Supplementary materials

«Novel derivatives propanesulfonic acids based on pyrimidine bases: synthesis, reactivity, structure»

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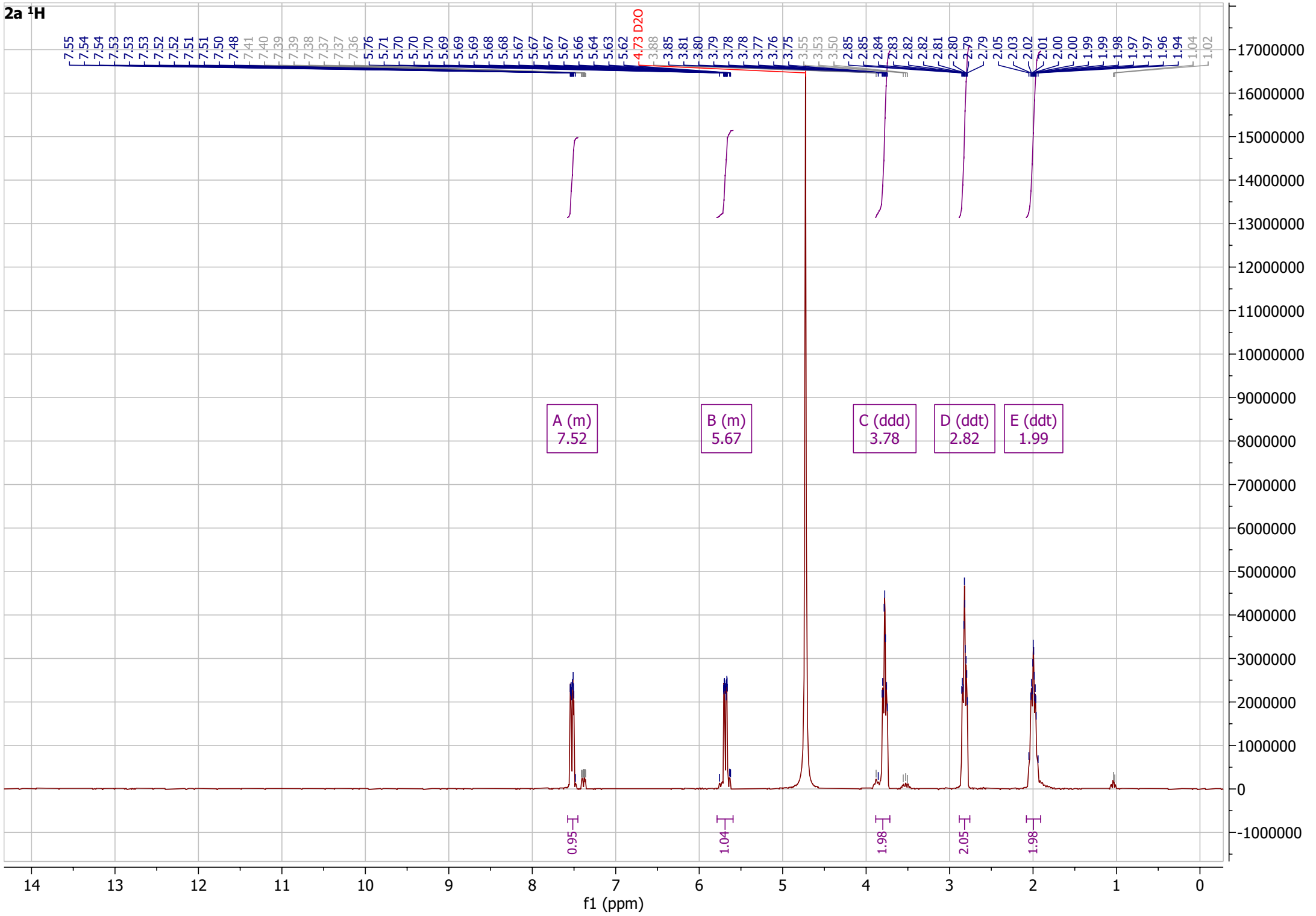
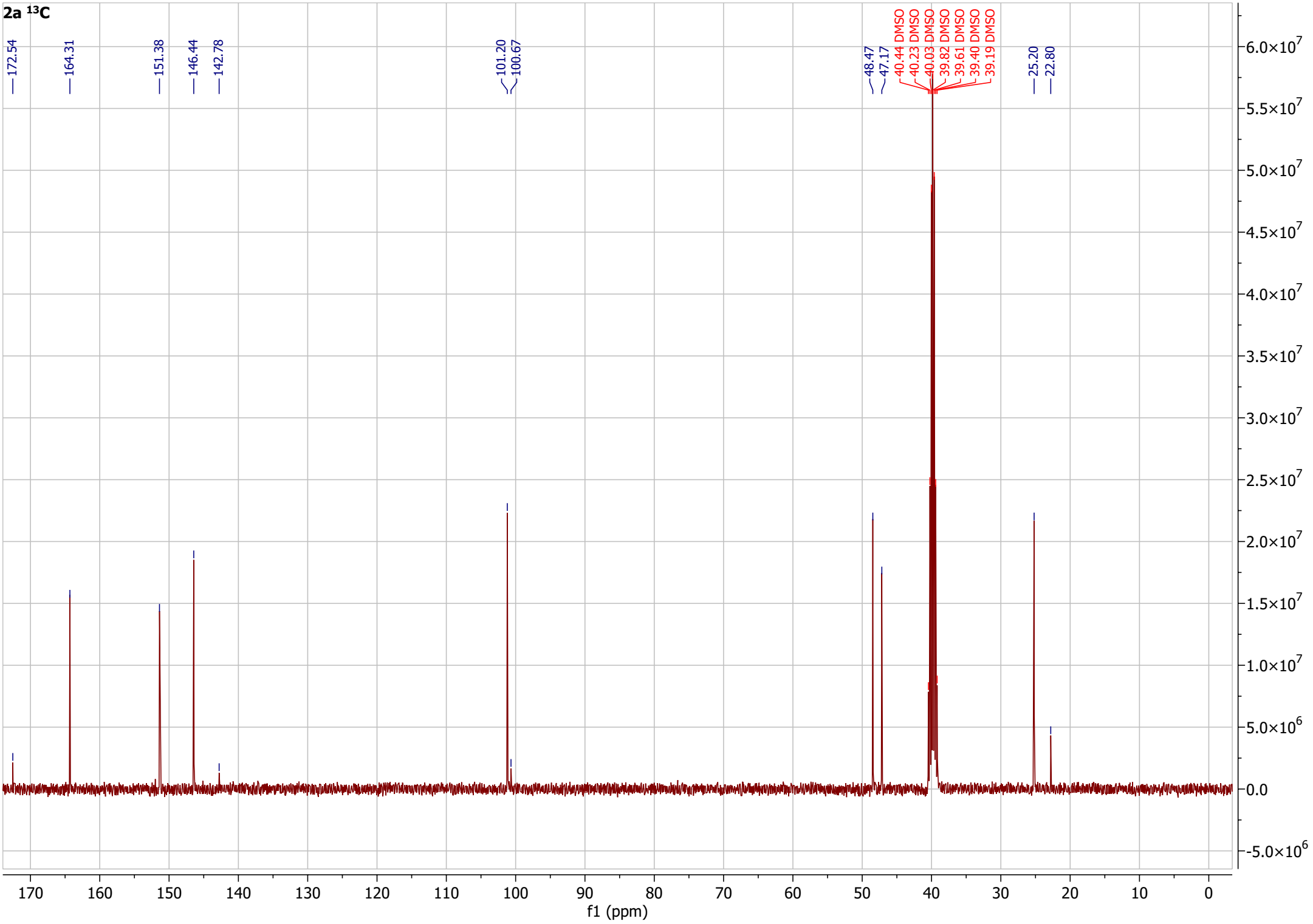
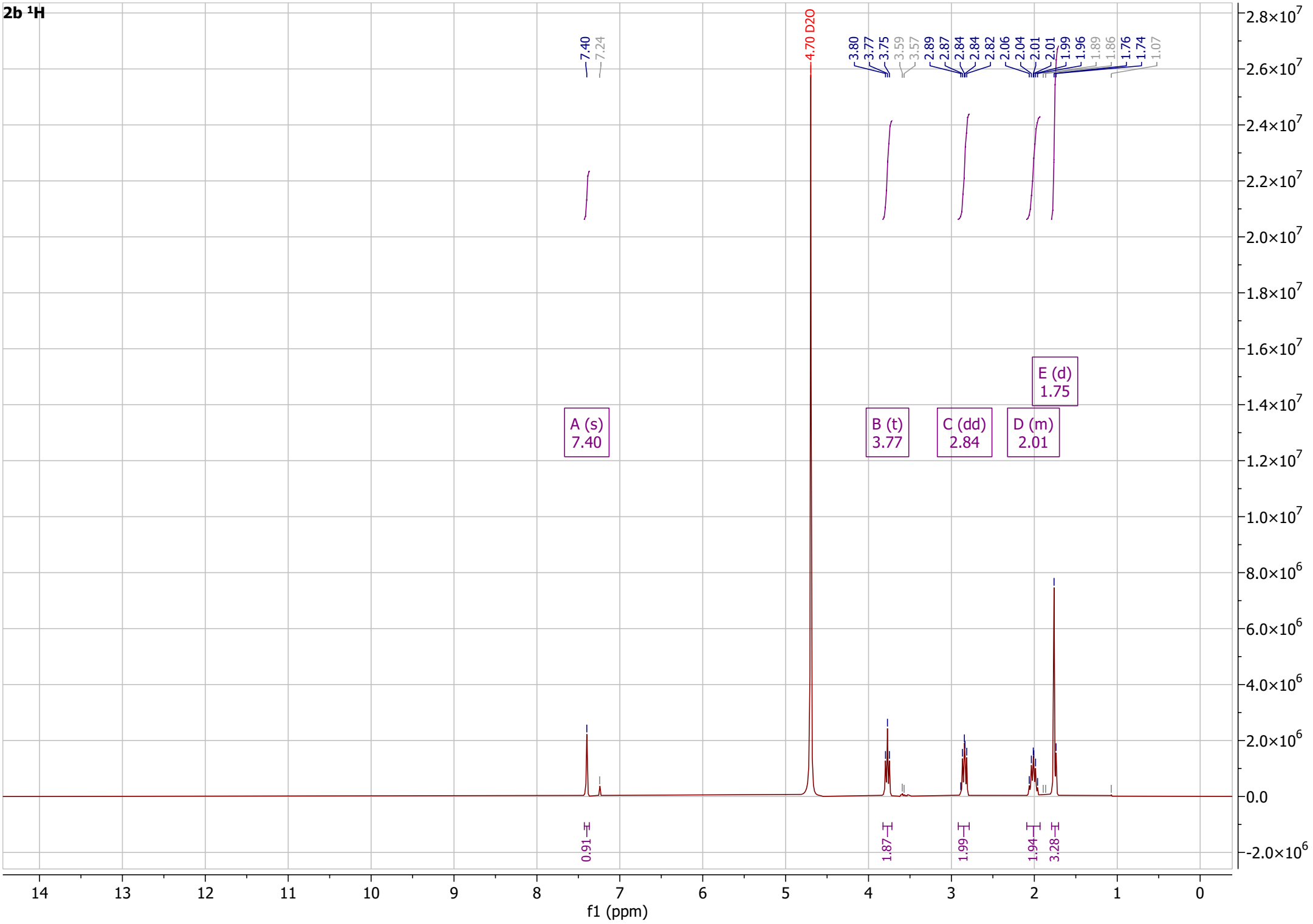
Email: negrebetsky1@rsmu.ru

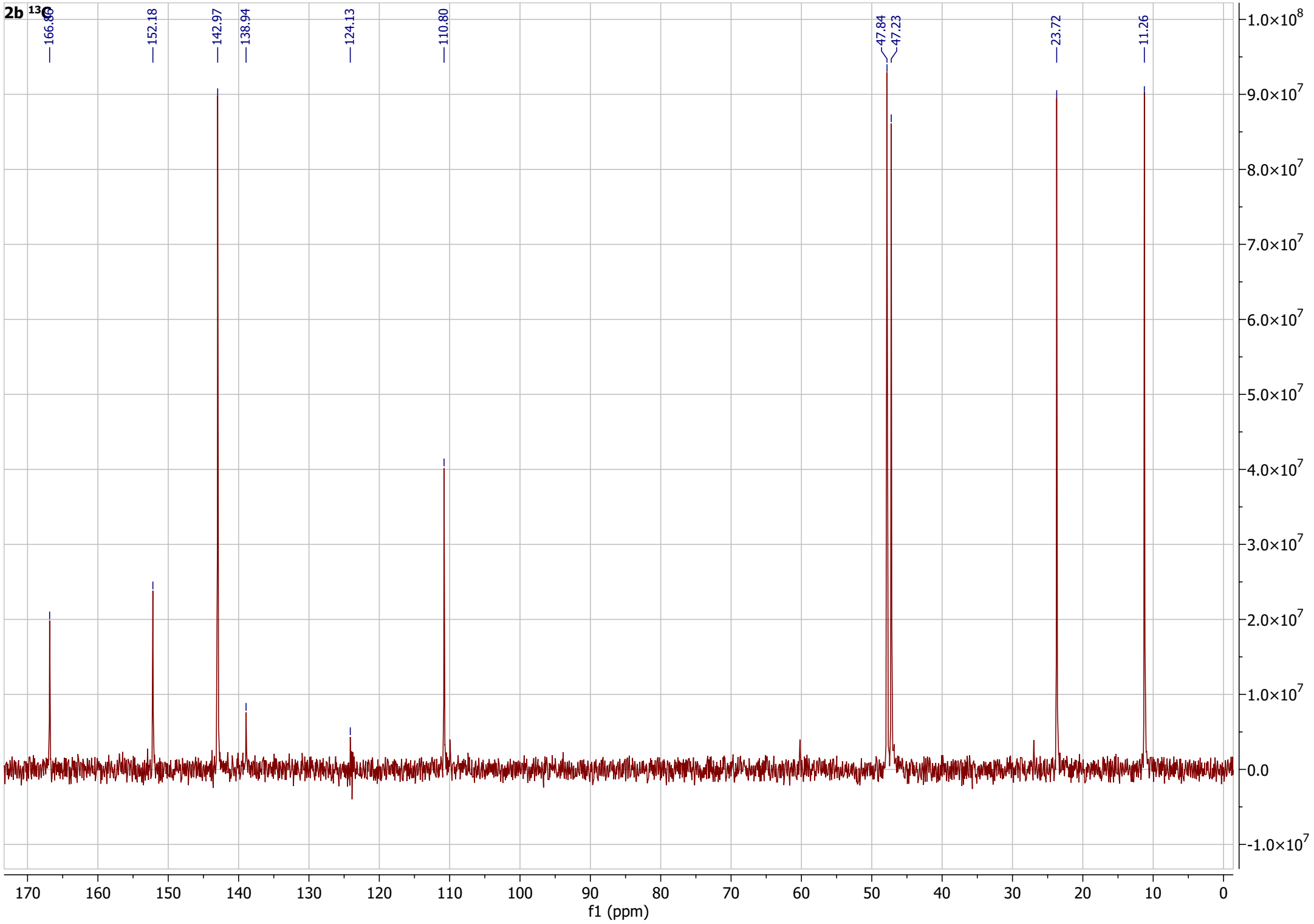
NMR spectra ^{1}H and ^{13}C

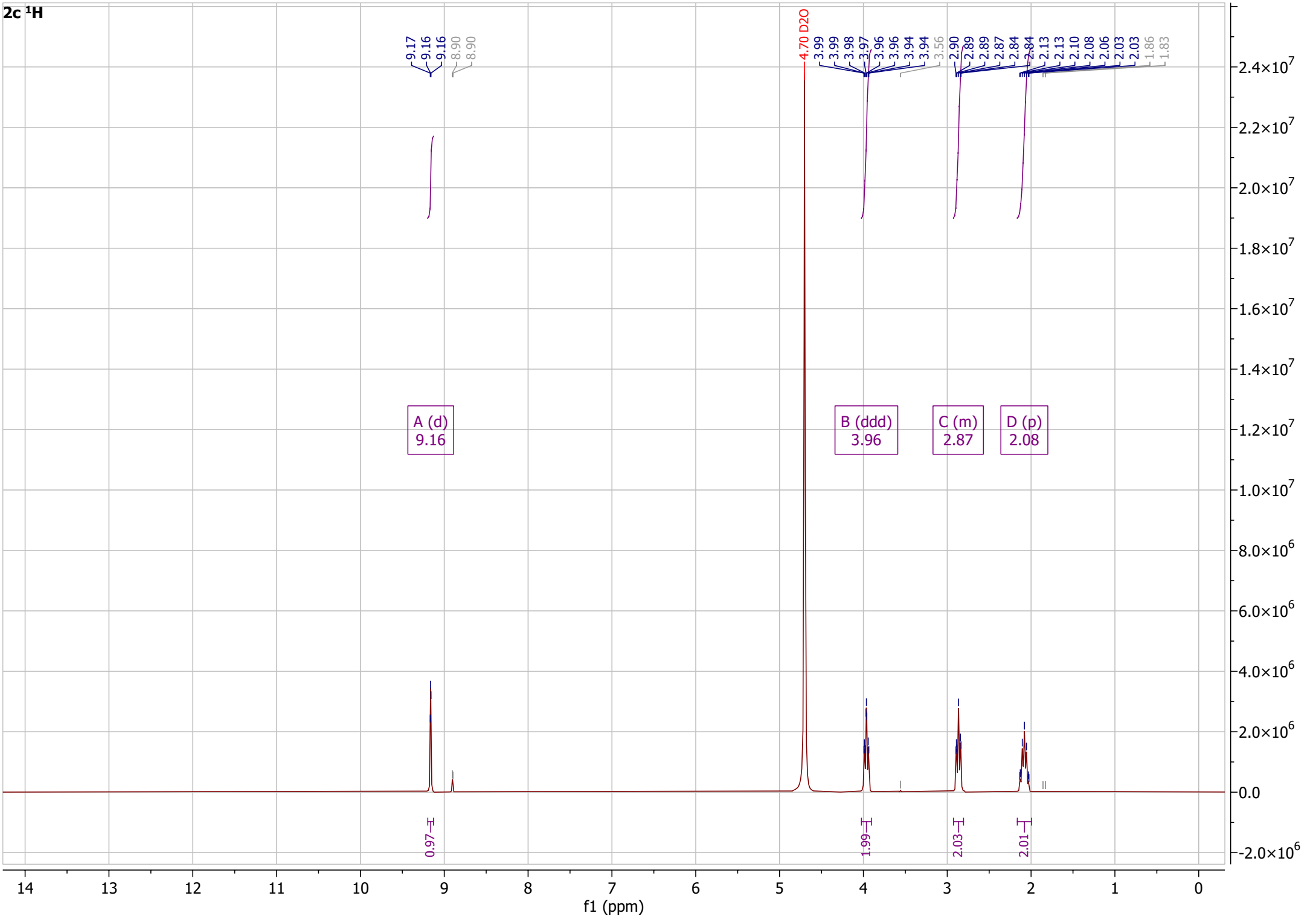
Compounds **2a-g**

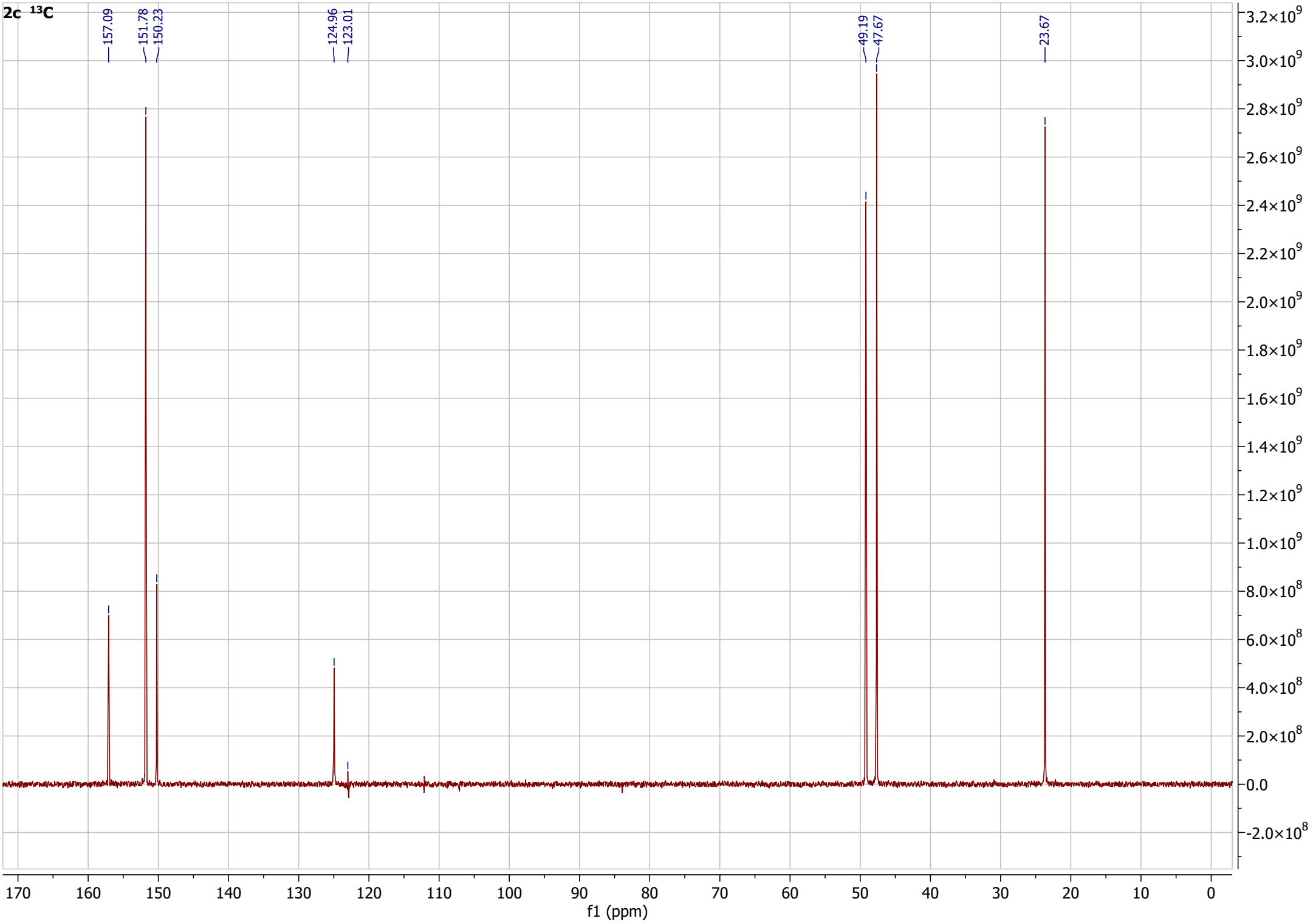

2a ¹H
A (m)
7.52
B (m)
5.67
C (ddd)
3.78
D (ddt)
2.82
E (ddt)
1.99
0.95
1.04
1.98
2.05
1.98
f1 (ppm)

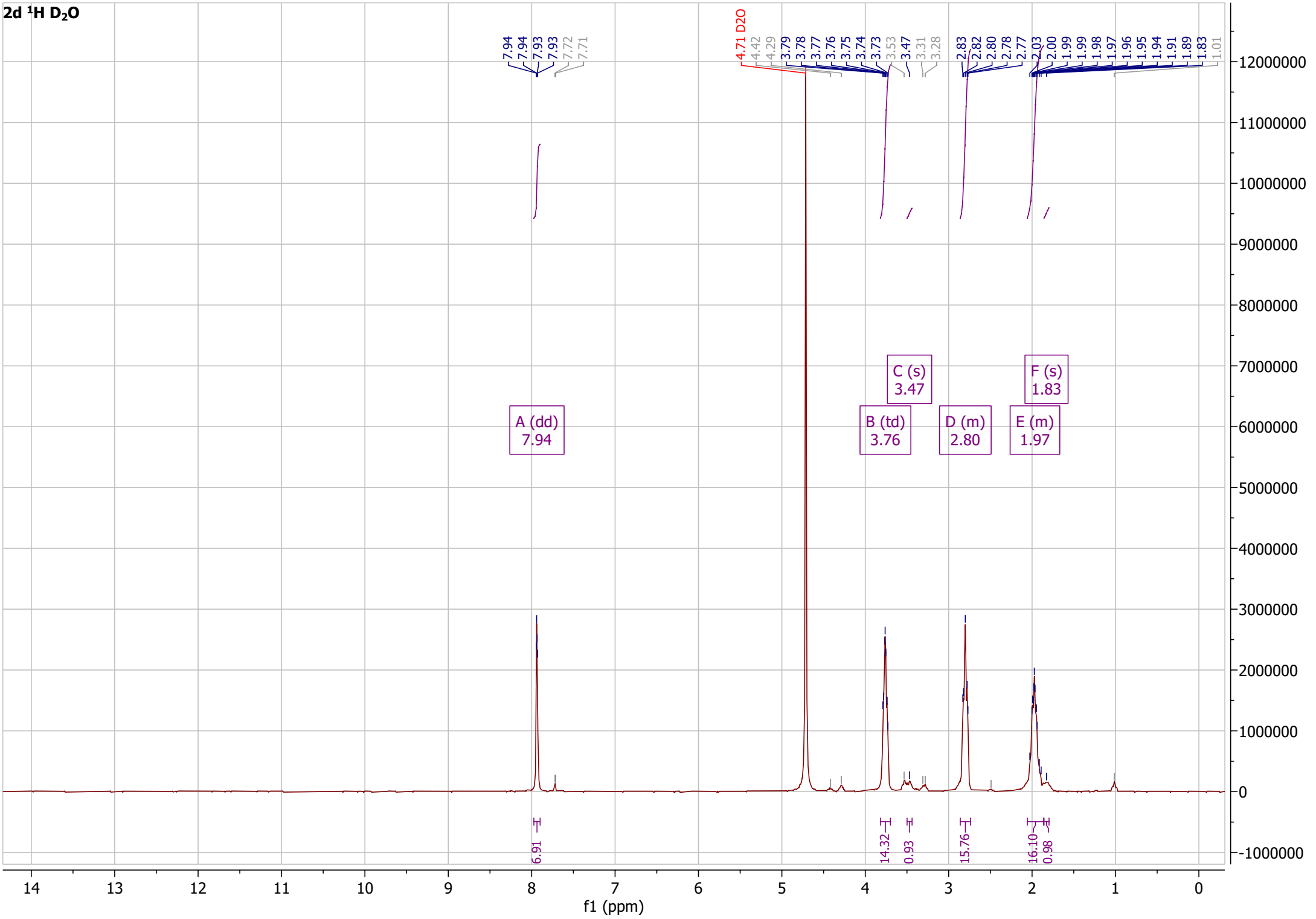

2a ¹³C
172.54
164.31
151.38
146.44
142.78
101.20
100.67
48.47
47.17
40.44 DMSO
40.23 DMSO
40.03 DMSO
39.82 DMSO
39.61 DMSO
39.40 DMSO
39.19 DMSO
25.20
22.80
6.0×10⁷
5.5×10⁷
5.0×10⁷
4.5×10⁷
4.0×10⁷
3.5×10⁷
3.0×10⁷
2.5×10⁷
2.0×10⁷
1.5×10⁷
1.0×10⁷
5.0×10⁶
0.0
-5.0×10⁶
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

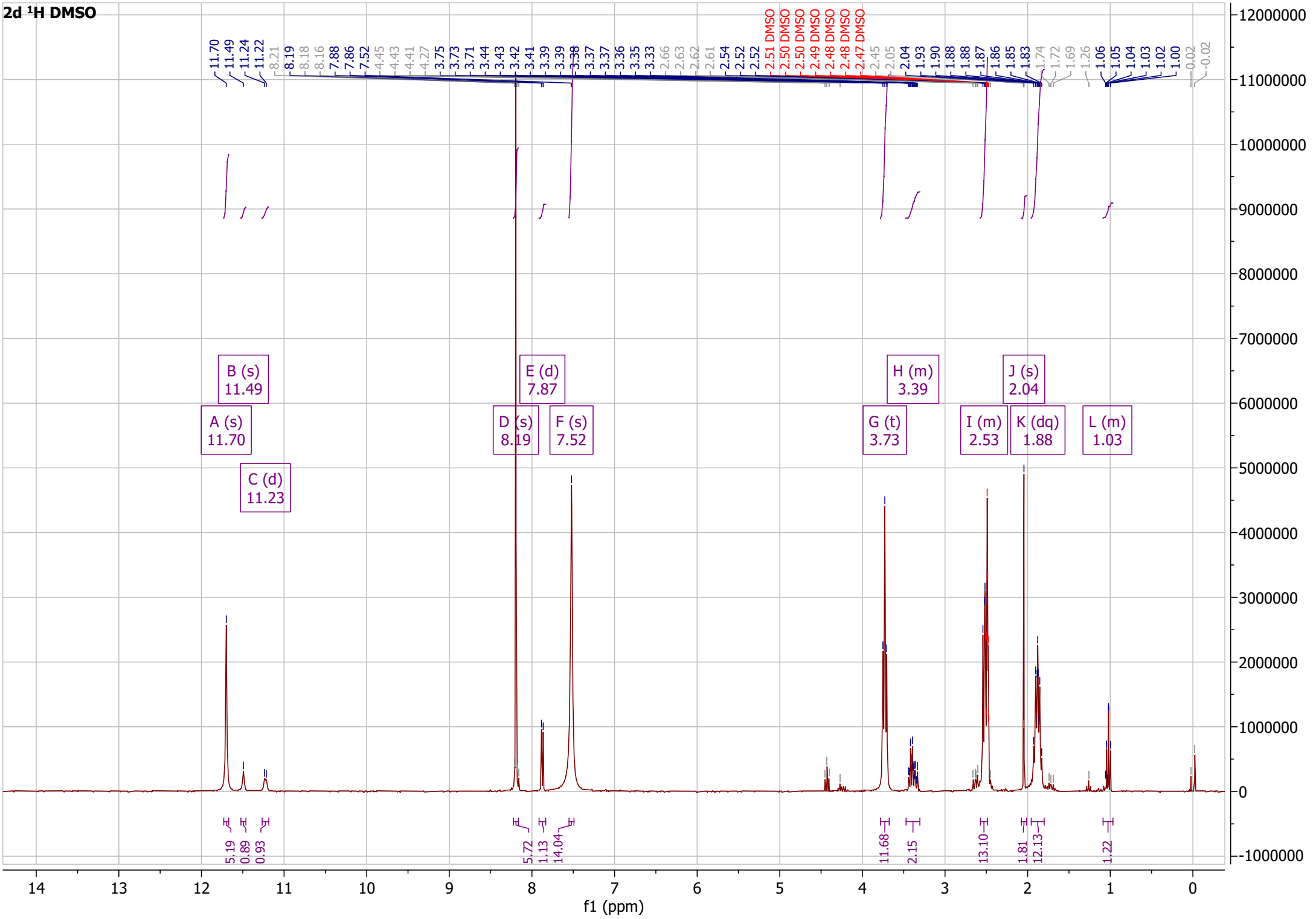

2b ¹H
7.40
7.24
4.70 D2O
3.80
3.77
3.75
3.59
3.57
2.89
2.87
2.84
2.84
2.82
2.06
2.04
2.01
2.01
1.99
1.96
1.89
1.86
1.76
1.74
1.07
A (s)
7.40
B (t)
3.77
C (dd)
2.84
D (m)
2.01
E (d)
1.75
0.91
1.87
1.99
1.94
3.28
f1 (ppm)

