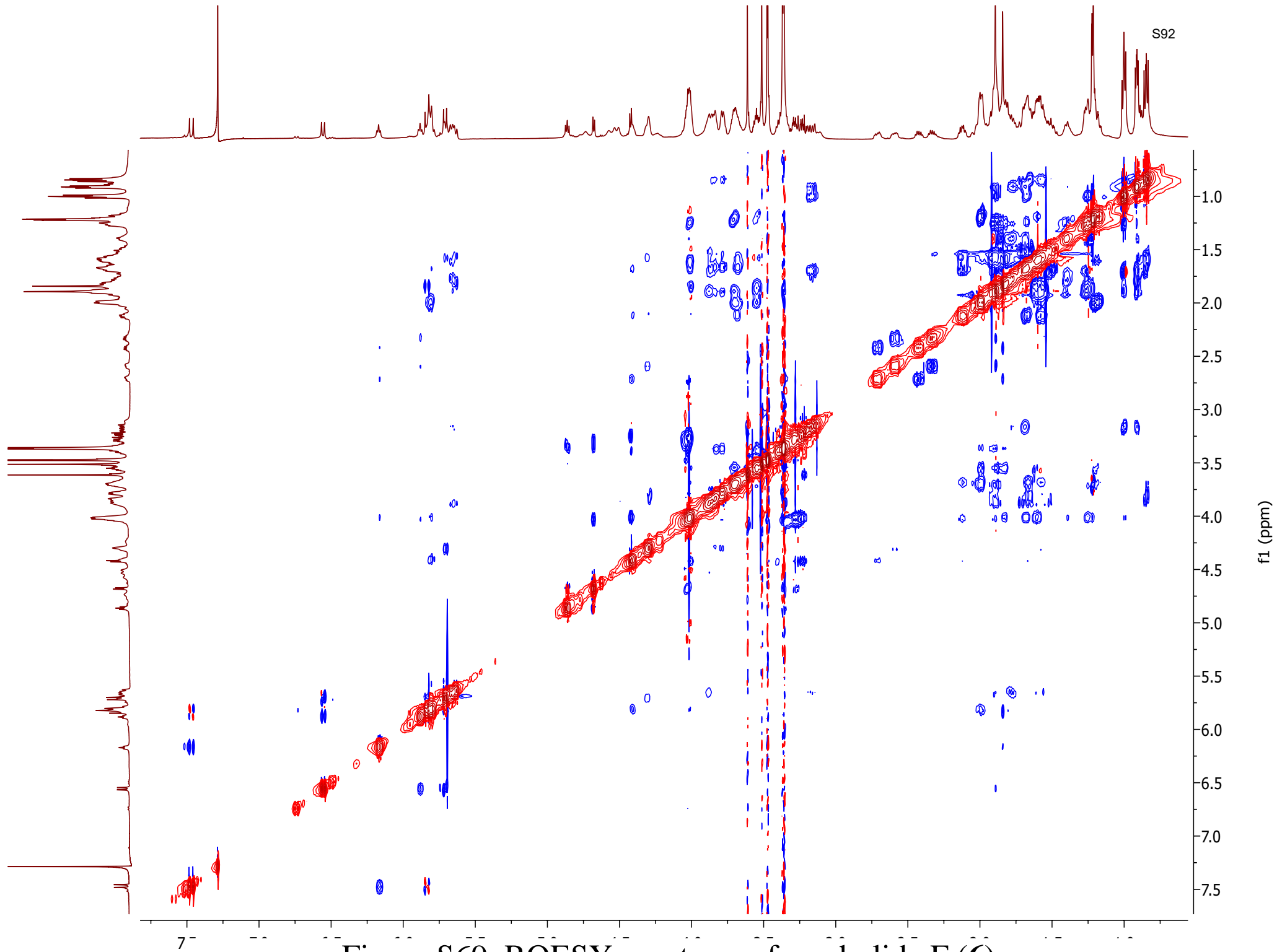


Figure S69 ROESY spectrum of samholide F (6)

2226H3C7A1.5.ser
UCSD_ROESY

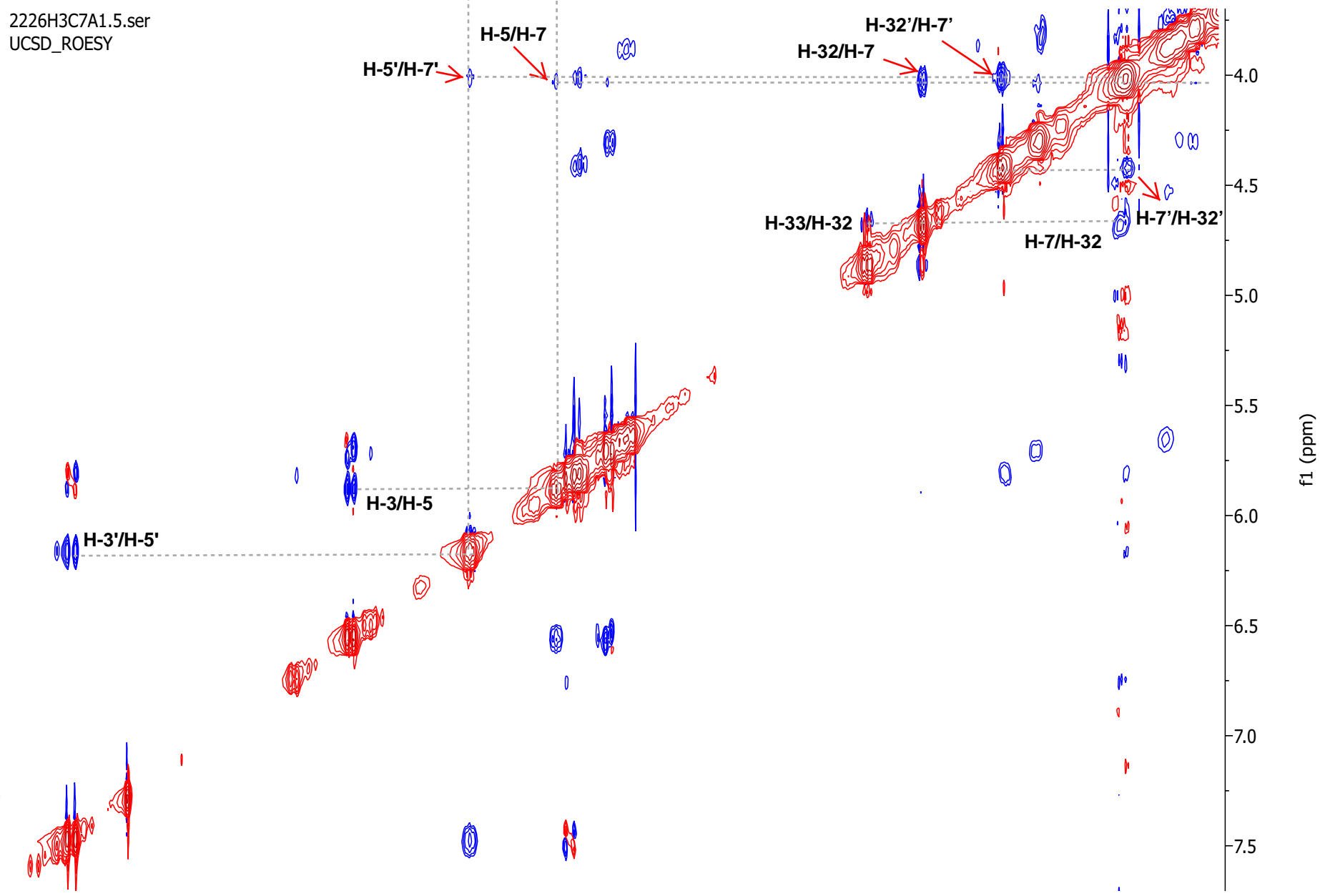


Figure S70 Amplified ROESY spectrum of samholide F (6)

2226H3C9A-a #17-21 RT: 0.41-0.50 AV: 5 SB: 4 0.26-0.33 NL: 9.29E7
T: + c Full ms [300.00-2000.00]

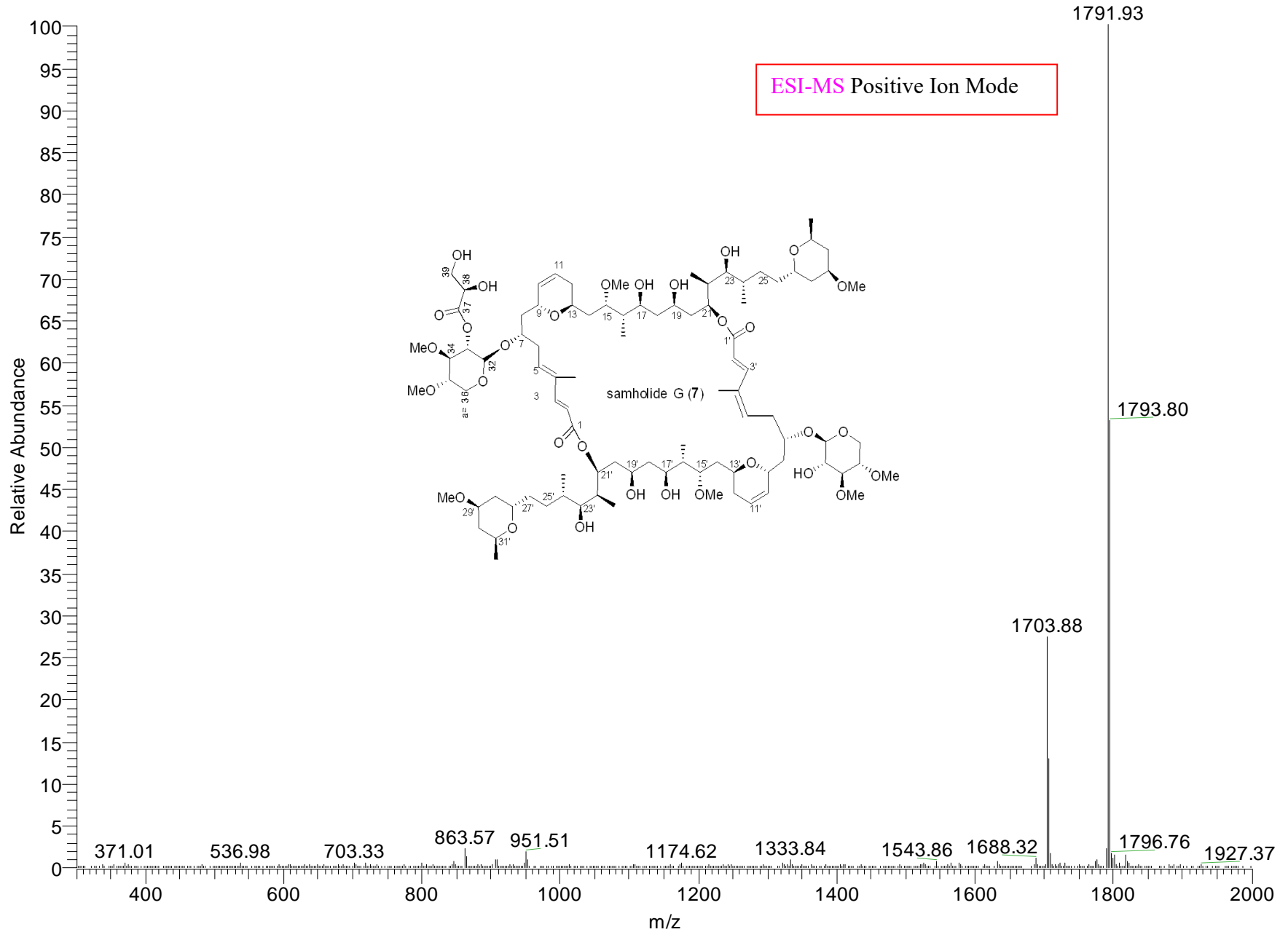


Figure S71 The ESI MS spectrum of samholide G (7)

2226H3C9A-a #33-36 RT: 0.75-0.80 AV: 4 NL: 2.96E7
F: + c Full ms2 1792.00@35.00 [490.00-2000.00]

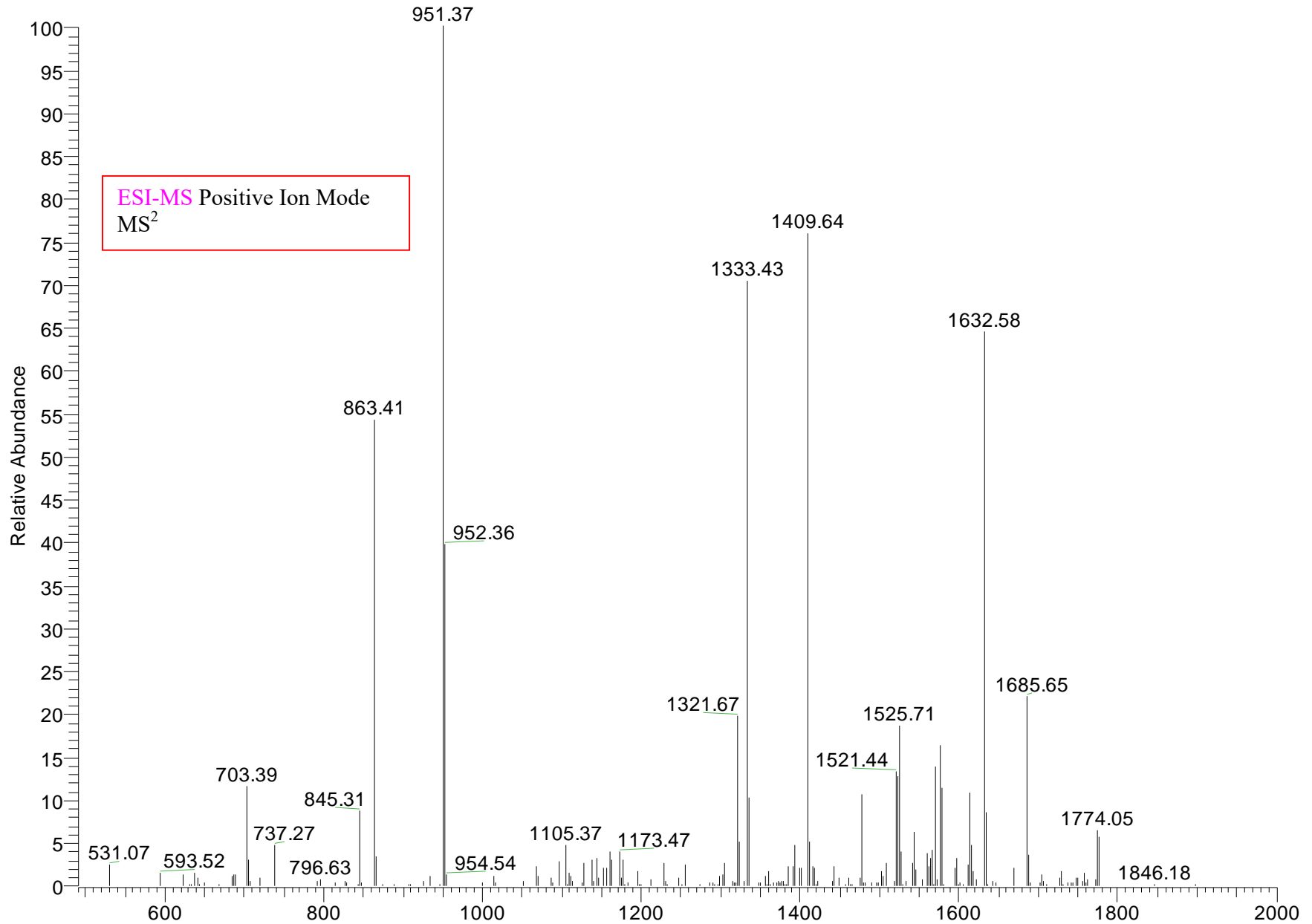


Figure S72 The ESI MS² spectrum of samholide G (7)

