SUPPLEMENTARY DATA

Structure-activity relationship studies of lipophilic teicoplanin pseudoaglycon derivatives as new anti-influenza virus agents

Zsolt Szűcs, Viktor Kelemen, Son Le Thai, Magdolna Csávás, Erzsébet Rőth, Gyula Batta, Annelies Stevaert, Evelien Vanderlinden, Lieve Naesens, Pál Herczegh* and Anikó Borbás**

Table of Contents

Table S1. ^{1}H and ^{13}C NMR data for teicoplanin pseudoaglycon bis-alkylthio maleimide derivatives **13**, **14** and **17** (Series 1)

	chemical shifts in ppm					
	13		**14**		**17**	
assignment	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H
x1	56.9	6.11	56.9	6.11	56.9	6.10
x2	55.5	5.00	55.5	5.00	55.5	4.98
x3	57.8	5.31	57.8	5.32	57.8	5.32
x4	54.5	5.65	54.5	5.66	54.5	5.66
x5	53.4	4.34	53.4	4.34	53.4	4.34
x6	60.8	4.12	60.8	4.13	60.8	4.10
x7	59.1	4.30	59.1	4.32	59.0	4.30
1e	118.2	6.92	118.1	6.94	118.2	6.92
2e	124.8	7.23	124.8	7.23	124.8	7.22
3b	109.7	6.34	109.7	6.34	109.7	6.33
3f	102.2	6.50	102.1	6.49	102.1	6.50
4b	107.8	5.59	107.8	5.59	107.8	5.58
5f	125.1	6.65	125.2	6.65	125.2	6.64
6b	128.3	7.86	128.3	7.86	128.4	7.86
7f	107.7	6.50	107.7	6.49	107.8	6.49
z6	75.4	5.43	75.7	5.40	75.0	5.46
z2 (z'2)	36.8	2.78/3.26	36.8	2.77/3.25	36.9	2.77/3.24
GlcNAc 1	98.6	4.39	98.9	4.38	98.3	4.40
GlcNAc CH_3	22.8	1.84	22.9	1.84	22.8	1.83
MI 2,5	165.2	-	165.9	-	165.9	-
MI 3,4	135.3	-	n.d.	-	n.d.	-
Propyl 1	-	-	-	-	32.7	3.25/3.15
Propyl 2	-	-	-	-	23.2	1.56
Propyl 3	-	-	-	-	12.5	0.92
Butyl 1, 1'	30.4	3.19/3.25	-	-	-	-
Butyl 2, 2'	31.7	1.53	-	-	-	-
Butyl 3, 3'	20.6	1.34	-	-	-	-
Butyl 4, 4'	13.1	0.86	-	-	-	-
Hexyl 1, 1'	-	-	30.7	3.19/3.23	-	-
Hexyl 2, 2'	-	-	29.7	1.53	-	-
Hexyl 3, 3'	-	-	27.1	1.32	-	-
Hexyl 4, 4'	-	-	30.4	1.22	-	-
Hexyl 5, 5'	-	-	21.7	1.23	-	-
Hexyl 6, 6'	-	-	13.6	0.84	-	-
Dodecyl 1	-	-	-	-	30.8	3.23/3.17
Dodecyl 2	-	-	-	-	29.7	1.55
Dodecyl 3	-	-	-	-	27.4	1.32
Dodecyl 4-9	-	-	-	-	29.1-28.1	1.25-1.20
Dodecyl 10	-	-	-	-	31.1	1.22
Dodecyl 11	-	-	-	-	21.9	1.25
Dodecyl 12	-	-	-	-	13.7	0.85

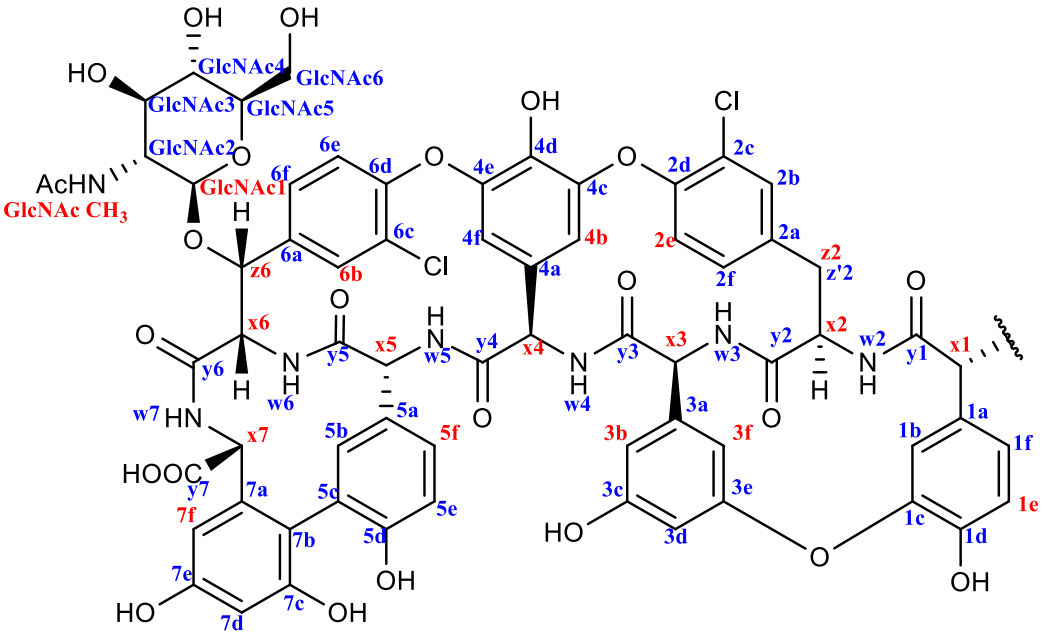


Figure S1. Atom numberings of teicoplanin pseudoaglycon for NMR assignment (used for all derivatives)

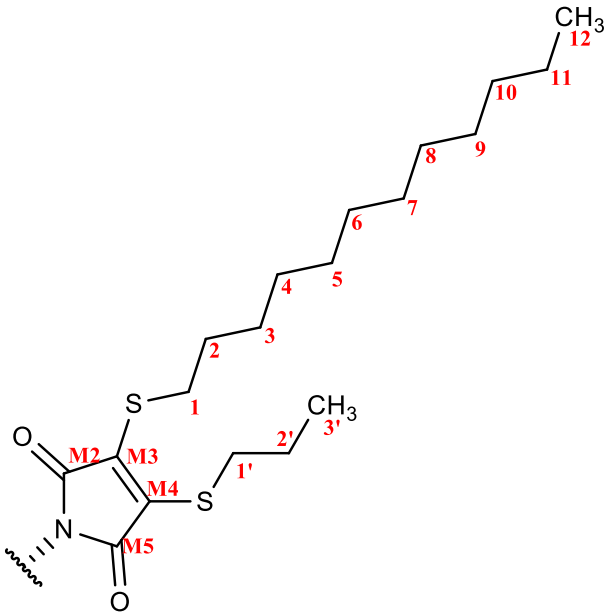


Figure S2. Atom numberings of Series 1 side chains for NMR assignment

Table S2. ^{1}H and ^{13}C NMR data for the triazole linked bis-alkylthio maleimide derivative **28** of teicoplanin pseudoaglycon (Series 2)

	chemical shifts in ppm	
	28	
assignment	^{1}H	^{13}C
x1	64.1	7.06
x2	55.5	4.87
x3	58.4	5.39
x4	54.7	5.62
x5	53.6	4.36
x6	60.9	4.14
x7	59.3	4.32
1b	119.6	7.01
1e	119.1	6.94
1f	125.7	6.83
2b	131.0	7.19
2e	125.2	7.15
2f	129.3	7.62
3b	110.1	6.33
3d	105.0	6.36
3f	104.0	6.54
4b	108.1	5.52
4f	104.6	5.08
5e	116.6	6.65
5f	125.5	6.63
6b	128.5	7.85
6e	123.4	7.26
6f	128.2	7.25
7d	101.7	6.30
7f	107.9	6.50
z6	76.1	5.40
z2/z'2	36.4	2.83/3.27
GlcNAc1	99.1	4.37
GlcNAc2	55.8	3.51
GlcNAc3	73.4	3.39
GlcNAc4	70.0	3.22
GlcNAc5	76.9	3.08
GlcNAc6	60.3	3.60
GlcNAc CH_3	23.0	1.84
Triazole 4	141.9	-
Triazole 5	123.0	7.69
M 2,5	165.7	-
M 3,4	135.8	-
M CH_2	33.5	4.59
Hexyl 1, 1'	31.1	3.22
Hexyl 2, 2'	29.9	1.54
Hexyl 3, 3'	27.4	1.32
Hexyl 4, 4'	30.6	1.23
Hexyl 5, 5'	21.9	1.23
Hexyl 6, 6'	13.8	0.83

Table S2. (continued) ^{1}H and ^{13}C NMR data* for the triazole linked bis-alkylthio maleimide derivatives **26, 27** of teicoplanin pseudoaglycon (Series 2)

	chemical shifts in ppm			
	26		**27**	
assignment	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.4	7.01	64.4	7.04
x2	55.3	4.93	55.5	4.88
x3	58.6	5.35	58.5	5.37
x4	54.6	5.59	54.8	5.61
x5	53.5	4.35	53.7	4.34
x6	60.9	4.11	61.1	4.13
x7	59.4	4.28	59.5	4.30
1e	118.9	6.87	119.2	6.92
2e	124.5	7.04	125.0	7.11
3b	109.8	6.30	110.2	6.32
3f	103.8	6.57	104.1	6.53
4b	107.9	5.53	108.1	5.52
5f	125.3	6.61	125.6	6.64
6b	128.5	7.85	128.7	7.84
7f	108.0	6.49	108.1	6.48
z6	75.4	5.44	76.3	5.38
z2/z’2	2.81/3.23	36.9	36.6	2.86/3.28
GlcNAc1	98.7	4.37	99.5	4.35
GlcNAc CH_3	23.0	1.83	23.1	1.85
Triazole 4	141.8	-	142.0	-
Triazole 5	123.3	7.67	123.1	7.66
M 2,5	165.6	-	165.8	-
M 3,4	135.6	-	135.8	-
M CH_2	33.5	4.60	33.6	4.59
Propyl 1, 1'	33.0	3.20	-	-
Propyl 2, 2'	23.4	1.56	-	-
Propyl 3, 3'	12.8	0.91	-	-
Butyl 1, 1'	-	-	30.9	3.22
Butyl 2, 2'	-	-	32.2	1.50
Butyl 3, 3'	-	-	21.1	1.31
Butyl 4, 4'	-	-	13.4	0.83

*only signals that are crucial for identification are listed

Table S2. (continued) ^{1}H and ^{13}C NMR data* for the triazole linked bis-alkylthio maleimide derivatives **29-31** of teicoplanin pseudoaglycon (Series 2)

	29		**30**		**31**	
assignment	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.6	7.05	64.7	7.01	64.0	7.07
x2	55.6	4.90	55.4	4.95	55.3	4.85
x3	58.7	5.37	58.9	5.34	58.4	5.39
x4	54.9	5.62	54.7	5.57	54.8	5.63
x5	53.9	4.35	53.6	4.36	53.7	4.34
x6	61.2	4.15	61.0	4.15	61.0	4.13
x7	59.6	4.31	59.6	4.26	59.2	4.31
1e	119.2	6.92	118.9	6.85	119.0	6.95
2e	125.0	7.11	124.6	6.99	125.3	7.14
3b	110.1	6.33	110.0	6.30	110.0	6.33
3f	104.0	6.56	103.8	6.56	103.9	6.53
4b	108.1	5.54	108.0	5.53	108.0	5.53
5f	125.6	6.65	125.5	6.62	125.4	6.63
6b	128.7	7.86	128.7	7.80	128.5	7.86
7f	108.1	6.49	108.1	6.47	107.9	6.50
z6	76.1	5.40	76.4	5.37	75.7	5.42
z2/z'2	36.7	3.27/2.85	37.3	2.78/3.21	36.1	2.88/3.29
GlcNAc1	99.3	4.38	99.7	4.34	98.9	4.38
GlcNAc CH_3	23.1	1.84	23.2	1.84	22.9	1.83
T4	141.8	-	142.1	-	141.9	-
T5	123.2	7.70	123.3	7.64	122.9	7.65
M 2,5	165.7	-	165.8	-	165.5	-
M 3,4	135.8	-	135.9	-	135.6	-
M CH_2	33.5	4.59	33.6	4.58	33.3	4.58
Alkyl α/α'	31.1	3.22	31.3	3.21	-	-
Alkyl β/β'	30.0	1.55	30.1	1.53	-	-
Alkyl γ/γ'	27.8	1.33	27.8	1.31	-	-
Alkyl bulk**	28.5	1.22	29.1	1.21	-	-
Alkyl ω-2/ω-2'	31.3	1.21	31.4	1.21	-	-
Alkyl ω-1/ω-1'	22.1	1.23	22.2	1.23	-	-
Alkyl ω/ω'	14.0	0.84	14.0	0.83	-	-
α-G1	-	-	-	-	95.8	5.38
α-G2	-	-	-	-	69.7	4.31
α-G3	-	-	-	-	70.2	4.59
α-G4	-	-	-	-	71.0	4.20
α-G5	-	-	-	-	67.3	3.80
α-G6	-	-	-	-	31.3	3.44 / 3.26
α-G-C_q	-	-	-	-	108.0/108.6	-
α-G-CH_3	-	-	-	-	25.6	1.28
	-	-	-	-	24.4	1.23

*only signals that are crucial for identification are listed

** δ to ω–3 methylene groups of alkyl substituents

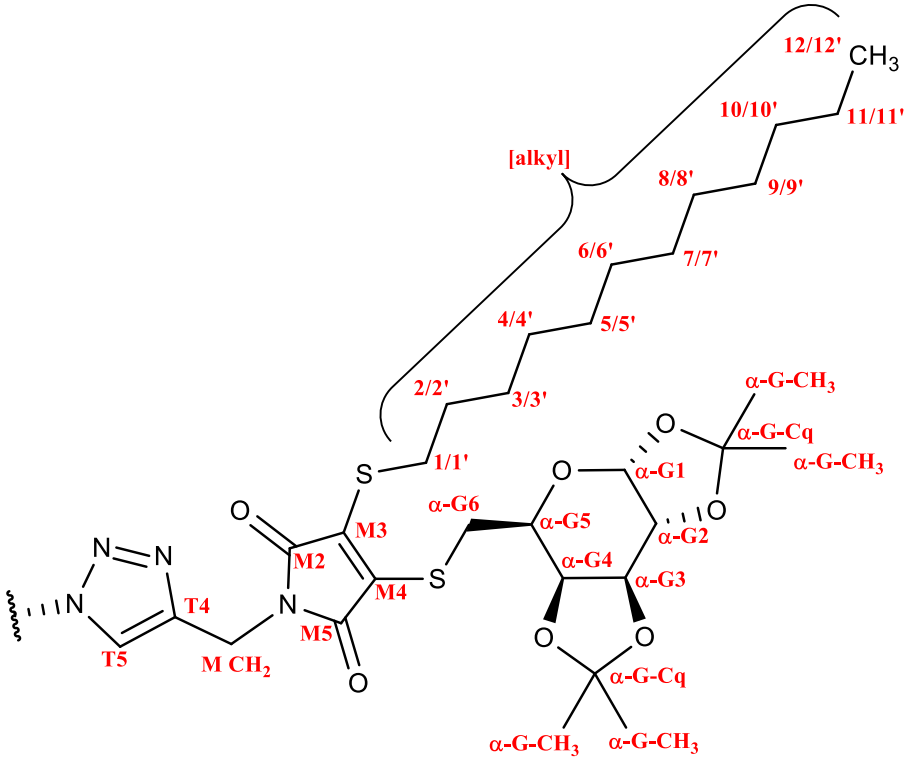


Figure S3. Atom numberings of Series 2 side chains for NMR assignment (This structure is only an illustration)

Table S3. ^{1}H and ^{13}C NMR data for the triazole-tetraethylene glycol linked bis-alkylthio maleimide derivative **42** of teicoplanin pseudoaglycon (Series 3)

			42		
assignment	^{1}H	^{13}C	assignment	^{1}H	^{13}C
x1	7.07	64.3	GlcNAc1	4.39	98.8
x2	4.91	55.4	GlcNAc2	3.52	55.9
x3	5.36	58.5	GlcNAc3	3.37	73.5
x4	5.61	54.7	GlcNAc4	3.20	69.9
x5	4.35	53.6	GlcNAc5	3.08	76.9
x6	4.13	61.0	GlcNAc6	3.58	60.3
x7	4.30	59.4	GlcNAc CH_3	1.83	23.0
1b	6.99	119.8			
1e	6.89	119.0	TEG a	4.44	63.4
1f	6.80	125.7	TEG h	3.49	66.9
2b	7.17	130.8	TEG i	3.55	37.8
2e	7.10	124.8	TEG bulk	3.48-3.38	70.0-69.0
3b	6.32	109.9			
3d	6.33	104.8	Triazole 4	-	143.7
3f	6.56	103.9	Triazole 5	7.71	124.2
4b	5.53	108.0			
4f	5.08	104.6	M 2,5	-	166.1
5e	6.61	116.5	M 3,4	-	135.5
5f	6.63	125.4			
6b	7.84	128.6	Hexyl 1, 1'	3.23	31.1
6e	7.25	123.3	Hexyl 2, 2'	1.55	30.0
6f	7.25	128.0	Hexyl 3, 3'	1.34	27.4
7d	6.27	101.6	Hexyl 4, 4'	1.24	30.7
7f	6.49	108.1	Hexyl 5, 5'	1.24	22.0
z6	5.43	75.7	Hexyl 6, 6'	0.84	13.9
z2/z’2	3.28/2.85	36.7			

Table S3. (continued) ^{1}H and ^{13}C NMR data* for the triazole-tetraethylene glycol linked bis-alkylthio maleimide derivatives of teicoplanin pseudoaglycon **40-46** (Series 3)

	chemical shifts in ppm			
	40		**41**	
assignment	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.3	7.06	64.1	7.07
x2	55.4	4.90	55.3	4.89
x3	58.5	5.37	58.3	5.37
x4	54.7	5.61	54.6	5.61
x5	53.7	4.34	53.5	4.35
x6	61.0	4.12	60.8	4.14
x7	59.2	4.32	59.3	4.29
1e	119.1	6.90	118.9	6.91
2e	124.6	7.10	124.8	7.11
3b	110.0	6.32	109.9	6.32
3f	104.0	6.57	103.8	6.55
4b	108.1	5.54	107.9	5.53
5f	125.4	6.63	125.2	6.63
6b	128.6	7.86	128.4	7.84
7f	108.2	6.52	107.9	6.48
z6	75.2	5.44	75.8	5.41
z2/z'2	36.7	2.86/3.28	36.5	2.86/3.28
GlcNAc1	98.4	4.39	98.9	4.38
GlcNAc CH_3	23.1	1.84	22.9	1.83
Triazole 4	143.7	-	n.d.	-
Triazole 5	124.2	7.71	124.5	7.72
M 2,5	166.0	-	n.d.	-
M 3,4	135.4	-	n.d.	-
TEG a	63.4	4.44	63.2	4.43
TEG h	66.9	3.50	66.7	3.49
TEG i	37.8	3.55	37.7	3.55
TEG bulk	70.2-69.2	3.49-3.41	69.8-68.8	3.49-3.41
Propyl 1, 1'	33.0	3.22	-	-
Propyl 2, 2'	23.5	1.59	-	-
Propyl 3, 3'	12.8	0.93	-	-
Butyl 1, 1'	-	-	30.7	3.23
Butyl 2, 2'	-	-	32.0	1.54
Butyl 3, 3'	-	-	20.9	1.36
Butyl 4, 4'	-	-	13.3	0.85

*only signals that are crucial for identification are listed

Table S3. (continued**)** ^{1}H and ^{13}C NMR data* for the triazole-TEG linked bis-alkylthio maleimide derivatives of teicoplanin pseudoaglycon **40-46** (Series 3)

	chemical shifts in ppm			
	43		**44**	
assignment	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.6	7.04	64.2	7.08
x2	55.4	4.96	55.5	4.87
x3	58.8	5.35	58.4	5.39
x4	54.7	5.59	54.8	5.63
x5	53.6	4.35	53.7	4.34
x6	61.0	4.16	61.1	4.12
x7	59.5	4.27	59.1	4.33
1e	119.0	6.88	119.2	6.95
2e	124.7	7.03	125.0	7.17
3b	110.0	6.31	110.2	6.34
3f	103.9	6.56	104.1	6.54
4b	108.0	5.53	108.2	5.54
5f	125.8	6.63	125.6	6.64
6b	128.7	7.81	128.7	7.85
7f	108.1	6.50	107.8	6.45
z6	76.4	5.36	75.8	5.40
z2/z'2	37.2	2.83/3.25	36.4	2.90/3.31
GlcNAc1	99.6	4.35	99.0	4.38
GlcNAc CH_3	23.2	1.84	23.1	1.83
Triazole 4	143.7	-	143.8	-
Triazole 5	124.3	7.68	124.1	7.72
M 2,5	166.1	-	166.1	-
M 3,4	135.6	-	135.6	-
TEG a	63.5	4.43	63.4	4.43
TEG h	67.0	3.49	67.0	3.49
TEG i	37.9	3.54	37.8	3.55
TEG bulk	69.8-68.9	3.49-3.39	69.8-69.0	3.49-3.39
Alkyl α, α'	31.2	3.22	31.1	3.22
Alkyl β, β'	30.2	1.55	30.1	1.55
Alkyl γ, γ'	27.9	1.32	27.8	1.33
Alkyl bulk**	28.7	1.22	29.0	1.21
Alkyl ω-2	31.3	1.21	31.4	1.20
Alkyl ω-1	22.3	1.25	22.1	1.24
Alkyl ω	14.1	0.83	13.9	0.84

*only signals that are crucial for identification are listed

** δ to ω–3 methylene groups of alkyl substituents

Table S3. (continued**)** ^{1}H and ^{13}C NMR data* for the triazole-TEG linked bis-alkylthio maleimide derivatives of teicoplanin pseudoaglycon **40-46** (Series 3)

	chemical shifts in ppm			
	45		**46**	
assignment	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.5	7.06	63.9	7.09
x2	55.2	4.96	55.4	4.84
x3	58.6	5.35	58.2	5.39
x4	54.4	5.59	54.6	5.67
x5	53.4	4.37	53.7	4.29
x6	60.7	4.17	60.9	4.12
x7	59.3	4.27	57.4	4.39
1e	118.9	6.89	119.1	6.94
2e	124.6	7.03	125.0	7.20
3b	109.8	6.32	110.2	6.33
3f	103.7	6.58	104.0	6.52
4b	108.0	5.54	108.2	5.53
5f	125.4	6.64	125.8	6.67
6b	128.7	7.82	128.7	7.85
7f	108.0	6.51	106.5	6.32
z6	76.2	5.37	75.5	5.33
z2/z'2	37.1	2.81/3.25	36.1	2.91/3.30
GlcNAc1	99.5	4.37	98.6	4.34
GlcNAc CH_3	22.9	1.85	23.1	1.86
Triazole 4	143.7	-	143.8	-
Triazole 5	124.2	7.69	124.1	7.74
M 2,5	166.0	-	166.1	-
M 3,4	135.5	-	135.4	-
TEG a	63.3	4.44	63.2	4.43
TEG h	66.9	3.48	66.8	3.49
TEG i	37.6	3.54	37.6	3.54
TEG bulk	70.2-69.0	3.53-3.40	70.0-69.0	.50-3.41
TEG1, 1'	-	-	30.7	3.42
TEG2, 2'	-	-	69.8	3.61
TEG7, 7'	-	-	72.3	3.40
TEG8, 8'	-	-	60.2	3.47
α-G1	95.9	5.44	-	-
α-G2-5	67.4	3.83	-	-
	69.7	4.34	-	-
	70.3	4.61	-	-
	71.1	4.22	-	-
α-G6	31.5	3.46 / 3.29	-	-
α-G-C_q	108.6/108.0	-	-	-
α-G-CH_3	25.8/25.6	1.38/1.33	-	-
	24.5	1.25		

*only signals that are crucial for identification are listed

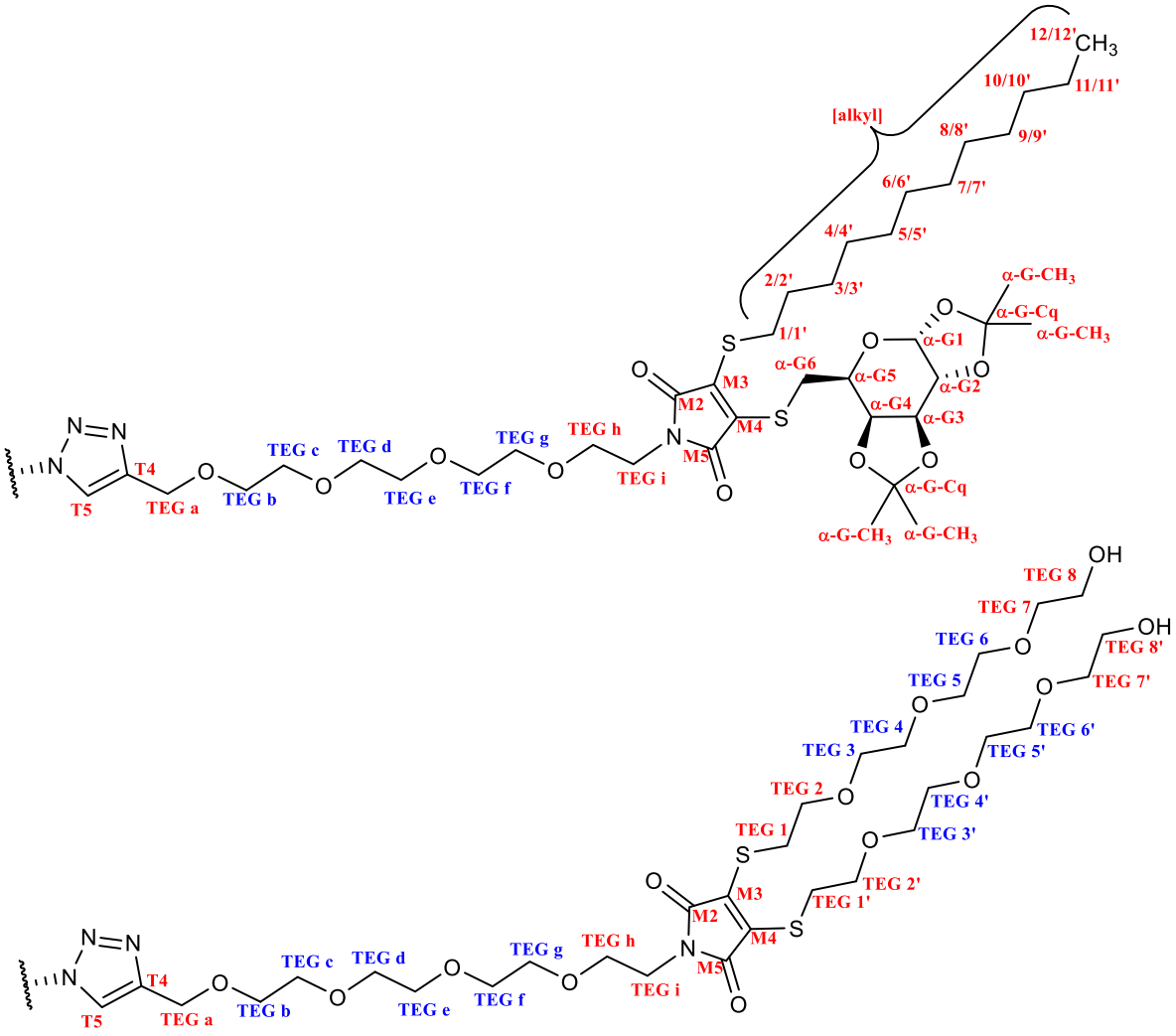


Figure S4. Atom numberings of Series 3 side chains for NMR assignment
(First structure is an illustration)

Table S4. ^{1}H and ^{13}C NMR data for teicoplanin pseudoaglycon TEG-monoalkyl derivatives **60-63** (Series 5)

assignment	**60**		**61**	
	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.1	7.07	64.2	7.07
x2	55.5	4.86	55.4	4.88
x3	58.4	5.38	58.3	5.38
x4	54.7	5.62	54.8	5.62
x5	53.6	4.34	53.7	4.34
x6	61.0	4.11	61.0	4.14
x7	59.4	4.30	59.4	4.30
1e	119.1	6.93	118.9	6.93
2e	124.9	7.15	124.9	7.14
3b	110.0	6.32	110.1	6.32
3f	104.0	6.55	104.0	6.56
4b	108.0	5.52	108.1	5.53
5f	125.3	6.61	125.4	6.62
6b	128.5	7.85	128.5	7.85
7f	107.9	6.48	108.0	6.48
z6	75.6	5.43	75.9	5.41
z2/z'2	36.4	2.88/3.30	36.5	2.88/3.28
G1	98.8	4.39	99.0	4.38
G-CH_3	23.1	1.82	23.1	1.83
TA 4	144.0	-	144.0	-
TA 5	124.1	7.71	124.1	7.71
TA Me	63.3	4.43	63.4	4.43
TB 4	143.8		143.8	-
TB 5	124.2	8.01	124.2	8.01
TB Me	63.3	4.45	63.4	4.45
TEG bulk	69.6	3.43	69.7	3.43
	69.5	3.47	69.5	3.47
TEG g	68.7	3.77	68.8	3.77
TEG h	49.3	4.49	49.4	4.48
Hexyl 1	-	-	69.6	3.39
Hexyl 2	-	-	29.2	1.47
Hexyl 3	-	-	25.4	1.25
Hexyl 4	-	-	31.2	1.22
Hexyl 5	-	-	22.1	1.23
Hexyl 6	-	-	14.0	0.83
Butyl 1	69.4	3.40	-	-
Butyl 2	31.6	1.48	-	-
Butyl 3	19.2	1.29	-	-
Butyl 4	14.1	0.85	-	-

Table S4. (continued) ^{1}H and ^{13}C NMR data for teicoplanin pseudoaglycon TEG-monoalkyl derivatives **60-63** (Series 5)

assignment	**62**		**63**	
	^{13}C	^{1}H	^{13}C	^{1}H
x1	64.6	7.03	64.5	7.04
x2	55.3	4.96	55.3	4.97
x3	58.8	5.33	58.8	5.34
x4	54.6	5.57	54.5	5.58
x5	53.5	4.35	53.5	4.36
x6	60.9	4.16	60.9	4.15
x7	59.6	4.27	59.5	4.27
1e	119.0	6.85	119.0	6.86
2e	124.7	7.00	124.6	7.00
3b	109.7	6.30	109.8	6.31
3f	103.7	6.56	103.7	6.58
4b	108.0	5.53	107.9	5.53
5f	125.5	6.63	125.4	6.62
6b	128.7	7.80	128.6	7.81
7f	108.0	6.47	108.0	6.48
z6	76.2	5.36	76.2	5.38
z2/z'2	37.3	2.79/3.22	37.2	2.80/3.23
G1	99.6	4.34	99.5	4.35
G-CH_3	23.1	1.84	23.0	1.84
TA 4	144.1	-	143.6	-
TA 5	124.2	7.67	124.3	7.67
TA Me	63.3	4.41	63.4	4.40
TB 4	144.4	-	144.0	-
TB 5	124.2	8.01	124.3	8.01
TB Me	63.3	4.44	63.4	4.44
TEG bulk	69.7	3.43	69.7	3.44
	69.6	3.47	69.5	3.48
TEG g	68.7	3.77	68.7	3.77
TEG h	49.4	4.47	49.3	4.48
Decyl 1	-	-	69.6	3.39
Decyl 2	-	-	29.2	1.46
Decyl 3	-	-	25.7	1.23
Decyl 4-7	-	-	28.9	1.22
Decyl 8	-	-	31.3	1.22
Decyl 9	-	-	22.1	1.23
Decyl 10	-	-	14.0	0.84
Octyl 1	69.5	3.39	-	-
Octyl 2	29.2	1.46	-	-
Octyl 3	25.6	1.25	-	-
Octyl 4-5	28.8	1.23	-	-
Octyl 6	31.3	1.20	-	-
Octyl 7	22.1	1.25	-	-
Octyl 8	13.6	0.84	-	-

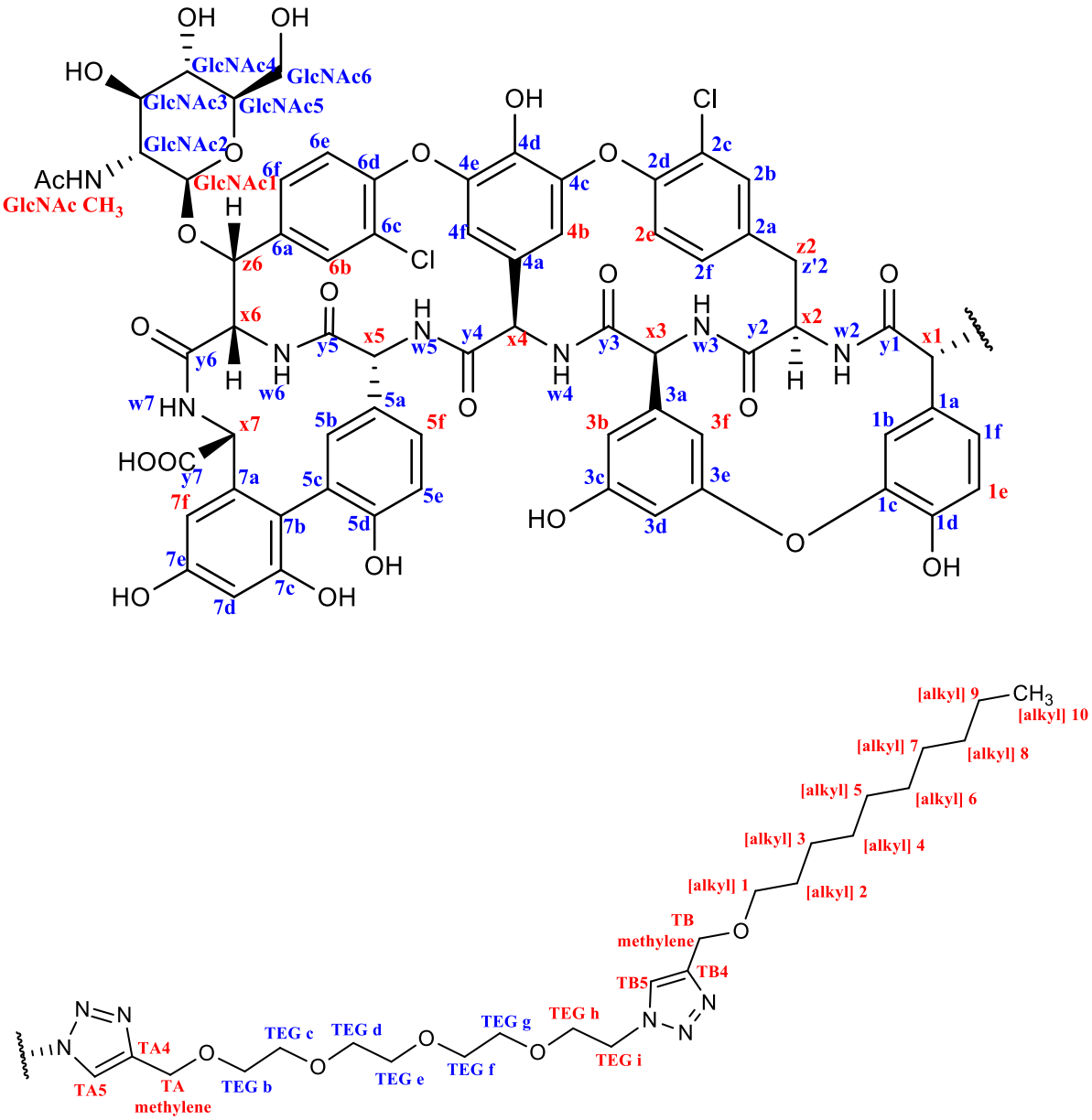


Figure S5. Atom numberings of Series 5 side chains for NMR assignment

Table S5. ^{1}H and ^{13}C NMR data for the sulfonamide derivatives **72-79** of teicoplanin pseudoaglycon (Series 6)

	chemical shifts in ppm			
assignment	**72**		**73**	
	^{13}C	^{1}H	^{13}C	^{1}H
x1	58.2 [a]	5.27 [a]	58.1[a]	5.27[a]
x2	55.2	4.25	55.2	4.24
x3	58.0[a]	5.20[a]	58.1[a]	5.27[a]
x4	54.7	5.60	54.7	5.60
x5	53.7	4.31	53.7	4.32
x6	61.0	4.11	61.0	4.13
x7	59.0	4.32	59.3	4.32
1e	118.5	6.92	118.6	6.68
2e	124.8	7.20	124.9	7.20
3b	110.0	6.27	110.1	6.27
3f	104.3	6.39	104.4	6.39
4b	107.7	5.45	107.8	5.46
5f	125.3	6.62	125.4	6.63
6b	128.5	7.85	128.7	7.86
7f	107.8	6.46	107.9	6.50
z6	75.8	5.39	76.1	5.38
z2/z'2	35.6	2.43/3.15	36.0	2.50/3.15
G1	99.0	4.38	99.3	4.36
G-CH_3	23.1	1.83	23.1	1.84
T2,6	127.1	7.73	-	-
T3,5	129.3	7.38	-	-
T-Me	21.0	2.37	-	-
BS1	-	-	140.9	-
BS2,6	-	-	127.0	7.86
BS3,5	-	-	128.9	7.59
BS4	-	-	132.6	7.64

[a]ambiguous

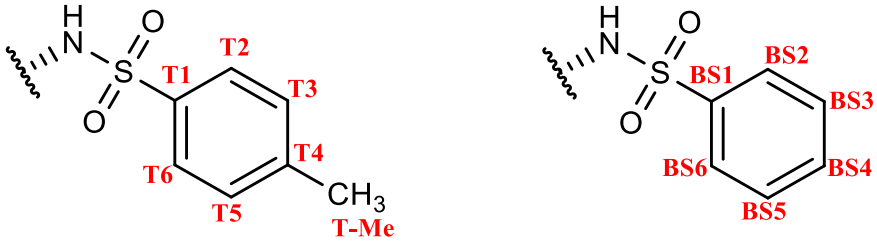


Figure S6. Atom numberings of Series 6 side chains for NMR assignment (for compounds **72** and **73**, respectively)

Table S5. (continued) ^{1}H and ^{13}C NMR data for the sulfonamide derivatives **72-79** of teicoplanin pseudoaglycon (Series 6)

	chemical shifts in ppm			
assignment	**74**		**75**	
	^{13}C	^{1}H	^{13}C	^{1}H
x1	58.2[a]	5.24[a]	58.1	5.29
x2	55.6	4.29	55.3	4.27
x3	58.4[a]	5.29[a]	58.3	5.28
x4	54.8	5.61	54.7	5.60
x5	53.8	4.33	53.7	4.32
x6	61.1	4.14	61.0	4.13
x7	59.5	4.32	59.3	4.33
1e	118.6	6.64	118.5	6.67
2e	125.0	7.18	124.8	7.20
3b	110.1	6.28	110.1	6.26
3f	104.4	6.40	104.4	6.40
4b	107.8	5.47	107.7	5.45
5f	125.5	6.64	125.4	6.63
6b	128.3	7.84	128.6	7.86
7f	108.0	6.48	107.9	6.50
z6	76.5	5.37	75.9	5.39
z2/z'2	36.0	2.52/3.14	35.9	2.50/3.07
G1	99.6	4.38	99.1	4.36
G-CH_3	23.2	1.85	23.2	1.85
P1	134.4	-	-	-
P2,6	128.2	7.77	-	-
P3,5	118.4	7.77	-	-
P4	144.9	-	-	-
P7	171.9	-	-	-
P8 (NHAc)	24.3	2.09	-	-
BPh1	-	-	139.6	-
BPh2,6	-	-	127.6	7.93
BPh3,5	-	-	127.0	7.89
BPh4	-	-	144.0	-
BPh7	-	-	138.6	-
BPh8,12	-	-	127.1	7.72
BPh9,11	-	-	129.3	7.52
BPh10	-	-	128.6	7.45

[a] ambiguous

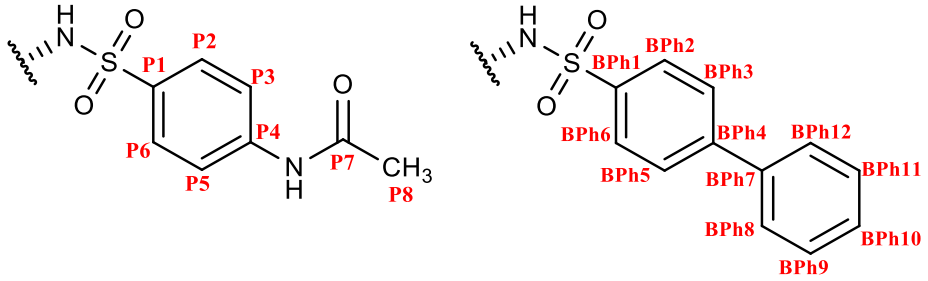


Figure S7. Atom numberings of Series 6 side chains for NMR assignment (for compounds **74** and **75**, respectively)

Table S5. (continued) ^{1}H and ^{13}C NMR data for the sulfonamide derivatives **72-79** of teicoplanin pseudoaglycon (Series 6)

	chemical shifts in ppm			
assignment	**76**		**77**	
	^{13}C	^{1}H	^{13}C	^{1}H
x1	58.2[a]	5.21[a]	58.16[a]	5.34[a]
x2	54.9	4.06	55.33	4.89
x3	58.2[a]	5.21[a]	58.16[a]	5.34[a]
x4	54.8	5.59	54.69	5.62
x5	53.7	4.30	53.66	4.32
x6	61.0	4.13	60.89	4.12
x7	59.3	4.33	59.20	4.30
1e	118.6	6.88	118.47	6.96
2e	124.9	7.20	124.83	7.19
3b	110.2	6.25	109.83	6.31
3f	104.2	6.34	103.83	6.41
4b	107.7	5.44	107.54	5.48
5f	125.5	6.63	125.29	6.63
6b	128.7	7.87	128.45	7.85
7f	108.0	6.50	107.83	6.48
z6	76.1	5.38	75.43	5.41
z2/z'2	36.0	2.20/3.02	36.47	2.78/3.33
G1	99.3	4.36	98.64	4.38
G-CH_3	23.1	1.85	23.03	1.83
Ds2	120.0	8.36	-	-
Ds3	127.8	7.56	-	-
Ds4	115.2	7.25	-	-
Ds5	151.1	-	-	-
Ds6-8	129.9	8.48	-	-
	128.9	8.31	-	-
	123.5	7.69	-	-
Ds11-12 (NMe_2)	45.2	2.82		
Hexyl 1	-	-	52.56	2.93
Hexyl 2	-	-	22.89	1.63
Hexyl 3	-	-	27.34	1.31
Hexyl 4	-	-	30.83	1.23
Hexyl 5	-	-	21.90	1.25
Hexyl 6	-	-	13.90	0.85

[a] ambiguous

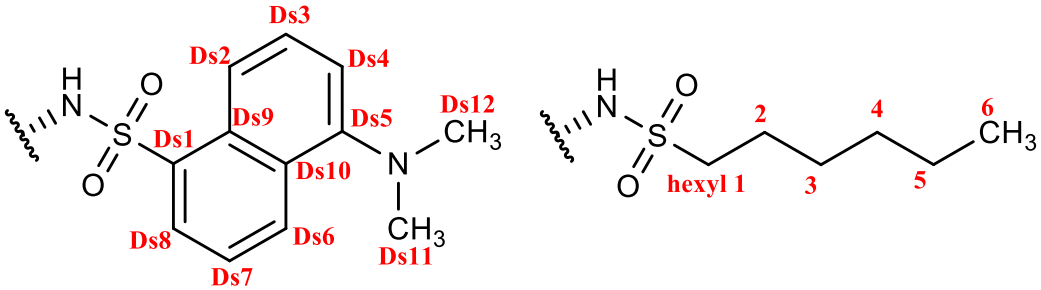


Figure S8. Atom numberings of Series 6 side chains for NMR assignment (for compounds **76** and **77**, respectively)

Table S5. (continued) ^{1}H and ^{13}C NMR data for the sulfonamide derivatives **72-79** of teicoplanin pseudoaglycon (Series 6)

	chemical shifts in ppm			
assignment	**78**		**79**	
	^{13}C	^{1}H	^{13}C	^{1}H
x1	58.2[a]	5.35[a]	58.1	5.35
x2	55.4	4.88	55.3	4.91
x3	58.2[a]	5.33[a]	58.1	5.35
x4	54.7	5.63	54.7	5.62
x5	53.7	4.32	53.6	4.32
x6	61.0	4.15	60.9	4.13
x7	58.9	4.31	59.2	4.30
1e	118.5	7.00	118.5	6.95
2e	125.0	7.19	124.8	7.19
3b	109.9	6.30	109.8	6.31
3f	103.9	6.38	103.8	6.42
4b	107.9	5.49	107.7	5.49
5f	125.5	6.64	125.3	6.62
6b	128.6	7.85	128.5	7.86
7f	107.7	6.43	107.9	6.50
z6	76.2	5.34	75.5	5.43
z2/z'2	36.5	2.77/3.33	36.6	2.79/3.34
G1	99.4	4.35	98.7	4.39
G-CH_3	23.1	1.82	23.0	1.83
Octyl 1	52.62	2.93	-	-
Octyl 2	22.98	1.63	-	-
Octyl 3	27.89	1.31	-	-
Octyl 4-5	28.71	1.23	-	-
Octyl 6	31.28	1.22	-	-
Octyl 7	22.10	1.24	-	-
Octyl 8	13.99	0.84	-	-
Dodecyl 1	-	-	52.5	2.94
Dodecyl 2	-	-	22.9	1.63
Dodecyl 3	-	-	27.6	1.31
Dodecyl 4-9	-	-	28.9	1.22
Dodecyl 10	-	-	31.2	1.21
Dodecyl 11	-	-	22.0	1.24
Dodecyl 12	-	-	13.9	0.84

[a] ambiguous

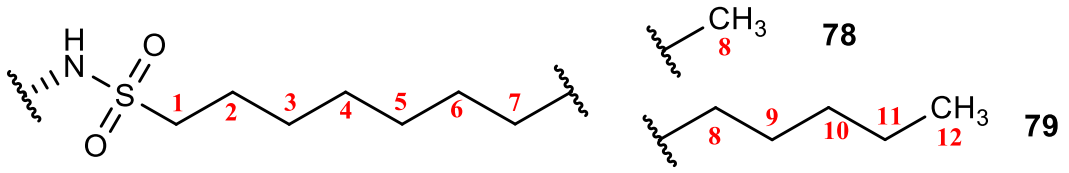


Figure S9. Atom numberings of Series 6 side chains for NMR assignment (for compounds **78** and **79**)

Table S6. Activity in human coronavirus 229E-infected human HEL[a] or A549[b] cells.

Compound	CPE reduction assay in HEL cells[a]		Virus yield assay in A549 cells[b]		
	EC_{50}	MCC	EC_{99}	EC_{90}	MCC
	μM				
13	5.4	≥20	10	4.1	50
14	5.4	≥20	9.4	5.8	50
27	5.4	≥20	11	5.9	>50
28	8.9	≥20	9.5	6.4	≥50
41	8.9	≥100	29	8.6	>50
42	5.4	≥20	21	7.6	>50
60	≥100	≥100	ND	ND	ND
61	44	≥100	44	25	>50
62	8.9	100	30	23	>50
72	5.2	≥100	10	4.9	>50
73	5.5	≥20	11	6.8	>50
74	>100	≥20	ND	ND	ND
75	>100	4	ND	ND	ND
76	>100	≥4	ND	ND	ND
77	1.5	20	ND	ND	ND
78	5.4	≥20	9.4	5.7	>50
79	1.8	20	4.7	2.8	50
UDA (μg/ml)[c]	1.8	>100	ND	ND	ND
K22 (μM)[c]	ND	ND	15	11	≥50

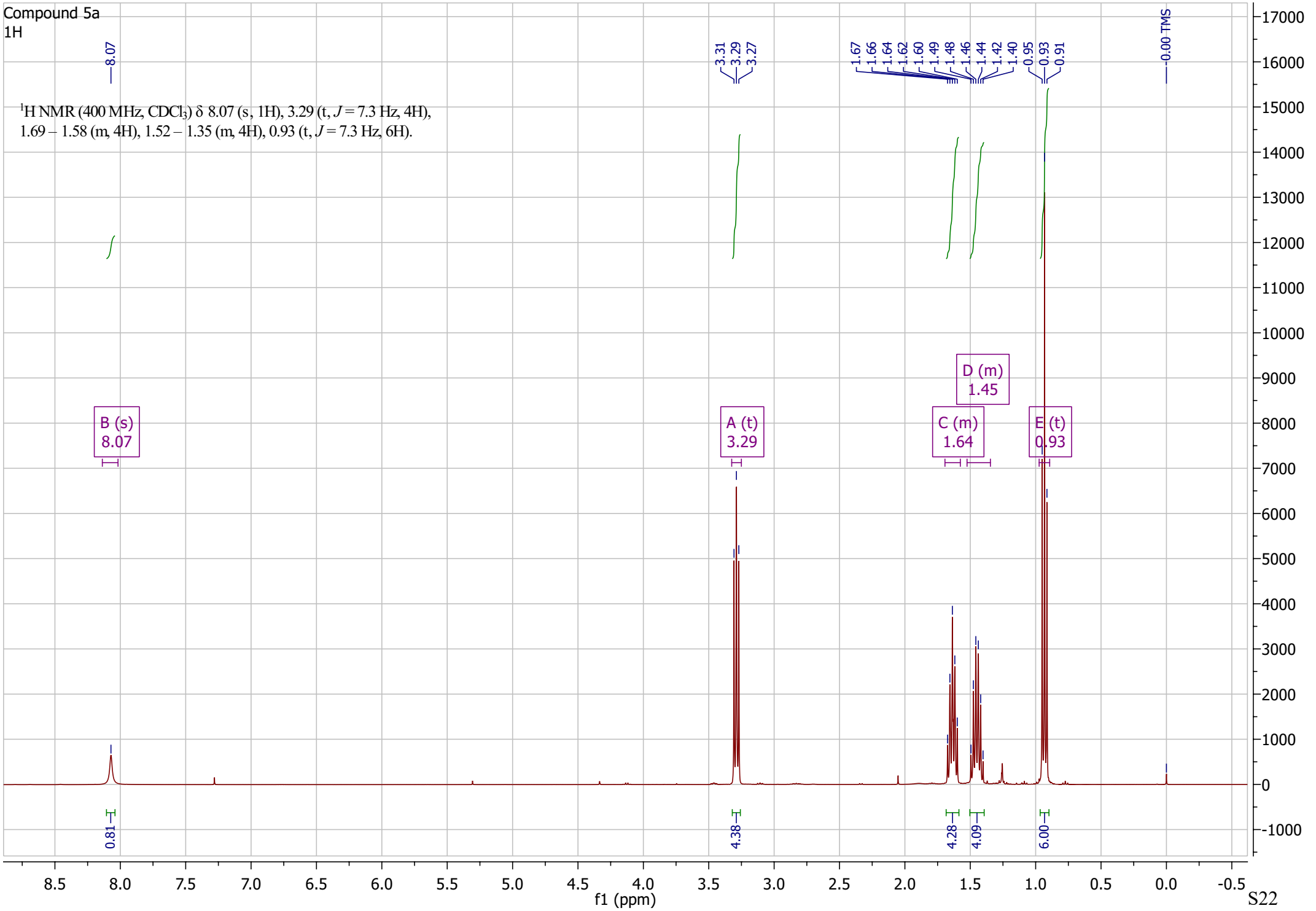
[a]HEL: human embryonic lung fibroblast cells. Antiviral EC_{50}: compound concentration producing 50% inhibition of virus replication, as estimated by microscopic scoring of the cytopathic effect (CPE). MCC: minimum cytotoxic concentration, i.e. compound concentration producing minimal changes in cell morphology, as estimated by microscopy.
[b]A549: human lung epithelial carcinoma cells. Antiviral activity expressed as the compound concentration causing a 2-$\log_{10}$ (EC_{99}) and 1-$\log_{10}$ (EC_{90}) reduction in virus yield at 72 h p.i., as determined by real-time RT-PCR.
[c]Reference compounds: UDA (Urtica dioica agglutinin) lectin, concentration expressed in μg/ml; K22 [(Z)-N-(3-(4-(4-bromophenyl)-4-hydroxypiperidin-1-yl)-3-oxo-1-phenylprop-1-en-2-yl)benzamide][1], concentration expressed in μM.
Data represent the averages of two independent tests. ND, not determined.

Table S7. Elemental analysis data (C, H, N, S) for teicoplanin derivatives.