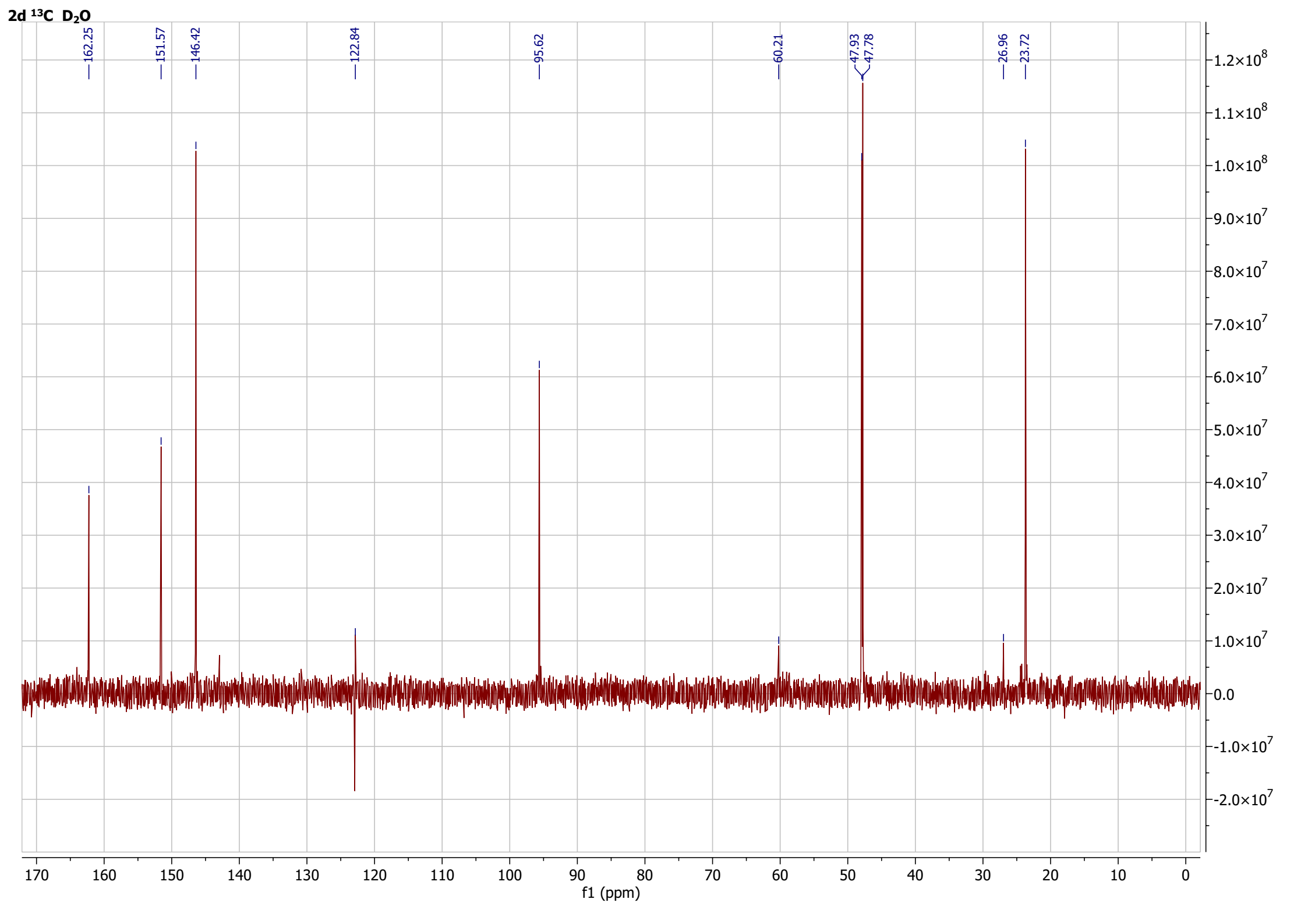

2b ^{13}C
166.80
152.18
142.97
138.94
124.13
110.80
47.84
47.23
23.72
11.26
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

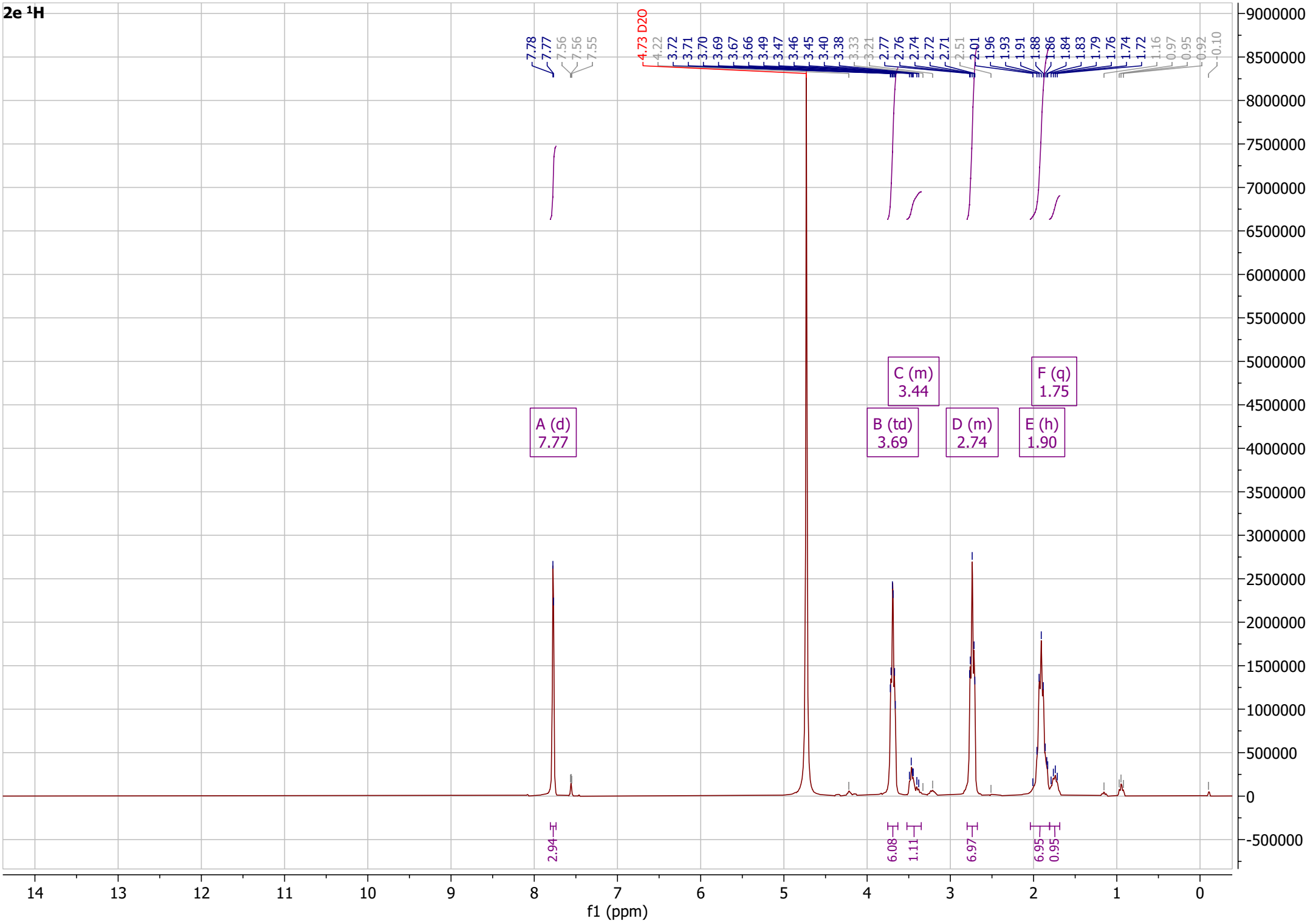

2c ¹H
9.17
9.16
9.16
8.90
8.90
4.70 D2O
3.99
3.99
3.98
3.97
3.96
3.96
3.94
3.94
3.56
2.90
2.89
2.89
2.87
2.84
2.84
2.13
2.13
2.10
2.08
2.06
2.03
2.03
1.86
1.83
A (d)
9.16
B (ddd)
3.96
C (m)
2.87
D (p)
2.08
0.97
1.99
2.03
2.01
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
-2.0×10^6
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

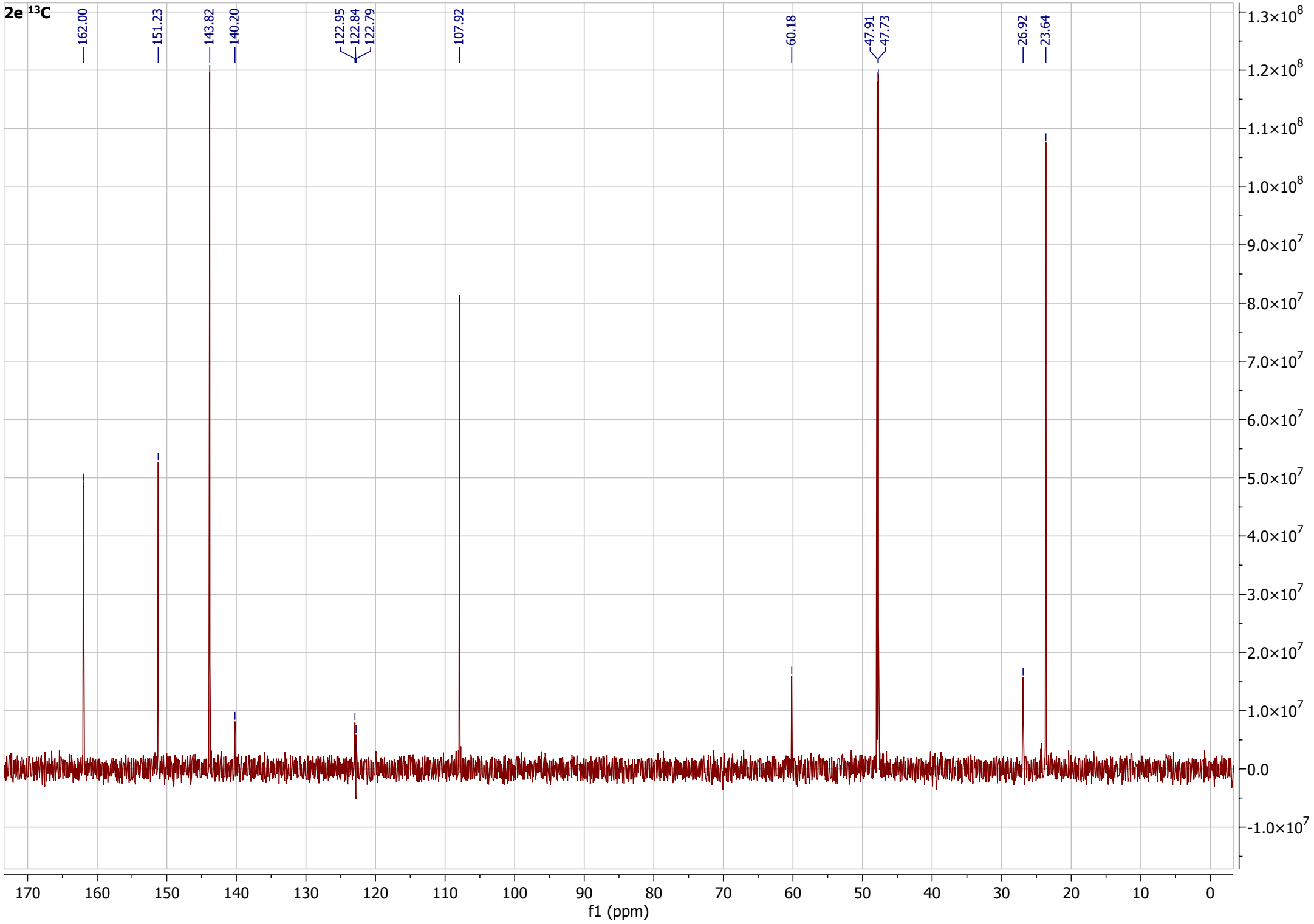

2c ¹³C
157.09
151.78
150.23
124.96
123.01
49.19
47.67
23.67
3.2×10⁹
3.0×10⁹
2.8×10⁹
2.6×10⁹
2.4×10⁹
2.2×10⁹
2.0×10⁹
1.8×10⁹
1.6×10⁹
1.4×10⁹
1.2×10⁹
1.0×10⁹
8.0×10⁸
6.0×10⁸
4.0×10⁸
2.0×10⁸
0.0
-2.0×10⁸
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

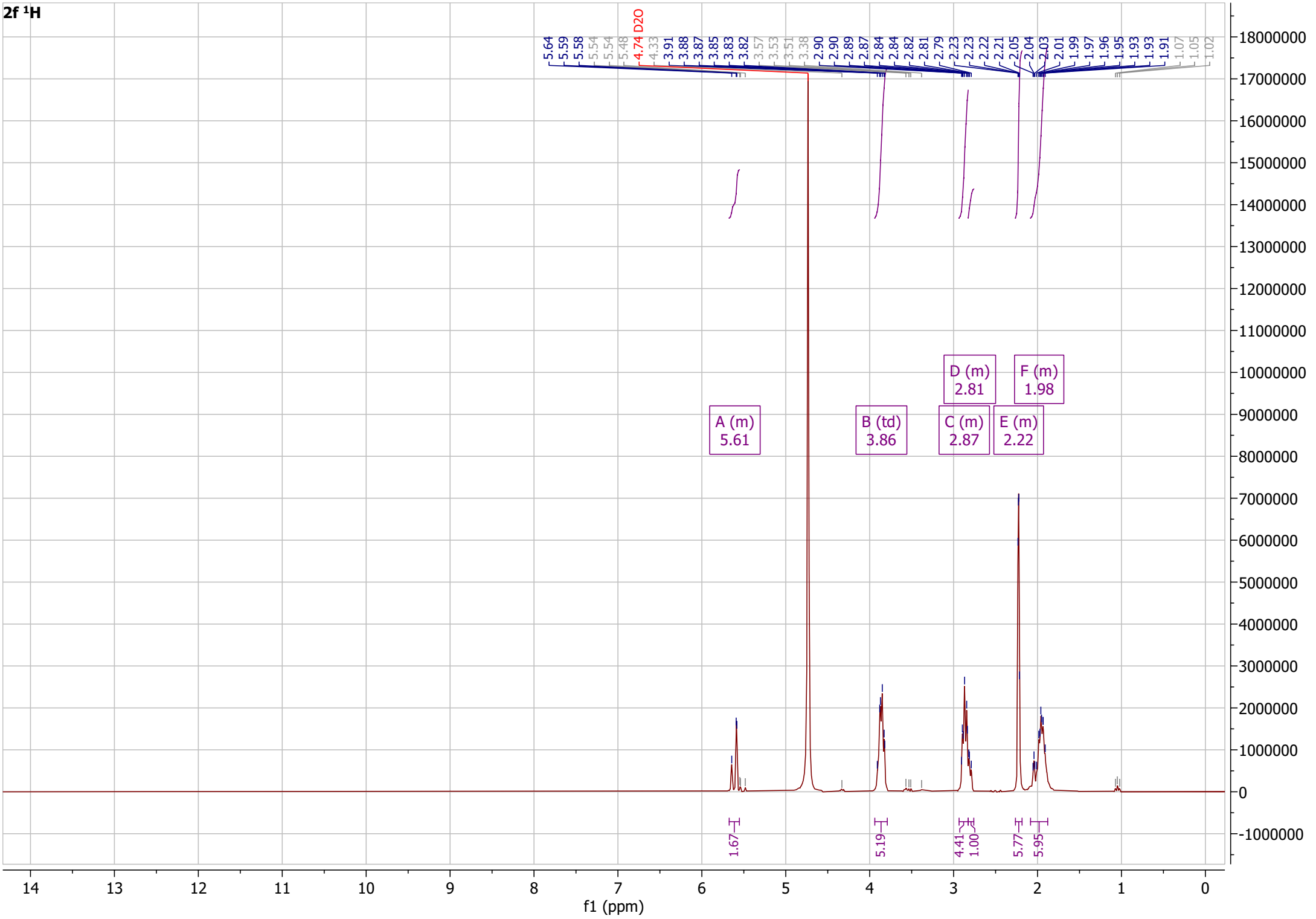

2d ¹H D₂O
7.94
7.94
7.93
7.93
7.72
7.71
4.71 D2O
4.42
4.29
3.79
3.78
3.77
3.76
3.75
3.74
3.73
3.53
3.47
3.31
3.28
2.83
2.82
2.80
2.78
2.77
2.03
2.00
1.99
1.99
1.98
1.97
1.96
1.95
1.94
1.91
1.89
1.83
1.01
A (dd)
7.94
B (td)
3.76
C (s)
3.47
D (m)
2.80
E (m)
1.97
F (s)
1.83
6.91
14.32
0.93
15.76
16.10
0.98
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

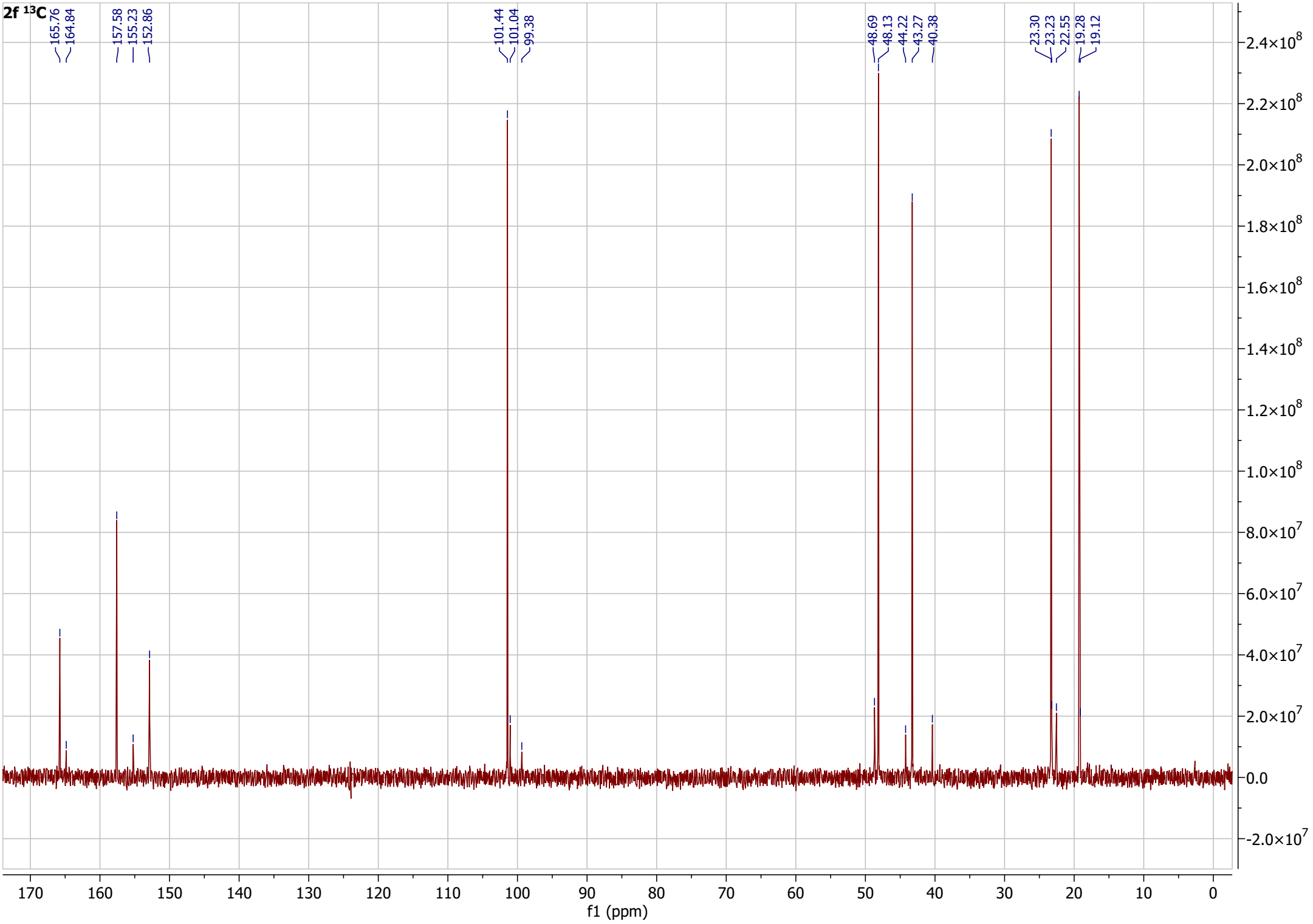

2d ¹H DMSO
B (s) 11.49
A (s) 11.70
C (d) 11.23
E (d) 7.87
D (s) 8.19
F (s) 7.52
H (m) 3.39
G (t) 3.73
J (s) 2.04
I (m) 2.53
K (dq) 1.88
L (m) 1.03
f1 (ppm)

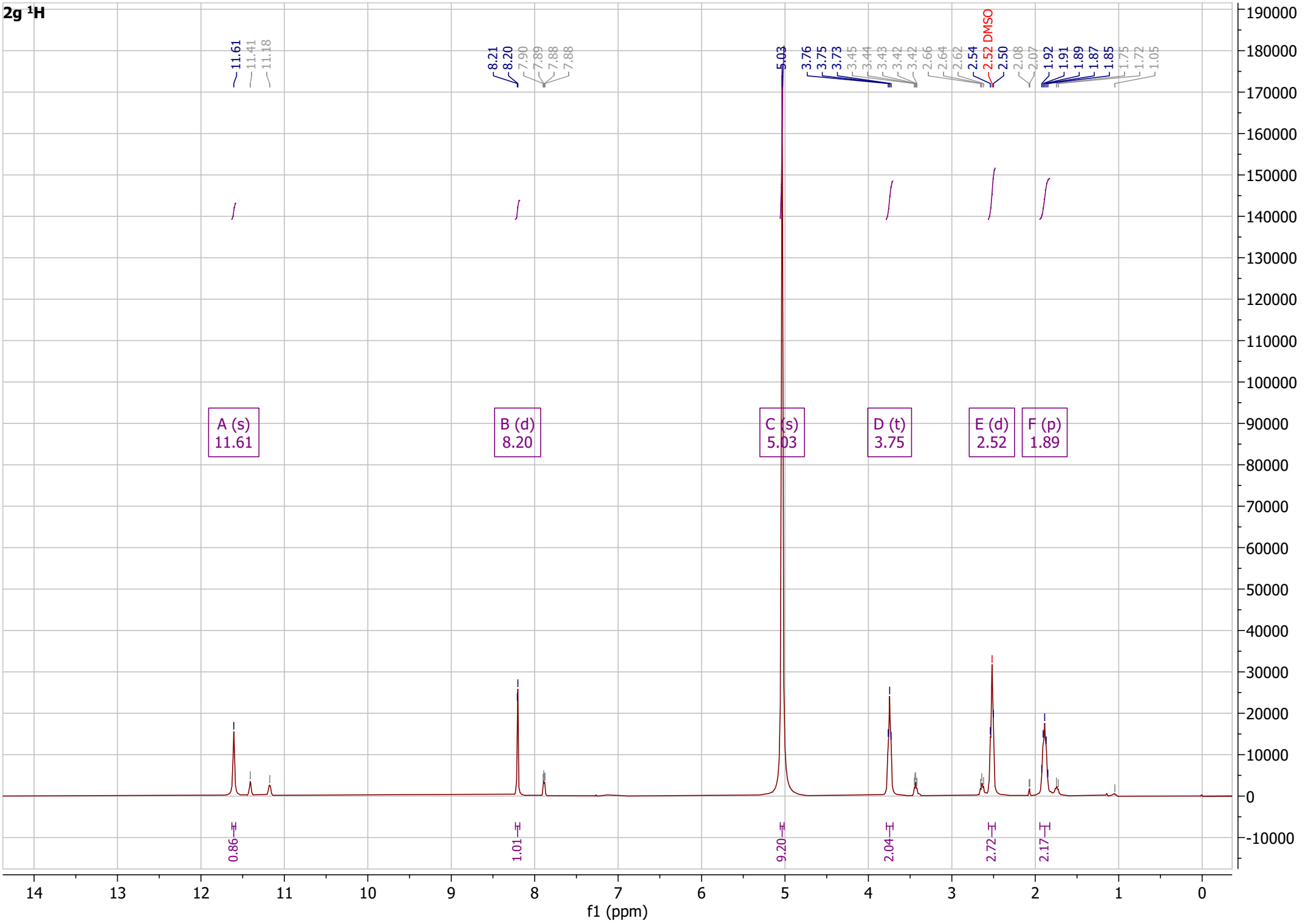

2d ^{13}C D_2O
162.25
151.57
146.42
122.84
95.62
60.21
47.93
47.78
26.96
23.72
1.2×10^8
1.1×10^8
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
-2.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

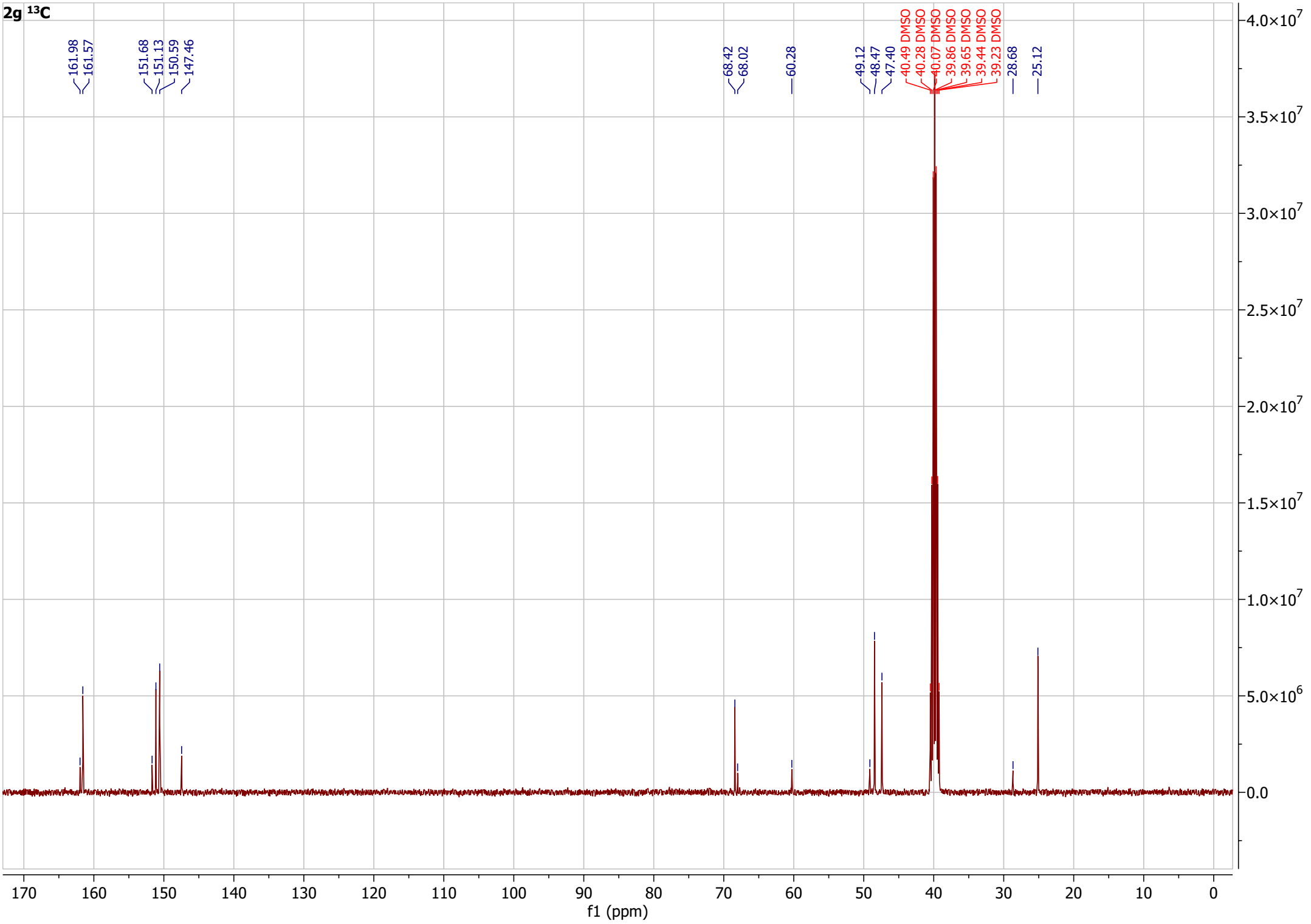

2e ¹H
7.78
7.77
7.56
7.56
7.55
4.73 D20
4.22
3.72
3.71
3.70
3.69
3.67
3.66
3.49
3.47
3.46
3.45
3.40
3.38
3.33
3.21
2.77
2.76
2.74
2.72
2.71
2.51
2.01
1.96
1.93
1.91
1.88
1.86
1.84
1.83
1.79
1.76
1.74
1.72
1.16
0.97
0.95
0.92
-0.10
A (d)
7.77
B (td)
3.69
C (m)
3.44
D (m)
2.74
E (h)
1.90
F (q)
1.75
2.94
6.08
1.11
6.97
6.95
0.95
f1 (ppm)


