Supporting Information

A Method for the Deprotection of Alkylpinacolyl Boronate Esters

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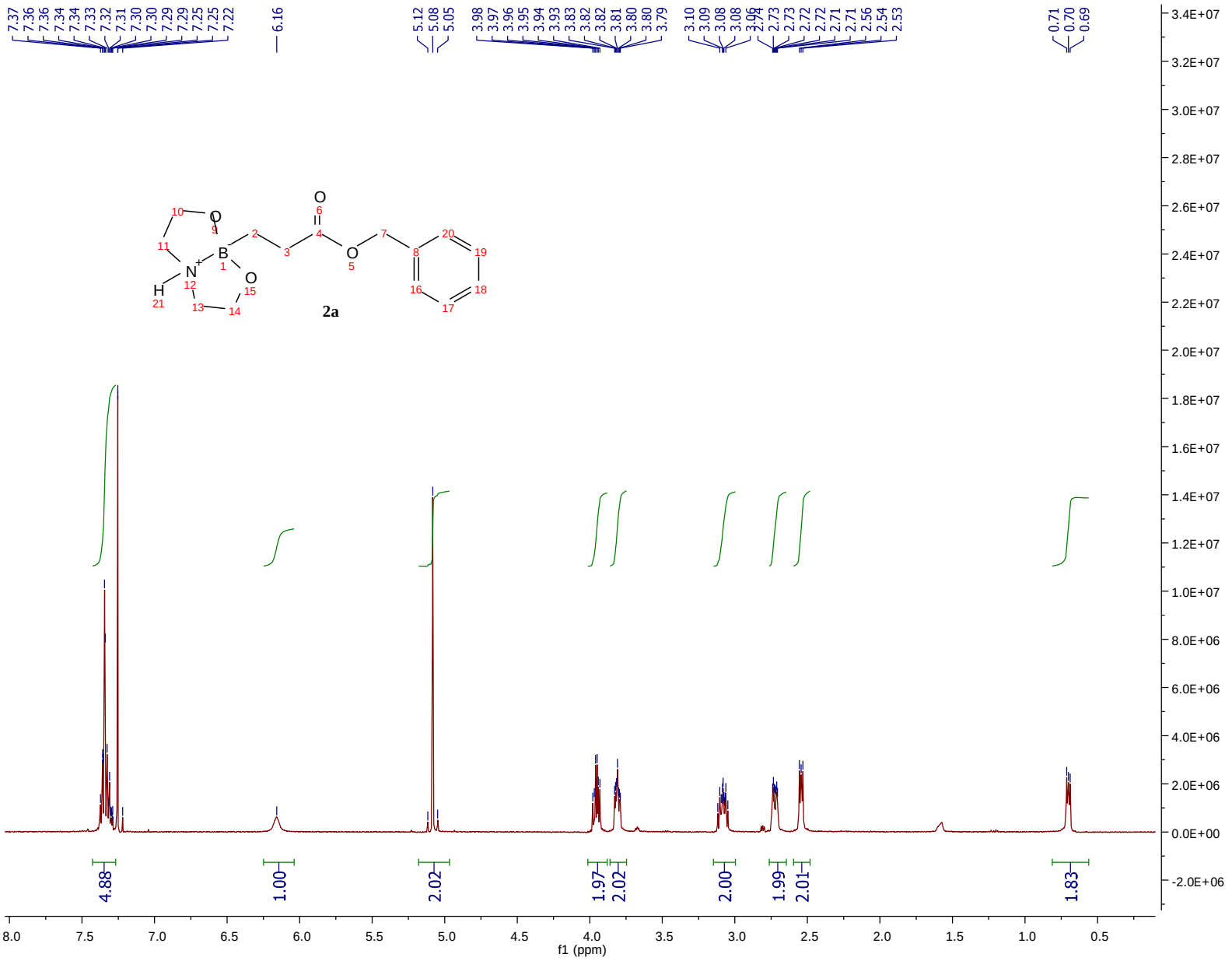
General Information:

^{1}H NMR spectra were recorded on either a 500 MHz or 400 MHz spectrometer. Chemical shifts are reported in ppm with the solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz), and assignment. ^{13}C NMR spectra were recorded on a 125 MHz spectrometer. Chemical shifts are reported in ppm with the solvent resonance as the internal standard ($CDCl_3$: 77.16 ppm). The carbon directly attached to boron was not observed due to quadrupolar relaxation. ^{11}B NMR spectra were recorded on a 160 MHz spectrometer. Chemical shifts are reported in ppm with boron trifluoride diethyl etherate as an external standard ($BF_3O(C_2H_5)_2$: 0 ppm).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5.12 5.08 5.05
3.98 3.97 3.96 3.95 3.94 3.93 3.83 3.82 3.82 3.81 3.80 3.80 3.79
3.10 3.09 3.08 3.08 3.06 2.74 2.73 2.73 2.72 2.72 2.71 2.71 2.56 2.54 2.53
0.71 0.70 0.69
2a
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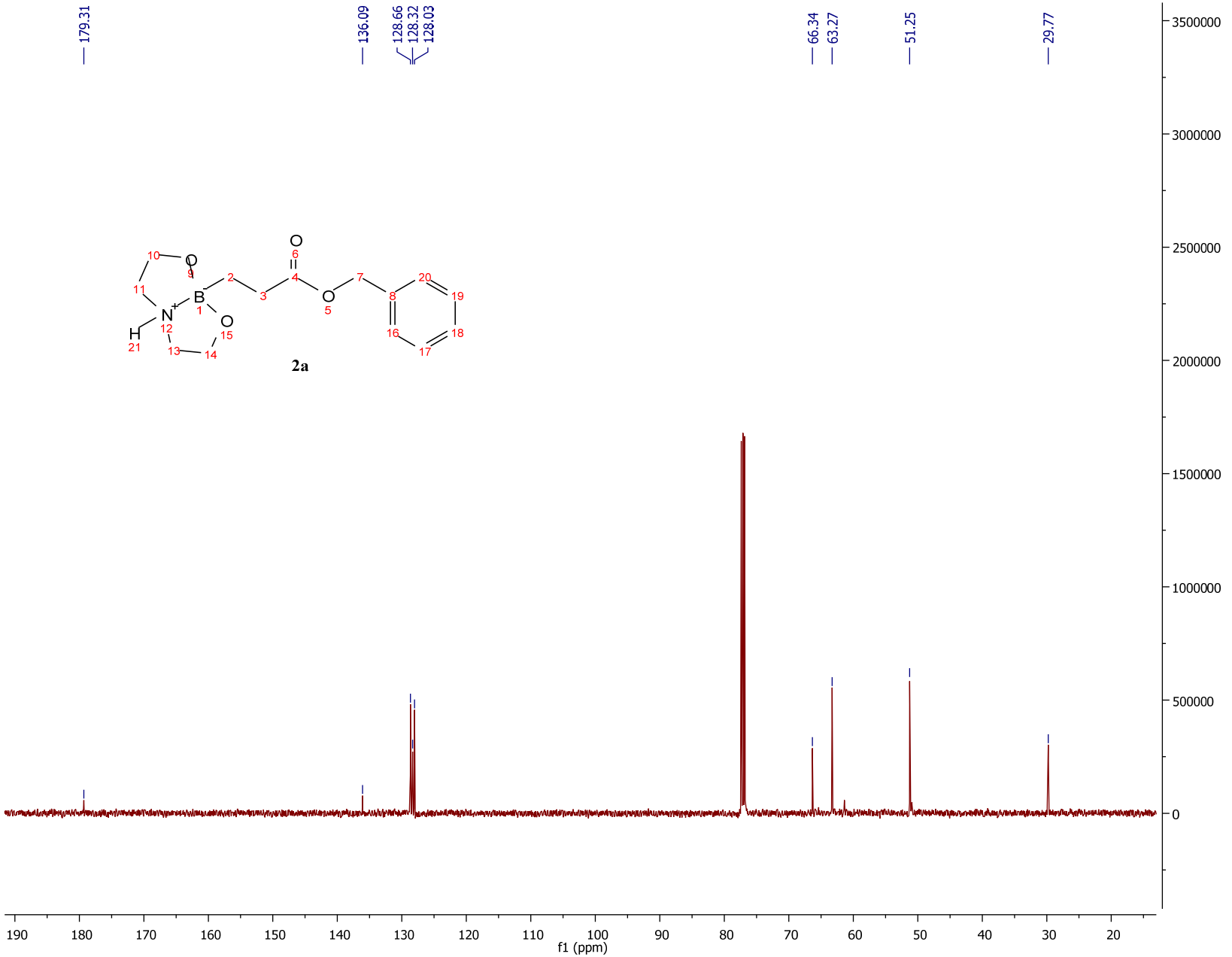
2.02
1.97
2.02
2.00
1.99
2.01
1.83
f1 (ppm)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128.32
128.03
66.34
63.27
51.25
29.77
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2500000
2000000
1500000
1000000
500000
0
190
180
170
160
150
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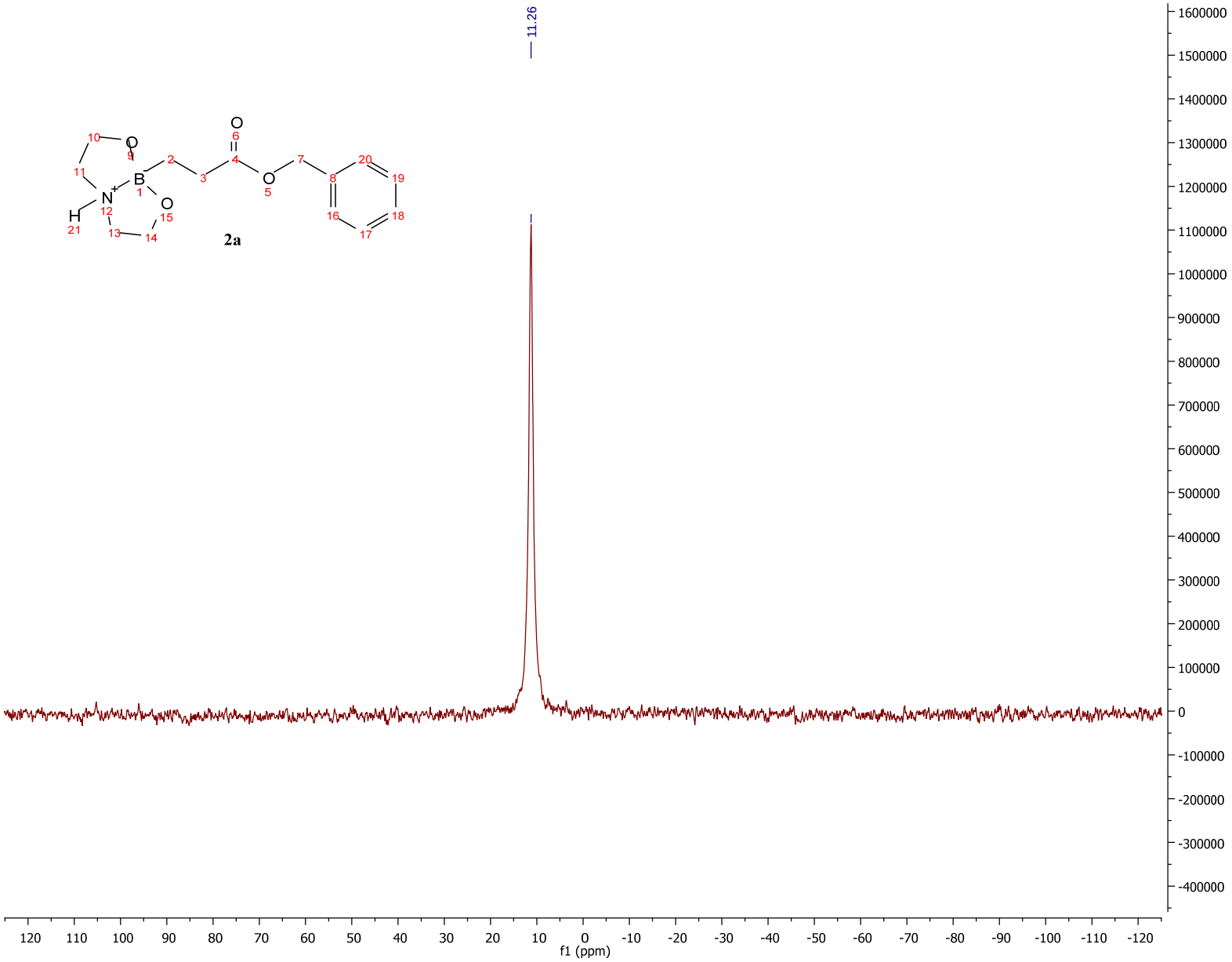
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

2a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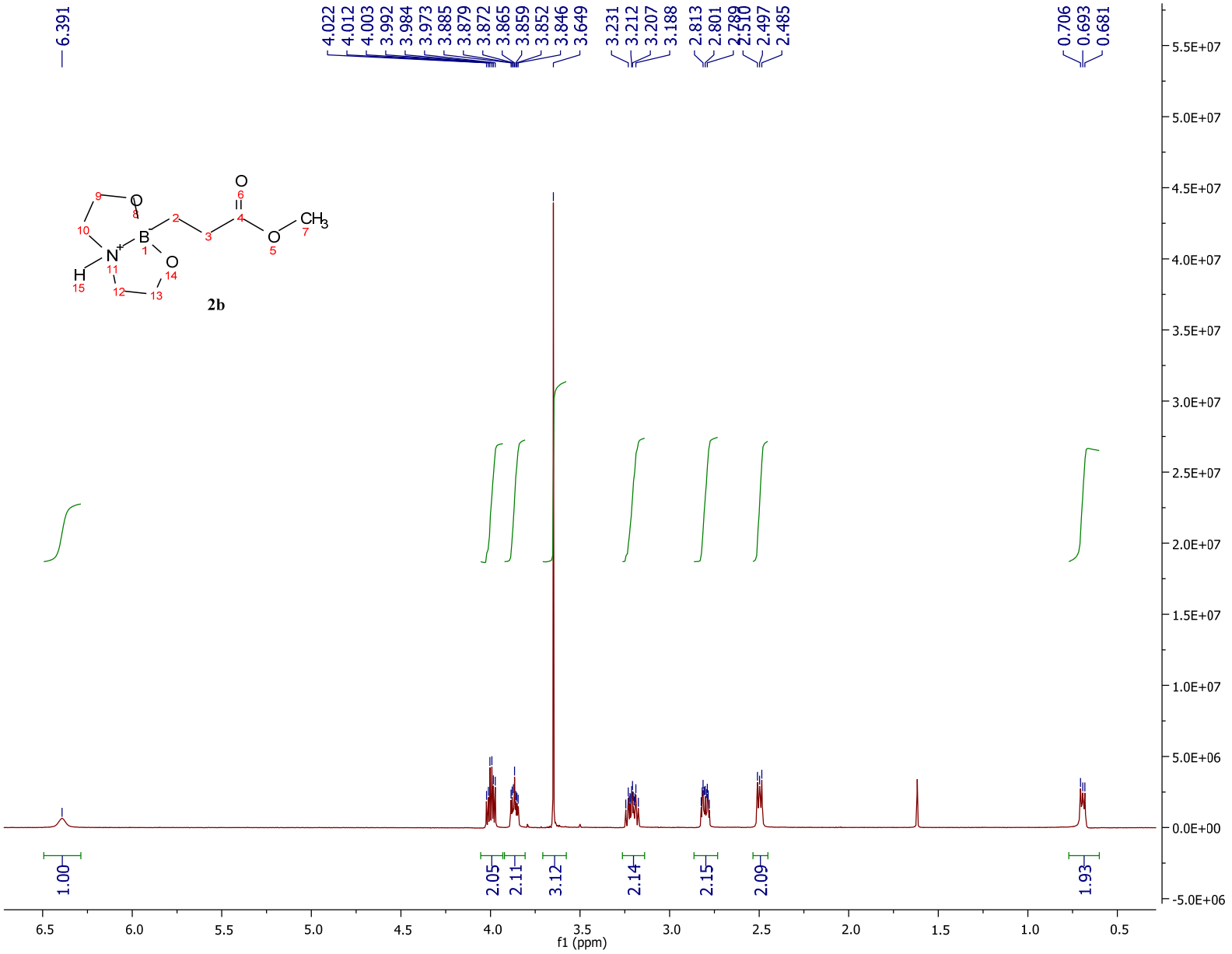
2a
f1 (ppm)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3.859
3.852
3.846
3.649
3.231
3.212
3.207
3.188
2.813
2.801
2.497
2.485
0.706
0.693
0.681
2b
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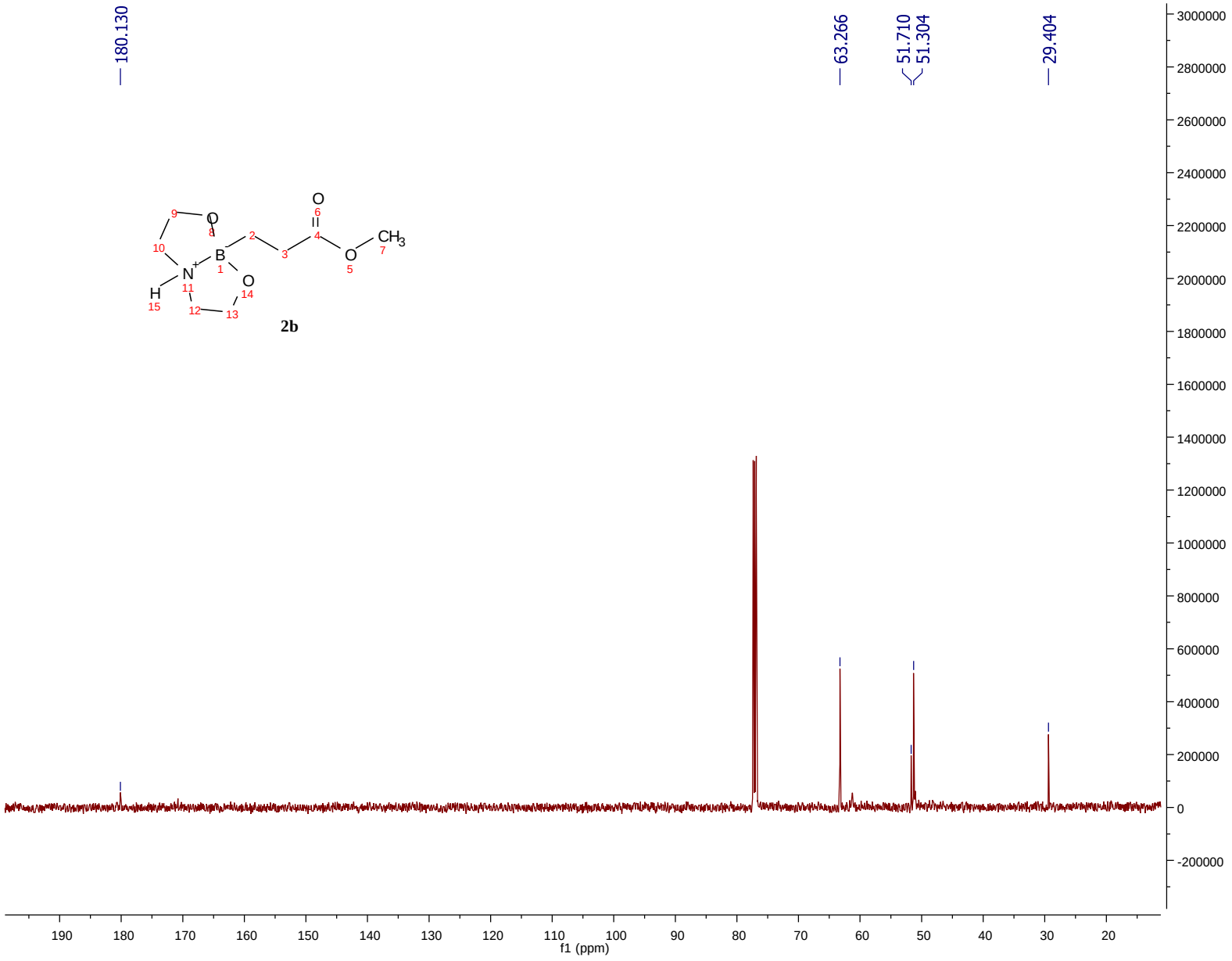
2.05
2.11
3.12
2.14
2.15
2.09
1.93
f1 (ppm)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51.304
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O
O
O
O
B
N
H
CH3
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
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1000000
800000
600000
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200000
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190
180
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120
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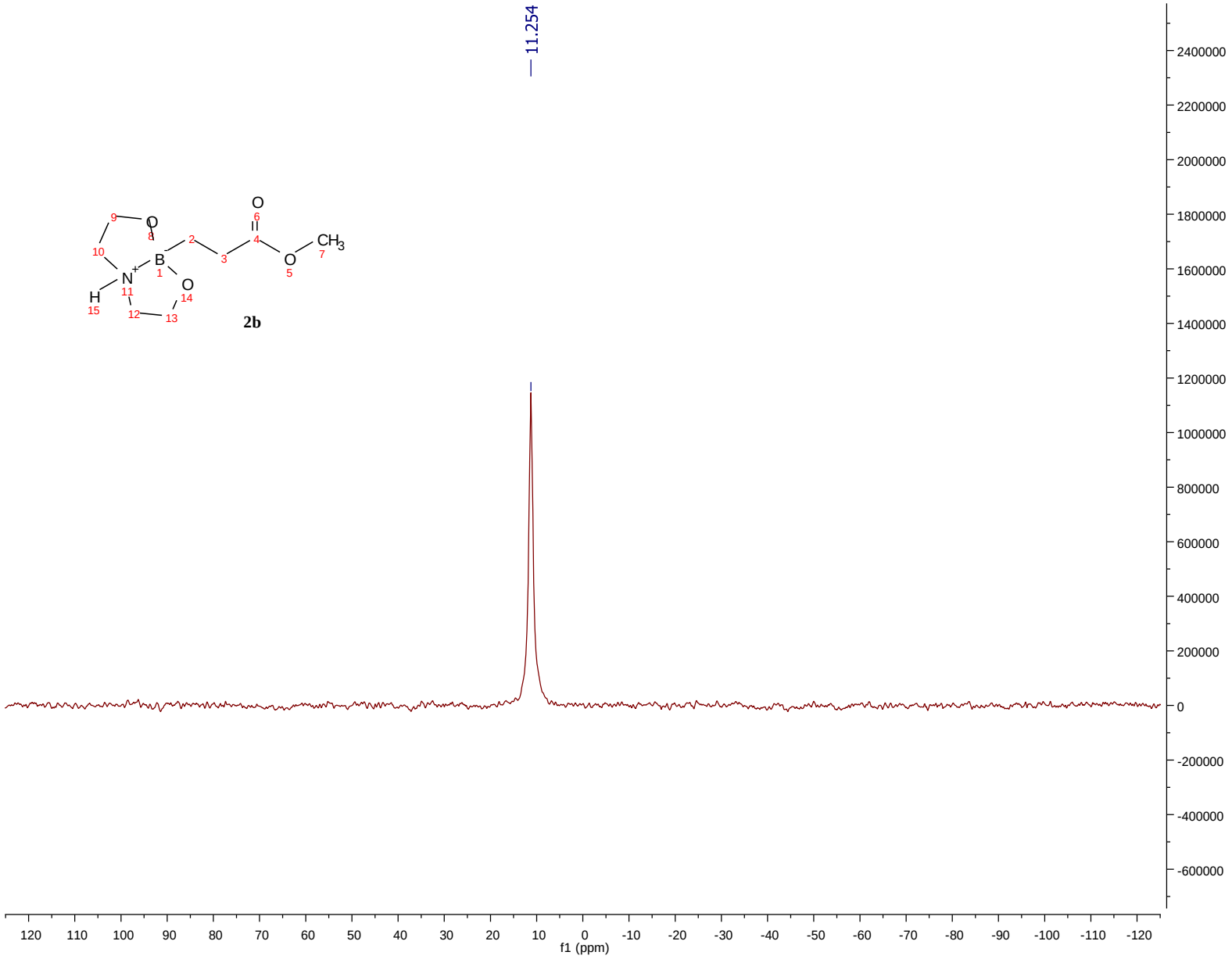
100
90
80
70
60
50
40
30
20
f1 (ppm)

2b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200000
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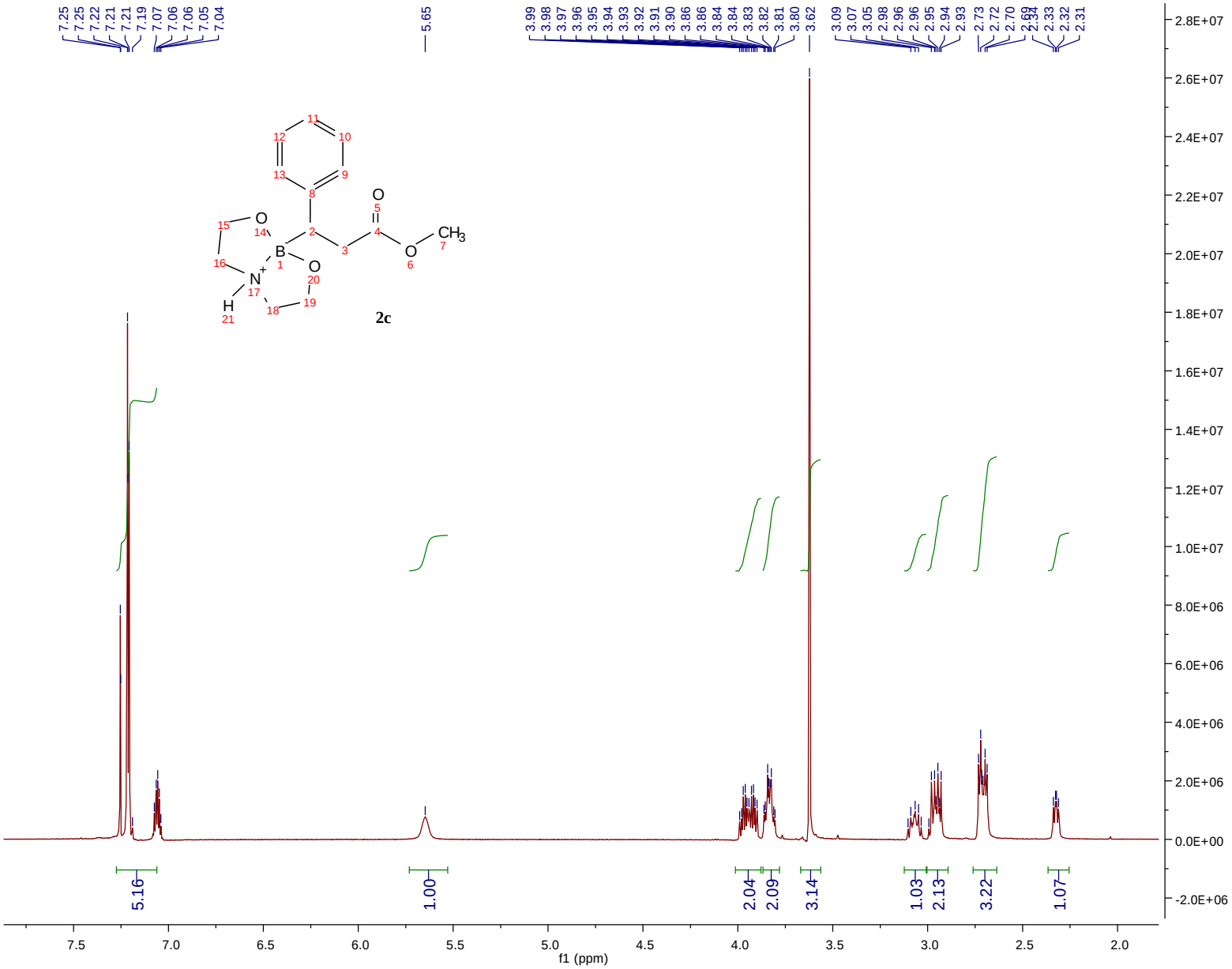
f1 (ppm)

