Supplementary Information

A novel approach for obtaining α,β-diaminophosphonates bearing structurally diverse side chains and their interactions with transitions metal ions studied by ITC

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1. Interaction of Zn^{2+} ion with three model aminophosponates 2e', 2f', 2g'

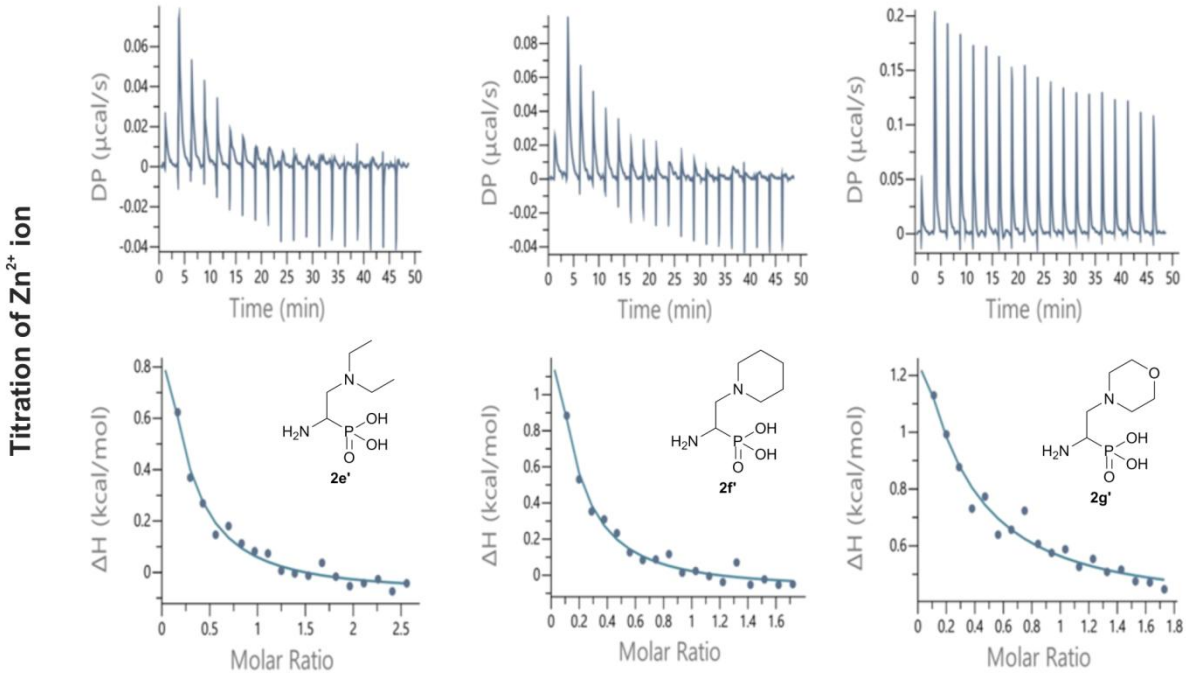
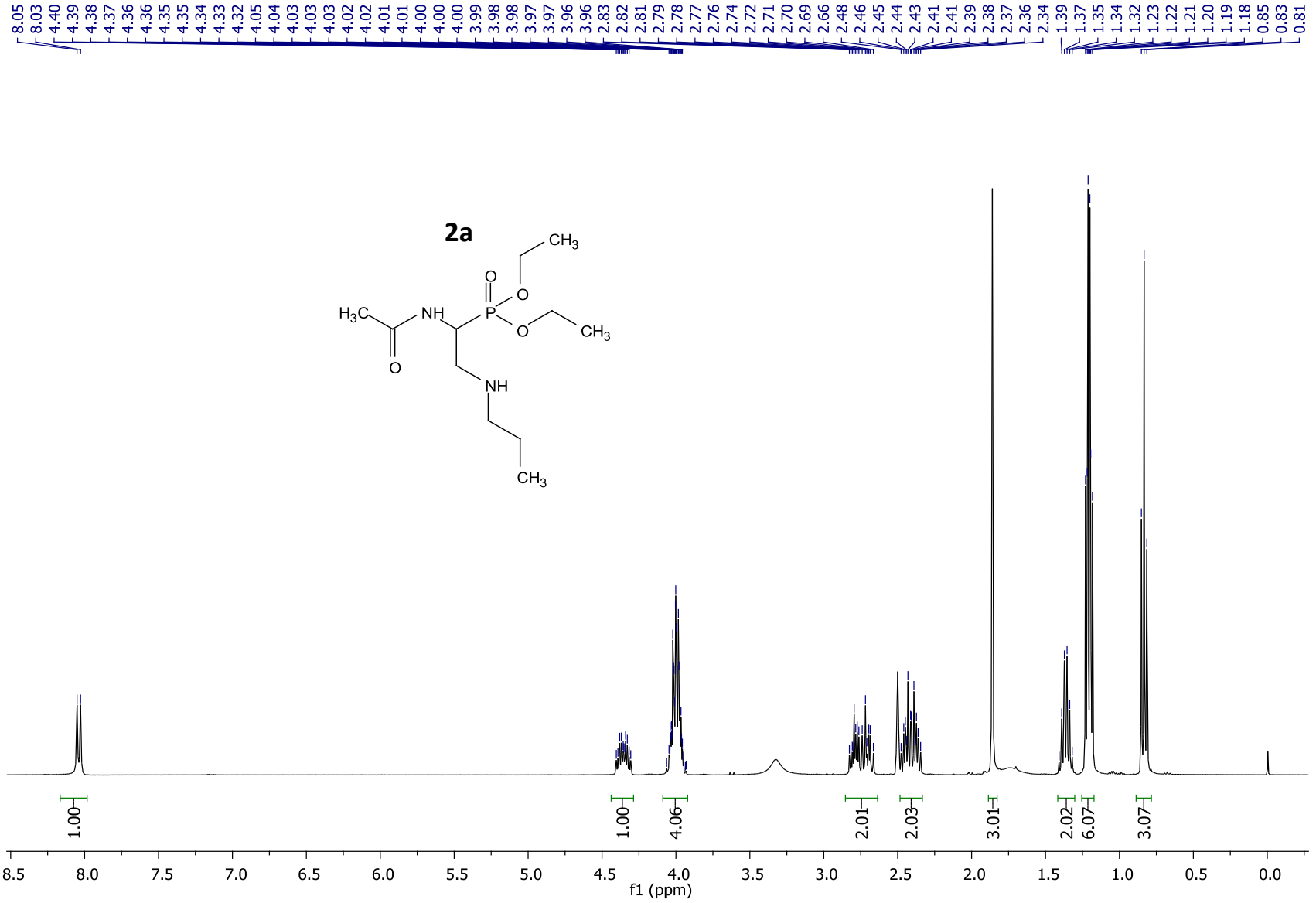
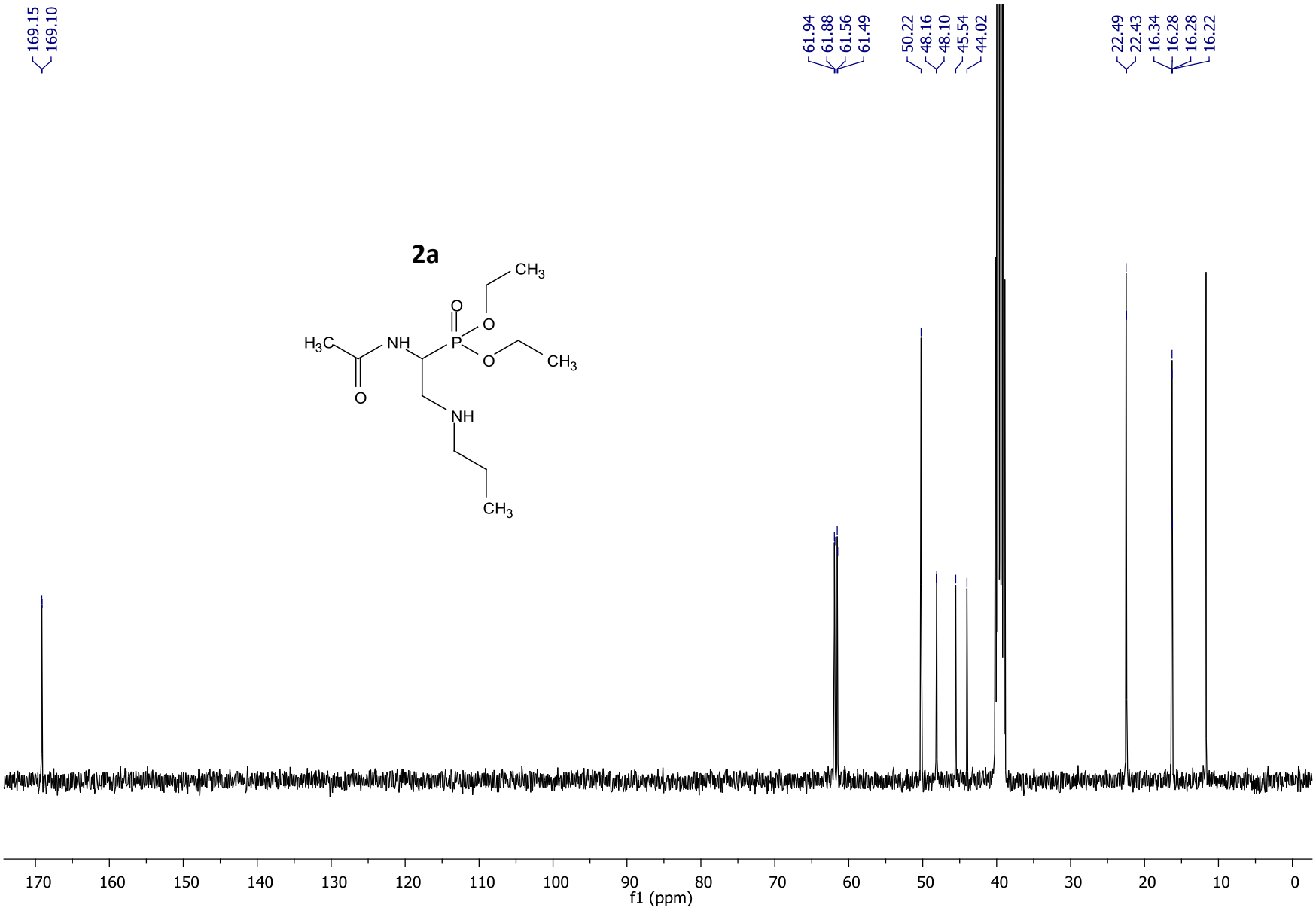


Fig. SI1 ITC titration (raw data above and corresponding plots below) of 3 mM Zn^{2+} to **2e'**, **2f'**and **2g'**

2. ^{1}H, ^{13}C, ^{31}P NMR spectra

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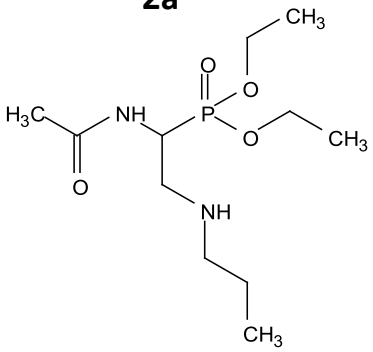
48.16
48.10
45.54
44.02
22.49
22.43
16.34
16.28
16.28
16.22
2a
CH3
O
O
H3C
NH
P
O
CH3
O
NH
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2a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P
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CH3
O
NH
CH3

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90
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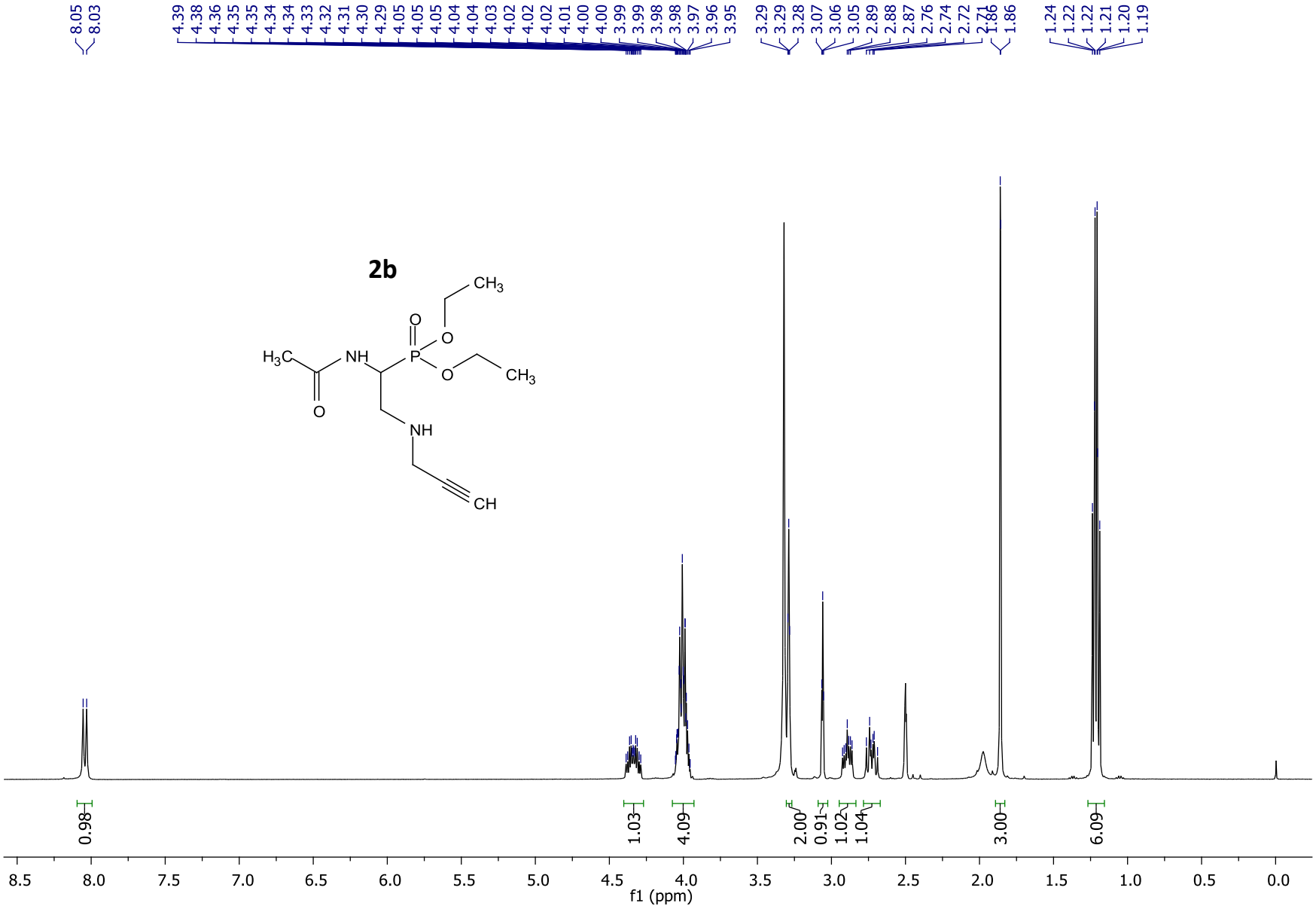
f1 (ppm)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4.35
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4.34
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4.32
4.31
4.30
4.29
4.05
4.05
4.05
4.04
4.04
4.03
4.02
4.02
4.02
4.01
4.00
4.00
3.99
3.99
3.98
3.98
3.97
3.96
3.95
3.29
3.29
3.28
3.07
3.06
3.05
2.89
2.88
2.87
2.76
2.74
2.72
2.71
1.86
1.86
1.24
1.22
1.22
1.21
1.20
1.19
2b
CH3
O
O
H3C
NH
P
O
CH3
O
NH
CH
0.98
1.03
4.09
2.00
0.91
1.02
1.04
3.00
6.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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1.0
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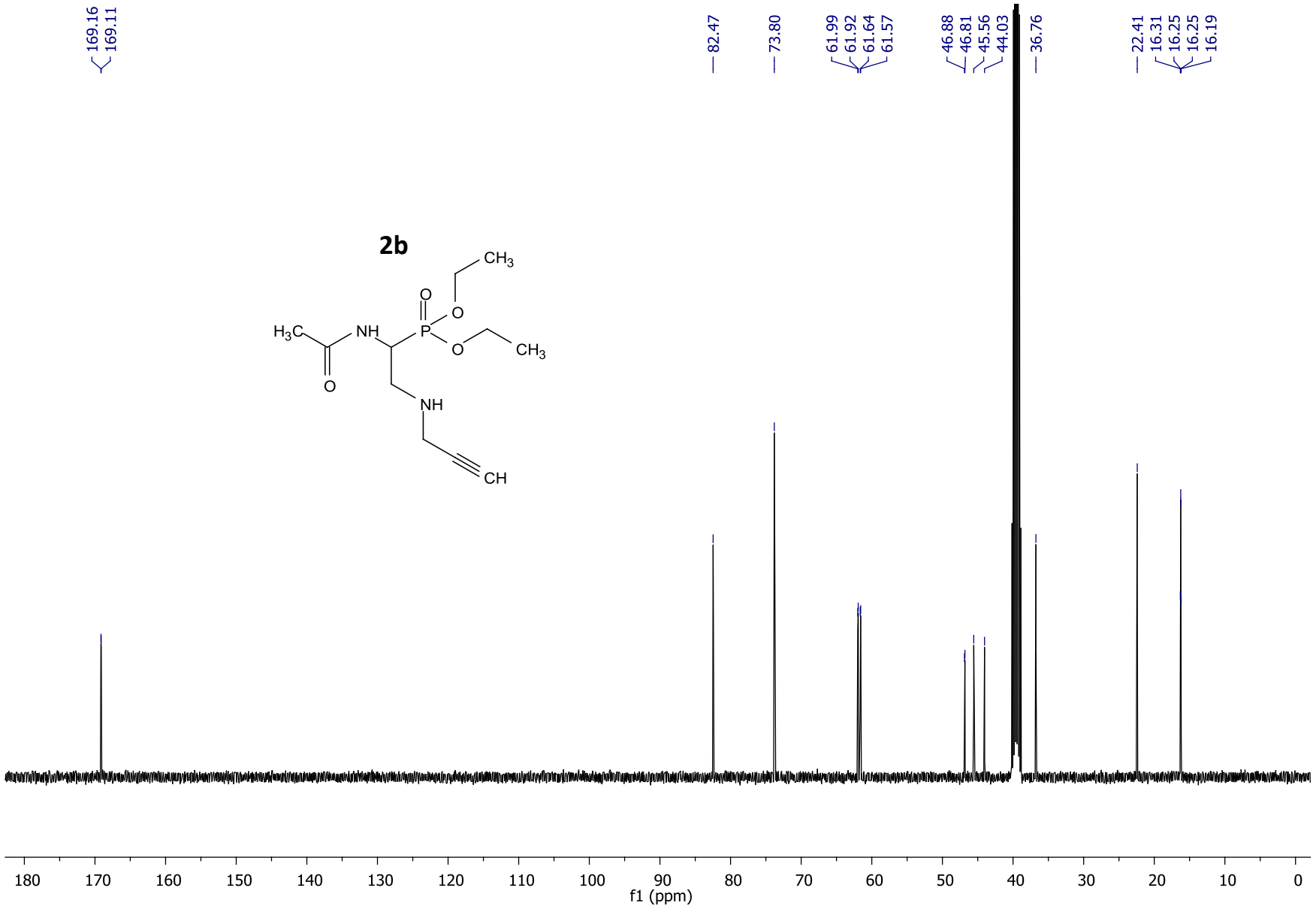
0.0
f1 (ppm)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73.80
61.99
61.92
61.64
61.57
46.88
46.81
45.56
44.03
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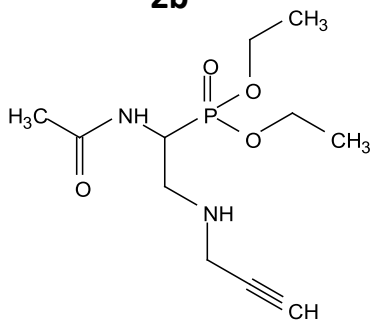
22.41
16.31
16.25
16.25
16.19
2b
CH3
O
O
H3C
NH
P
O
CH3
O
NH
CH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2b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H3C
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P
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CH3
O
NH
CH

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90
80
70
60
50
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0
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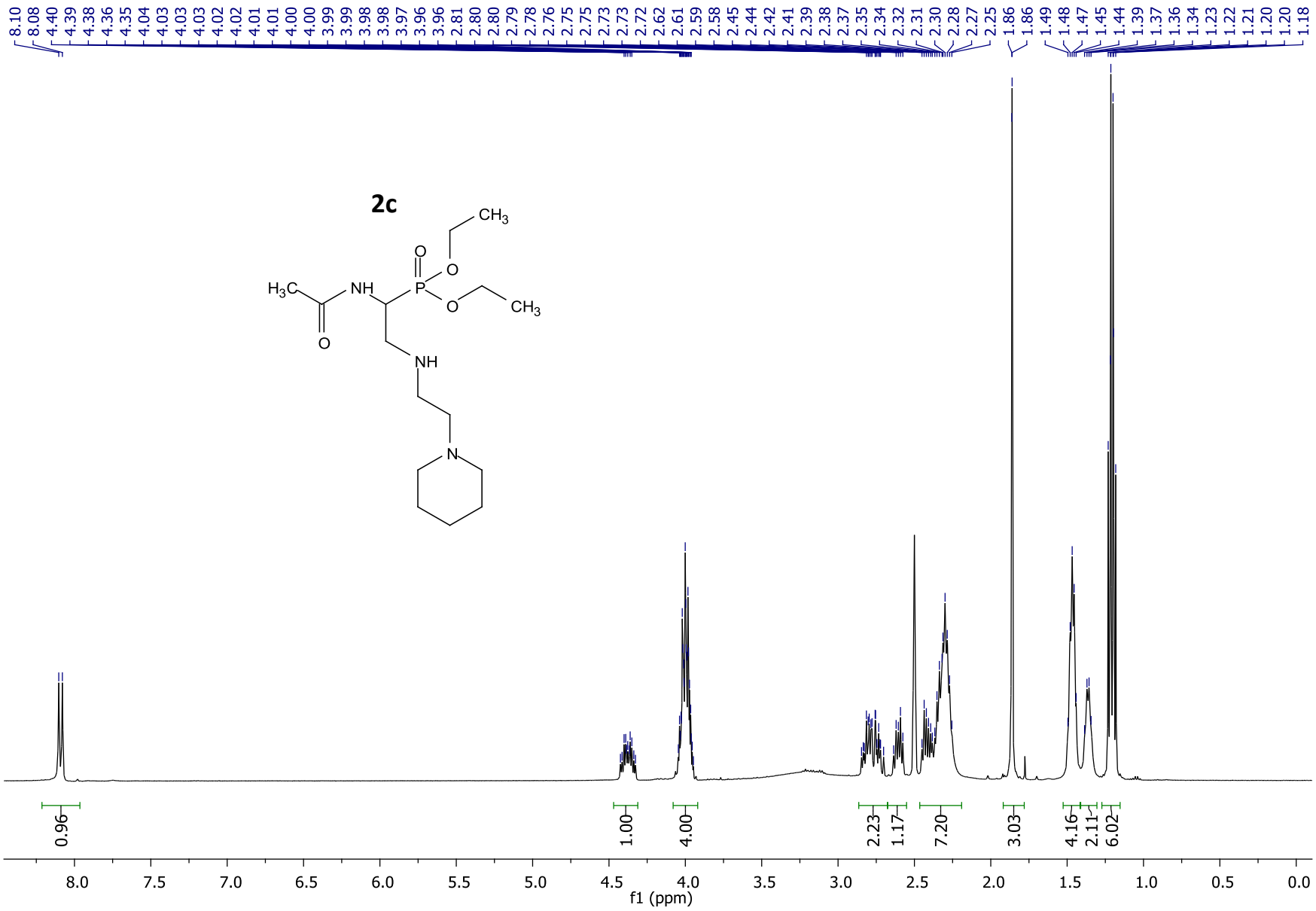
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0.96 1.00 4.00 2.23 1.17 7.20 3.03 4.16 2.11 6.02
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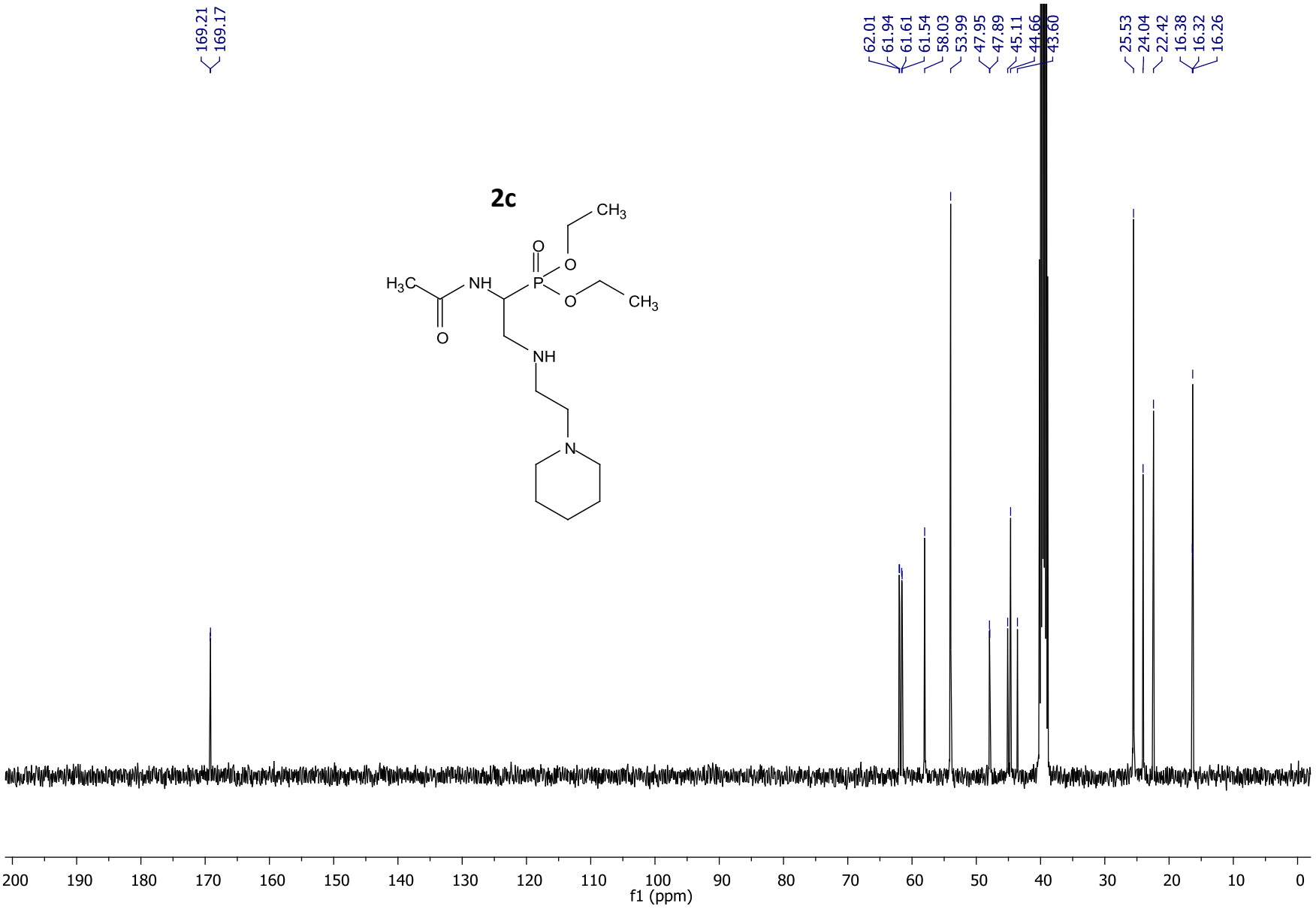
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47.89
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43.60
25.53
24.04
22.42
16.38
16.32
16.26
2c
CH3
O
O
H3C
NH
P
O
CH3
O
NH
N
200
190
180
170
160
150
140
130
120
110
100
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20
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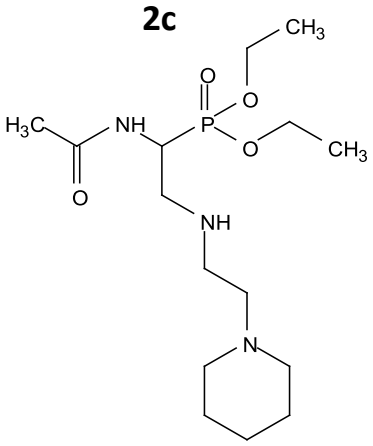
0
f1 (ppm)

2c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H3C
NH
P
O
CH3
O
NH
N

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100
90
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50
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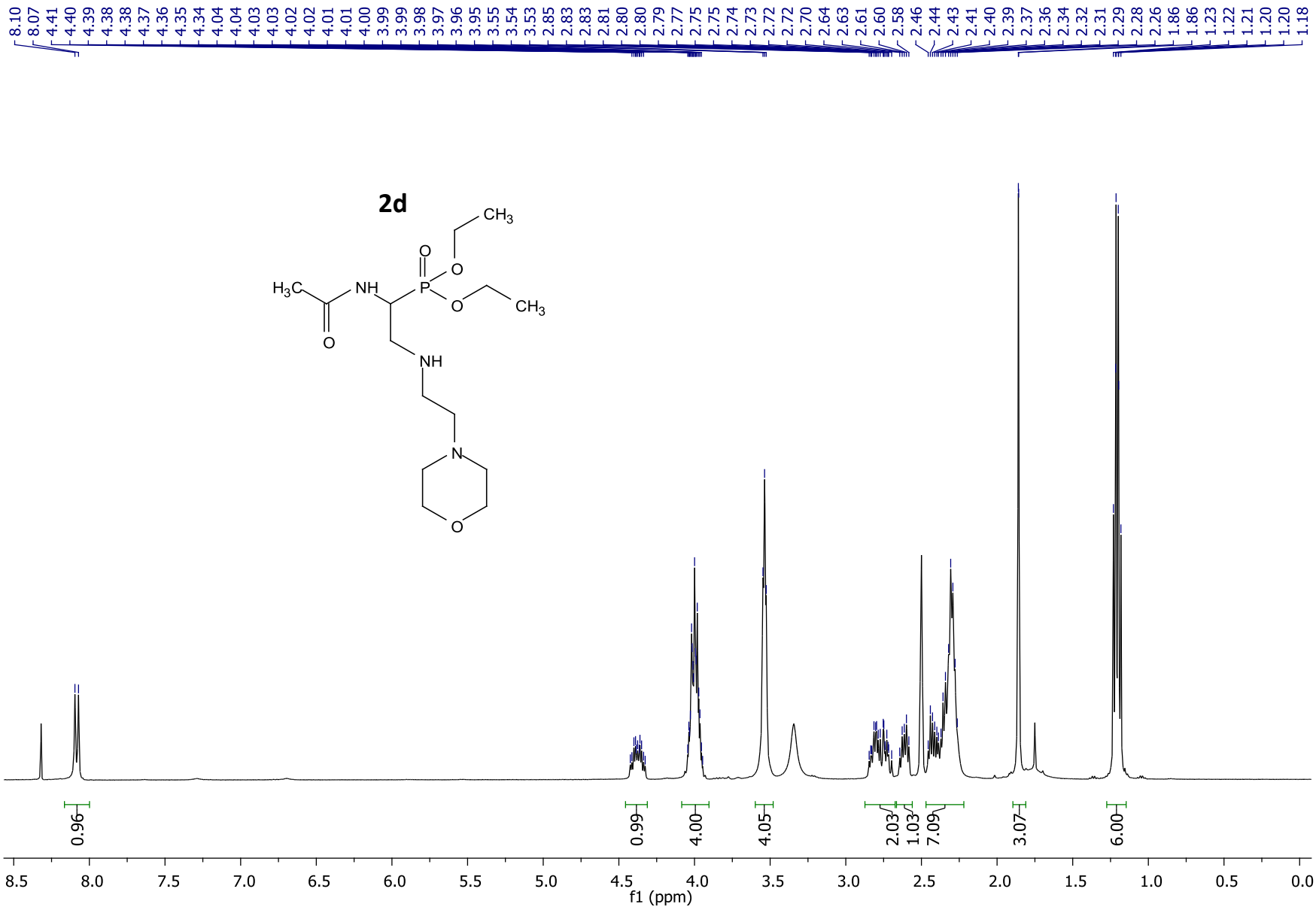
10
0
f1 (ppm)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2d
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O
O
H3C
NH
P
O
CH3
O
NH
N
O
0.96
0.99
4.00
4.05
2.03
1.03
7.09
3.07
6.00
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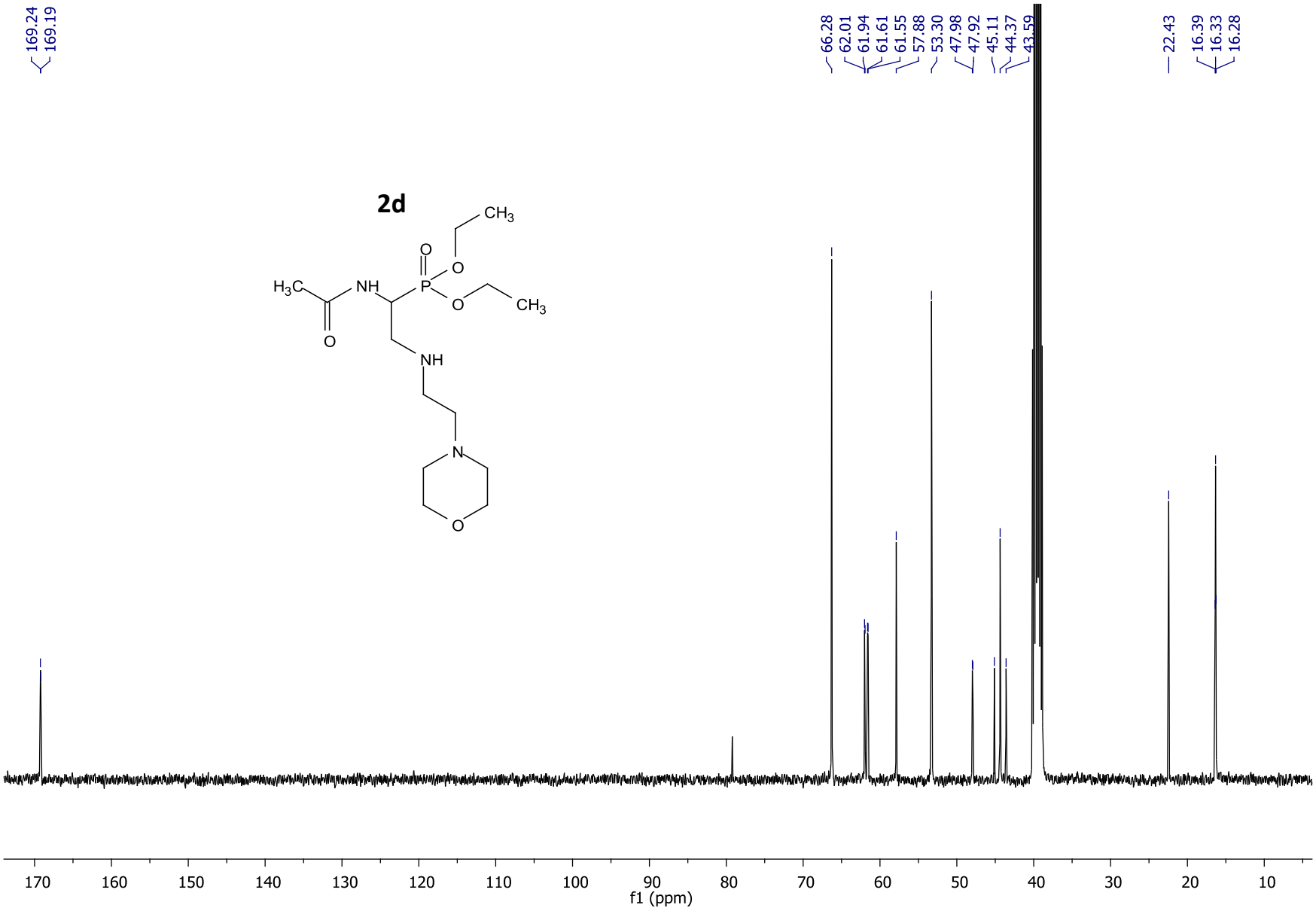
f1 (ppm)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CH3
O
NH
N
O
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120
110
100
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40
30
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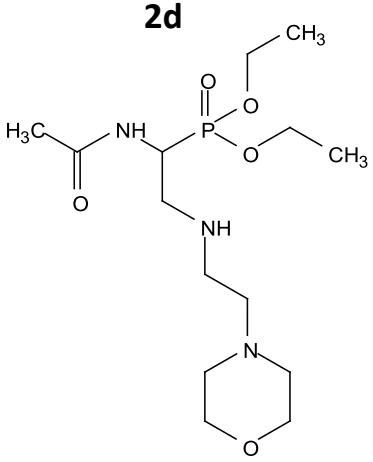
10
f1 (ppm)

2d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NH
P
O
CH3
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NH
N
O