2e ¹³C
162.00
151.23
143.82
140.20
122.95
122.84
122.79
107.92
60.18
47.91
47.73
26.92
23.64
1.3×10⁸
1.2×10⁸
1.1×10⁸
1.0×10⁸
9.0×10⁷
8.0×10⁷
7.0×10⁷
6.0×10⁷
5.0×10⁷
4.0×10⁷
3.0×10⁷
2.0×10⁷
1.0×10⁷
0.0
-1.0×10⁷
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

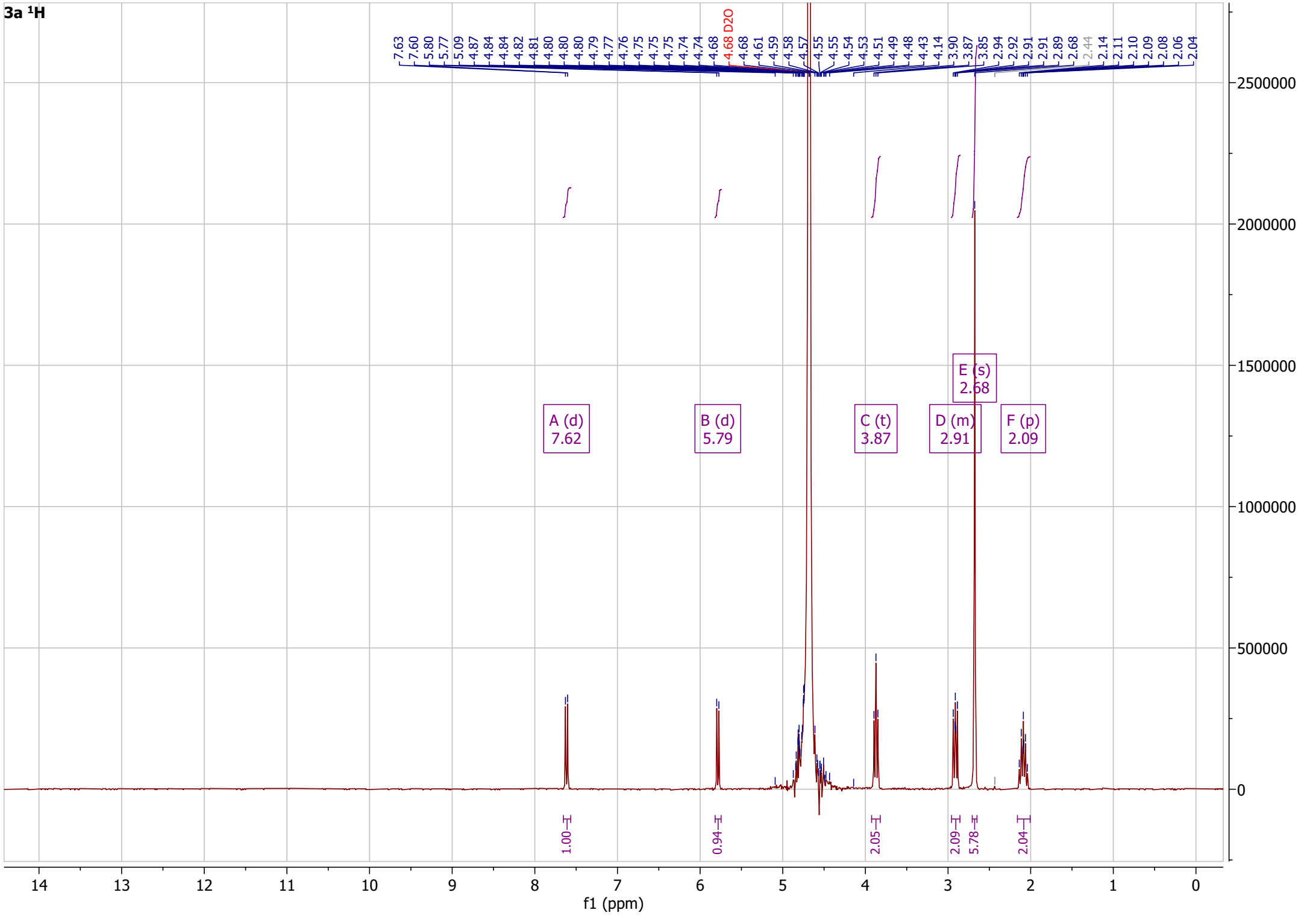

2f ¹H
5.64 5.59 5.58 5.54 5.54 5.48 4.74 D2O 4.33 3.91 3.88 3.87 3.85 3.83 3.82 3.57 3.53 3.51 3.38 2.90 2.90 2.89 2.87 2.84 2.84 2.82 2.81 2.79 2.23 2.23 2.22 2.21 2.05 2.04 2.03 2.01 1.99 1.97 1.96 1.95 1.93 1.93 1.91 1.07 1.05 1.02
A (m) 5.61
B (td) 3.86
C (m) 2.87
D (m) 2.81
E (m) 2.22
F (m) 1.98
1.67
5.19
4.41
1.00
5.77
5.95
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

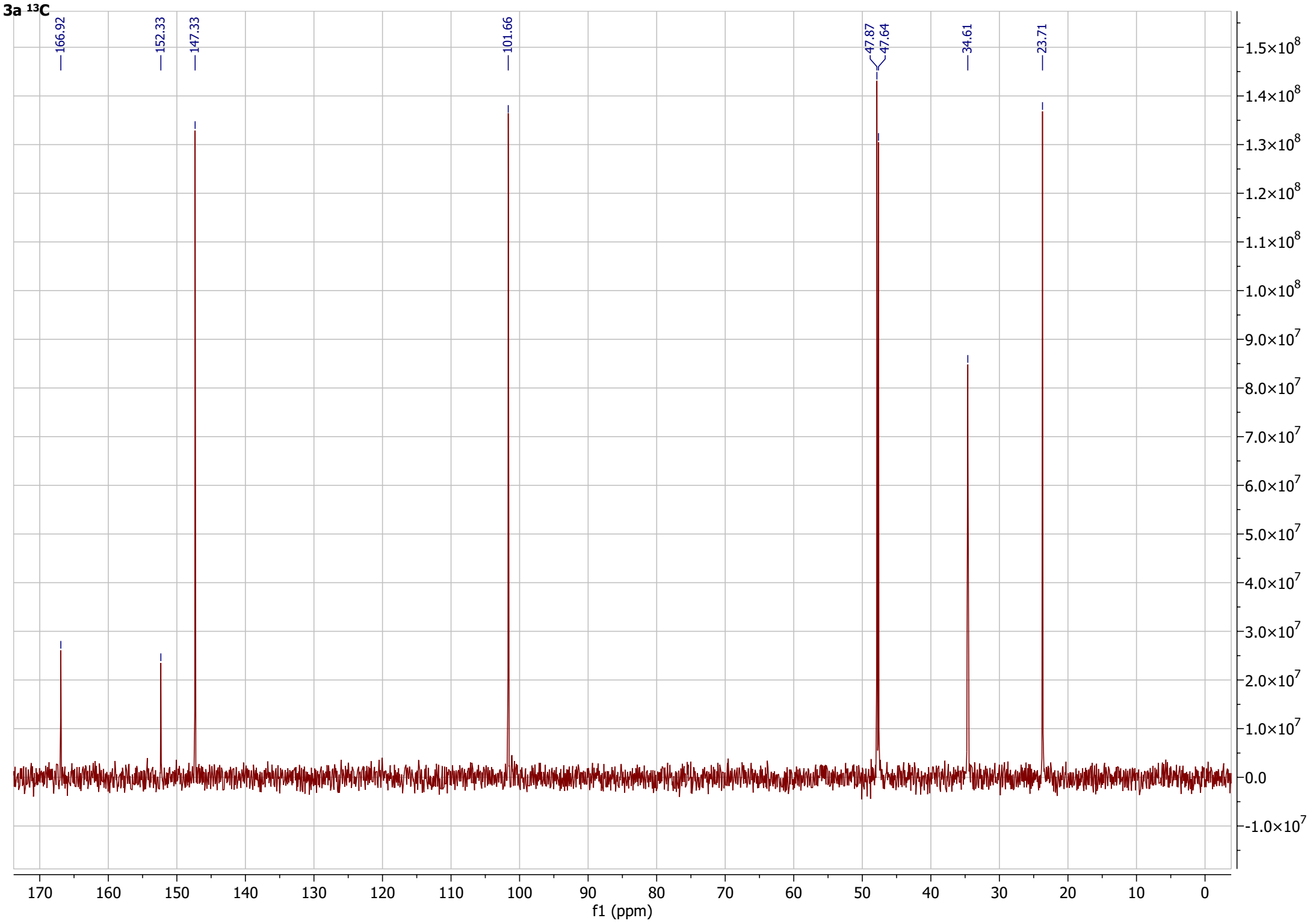

2f ^{13}C
165.76
164.84
157.58
155.23
152.86
101.44
101.04
99.38
48.69
48.13
44.22
43.27
40.38
23.30
23.23
22.55
19.28
19.12
2.4×10^8
2.2×10^8
2.0×10^8
1.8×10^8
1.6×10^8
1.4×10^8
1.2×10^8
1.0×10^8
8.0×10^7
6.0×10^7
4.0×10^7
2.0×10^7
0.0
-2.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

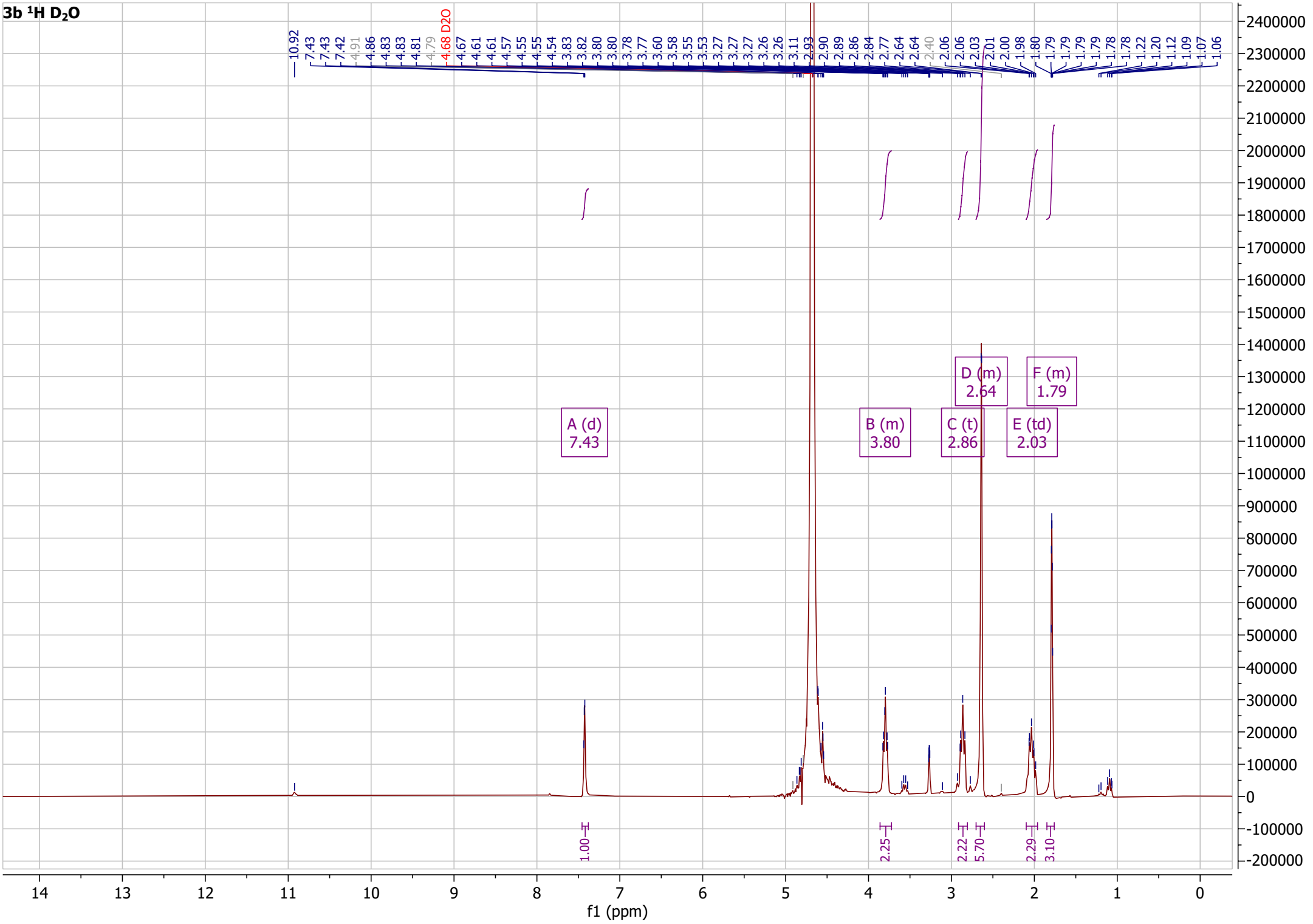

2g ¹H
11.61
11.41
11.18
8.21
8.20
7.90
7.89
7.88
7.88
5.03
3.76
3.75
3.73
3.45
3.44
3.43
3.42
3.42
2.66
2.64
2.62
2.54
2.52 DMSO
2.50
2.08
2.07
1.92
1.91
1.89
1.87
1.85
1.75
1.72
1.05
A (s) 11.61
B (d) 8.20
C (s) 5.03
D (t) 3.75
E (d) 2.52
F (p) 1.89
0.86
1.01
9.20
2.04
2.72
2.17
f1 (ppm)


2g ^{13}C
161.98
161.57
151.68
151.13
150.59
147.46
68.42
68.02
60.28
49.12
48.47
47.40
40.49 DMSO
40.28 DMSO
40.07 DMSO
39.86 DMSO
39.65 DMSO
39.44 DMSO
39.23 DMSO
28.68
25.12
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

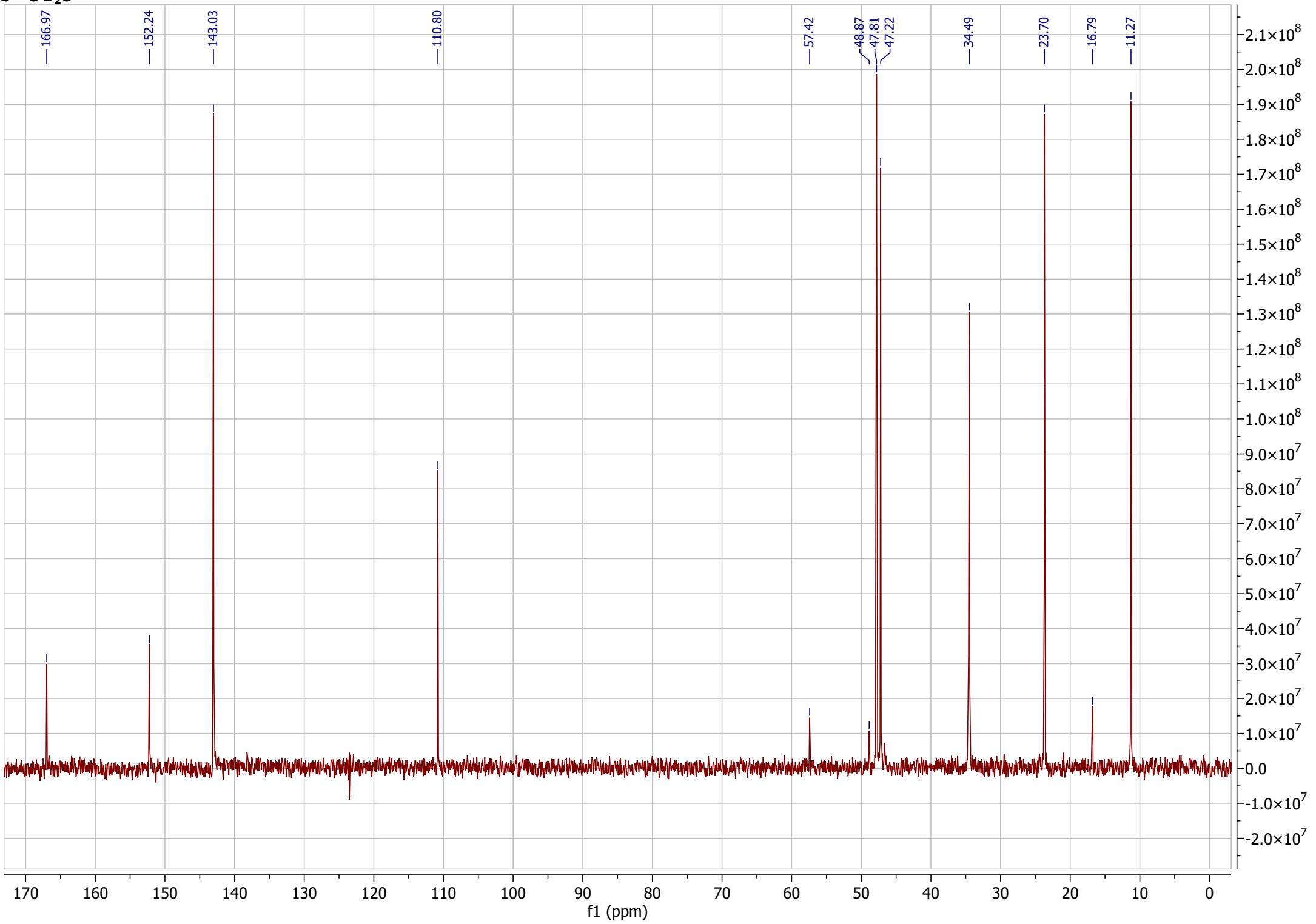
Compounds **3a-g**

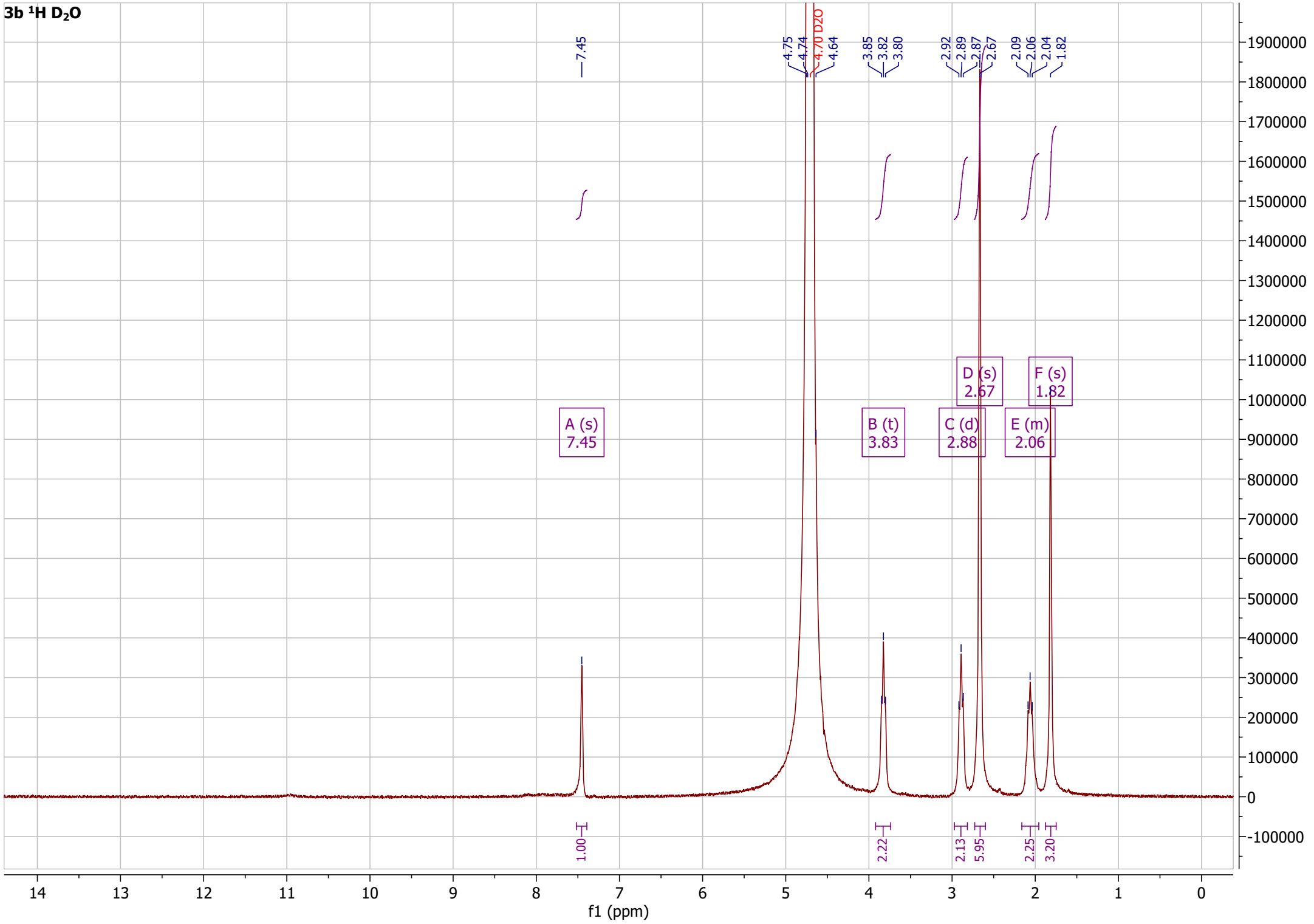

3a ¹H
7.63 7.60 5.80 5.77 5.09 4.87 4.84 4.84 4.82 4.81 4.80 4.80 4.80 4.79 4.77 4.76 4.75 4.75 4.75 4.74 4.74 4.68 4.68 D2O 4.68 4.61 4.59 4.58 4.57 4.55 4.55 4.54 4.53 4.51 4.49 4.48 4.43 4.14 3.90 3.87 3.85 2.94 2.92 2.91 2.91 2.89 2.68 2.44 2.14 2.11 2.10 2.09 2.08 2.06 2.04
A (d) 7.62
B (d) 5.79
C (t) 3.87
D (m) 2.91
E (s) 2.68
F (p) 2.09
1.00
0.94
2.05
2.09
5.78
2.04
2500000
2000000
1500000
1000000
500000
0
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

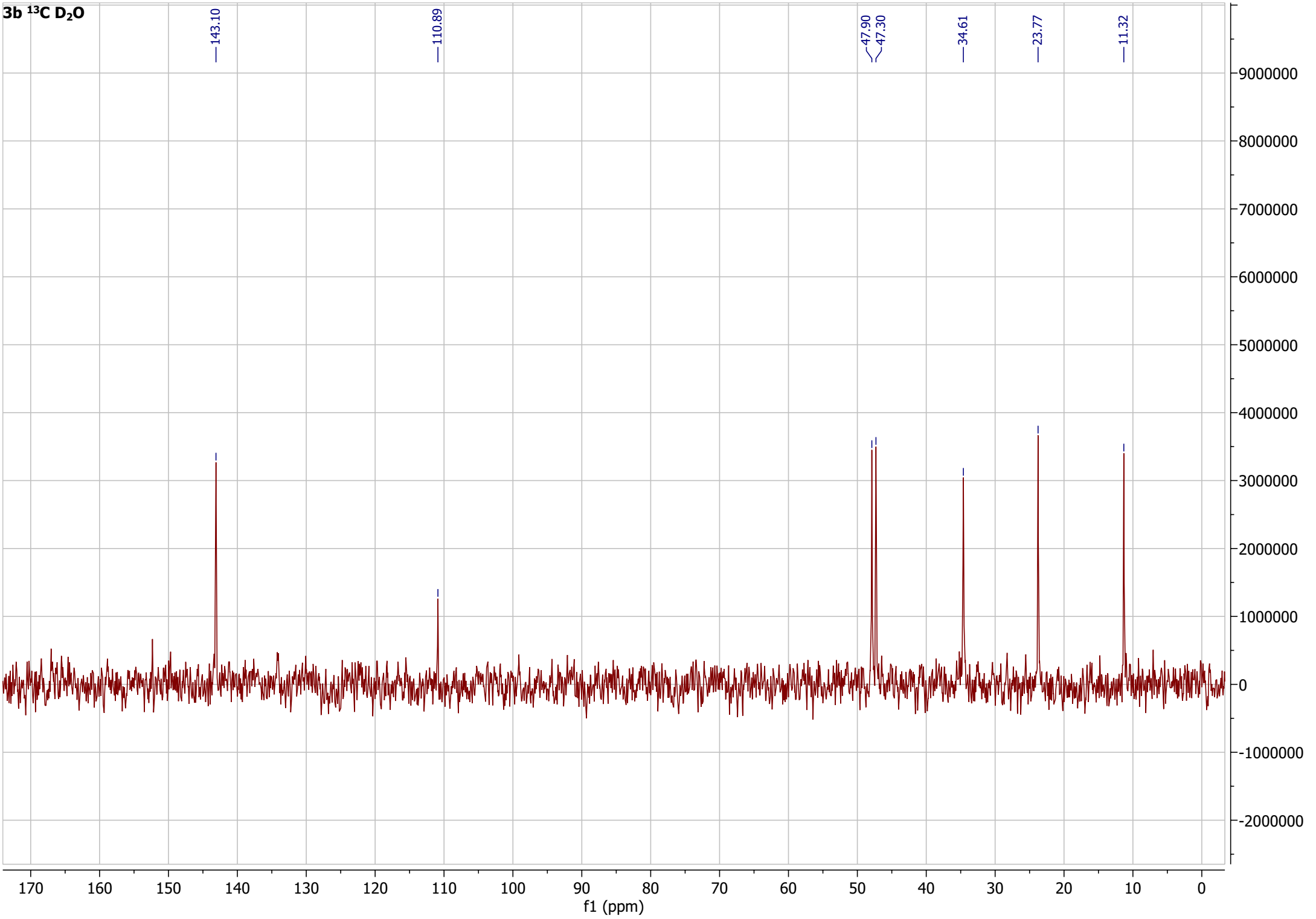

3a ^{13}C
166.92
152.33
147.33
101.66
47.87
47.64
34.61
23.71
1.5×10^8
1.4×10^8
1.3×10^8
1.2×10^8
1.1×10^8
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

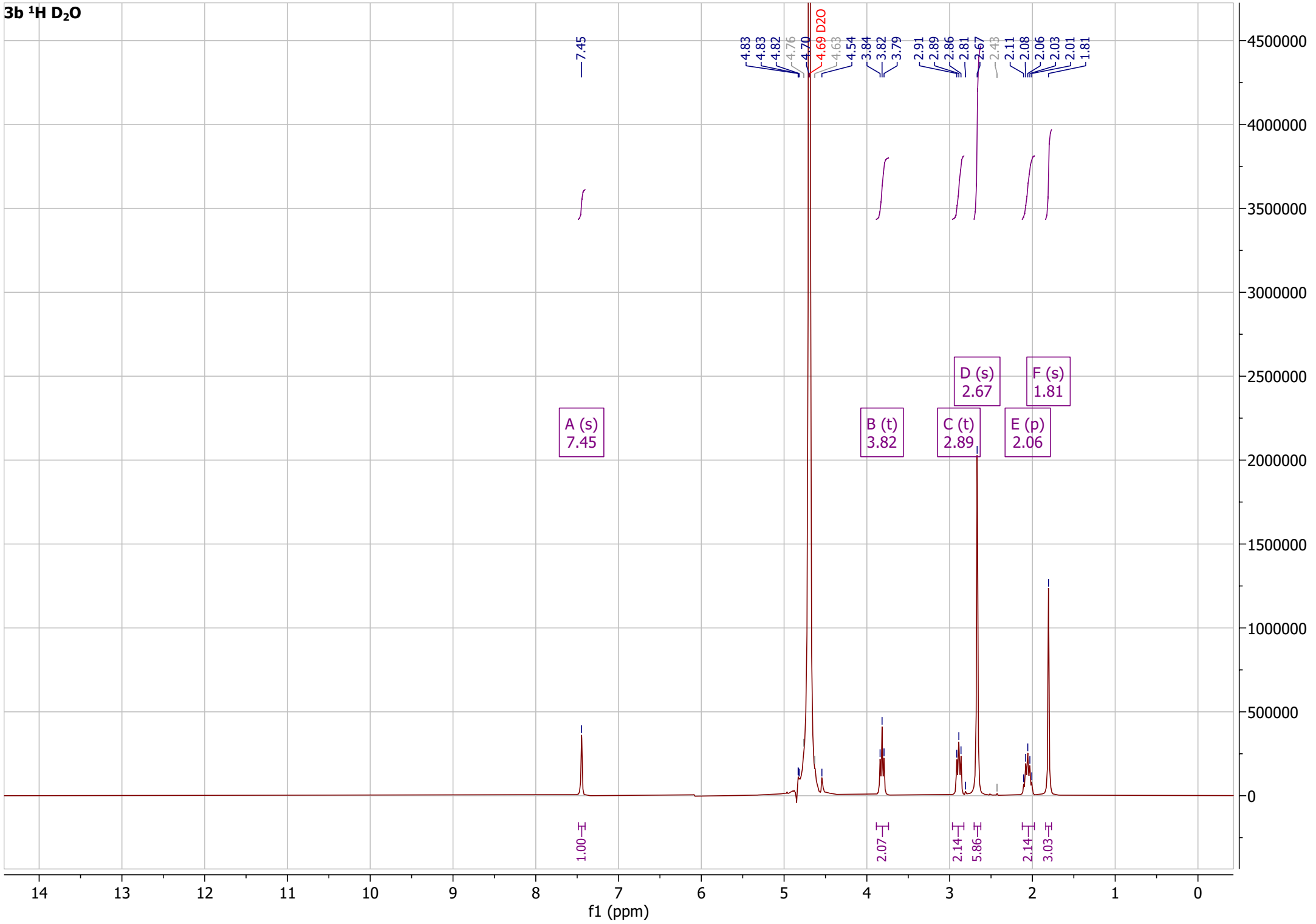

3b ¹H D₂O
10.92
7.43
7.43
7.42
4.91
4.86
4.83
4.83
4.81
4.79
4.68 D2O
4.67
4.61
4.61
4.57
4.55
4.55
4.54
3.83
3.82
3.80
3.80
3.78
3.77
3.60
3.58
3.55
3.53
3.27
3.27
3.27
3.26
3.26
3.11
2.93
2.90
2.89
2.86
2.84
2.77
2.64
2.64
2.40
2.06
2.06
2.03
2.01
2.00
1.98
1.80
1.79
1.79
1.79
1.79
1.78
1.78
1.22
1.20
1.12
1.09
1.07
1.06
A (d) 7.43
B (m) 3.80
C (t) 2.86
D (m) 2.64
E (td) 2.03
F (m) 1.79
1.00
2.25
2.22
5.70
2.29
3.10
f1 (ppm)