#	formula	C		H		N		S	
		Calcd.	Found	Calcd.	Found	Calcd.	Found	Calcd.	Found
13	$C_{78}H_{74}Cl_2N_8O_{25}S_2$	56.49	56.35	4.50	4.65	6.76	6.63	3.87	3.75
14	$C_{82}H_{82}Cl_2N_8O_{25}S_2$	57.44	57.39	4.82	5.09	6.54	6.40	3.74	3.67
17	$C_{85}H_{88}Cl_2N_8O_{25}S_2$	58.12	57.95	5.05	5.21	6.38	6.25	3.65	3.44
26	$C_{79}H_{73}Cl_2N_{11}O_{25}S_2$	55.44	55.32	4.30	4.48	9.00	8.87	3.75	3.63
27	$C_{81}H_{77}Cl_2N_{11}O_{25}S_2$	55.93	55.68	4.46	4.69	8.86	8.80	3.69	3.59
28	$C_{85}H_{85}Cl_2N_{11}O_{25}S_2$	56.85	56.57	4.77	5.02	8.58	8.45	3.57	3.51
29	$C_{89}H_{93}Cl_2N_{11}O_{25}S_2$	57.73	57.57	5.06	5.28	8.32	8.28	3.46	3.38
30	$C_{97}H_{109}Cl_2N_{11}O_{25}S_2$	59.32	59.22	5.59	5.84	7.85	7.65	3.26	3.14
31	$C_{97}H_{97}Cl_2N_{11}O_{35}S_2$	55.17	55.25	4.63	4.91	7.30	7.13	3.04	2.92
40	$C_{87}H_{89}Cl_2N_{11}O_{29}S_2$	55.36	55.18	4.75	4.98	8.16	8.10	3.40	3.29
41	$C_{89}H_{93}Cl_2N_{11}O_{29}S_2$	55.80	55.62	4.89	5.05	8.04	7.92	3.35	3.27
42	$C_{93}H_{101}Cl_2N_{11}O_{29}S_2$	56.65	55.48	5.16	5.34	7.81	7.67	3.25	3.18
43	$C_{97}H_{109}Cl_2N_{11}O_{29}S_2$	57.45	57.32	5.42	5.53	7.60	7.54	3.16	3.05
44	$C_{105}H_{125}Cl_2N_{11}O_{29}S_2$	58.93	58.70	5.89	6.02	7.20	7.11	3.00	2.91
45	$C_{105}H_{113}Cl_2N_{11}O_{39}S_2$	55.12	54.95	4.98	5.09	6.73	6.61	2.80	2.70
46	$C_{97}H_{109}Cl_2N_{11}O_{37}S_2$	54.04	53.85	5.10	5.18	7.15	7.07	2.97	2.83
60	$C_{84}H_{87}Cl_2N_{13}O_{28}$	56.13	55.89	4.88	5.03	10.13	10.02	-	-
61	$C_{86}H_{91}Cl_2N_{13}O_{28}$	56.58	56.35	5.02	5.11	9.97	9.80	-	-
62	$C_{88}H_{95}Cl_2N_{13}O_{28}$	57.02	56.88	5.17	5.29	9.82	9.64	-	-
63	$C_{90}H_{99}Cl_2N_{13}O_{28}$	57.45	57.35	5.30	5.47	9.68	9.49	-	-
72	$C_{73}H_{64}Cl_2N_8O_{25}S$	56.34	56.32	4.15	4.36	7.20	7.08	2.06	1.95
73	$C_{72}H_{62}Cl_2N_8O_{25}S$	56.07	56.11	4.05	4.24	7.27	7.13	2.08	1.94
74	$C_{74}H_{65}Cl_2N_9O_{26}S$	55.57	55.34	4.10	4.18	7.88	7.66	2.00	1.94
75	$C_{78}H_{66}Cl_2N_8O_{25}S$	57.89	57.95	4.11	4.22	6.92	6.75	1.98	1.90
76	$C_{78}H_{69}Cl_2N_9O_{25}S$	57.29	57.32	4.25	4.50	7.71	7.44	1.96	1.88
77	$C_{72}H_{70}Cl_2N_8O_{25}S$	55.78	55.57	4.55	4.78	7.23	7.10	2.07	1.97
78	$C_{74}H_{74}Cl_2N_8O_{25}S$	56.31	56.08	4.73	4.88	7.10	6.98	2.03	1.96
79	$C_{78}H_{82}Cl_2N_8O_{25}S$	57.32	57.04	5.06	5.11	6.86	6.82	1.96	1.91

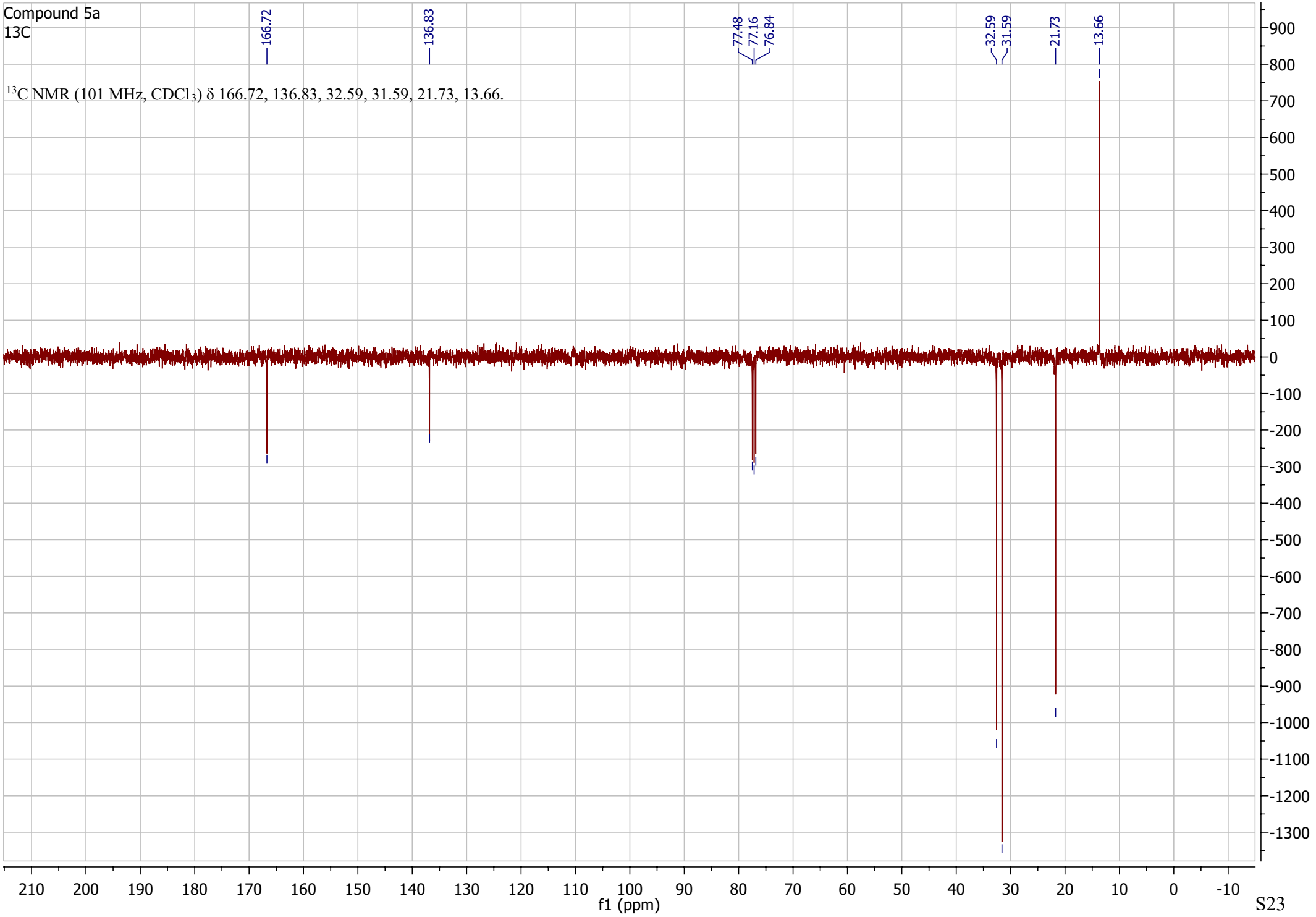
References

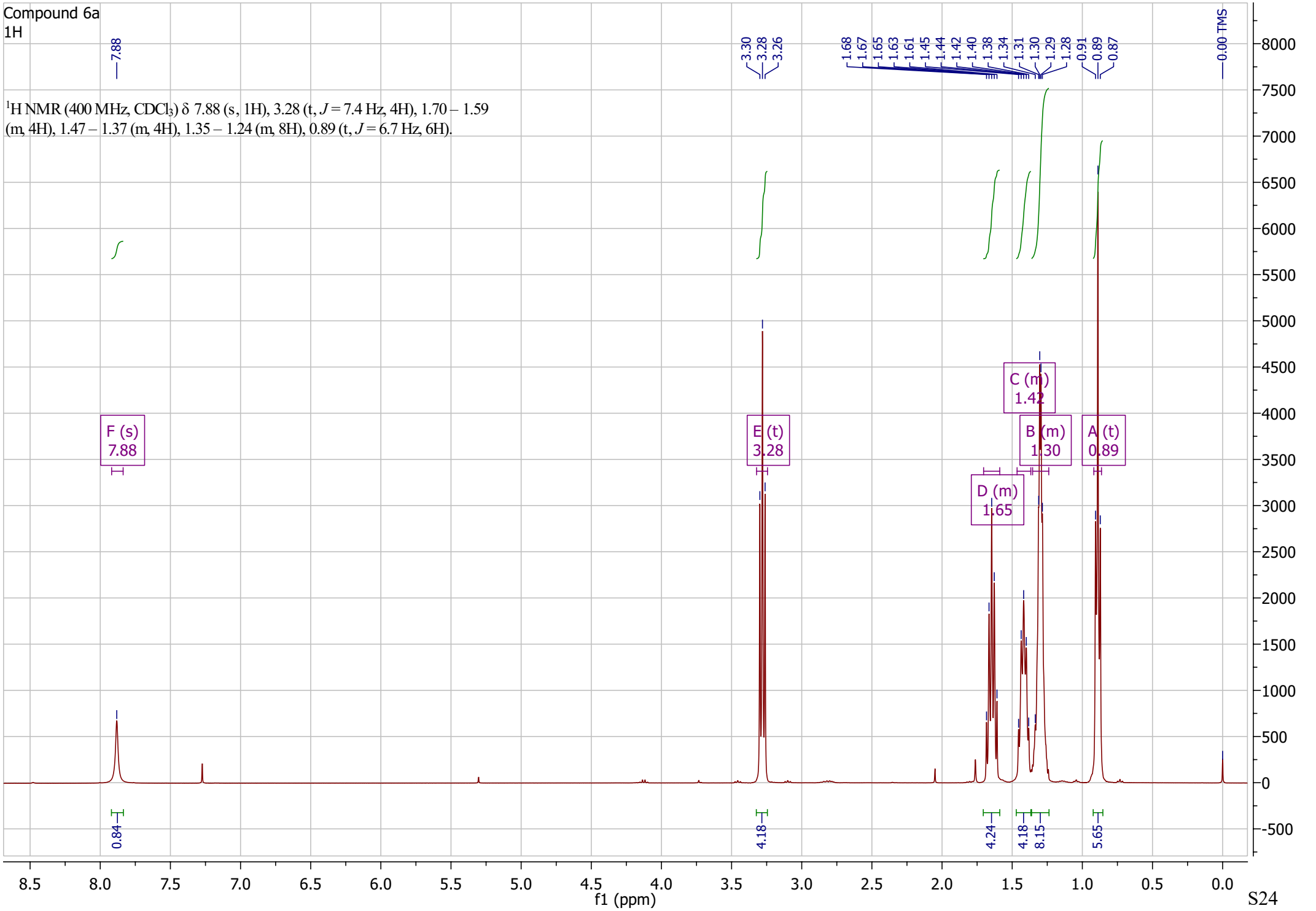
1. Lundin, A.; Dijkman, R.; Bergström, T.; Kann, N.; Adamiak, B.; Hannoun, C.; Kindler, E.; Jónsdóttir, H. R.; Muth, D.; Kint, J.; Forlenza, M.; Müller, M. A.; Drosten, C.; Thiel, V.; Trybala, E. Targeting membrane-bound viral RNA synthesis reveals potent inhibition of diverse coronaviruses including the middle East respiratory syndrome virus. *PLoS Pathog.* **2014**, *10*, e1004166.


Compound 5a
1H
8.07
3.31
3.29
3.27
1.67
1.66
1.64
1.62
1.60
1.49
1.48
1.46
1.44
1.42
1.40
0.95
0.93
0.91
-0.00 TMS
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 3.29 (t, J = 7.3 Hz, 4H), 1.69 – 1.58 (m, 4H), 1.52 – 1.35 (m, 4H), 0.93 (t, J = 7.3 Hz, 6H).
B (s) 8.07
A (t) 3.29
D (m) 1.45
C (m) 1.64
E (t) 0.93
0.81
4.38
4.28
4.09
6.00
f1 (ppm)

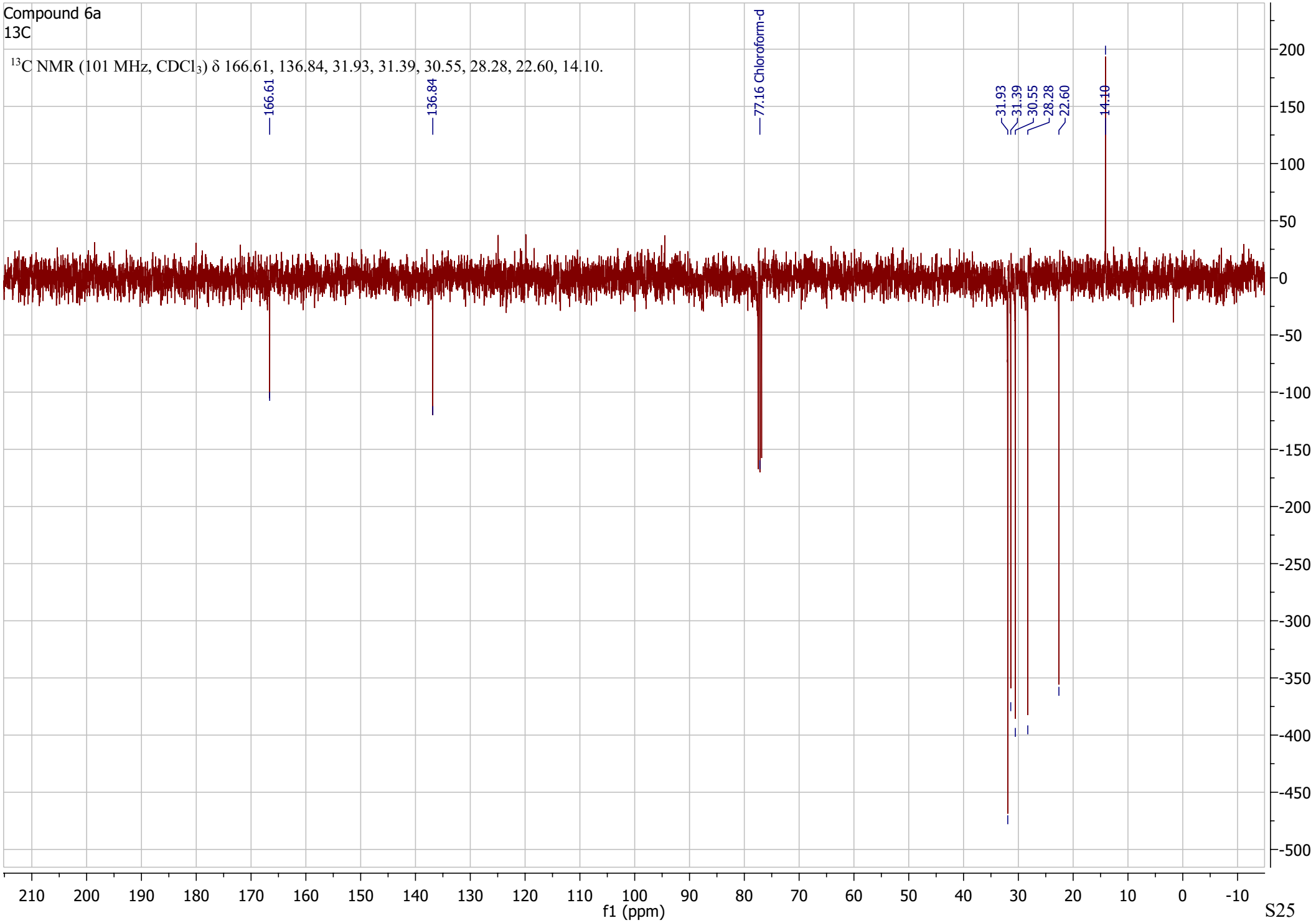
Compound 5a
13C

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.72, 136.83, 32.59, 31.59, 21.73, 13.66.



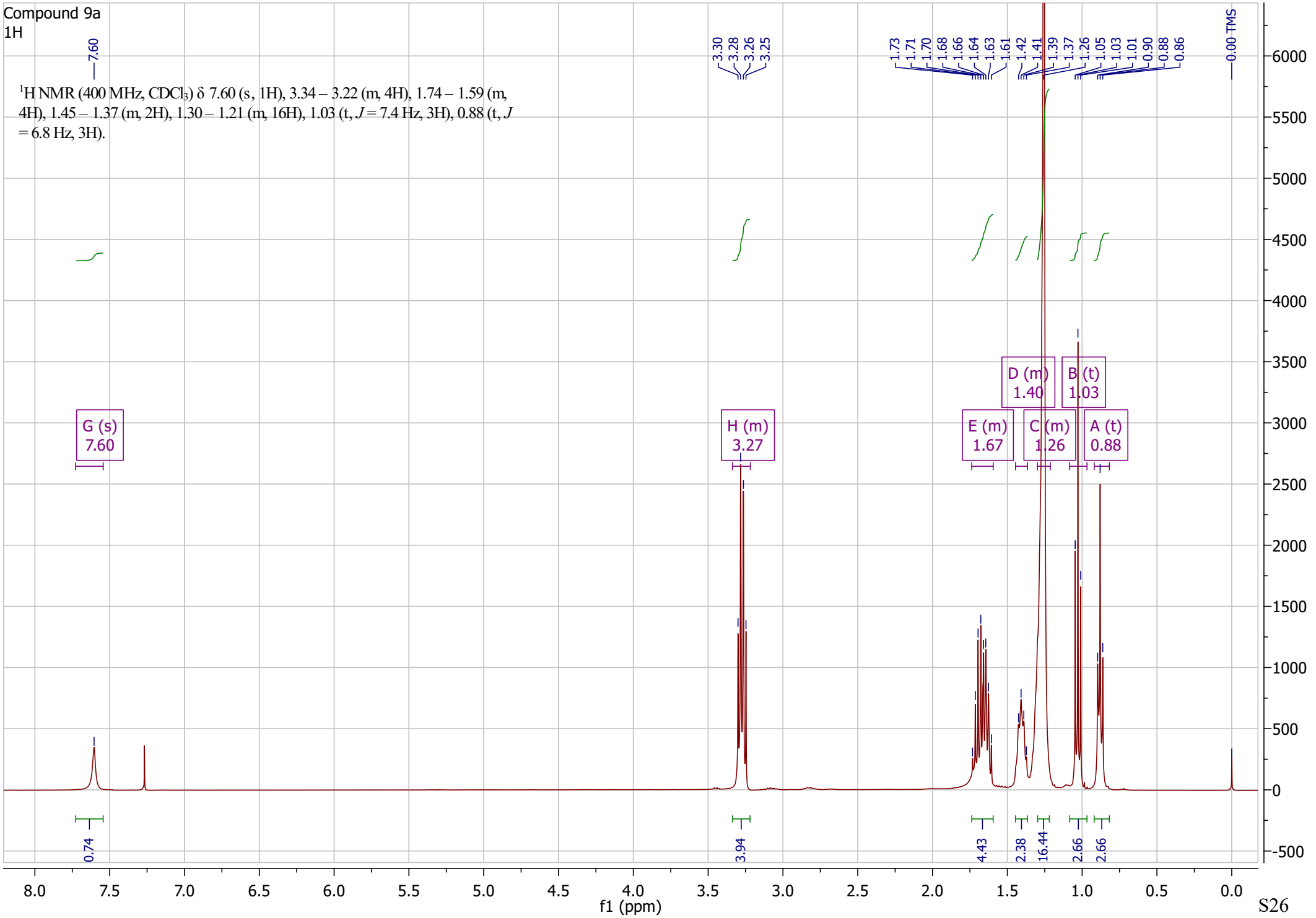


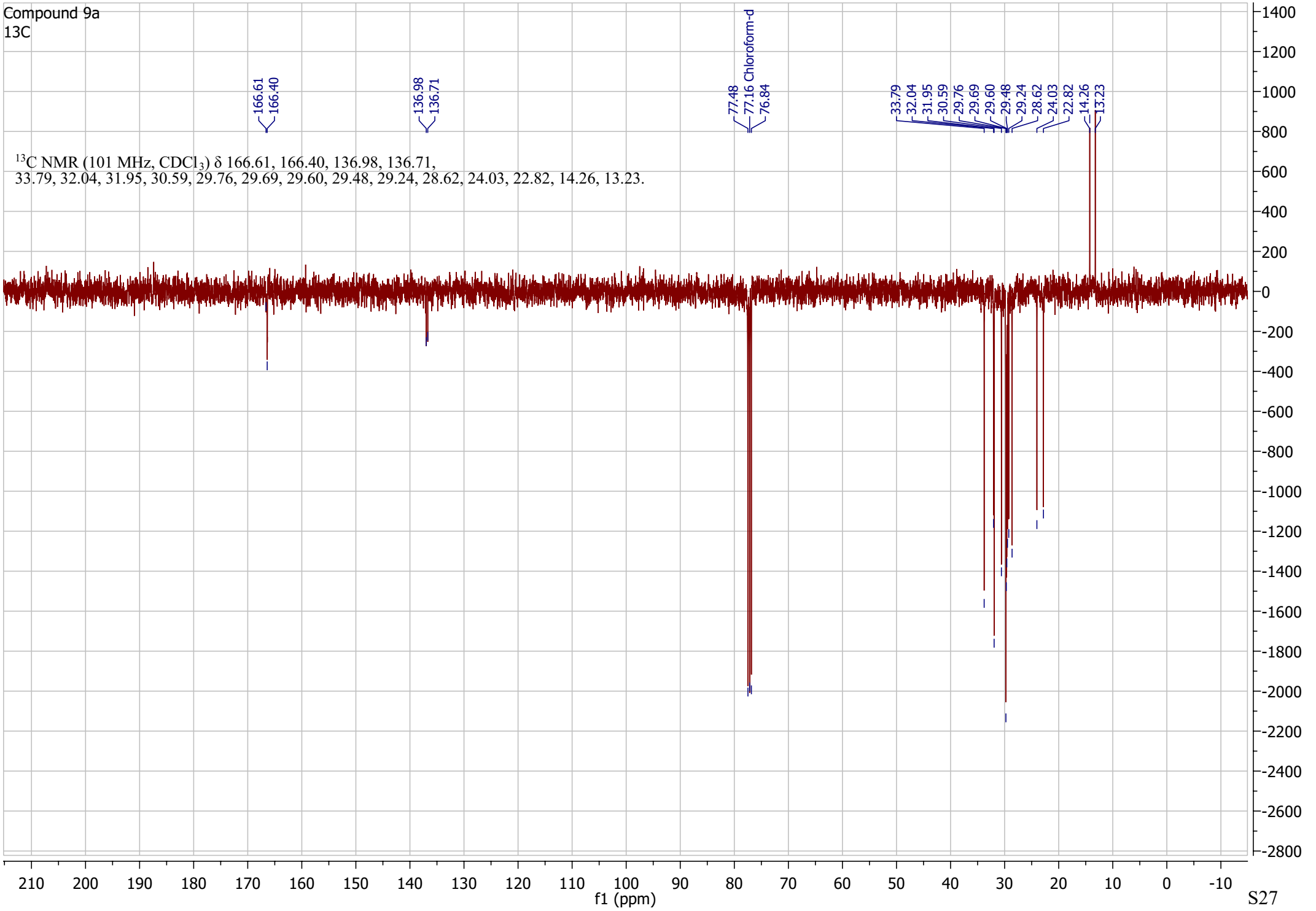
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 3.28 (t, *J* = 7.4 Hz, 4H), 1.70 – 1.59 (m, 4H), 1.47 – 1.37 (m, 4H), 1.35 – 1.24 (m, 8H), 0.89 (t, *J* = 6.7 Hz, 6H).

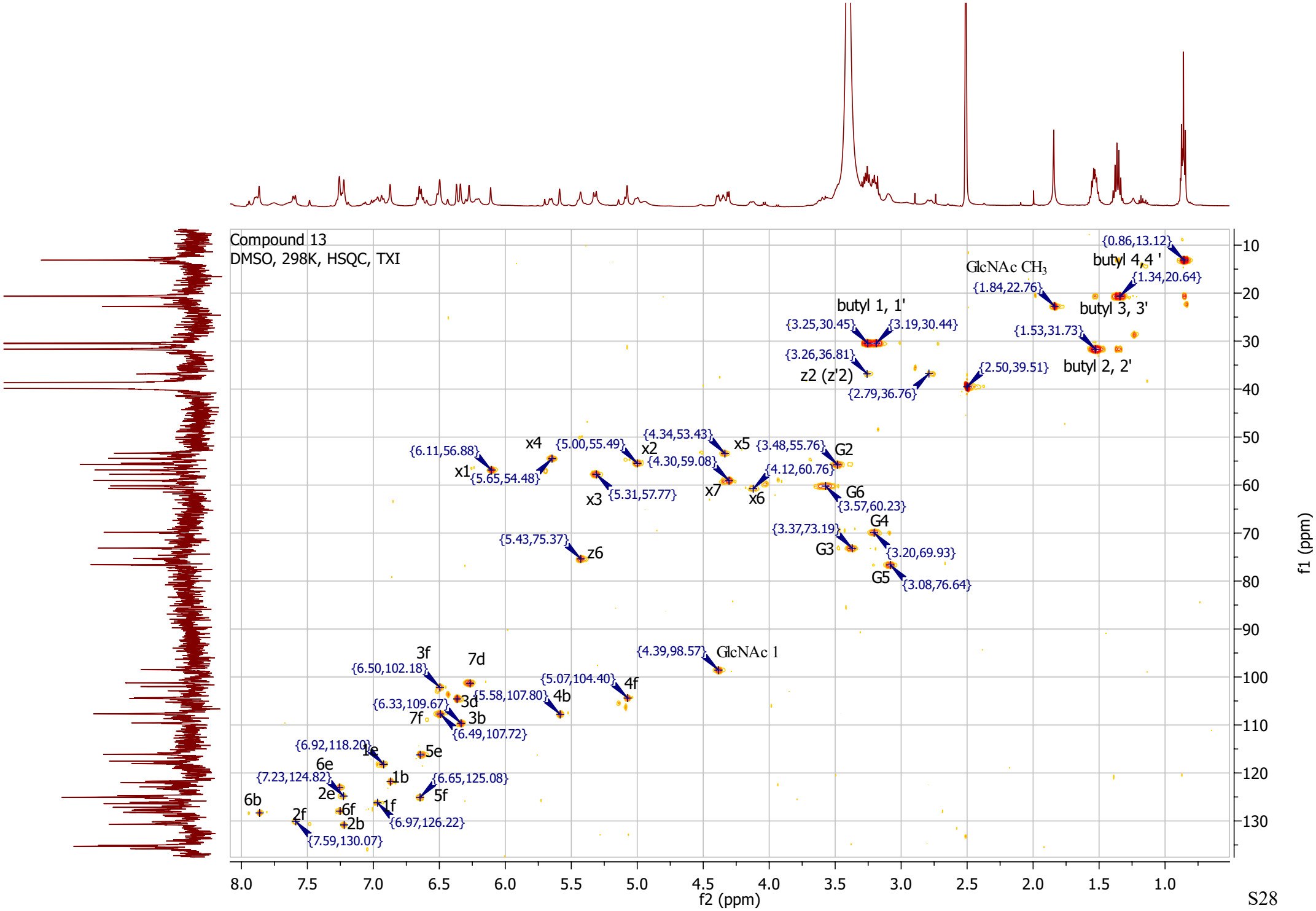

Compound 6a
13C
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.61, 136.84, 31.93, 31.39, 30.55, 28.28, 22.60, 14.10.
166.61
136.84
77.16 Chloroform-d
31.93
31.39
30.55
28.28
22.60
14.10
f1 (ppm)

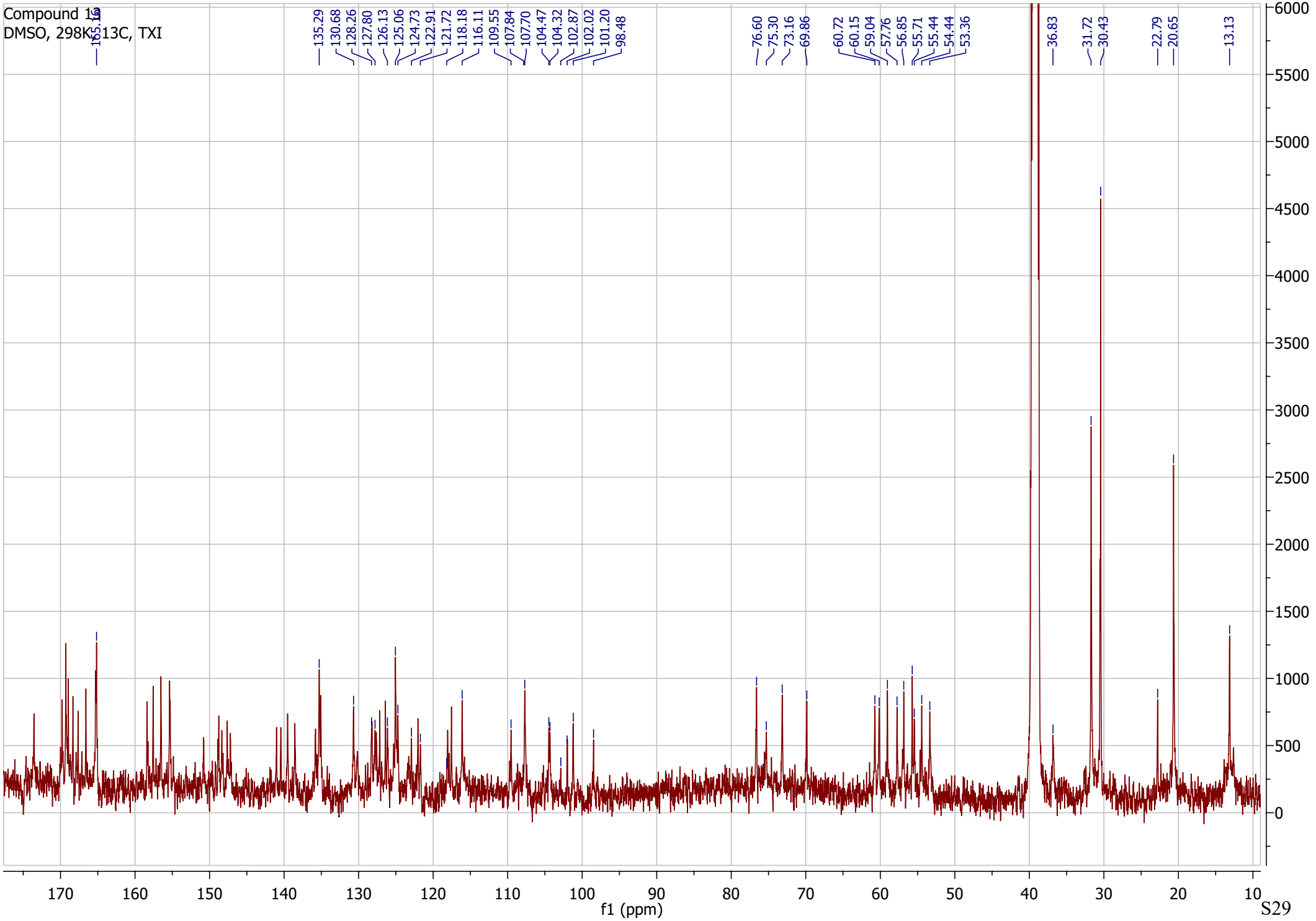
Compound 9a
1H

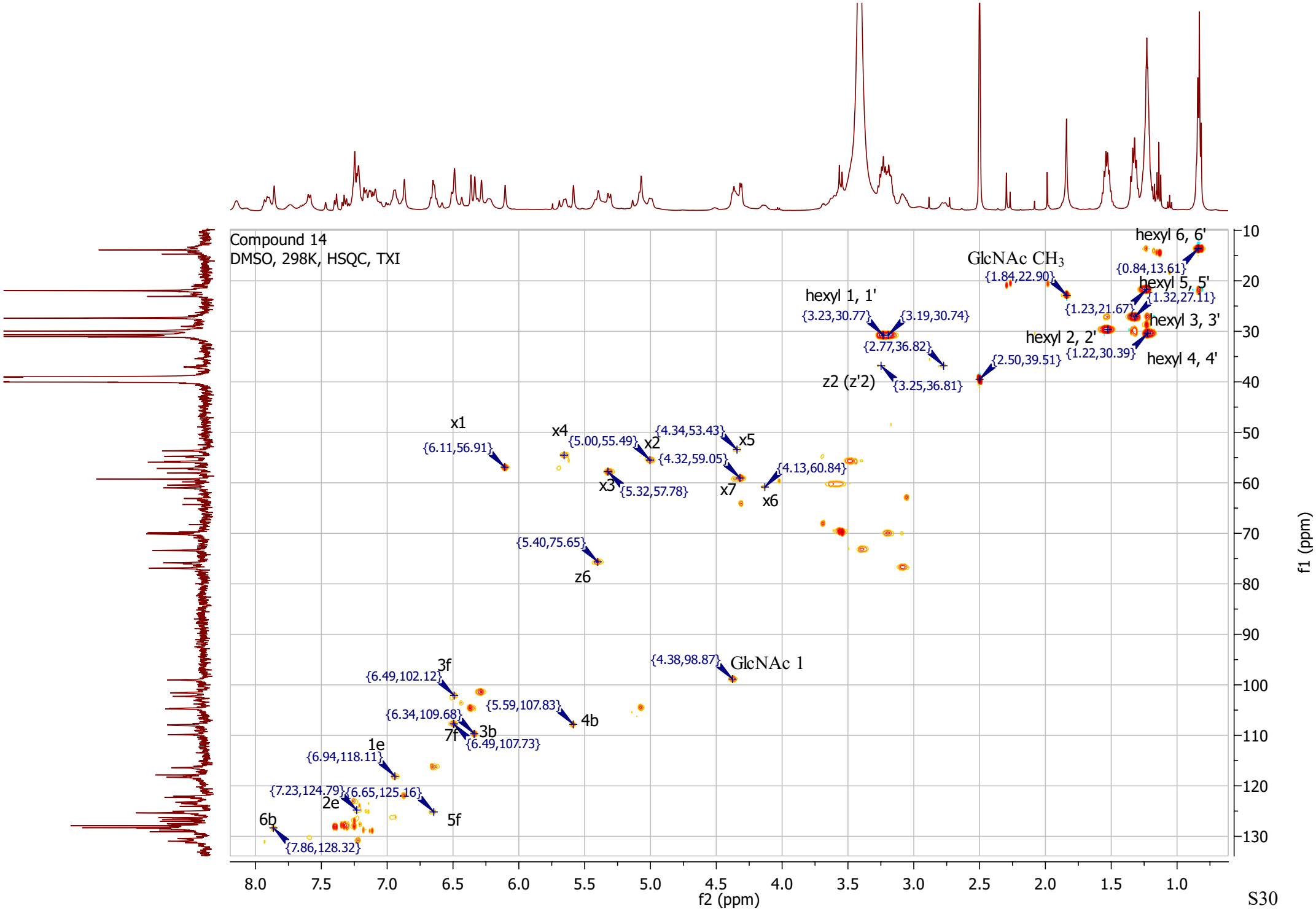
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 3.34 – 3.22 (m, 4H), 1.74 – 1.59 (m, 4H), 1.45 – 1.37 (m, 2H), 1.30 – 1.21 (m, 16H), 1.03 (t, *J* = 7.4 Hz, 3H), 0.88 (t, *J* = 6.8 Hz, 3H).

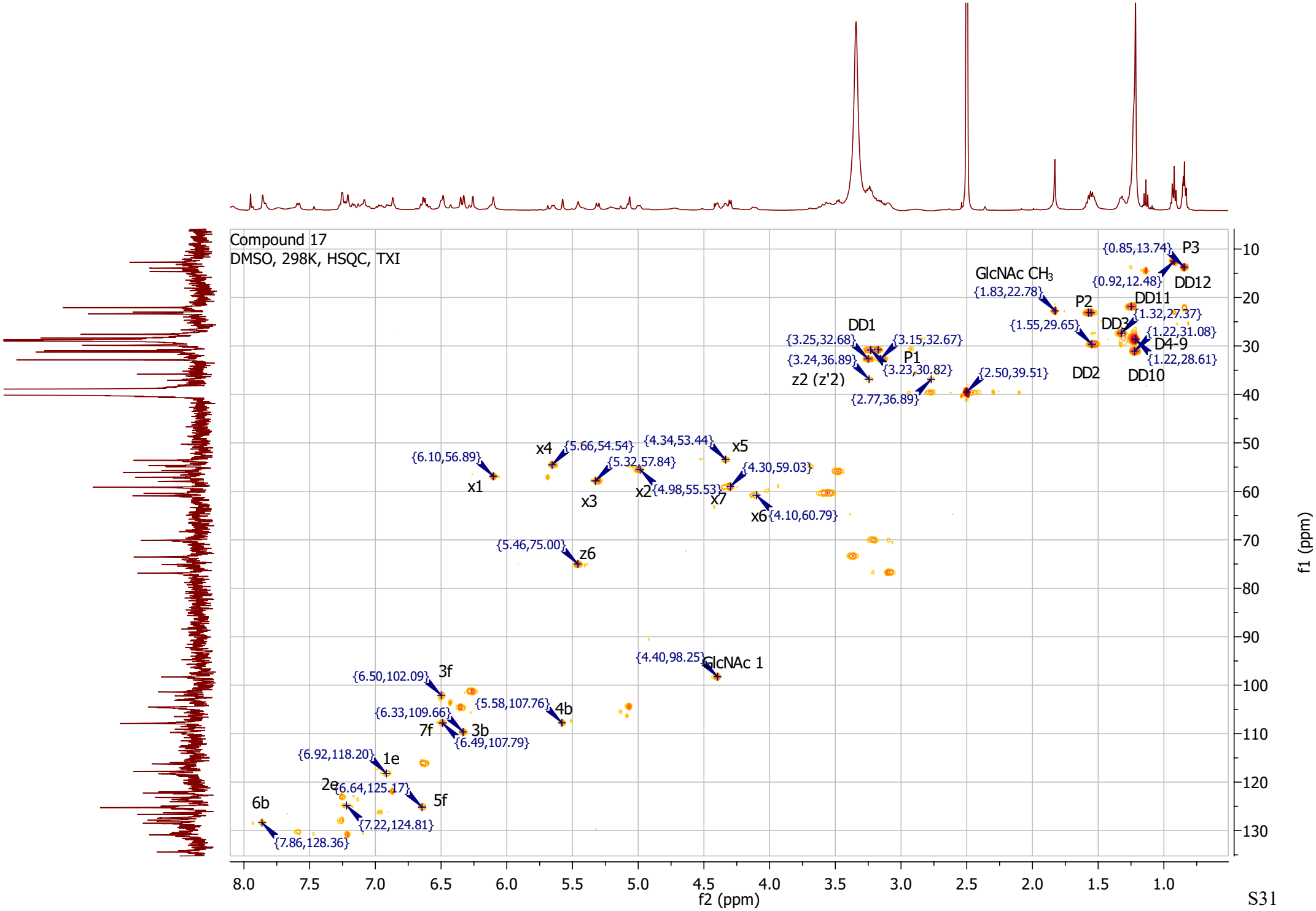



Compound 9a
13C
166.61
166.40
136.98
136.71
77.48
77.16 Chloroform-d
76.84
33.79
32.04
31.95
30.59
29.76
29.69
29.60
29.48
29.24
28.62
24.03
22.82
14.26
13.23
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.61, 166.40, 136.98, 136.71,
33.79, 32.04, 31.95, 30.59, 29.76, 29.69, 29.60, 29.48, 29.24, 28.62, 24.03, 22.82, 14.26, 13.23.
f1 (ppm)


Compound 13
DMSO, 298K, HSQC, TXI
GlcNAc CH3
{0.86,13.12}
butyl 4, 4'
{1.34,20.64}
{1.84,22.76}
butyl 3, 3'
butyl 1, 1'
{3.25,30.45}
{3.19,30.44}
{1.53,31.73}
{3.26,36.81}
butyl 2, 2'
z2 (z'2)
{2.50,39.51}
{2.79,36.76}
{4.34,53.43}
x5
{3.48,55.76}
G2
x4
{5.00,55.49}
x2
{6.11,56.88}
{4.30,59.08}
{4.12,60.76}
x1
{5.65,54.48}
x7
x6
G6
x3
{5.31,57.77}
{3.57,60.23}
G4
{3.37,73.19}
{5.43,75.37}
G3
{3.20,69.93}
z6
G5
{3.08,76.64}
{4.39,98.57}
GlcNAc 1
3f
7d
{6.50,102.18}
{5.07,104.40}
4f
{5.58,107.80}
4b
{6.33,109.67}
3d
7f
3b
{6.49,107.72}
{6.92,118.20}
1e
5e
6e
{7.23,124.82}
1b
{6.65,125.08}
2e
5f
6b
2f
6f
1f
2b
{6.97,126.22}
{7.59,130.07}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

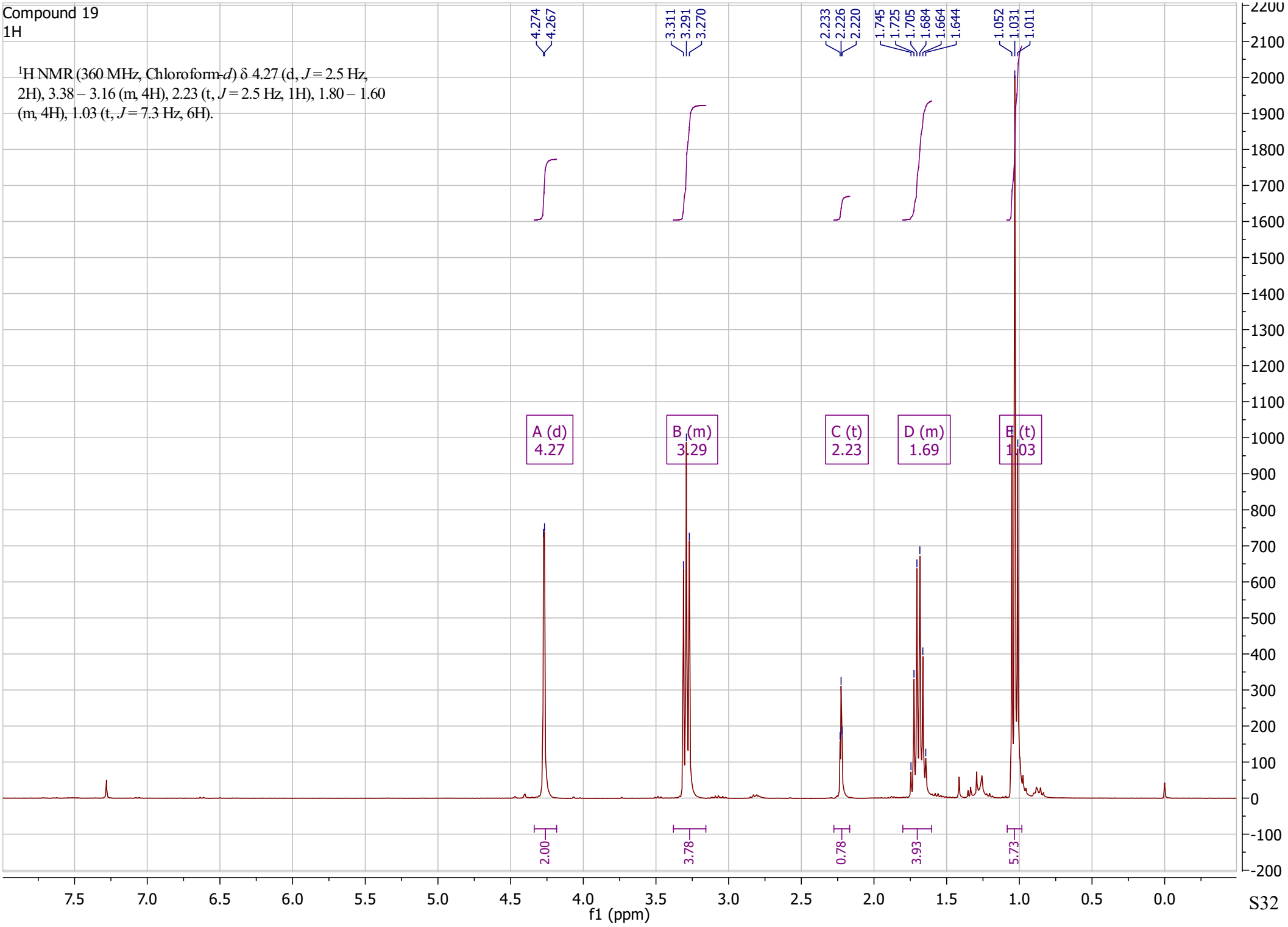

Compound 1a
DMSO, 298K, 13C, TXI
165.14
135.29
130.68
128.26
127.80
126.13
125.06
124.73
122.91
121.72
118.18
116.11
109.55
107.84
107.70
104.47
104.32
102.87
102.02
101.20
98.48
76.60
75.30
73.16
69.86
60.72
60.15
59.04
57.76
56.85
55.71
55.44
54.44
53.36
36.83
31.72
30.43
22.79
20.65
13.13
f1 (ppm)

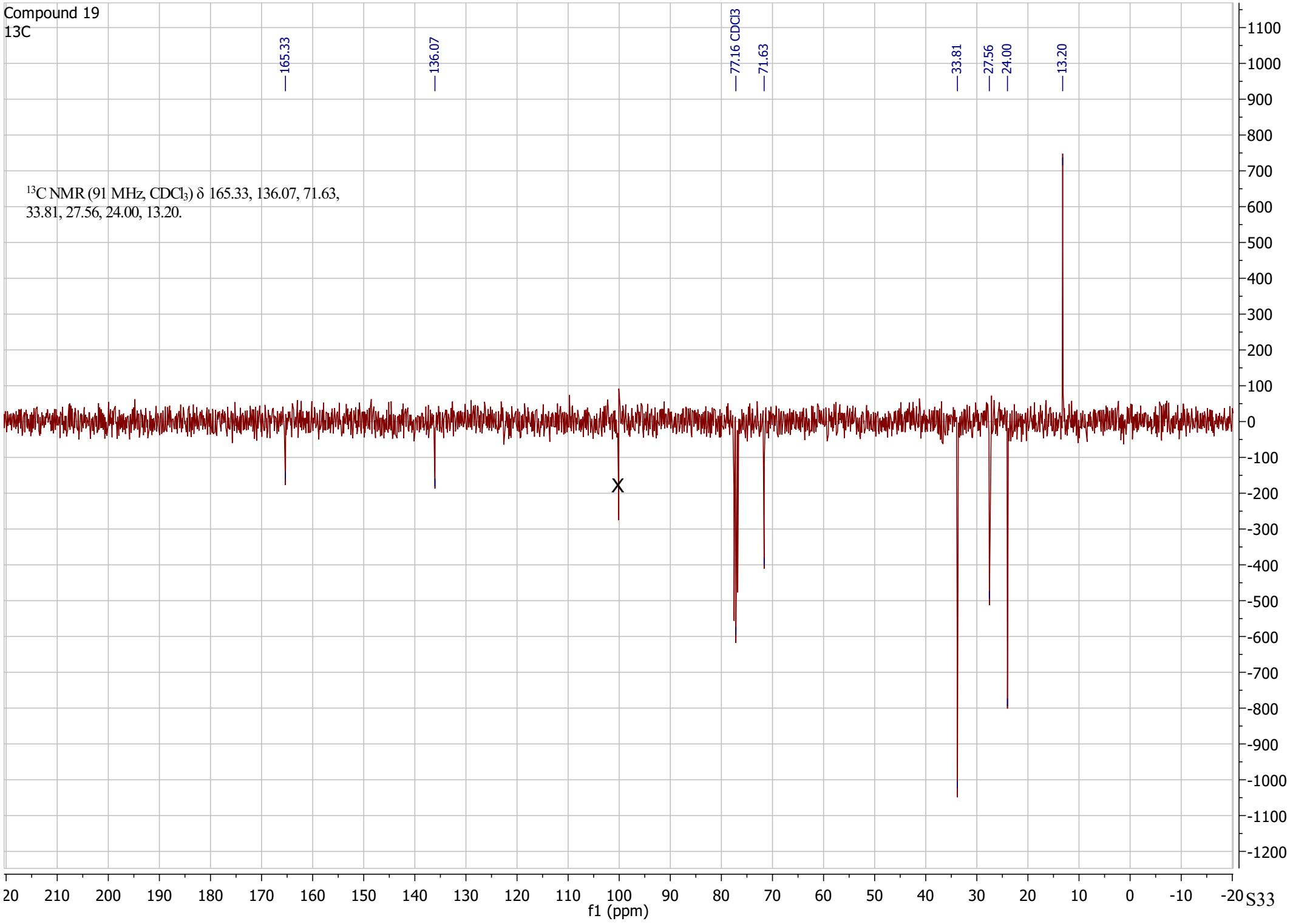

Compound 14
DMSO, 298K, HSQC, TXI
hexyl 6, 6'
{0.84,13.61}
GlcNAc CH3
{1.84,22.90}
hexyl 5, 5'
{1.32,27.11}
{1.23,21.67}
hexyl 1, 1'
{3.23,30.77}
{3.19,30.74}
hexyl 3, 3'
hexyl 2, 2'
{2.77,36.82}
{1.22,30.39}
hexyl 4, 4'
{2.50,39.51}
z2 (z'2)
{3.25,36.81}
x1
{6.11,56.91}
x4
{5.00,55.49}
x2
{4.34,53.43}
x5
{4.32,59.05}
{4.13,60.84}
x3
{5.32,57.78}
x7
x6
{5.40,75.65}
z6
{4.38,98.87}
GlcNAc 1
3f
{6.49,102.12}
{5.59,107.83}
4b
{6.34,109.68}
7f
3b
{6.49,107.73}
1e
{6.94,118.11}
{7.23,124.79}
{6.65,125.16}
2e
5f
6b
{7.86,128.32}
f2 (ppm)
f1 (ppm)

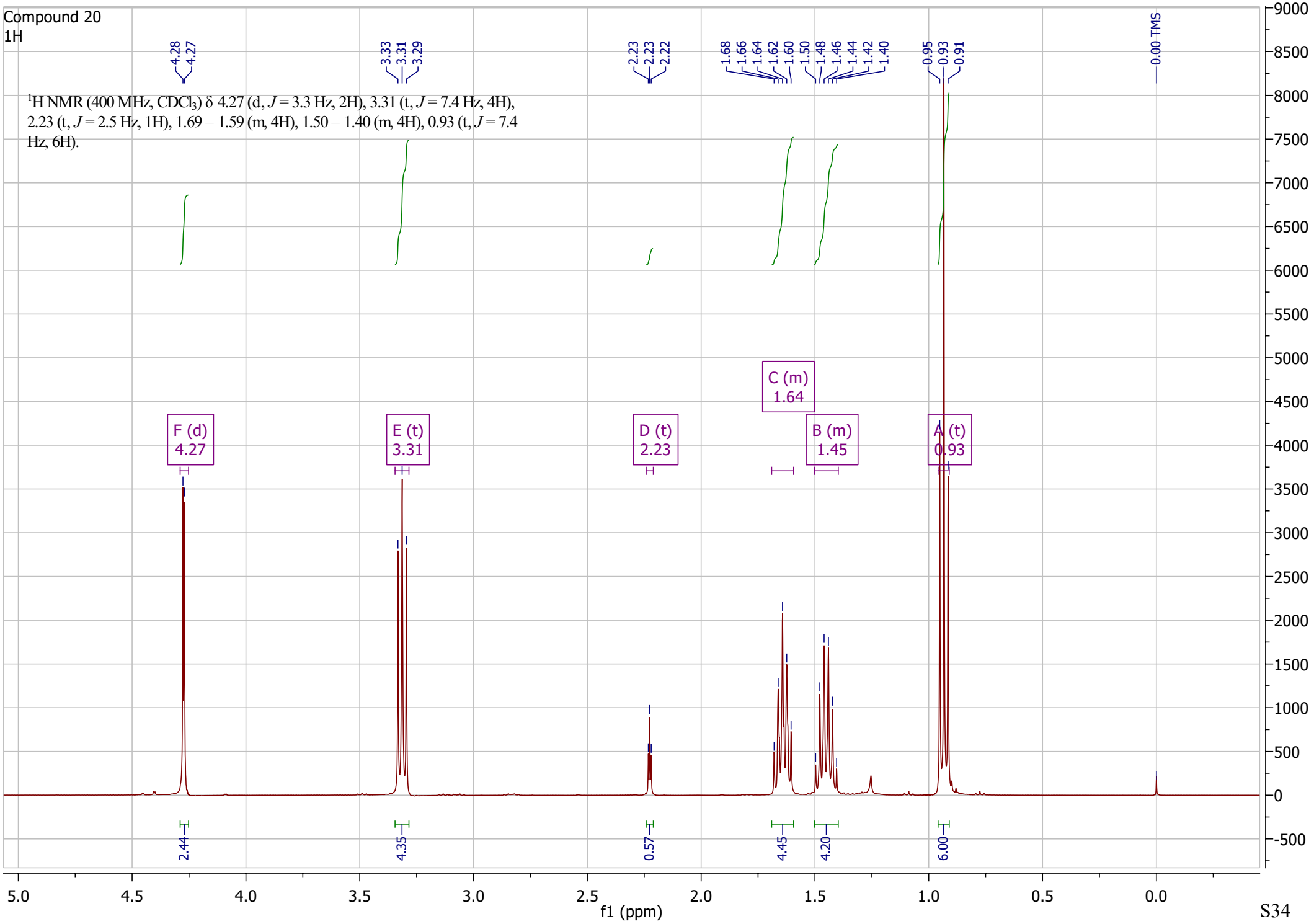

Compound 17
DMSO, 298K, HSQC, TXI
{0.85,13.74}
P3
{0.92,12.48}
DD12
GlcNAc CH3
{1.83,22.78}
P2
DD11
{1.32,27.37}
{1.55,29.65}
DD3
{1.22,31.08}
DD1
{3.25,32.68}
{3.15,32.67}
D4-9
{3.24,36.89}
P1
{3.23,30.82}
{1.22,28.61}
z2 (z'2)
{2.50,39.51}
DD2
DD10
{2.77,36.89}
{6.10,56.89}
x4
{5.66,54.54}
{4.34,53.44}
x5
x1
{5.32,57.84}
{4.30,59.03}
x3
x2
{4.98,55.53}
x7
x6
{4.10,60.79}
{5.46,75.00}
z6
{4.40,98.25}
GlcNAc 1
{6.50,102.09}
3f
{5.58,107.76}
4b
{6.33,109.66}
7f
3b
{6.49,107.79}
{6.92,118.20}
1e
2e
{6.64,125.17}
5f
6b
{7.22,124.81}
{7.86,128.36}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

Compound 19
1H

^{1}H NMR (360 MHz, Chloroform-*d*) δ 4.27 (d, *J* = 2.5 Hz, 2H), 3.38 – 3.16 (m, 4H), 2.23 (t, *J* = 2.5 Hz, 1H), 1.80 – 1.60 (m, 4H), 1.03 (t, *J* = 7.3 Hz, 6H).