2b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3.62
3.09 3.07 3.05 2.98 2.96 2.96 2.95 2.94 2.93
2.73 2.72 2.70 2.69 2.34 2.33 2.32 2.31
2c
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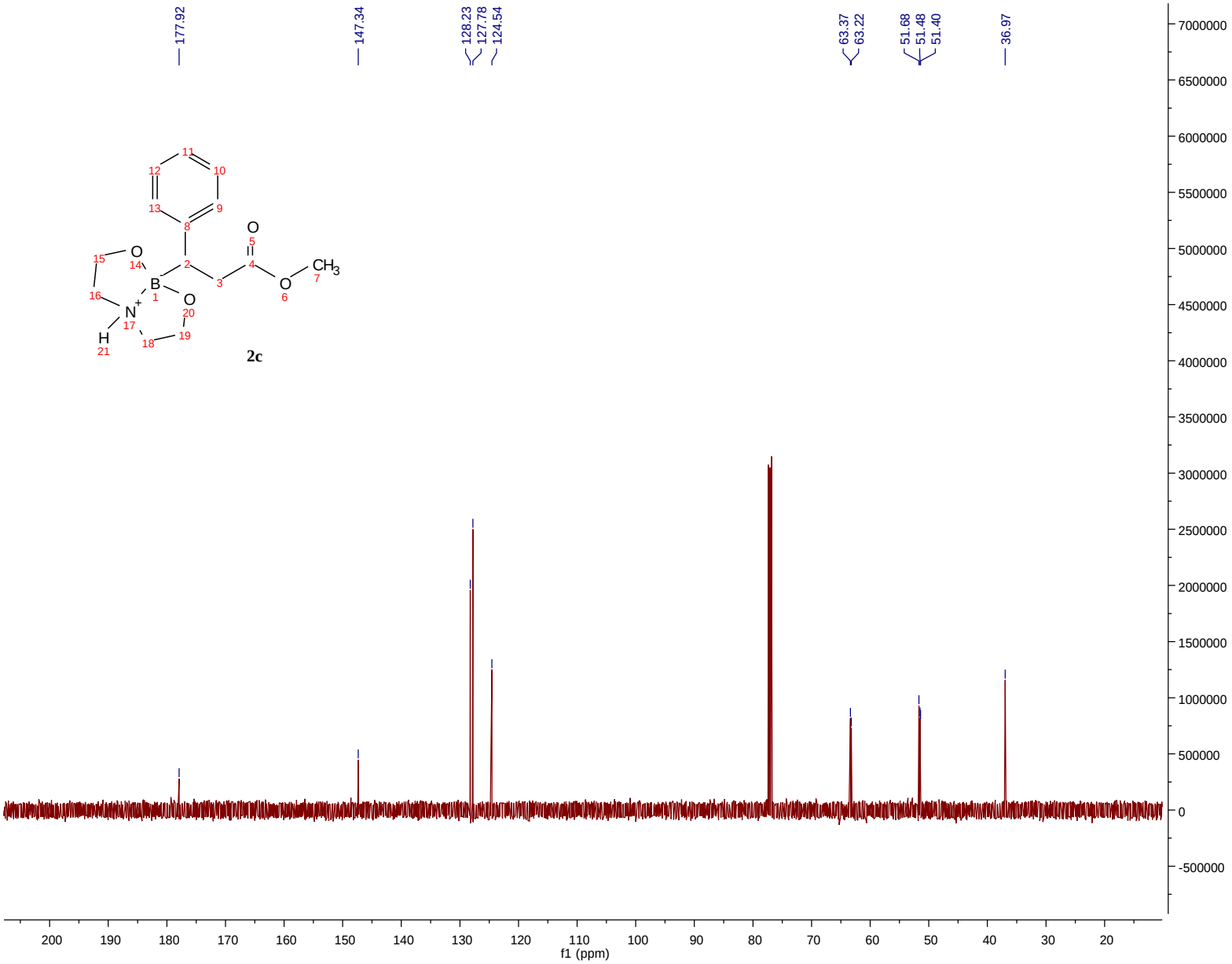
1.00
2.04
2.09
3.14
1.03
2.13
3.22
1.07
f1 (ppm)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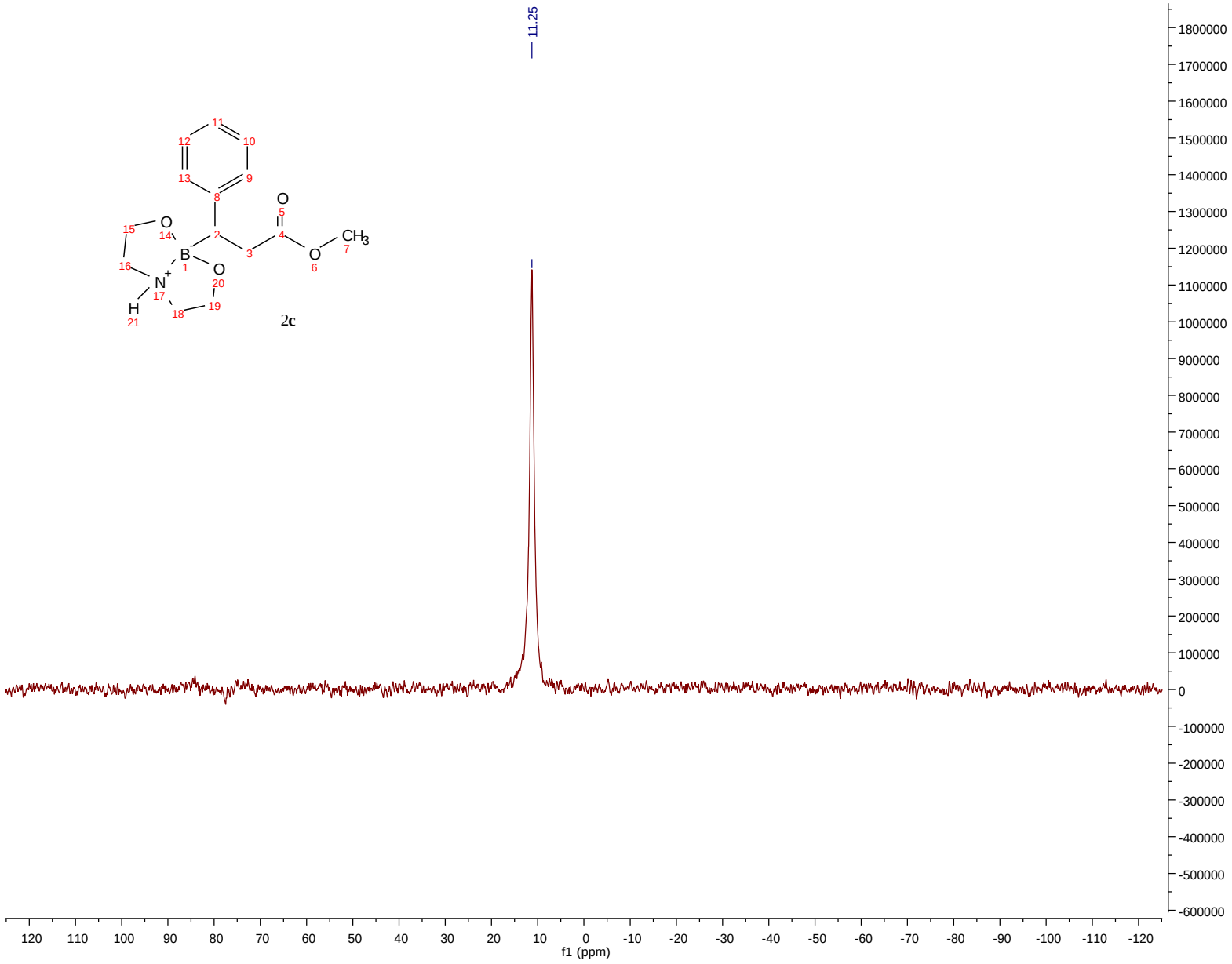
51.68
51.48
51.40
36.97
2c
f1 (ppm)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1500000
1400000
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1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
-200000
-300000
-400000
-500000
-600000
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120
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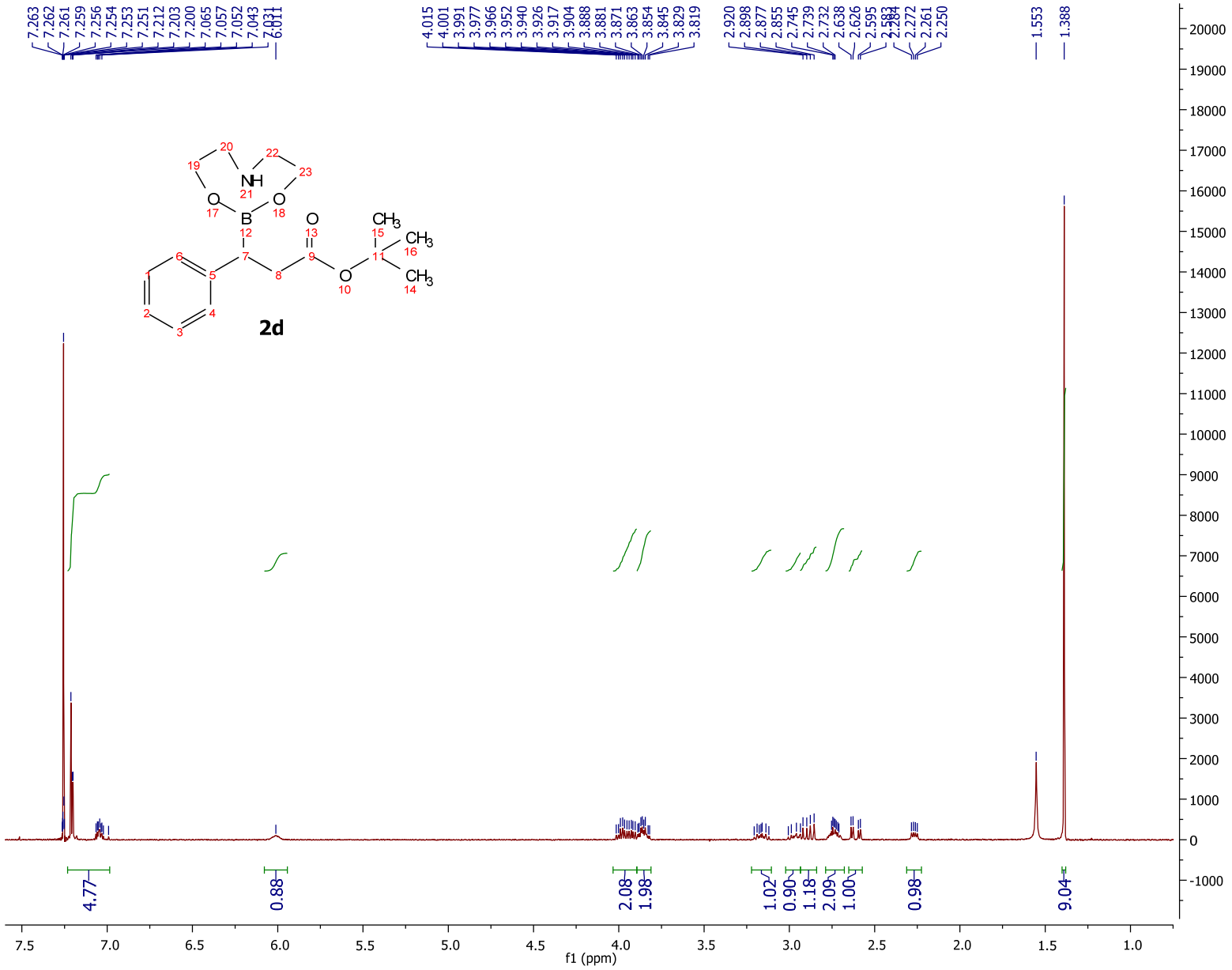
O
O
O
O
B
N+
H
CH3
2c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7.057
7.052
7.043
7.031
6.011
4.015
4.001
3.991
3.977
3.966
3.952
3.940
3.926
3.917
3.904
3.888
3.881
3.871
3.863
3.854
3.845
3.829
3.819
2.920
2.898
2.877
2.855
2.745
2.739
2.732
2.638
2.626
2.595
2.272
2.261
2.250
1.553
1.388
2d
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0.88
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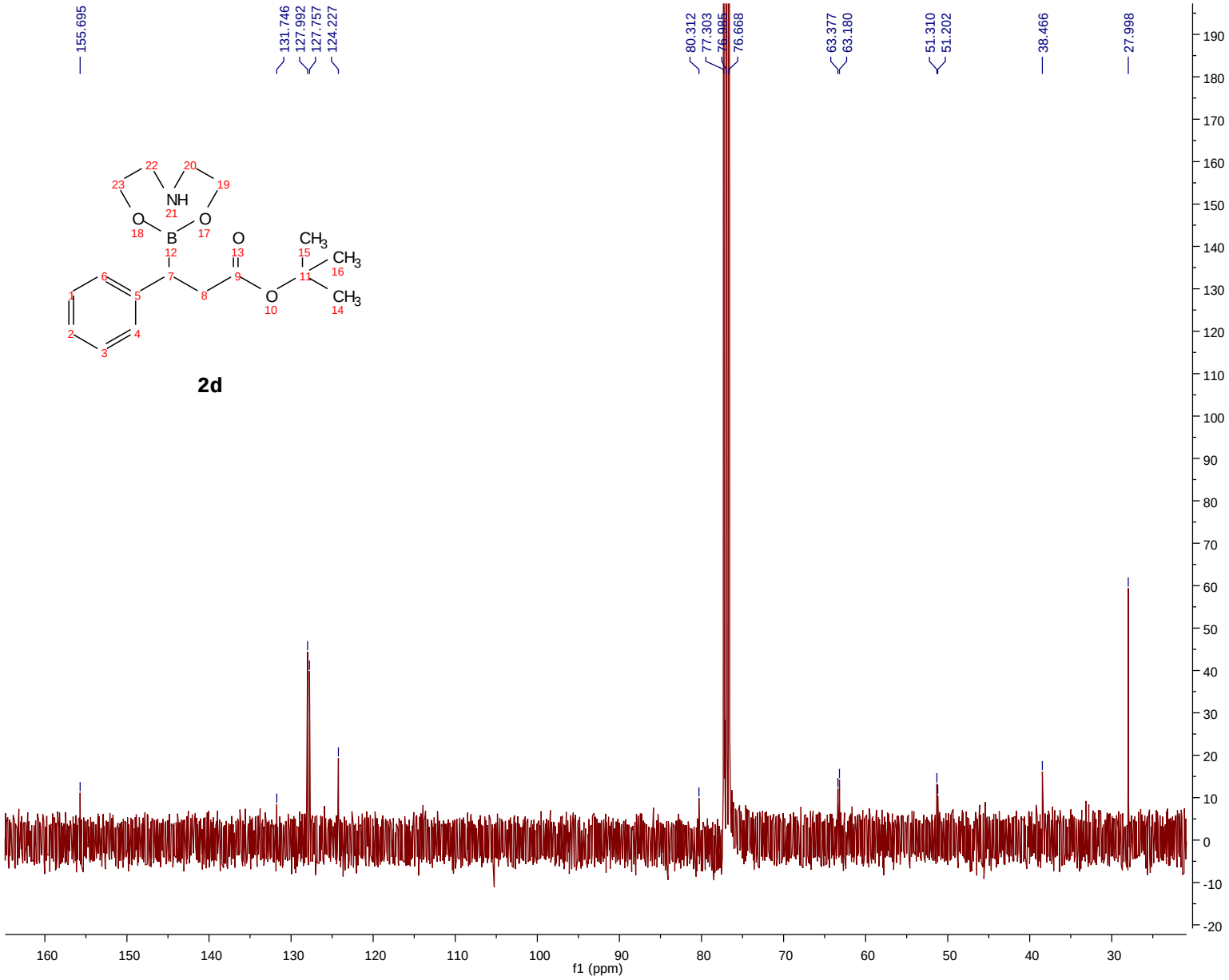
1.98
1.02
0.90
1.18
2.09
1.00
0.98
9.04
f1 (ppm)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76.668
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27.998
NH
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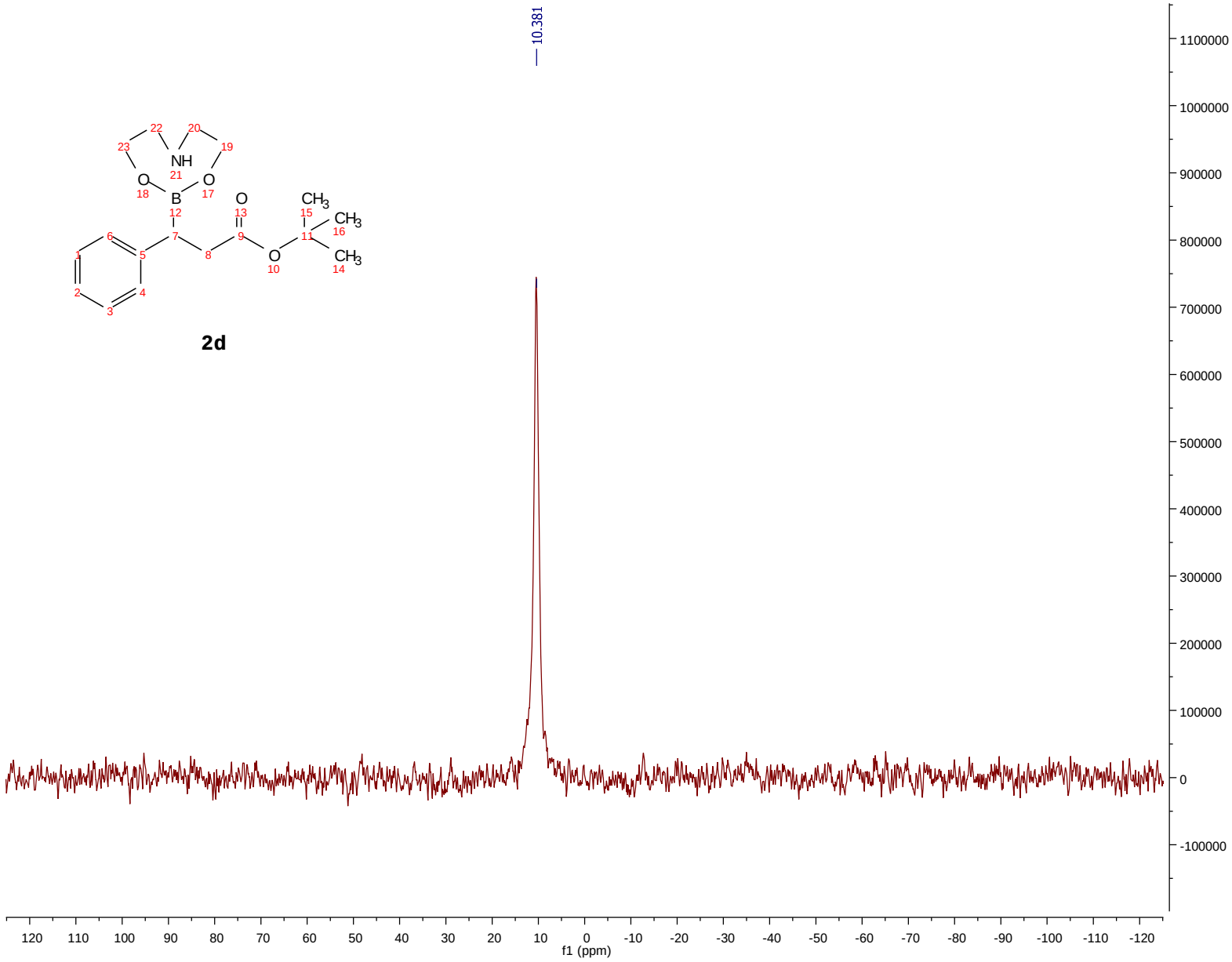
B
O
O
O
CH3
CH3
CH3
f1 (ppm)