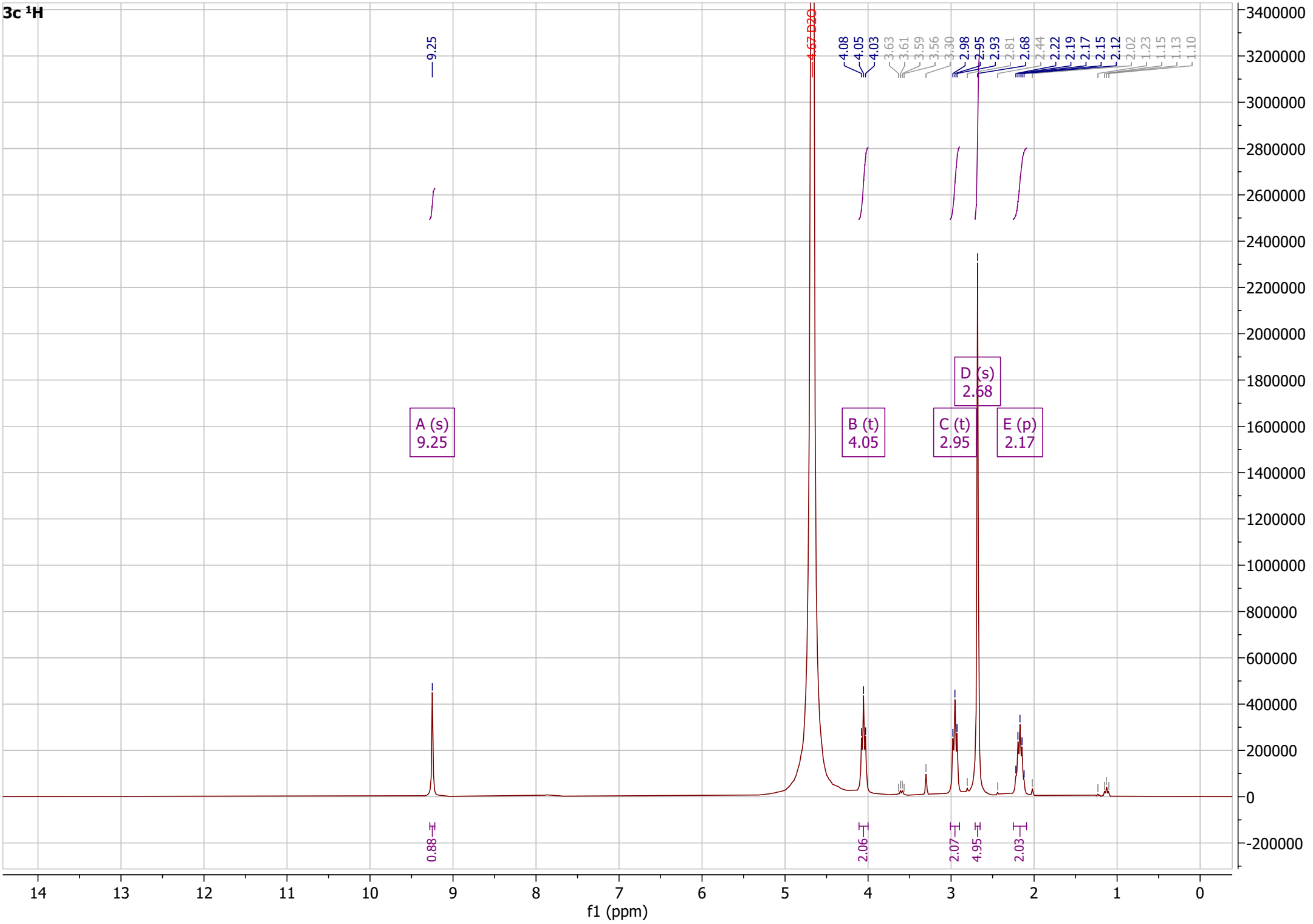
3b ^{13}C D_2O

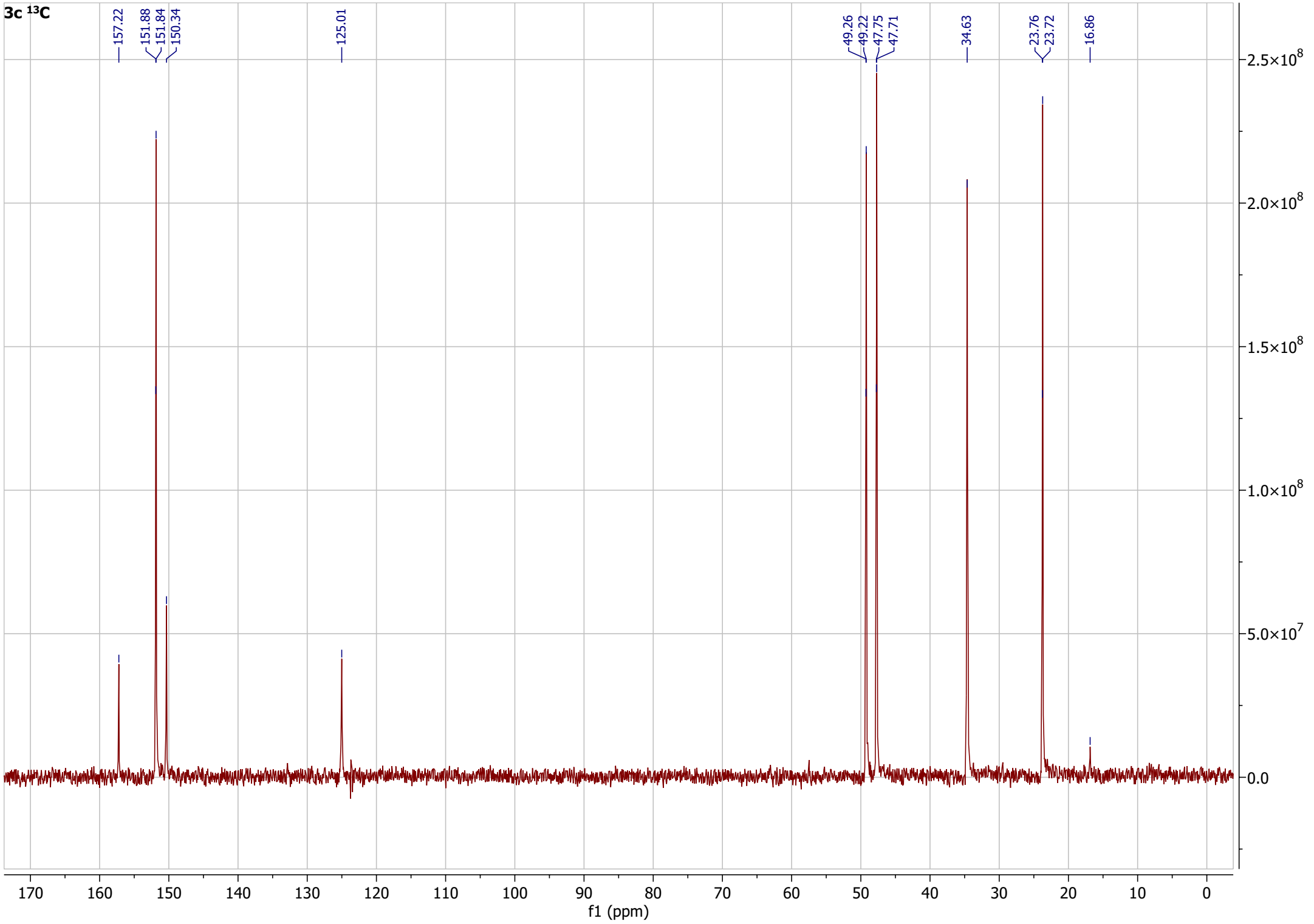

166.97
152.24
143.03
110.80
57.42
48.87
47.81
47.22
34.49
23.70
16.79
11.27
2.1×10^8
2.0×10^8
1.9×10^8
1.8×10^8
1.7×10^8
1.6×10^8
1.5×10^8
1.4×10^8
1.3×10^8
1.2×10^8
1.1×10^8
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
-2.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

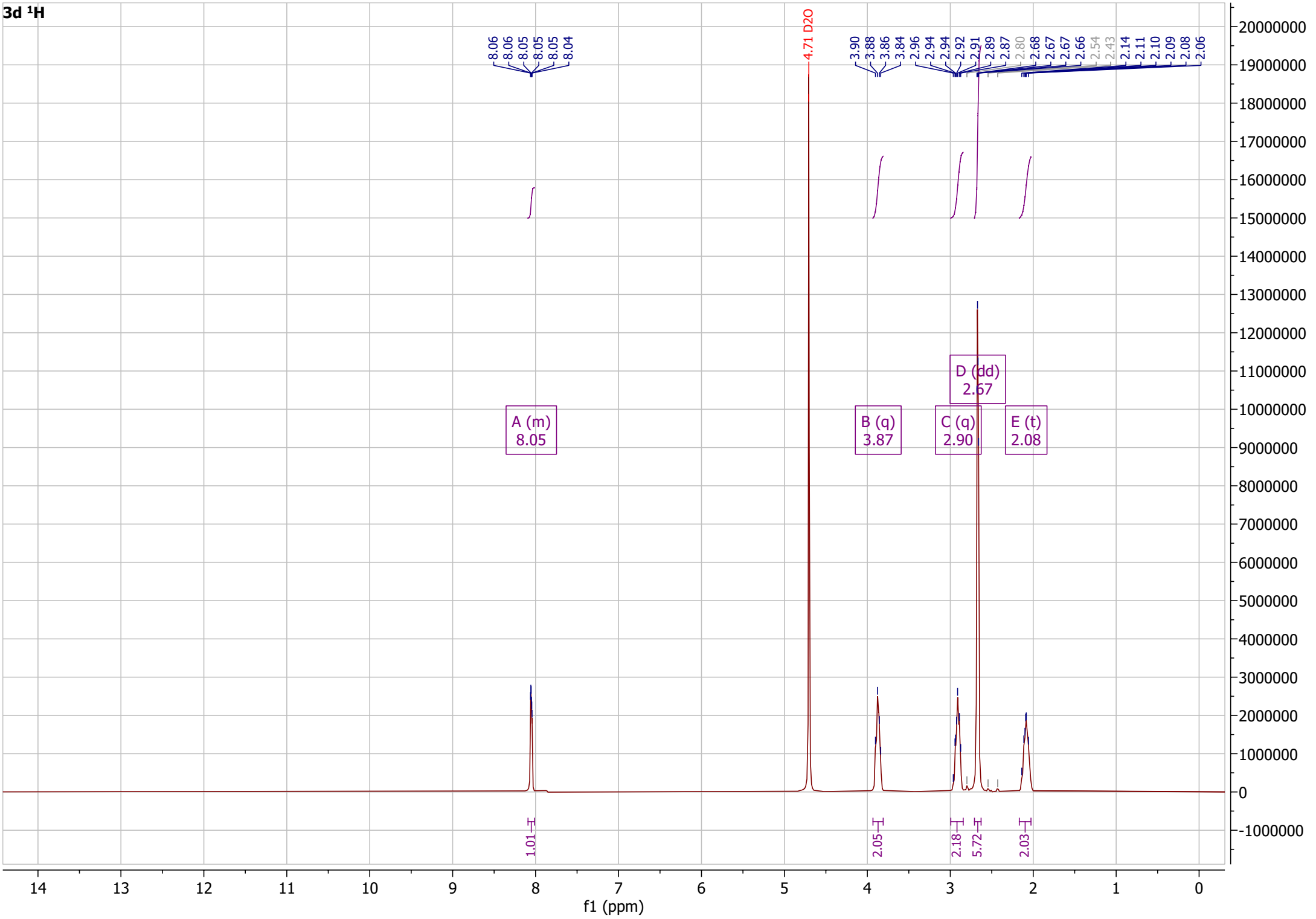

3b ¹H D₂O
7.45
4.75
4.74
4.70 D2O
4.64
3.85
3.82
3.80
2.92
2.89
2.87
2.67
2.09
2.06
2.04
1.82
A (s)
7.45
B (t)
3.83
C (d)
2.88
D (s)
2.67
E (m)
2.06
F (s)
1.82
1.00
2.22
2.13
5.95
2.25
3.20
f1 (ppm)

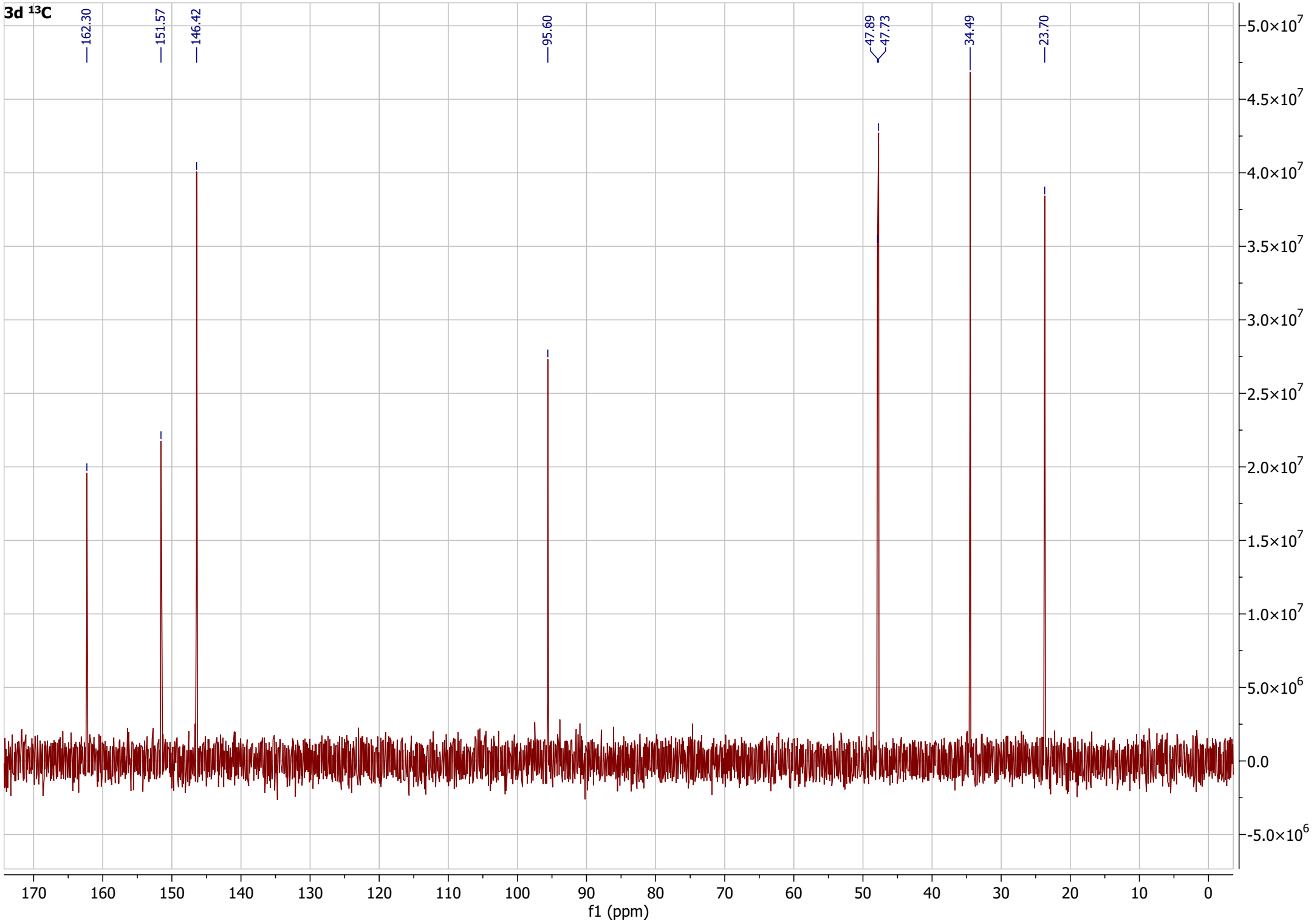

3b ^{13}C D_2O
143.10
110.89
47.90
47.30
34.61
23.77
11.32
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

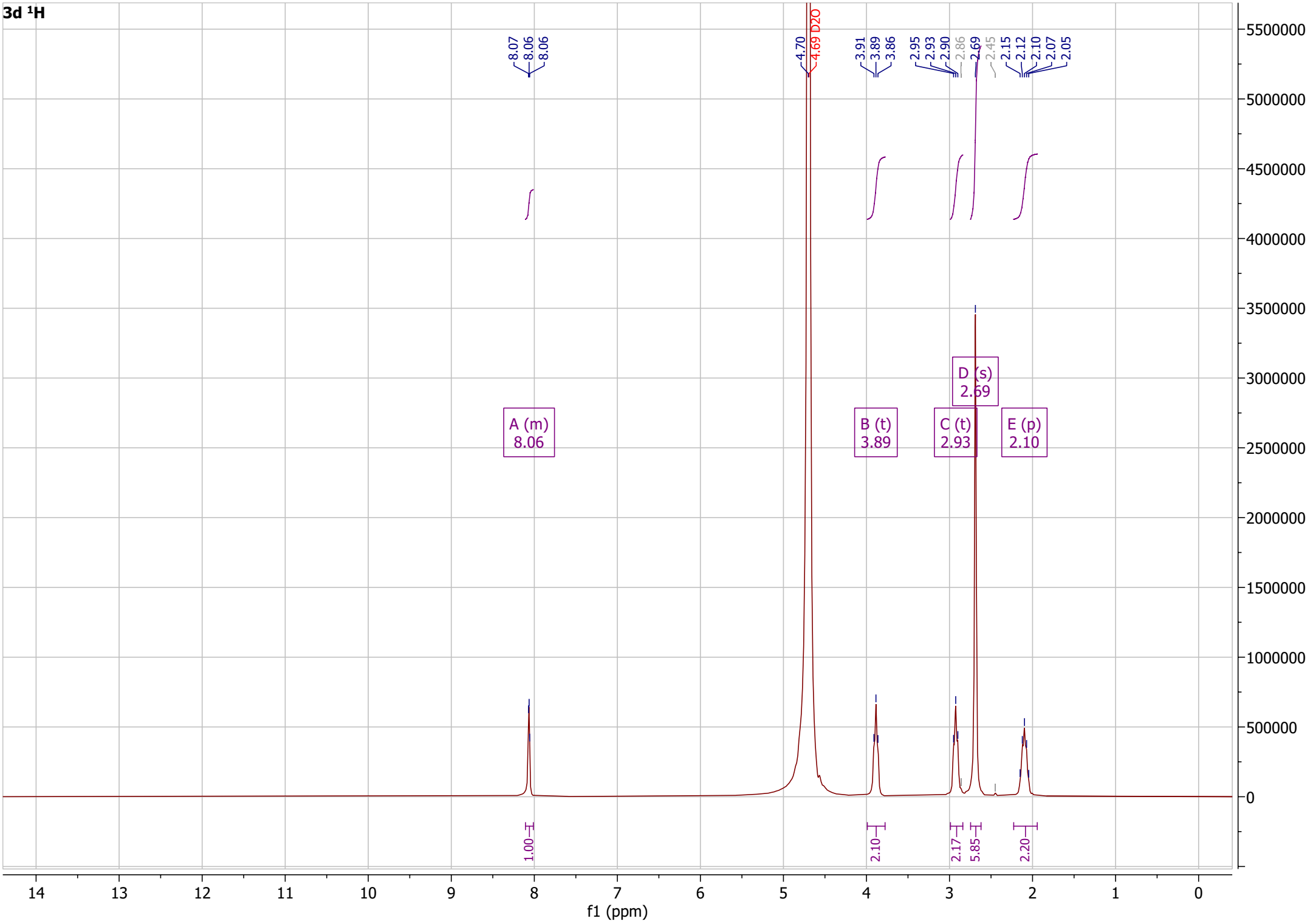

3b ¹H D₂O
7.45
4.83
4.83
4.82
4.76
4.70
4.69 D2O
4.63
4.54
3.84
3.82
3.79
2.91
2.89
2.86
2.81
2.67
2.43
2.11
2.08
2.06
2.03
2.01
1.81
A (s) 7.45
B (t) 3.82
C (t) 2.89
D (s) 2.67
E (p) 2.06
F (s) 1.81
1.00
2.07
2.14
5.86
2.14
3.03
f1 (ppm)

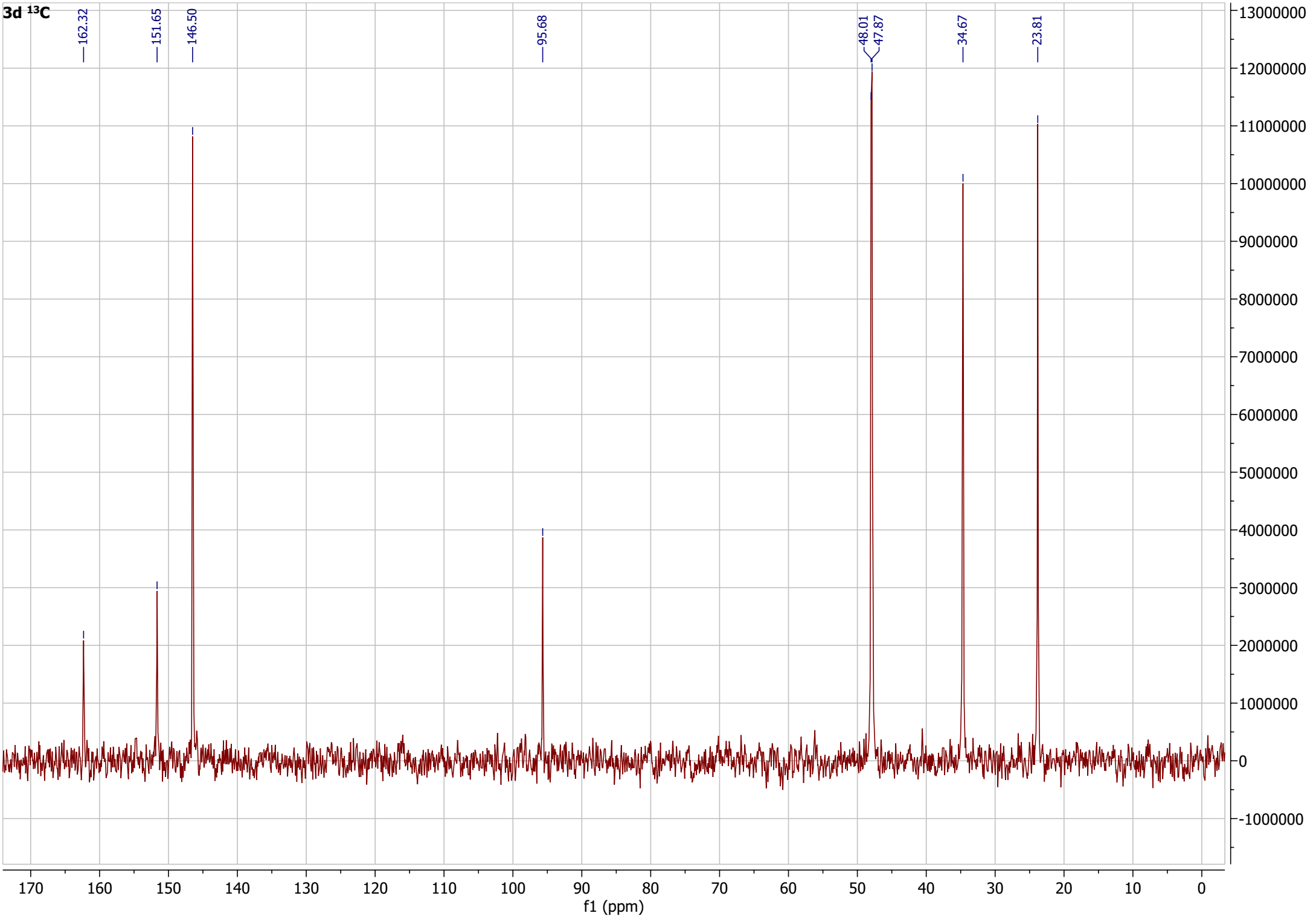

3c ¹H
9.25
4.67 D2O
4.08
4.05
4.03
3.63
3.61
3.59
3.56
3.30
2.98
2.95
2.93
2.81
2.68
2.44
2.22
2.19
2.17
2.15
2.12
2.02
1.23
1.15
1.13
1.10
A (s)
9.25
B (t)
4.05
C (t)
2.95
D (s)
2.68
E (p)
2.17
0.88
2.06
2.07
4.95
2.03
f1 (ppm)

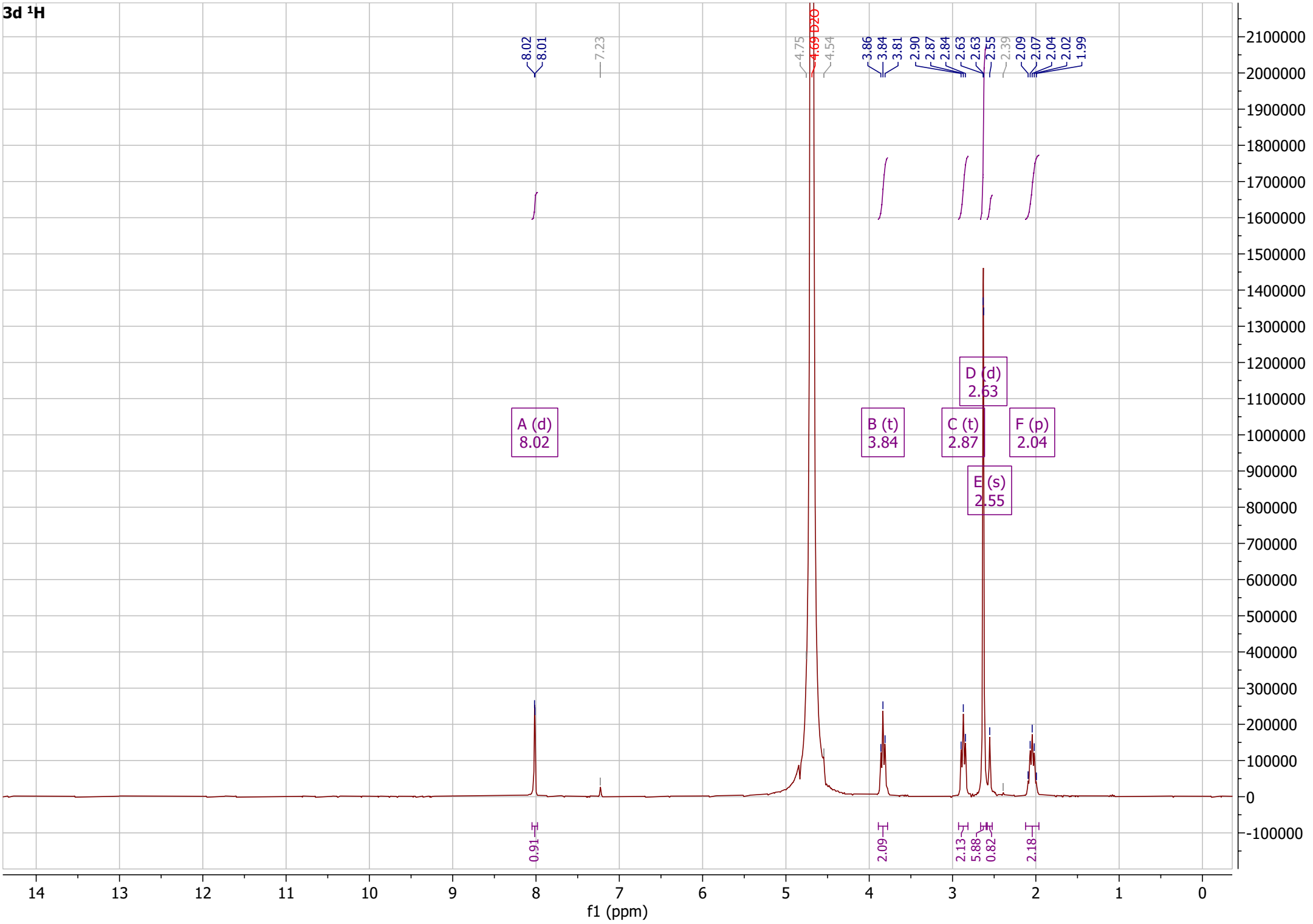

3c ^{13}C
157.22
151.88
151.84
150.34
125.01
49.26
49.22
47.75
47.71
34.63
23.76
23.72
16.86
2.5×10^8
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