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110
100
90
80
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60
50
40
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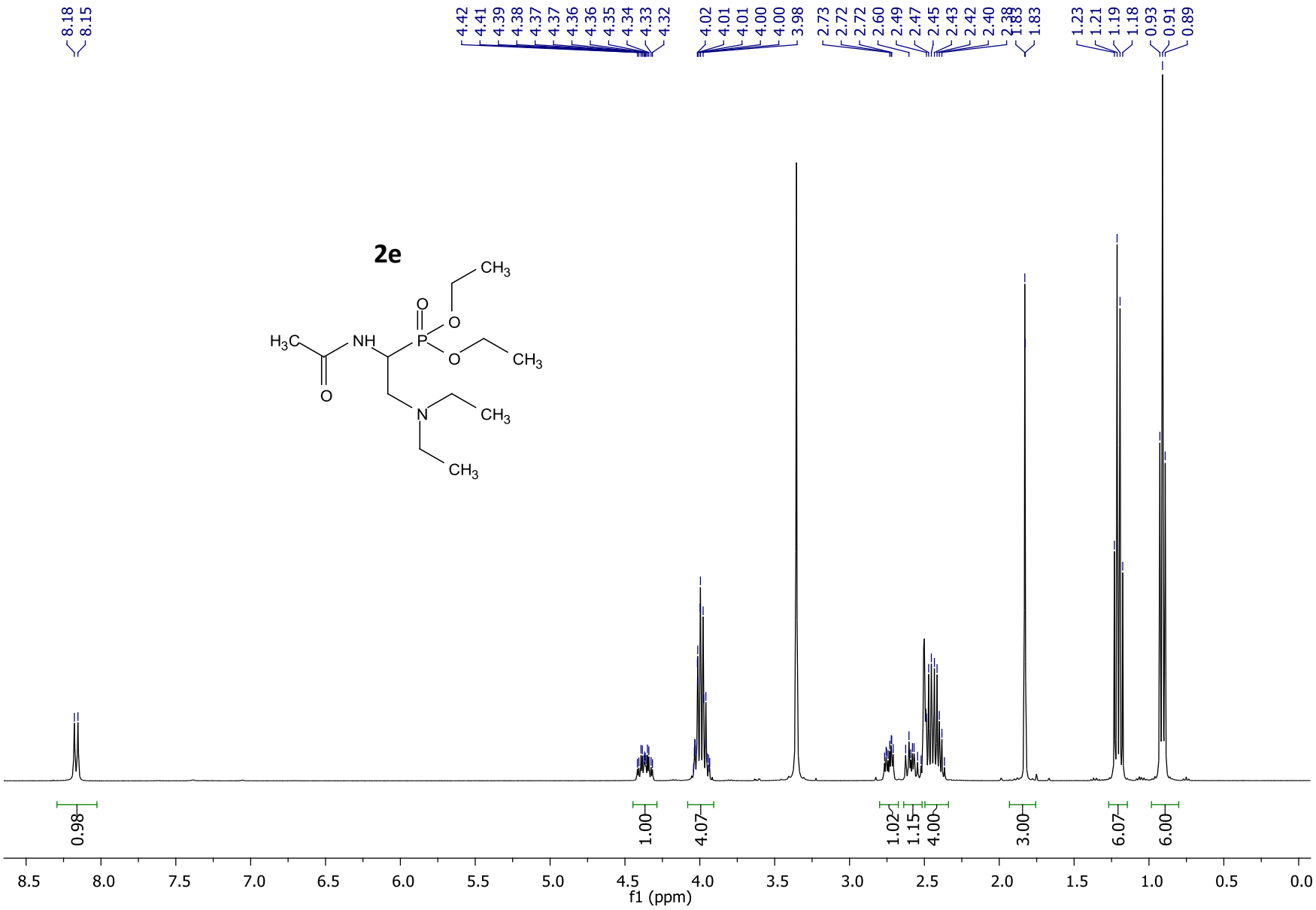
10
0
f1 (ppm)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4.36
4.35
4.34
4.33
4.32
4.02
4.01
4.01
4.00
4.00
3.98
2.73
2.72
2.72
2.60
2.49
2.47
2.45
2.43
2.42
2.40
1.83
1.23
1.21
1.19
1.18
0.93
0.91
0.89
2e
CH3
O
O
H3C
NH
P
O
CH3
O
N
CH3
CH3
0.98
1.00
4.07
1.02
1.15
4.00
3.00
6.07
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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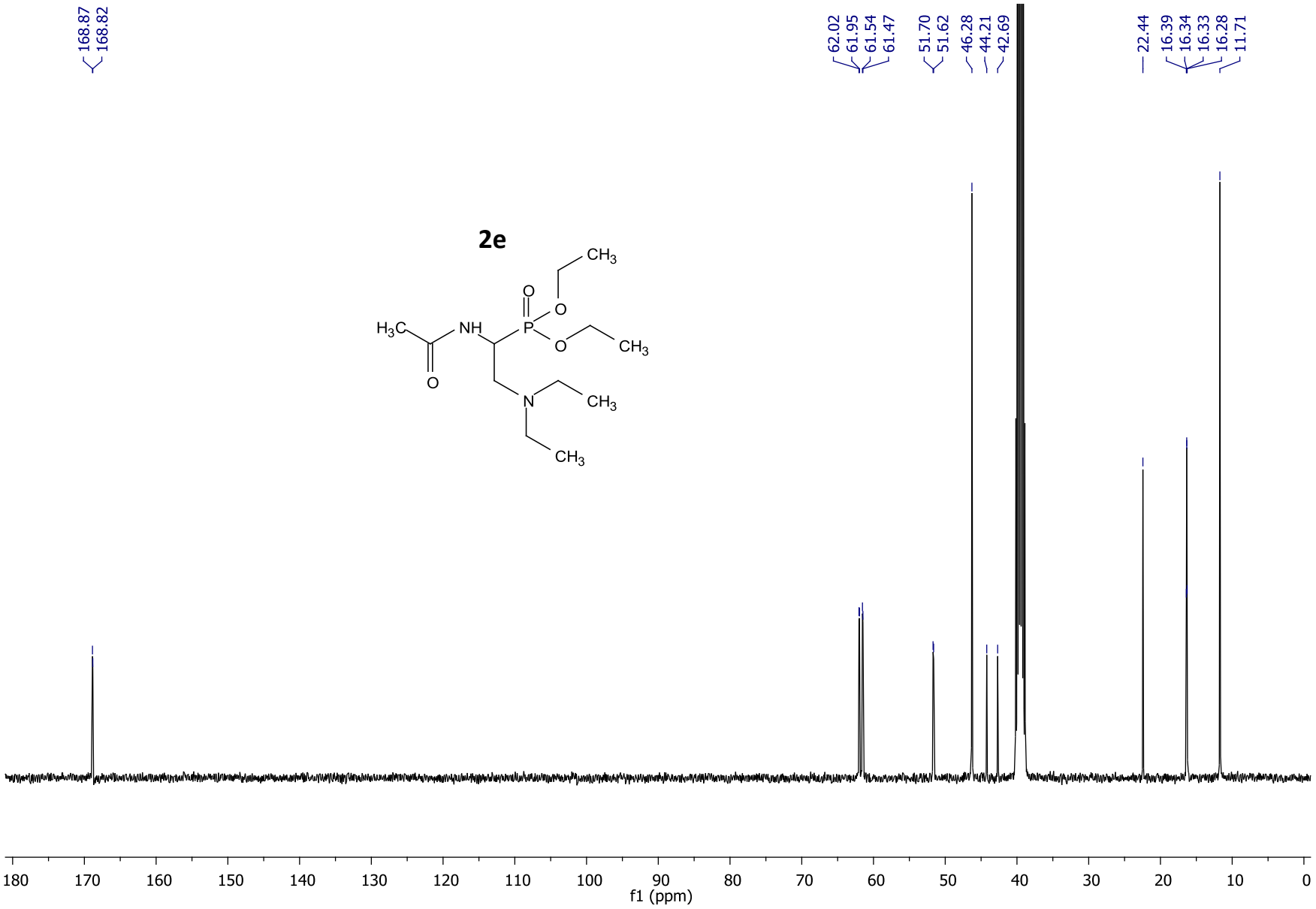
f1 (ppm)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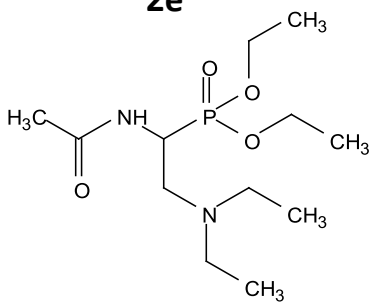
22.44
16.39
16.34
16.33
16.28
11.71
2e
CH3
O
O
H3C
NH
P
O
CH3
O
N
CH3
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2e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NH
P
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CH3
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CH3
CH3

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120
110
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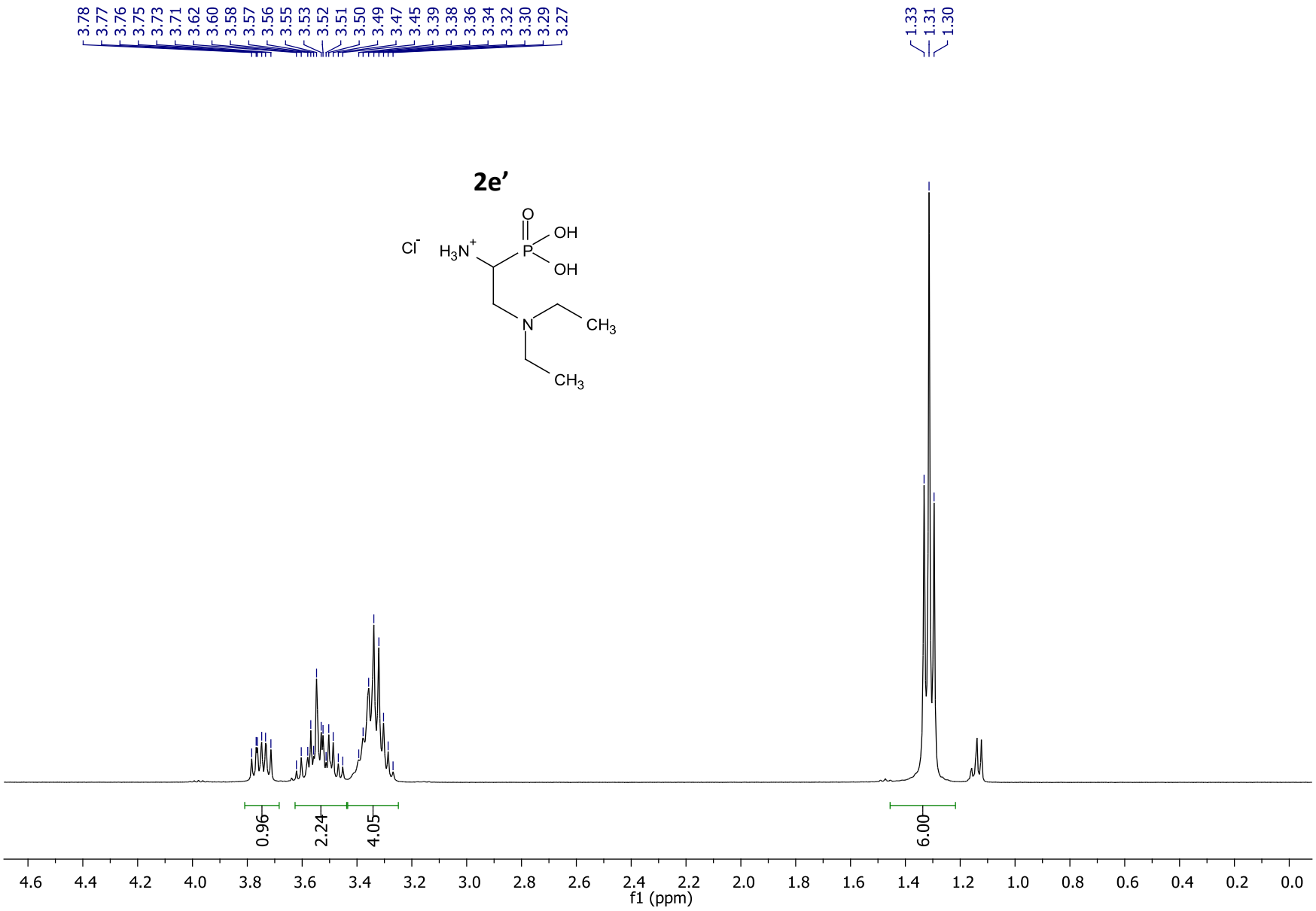
0
f1 (ppm)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3.47
3.45
3.39
3.38
3.36
3.34
3.32
3.30
3.29
3.27
1.33
1.31
1.30
2e’
Cl-
H3N+
O
OH
P
OH
N
CH3
CH3
0.96
2.24
4.05
6.00
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
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1.4
1.2
1.0
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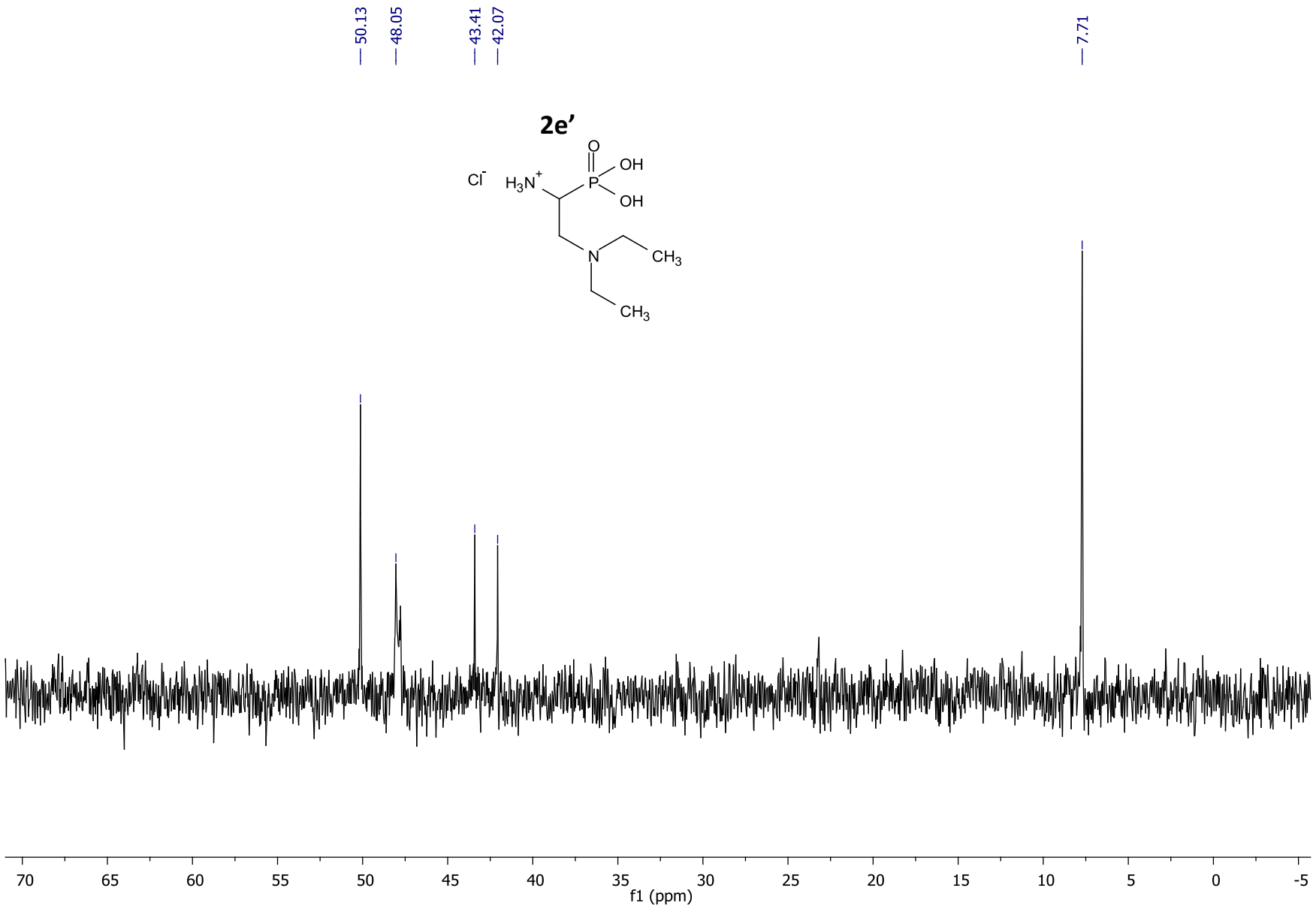
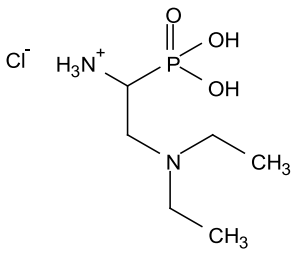
0.4
0.2
0.0
f1 (ppm)


50.13
48.05
43.41
42.07
7.71
2e'
Cl-
H3N+
O
OH
P
OH
N
CH3
CH3
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
f1 (ppm)

2e’


O
OH
Cl-
H3N+
P
OH
N
CH3
CH3

10.44
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140
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80
70
60
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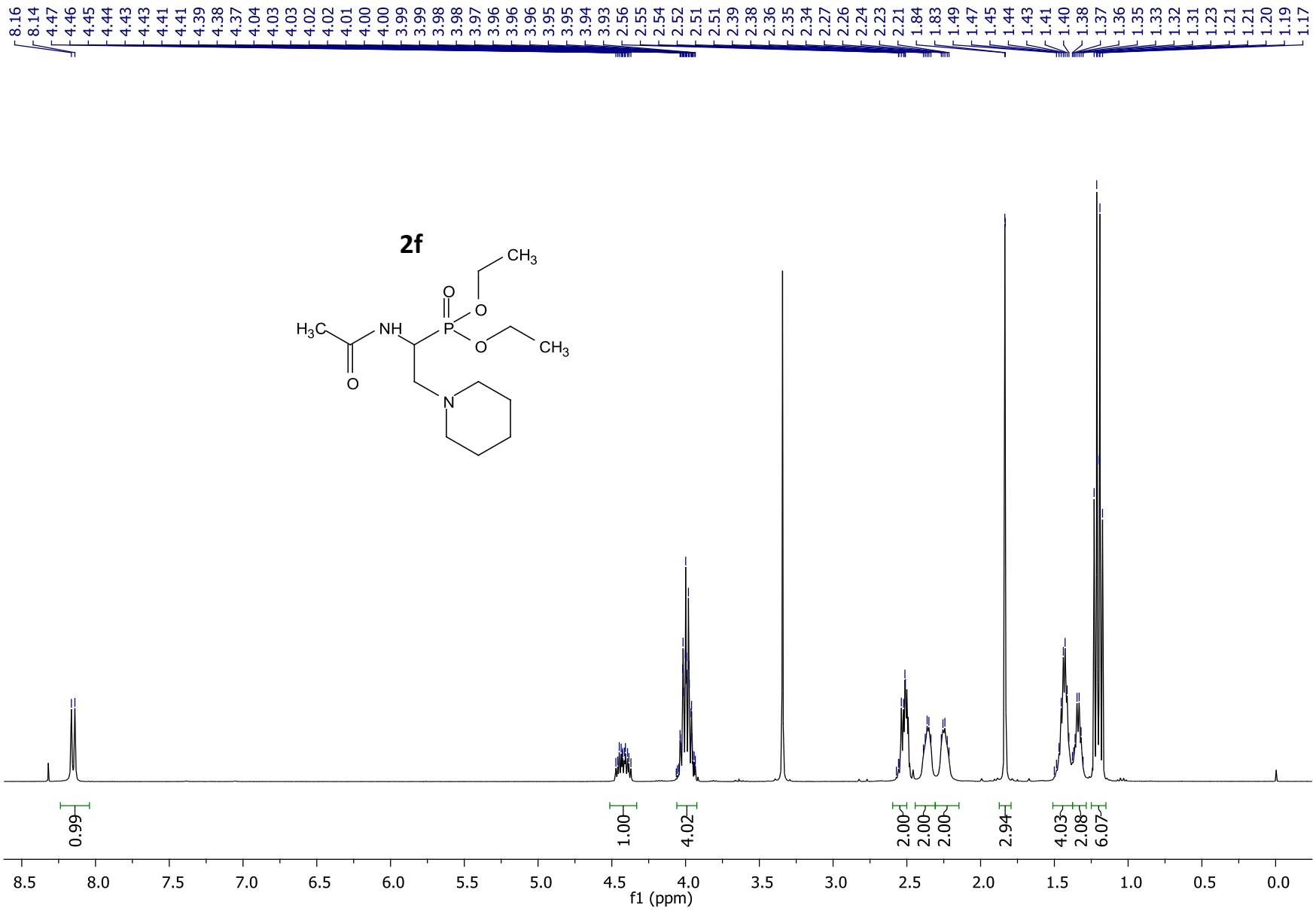
40
30
20
10
0
-10
f1 (ppm)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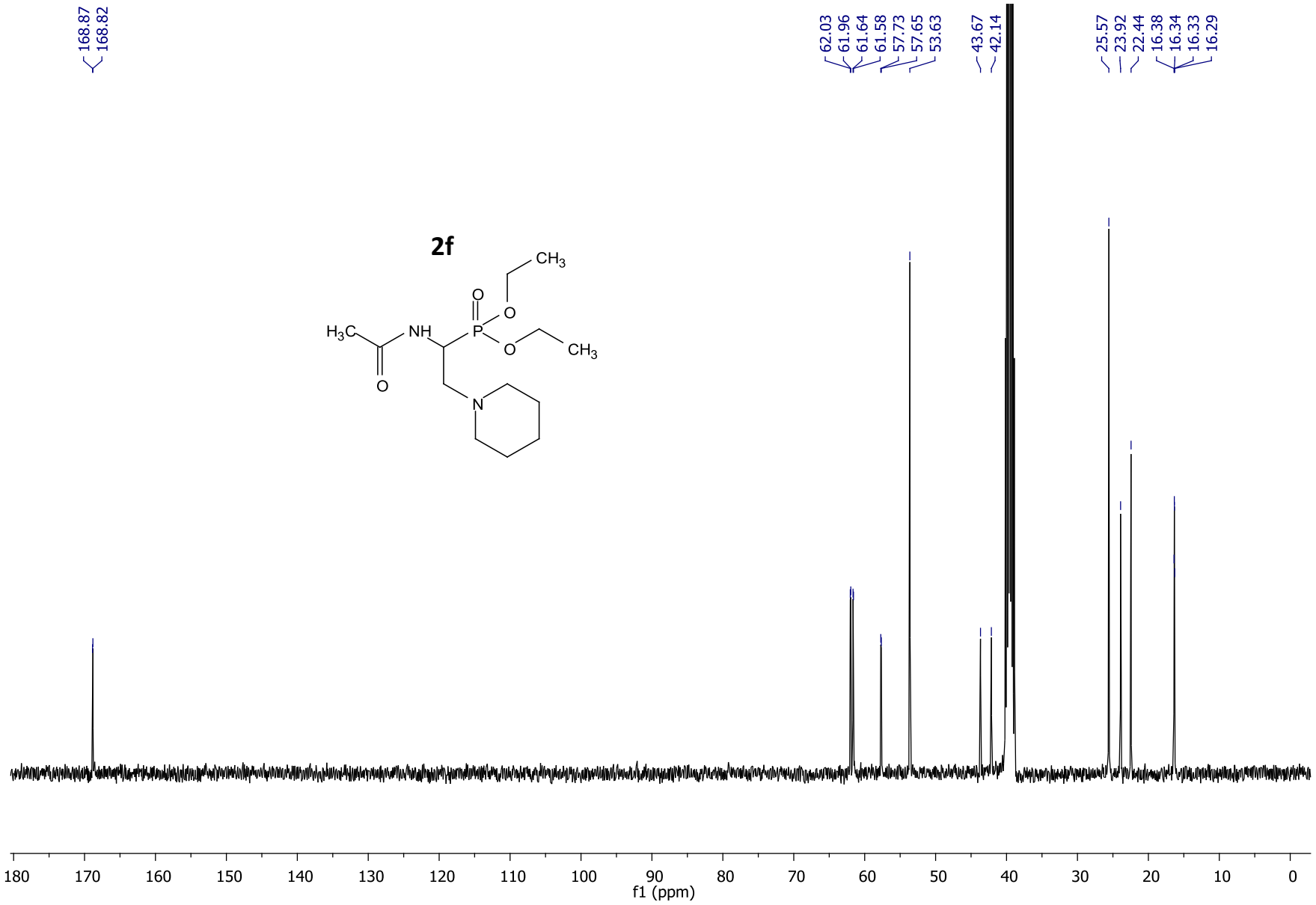
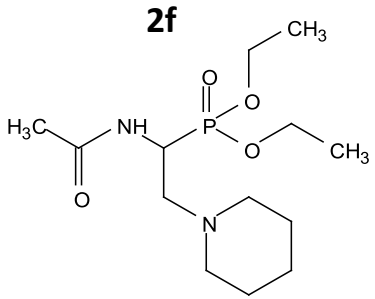
2f
CH3
O
O
H3C
NH
P
O
CH3
O
N
0.99
1.00
4.02
2.00
2.00
2.00
2.94
4.03
2.08
6.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.87
168.82
62.03
61.96
61.64
61.58
57.73
57.65
53.63
43.67
42.14
25.57
23.92
22.44
16.38
16.34
16.33
16.29
2f
CH3
O
O
H3C
NH
P
O
CH3
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2f


CH3
O
O
H3C
NH
P
O
CH3
O
N

25.80
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150
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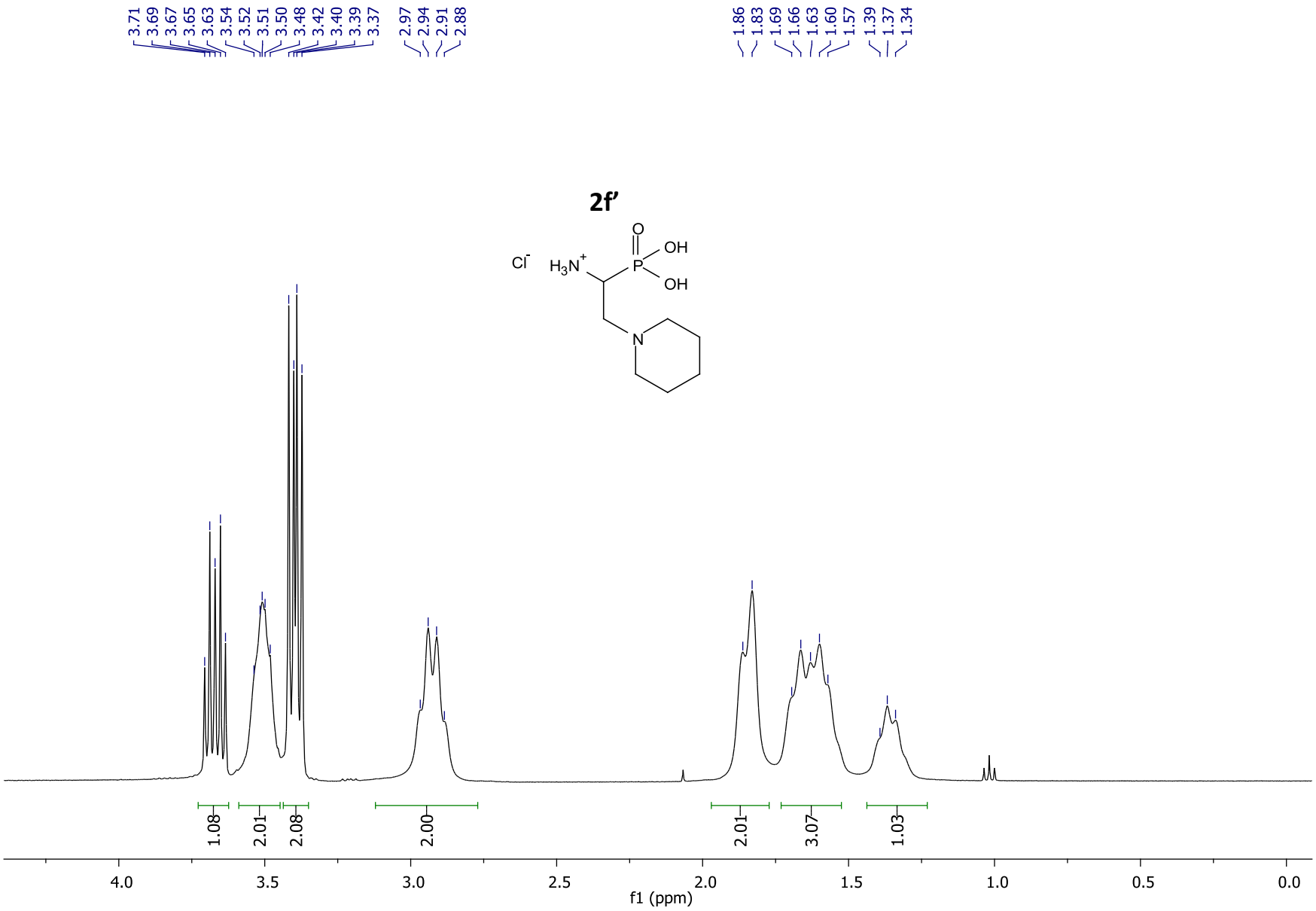
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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3.69
3.67
3.65
3.63
3.54
3.52
3.51
3.50
3.48
3.42
3.40
3.39
3.37
2.97
2.94
2.91
2.88
1.86
1.83
1.69
1.66
1.63
1.60
1.57
1.39
1.37
1.34
2f'
Cl-
H3N+
O
OH
P
OH
N
1.08
2.01
2.08
2.00
2.01
3.07
1.03
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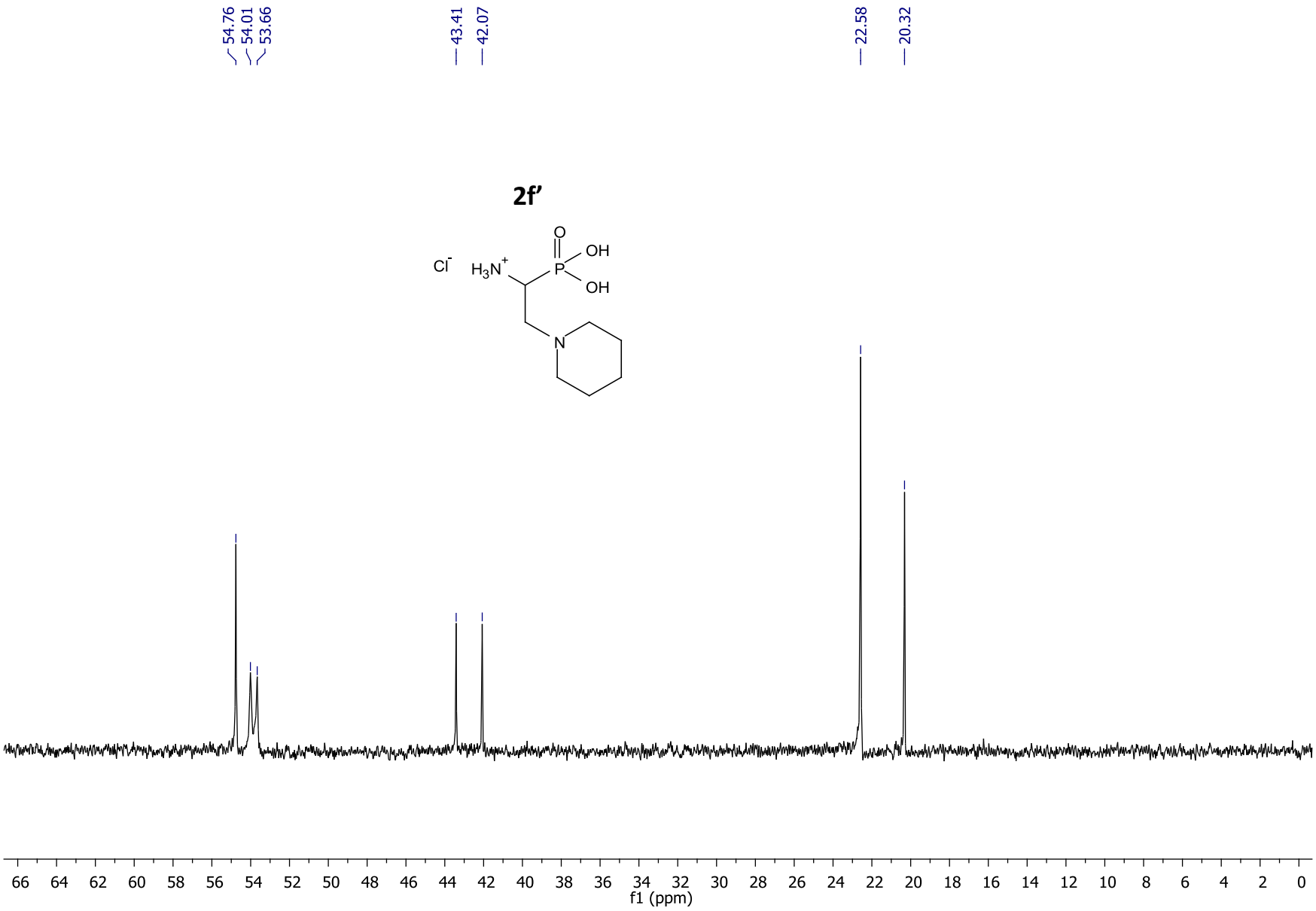
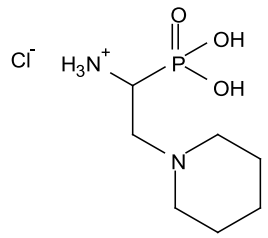
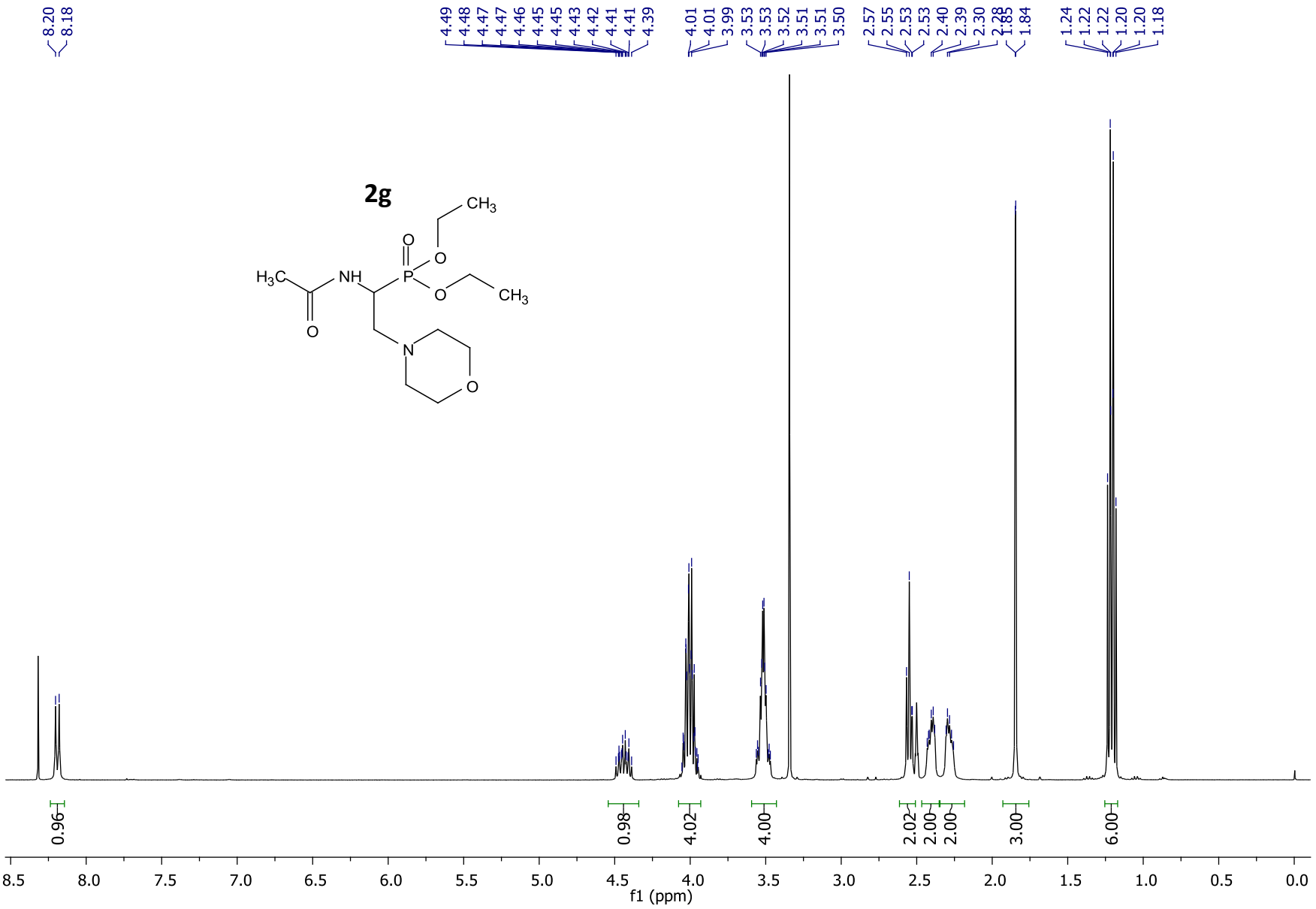
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

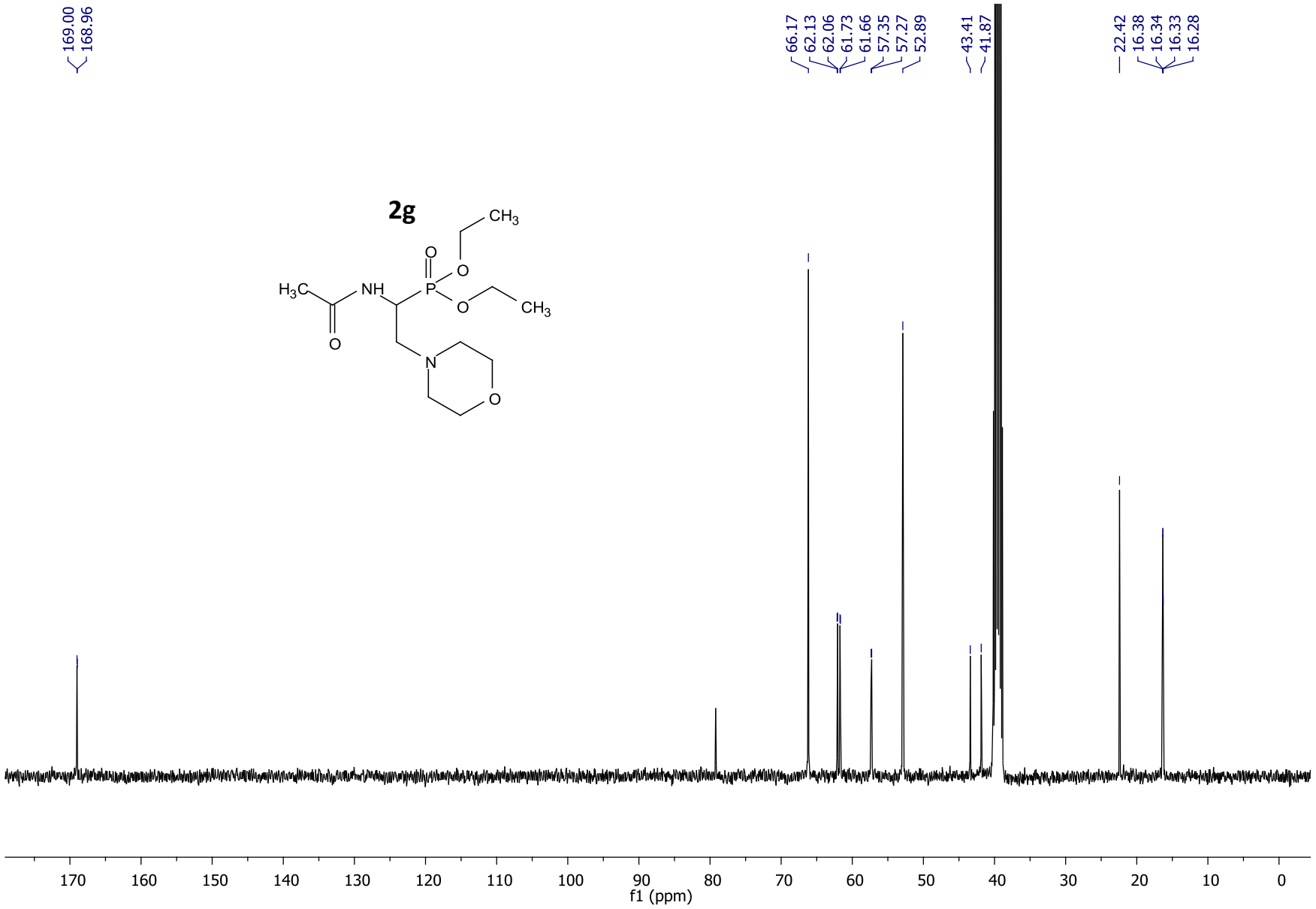

54.76
54.01
53.66
43.41
42.07
22.58
20.32
2f'
Cl-
H3N+
O
OH
OH
P
N
66 64 62 60 58 56 54 52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20 18 16 14 12 10 8 6 4 2 0
f1 (ppm)

2f'

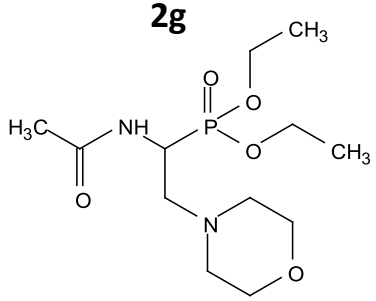

Cl-
H3N+
O
OH
P
OH
N

9.99
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

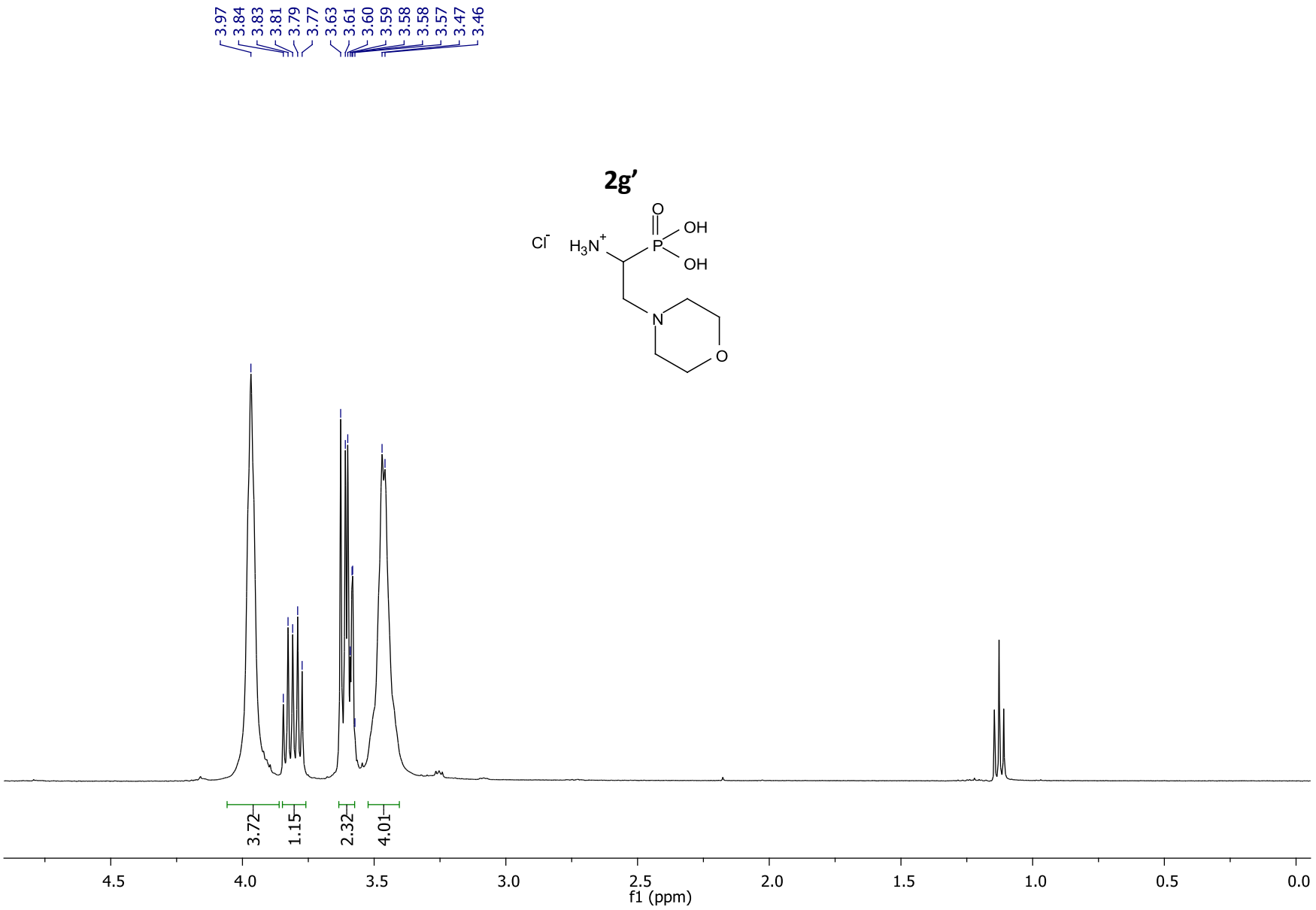

8.20
8.18
4.49
4.48
4.47
4.47
4.46
4.45
4.45
4.43
4.42
4.41
4.41
4.39
4.01
4.01
3.99
3.53
3.53
3.52
3.51
3.51
3.50
2.57
2.55
2.53
2.53
2.40
2.39
2.30
1.84
1.24
1.22
1.20
1.20
1.18
2g
CH3
O
O
H3C
NH
P
O
CH3
O
N
O
0.96
0.98
4.02
4.00
2.02
2.00
2.00
3.00
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