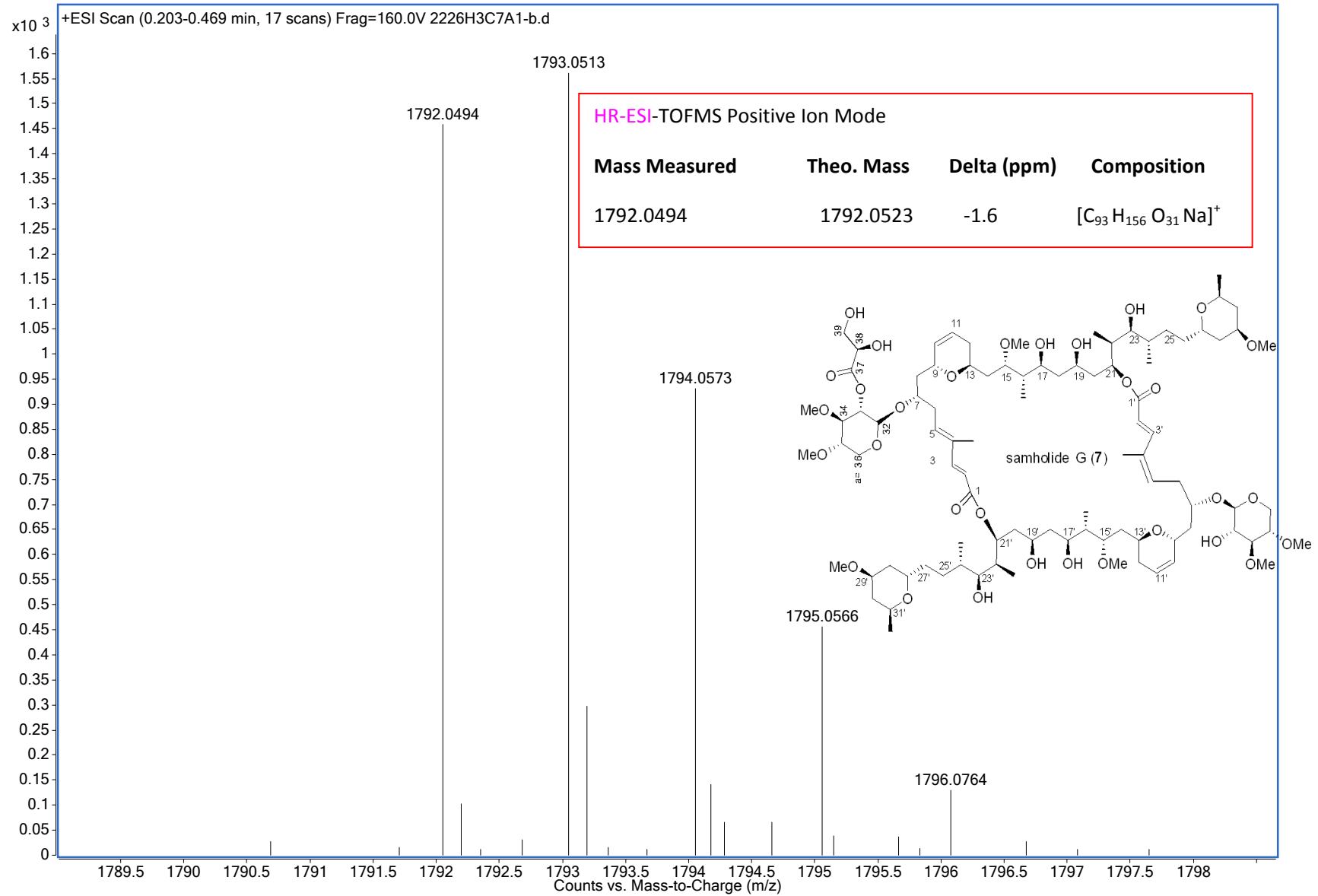


Figure S73 The positive HRESIMS spectrum of samholide G (7)

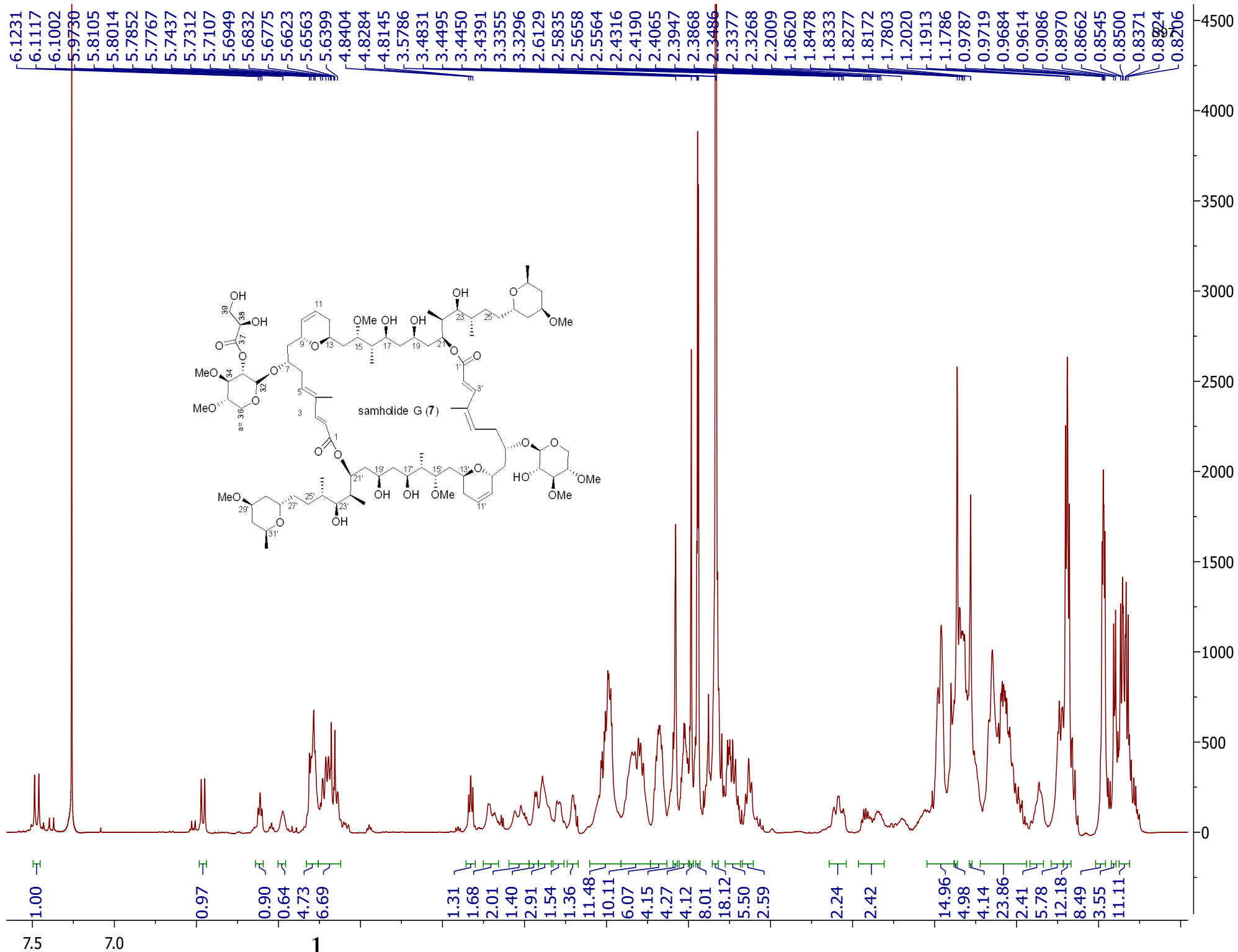
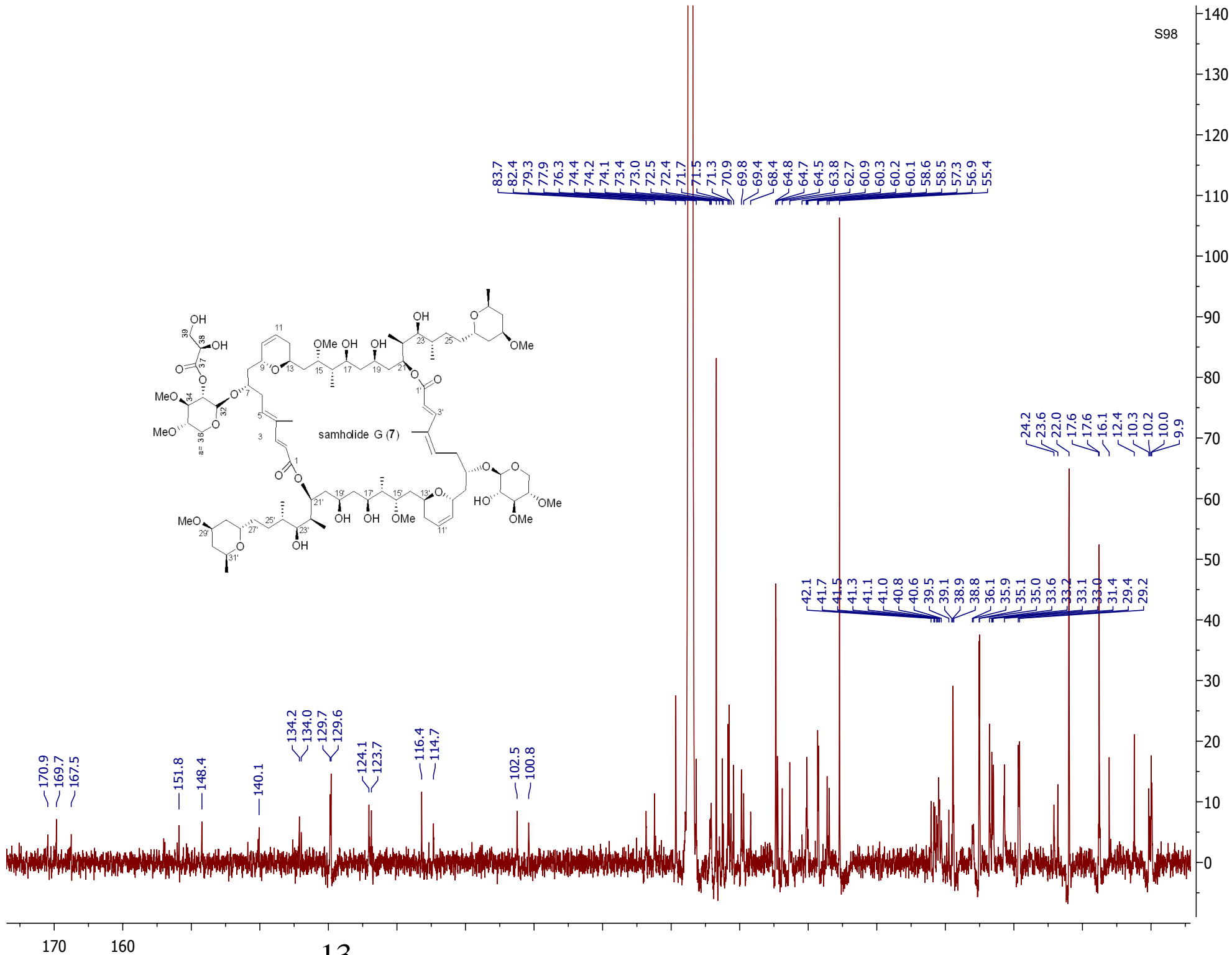


Figure S74 ^1H NMR (600 MHz, DMSO) spectrum of samholide G (7)



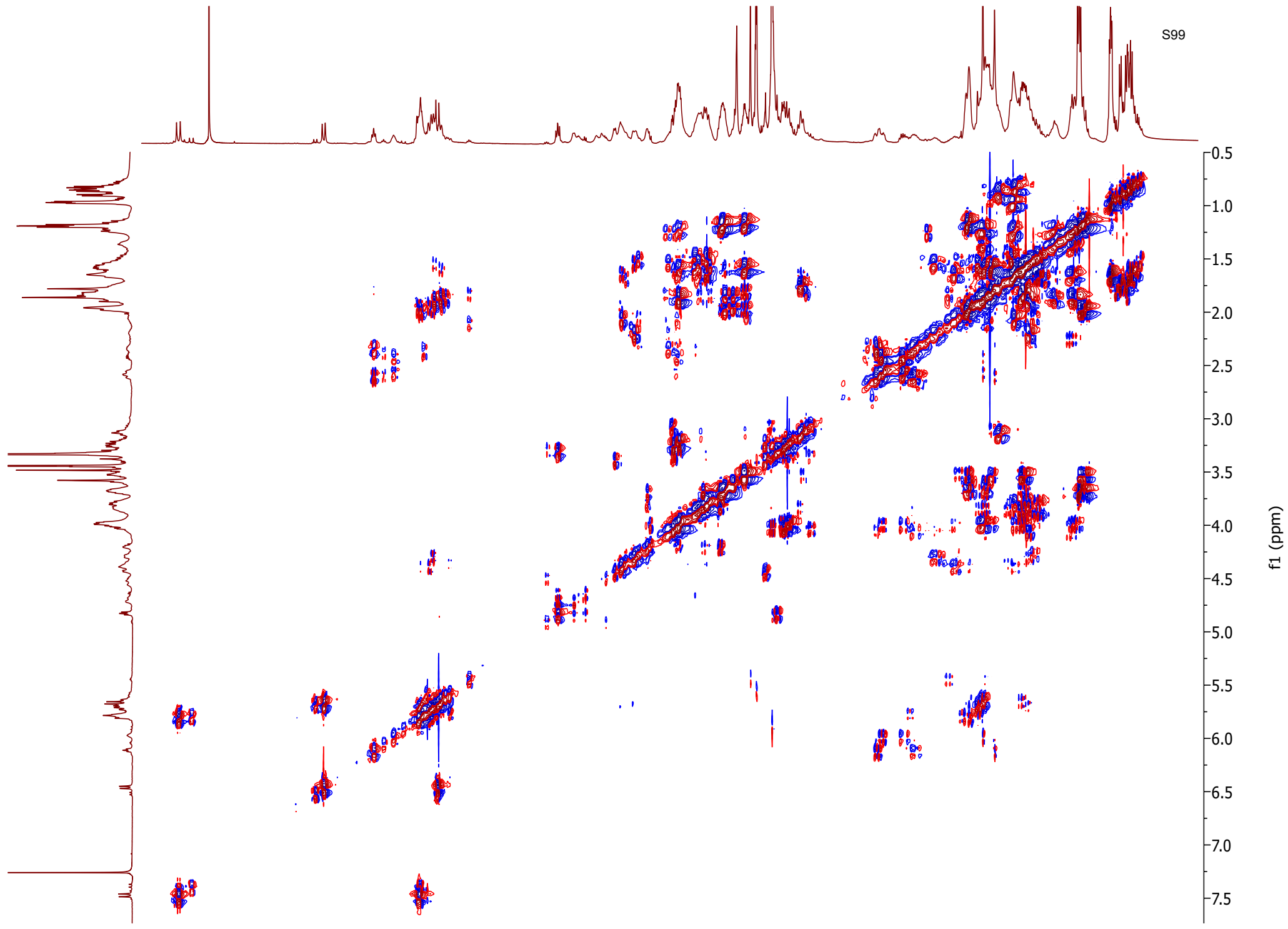


Figure S76 ^1H - ^1H COSY spectrum of samholide G (7)

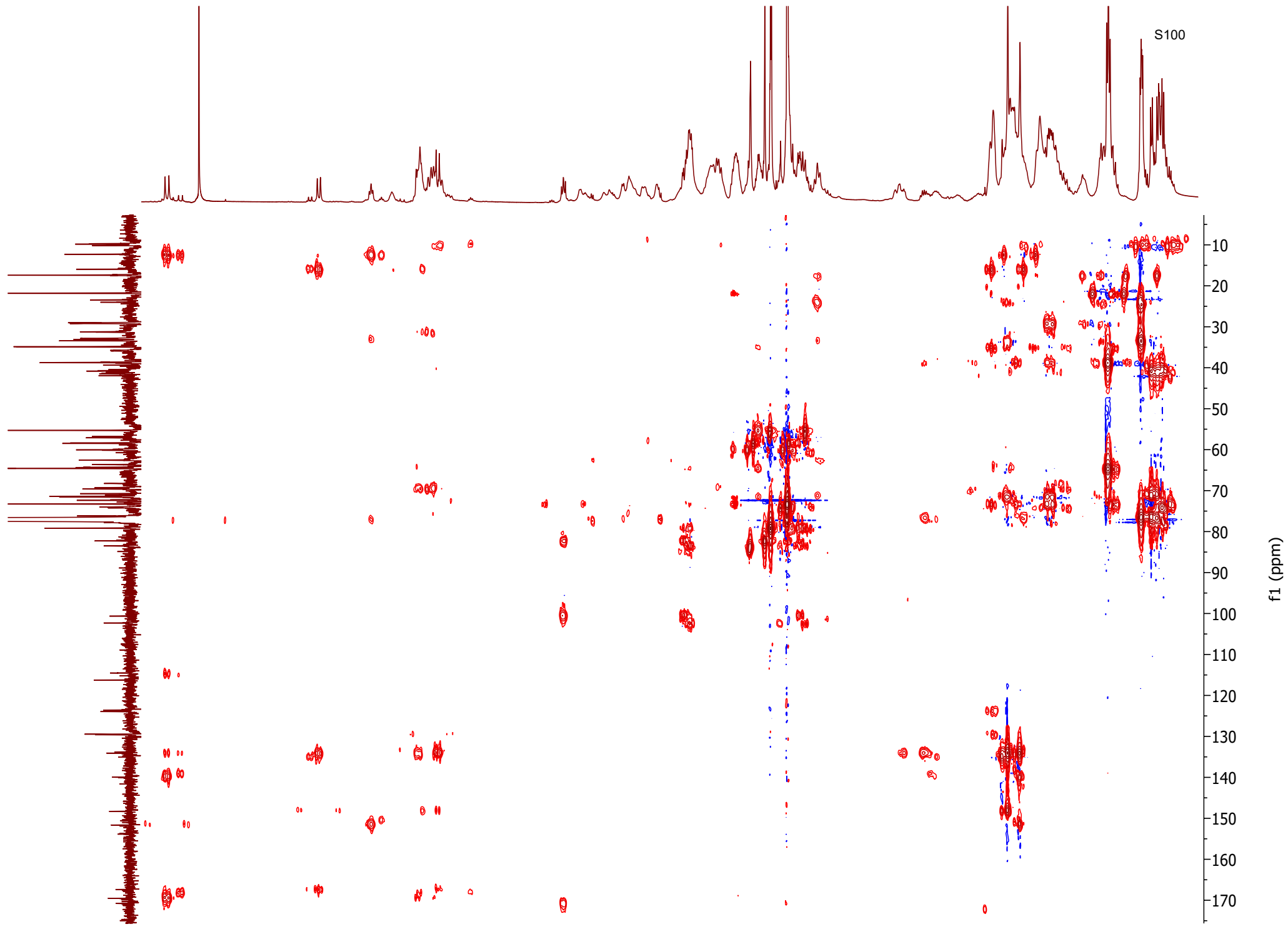


Figure S77 HMBC spectrum of samholide G (7)