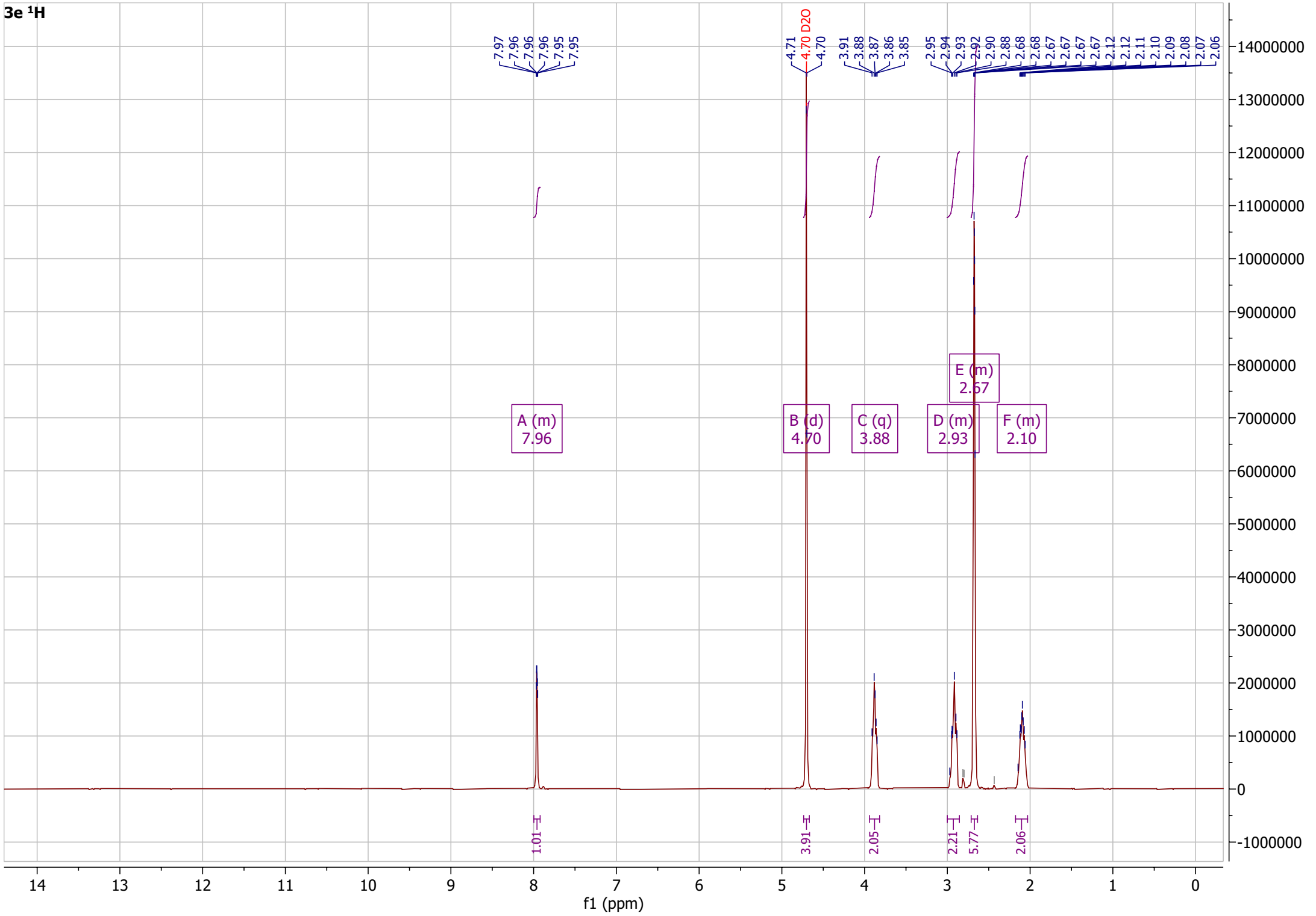

3d ¹H
8.06
8.06
8.05
8.05
8.05
8.04
4.71 D2O
3.90
3.88
3.86
3.84
2.96
2.94
2.94
2.92
2.91
2.89
2.87
2.80
2.68
2.67
2.67
2.66
2.54
2.43
2.14
2.11
2.10
2.09
2.08
2.06
A (m)
8.05
B (q)
3.87
C (q)
2.90
D (dd)
2.67
E (t)
2.08
1.01
2.05
2.18
5.72
2.03
f1 (ppm)

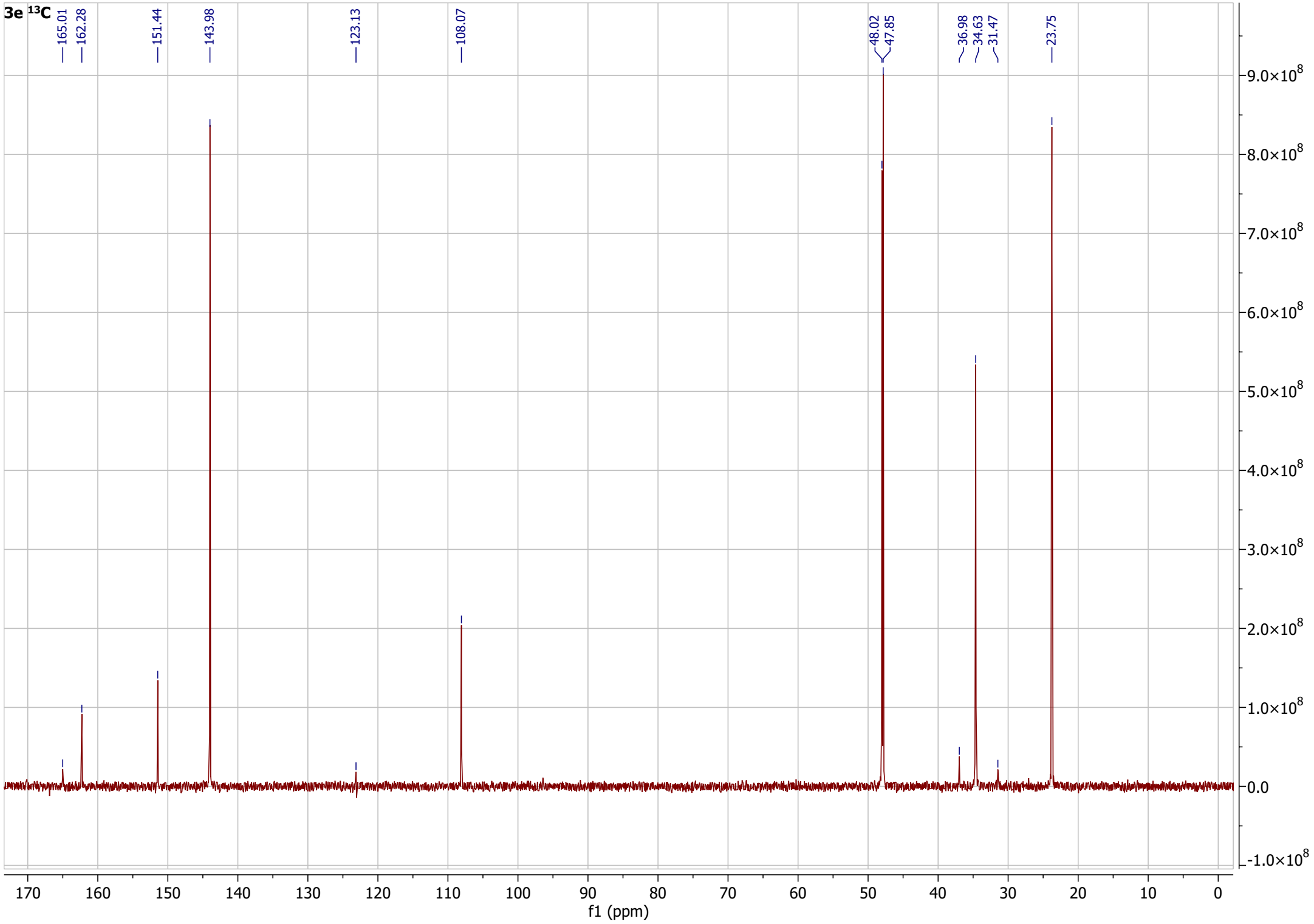

3d ^{13}C
162.30
151.57
146.42
95.60
47.89
47.73
34.49
23.70
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

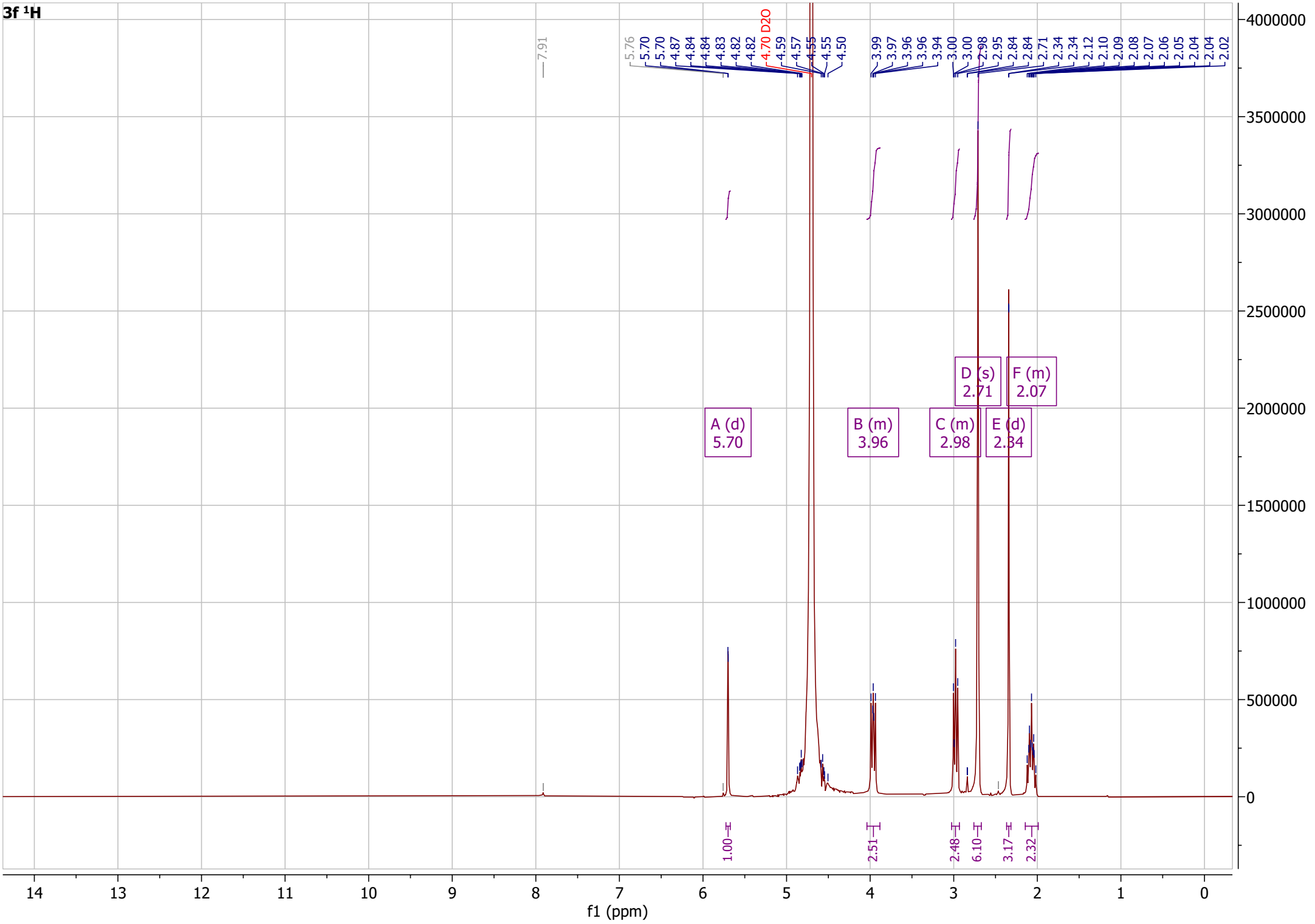

3d ¹H
8.07
8.06
8.06
4.70
4.69 D2O
3.91
3.89
3.86
2.95
2.93
2.90
2.86
2.69
2.45
2.15
2.12
2.10
2.07
2.05
A (m)
8.06
B (t)
3.89
C (t)
2.93
D (s)
2.69
E (p)
2.10
1.00
2.10
2.17
5.85
2.20
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

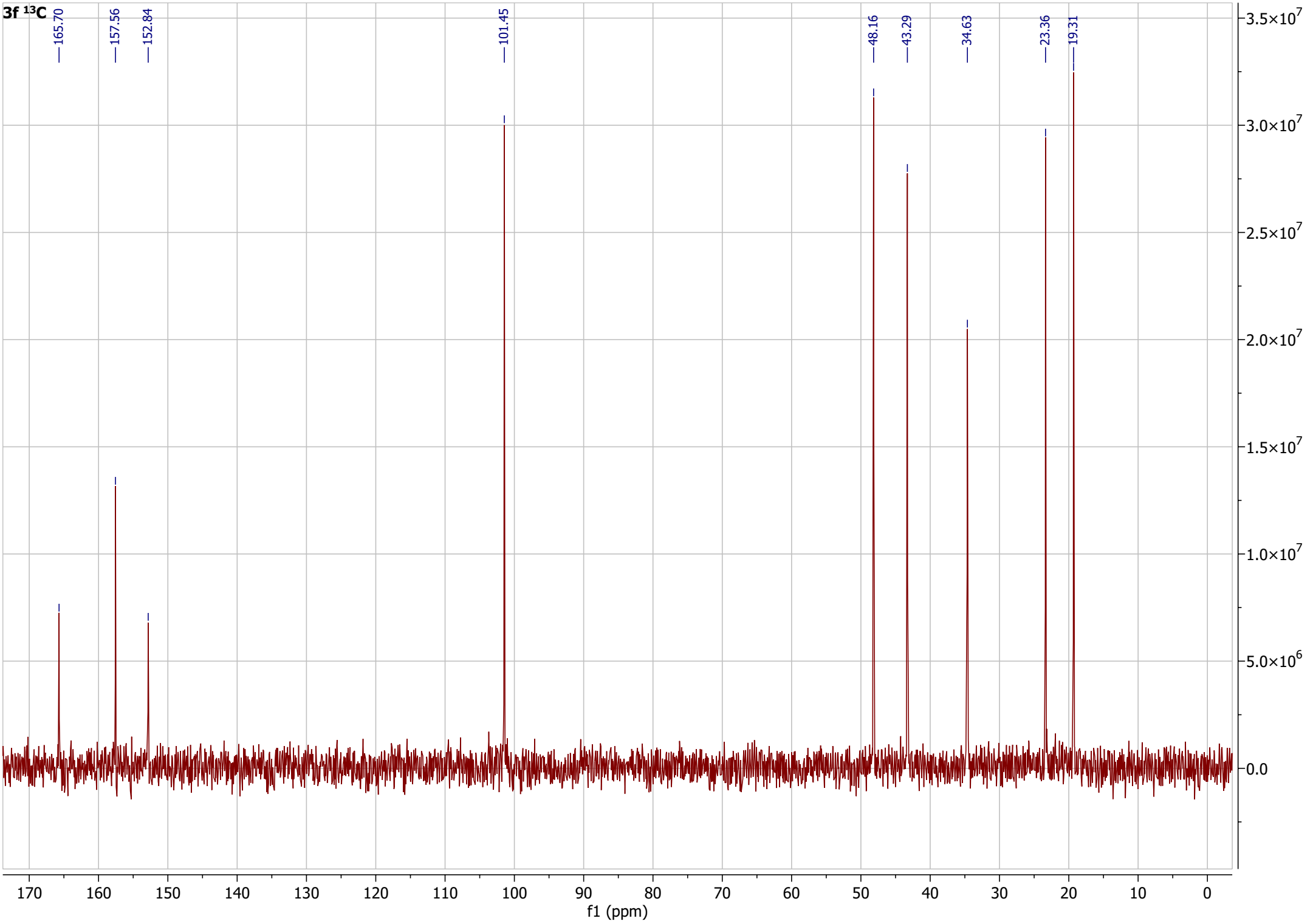

3d ^{13}C
162.32
151.65
146.50
95.68
48.01
47.87
34.67
23.81
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

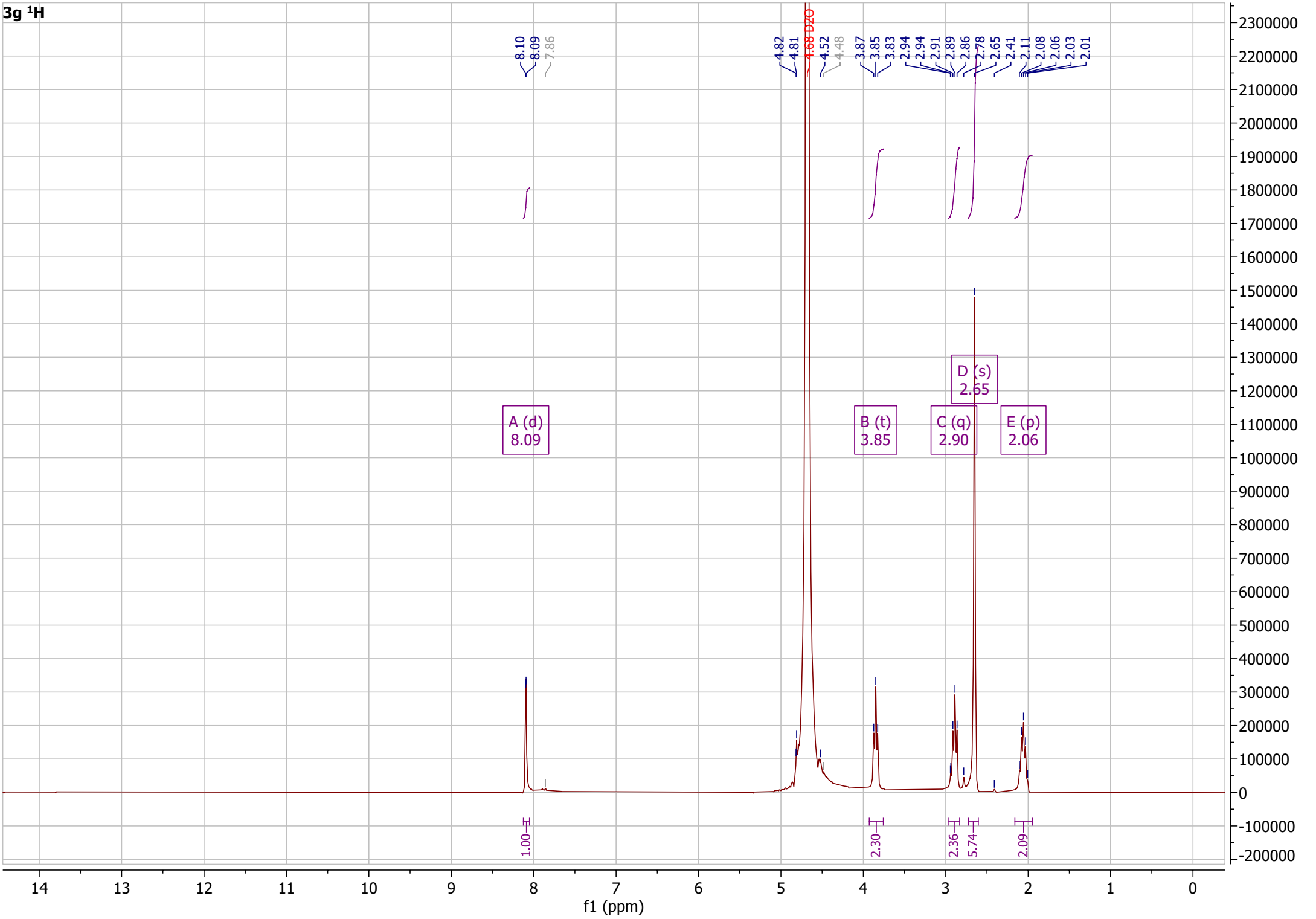

3d ¹H
8.02
8.01
7.23
4.75
4.69 D2O
4.54
3.86
3.84
3.81
2.90
2.87
2.84
2.63
2.63
2.55
2.39
2.09
2.07
2.04
2.02
1.99
A (d) 8.02
B (t) 3.84
C (t) 2.87
D (d) 2.63
E (s) 2.55
F (p) 2.04
0.91
2.09
2.13
5.88
0.82
2.18
f1 (ppm)

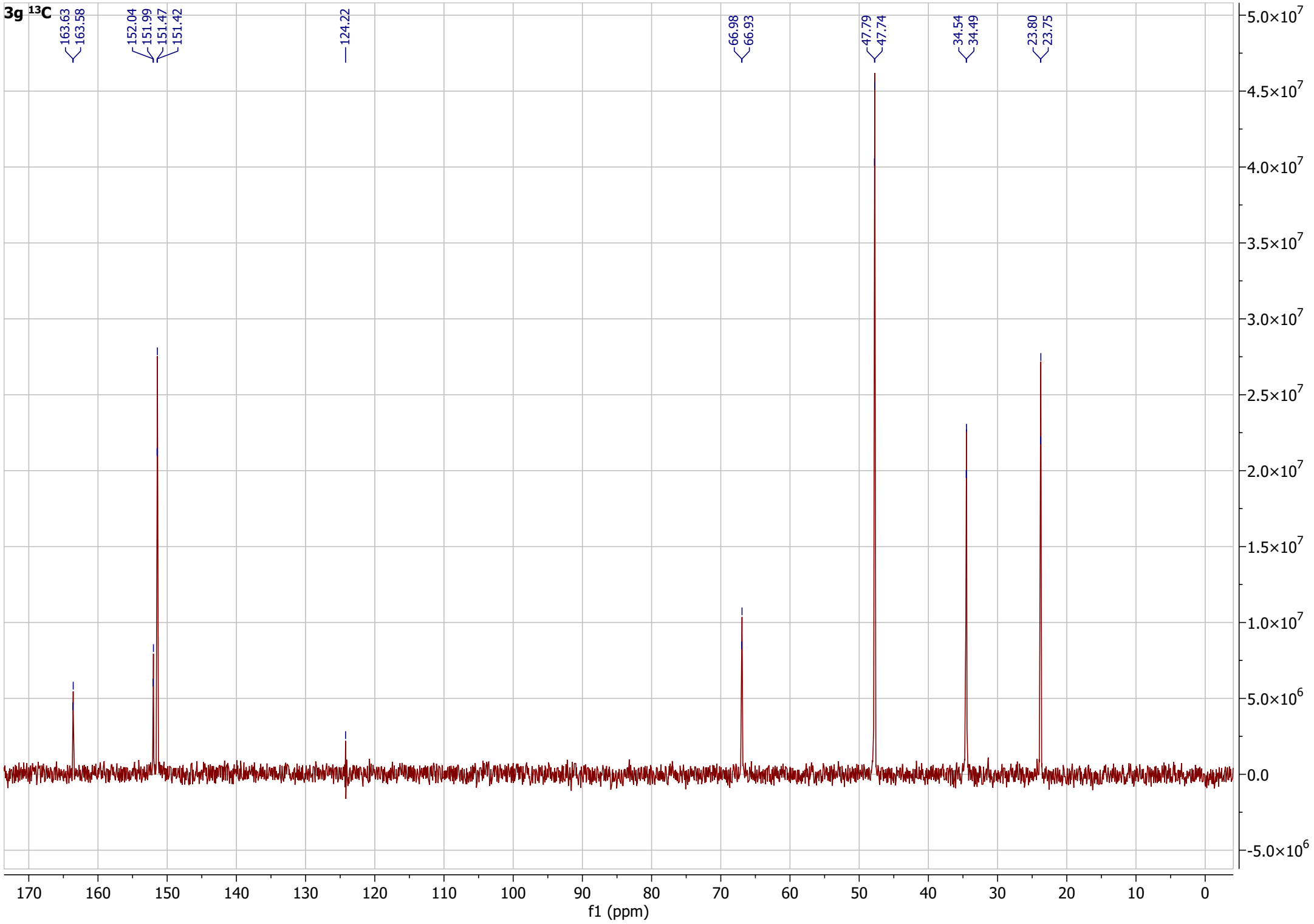

3e ¹H
7.97
7.96
7.96
7.96
7.95
7.95
4.71
4.70 D2O
4.70
3.91
3.88
3.87
3.86
3.85
2.95
2.94
2.93
2.92
2.90
2.88
2.68
2.68
2.67
2.67
2.67
2.67
2.12
2.12
2.11
2.10
2.09
2.08
2.07
2.06
A (m)
7.96
B (d)
4.70
C (q)
3.88
D (m)
2.93
E (m)
2.67
F (m)
2.10
1.01
3.91
2.05
2.21
5.77
2.06
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


3e ^{13}C
165.01
162.28
151.44
143.98
123.13
108.07
48.02
47.85
36.98
34.63
31.47
23.75
9.0×10^8
8.0×10^8
7.0×10^8
6.0×10^8
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
-1.0×10^8
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

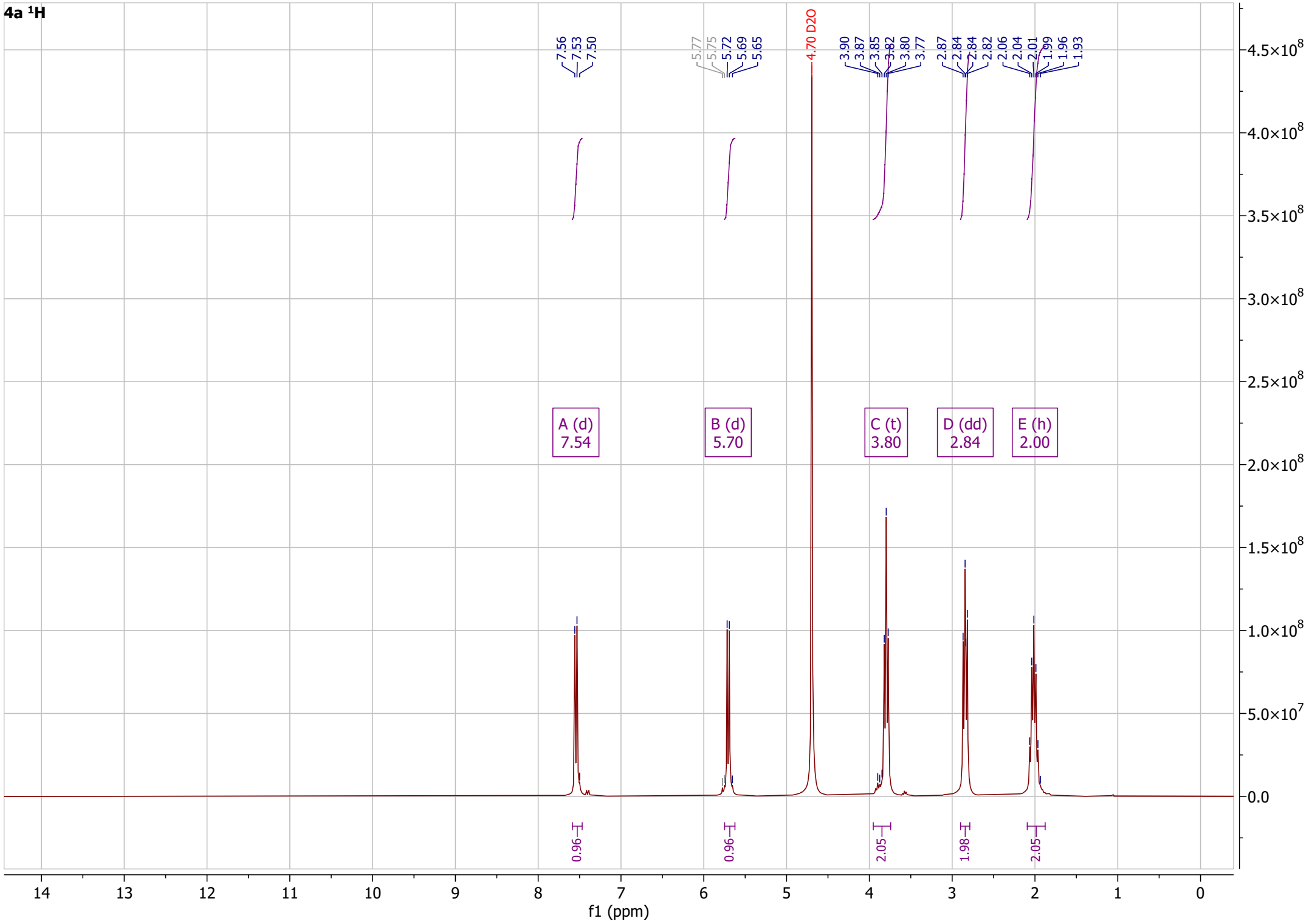

3f ¹H
7.91
5.76
5.70
5.70
4.87
4.84
4.84
4.83
4.82
4.82
4.70 D2O
4.59
4.57
4.55
4.55
4.50
3.99
3.97
3.96
3.96
3.94
3.00
3.00
2.98
2.95
2.84
2.84
2.71
2.34
2.34
2.12
2.10
2.09
2.08
2.07
2.06
2.05
2.04
2.04
2.02
A (d)
5.70
B (m)
3.96
C (m)
2.98
D (s)
2.71
E (d)
2.84
F (m)
2.07
1.00
2.51
2.48
6.10
3.17
2.32
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