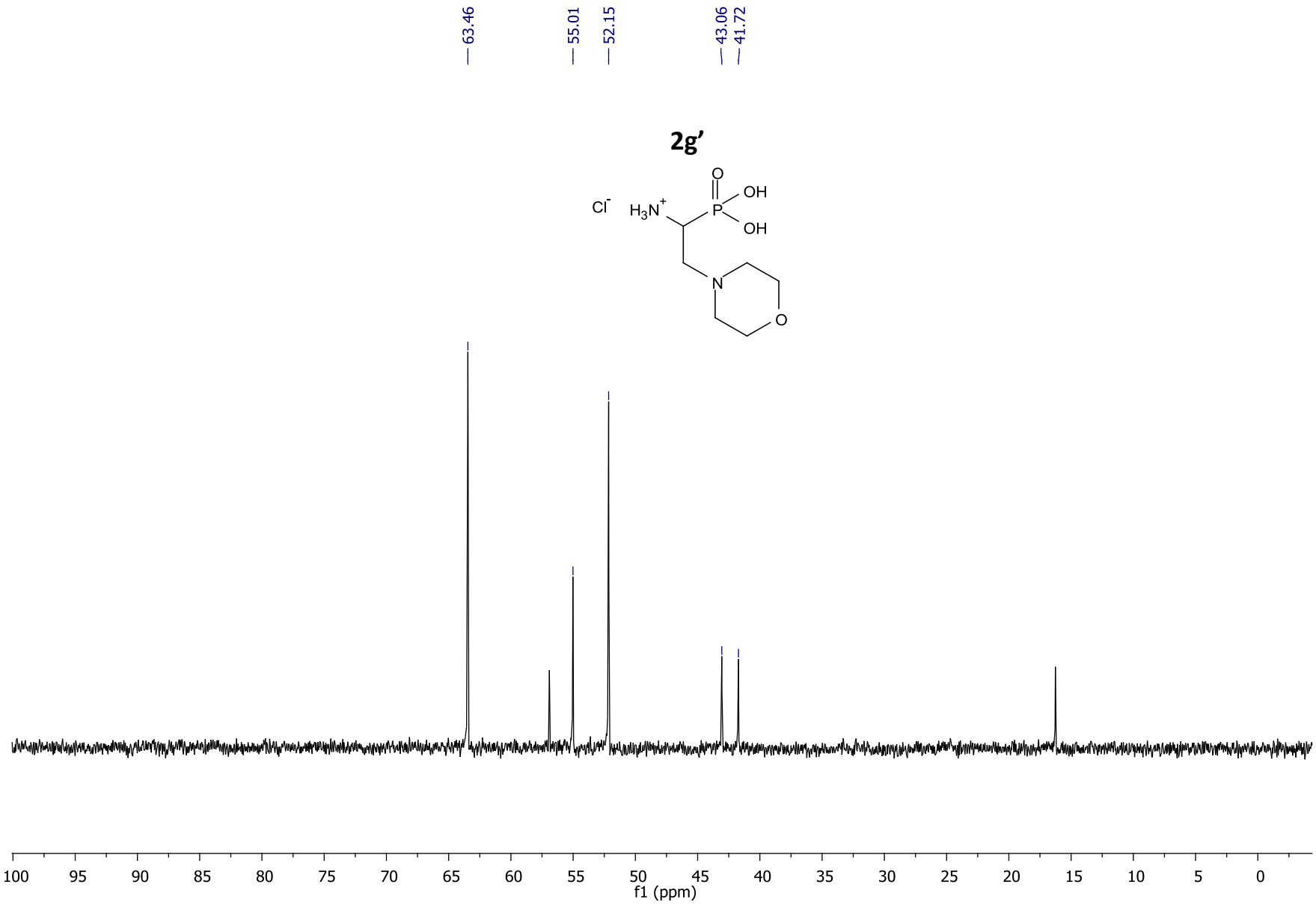

169.00
168.96
66.17
62.13
62.06
61.73
61.66
57.35
57.27
52.89
43.41
41.87
22.42
16.38
16.34
16.33
16.28
2g
CH3
O
O
H3C
NH
P
O
CH3
O
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2g

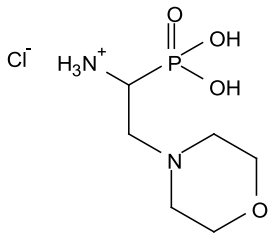

CH3
O
O
H3C
NH
P
O
CH3
O
N
O

25.51
130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

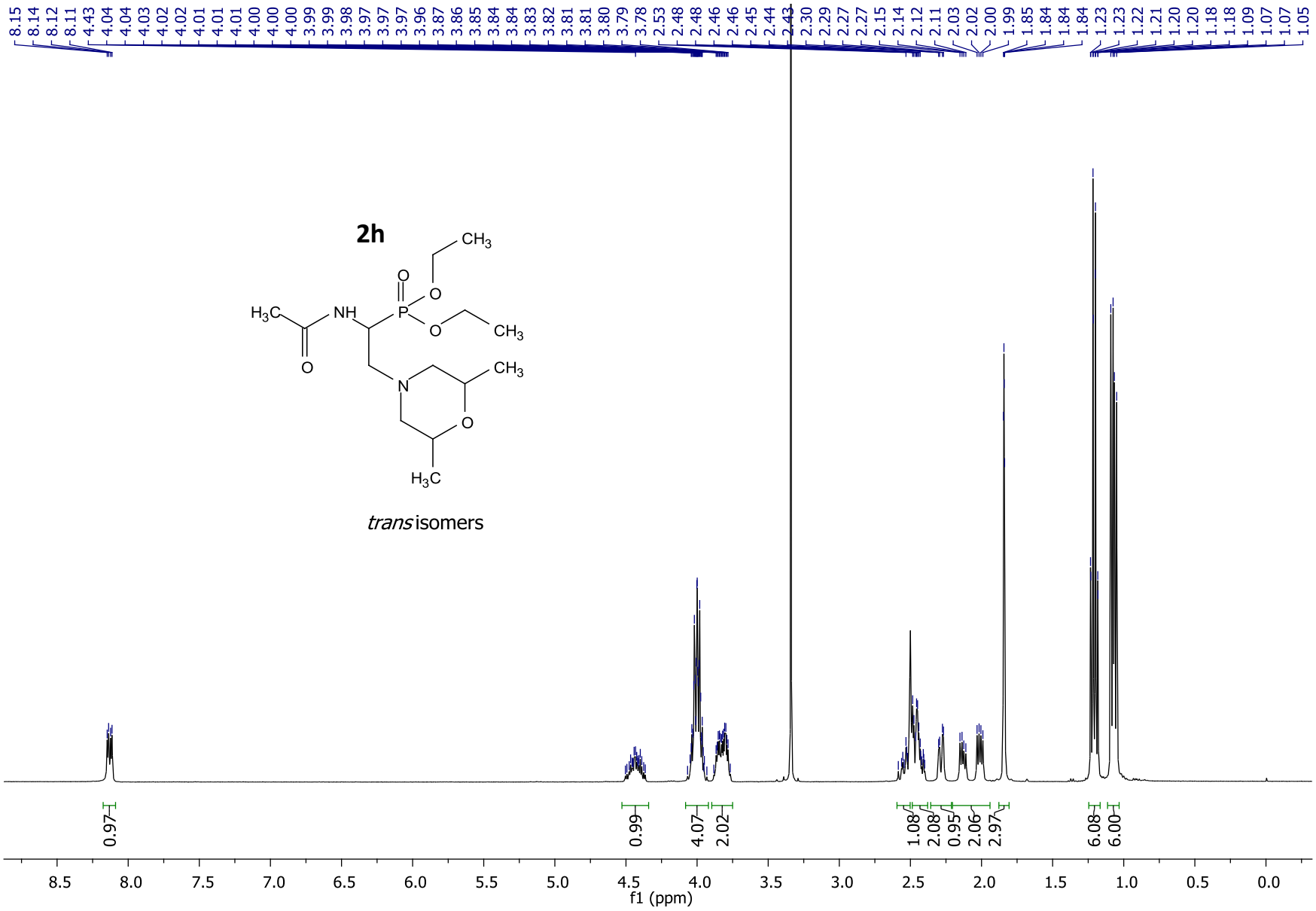

3.97
3.84
3.83
3.81
3.79
3.77
3.63
3.61
3.60
3.59
3.58
3.58
3.57
3.47
3.46
2g'
Cl-
H3N+
O
OH
P
OH
N
O
3.72
1.15
2.32
4.01
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

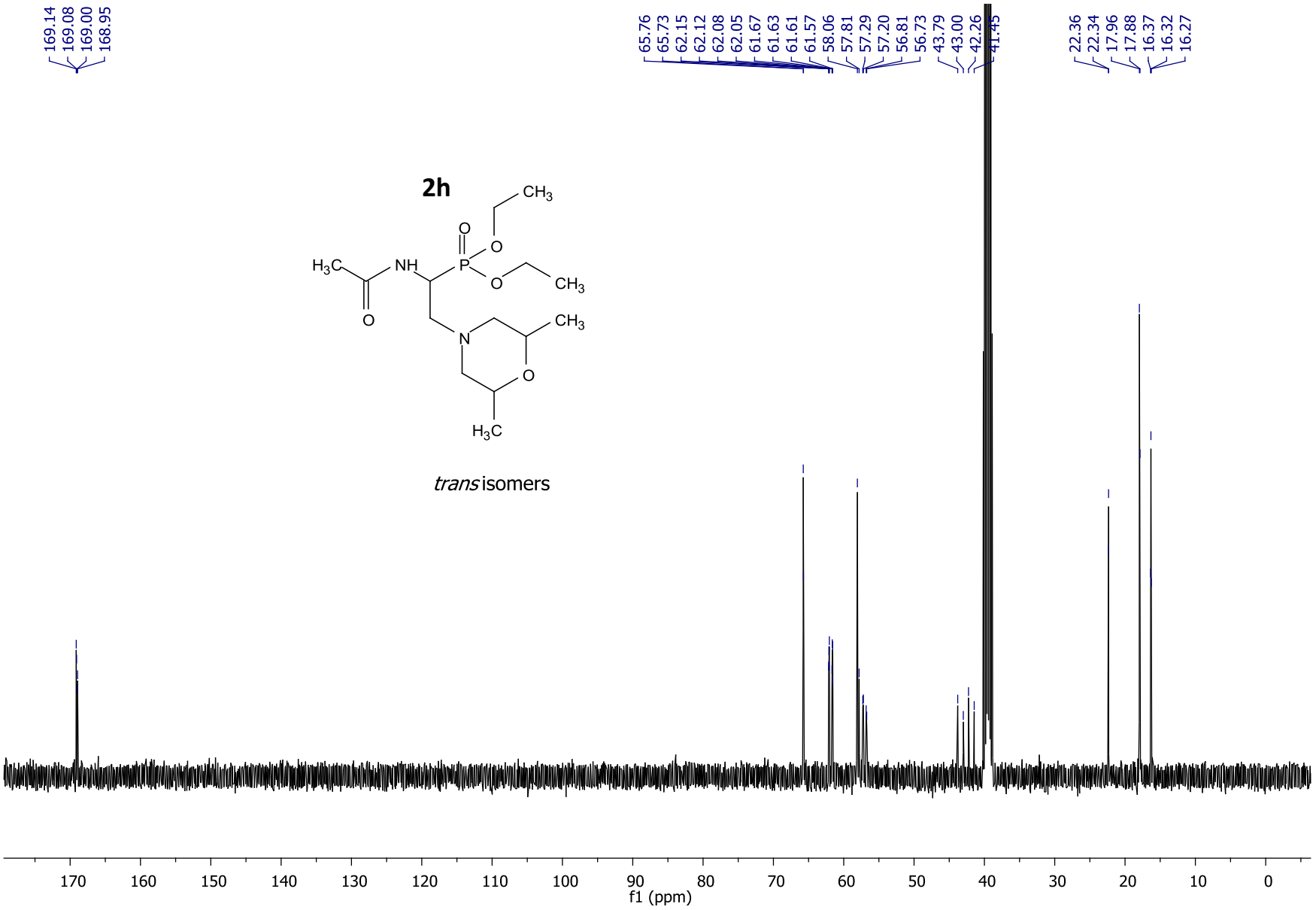

63.46
55.01
52.15
43.06
41.72
2g'
Cl-
H3N+
O
OH
P
OH
N
O
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

2g’

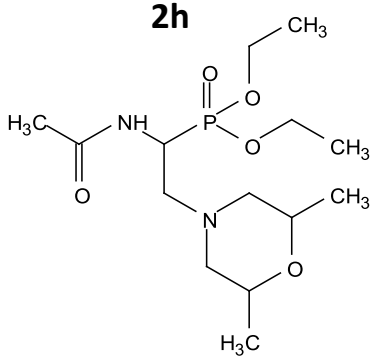

Cl-
H3N+
O
P
OH
OH
N
O

9.76
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

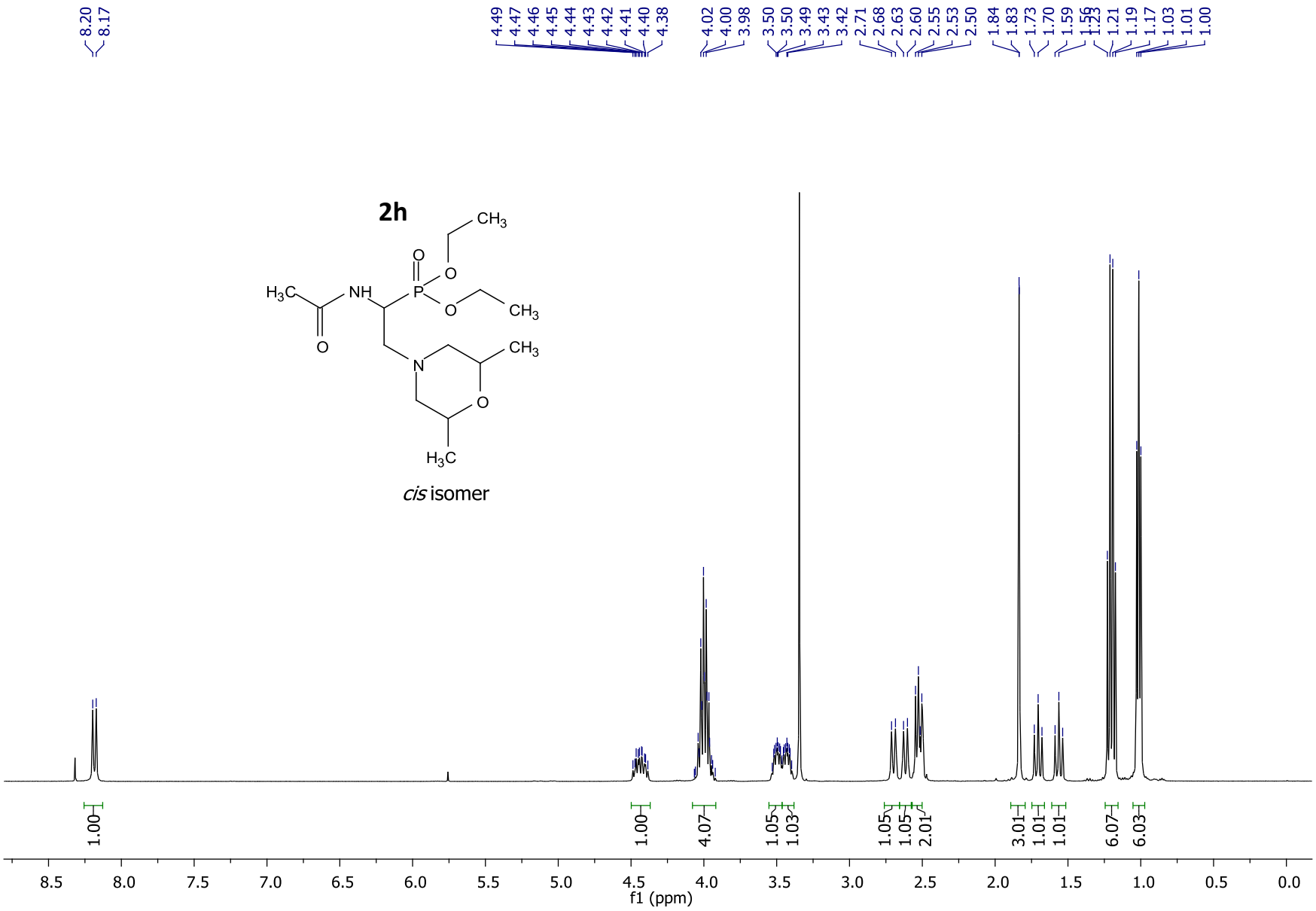

8.15 8.14 8.12 8.11 4.43 4.04 4.04 4.03 4.02 4.02 4.01 4.01 4.01 4.00 4.00 4.00 3.99 3.99 3.98 3.97 3.97 3.97 3.96 3.87 3.86 3.85 3.84 3.84 3.83 3.82 3.81 3.81 3.80 3.79 3.78 2.53 2.48 2.48 2.46 2.46 2.45 2.44 2.43 2.30 2.29 2.27 2.27 2.15 2.14 2.12 2.11 2.03 2.02 2.00 1.99 1.85 1.84 1.84 1.84 1.23 1.23 1.22 1.21 1.20 1.20 1.18 1.18 1.09 1.07 1.07 1.05
2h
CH3
O
O
H3C
NH
P
O
CH3
O
CH3
N
O
H3C
trans isomers
0.97
0.99
4.07
2.02
1.08
2.08
0.95
2.06
2.97
6.08
6.00
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 0.5 0.0
f1 (ppm)

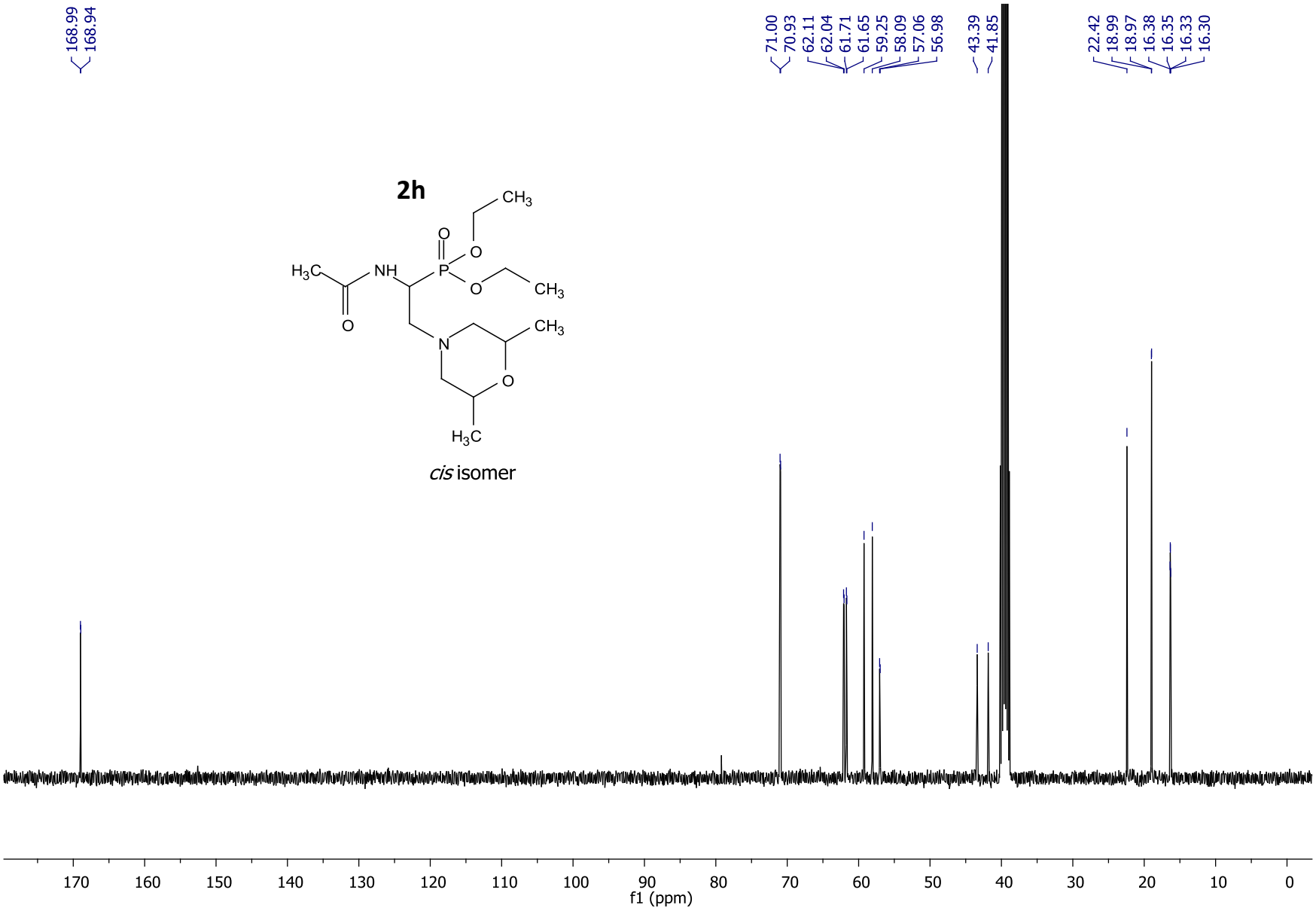

169.14
169.08
169.00
168.95
65.76
65.73
62.15
62.12
62.08
62.05
61.67
61.63
61.61
61.57
58.06
57.81
57.29
57.20
56.81
56.73
43.79
43.00
42.26
41.45
22.36
22.34
17.96
17.88
16.37
16.32
16.27
2h
CH3
O
O
H3C
NH
P
O
CH3
O
CH3
N
O
H3C
trans isomers
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2h

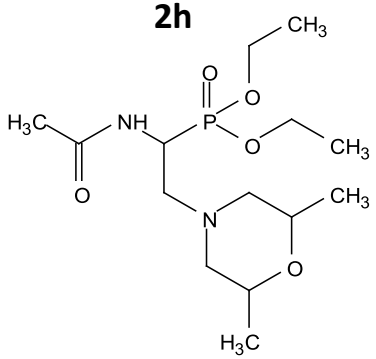


trans isomers

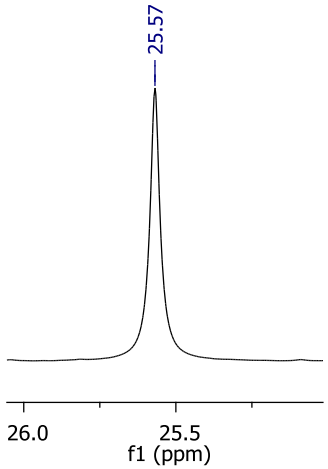

8.20
8.17
4.49
4.47
4.46
4.45
4.44
4.43
4.42
4.41
4.40
4.38
4.02
4.00
3.98
3.50
3.50
3.49
3.43
3.42
2.71
2.68
2.63
2.60
2.55
2.53
2.50
1.84
1.83
1.73
1.70
1.59
1.56
1.23
1.21
1.19
1.17
1.03
1.01
1.00
2h
CH3
O
O
H3C
NH
P
O
CH3
O
CH3
N
O
H3C
cis isomer
1.00
1.00
4.07
1.05
1.03
1.05
1.05
2.01
3.01
1.01
1.01
6.07
6.03
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
0.5
0.0
f1 (ppm)

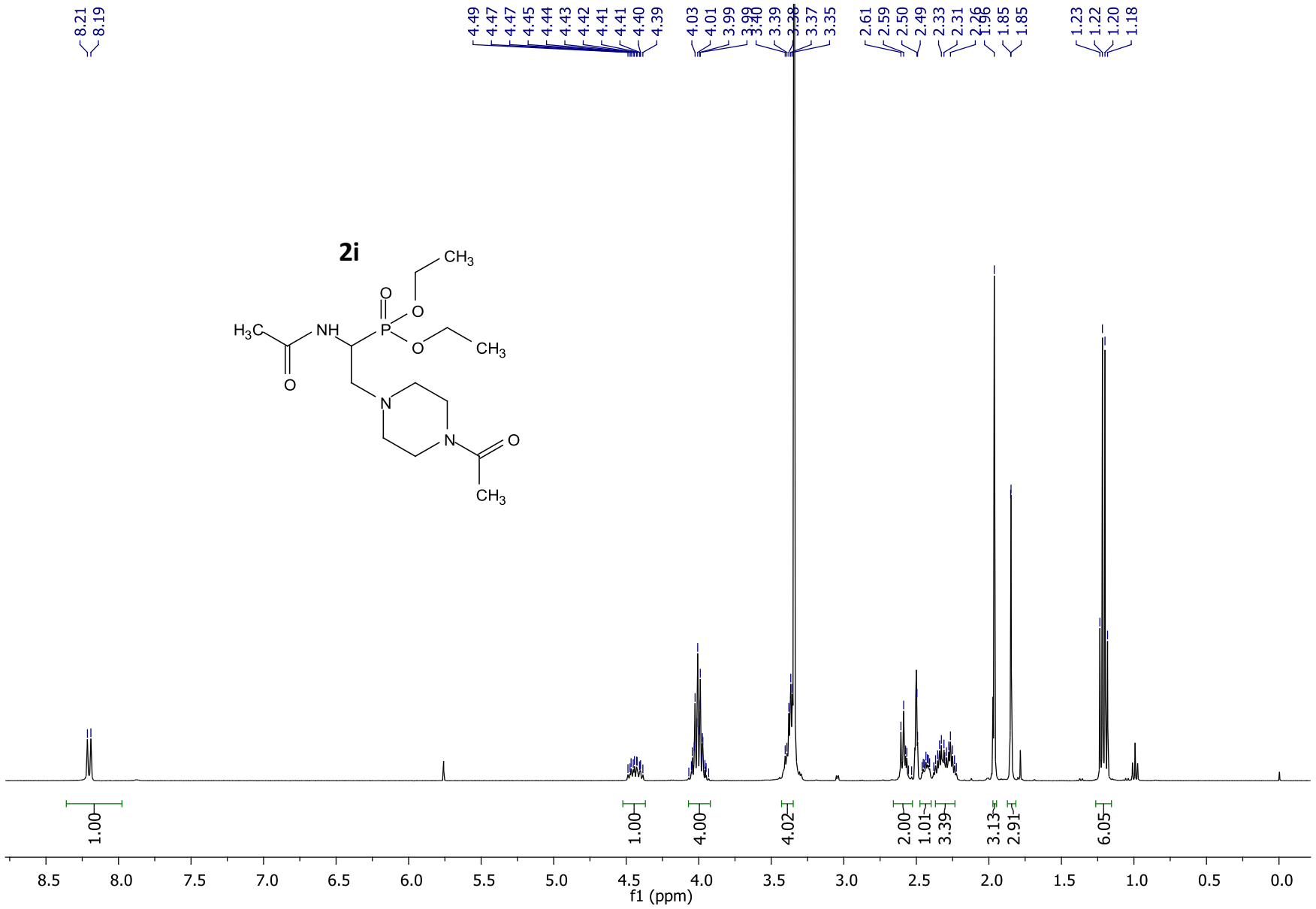

168.99
168.94
71.00
70.93
62.11
62.04
61.71
61.65
59.25
58.09
57.06
56.98
43.39
41.85
22.42
18.99
18.97
16.38
16.35
16.33
16.30
2h
cis isomer
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

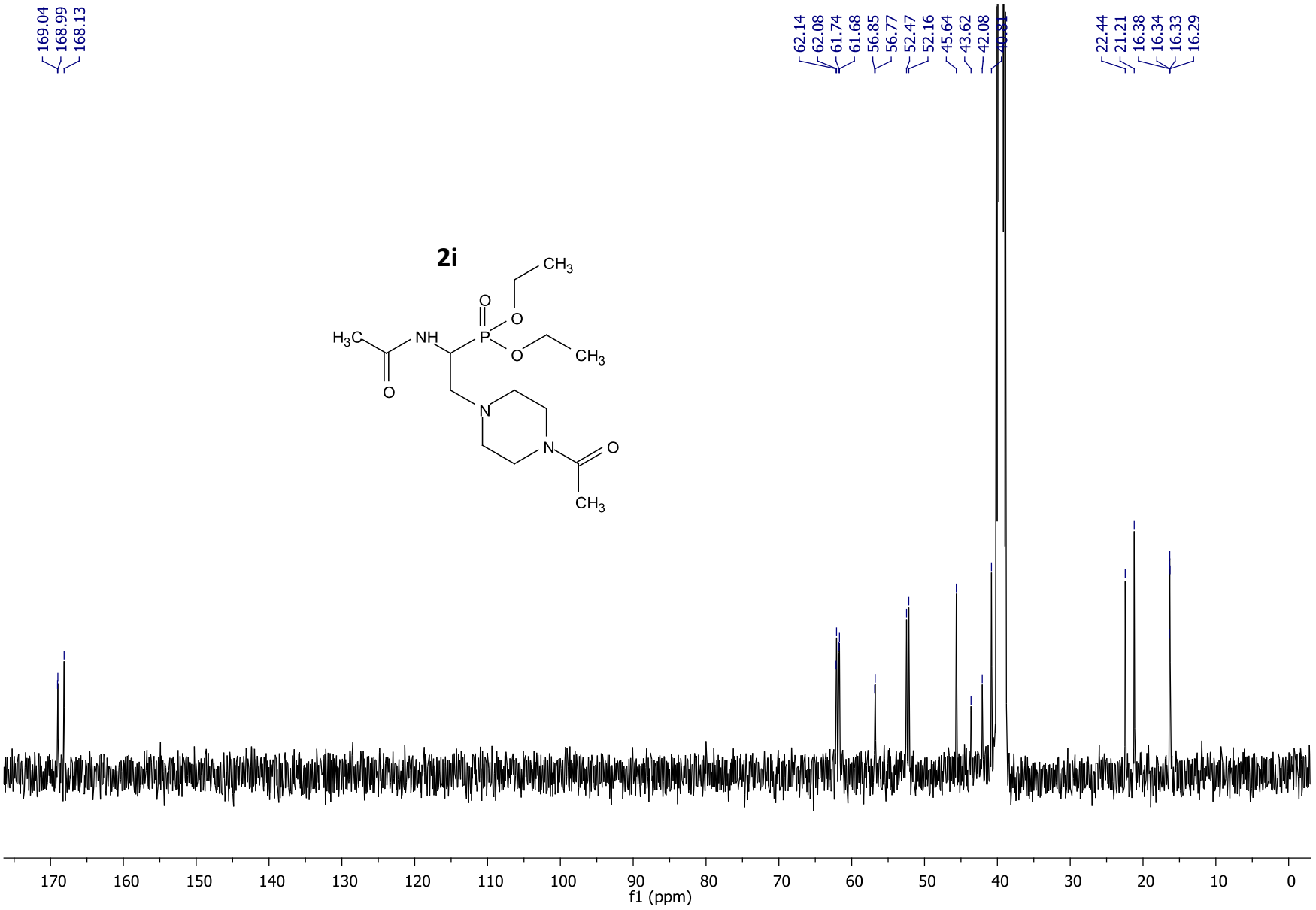
2h



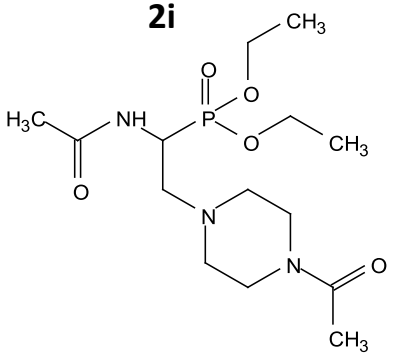
cis isomer



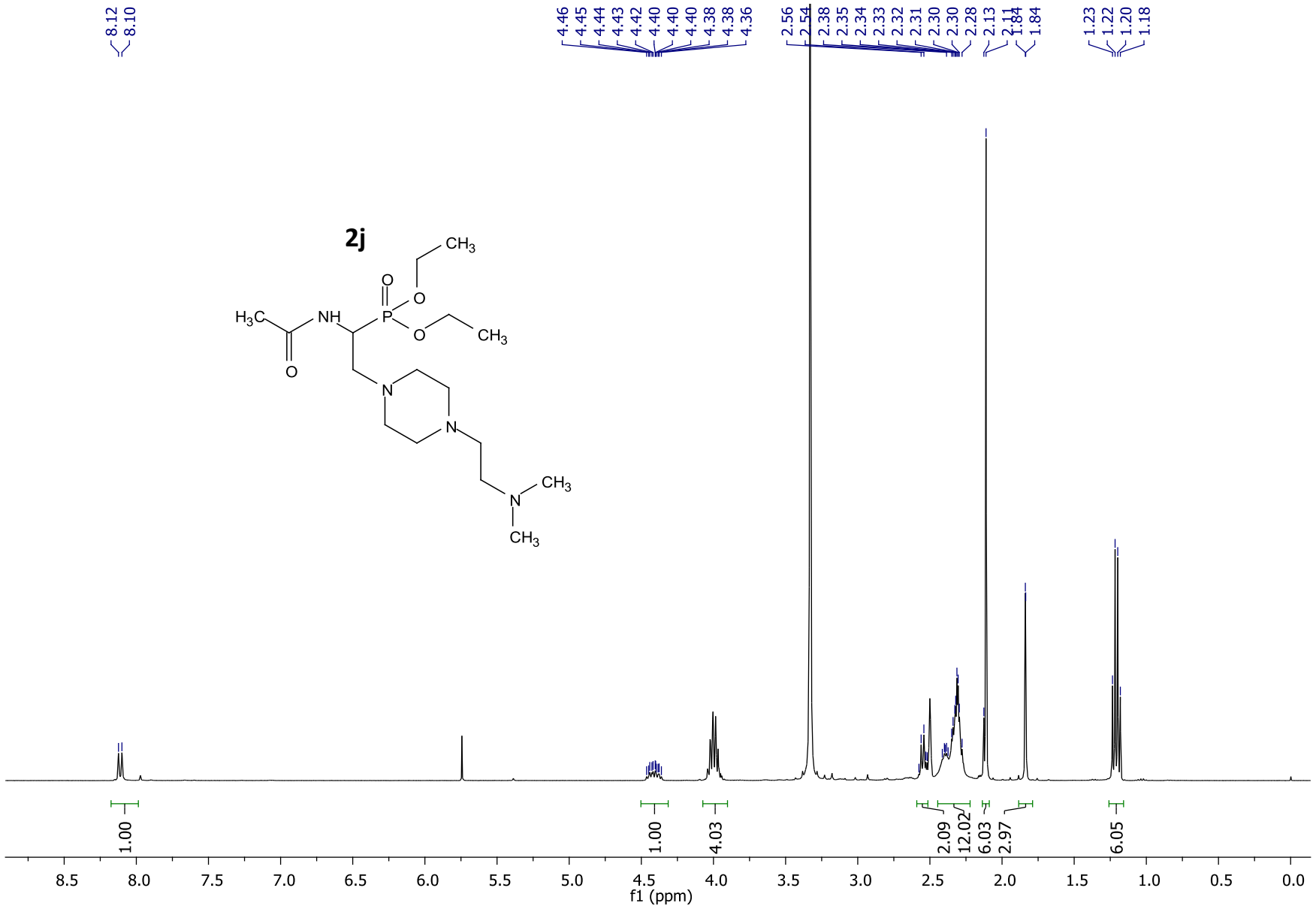

2i
8.21
8.19
4.49
4.47
4.47
4.45
4.44
4.43
4.42
4.41
4.41
4.40
4.39
4.03
4.01
3.99
3.99
3.40
3.39
3.38
3.37
3.35
2.61
2.59
2.50
2.49
2.33
2.31
1.85
1.85
1.23
1.22
1.20
1.18
1.00
1.00
4.00
4.02
2.00
1.01
3.39
3.13
2.91
6.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

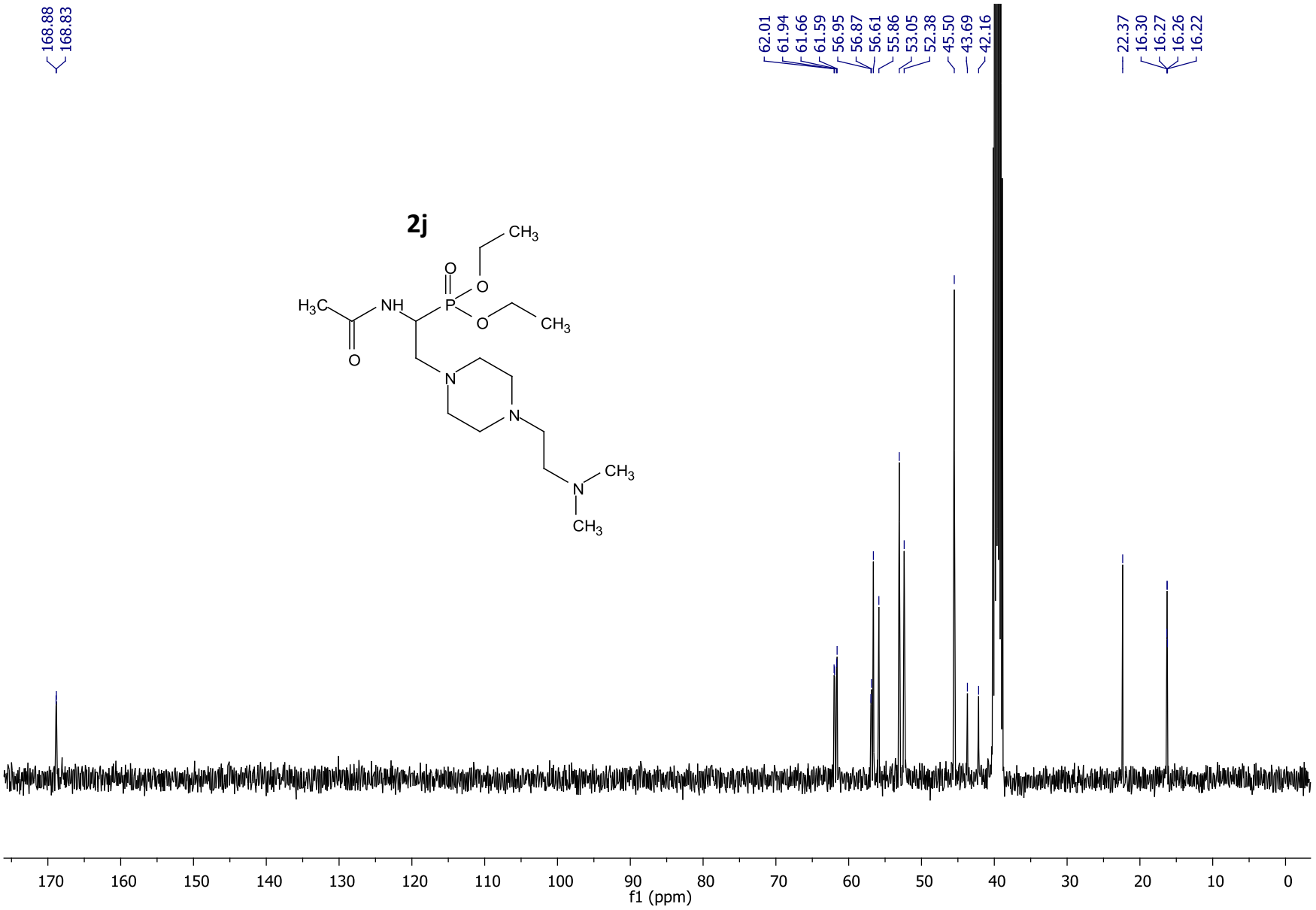

169.04
168.99
168.13
62.14
62.08
61.74
61.68
56.85
56.77
52.47
52.16
45.64
43.62
42.08
22.44
21.21
16.38
16.34
16.33
16.29
2i
CH3
O
O
H3C
NH
P
O
CH3
O
N
N
O
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2i