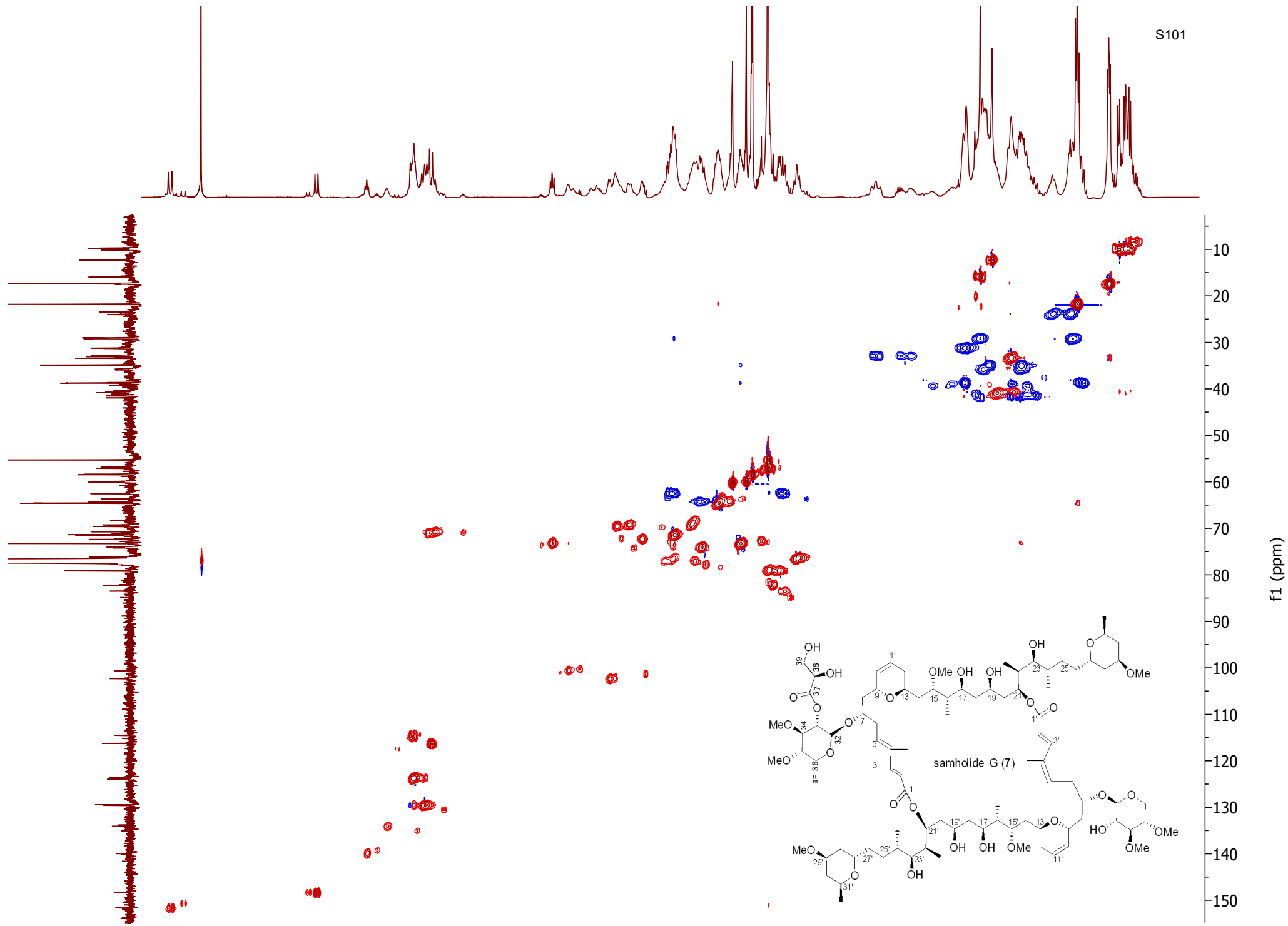


Figure S78 HMBC spectrum of samholide G (7)

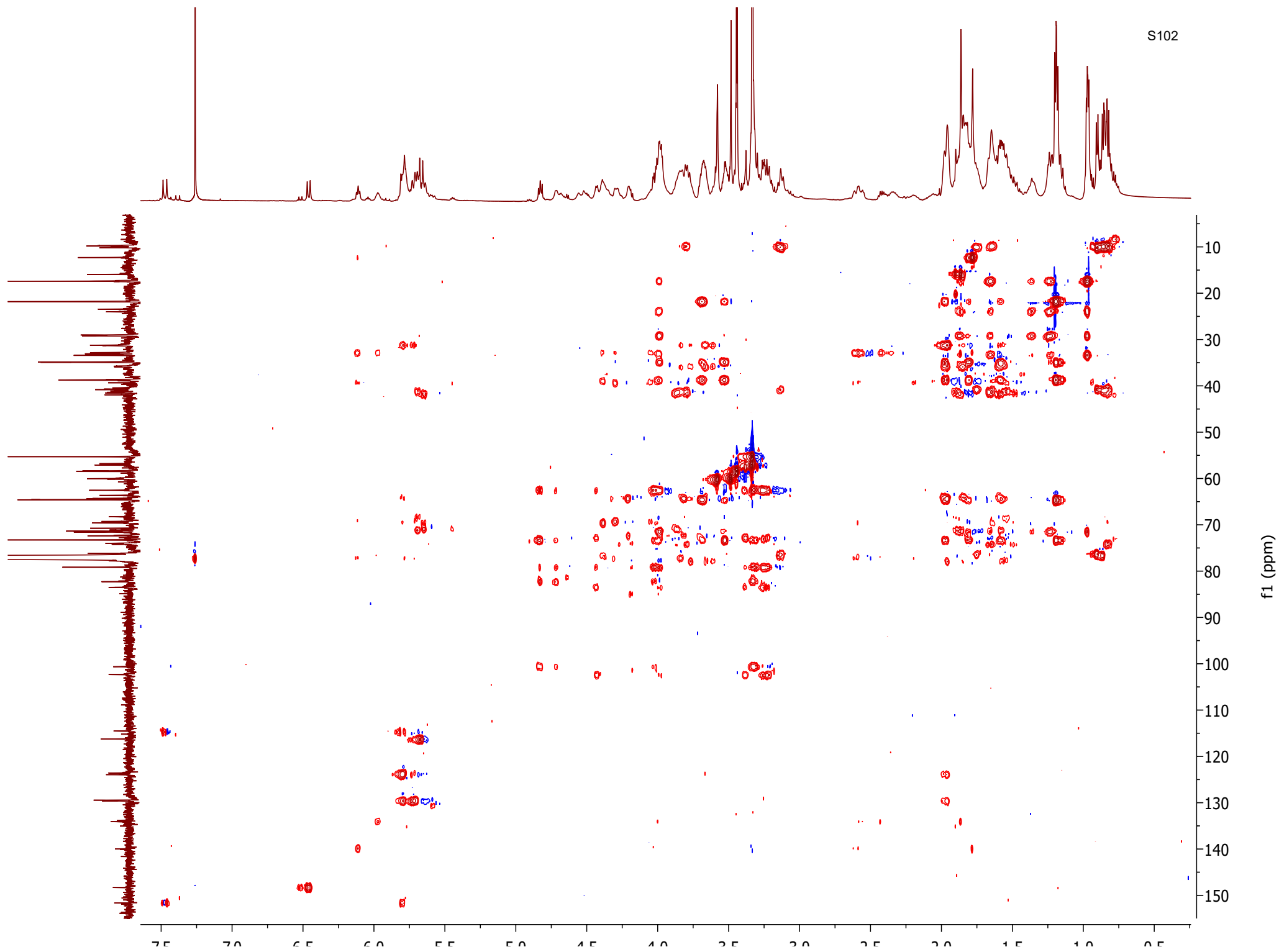


Figure S79 HSQC-TOCSY spectrum of samholide G (7)

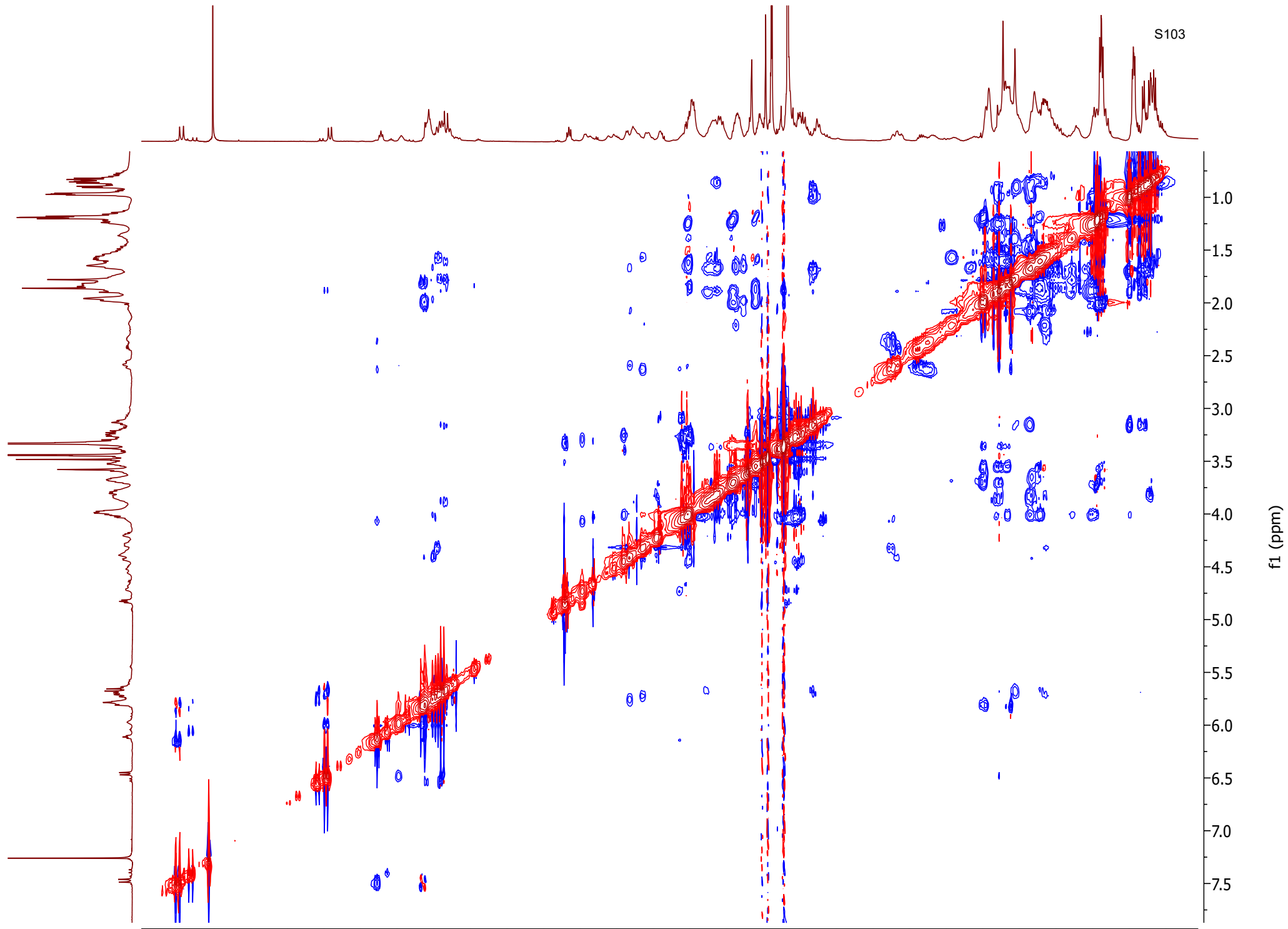


Figure S80 ROESY spectrum of samholide G (7)

2226H3CB4A-a #12-15 RT: 0.28-0.35 AV: 4 SB: 3 0.18-0.23 NL: 1.72E6

T: + c Full ms [300.00-2000.00]

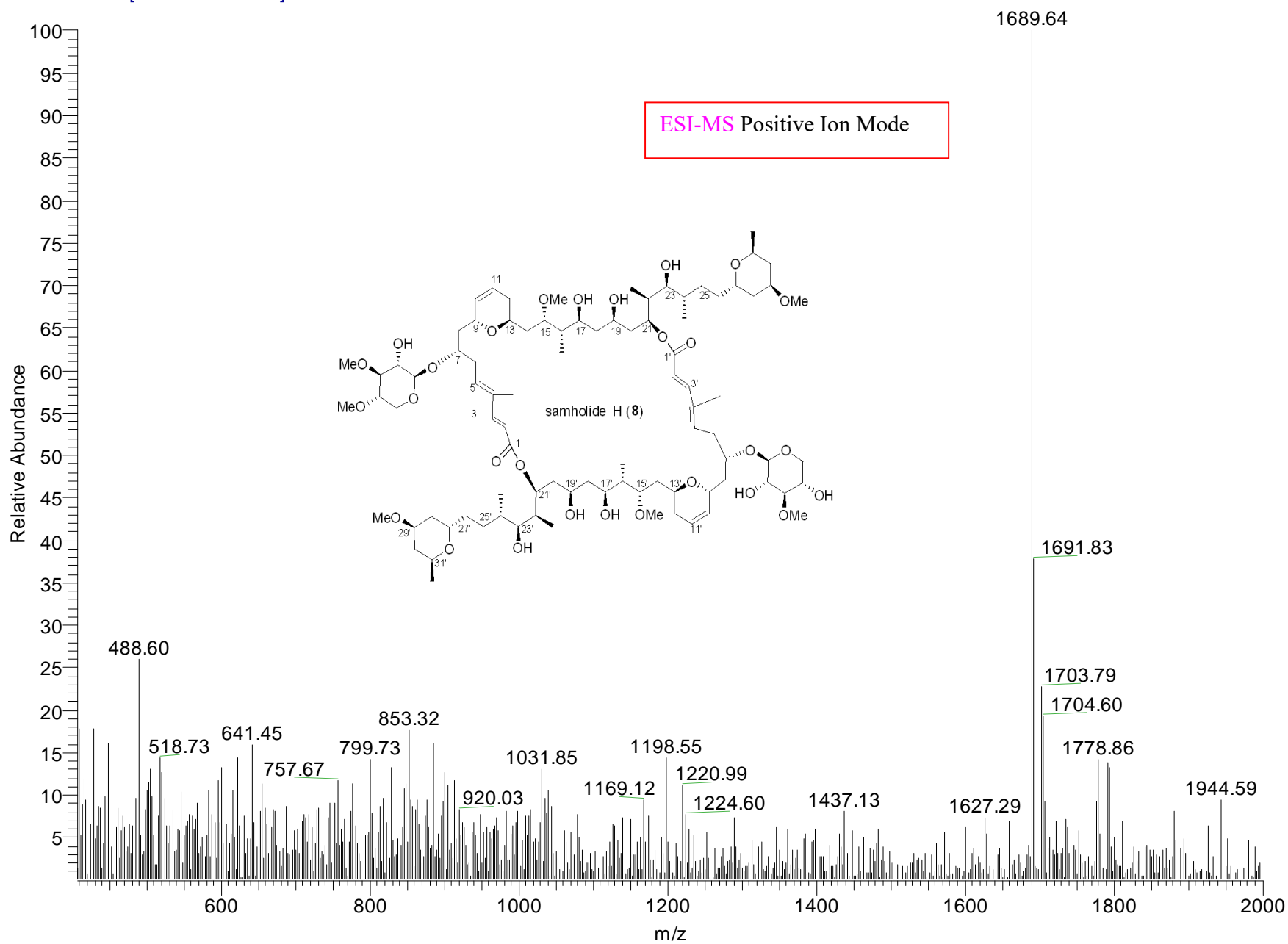
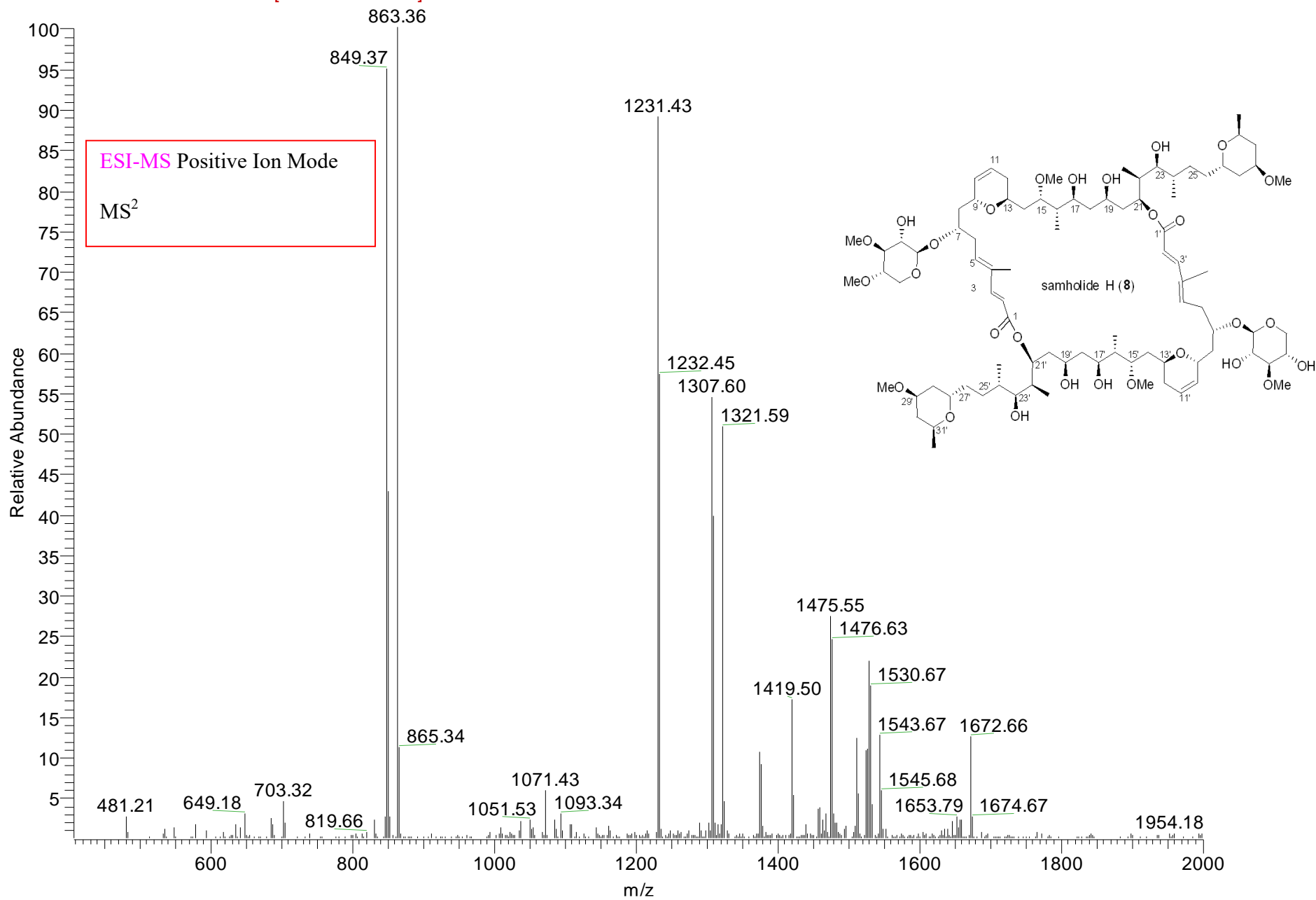