2d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f1 (ppm)
NH
O
B
O
O
O
CH3
CH3
CH3
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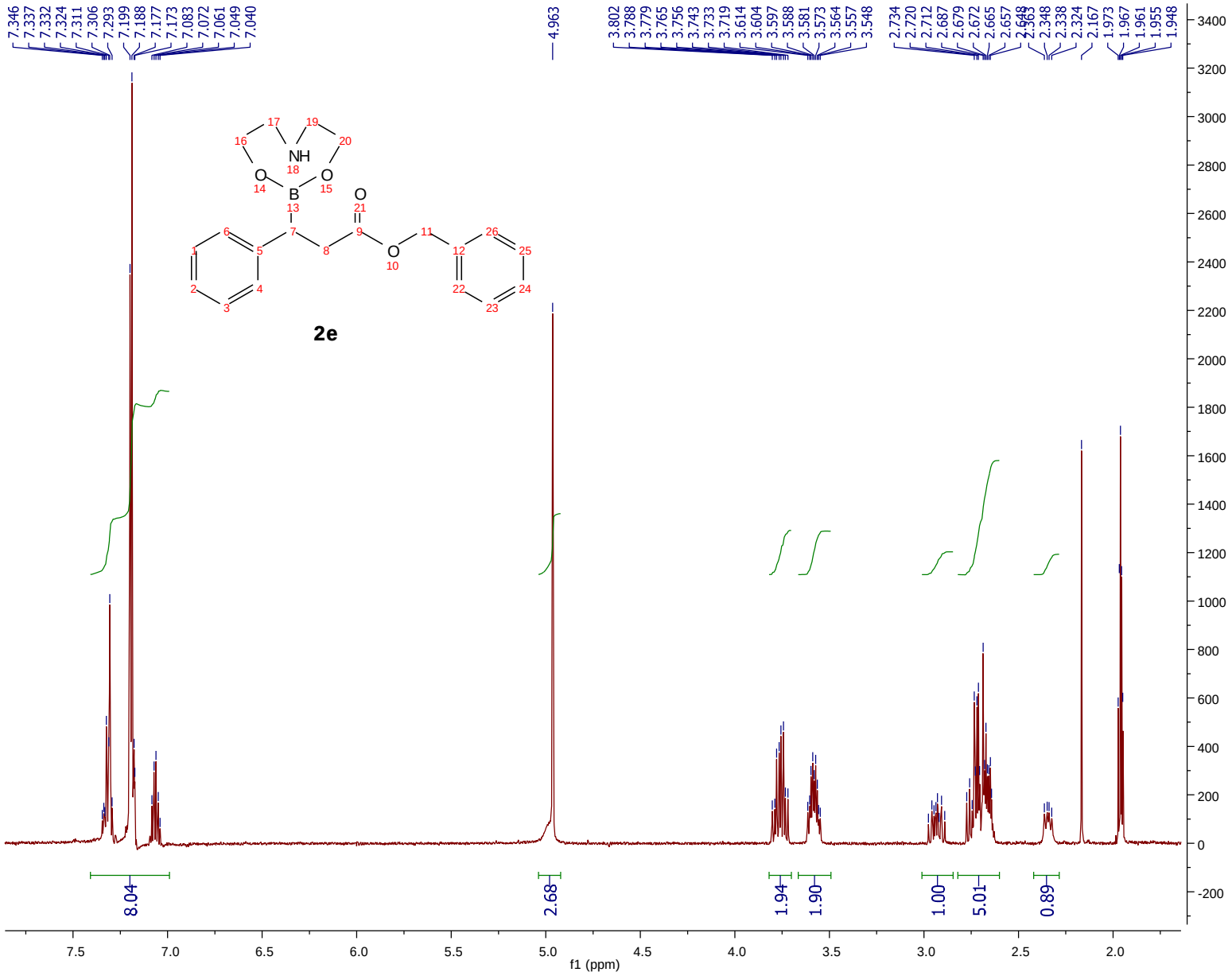
2d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7.177
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7.072
7.061
7.049
7.040
4.963
3.802
3.788
3.779
3.765
3.756
3.743
3.733
3.719
3.614
3.604
3.597
3.588
3.581
3.573
3.564
3.557
3.548
2.734
2.720
2.712
2.687
2.679
2.672
2.665
2.657
2.648
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2.348
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1.955
1.948
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O
B
O
2e
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1.94
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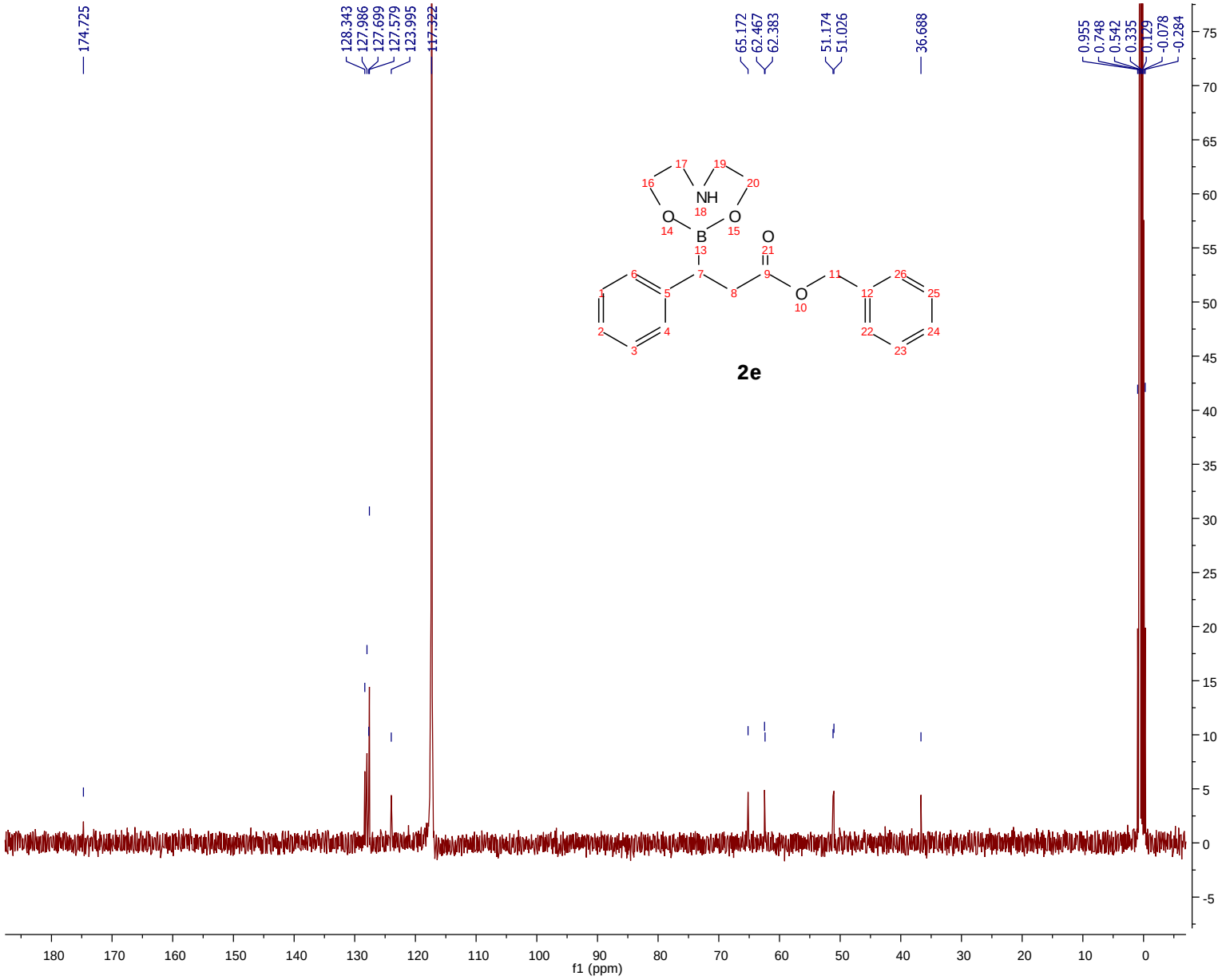
1.00
5.01
0.89
f1 (ppm)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127.699
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65.172
62.467
62.383
51.174
51.026
36.688
0.955
0.748
0.542
0.335
0.129
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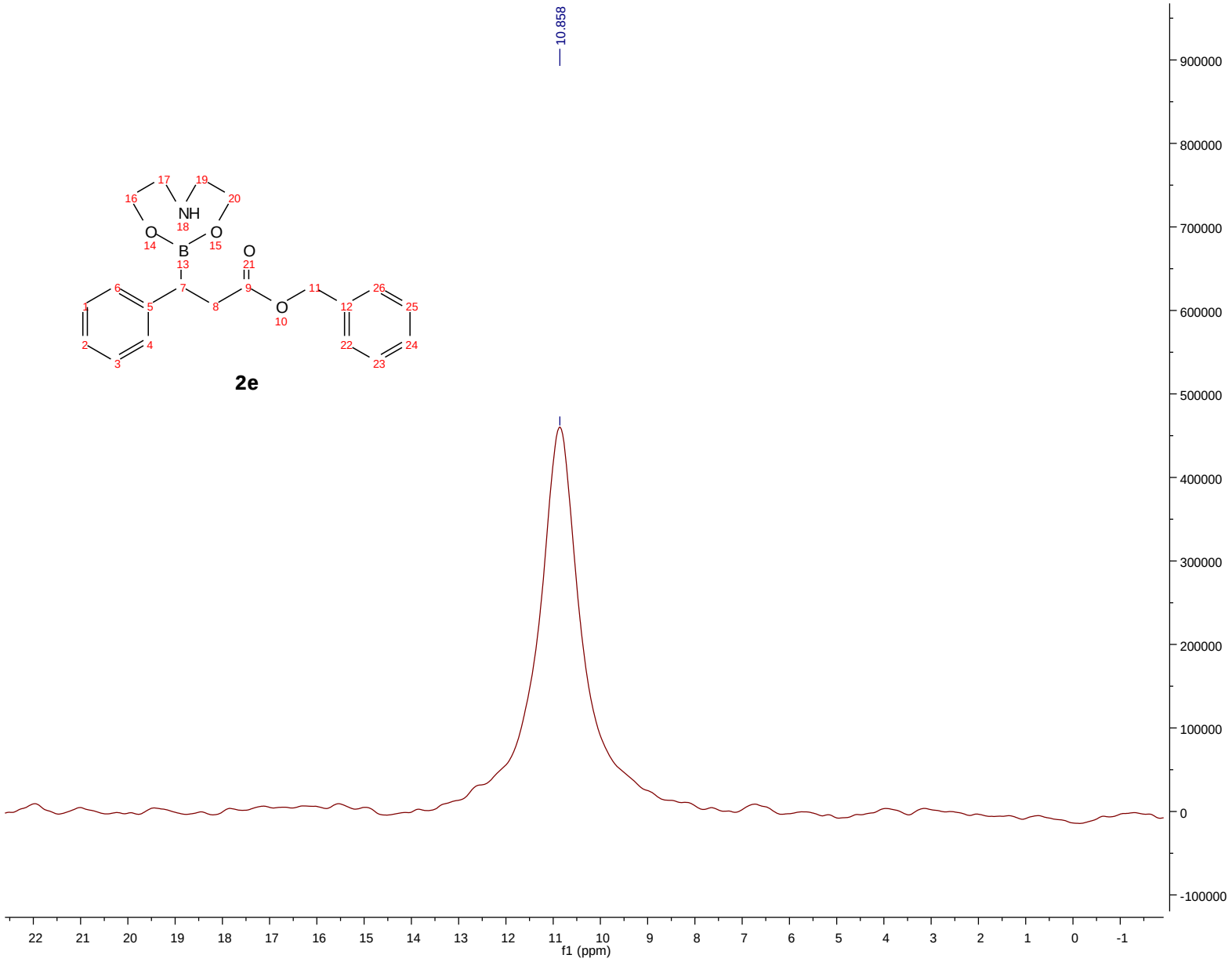
-0.284
NH
O
O
B
O
O
2e
f1 (ppm)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600000
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300000
200000
100000
0
-100000
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f1 (ppm)
NH
O
B
O
O
O
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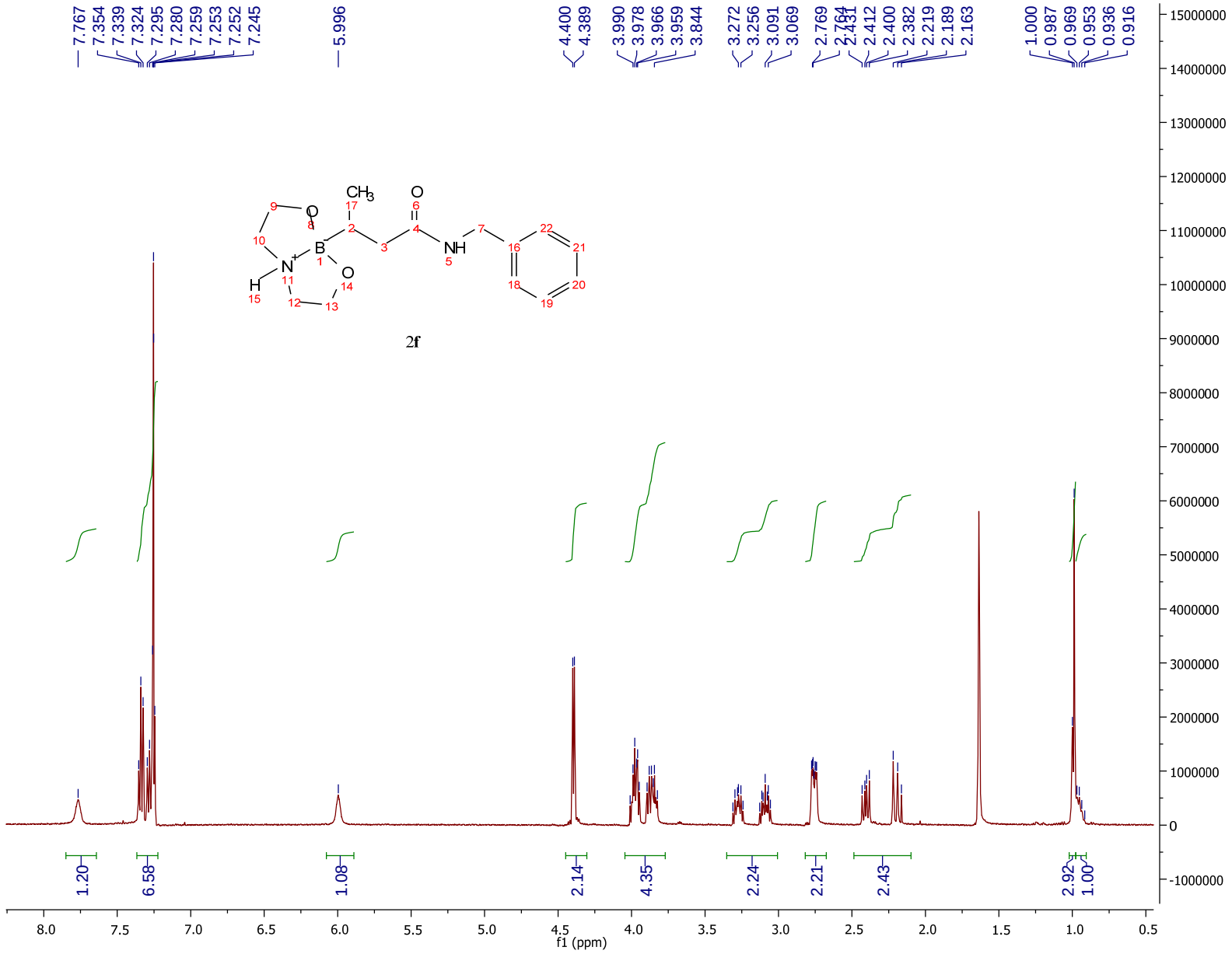
2e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7.253
7.252
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4.389
3.990
3.978
3.966
3.959
3.844
3.272
3.256
3.091
3.069
2.769
2.764
2.431
2.412
2.400
2.382
2.219
2.189
2.163
1.000
0.987
0.969
0.953
0.936
0.916
CH3
O
NH
B
N+
H
1.20
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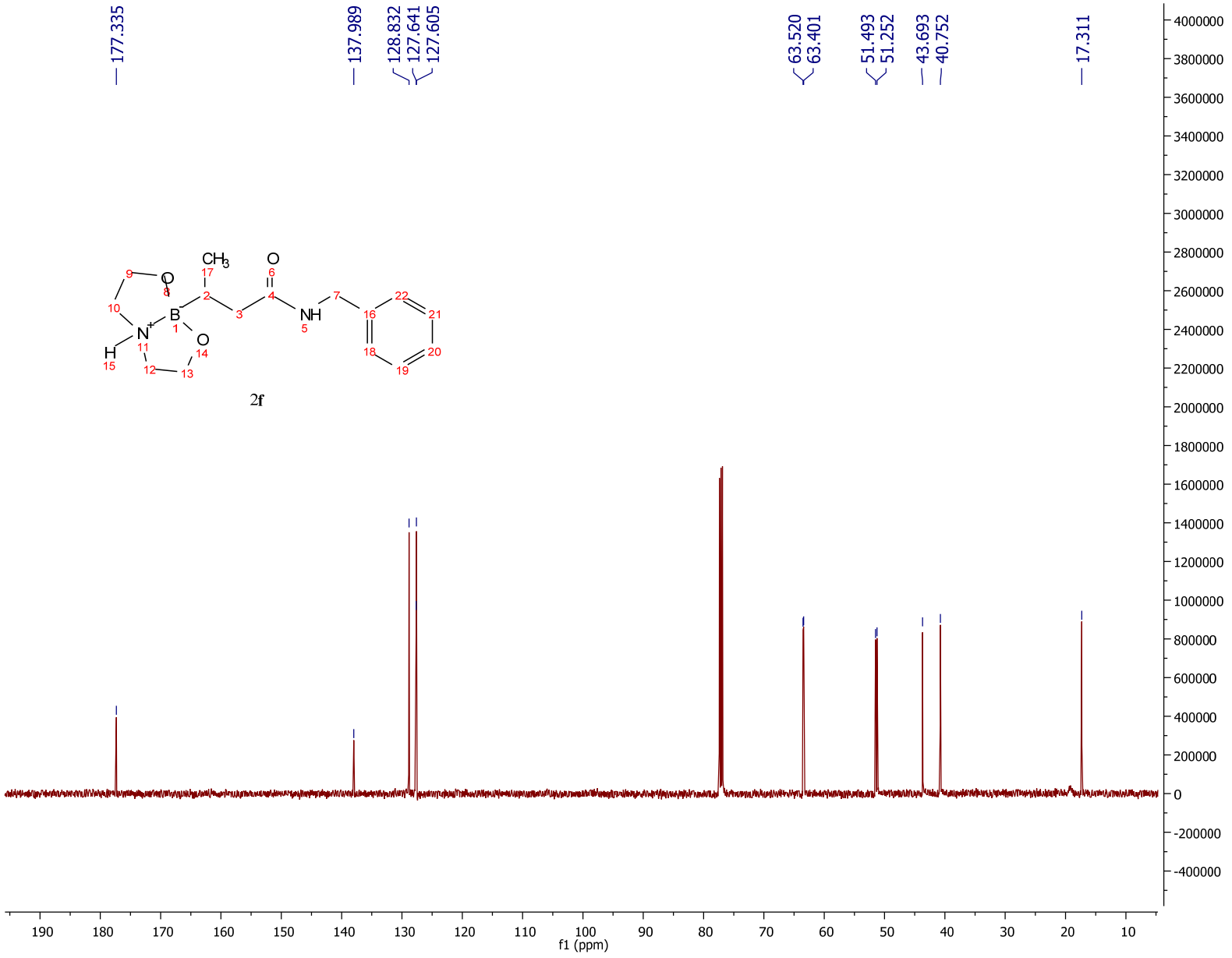
2.14
4.35
2.24
2.21
2.43
2.92
1.00
f1 (ppm)

2f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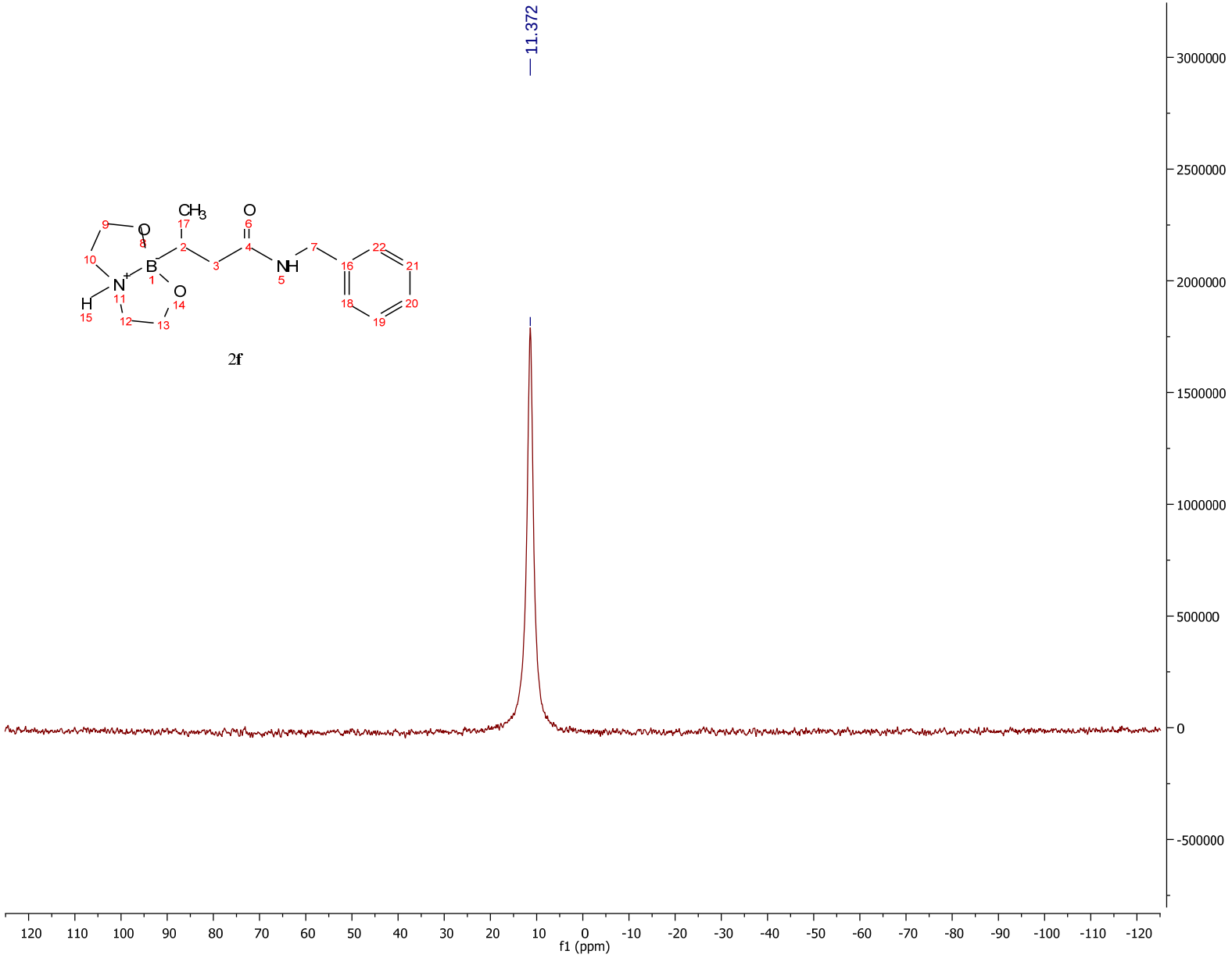
f1 (ppm)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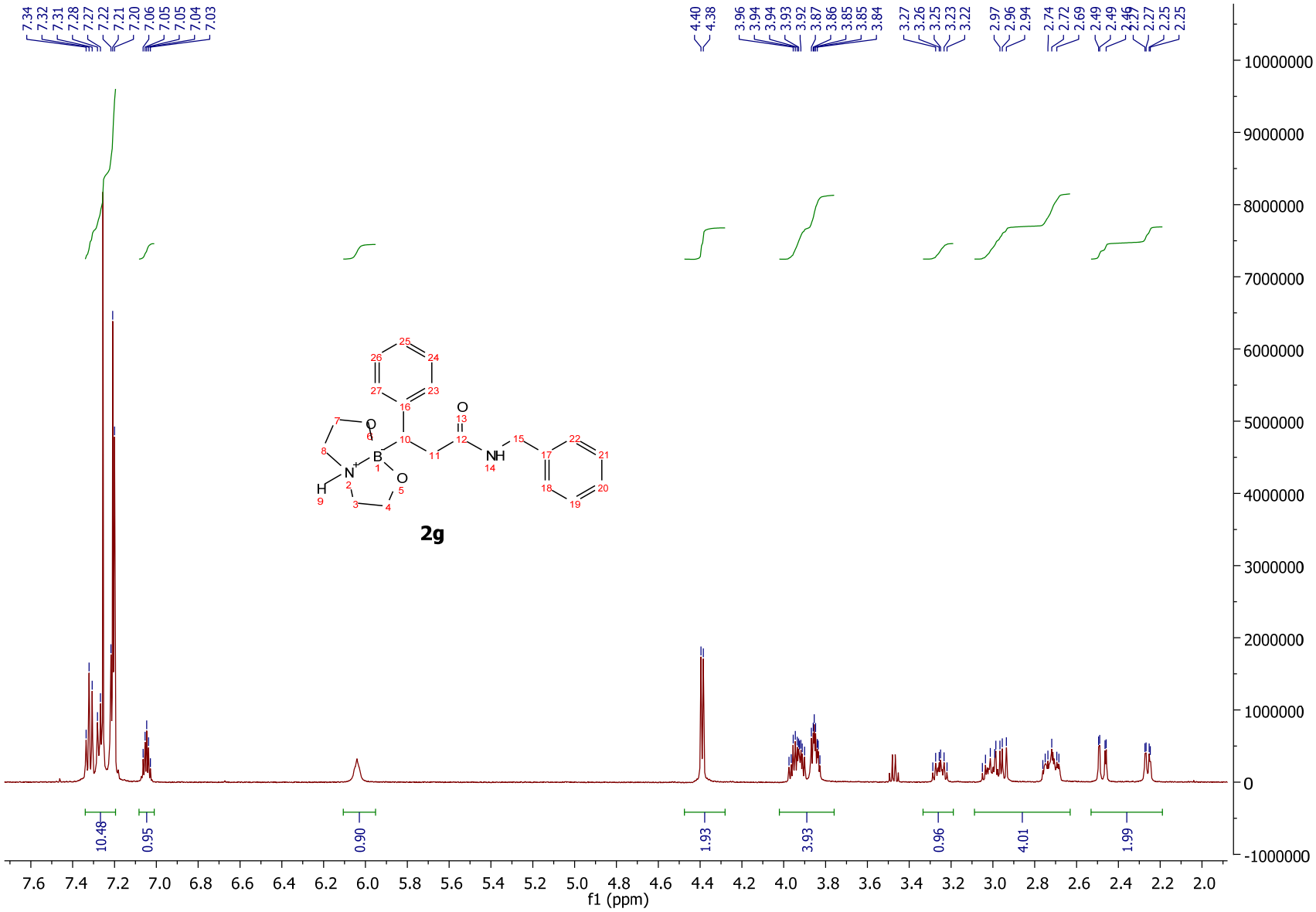
f1 (ppm)

2f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7.21
7.20
7.06
7.05
7.05
7.04
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4.40
4.38
3.96
3.94
3.94
3.93
3.92
3.87
3.86
3.85
3.85
3.84
3.27
3.26
3.25
3.23
3.22
2.97
2.96
2.94
2.74
2.72
2.69
2.49
2.49
2.27
2.27
2.25
2.25
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4000000
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0.90
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3.93
0.96
4.01
1.99
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
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2.8
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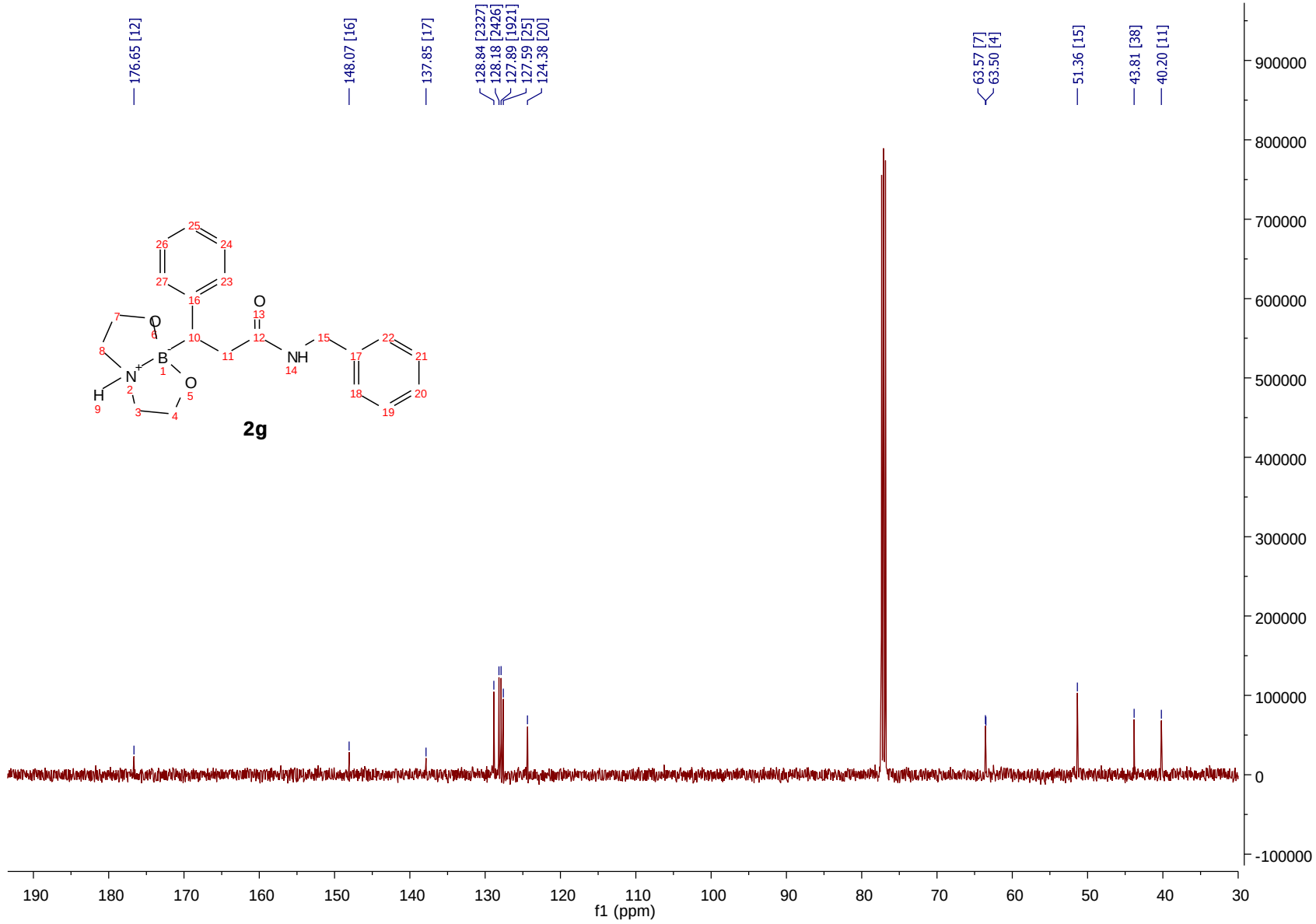
2.4
2.2
2.0
f1 (ppm)

