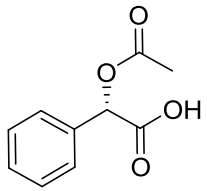
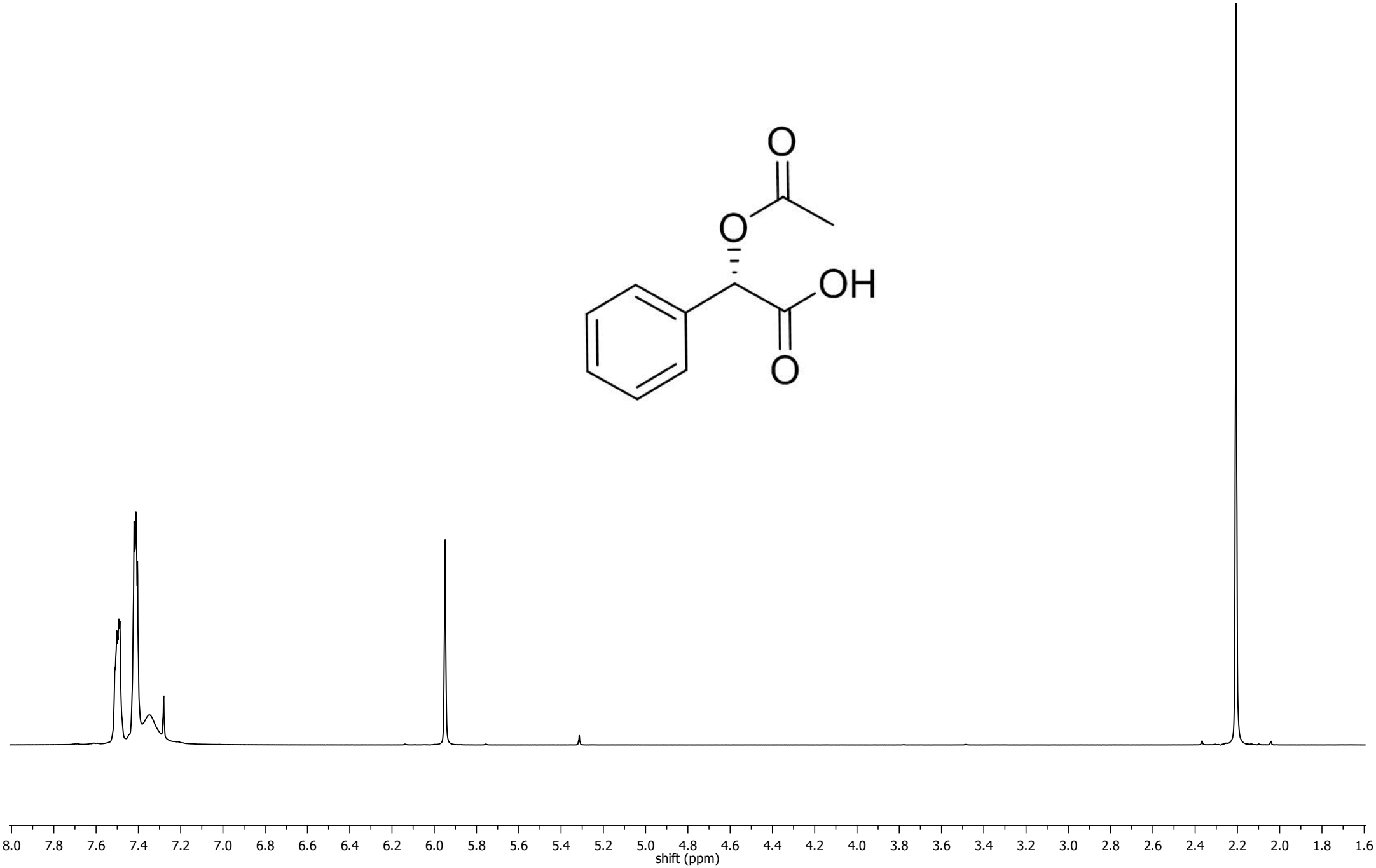
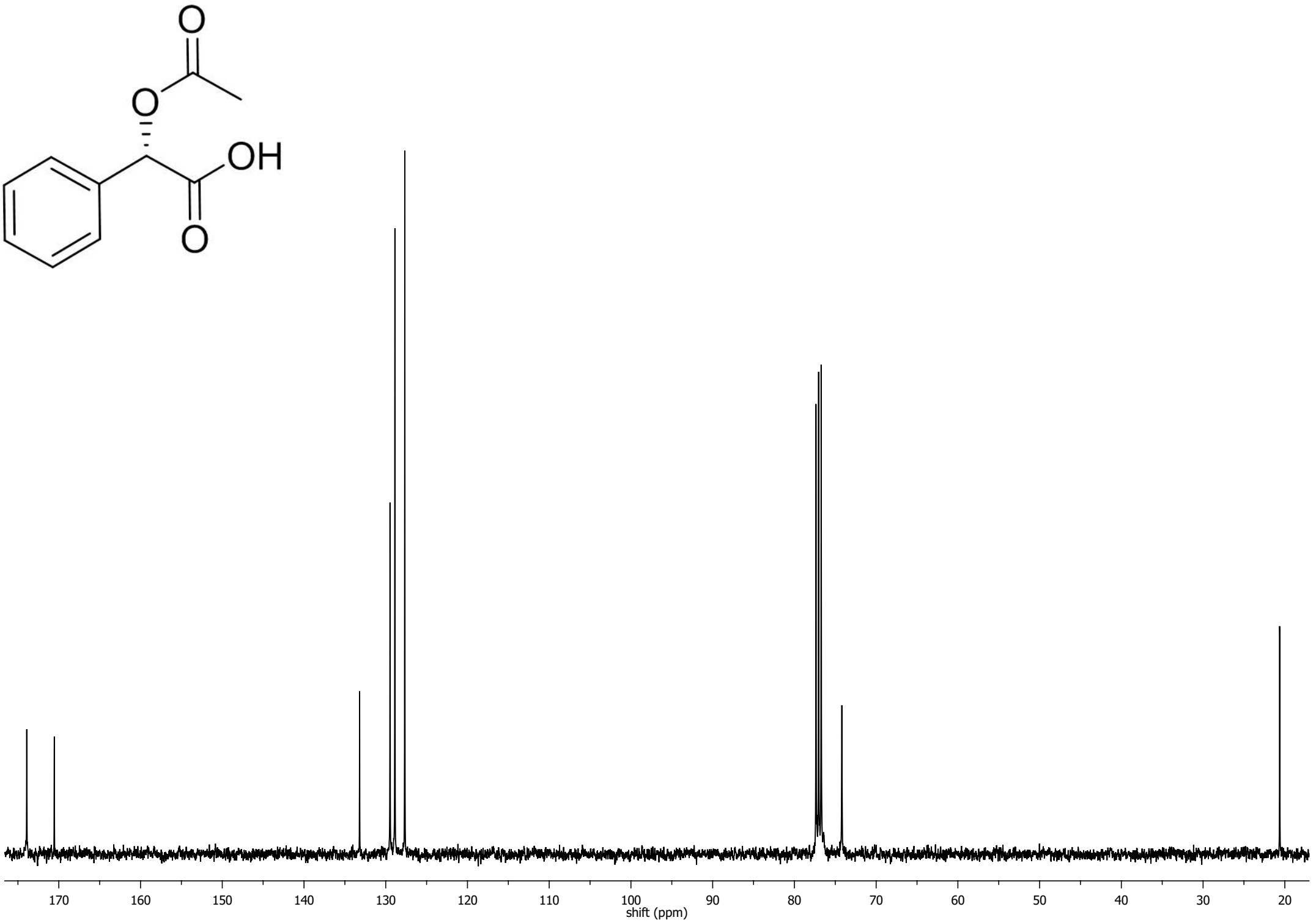
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

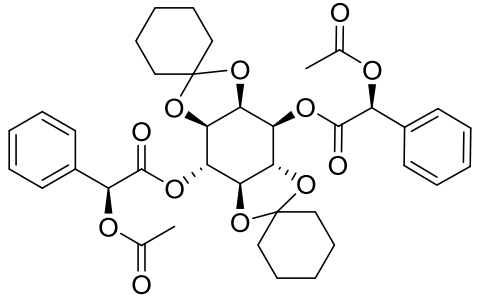


_S_-Acetyl Mandelic Acid, 8a.

HRMS (EI+) *m/z* found $[M]^{\cdot+}$ = 194·0581, $C_{10}H_9O_4$ requires 194·0579.

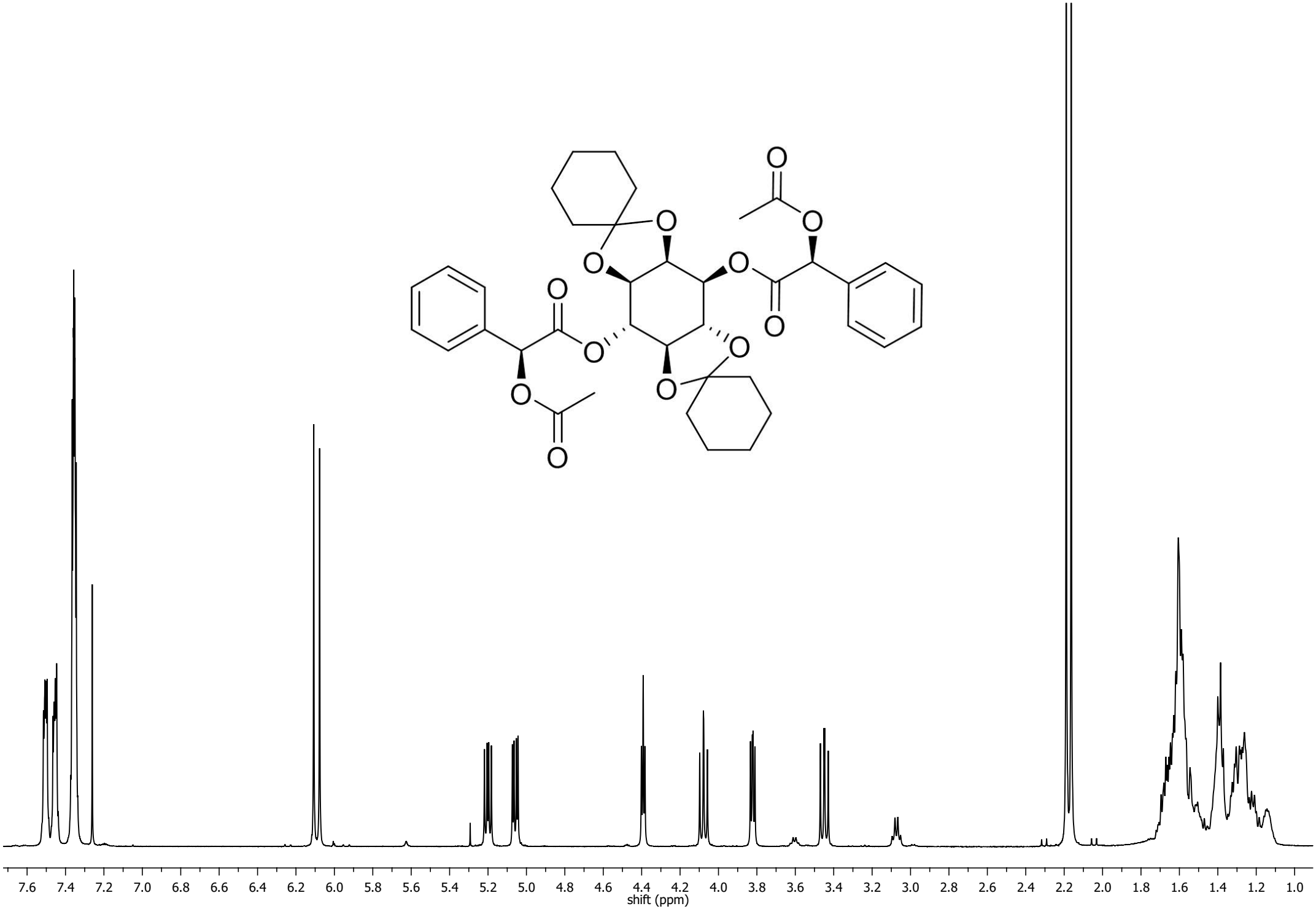

O
O
OH
O
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6
shift (ppm)

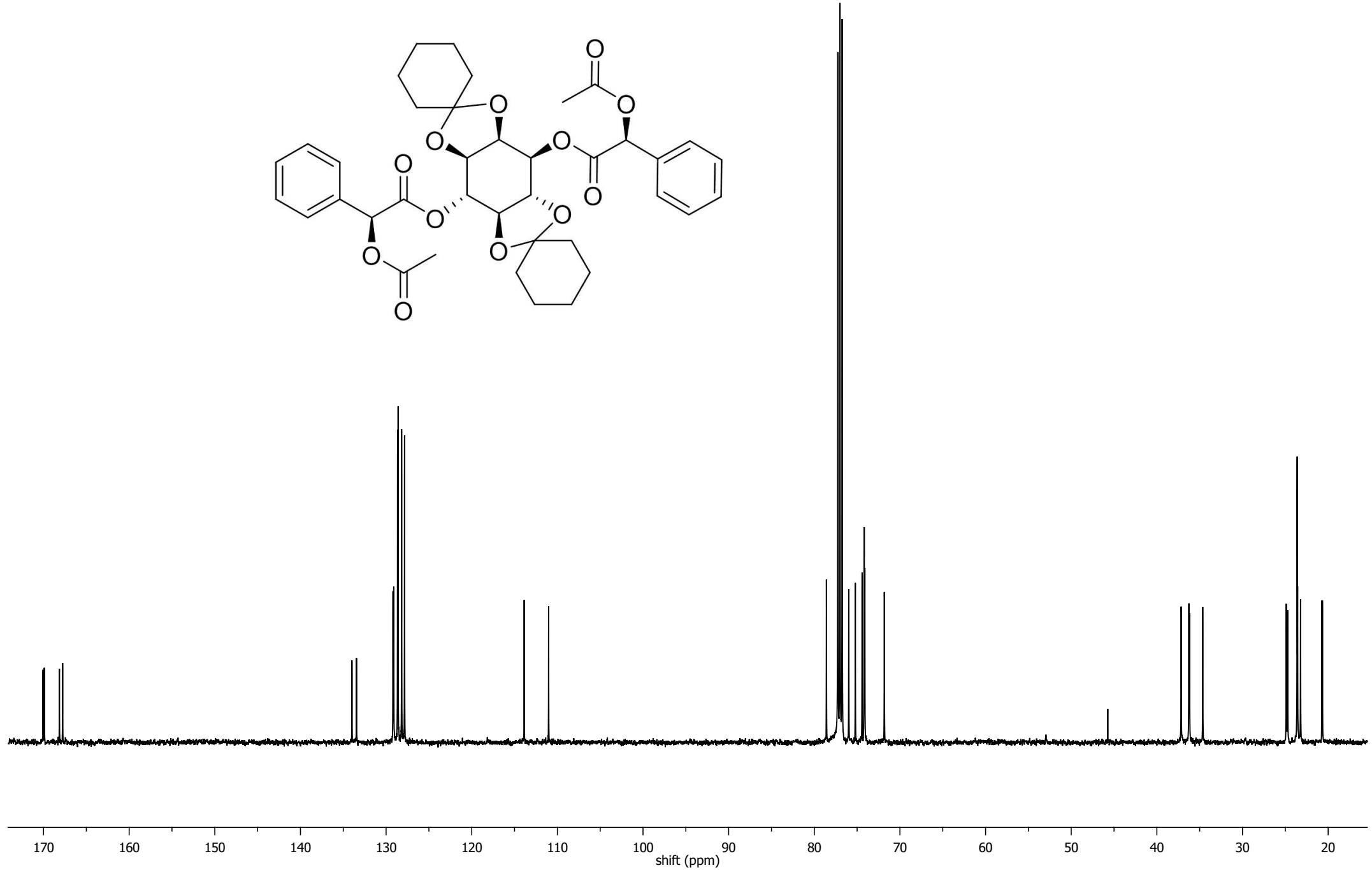

O
O
OH
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
shift (ppm)