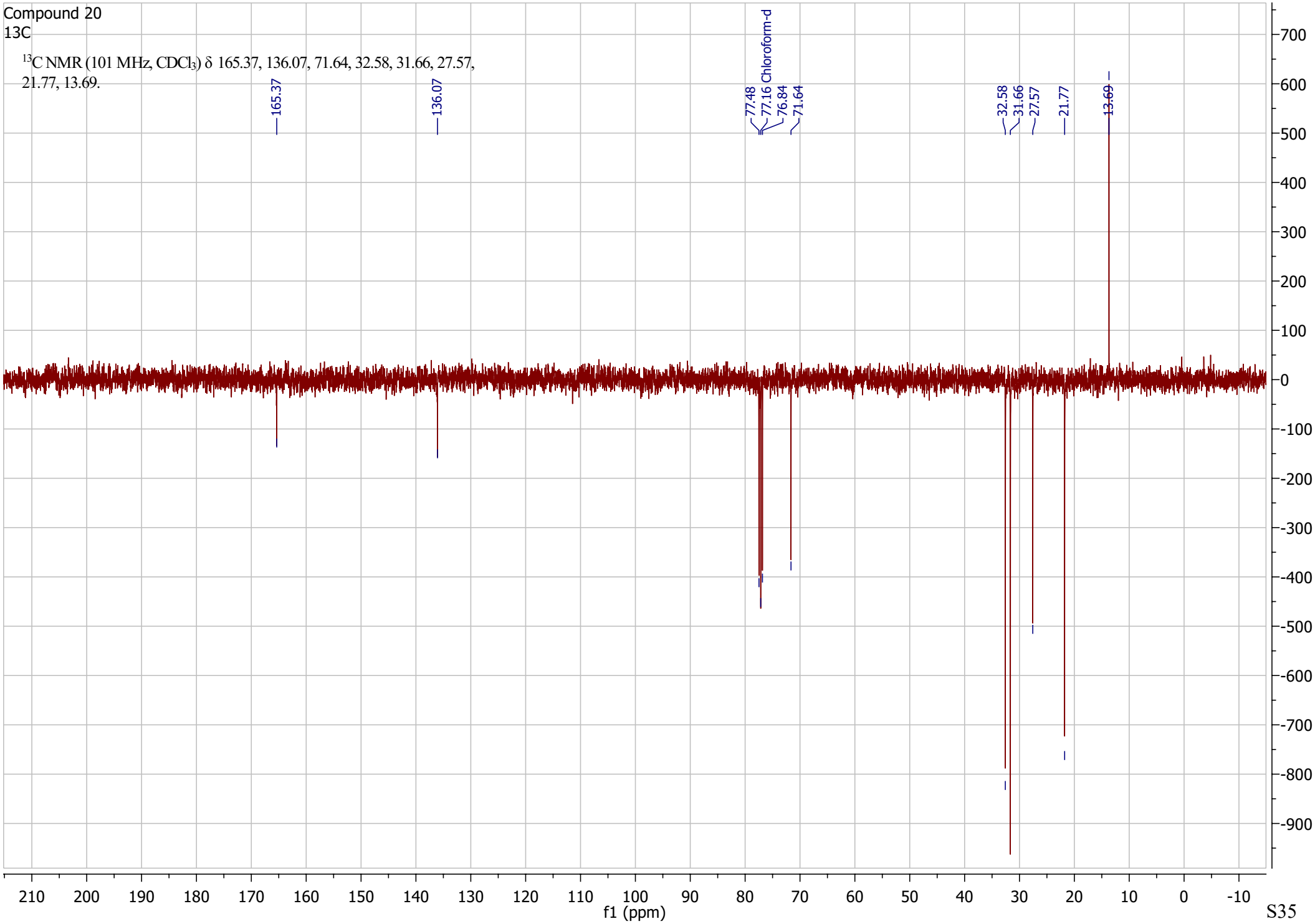


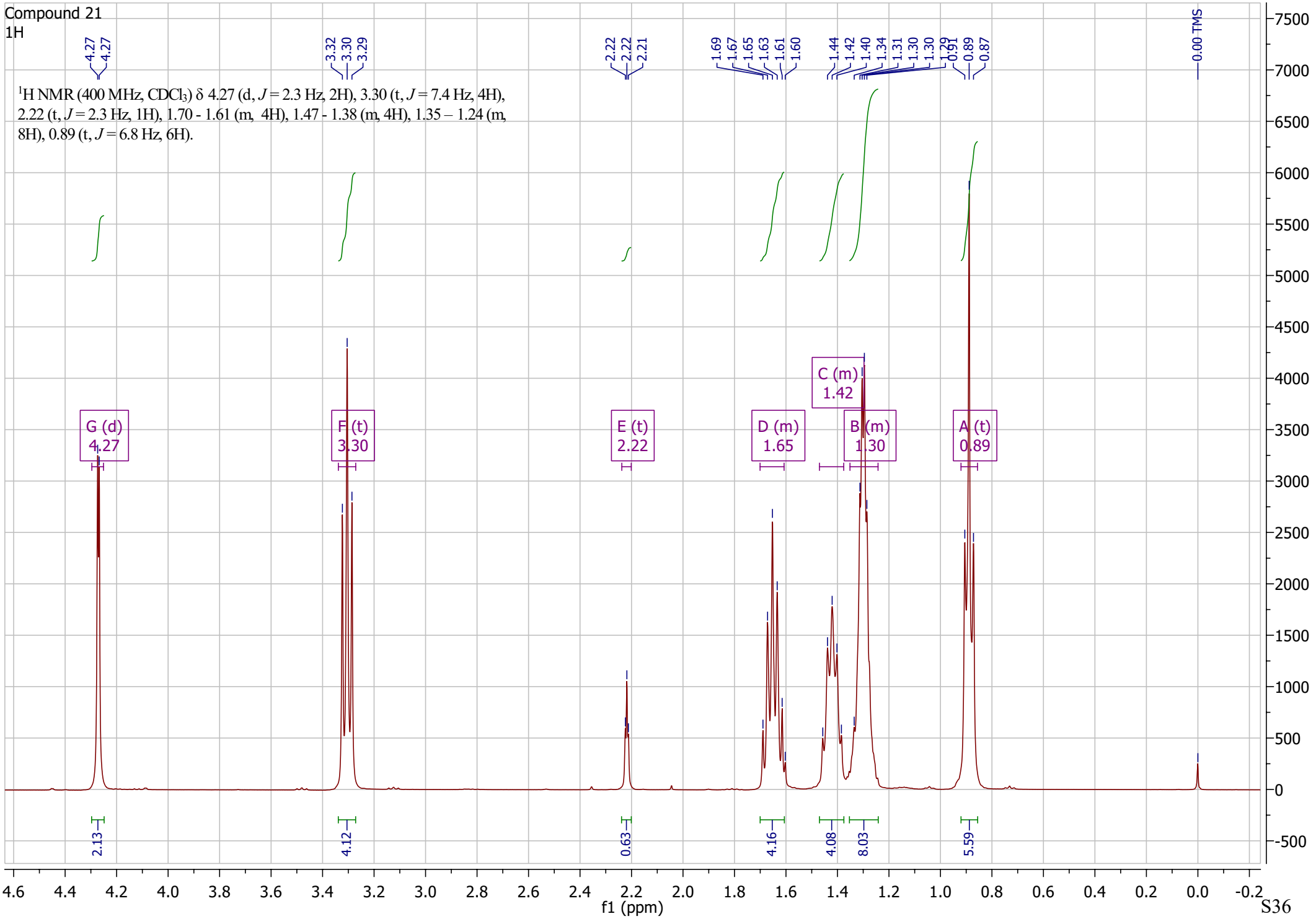

Compound 19
13C
165.33
136.07
77.16 CDCl3
71.63
33.81
27.56
24.00
13.20
^{13}C NMR (91 MHz, $CDCl_3$) δ 165.33, 136.07, 71.63, 33.81, 27.56, 24.00, 13.20.
X
f1 (ppm)

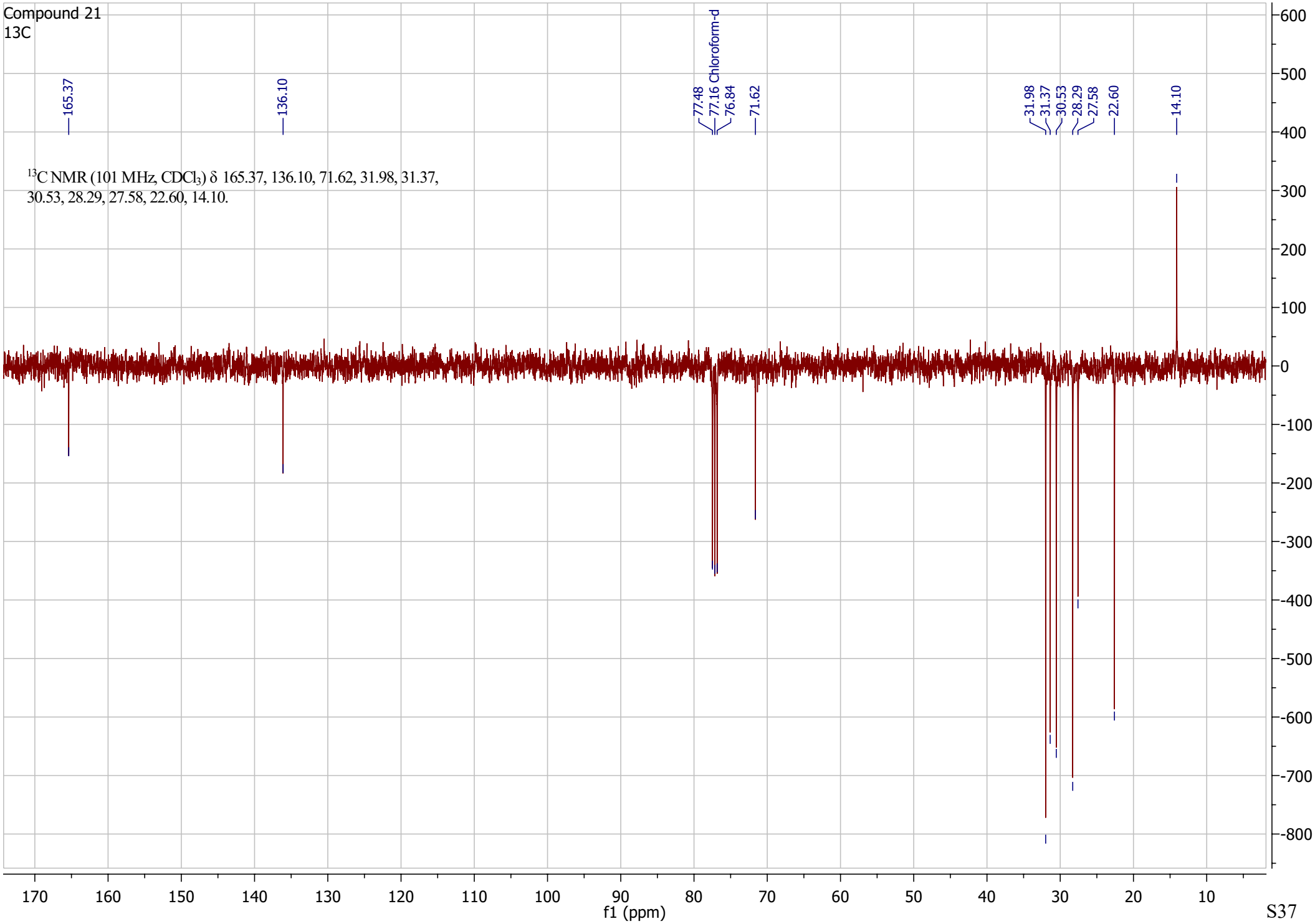

Compound 20
1H
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.27 (d, J = 3.3 Hz, 2H), 3.31 (t, J = 7.4 Hz, 4H), 2.23 (t, J = 2.5 Hz, 1H), 1.69 – 1.59 (m, 4H), 1.50 – 1.40 (m, 4H), 0.93 (t, J = 7.4 Hz, 6H).
4.28
4.27
3.33
3.31
3.29
2.23
2.23
2.22
1.68
1.66
1.64
1.62
1.60
1.50
1.48
1.46
1.44
1.42
1.40
0.95
0.93
0.91
0.00 TMS
F (d) 4.27
E (t) 3.31
D (t) 2.23
C (m) 1.64
B (m) 1.45
A (t) 0.93
2.44
4.35
0.57
4.45
4.20
6.00
f1 (ppm)

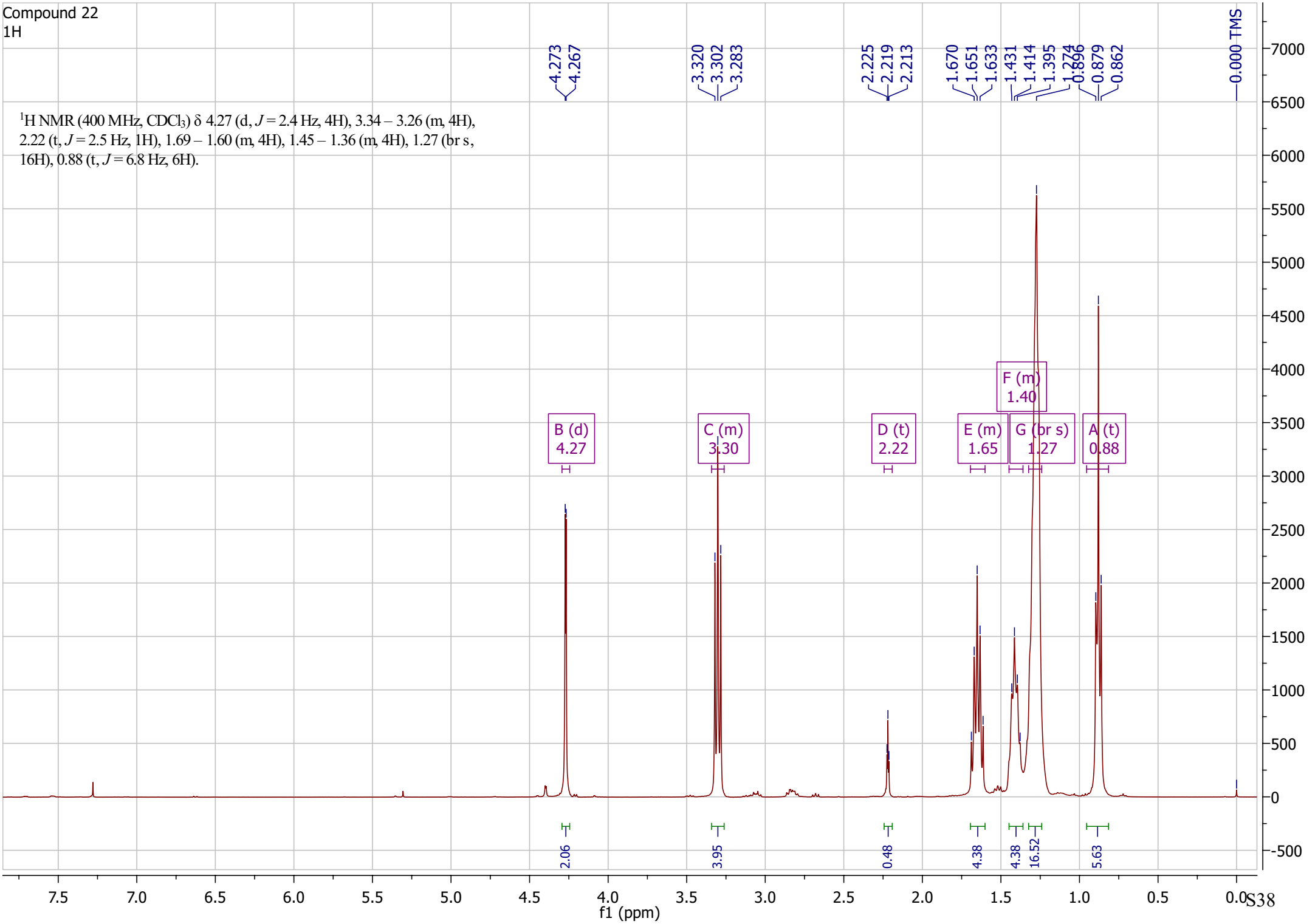
Compound 20
13C

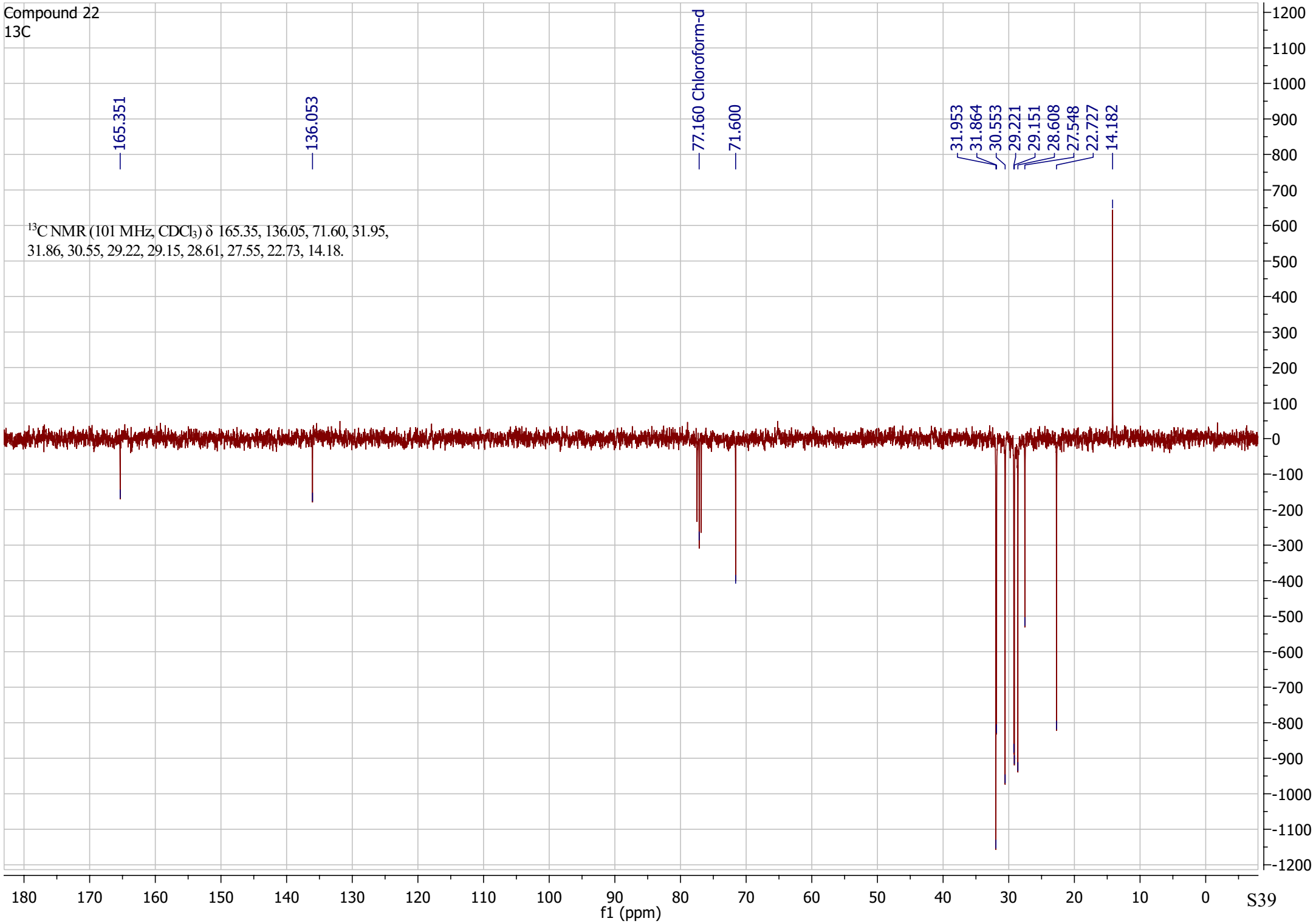
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.37, 136.07, 71.64, 32.58, 31.66, 27.57, 21.77, 13.69.




Compound 21
1H
[1]H NMR (400 MHz, CDCl3) δ 4.27 (d, J = 2.3 Hz, 2H), 3.30 (t, J = 7.4 Hz, 4H), 2.22 (t, J = 2.3 Hz, 1H), 1.70 - 1.61 (m, 4H), 1.47 - 1.38 (m, 4H), 1.35 – 1.24 (m, 8H), 0.89 (t, J = 6.8 Hz, 6H).
4.27
4.27
3.32
3.30
3.29
2.22
2.22
2.21
1.69
1.67
1.65
1.63
1.61
1.60
1.44
1.42
1.40
1.34
1.31
1.30
1.30
1.29
0.91
0.89
0.87
0.00 TMS
G (d) 4.27
F (t) 3.30
E (t) 2.22
D (m) 1.65
C (m) 1.42
B (m) 1.30
A (t) 0.89
2.13
4.12
0.63
4.16
4.08
8.03
5.59
f1 (ppm)

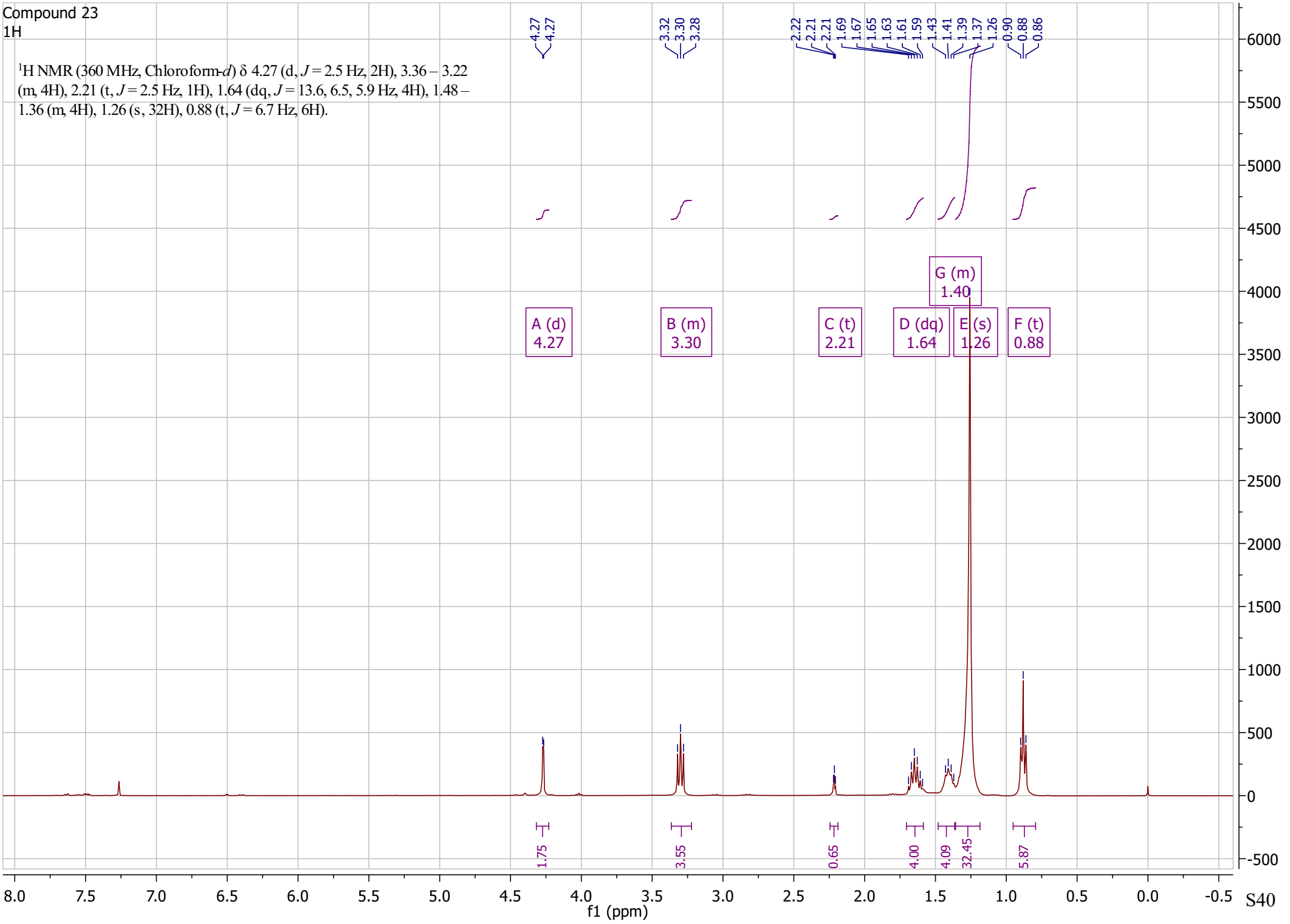

Compound 21
13C
165.37
136.10
77.48
77.16 Chloroform-d
76.84
71.62
31.98
31.37
30.53
28.29
27.58
22.60
14.10
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.37, 136.10, 71.62, 31.98, 31.37, 30.53, 28.29, 27.58, 22.60, 14.10.
f1 (ppm)

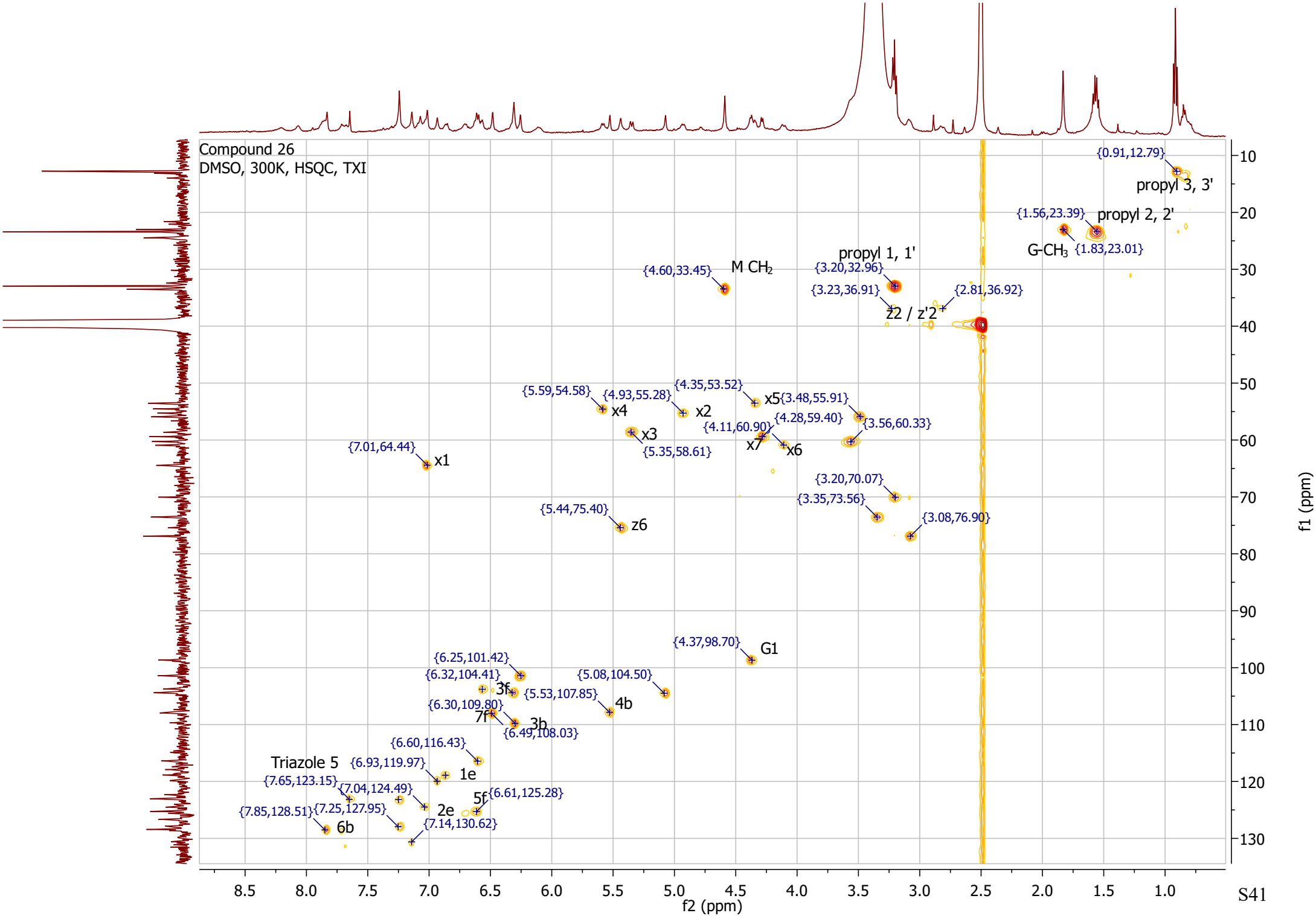

Compound 22
1H
[1]H NMR (400 MHz, CDCl3) δ 4.27 (d, J = 2.4 Hz, 4H), 3.34 – 3.26 (m, 4H), 2.22 (t, J = 2.5 Hz, 1H), 1.69 – 1.60 (m, 4H), 1.45 – 1.36 (m, 4H), 1.27 (br s, 16H), 0.88 (t, J = 6.8 Hz, 6H).
4.273
4.267
3.320
3.302
3.283
2.225
2.219
2.213
1.670
1.651
1.633
1.431
1.414
1.395
1.274
0.896
0.879
0.862
0.000 TMS
B (d) 4.27
C (m) 3.30
D (t) 2.22
E (m) 1.65
F (m) 1.40
G (br s) 1.27
A (t) 0.88
2.06
3.95
0.48
4.38
4.38
16.52
5.63
f1 (ppm)

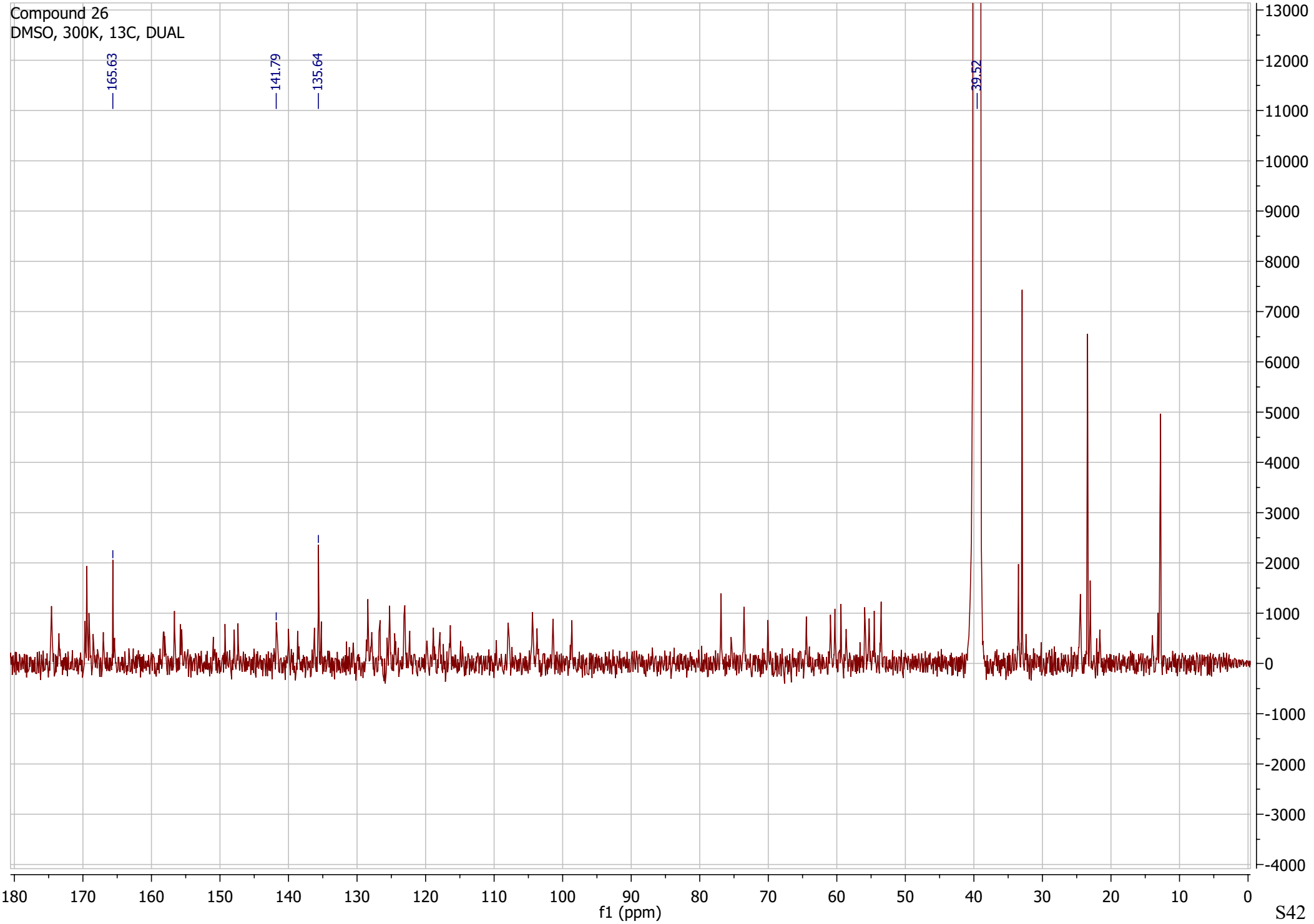

Compound 22
13C
165.351
136.053
77.160 Chloroform-d
71.600
31.953
31.864
30.553
29.221
29.151
28.608
27.548
22.727
14.182
13C NMR (101 MHz, CDCl3) δ 165.35, 136.05, 71.60, 31.95, 31.86, 30.55, 29.22, 29.15, 28.61, 27.55, 22.73, 14.18.
f1 (ppm)

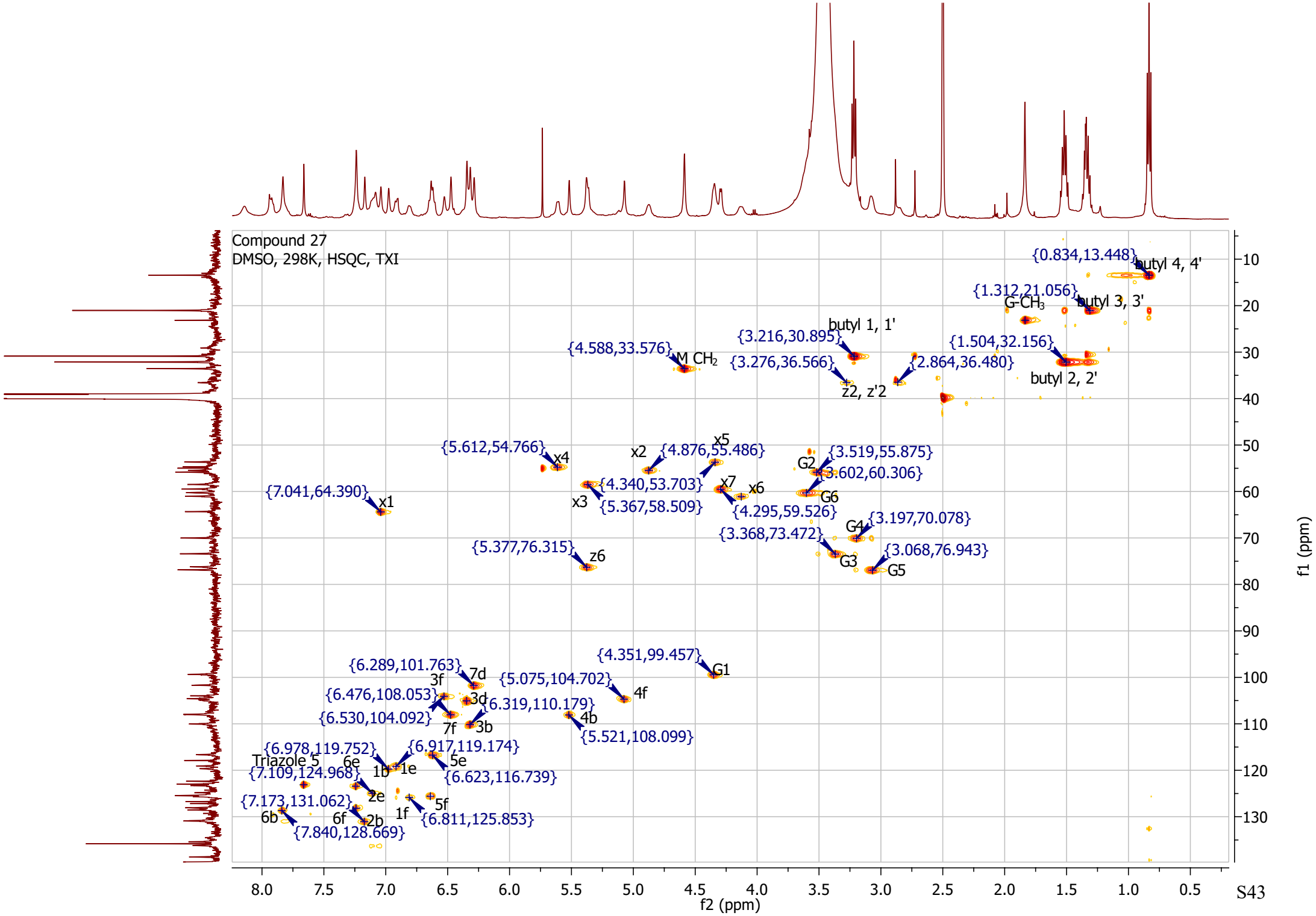
Compound 23
1H

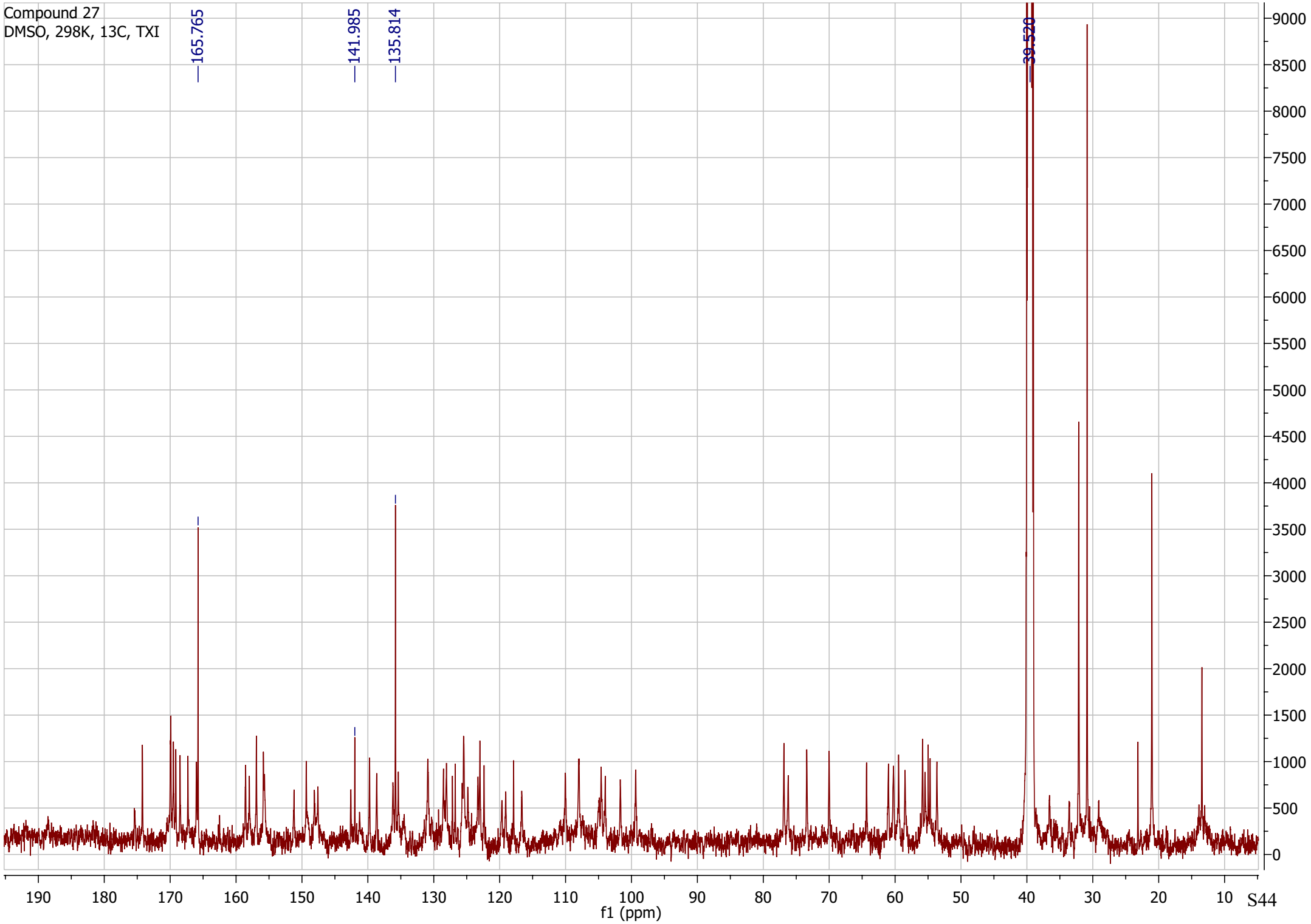
^{1}H NMR (360 MHz, Chloroform-*d*) δ 4.27 (d, *J* = 2.5 Hz, 2H), 3.36 – 3.22 (m, 4H), 2.21 (t, *J* = 2.5 Hz, 1H), 1.64 (dq, *J* = 13.6, 6.5, 5.9 Hz, 4H), 1.48 – 1.36 (m, 4H), 1.26 (s, 32H), 0.88 (t, *J* = 6.7 Hz, 6H).

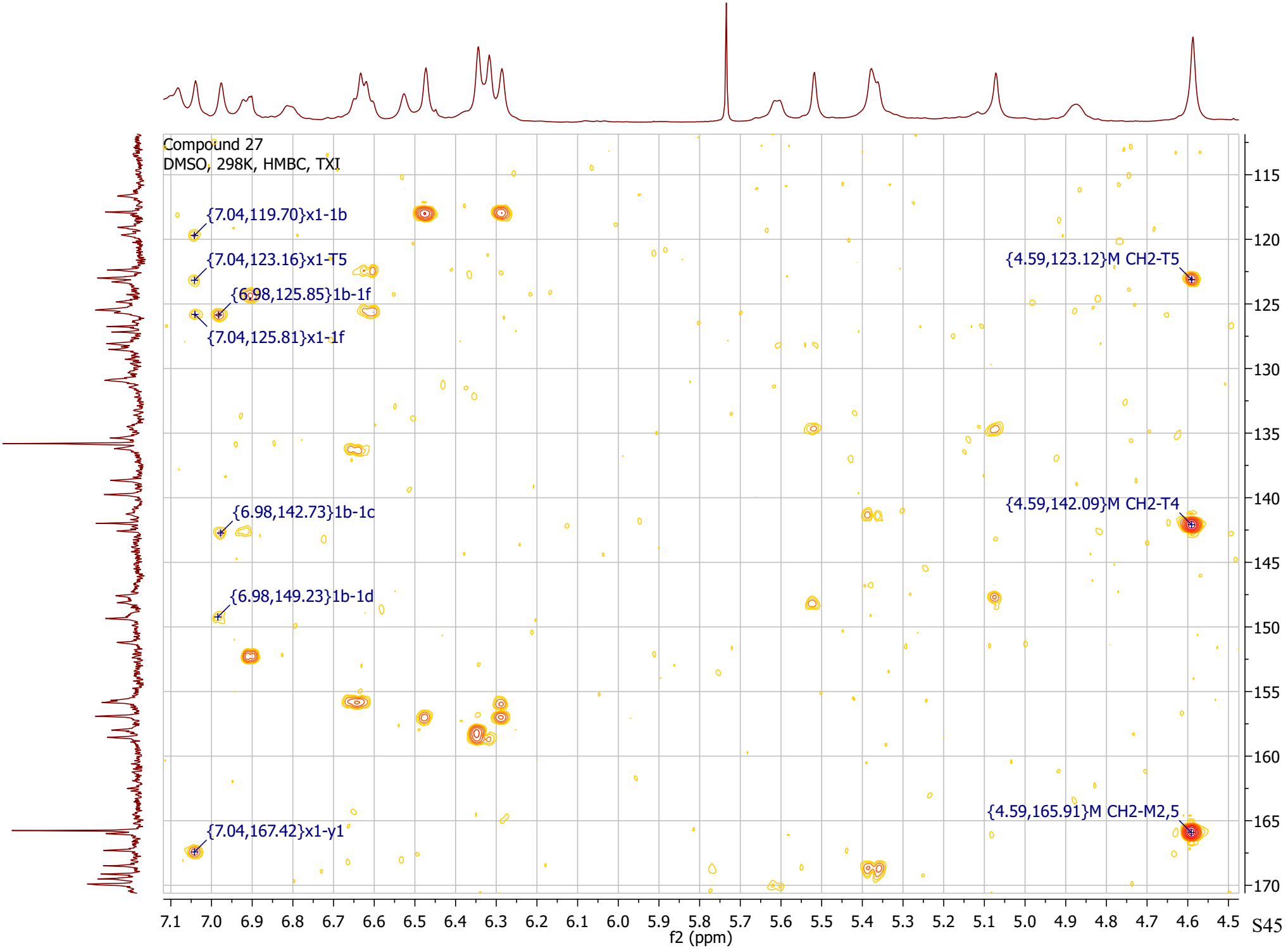


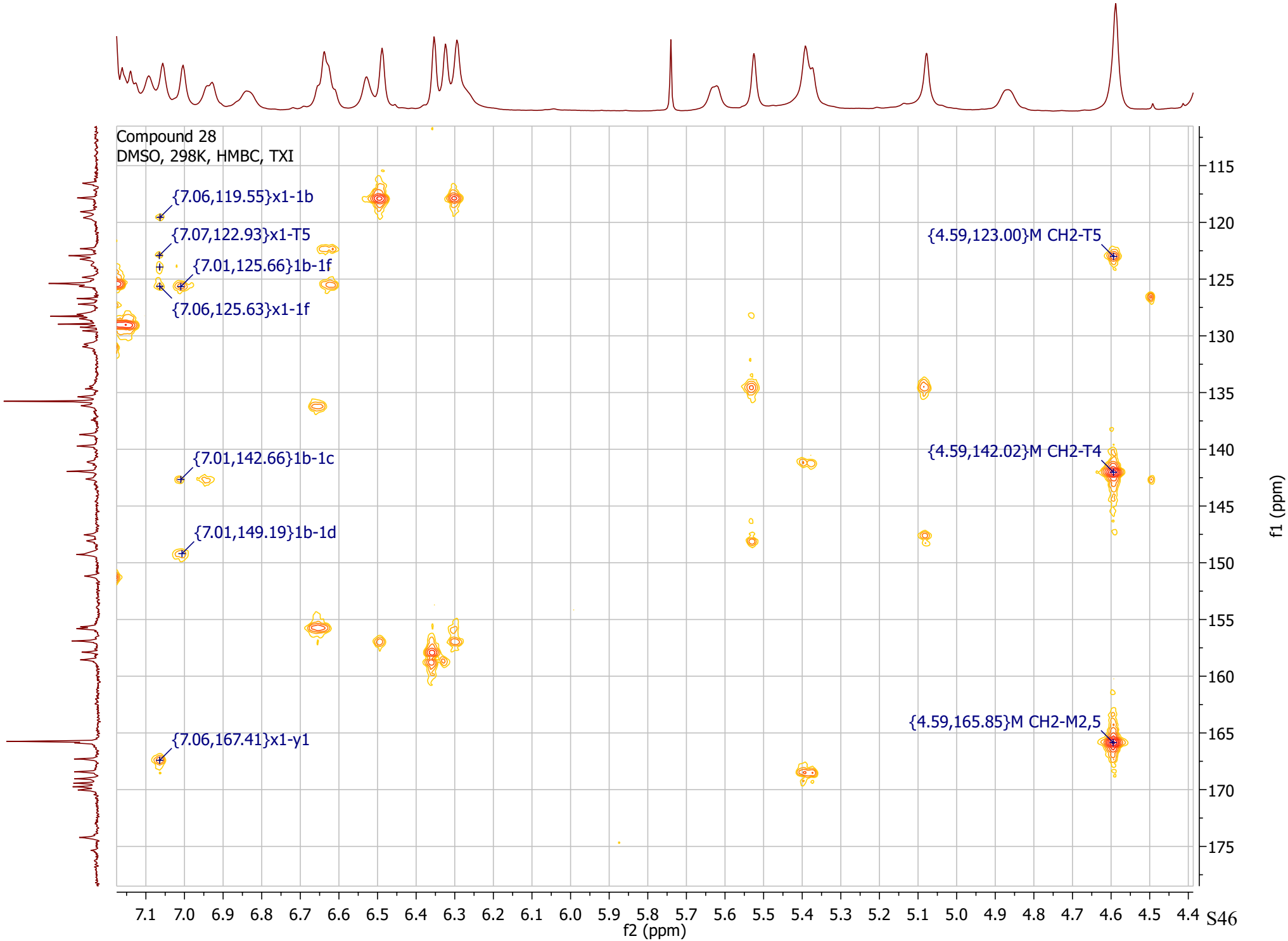

Compound 26
DMSO, 300K, HSQC, TXI
{0.91,12.79}
propyl 3, 3'
{1.56,23.39}
propyl 2, 2'
G-CH3
{1.83,23.01}
propyl 1, 1'
{4.60,33.45}
M CH2
{3.20,32.96}
{3.23,36.91}
{2.81,36.92}
z2 / z'2
{5.59,54.58}
{4.93,55.28}
{4.35,53.52}
x5
{3.48,55.91}
x4
x2
{4.28,59.40}
{4.11,60.90}
{3.56,60.33}
x3
x7
x6
{5.35,58.61}
{7.01,64.44}
x1
{3.20,70.07}
{3.35,73.56}
{3.08,76.90}
{5.44,75.40}
z6
{4.37,98.70}
G1
{6.25,101.42}
{6.32,104.41}
{5.08,104.50}
3f
{5.53,107.85}
4b
{6.30,109.80}
7f
3b
{6.49,108.03}
{6.60,116.43}
Triazole 5
{6.93,119.97}
1e
{7.65,123.15}
{7.04,124.49}
5f
{6.61,125.28}
{7.85,128.51}
{7.25,127.95}
2e
{7.14,130.62}
6b
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

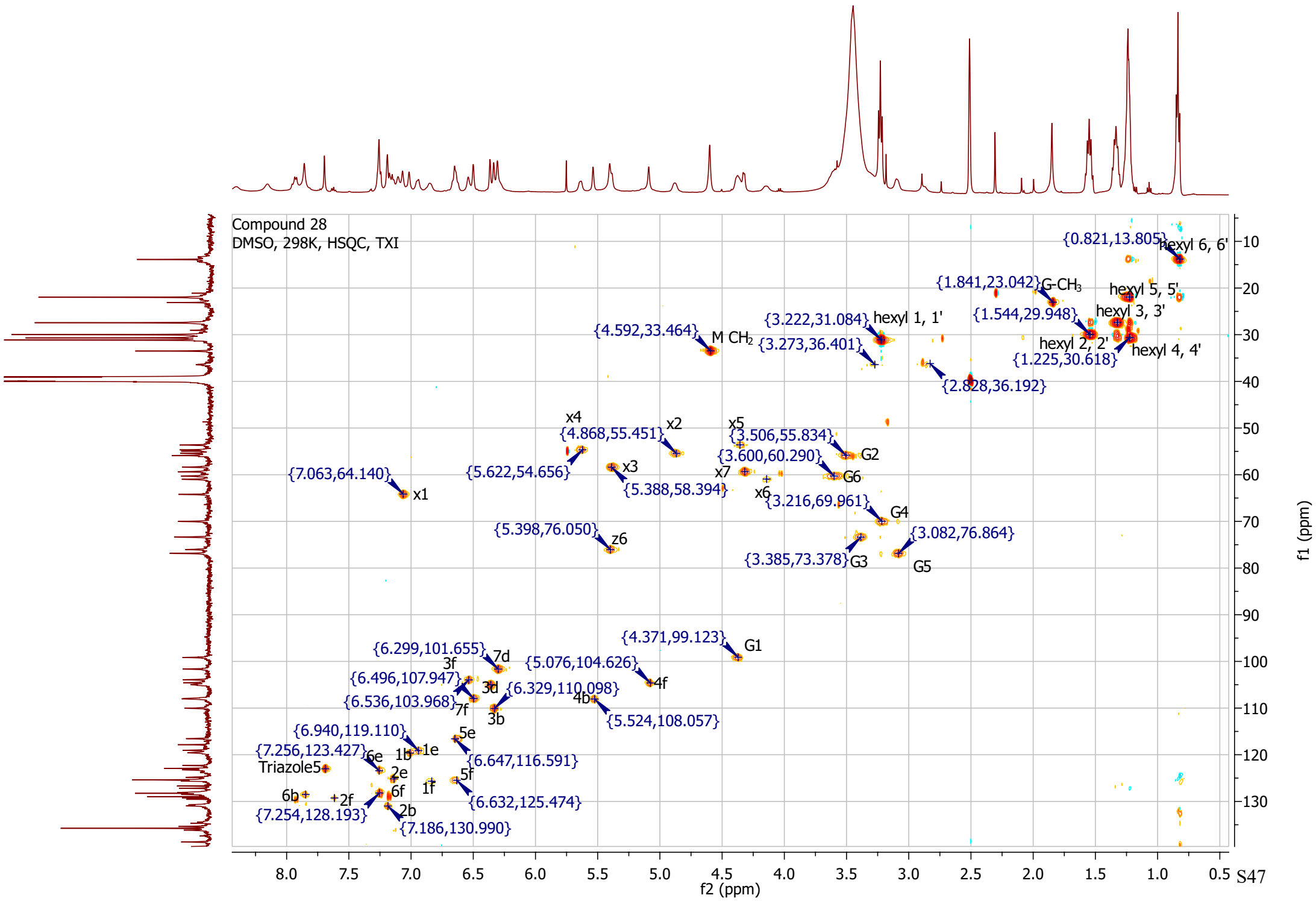

Compound 26
DMSO, 300K, 13C, DUAL
165.63
141.79
135.64
39.52
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

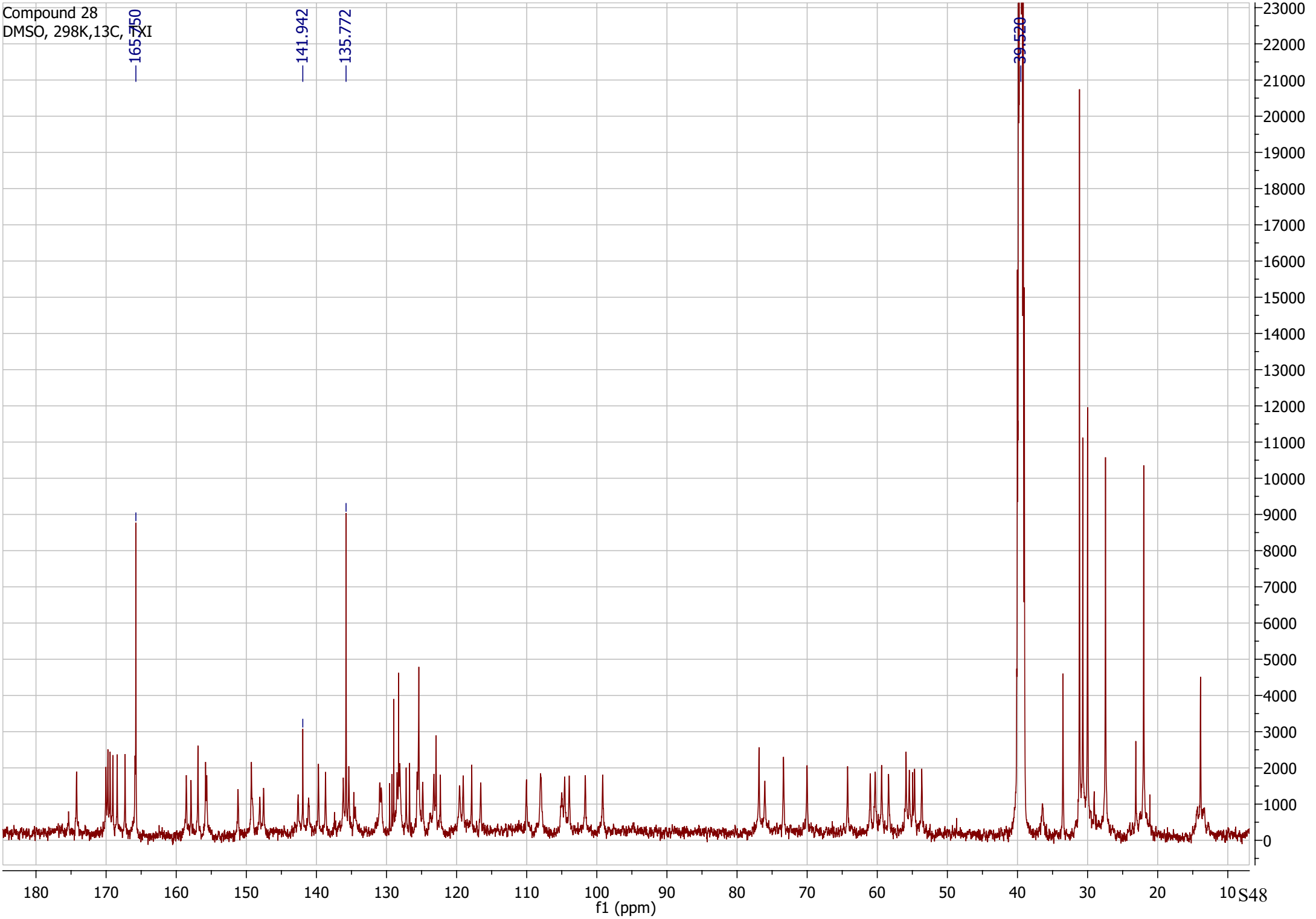

Compound 27
DMSO, 298K, HSQC, TXI
{0.834,13.448}
butyl 4, 4'
{1.312,21.056}
G-CH3
butyl 3, 3'
butyl 1, 1'
{3.216,30.895}
{4.588,33.576}
M CH2
{3.276,36.566}
{2.864,36.480}
{1.504,32.156}
butyl 2, 2'
z2, z'2
{5.612,54.766}
x4
x2
{4.876,55.486}
x5
G2
{3.519,55.875}
{3.602,60.306}
{4.340,53.703}
x7
x6
G6
{7.041,64.390}
x1
x3
{5.367,58.509}
{4.295,59.526}
{3.197,70.078}
G4
{3.368,73.472}
{5.377,76.315}
z6
G3
{3.068,76.943}
G5
{4.351,99.457}
G1
{6.289,101.763}
7d
3f
{5.075,104.702}
4f
{6.476,108.053}
3d
{6.319,110.179}
{6.530,104.092}
4b
7f
3b
{5.521,108.099}
{6.978,119.752}
{6.917,119.174}
Triazole 5
6e
1b
1e
5e
{7.109,124.968}
{6.623,116.739}
2e
{7.173,131.062}
5f
6b
6f
2b
1f
{6.811,125.853}
{7.840,128.669}
f2 (ppm)
f1 (ppm)
S43

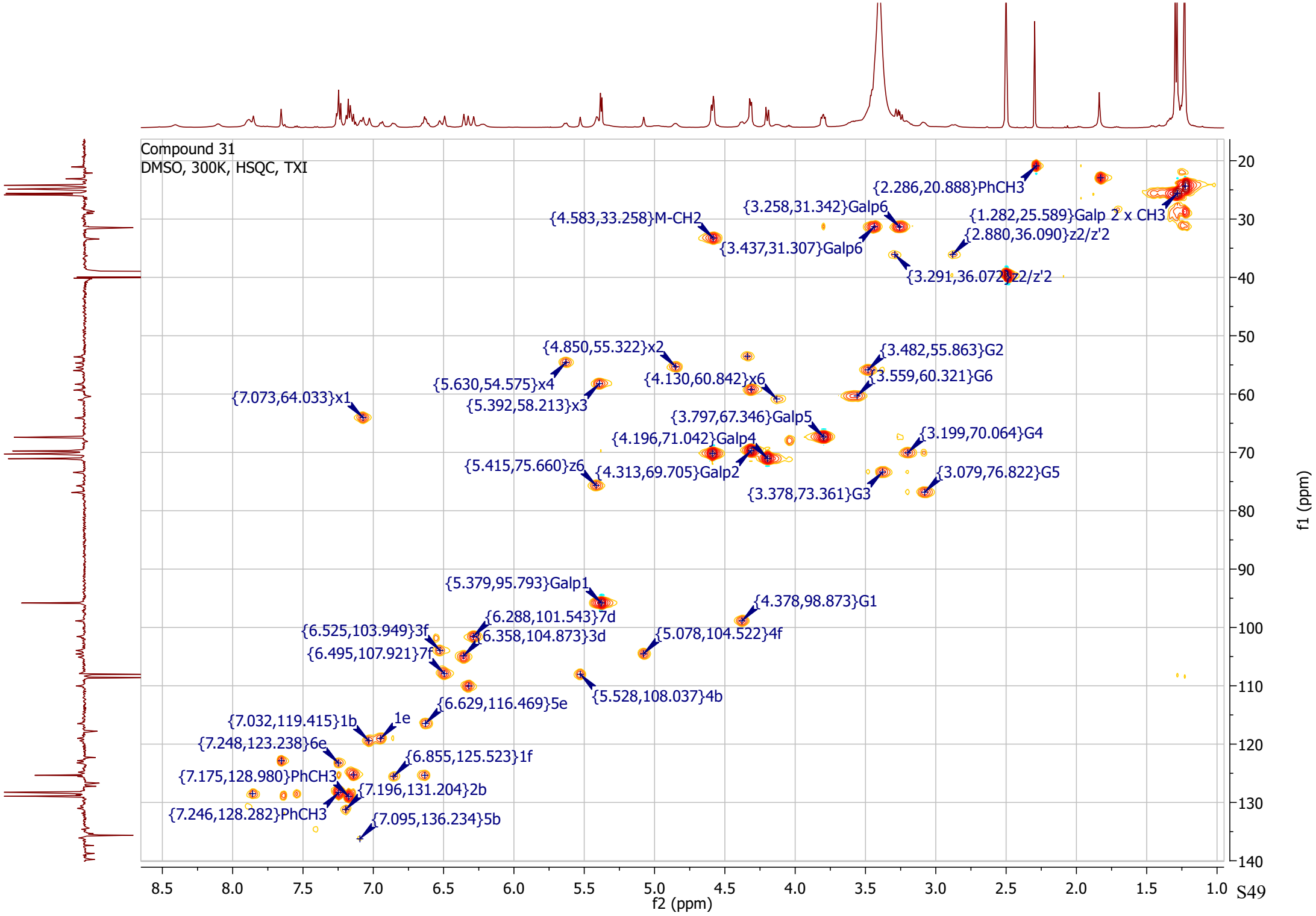

Compound 27
DMSO, 298K, 13C, TXI
165.765
141.985
135.814
39.520
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