2g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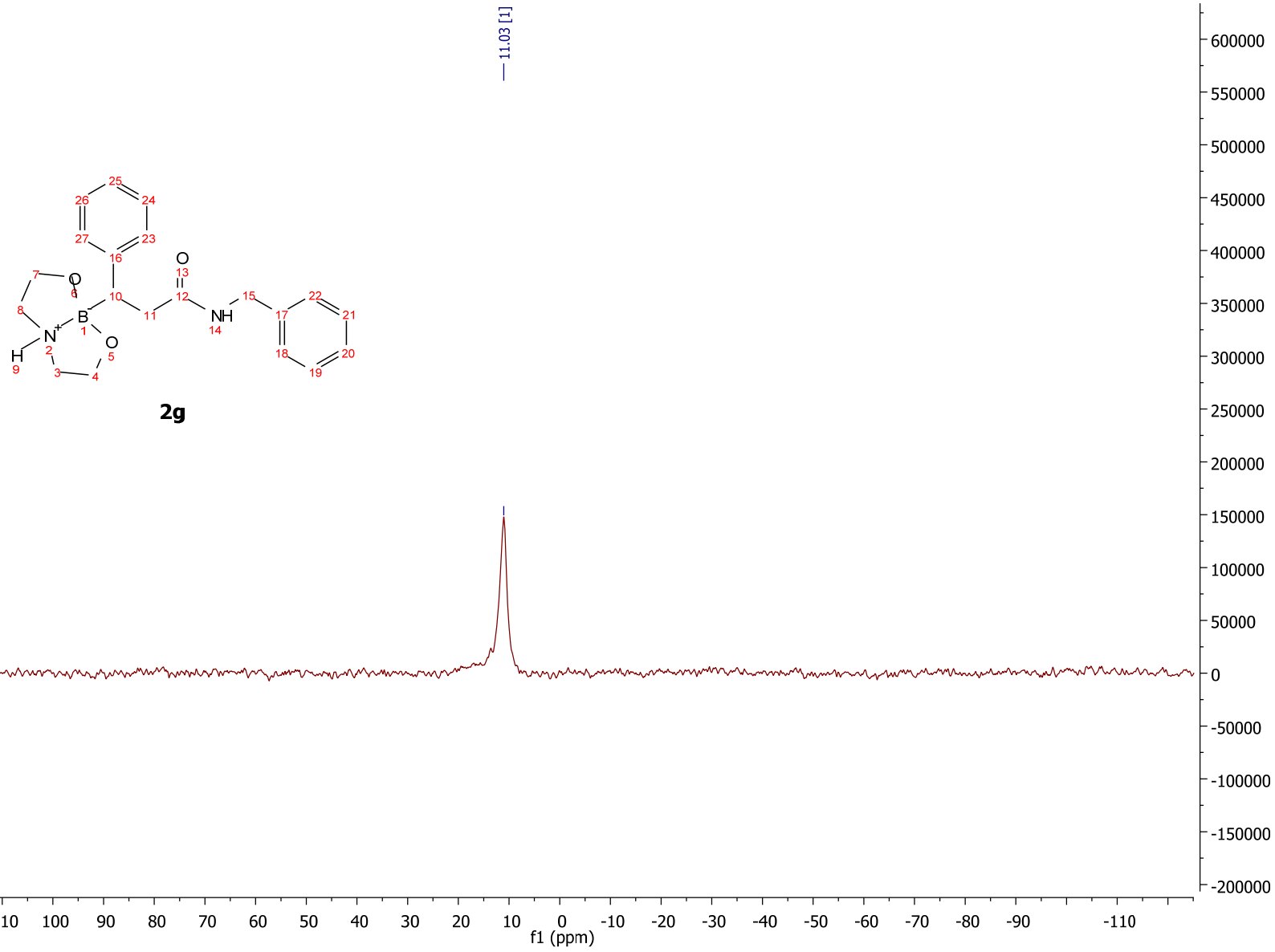
40.20 [11]
2g
f1 (ppm)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350000
300000
250000
200000
150000
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0
-50000
-100000
-150000
-200000
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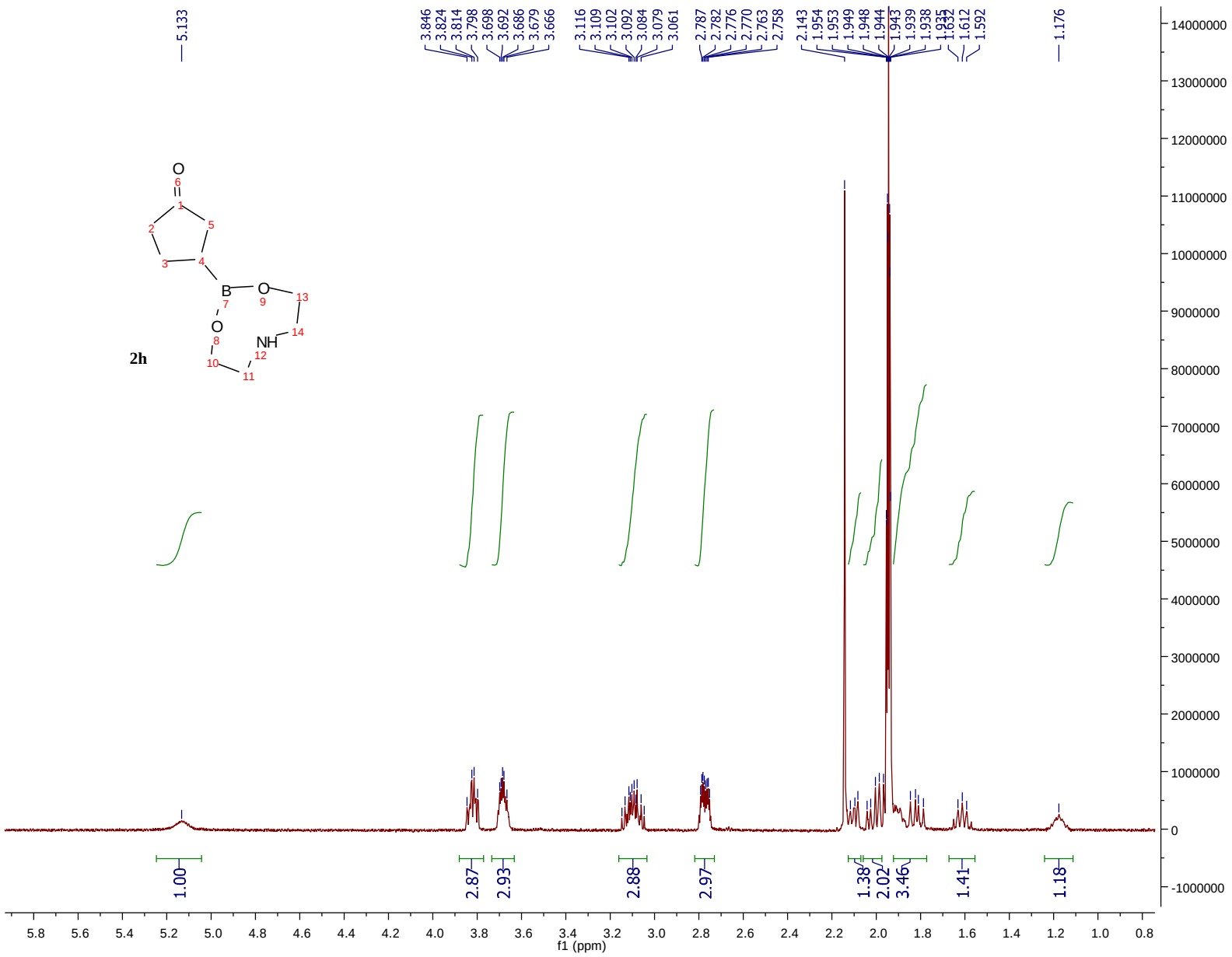
f1 (ppm)

2g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3.814
3.798
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3.692
3.686
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3.102
3.092
3.084
3.079
3.061
2.787
2.782
2.776
2.770
2.763
2.758
2.143
1.954
1.953
1.949
1.948
1.944
1.943
1.939
1.938
1.935
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1.612
1.592
1.176
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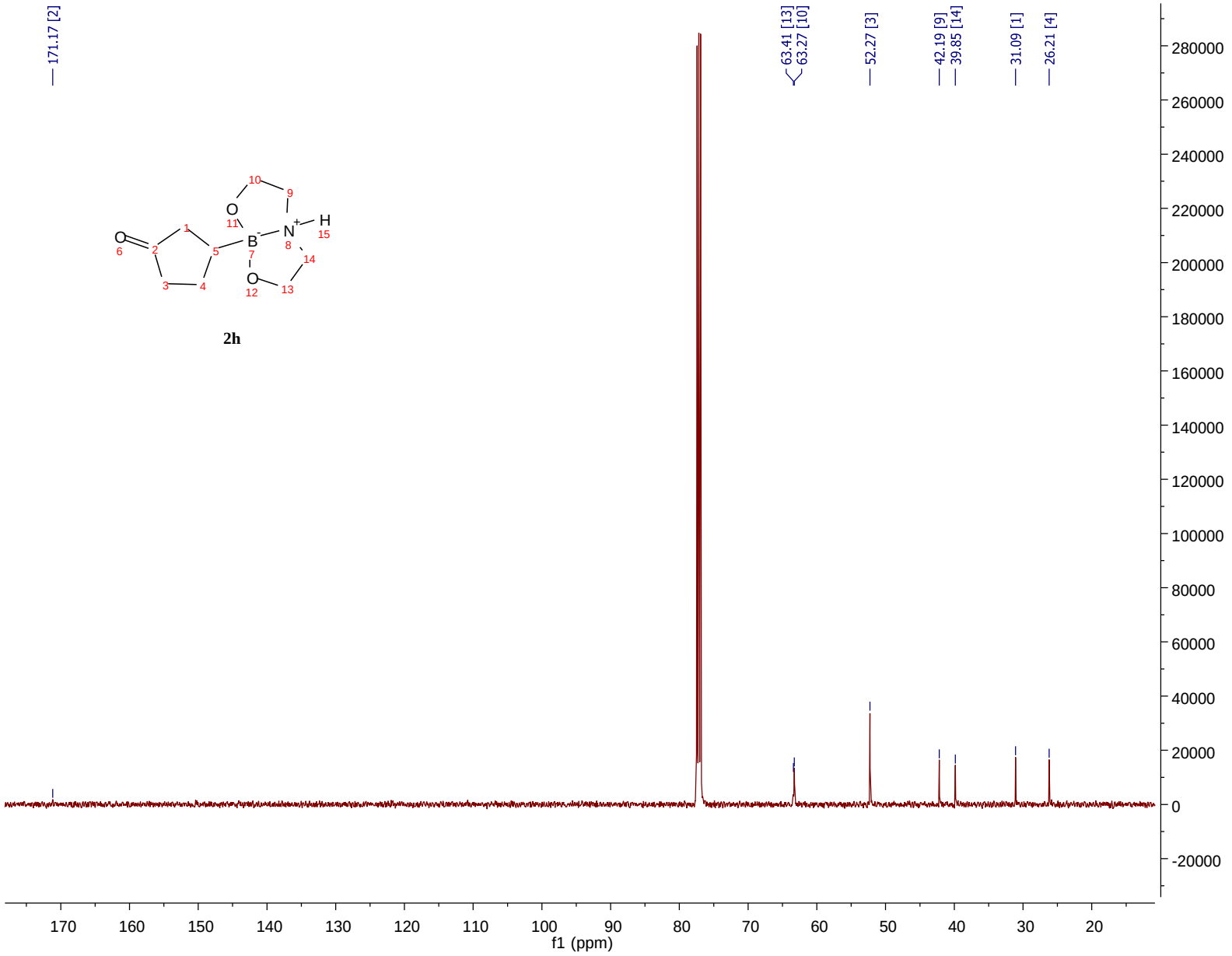
1.38
2.02
3.46
1.41
1.18
f1 (ppm)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63.41 [13]
63.27 [10]
52.27 [3]
42.19 [9]
39.85 [14]
31.09 [1]
26.21 [4]
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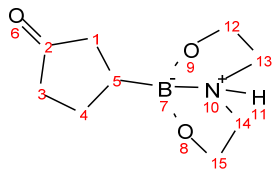
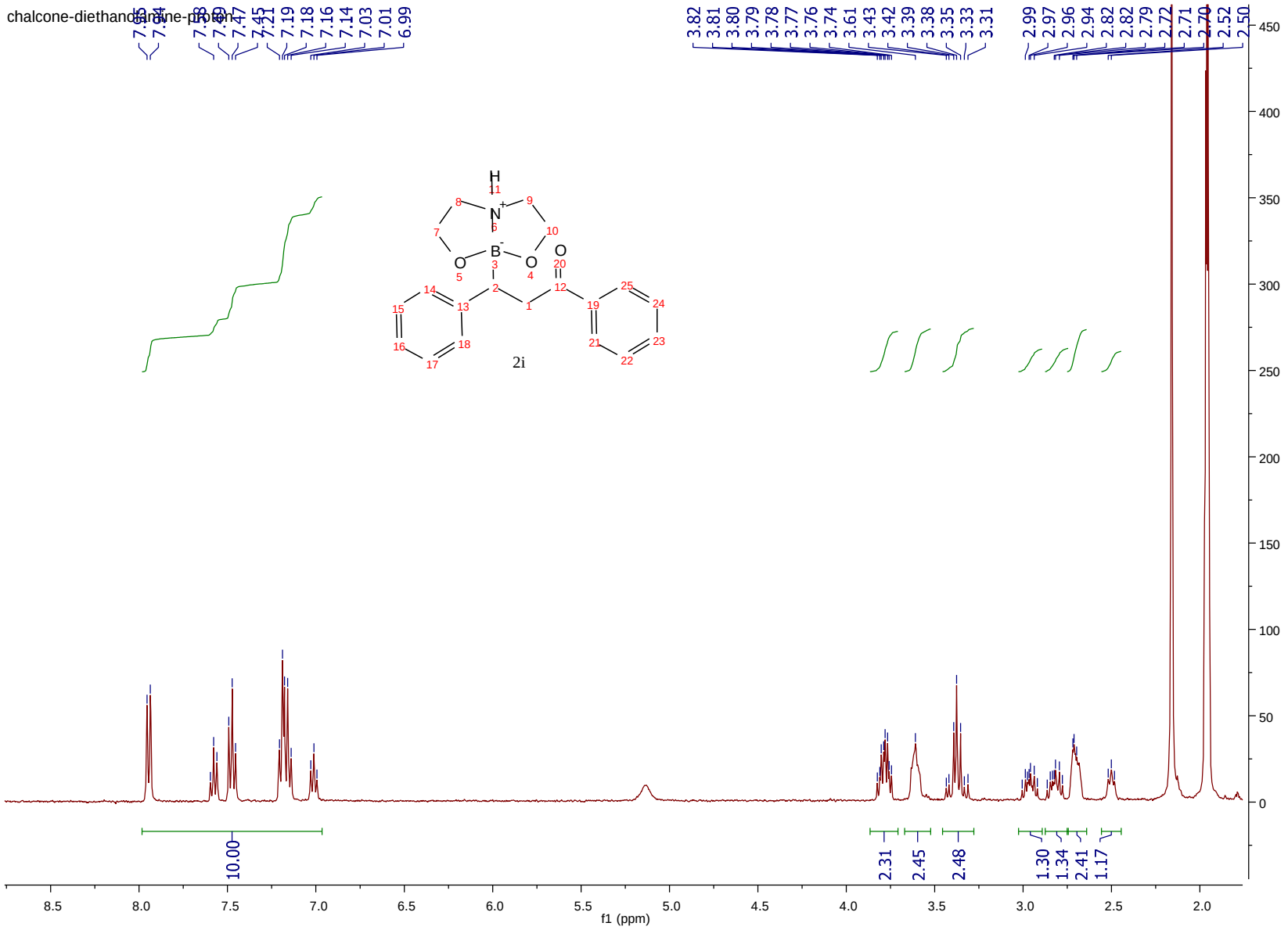
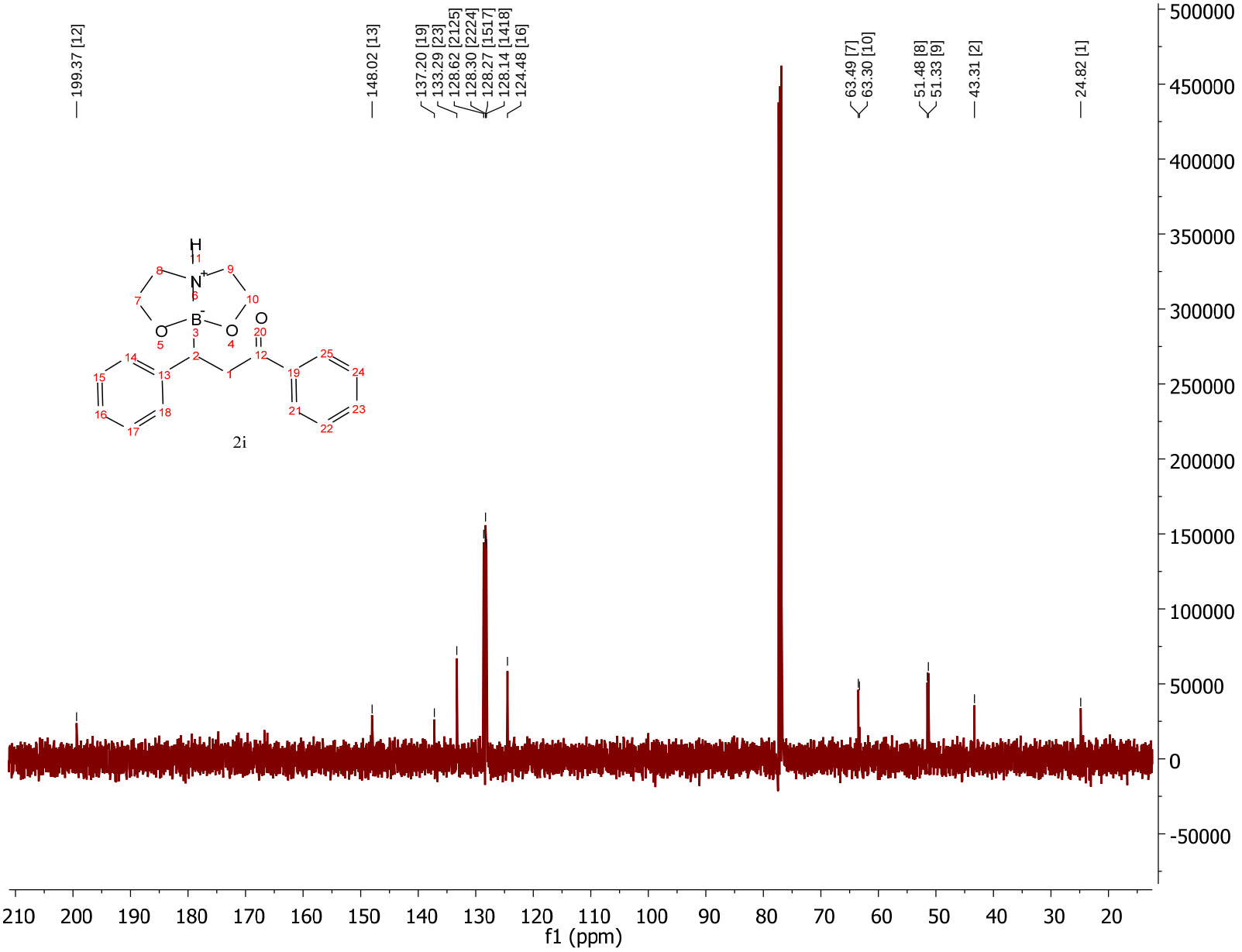
6
1
2
3
4
5
B
7
O
12
13
14
N
8
O
11
10
9
H
15
2h
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

S#424654
Single Pulse with Broadband Decoupling

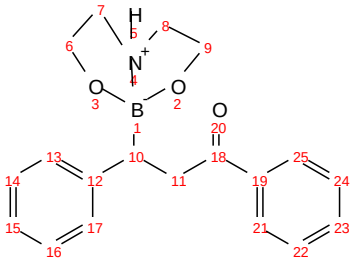


2h

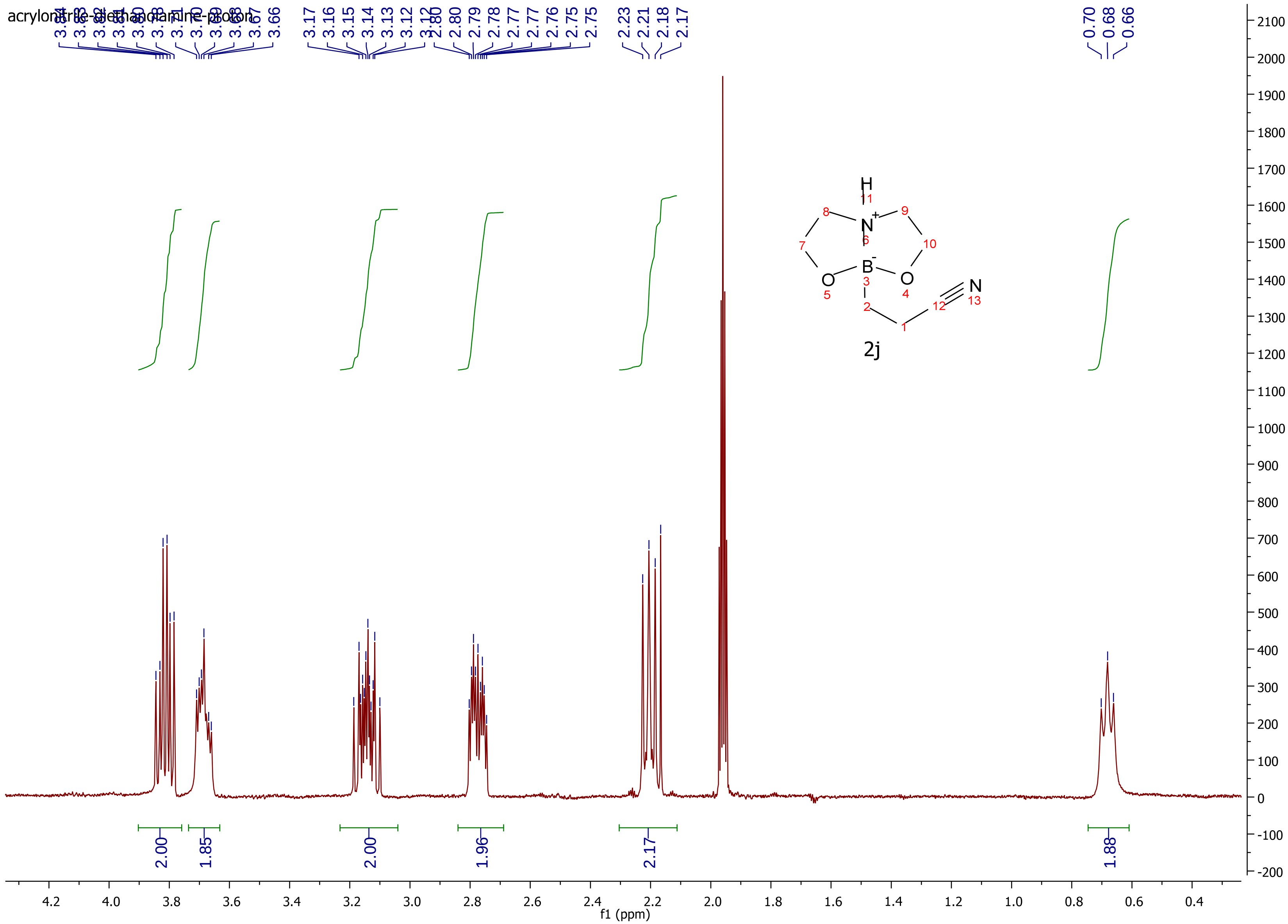

chalcone-diethanolamine-proton
7.95
7.94
7.88
7.89
7.87
7.45
7.21
7.19
7.18
7.16
7.14
7.03
7.01
6.99
3.82
3.81
3.80
3.79
3.78
3.77
3.76
3.74
3.61
3.43
3.42
3.39
3.38
3.35
3.33
3.31
2.99
2.97
2.96
2.94
2.82
2.82
2.79
2.72
2.71
2.70
2.52
2.50
2i
10.00
2.31
2.45
2.48
1.30
1.34
2.41
1.17
f1 (ppm)

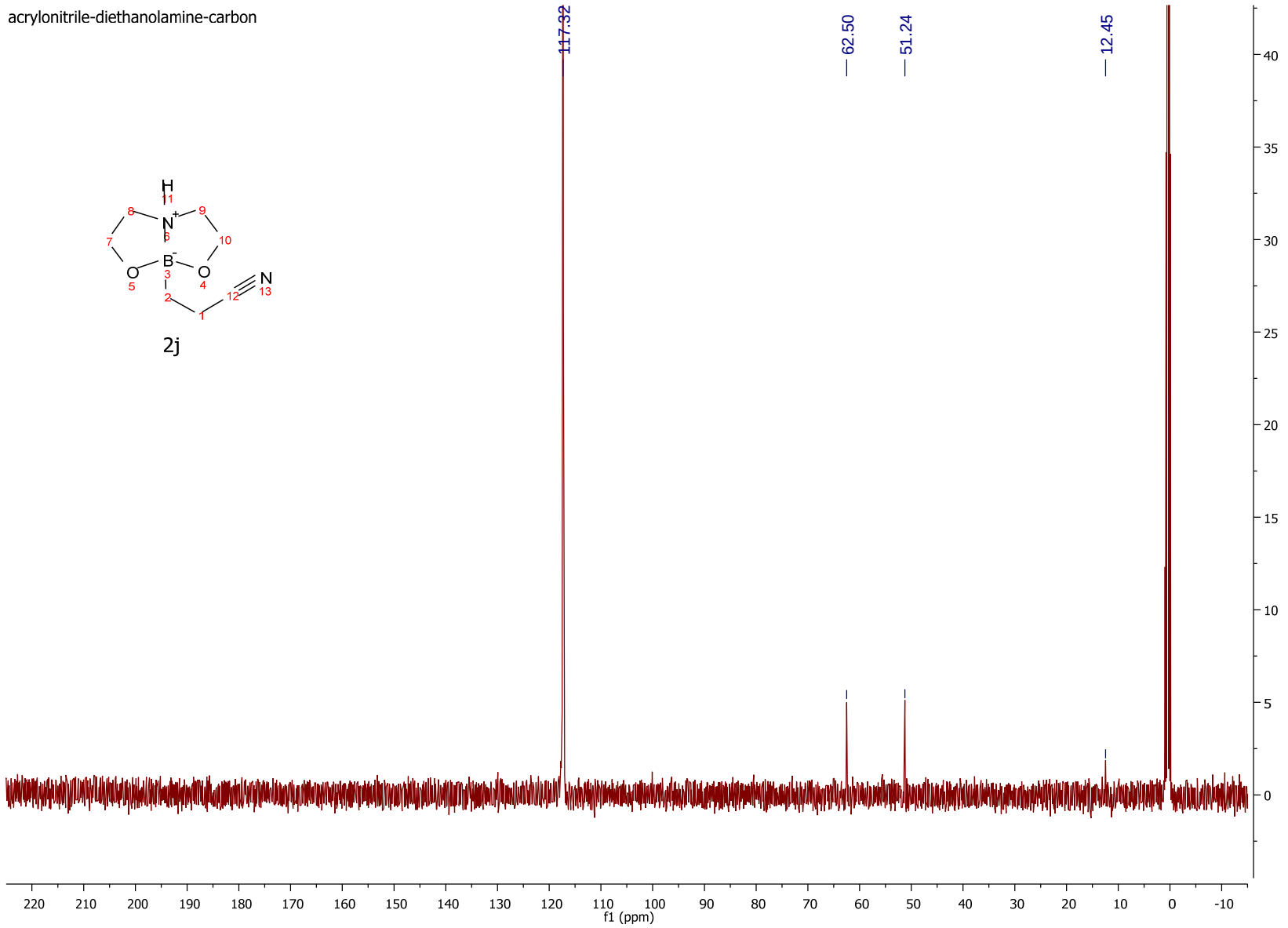

199.37 [12]
148.02 [13]
137.20 [19]
133.29 [23]
128.62 [2125]
128.30 [2224]
128.27 [1517]
128.14 [1418]
124.48 [16]
63.49 [7]
63.30 [10]
51.48 [8]
51.33 [9]
43.31 [2]
24.82 [1]
2i
f1 (ppm)