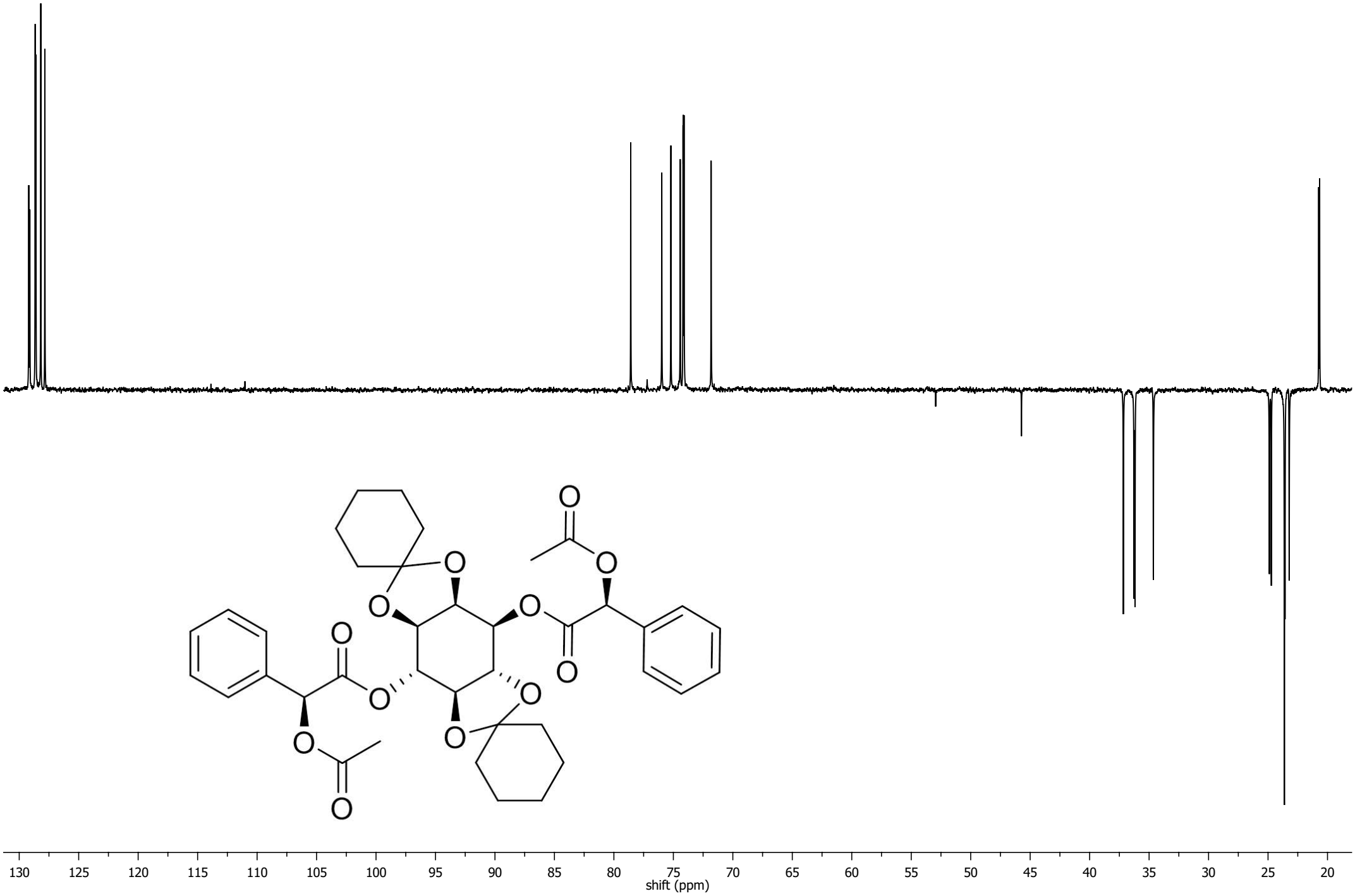


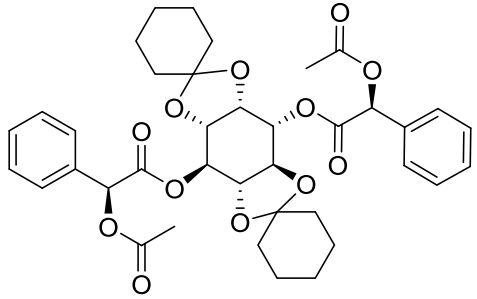
1,4-*O*-Di(*S*-acetylmandelyl)-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 6.

HRMS (ESI+) *m/z* found $[M+H]^+$ = 693·2911, $C_{38}H_{45}O_{12}^+$ requires 693·2900.


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 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0
shift (ppm)


O
O
O
O
O
O
O
O
O
O
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
shift (ppm)

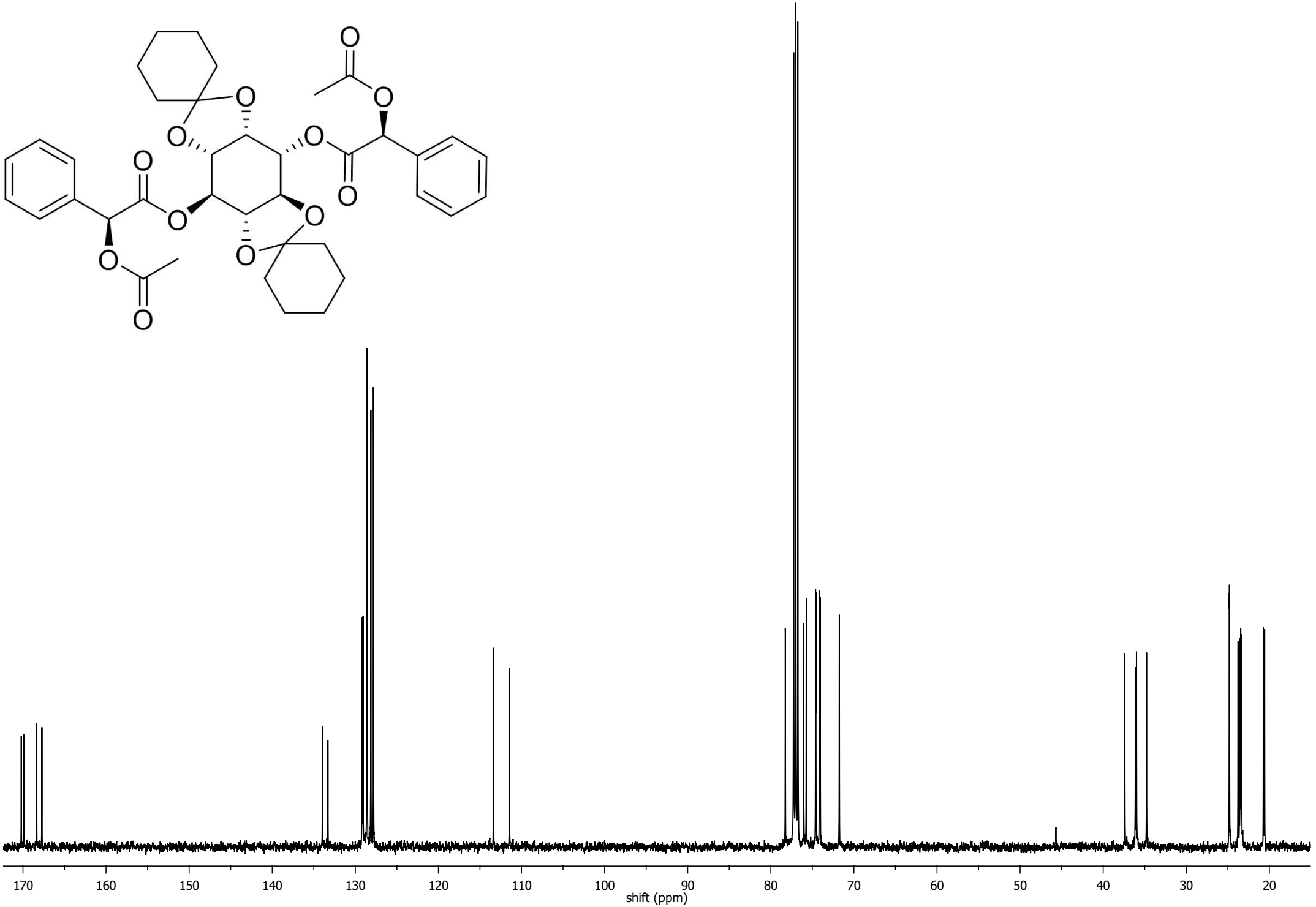

130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
shift (ppm)

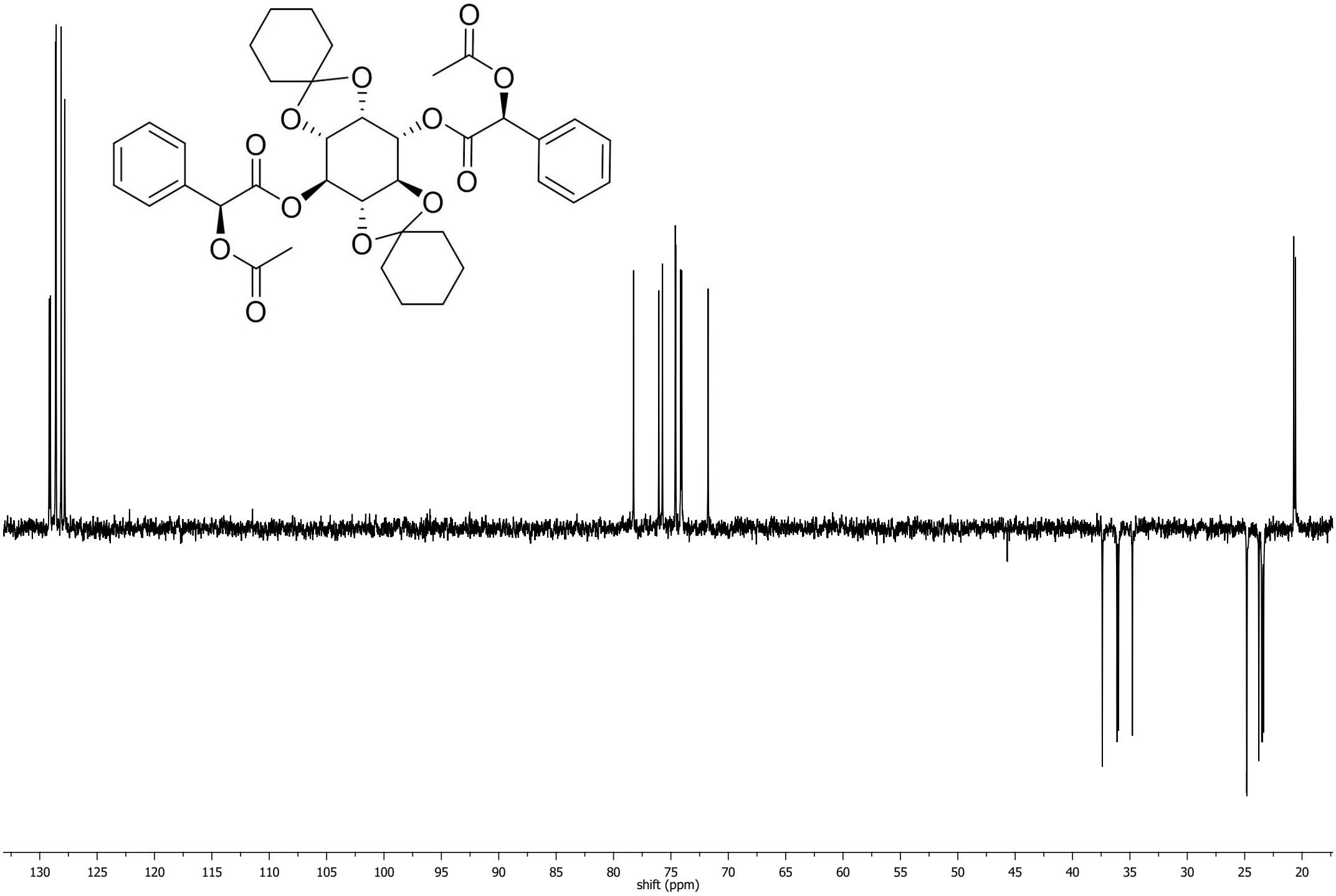


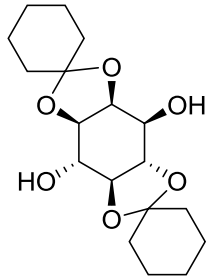
3,6-*O*-Di(*S*-acetylmandelyl)-(1,2)(4,5)-*O*-dicyclohexylidene-*myo*-inositol, 7.

HRMS (ESI+) *m/z* found $[M+H]^+$ = 693·2911, $C_{38}H_{45}O_{12}^+$ requires 693·2927.


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
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
shift (ppm)


O
O
O
O
O
O
O
O
O
O
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
shift (ppm)

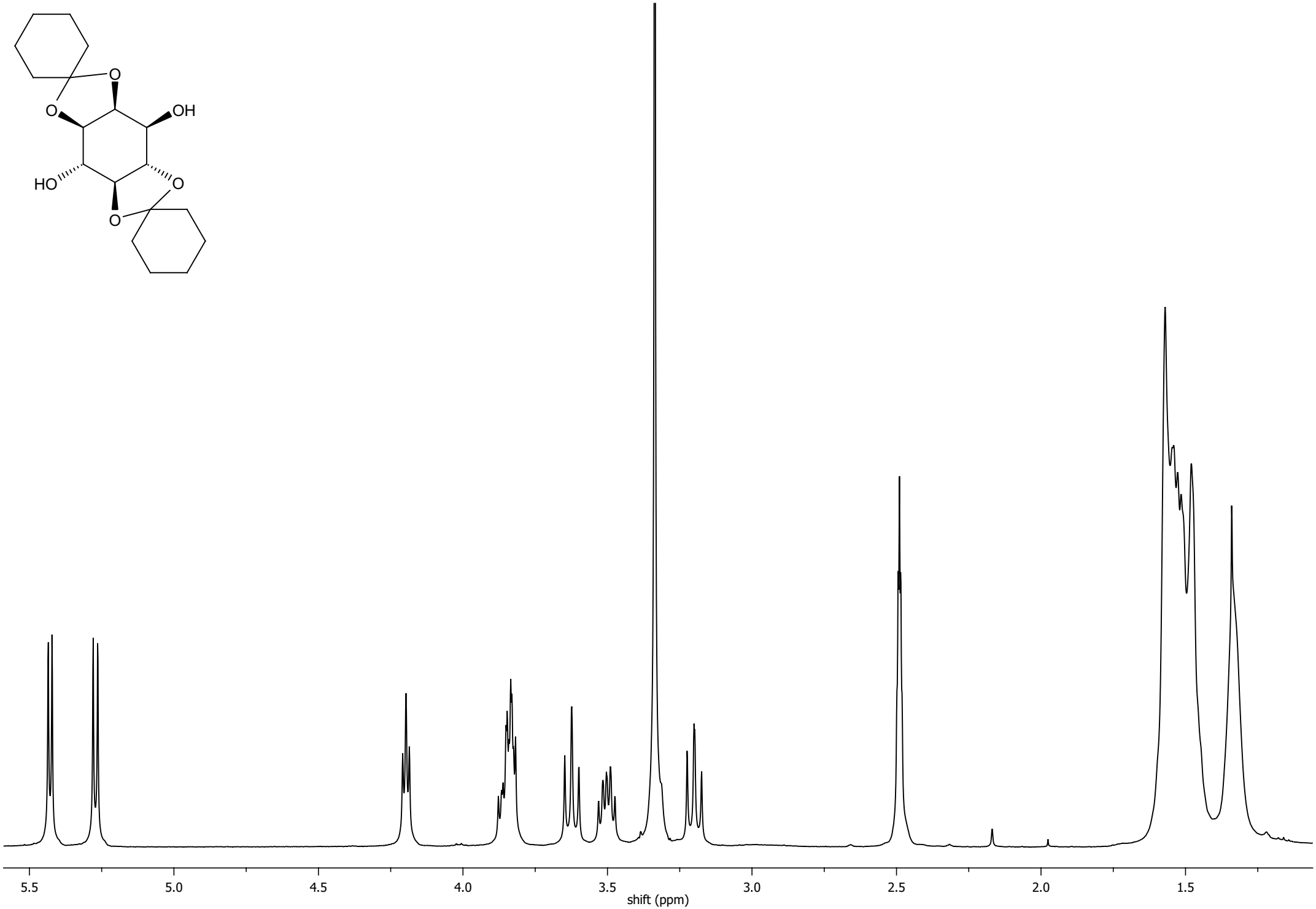

130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
shift (ppm)