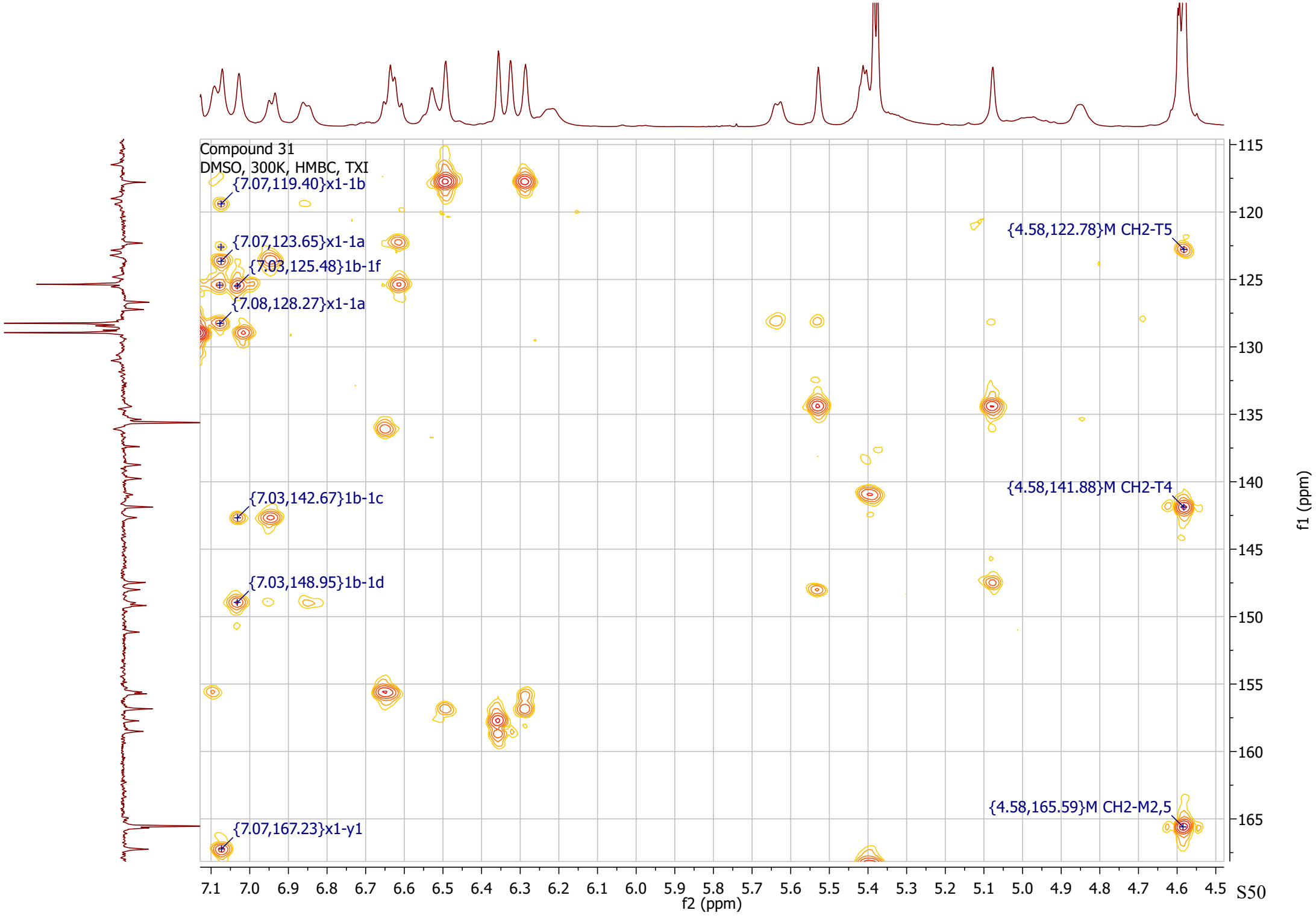

Compound 27
DMSO, 298K, HMBC, TXI
{7.04,119.70}x1-1b
{7.04,123.16}x1-T5
{6.98,125.85}1b-1f
{7.04,125.81}x1-1f
{6.98,142.73}1b-1c
{6.98,149.23}1b-1d
{7.04,167.42}x1-y1
{4.59,123.12}M CH2-T5
{4.59,142.09}M CH2-T4
{4.59,165.91}M CH2-M2,5
f2 (ppm)
f1 (ppm)
S45

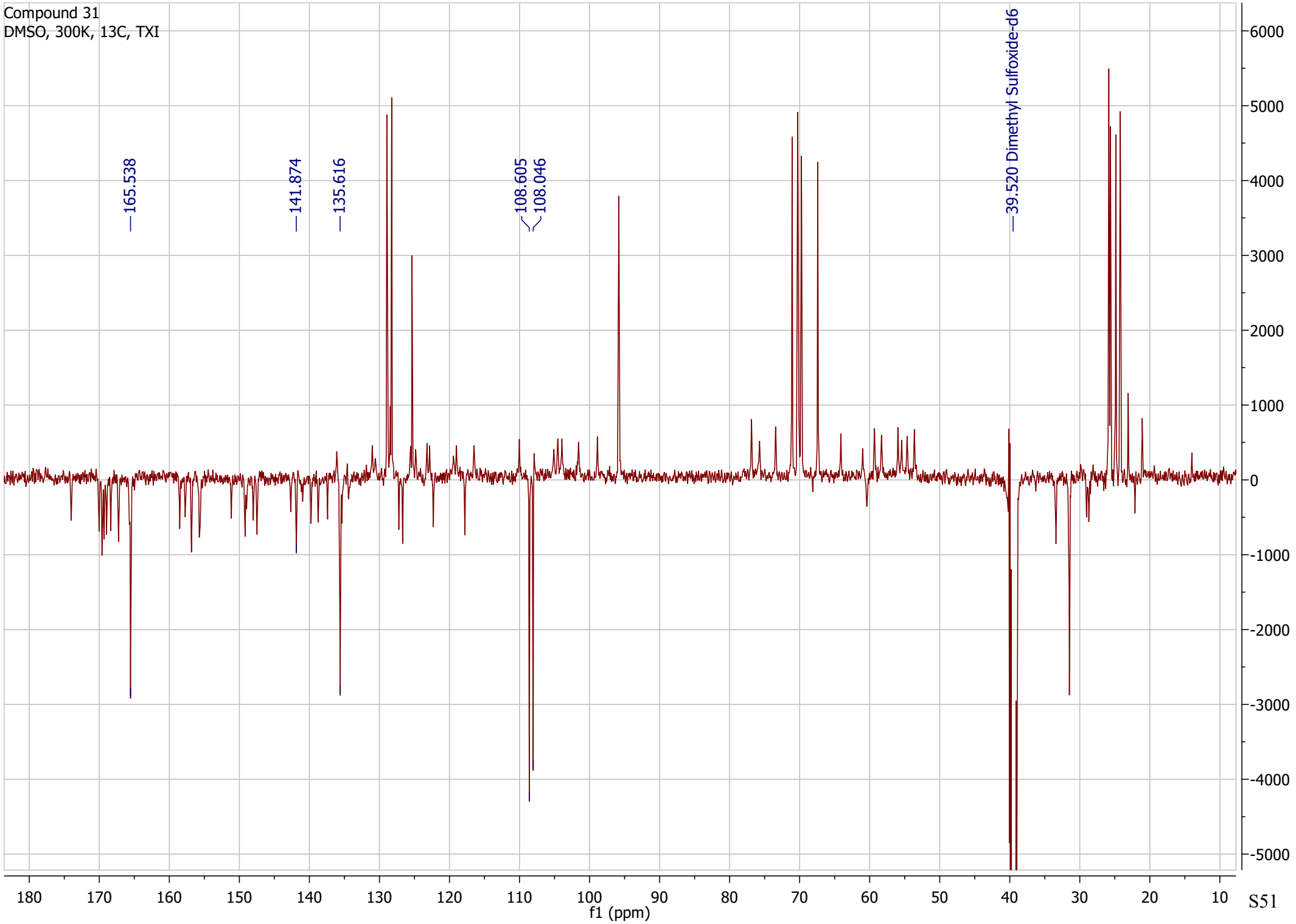

Compound 28
DMSO, 298K, HMBC, TXI
{7.06,119.55}x1-1b
{7.07,122.93}x1-T5
{7.01,125.66}1b-1f
{7.06,125.63}x1-1f
{7.01,142.66}1b-1c
{7.01,149.19}1b-1d
{7.06,167.41}x1-y1
{4.59,123.00}M CH2-T5
{4.59,142.02}M CH2-T4
{4.59,165.85}M CH2-M2,5
f2 (ppm)
f1 (ppm)

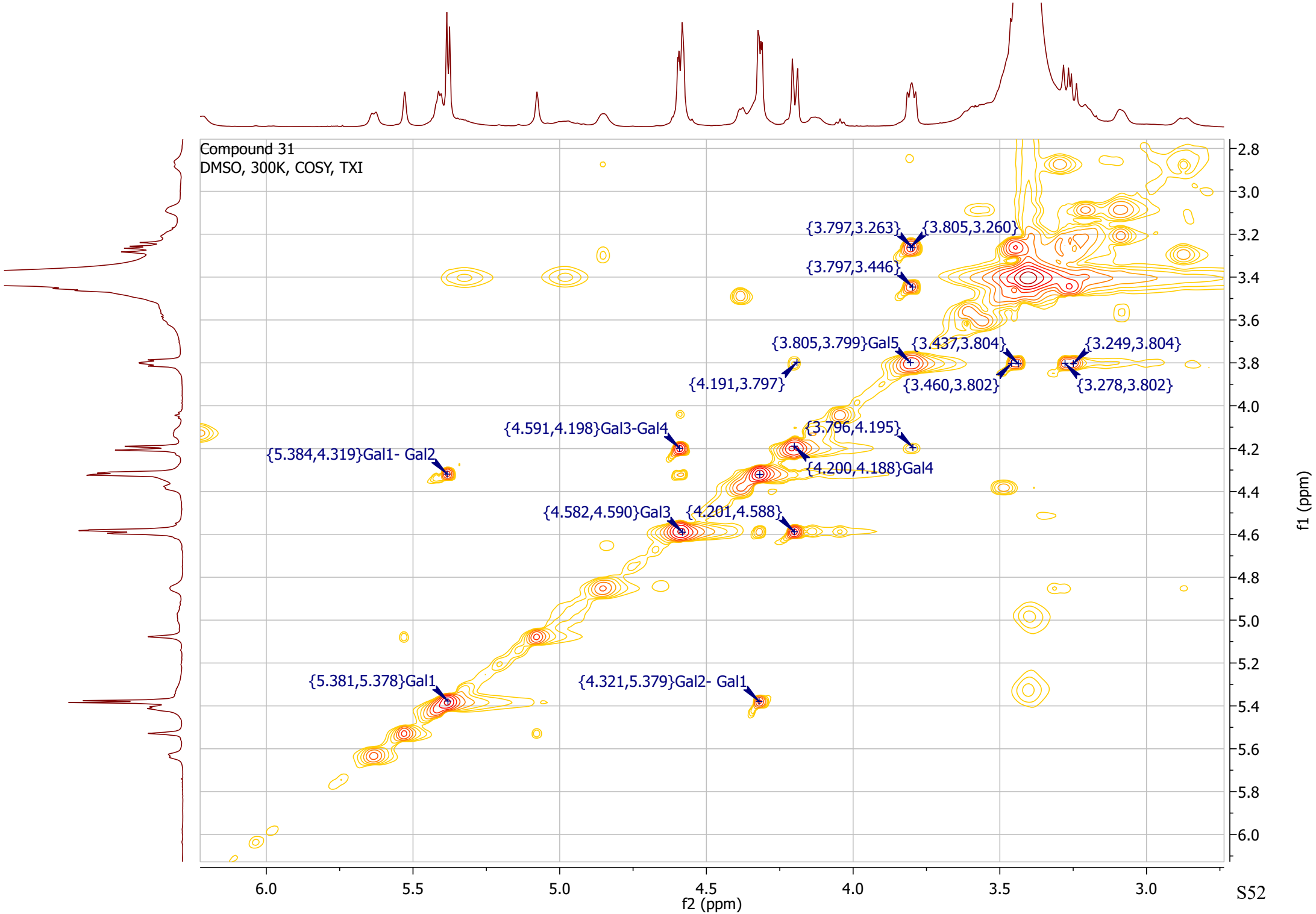

Compound 28
DMSO, 298K, HSQC, TXI
{0.821,13.805}
hexyl 6, 6'
{1.841,23.042}
G-CH3
hexyl 5, 5'
{1.544,29.948}
hexyl 3, 3'
{3.222,31.084}
hexyl 1, 1'
{4.592,33.464}
M CH2
{3.273,36.401}
hexyl 2, 2'
hexyl 4, 4'
{1.225,30.618}
{2.828,36.192}
x4
{4.868,55.451}
x2
x5
{3.506,55.834}
G2
{3.600,60.290}
{7.063,64.140}
x1
{5.622,54.656}
x3
x7
G6
{5.388,58.394}
x6
{3.216,69.961}
G4
{5.398,76.050}
z6
{3.082,76.864}
{3.385,73.378}
G3
G5
{4.371,99.123}
G1
{6.299,101.655}
7d
3f
{5.076,104.626}
4f
{6.496,107.947}
3d
{6.329,110.098}
4b
{6.536,103.968}
7f
3b
{5.524,108.057}
{6.940,119.110}
5e
{7.256,123.427}
6e
1b
1e
{6.647,116.591}
Triazole5
2e
5f
1f
6b
2f
6f
{6.632,125.474}
{7.254,128.193}
2b
{7.186,130.990}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)


Compound 28
DMSO, 298K,13C, ZXI
165.750
141.942
135.772
39.520
f1 (ppm)


Compound 31
DMSO, 300K, HSQC, TXI
{2.286,20.888}PhCH3
{3.258,31.342}Galp6
{1.282,25.589}Galp 2 x CH3
{4.583,33.258}M-CH2
{2.880,36.090}z2/z'2
{3.437,31.307}Galp6
{3.291,36.072}z2/z'2
{4.850,55.322}x2
{3.482,55.863}G2
{4.130,60.842}x6
{5.630,54.575}x4
{3.559,60.321}G6
{7.073,64.033}x1
{5.392,58.213}x3
{3.797,67.346}Galp5
{4.196,71.042}Galp4
{3.199,70.064}G4
{5.415,75.660}z6
{4.313,69.705}Galp2
{3.079,76.822}G5
{3.378,73.361}G3
{5.379,95.793}Galp1
{4.378,98.873}G1
{6.288,101.543}7d
{6.525,103.949}3f
{6.358,104.873}3d
{5.078,104.522}4f
{6.495,107.921}7f
{5.528,108.037}4b
{6.629,116.469}5e
{7.032,119.415}1b
1e
{7.248,123.238}6e
{6.855,125.523}1f
{7.175,128.980}PhCH3
{7.196,131.204}2b
{7.246,128.282}PhCH3
{7.095,136.234}5b
f2 (ppm)
f1 (ppm)
S49

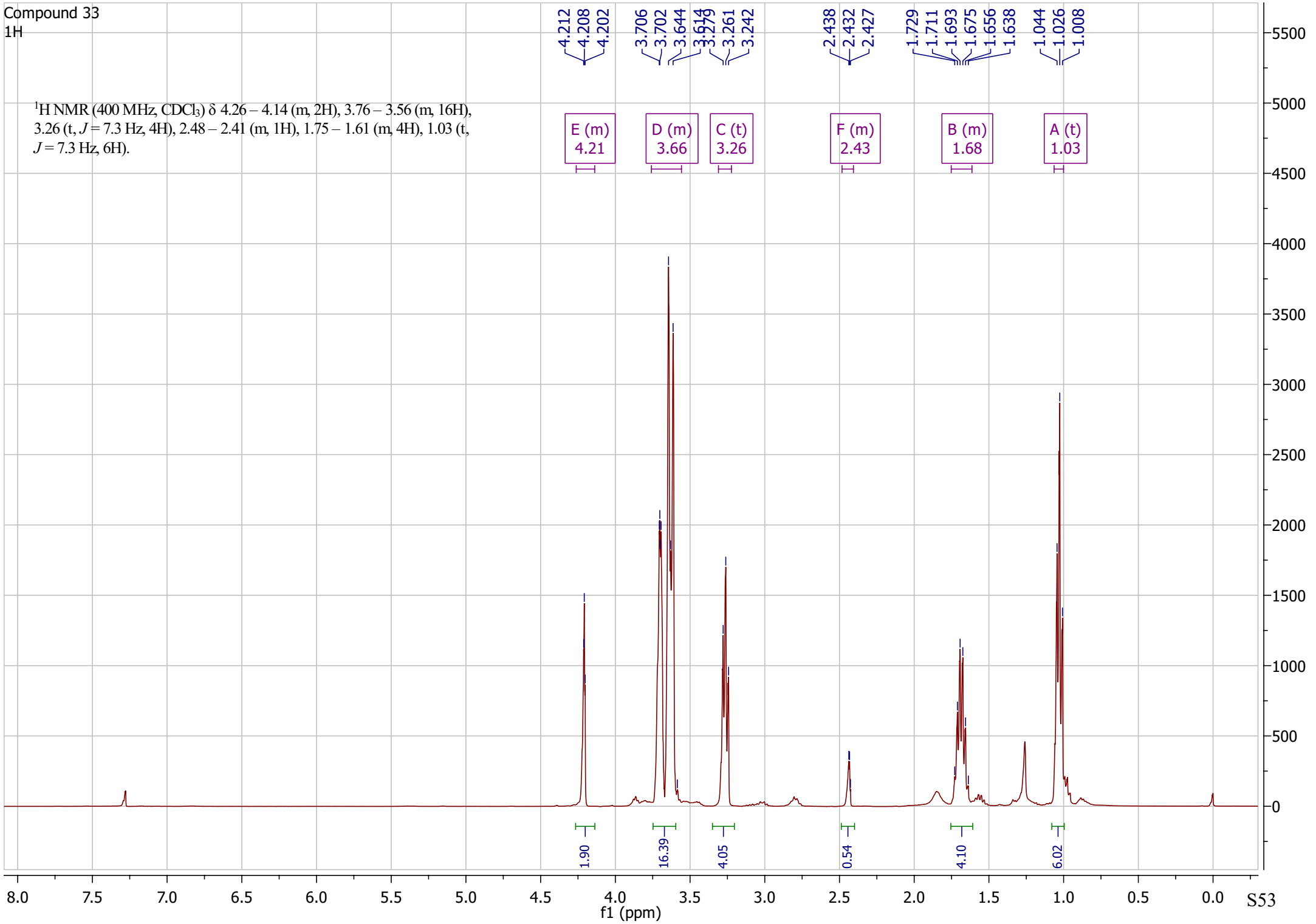

Compound 31
DMSO, 300K, HMBC, TXI
{7.07,119.40}x1-1b
{7.07,123.65}x1-1a
{7.03,125.48}1b-1f
{7.08,128.27}x1-1a
{4.58,122.78}M CH2-T5
{4.58,141.88}M CH2-T4
{7.03,142.67}1b-1c
{7.03,148.95}1b-1d
{4.58,165.59}M CH2-M2,5
{7.07,167.23}x1-y1
f2 (ppm)
f1 (ppm)
S50

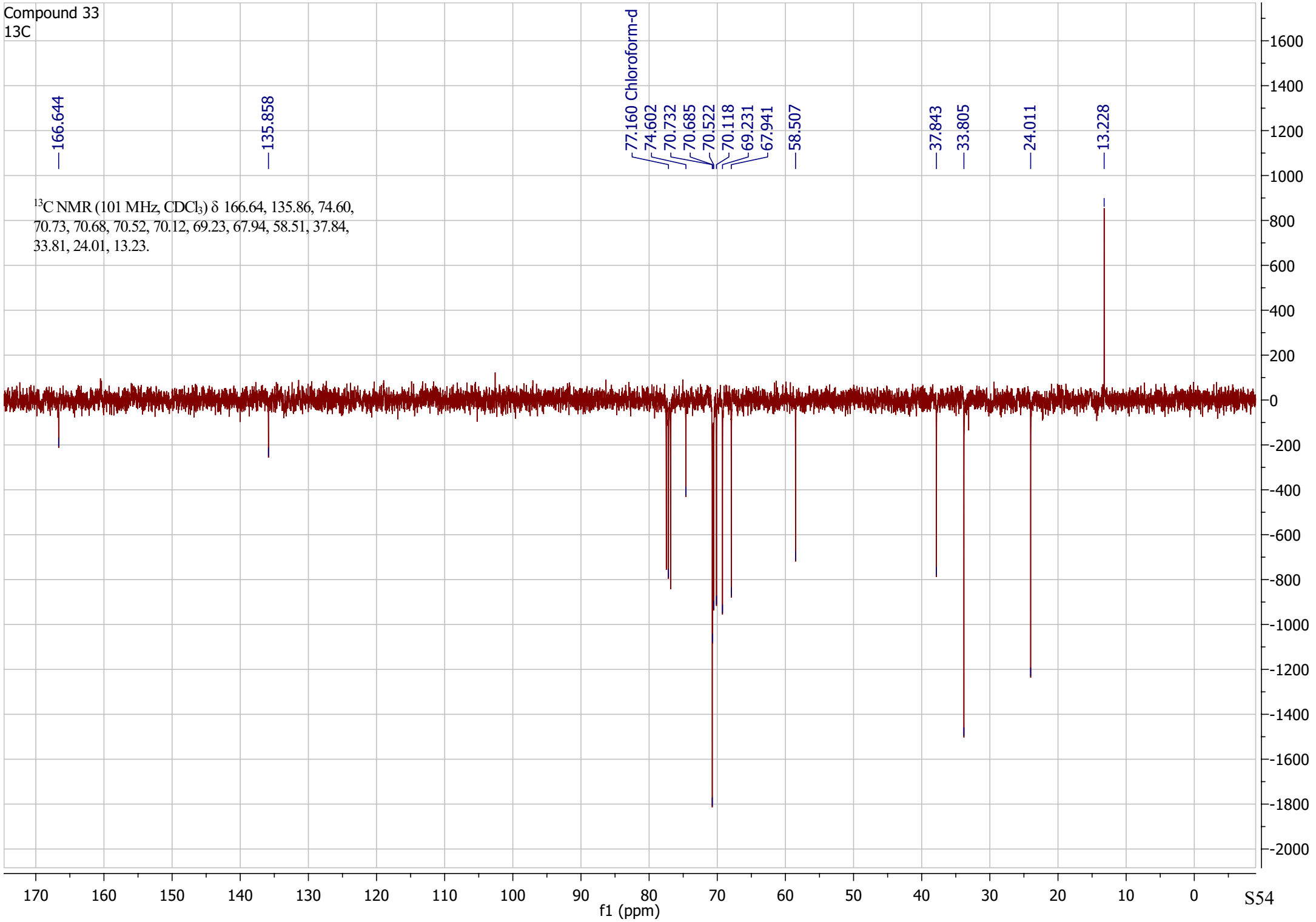

Compound 31
DMSO, 300K, 13C, TXI
165.538
141.874
135.616
108.605
108.046
39.520 Dimethyl Sulfoxide-d6
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


Compound 31
DMSO, 300K, COSY, TXI
{3.797,3.263}
{3.805,3.260}
{3.797,3.446}
{3.805,3.799}Gal5
{3.437,3.804}
{3.249,3.804}
{4.191,3.797}
{3.460,3.802}
{3.278,3.802}
{4.591,4.198}Gal3-Gal4
{3.796,4.195}
{5.384,4.319}Gal1- Gal2
{4.200,4.188}Gal4
{4.582,4.590}Gal3
{4.201,4.588}
{5.381,5.378}Gal1
{4.321,5.379}Gal2- Gal1
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f2 (ppm)
2.8
3.0
3.2
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
5.0
5.2
5.4
5.6
5.8
6.0
f1 (ppm)

Compound 33
1H

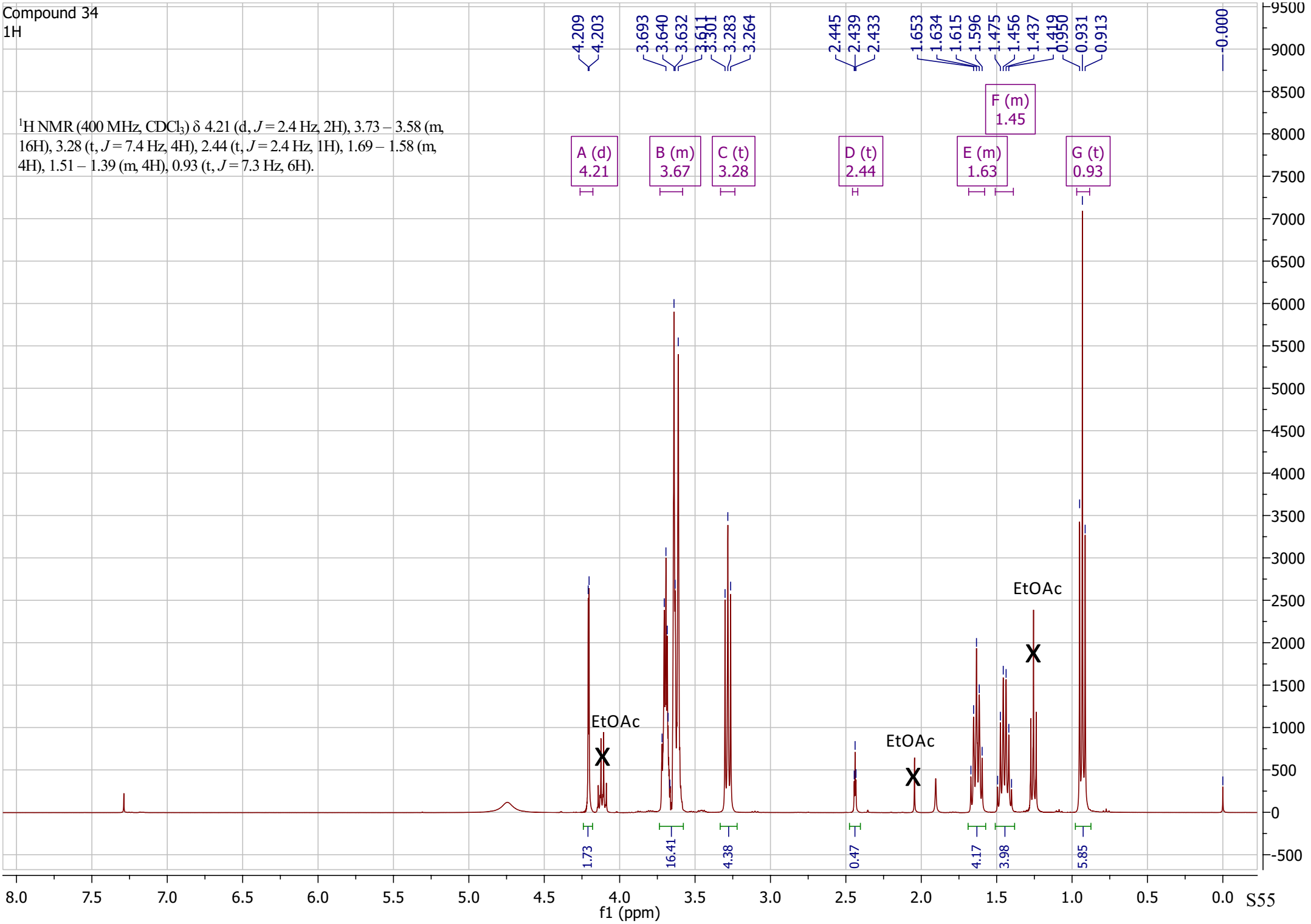
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 – 4.14 (m, 2H), 3.76 – 3.56 (m, 16H), 3.26 (t, *J* = 7.3 Hz, 4H), 2.48 – 2.41 (m, 1H), 1.75 – 1.61 (m, 4H), 1.03 (t, *J* = 7.3 Hz, 6H).

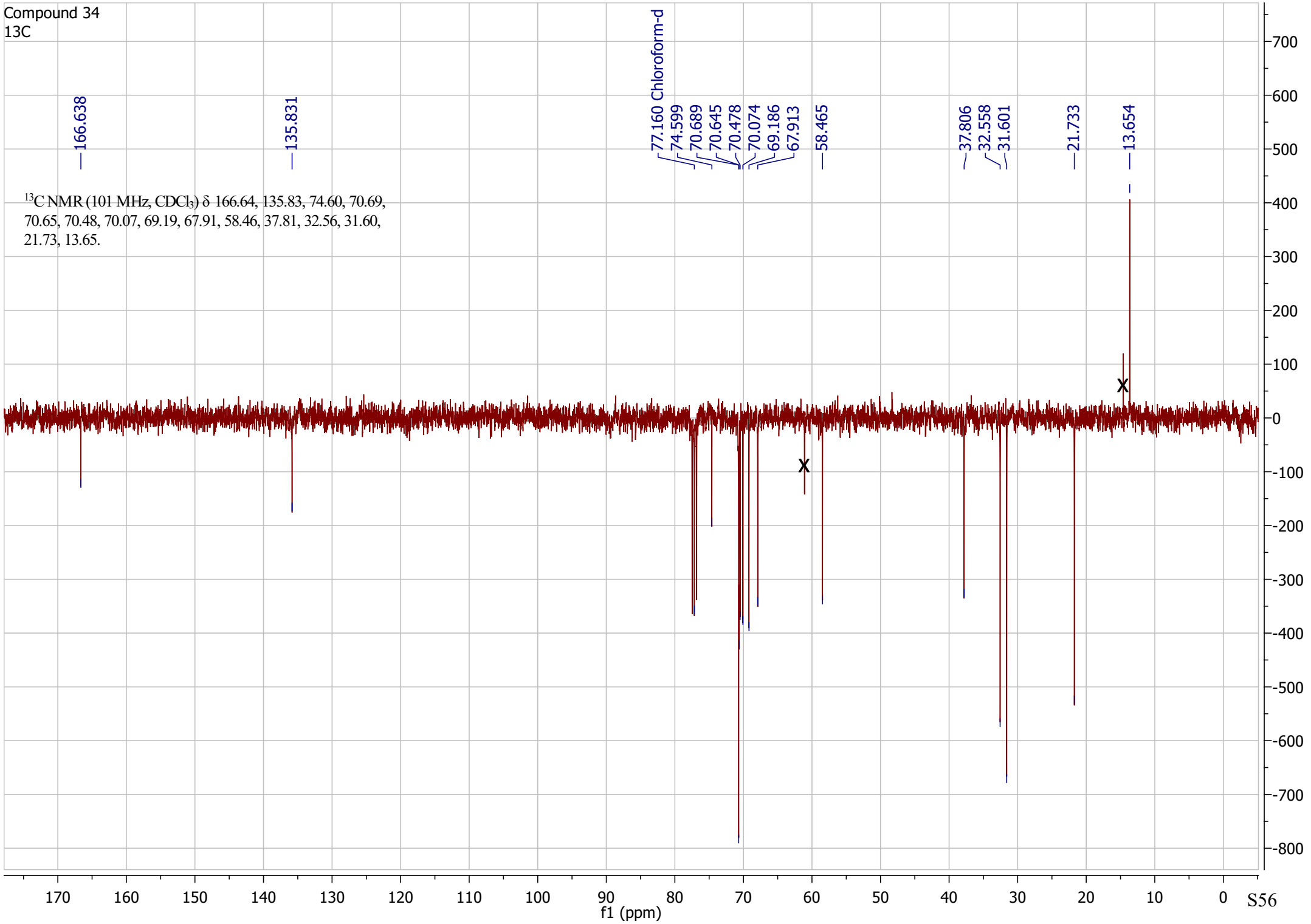


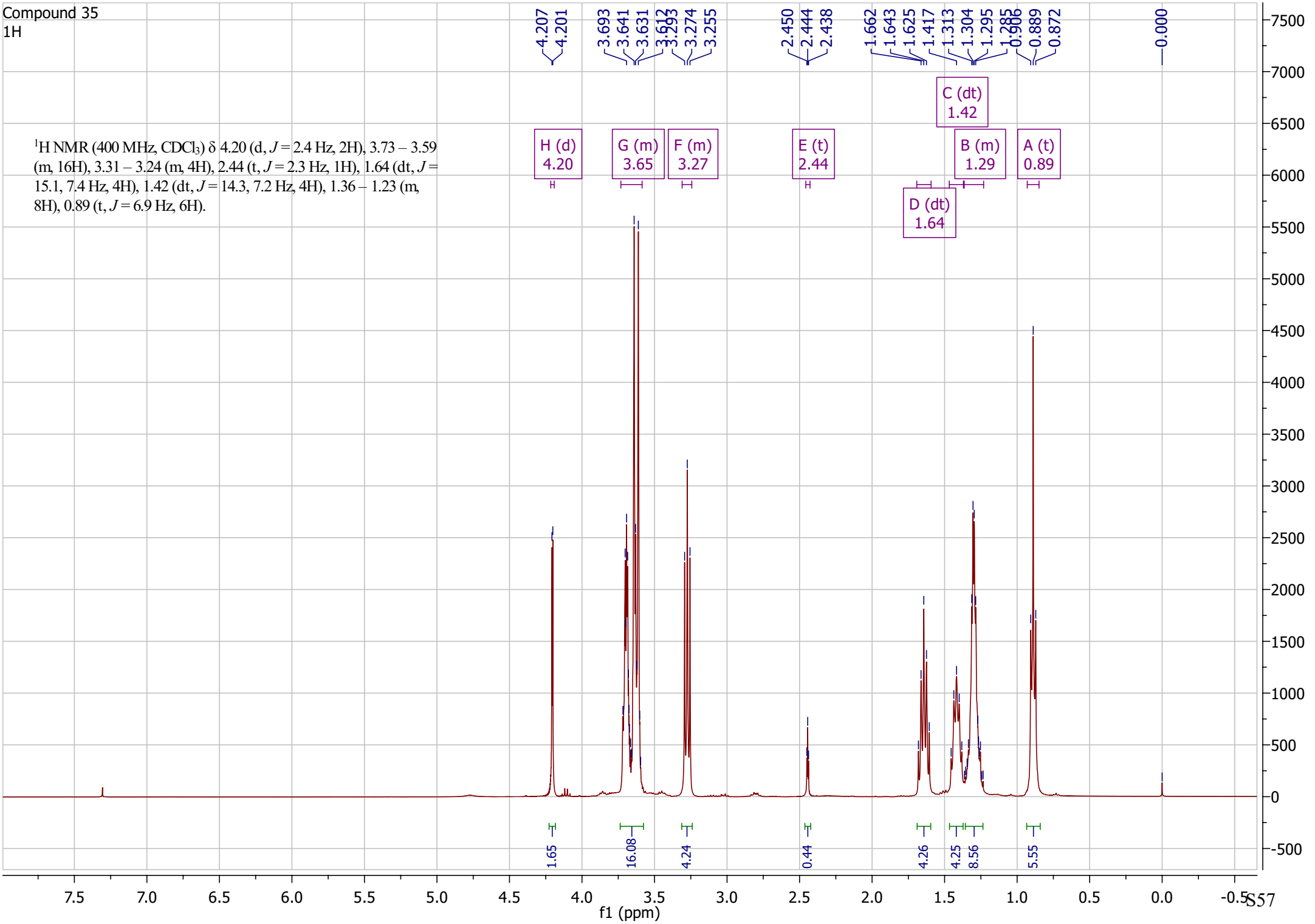

Compound 33
13C
166.644
135.858
77.160 Chloroform-d
74.602
70.732
70.685
70.522
70.118
69.231
67.941
58.507
37.843
33.805
24.011
13.228
13C NMR (101 MHz, CDCl3) δ 166.64, 135.86, 74.60, 70.73, 70.68, 70.52, 70.12, 69.23, 67.94, 58.51, 37.84, 33.81, 24.01, 13.23.
f1 (ppm)

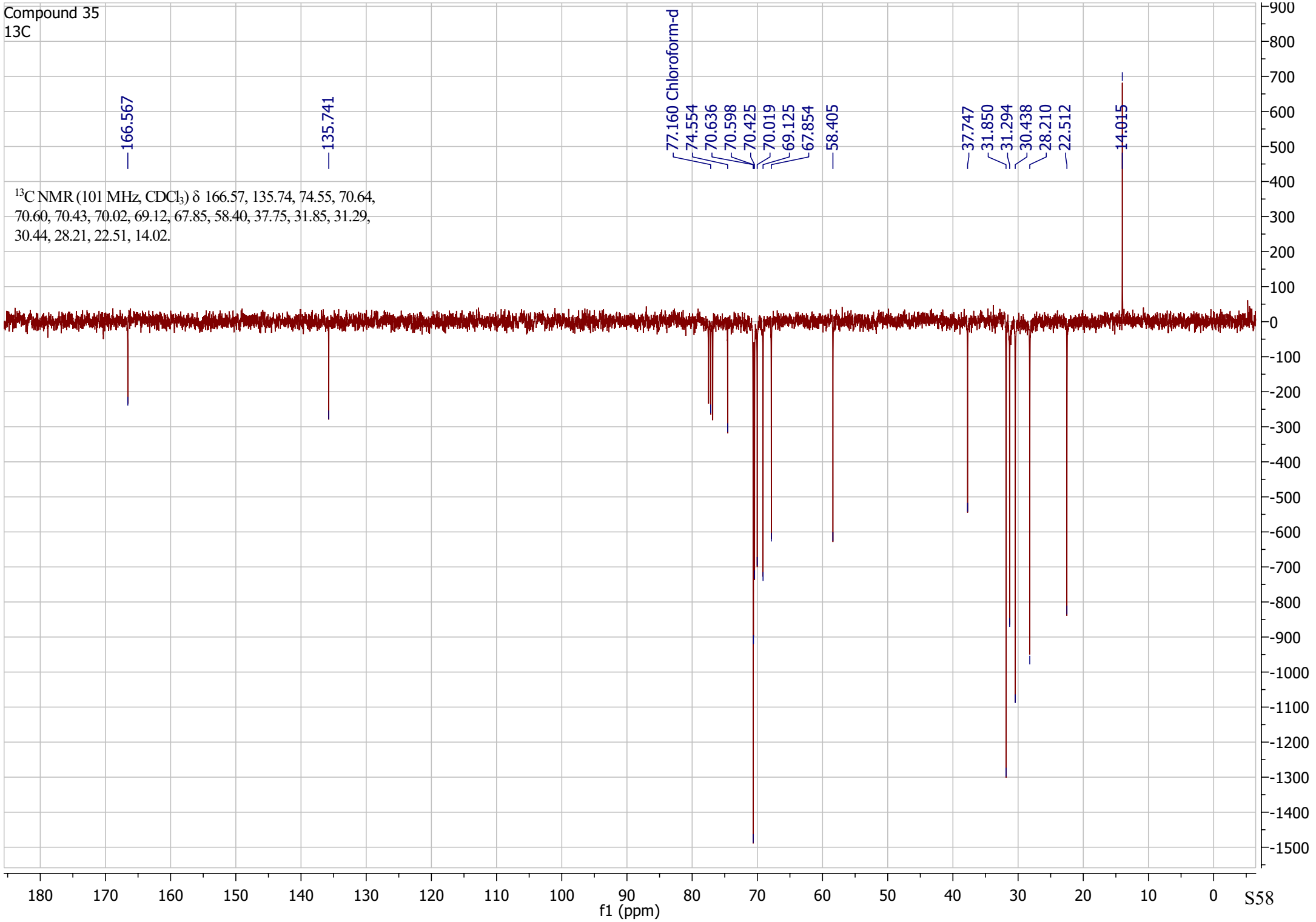
Compound 34
1H

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.21 (d, *J* = 2.4 Hz, 2H), 3.73 – 3.58 (m, 16H), 3.28 (t, *J* = 7.4 Hz, 4H), 2.44 (t, *J* = 2.4 Hz, 1H), 1.69 – 1.58 (m, 4H), 1.51 – 1.39 (m, 4H), 0.93 (t, *J* = 7.3 Hz, 6H).



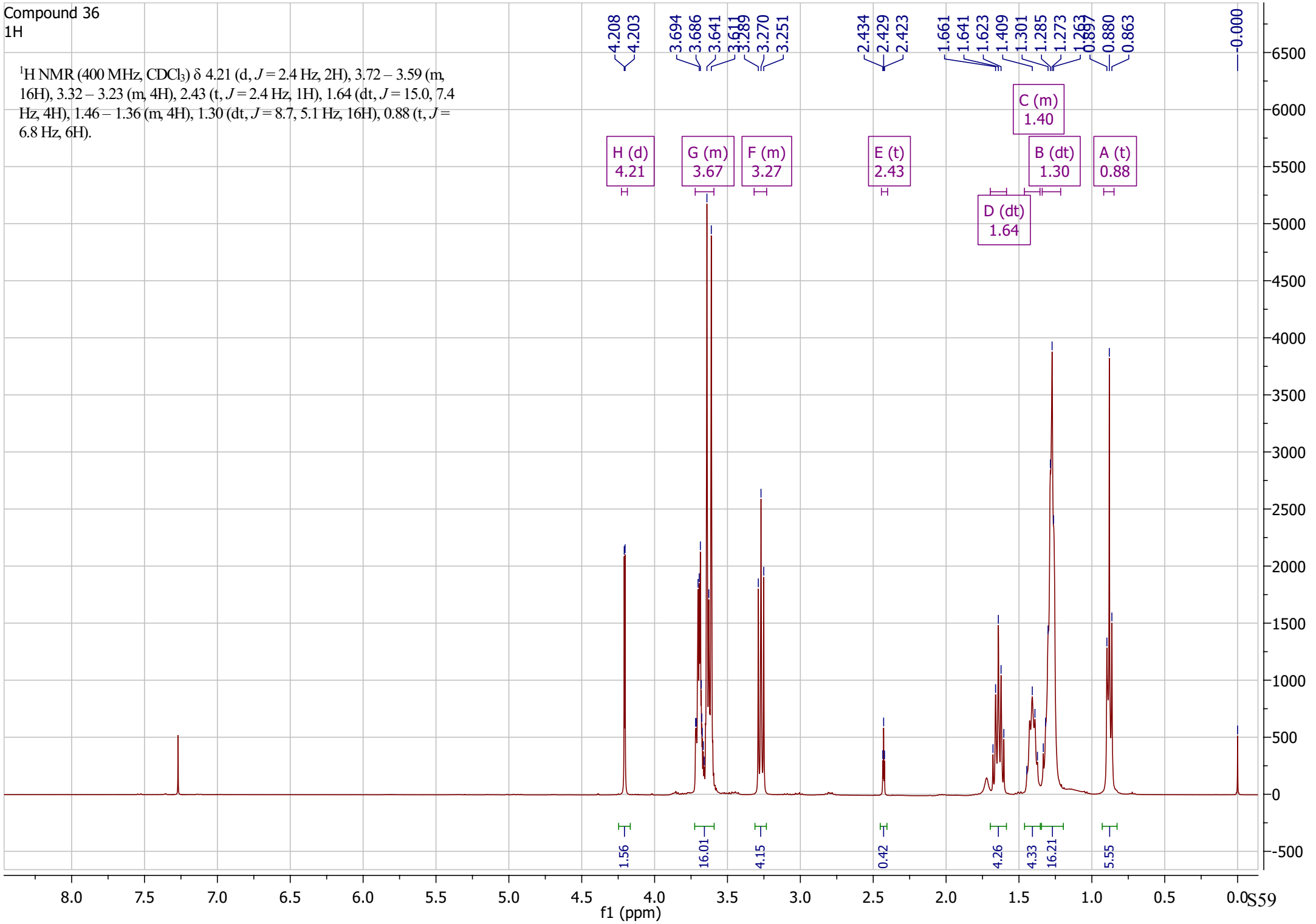

Compound 34
13C
166.638
135.831
77.160 Chloroform-d
74.599
70.689
70.645
70.478
70.074
69.186
67.913
58.465
37.806
32.558
31.601
21.733
13.654
13C NMR (101 MHz, CDCl3) δ 166.64, 135.83, 74.60, 70.69, 70.65, 70.48, 70.07, 69.19, 67.91, 58.46, 37.81, 32.56, 31.60, 21.73, 13.65.
f1 (ppm)

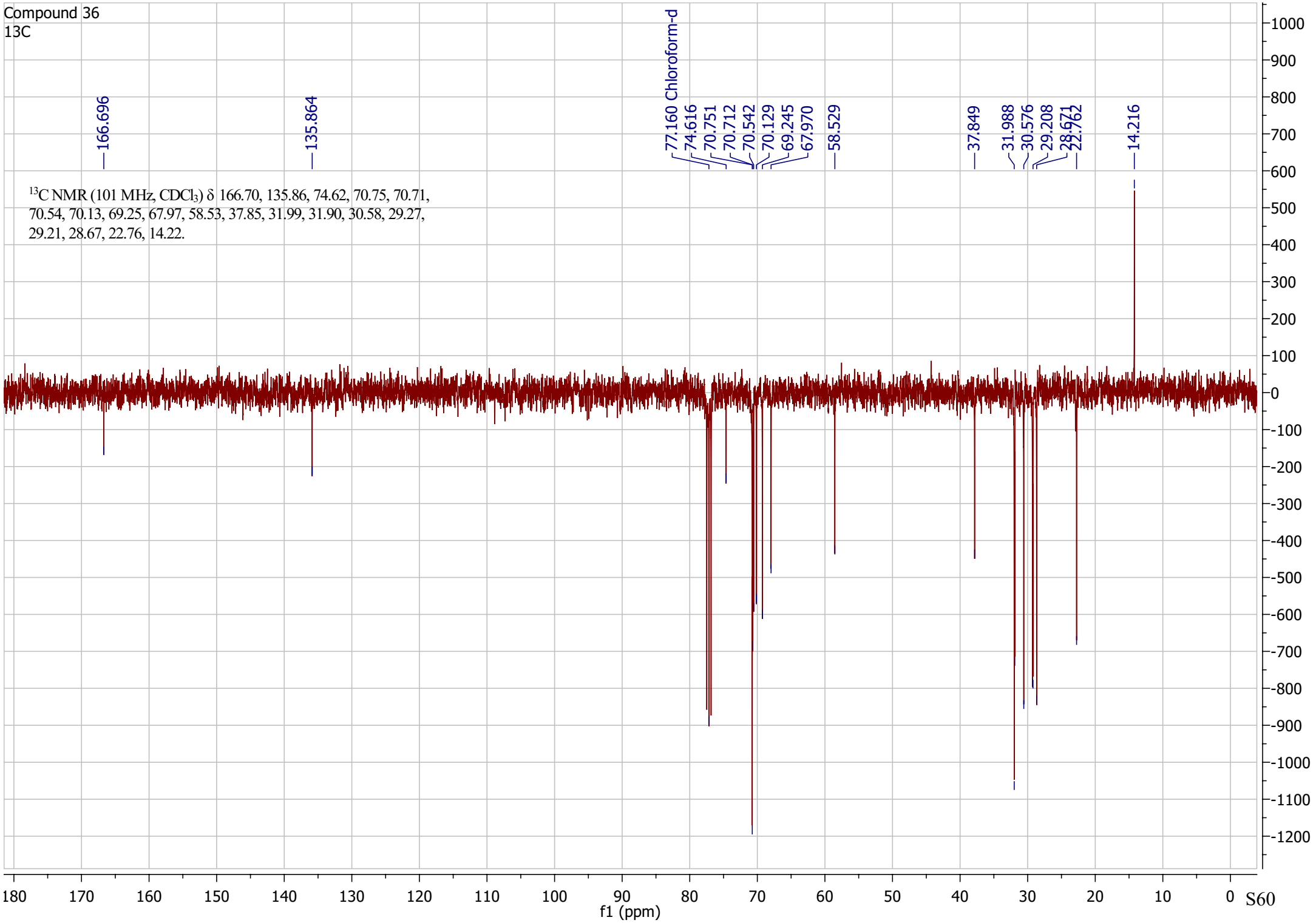

Compound 35
1H
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20 (d, J = 2.4 Hz, 2H), 3.73 – 3.59 (m, 16H), 3.31 – 3.24 (m, 4H), 2.44 (t, J = 2.3 Hz, 1H), 1.64 (dt, J = 15.1, 7.4 Hz, 4H), 1.42 (dt, J = 14.3, 7.2 Hz, 4H), 1.36 – 1.23 (m, 8H), 0.89 (t, J = 6.9 Hz, 6H).
H (d) 4.20
G (m) 3.65
F (m) 3.27
E (t) 2.44
C (dt) 1.42
B (m) 1.29
A (t) 0.89
D (dt) 1.64
4.207
4.201
3.693
3.641
3.631
3.612
3.293
3.274
3.255
2.450
2.444
2.438
1.662
1.643
1.625
1.417
1.313
1.304
1.295
1.285
0.906
0.889
0.872
0.000
1.65
16.08
4.24
0.44
4.26
4.25
8.56
5.55
f1 (ppm)

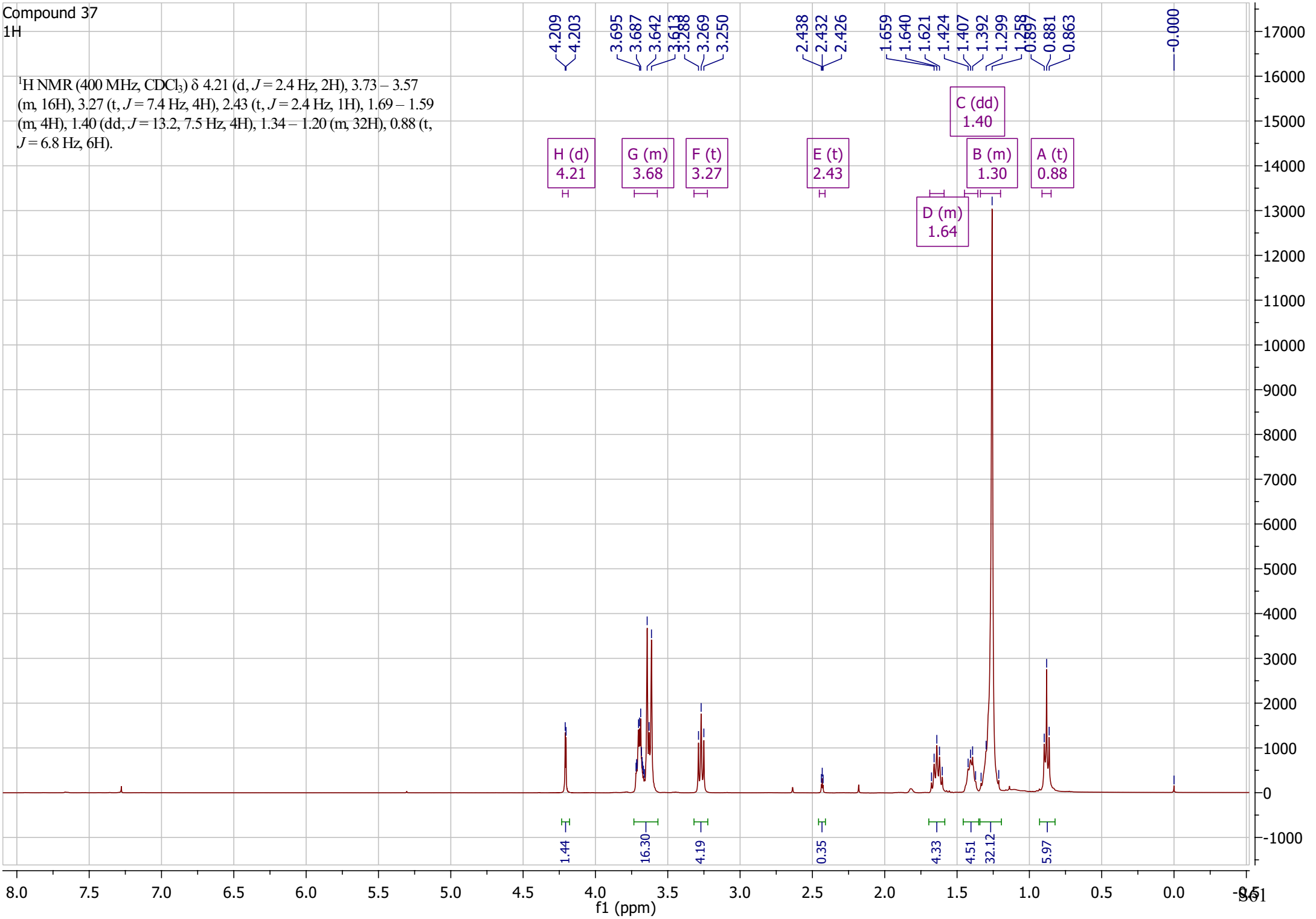

Compound 35
13C
166.567
135.741
77.160 Chloroform-d
74.554
70.636
70.598
70.425
70.019
69.125
67.854
58.405
37.747
31.850
31.294
30.438
28.210
22.512
14.015
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.57, 135.74, 74.55, 70.64, 70.60, 70.43, 70.02, 69.12, 67.85, 58.40, 37.75, 31.85, 31.29, 30.44, 28.21, 22.51, 14.02.
f1 (ppm)

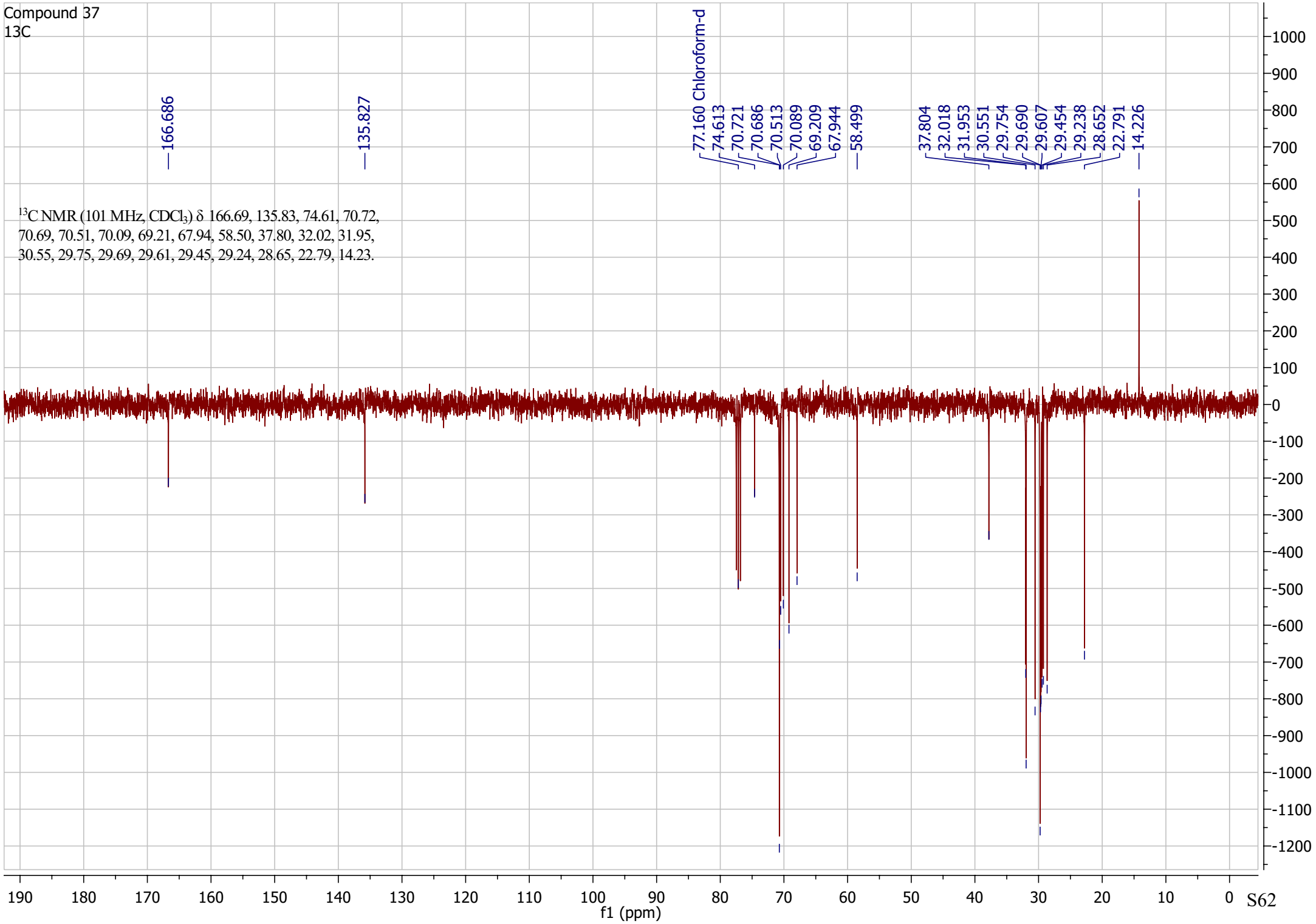
Compound 36
1H

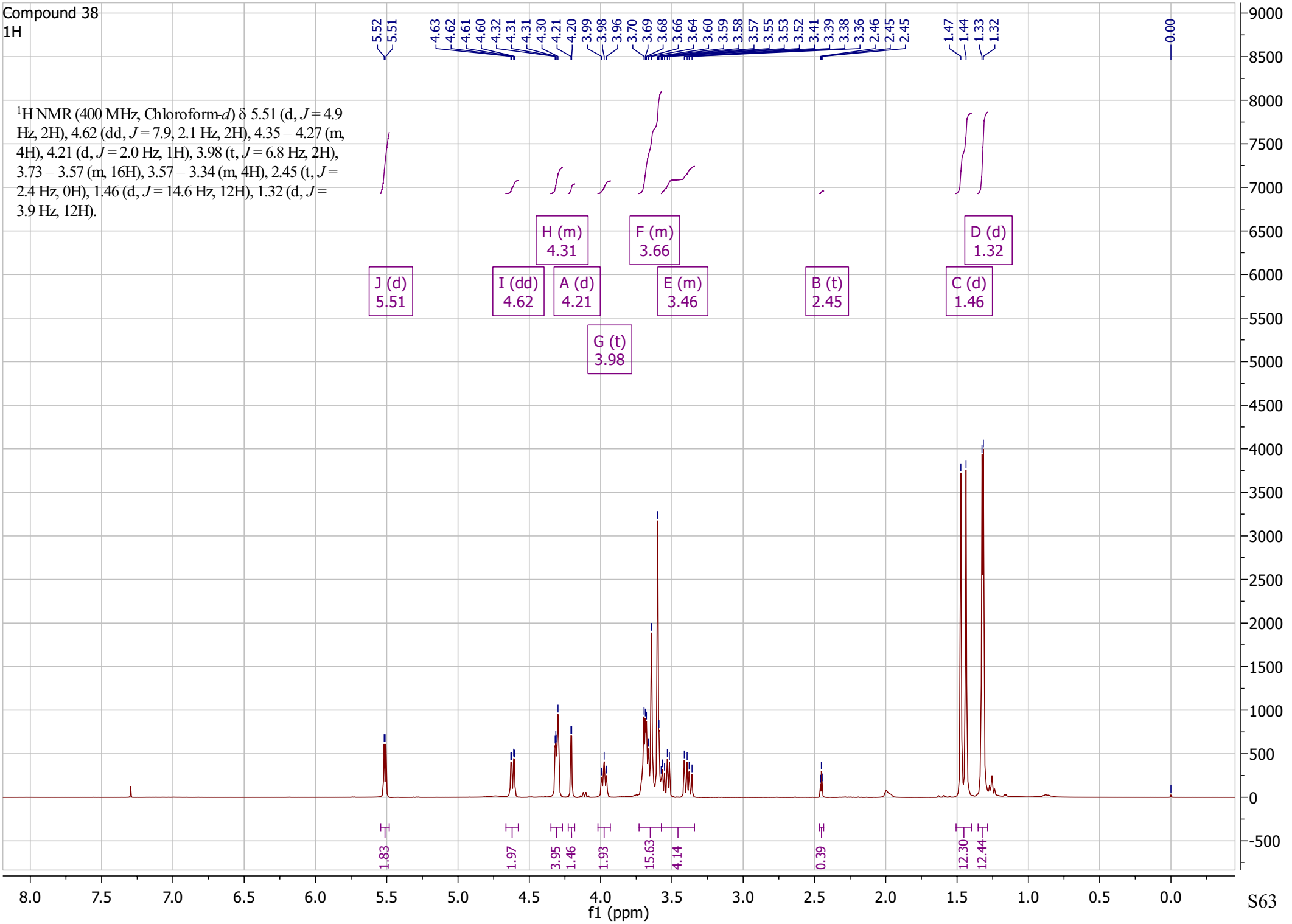
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.21 (d, *J* = 2.4 Hz, 2H), 3.72 – 3.59 (m, 16H), 3.32 – 3.23 (m, 4H), 2.43 (t, *J* = 2.4 Hz, 1H), 1.64 (dt, *J* = 15.0, 7.4 Hz, 4H), 1.46 – 1.36 (m, 4H), 1.30 (dt, *J* = 8.7, 5.1 Hz, 16H), 0.88 (t, *J* = 6.8 Hz, 6H).