S#433639
Single Pulse with Broadband Decoupling

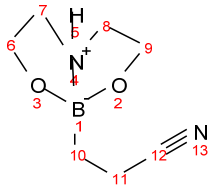


2i

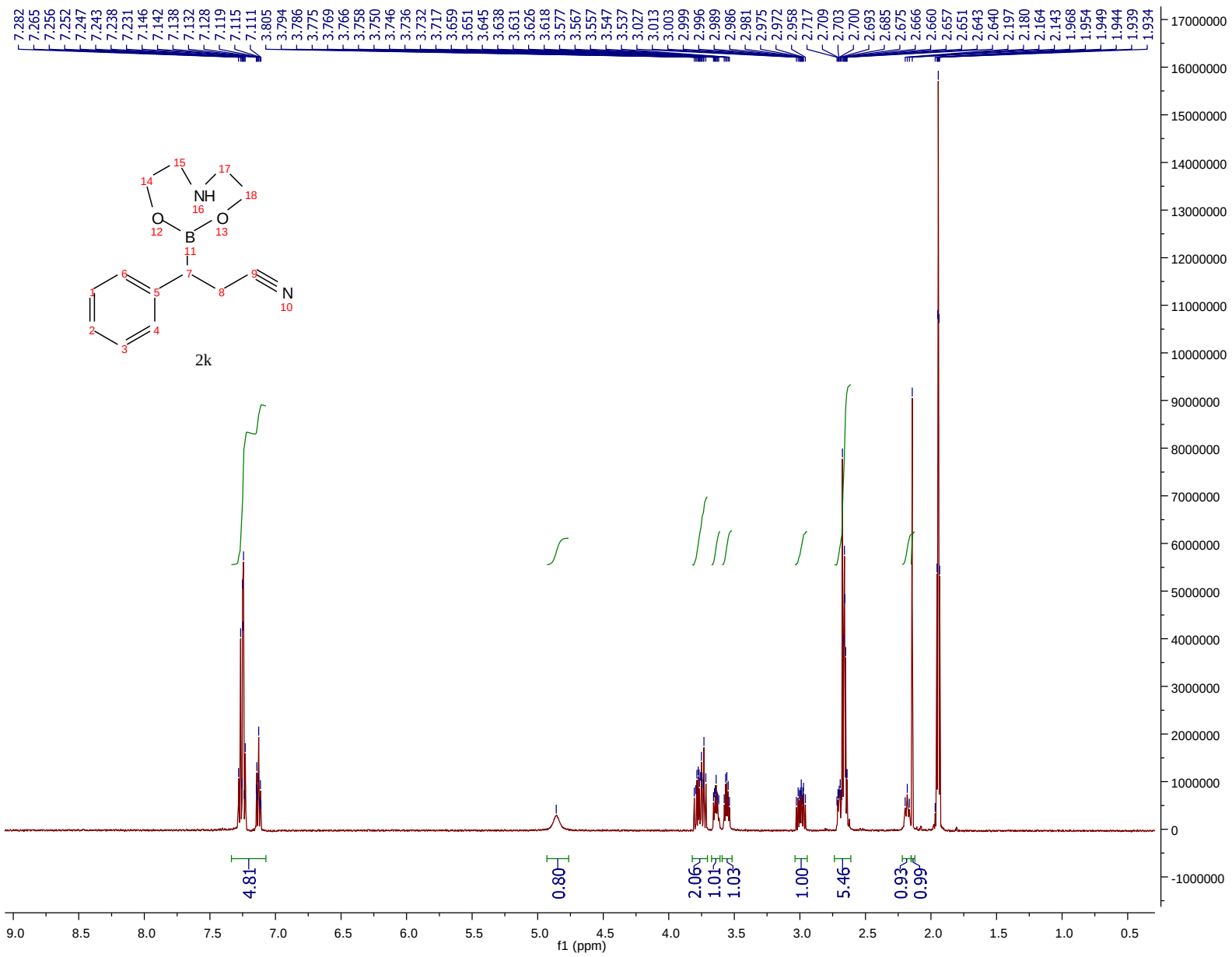

acrylonitrile-diethanolamine-proton
3.84 3.83 3.82 3.81 3.80 3.78 3.71 3.70 3.69 3.68 3.67 3.66
3.17 3.16 3.15 3.14 3.13 3.12 3.12
2.80 2.80 2.79 2.78 2.77 2.77 2.76 2.75 2.75
2.23 2.21 2.18 2.17
0.70 0.68 0.66
2.00 1.85 2.00 1.96 2.17 1.88
f1 (ppm)
2j

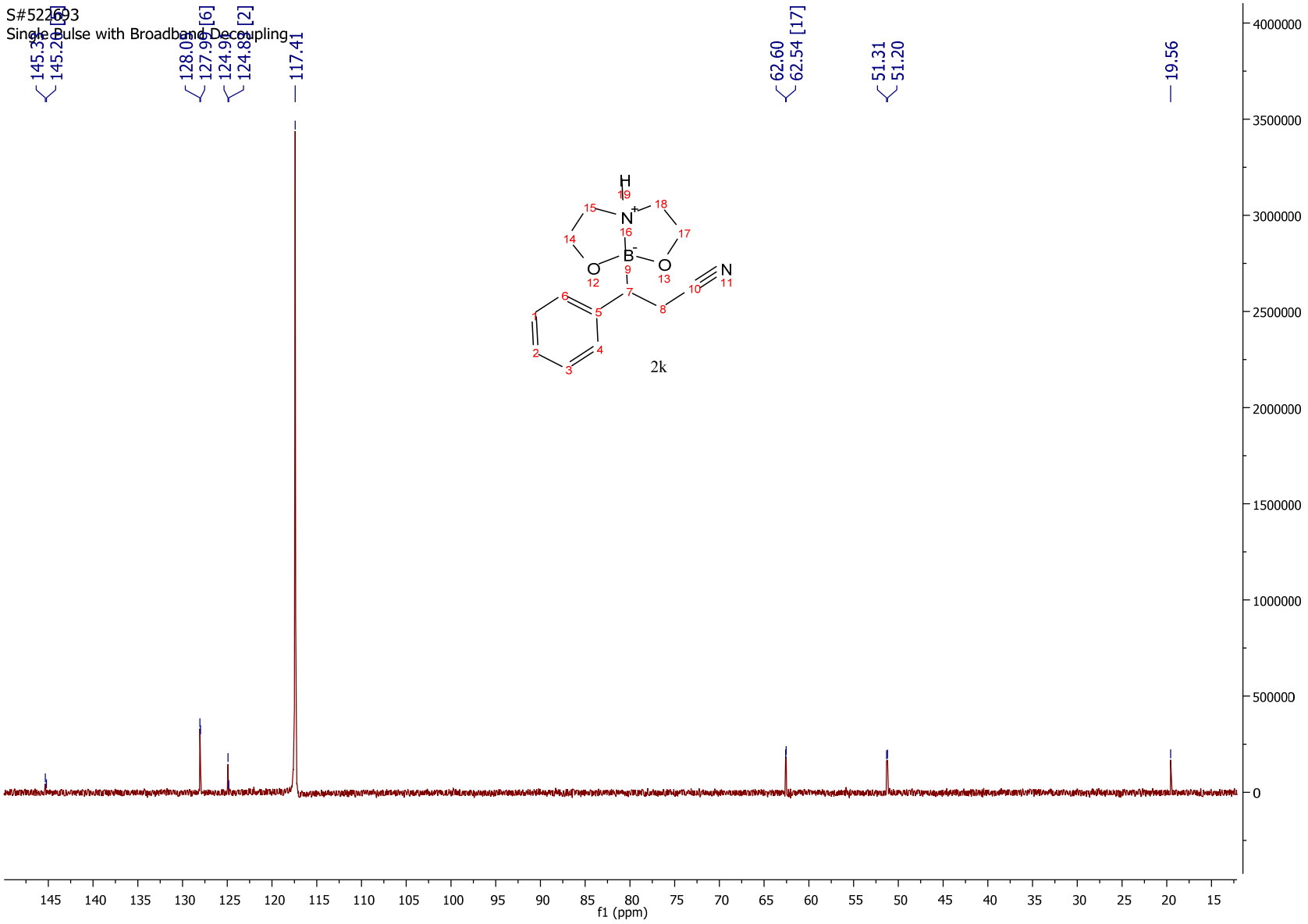

acrylonitrile-diethanolamine-carbon
117.32
62.50
51.24
12.45
2j
f1 (ppm)

S#381680
Single Pulse with Broadband Decoupling

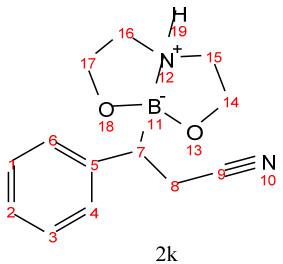


2j


7.282 7.265 7.256 7.252 7.247 7.243 7.238 7.231 7.146 7.142 7.138 7.132 7.128 7.119 7.115 7.111 3.805 3.794 3.786 3.775 3.769 3.766 3.758 3.750 3.746 3.736 3.732 3.717 3.659 3.651 3.645 3.638 3.631 3.626 3.618 3.577 3.567 3.557 3.547 3.537 3.027 3.013 3.003 2.999 2.996 2.989 2.986 2.981 2.975 2.972 2.958 2.717 2.709 2.703 2.700 2.693 2.685 2.675 2.666 2.660 2.657 2.651 2.643 2.640 2.197 2.180 2.164 2.143 1.968 1.954 1.949 1.944 1.939 1.934
NH
O
O
B
N
2k
4.81
0.80
2.06
1.01
1.03
1.00
5.46
0.93
0.99
f1 (ppm)

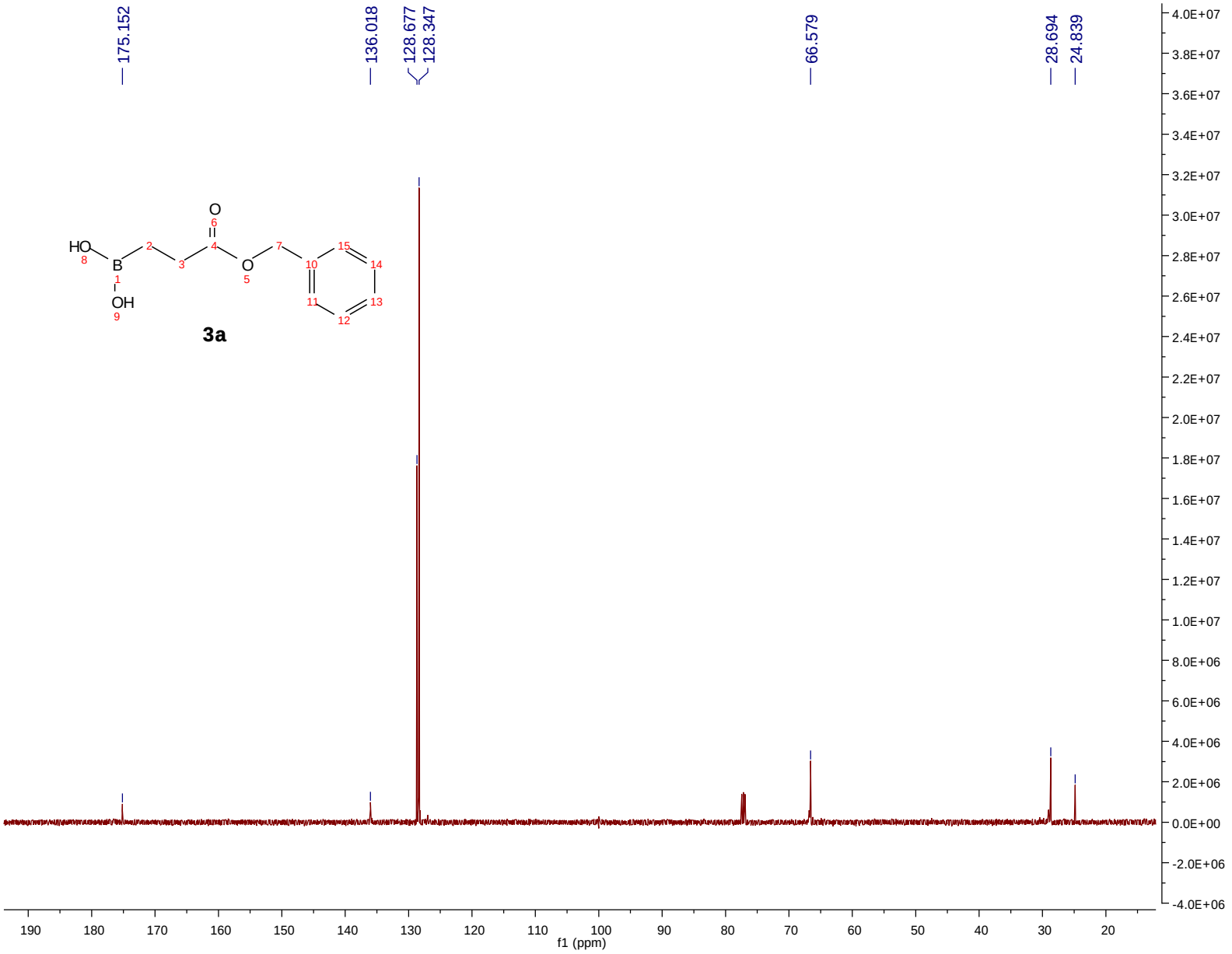

S#522693
Single Pulse with Broadband Decoupling
145.39
145.20 [2]
128.08
127.99 [6]
124.91
124.82 [2]
117.41
62.60
62.54 [17]
51.31
51.20
19.56
2k
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15
f1 (ppm)

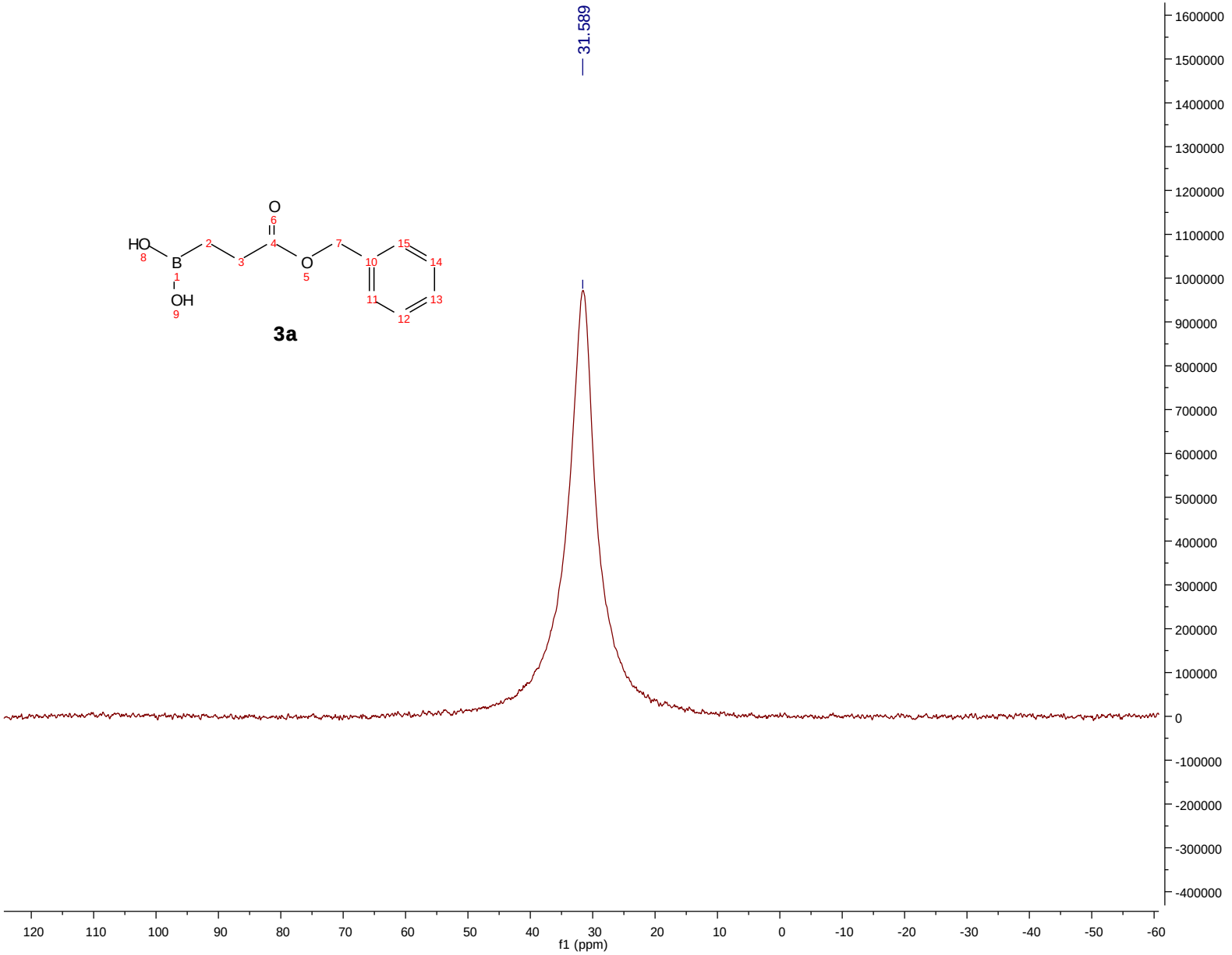
S#370674
Single Pulse with Broadband Decoupling

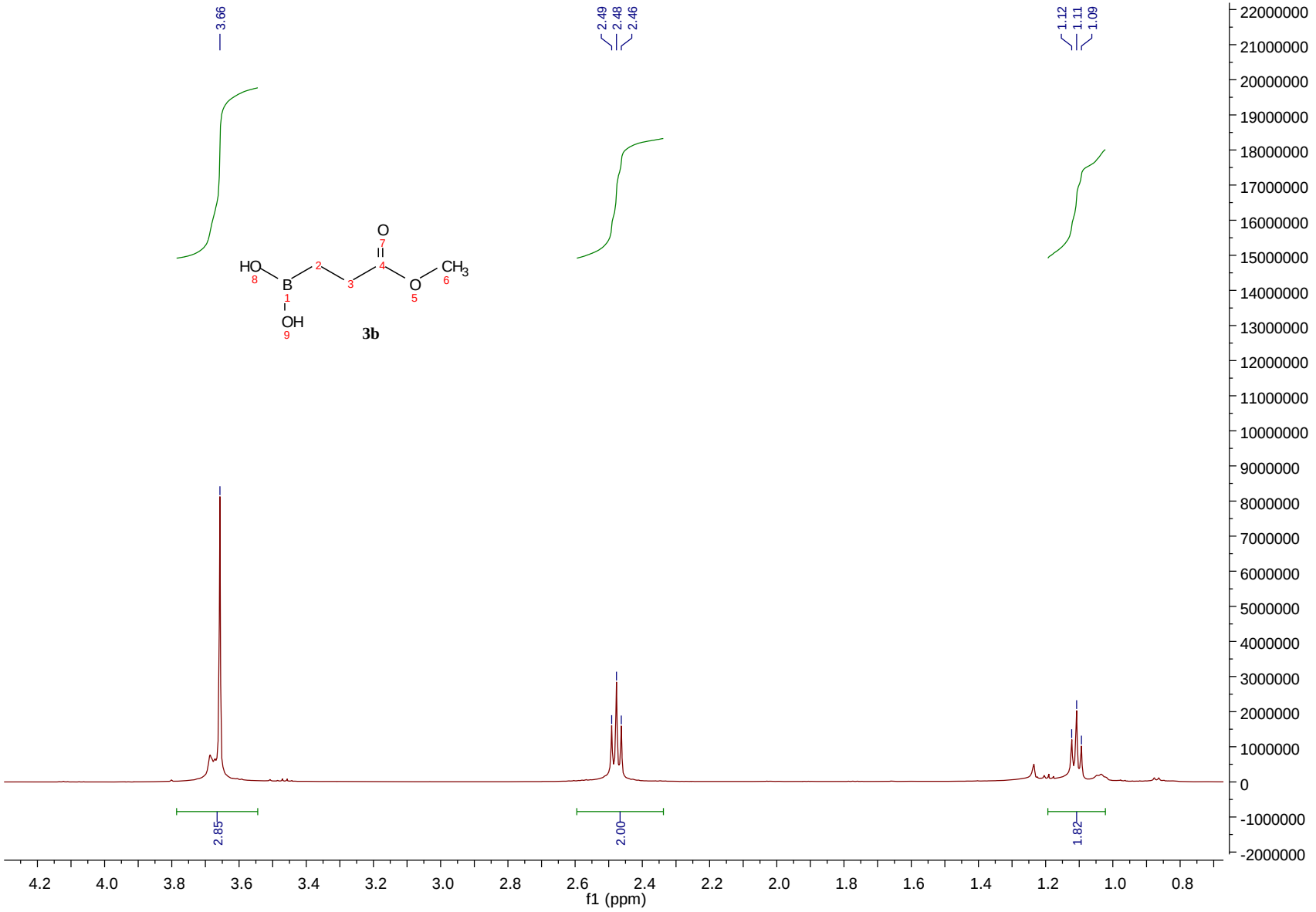


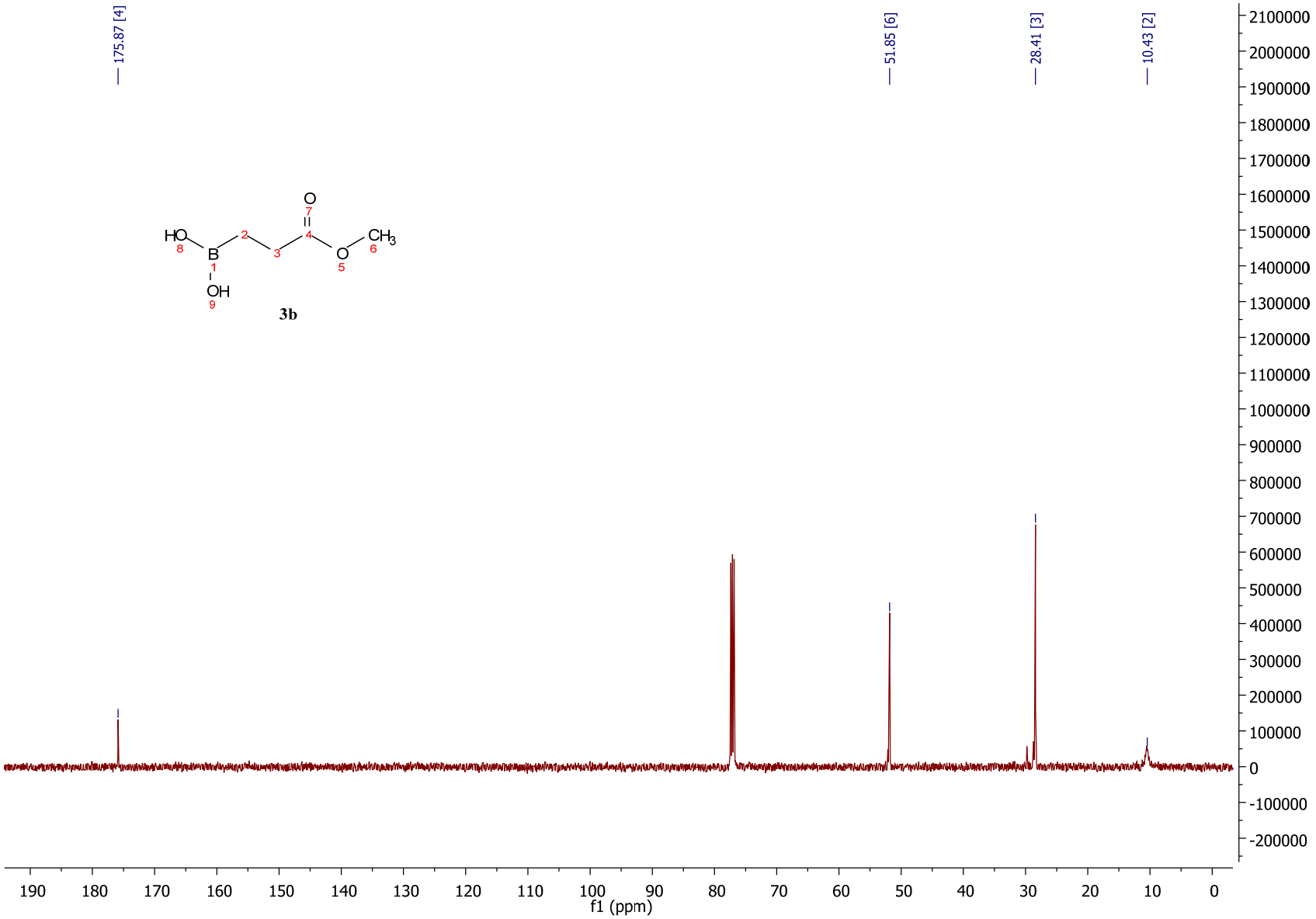
2k

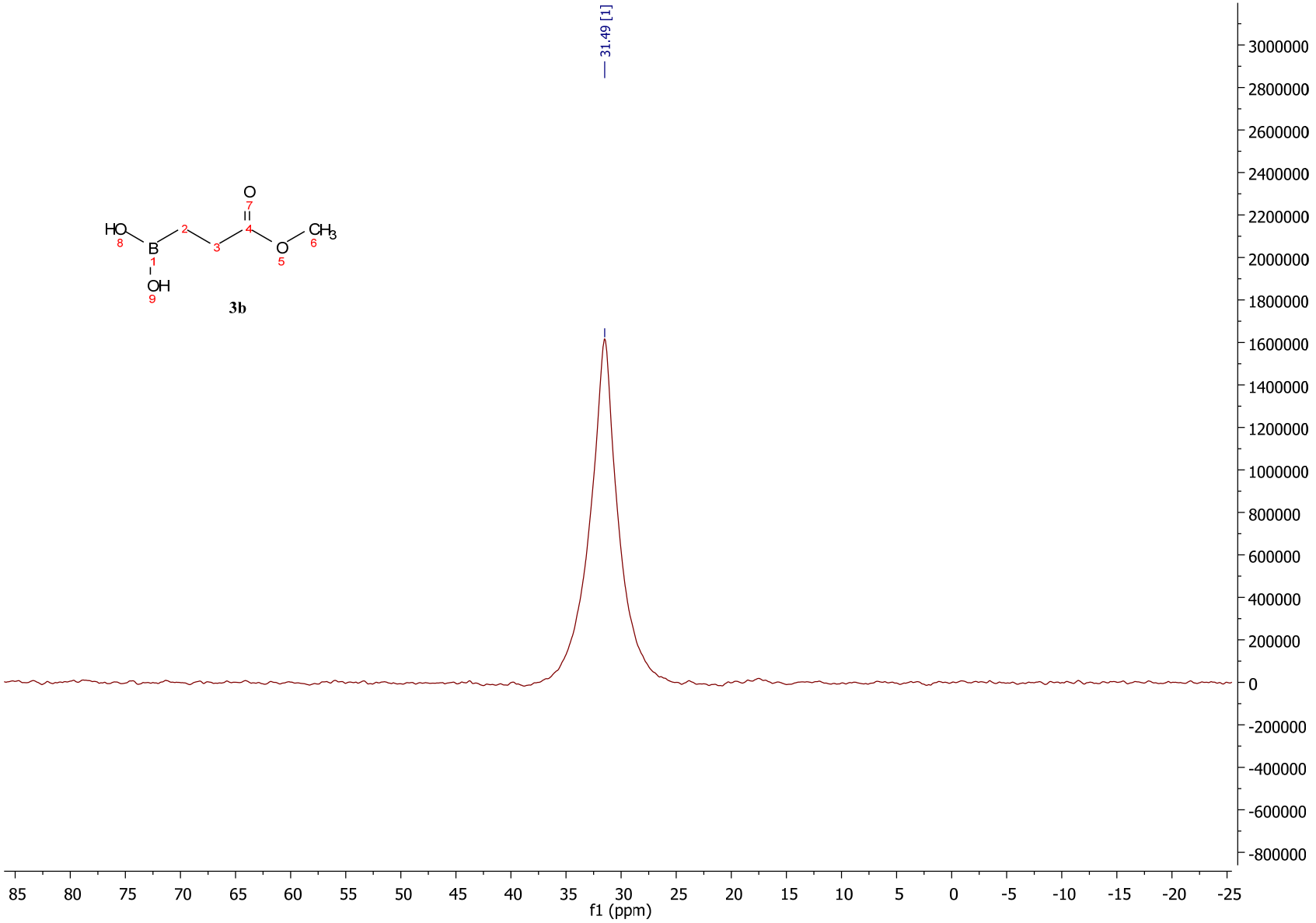

7.377
7.359
7.351
7.335
7.329
7.318
7.308
5.126
2.547
2.532
2.518
1.133
1.119
1.105
HO
B
OH
O
O
3a
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
4.97
2.07
2.10
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