Figure S81 The ESI MS spectrum of samholide H (8)

2226H3CB4A-a #55-73 RT: 1.30-1.62 AV: 19 NL: 3.56E5

F: + c Full ms2 1690.00@35.00 [465.00-2000.00]

Figure S82 The ESI MS² spectrum of samholide H (8)

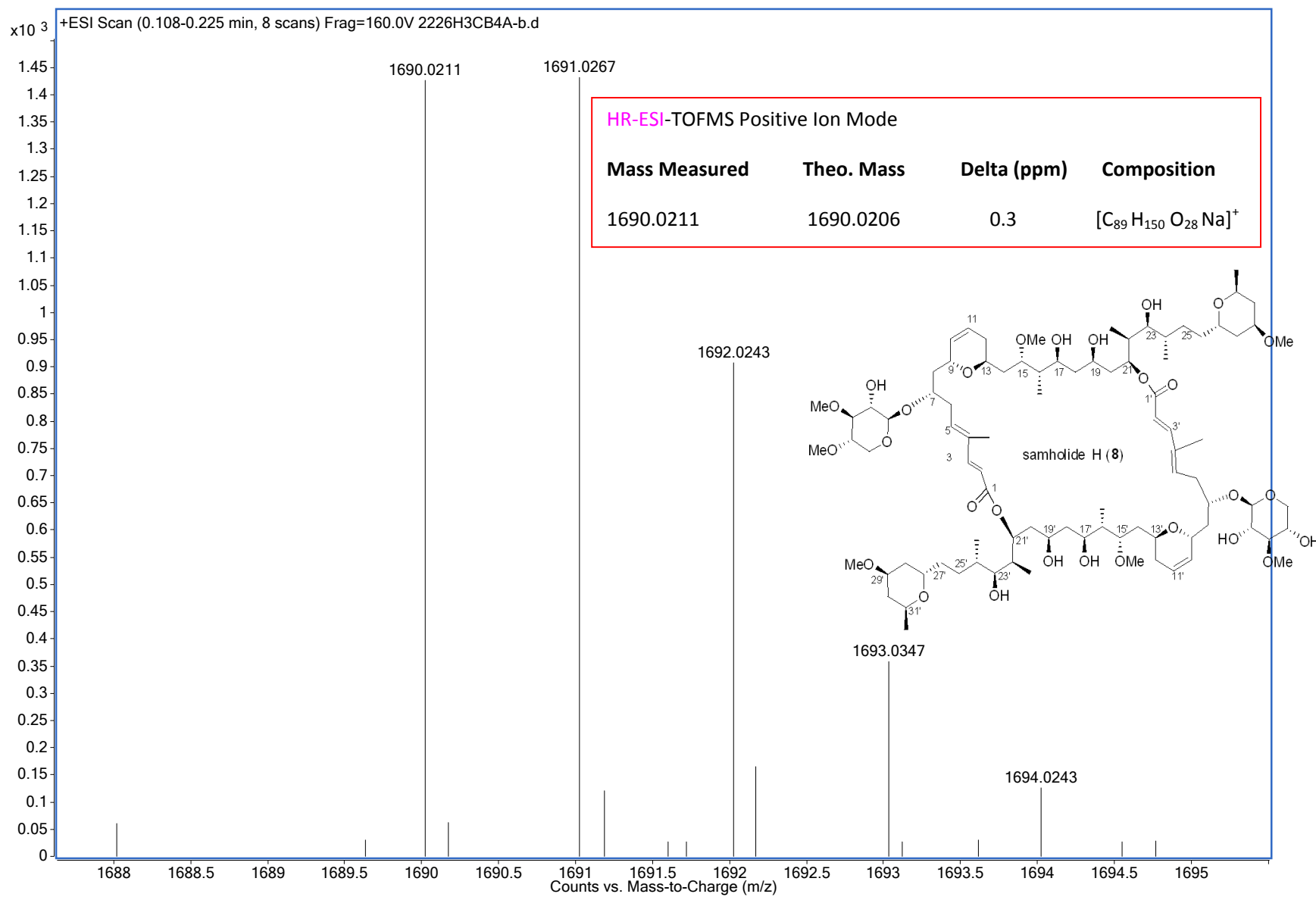


Figure S83 The positive HRESIMS spectrum of samholide H (8)

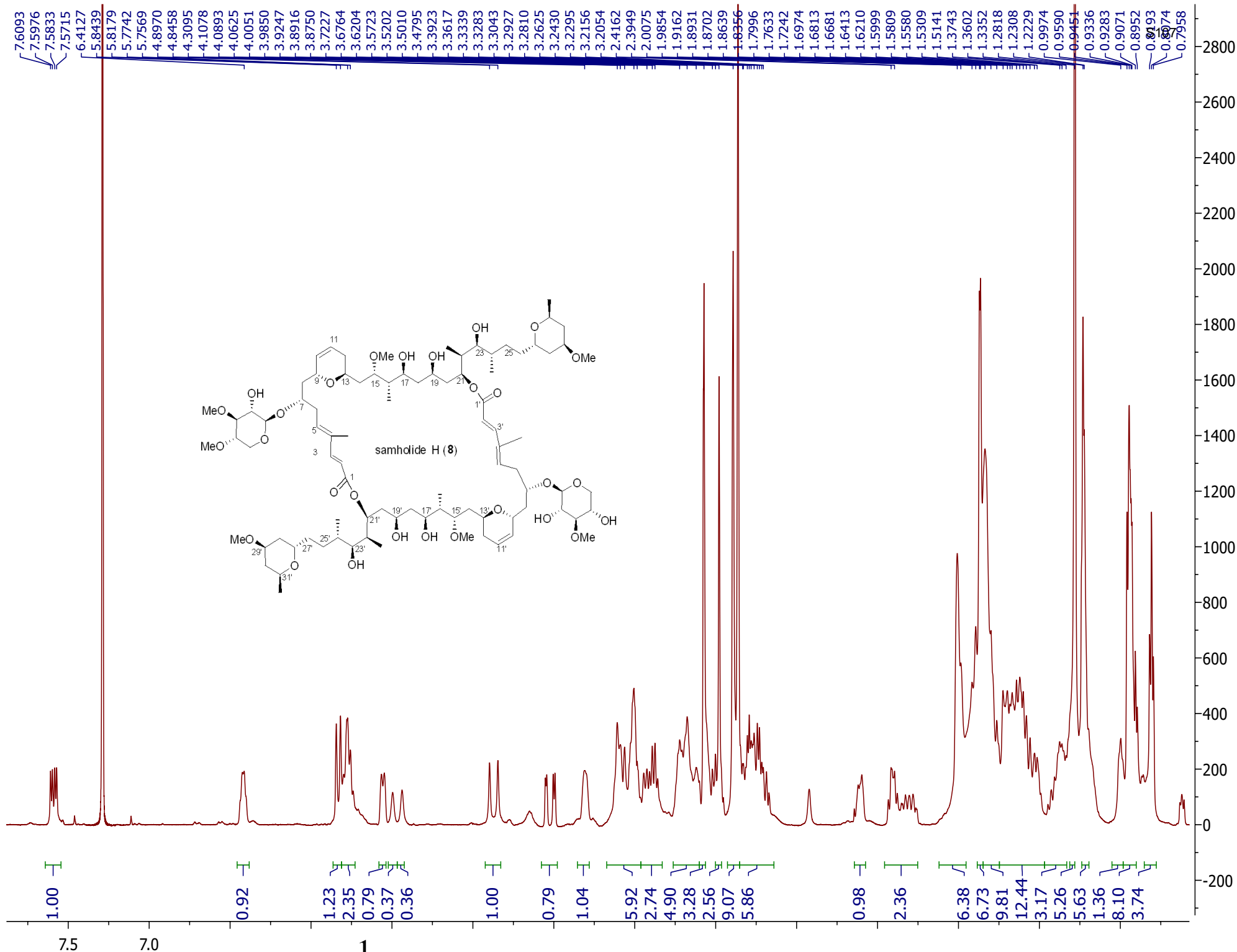


Figure S84 ^1H NMR (600 MHz, DMSO) spectrum of samholide H (**8**)

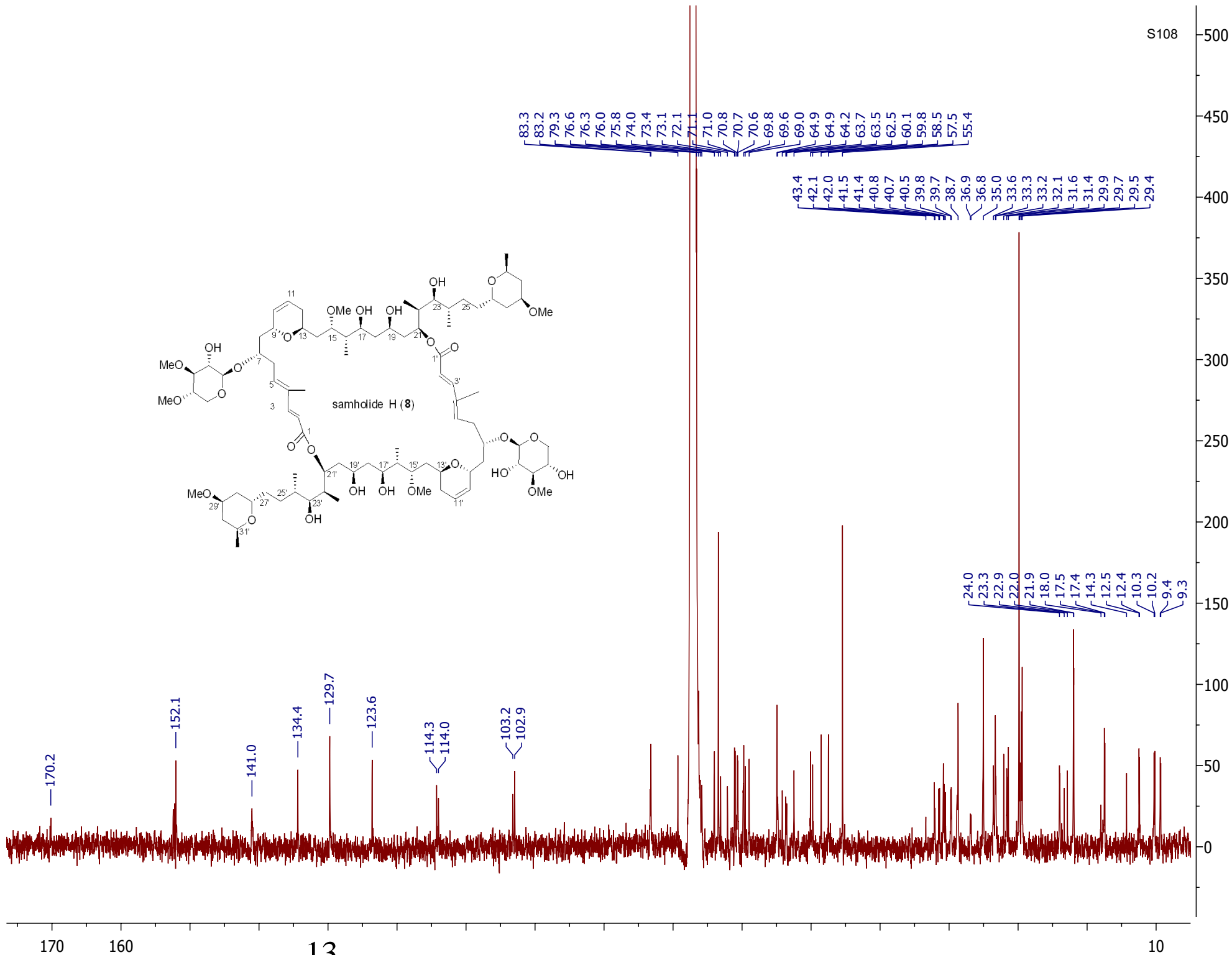


Figure S85 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide H (8)

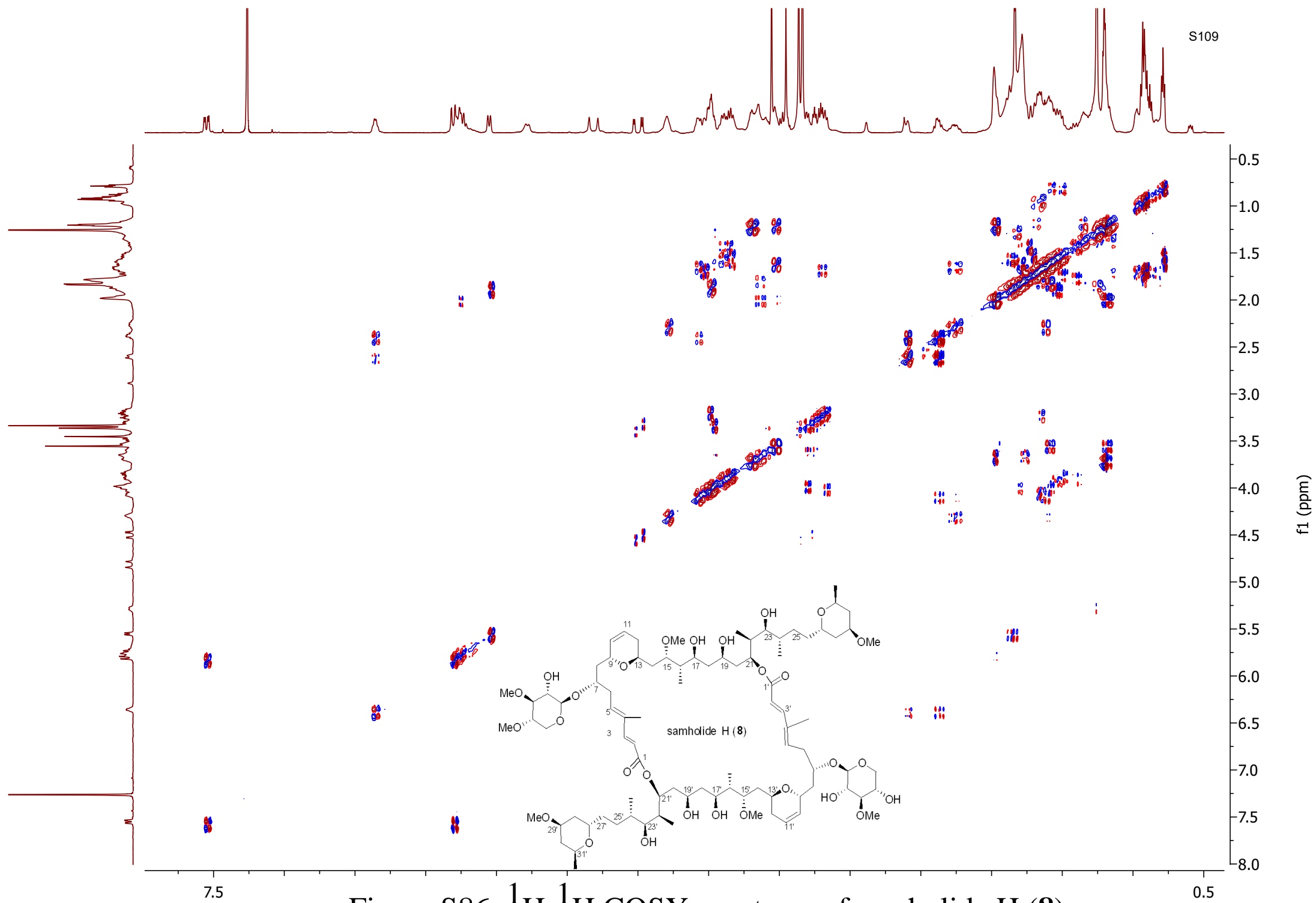


Figure S86 ^1H - ^1H COSY spectrum of samholide H (8)