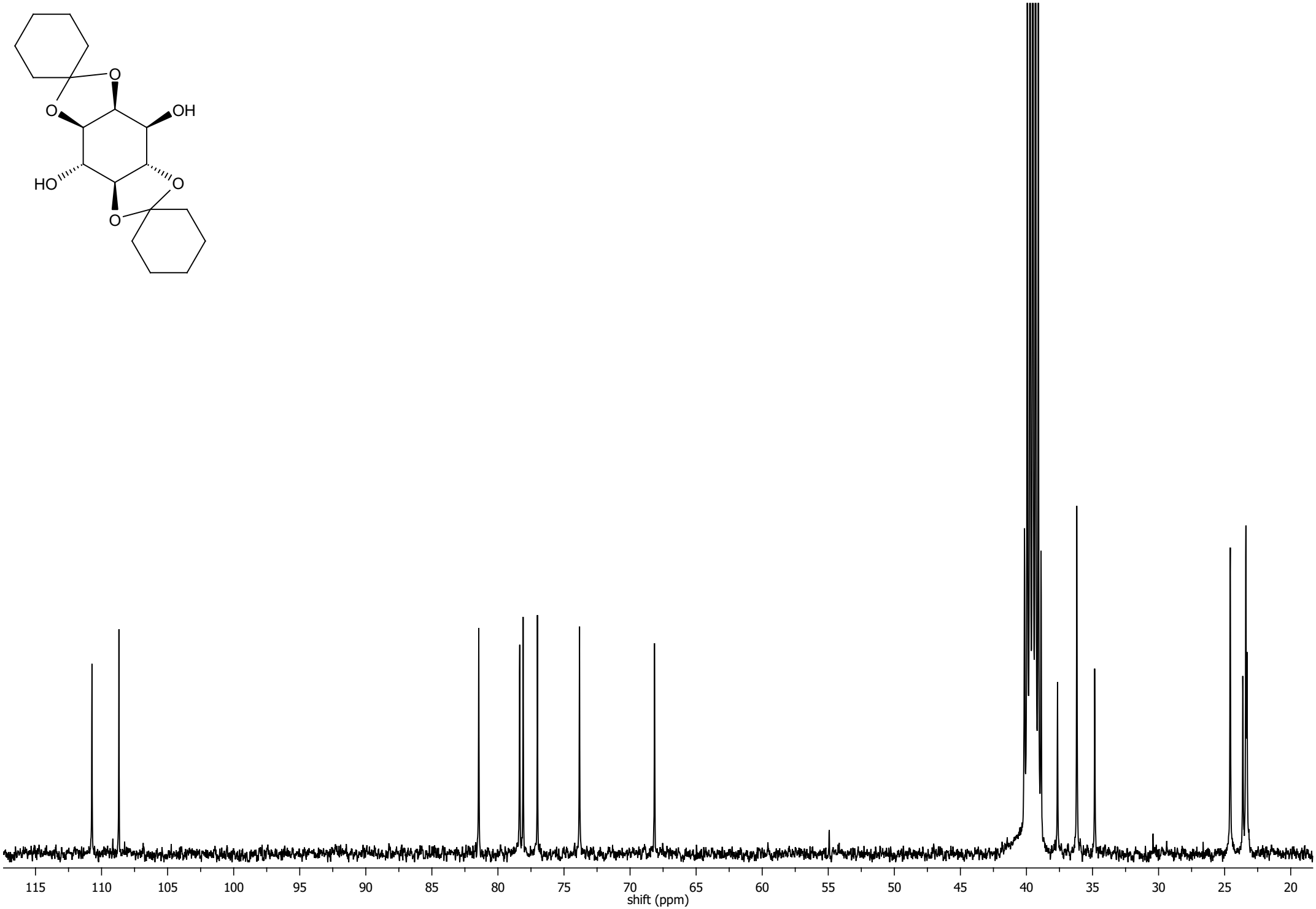
(+)-(2,3)(5,6)-*O*-Dicyclohexylidene-*myo*-inositol, D-5 *from* **6.**

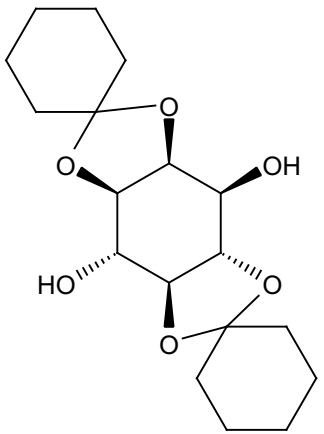
HRMS (ESI+) *m/z* found $[M+H]^+$ = 341·1956, $C_{18}H_{29}O_6^+$ requires 341·1964.

O
O
OH
HO
O
O


5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
shift (ppm)

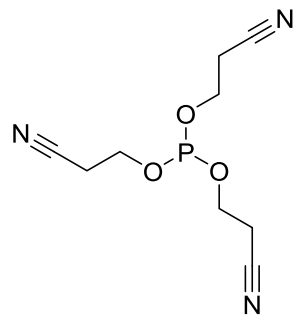
O
O
OH
HO
O
O


115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
shift (ppm)



84 82 80 78 76 74 72 70 68 66 64 62 60 58 56 54 52 50 48 46 44 42 40 38 36 34 32 30 28 26 24 22 20

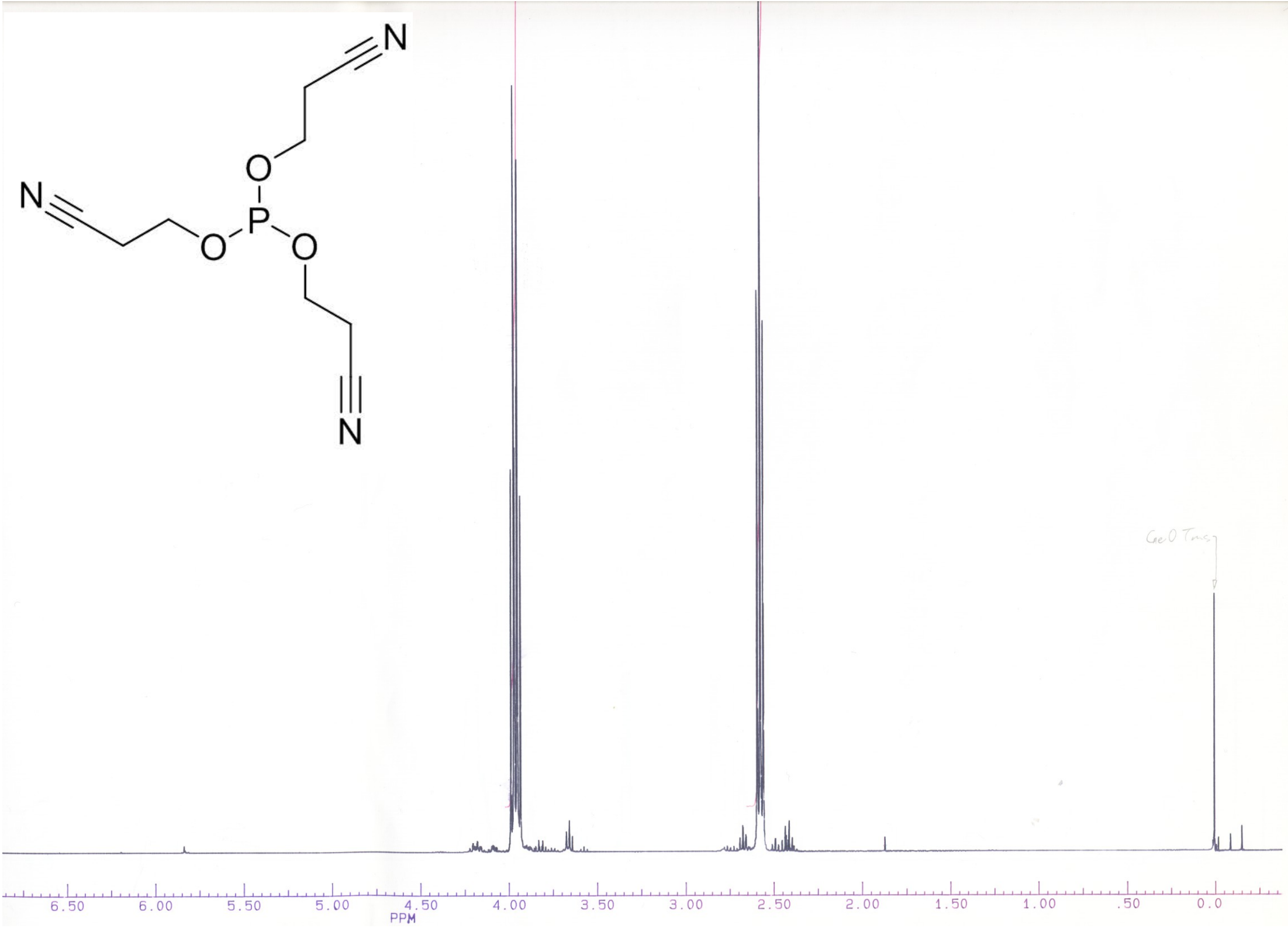
shift (ppm)



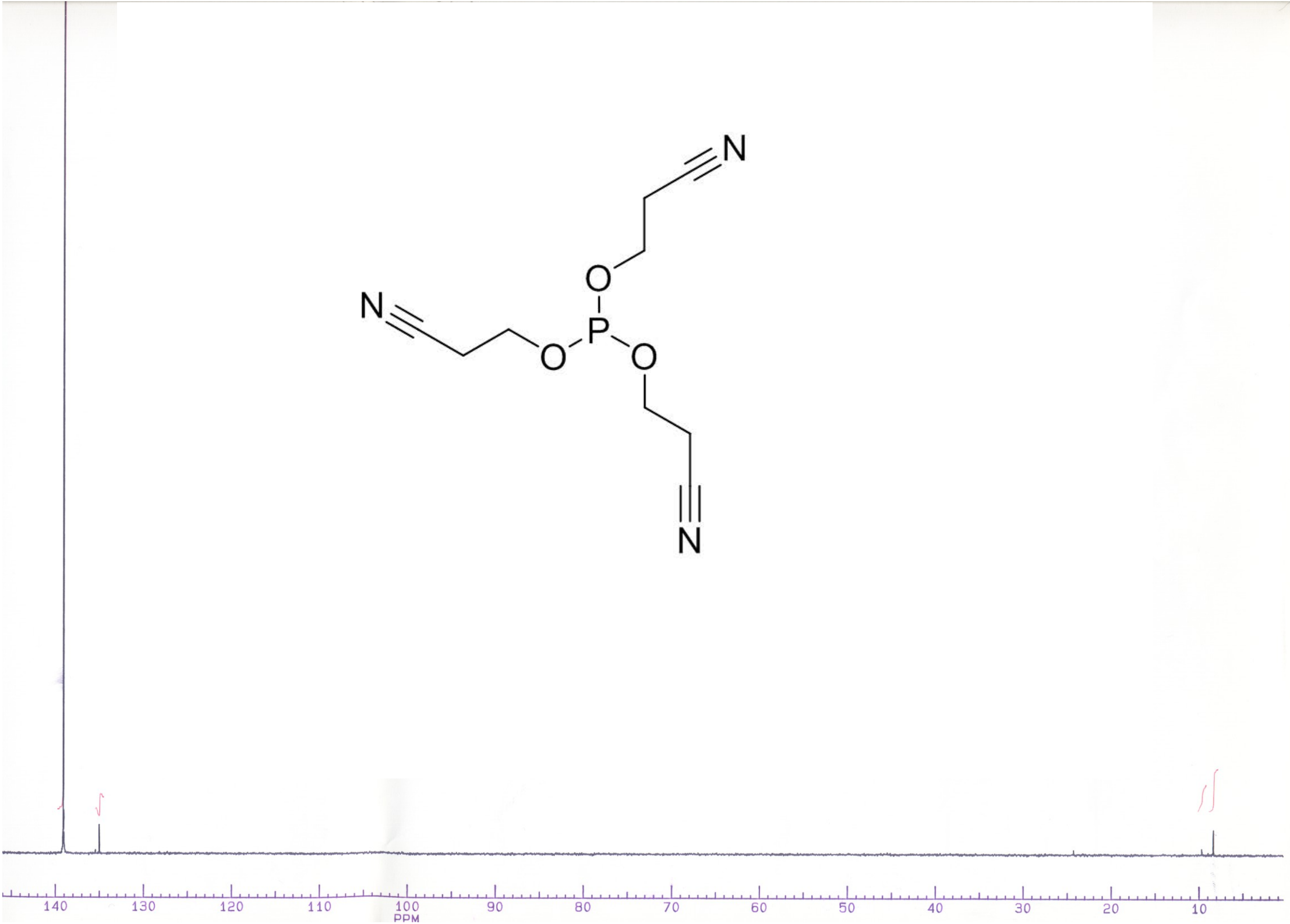
Tricyanoethyl phosphite, 13.

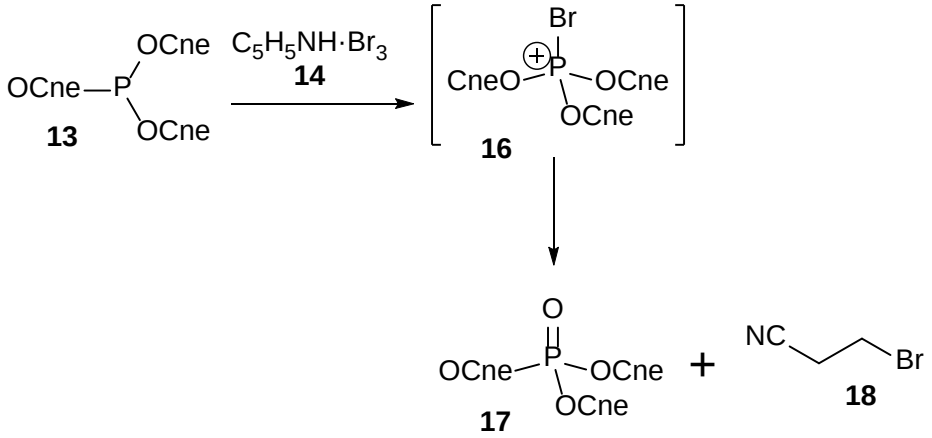
HRMS (ESI+) *m/z* found $[M+Na]^+$ = 264·0513, $C_9H_{12}O_3N_3PNa$ requires 264·0514.