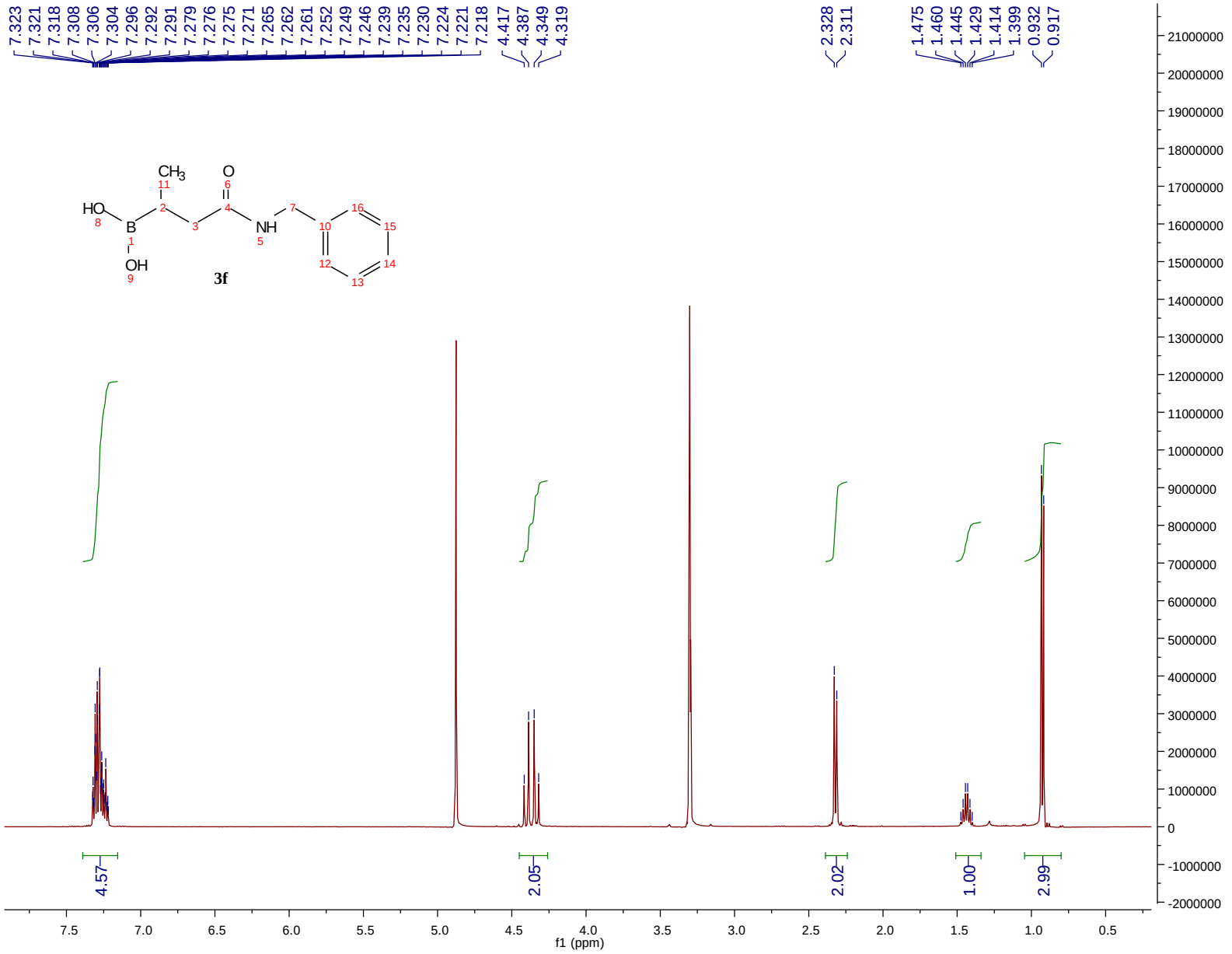

175.152
136.018
128.677
128.347
66.579
28.694
24.839
HO
B
OH
O
O
3a
f1 (ppm)

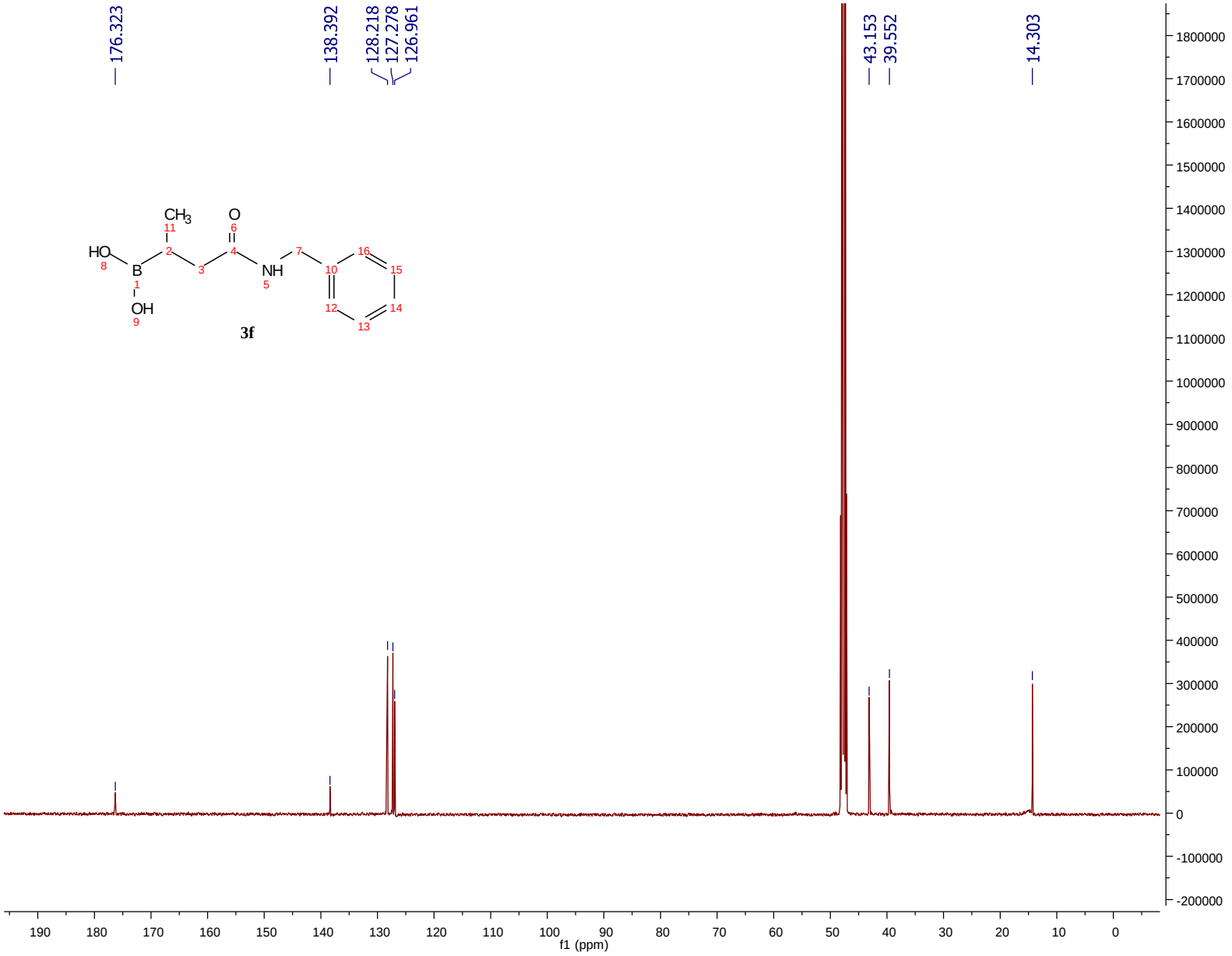

31.589
HO
B
OH
O
O
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
3a
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
-200000
-300000
-400000
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
f1 (ppm)

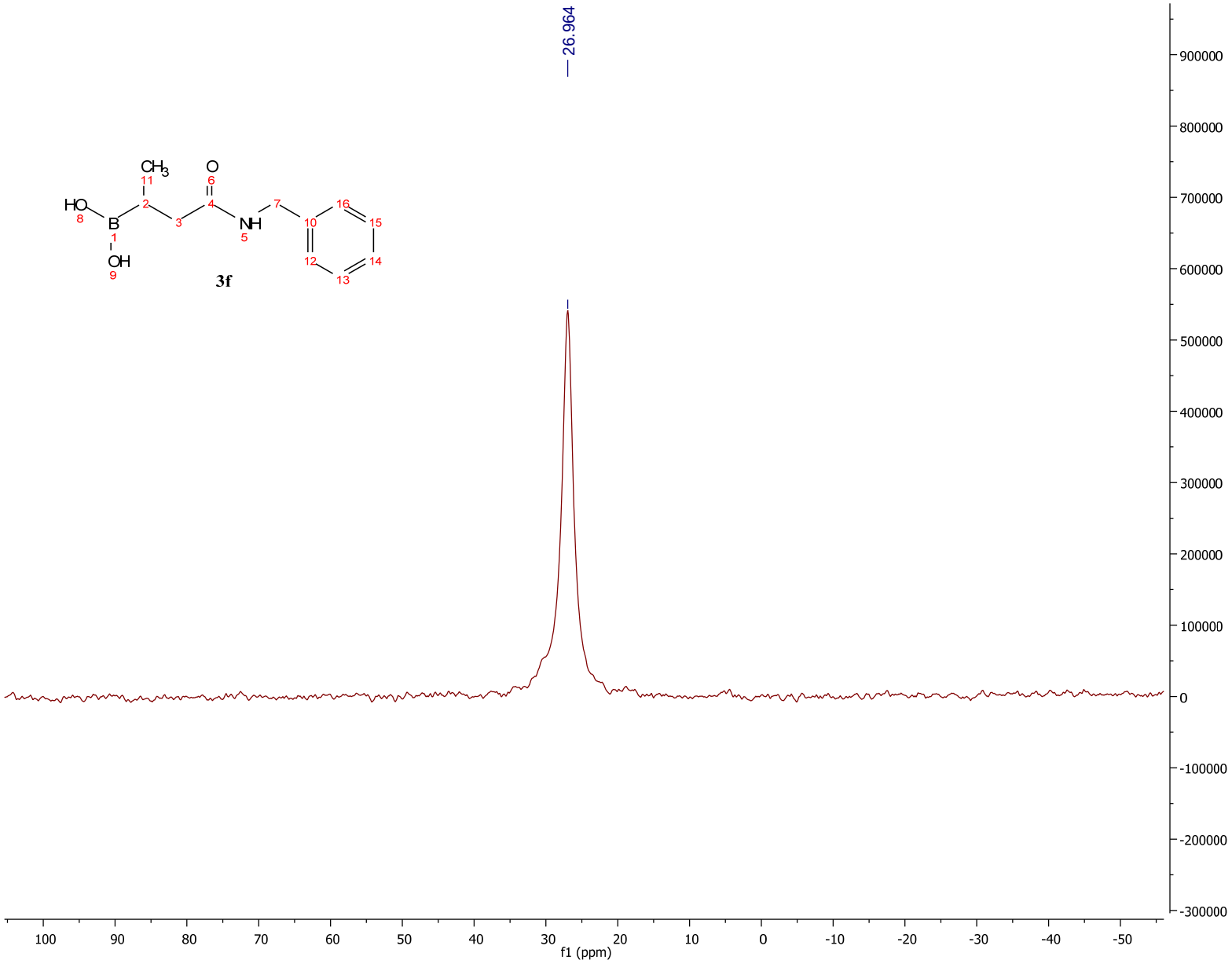

3.66
2.49
2.48
2.46
1.12
1.11
1.09
HO
B
OH
O
O
CH3
1
2
3
4
5
6
7
8
9
3b
2.85
2.00
1.82
f1 (ppm)

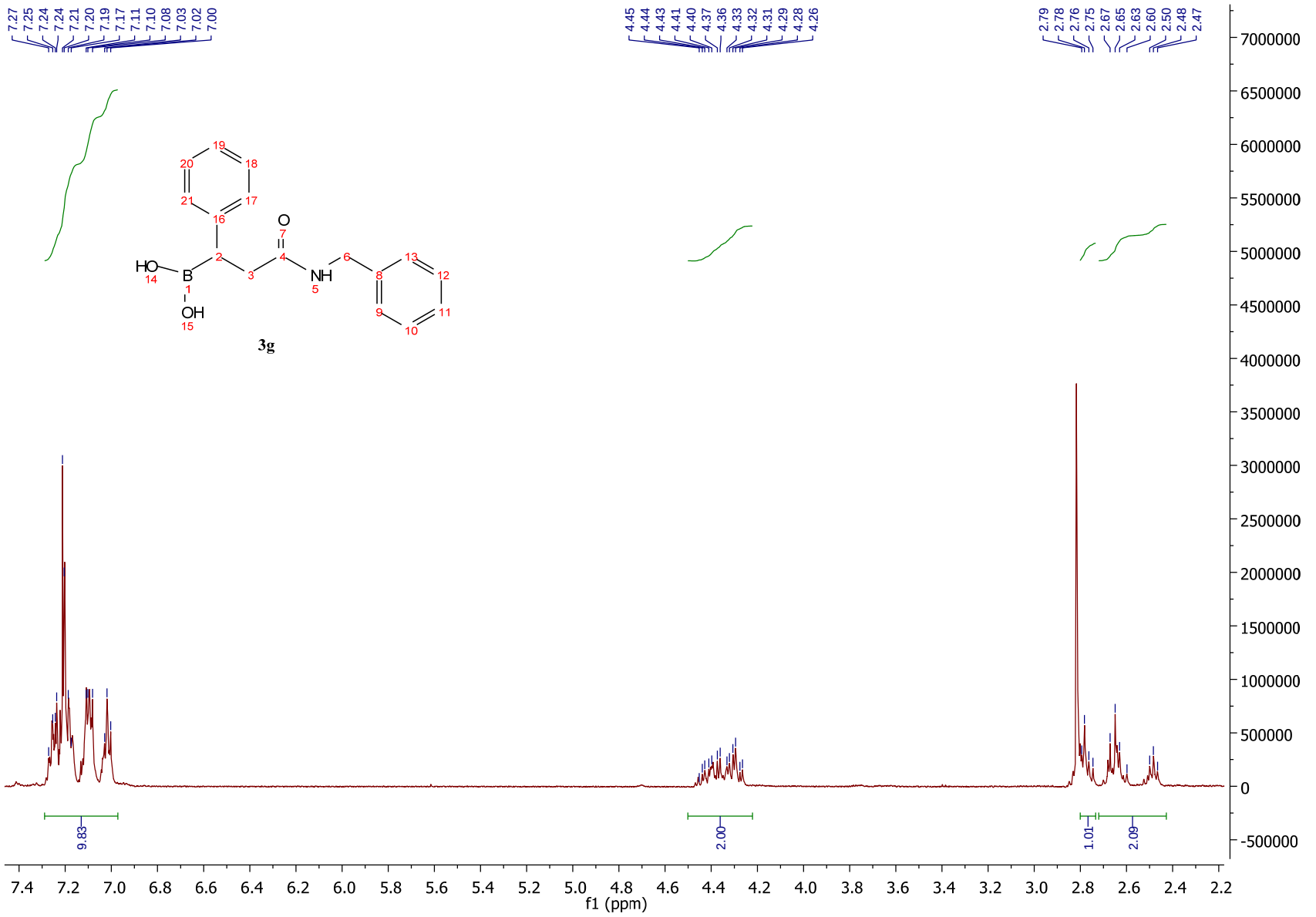

175.87 [4]
51.85 [6]
28.41 [3]
10.43 [2]
HO
B
OH
O
CH3
1
2
3
4
5
6
7
8
9
3b
2100000
2000000
1900000
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
-200000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

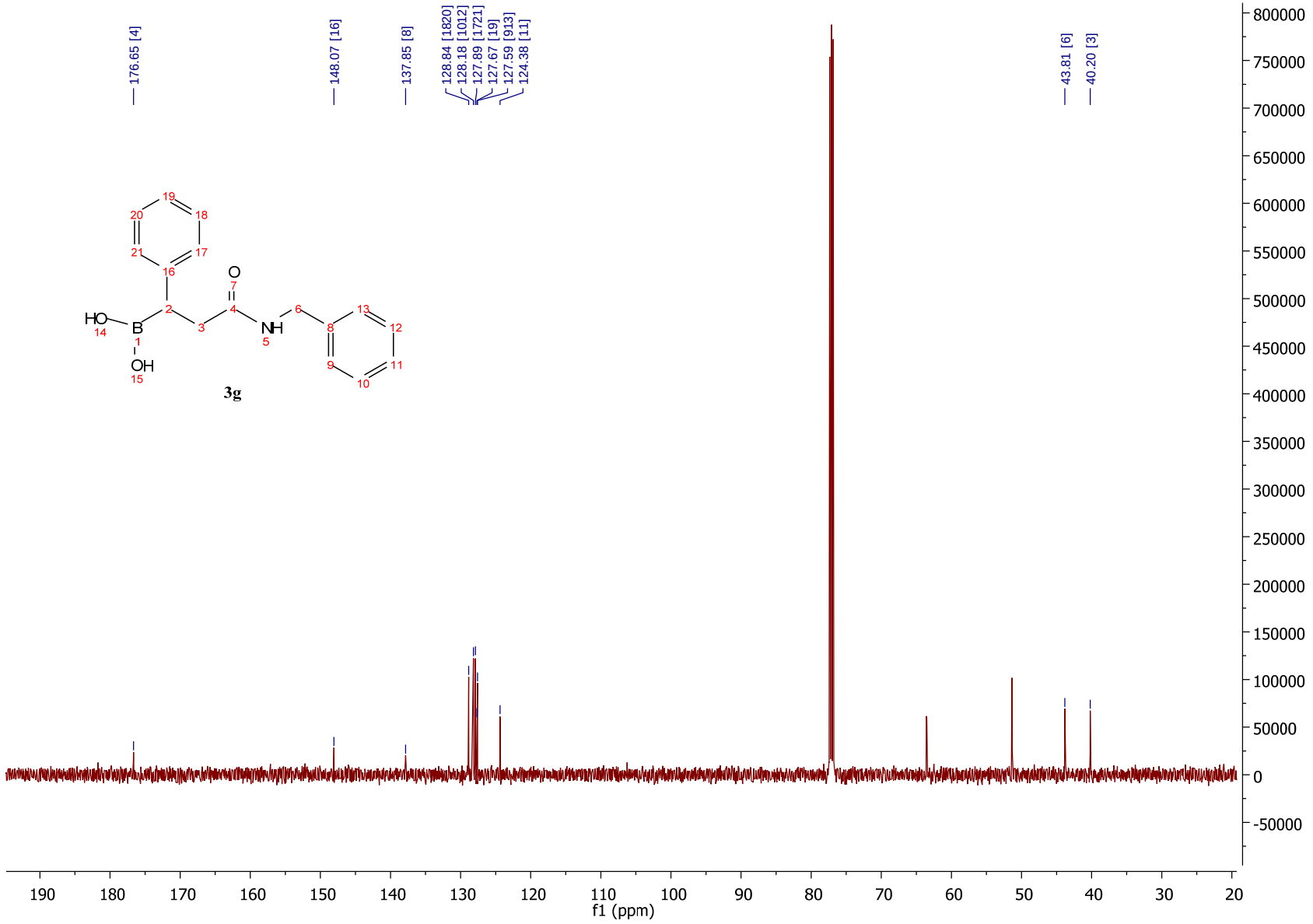

31.49 [1]
HO
B
OH
O
O
CH3
1
2
3
4
5
6
7
8
9
3b
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
-200000
-400000
-600000
-800000
85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25
f1 (ppm)

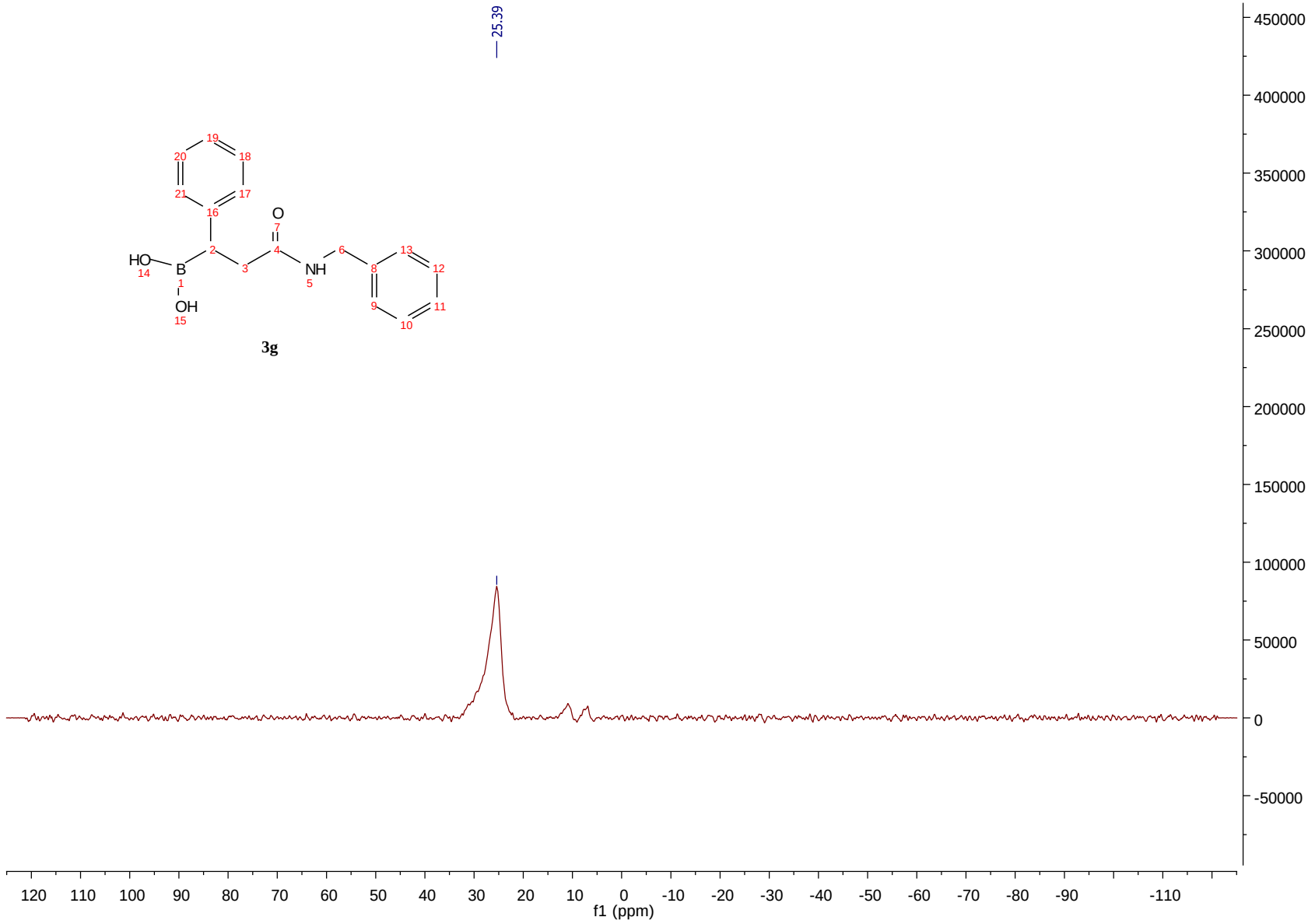

7.323
7.321
7.318
7.308
7.306
7.304
7.296
7.292
7.291
7.279
7.276
7.275
7.271
7.265
7.262
7.261
7.252
7.249
7.246
7.239
7.235
7.230
7.224
7.221
7.218
4.417
4.387
4.349
4.319
2.328
2.311
1.475
1.460
1.445
1.429
1.414
1.399
0.932
0.917
CH3
11
O
6
HO
8
B
1
OH
9
2
3
4
NH
5
7
10
16
15
12
14
13
3f
4.57
2.05
2.02
1.00
2.99
f1 (ppm)