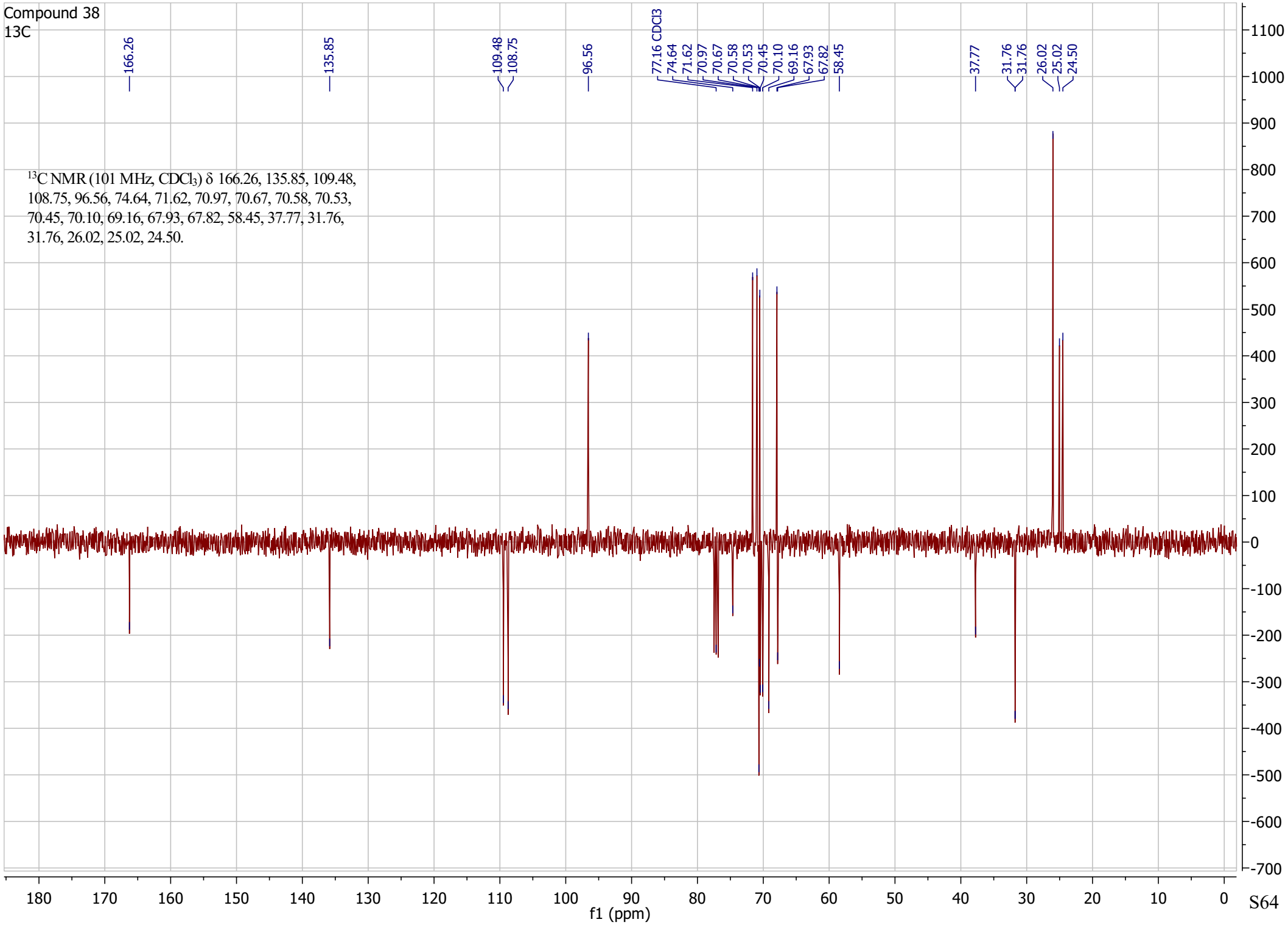


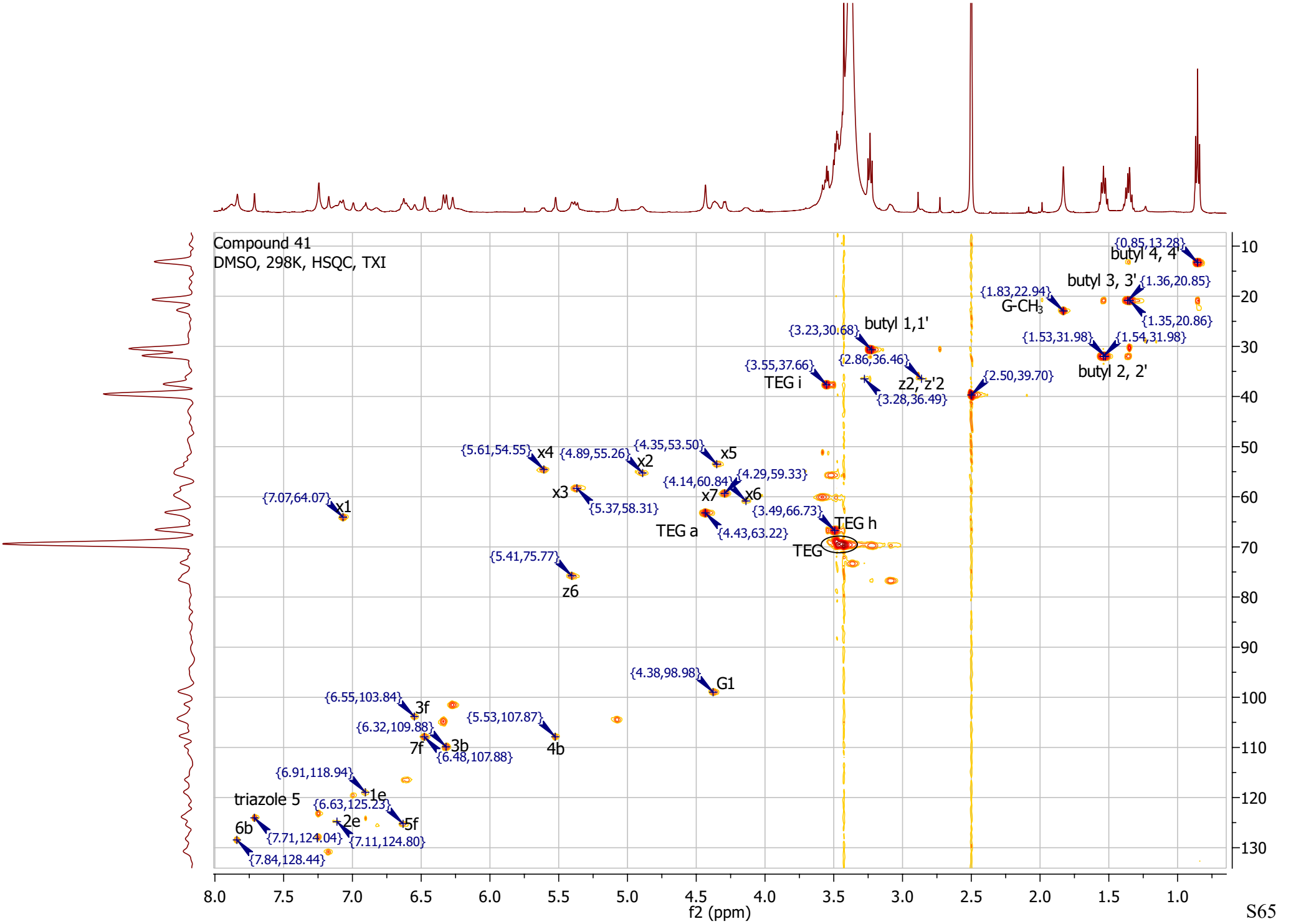

Compound 36
13C
166.696
135.864
77.160 Chloroform-d
74.616
70.751
70.712
70.542
70.129
69.245
67.970
58.529
37.849
31.988
30.576
29.208
28.671
22.762
14.216
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.70, 135.86, 74.62, 70.75, 70.71, 70.54, 70.13, 69.25, 67.97, 58.53, 37.85, 31.99, 31.90, 30.58, 29.27, 29.21, 28.67, 22.76, 14.22.
f1 (ppm)
S60

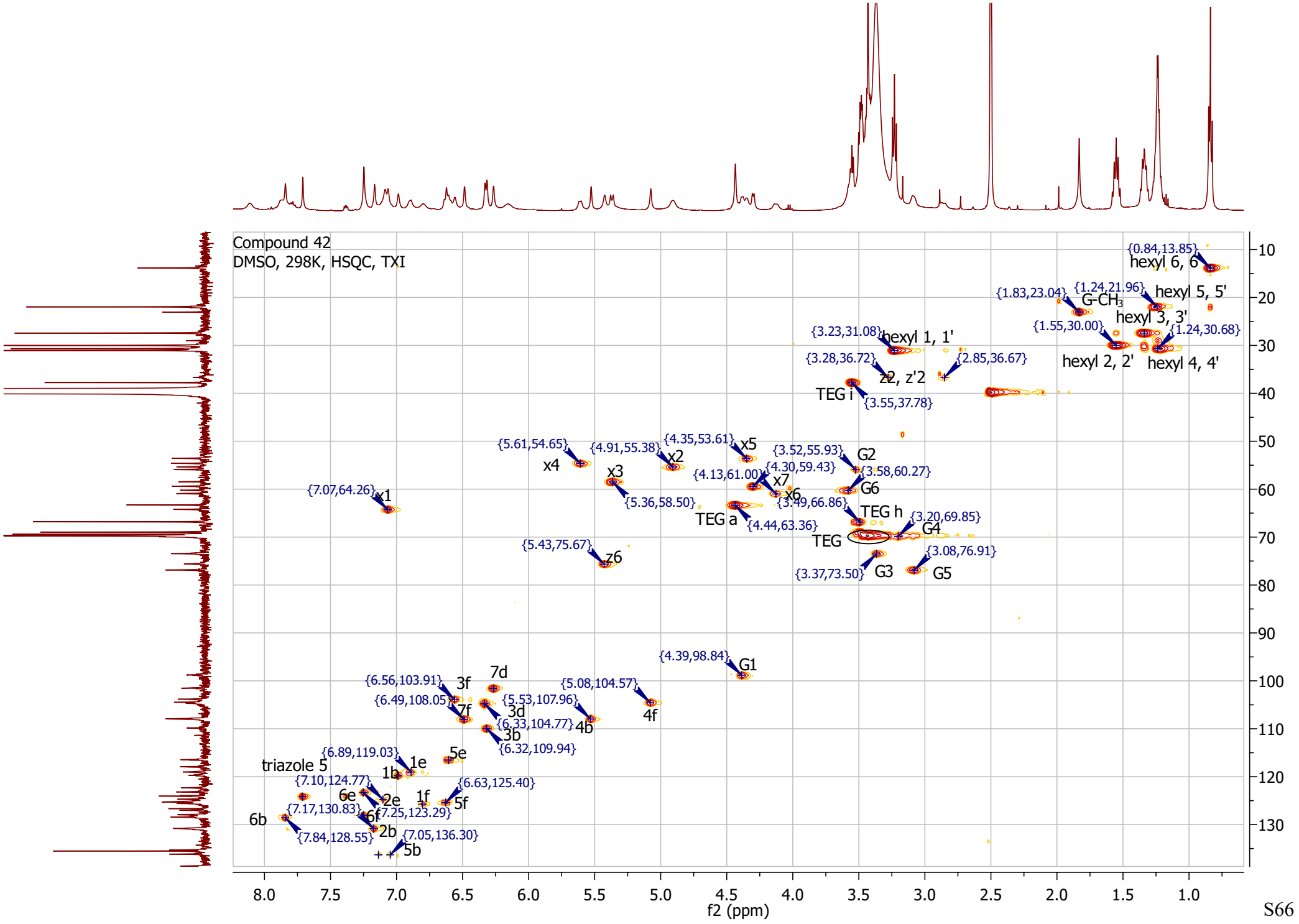

Compound 37
1H
[1]H NMR (400 MHz, CDCl3) δ 4.21 (d, J = 2.4 Hz, 2H), 3.73 – 3.57 (m, 16H), 3.27 (t, J = 7.4 Hz, 4H), 2.43 (t, J = 2.4 Hz, 1H), 1.69 – 1.59 (m, 4H), 1.40 (dd, J = 13.2, 7.5 Hz, 4H), 1.34 – 1.20 (m, 32H), 0.88 (t, J = 6.8 Hz, 6H).
4.209
4.203
3.695
3.687
3.642
3.613
3.288
3.269
3.250
2.438
2.432
2.426
1.659
1.640
1.621
1.424
1.407
1.392
1.299
1.258
0.897
0.881
0.863
-0.000
H (d) 4.21
G (m) 3.68
F (t) 3.27
E (t) 2.43
C (dd) 1.40
B (m) 1.30
D (m) 1.64
A (t) 0.88
1.44
16.30
4.19
0.35
4.33
4.51
32.12
5.97
f1 (ppm)

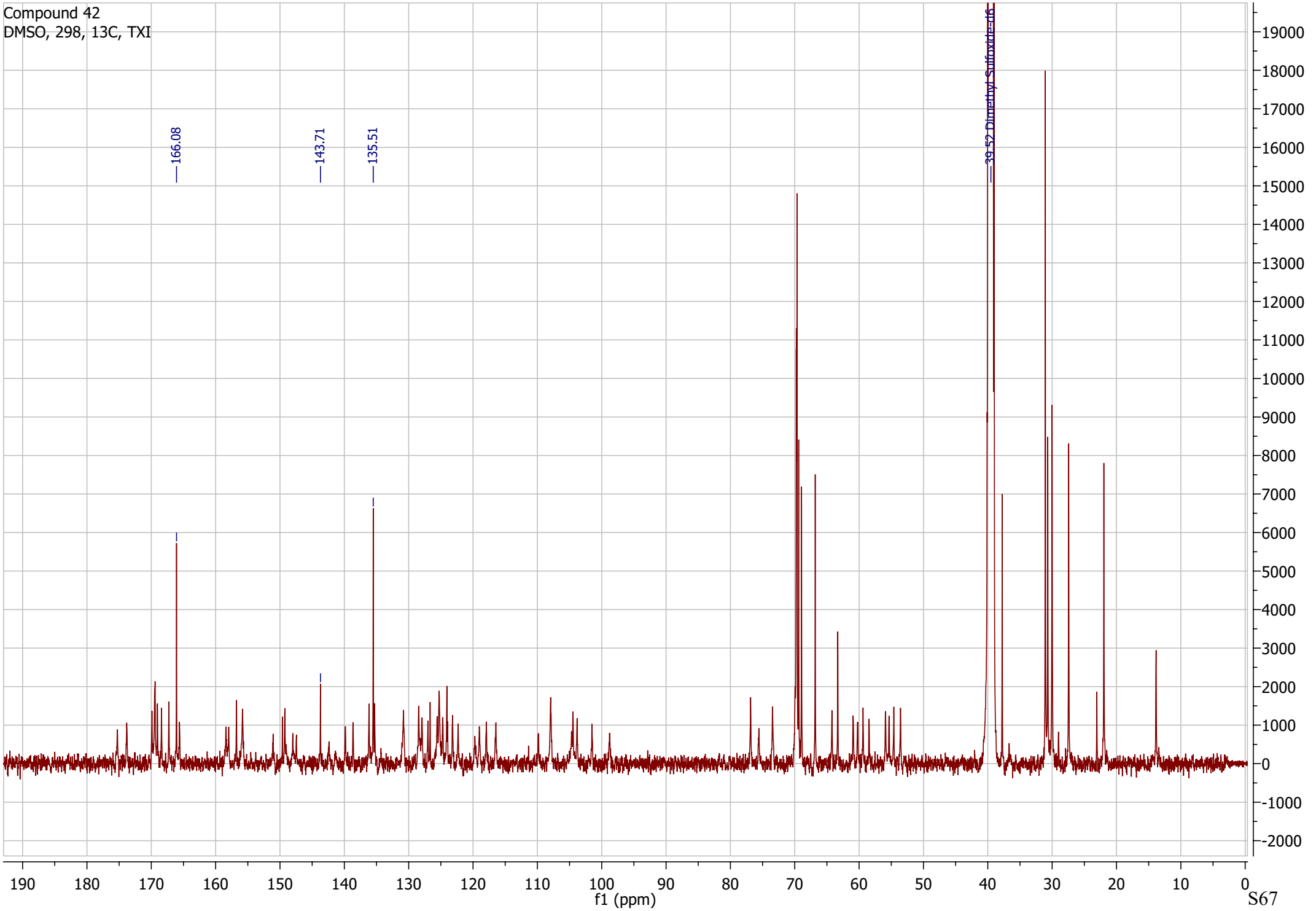

Compound 37
13C
166.686
135.827
77.160 Chloroform-d
74.613
70.721
70.686
70.513
70.089
69.209
67.944
58.499
37.804
32.018
31.953
30.551
29.754
29.690
29.607
29.454
29.238
28.652
22.791
14.226
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.69, 135.83, 74.61, 70.72, 70.69, 70.51, 70.09, 69.21, 67.94, 58.50, 37.80, 32.02, 31.95, 30.55, 29.75, 29.69, 29.61, 29.45, 29.24, 28.65, 22.79, 14.23.
f1 (ppm)

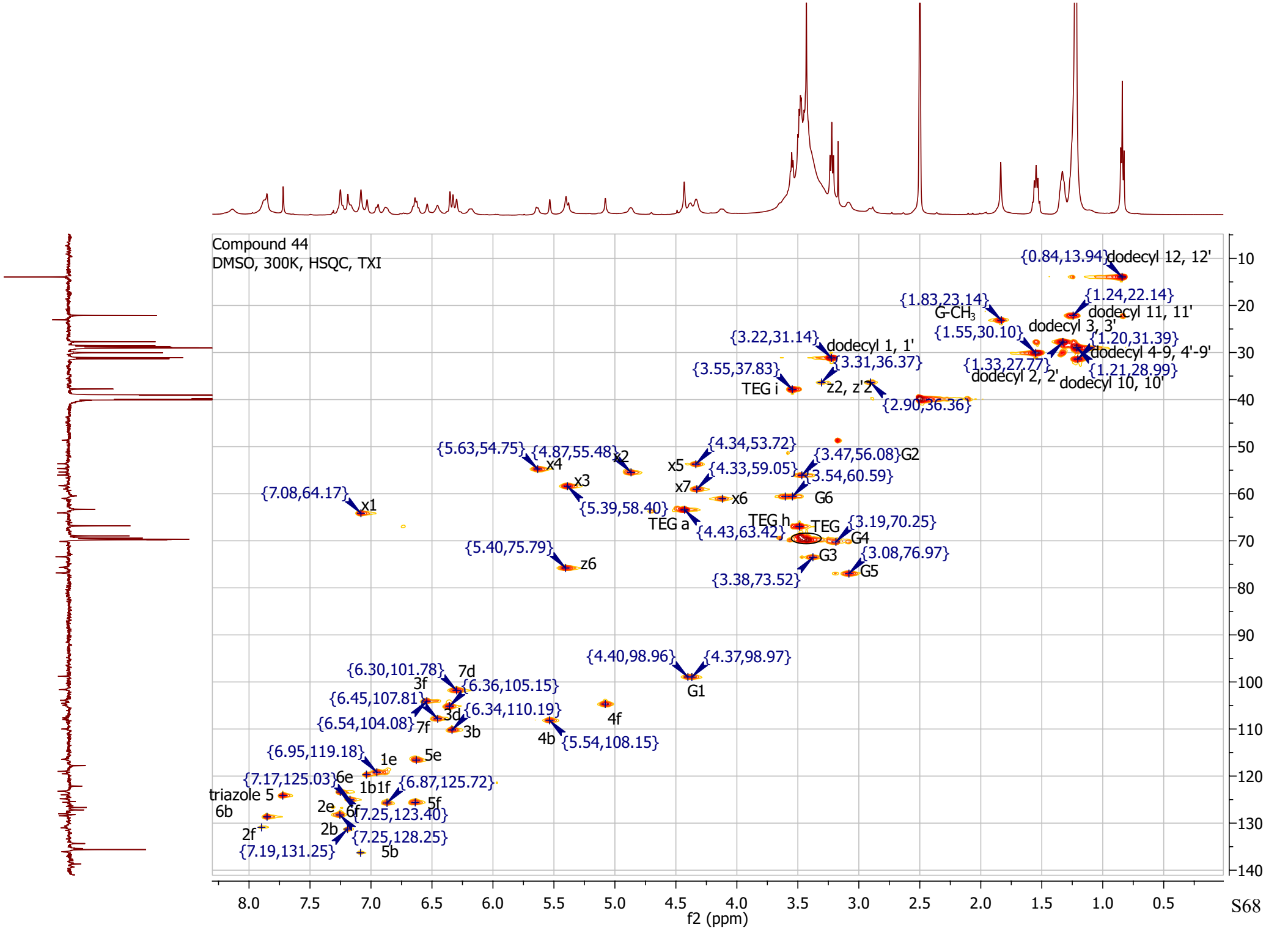

Compound 38
1H
[1]H NMR (400 MHz, Chloroform-d) δ 5.51 (d, J = 4.9 Hz, 2H), 4.62 (dd, J = 7.9, 2.1 Hz, 2H), 4.35 – 4.27 (m, 4H), 4.21 (d, J = 2.0 Hz, 1H), 3.98 (t, J = 6.8 Hz, 2H), 3.73 – 3.57 (m, 16H), 3.57 – 3.34 (m, 4H), 2.45 (t, J = 2.4 Hz, 0H), 1.46 (d, J = 14.6 Hz, 12H), 1.32 (d, J = 3.9 Hz, 12H).
J (d) 5.51
I (dd) 4.62
H (m) 4.31
A (d) 4.21
G (t) 3.98
F (m) 3.66
E (m) 3.46
B (t) 2.45
C (d) 1.46
D (d) 1.32
f1 (ppm)

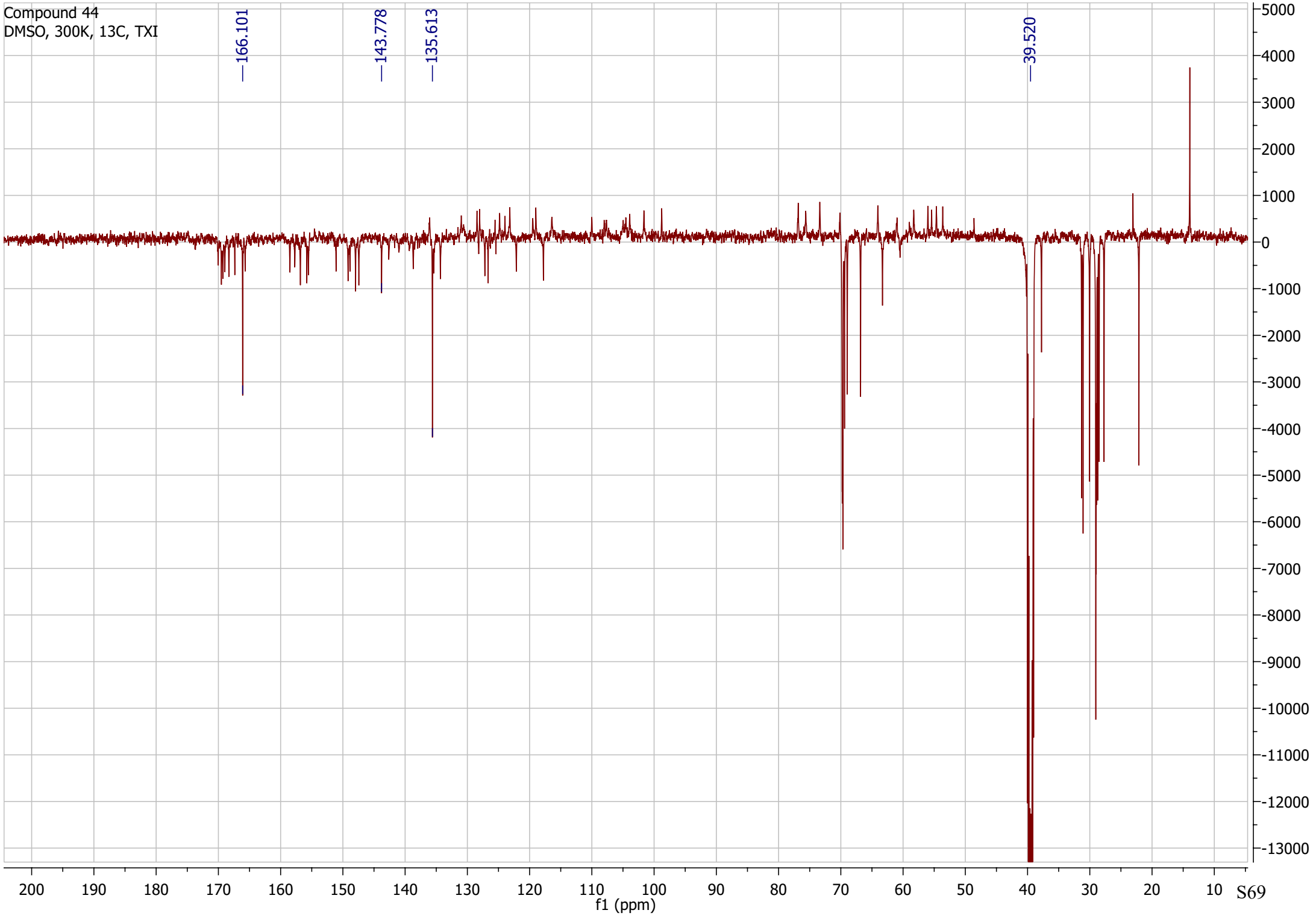

Compound 38
13C
166.26
135.85
109.48
108.75
96.56
77.16 CDCl3
74.64
71.62
70.97
70.67
70.58
70.53
70.45
70.10
69.16
67.93
67.82
58.45
37.77
31.76
31.76
26.02
25.02
24.50
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.26, 135.85, 109.48, 108.75, 96.56, 74.64, 71.62, 70.97, 70.67, 70.58, 70.53, 70.45, 70.10, 69.16, 67.93, 67.82, 58.45, 37.77, 31.76, 31.76, 26.02, 25.02, 24.50.
f1 (ppm)

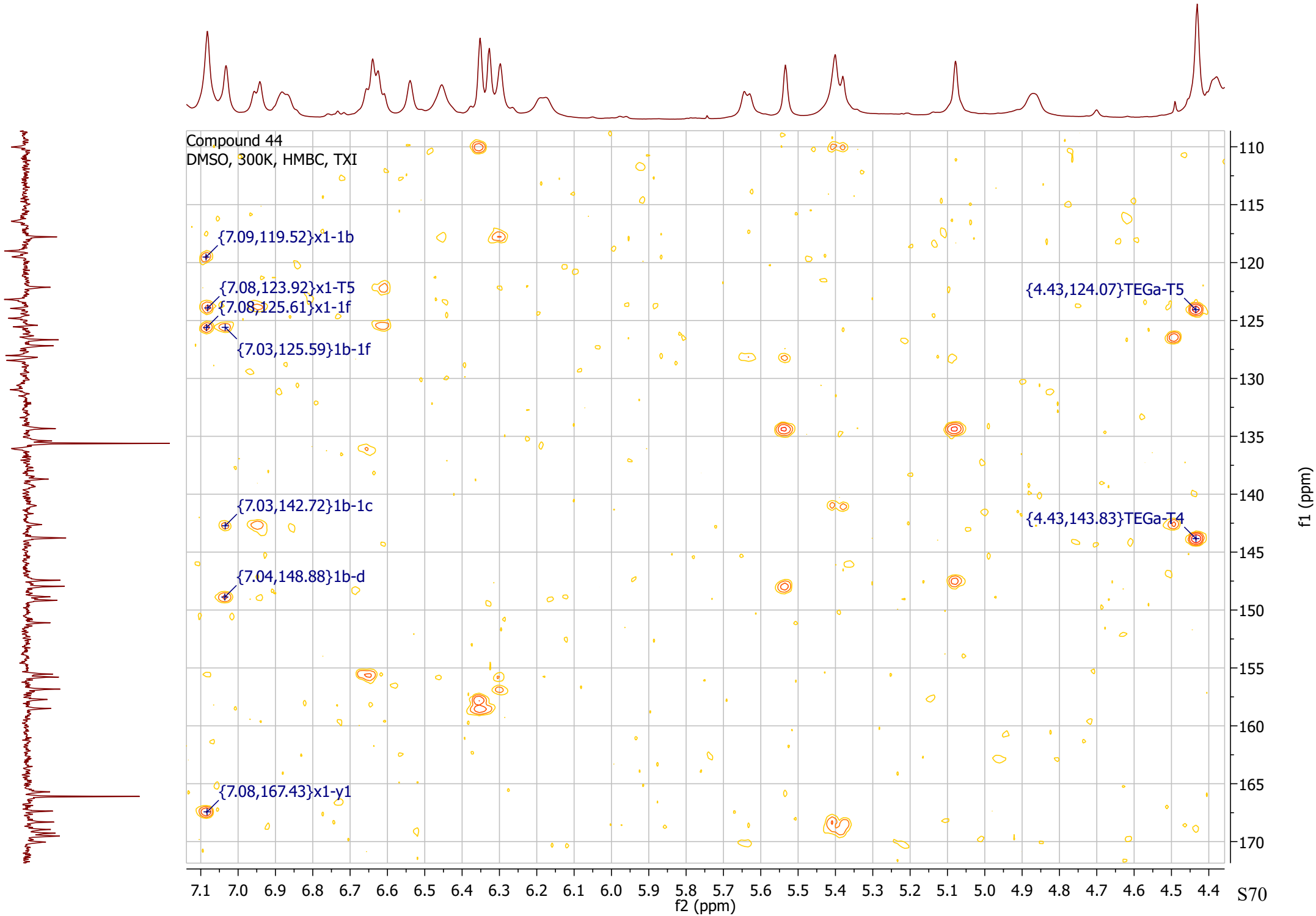

Compound 41
DMSO, 298K, HSQC, TXI
{0.85,13.28}
butyl 4, 4'
butyl 3, 3'
{1.36,20.85}
{1.83,22.94}
G-CH3
{1.35,20.86}
{3.23,30.68}
butyl 1,1'
{1.53,31.98}
{1.54,31.98}
{2.86,36.46}
{3.55,37.66}
TEG i
z2, z'2
butyl 2, 2'
{2.50,39.70}
{3.28,36.49}
{5.61,54.55}
x4
{4.89,55.26}
x2
{4.35,53.50}
x5
{4.29,59.33}
{4.14,60.84}
x6
x7
x3
{5.37,58.31}
{7.07,64.07}
x1
{3.49,66.73}
TEG h
TEG a
{4.43,63.22}
TEG
{5.41,75.77}
z6
{4.38,98.98}
G1
{6.55,103.84}
3f
{5.53,107.87}
{6.32,109.88}
7f
3b
4b
{6.48,107.88}
{6.91,118.94}
1e
triazole 5
{6.63,125.23}
2e
5f
6b
{7.71,124.04}
{7.11,124.80}
{7.84,128.44}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

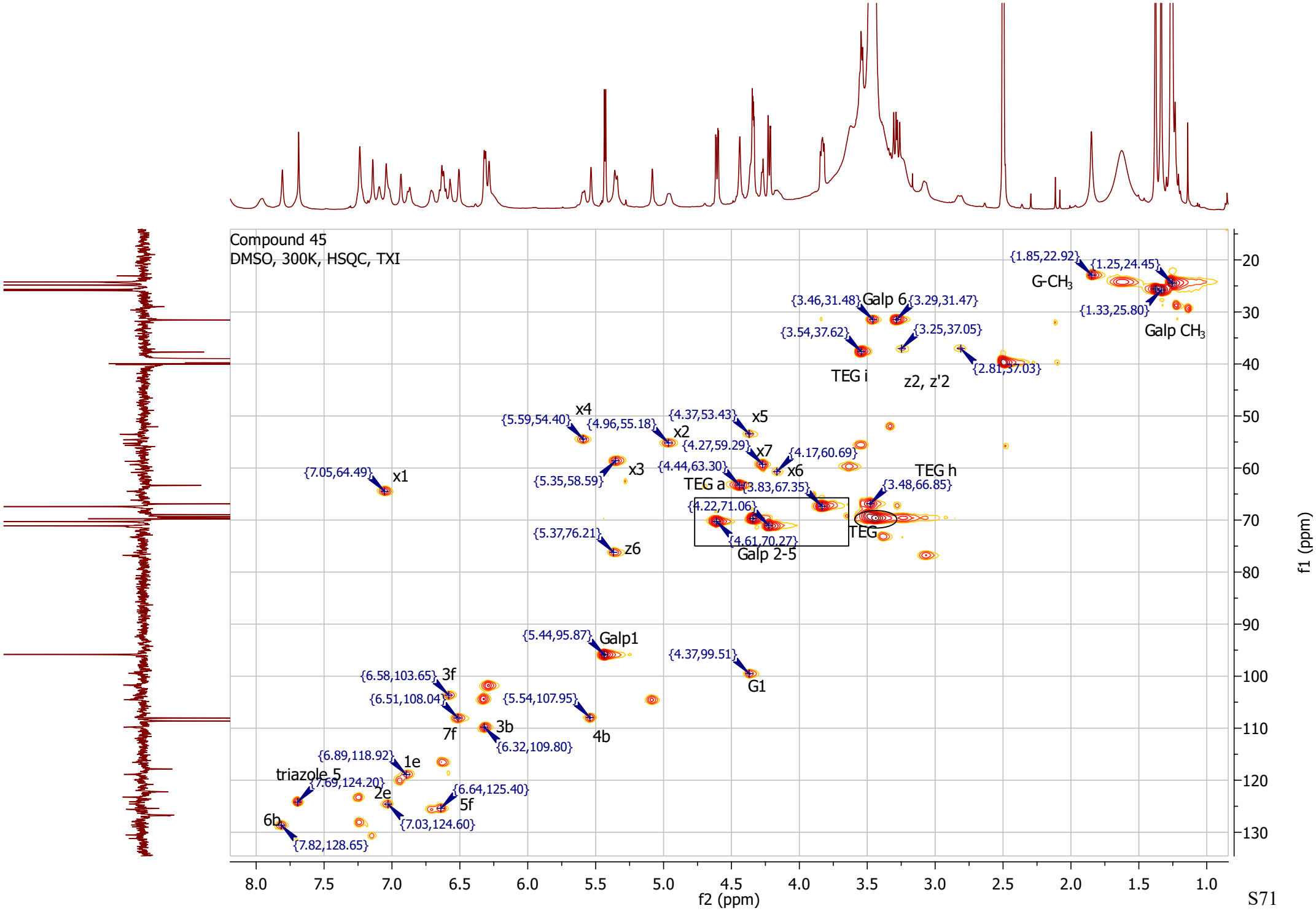

Compound 42
DMSO, 298K, HSQC, TXI
{0.84,13.85}
hexyl 6, 6
{1.83,23.04}
{1.24,21.96}
hexyl 5, 5'
G-CH3
hexyl 3, 3'
{1.55,30.00}
{1.24,30.68}
{3.23,31.08}
hexyl 1, 1'
hexyl 2, 2'
hexyl 4, 4'
{3.28,36.72}
{2.85,36.67}
z2, z'2
TEG i
{3.55,37.78}
{5.61,54.65}
{4.91,55.38}
{4.35,53.61}
x5
{3.52,55.93}
G2
x4
x2
x3
{4.13,61.00}
{4.30,59.43}
{3.58,60.27}
x7
G6
{7.07,64.26}
x1
x6
{5.36,58.50}
{3.49,66.86}
TEG h
TEG a
{4.44,63.36}
{3.20,69.85}
G4
TEG
{5.43,75.67}
z6
{3.08,76.91}
{3.37,73.50}
G3
G5
{4.39,98.84}
G1
{6.56,103.91}
3f
7d
{5.08,104.57}
{6.49,108.05}
7f
{5.53,107.96}
3d
4f
{6.33,104.77}
4b
3b
{6.32,109.94}
{6.89,119.03}
5e
triazole 5
1e
1b
{7.10,124.77}
{6.63,125.40}
6e
2e
1f
5f
{7.17,130.83}
{7.25,123.29}
6b
6f
2b
{7.84,128.55}
{7.05,136.30}
5b
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

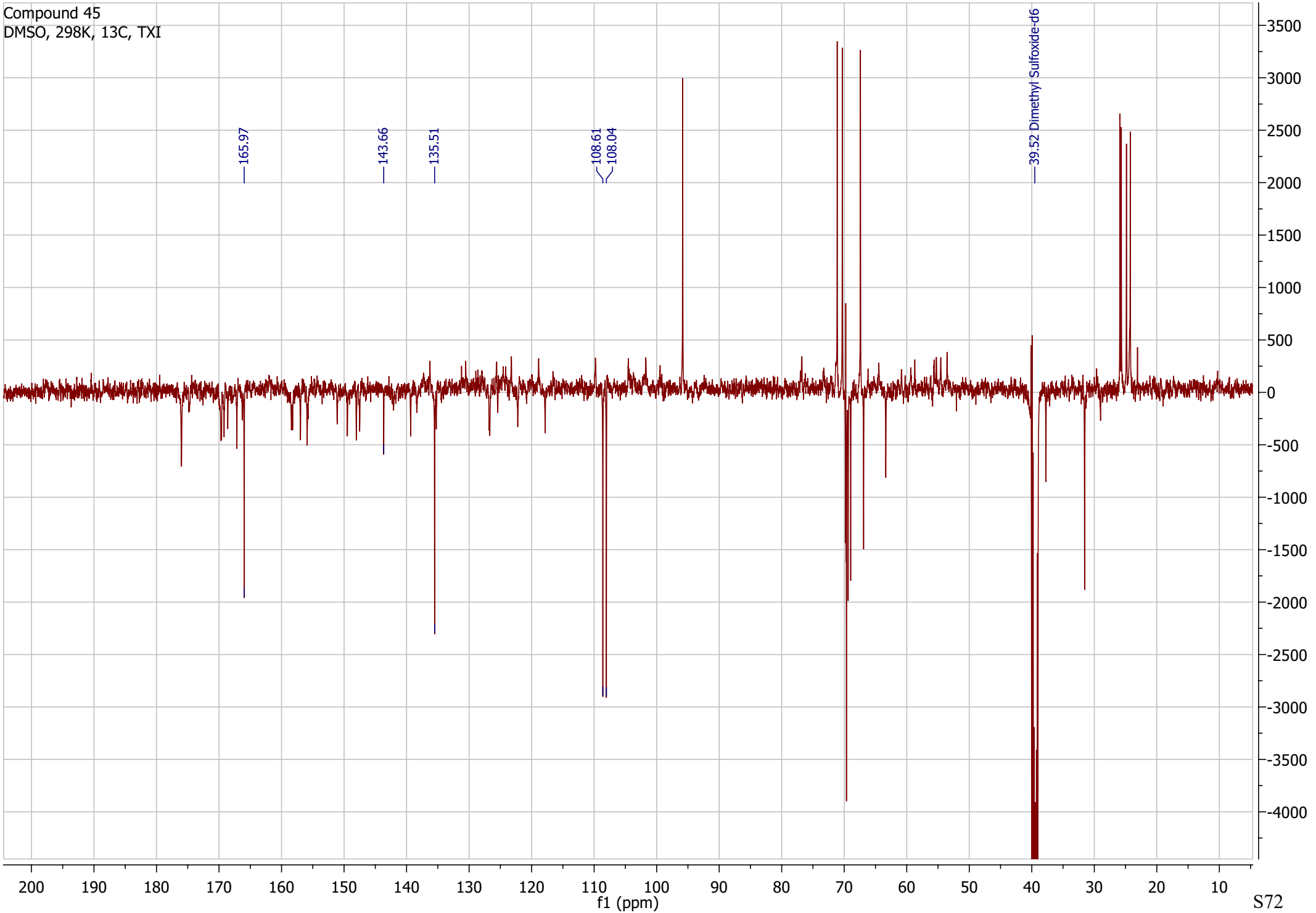

Compound 42
DMSO, 298, 13C, TXI
166.08
143.71
135.51
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)

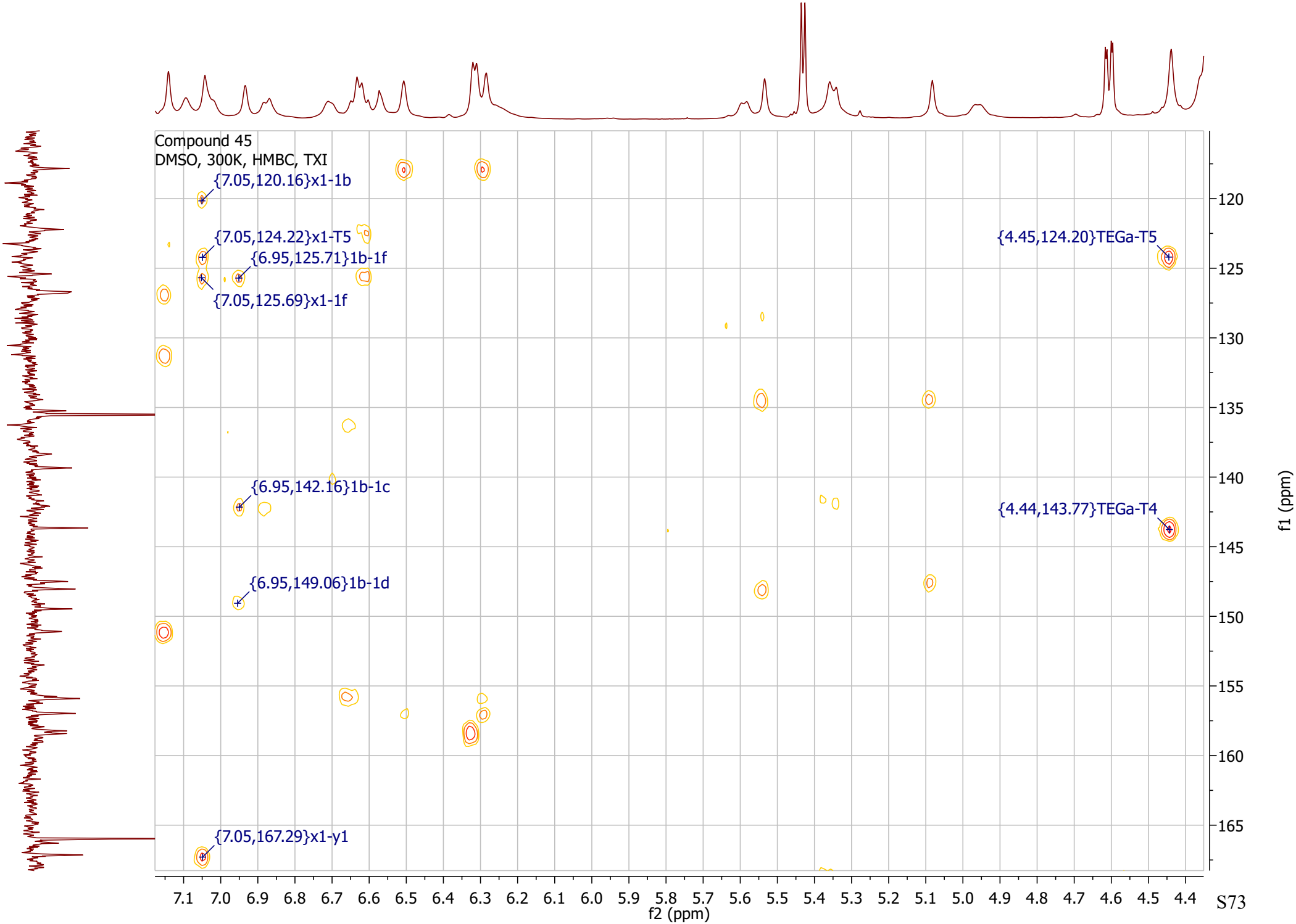

Compound 44
DMSO, 300K, HSQC, TXI
{0.84,13.94}dodecyl 12, 12'
{1.24,22.14}
dodecyl 11, 11'
{1.83,23.14}
G-CH3
{1.55,30.10}
dodecyl 3, 3'
{1.20,31.39}
dodecyl 4-9, 4'-9'
{1.33,27.77}
dodecyl 2, 2'
{1.21,28.99}
dodecyl 10, 10'
{3.22,31.14}
dodecyl 1, 1'
{3.31,36.37}
{3.55,37.83}
TEG i
z2, z'2
{2.90,36.36}
{5.63,54.75}
{4.87,55.48}
x2
x4
x5
{4.34,53.72}
{3.47,56.08}G2
{4.33,59.05}
{3.54,60.59}
x3
x7
x6
G6
{7.08,64.17}
x1
{5.39,58.40}
TEG a
TEG h
TEG
{3.19,70.25}
{4.43,63.42}
G4
{5.40,75.79}
z6
G3
{3.08,76.97}
G5
{3.38,73.52}
{4.40,98.96}
{4.37,98.97}
G1
{6.30,101.78}
7d
3f
{6.36,105.15}
{6.45,107.81}
4
{6.34,110.19}
3d
{6.54,104.08}
7f
3b
4f
4b
{5.54,108.15}
{6.95,119.18}
1e
5e
{7.17,125.03}
6e
1b
1f
{6.87,125.72}
triazole 5
6b
2e
6f
5f
{7.25,123.40}
2f
2b
{7.25,128.25}
{7.19,131.25}
5b
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (ppm)


Compound 44
DMSO, 300K, 13C, TXI
166.101
143.778
135.613
39.520
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
-6000
-7000
-8000
-9000
-10000
-11000
-12000
-13000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

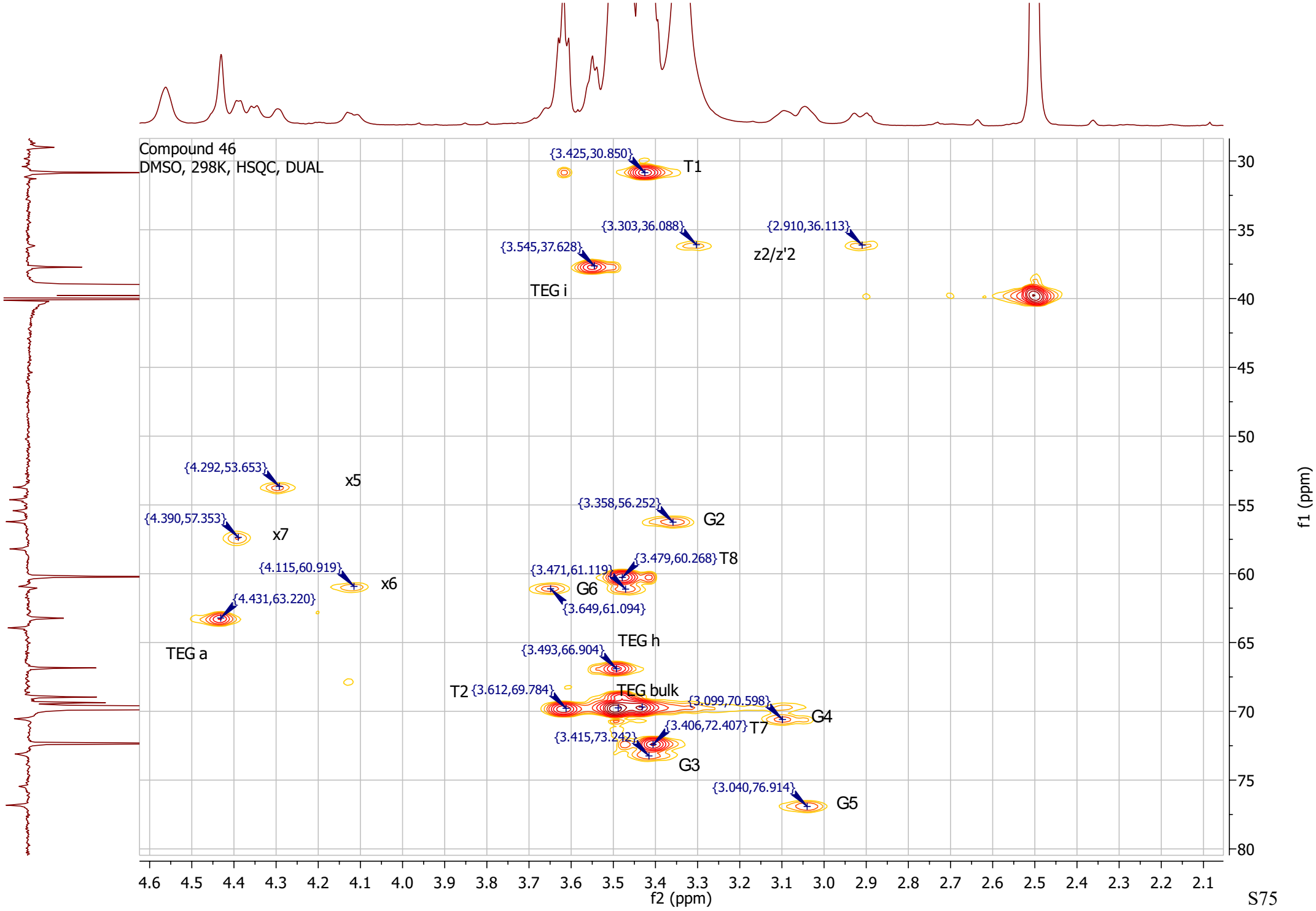

Compound 44
DMSO, 300K, HMBC, TXI
{7.09,119.52}x1-1b
{7.08,123.92}x1-T5
{7.08,125.61}x1-1f
{7.03,125.59}1b-1f
{7.03,142.72}1b-1c
{7.04,148.88}1b-d
{7.08,167.43}x1-y1
{4.43,124.07}TEGa-T5
{4.43,143.83}TEGa-T4
f2 (ppm)
f1 (ppm)
S70

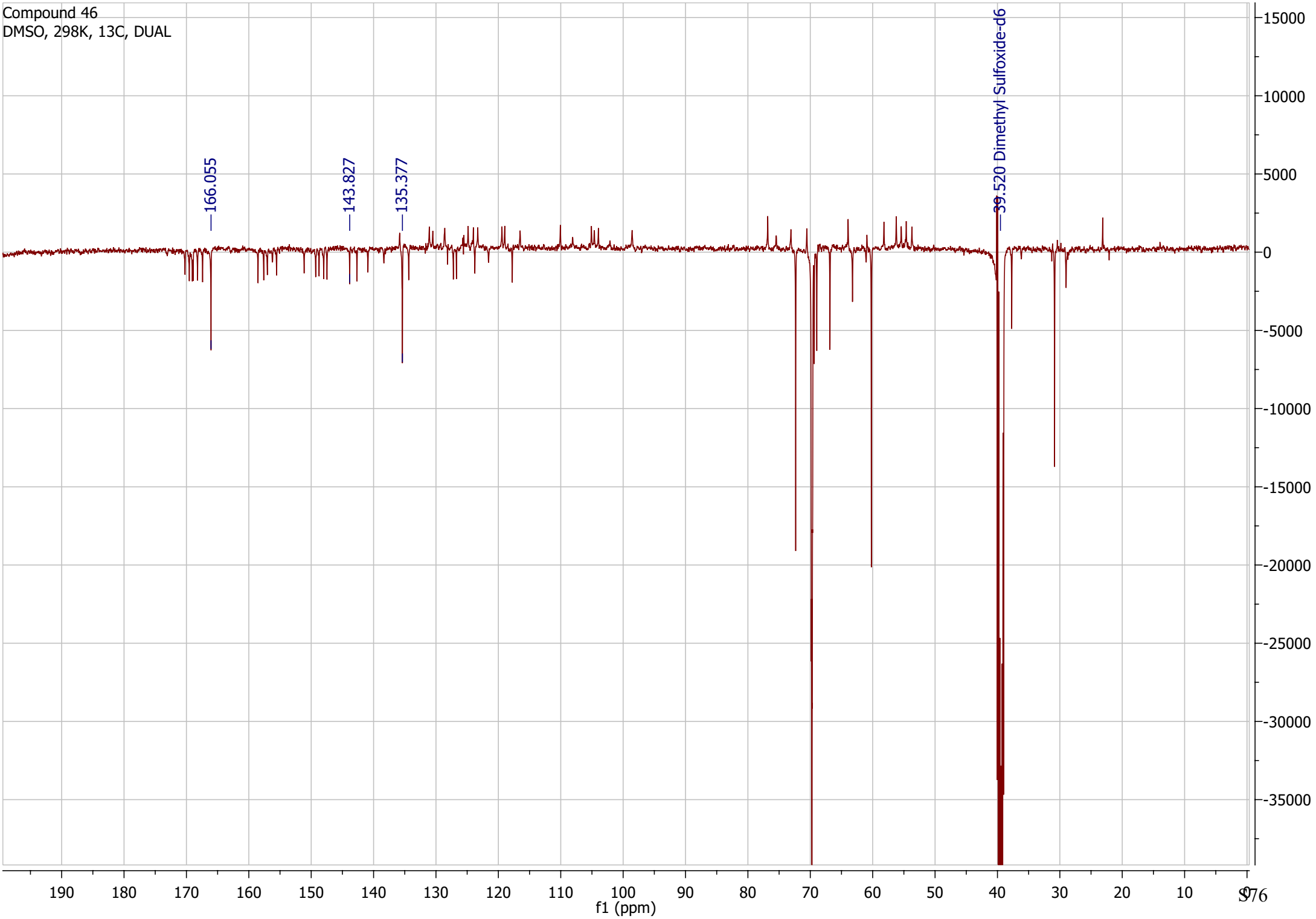

Compound 45
DMSO, 300K, HSQC, TXI
{1.85,22.92}
{1.25,24.45}
G-CH3
{1.33,25.80}
Galp CH3
{3.46,31.48}
Galp 6
{3.29,31.47}
{3.54,37.62}
{3.25,37.05}
{2.81,37.03}
TEG i
z2, z'2
x4
{5.59,54.40}
{4.96,55.18}
x2
{4.37,53.43}
x5
{4.27,59.29}
x7
{4.17,60.69}
{7.05,64.49}
x1
{5.35,58.59}
x3
{4.44,63.30}
x6
TEG a
{3.83,67.35}
TEG h
{3.48,66.85}
{4.22,71.06}
TEG
{5.37,76.21}
z6
{4.61,70.27}
Galp 2-5
{5.44,95.87}
Galp1
{4.37,99.51}
G1
{6.58,103.65}
3f
{6.51,108.04}
{5.54,107.95}
7f
3b
4b
{6.32,109.80}
{6.89,118.92}
1e
triazole 5
{7.69,124.20}
2e
{6.64,125.40}
5f
6b
{7.03,124.60}
{7.82,128.65}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)