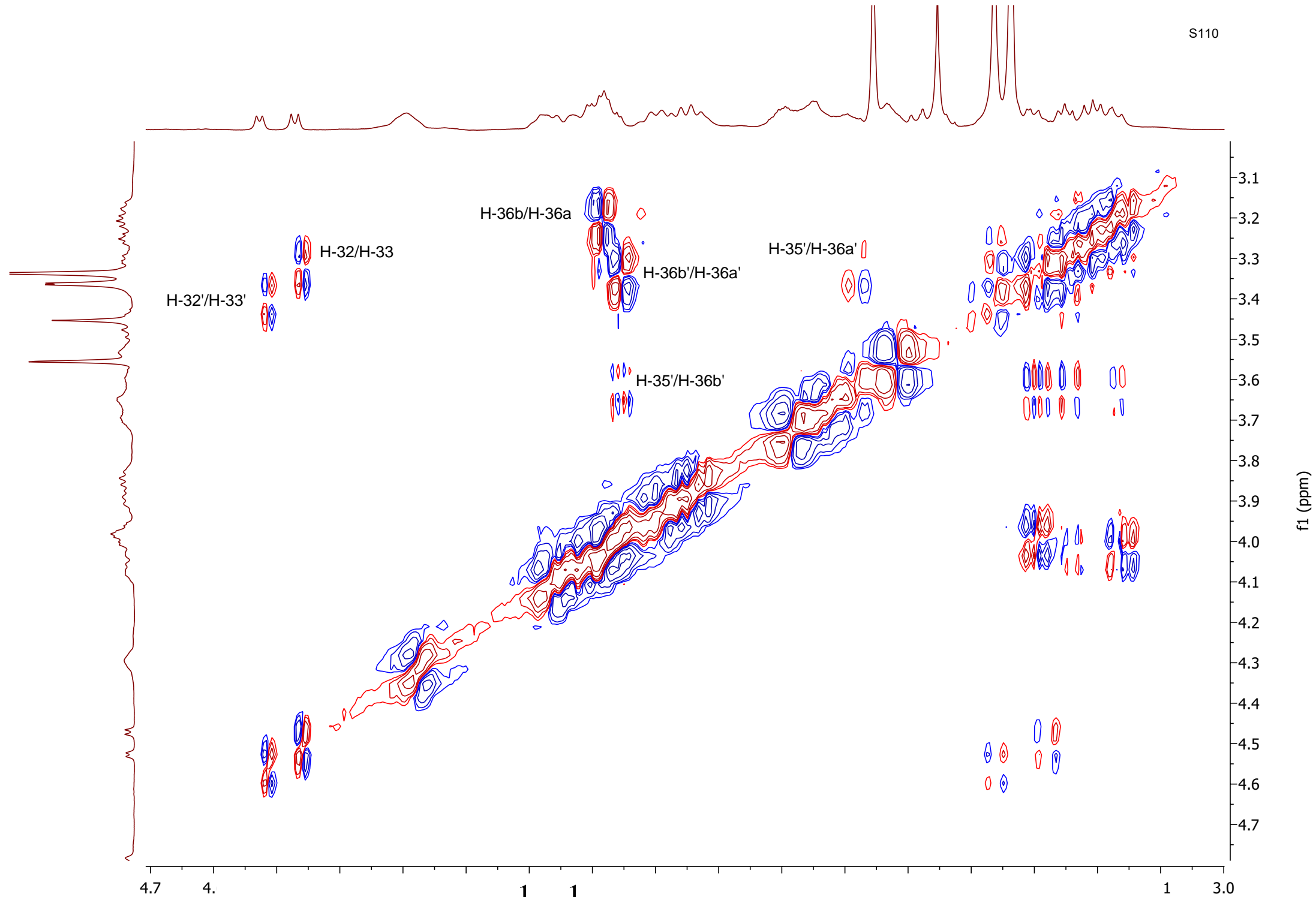


Figure S87 Amplified ^1H - ^1H COSY spectrum of samholide H (**8**)

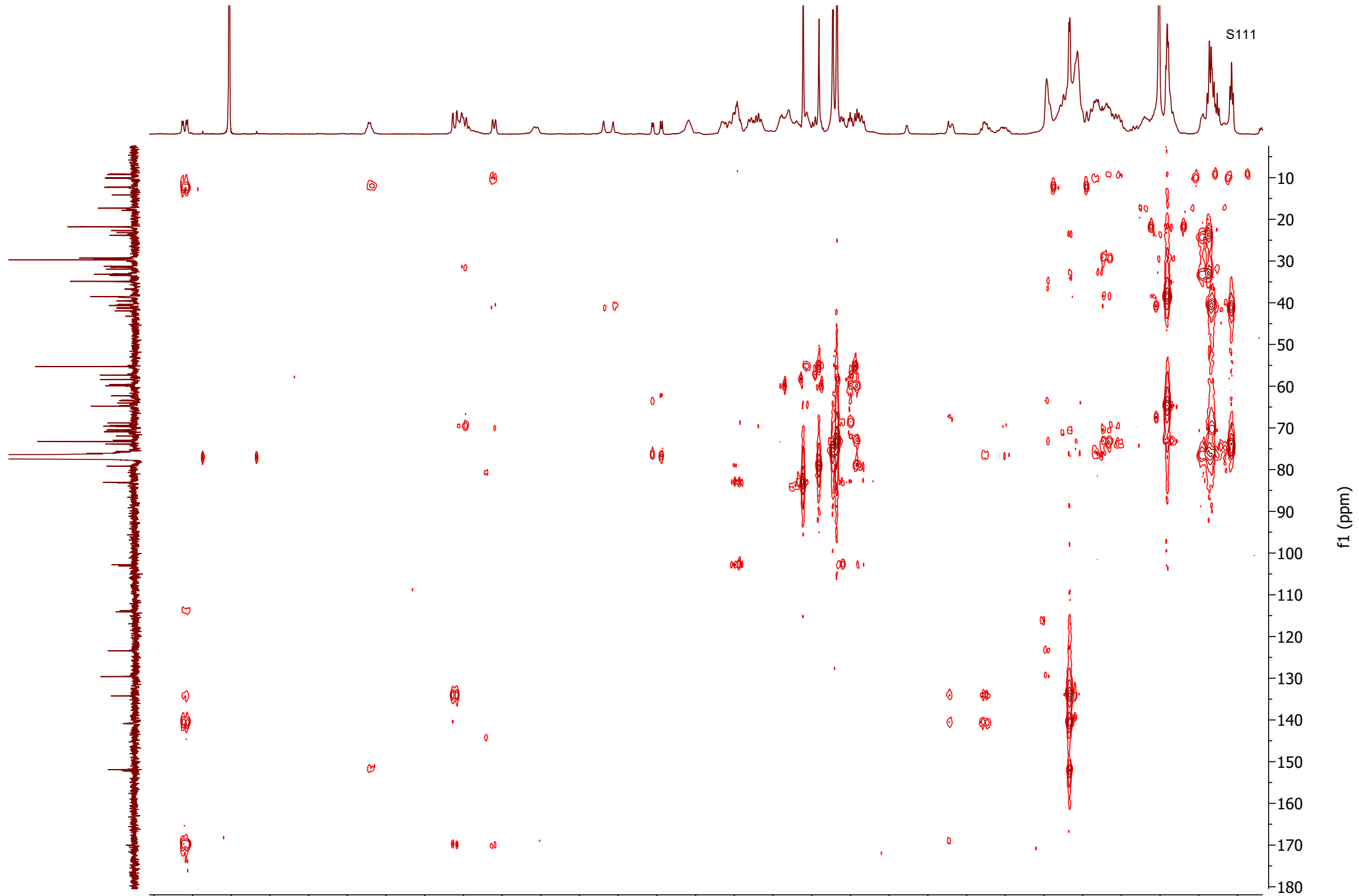
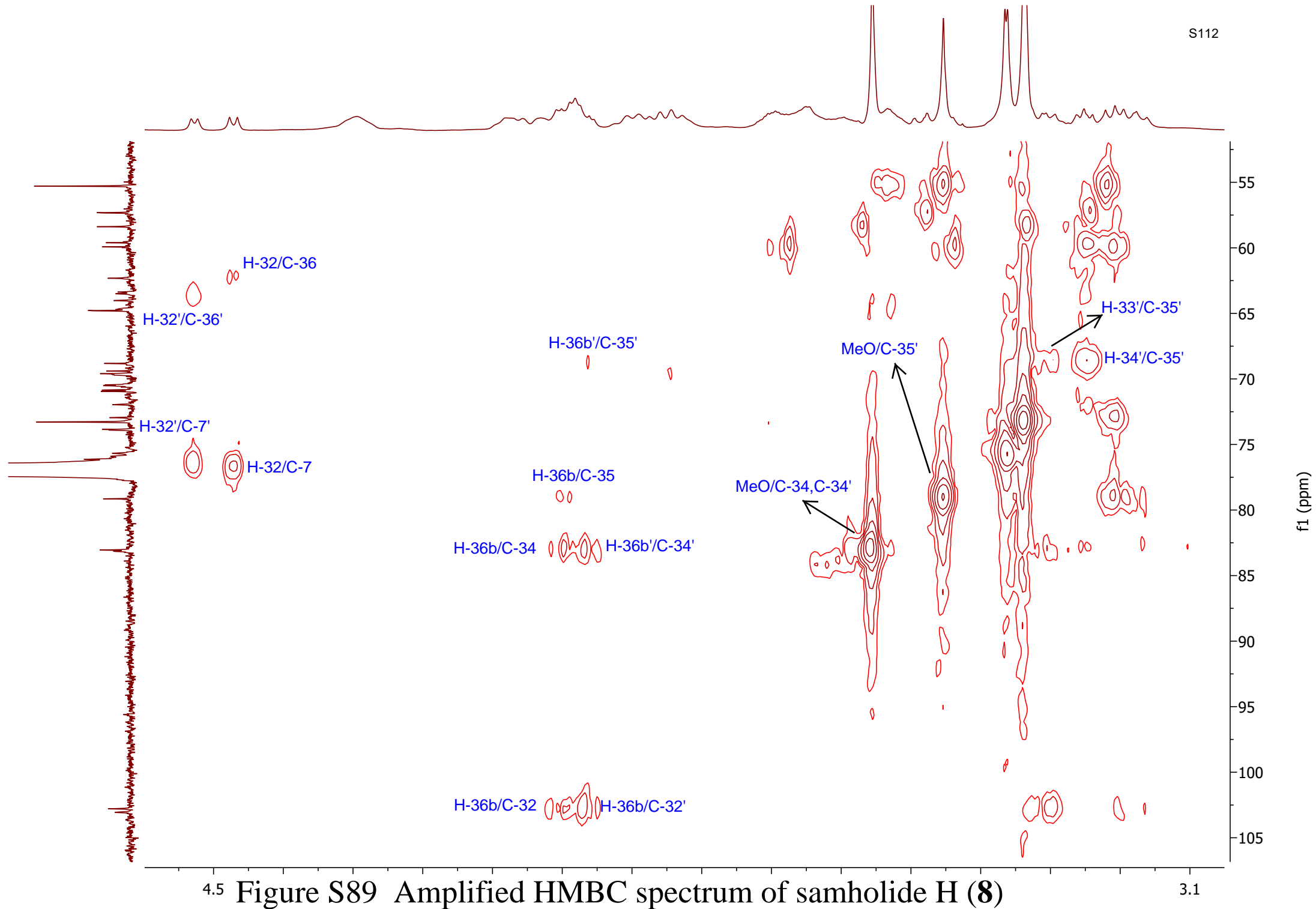
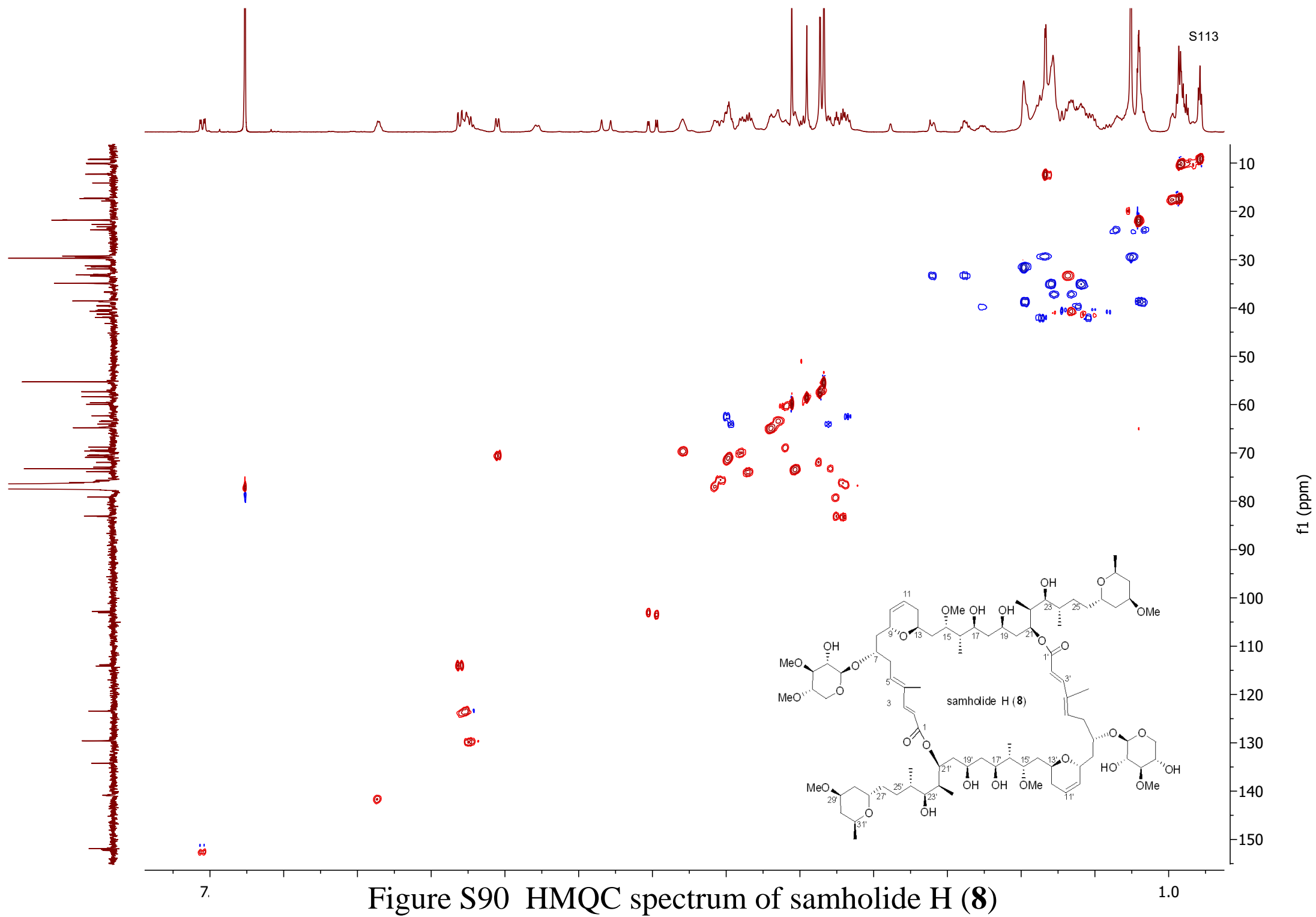


Figure S88 HMBC spectrum of samholide H (**8**)



4.5 Figure S89 Amplified HMBC spectrum of samholide H (8)



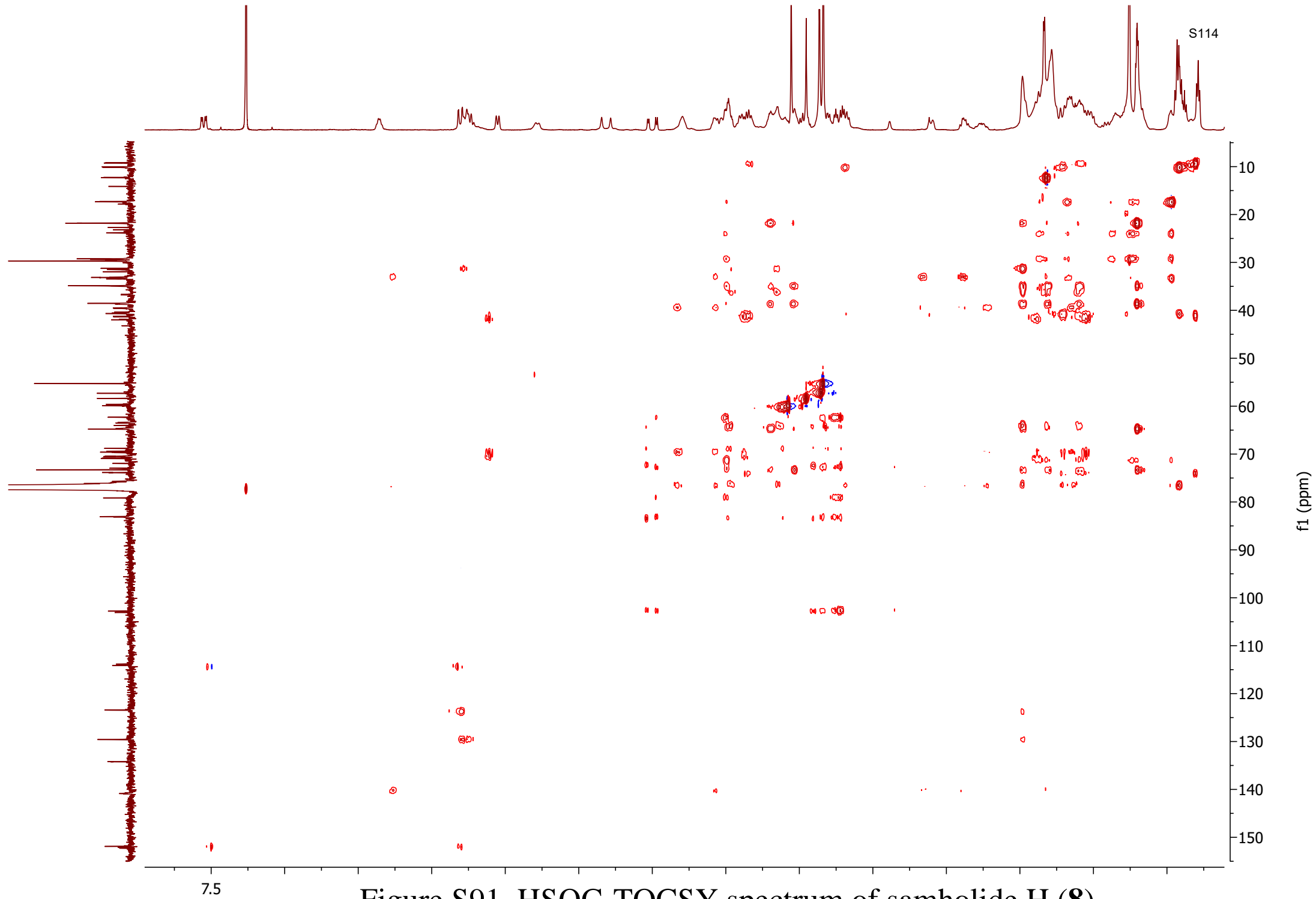


Figure S91 HSQC-TOCSY spectrum of samholide H (**8**)