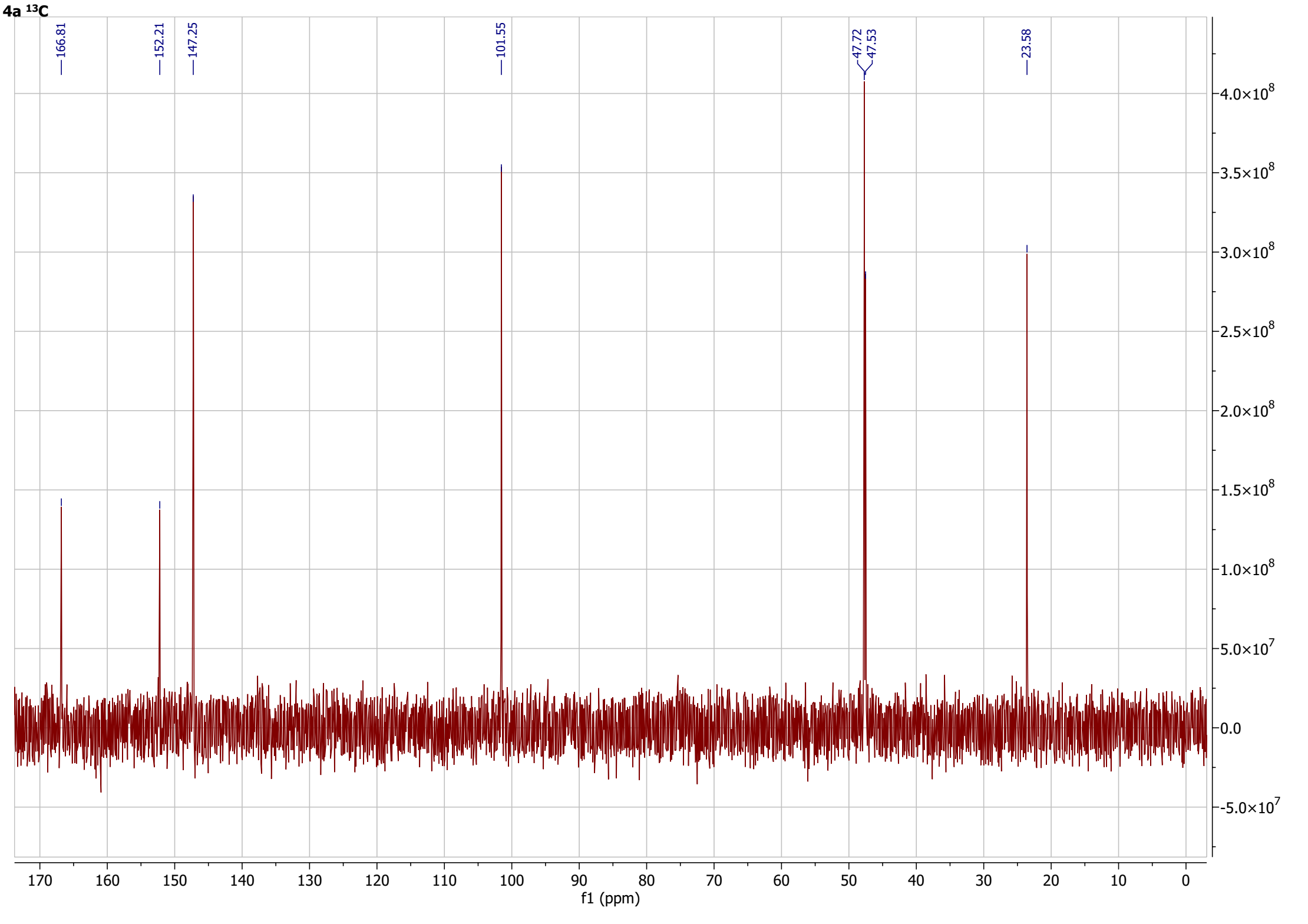

3f ^{13}C
165.70
157.56
152.84
101.45
48.16
43.29
34.63
23.36
19.31
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

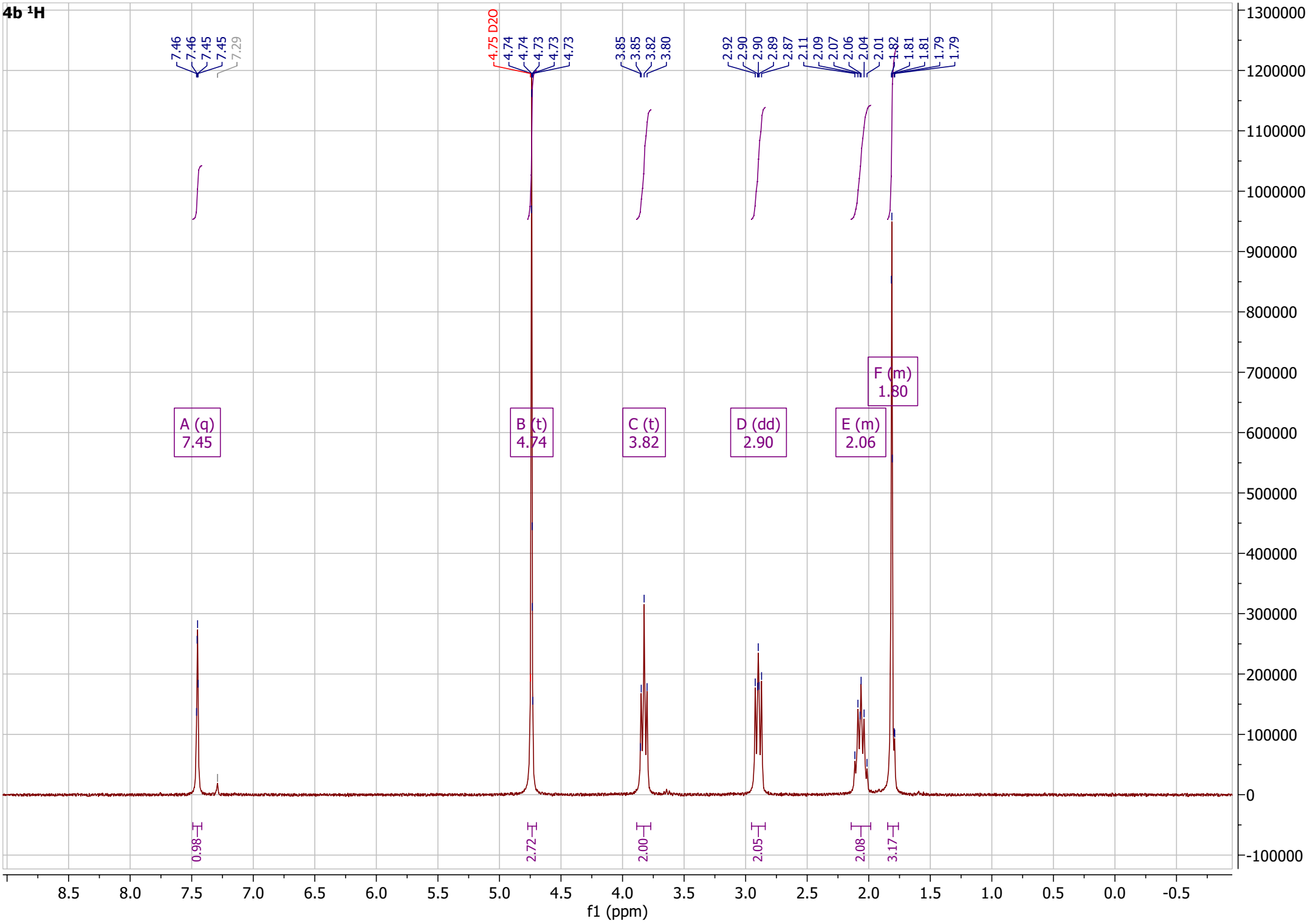

3g ¹H
8.10
8.09
7.86
4.82
4.81
4.68 D2O
4.52
4.48
3.87
3.85
3.83
2.94
2.94
2.91
2.89
2.86
2.78
2.65
2.41
2.11
2.08
2.06
2.03
2.01
A (d)
8.09
B (t)
3.85
C (q)
2.90
D (s)
2.65
E (p)
2.06
1.00
2.30
2.36
5.74
2.09
f1 (ppm)

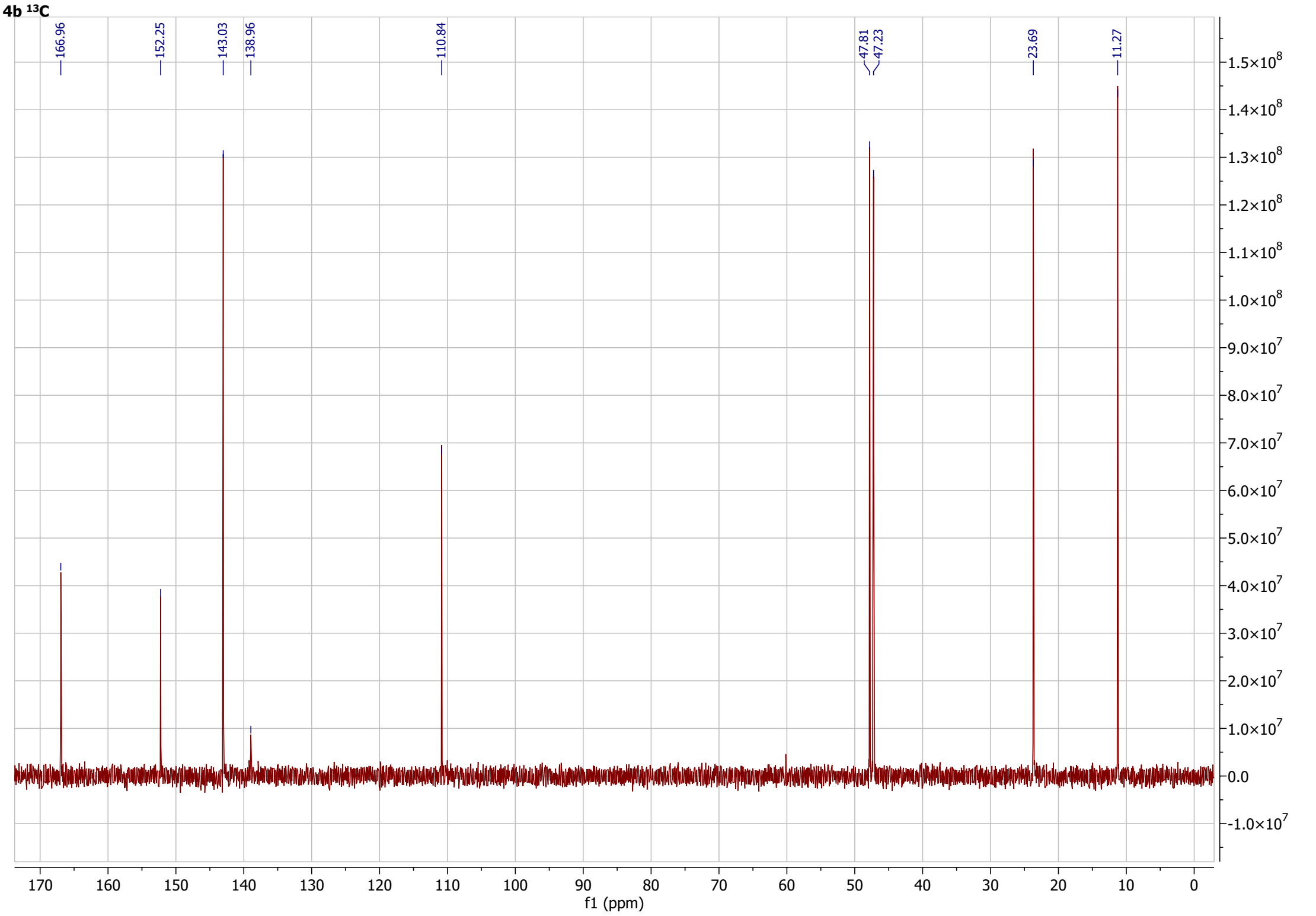

3g ^{13}C
163.63
163.58
152.04
151.99
151.47
151.42
124.22
66.98
66.93
47.79
47.74
34.54
34.49
23.80
23.75
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

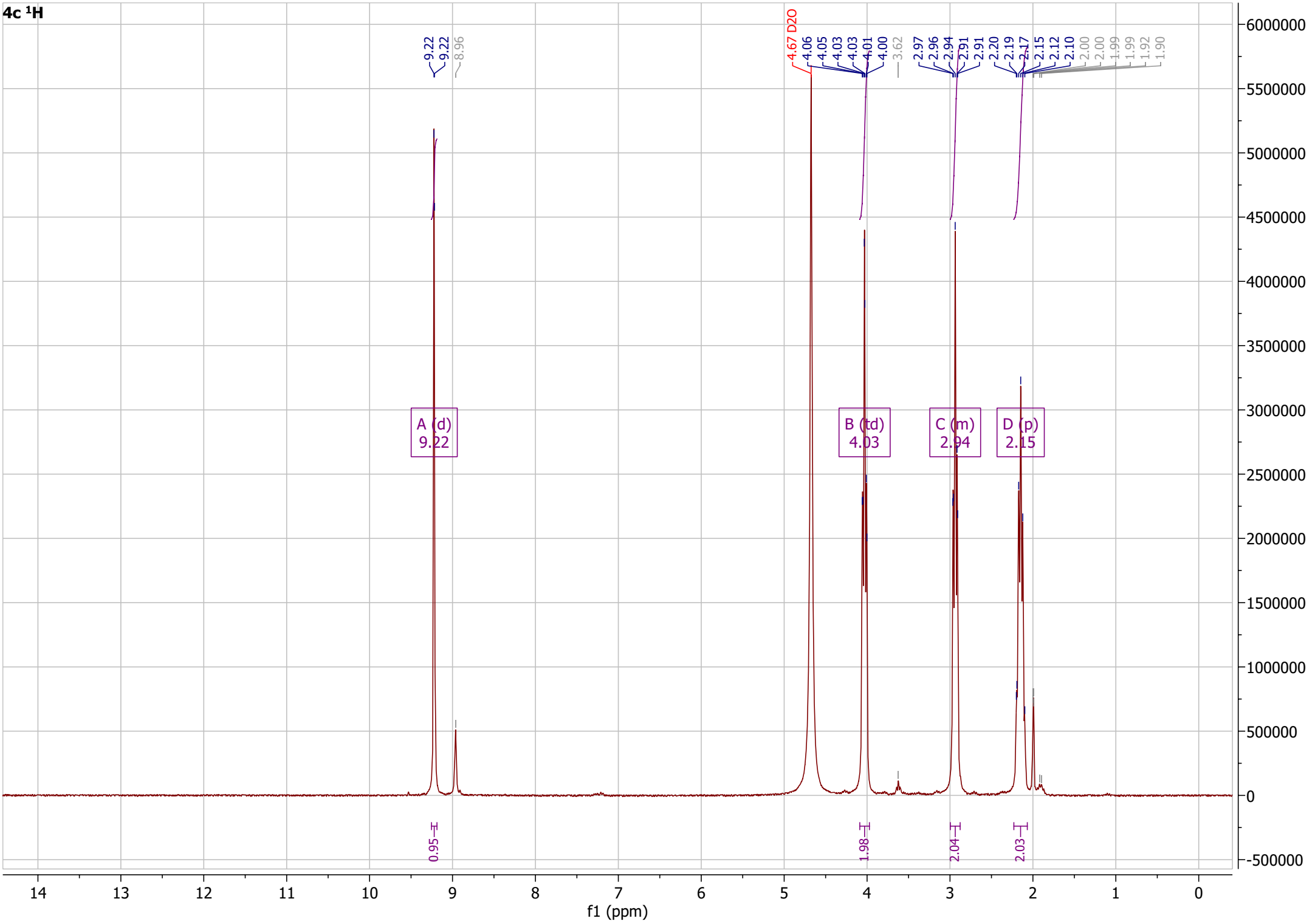
Compounds **4a-g**

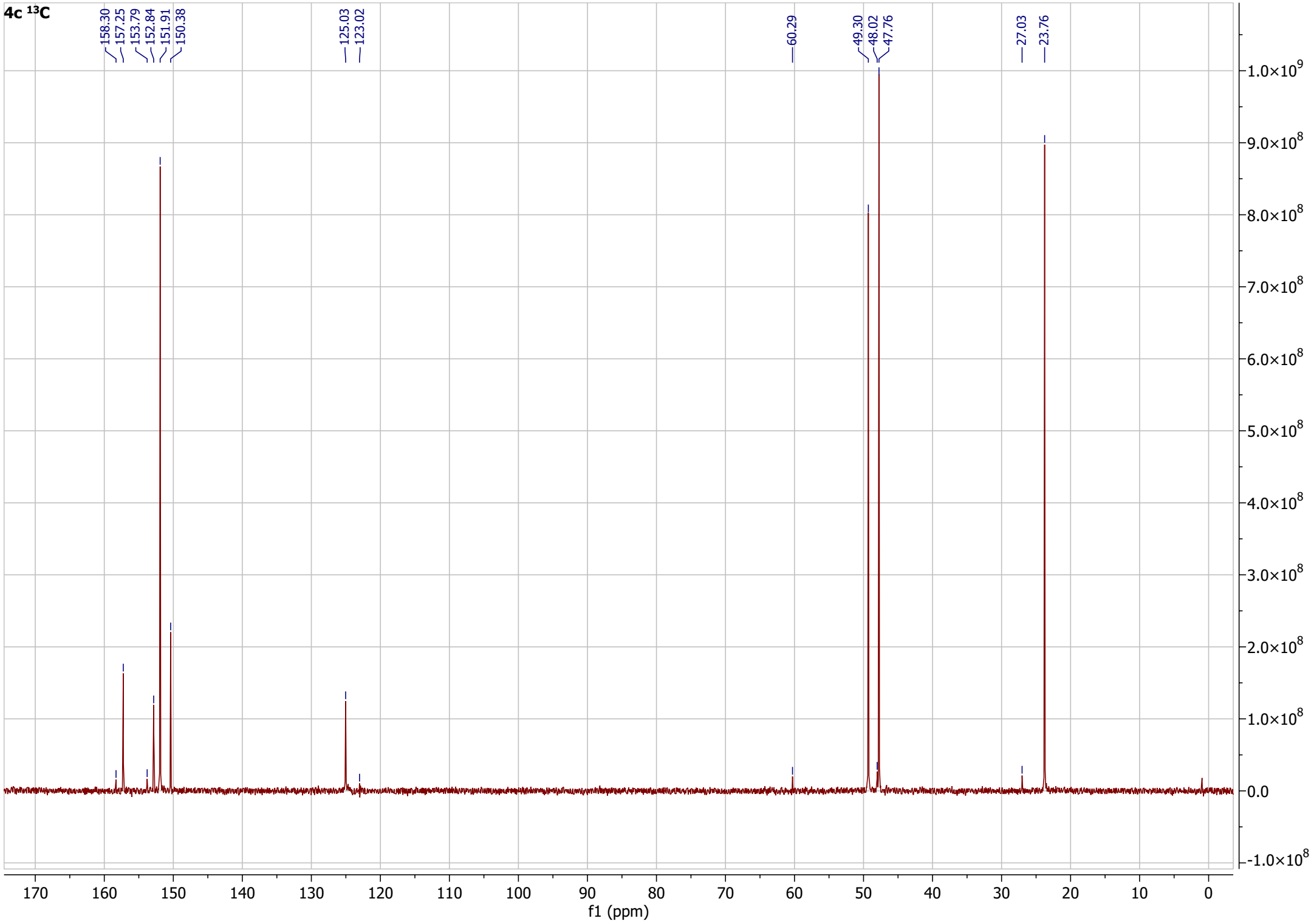

4a ¹H
7.56
7.53
7.50
5.77
5.75
5.72
5.69
5.65
4.70 D2O
3.90
3.87
3.85
3.82
3.80
3.77
2.87
2.84
2.84
2.82
2.06
2.04
2.01
1.99
1.96
1.93
A (d)
7.54
B (d)
5.70
C (t)
3.80
D (dd)
2.84
E (h)
2.00
0.96
0.96
2.05
1.98
2.05
4.5×10^8
4.0×10^8
3.5×10^8
3.0×10^8
2.5×10^8
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0.0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

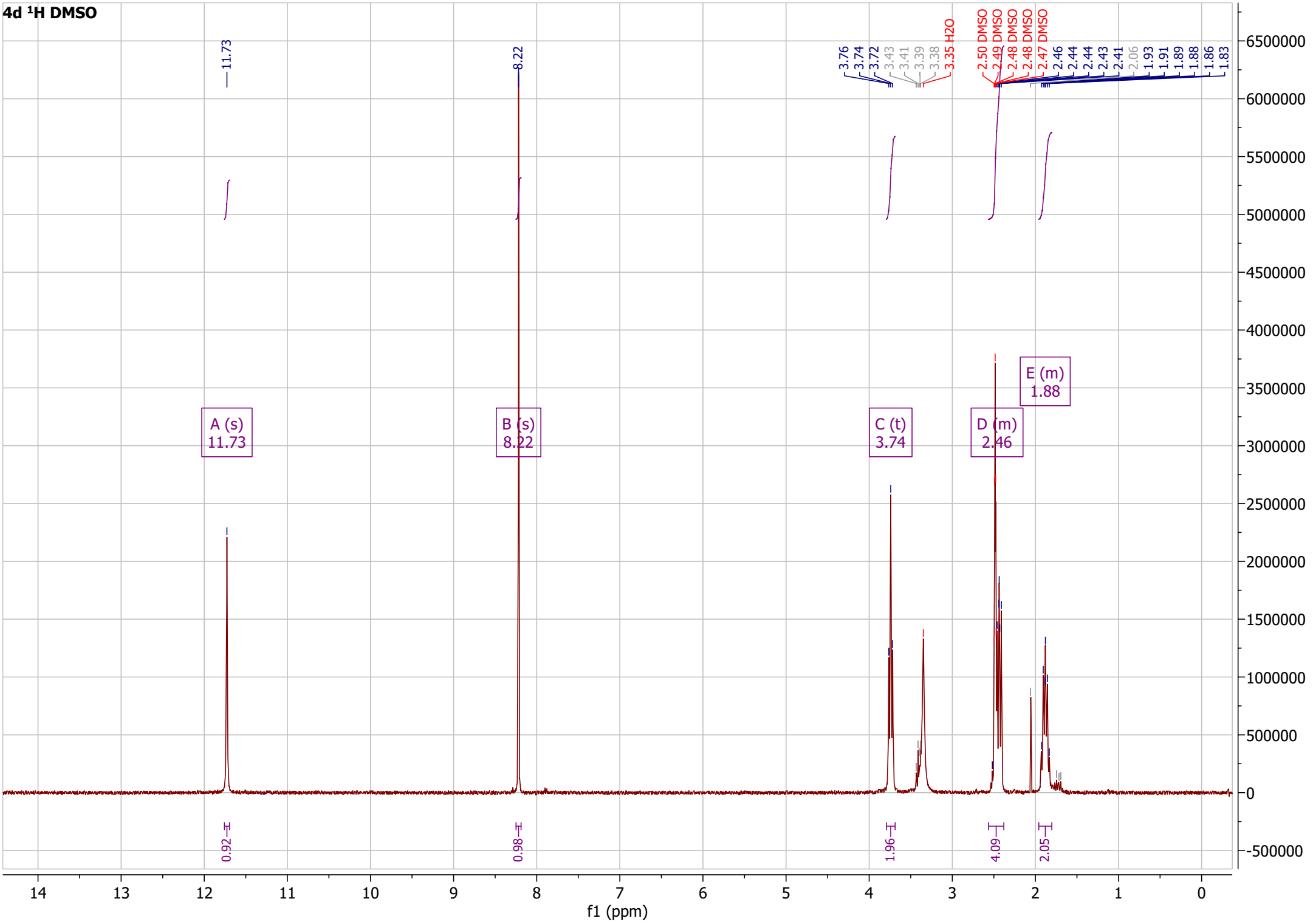

4a ^{13}C
166.81
152.21
147.25
101.55
47.72
47.53
23.58
4.0×10^8
3.5×10^8
3.0×10^8
2.5×10^8
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0.0
-5.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

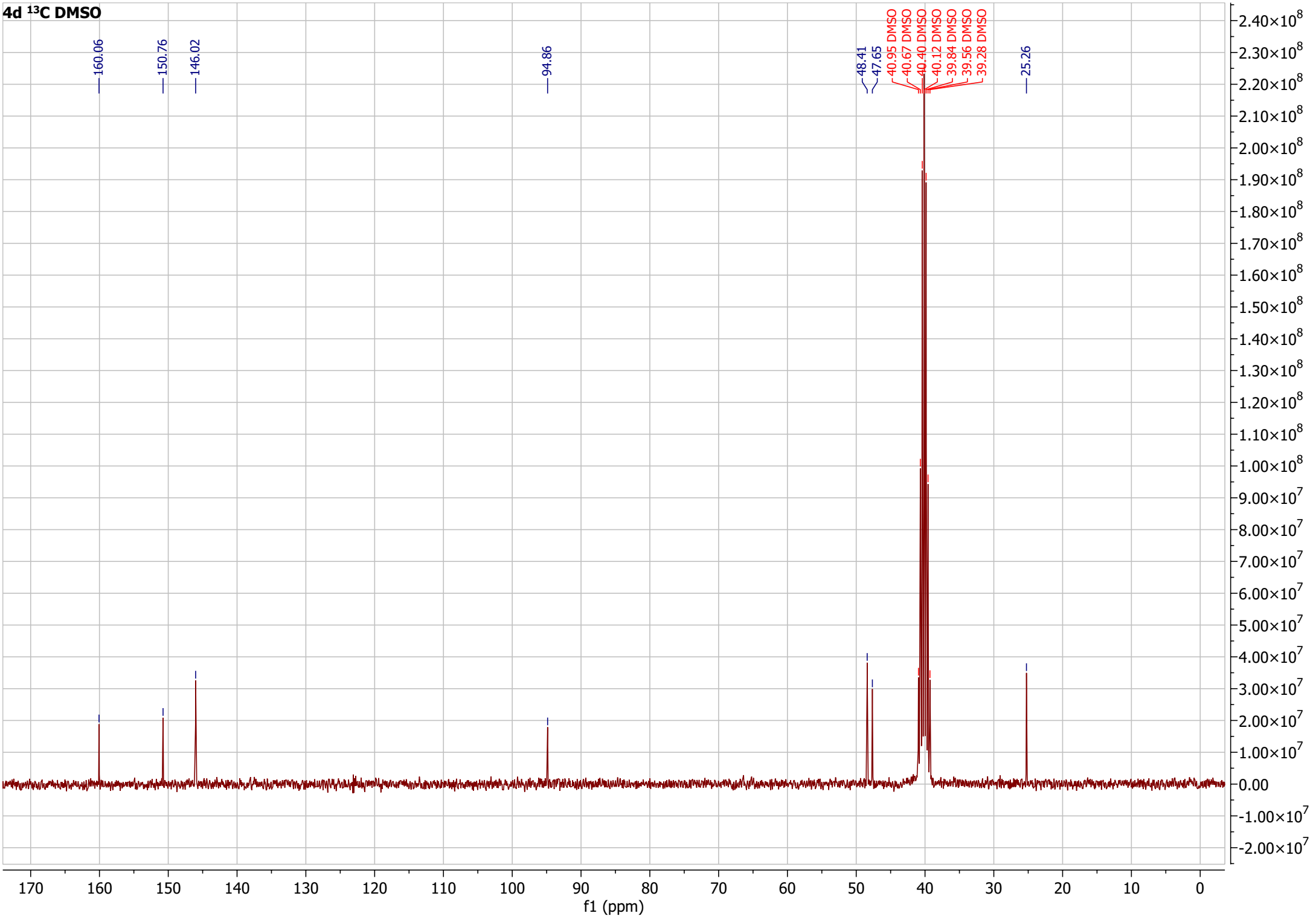

4b ¹H
7.46
7.46
7.45
7.45
7.29
4.75 D2O
4.74
4.74
4.73
4.73
4.73
3.85
3.85
3.82
3.80
2.92
2.90
2.90
2.89
2.87
2.11
2.09
2.07
2.06
2.04
2.01
1.82
1.81
1.81
1.79
1.79
A (q)
7.45
B (t)
4.74
C (t)
3.82
D (dd)
2.90
E (m)
2.06
F (m)
1.80
0.98
2.72
2.00
2.05
2.08
3.17
f1 (ppm)

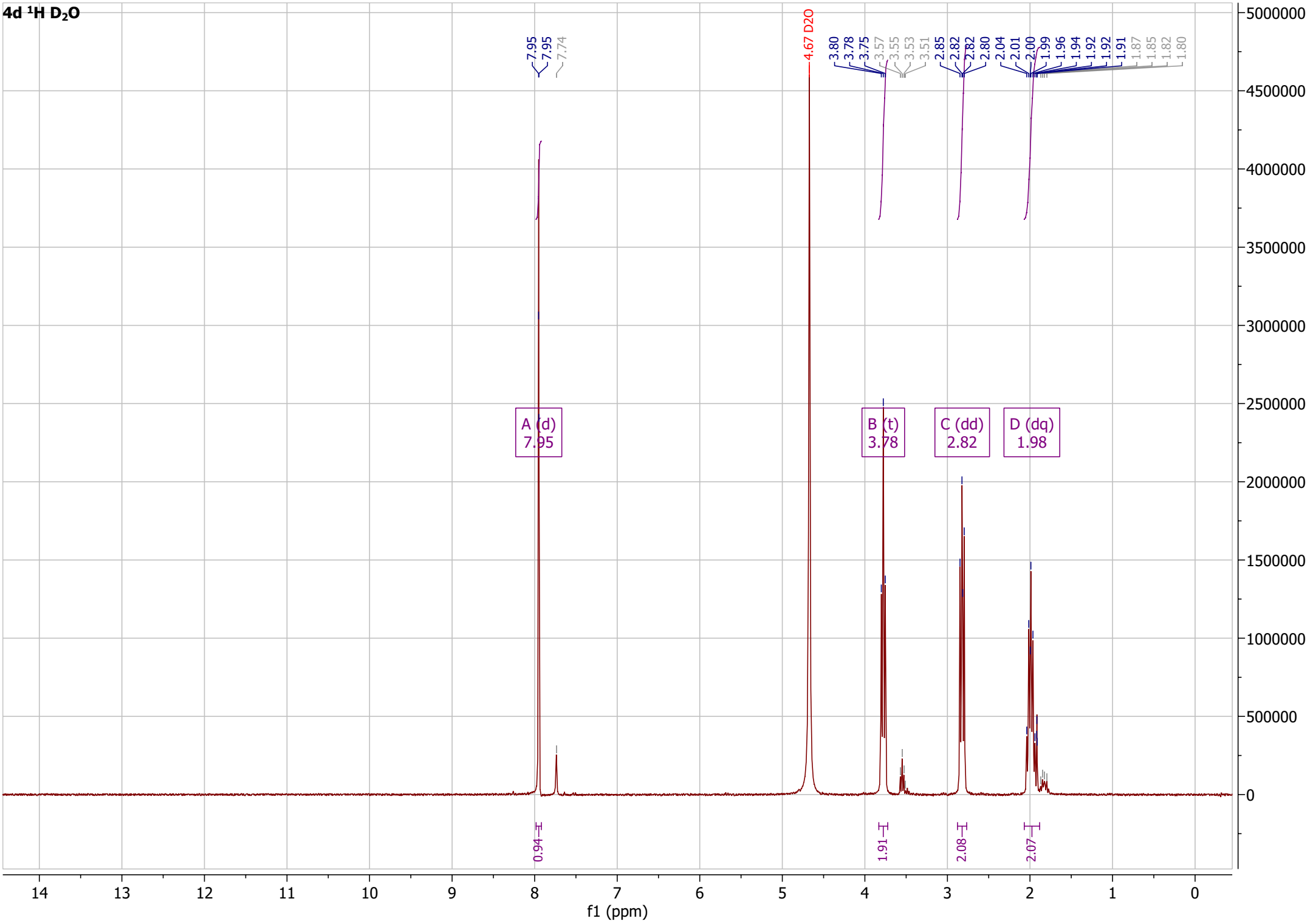

4b ¹³C
166.96
152.25
143.03
138.96
110.84
47.81
47.23
23.69
11.27
1.5×10^8
1.4×10^8
1.3×10^8
1.2×10^8
1.1×10^8
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4c ¹H
9.22
9.22
8.96
4.67 D2O
4.06
4.05
4.03
4.03
4.01
4.00
3.62
2.97
2.96
2.94
2.91
2.91
2.20
2.19
2.17
2.15
2.12
2.10
2.00
2.00
1.99
1.99
1.92
1.90
A (d)
9.22
B (td)
4.03
C (m)
2.94
D (p)
2.15
0.95
1.98
2.04
2.03
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
-500000
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