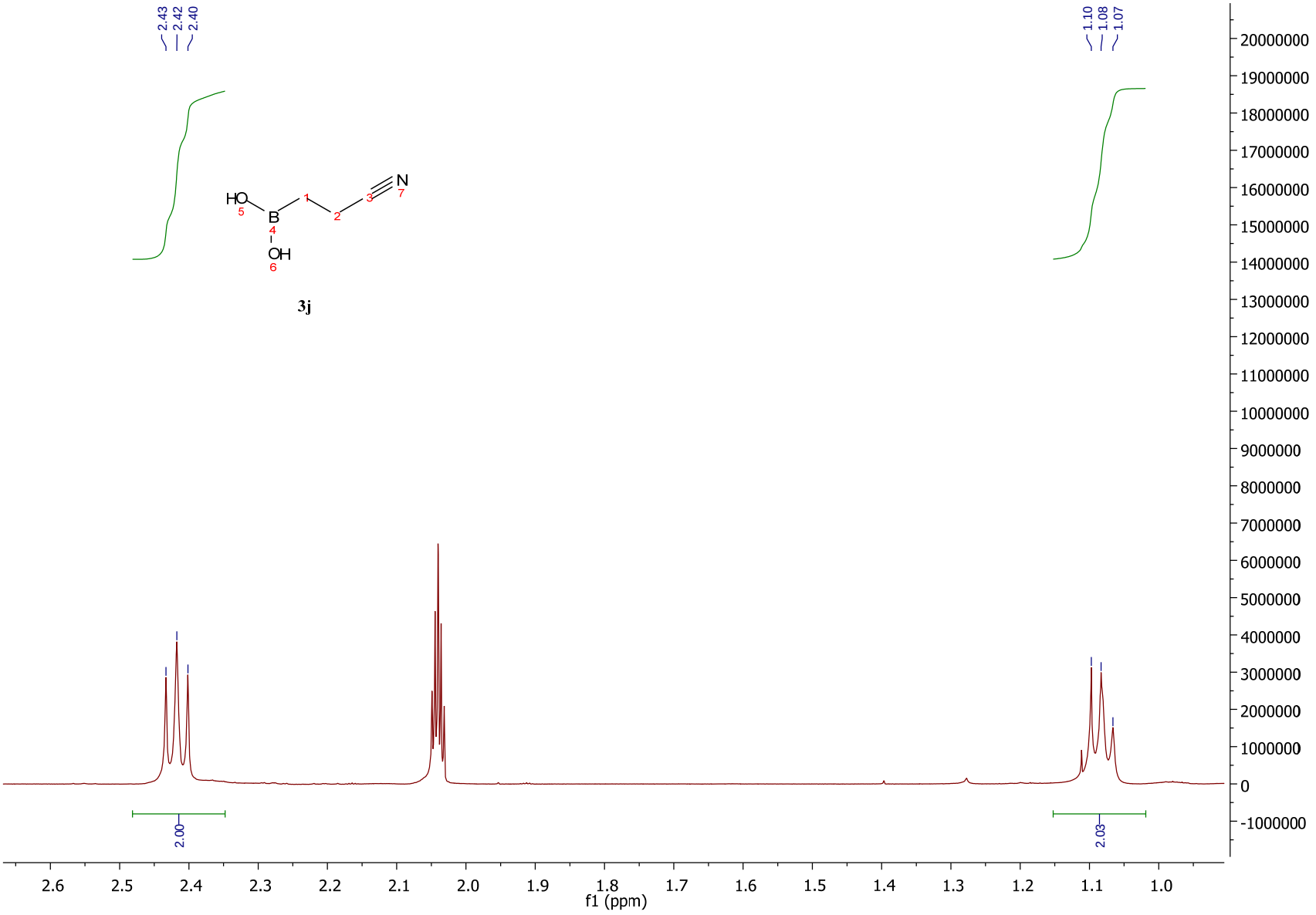

176.323
138.392
128.218
127.278
126.961
43.153
39.552
14.303
CH3
O
HO
B
NH
OH
3f
f1 (ppm)


26.964
HO
B
OH
CH3
O
NH
3f
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
-200000
-300000
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
f1 (ppm)

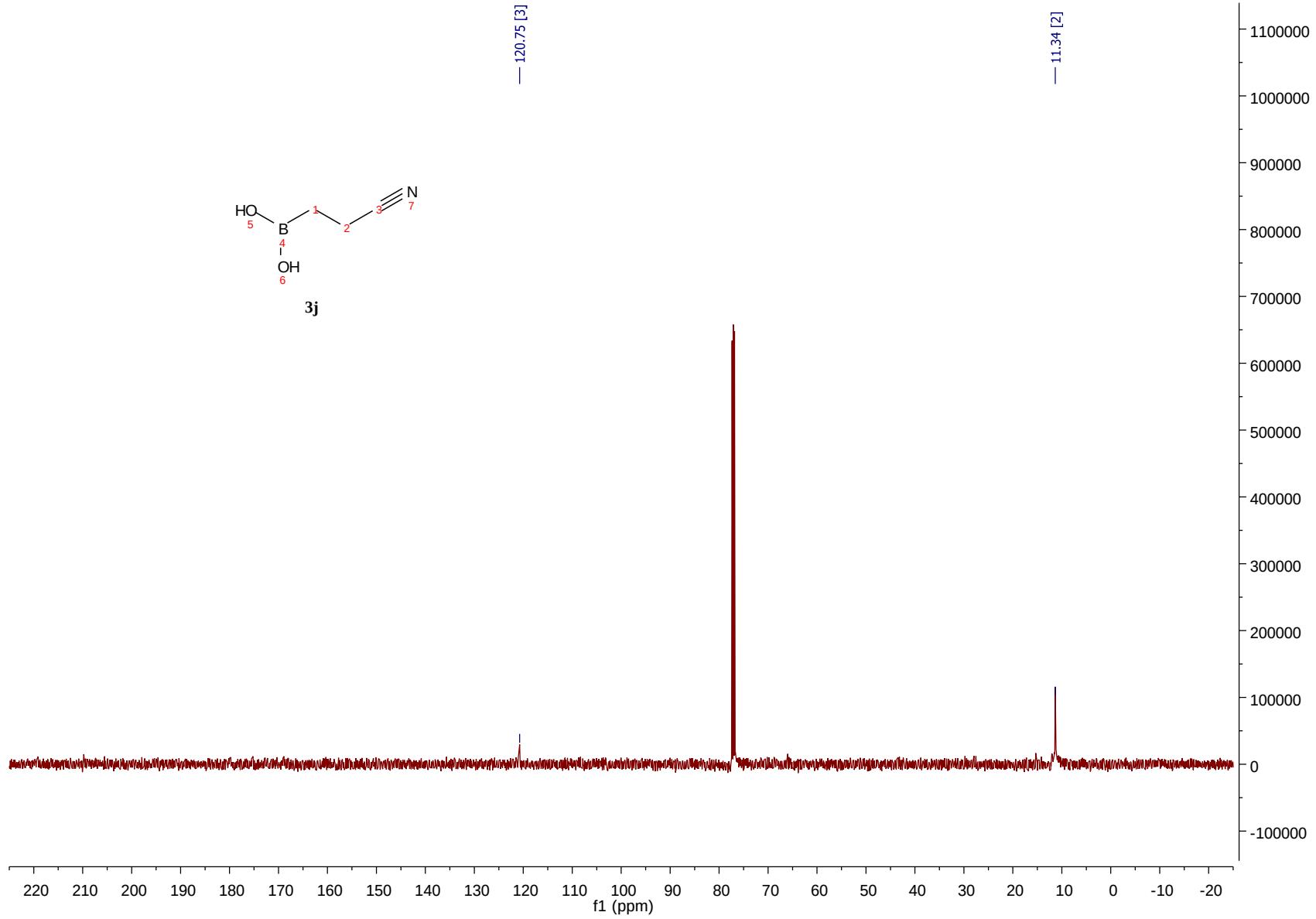

7.27
7.25
7.24
7.24
7.21
7.20
7.19
7.17
7.11
7.10
7.08
7.03
7.02
7.00
4.45
4.44
4.43
4.41
4.40
4.37
4.36
4.33
4.32
4.31
4.29
4.28
4.26
2.79
2.78
2.76
2.75
2.67
2.65
2.63
2.60
2.50
2.48
2.47
HO
B
OH
NH
O
3g
9.83
2.00
1.01
2.09
f1 (ppm)

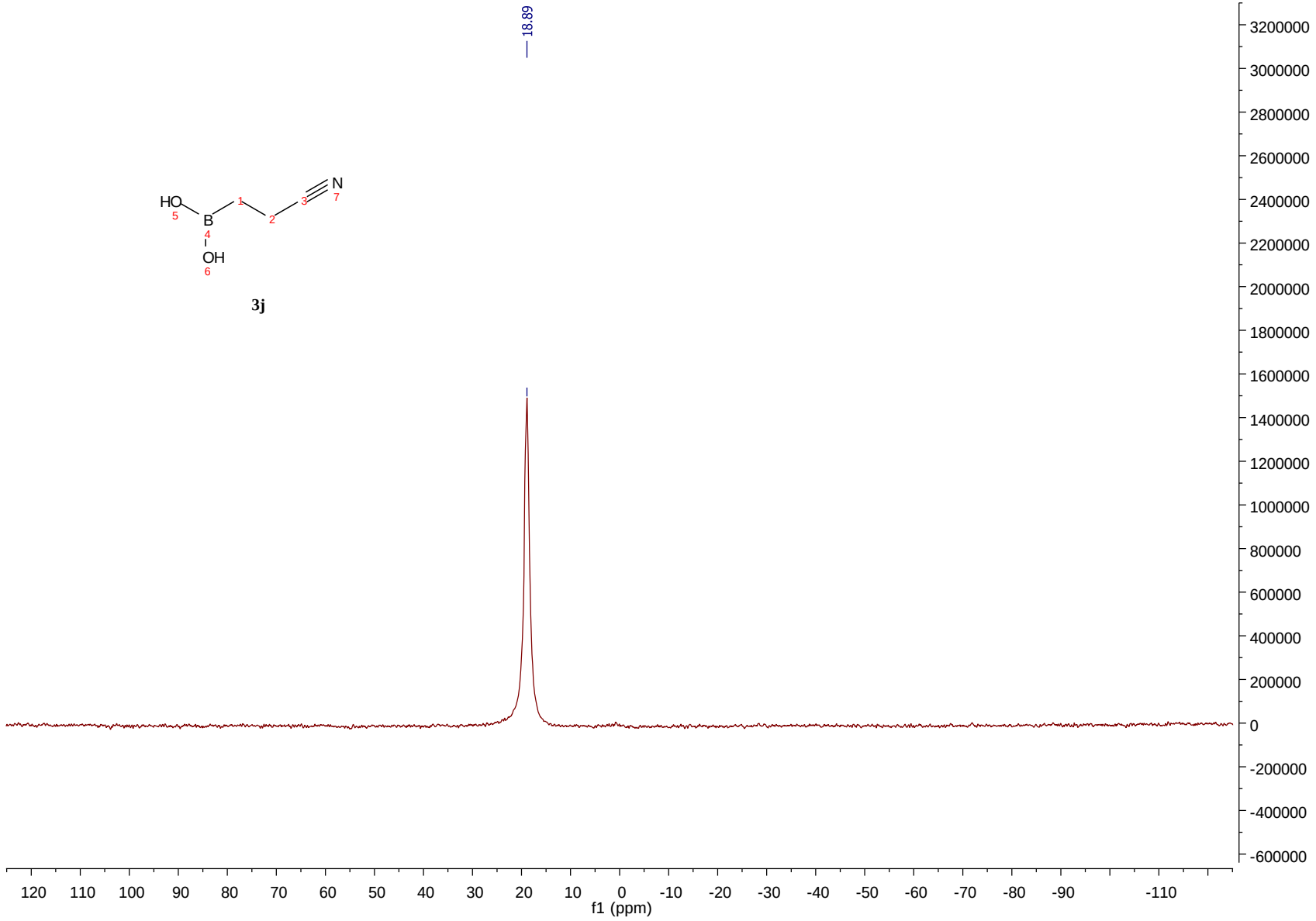

176.65 [4]
148.07 [16]
137.85 [8]
128.84 [1820]
128.18 [1012]
127.89 [1721]
127.67 [19]
127.59 [913]
124.38 [11]
43.81 [6]
40.20 [3]
HO
B
OH
NH
O
3g
f1 (ppm)


25.39
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)
HO
B
OH
NH
O
3g



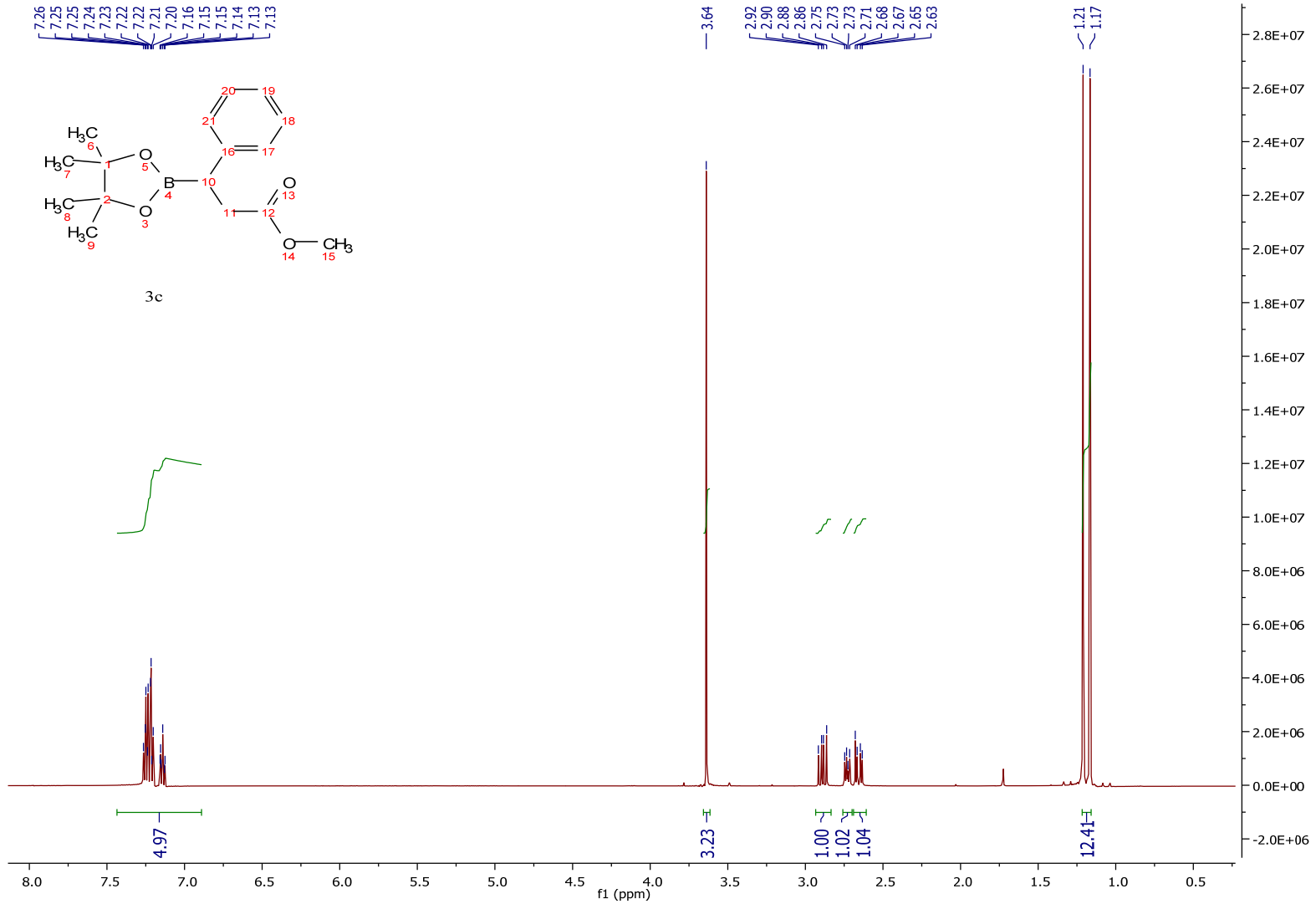
3j

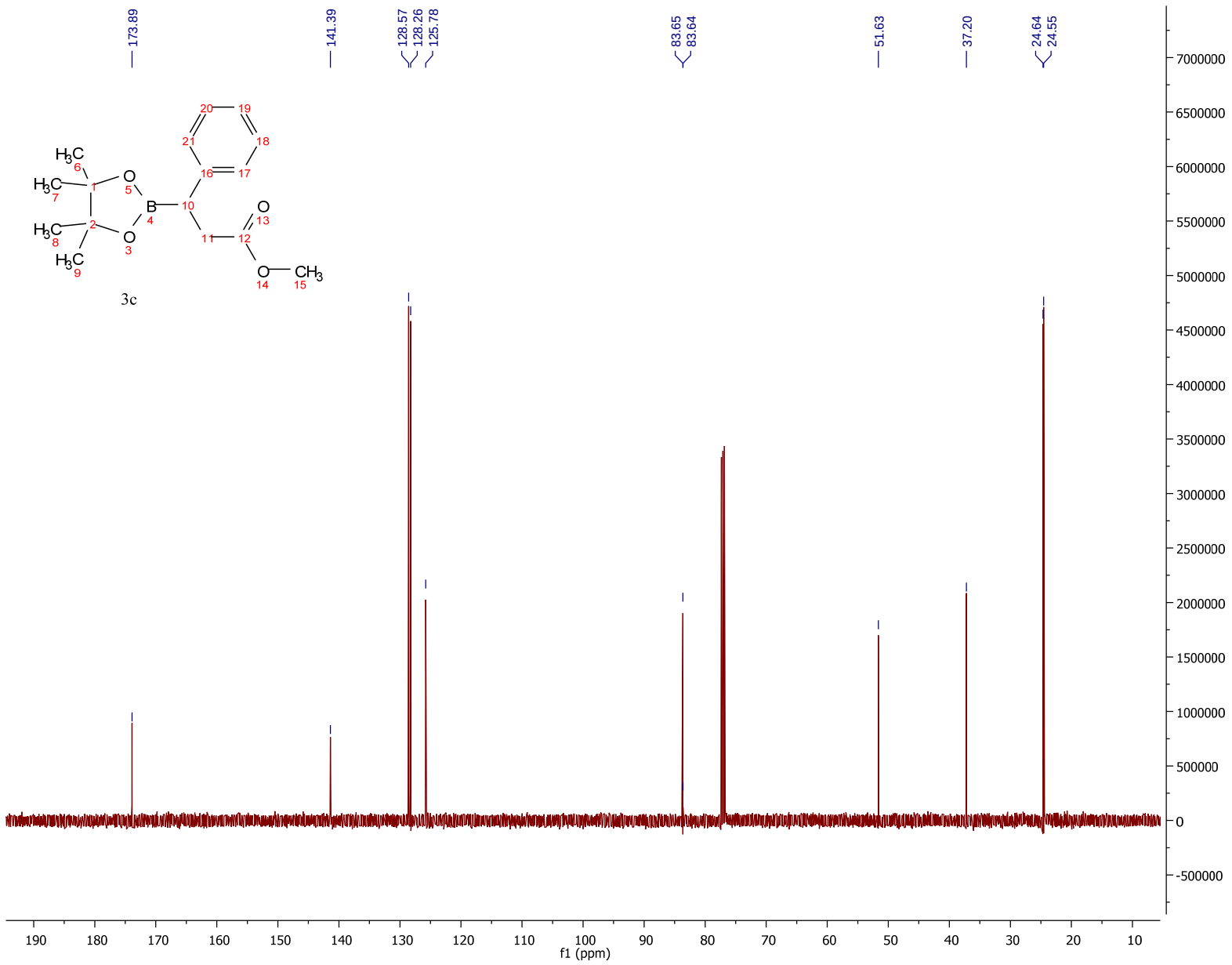

120.75 [3]
11.34 [2]
HO
5
B
4
OH
6
1
2
3
N
7
3j
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
-100000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

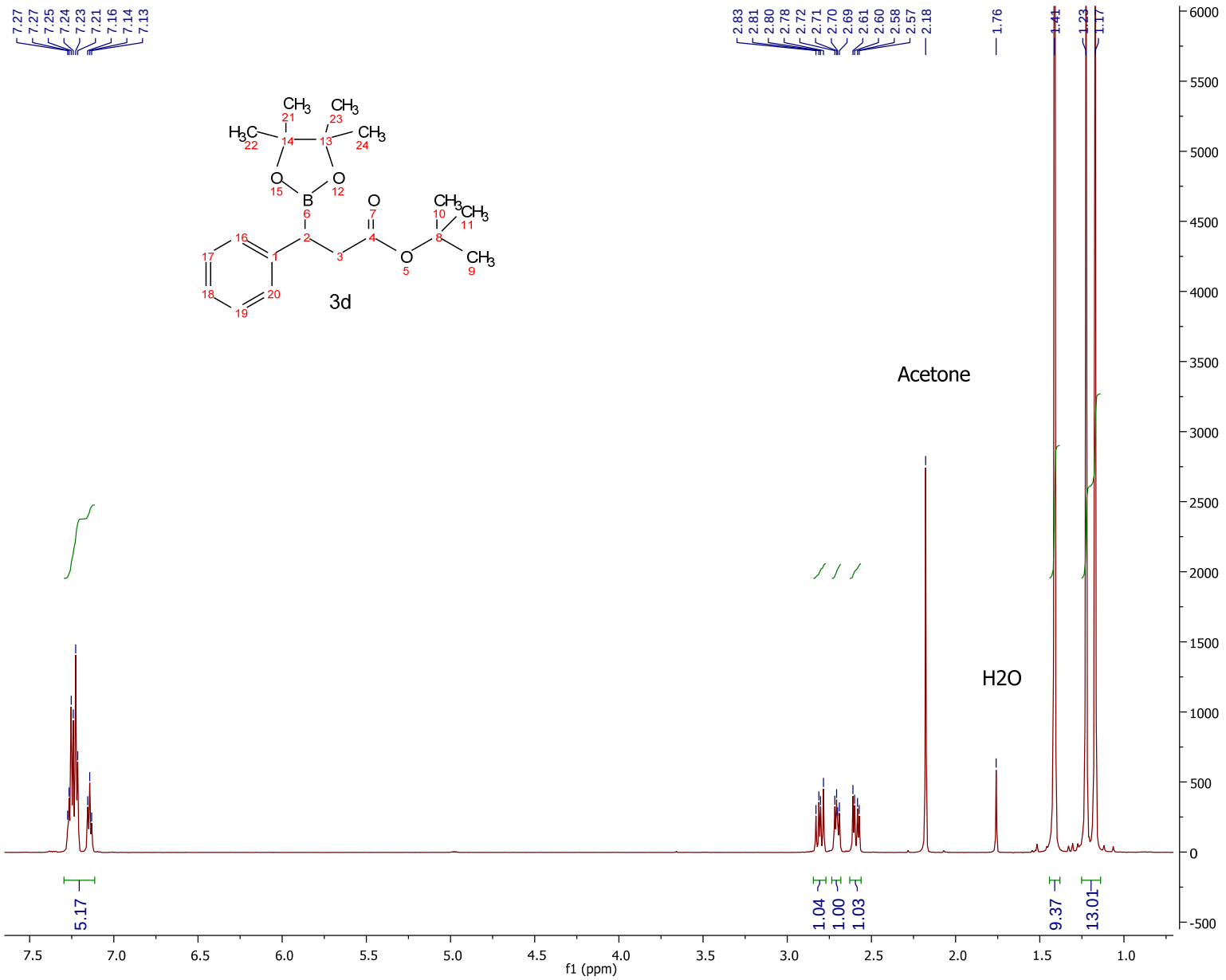

18.89
HO
5
B
4
OH
6
1
2
3
N
7
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
-200000
-400000
-600000
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110
f1 (ppm)