N
O
P
O
O
N
N

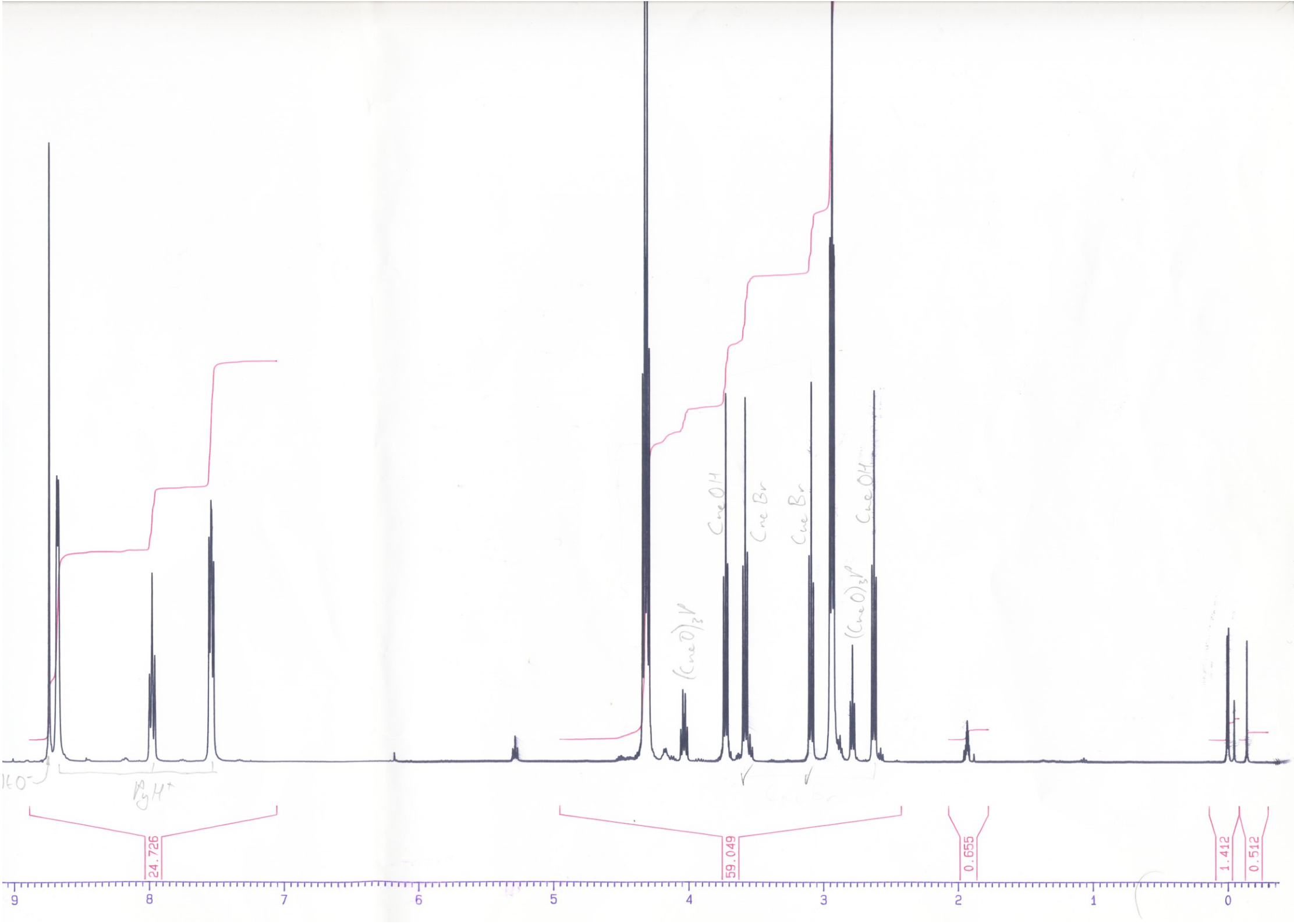

6.50
6.00
5.50
5.00
4.50
PPM
4.00
3.50
3.00
2.50
2.00
1.50
1.00
.50
0.0

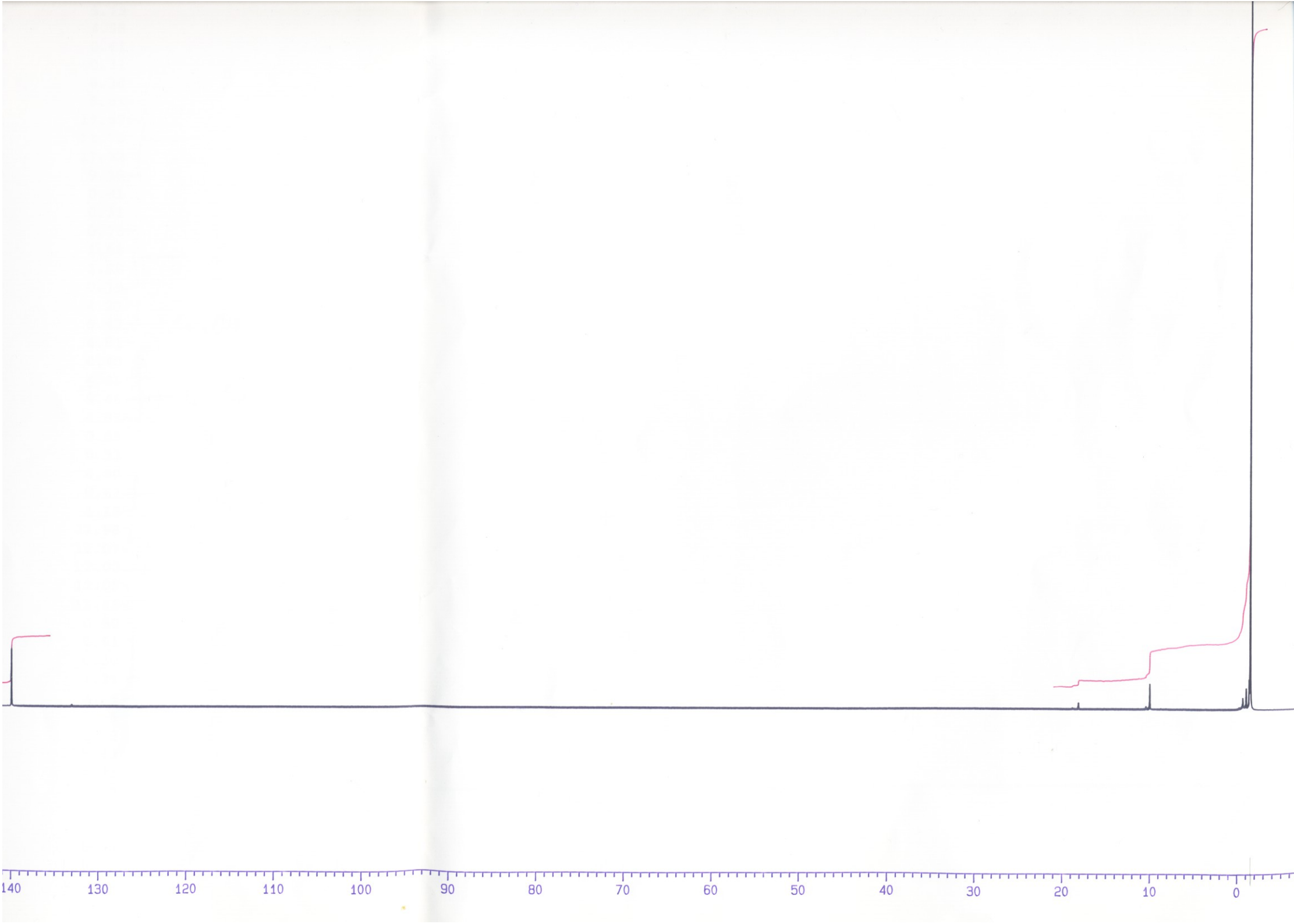
N
O
N
O
P
O
N

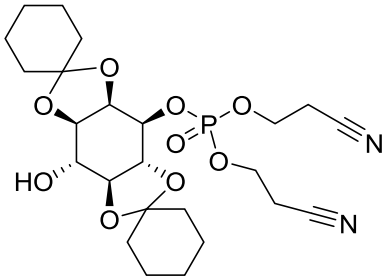

140
130
120
110
100
90
80
70
60
50
40
30
20
10
PPM



^{1}H NMR and ^{31}P NMR spectra relating to the reaction between tricyanotheyl phosphite, cyanoethanol and pyridinium bromide perbromide.