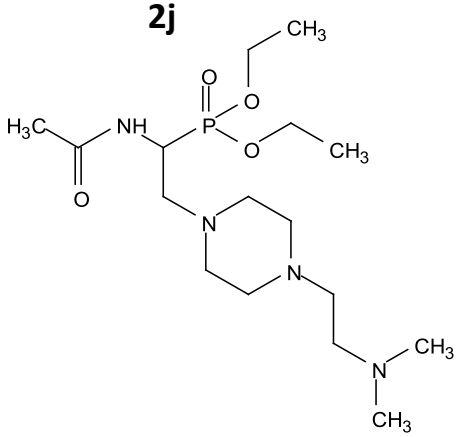

CH3
O
O
H3C
NH
P
O
CH3
O
N
N
O
CH3

25.43
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

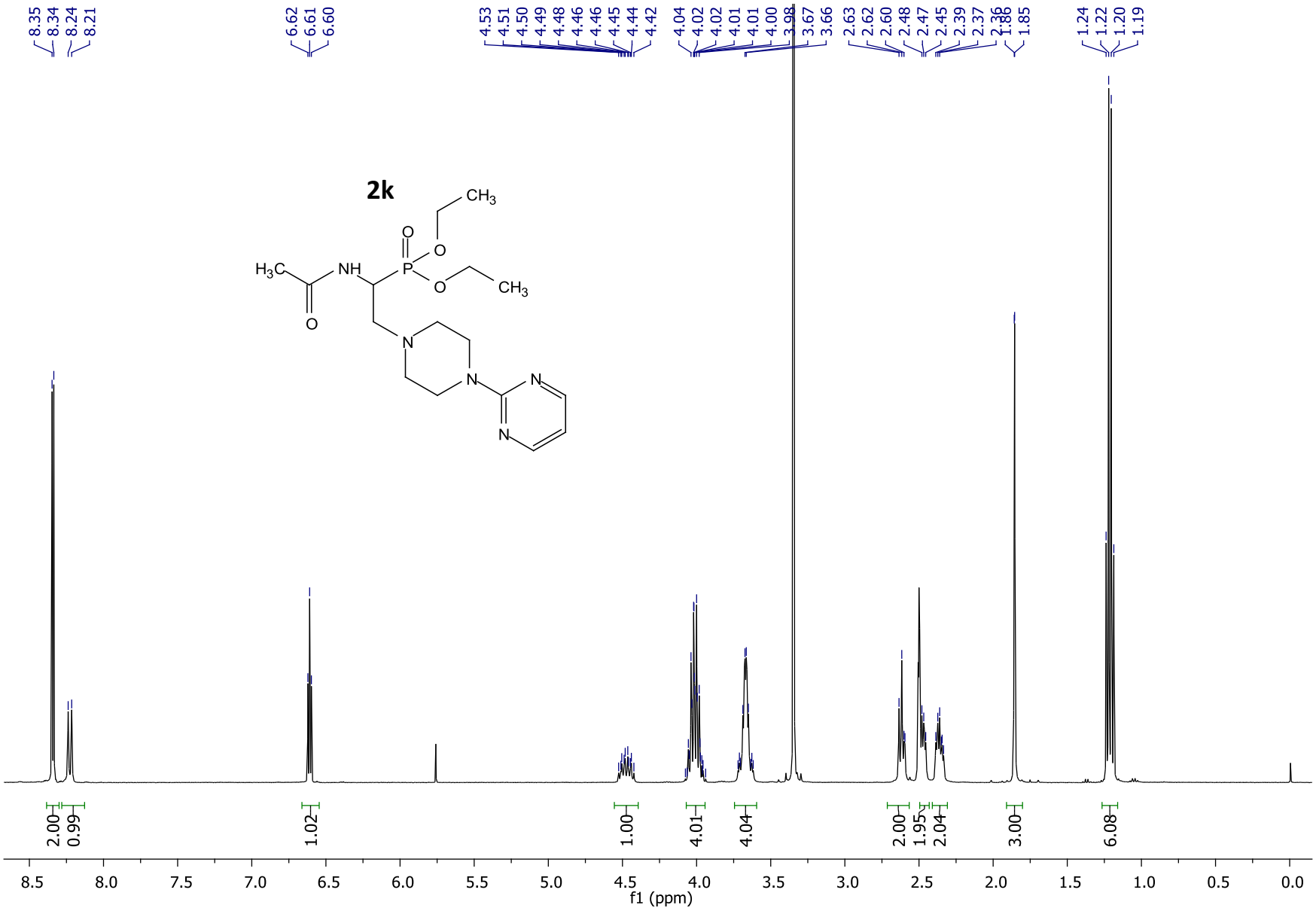

2j
8.12
8.10
4.46
4.45
4.44
4.43
4.42
4.40
4.40
4.40
4.38
4.38
4.36
2.56
2.54
2.38
2.35
2.34
2.33
2.32
2.31
2.30
2.30
2.28
2.13
2.11
1.84
1.23
1.22
1.20
1.18
1.00
1.00
4.03
2.09
12.02
6.03
2.97
6.05
f1 (ppm)

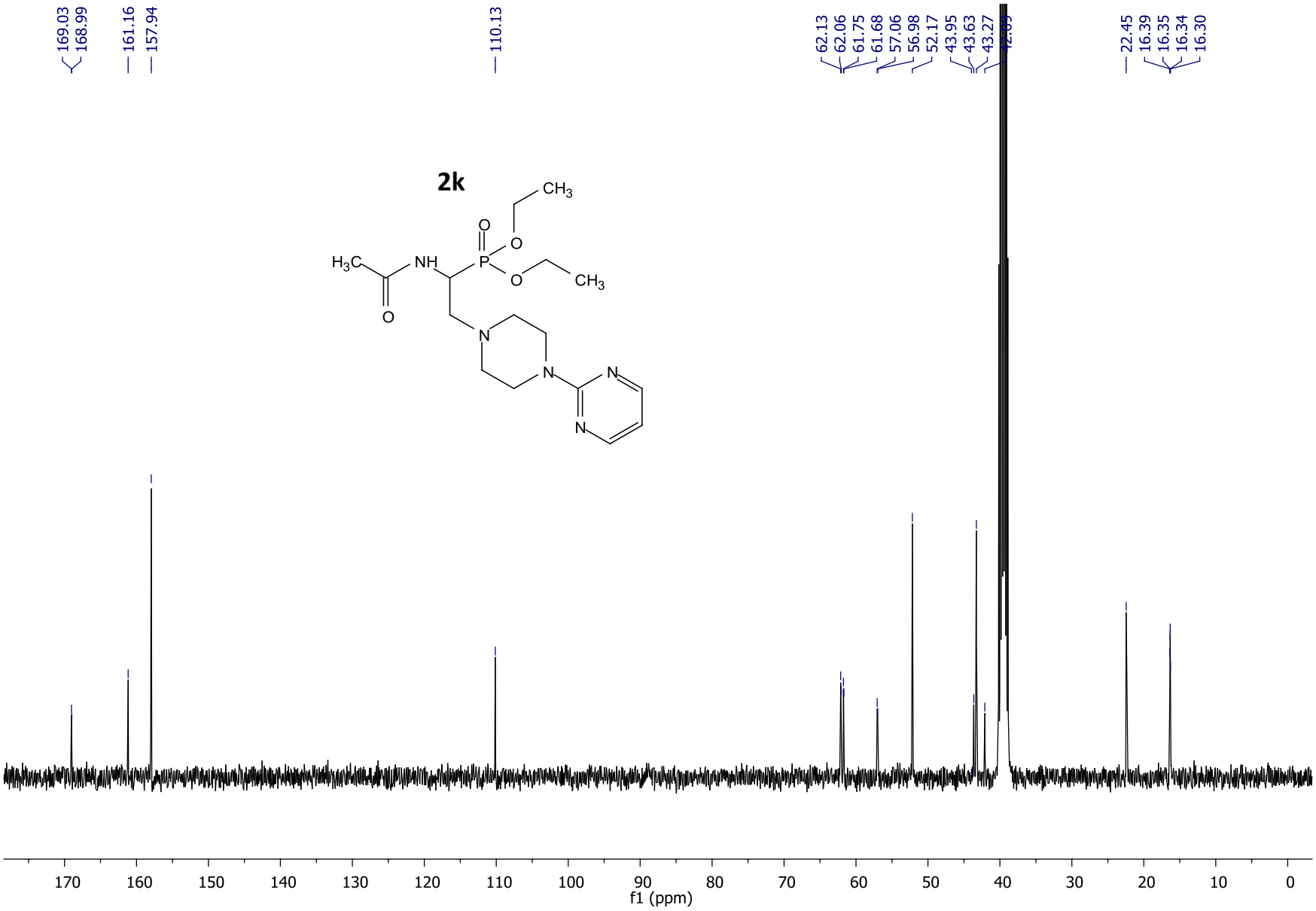

168.88
168.83
62.01
61.94
61.66
61.59
56.95
56.87
56.61
55.86
53.05
52.38
45.50
43.69
42.16
22.37
16.30
16.27
16.26
16.22
2j
CH3
O
O
H3C
NH
P
O
CH3
O
N
N
CH3
N
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2j

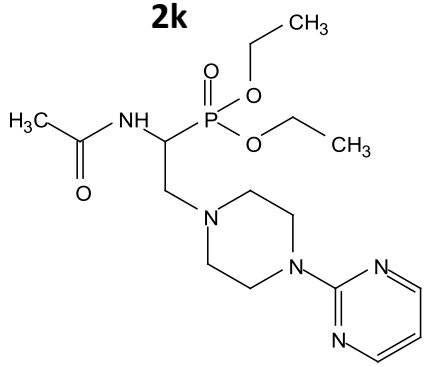

CH3
O
O
H3C
NH
P
O
CH3
O
N
N
CH3
N
CH3

25.63
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

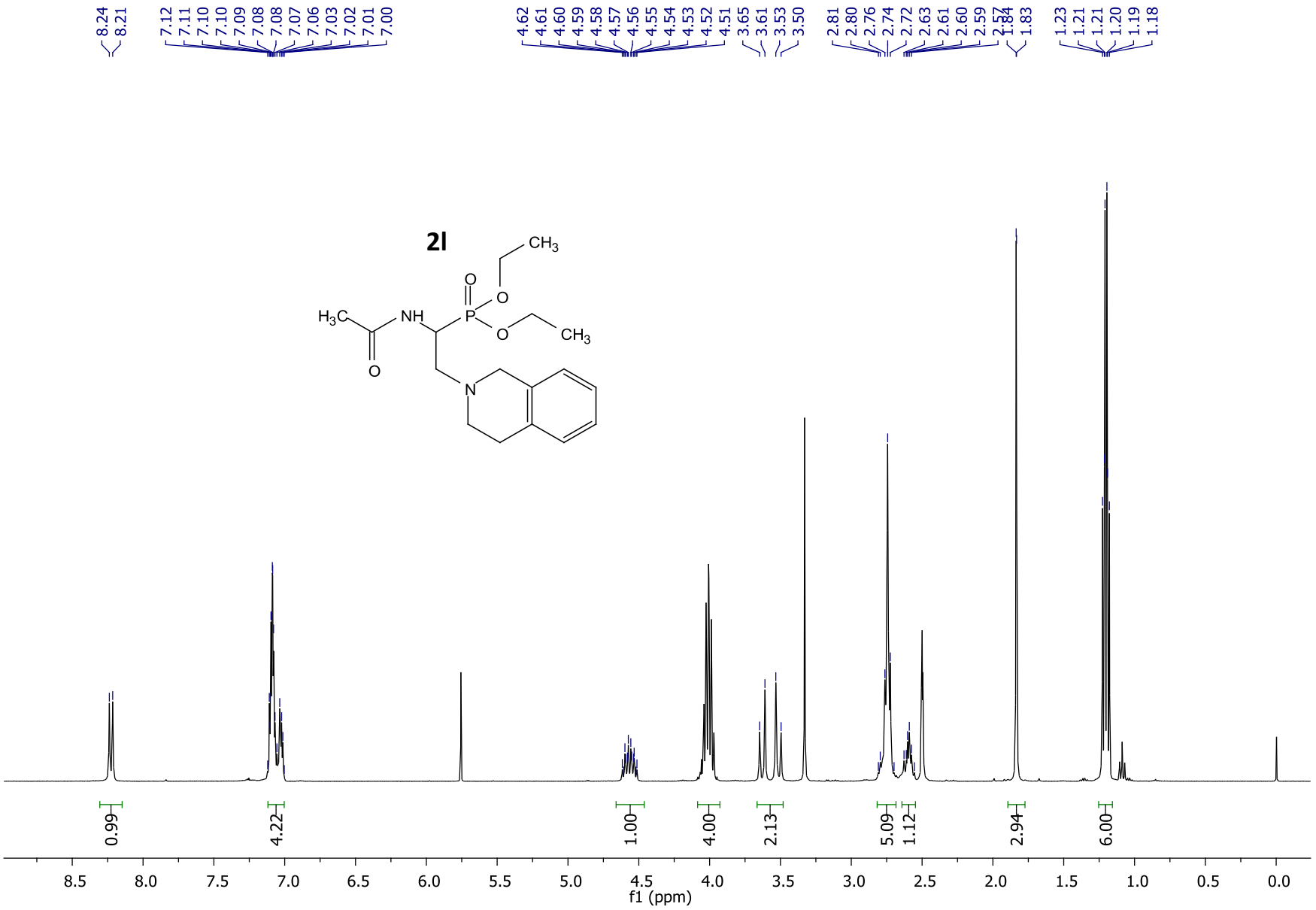

8.35
8.34
8.24
8.21
6.62
6.61
6.60
4.53
4.51
4.50
4.49
4.48
4.46
4.46
4.45
4.44
4.42
4.04
4.02
4.02
4.01
4.01
4.00
3.98
3.67
3.66
2.63
2.62
2.60
2.48
2.47
2.45
2.39
2.37
1.85
1.24
1.22
1.20
1.19
2k
CH3
O
O
H3C
NH
P
O
CH3
O
N
N
N
N
2.00
0.99
1.02
1.00
4.01
4.04
2.00
1.95
2.04
3.00
6.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

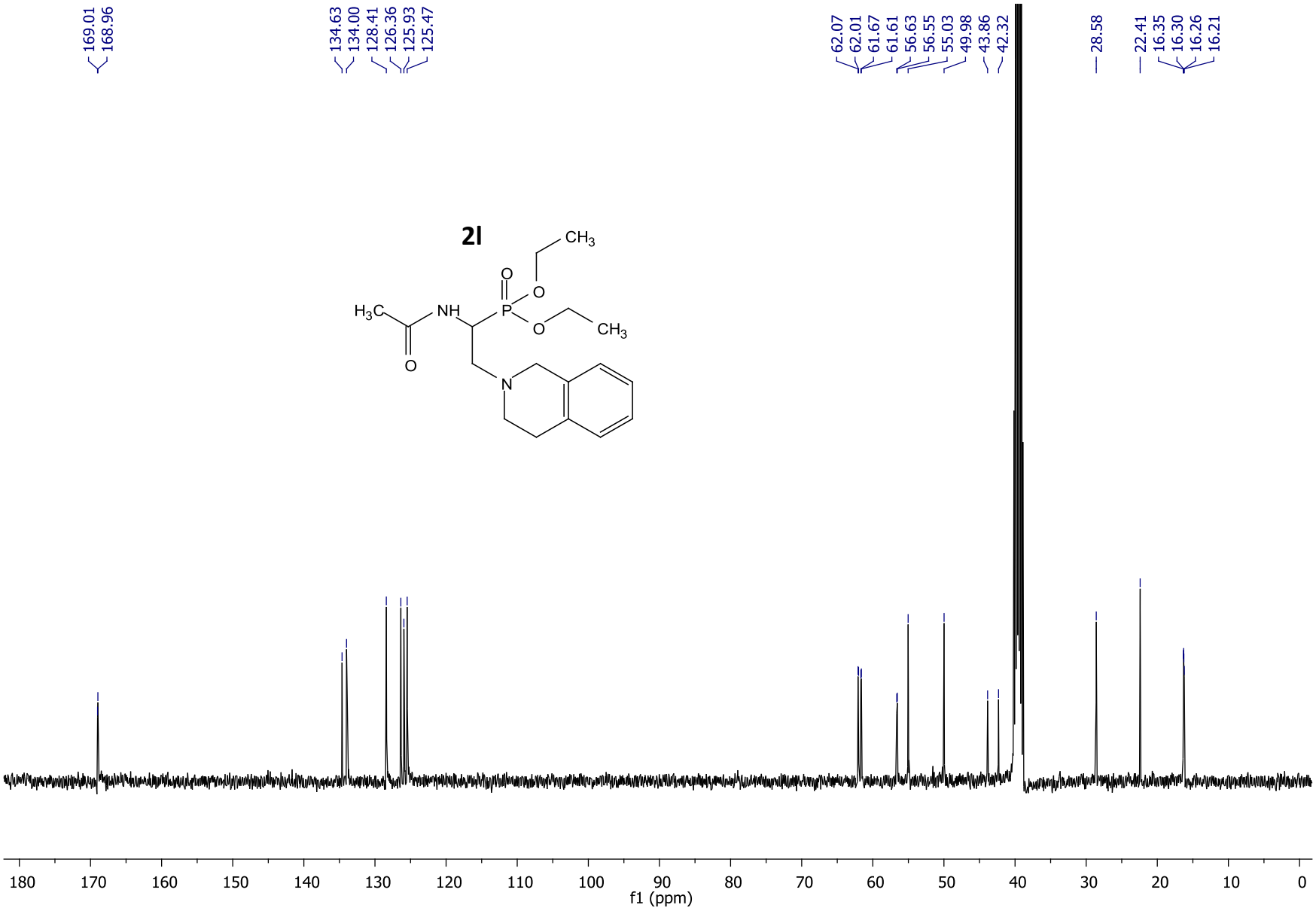

169.03
168.99
161.16
157.94
110.13
62.13
62.06
61.75
61.68
57.06
56.98
52.17
43.95
43.63
43.27
22.45
16.39
16.35
16.34
16.30
2k
CH3
O
O
H3C
NH
P
O
CH3
O
N
N
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2k

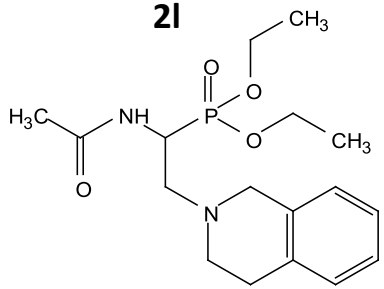

CH3
O
O
H3C
NH
P
O
CH3
O
N
N
N
N

25.52
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

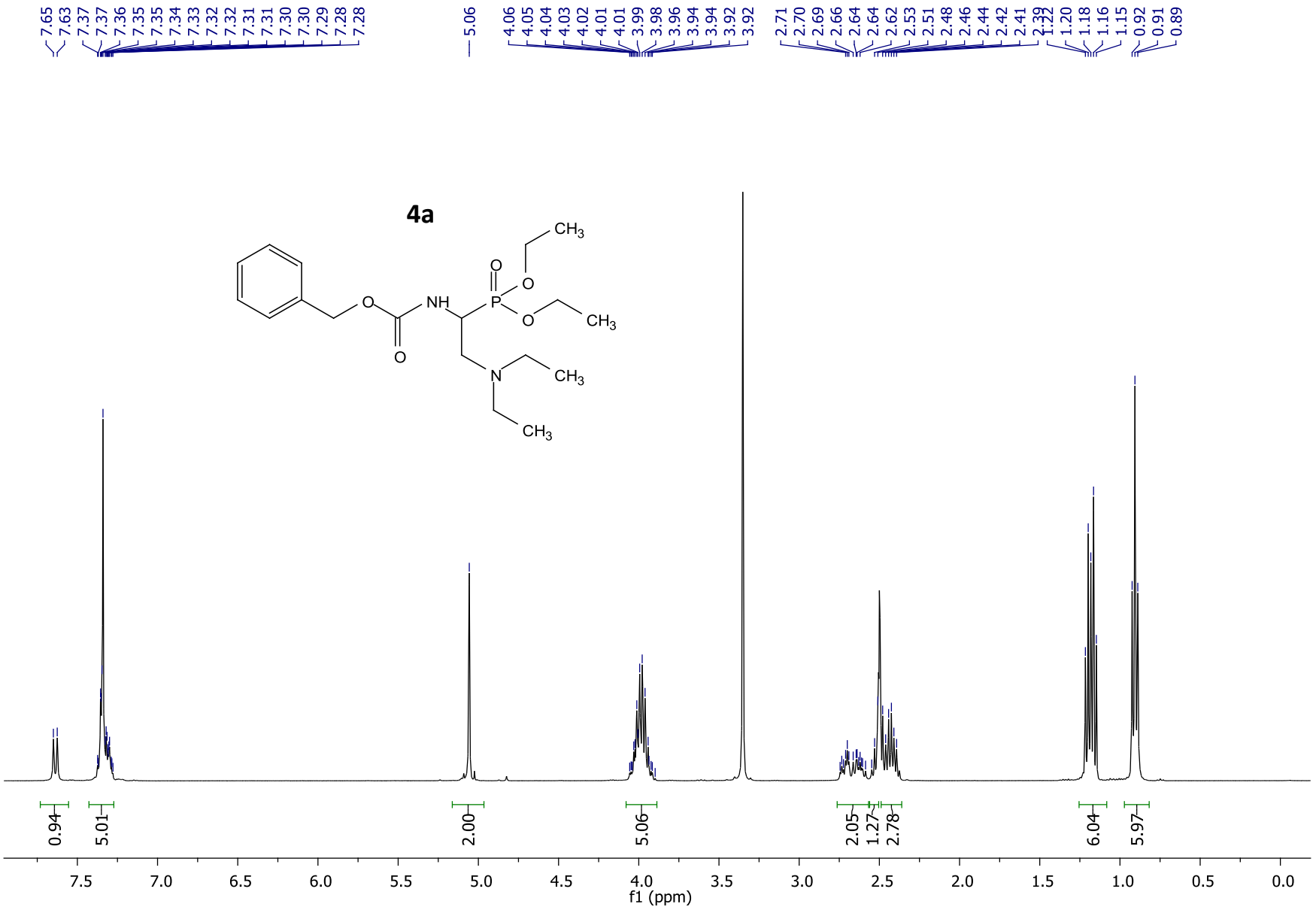

8.24
8.21
7.12
7.11
7.10
7.10
7.09
7.08
7.08
7.07
7.06
7.03
7.02
7.01
7.00
4.62
4.61
4.60
4.59
4.58
4.57
4.56
4.55
4.54
4.53
4.52
4.51
3.65
3.61
3.53
3.50
2.81
2.80
2.76
2.74
2.72
2.63
2.61
2.60
2.59
2.57
1.84
1.83
1.23
1.21
1.21
1.20
1.19
1.18
2l
CH3
O
O
H3C
NH
P
O
CH3
O
N
0.99
4.22
1.00
4.00
2.13
5.09
1.12
2.94
6.00
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
0.5
0.0
f1 (ppm)

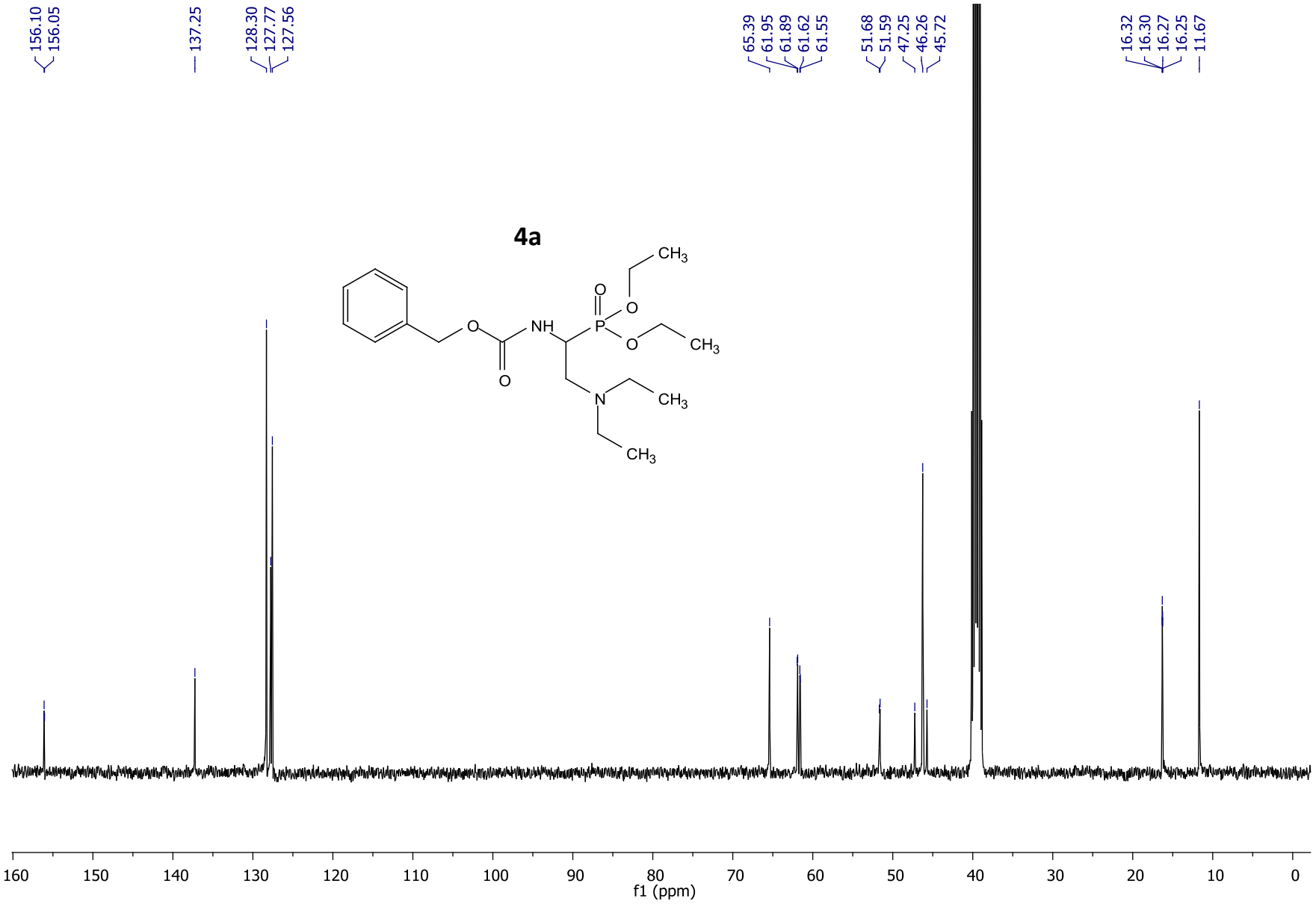

169.01
168.96
134.63
134.00
128.41
126.36
125.93
125.47
62.07
62.01
61.67
61.61
56.63
56.55
55.03
49.98
43.86
42.32
28.58
22.41
16.35
16.30
16.26
16.21
2l
CH3
O
O
H3C
NH
P
O
CH3
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

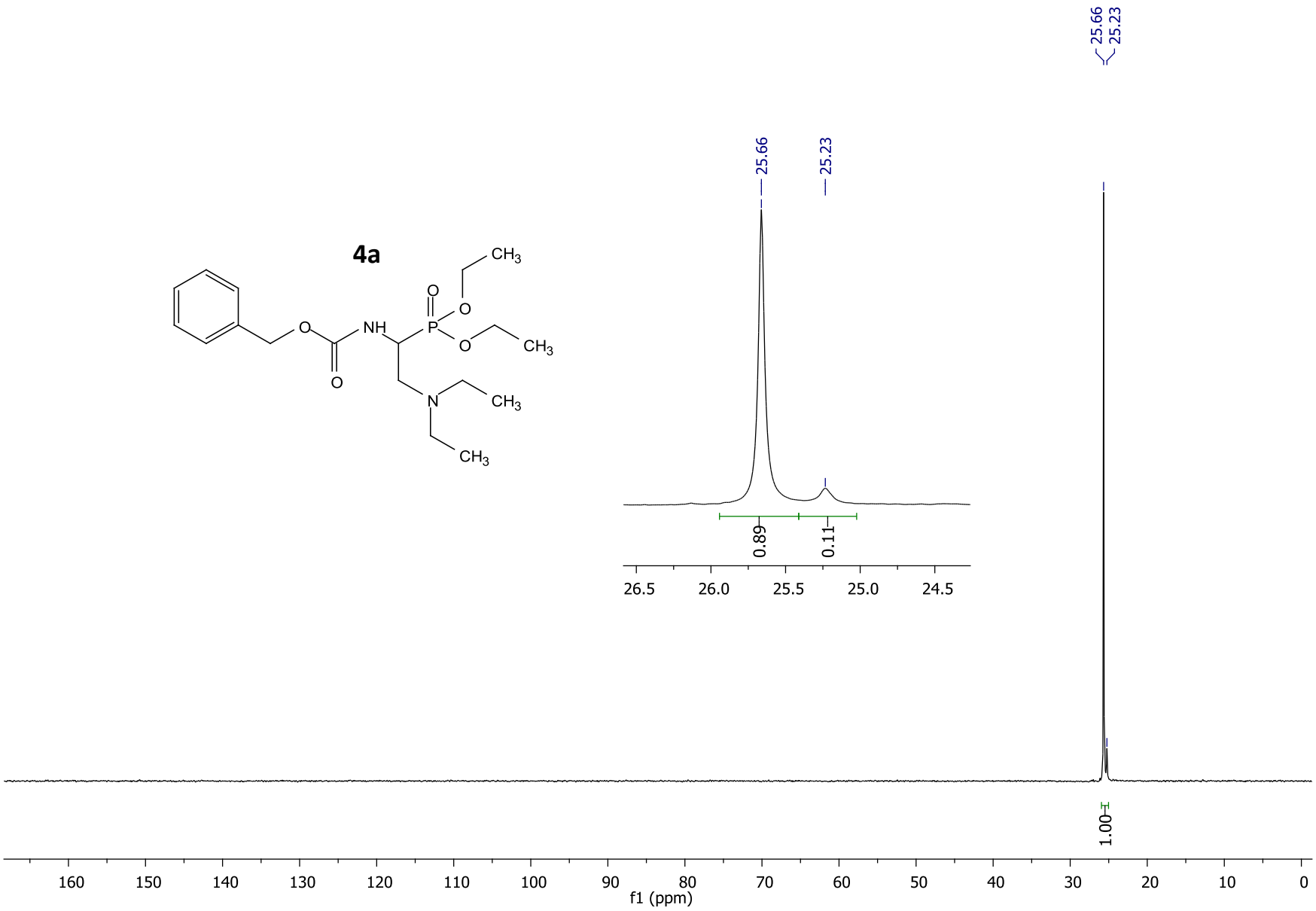
2l

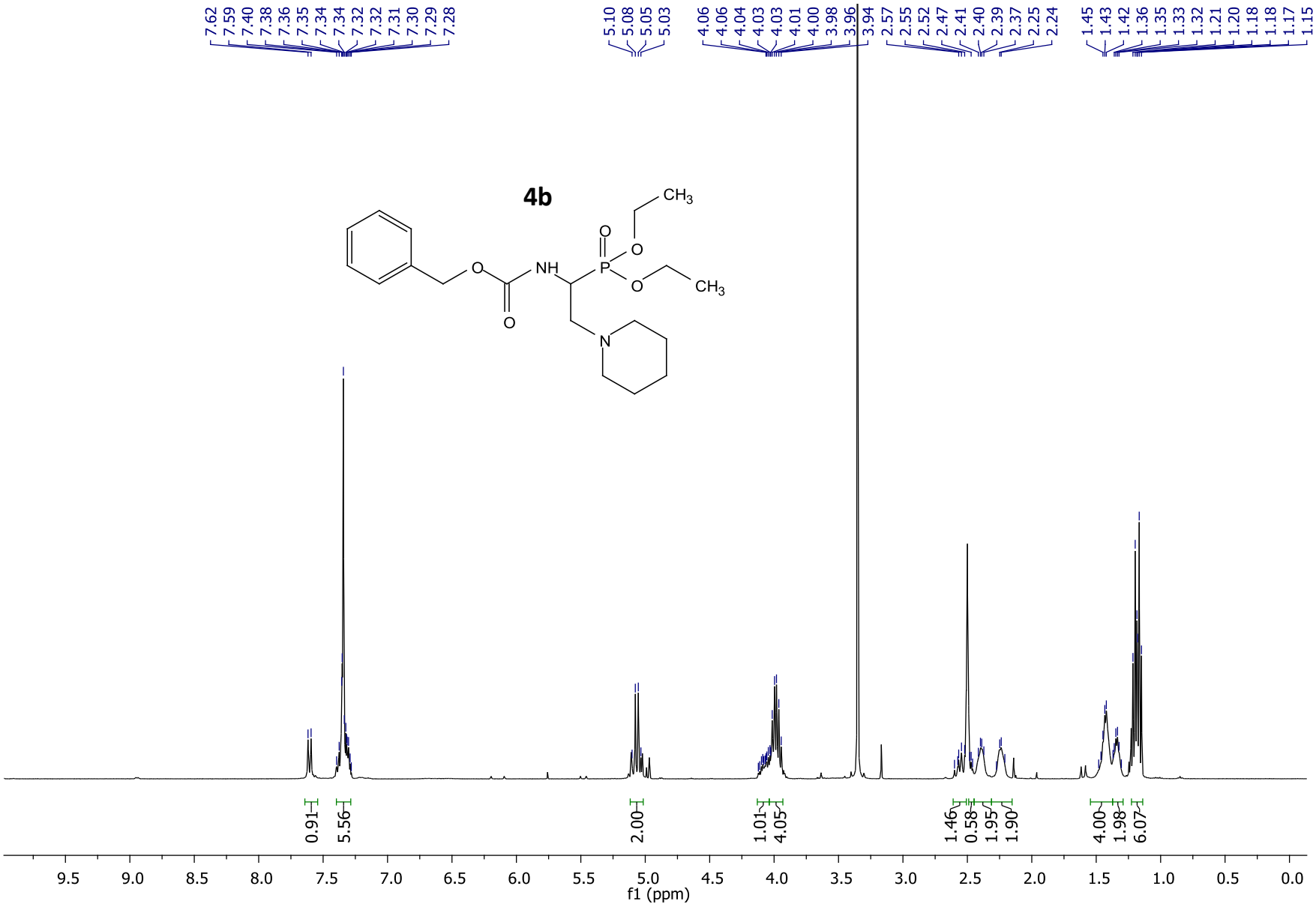

CH3
O
O
H3C
NH
P
O
CH3
O
N

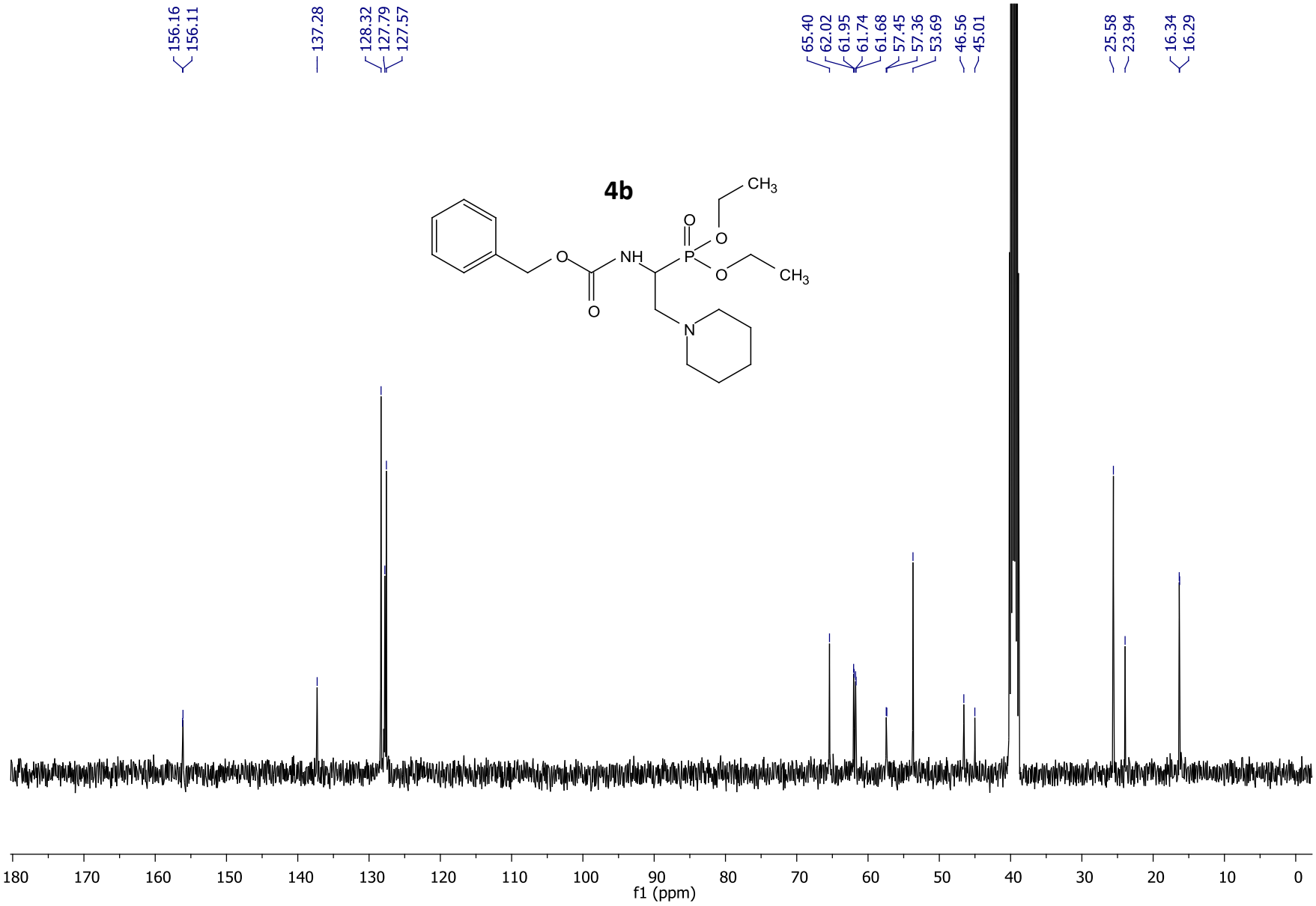
25.54
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

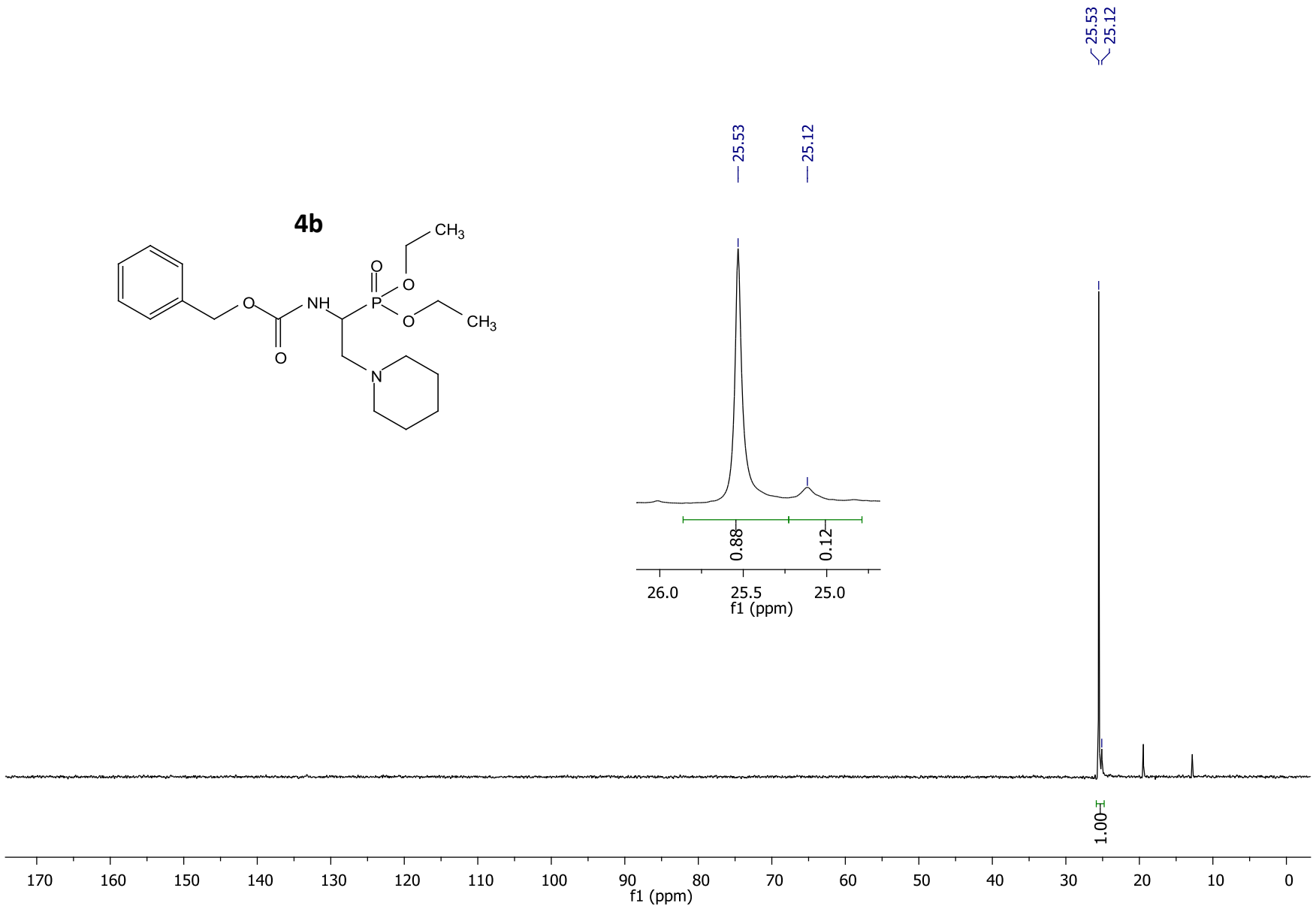

7.65 7.63 7.37 7.37 7.36 7.35 7.35 7.34 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.28
5.06
4.06 4.05 4.04 4.03 4.02 4.01 4.01 3.99 3.98 3.96 3.94 3.94 3.92 3.92
2.71 2.70 2.69 2.66 2.64 2.64 2.62 2.53 2.51 2.48 2.46 2.44 2.42 2.41 2.39 2.32 1.20 1.18 1.16 1.15 0.92 0.91 0.89
4a
CH3
O
O
NH
P
O
CH3
O
N
CH3
CH3
0.94 5.01 2.00 5.06 2.05 1.27 2.78 6.04 5.97
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 0.0
f1 (ppm)