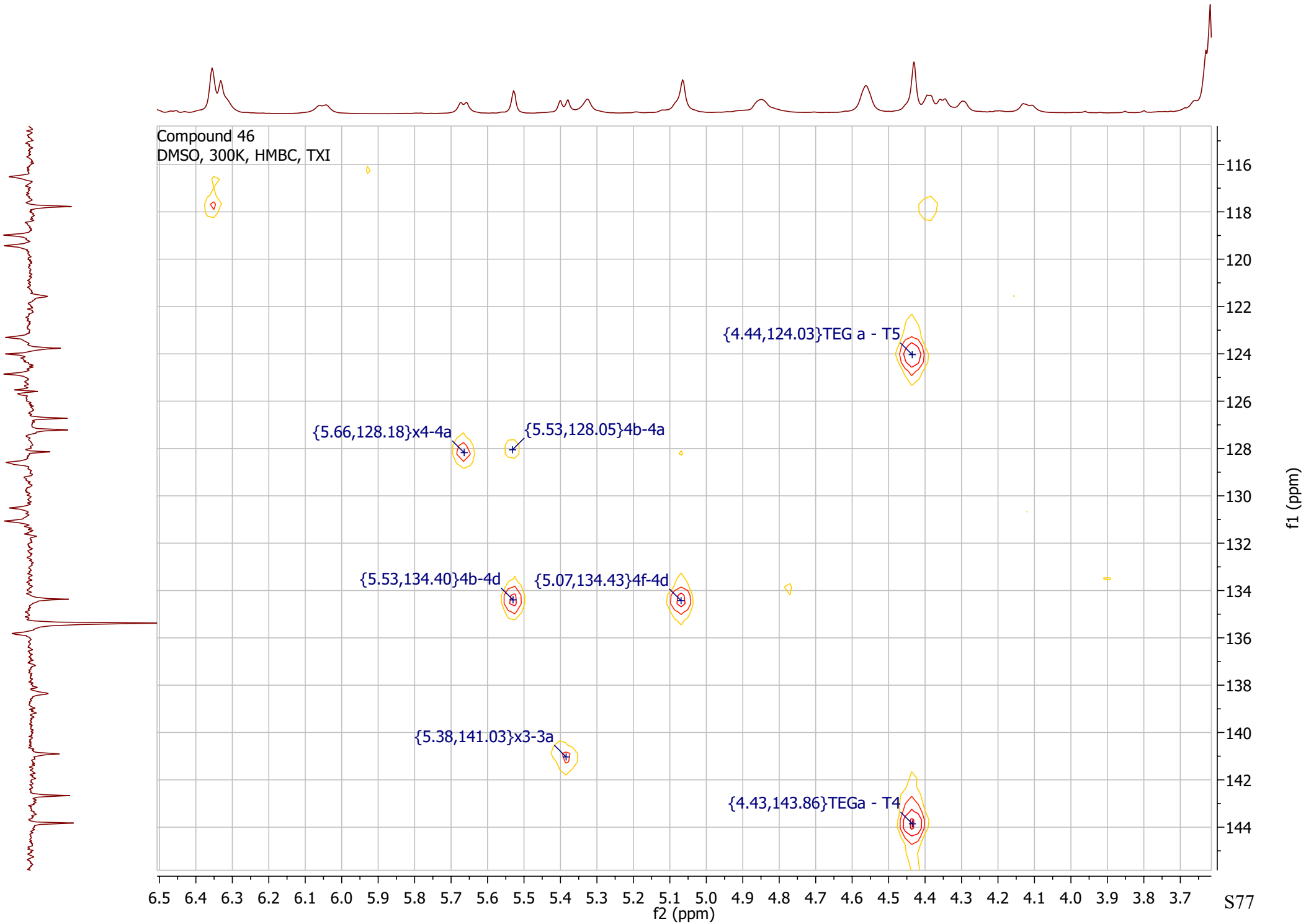

Compound 45
DMSO, 298K, 13C, TXI
165.97
143.66
135.51
108.61
108.04
39.52 Dimethyl Sulfoxide-d6
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
-3500
-4000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

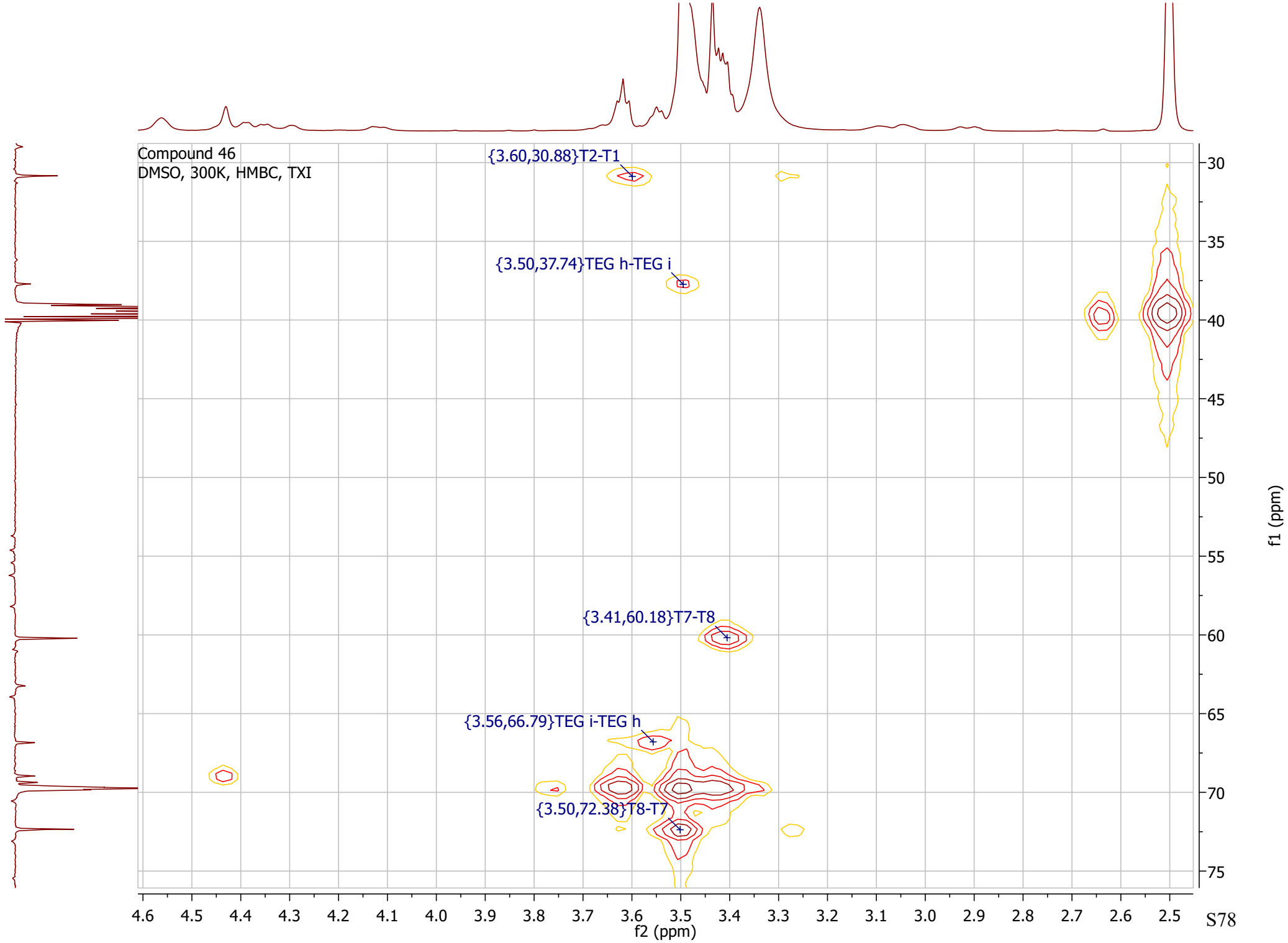

Compound 45
DMSO, 300K, HMBC, TXI
{7.05,120.16}x1-1b
{7.05,124.22}x1-T5
{6.95,125.71}1b-1f
{7.05,125.69}x1-1f
{4.45,124.20}TEGa-T5
{6.95,142.16}1b-1c
{4.44,143.77}TEGa-T4
{6.95,149.06}1b-1d
{7.05,167.29}x1-y1
f2 (ppm)
f1 (ppm)


Compound 46
DMSO, 298K, HSQC, DUAL
{1.864,23.116}
G-CH3
{3.425,30.850}
T1
{2.910,36.113}
{3.545,37.628}
z2/z'2
TEG i
{3.303,36.088}
{5.667,54.582}
x4
{4.292,53.653}
x5
{3.358,56.252}
G2
{4.390,57.353}
x2
x7
x3
{5.386,58.162}
{3.471,61.119}
T8
{4.431,63.220}
x6
G6
{7.090,63.888}
x1
{3.493,66.904}
TEG h
{3.479,60.268}
TEG a
{3.612,69.784}
{3.488,69.751}
TEG bulk
T2
{3.406,72.407}
G4
{5.331,75.507}
z6
{3.432,69.691}
G3
{3.040,76.914}
{3.415,73.242}
T7
G5
{4.344,98.610}
G1
{6.524,104.045}
3f
{5.063,104.684}
{5.530,108.230}
{6.332,110.165}
7f
4b
{6.315,106.538}
3b
{6.649,116.677}
5e
{7.054,119.527}
1b
triazole 5
1e
{7.743,124.129}
{6.673,125.811}
2e
1f
5f
{7.849,128.735}
6b
{6.919,125.693}
{7.075,135.960}
f2 (ppm)
f1 (ppm)


Compound 46
DMSO, 298K, HSQC, DUAL
{3.425,30.850}
T1
{3.303,36.088}
{2.910,36.113}
{3.545,37.628}
z2/z'2
TEG i
{4.292,53.653}
x5
{3.358,56.252}
G2
{4.390,57.353}
x7
{3.479,60.268}
T8
{4.115,60.919}
{3.471,61.119}
x6
G6
{4.431,63.220}
{3.649,61.094}
TEG h
TEG a
{3.493,66.904}
T2
{3.612,69.784}
TEG bulk
{3.099,70.598}
G4
{3.406,72.407}
T7
{3.415,73.242}
G3
{3.040,76.914}
G5
f2 (ppm)
f1 (ppm)

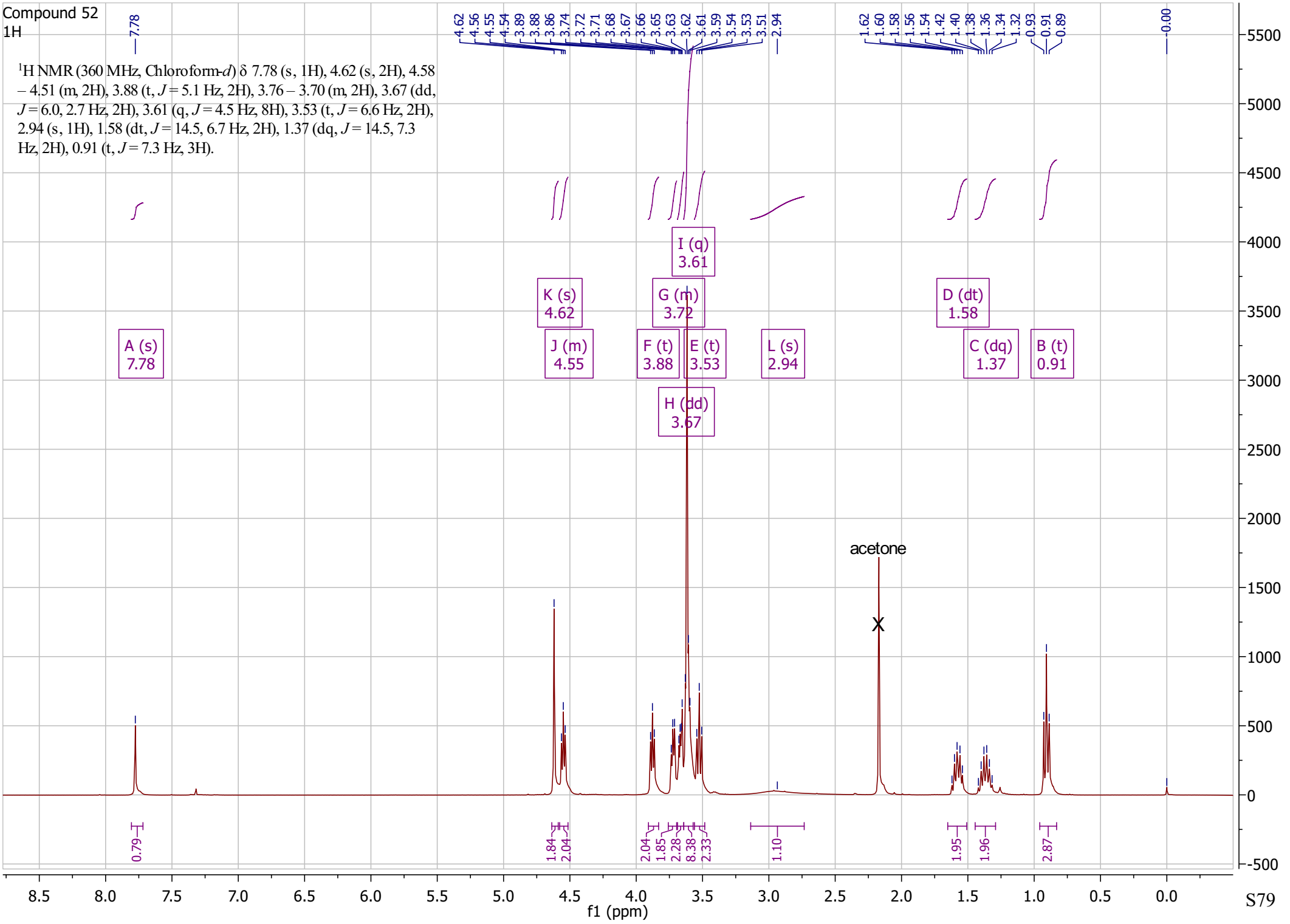

Compound 46
DMSO, 298K, 13C, DUAL
166.055
143.827
135.377
39.520 Dimethyl Sulfoxide-d6
15000
10000
5000
0
-5000
-10000
-15000
-20000
-25000
-30000
-35000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

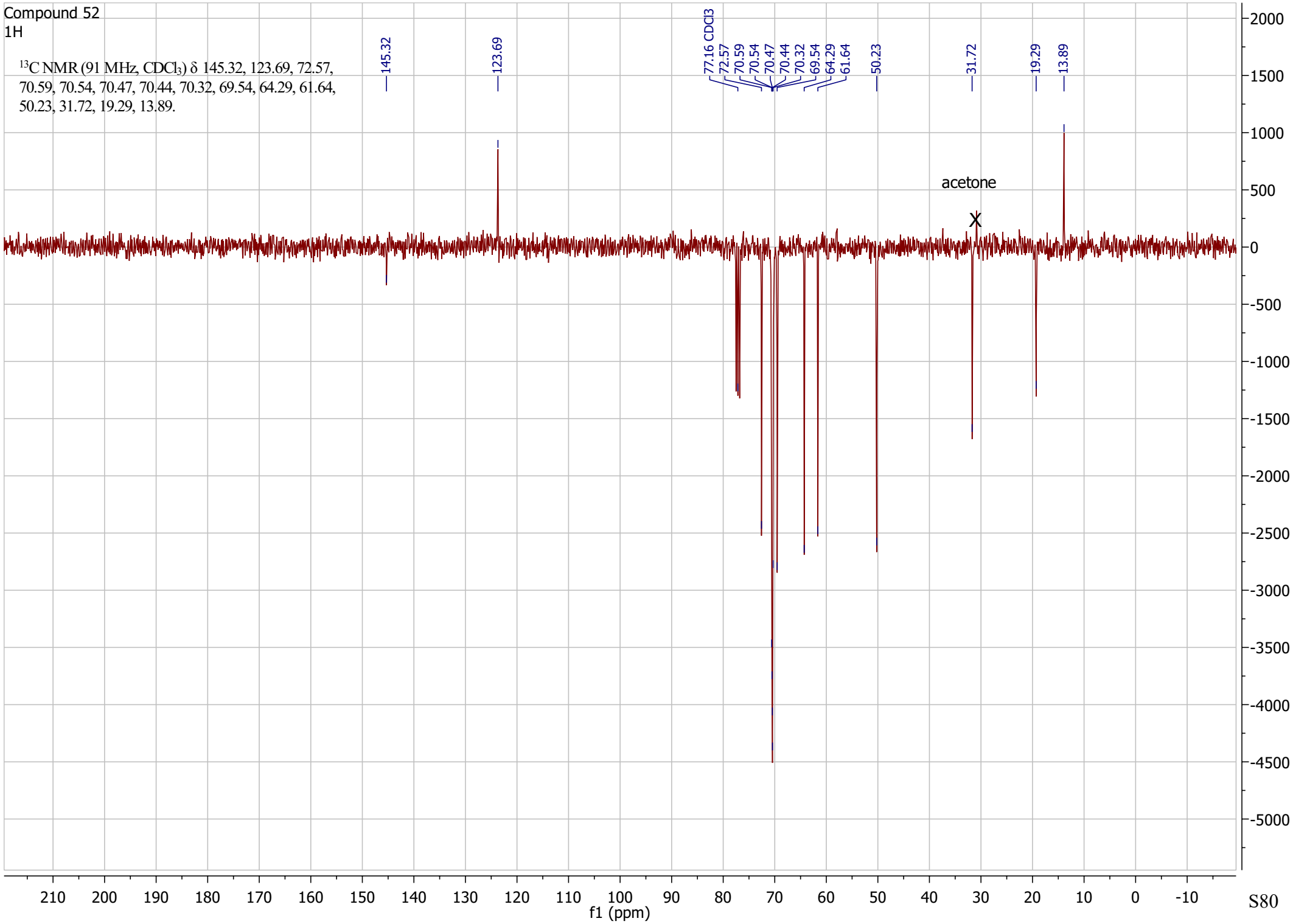

Compound 46
DMSO, 300K, HMBC, TXI
{4.44,124.03}TEG a - T5
{5.66,128.18}x4-4a
{5.53,128.05}4b-4a
{5.53,134.40}4b-4d
{5.07,134.43}4f-4d
{5.38,141.03}x3-3a
{4.43,143.86}TEGa - T4
f1 (ppm)
f2 (ppm)
116
118
120
122
124
126
128
130
132
134
136
138
140
142
144
6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7

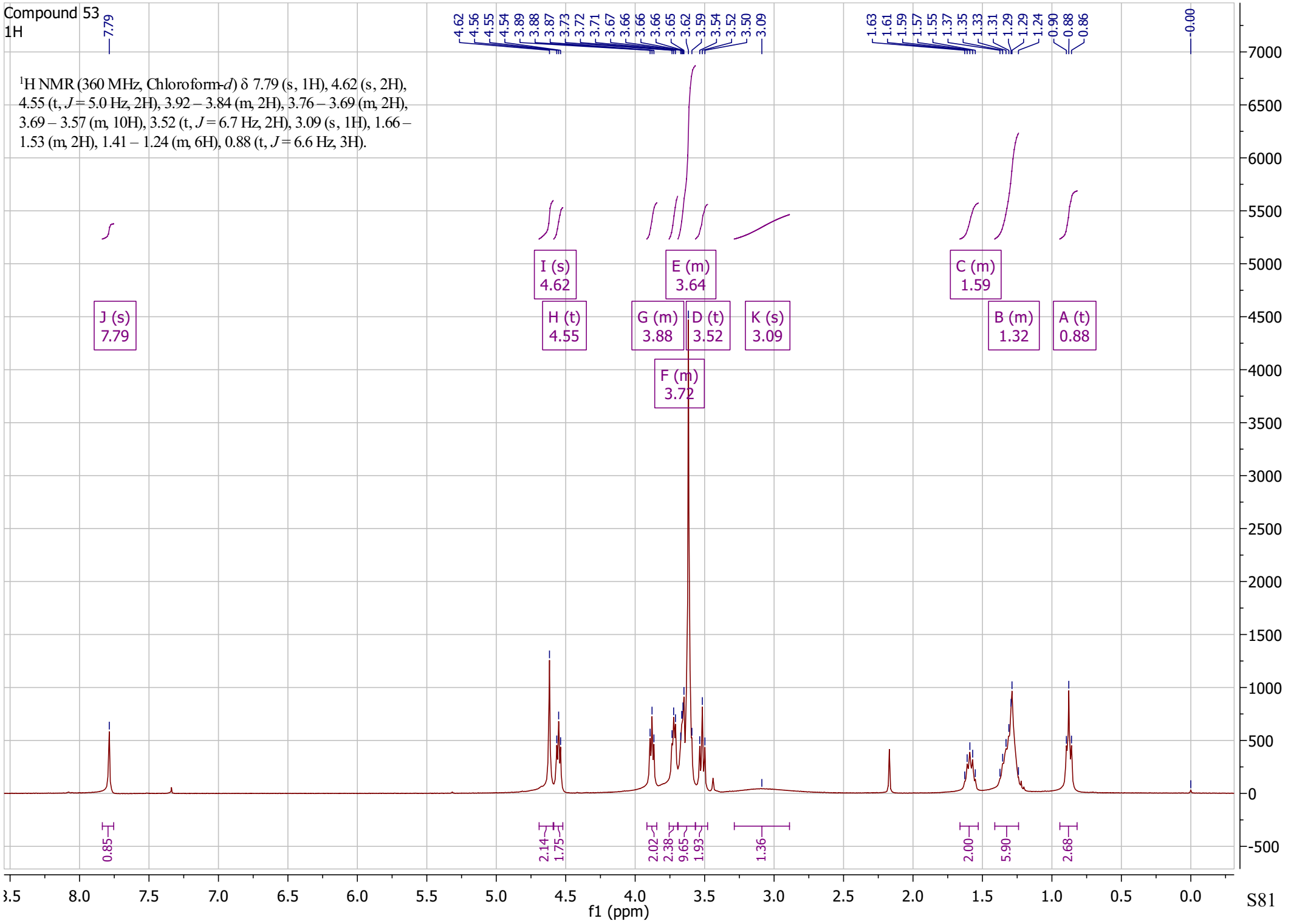

Compound 46
DMSO, 300K, HMBC, TXI
{3.60,30.88}T2-T1
{3.50,37.74}TEG h-TEG i
{3.41,60.18}T7-T8
{3.56,66.79}TEG i-TEG h
{3.50,72.38}T8-T7
f2 (ppm)
f1 (ppm)

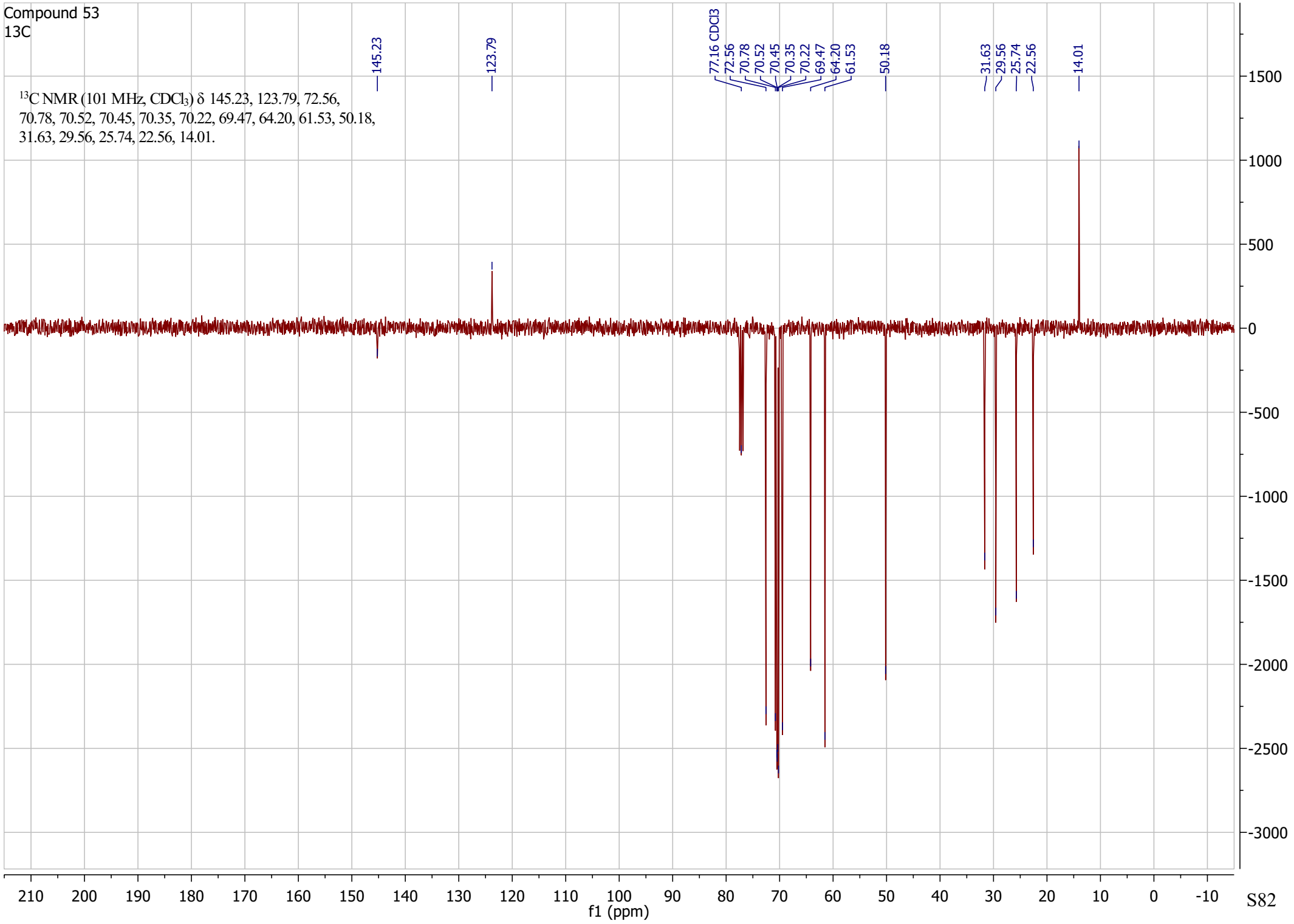
Compound 52
1H

^{1}H NMR (360 MHz, Chloroform-*d*) δ 7.78 (s, 1H), 4.62 (s, 2H), 4.58 – 4.51 (m, 2H), 3.88 (t, *J* = 5.1 Hz, 2H), 3.76 – 3.70 (m, 2H), 3.67 (dd, *J* = 6.0, 2.7 Hz, 2H), 3.61 (q, *J* = 4.5 Hz, 8H), 3.53 (t, *J* = 6.6 Hz, 2H), 2.94 (s, 1H), 1.58 (dt, *J* = 14.5, 6.7 Hz, 2H), 1.37 (dq, *J* = 14.5, 7.3 Hz, 2H), 0.91 (t, *J* = 7.3 Hz, 3H).



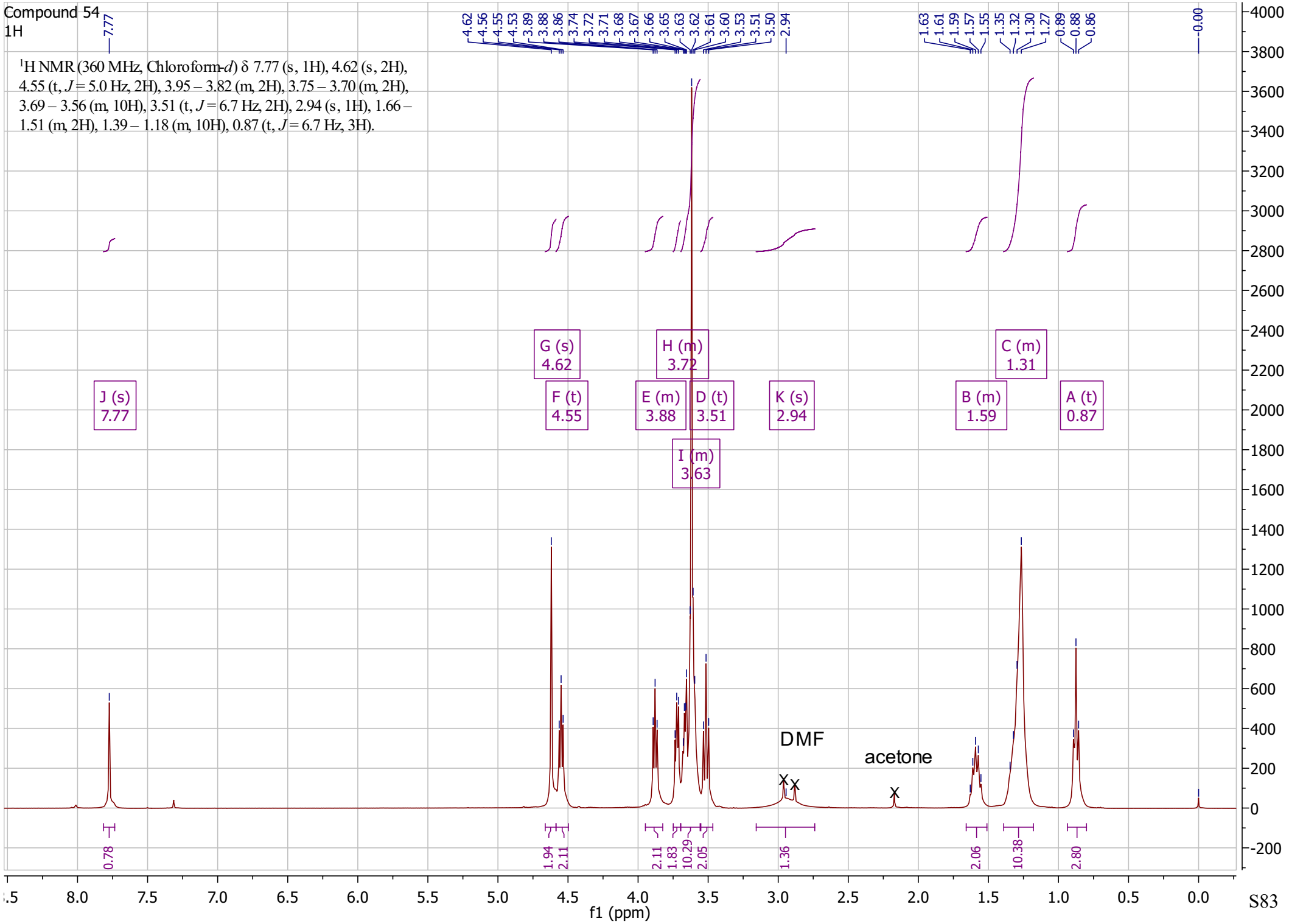

Compound 52
1H
^{13}C NMR (91 MHz, $CDCl_3$) δ 145.32, 123.69, 72.57, 70.59, 70.54, 70.47, 70.44, 70.32, 69.54, 64.29, 61.64, 50.23, 31.72, 19.29, 13.89.
145.32
123.69
77.16 CDCl3
72.57
70.59
70.54
70.47
70.44
70.32
69.54
64.29
61.64
50.23
31.72
19.29
13.89
acetone
f1 (ppm)

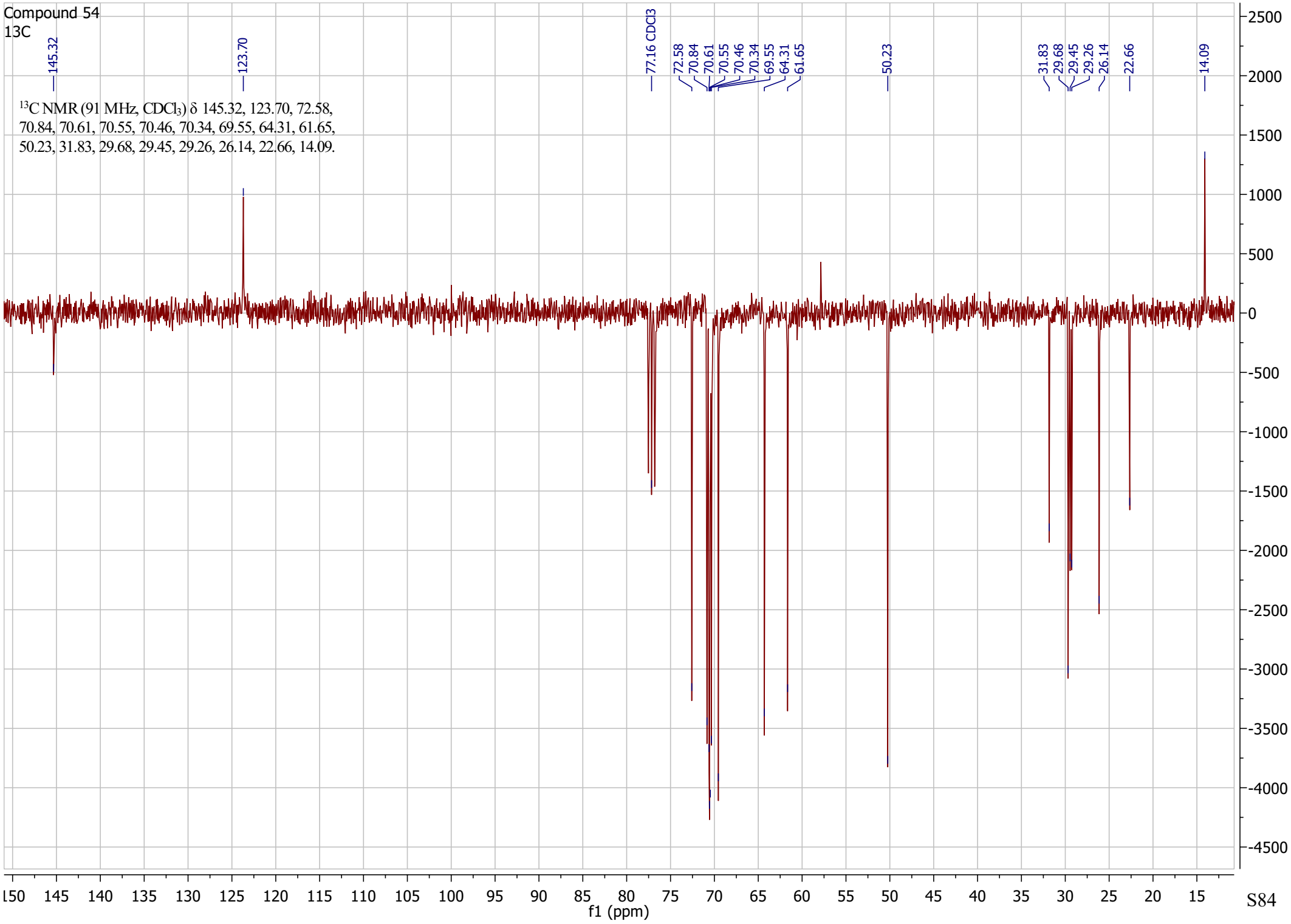

Compound 53
1H
[1]H NMR (360 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 4.62 (s, 2H), 4.55 (t, *J* = 5.0 Hz, 2H), 3.92 – 3.84 (m, 2H), 3.76 – 3.69 (m, 2H), 3.69 – 3.57 (m, 10H), 3.52 (t, *J* = 6.7 Hz, 2H), 3.09 (s, 1H), 1.66 – 1.53 (m, 2H), 1.41 – 1.24 (m, 6H), 0.88 (t, *J* = 6.6 Hz, 3H).
7.79
4.62 4.56 4.55 4.54 3.89 3.88 3.87 3.73 3.72 3.71 3.67 3.66 3.66 3.66 3.65 3.62 3.59 3.54 3.52 3.50 3.09
1.63 1.61 1.59 1.57 1.55 1.37 1.35 1.33 1.31 1.29 1.29 1.24 0.90 0.88 0.86
0.00
I (s) 4.62
E (m) 3.64
C (m) 1.59
J (s) 7.79
H (t) 4.55
G (m) 3.88
D (t) 3.52
K (s) 3.09
B (m) 1.32
A (t) 0.88
F (m) 3.72
0.85
2.14
1.75
2.02
2.38
9.65
1.93
1.36
2.00
5.90
2.68
f1 (ppm)

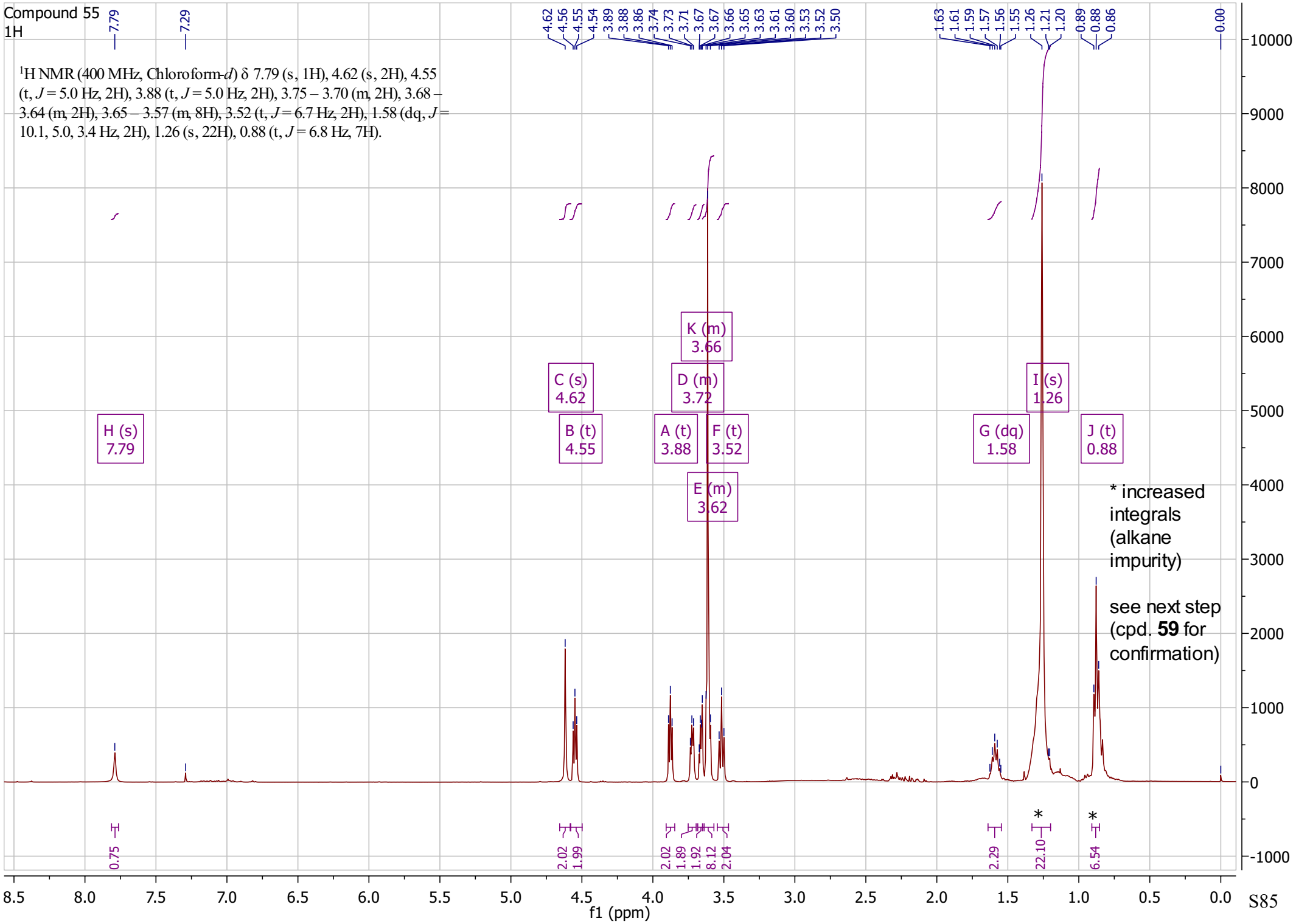

Compound 53
13C
145.23
123.79
77.16 CDCl3
72.56
70.78
70.52
70.45
70.35
70.22
69.47
64.20
61.53
50.18
31.63
29.56
25.74
22.56
14.01
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.23, 123.79, 72.56, 70.78, 70.52, 70.45, 70.35, 70.22, 69.47, 64.20, 61.53, 50.18, 31.63, 29.56, 25.74, 22.56, 14.01.
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

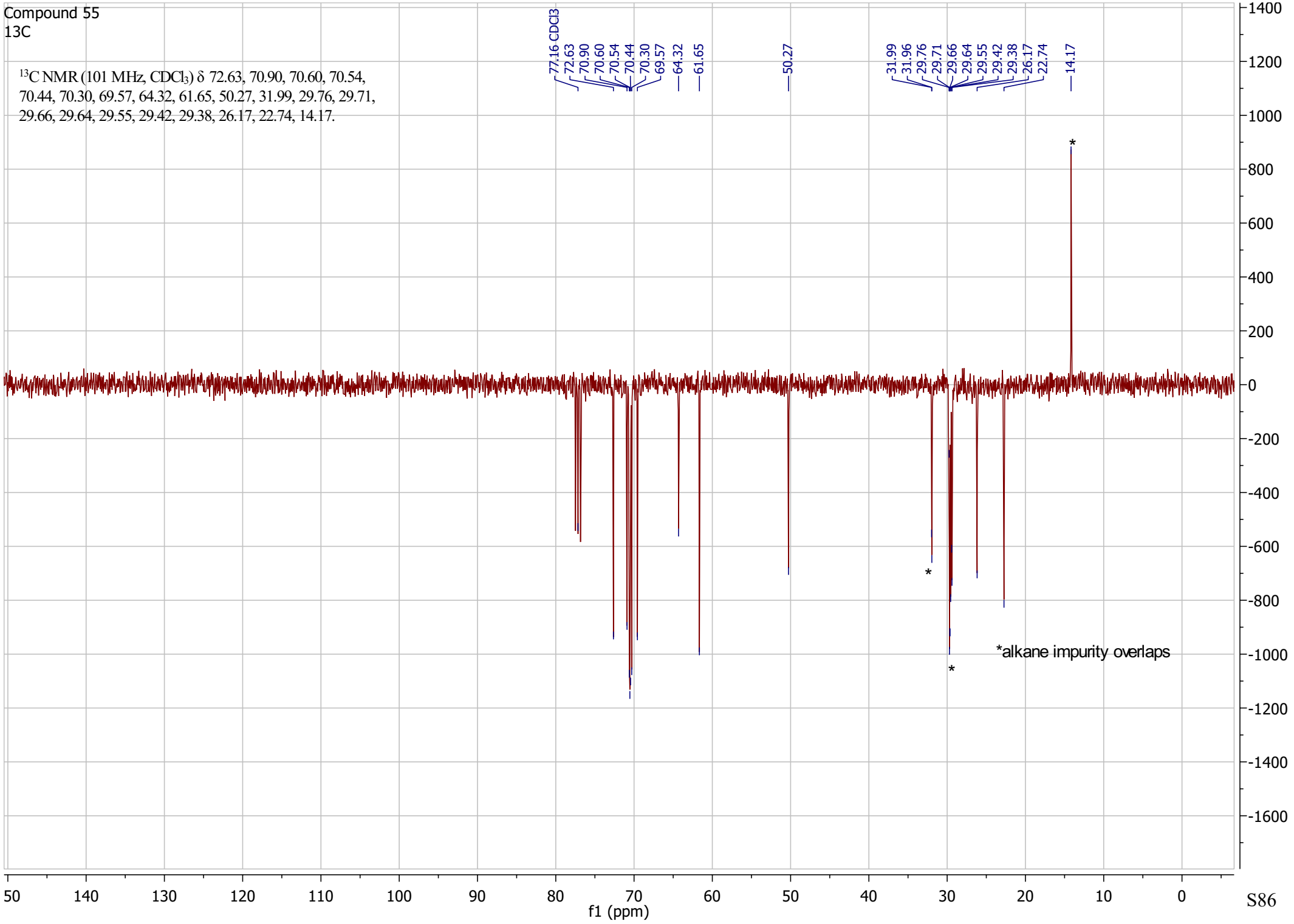
Compound 54
1H

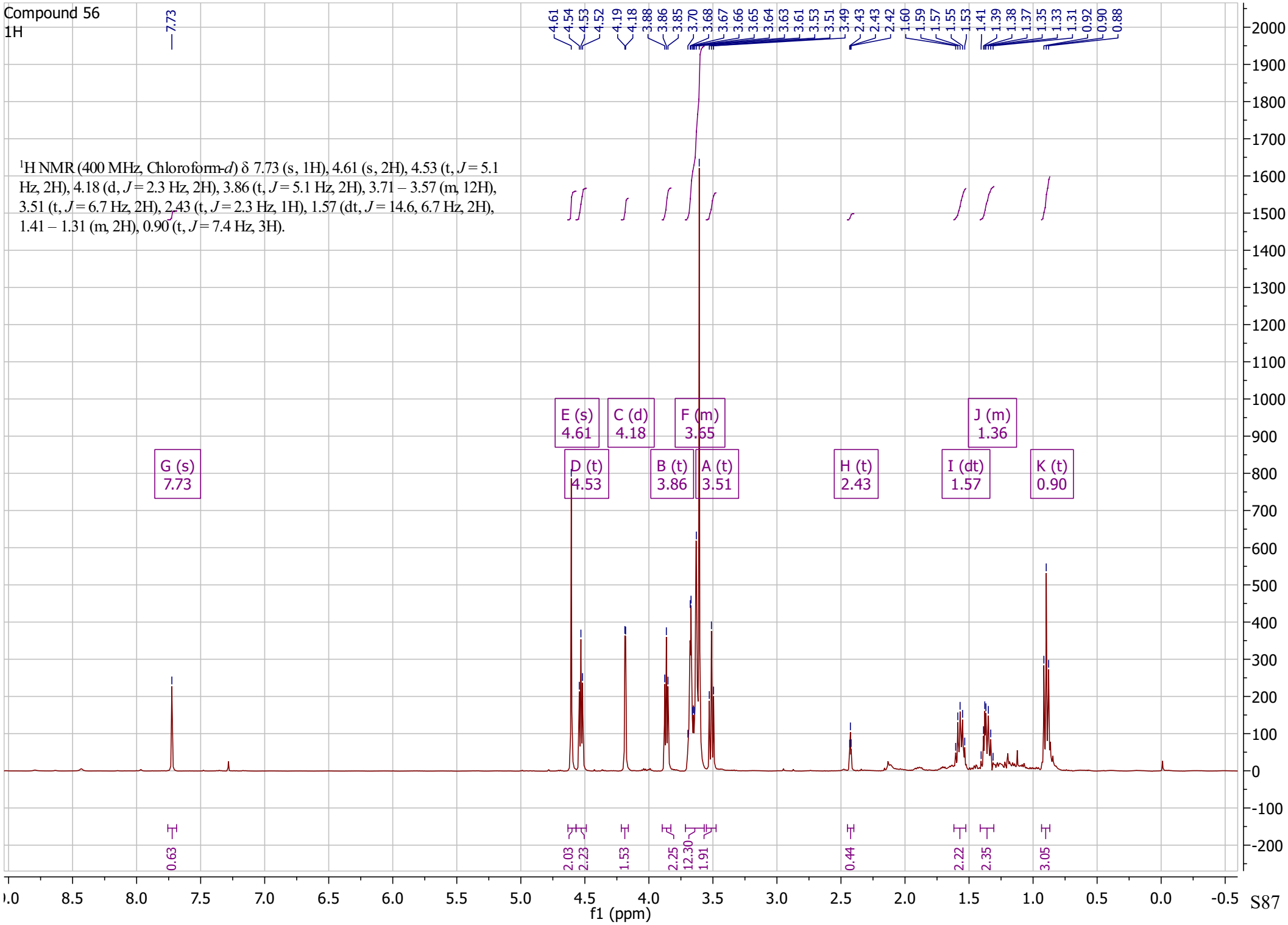
^{1}H NMR (360 MHz, Chloroform-*d*) δ 7.77 (s, 1H), 4.62 (s, 2H), 4.55 (t, *J* = 5.0 Hz, 2H), 3.95 – 3.82 (m, 2H), 3.75 – 3.70 (m, 2H), 3.69 – 3.56 (m, 10H), 3.51 (t, *J* = 6.7 Hz, 2H), 2.94 (s, 1H), 1.66 – 1.51 (m, 2H), 1.39 – 1.18 (m, 10H), 0.87 (t, *J* = 6.7 Hz, 3H).

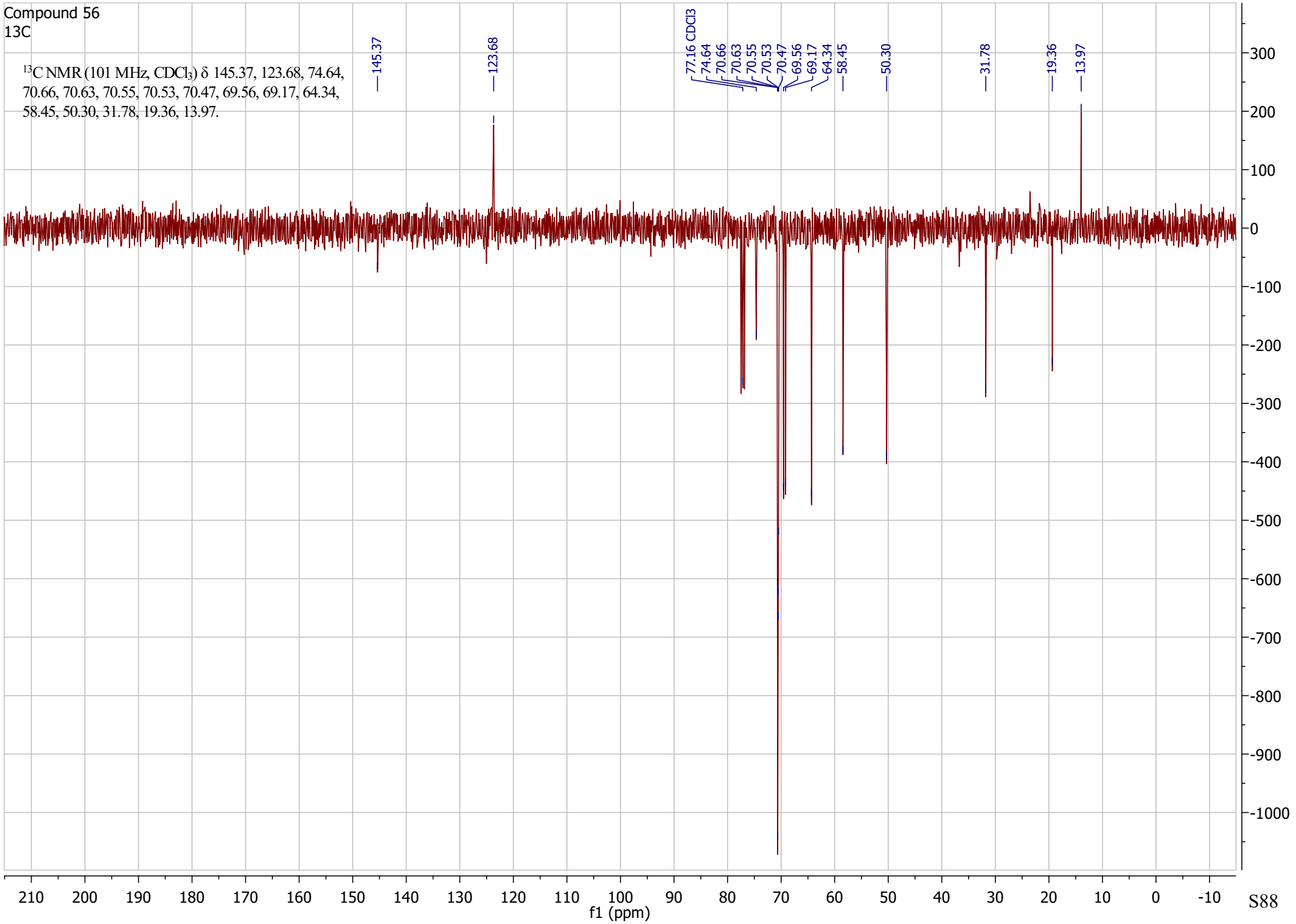


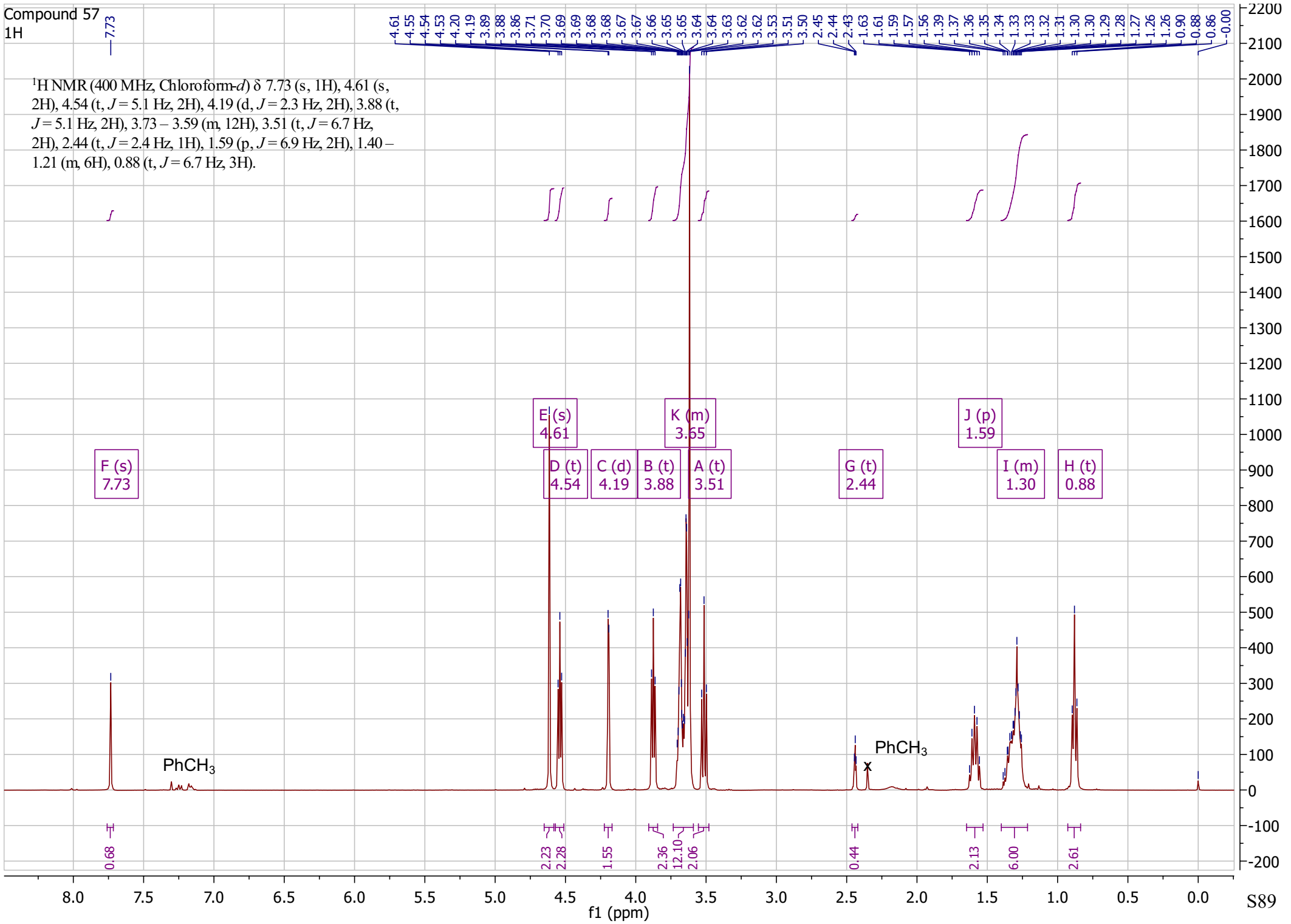

Compound 54
13C
145.32
123.70
77.16 CDCl3
72.58
70.84
70.61
70.55
70.46
70.34
69.55
64.31
61.65
50.23
31.83
29.68
29.45
29.26
26.14
22.66
14.09
13C NMR (91 MHz, CDCl3) δ 145.32, 123.70, 72.58, 70.84, 70.61, 70.55, 70.46, 70.34, 69.55, 64.31, 61.65, 50.23, 31.83, 29.68, 29.45, 29.26, 26.14, 22.66, 14.09.
f1 (ppm)

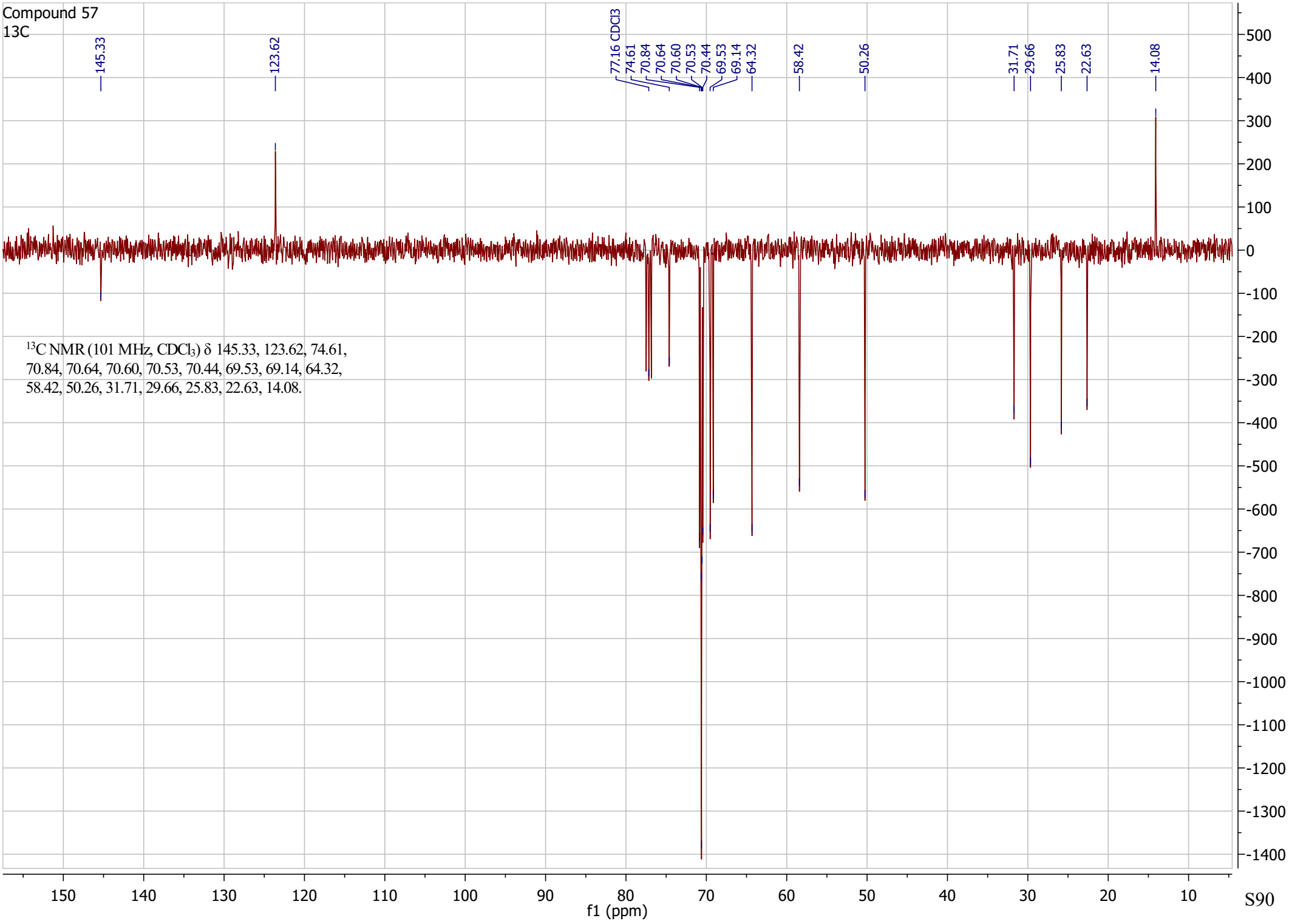

Compound 55
1H
[1]H NMR (400 MHz, Chloroform-d) δ 7.79 (s, 1H), 4.62 (s, 2H), 4.55 (t, J = 5.0 Hz, 2H), 3.88 (t, J = 5.0 Hz, 2H), 3.75 – 3.70 (m, 2H), 3.68 – 3.64 (m, 2H), 3.65 – 3.57 (m, 8H), 3.52 (t, J = 6.7 Hz, 2H), 1.58 (dq, J = 10.1, 5.0, 3.4 Hz, 2H), 1.26 (s, 22H), 0.88 (t, J = 6.8 Hz, 7H).
H (s) 7.79
C (s) 4.62
B (t) 4.55
K (m) 3.66
D (m) 3.72
A (t) 3.88
F (t) 3.52
E (m) 3.62
G (dq) 1.58
I (s) 1.26
J (t) 0.88
* increased integrals (alkane impurity)
see next step (cpd. 59 for confirmation)
f1 (ppm)