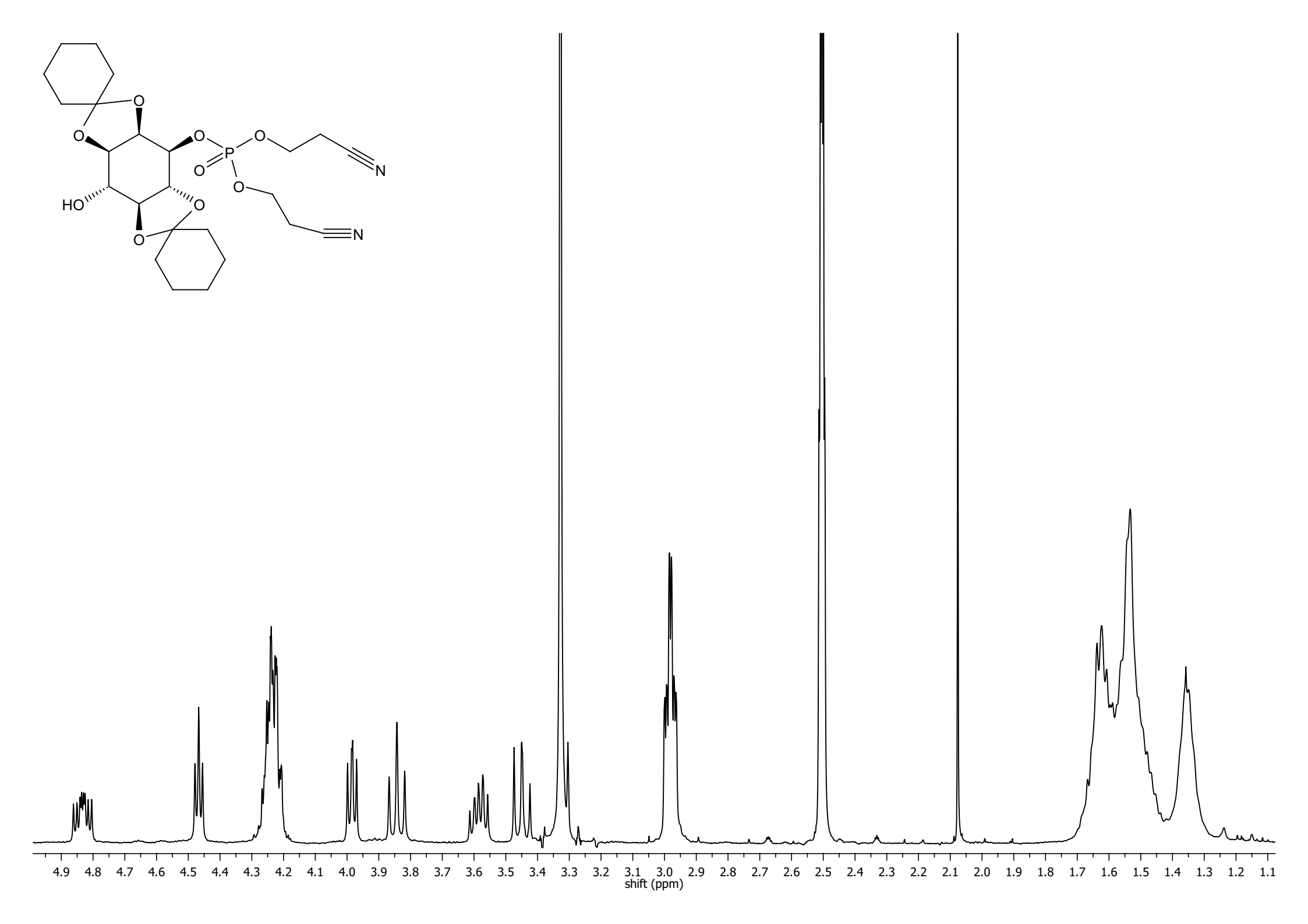


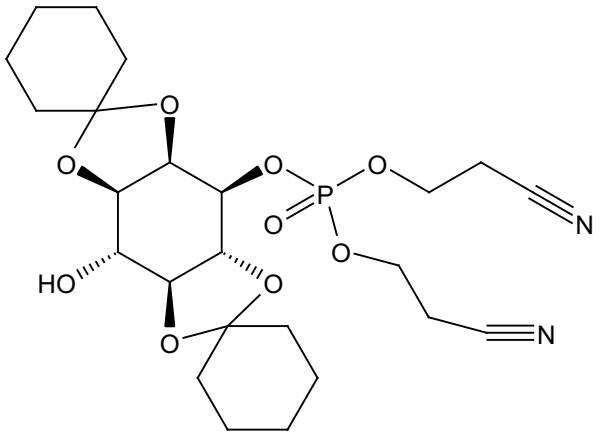


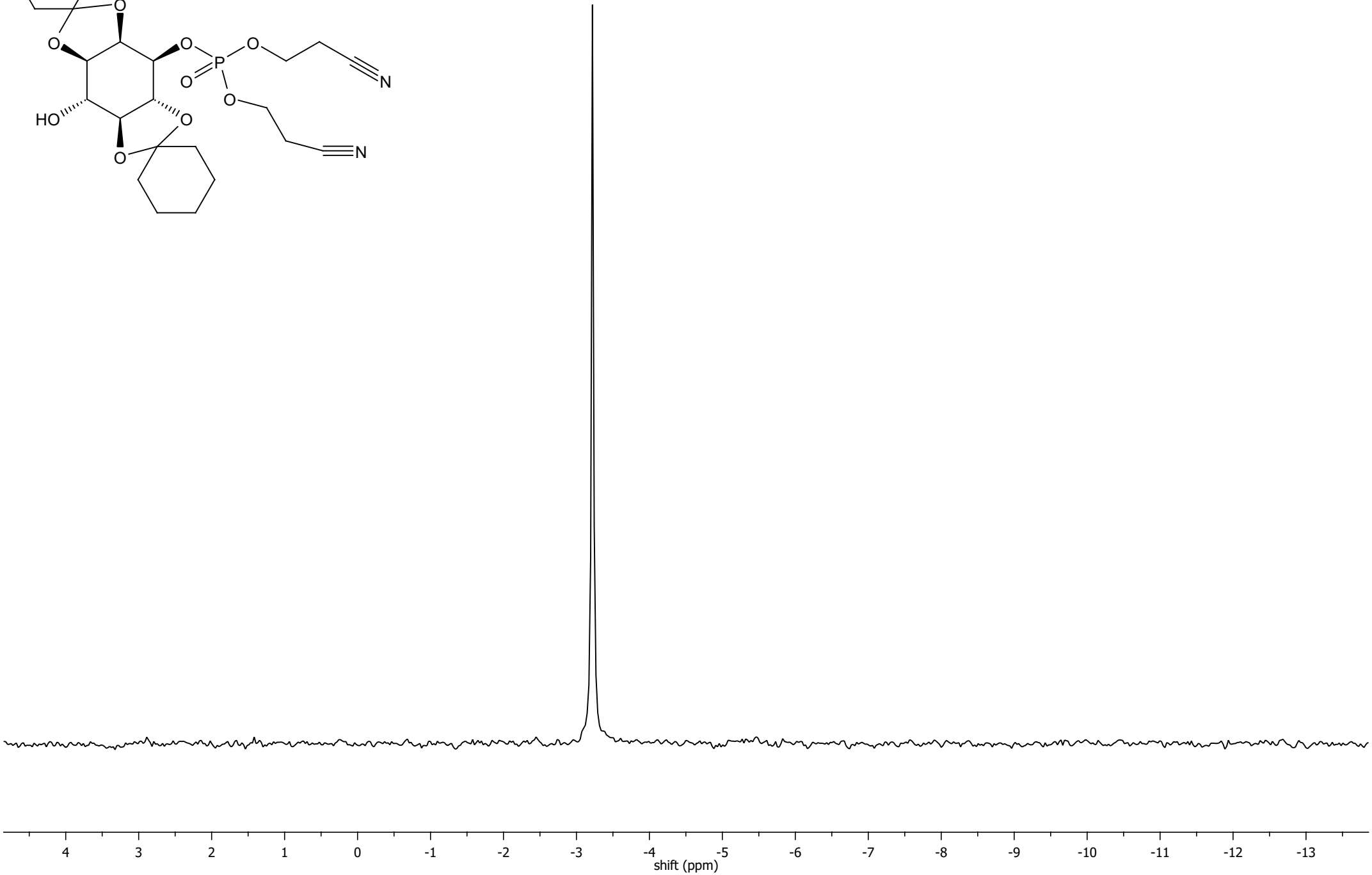


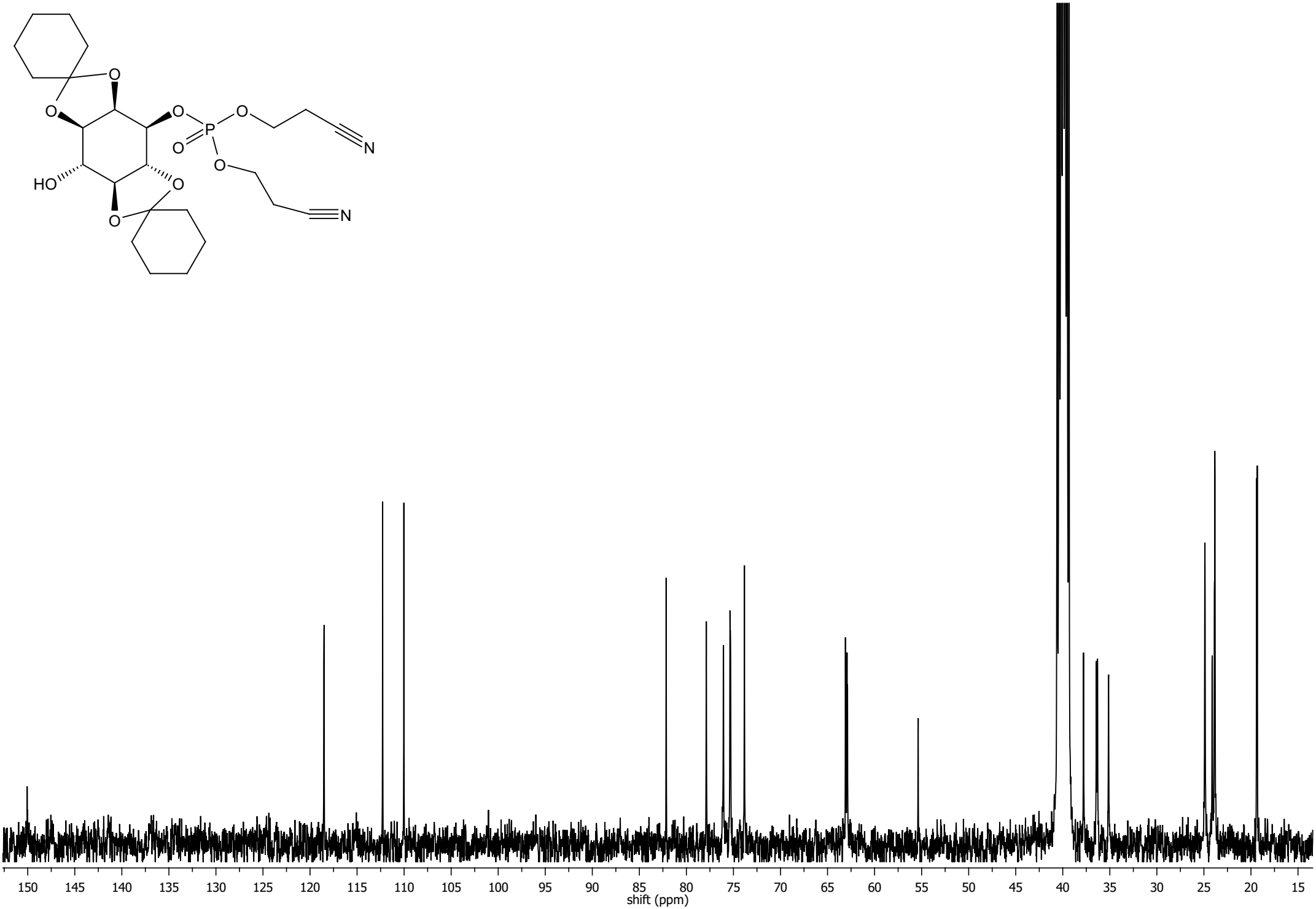
(-)-1-*O*-(Dicyanoethyloxy)phosphoryl-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 11.

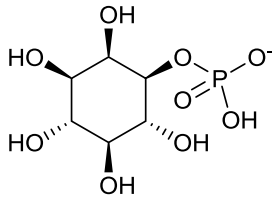
HRMS (ESI+) *m/z* found $[M+H]^+$ = 527·2141, $C_{24}H_{36}O_9N_2P$ requires 527·2158.


O
O
O
O
P
O
O
O
N
HO
O
O
O
N
4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1
shift (ppm)


O
O
O
O
P
O
O
O
N
HO
O
O
N

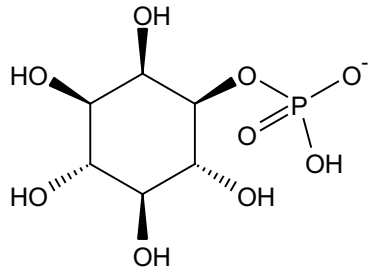

4
3
2
1
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
shift (ppm)

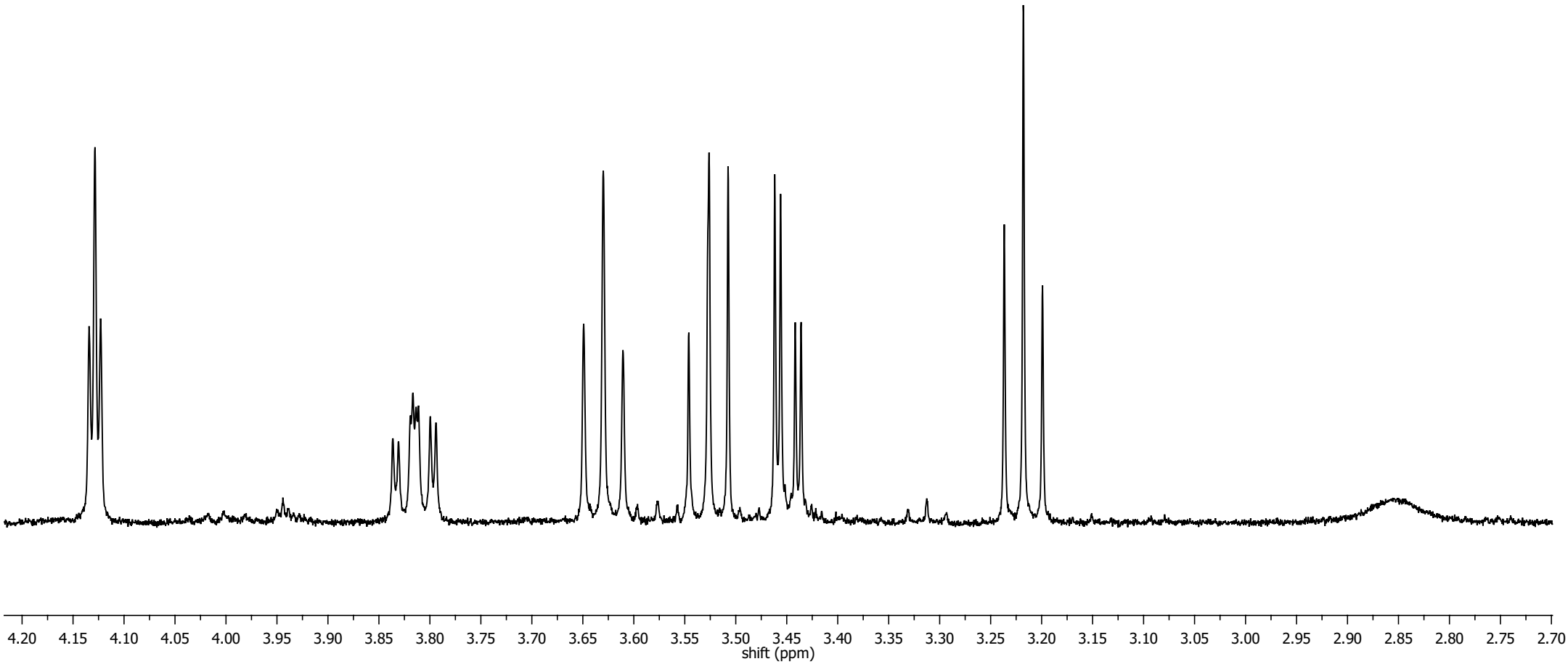

O
O
O
P
O
O
O
N
HO
O
O
N
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
shift (ppm)



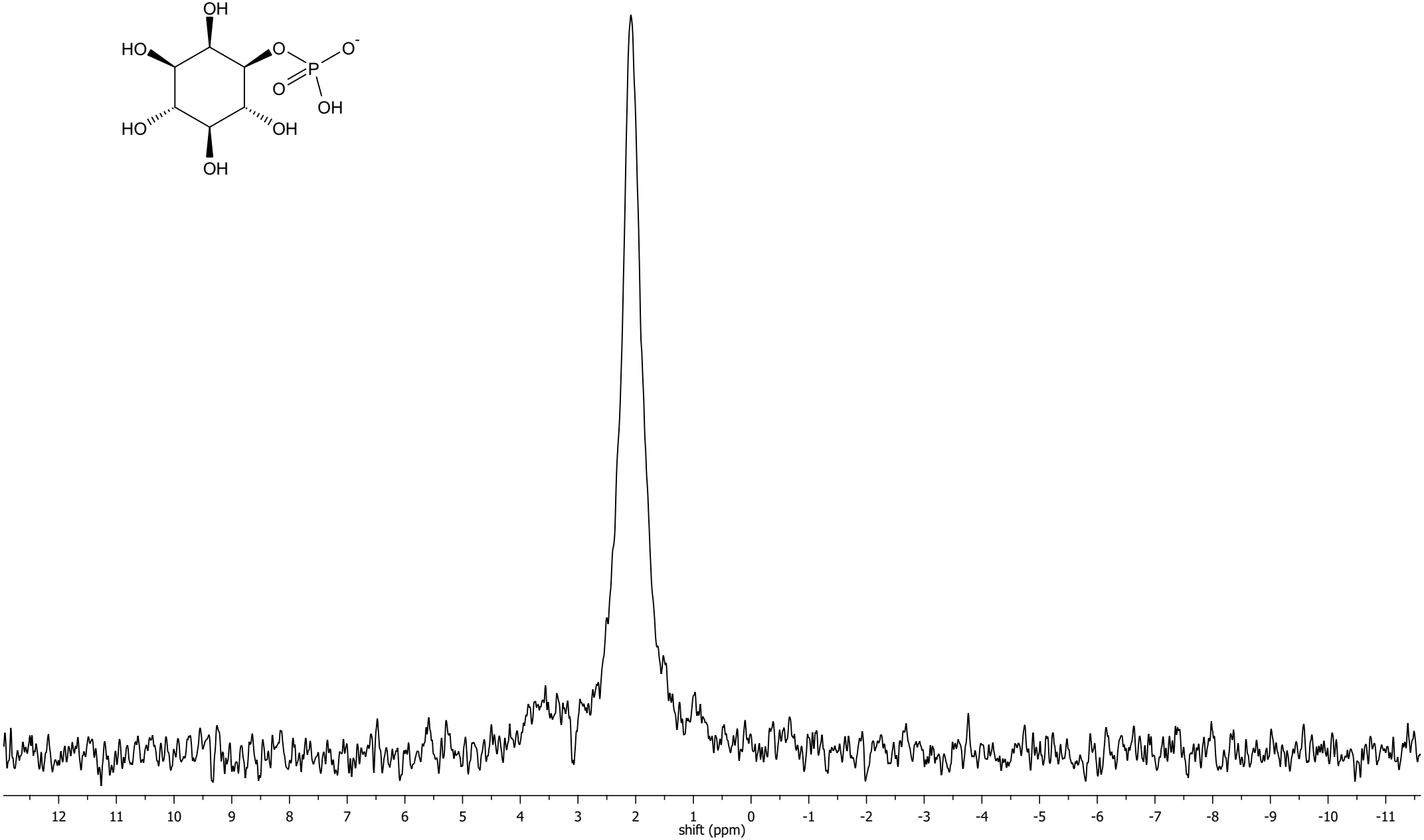
***myo*-Inositol-1-phosphate, 26.**

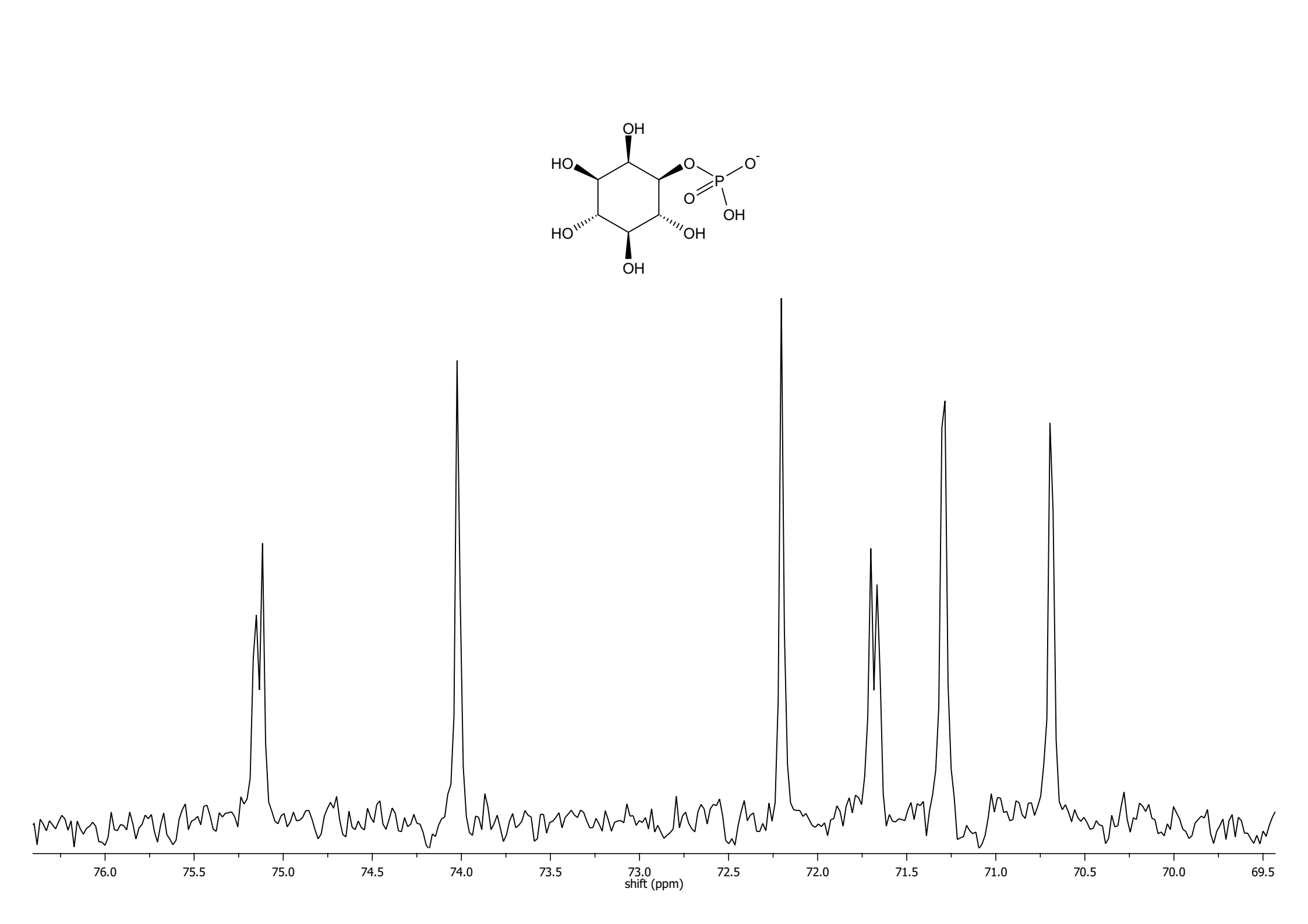
HRMS (ESI-) *m/z* found $[M-H]^-$ = 259·0210, $C_6H_{12}O_9P^-$ requires 259·0219.