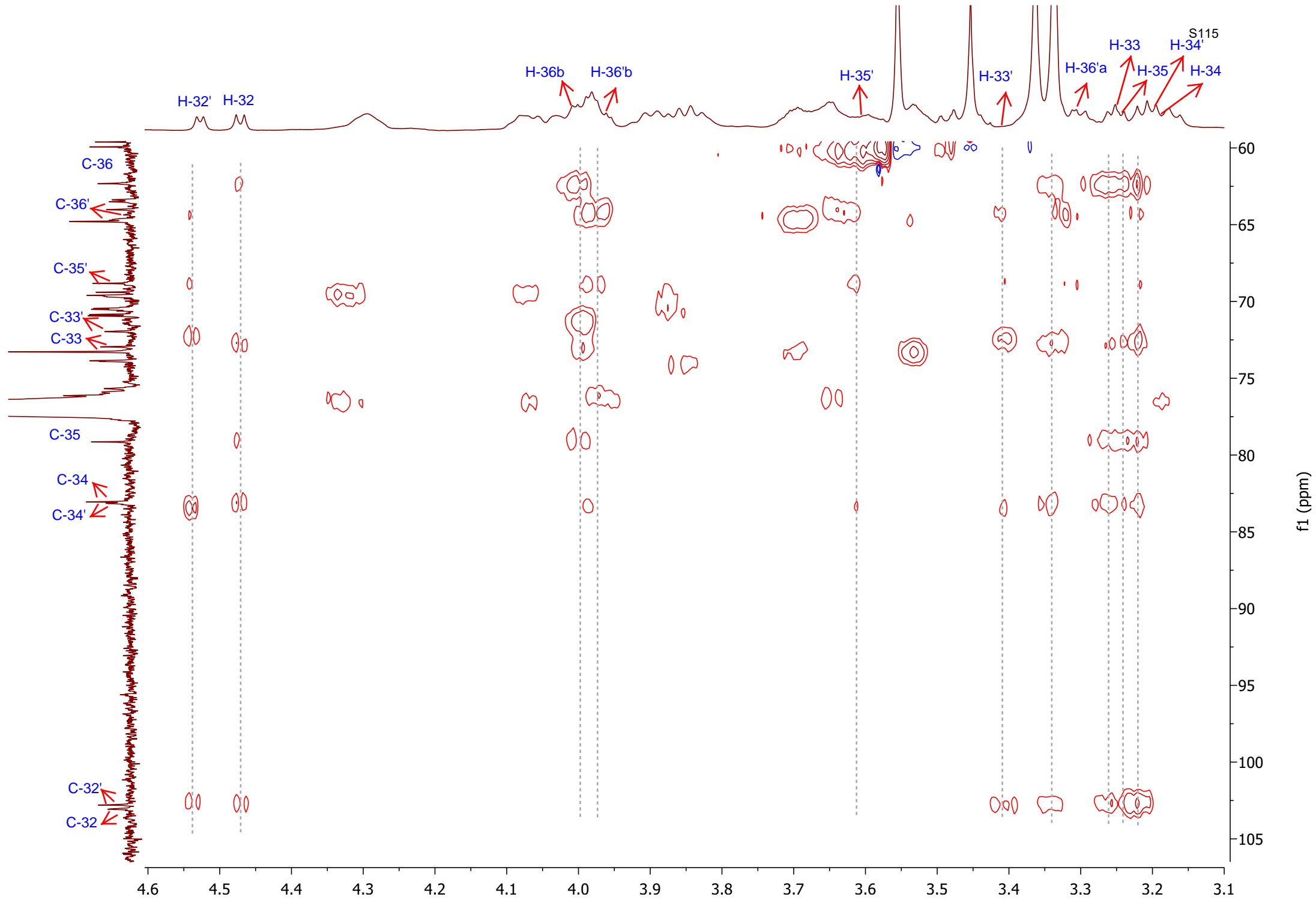


Figure S92 Amplified HSQC-TOCSY spectrum of samholide H (**8**)

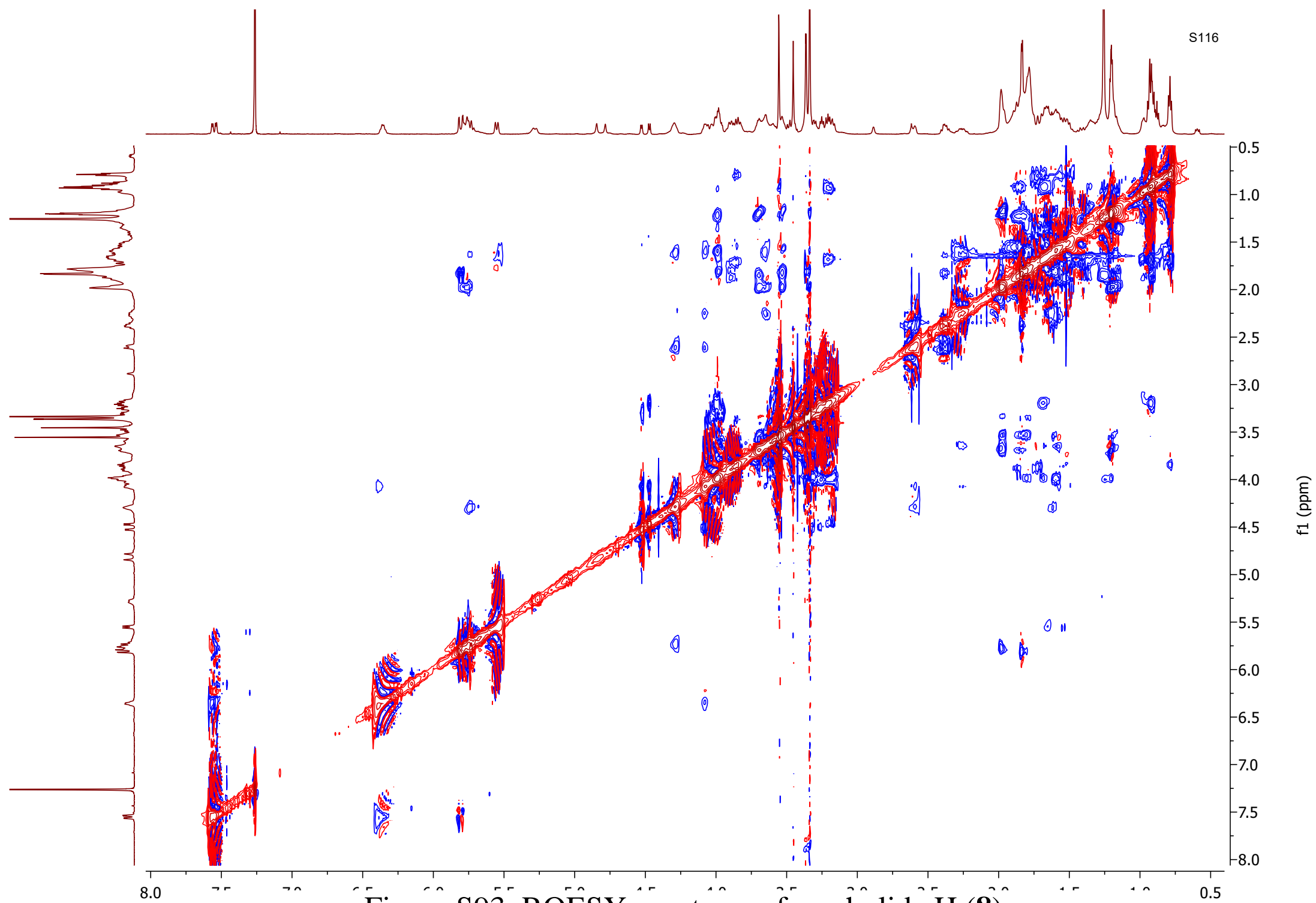


Figure S93 ROESY spectrum of samholide H (8)

2226H3C3-a #13-15 RT: 0.34-0.39 AV: 3 SB: 2 0.27-0.29 NL: 1.71E7

F: + c Full ms [200.00-2000.00]

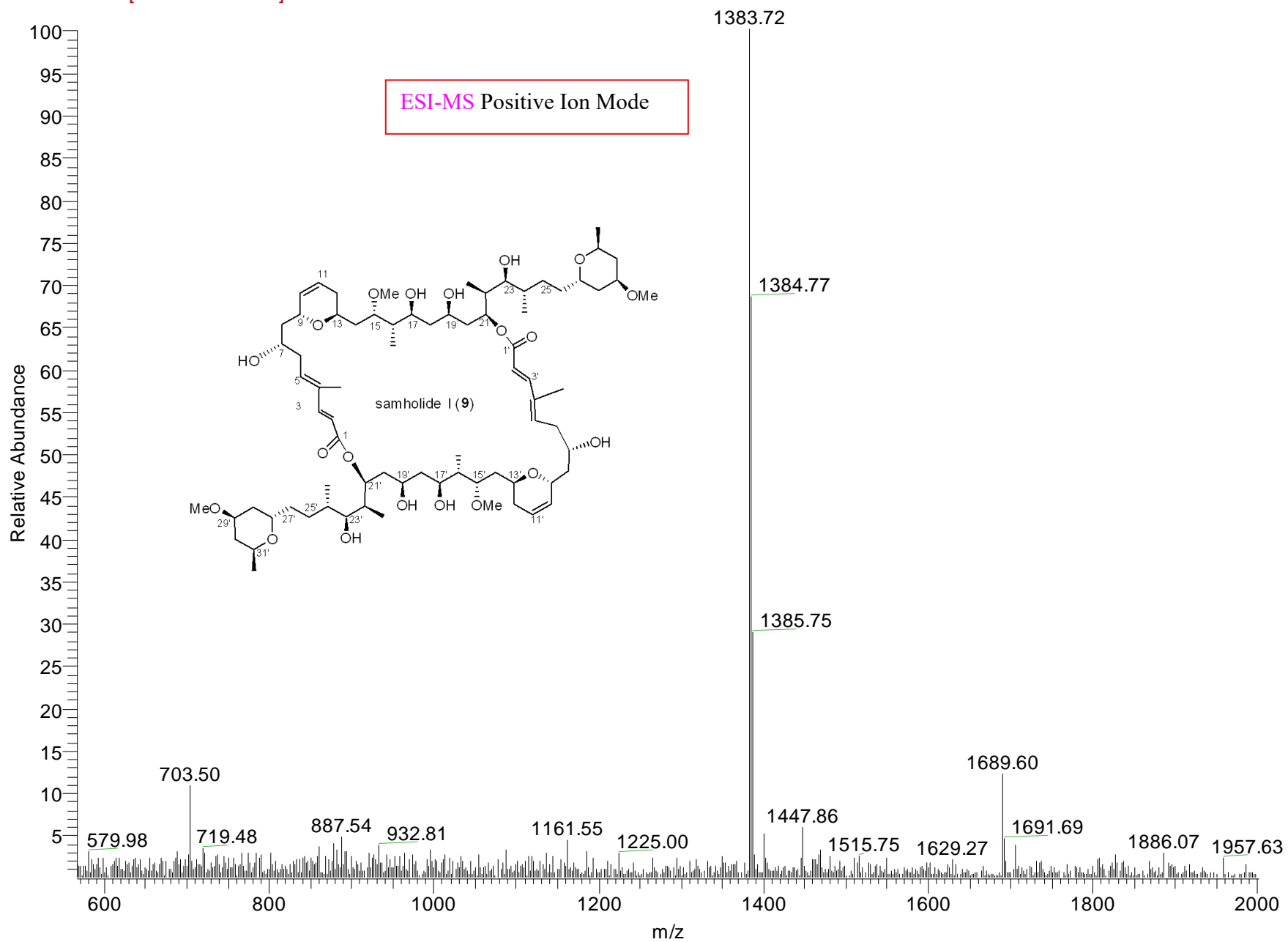
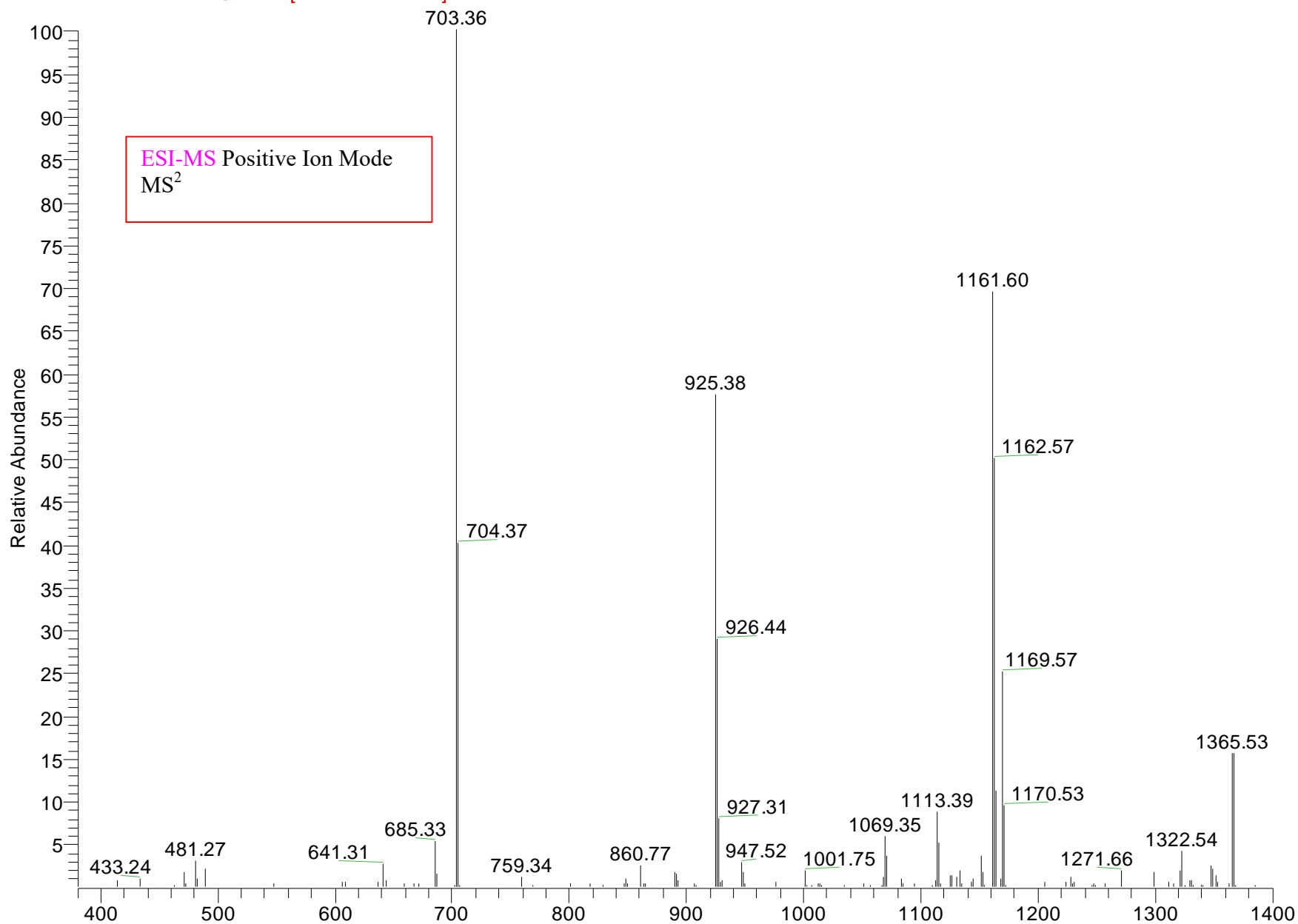


Figure S94 The ESI MS spectrum of samholide I (9)