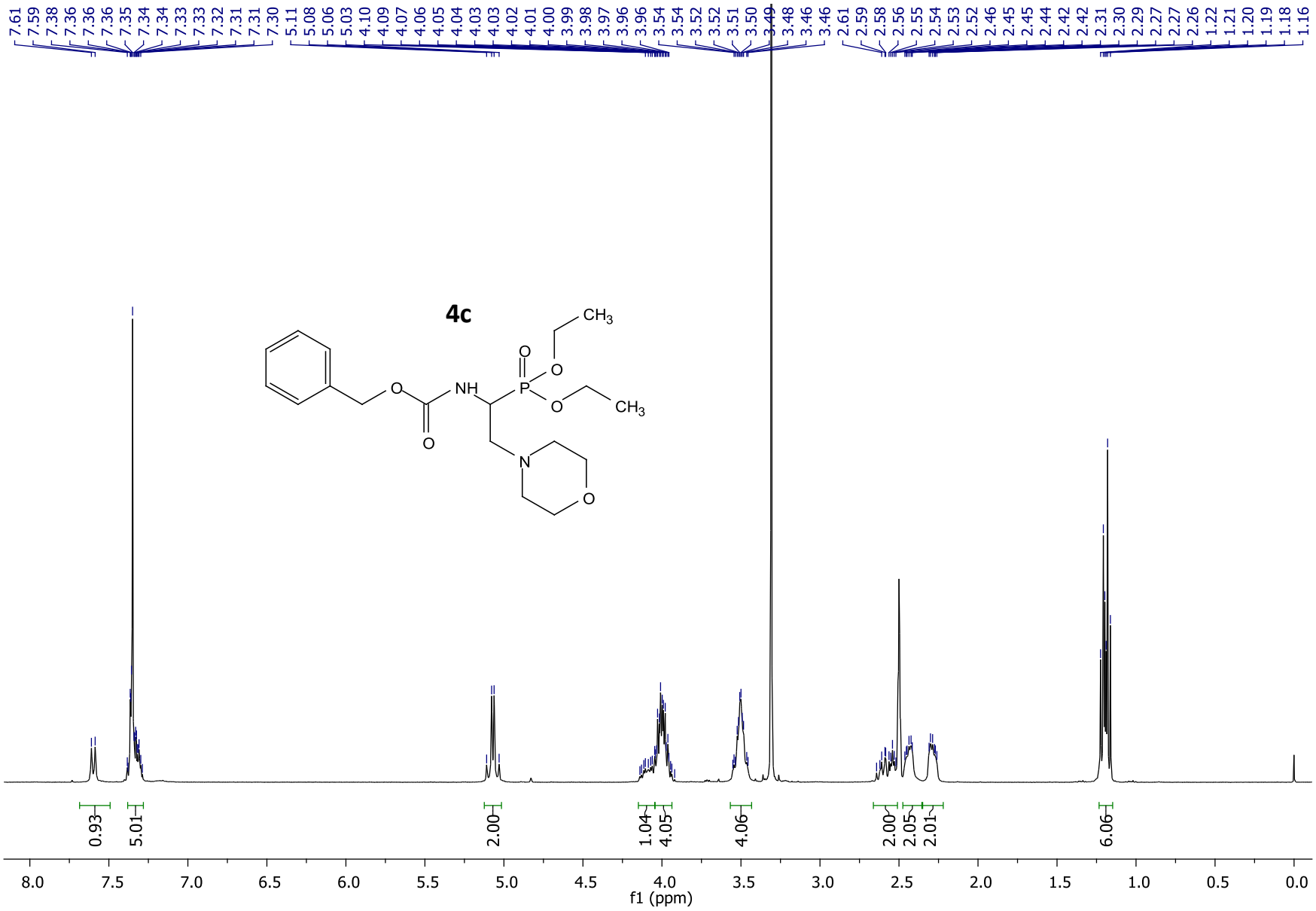

156.10
156.05
137.25
128.30
127.77
127.56
65.39
61.95
61.89
61.62
61.55
51.68
51.59
47.25
46.26
45.72
16.32
16.30
16.27
16.25
11.67
4a
CH3
O
O
NH
P
O
CH3
O
CH3
N
CH3
CH3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

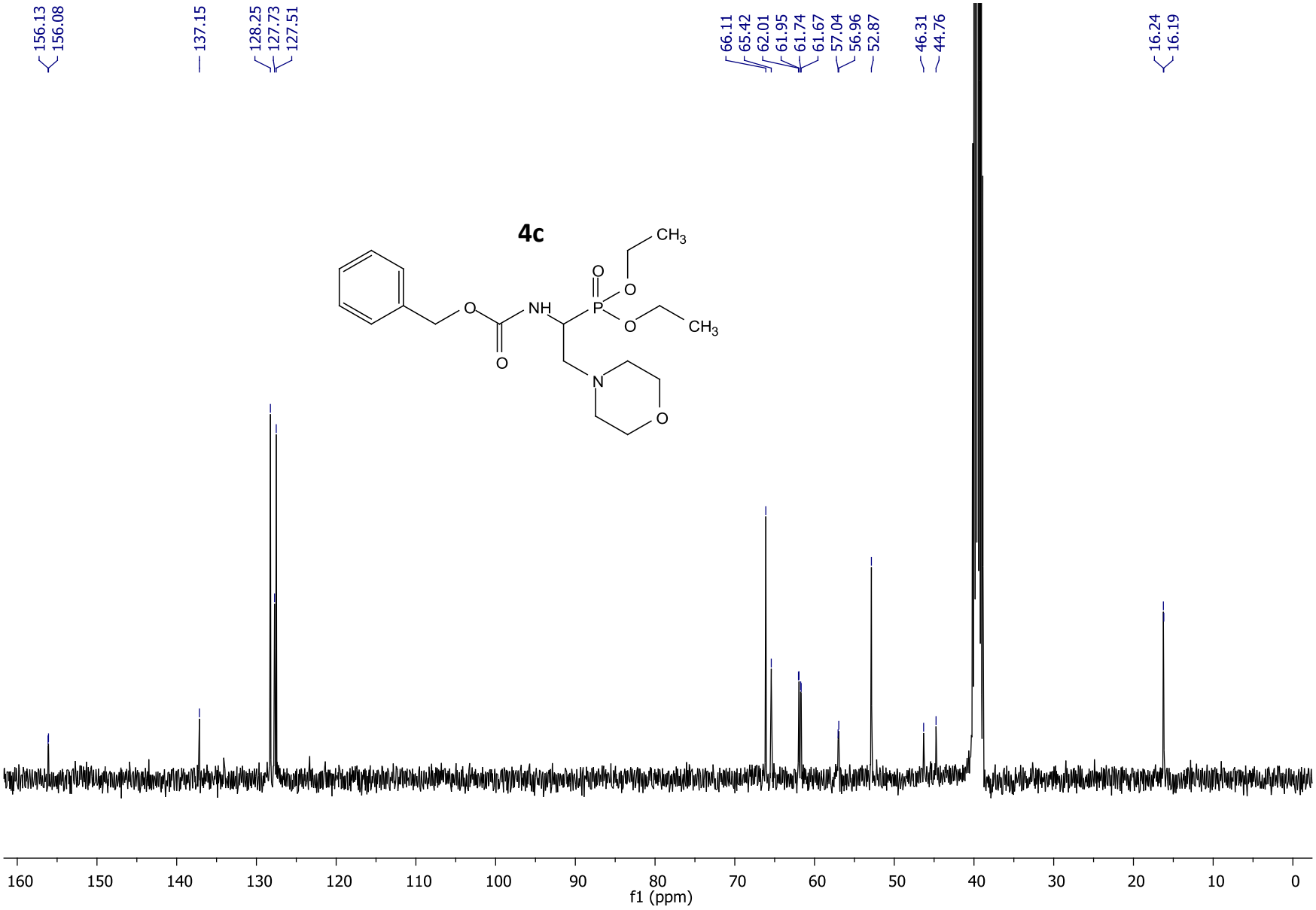

4a
CH3
O
O
NH
P
O
CH3
O
N
CH3
CH3
25.66
25.23
25.66
25.23
0.89
0.11
26.5
26.0
25.5
25.0
24.5
1.00
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

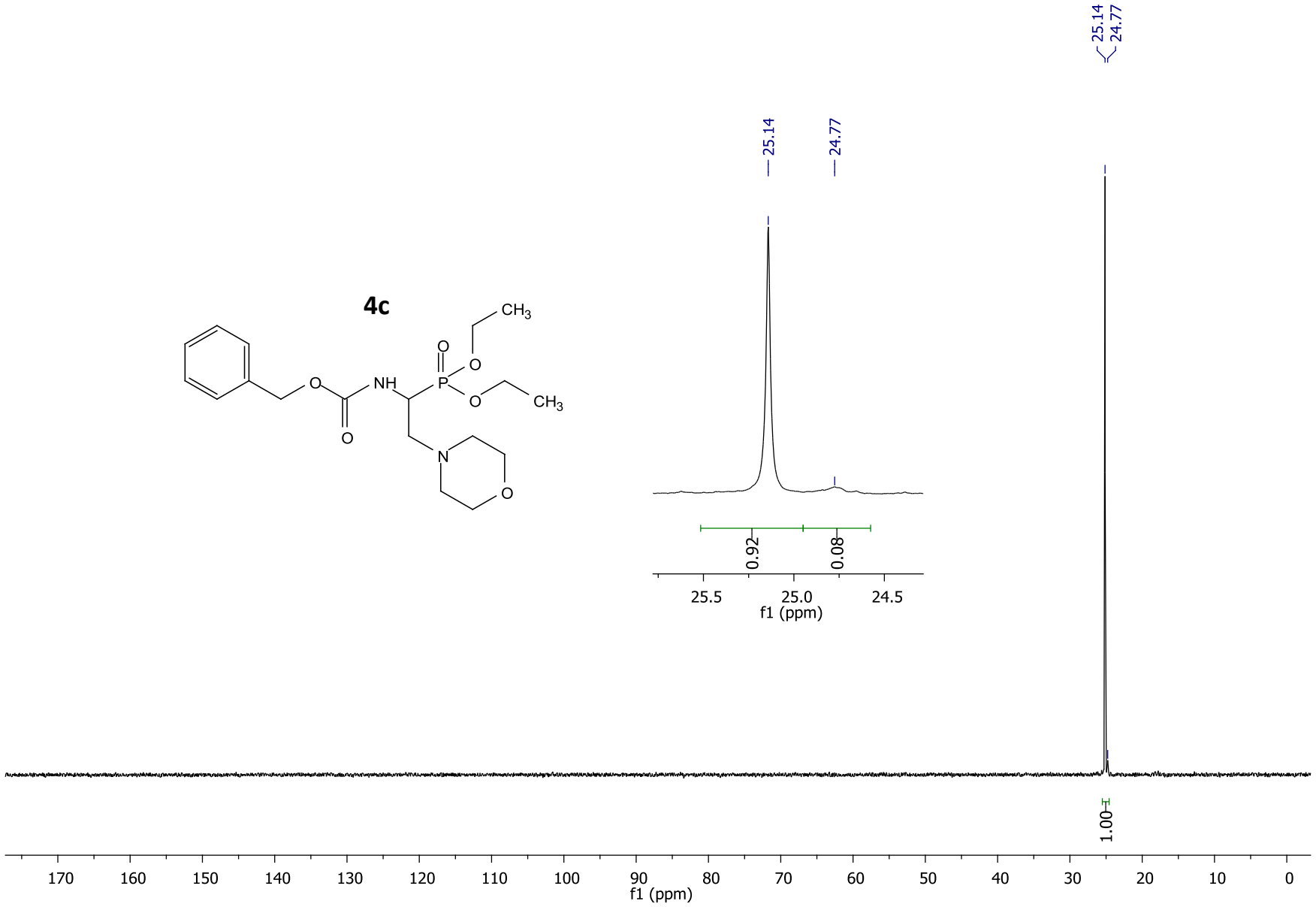

7.62 7.59 7.40 7.38 7.36 7.35 7.34 7.34 7.32 7.32 7.31 7.30 7.29 7.28
5.10 5.08 5.05 5.03
4.06 4.06 4.04 4.03 4.03 4.01 4.00 3.98 3.96 3.94
2.57 2.55 2.52 2.47 2.41 2.40 2.39 2.37 2.25 2.24
1.45 1.43 1.42 1.36 1.35 1.33 1.32 1.21 1.20 1.18 1.18 1.17 1.15
4b
CH3
O
O
NH
P
O
CH3
O
O
N
0.91 5.56 2.00 1.01 4.05 1.46 0.58 1.95 1.90 4.00 1.98 6.07
9.5 9.0 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 0.5 0.0
f1 (ppm)

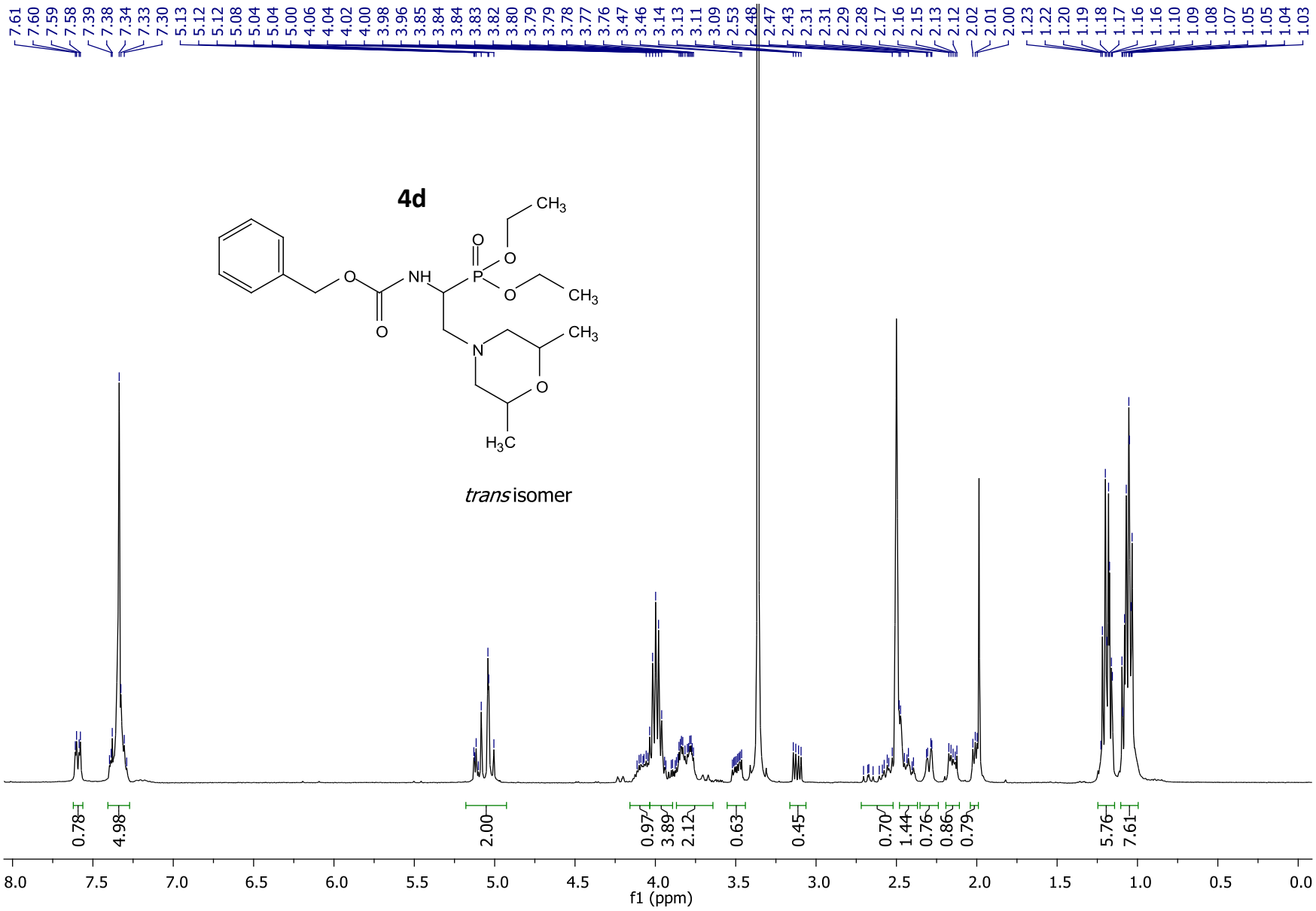

156.16
156.11
137.28
128.32
127.79
127.57
65.40
62.02
61.95
61.74
61.68
57.45
57.36
53.69
46.56
45.01
25.58
23.94
16.34
16.29
4b
CH3
O
O
NH
P
O
CH3
O
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

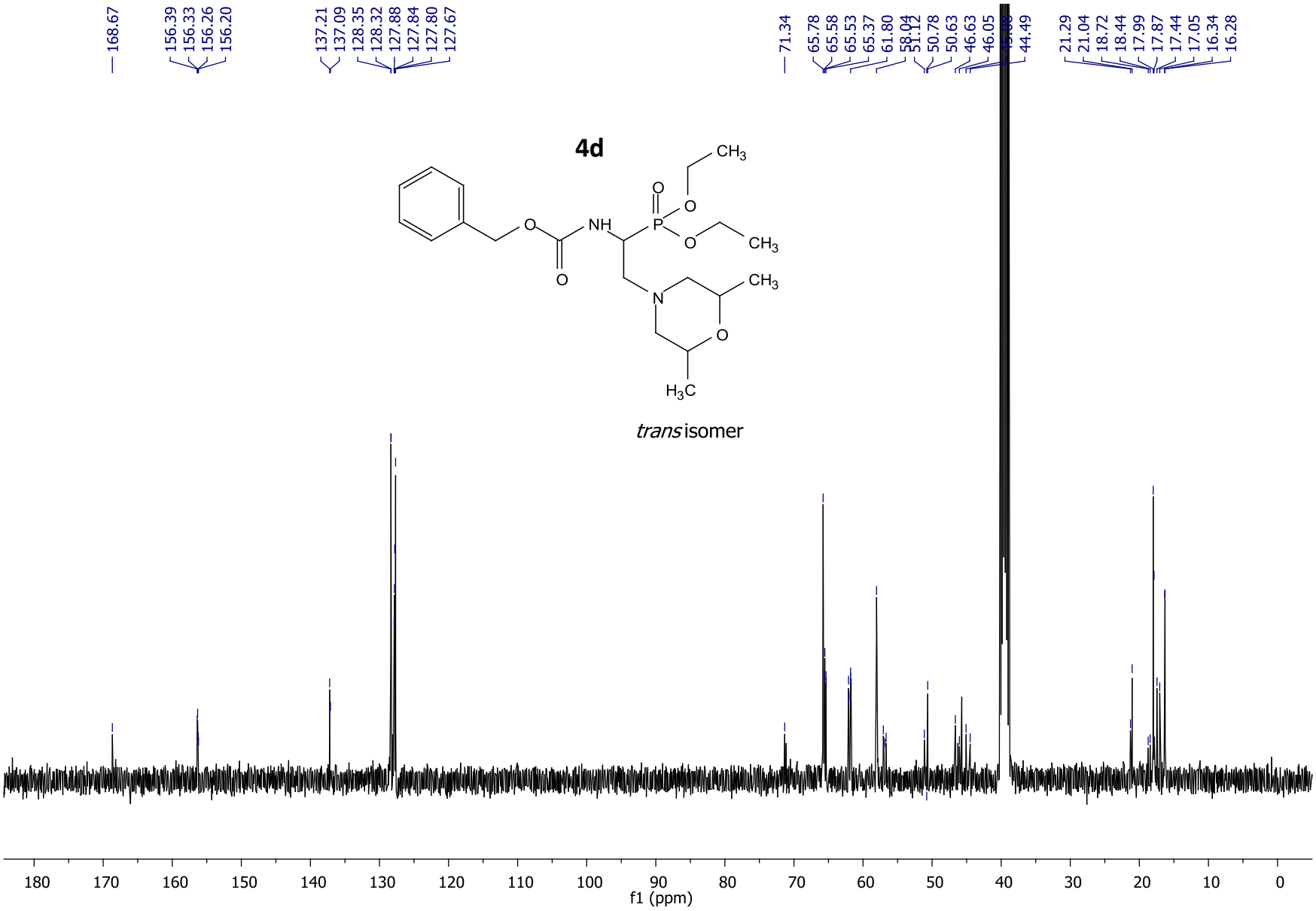

4b
CH3
O
O
NH
P
O
O
CH3
O
O
N
25.53
25.12
25.53
25.12
0.88
0.12
26.0
25.5
25.0
f1 (ppm)
1.00
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.61 7.59 7.38 7.36 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.31 7.31 7.30
5.11 5.08 5.06 5.03 4.10 4.09 4.07 4.06 4.05 4.04 4.03 4.03 4.02 4.01 4.00 3.99 3.98 3.97 3.96 3.96 3.54 3.54 3.52 3.52 3.51 3.50 3.49 3.48 3.46 3.46
2.61 2.59 2.58 2.56 2.55 2.54 2.53 2.52 2.46 2.45 2.45 2.44 2.42 2.42 2.31 2.30 2.29 2.27 2.27 2.26 1.22 1.21 1.20 1.19 1.18 1.16
4c
CH3
O
O
NH
P
O
CH3
O
O
N
O
0.93
5.01
2.00
1.04
4.05
4.06
2.00
2.05
2.01
6.06
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 0.0
f1 (ppm)

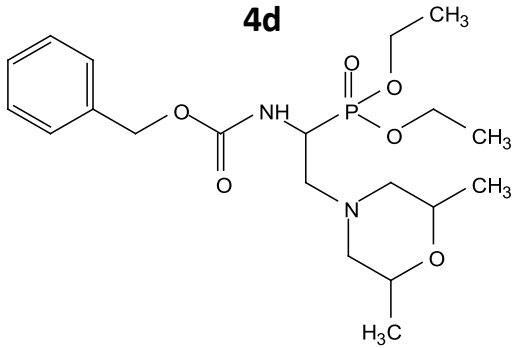

156.13
156.08
137.15
128.25
127.73
127.51
66.11
65.42
62.01
61.95
61.74
61.67
57.04
56.96
52.87
46.31
44.76
16.24
16.19
4c
CH3
O
O
NH
P
O
CH3
O
O
N
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4c
CH3
O
O
NH
P
O
O
CH3
O
O
N
O
25.14
24.77
25.14
24.77
0.92
0.08
25.5
25.0
24.5
f1 (ppm)
1.00
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

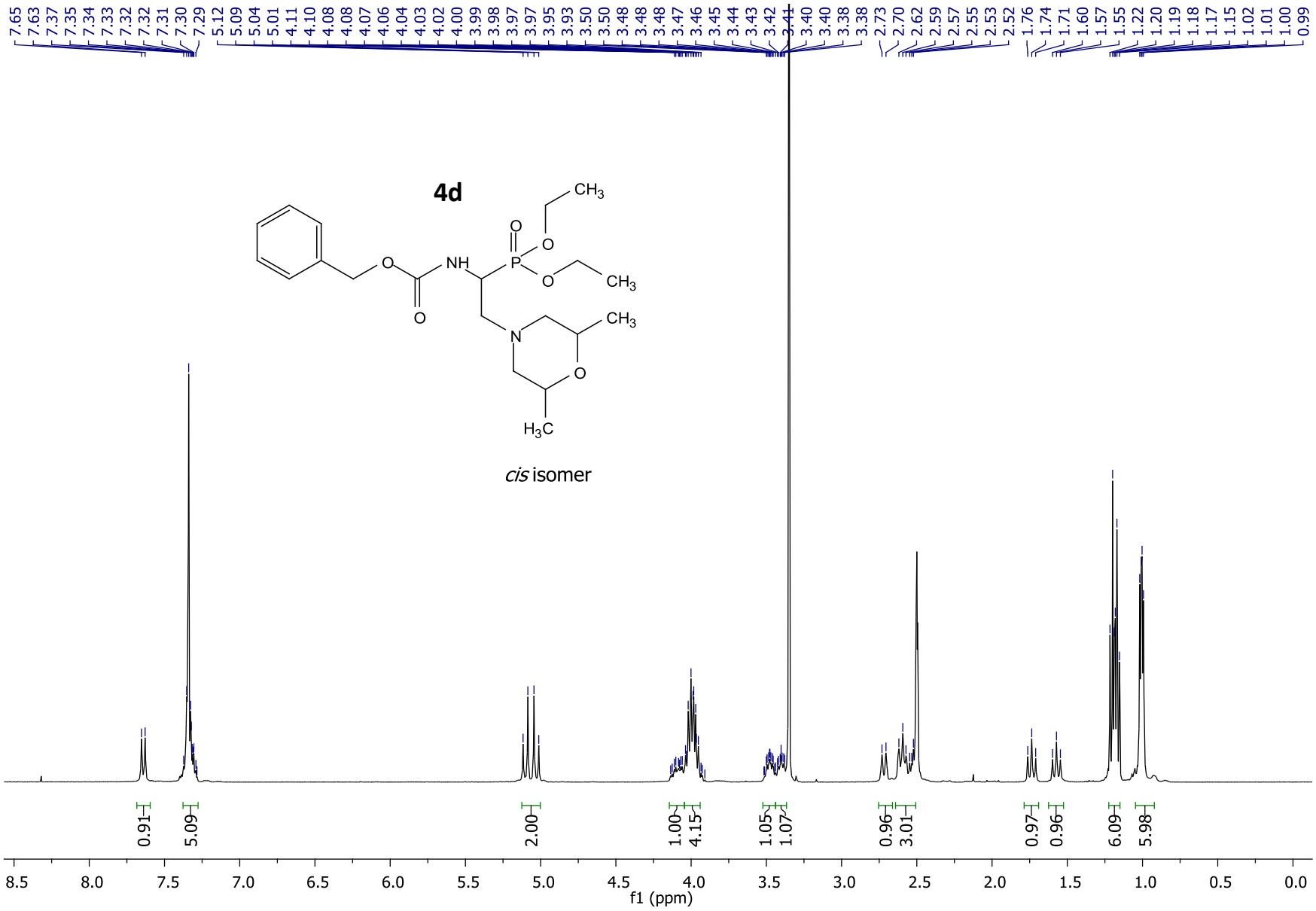

4d
CH3
O
O
NH
P
O
CH3
O
O
CH3
N
O
H3C
trans isomer
7.61 7.60 7.59 7.58 7.39 7.38 7.34 7.33 7.30 5.13 5.12 5.12 5.08 5.04 5.04 5.00 4.06 4.04 4.02 4.00 3.98 3.96 3.85 3.84 3.84 3.83 3.82 3.80 3.79 3.79 3.78 3.77 3.76 3.47 3.46 3.14 3.13 3.11 3.09 2.53 2.48 2.47 2.43 2.31 2.31 2.29 2.28 2.17 2.16 2.15 2.13 2.12 2.02 2.01 2.00 1.23 1.22 1.20 1.19 1.18 1.17 1.16 1.16 1.10 1.09 1.08 1.07 1.05 1.05 1.04 1.03
0.78 4.98 2.00 0.97 3.89 2.12 0.63 0.45 0.70 1.44 0.76 0.86 0.79 5.76 7.61
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 0.0
f1 (ppm)

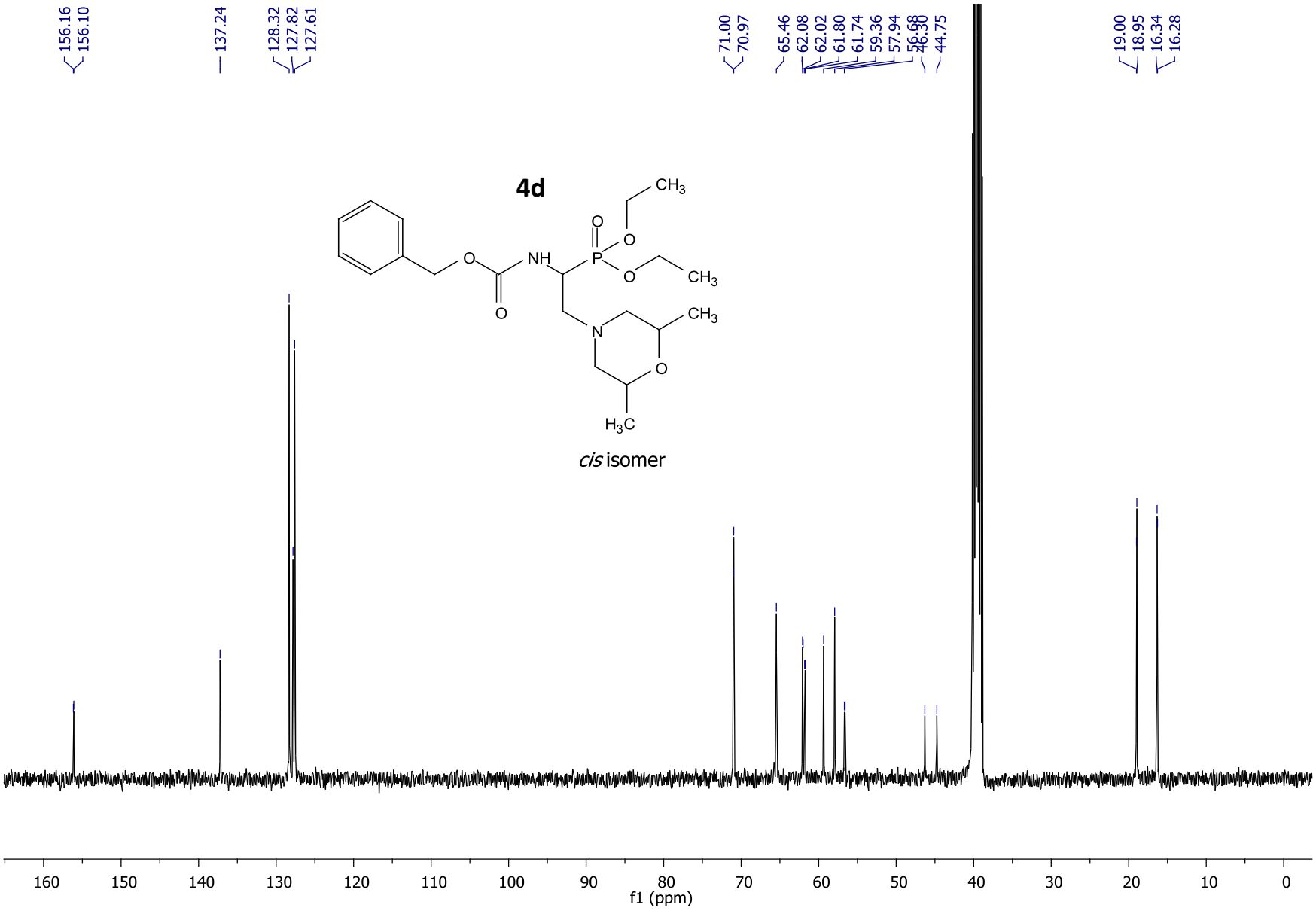

168.67
156.39
156.33
156.26
156.20
137.21
137.09
128.35
128.32
127.88
127.84
127.80
127.67
71.34
65.78
65.58
65.53
65.37
61.80
58.04
51.12
50.78
50.63
46.63
46.05
44.49
21.29
21.04
18.72
18.44
17.99
17.87
17.44
17.05
16.34
16.28
4d
CH3
O
O
NH
P
O
CH3
O
CH3
N
O
H3C
trans isomer
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4d

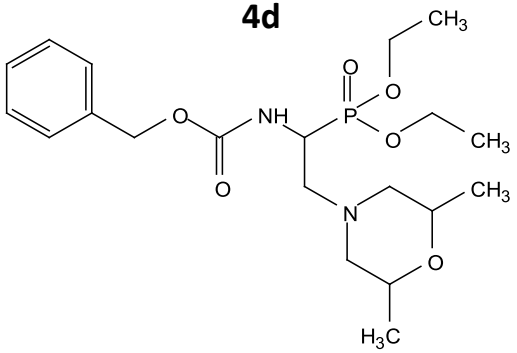


trans isomer

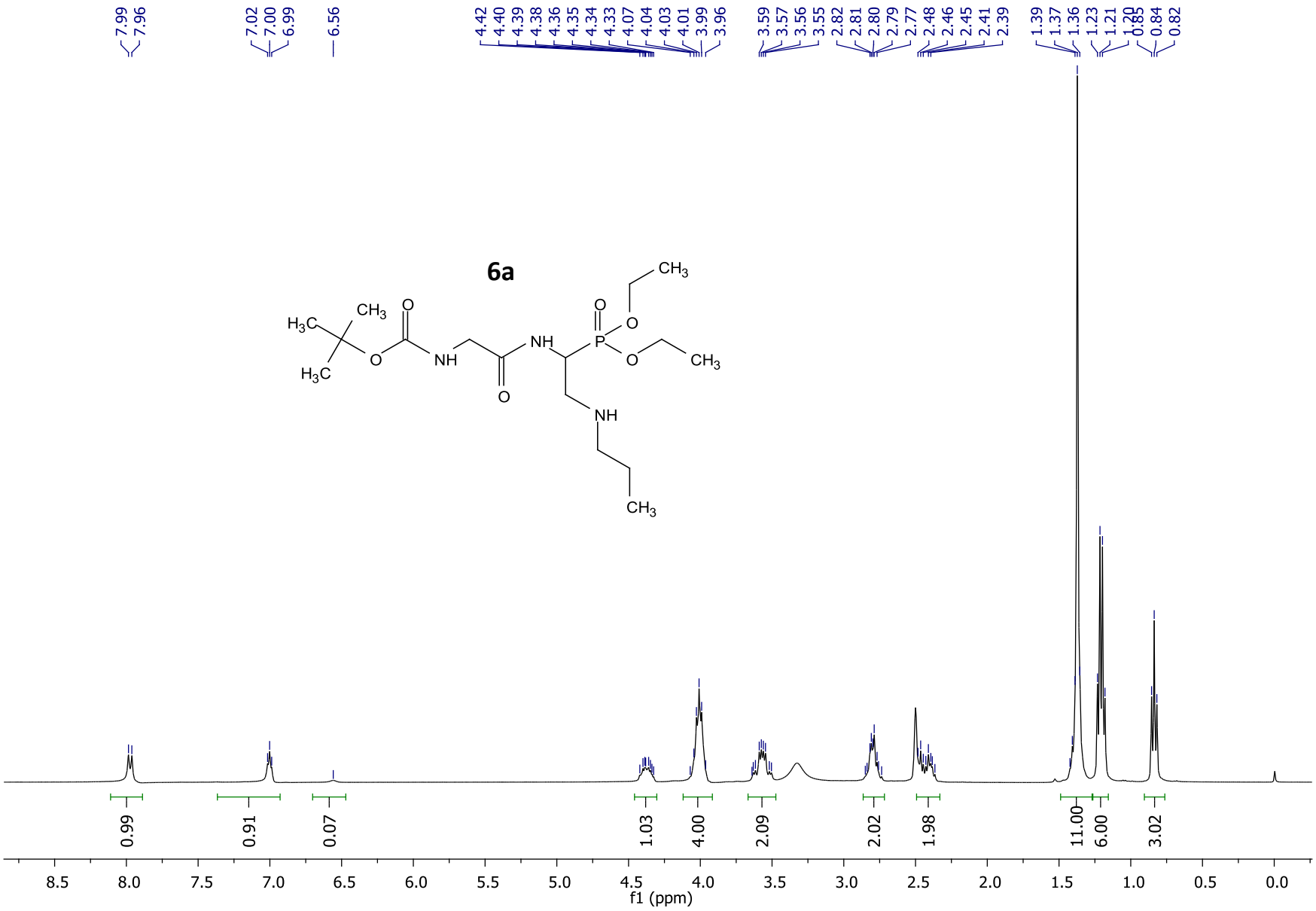

4d
cis isomer
f1 (ppm)

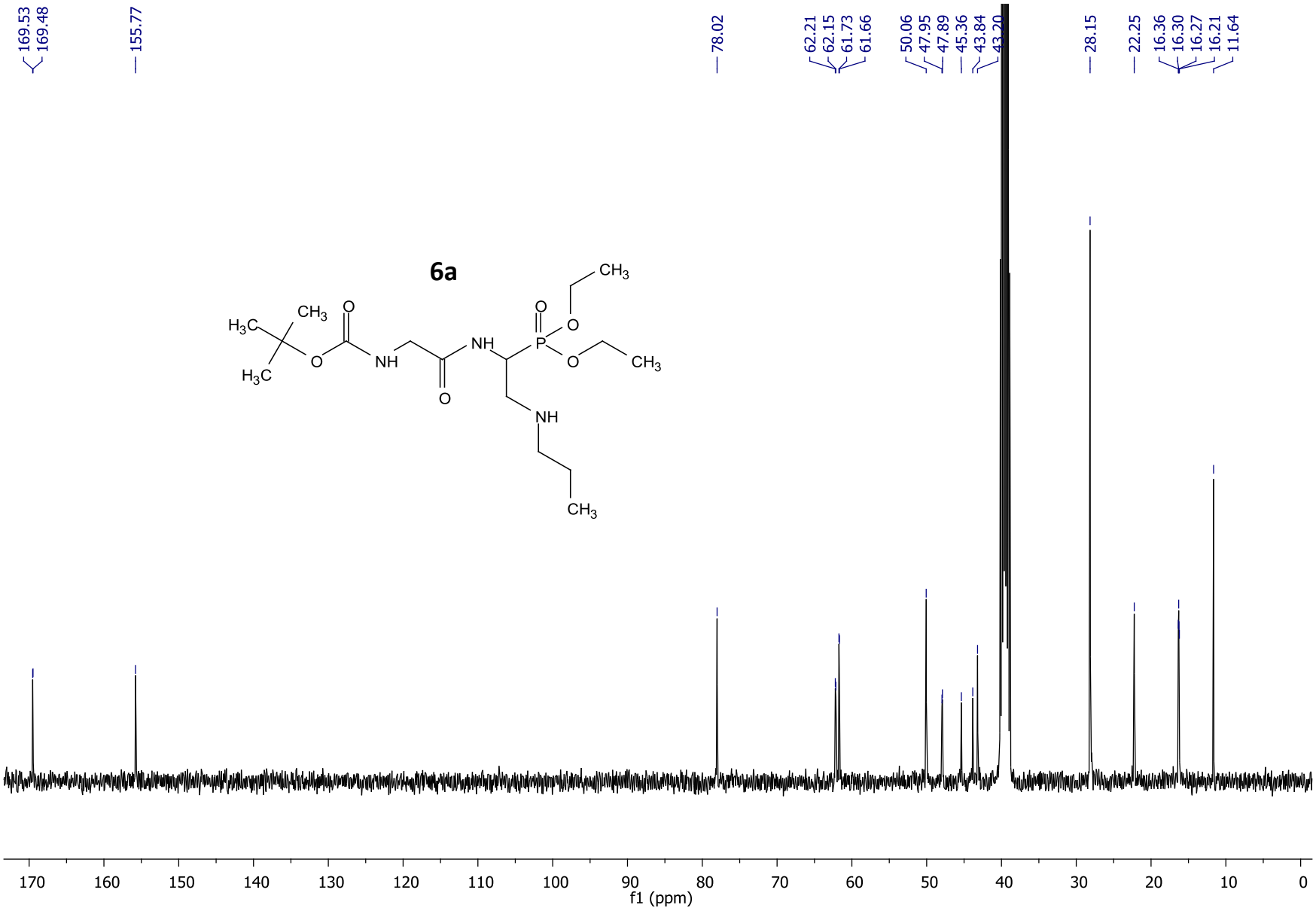

156.16
156.10
137.24
128.32
127.82
127.61
71.00
70.97
65.46
62.08
62.02
61.80
61.74
59.36
57.94
44.75
19.00
18.95
16.34
16.28
4d
CH3
O
O
NH
P
O
CH3
O
CH3
N
O
H3C
cis isomer
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