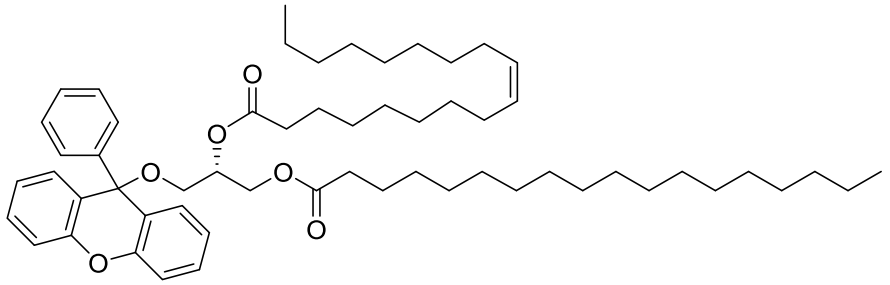

OH
HO
O
O-
P
O
OH
HO
OH
OH


4.20 4.15 4.10 4.05 4.00 3.95 3.90 3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25 3.20 3.15 3.10 3.05 3.00 2.95 2.90 2.85 2.80 2.75 2.70
shift (ppm)

OH
HO
O
O-
P
O
OH
HO
OH
OH

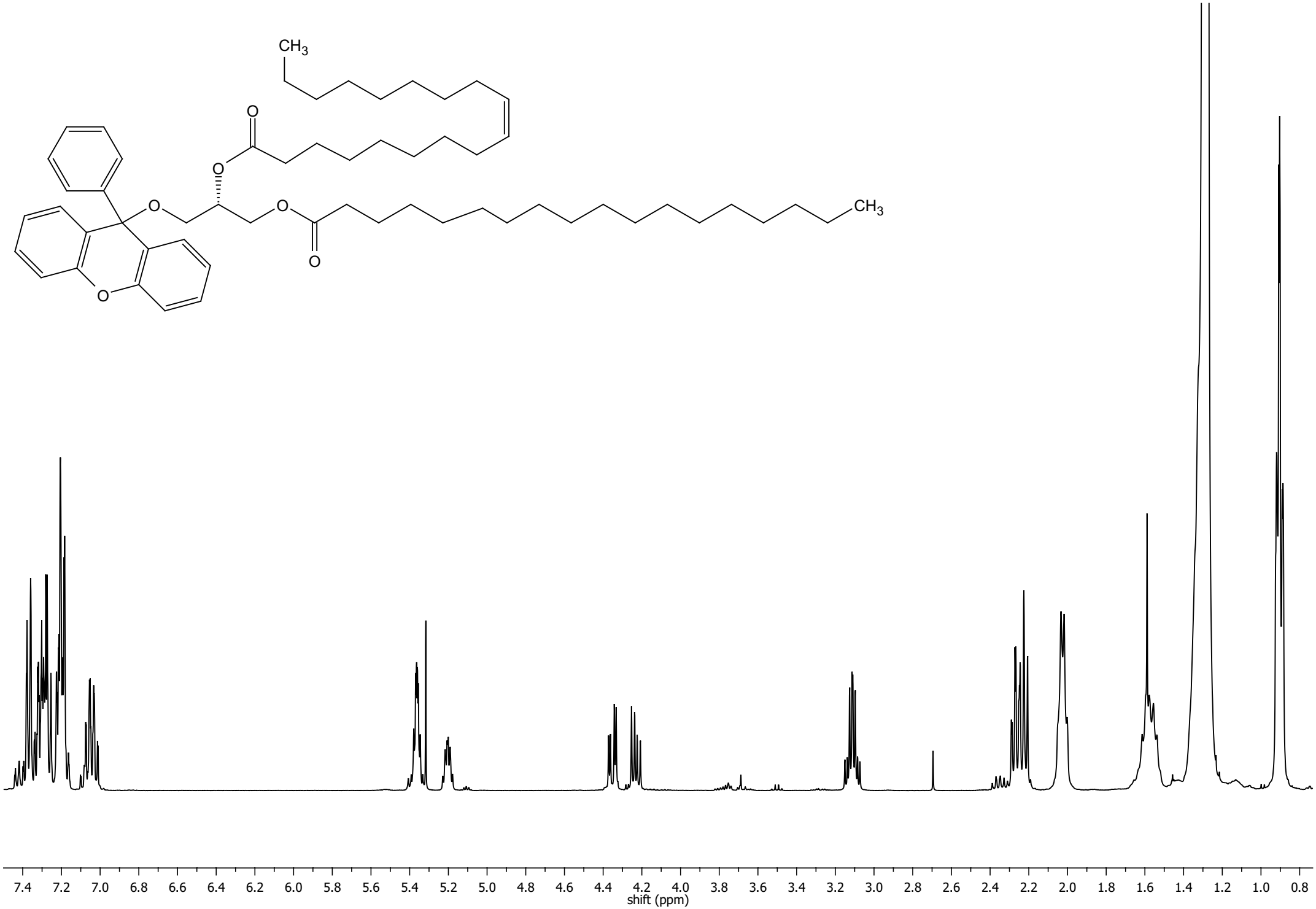

12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
shift (ppm)

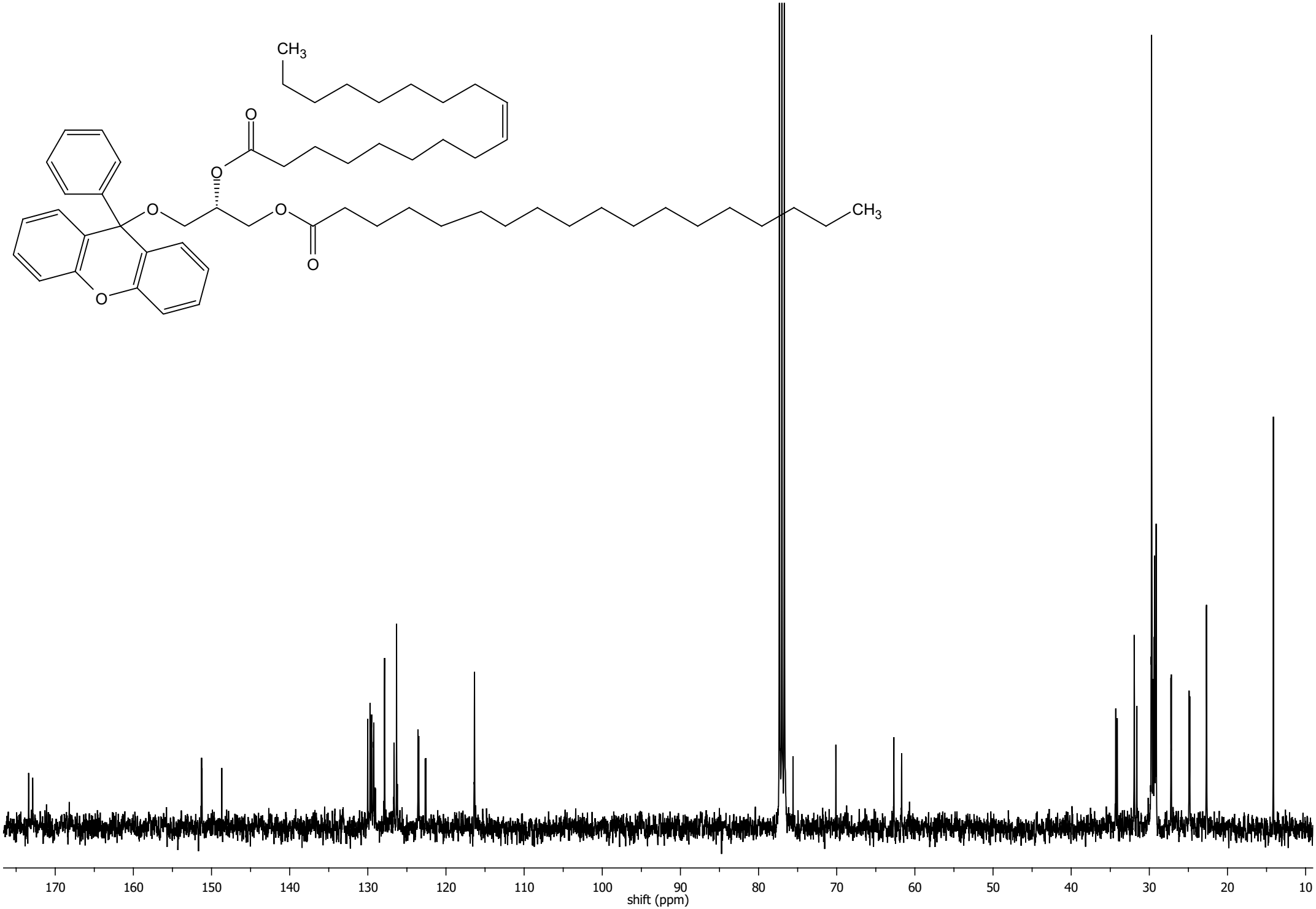

OH
HO
O
O
P
O
OH
HO
OH
OH
76.0
75.5
75.0
74.5
74.0
73.5
73.0
72.5
72.0
71.5
71.0
70.5
70.0
69.5
shift (ppm)

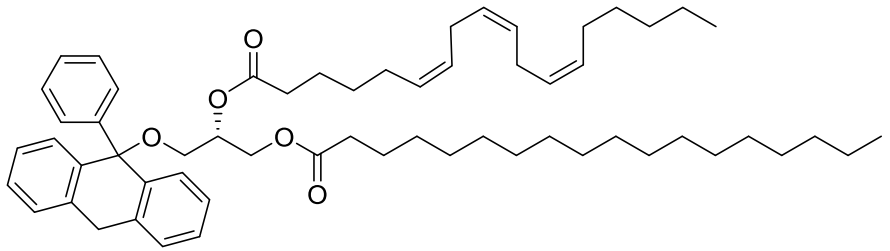


***sn*-1-*O*-Stearoyl-2-*O*-oleoyl-3-*O*-(9-phenylxanthen-9-yl) glycerol.**

HRMS (ESI+) *m/z* found $[M+Na]^+$ = 901·6354, $C_{58}H_{86}O_6Na$ requires 901·6322.

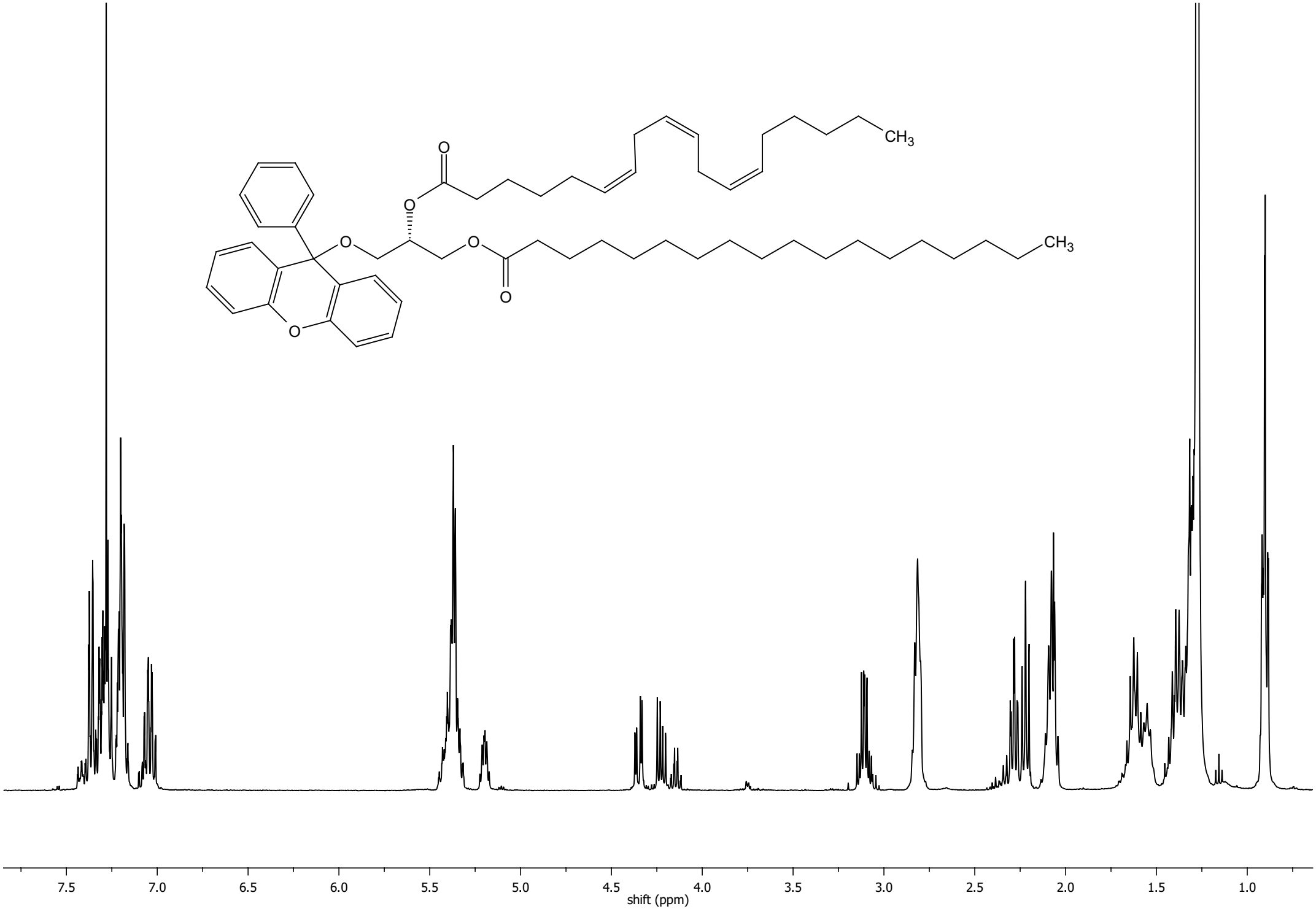

CH3
O
O
O
O
O
O
CH3
7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
shift (ppm)


CH3
O
O
O
O
O
O
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)