2226H3C3-a #31-34 RT: 0.73-0.77 AV: 4 NL: 8.51E6

F: + c Full ms2 1384.00@35.00 [380.00-1400.00]

Figure S95 The ESI MS² spectrum of samholide I (9)

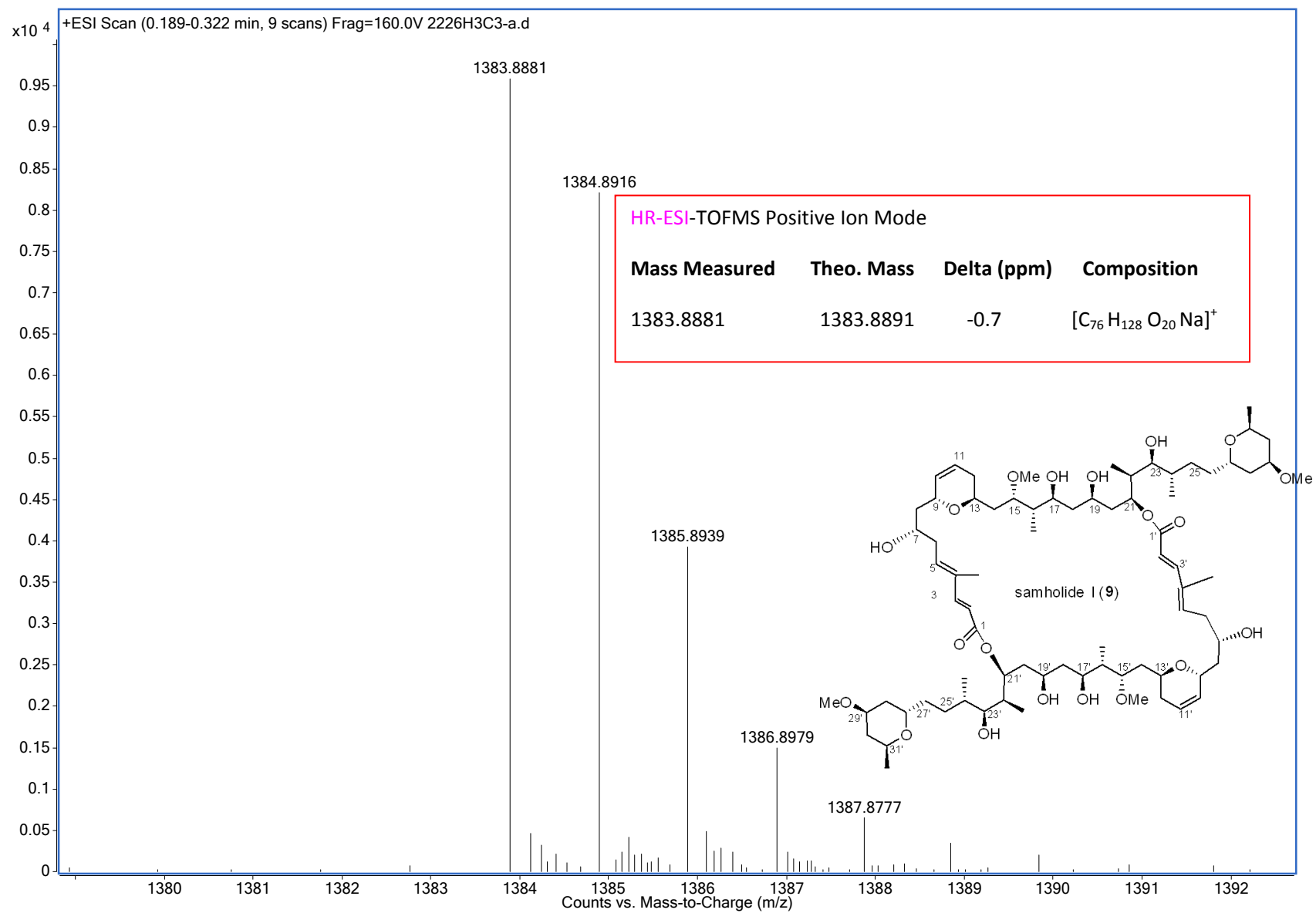
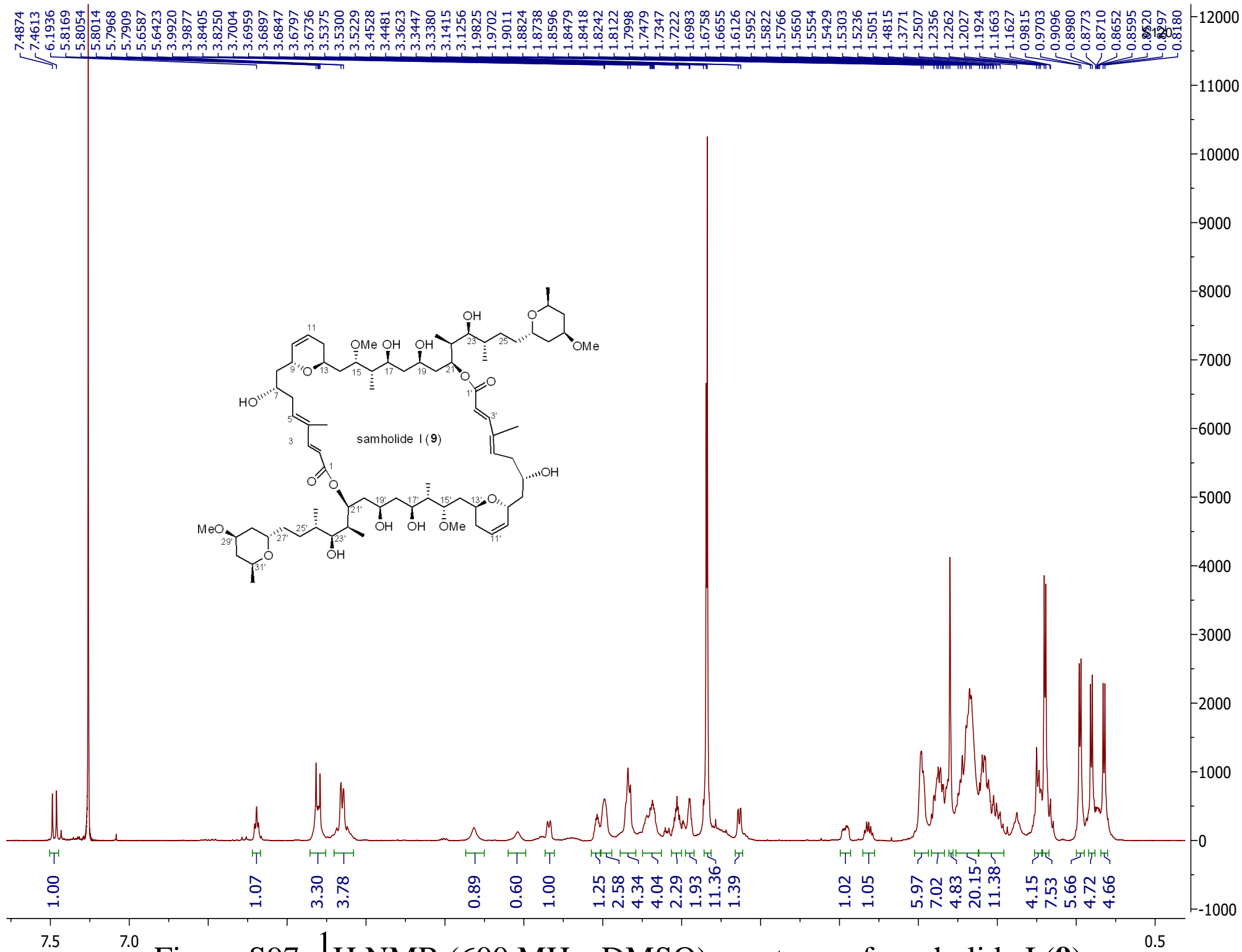


Figure S96 The positive HRESIMS spectrum of samholide I (9)



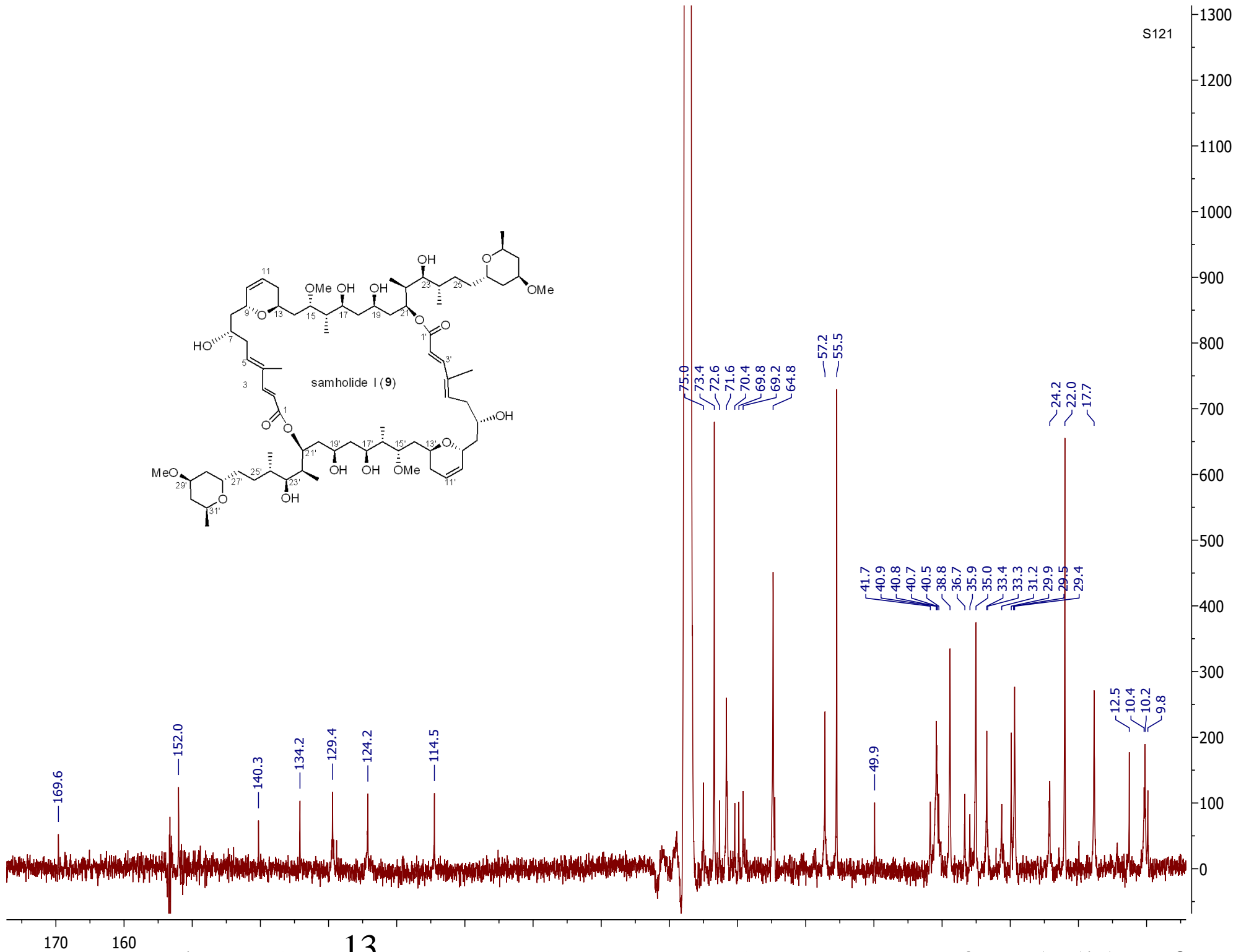


Figure S98 ^{13}C NMR (150 MHz, DMSO) spectrum of samholide I (9)

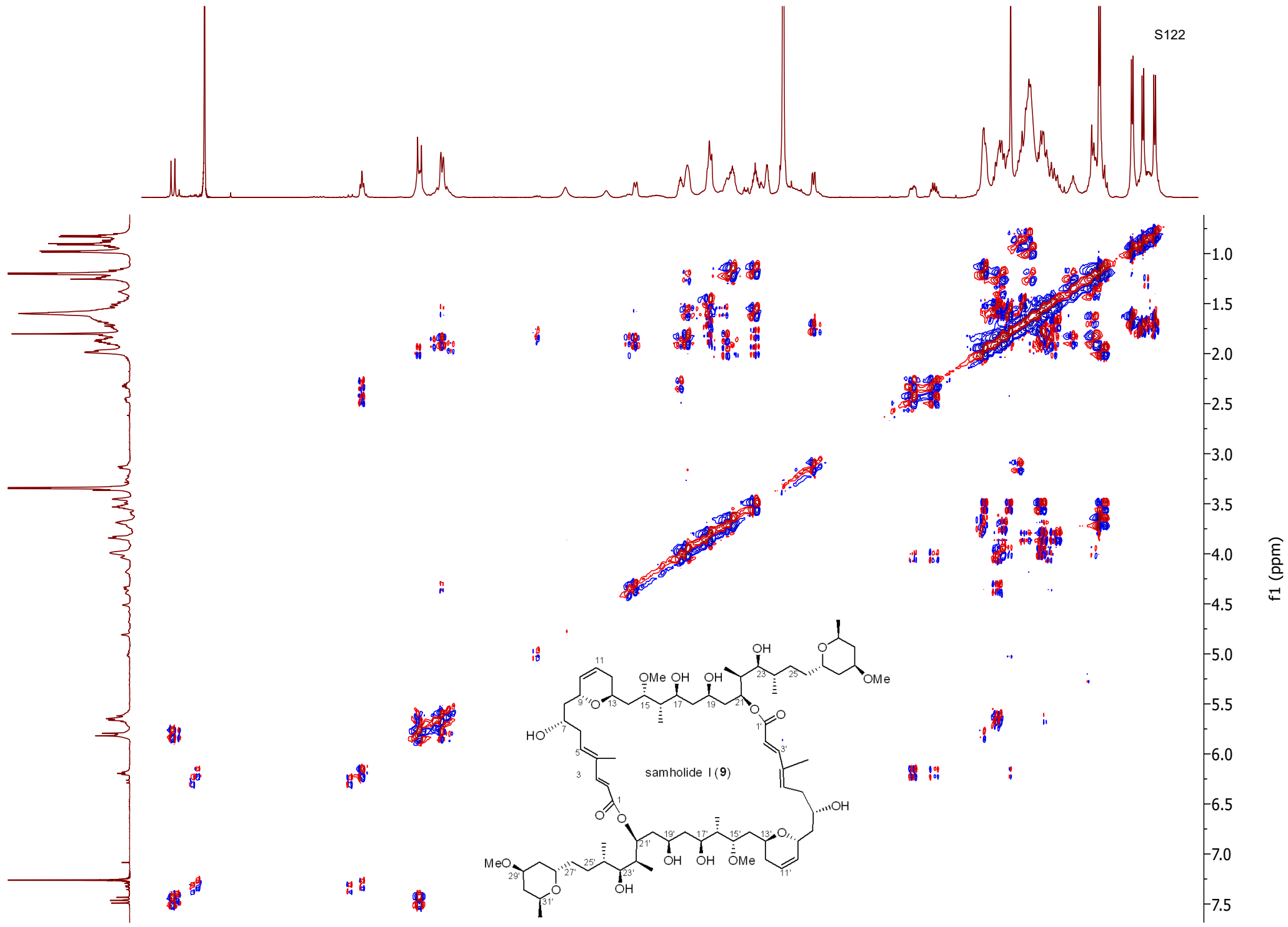


Figure S99 ^1H - ^1H COSY spectrum of samholide I (9)