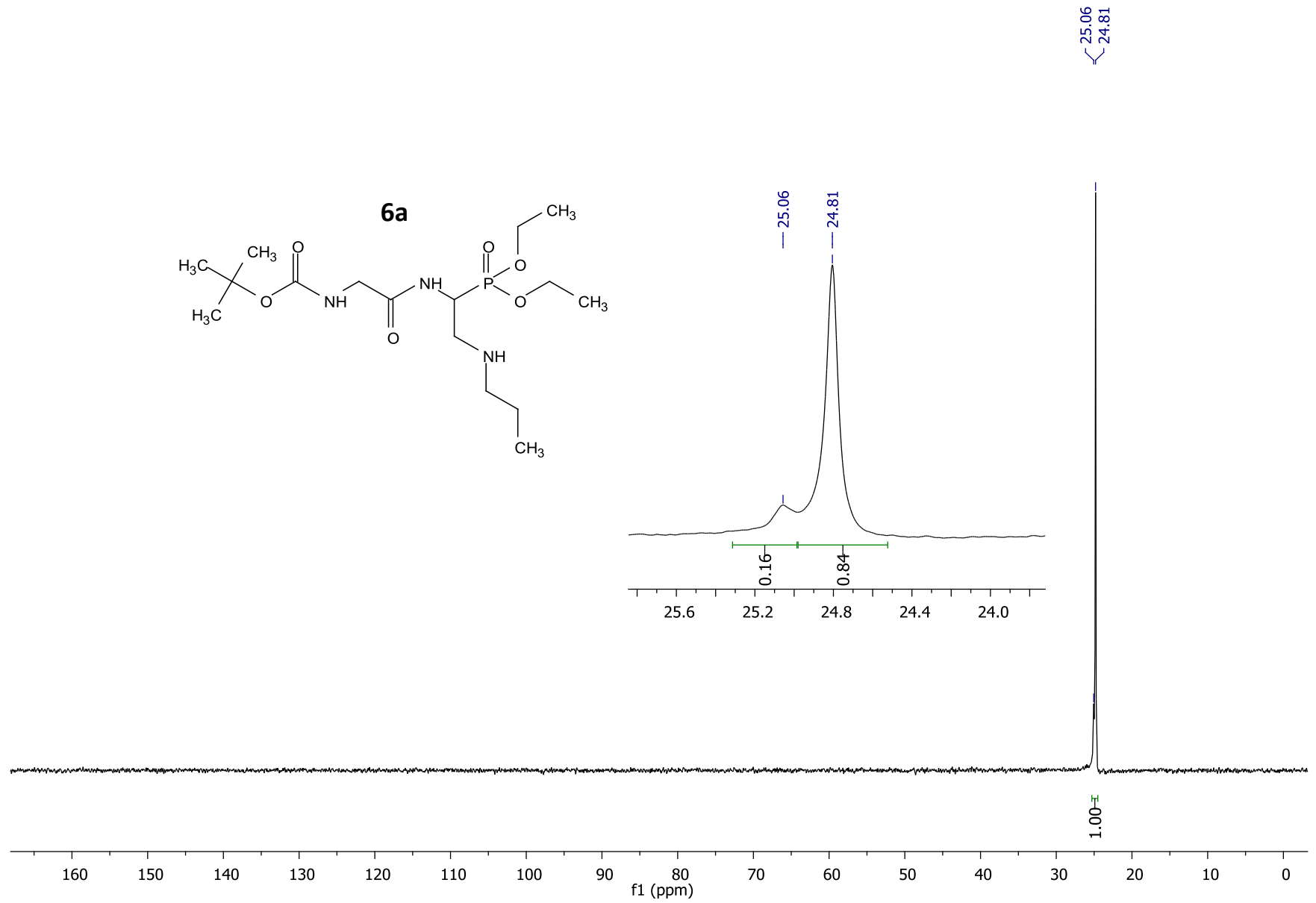
4d

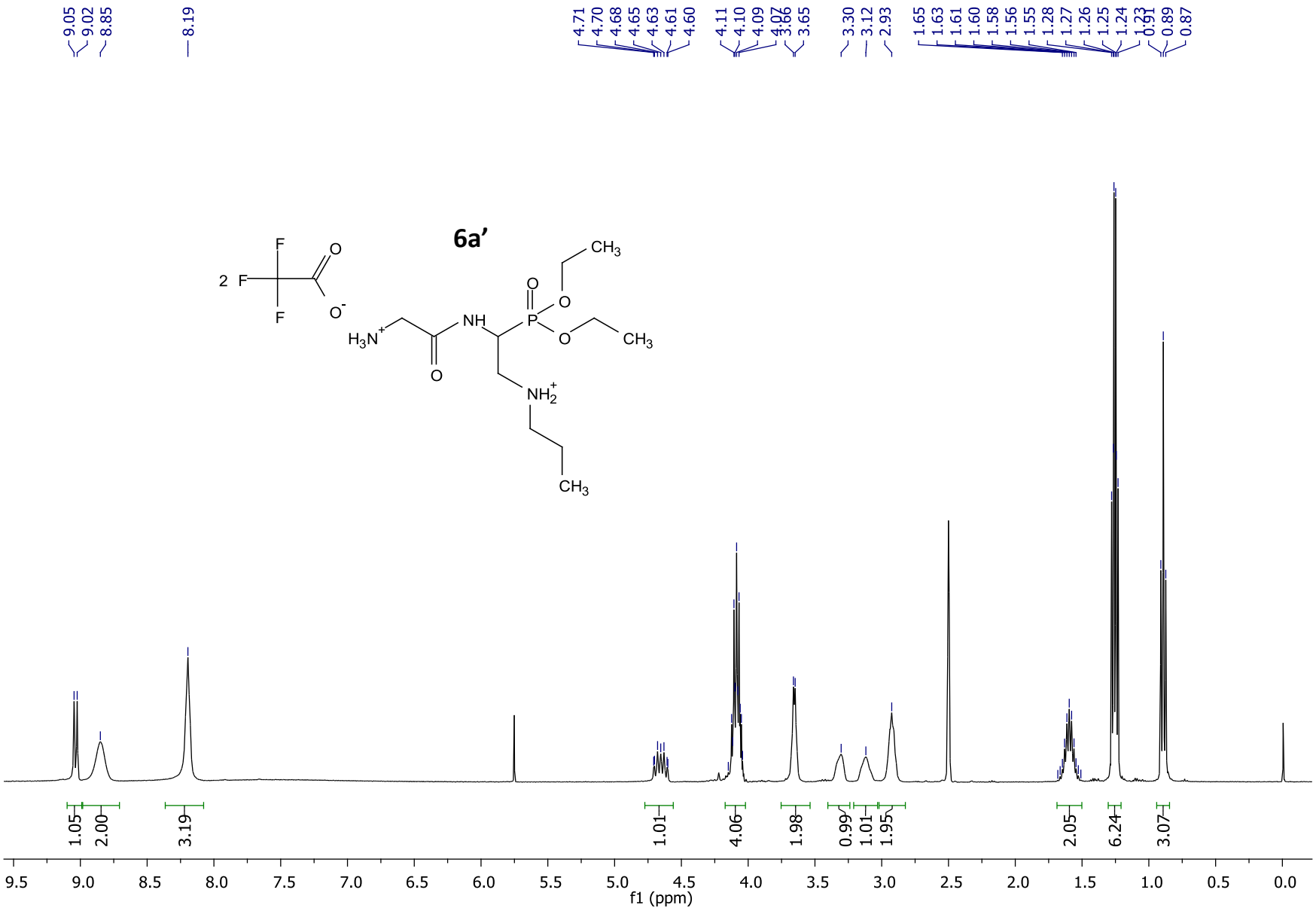


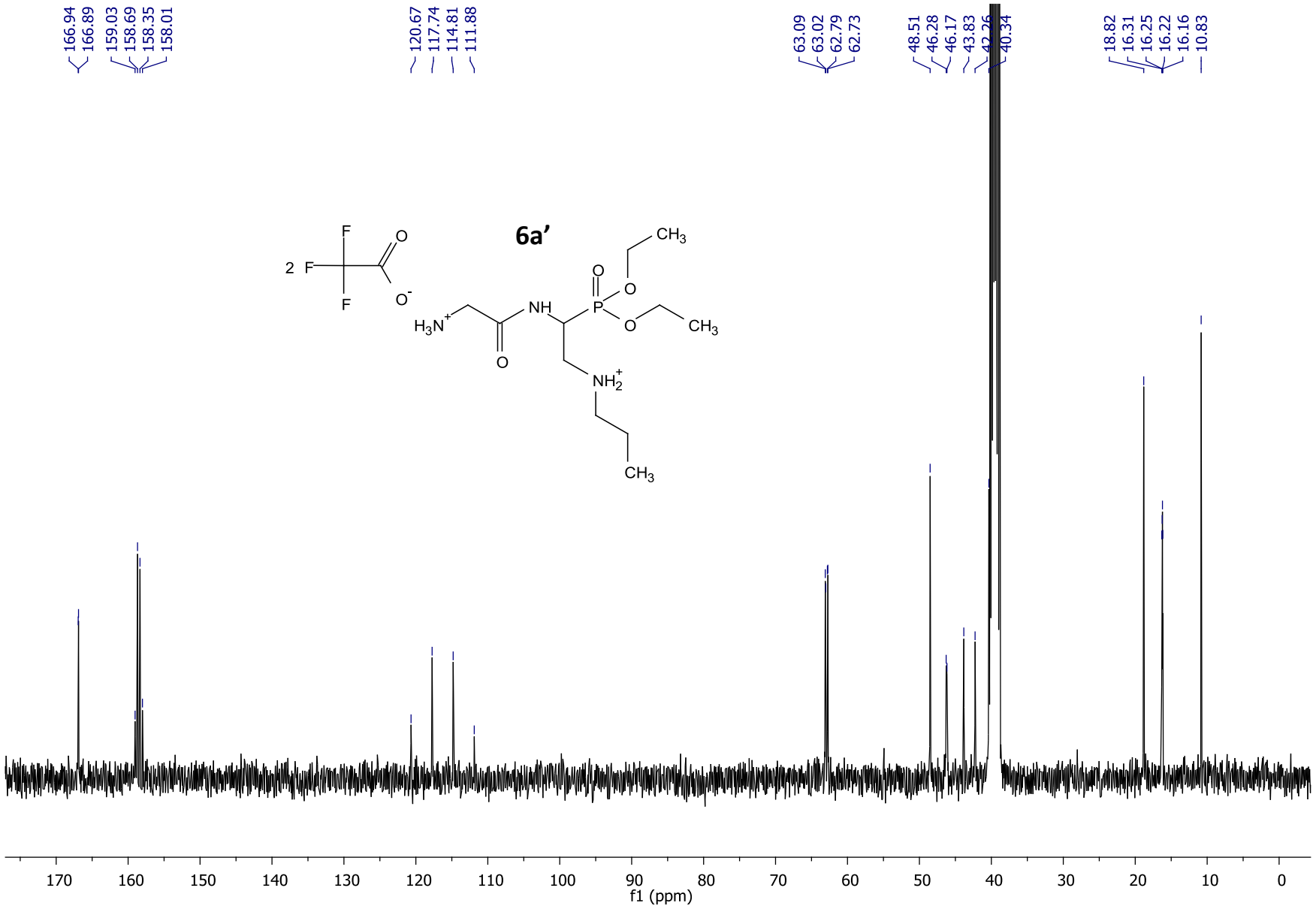
cis isomer

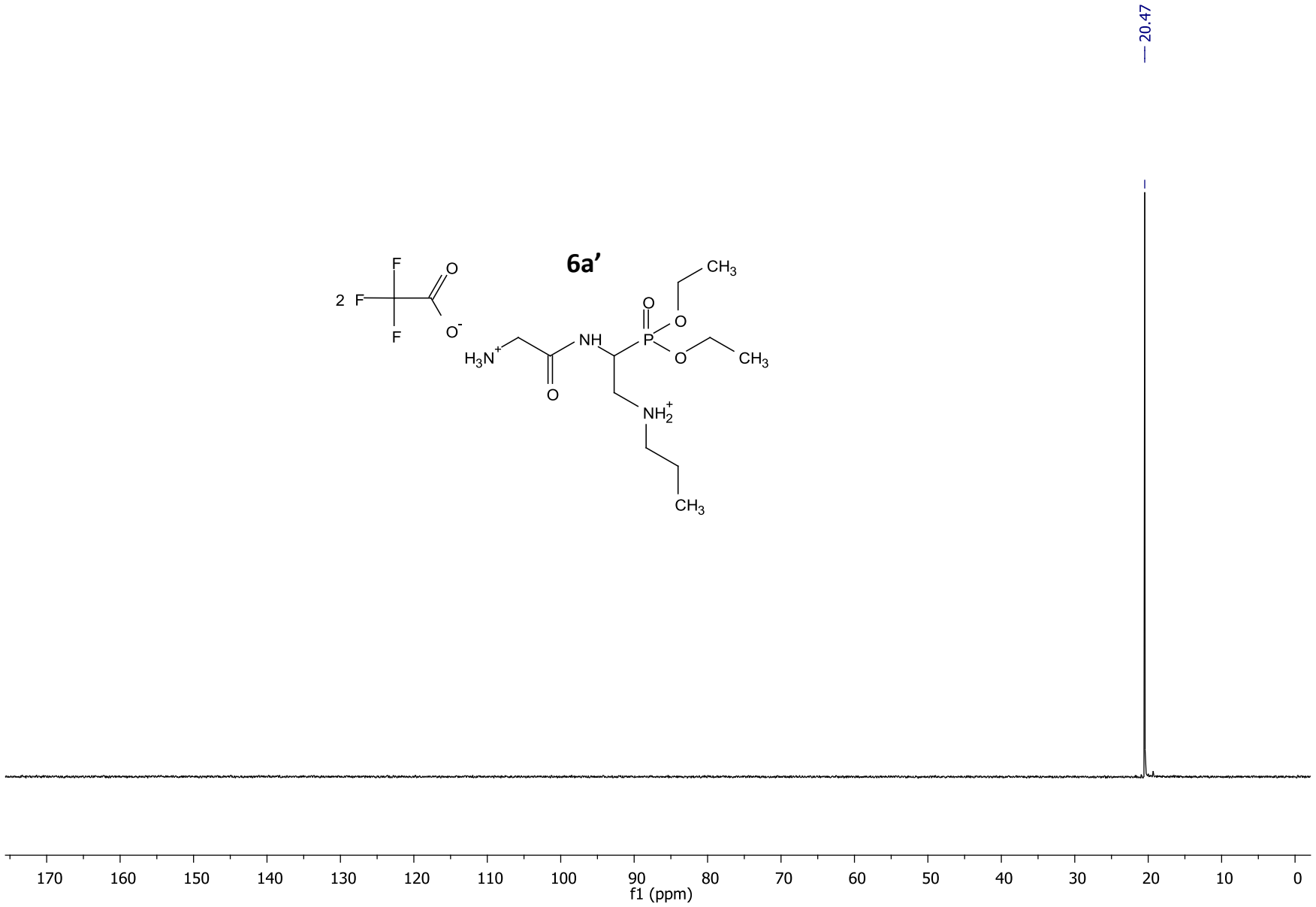

7.99
7.96
7.02
7.00
6.99
6.56
4.42
4.40
4.39
4.38
4.36
4.35
4.34
4.33
4.07
4.04
4.03
4.01
3.99
3.96
3.59
3.57
3.56
3.55
2.82
2.81
2.80
2.79
2.77
2.48
2.46
2.45
2.41
2.39
1.39
1.37
1.36
1.23
1.21
1.20
0.85
0.84
0.82
6a
0.99
0.91
0.07
1.03
4.00
2.09
2.02
1.98
11.00
6.00
3.02
f1 (ppm)

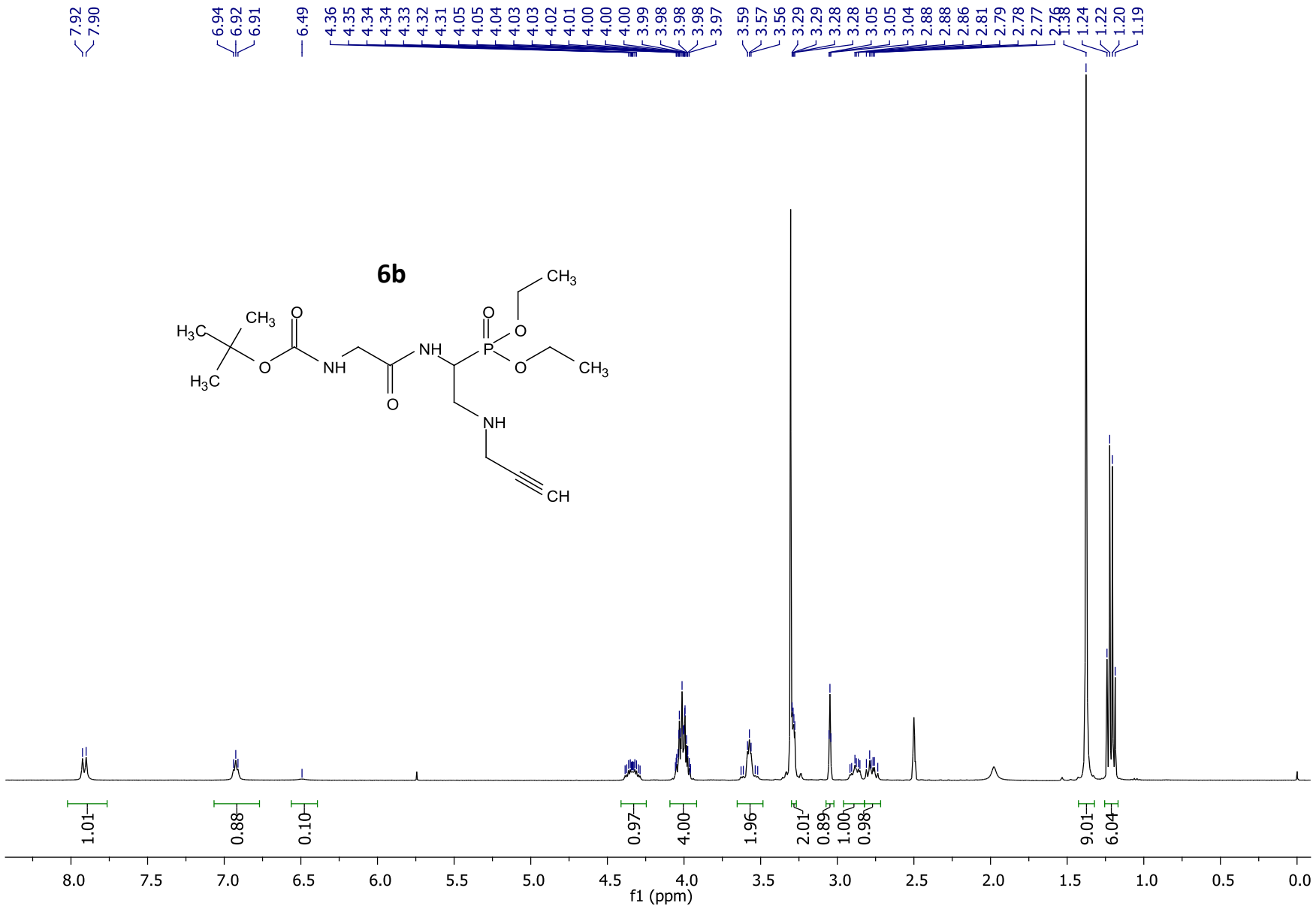

169.53
169.48
155.77
78.02
62.21
62.15
61.73
61.66
50.06
47.95
47.89
45.36
43.84
43.20
28.15
22.25
16.36
16.30
16.27
16.21
11.64
6a
CH3
H3C
CH3
H3C
O
O
NH
O
NH
O
P
O
O
CH3
NH
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

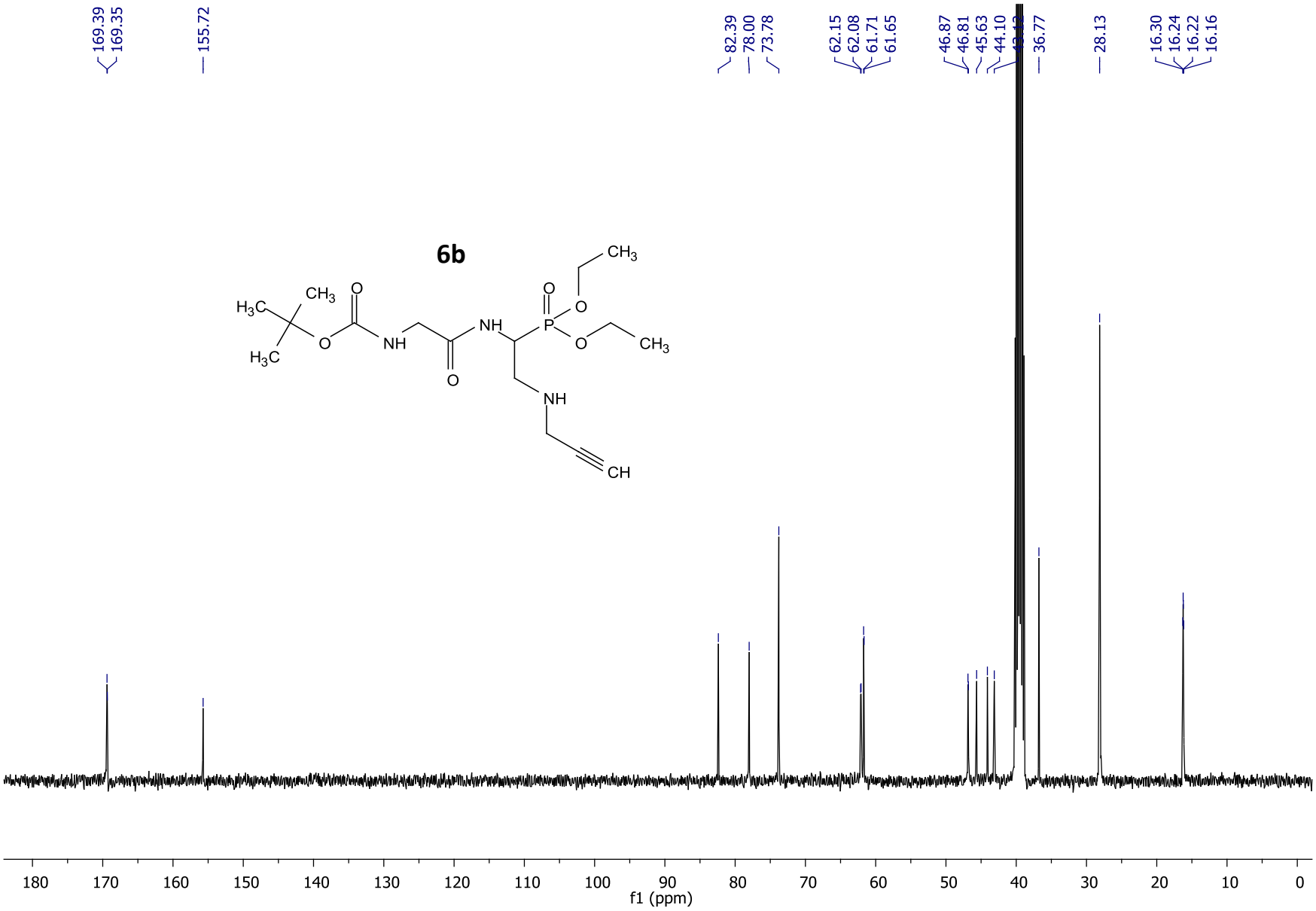

6a
25.06
24.81
0.16
0.84
1.00
f1 (ppm)

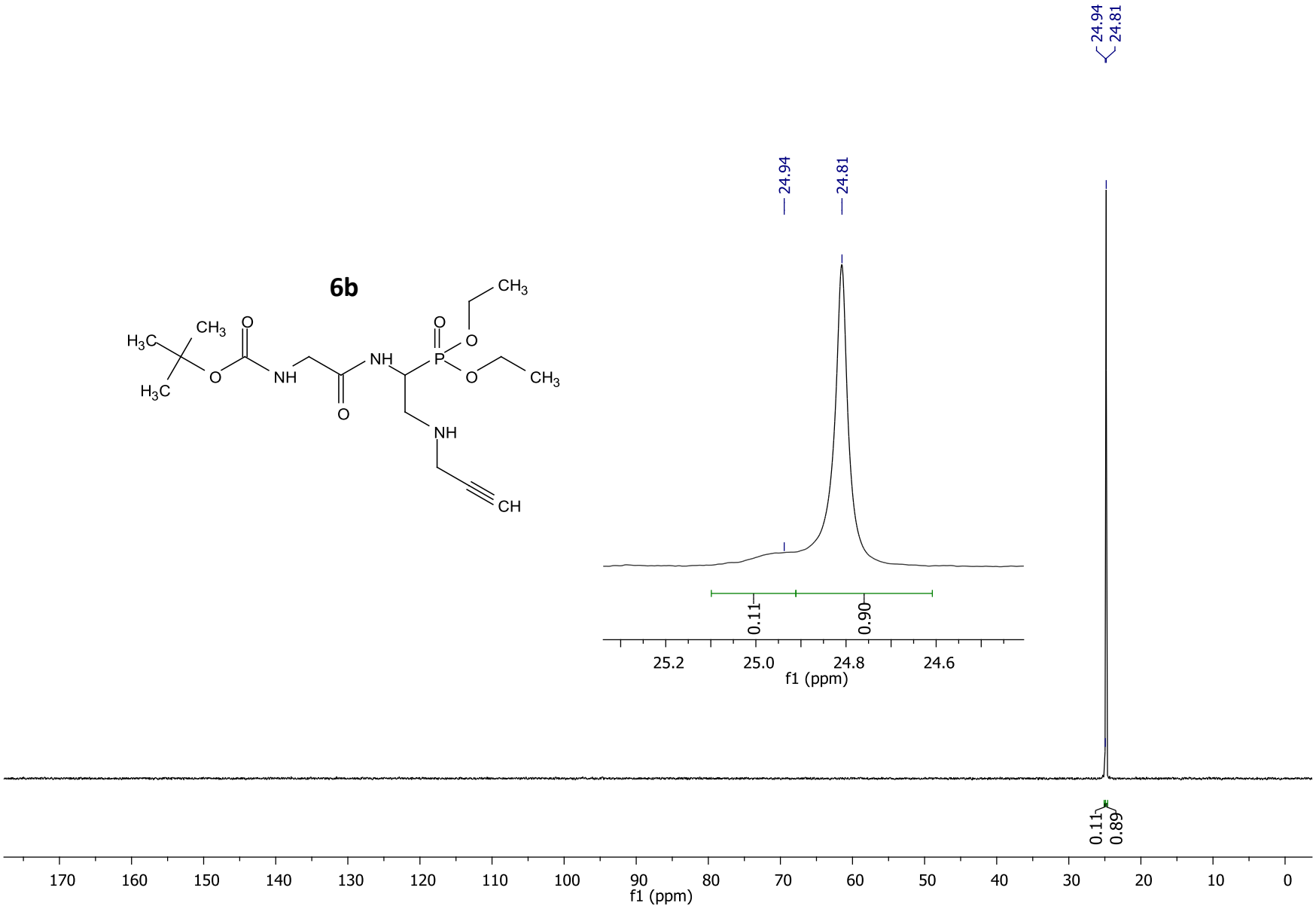

9.05
9.02
8.85
8.19
4.71
4.70
4.68
4.65
4.63
4.61
4.60
4.11
4.10
4.09
3.86
3.65
3.30
3.12
2.93
1.65
1.63
1.61
1.60
1.58
1.56
1.55
1.28
1.27
1.26
1.25
1.24
0.91
0.89
0.87
6a’
2 F
F
F
O
O-
H3N+
NH
O
O
P
O
O
CH3
CH3
NH2+
CH3
1.05
2.00
3.19
1.01
4.06
1.98
0.99
1.01
1.95
2.05
6.24
3.07
9.5
9.0
8.5
8.0
7.5
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
0.5
0.0
f1 (ppm)

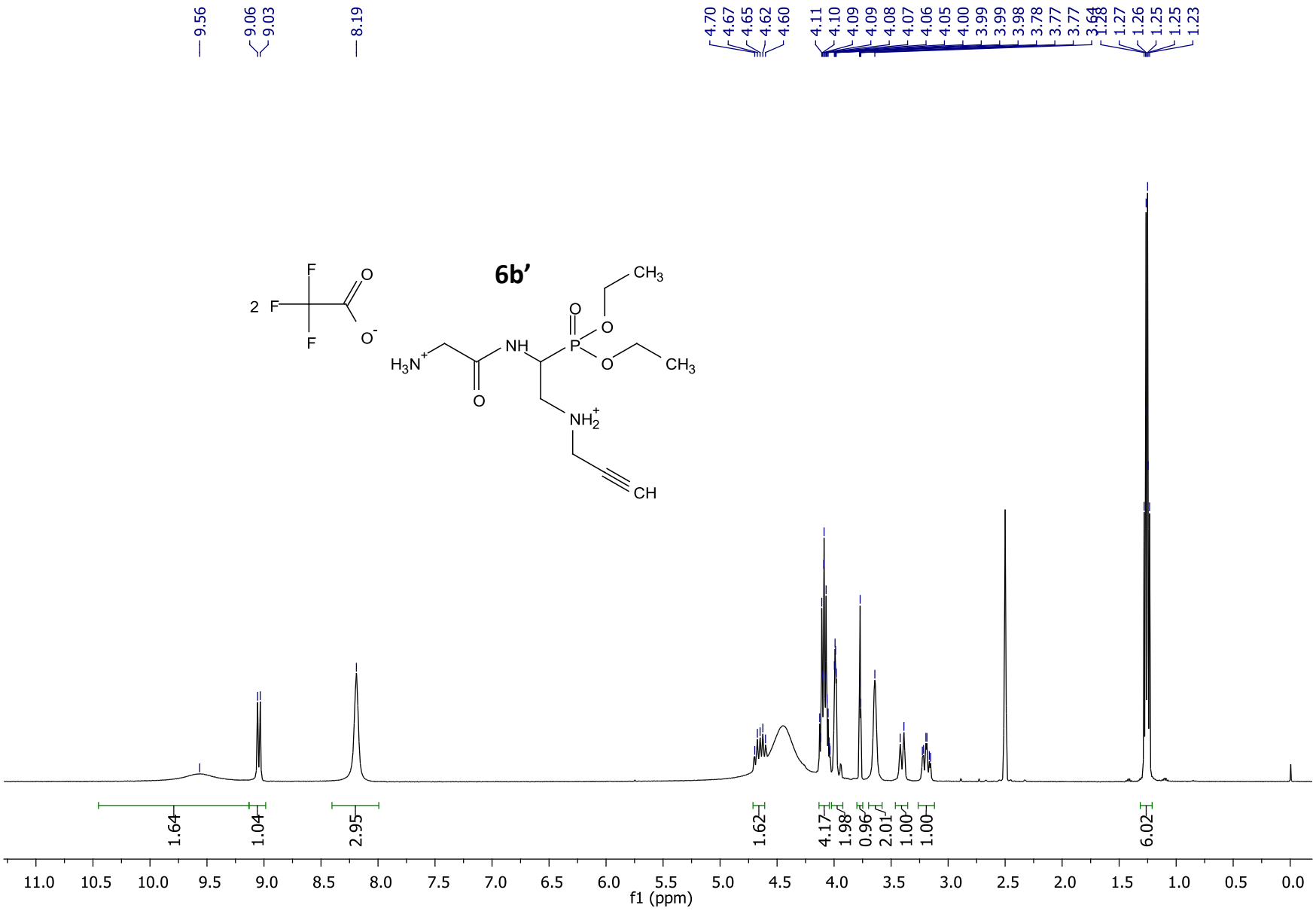

166.94
166.89
159.03
158.69
158.35
158.01
120.67
117.74
114.81
111.88
63.09
63.02
62.79
62.73
48.51
46.28
46.17
43.83
42.26
40.34
18.82
16.31
16.25
16.22
16.16
10.83
6a’
2 F
F
F
O
O-
H3N+
NH
O
P
O
O
O
CH3
CH3
NH2+
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

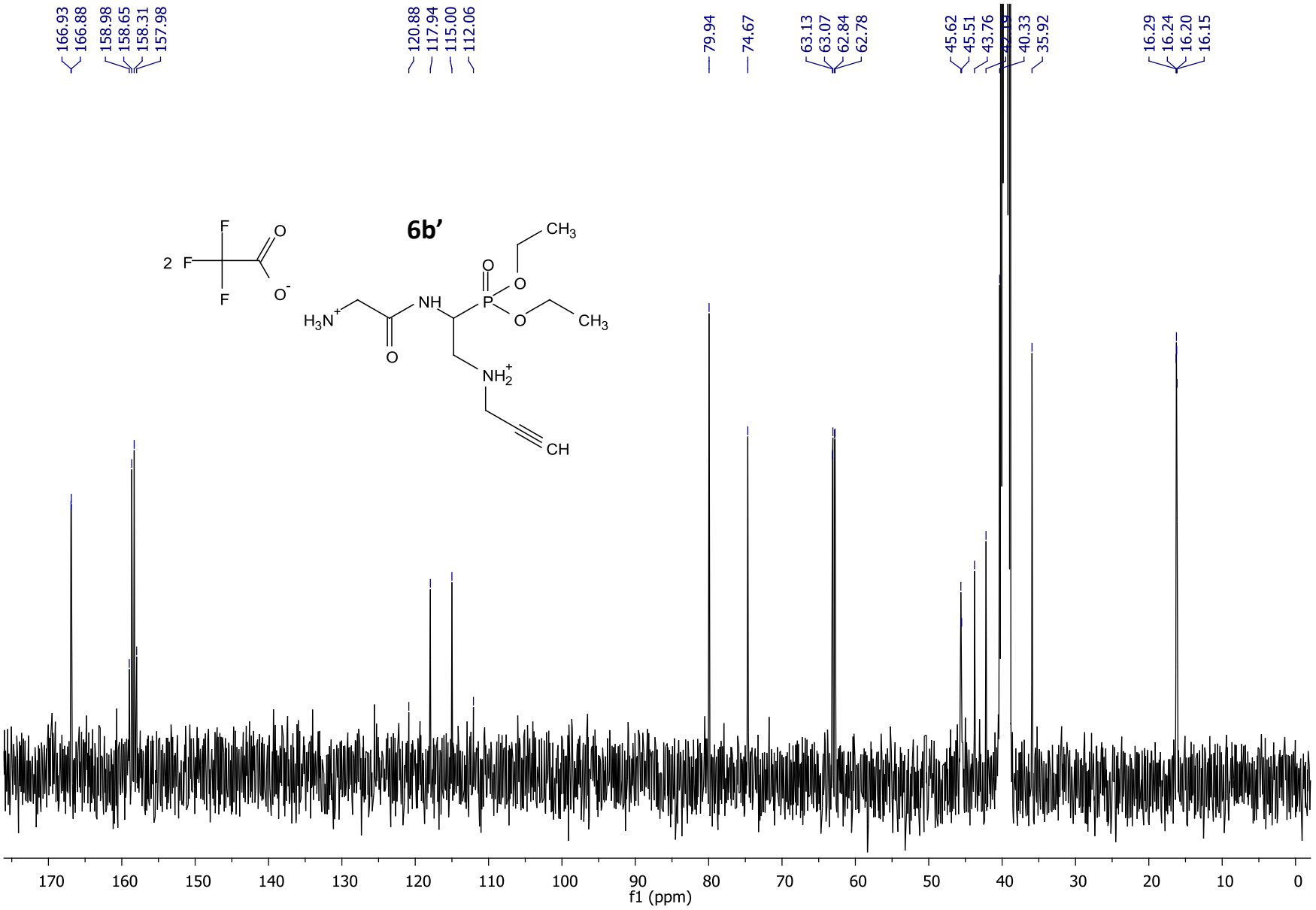

20.47
6a’
2 F
F
F
O
O-
H3N+
NH
O
P
O
O
O
CH3
CH3
NH2+
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.92
7.90
6.94
6.92
6.91
6.49
4.36
4.35
4.34
4.34
4.33
4.32
4.31
4.05
4.05
4.04
4.03
4.03
4.02
4.01
4.00
4.00
4.00
3.99
3.98
3.98
3.98
3.97
3.59
3.57
3.56
3.29
3.29
3.28
3.28
3.05
3.05
3.04
2.88
2.88
2.86
2.81
2.79
2.78
2.77
2.76
1.38
1.24
1.22
1.20
1.19
6b
1.01
0.88
0.10
0.97
4.00
1.96
2.01
0.89
1.00
0.98
9.01
6.04
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
0.0
f1 (ppm)