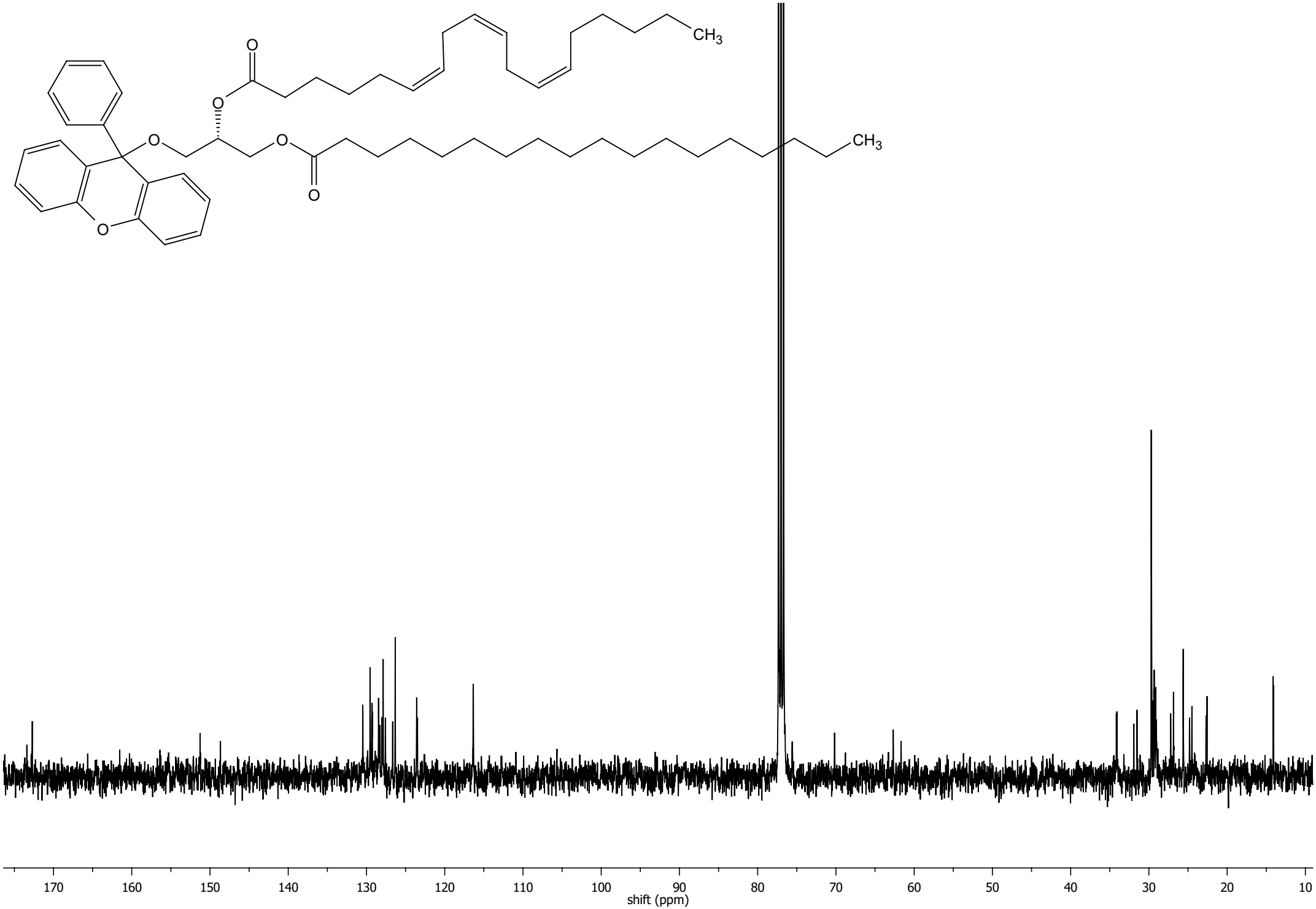


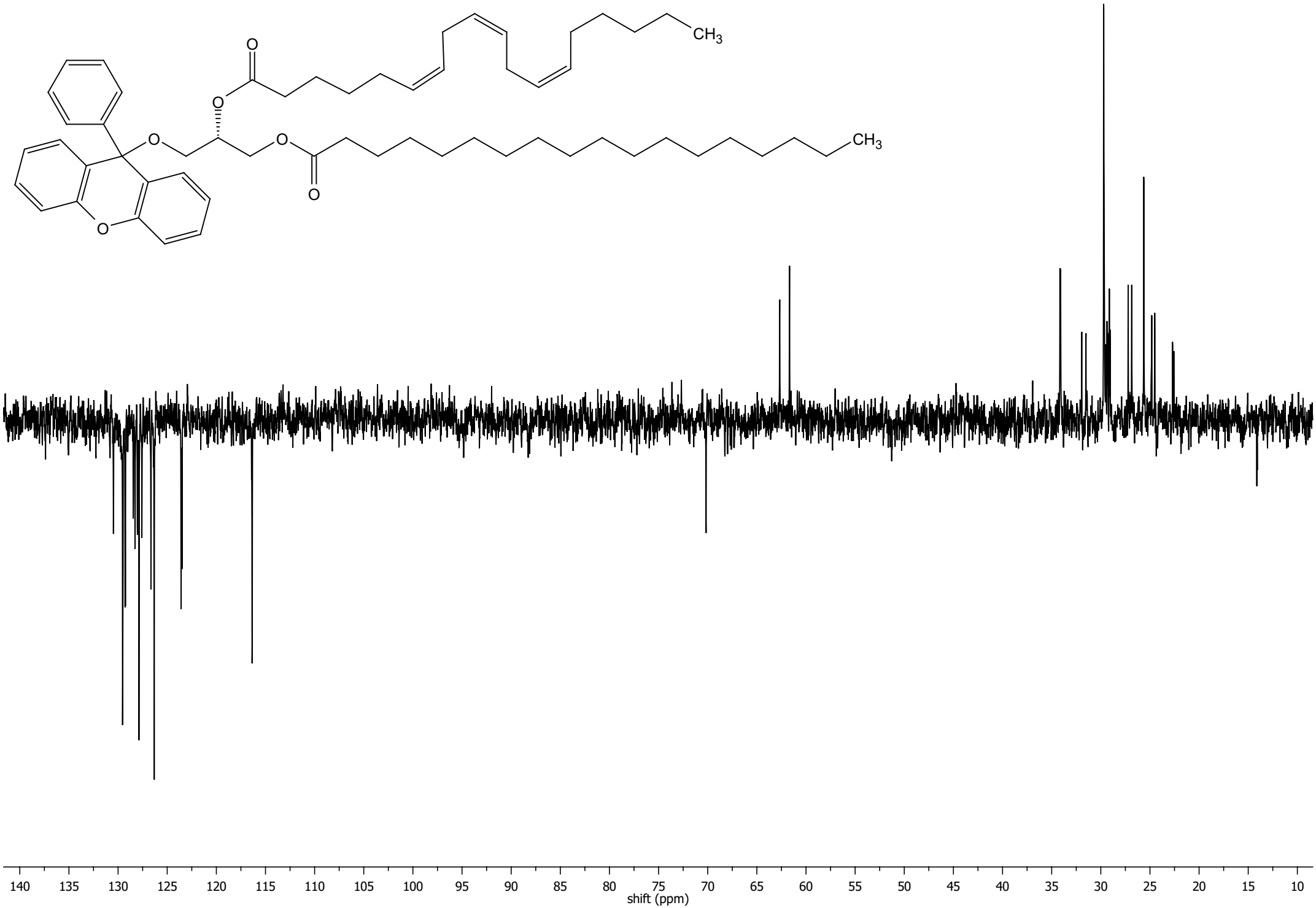
_sn_-1-_O_-Stearoyl-2-_O_-γ-linolenoyl-3-_O_-(9-phenylxanthen-9-yl) glycerol.

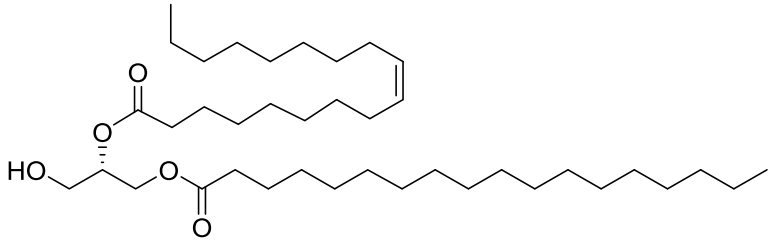
HRMS (ESI+) *m/z* found $[M+Na]^+$ = 897·6018, $C_{58}H_{82}O_6Na$ requires 897·6009.


CH3
O
O
O
O
O
O
O
CH3
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
shift (ppm)

CH3
O
O
O
O
O
O
CH3

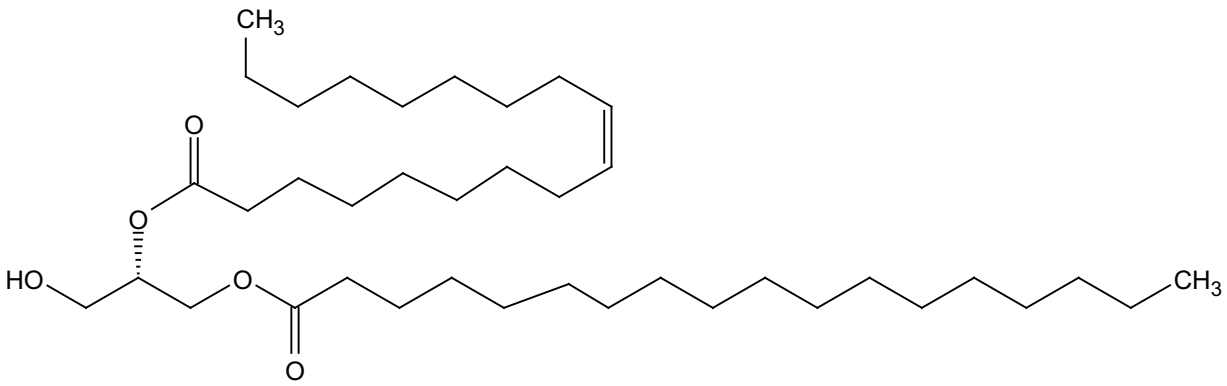

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)


CH3
O
O
O
O
O
O
O
CH3
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 10
shift (ppm)

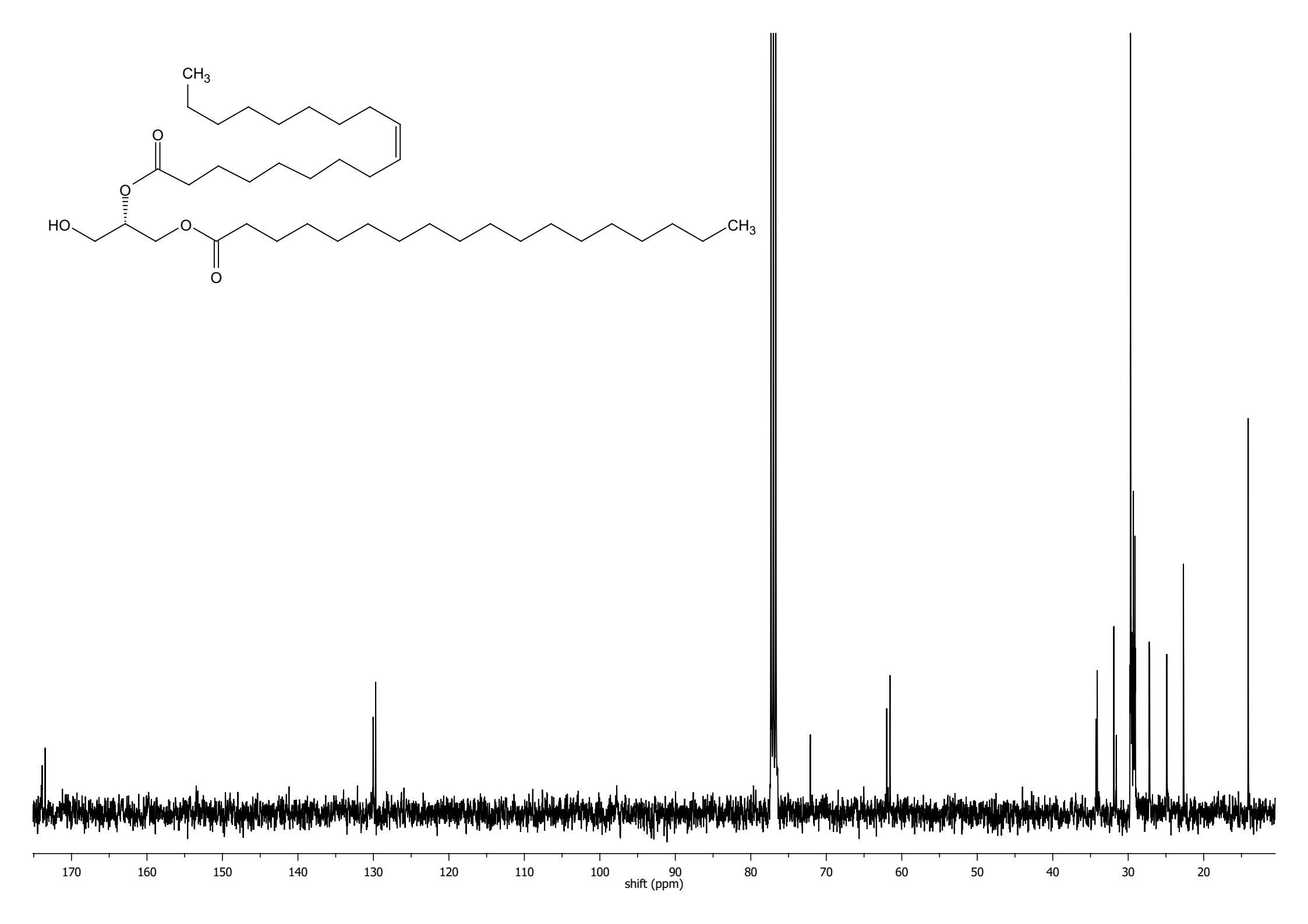


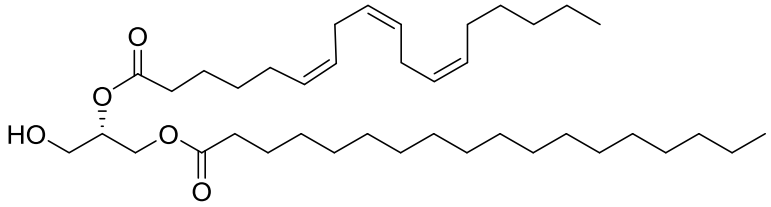
***sn*-1-*O*-Stearoyl-2-*O*-oleoyl glycerol, 19b**.

HRMS (ESI+) *m/z* $[M+H]^+$ = 623·5623, $C_{39}H_{75}O_5^+$ requires 623·5610.


CH3
O
O
HO
O
CH3
O

5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
shift (ppm)

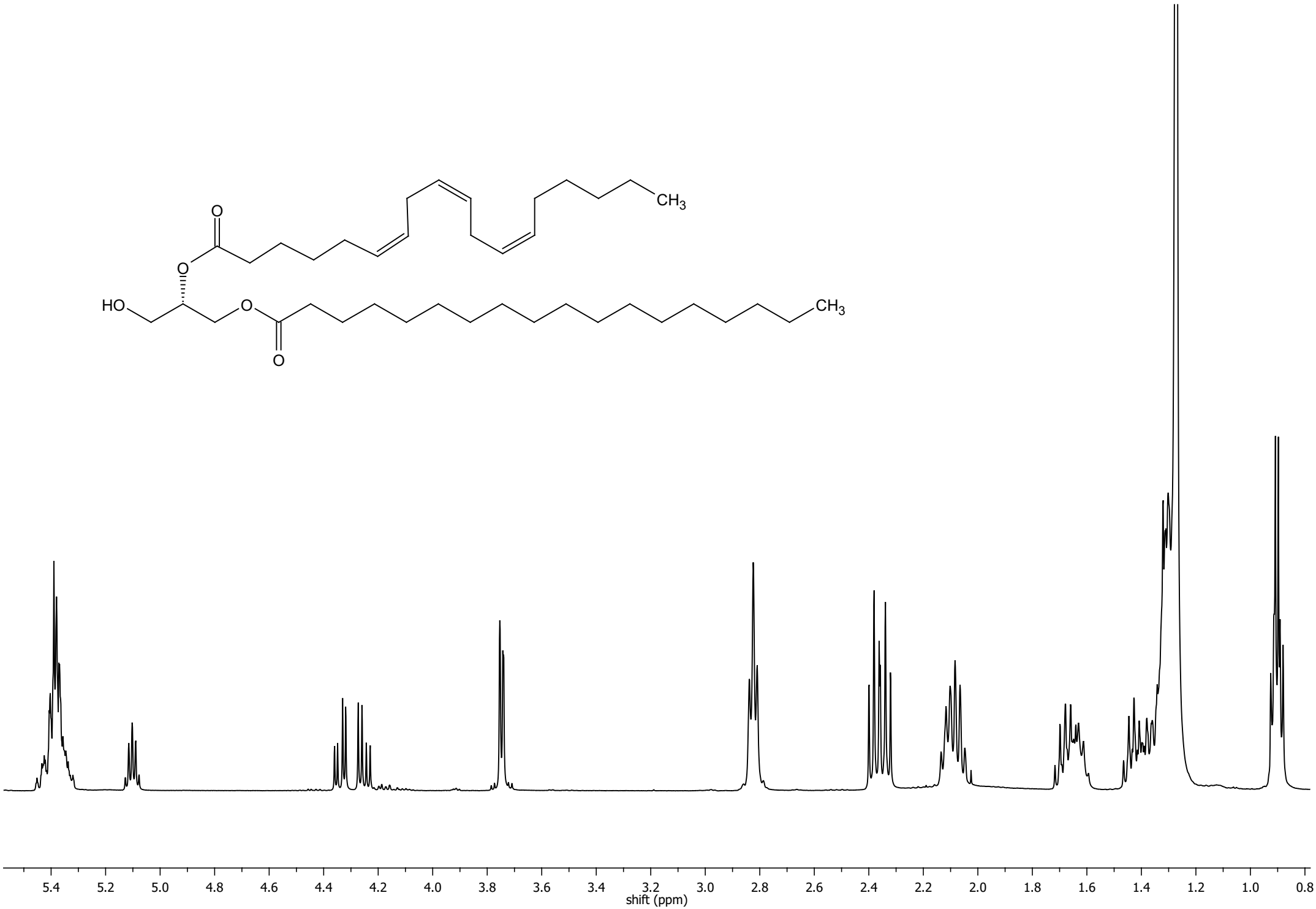

CH3
O
O
HO
O
CH3
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
shift (ppm)