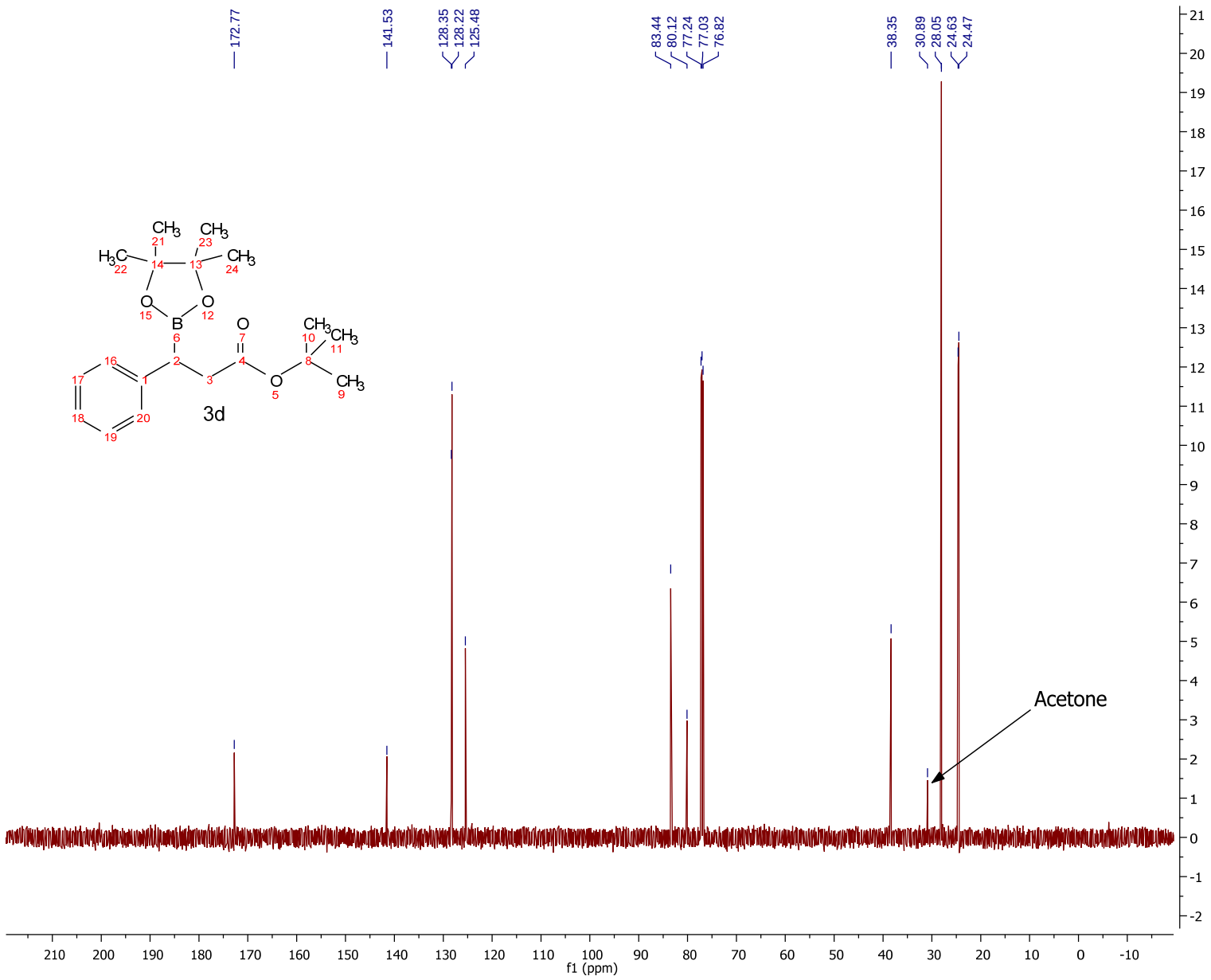
3j

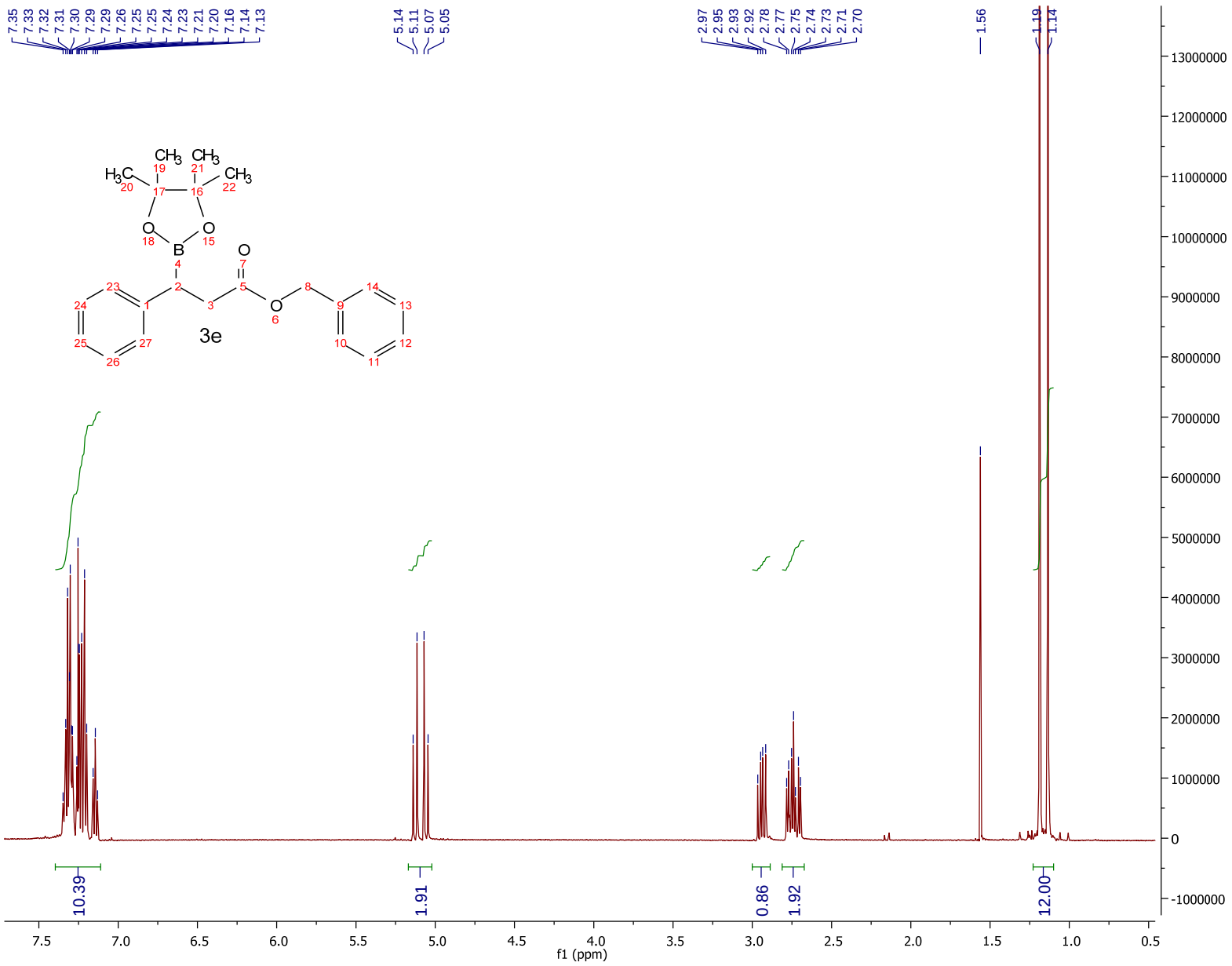
The following spectra (3c-e, 3h, 3i) represent the reisolated pinacol protected boronic ester from the corresponding DEA-adduct (see Table 1).

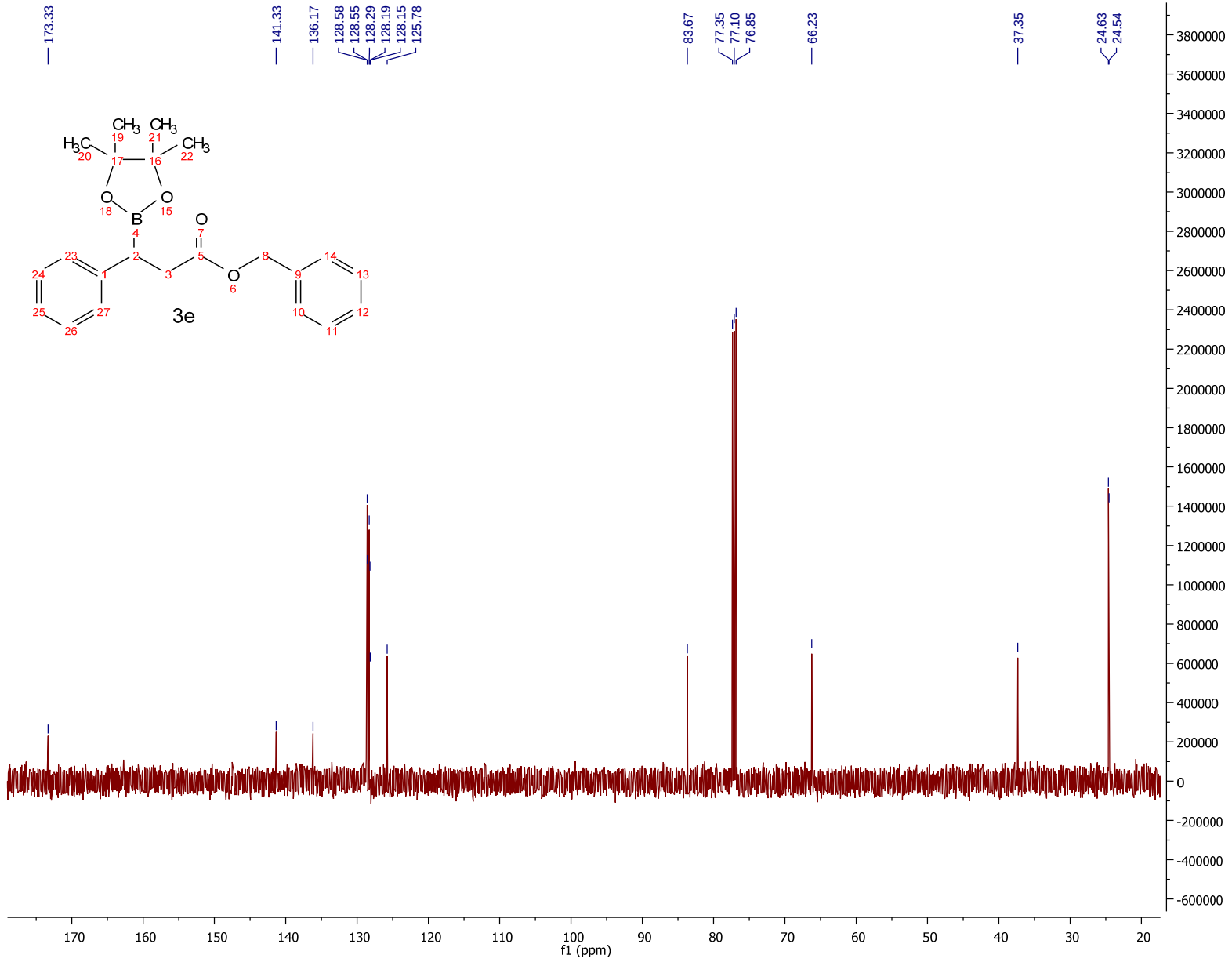


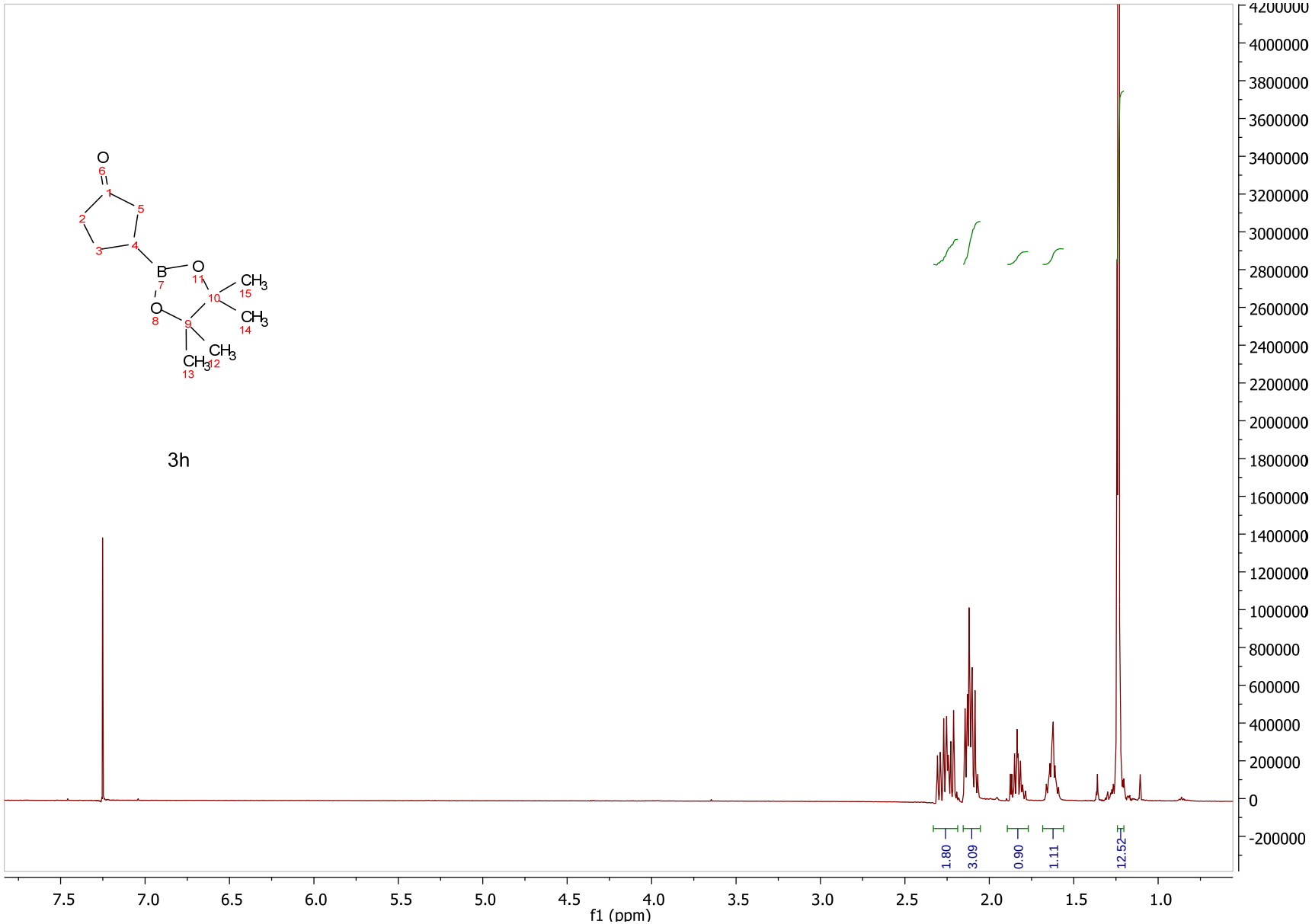

173.89
141.39
128.57
128.26
125.78
83.65
83.64
51.63
37.20
24.64
24.55
3c
f1 (ppm)

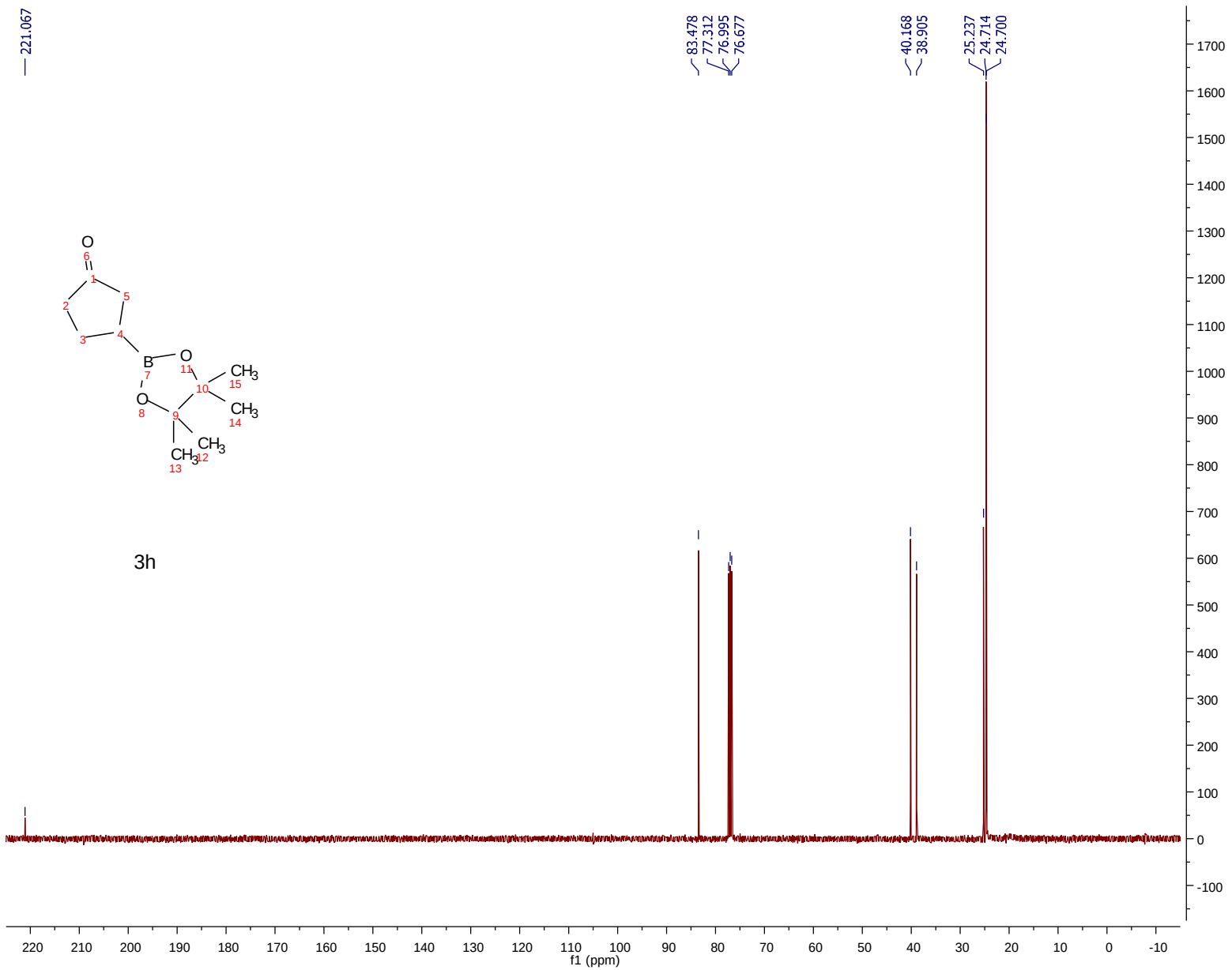

7.27
7.27
7.25
7.24
7.23
7.21
7.16
7.14
7.13
2.83
2.81
2.80
2.78
2.72
2.71
2.70
2.69
2.61
2.60
2.58
2.57
2.18
1.76
1.41
1.23
1.17
3d
Acetone
H2O
5.17
1.04
1.00
1.03
9.37
13.01
f1 (ppm)

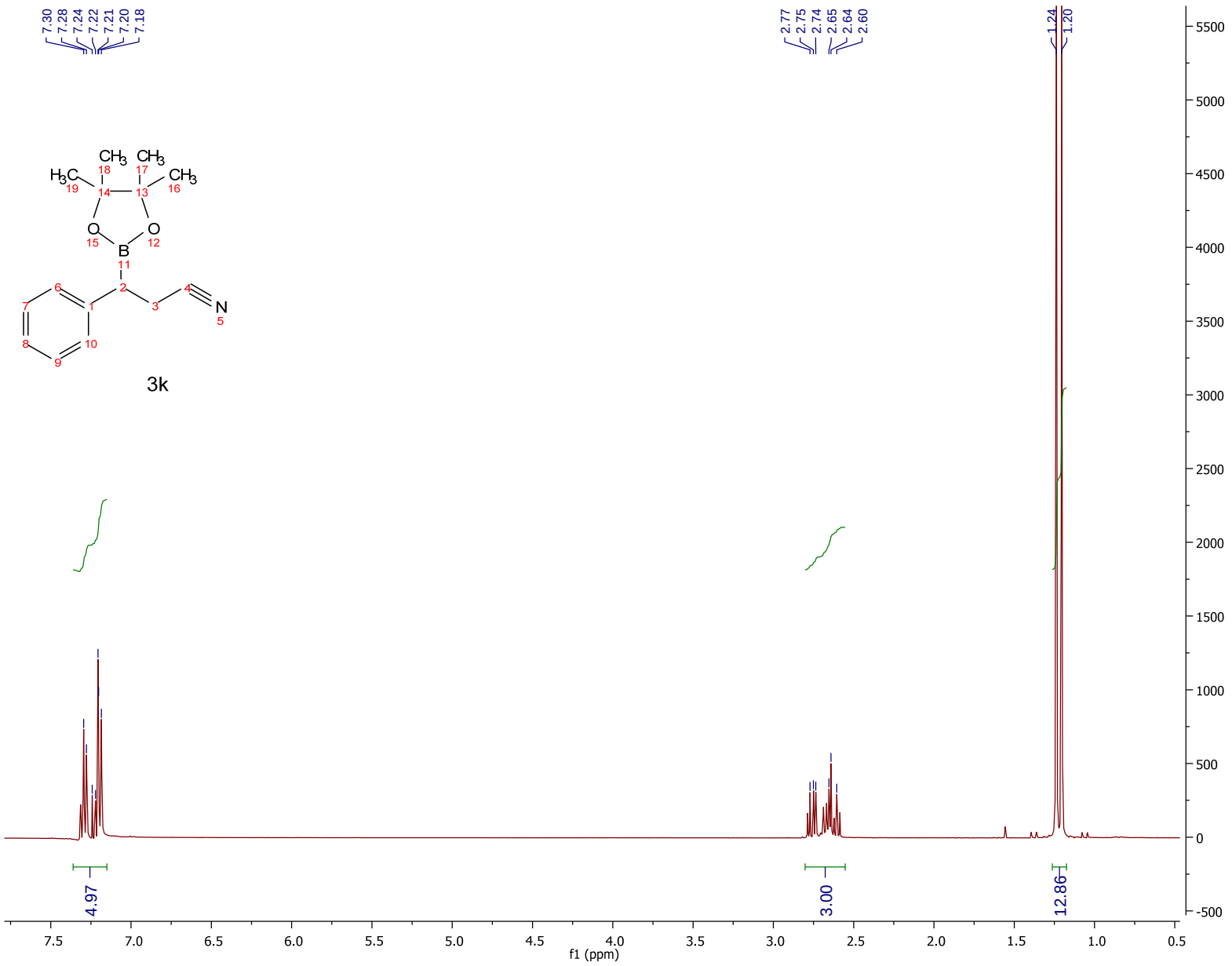

172.77
141.53
128.35
128.22
125.48
83.44
80.12
77.24
77.03
76.82
38.35
30.89
28.05
24.63
24.47
3d
Acetone
f1 (ppm)

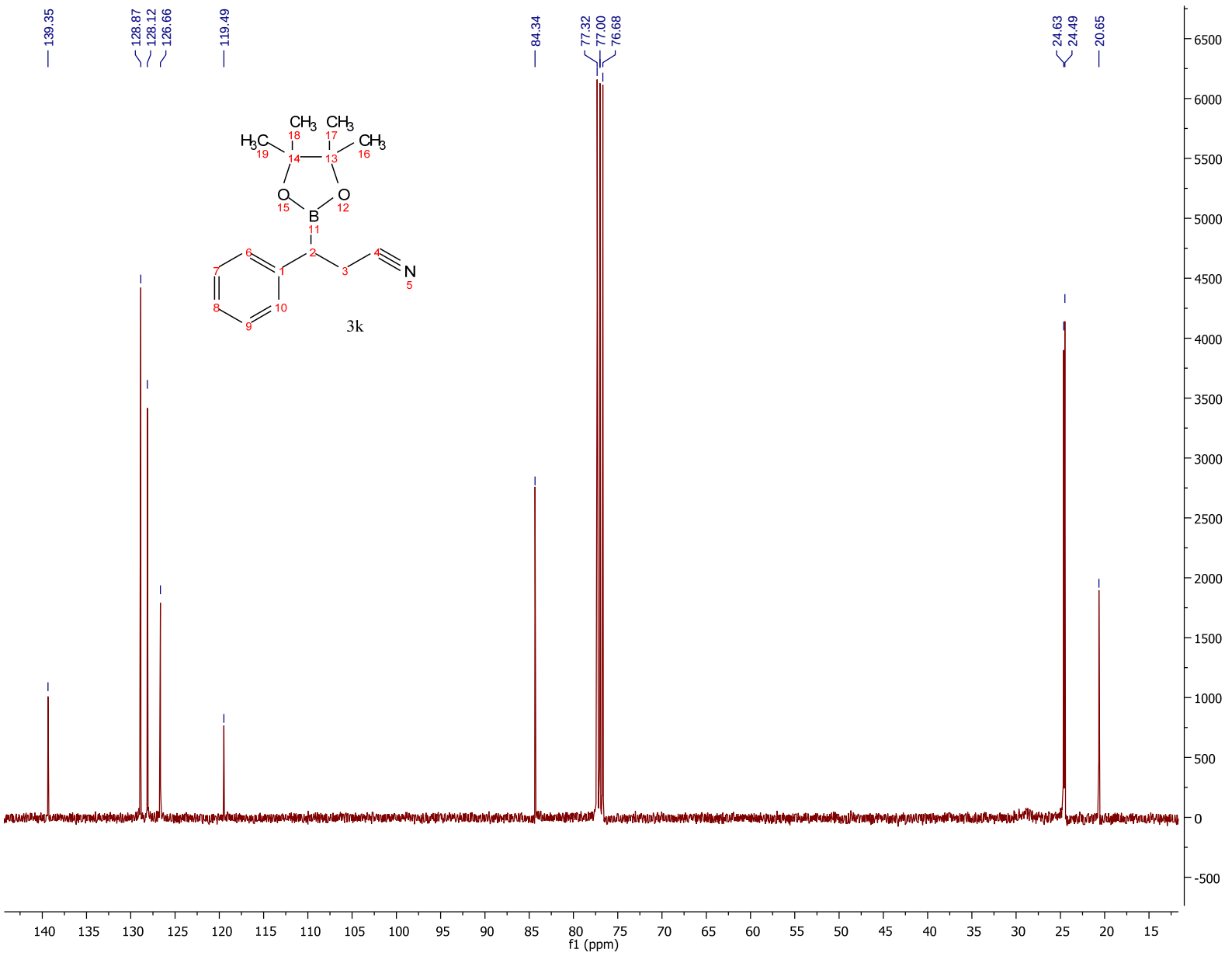

7.35
7.33
7.32
7.31
7.30
7.29
7.29
7.26
7.25
7.25
7.24
7.23
7.21
7.20
7.16
7.14
7.13
5.14
5.11
5.07
5.05
2.97
2.95
2.93
2.92
2.78
2.77
2.75
2.74
2.73
2.71
2.70
1.56
1.19
1.14
3e
10.39
1.91
0.86
1.92
12.00
f1 (ppm)


173.33
141.33
136.17
128.58
128.55
128.29
128.19
128.15
125.78
83.67
77.35
77.10
76.85
66.23
37.35
24.63
24.54
3e
f1 (ppm)


3h
1.80
3.09
0.90
1.11
12.52
f1 (ppm)


221.067
83.478
77.312
76.995
76.677
40.168
38.905
25.237
24.714
24.700
O
6
1
5
2
3
4
B
7
O
11
CH3
15
10
O
8
9
CH3
14
CH3
13
12
3h
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
220
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)


7.30
7.28
7.24
7.22
7.21
7.20
7.18
2.77
2.75
2.74
2.65
2.64
2.60
1.24
1.20
3k
4.97
3.00
12.86
f1 (ppm)


139.35
128.87
128.12
126.66
119.49
84.34
77.32
77.00
76.68
24.63
24.49
20.65
3k
f1 (ppm)