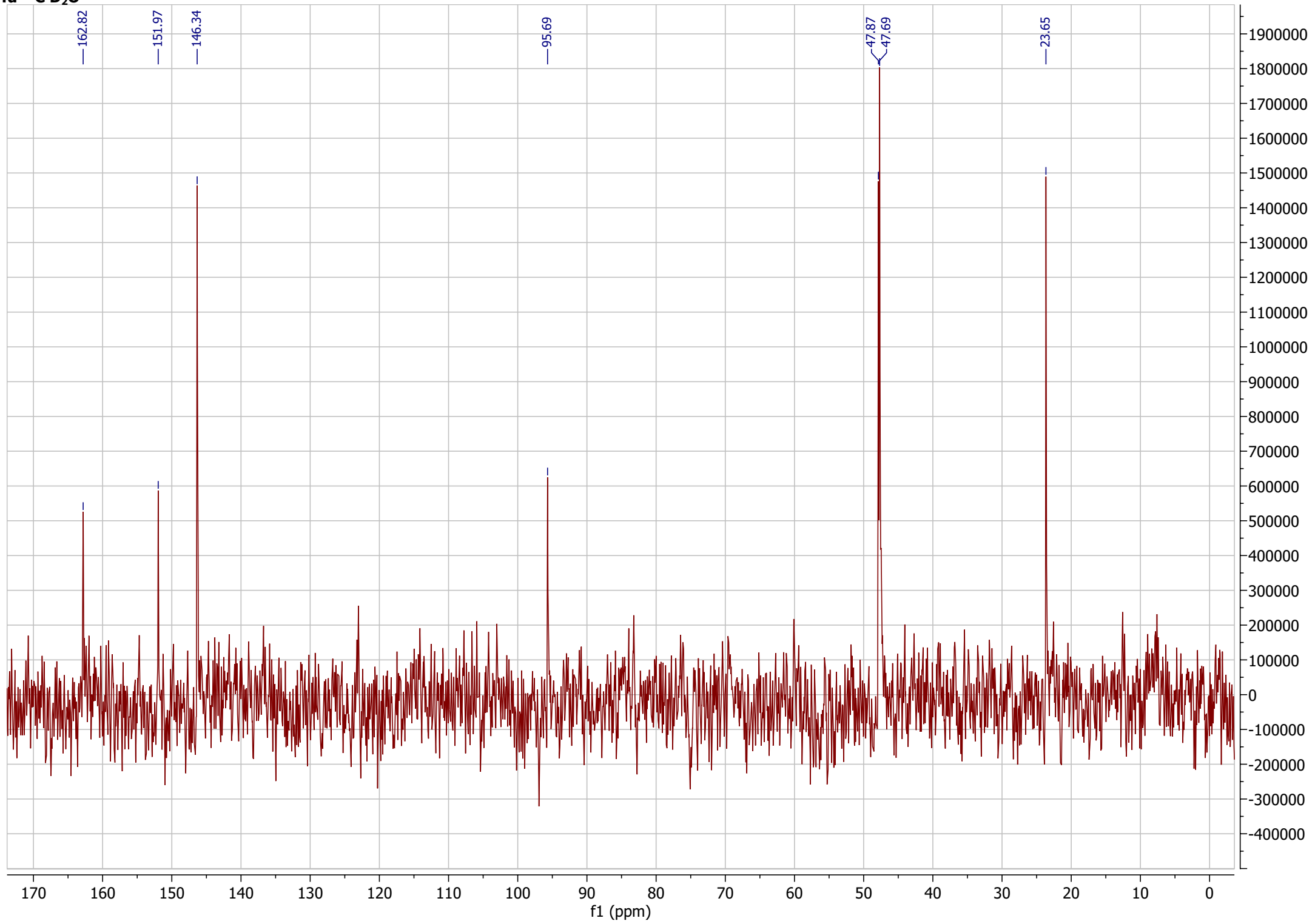

4c ^{13}C
158.30
157.25
153.79
152.84
151.91
150.38
125.03
123.02
60.29
49.30
48.02
47.76
27.03
23.76
1.0×10^9
9.0×10^8
8.0×10^8
7.0×10^8
6.0×10^8
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
-1.0×10^8
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

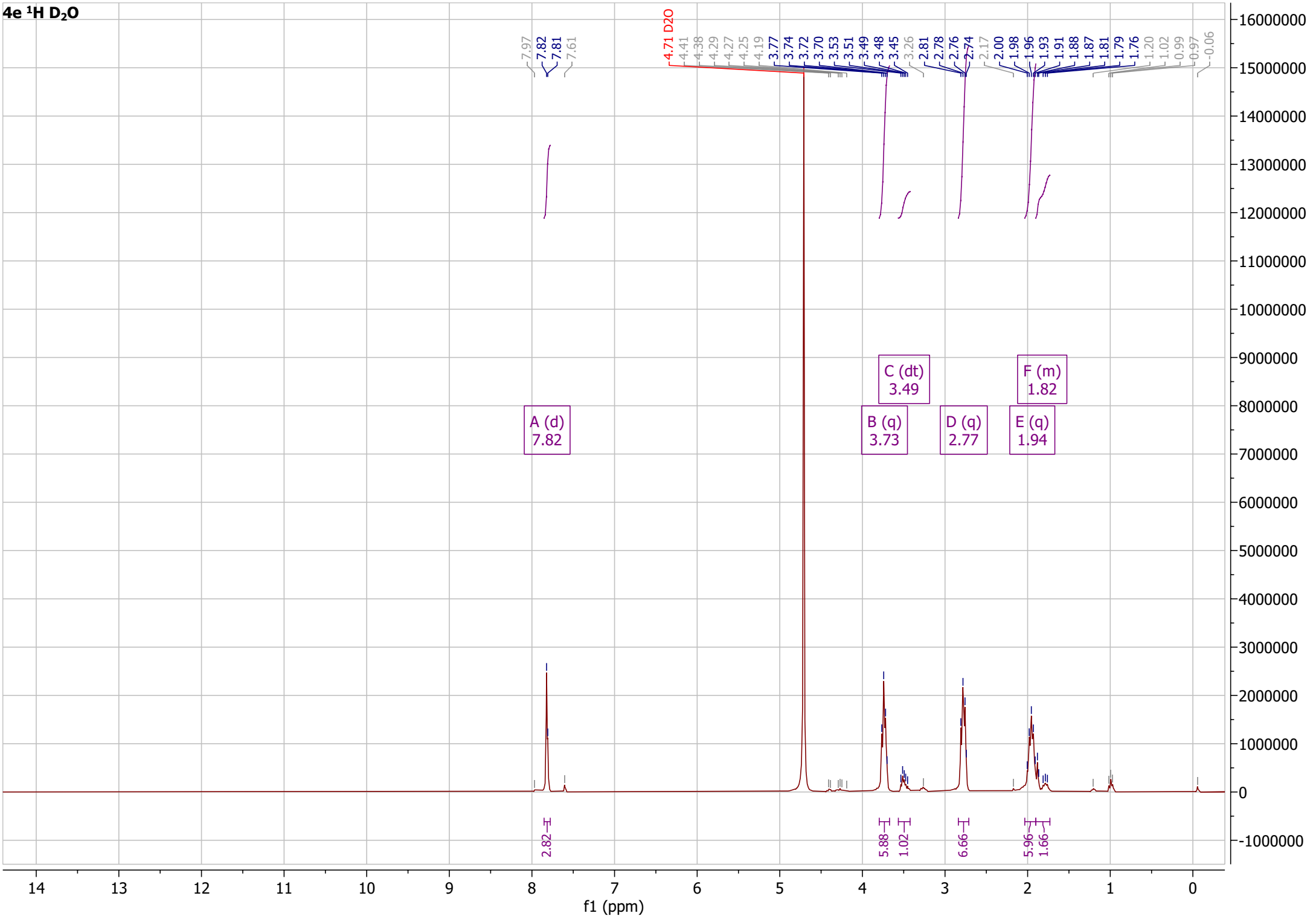

4d ¹H DMSO
11.73
8.22
3.76
3.74
3.72
3.43
3.41
3.39
3.38
3.35 H2O
2.50 DMSO
2.49 DMSO
2.48 DMSO
2.48 DMSO
2.47 DMSO
2.46
2.44
2.44
2.43
2.41
2.06
1.93
1.91
1.89
1.88
1.86
1.83
A (s)
11.73
B (s)
8.22
C (t)
3.74
D (m)
2.46
E (m)
1.88
0.92
0.98
1.96
4.09
2.05
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
-500000
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

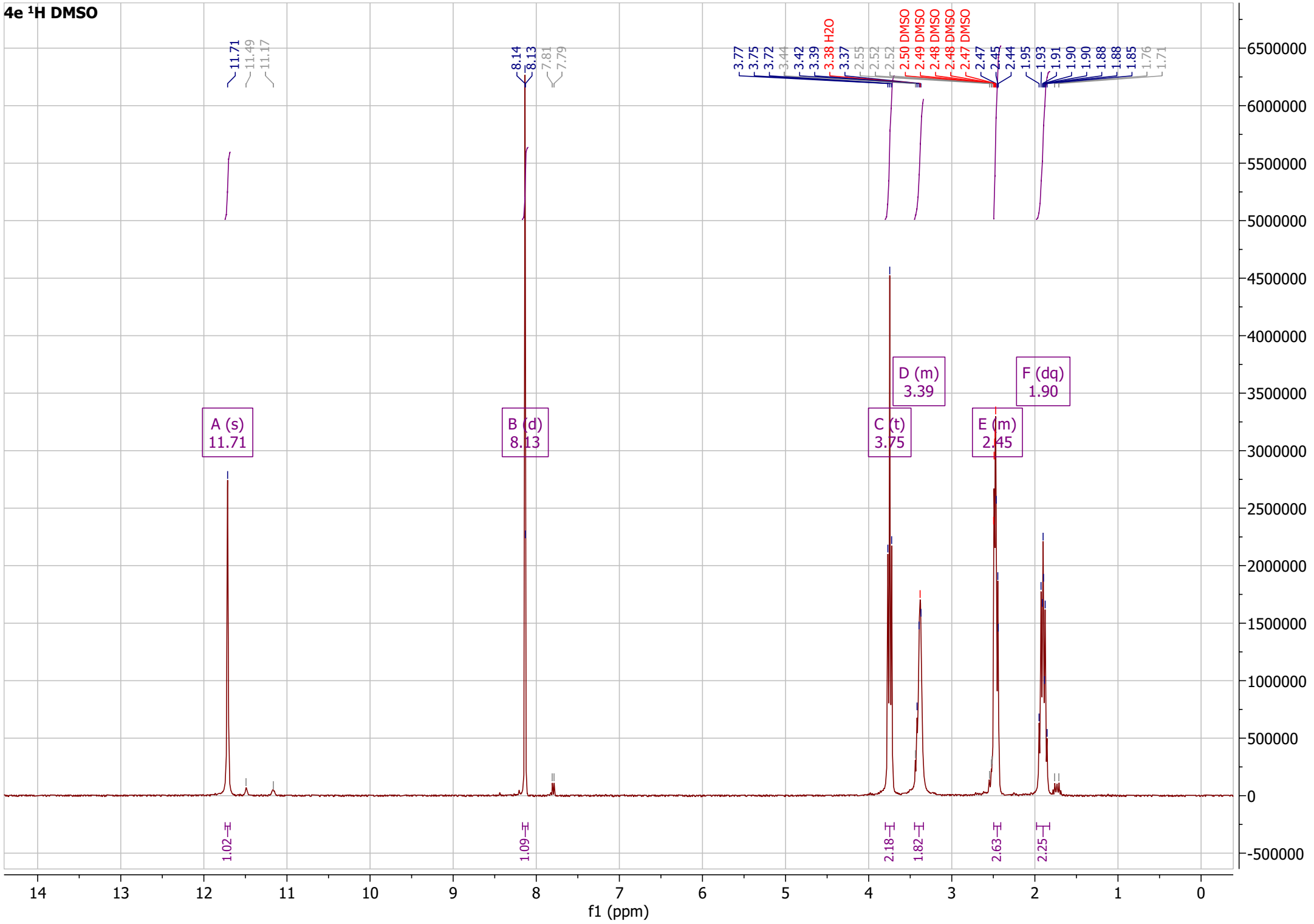

4d ¹³C DMSO
160.06
150.76
146.02
94.86
48.41
47.65
40.95 DMSO
40.67 DMSO
40.40 DMSO
40.12 DMSO
39.84 DMSO
39.56 DMSO
39.28 DMSO
25.26
f1 (ppm)

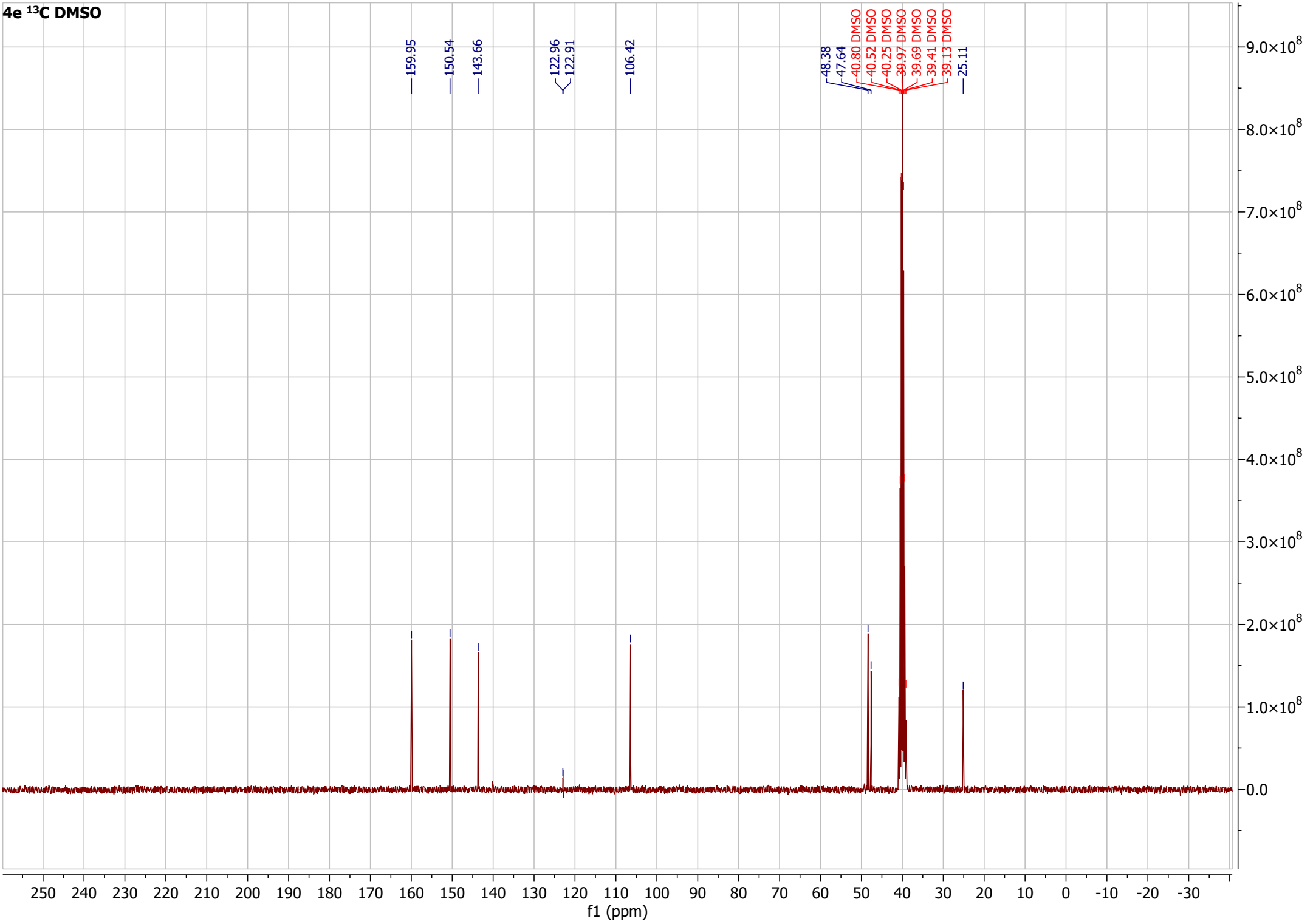

4d ¹H D₂O
7.95
7.95
7.74
4.67 D2O
3.80
3.78
3.75
3.57
3.55
3.53
3.51
2.85
2.82
2.82
2.80
2.04
2.01
2.00
1.99
1.96
1.94
1.92
1.92
1.91
1.87
1.85
1.82
1.80
A (d)
7.95
B (t)
3.78
C (dd)
2.82
D (dq)
1.98
0.94
1.91
2.08
2.07
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

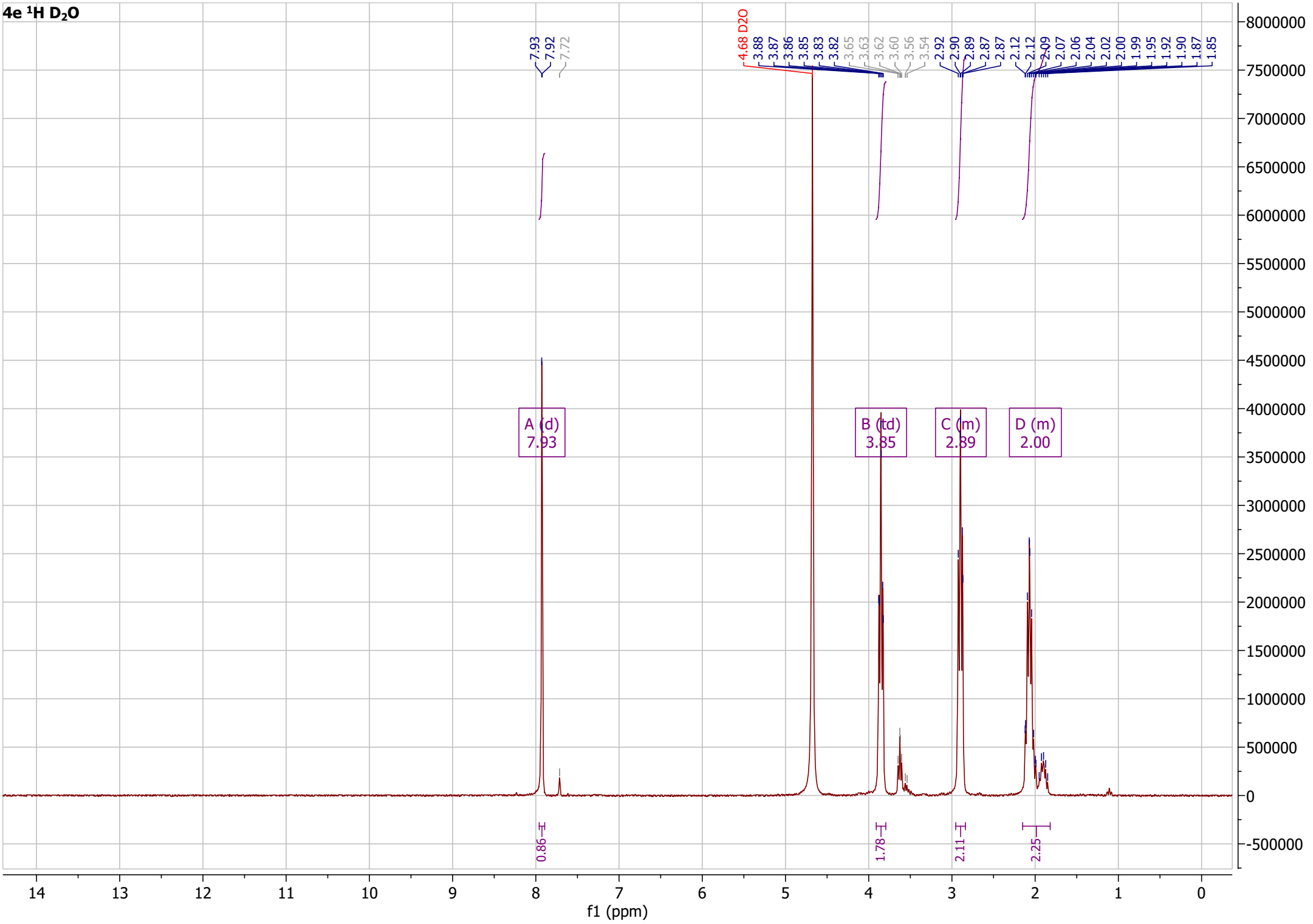
4d ^{13}C D_2O

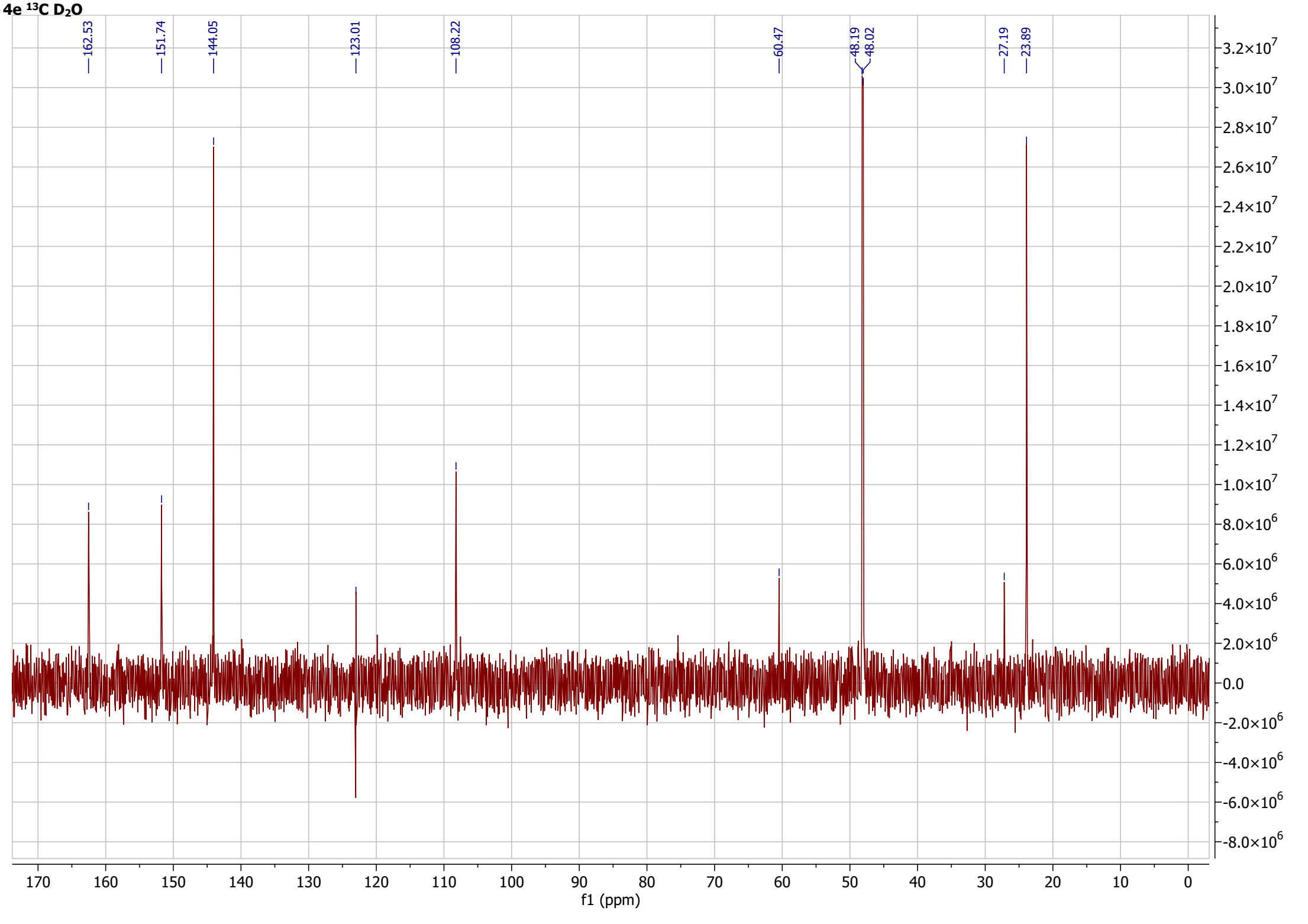

162.82
151.97
146.34
95.69
47.87
47.69
23.65
1900000
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
-200000
-300000
-400000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

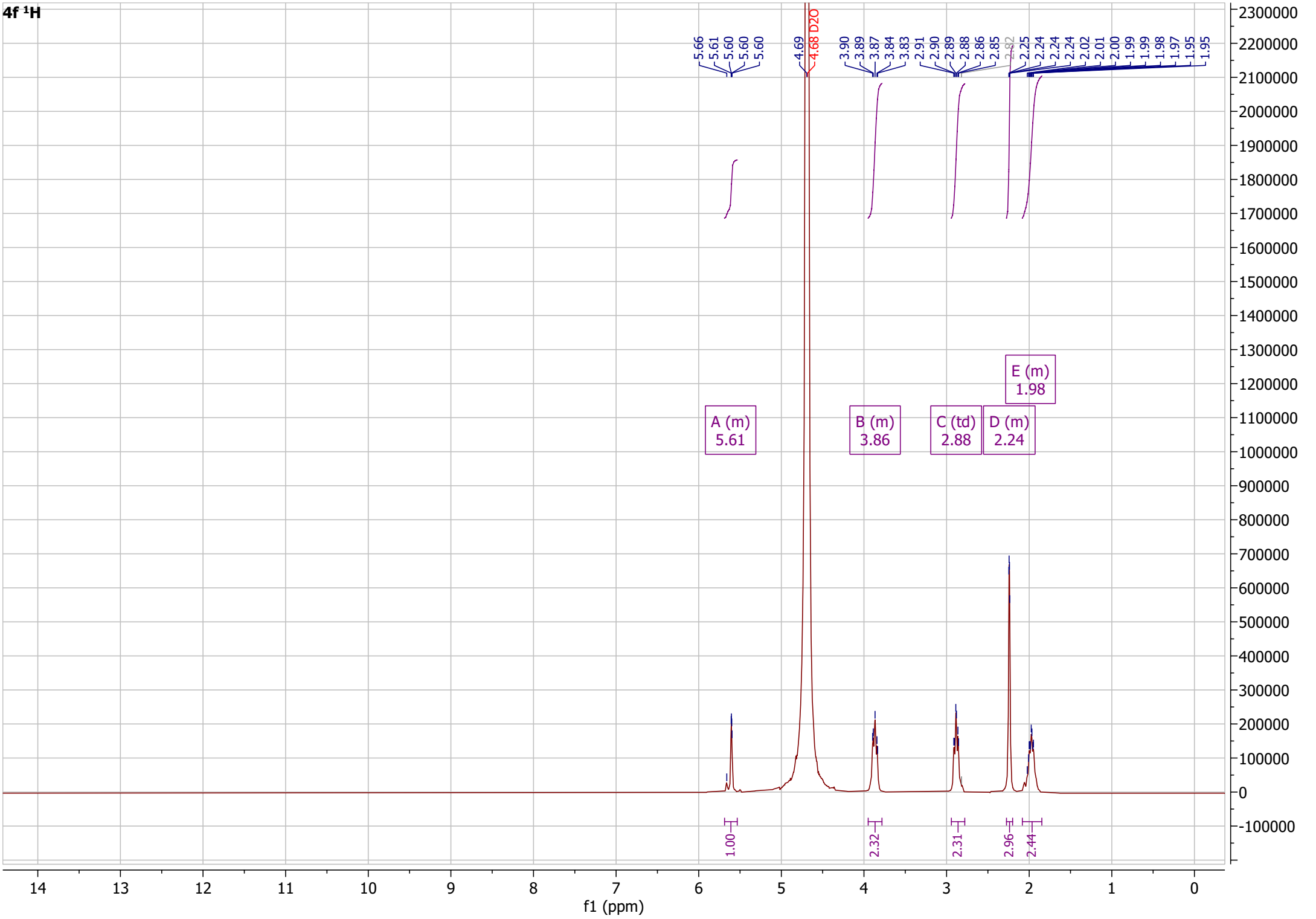

4e ¹H D₂O
4.71 D2O
A (d)
7.82
B (q)
3.73
C (dt)
3.49
D (q)
2.77
E (q)
1.94
F (m)
1.82
2.82
5.88
1.02
6.66
5.96
1.66
f1 (ppm)