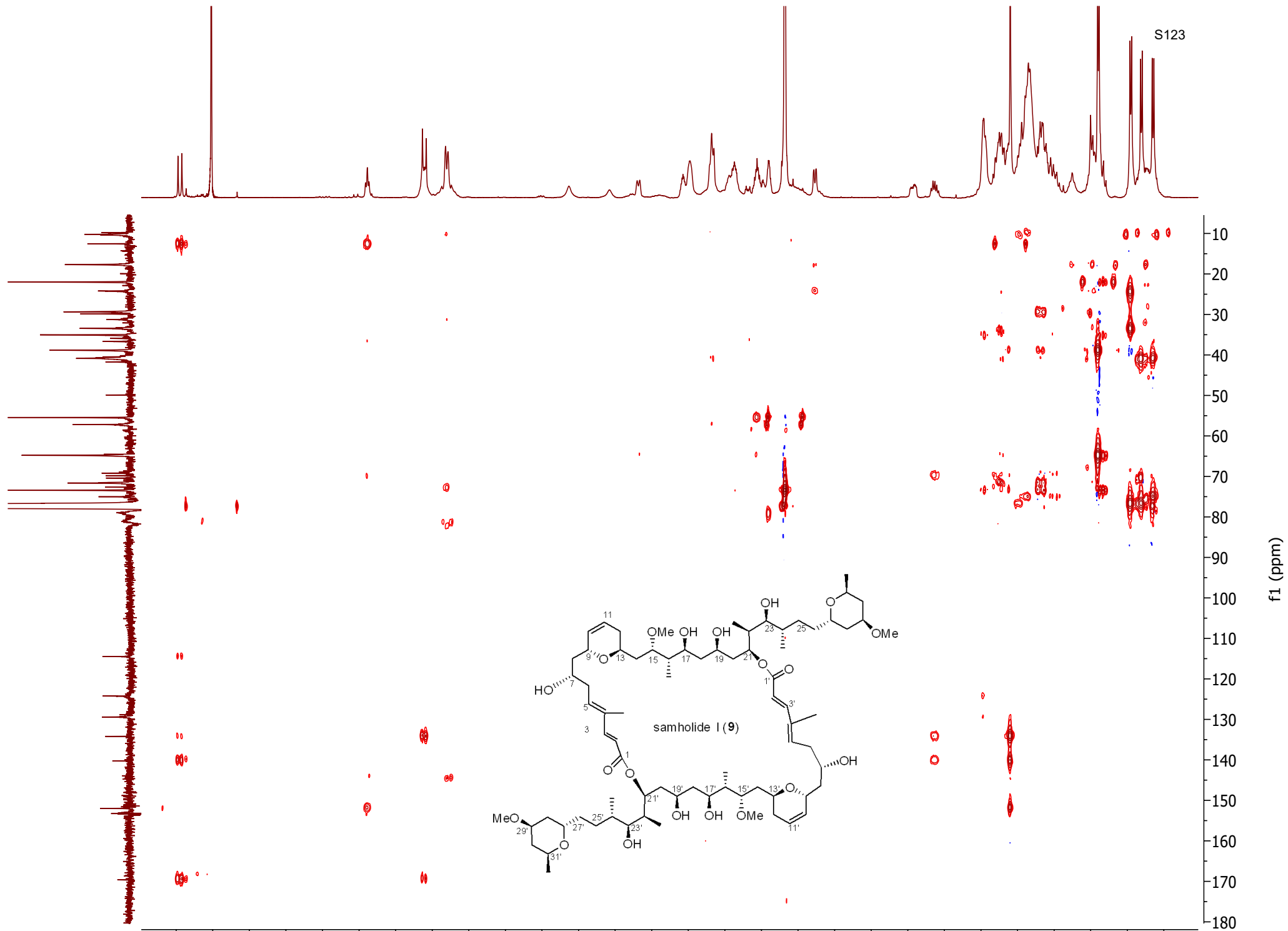


Figure S100 HMBC spectrum of samholide I (9)

S124

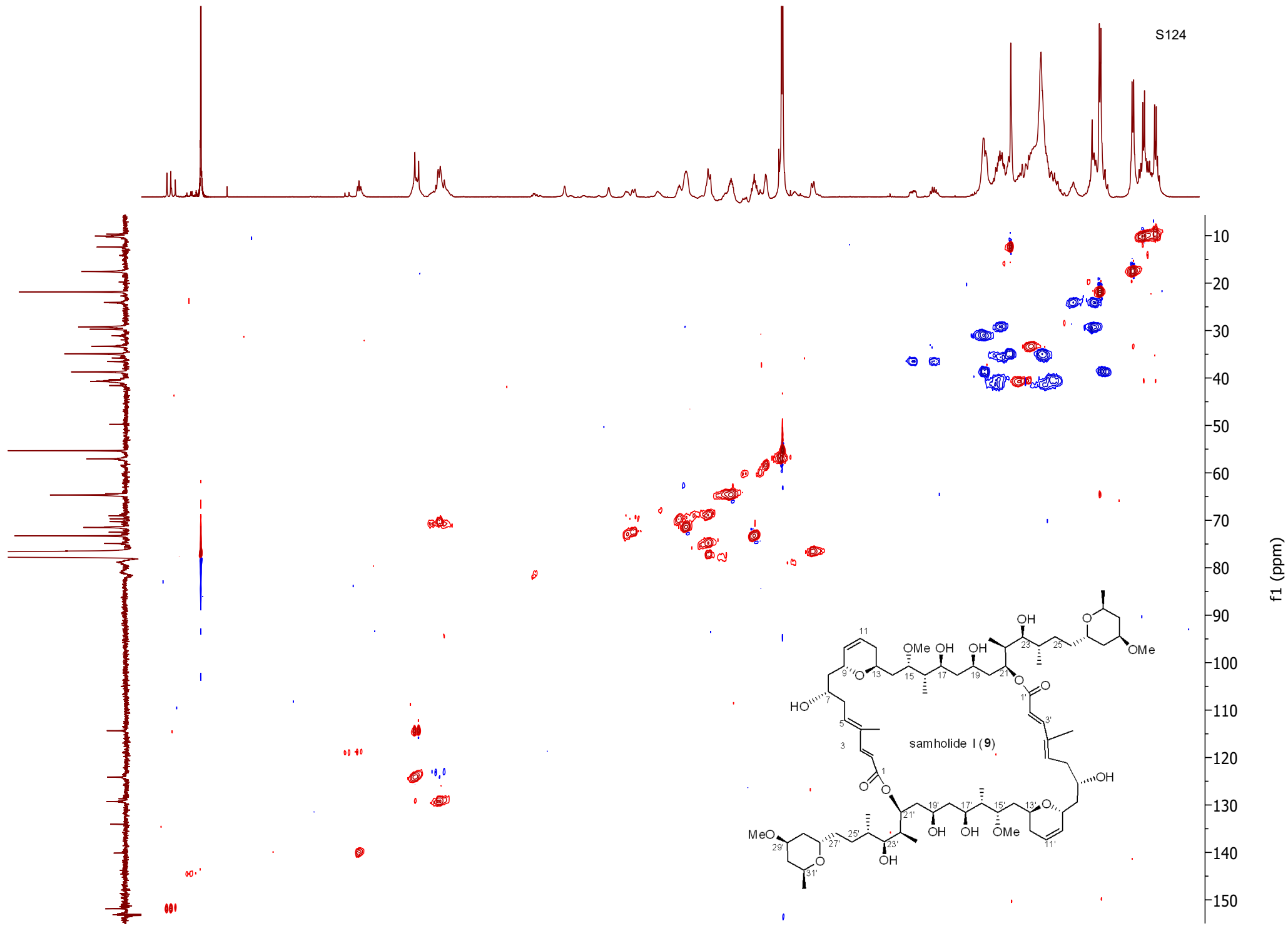


Figure S101 HMQC spectrum of samholide I (9)

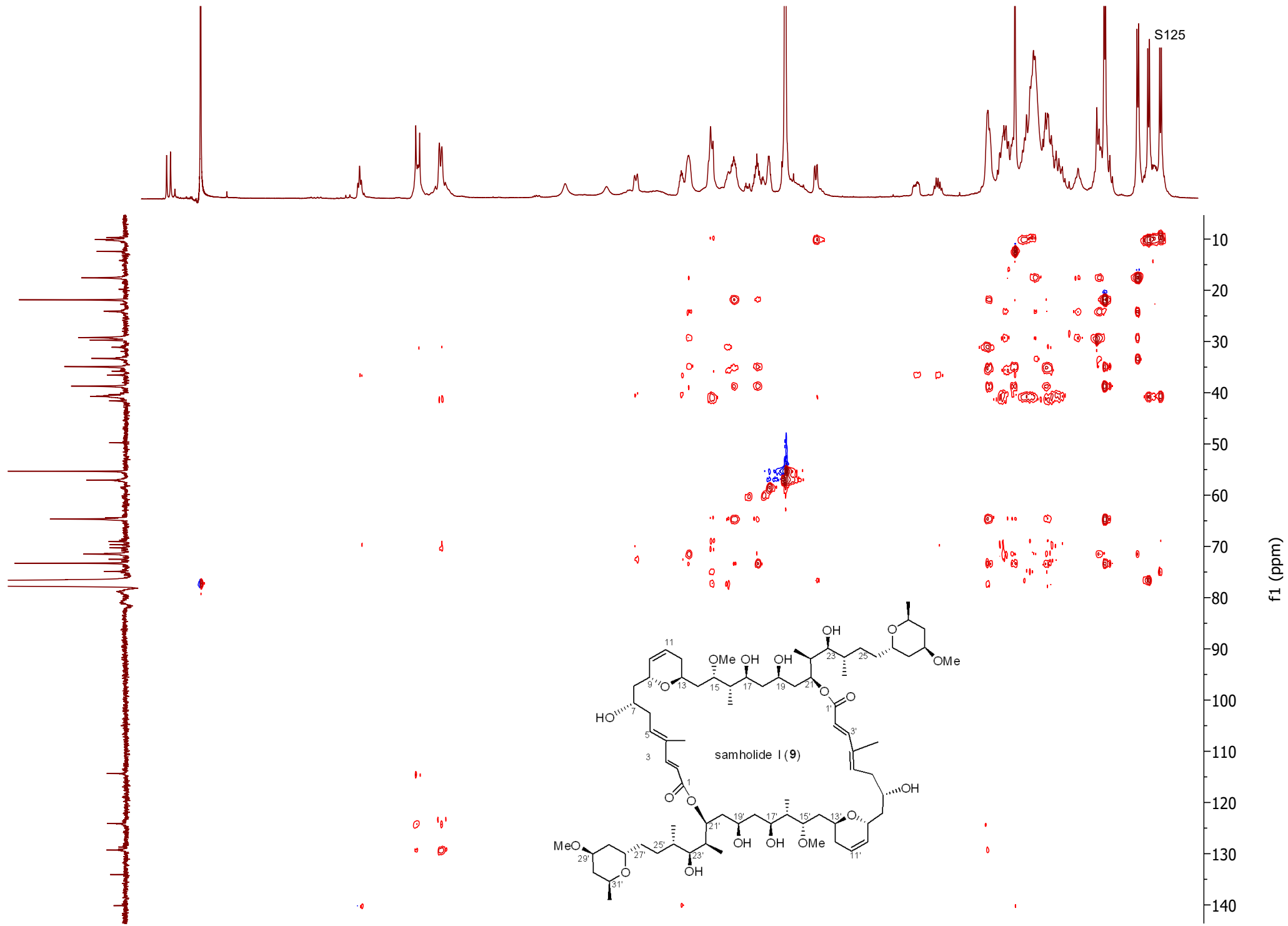


Figure S102 HSQC-TOCSY spectrum of samholide I (9)

S126

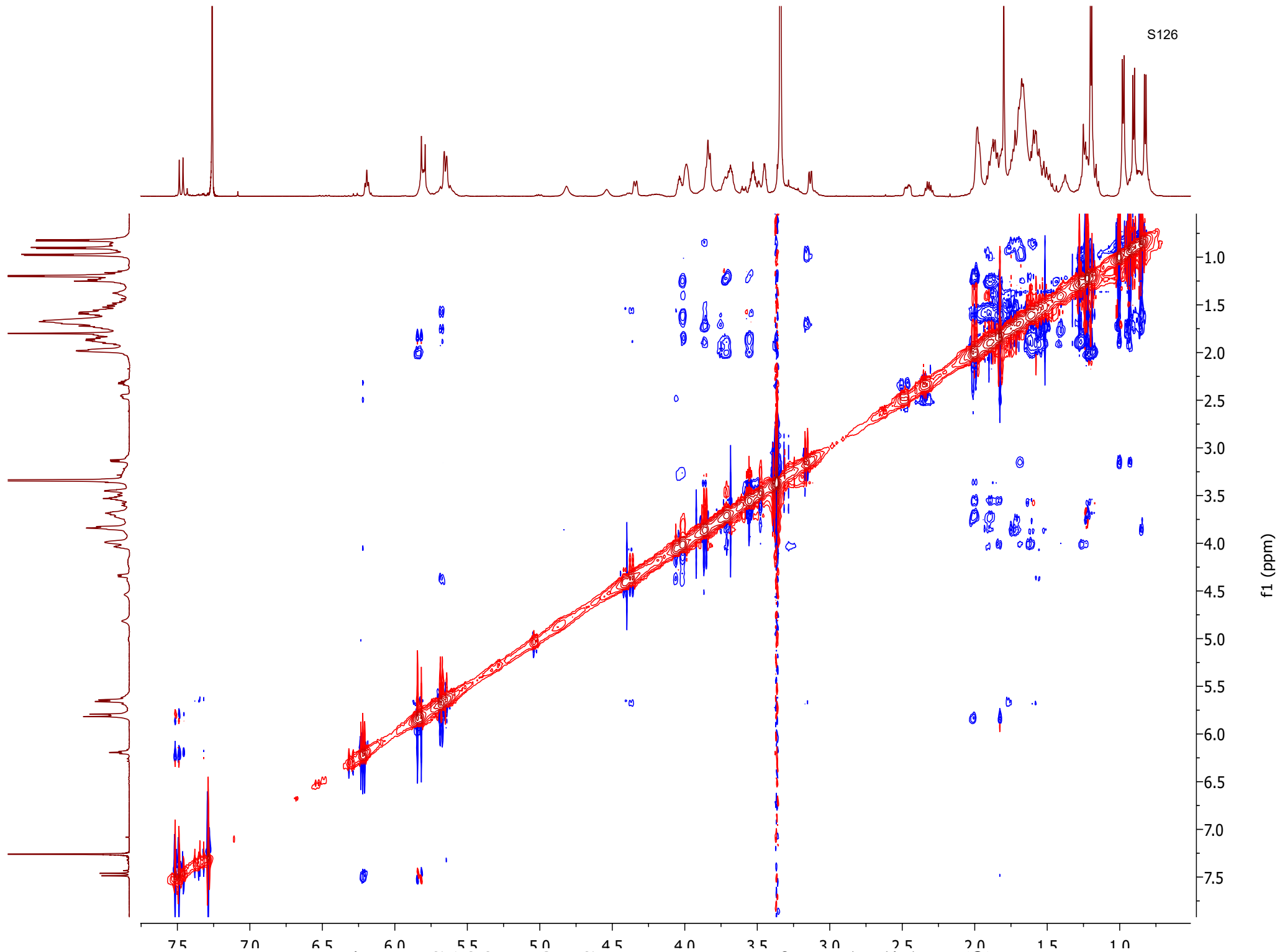


Figure S103 ROESY spectrum of samholide I (9)

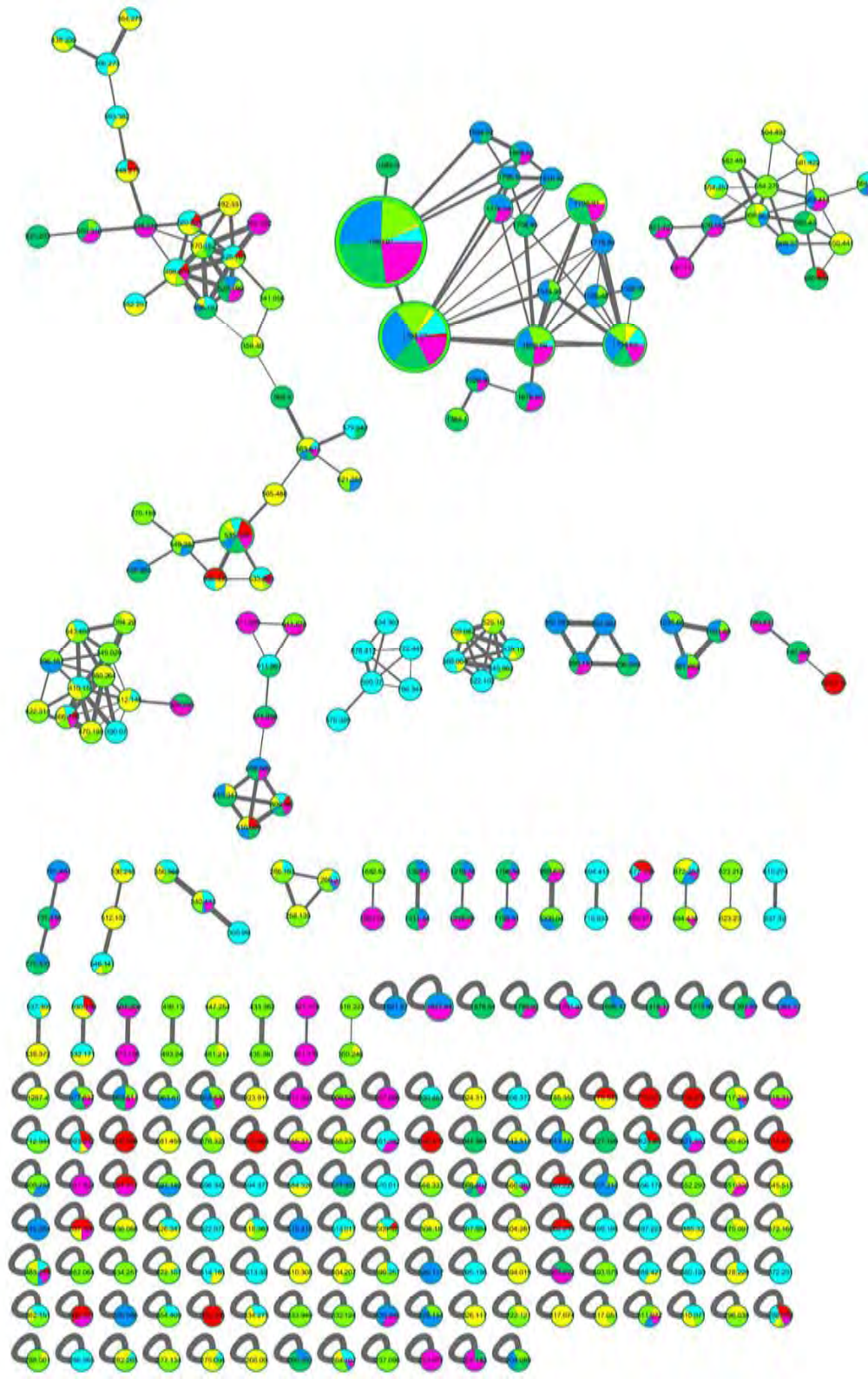


Figure S104 MS²-
based molecular
networking of fractions
D-I of cf. *Phormidium*
sp.