169.39
169.35
155.72
82.39
78.00
73.78
62.15
62.08
61.71
61.65
46.87
46.81
45.63
44.10
36.77
28.13
16.30
16.24
16.22
16.16
6b
CH3
O
O
H3C
CH3
O
NH
NH
P
O
CH3
H3C
O
O
NH
CH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6b
24.94
24.81
0.11
0.90
25.2
25.0
24.8
24.6
f1 (ppm)
0.11
0.89
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.56
9.06
9.03
8.19
4.70
4.67
4.65
4.62
4.60
4.11
4.10
4.09
4.09
4.08
4.07
4.06
4.05
4.00
3.99
3.99
3.98
3.78
3.77
3.77
3.64
1.28
1.27
1.26
1.25
1.25
1.23
6b’
2
F
F
F
O
O-
H3N+
NH
O
O
P
O
O
CH3
CH3
NH2+
CH
1.64
1.04
2.95
1.62
4.17
1.98
0.96
2.01
1.00
1.00
6.02
11.0
10.5
10.0
9.5
9.0
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
0.5
0.0
f1 (ppm)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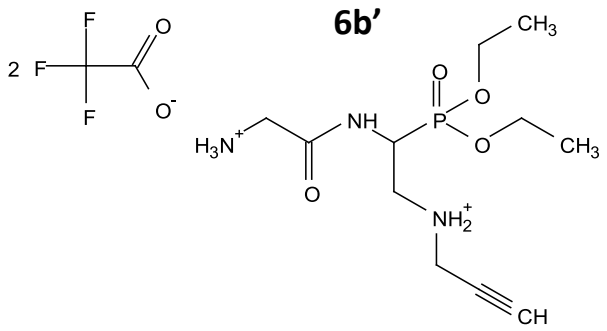
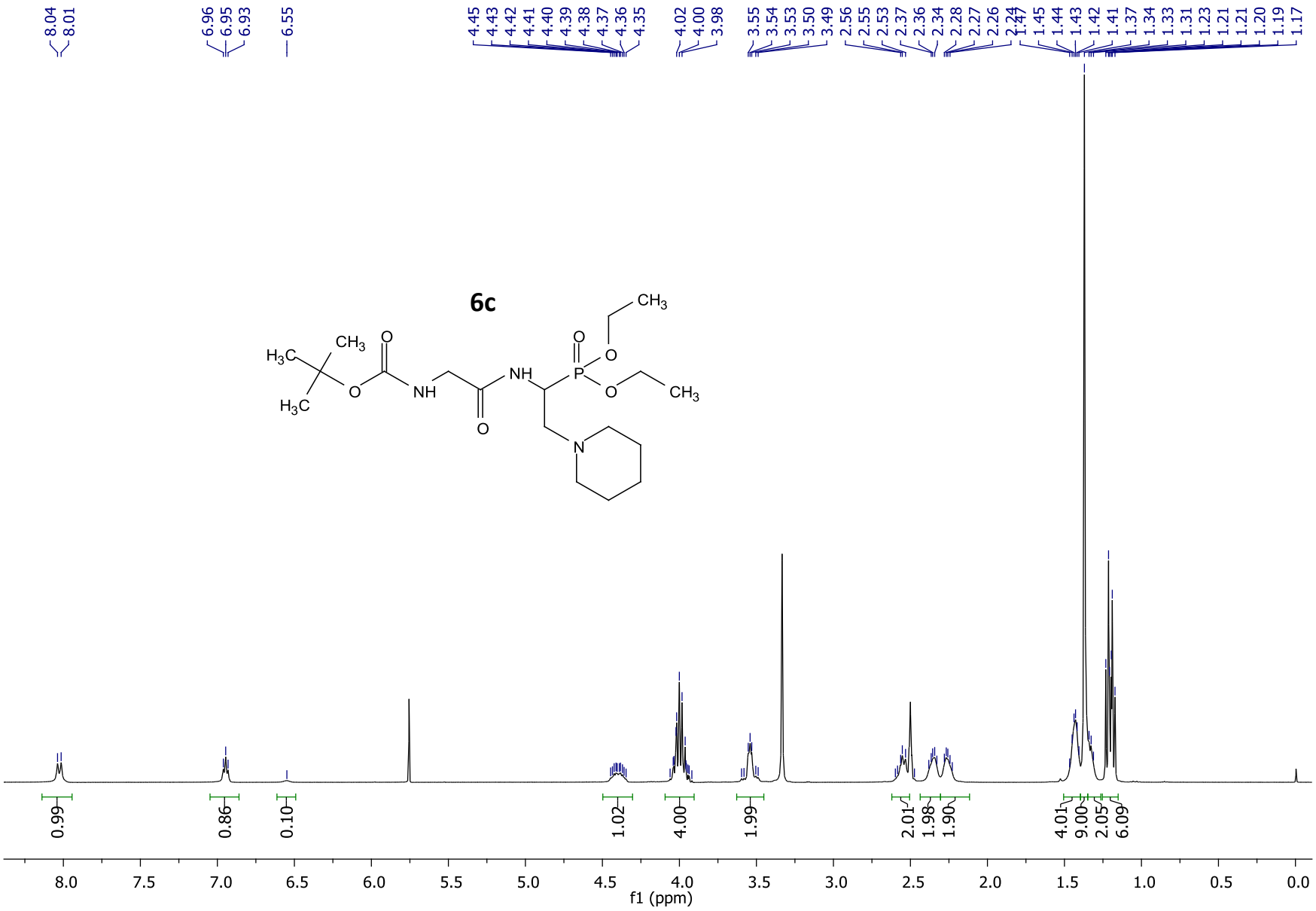
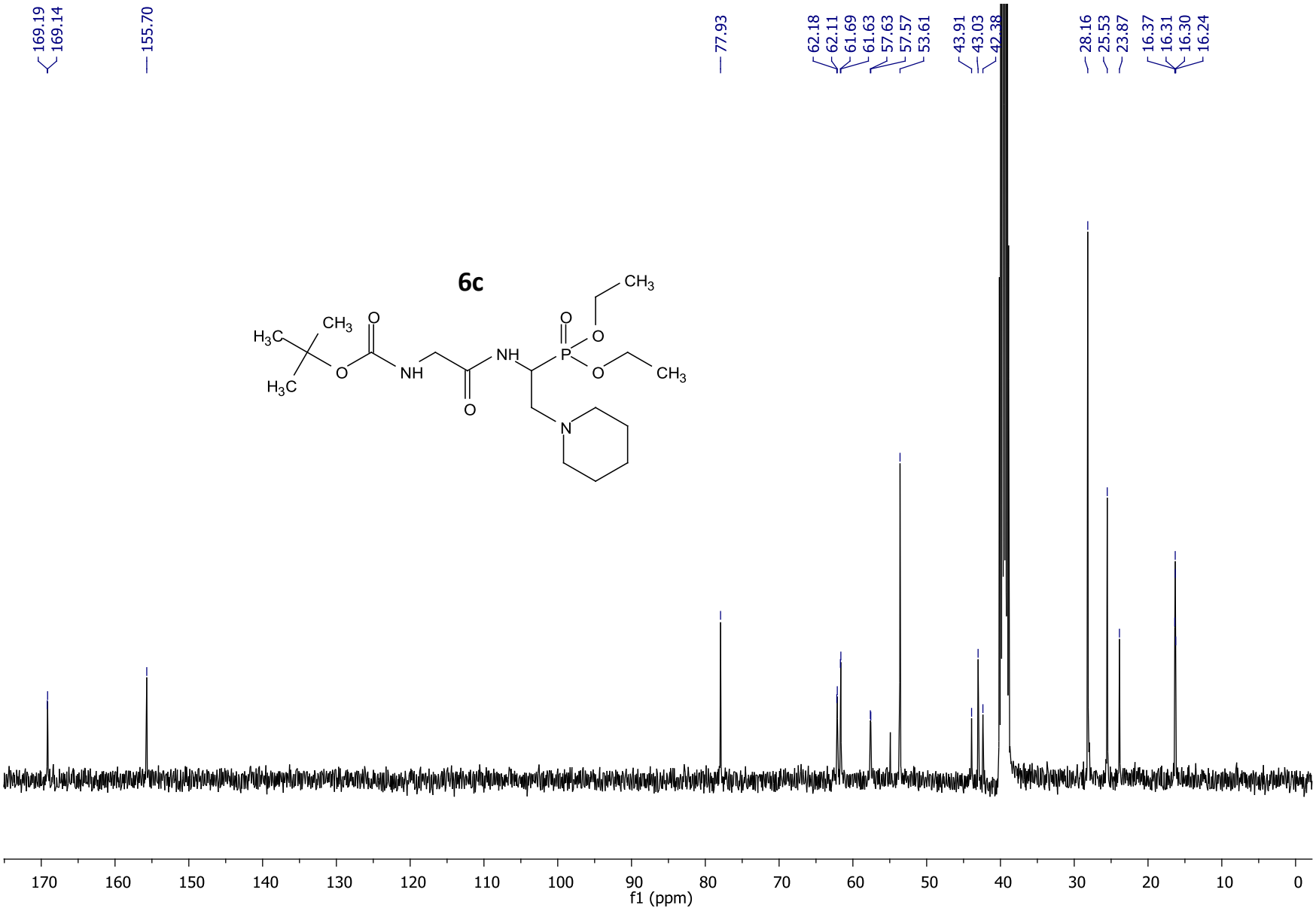
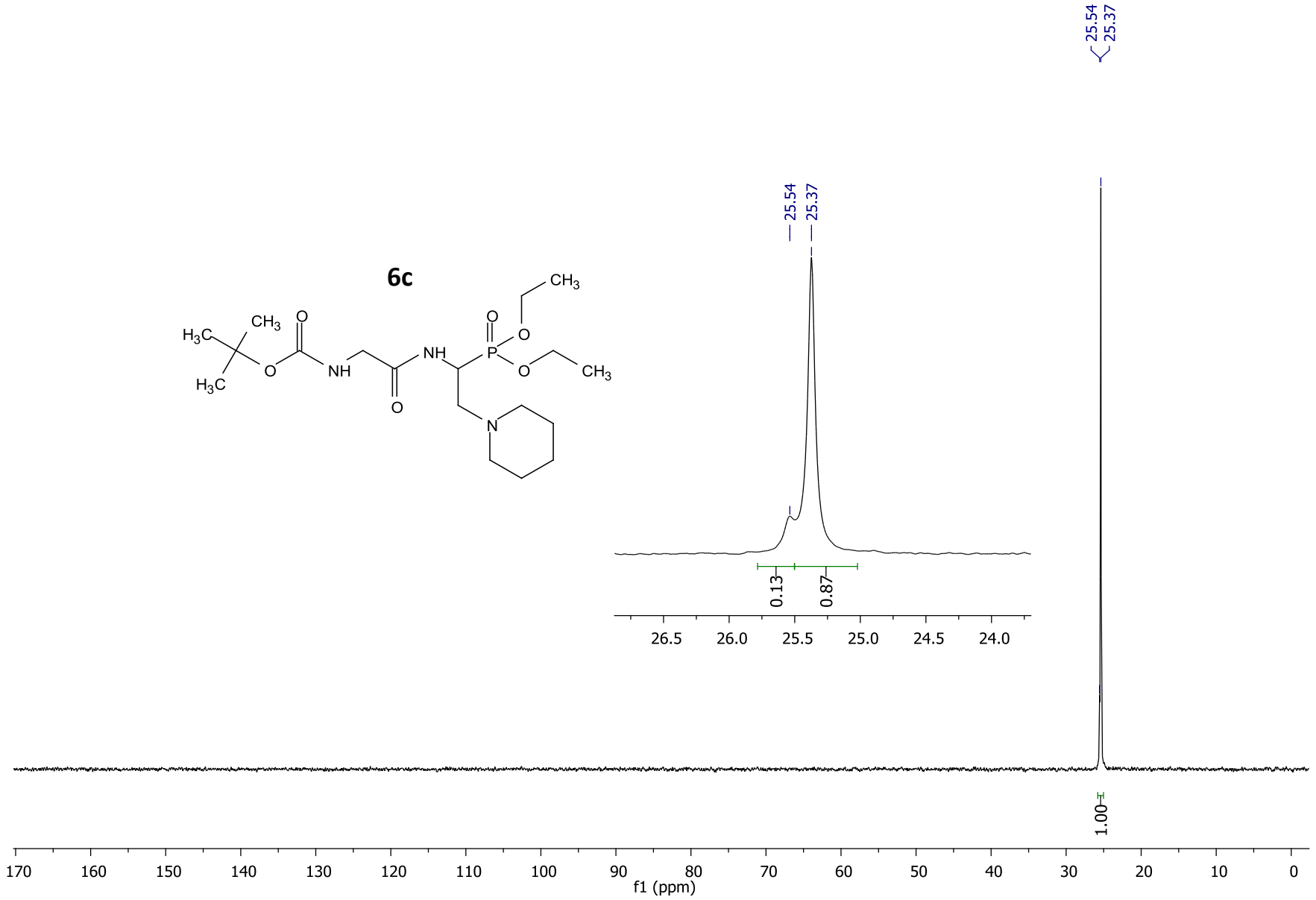
166.88
158.98
158.65
158.31
157.98
120.88
117.94
115.00
112.06
79.94
74.67
63.13
63.07
62.84
62.78
45.62
45.51
43.76
40.33
35.92
16.29
16.24
16.20
16.15
6b'
2 F
F
F
O
O-
H3N+
NH
P
O
O
O
CH3
CH3
NH2+
CH
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

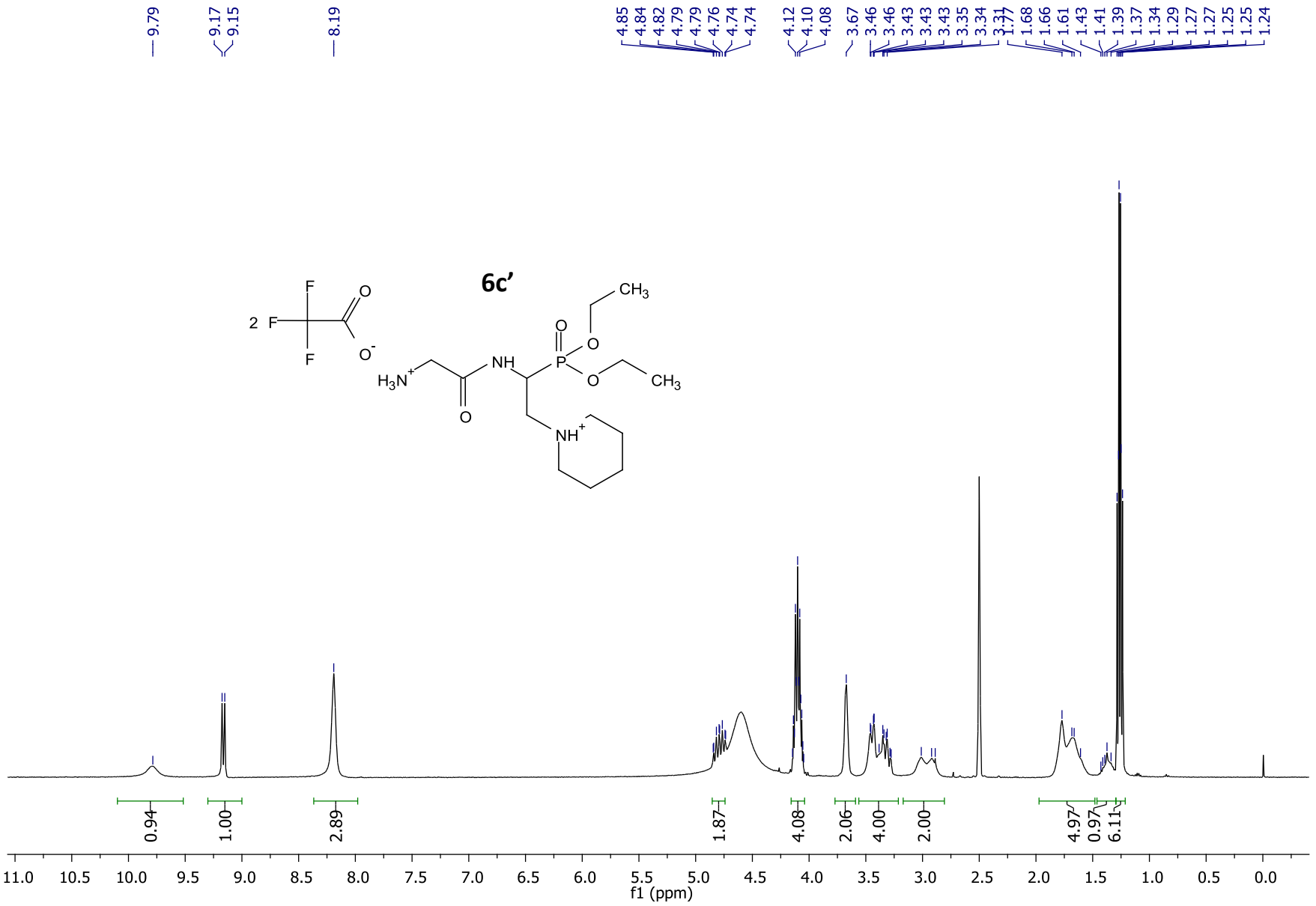

6b’
2
F
F
F
O
O-
H3N+
NH
O
P
O
O
CH3
CH3
NH2+
CH

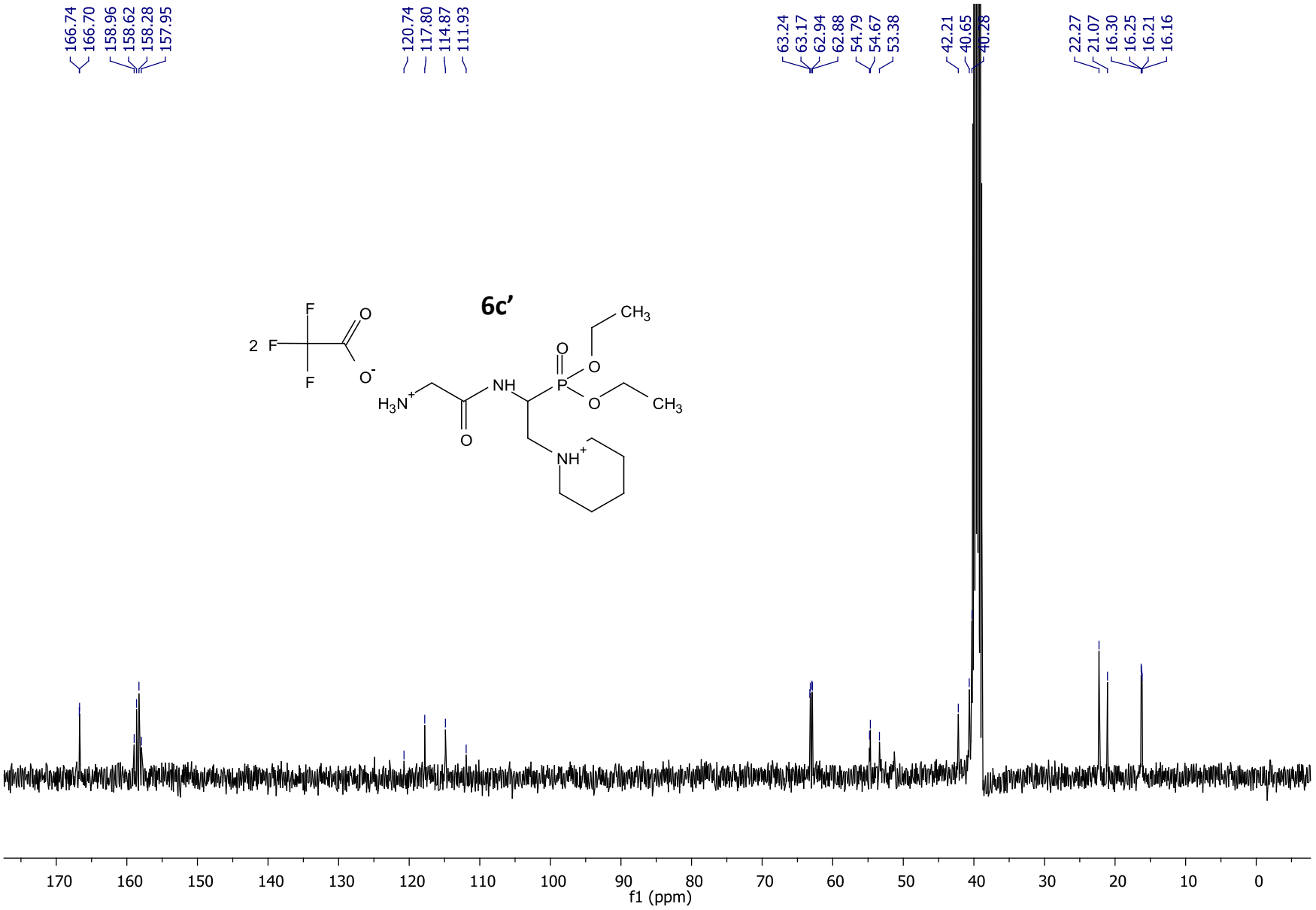
20.28
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.04
8.01
6.96
6.95
6.93
6.55
4.45
4.43
4.42
4.41
4.40
4.39
4.38
4.37
4.36
4.35
4.02
4.00
3.98
3.55
3.54
3.53
3.50
3.49
2.56
2.55
2.53
2.37
2.36
2.34
2.28
2.27
2.26
2.24
1.47
1.45
1.44
1.43
1.42
1.41
1.37
1.34
1.33
1.31
1.23
1.21
1.21
1.20
1.19
1.17
6c
CH3
H3C
CH3
O
O
NH
NH
P
O
O
O
CH3
H3C
O
O
N
0.99
0.86
0.10
1.02
4.00
1.99
2.01
1.98
1.90
4.01
9.00
2.05
6.09
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
0.0
f1 (ppm)

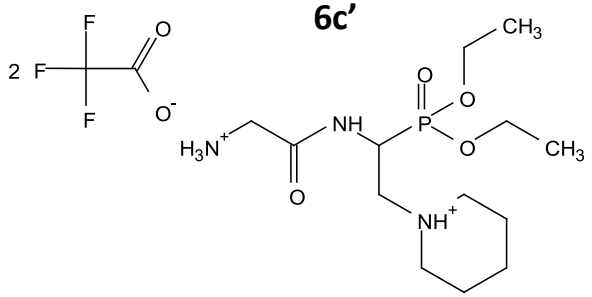

169.19
169.14
155.70
77.93
62.18
62.11
61.69
61.63
57.63
57.57
53.61
43.91
43.03
42.38
28.16
25.53
23.87
16.37
16.31
16.30
16.24
6c
CH3
H3C
CH3
O
O
NH
NH
P
O
O
O
CH3
H3C
O
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6c
25.54
25.37
0.13
0.87
1.00
26.5
26.0
25.5
25.0
24.5
24.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

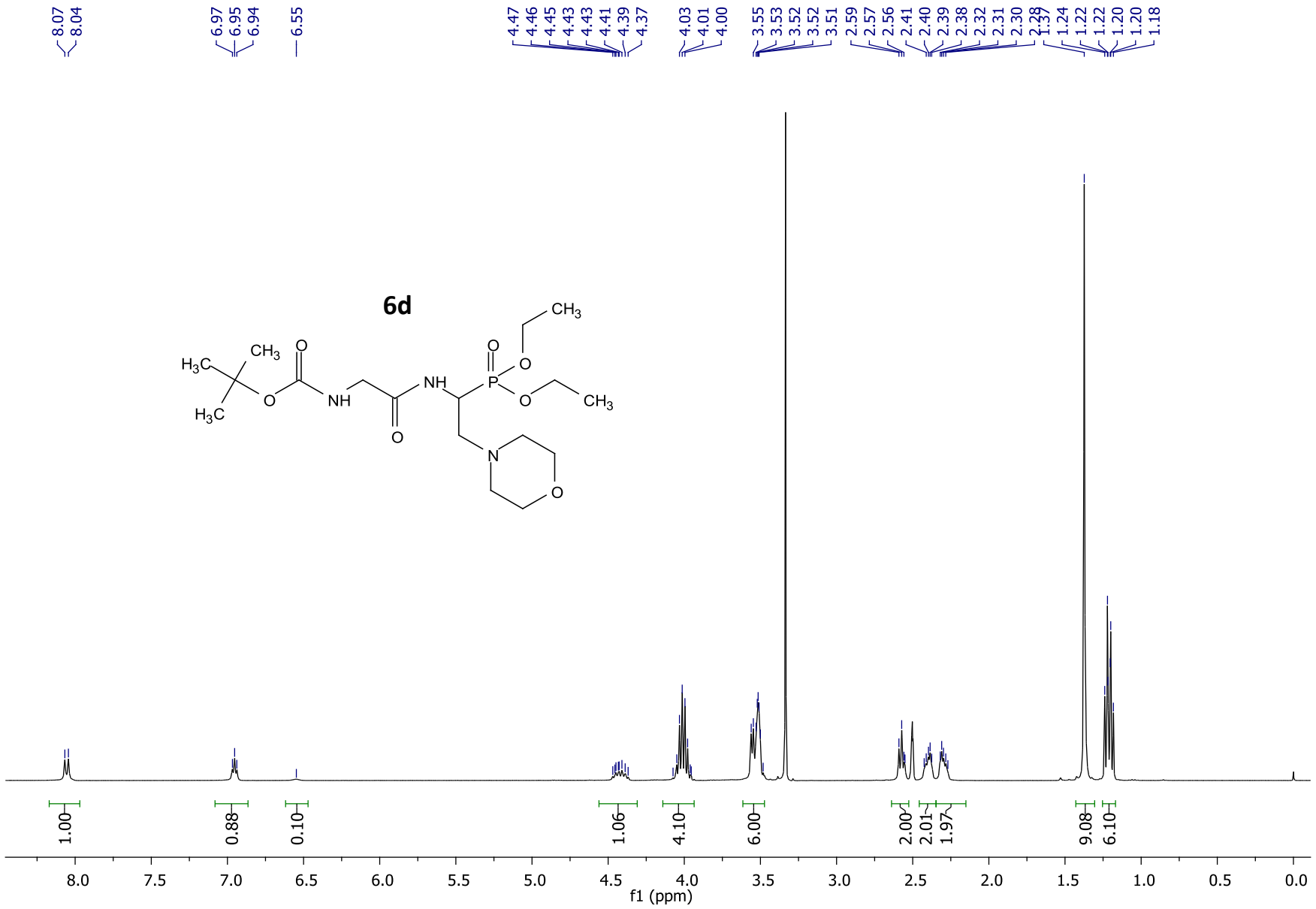

9.79
9.17
9.15
8.19
4.85
4.84
4.82
4.79
4.79
4.76
4.74
4.74
4.12
4.10
4.08
3.67
3.46
3.46
3.43
3.43
3.43
3.35
3.34
3.31
1.77
1.68
1.66
1.61
1.43
1.41
1.39
1.37
1.34
1.29
1.27
1.27
1.25
1.25
1.24
6c’
2 F
F
F
O
O-
H3N+
NH
P
O
O
O
CH3
CH3
NH+
0.94
1.00
2.89
1.87
4.08
2.06
4.00
2.00
4.97
0.97
6.11
11.0
10.5
10.0
9.5
9.0
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
0.5
0.0
f1 (ppm)

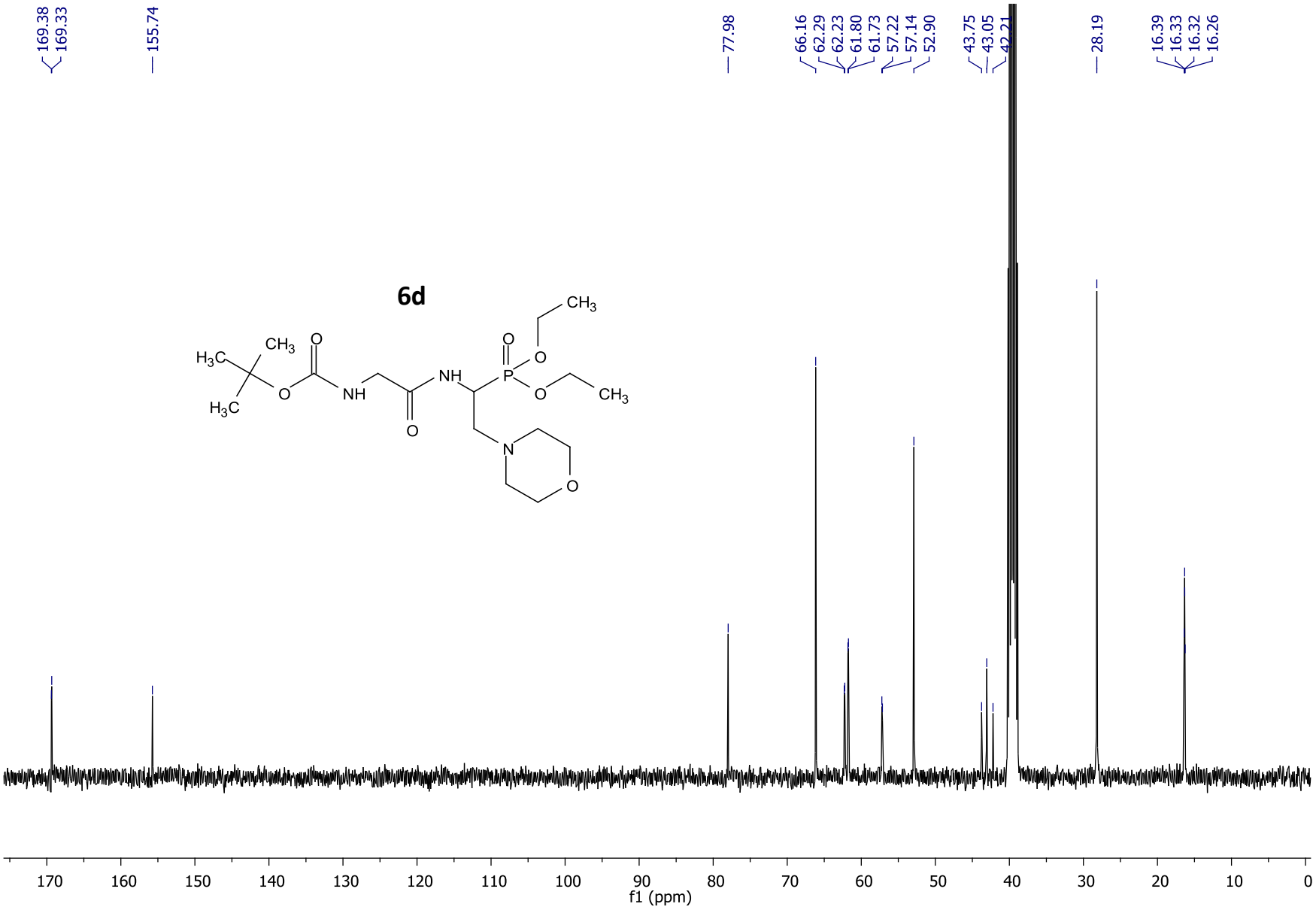

166.74
166.70
158.96
158.62
158.28
157.95
120.74
117.80
114.87
111.93
63.24
63.17
62.94
62.88
54.79
54.67
53.38
42.21
40.65
40.28
22.27
21.07
16.30
16.25
16.21
16.16
6c'
2 F
F
F
O
O-
H3N+
NH
P
O
O
O
CH3
CH3
NH+
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

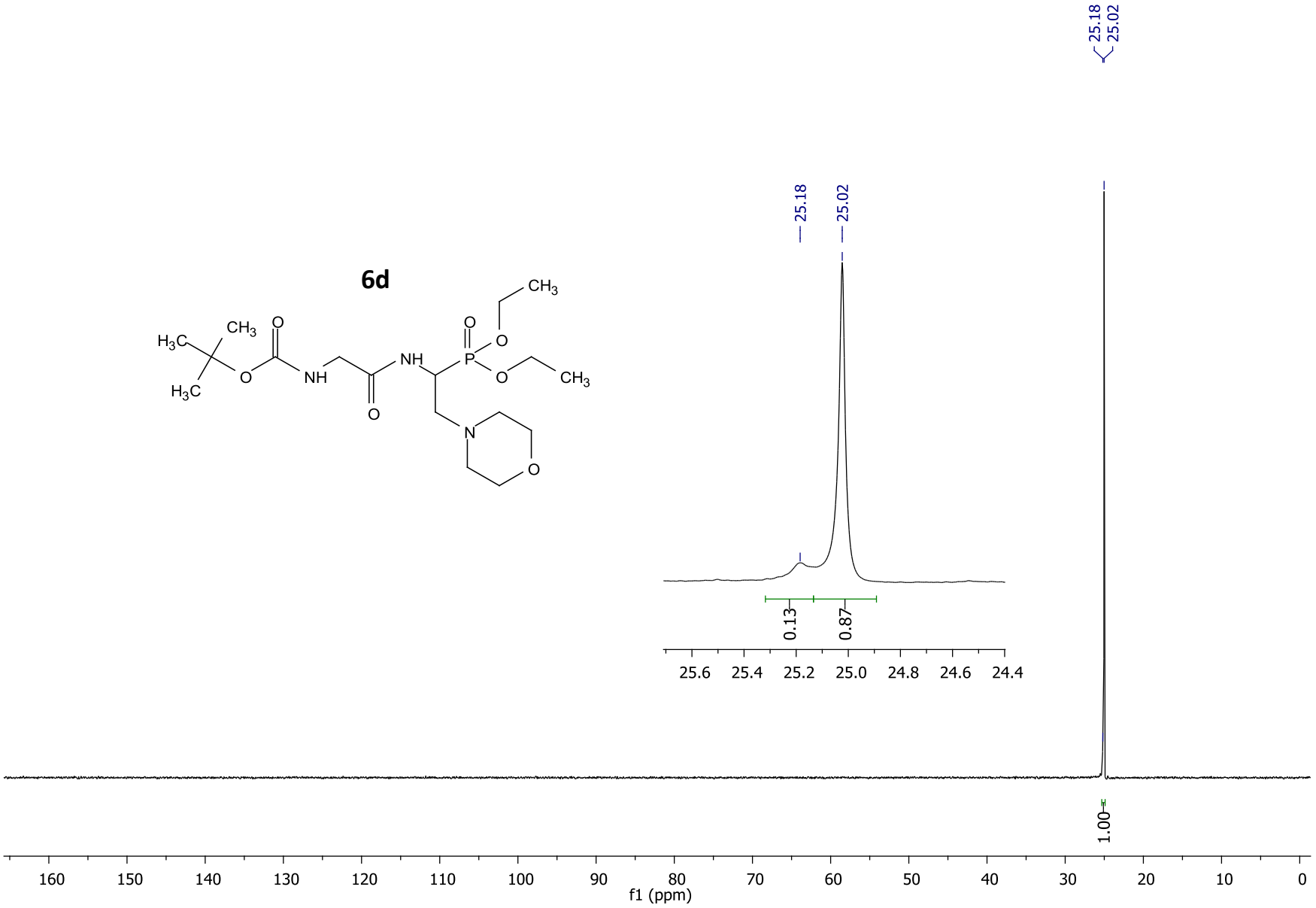
6c’

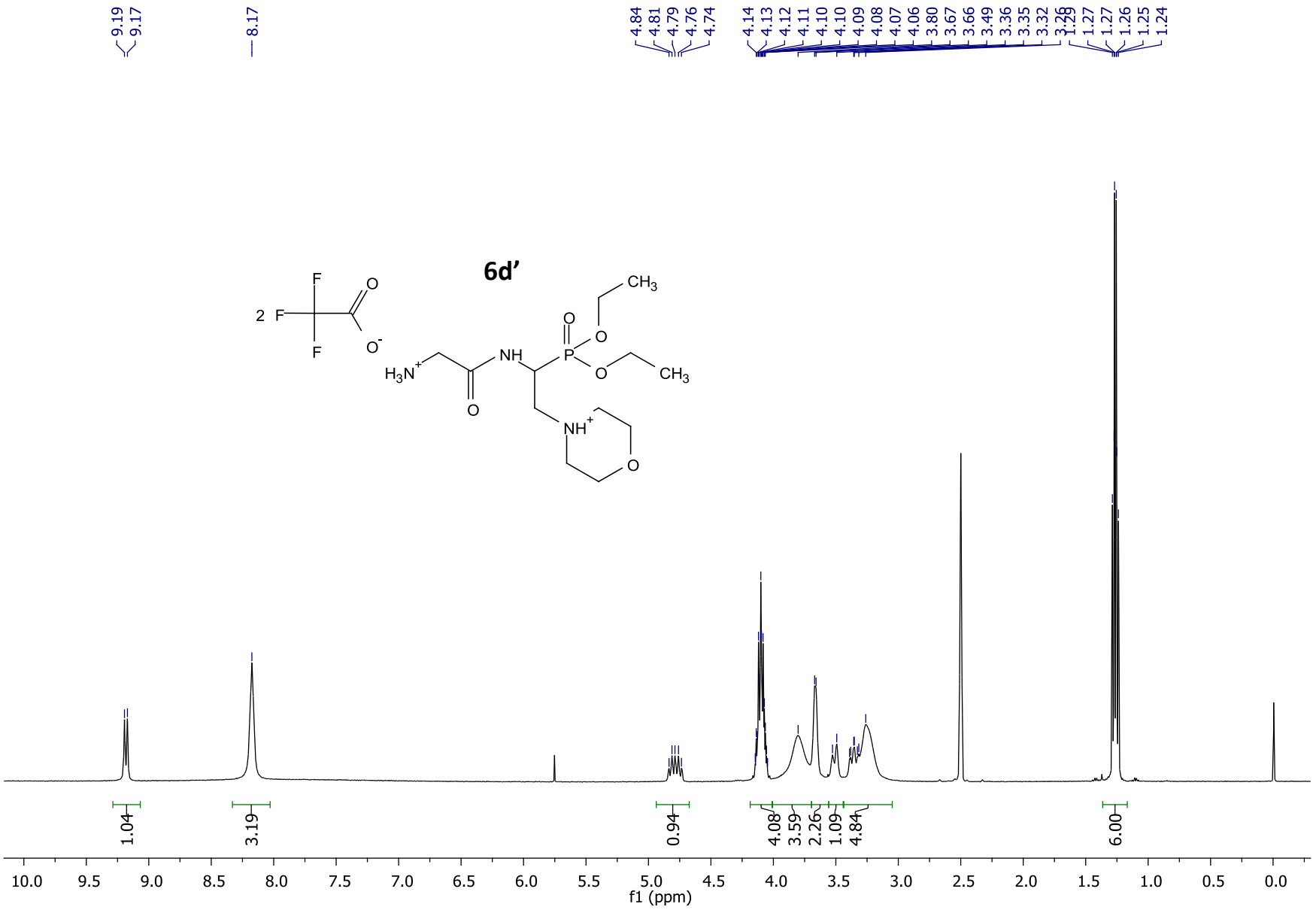

2
F
F
F
O
O-
H3N+
NH
O
O
P
O
CH3
O
CH3
NH+

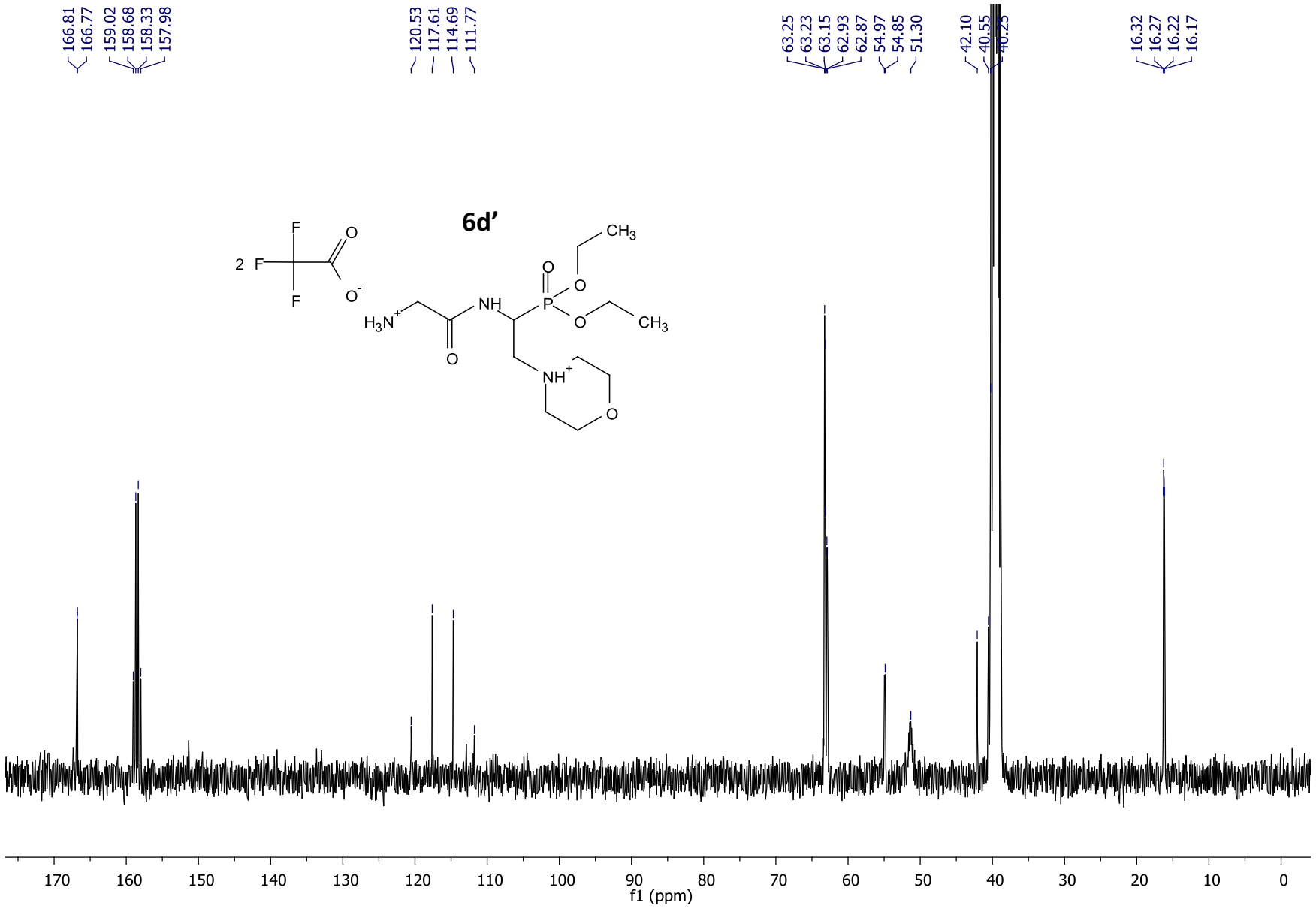
20.55
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

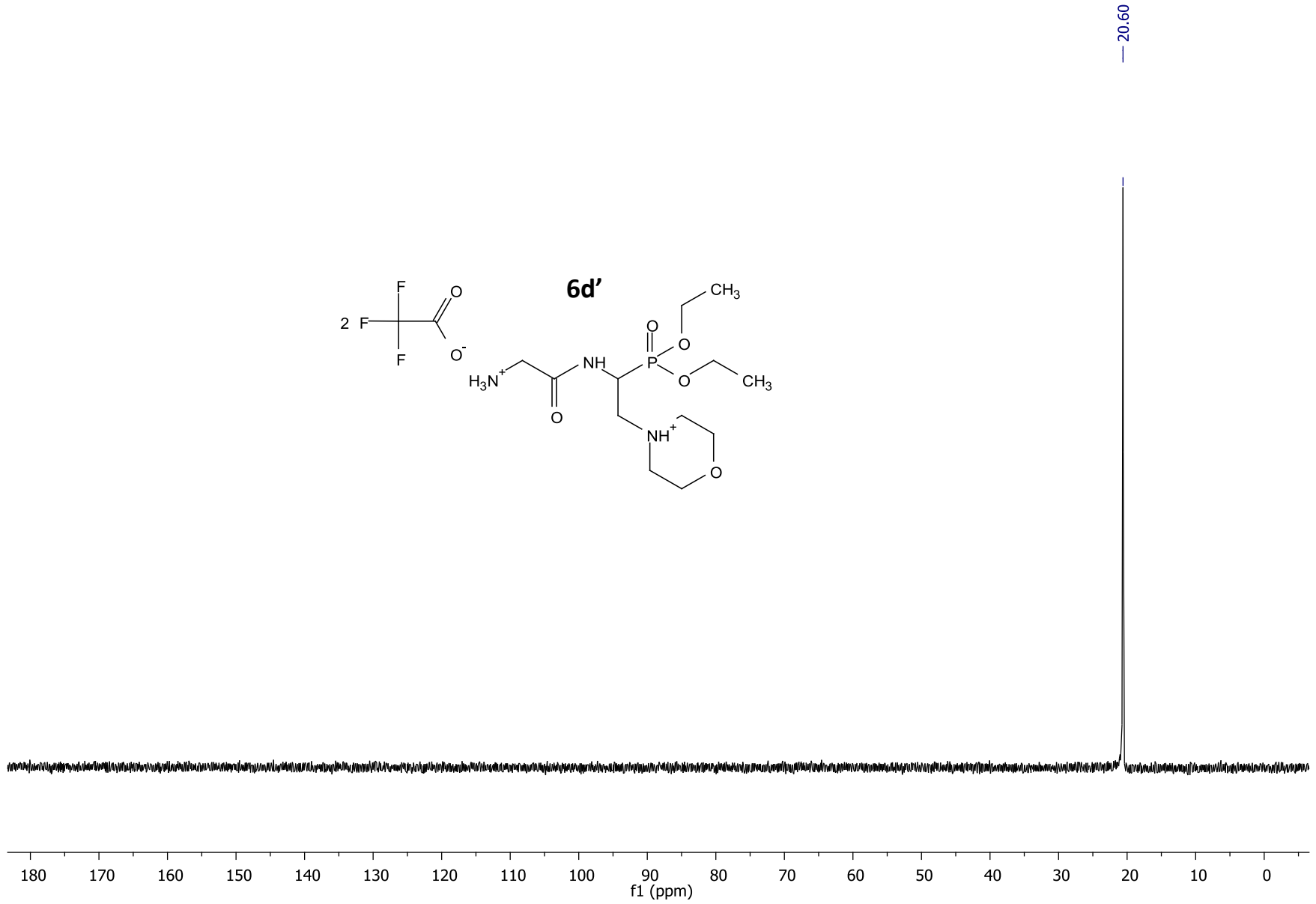

8.07
8.04
6.97
6.95
6.94
6.55
4.47
4.46
4.45
4.43
4.43
4.41
4.39
4.37
4.03
4.01
4.00
3.55
3.53
3.52
3.52
3.51
2.59
2.57
2.56
2.41
2.40
2.39
2.38
2.32
2.31
2.30
1.24
1.22
1.22
1.20
1.20
1.18
6d
1.00
0.88
0.10
1.06
4.10
6.00
2.00
2.01
1.97
9.08
6.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