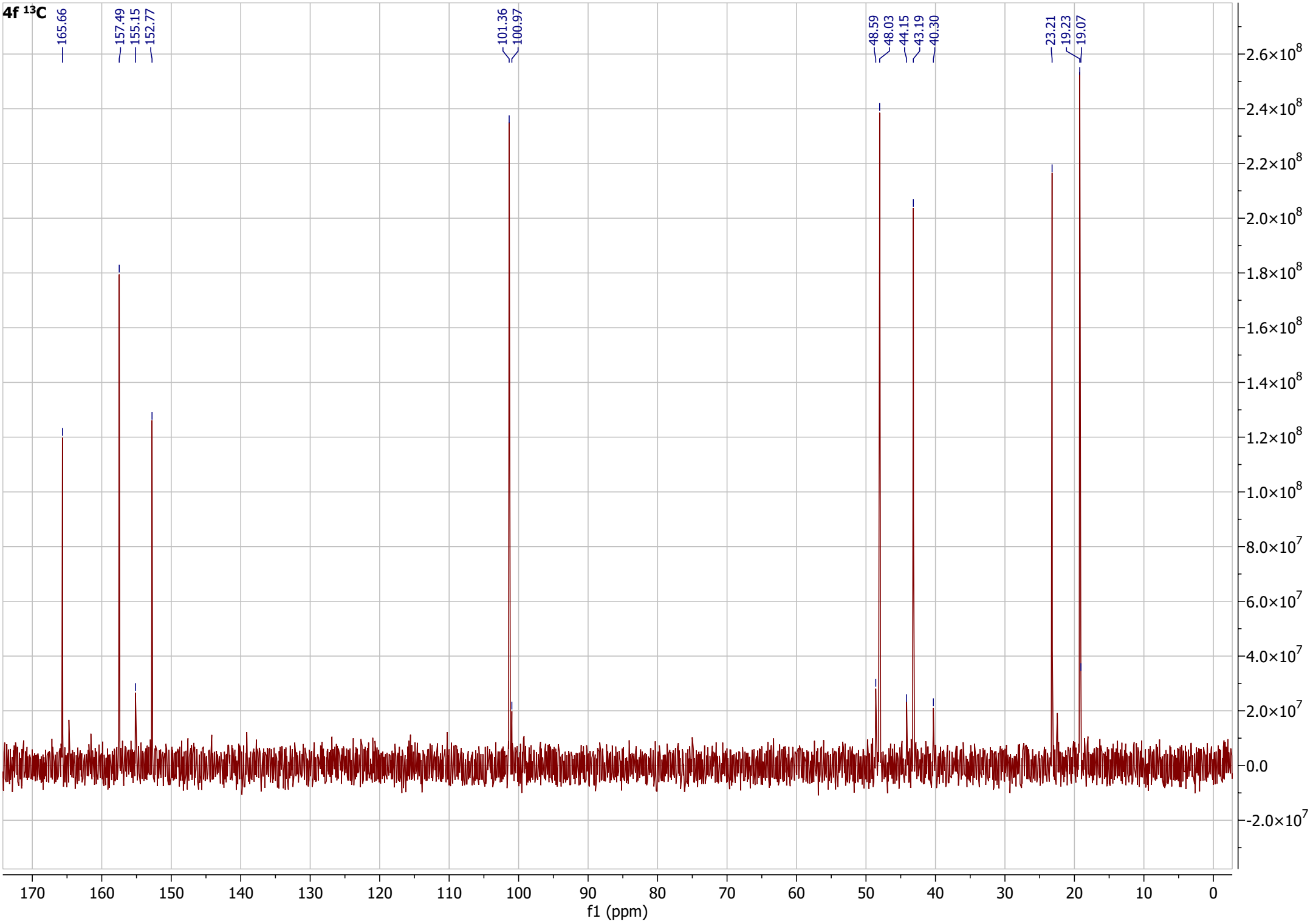

4e ¹H DMSO
11.71
11.49
11.17
8.14
8.13
7.81
7.79
3.77
3.75
3.72
3.44
3.42
3.39
3.38 H2O
3.37
2.55
2.52
2.52
2.50 DMSO
2.49 DMSO
2.48 DMSO
2.48 DMSO
2.47 DMSO
2.47
2.45
2.44
1.95
1.93
1.91
1.90
1.90
1.88
1.88
1.85
1.76
1.71
A (s)
11.71
B (d)
8.13
C (t)
3.75
D (m)
3.39
E (m)
2.45
F (dq)
1.90
1.02
1.09
2.18
1.82
2.63
2.25
f1 (ppm)

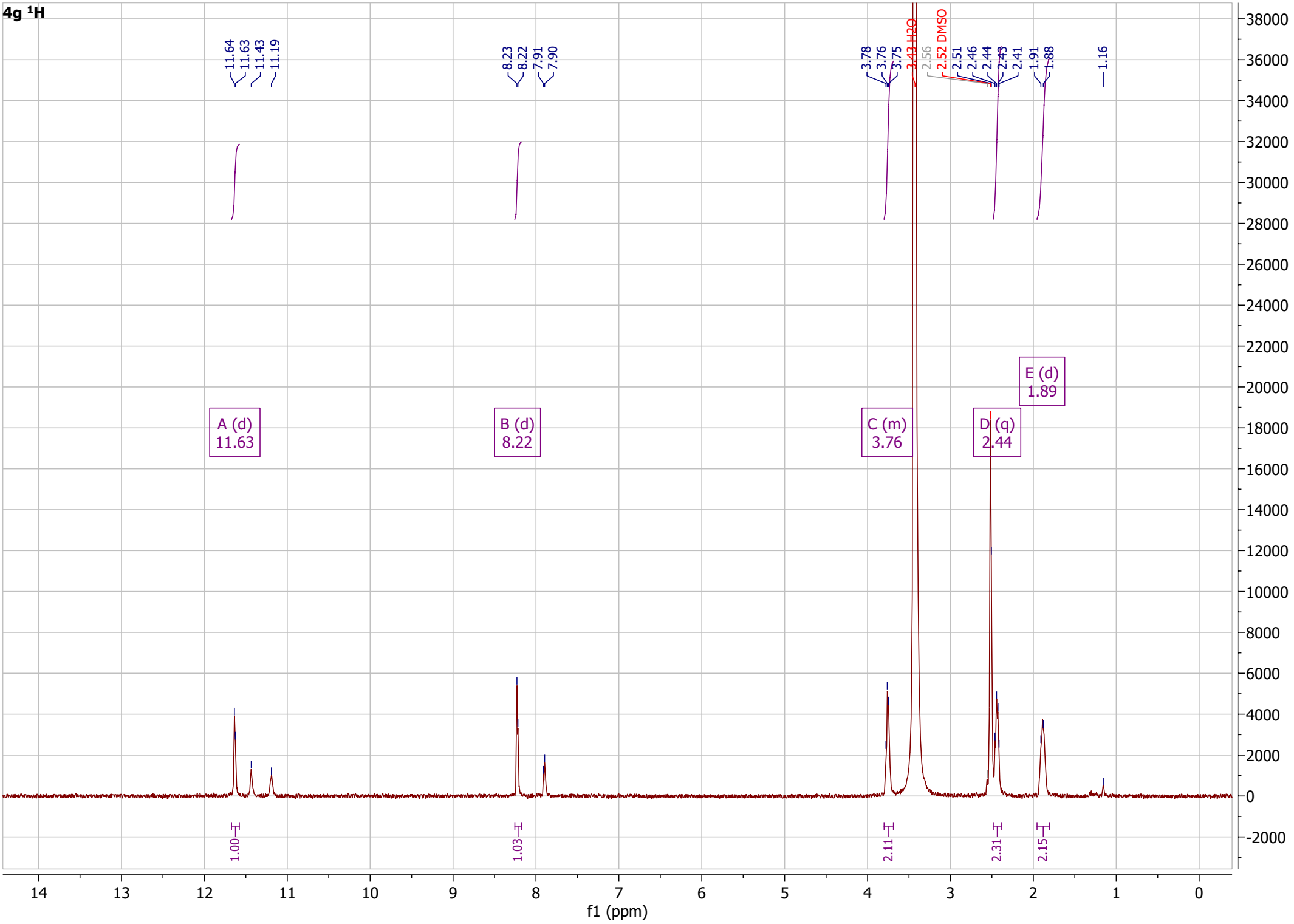

4e ¹³C DMSO
159.95
150.54
143.66
122.96
122.91
106.42
48.38
47.64
40.80 DMSO
40.52 DMSO
40.25 DMSO
39.97 DMSO
39.69 DMSO
39.41 DMSO
39.13 DMSO
25.11
9.0×10⁸
8.0×10⁸
7.0×10⁸
6.0×10⁸
5.0×10⁸
4.0×10⁸
3.0×10⁸
2.0×10⁸
1.0×10⁸
0.0
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)

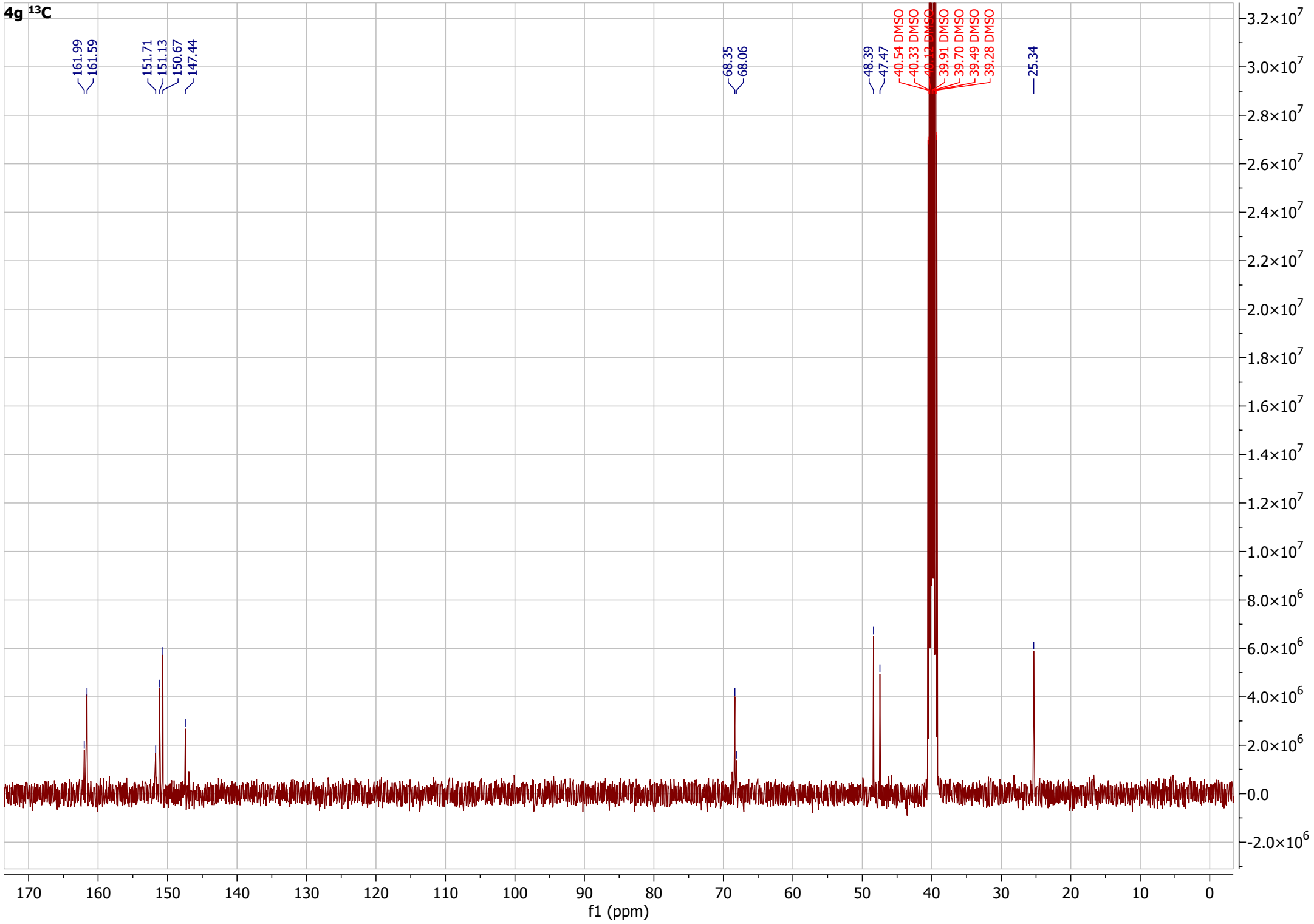

4e ¹H D₂O
4.68 D2O
3.88
3.87
3.86
3.85
3.83
3.82
3.65
3.63
3.62
3.60
3.56
3.54
2.92
2.90
2.89
2.87
2.87
2.12
2.12
2.09
2.07
2.06
2.04
2.02
2.00
1.99
1.95
1.92
1.90
1.87
1.85
7.93
7.92
7.72
A (d)
7.93
B (td)
3.85
C (m)
2.89
D (m)
2.00
0.86
1.78
2.11
2.25
f1 (ppm)


4e ^{13}C D_2O
162.53
151.74
144.05
123.01
108.22
60.47
48.19
48.02
27.19
23.89
3.2×10^7
3.0×10^7
2.8×10^7
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
-2.0×10^6
-4.0×10^6
-6.0×10^6
-8.0×10^6
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4f ¹H
5.66
5.61
5.60
5.60
5.60
4.69
4.68 D2O
3.90
3.89
3.87
3.84
3.83
2.91
2.90
2.89
2.88
2.86
2.85
2.82
2.25
2.24
2.24
2.24
2.02
2.01
2.00
1.99
1.99
1.98
1.97
1.95
1.95
A (m)
5.61
B (m)
3.86
C (td)
2.88
D (m)
2.24
E (m)
1.98
1.00
2.32
2.31
2.96
2.44
f1 (ppm)


4f ^{13}C
165.66
157.49
155.15
152.77
101.36
100.97
48.59
48.03
44.15
43.19
40.30
23.21
19.23
19.07
2.6×10^8
2.4×10^8
2.2×10^8
2.0×10^8
1.8×10^8
1.6×10^8
1.4×10^8
1.2×10^8
1.0×10^8
8.0×10^7
6.0×10^7
4.0×10^7
2.0×10^7
0.0
-2.0×10^7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4g ¹H
11.64
11.63
11.43
11.19
8.23
8.22
7.91
7.90
3.78
3.76
3.75
3.43 H2O
2.56
2.52 DMSO
2.51
2.46
2.44
2.43
2.41
1.91
1.88
1.16
A (d)
11.63
B (d)
8.22
C (m)
3.76
D (q)
2.44
E (d)
1.89
1.00
1.03
2.11
2.31
2.15
f1 (ppm)


4g ^{13}C
161.99
161.59
151.71
151.13
150.67
147.44
68.35
68.06
48.39
47.47
40.54 DMSO
40.33 DMSO
40.13 DMSO
39.91 DMSO
39.70 DMSO
39.49 DMSO
39.28 DMSO
25.34
3.2×10^7
3.0×10^7
2.8×10^7
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
-2.0×10^6
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2d

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2d

```
Bond precision:   C-C = 0.0030 A           Wavelength=0.71073

Cell:             a=19.1694(14)     b=7.9541(7)         c=17.1543(19)
                  alpha=90          beta=122.616(2)     gamma=90
Temperature:      140 K

                  Calculated                  Reported
Volume            2203.1(4)                   2203.1(4)
Space group       C 2/c                       C 1 2/c 1
Hall group        -C 2yc                      -C 2yc
Moiety formula    2(C7 H9 Br N2 O5 S), H2 O   C7 H9 Br N2 O5 S, 0.5(H2 O)
Sum formula       C14 H20 Br2 N4 O11 S2       C7 H10 Br N2 O5.50 S
Mr                644.26                      322.14
Dx,g cm-3         1.942                       1.942
Z                 4                           8
Mu (mm-1)         3.935                       3.935
F000              1288.0                      1288.0
F000'             1287.38
h,k,lmax          27,11,24                    27,11,24
Nref              3375                        3211
Tmin,Tmax         0.453,0.554                 0.578,0.746
Tmin'             0.356

Correction method= # Reported T Limits: Tmin=0.578 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.951            Theta(max)= 30.533

R(reflections)= 0.0262( 2683)                    wR2(reflections)=
                                                 0.0694( 3211)
S = 1.093                  Npar= 156
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
PLAT431_ALERT_2_B Short Inter HL..A Contact  Br1      ..O5       .       2.99 Ang.
                                          x,1-y,1/2+z  =      6_566 Check
```

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C14 H20 Br2 N4 O11 S2
             Rep.: C7 H10 Br N2 O5.50 S
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C7 H9 Br N2 O5 S), H2 O
             Rep.: C7 H9 Br N2 O5 S, 0.5(H2 O)
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         27 Report
               0  2  0,   1  1  0,   2  2  0,   3  1  0,   4  0  0,  -2  2  1,
             -16  0  2,   0  0  2,   4  0  2, -19  3  3, -17  5  3,  10  2  3,
             -20  2  4,  -7  3  4,  -6  2  4,  -4  0  4,  -1  1  4, -21  3  8,
             -22  2  9,  10  0 10,  10  2 10,   9  1 11,   8  0 12, -21  1 16,
             -20  0 16,  -2  0 18,  -7  1 19,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
               0  2  0,   2  2  0,   4  0  2,  -6  2  4,  -1  1  4,
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From O1      .       0.47 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.47Ang From O1      .      -0.59 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.65Ang From O1      .      -0.59 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4B       .      -0.33 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          5 Report
             H2    H4A   H4B   H1C   H1D
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c       I2/a Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             H4A     H4B     H1C     H1D
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          4 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          3 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        136 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
               1  1  0,  -7  3  4,   0  0  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.353 Note
             Predicted wR2: Based on SigI**2  2.95 or SHELX Weight  6.35
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully

```
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 15 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  8 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

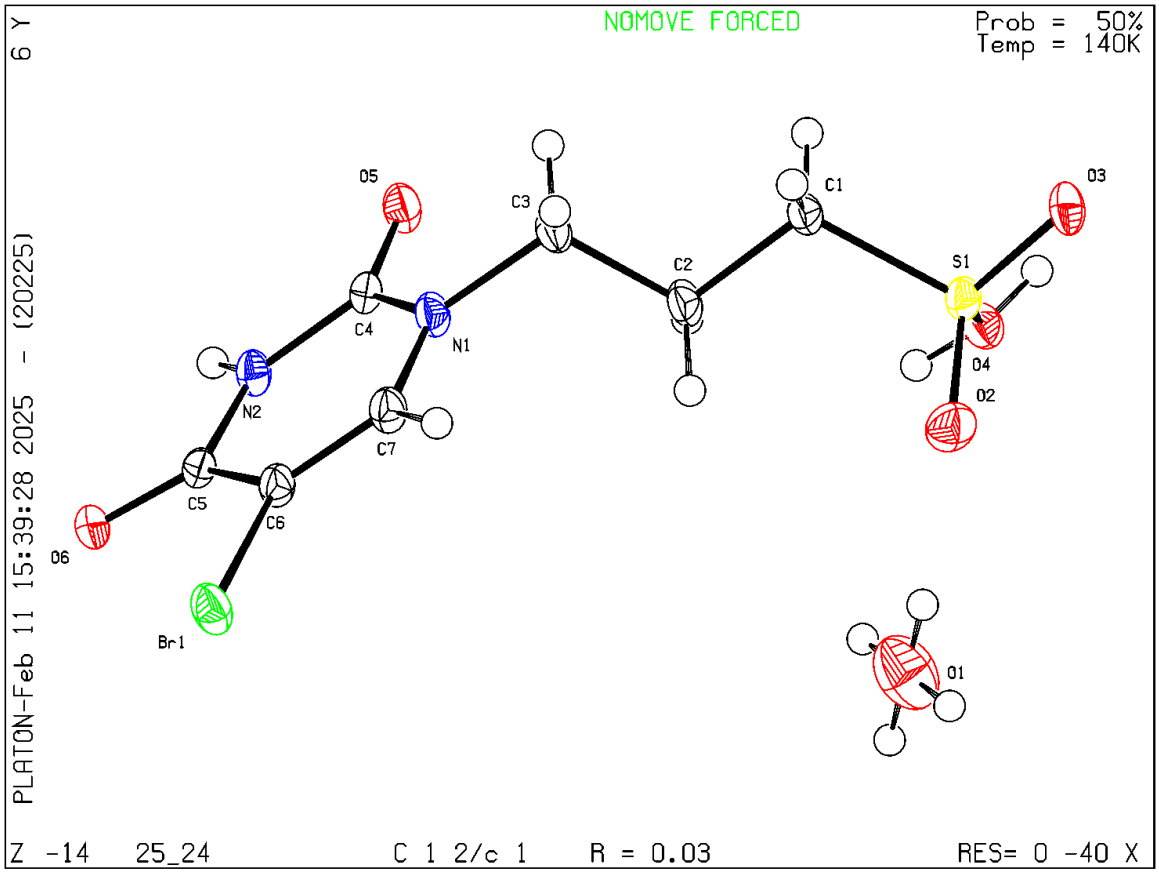
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock 2d - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3d

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3d

```
Bond precision:   C-C = 0.0045 A           Wavelength=0.75170

Cell:             a=5.4130(11)       b=9.910(2)        c=12.756(3)
                  alpha=81.88(3)     beta=81.24(3)     gamma=88.37(3)
Temperature:      100 K

                  Calculated                  Reported
Volume            669.5(3)                    669.5(2)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C7 H8 Br N2 O5 S, C2 H8 N   C7 H8 Br N2 O5 S, C2 H8 N
Sum formula       C9 H16 Br N3 O5 S           C9 H16 Br N3 O5 S
Mr                358.21                      358.22
Dx,g cm-3         1.777                       1.777
Z                 2                           2
Mu (mm-1)         3.712                       3.743
F000              364.0                       364.0
F000'             363.30
h,k,lmax          7,13,17                     7,13,17
Nref              3659                        3618
Tmin,Tmax         0.722,0.829                 0.540,1.000
Tmin'             0.655

Correction method= # Reported T Limits: Tmin=0.540 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.989            Theta(max)= 31.122

R(reflections)= 0.0516( 3201)                    wR2(reflections)=
                                                 0.1393( 3618)
S = 1.066                  Npar= 176
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
PLAT434_ALERT_2_B Short Inter HL..HL Contact Br1      ..Br1      .       3.20 Ang.
                                                  -x,-y,2-z  =      2_557 Check
```

Alert level C

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         17 Report
               -1  2  0,   1  2  1,   0 -2  2,  -1 -1  2,   0  0  2,  -1  1  2,
                1  0  3,   0  1  3,   1  1  3,   0  2  3,  -1 11  4,   4  8  8,
                1 -1  9,   2  3  9,   0 -3 10,   2  2 11,   3 -1 13,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
               -1  2  0,   1  2  1,   0  0  2,   0  2  3,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From Br1              1.97 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.14Ang From Br1              1.78 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.02Ang From O3      .        0.61 eA-3
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
              H2    H3C   H3D
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.03 Degree
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         25 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.181 Note
              Predicted wR2: Based on SigI**2  3.33 or SHELX Weight 13.07
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
PLAT984_ALERT_1_G The Br-f'=   -0.6336 Deviates from the B&C-Value    -0.5915 Check
PLAT984_ALERT_1_G The  N-f'=    0.0051 Deviates from the B&C-Value     0.0071 Check
PLAT984_ALERT_1_G The  O-f'=    0.0094 Deviates from the B&C-Value     0.0124 Check
PLAT984_ALERT_1_G The  S-f'=    0.1227 Deviates from the B&C-Value     0.1365 Check
PLAT985_ALERT_1_G The Br-f"=    2.7055 Deviates from the B&C-Value     2.6633 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

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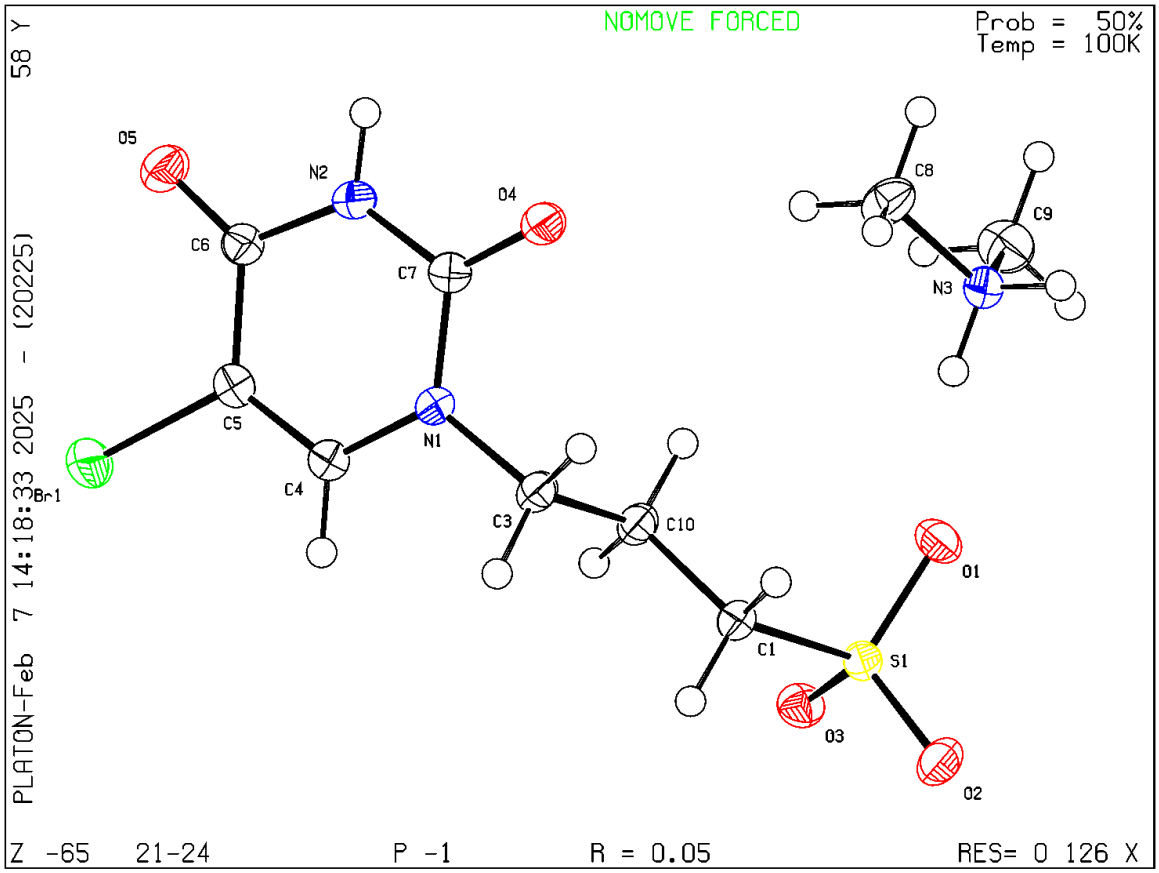
PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock 3d- ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3e

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3e

```
Bond precision:   C-C = 0.0052 A           Wavelength=0.75170

Cell:             a=5.3800(11)       b=9.789(2)        c=12.738(3)
                  alpha=82.08(3)     beta=80.63(3)     gamma=89.38(3)
Temperature:      100 K

                  Calculated                  Reported
Volume            655.5(3)                    655.5(2)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C7 H8 Cl N2 O5 S, C2 H8 N   C7 H8 Cl N2 O5 S, C2 H8 N
Sum formula       C9 H16 Cl N3 O5 S           C9 H16 Cl N3 O5 S
Mr                313.76                      313.76
Dx,g cm-3         1.590                       1.590
Z                 2                           2
Mu (mm-1)         0.543                       0.548
F000              328.0                       328.0
F000'             328.78
h,k,lmax          7,13,17                     7,13,17
Nref              3580                        3482
Tmin,Tmax         0.947,0.973                 0.774,1.000
Tmin'             0.947

Correction method= # Reported T Limits: Tmin=0.774 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.973            Theta(max)= 31.127

R(reflections)= 0.0767( 2951)                    wR2(reflections)=
                                                 0.2409( 3482)
S = 1.151                  Npar= 177
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.979 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.43 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       1.44 eA-3
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00525 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.205 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         51 Report
               -5  2  0,  -1  2  0,   1  3  0,  -1  0  1,  -1  1  1,  -1  2  1,
                1  2  1,   0 -2  2,  -1 -1  2,  -4  0  2,  -1  0  2,   0  0  2,
                0  2  2,  -5  3  2,  -1  8  2,  -4  0  3,   1  0  3,  -5  1  3,
               -5  2  3,   0  2  3,  -5  3  3,  -4  1  4,  -5  3  4,  -1 10  4,
               -5 -1  5,  -4 -1  5,  -5  0  5,  -5  2  5,   0 10  5,  -4 -1  6,
               -5  0  6,  -5  1  6,  -5  3  6,  -1  9  6,  -4 -5  7,  -2 -3  7,
               -5  0  7,  -5  1  7,   1  7  7,  -2 -2  8,  -4  1  8,  -3  1  8,
               -1 -1  9,  -4  0  9,  -4  1  9,  -4  2  9,   5  4  9,  -4  1 10,
               -4  2 10,  -4  3 10,  -3  3 12,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
               -1  2  0,   1  2  1,   0  2  2,   0  2  3,
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
             not performed for this radiation type.
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            H2    H3C   H3D
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.03 Degree
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1      ..Cl1      .       3.17 Ang.
                                                  -x,-y,2-z  =      2_557 Check
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         47 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      6.623 Note
            Predicted wR2: Based on SigI**2  3.64 or SHELX Weight 20.92
PLAT984_ALERT_1_G The Cl-f'=    0.1458 Deviates from the B&C-Value     0.1623 Check
PLAT984_ALERT_1_G The  N-f'=    0.0051 Deviates from the B&C-Value     0.0071 Check
PLAT984_ALERT_1_G The  O-f'=    0.0094 Deviates from the B&C-Value     0.0124 Check
PLAT984_ALERT_1_G The  S-f'=    0.1227 Deviates from the B&C-Value     0.1365 Check
```

---

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Datablock 3e- ellipsoid plot