Compound 55
13C
^{13}C NMR (101 MHz, $CDCl_3$) δ 72.63, 70.90, 70.60, 70.54, 70.44, 70.30, 69.57, 64.32, 61.65, 50.27, 31.99, 29.76, 29.71, 29.66, 29.64, 29.55, 29.42, 29.38, 26.17, 22.74, 14.17.
77.16 CDCl3
72.63
70.90
70.60
70.54
70.44
70.30
69.57
64.32
61.65
50.27
31.99
31.96
29.76
29.71
29.66
29.64
29.55
29.42
29.38
26.17
22.74
14.17
*alkane impurity overlaps
f1 (ppm)


Compound 56
1H
7.73
4.61 4.54 4.53 4.52 4.19 4.18 3.88 3.86 3.85 3.70 3.68 3.67 3.66 3.65 3.64 3.63 3.61 3.53 3.51 3.49 2.43 2.43 2.42 1.60 1.59 1.57 1.55 1.53 1.41 1.39 1.38 1.37 1.35 1.33 1.31 0.92 0.90 0.88
[1]H NMR (400 MHz, Chloroform-d) δ 7.73 (s, 1H), 4.61 (s, 2H), 4.53 (t, J = 5.1 Hz, 2H), 4.18 (d, J = 2.3 Hz, 2H), 3.86 (t, J = 5.1 Hz, 2H), 3.71 – 3.57 (m, 12H), 3.51 (t, J = 6.7 Hz, 2H), 2.43 (t, J = 2.3 Hz, 1H), 1.57 (dt, J = 14.6, 6.7 Hz, 2H), 1.41 – 1.31 (m, 2H), 0.90 (t, J = 7.4 Hz, 3H).
E (s) 4.61
C (d) 4.18
F (m) 3.65
J (m) 1.36
G (s) 7.73
D (t) 4.53
B (t) 3.86
A (t) 3.51
H (t) 2.43
I (dt) 1.57
K (t) 0.90
0.63
2.03 2.23 1.53 2.25 12.30 1.91 0.44 2.22 2.35 3.05
f1 (ppm)

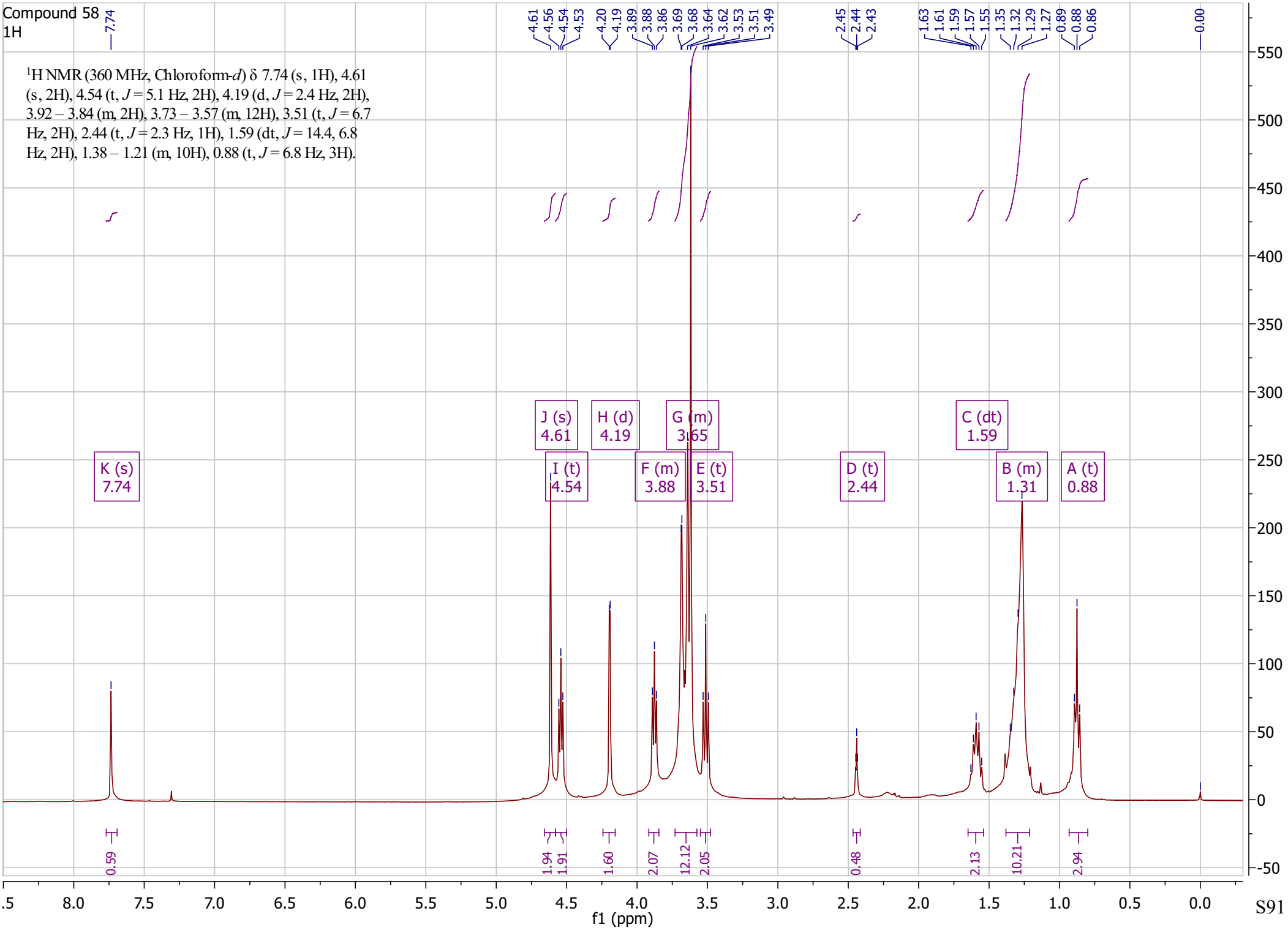

Compound 56
13C
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.37, 123.68, 74.64, 70.66, 70.63, 70.55, 70.53, 70.47, 69.56, 69.17, 64.34, 58.45, 50.30, 31.78, 19.36, 13.97.
145.37
123.68
77.16 CDCl3
74.64
70.66
70.63
70.55
70.53
70.47
69.56
69.17
64.34
58.45
50.30
31.78
19.36
13.97
f1 (ppm)

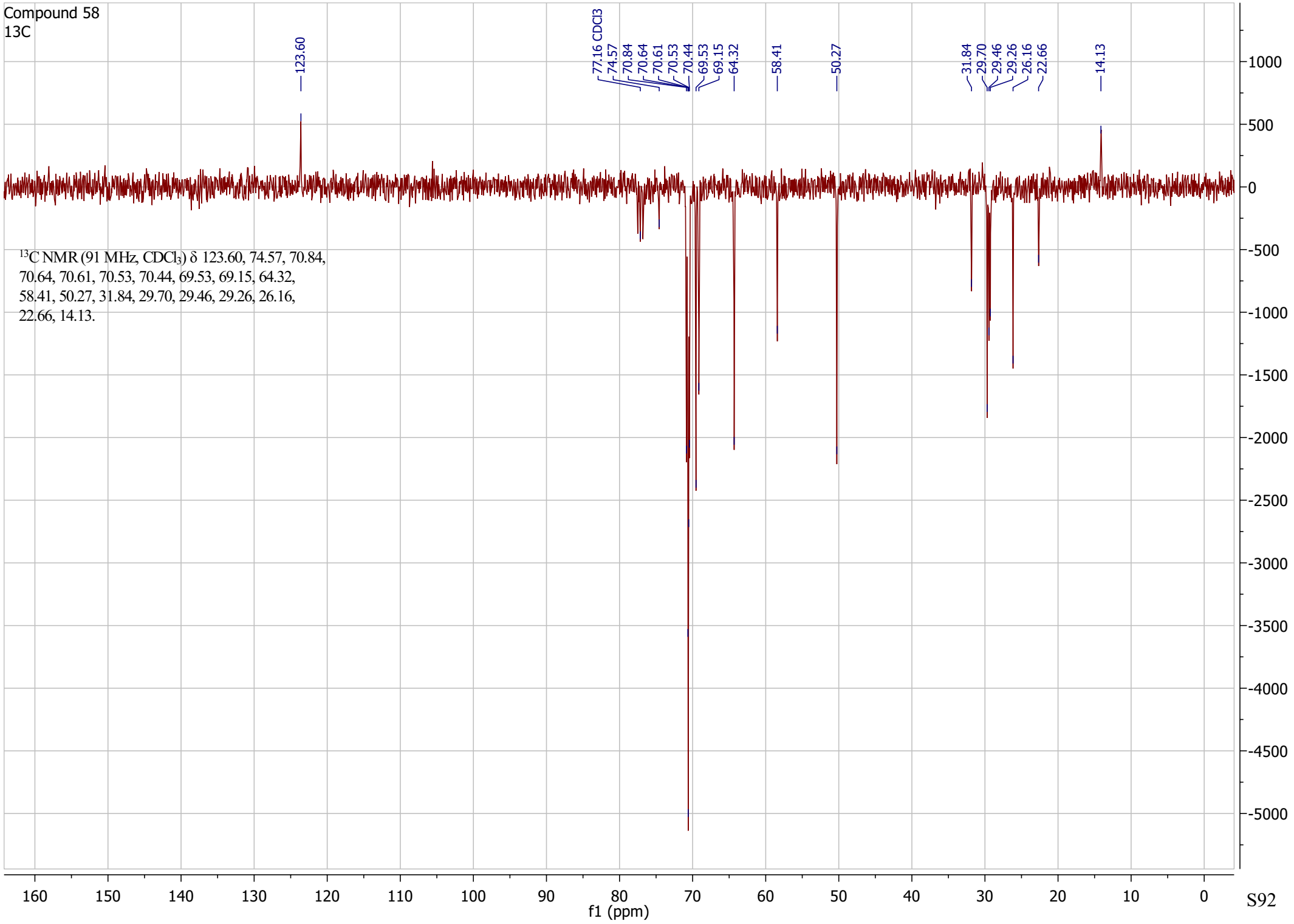

Compound 57
1H
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (s, 1H), 4.61 (s, 2H), 4.54 (t, *J* = 5.1 Hz, 2H), 4.19 (d, *J* = 2.3 Hz, 2H), 3.88 (t, *J* = 5.1 Hz, 2H), 3.73 – 3.59 (m, 12H), 3.51 (t, *J* = 6.7 Hz, 2H), 2.44 (t, *J* = 2.4 Hz, 1H), 1.59 (p, *J* = 6.9 Hz, 2H), 1.40 – 1.21 (m, 6H), 0.88 (t, *J* = 6.7 Hz, 3H).
F (s) 7.73
E (s) 4.61
D (t) 4.54
C (d) 4.19
B (t) 3.88
K (m) 3.65
A (t) 3.51
G (t) 2.44
J (p) 1.59
I (m) 1.30
H (t) 0.88
PhCH3
PhCH3
0.68
2.23
2.28
1.55
2.36
12.10
2.06
0.44
2.13
6.00
2.61
f1 (ppm)

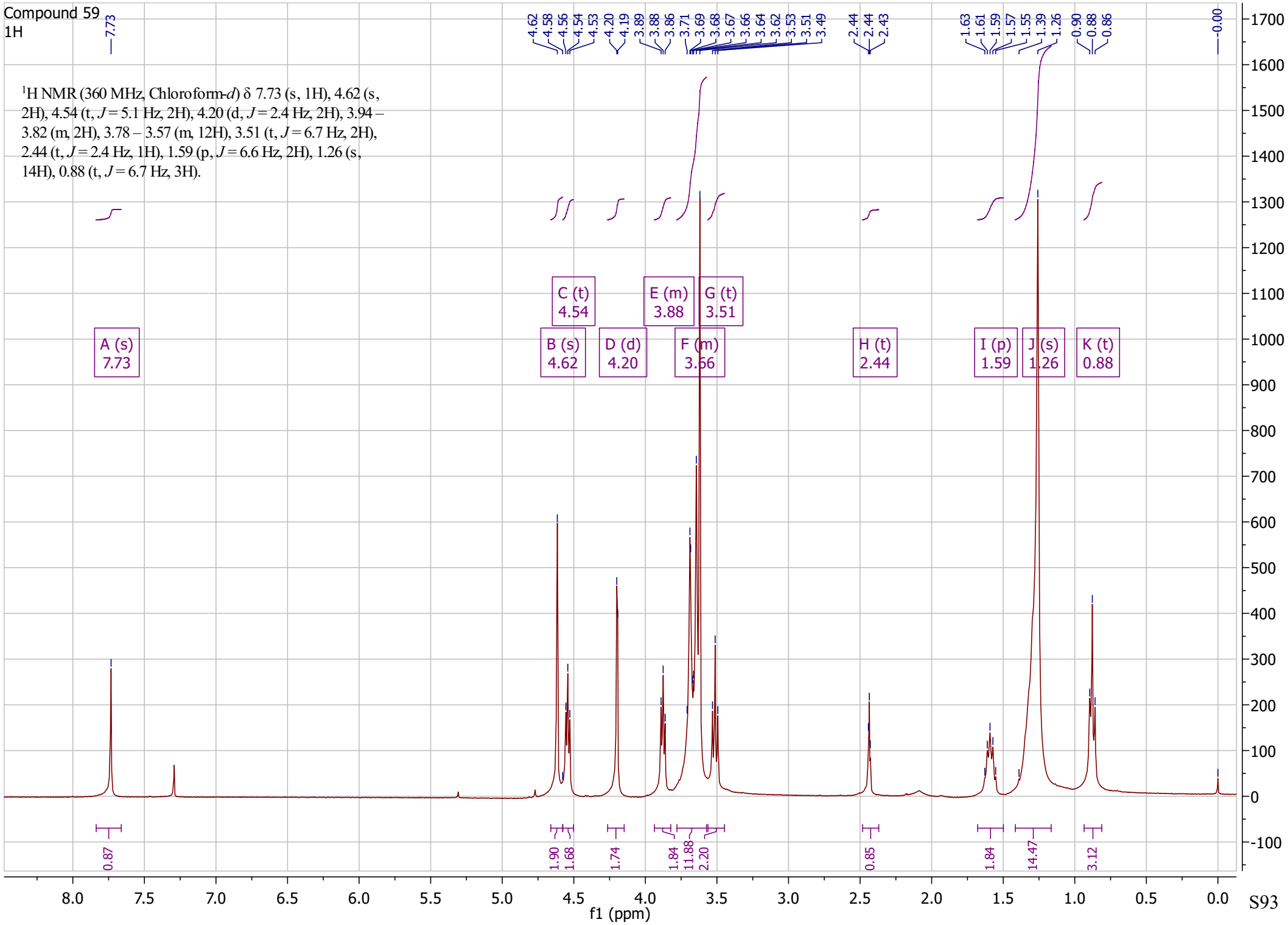

Compound 57
13C
145.33
123.62
77.16 CDCl3
74.61
70.84
70.64
70.60
70.53
70.44
69.53
69.14
64.32
58.42
50.26
31.71
29.66
25.83
22.63
14.08
13C NMR (101 MHz, CDCl3) δ 145.33, 123.62, 74.61,
70.84, 70.64, 70.60, 70.53, 70.44, 69.53, 69.14, 64.32,
58.42, 50.26, 31.71, 29.66, 25.83, 22.63, 14.08.
f1 (ppm)

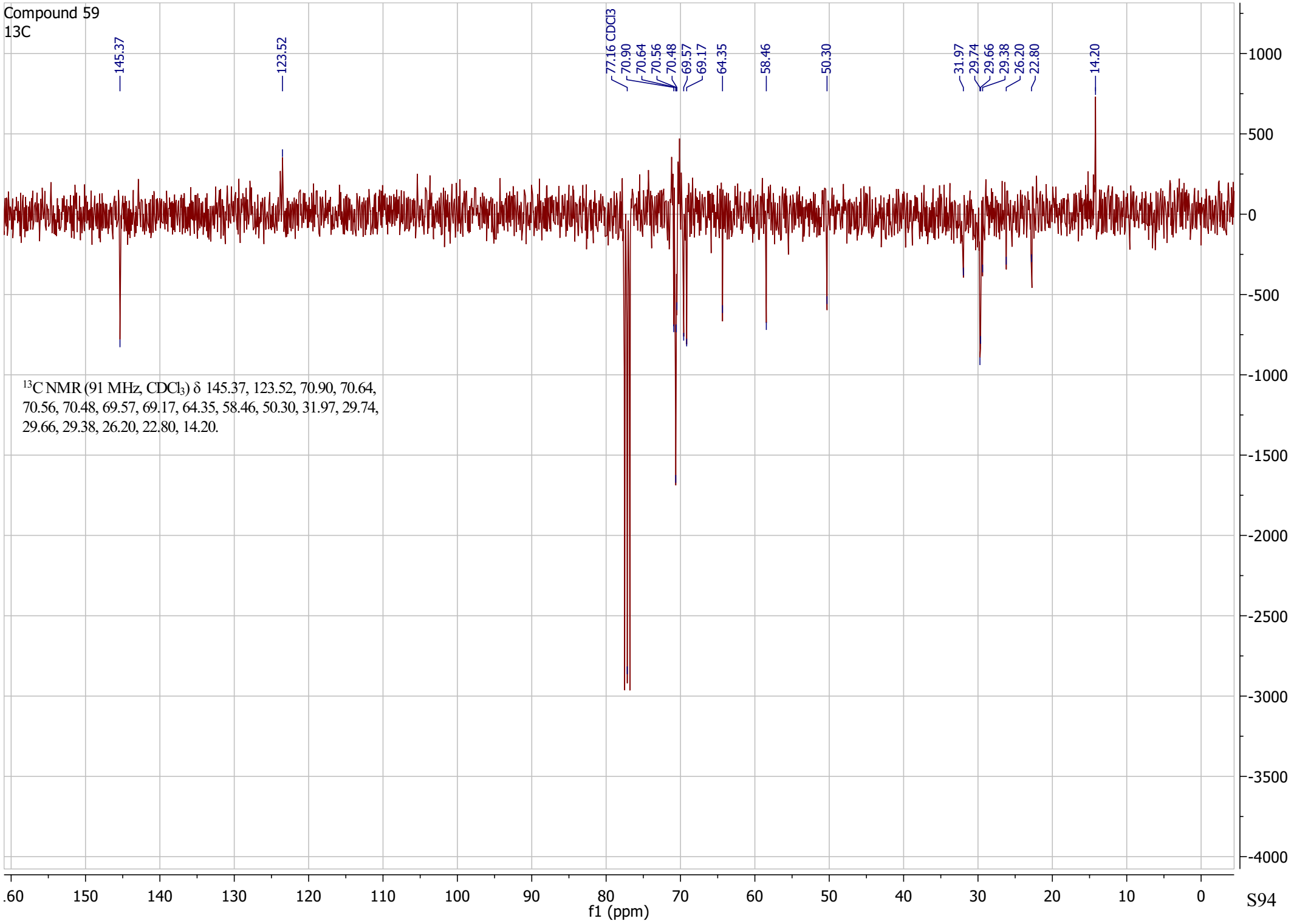
Compound 58
1H

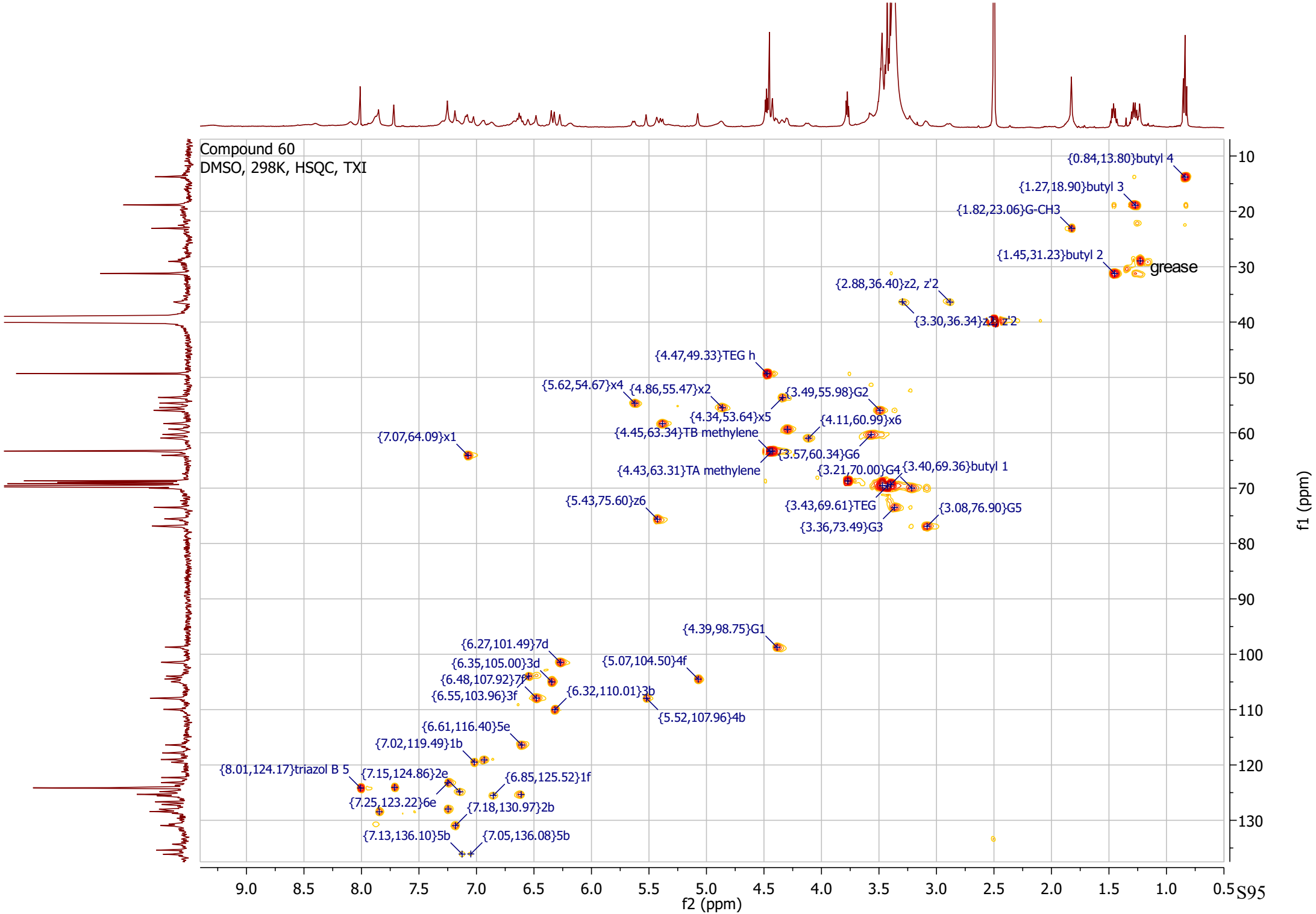
^{1}H NMR (360 MHz, Chloroform-*d*) δ 7.74 (s, 1H), 4.61 (s, 2H), 4.54 (t, *J* = 5.1 Hz, 2H), 4.19 (d, *J* = 2.4 Hz, 2H), 3.92 – 3.84 (m, 2H), 3.73 – 3.57 (m, 12H), 3.51 (t, *J* = 6.7 Hz, 2H), 2.44 (t, *J* = 2.3 Hz, 1H), 1.59 (dt, *J* = 14.4, 6.8 Hz, 2H), 1.38 – 1.21 (m, 10H), 0.88 (t, *J* = 6.8 Hz, 3H).

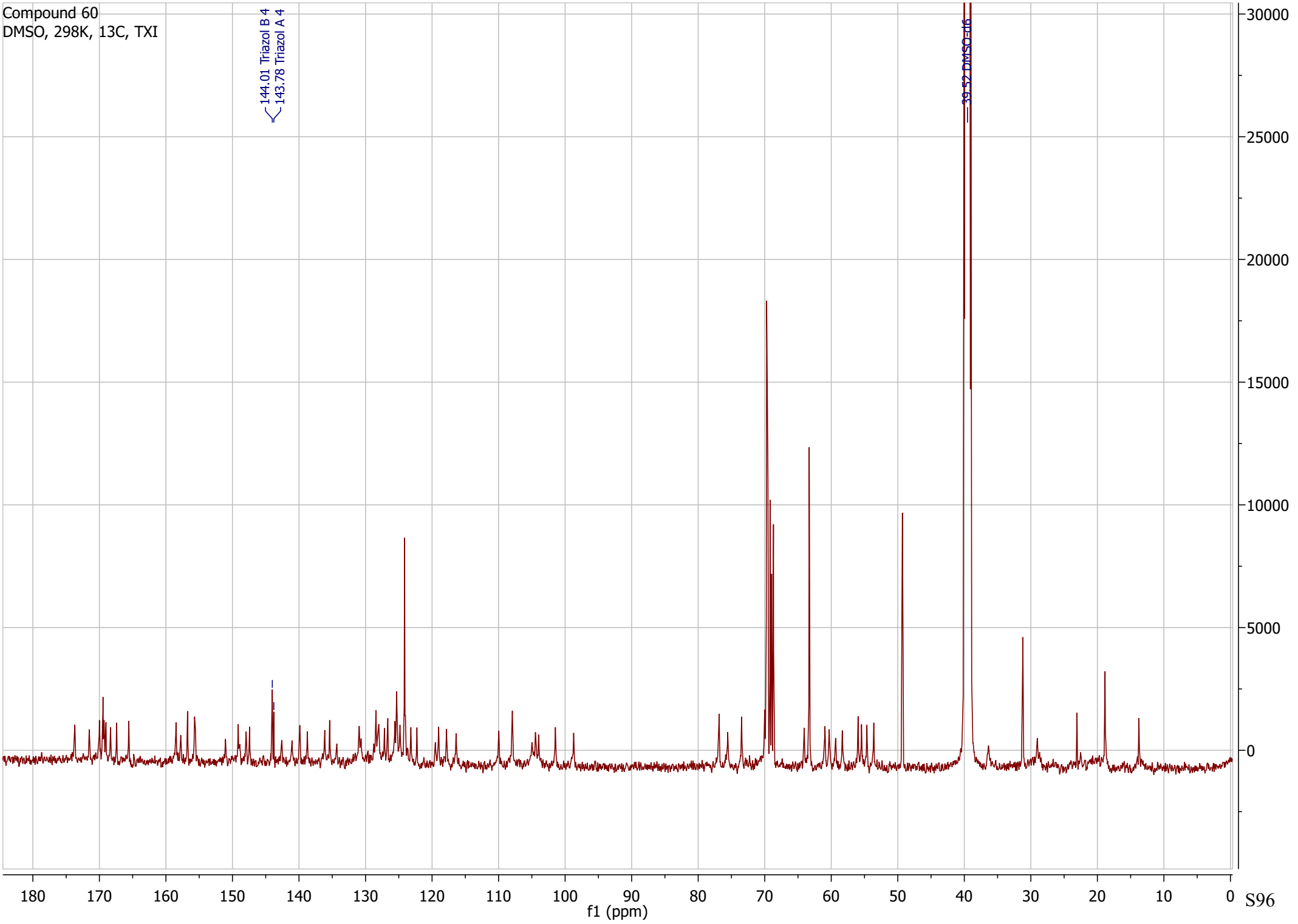


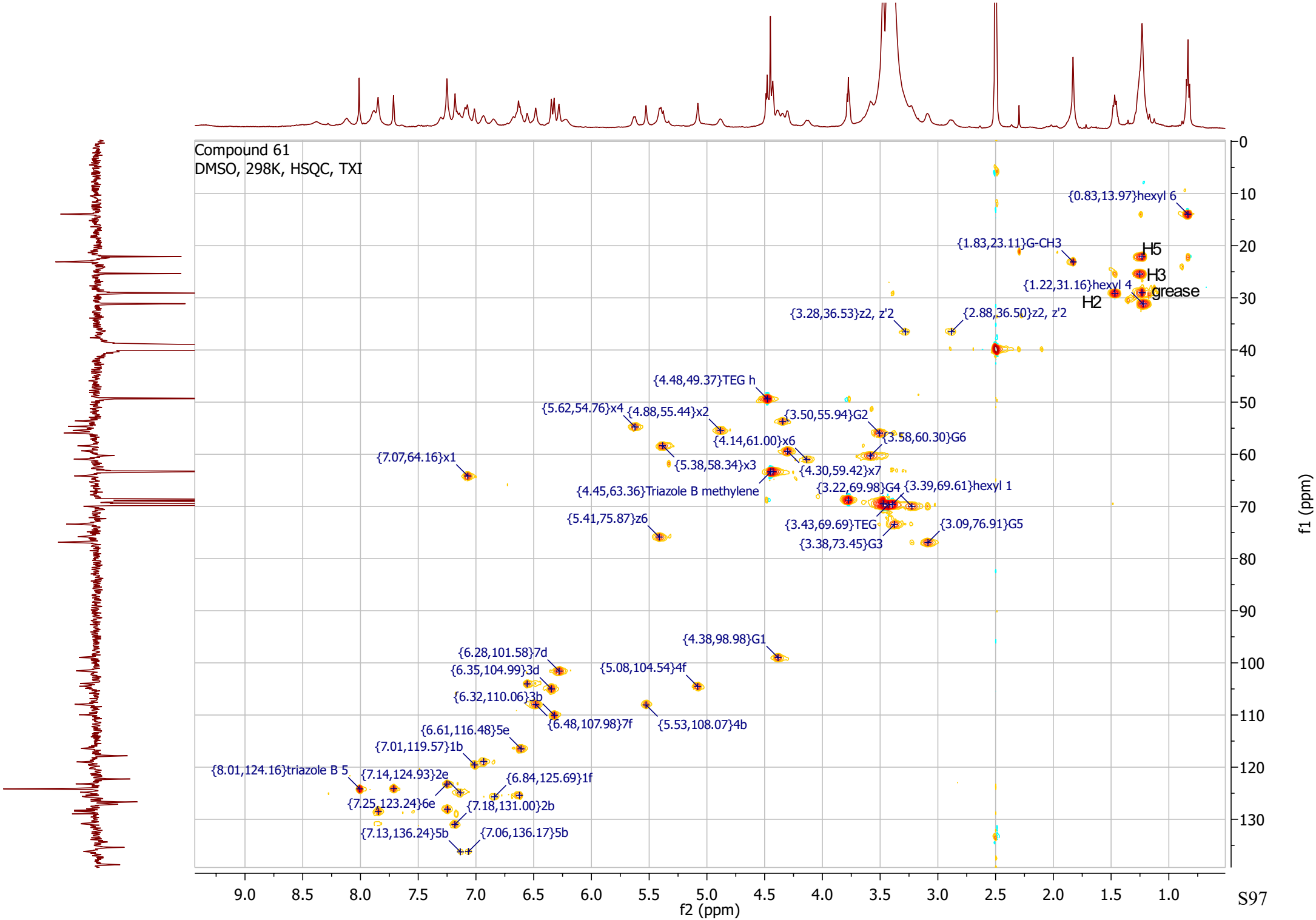

Compound 58
13C
123.60
77.16 CDCl3
74.57
70.84
70.64
70.61
70.53
70.44
69.53
69.15
64.32
58.41
50.27
31.84
29.70
29.46
29.26
26.16
22.66
14.13
^{13}C NMR (91 MHz, $CDCl_3$) δ 123.60, 74.57, 70.84, 70.64, 70.61, 70.53, 70.44, 69.53, 69.15, 64.32, 58.41, 50.27, 31.84, 29.70, 29.46, 29.26, 26.16, 22.66, 14.13.
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
-3500
-4000
-4500
-5000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

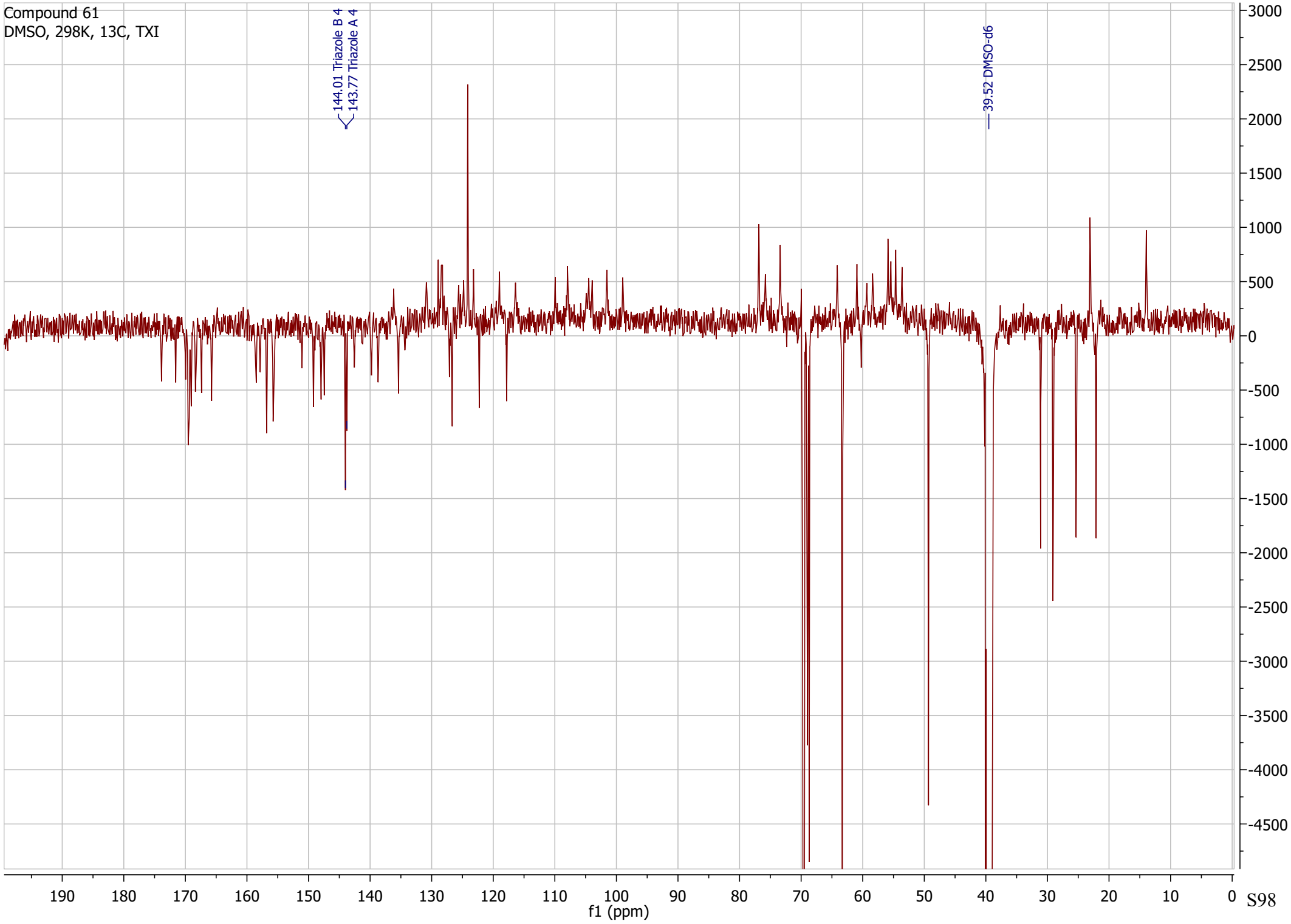

Compound 59
1H
[1]H NMR (360 MHz, Chloroform-*d*) δ 7.73 (s, 1H), 4.62 (s, 2H), 4.54 (t, *J* = 5.1 Hz, 2H), 4.20 (d, *J* = 2.4 Hz, 2H), 3.94 – 3.82 (m, 2H), 3.78 – 3.57 (m, 12H), 3.51 (t, *J* = 6.7 Hz, 2H), 2.44 (t, *J* = 2.4 Hz, 1H), 1.59 (p, *J* = 6.6 Hz, 2H), 1.26 (s, 14H), 0.88 (t, *J* = 6.7 Hz, 3H).
A (s) 7.73
B (s) 4.62
C (t) 4.54
D (d) 4.20
E (m) 3.88
F (m) 3.66
G (t) 3.51
H (t) 2.44
I (p) 1.59
J (s) 1.26
K (t) 0.88
f1 (ppm)

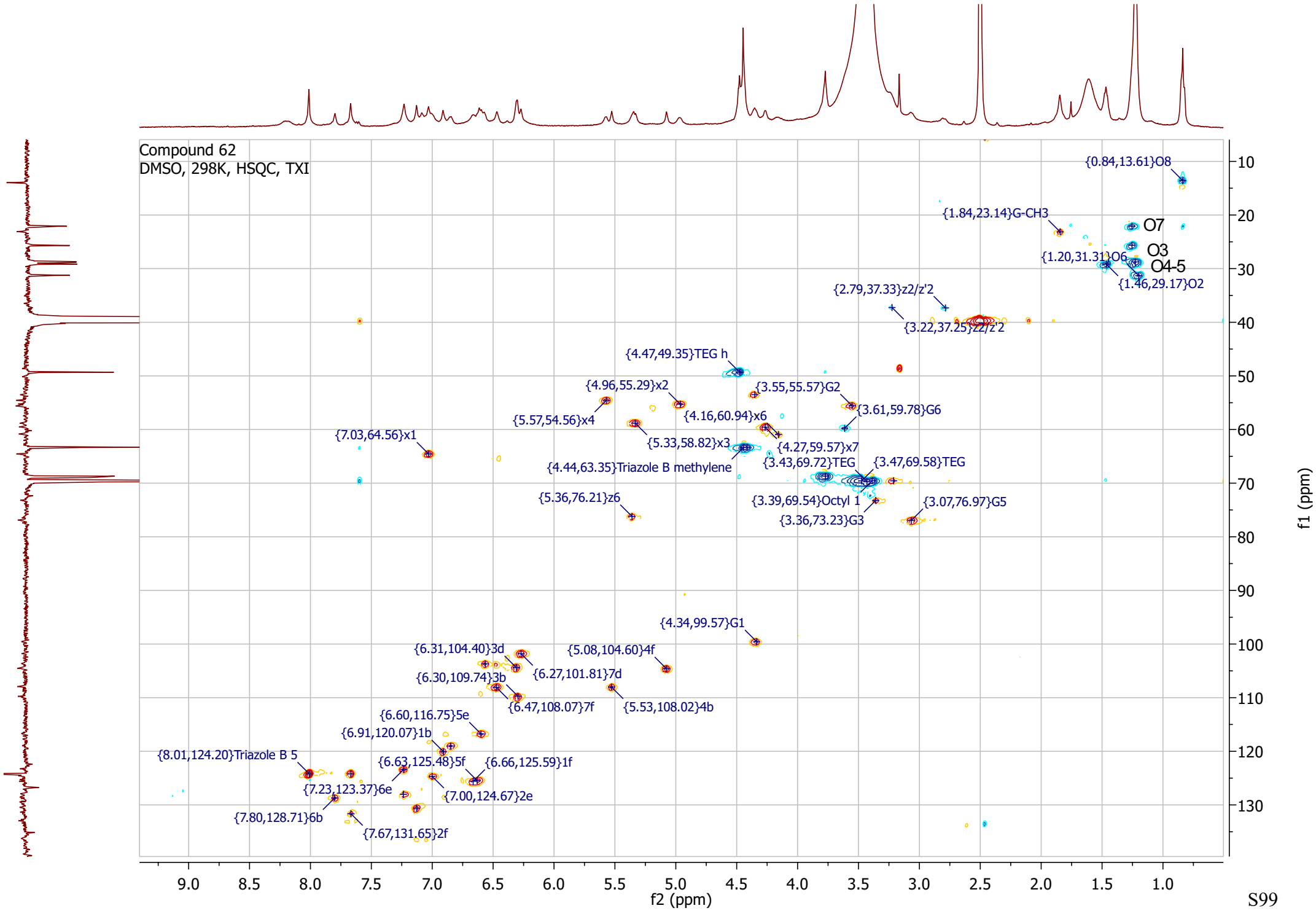

Compound 59
13C
145.37
123.52
77.16 CDCl3
70.90
70.64
70.56
70.48
69.57
69.17
64.35
58.46
50.30
31.97
29.74
29.66
29.38
26.20
22.80
14.20
^{13}C NMR (91 MHz, $CDCl_3$) δ 145.37, 123.52, 70.90, 70.64, 70.56, 70.48, 69.57, 69.17, 64.35, 58.46, 50.30, 31.97, 29.74, 29.66, 29.38, 26.20, 22.80, 14.20.
f1 (ppm)

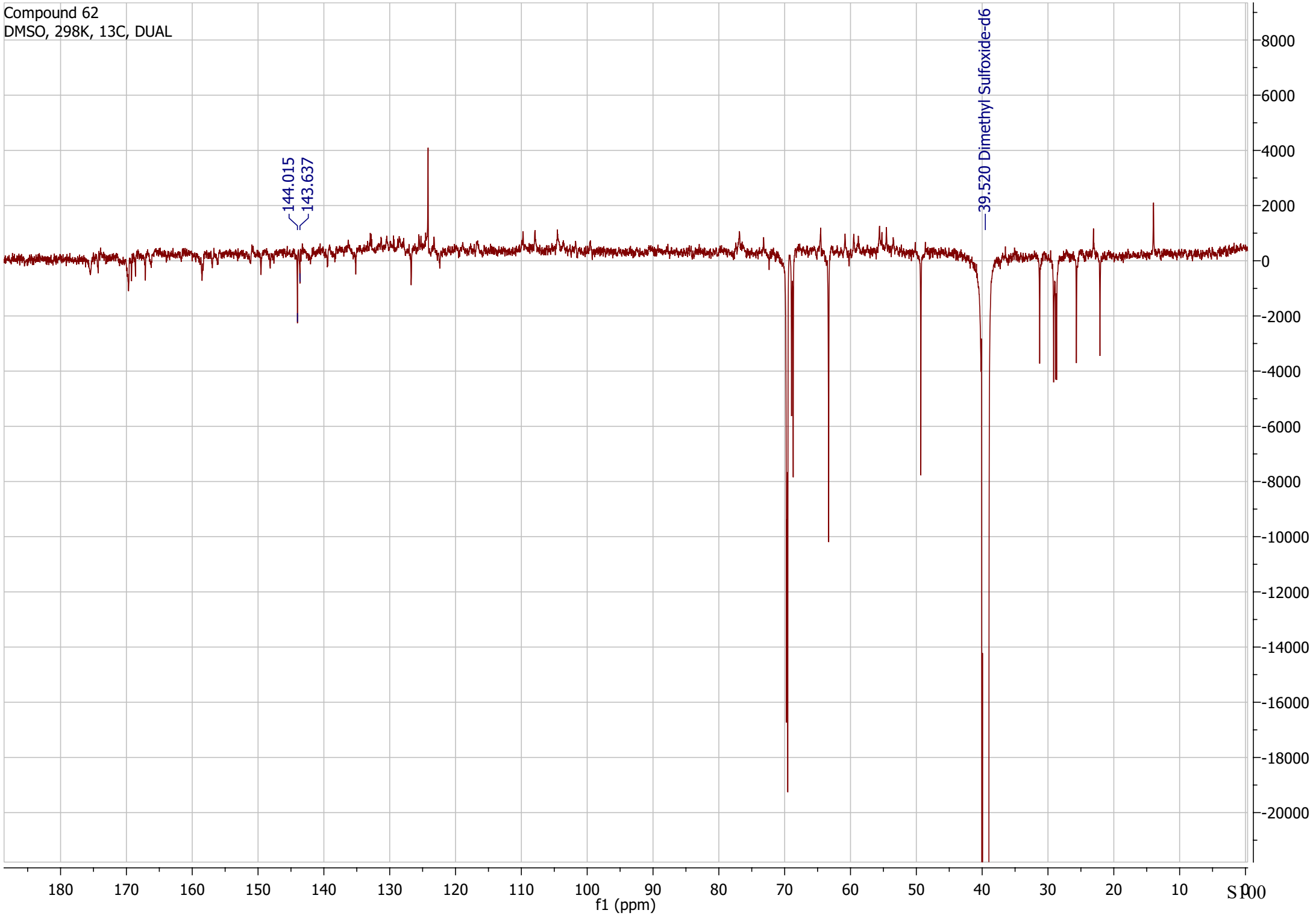

Compound 60
DMSO, 298K, HSQC, TXI
{0.84,13.80}butyl 4
{1.27,18.90}butyl 3
{1.82,23.06}G-CH3
{1.45,31.23}butyl 2
grease
{2.88,36.40}z2, z'2
{3.30,36.34}z2, z'2
{4.47,49.33}TEG h
{5.62,54.67}x4
{4.86,55.47}x2
{3.49,55.98}G2
{4.34,53.64}x5
{4.11,60.99}x6
{4.45,63.34}TB methylene
{7.07,64.09}x1
{3.57,60.34}G6
{4.43,63.31}TA methylene
{3.21,70.00}G4
{3.40,69.36}butyl 1
{5.43,75.60}z6
{3.43,69.61}TEG
{3.08,76.90}G5
{3.36,73.49}G3
{4.39,98.75}G1
{6.27,101.49}7d
{6.35,105.00}3d
{5.07,104.50}4f
{6.48,107.92}7f
{6.55,103.96}3f
{6.32,110.01}3b
{5.52,107.96}4b
{6.61,116.40}5e
{7.02,119.49}1b
{8.01,124.17}triazol B 5
{7.15,124.86}2e
{6.85,125.52}1f
{7.25,123.22}6e
{7.18,130.97}2b
{7.13,136.10}5b
{7.05,136.08}5b
f2 (ppm)
f1 (ppm)

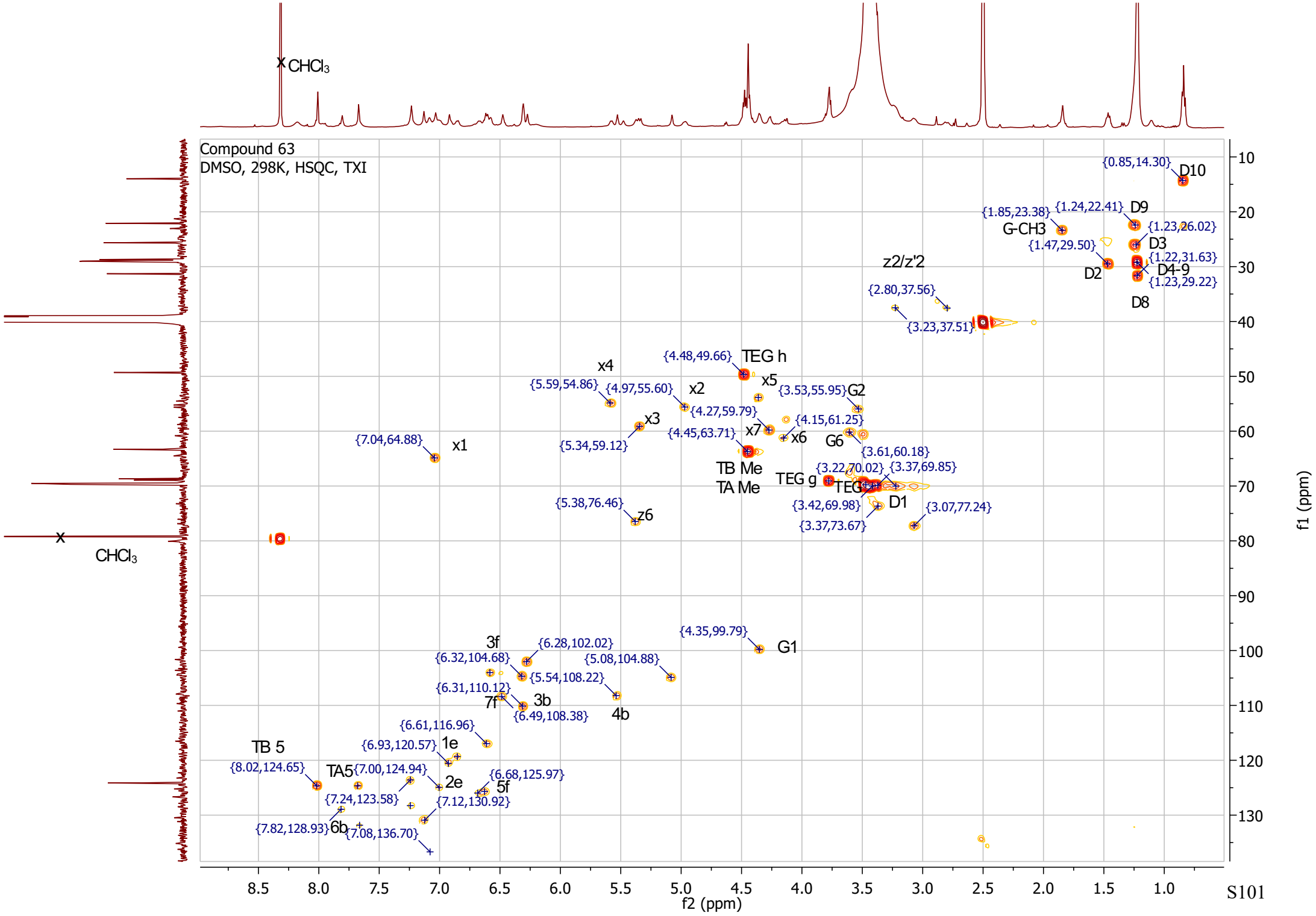

Compound 60
DMSO, 298K, 13C, TXI
144.01 Triazol B 4
143.78 Triazol A 4
39.52 DMSO-d6
30000
25000
20000
15000
10000
5000
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

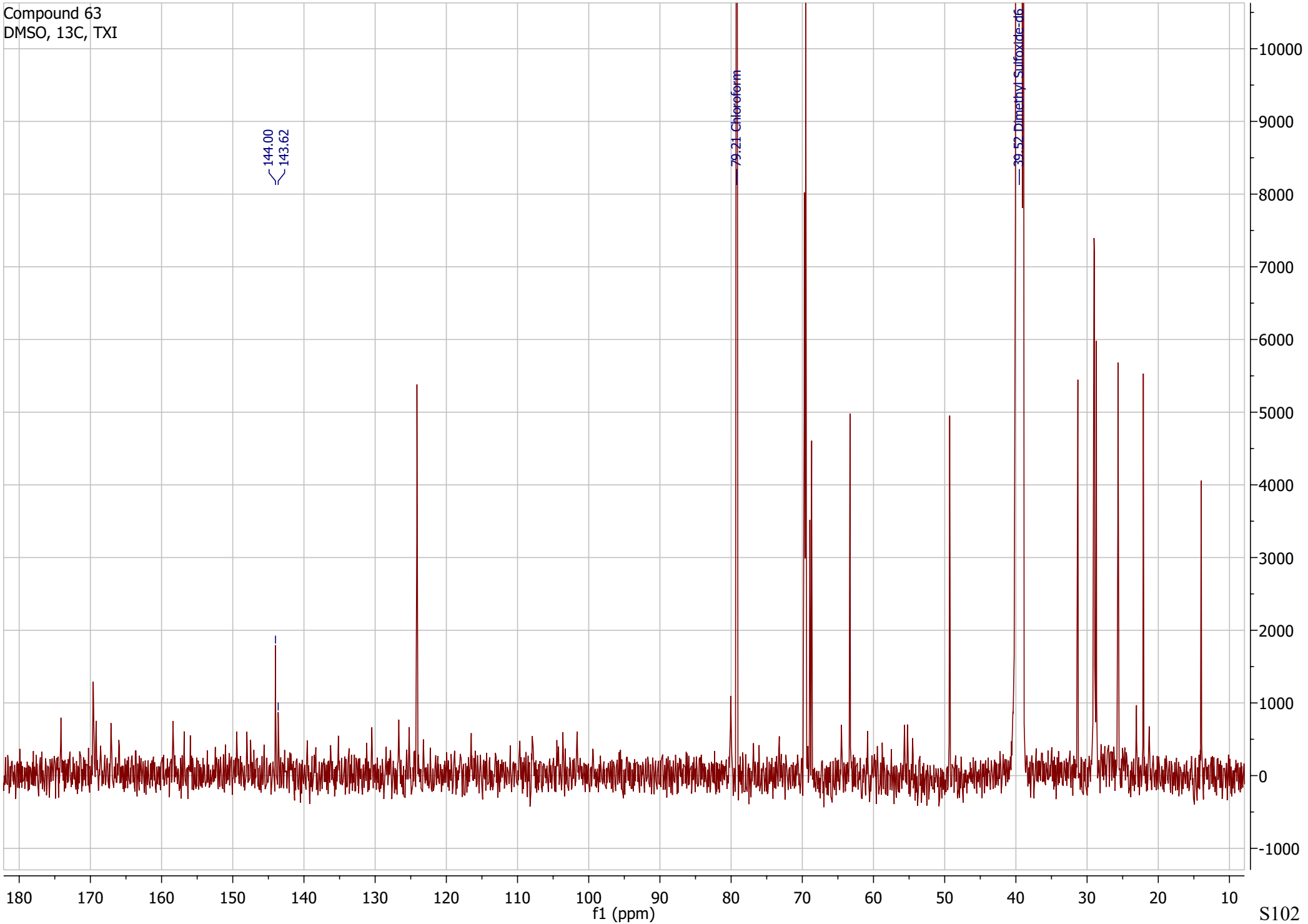

Compound 61
DMSO, 298K, HSQC, TXI
{0.83,13.97}hexyl 6
{1.83,23.11}G-CH3
H5
H3
{1.22,31.16}hexyl 4
grease
H2
{3.28,36.53}z2, z'2
{2.88,36.50}z2, z'2
{4.48,49.37}TEG h
{5.62,54.76}x4
{4.88,55.44}x2
{3.50,55.94}G2
{3.58,60.30}G6
{4.14,61.00}x6
{7.07,64.16}x1
{5.38,58.34}x3
{4.30,59.42}x7
{4.45,63.36}Triazole B methylene
{3.22,69.98}G4
{3.39,69.61}hexyl 1
{5.41,75.87}z6
{3.43,69.69}TEG
{3.09,76.91}G5
{3.38,73.45}G3
{4.38,98.98}G1
{6.28,101.58}7d
{6.35,104.99}3d
{5.08,104.54}4f
{6.32,110.06}3b
{6.48,107.98}7f
{5.53,108.07}4b
{6.61,116.48}5e
{7.01,119.57}1b
{8.01,124.16}triazole B 5
{7.14,124.93}2e
{6.84,125.69}1f
{7.25,123.24}6e
{7.18,131.00}2b
{7.13,136.24}5b
{7.06,136.17}5b
f2 (ppm)
f1 (ppm)