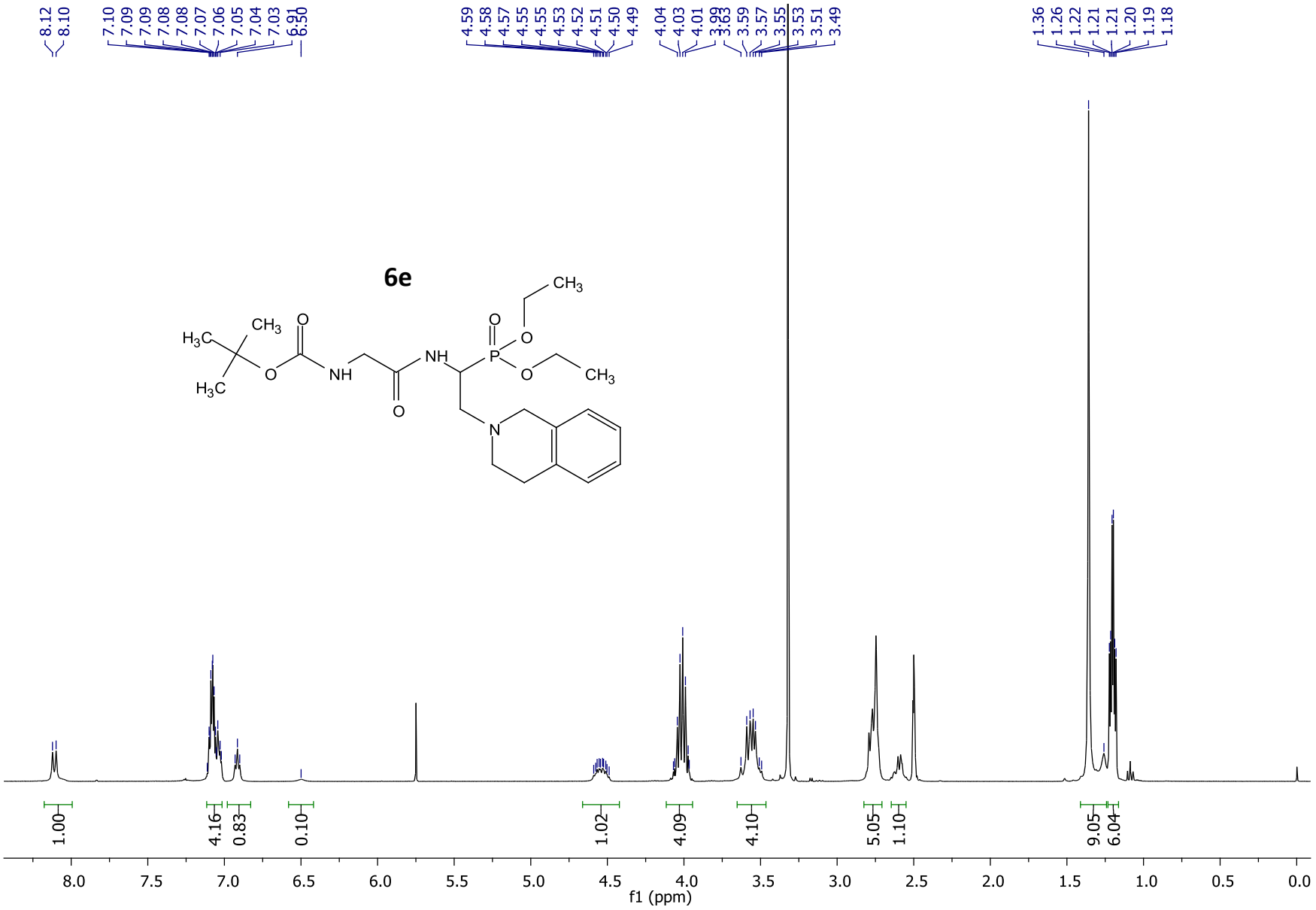

169.38
169.33
155.74
77.98
66.16
62.29
62.23
61.80
61.73
57.22
57.14
52.90
43.75
43.05
42.21
28.19
16.39
16.33
16.32
16.26
6d
CH3
H3C
CH3
O
O
NH
NH
O
P
O
O
CH3
H3C
O
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

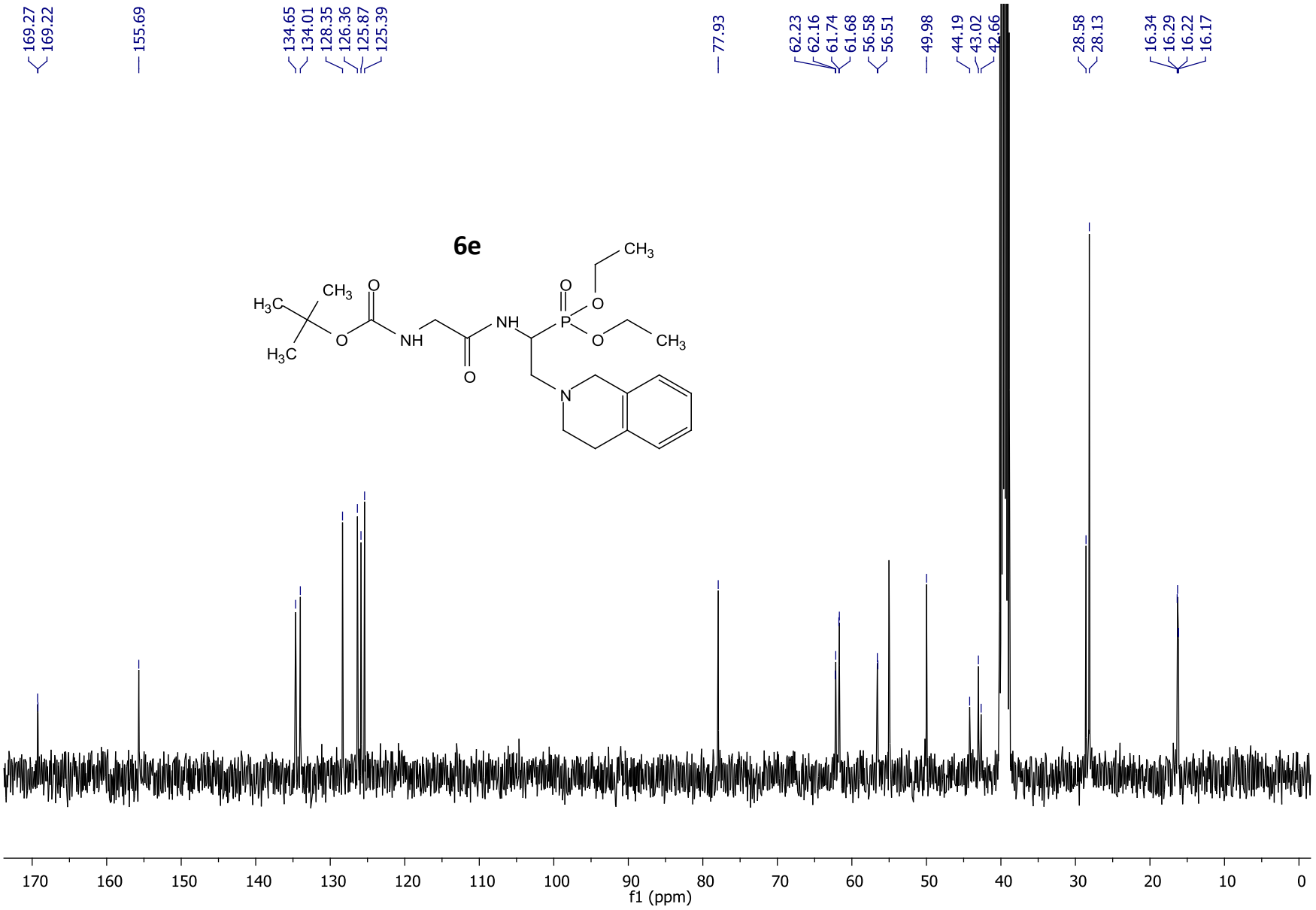

6d
25.18
25.02
0.13
0.87
1.00
f1 (ppm)

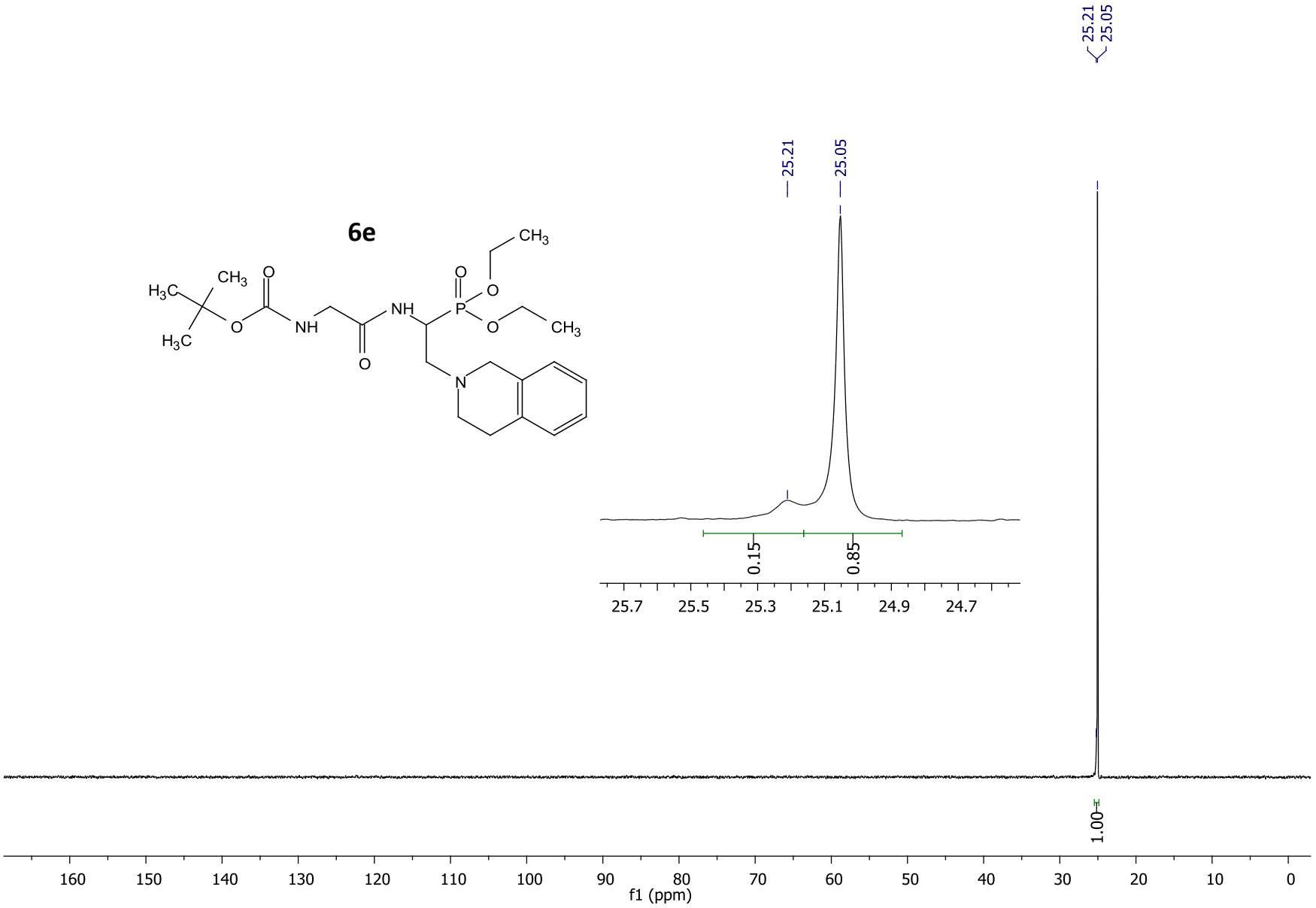

9.19
9.17
8.17
4.84
4.81
4.79
4.76
4.74
4.14
4.13
4.12
4.11
4.10
4.10
4.09
4.08
4.07
4.06
3.80
3.67
3.66
3.49
3.36
3.35
3.32
1.27
1.27
1.26
1.25
1.24
6d’
2
F
F
F
O
O-
H3N+
NH
O
P
O
O
CH3
CH3
NH+
O
1.04
3.19
0.94
4.08
3.59
2.26
1.09
4.84
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

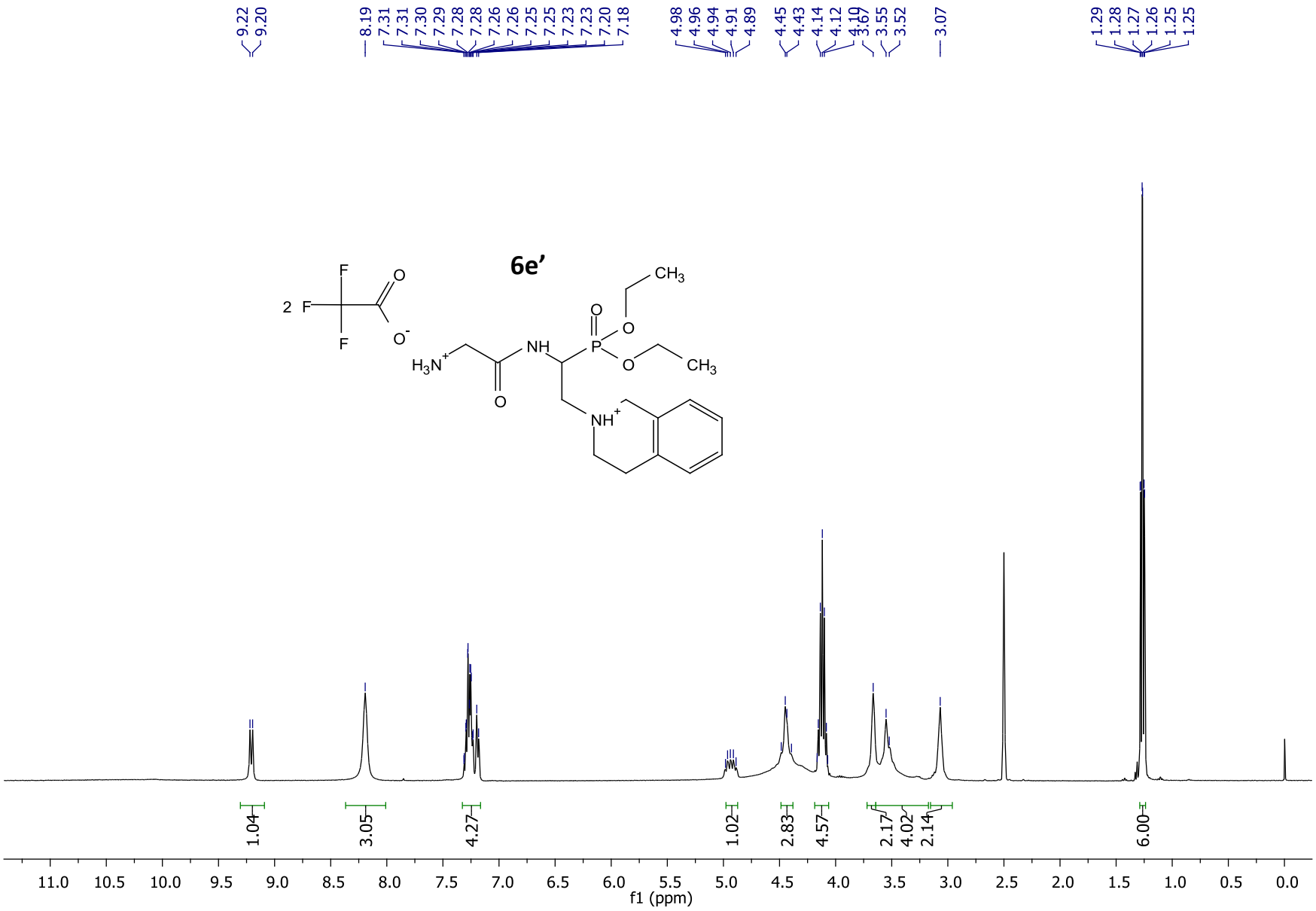

166.81
166.77
159.02
158.68
158.33
157.98
120.53
117.61
114.69
111.77
63.25
63.23
63.15
62.93
62.87
54.97
54.85
51.30
42.10
40.55
40.25
16.32
16.27
16.22
16.17
6d'
2
F
F
F
O
O-
H3N+
NH
P
O
O
CH3
O
CH3
O
NH+
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

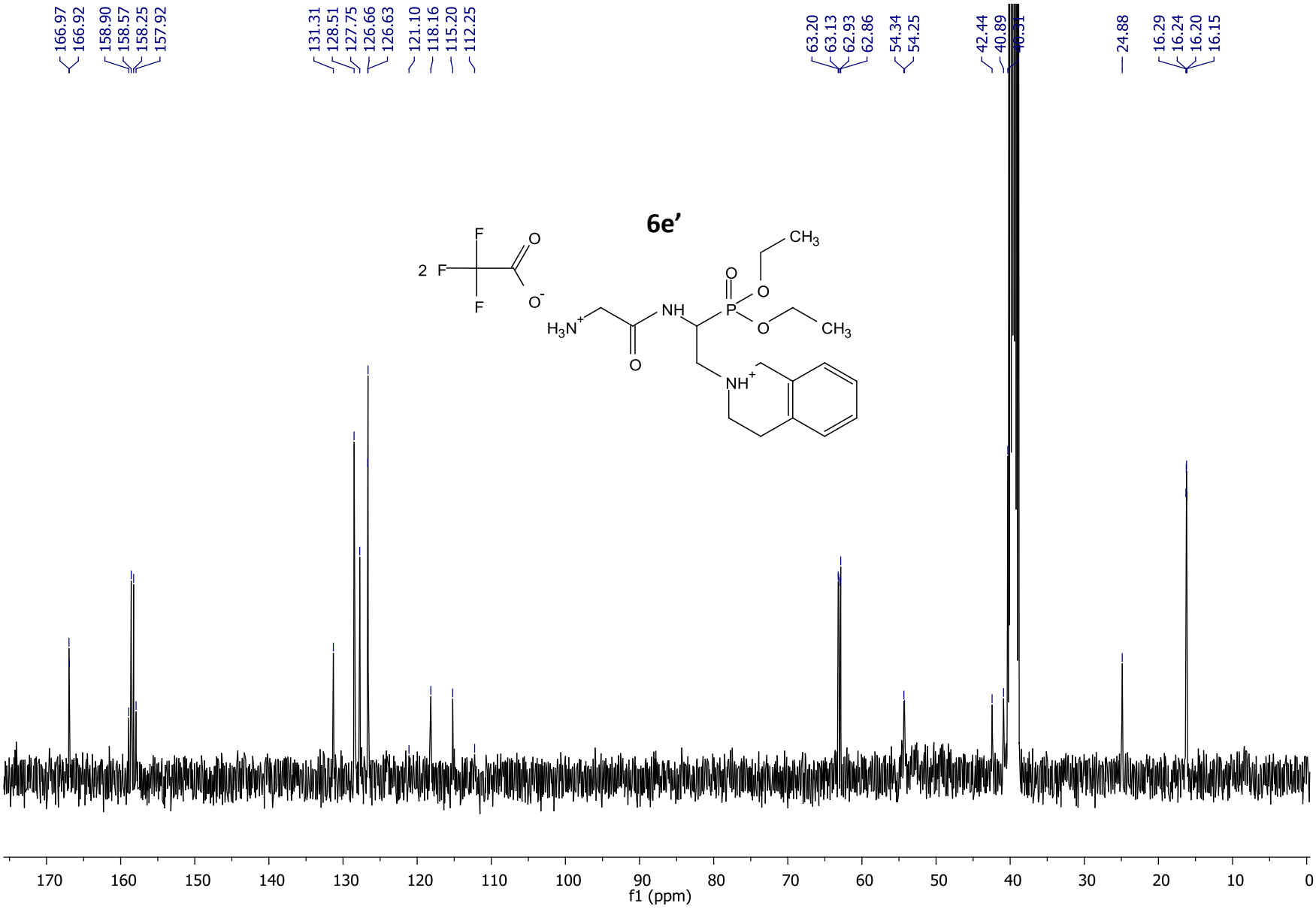

20.60
6d’
2
F
F
F
O
O-
H3N+
NH
O
P
O
O
O
CH3
CH3
NH+
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

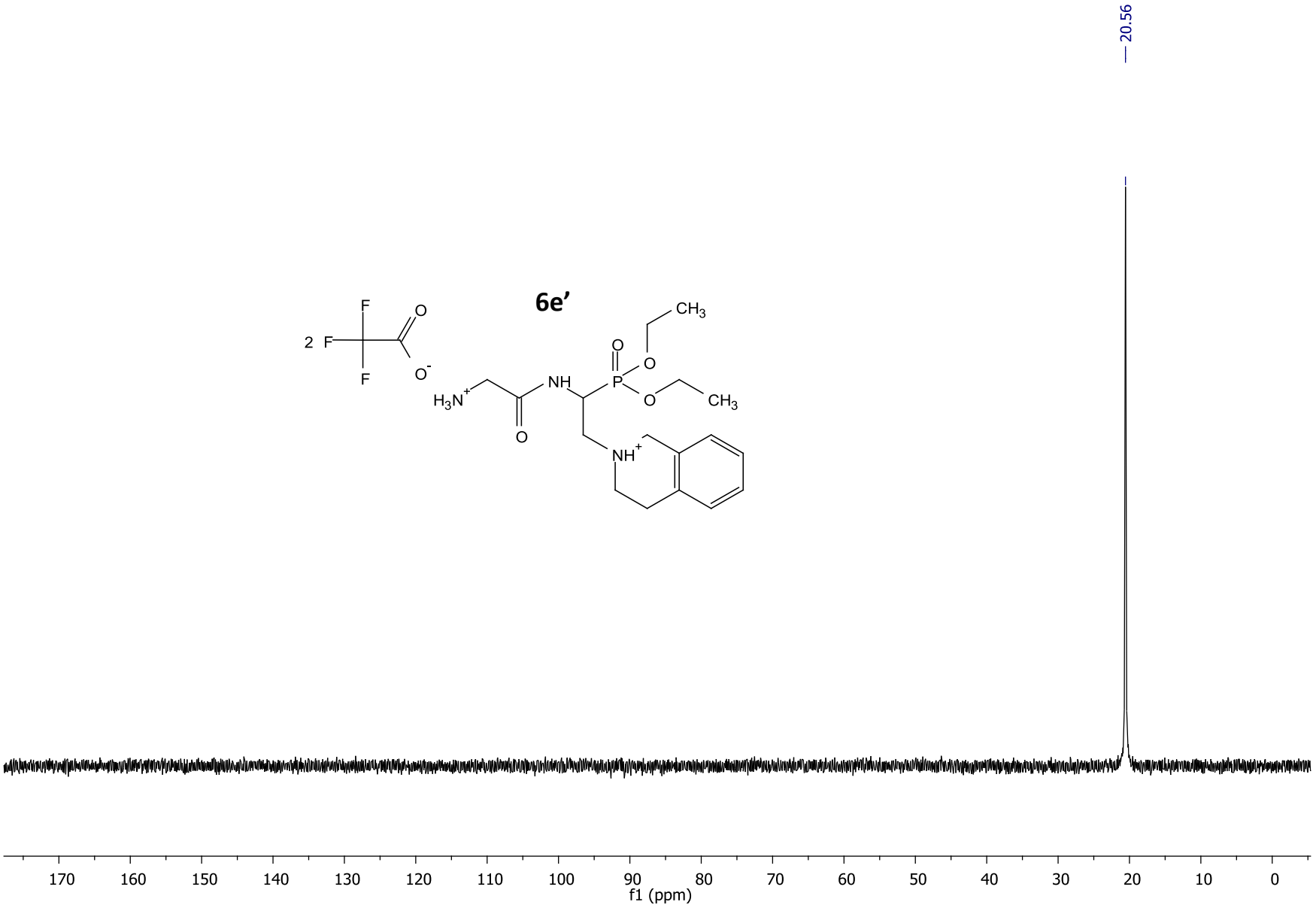

8.12
8.10
7.10
7.09
7.09
7.08
7.08
7.07
7.06
7.05
7.04
7.03
6.91
6.90
4.59
4.58
4.57
4.55
4.55
4.53
4.52
4.51
4.50
4.49
4.04
4.03
4.01
3.99
3.63
3.59
3.57
3.55
3.53
3.51
3.49
1.36
1.26
1.22
1.21
1.21
1.20
1.19
1.18
6e
CH3
H3C
CH3
O
O
NH
NH
P
O
O
CH3
H3C
O
O
N
1.00
4.16
0.83
0.10
1.02
4.09
4.10
5.05
1.10
9.05
6.04
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
0.0
f1 (ppm)


169.27
169.22
155.69
134.65
134.01
128.35
126.36
125.87
125.39
77.93
62.23
62.16
61.74
61.68
56.58
56.51
49.98
44.19
43.02
42.66
28.58
28.13
16.34
16.29
16.22
16.17
6e
CH3
H3C
CH3
H3C
O
O
NH
O
NH
O
P
O
O
CH3
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6e
25.21
25.05
0.15
0.85
1.00
f1 (ppm)


9.22
9.20
8.19
7.31
7.31
7.30
7.29
7.28
7.28
7.26
7.26
7.25
7.25
7.23
7.23
7.20
7.18
4.98
4.96
4.94
4.91
4.89
4.45
4.43
4.14
4.12
4.10
3.60
3.55
3.52
3.07
1.29
1.28
1.27
1.26
1.25
1.25
6e’
2 F
F
F
O
O-
H3N+
NH
O
P
O
O
CH3
CH3
NH+
1.04
3.05
4.27
1.02
2.83
4.57
2.17
4.02
2.14
6.00
11.0
10.5
10.0
9.5
9.0
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
0.5
0.0
f1 (ppm)


166.97
166.92
158.90
158.57
158.25
157.92
131.31
128.51
127.75
126.66
126.63
121.10
118.16
115.20
112.25
63.20
63.13
62.93
62.86
54.34
54.25
42.44
40.89
40.51
24.88
16.29
16.24
16.20
16.15
6e'
2
F
F
F
O
O-
H3N+
NH
P
O
O
O
CH3
CH3
NH+
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6e’
20.56
2 F
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H3N+
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CH3
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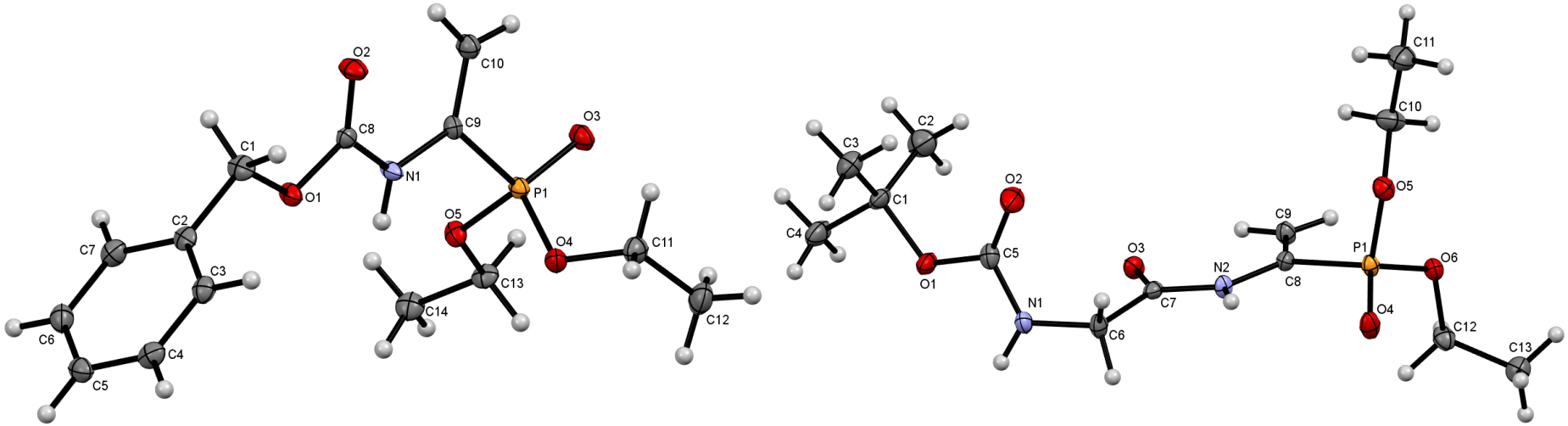
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3. Crystallographic data

Table S1: Experimental details for **3** and **5**

	3	**5**
CCDC No.	1935968	1935969
Crystal data		
Chemical formula	$C_{14}H_{20}NO_5P$	$C_{13}H_{25}N_2O_6P$
M_r	313.28	336.32
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
a, b, c (Å)	10.7418 (3), 10.0430 (2), 14.6765 (4)	9.9692 (3), 17.6005 (5), 10.3762 (3)
β (°)	104.329 (3)	111.329 (4)
V (Å^3)	1534.04 (7)	1695.94 (10)
μ (mm^{-1})	0.20	0.19
Z	4	4
μ (mm^{-1})	0.20	0.19
Crystal size (mm)	0.4 × 0.3 × 0.2	0.5 × 0.3 × 0.1
Data collection		

Absorption correction	–	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10172, 2987, 2459	11346, 3315, 2510
R_{int}	0.019	0.028
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.617	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.077, 1.07	0.031, 0.071, 0.94
No. of reflections	2987	3315
No. of parameters	192	204
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.38, −0.34	0.36, −0.37



3 **5**

Fig. SI2 Molecular structures of the studied molecules in the asymmetric part of unit cell. Displacement ellipsoids are drawn at the 50% probability level.

Table S2: Selected geometric parameters (Å, º) for **3** and **5**.

3			
P1—O3	1.4673 (9)	C5—H5	0.9300
P1—O5	1.5666 (9)	O5—C13	1.4707 (14)
P1—O4	1.5816 (9)	C6—C7	1.3879 (18)

P1—C9	1.7977 (13)	C6—H6	0.9300
O1—C8	1.3542 (15)	C7—H7	0.9300
O1—C1	1.4532 (15)	C9—C10	1.3296 (17)
N1—C8	1.3597 (16)	C10—H10A	0.9300
N1—C9	1.4088 (16)	C10—H10B	0.9300
N1—H1	0.8600	C11—C12	1.5032 (19)
C1—C2	1.4991 (18)	C11—H11A	0.9700
C1—H1A	0.9700	C11—H11B	0.9700
C1—H1B	0.9700	C12—H12A	0.9600
O2—C8	1.2099 (15)	C12—H12B	0.9600
C2—C7	1.3894 (19)	C12—H12C	0.9600
C2—C3	1.3933 (18)	C13—C14	1.5019 (18)
C3—C4	1.3896 (19)	C13—H13A	0.9700
C3—H3	0.9300	C13—H13B	0.9700
C4—C5	1.3838 (19)	C14—H14A	0.9600

C4—H4	0.9300	C14—H14B	0.9600
O4—C11	1.4579 (15)	C14—H14C	0.9600
C5—C6	1.386 (2)		
O3—P1—O5	116.33 (5)	C2—C7—H7	119.8
O3—P1—O4	114.28 (5)	O2—C8—O1	123.66 (12)
O5—P1—O4	102.90 (5)	O2—C8—N1	126.98 (12)
O3—P1—C9	112.34 (6)	O1—C8—N1	109.36 (10)
O5—P1—C9	102.63 (5)	C10—C9—N1	126.85 (12)
O4—P1—C9	107.16 (5)	C10—C9—P1	116.47 (10)
C8—O1—C1	114.44 (10)	N1—C9—P1	116.67 (9)
C8—N1—C9	124.25 (11)	C9—C10—H10A	120.0
C8—N1—H1	117.9	C9—C10—H10B	120.0
C9—N1—H1	117.9	H10A—C10—H10B	120.0
O1—C1—C2	107.07 (10)	O4—C11—C12	109.80 (11)
O1—C1—H1A	110.3	O4—C11—H11A	109.7

C2—C1—H1A	110.3	C12—C11—H11A	109.7
O1—C1—H1B	110.3	O4—C11—H11B	109.7
C2—C1—H1B	110.3	C12—C11—H11B	109.7
H1A—C1—H1B	108.6	H11A—C11—H11B	108.2
C7—C2—C3	119.17 (13)	C11—C12—H12A	109.5
C7—C2—C1	120.45 (12)	C11—C12—H12B	109.5
C3—C2—C1	120.38 (12)	H12A—C12—H12B	109.5
C4—C3—C2	120.25 (12)	C11—C12—H12C	109.5
C4—C3—H3	119.9	H12A—C12—H12C	109.5
C2—C3—H3	119.9	H12B—C12—H12C	109.5
C5—C4—C3	120.20 (13)	O5—C13—C14	107.14 (10)
C5—C4—H4	119.9	O5—C13—H13A	110.3
C3—C4—H4	119.9	C14—C13—H13A	110.3
C11—O4—P1	120.06 (8)	O5—C13—H13B	110.3
C4—C5—C6	119.81 (13)	C14—C13—H13B	110.3

C4—C5—H5	120.1	H13A—C13—H13B	108.5
C6—C5—H5	120.1	C13—C14—H14A	109.5
C13—O5—P1	119.53 (8)	C13—C14—H14B	109.5
C5—C6—C7	120.15 (13)	H14A—C14—H14B	109.5
C5—C6—H6	119.9	C13—C14—H14C	109.5
C7—C6—H6	119.9	H14A—C14—H14C	109.5
C6—C7—C2	120.43 (13)	H14B—C14—H14C	109.5
C6—C7—H7	119.8		
C8—O1—C1—C2	−178.57 (10)	C1—C2—C7—C6	179.86 (12)
O1—C1—C2—C7	−78.83 (15)	C1—O1—C8—O2	−3.16 (18)
O1—C1—C2—C3	101.51 (14)	C1—O1—C8—N1	177.01 (10)
C7—C2—C3—C4	0.54 (19)	C9—N1—C8—O2	−2.2 (2)
C1—C2—C3—C4	−179.79 (12)	C9—N1—C8—O1	177.62 (11)
C2—C3—C4—C5	0.0 (2)	C8—N1—C9—C10	−11.3 (2)
O3—P1—O4—C11	32.10 (11)	C8—N1—C9—P1	167.72 (10)

O5—P1—O4—C11	159.15 (9)	O3—P1—C9—C10	0.06 (13)
C9—P1—O4—C11	−93.06 (10)	O5—P1—C9—C10	−125.65 (11)
C3—C4—C5—C6	−0.69 (19)	O4—P1—C9—C10	126.38 (10)
O3—P1—O5—C13	43.69 (11)	O3—P1—C9—N1	−179.06 (9)
O4—P1—O5—C13	−82.04 (9)	O5—P1—C9—N1	55.24 (10)
C9—P1—O5—C13	166.76 (9)	O4—P1—C9—N1	−52.74 (10)
C4—C5—C6—C7	0.7 (2)	P1—O4—C11—C12	−104.59 (11)
C5—C6—C7—C2	−0.2 (2)	P1—O5—C13—C14	−174.30 (9)
C3—C2—C7—C6	−0.48 (19)		

5

P1—O4	1.4629 (10)	C3—H3B	0.9600
P1—O5	1.5649 (10)	C3—H3C	0.9600
P1—O6	1.5696 (10)	C4—H4A	0.9600
P1—C8	1.8042 (14)	C4—H4B	0.9600
N1—C5	1.3498 (18)	C4—H4C	0.9600

N1—C6	1.4379 (18)	C6—C7	1.5279 (19)
N1—H1	0.8600	C6—H6A	0.9700
N2—C7	1.3560 (17)	C6—H6B	0.9700
N2—C8	1.4089 (17)	C8—C9	1.3316 (19)
N2—H2	0.8600	C9—H9A	0.9300
O1—C5	1.3522 (17)	C9—H9B	0.9300
O1—C1	1.4785 (17)	C10—C11	1.495 (2)
O2—C5	1.2099 (17)	C10—H10A	0.9700
O3—C7	1.2230 (16)	C10—H10B	0.9700
O5—C10	1.4571 (17)	C11—H11A	0.9600
O6—C12	1.4623 (17)	C11—H11B	0.9600
C1—C2	1.511 (2)	C11—H11C	0.9600
C1—C3	1.516 (2)	C12—C13	1.493 (2)
C1—C4	1.517 (2)	C12—H12A	0.9700
C2—H2A	0.9600	C12—H12B	0.9700

C2—H2B	0.9600	C13—H13A	0.9600
C2—H2C	0.9600	C13—H13B	0.9600
C3—H3A	0.9600	C13—H13C	0.9600
O4—P1—O5	111.55 (6)	N1—C5—O1	109.44 (12)
O4—P1—O6	115.90 (6)	N1—C6—C7	112.30 (11)
O5—P1—O6	102.84 (5)	N1—C6—H6A	109.1
O4—P1—C8	112.12 (6)	C7—C6—H6A	109.1
O5—P1—C8	108.05 (6)	N1—C6—H6B	109.1
O6—P1—C8	105.68 (6)	C7—C6—H6B	109.1
C5—N1—C6	119.26 (12)	H6A—C6—H6B	107.9
C5—N1—H1	120.4	O3—C7—N2	124.28 (13)
C6—N1—H1	120.4	O3—C7—C6	121.81 (12)
C7—N2—C8	125.70 (12)	N2—C7—C6	113.91 (12)
C7—N2—H2	117.2	C9—C8—N2	127.15 (13)
C8—N2—H2	117.2	C9—C8—P1	119.33 (11)

C5—O1—C1	121.05 (11)	N2—C8—P1	113.49 (10)
C10—O5—P1	122.64 (9)	C8—C9—H9A	120.0
C12—O6—P1	118.76 (9)	C8—C9—H9B	120.0
O1—C1—C2	110.53 (12)	H9A—C9—H9B	120.0
O1—C1—C3	110.55 (12)	O5—C10—C11	108.17 (12)
C2—C1—C3	111.86 (13)	O5—C10—H10A	110.1
O1—C1—C4	101.93 (11)	C11—C10—H10A	110.1
C2—C1—C4	111.05 (13)	O5—C10—H10B	110.1
C3—C1—C4	110.49 (13)	C11—C10—H10B	110.1
C1—C2—H2A	109.5	H10A—C10—H10B	108.4
C1—C2—H2B	109.5	C10—C11—H11A	109.5
H2A—C2—H2B	109.5	C10—C11—H11B	109.5
C1—C2—H2C	109.5	H11A—C11—H11B	109.5
H2A—C2—H2C	109.5	C10—C11—H11C	109.5
H2B—C2—H2C	109.5	H11A—C11—H11C	109.5

C1—C3—H3A	109.5	H11B—C11—H11C	109.5
C1—C3—H3B	109.5	O6—C12—C13	109.27 (12)
H3A—C3—H3B	109.5	O6—C12—H12A	109.8
C1—C3—H3C	109.5	C13—C12—H12A	109.8
H3A—C3—H3C	109.5	O6—C12—H12B	109.8
H3B—C3—H3C	109.5	C13—C12—H12B	109.8
C1—C4—H4A	109.5	H12A—C12—H12B	108.3
C1—C4—H4B	109.5	C12—C13—H13A	109.5
H4A—C4—H4B	109.5	C12—C13—H13B	109.5
C1—C4—H4C	109.5	H13A—C13—H13B	109.5
H4A—C4—H4C	109.5	C12—C13—H13C	109.5
H4B—C4—H4C	109.5	H13A—C13—H13C	109.5
O2—C5—N1	124.57 (14)	H13B—C13—H13C	109.5
O2—C5—O1	125.98 (14)		
O4—P1—O5—C10	176.90 (11)	C8—N2—C7—O3	−3.7 (2)

O6—P1—O5—C10	52.03 (12)	C8—N2—C7—C6	175.79 (12)
C8—P1—O5—C10	−59.44 (13)	N1—C6—C7—O3	−5.60 (19)
O4—P1—O6—C12	51.58 (11)	N1—C6—C7—N2	174.88 (12)
O5—P1—O6—C12	173.55 (9)	C7—N2—C8—C9	2.5 (2)
C8—P1—O6—C12	−73.24 (11)	C7—N2—C8—P1	−179.20 (11)
C5—O1—C1—C2	61.35 (17)	O4—P1—C8—C9	−152.90 (11)
C5—O1—C1—C3	−63.06 (17)	O5—P1—C8—C9	83.77 (13)
C5—O1—C1—C4	179.46 (12)	O6—P1—C8—C9	−25.76 (13)
C6—N1—C5—O2	−13.2 (2)	O4—P1—C8—N2	28.64 (12)
C6—N1—C5—O1	167.57 (11)	O5—P1—C8—N2	−94.68 (10)
C1—O1—C5—O2	3.9 (2)	O6—P1—C8—N2	155.78 (9)
C1—O1—C5—N1	−176.89 (11)	P1—O5—C10—C11	179.43 (10)
C5—N1—C6—C7	−68.01 (17)	P1—O6—C12—C13	−115.75 (11)

Table S3: Selected hydrogen-bond parameters for **3** and **5**.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
3				
N1—H1···O3^{i}	0.86	2.00	2.8401 (14)	166.9
C10—H10A···O2	0.93	2.29	2.8695 (16)	120.1
C14—H14A···O1^{ii}	0.96	2.63	3.5318 (17)	157.0
5				
N1—H1···O3^{iii}	0.86	2.16	2.9800 (15)	159.6
N2—H2···O4	0.86	2.58	2.9898 (15)	110.5
N2—H2···O4^{iv}	0.86	2.07	2.8633 (15)	153.8
C2—H2B···O2	0.96	2.49	3.041 (2)	116.7
C3—H3B···O2	0.96	2.46	3.0163 (19)	116.8
C4—H4A···O2^{v}	0.96	2.44	3.3504 (19)	157.2
C9—H9A···O3	0.93	2.25	2.8474 (17)	121.3
C12—H12A···O3^{vi}	0.97	2.46	3.4329 (18)	178.3

Symmetry code(s): (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+2; (v) *x*−1/2, −*y*+3/2, *z*−1/2; (vi) −*x*+1, −*y*+1, −*z*+1.