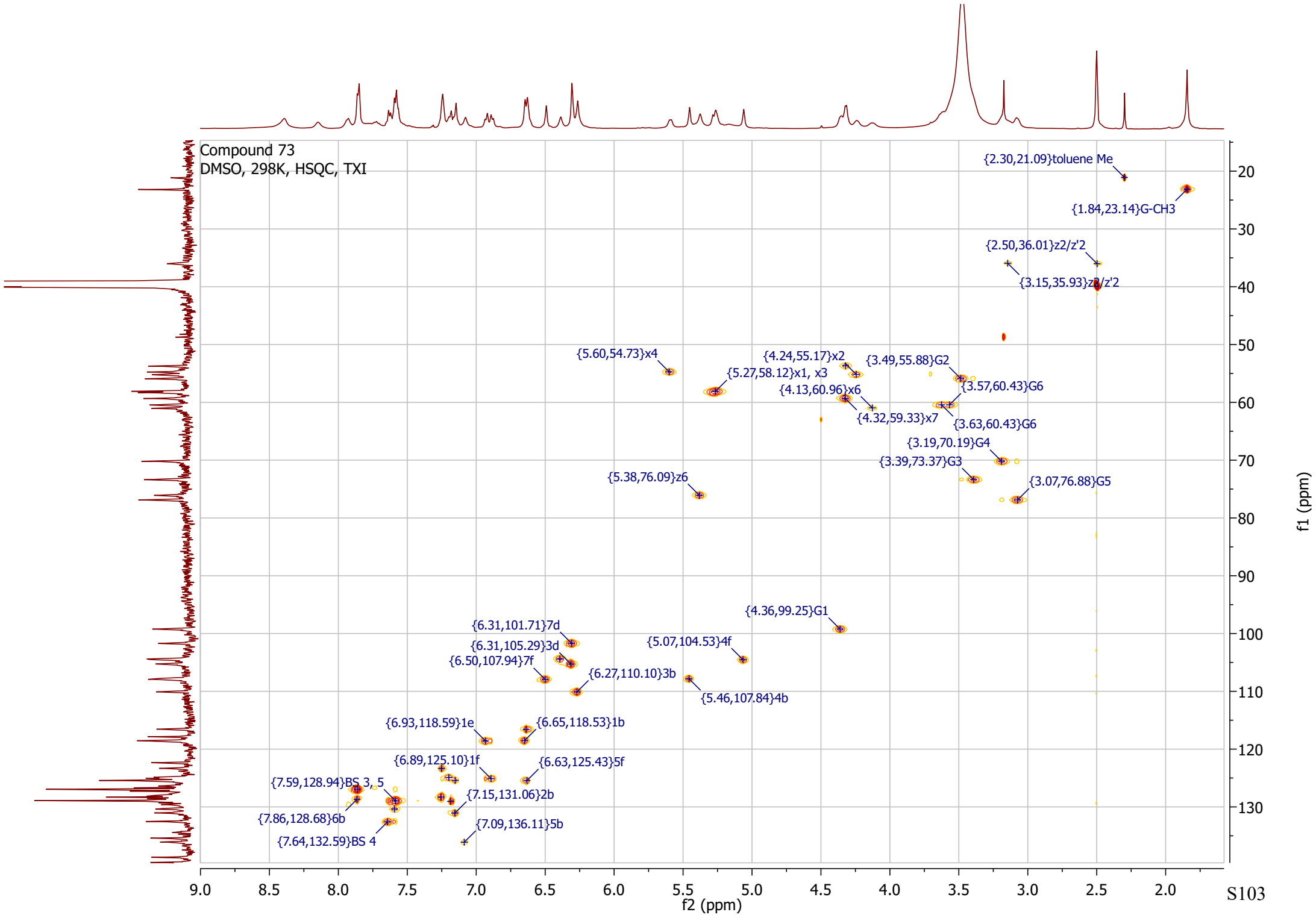

Compound 61
DMSO, 298K, 13C, TXI
144.01 Triazole B 4
143.77 Triazole A 4
39.52 DMSO-d6
f1 (ppm)

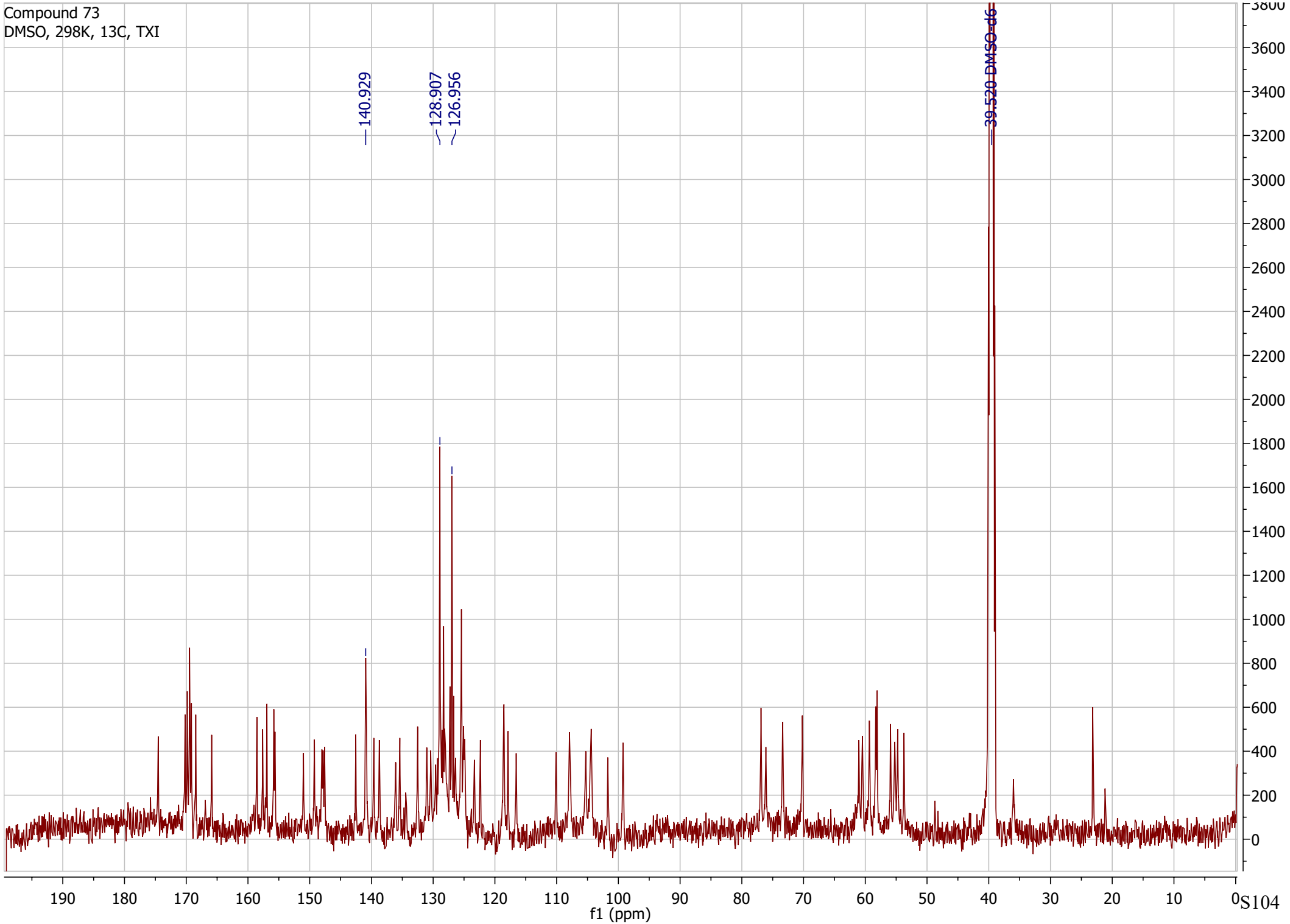

Compound 62
DMSO, 298K, HSQC, TXI
{0.84,13.61}O8
{1.84,23.14}G-CH3
O7
O3
{1.20,31.31}O6
O4-5
{1.46,29.17}O2
{2.79,37.33}z2/z'2
{3.22,37.25}z2/z'2
{4.47,49.35}TEG h
{4.96,55.29}x2
{3.55,55.57}G2
{5.57,54.56}x4
{4.16,60.94}x6
{3.61,59.78}G6
{7.03,64.56}x1
{5.33,58.82}x3
{4.27,59.57}x7
{4.44,63.35}Triazole B methylene
{3.43,69.72}TEG
{3.47,69.58}TEG
{5.36,76.21}z6
{3.39,69.54}Octyl 1
{3.07,76.97}G5
{3.36,73.23}G3
{4.34,99.57}G1
{6.31,104.40}3d
{5.08,104.60}4f
{6.27,101.81}7d
{6.30,109.74}3b
{6.47,108.07}7f
{5.53,108.02}4b
{6.60,116.75}5e
{6.91,120.07}1b
{8.01,124.20}Triazole B 5
{6.63,125.48}5f
{6.66,125.59}1f
{7.23,123.37}6e
{7.00,124.67}2e
{7.80,128.71}6b
{7.67,131.65}2f
f2 (ppm)
f1 (ppm)

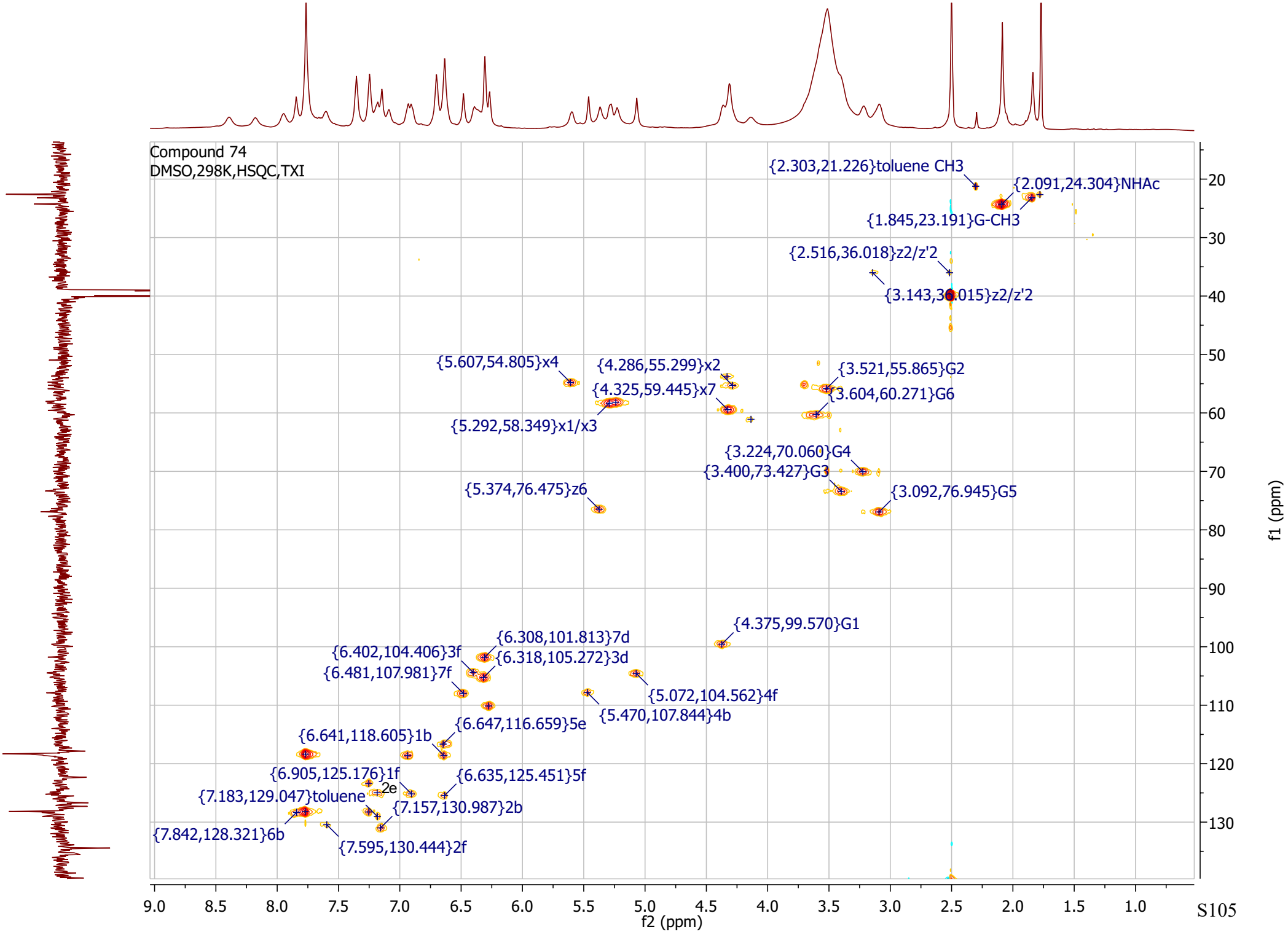

Compound 62
DMSO, 298K, 13C, DUAL
144.015
143.637
39.520 Dimethyl Sulfoxide-d6
8000
6000
4000
2000
0
-2000
-4000
-6000
-8000
-10000
-12000
-14000
-16000
-18000
-20000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

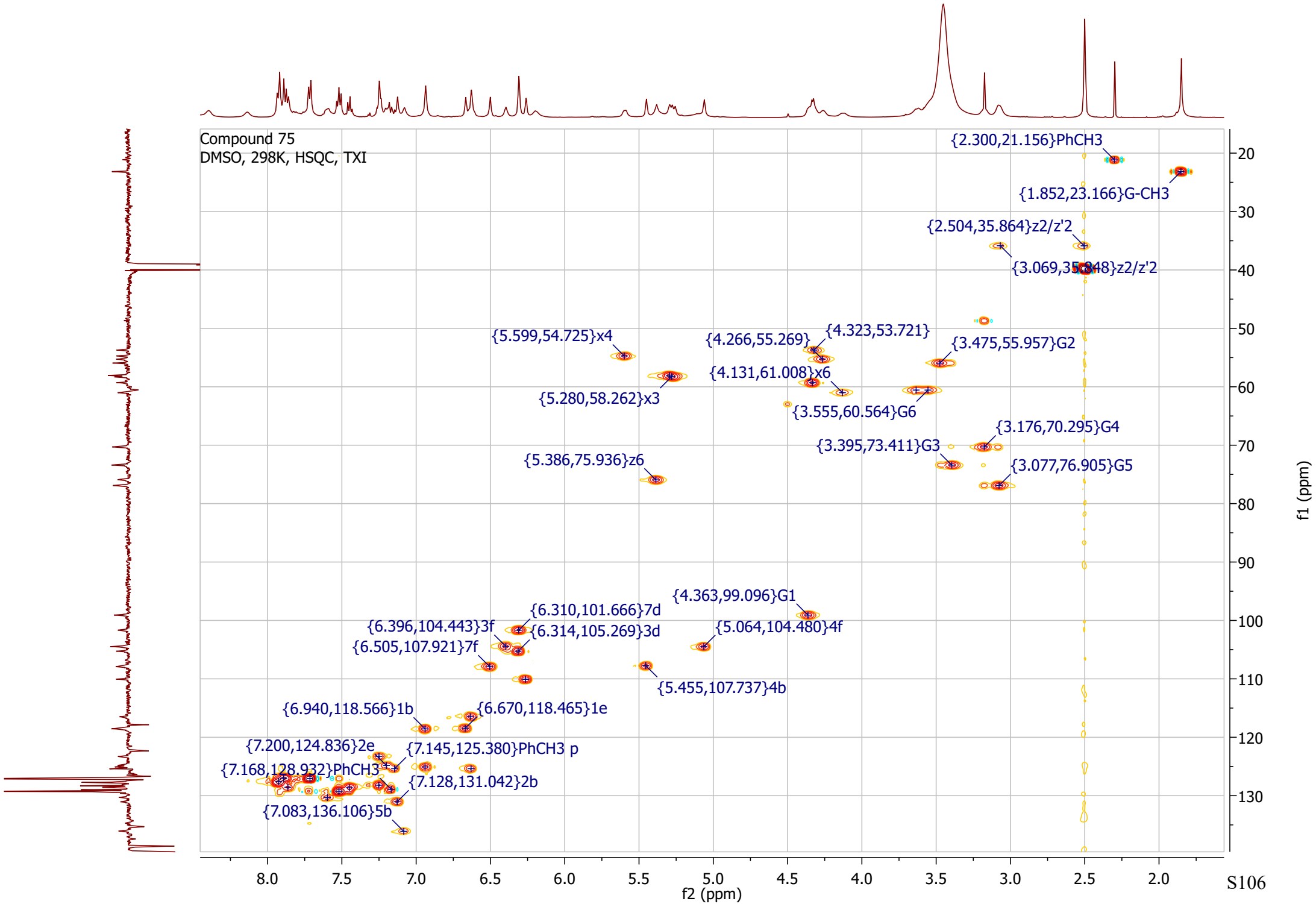

Compound 63
DMSO, 298K, HSQC, TXI
X CHCl3
X
CHCl3
{0.85,14.30} D10
{1.85,23.38} {1.24,22.41} D9
G-CH3
{1.23,26.02}
{1.47,29.50} D3
{1.22,31.63}
D2 D4-9
{1.23,29.22}
D8
z2/z'2
{2.80,37.56}
{3.23,37.51}
{4.48,49.66} TEG h
x4
x5
{5.59,54.86} {4.97,55.60} x2
{3.53,55.95} G2
{4.27,59.79}
x3
{4.15,61.25}
{4.45,63.71} x7 x6
G6
{7.04,64.88} x1
{5.34,59.12}
{3.61,60.18}
TB Me
TA Me
{3.22,70.02} {3.37,69.85}
TEG g
TEG
{5.38,76.46} z6
{3.42,69.98} D1
{3.07,77.24}
{3.37,73.67}
{4.35,99.79} G1
3f
{6.28,102.02}
{6.32,104.68}
{5.08,104.88}
{5.54,108.22}
{6.31,110.12}
7f 3b
{6.49,108.38}
4b
{6.61,116.96}
TB 5
{6.93,120.57} 1e
{8.02,124.65}
TA5 {7.00,124.94}
2e
{6.68,125.97}
5f
{7.24,123.58}
{7.12,130.92}
{7.82,128.93} 6b
{7.08,136.70}
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f2 (ppm)
10 20 30 40 50 60 70 80 90 100 110 120 130
f1 (ppm)
S101

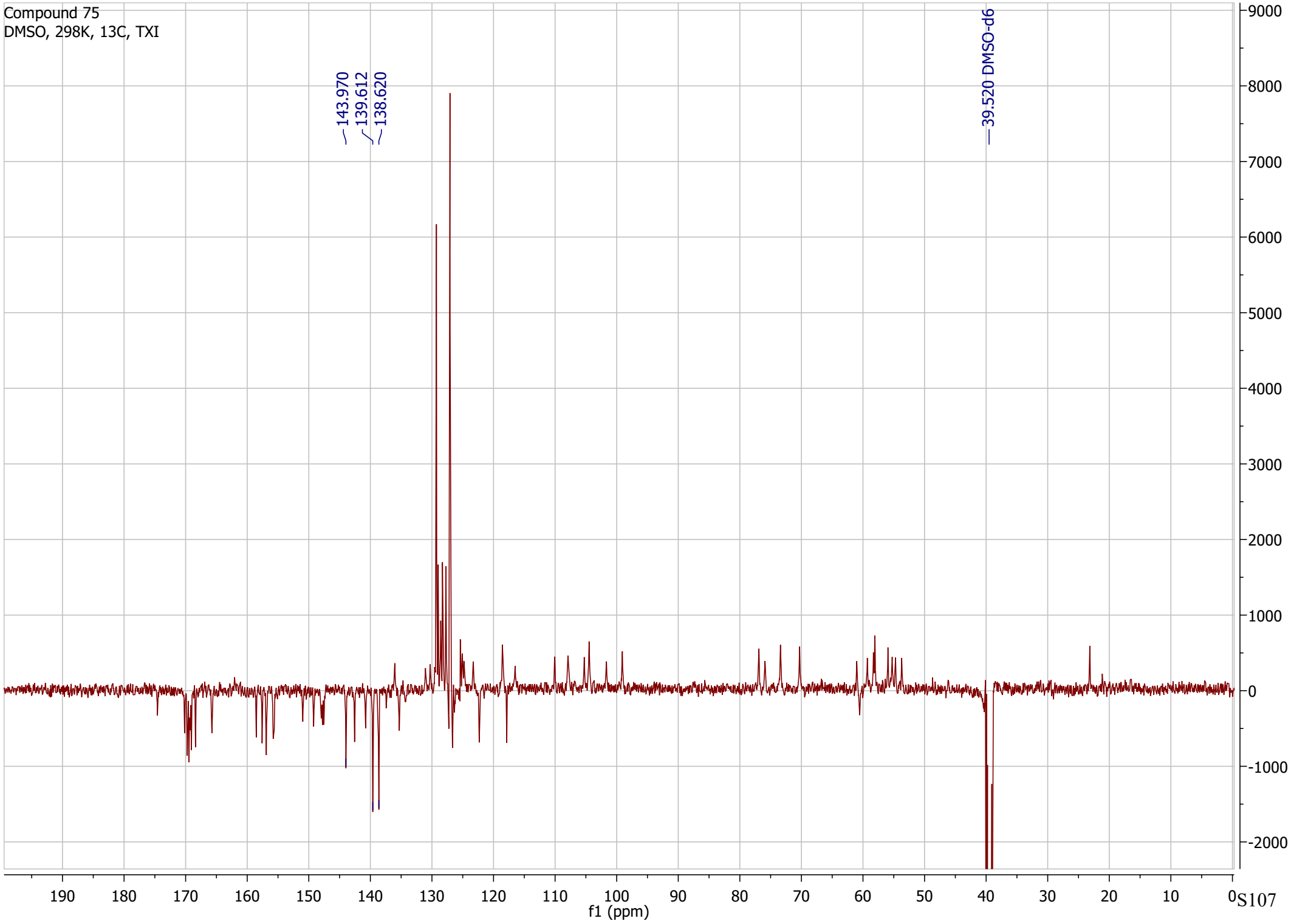

Compound 63
DMSO, 13C, TXI
144.00
143.62
79.21 Chloroform
39.52 Dimethyl Sulfoxide-d6
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


Compound 73
DMSO, 298K, HSQC, TXI
{2.30,21.09}toluene Me
{1.84,23.14}G-CH3
{2.50,36.01}z2/z'2
{3.15,35.93}z2/z'2
{5.60,54.73}x4
{4.24,55.17}x2
{3.49,55.88}G2
{5.27,58.12}x1, x3
{3.57,60.43}G6
{4.13,60.96}x6
{4.32,59.33}x7
{3.63,60.43}G6
{3.19,70.19}G4
{3.39,73.37}G3
{5.38,76.09}z6
{3.07,76.88}G5
{4.36,99.25}G1
{6.31,101.71}7d
{6.31,105.29}3d
{6.50,107.94}7f
{5.07,104.53}4f
{6.27,110.10}3b
{5.46,107.84}4b
{6.93,118.59}1e
{6.65,118.53}1b
{6.89,125.10}1f
{6.63,125.43}5f
{7.59,128.94}BS 3, 5
{7.15,131.06}2b
{7.86,128.68}6b
{7.09,136.11}5b
{7.64,132.59}BS 4
f2 (ppm)
f1 (ppm)
S103

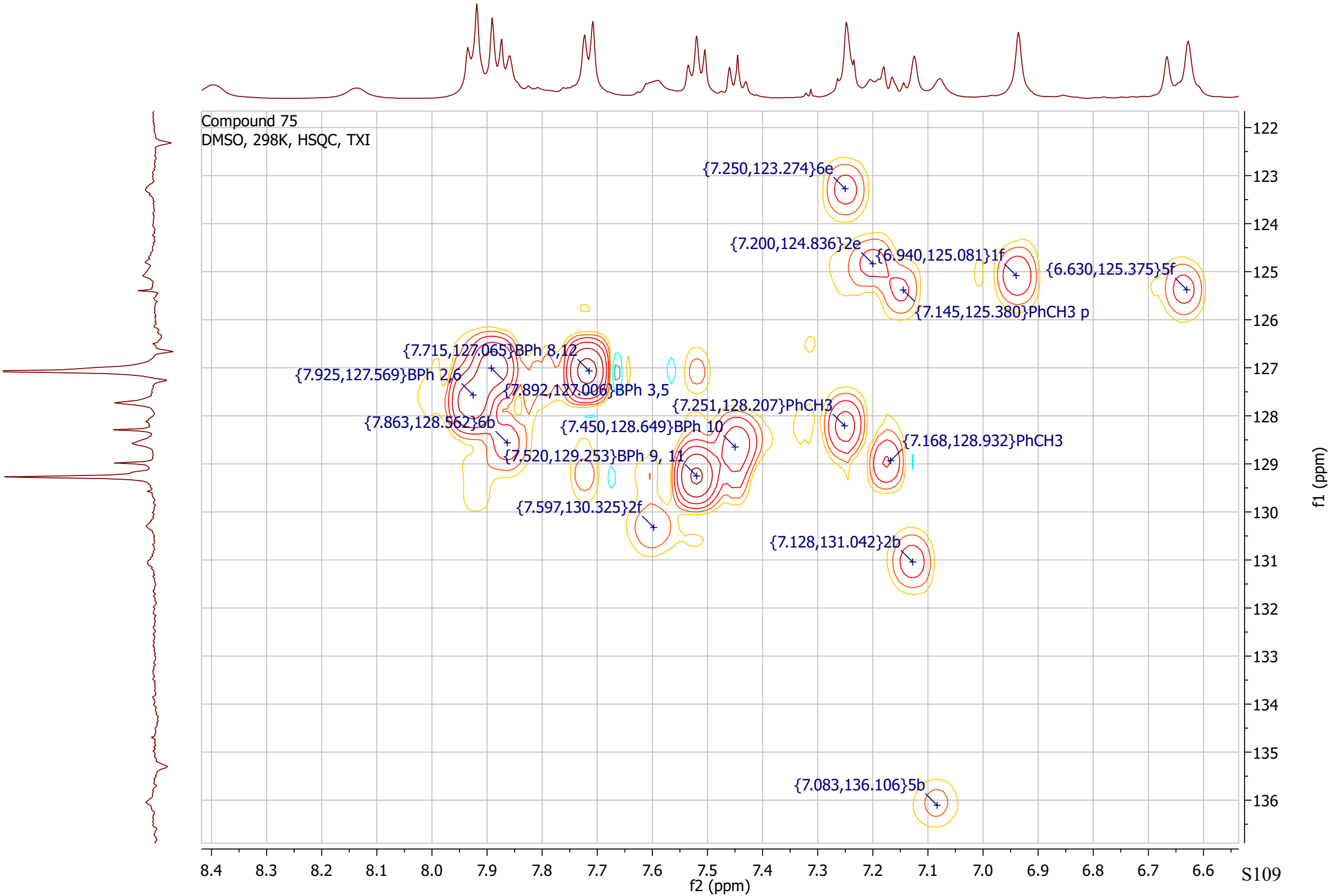

Compound 73
DMSO, 298K, 13C, TXI
140.929
128.907
126.956
39.520 DMSO-d6
f1 (ppm)

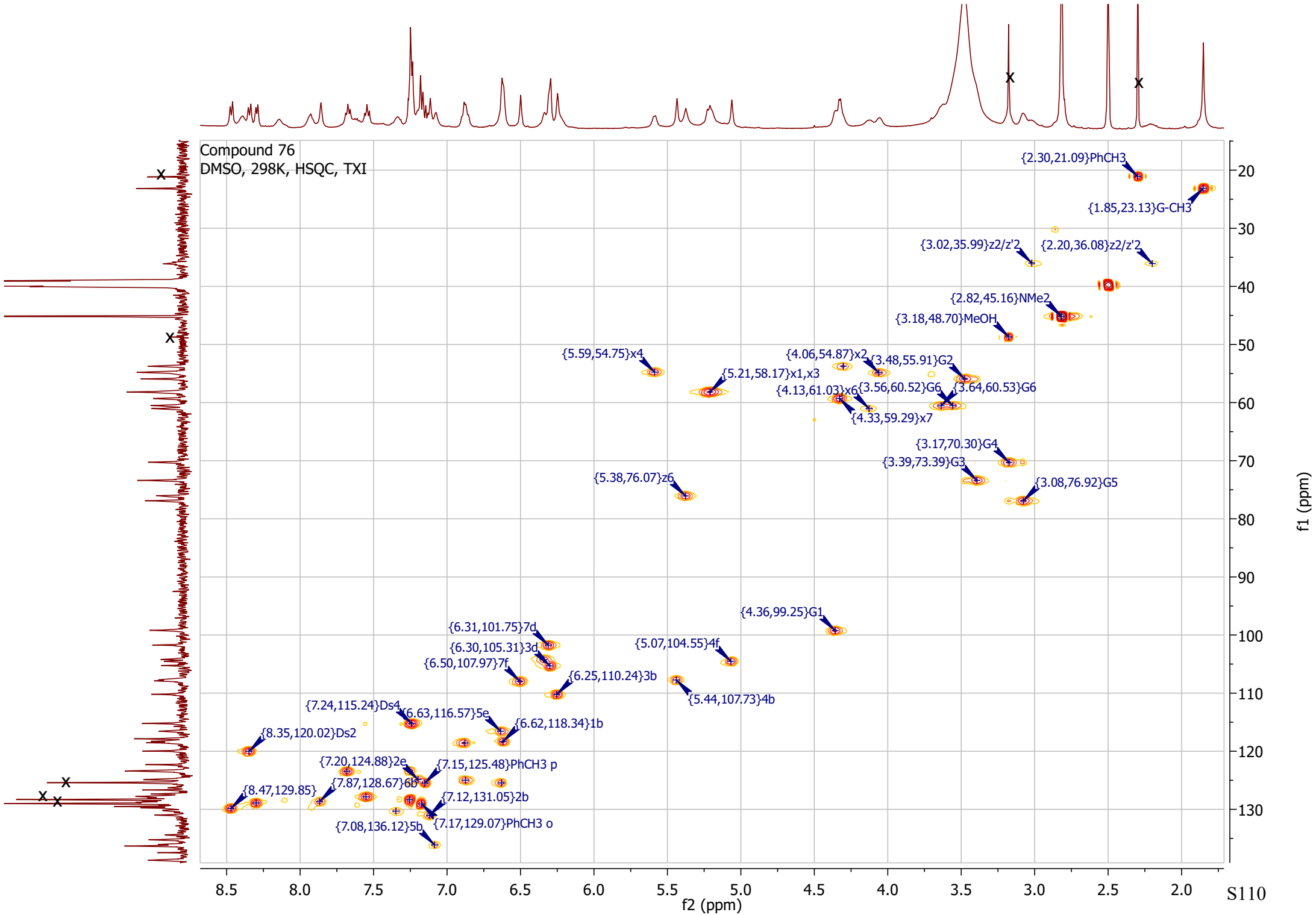

Compound 74
DMSO,298K,HSQC,TXI
{2.303,21.226}toluene CH3
{2.091,24.304}NHAc
{1.845,23.191}G-CH3
{2.516,36.018}z2/z'2
{3.143,36.015}z2/z'2
{5.607,54.805}x4
{4.286,55.299}x2
{3.521,55.865}G2
{4.325,59.445}x7
{3.604,60.271}G6
{5.292,58.349}x1/x3
{3.224,70.060}G4
{3.400,73.427}G3
{5.374,76.475}z6
{3.092,76.945}G5
{4.375,99.570}G1
{6.308,101.813}7d
{6.402,104.406}3f
{6.318,105.272}3d
{6.481,107.981}7f
{5.072,104.562}4f
{5.470,107.844}4b
{6.647,116.659}5e
{6.641,118.605}1b
{6.905,125.176}1f
{6.635,125.451}5f
2e
{7.183,129.047}toluene
{7.157,130.987}2b
{7.842,128.321}6b
{7.595,130.444}2f
f2 (ppm)
f1 (ppm)
S105

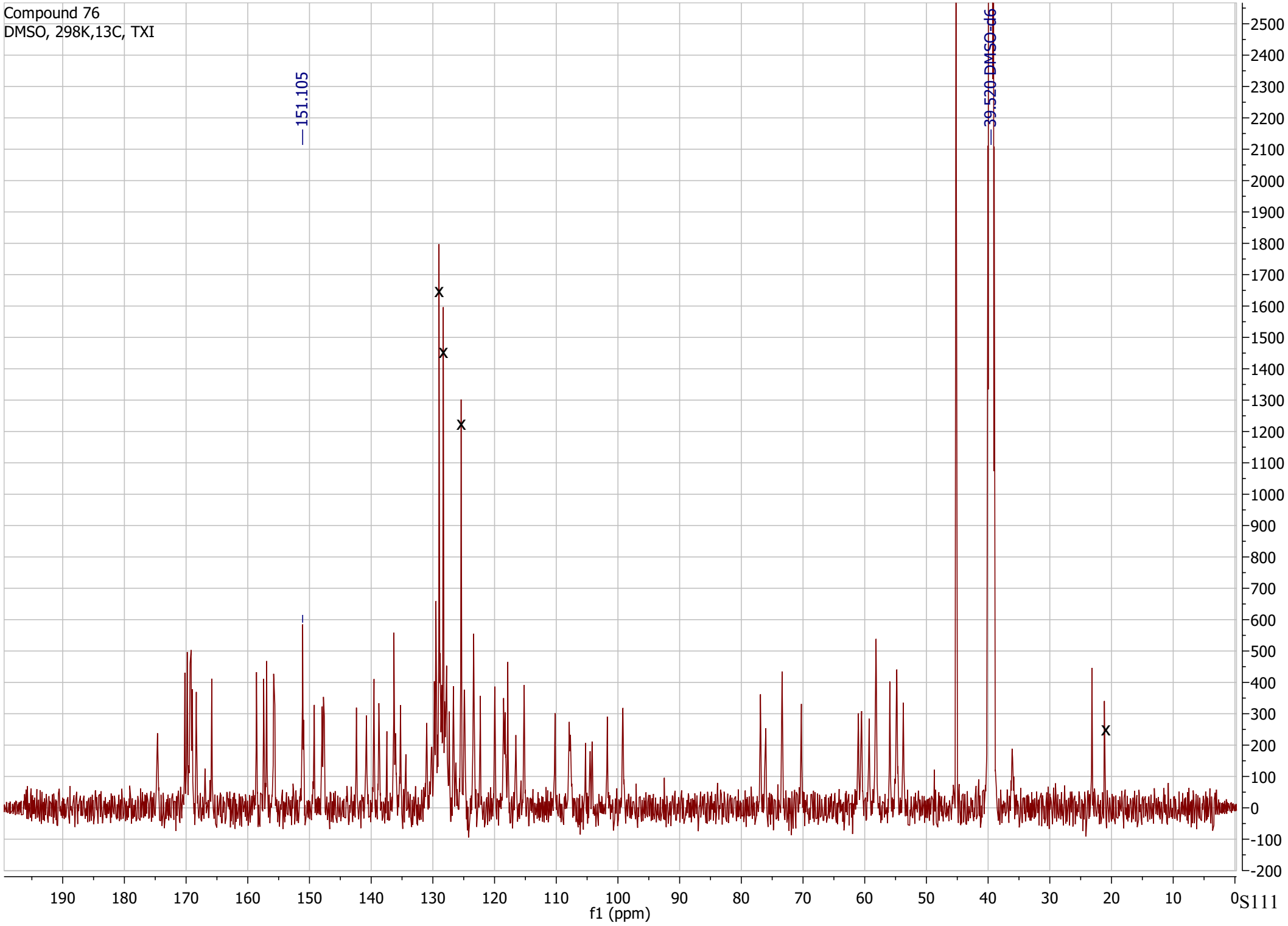

Compound 75
DMSO, 298K, HSQC, TXI
{2.300,21.156}PhCH3
{1.852,23.166}G-CH3
{2.504,35.864}z2/z'2
{3.069,35.848}z2/z'2
{5.599,54.725}x4
{4.266,55.269}
{4.323,53.721}
{3.475,55.957}G2
{4.131,61.008}x6
{5.280,58.262}x3
{3.555,60.564}G6
{3.176,70.295}G4
{3.395,73.411}G3
{5.386,75.936}z6
{3.077,76.905}G5
{4.363,99.096}G1
{6.310,101.666}7d
{6.396,104.443}3f
{6.314,105.269}3d
{5.064,104.480}4f
{6.505,107.921}7f
{5.455,107.737}4b
{6.940,118.566}1b
{6.670,118.465}1e
{7.200,124.836}2e
{7.145,125.380}PhCH3 p
{7.168,128.932}PhCH3
{7.128,131.042}2b
{7.083,136.106}5b
f2 (ppm)
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
20
30
40
50
60
70
80
90
100
110
120
130

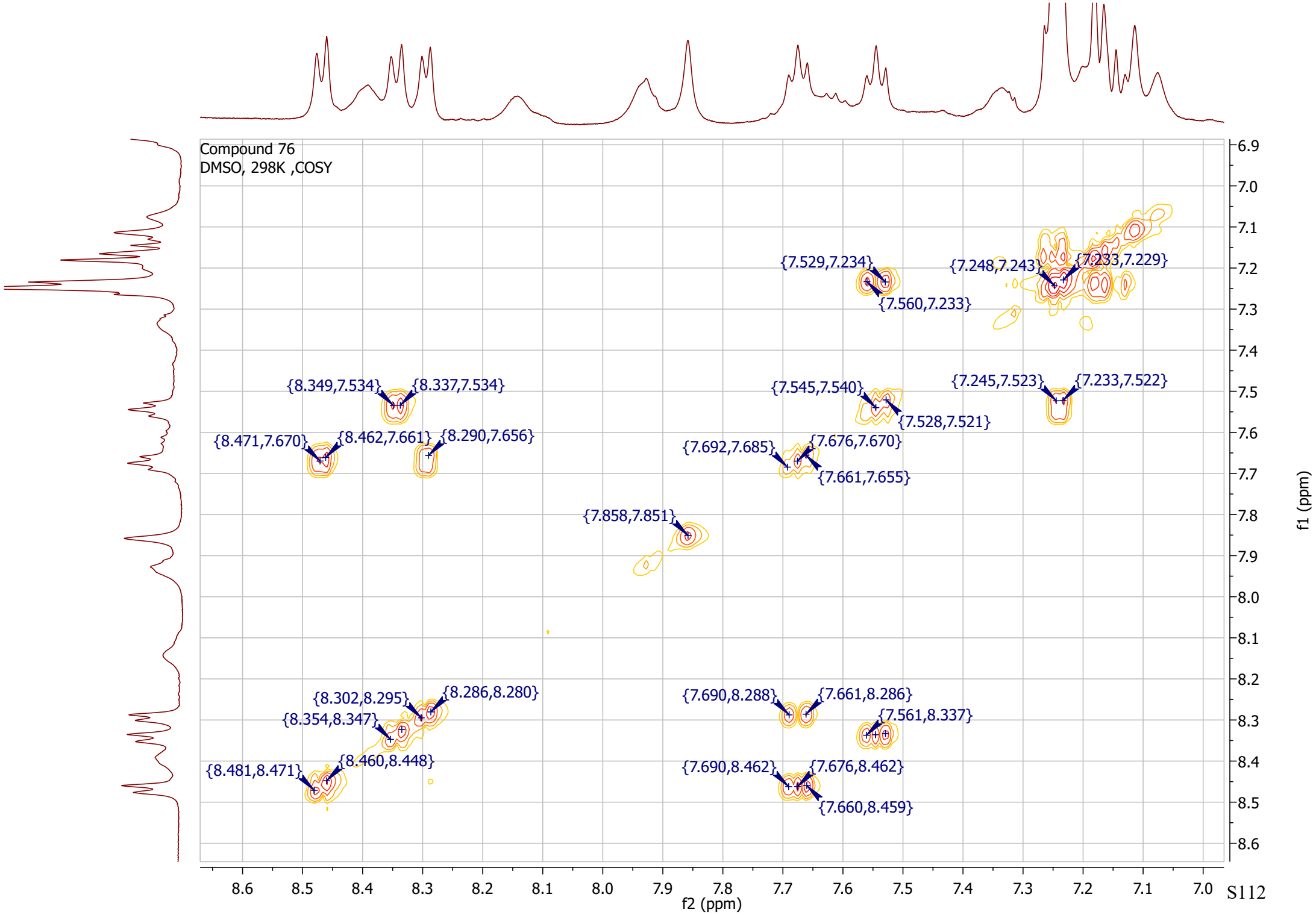

Compound 75
DMSO, 298K, 13C, TXI
143.970
139.612
138.620
39.520 DMSO-d6
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

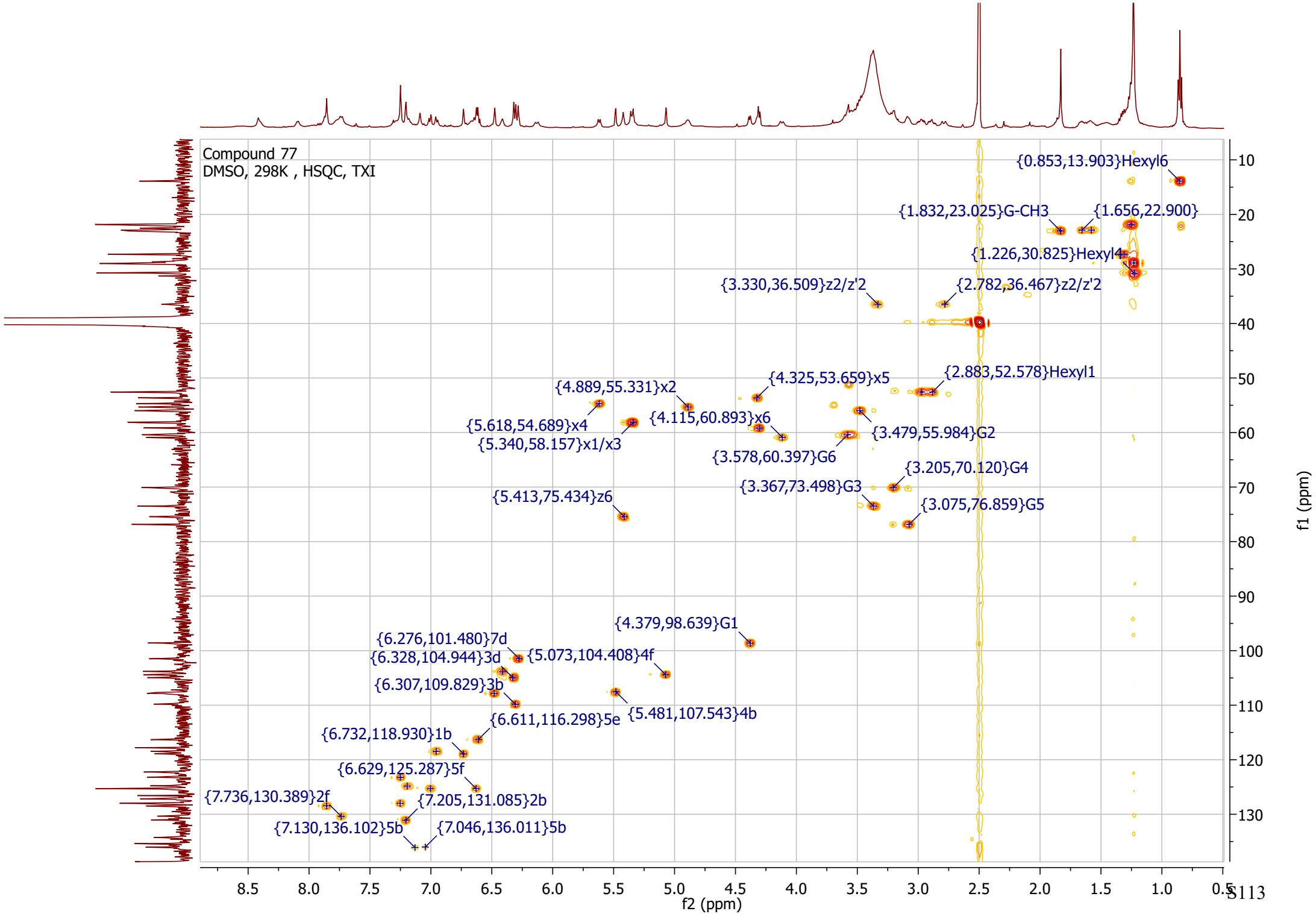

Compound 75
DMSO, 298K, HMBC, TXI
{7.874,138.695}BPh 3,5 - BPh 7
{7.881,139.641}BPh 3,5 - BPh 1
{7.895,138.604}BPh 3,5 - BPh 7
{7.520,138.614}BPh 9,11-BPh 7
{7.712,144.014}BPh 8,12 - BPh 4
{7.926,144.009}BPh 2,6 - BPh 4
f2 (ppm)
f1 (ppm)

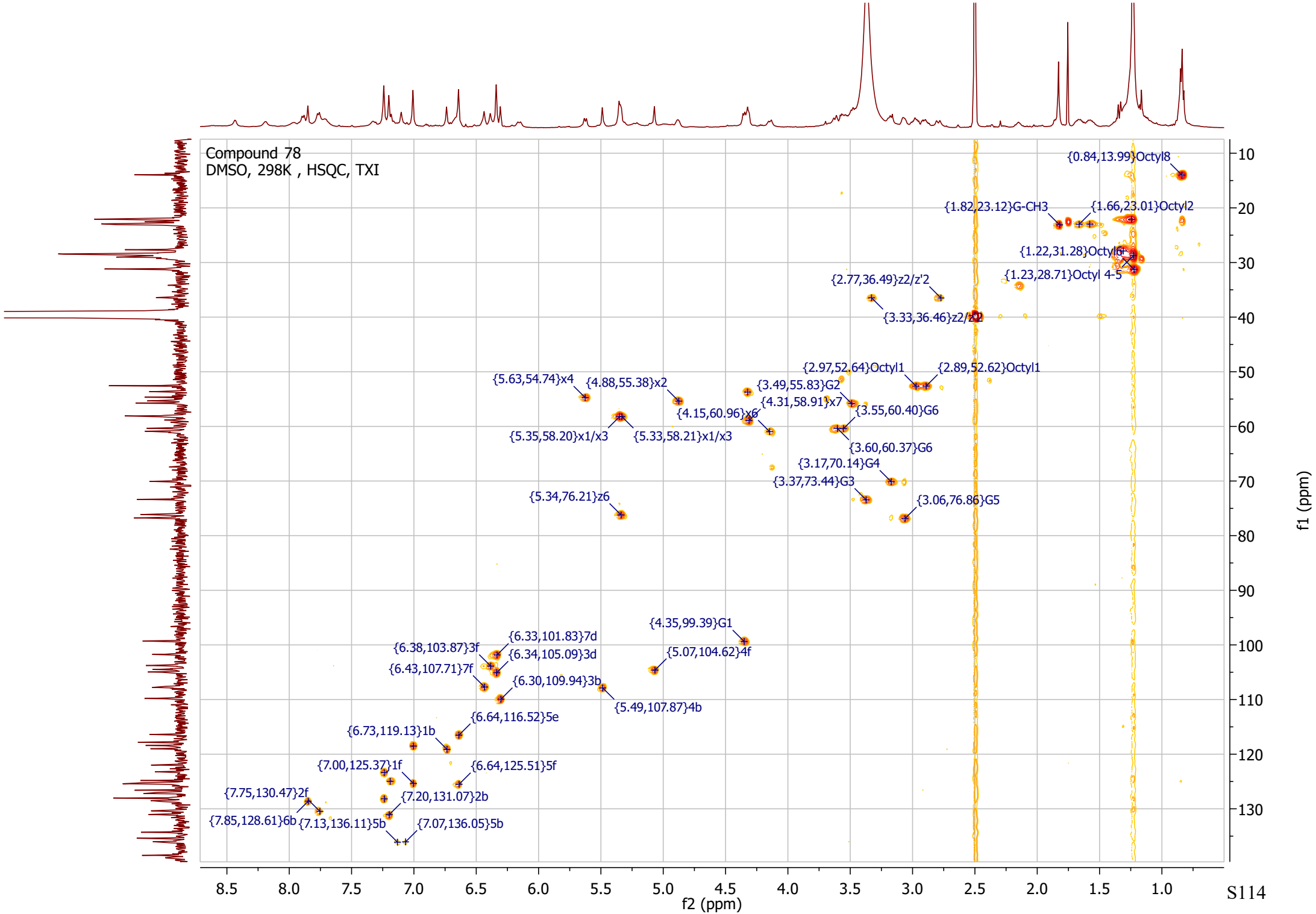

Compound 75
DMSO, 298K, HSQC, TXI
{7.250,123.274}6e
{7.200,124.836}2e
{6.940,125.081}1f
{6.630,125.375}5f
{7.145,125.380}PhCH3 p
{7.715,127.065}BPh 8,12
{7.925,127.569}BPh 2,6
{7.892,127.006}BPh 3,5
{7.863,128.562}6b
{7.251,128.207}PhCH3
{7.450,128.649}BPh 10
{7.168,128.932}PhCH3
{7.520,129.253}BPh 9, 11
{7.597,130.325}2f
{7.128,131.042}2b
{7.083,136.106}5b
f2 (ppm)
f1 (ppm)
S109

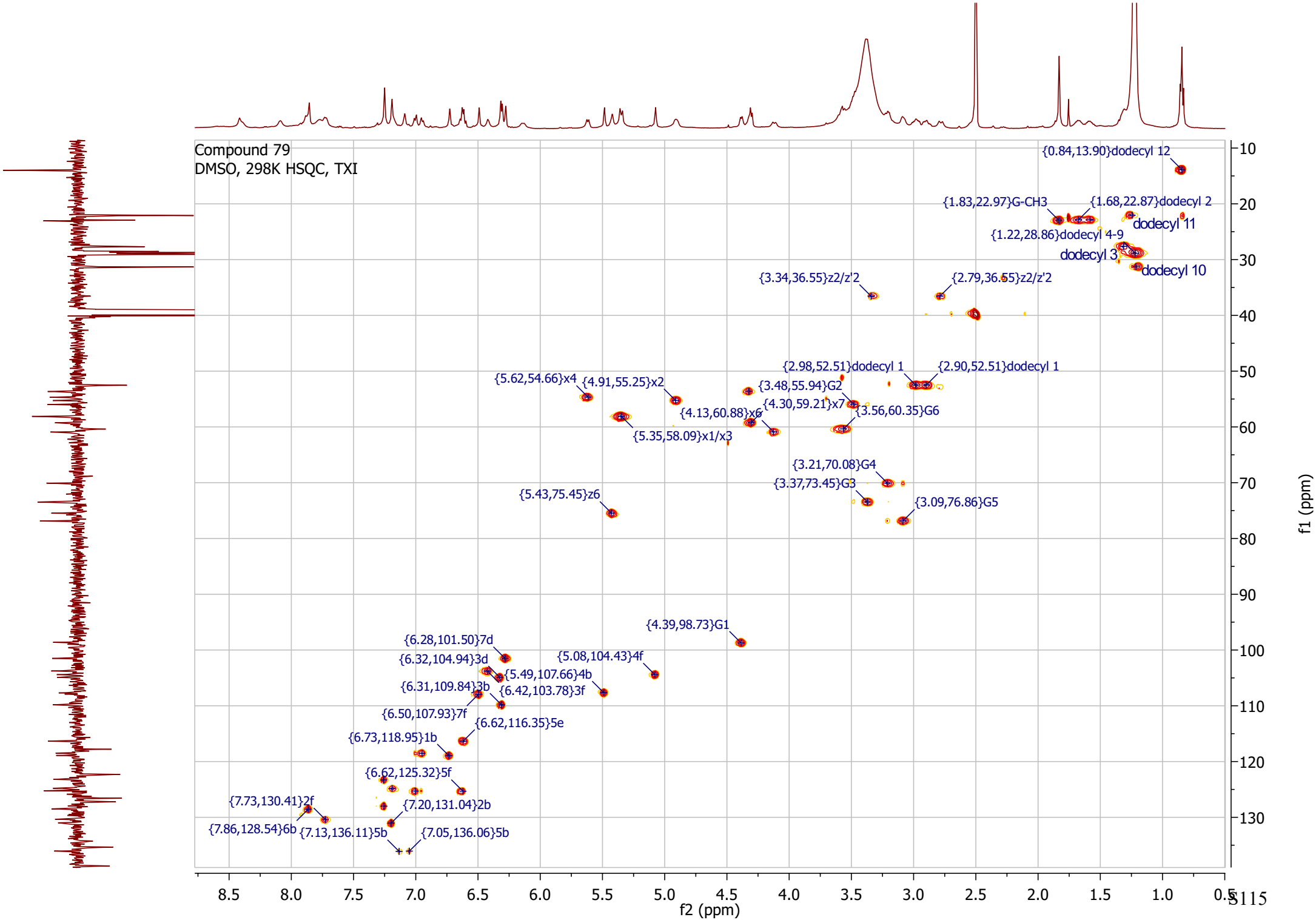

Compound 76
DMSO, 298K, HSQC, TXI
{2.30,21.09}PhCH3
{1.85,23.13}G-CH3
{3.02,35.99}z2/z'2
{2.20,36.08}z2/z'2
{2.82,45.16}NMe2
{3.18,48.70}MeOH
{5.59,54.75}x4
{5.21,58.17}x1,x3
{4.06,54.87}x2
{3.48,55.91}G2
{4.13,61.03}x6
{3.56,60.52}G6
{3.64,60.53}G6
{4.33,59.29}x7
{3.17,70.30}G4
{3.39,73.39}G3
{5.38,76.07}z6
{3.08,76.92}G5
{4.36,99.25}G1
{6.31,101.75}7d
{6.30,105.31}3d
{6.50,107.97}7f
{5.07,104.55}4f
{6.25,110.24}3b
{5.44,107.73}4b
{7.24,115.24}Ds4
{6.63,116.57}5e
{6.62,118.34}1b
{8.35,120.02}Ds2
{7.20,124.88}2e
{7.15,125.48}PhCH3 p
{8.47,129.85}
{7.87,128.67}6b
{7.12,131.05}2b
{7.08,136.12}5b
{7.17,129.07}PhCH3 o
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f2 (ppm)
20
30
40
50
60
70
80
90
100
110
120
130
f1 (ppm)
S110


Compound 76
DMSO, 298K,13C, TXI
151.105
39.520 DMSO-d6
f1 (ppm)


Compound 76
DMSO, 298K ,COSY
{7.529,7.234}
{7.560,7.233}
{7.248,7.243}
{7.233,7.229}
{8.349,7.534}
{8.337,7.534}
{8.471,7.670}
{8.462,7.661}
{8.290,7.656}
{7.545,7.540}
{7.528,7.521}
{7.245,7.523}
{7.233,7.522}
{7.692,7.685}
{7.676,7.670}
{7.661,7.655}
{7.858,7.851}
{8.302,8.295}
{8.286,8.280}
{8.354,8.347}
{8.481,8.471}
{8.460,8.448}
{7.690,8.288}
{7.661,8.286}
{7.561,8.337}
{7.690,8.462}
{7.676,8.462}
{7.660,8.459}
f2 (ppm)
f1 (ppm)
S112


Compound 77
DMSO, 298K , HSQC, TXI
{0.853,13.903}Hexyl6
{1.832,23.025}G-CH3
{1.656,22.900}
{1.226,30.825}Hexyl4
{3.330,36.509}z2/z'2
{2.782,36.467}z2/z'2
{4.325,53.659}x5
{2.883,52.578}Hexyl1
{4.889,55.331}x2
{4.115,60.893}x6
{5.618,54.689}x4
{5.340,58.157}x1/x3
{3.479,55.984}G2
{3.578,60.397}G6
{3.205,70.120}G4
{3.367,73.498}G3
{5.413,75.434}z6
{3.075,76.859}G5
{4.379,98.639}G1
{6.276,101.480}7d
{6.328,104.944}3d
{5.073,104.408}4f
{6.307,109.829}3b
{5.481,107.543}4b
{6.611,116.298}5e
{6.732,118.930}1b
{6.629,125.287}5f
{7.736,130.389}2f
{7.205,131.085}2b
{7.130,136.102}5b
{7.046,136.011}5b
f2 (ppm)
f1 (ppm)


Compound 78
DMSO, 298K , HSQC, TXI
{0.84,13.99}Octyl8
{1.82,23.12}G-CH3
{1.66,23.01}Octyl2
{1.22,31.28}Octyl6
{1.23,28.71}Octyl 4-5
{2.77,36.49}z2/z'2
{3.33,36.46}z2/z'2
{2.97,52.64}Octyl1
{2.89,52.62}Octyl1
{5.63,54.74}x4
{4.88,55.38}x2
{3.49,55.83}G2
{4.31,58.91}x7
{3.55,60.40}G6
{4.15,60.96}x6
{5.35,58.20}x1/x3
{5.33,58.21}x1/x3
{3.60,60.37}G6
{3.17,70.14}G4
{3.37,73.44}G3
{5.34,76.21}z6
{3.06,76.86}G5
{4.35,99.39}G1
{6.33,101.83}7d
{6.38,103.87}3f
{6.34,105.09}3d
{5.07,104.62}4f
{6.43,107.71}7f
{6.30,109.94}3b
{5.49,107.87}4b
{6.64,116.52}5e
{6.73,119.13}1b
{7.00,125.37}1f
{6.64,125.51}5f
{7.75,130.47}2f
{7.20,131.07}2b
{7.85,128.61}6b
{7.13,136.11}5b
{7.07,136.05}5b
f2 (ppm)
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
10
20
30
40
50
60
70
80
90
100
110
120
130


Compound 79
DMSO, 298K HSQC, TXI
{0.84,13.90}dodecyl 12
{1.83,22.97}G-CH3
{1.68,22.87}dodecyl 2
dodecyl 11
{1.22,28.86}dodecyl 4-9
dodecyl 3
dodecyl 10
{3.34,36.55}z2/z'2
{2.79,36.55}z2/z'2
{2.98,52.51}dodecyl 1
{2.90,52.51}dodecyl 1
{5.62,54.66}x4
{4.91,55.25}x2
{3.48,55.94}G2
{4.30,59.21}x7
{3.56,60.35}G6
{4.13,60.88}x6
{5.35,58.09}x1/x3
{3.21,70.08}G4
{3.37,73.45}G3
{5.43,75.45}z6
{3.09,76.86}G5
{4.39,98.73}G1
{6.28,101.50}7d
{6.32,104.94}3d
{5.08,104.43}4f
{5.49,107.66}4b
{6.31,109.84}3b
{6.42,103.78}3f
{6.50,107.93}7f
{6.62,116.35}5e
{6.73,118.95}1b
{6.62,125.32}5f
{7.73,130.41}2f
{7.20,131.04}2b
{7.86,128.54}6b
{7.13,136.11}5b
{7.05,136.06}5b
f2 (ppm)
f1 (ppm)