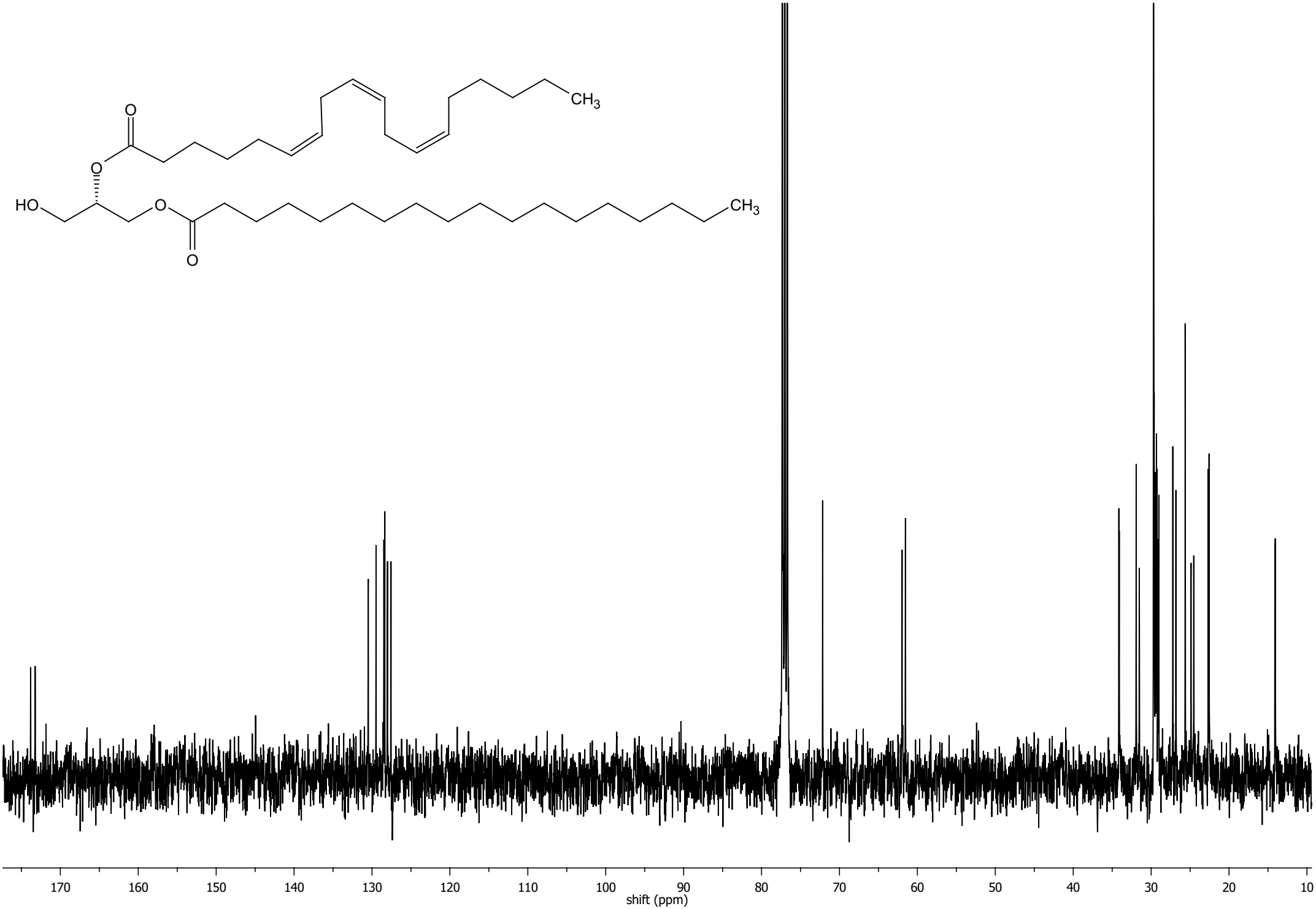


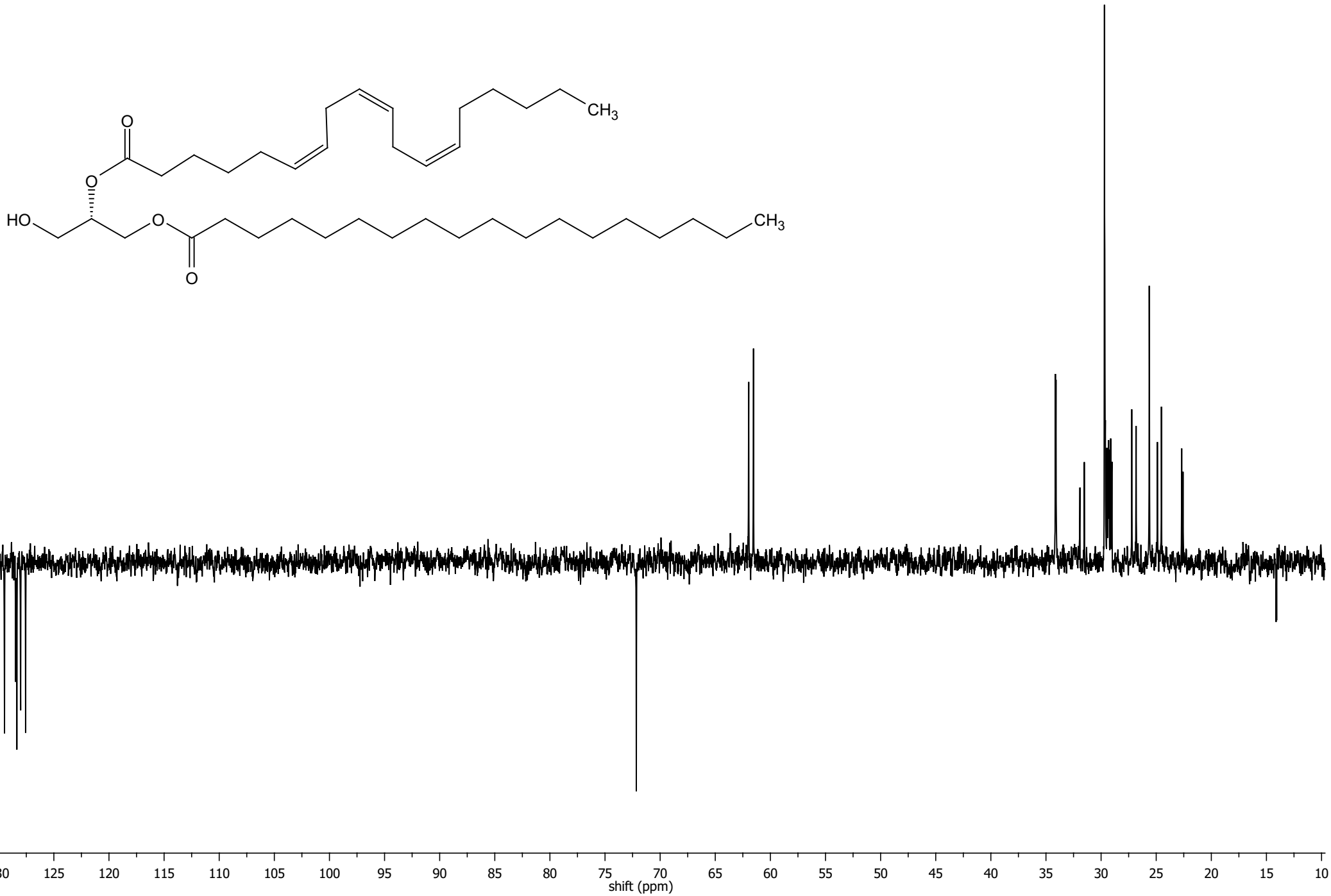
***sn*-1-*O*-Stearoyl-2-*O*-*γ*-linolenoyl glycerol, 19c.**

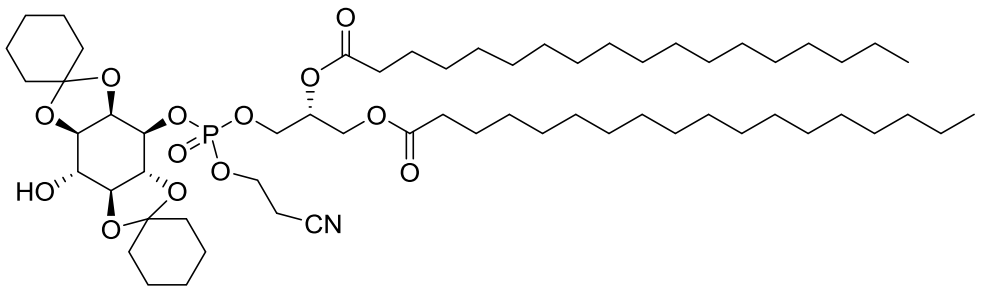
HRMS (ESI+) *m/z* found $[M+H]^+$ = 619·5006, $C_{39}H_{71}O_5$ requires 619·5050.

HO
O
O
O
O
O
CH3
CH3


5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
shift (ppm)

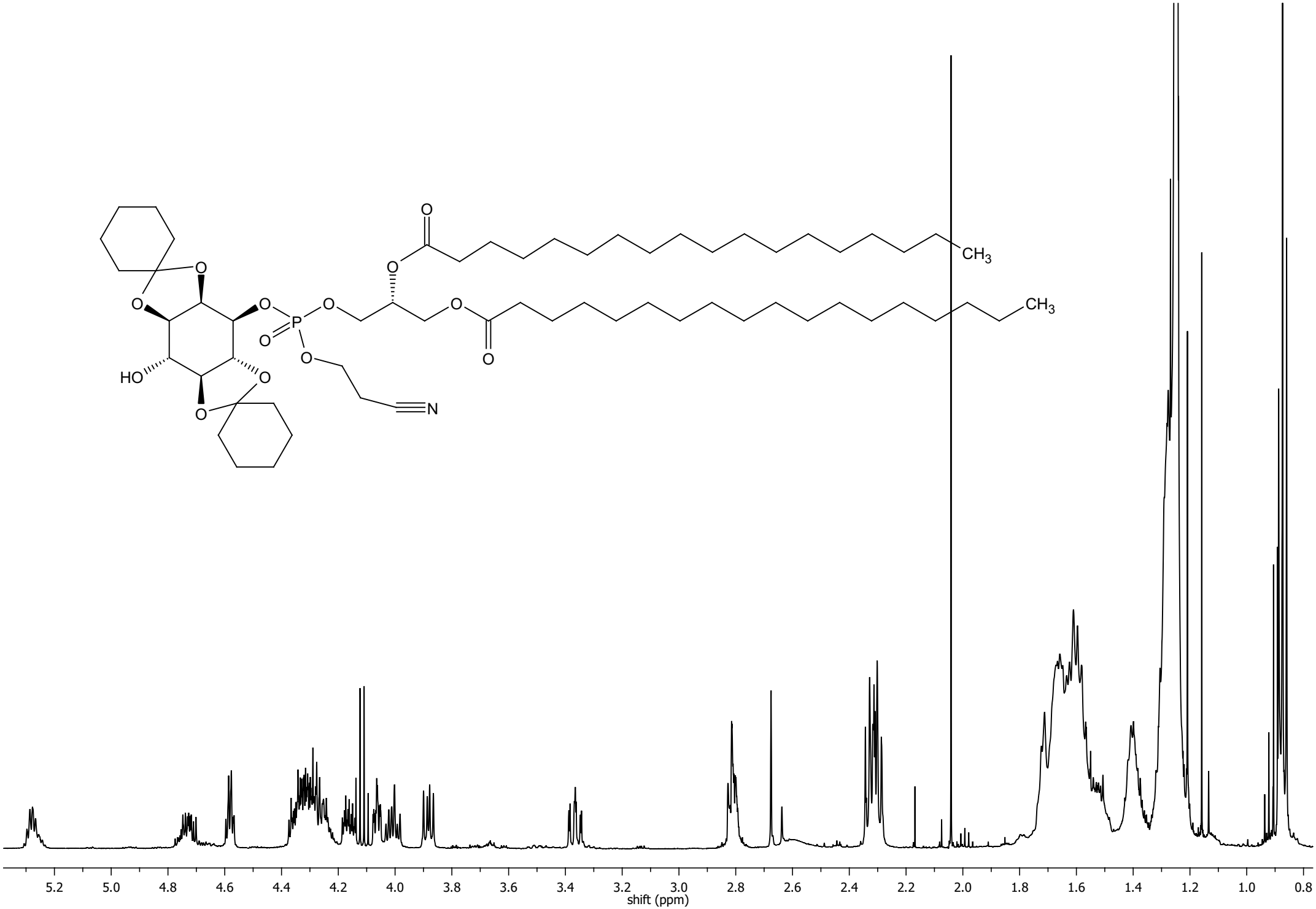

HO
O
O
O
O
O
CH3
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)

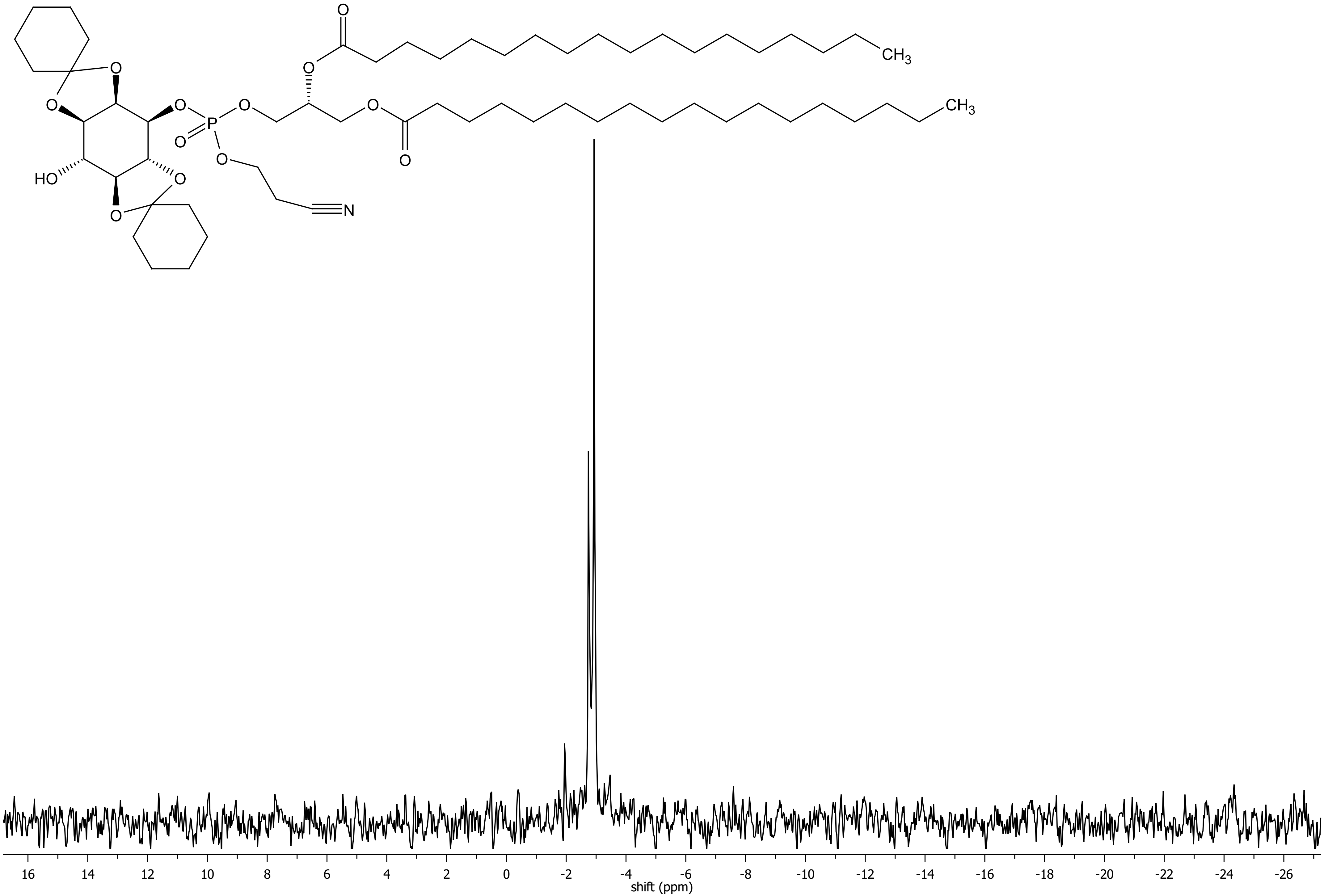

HO
O
O
O
O
O
CH3
CH3
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
shift (ppm)



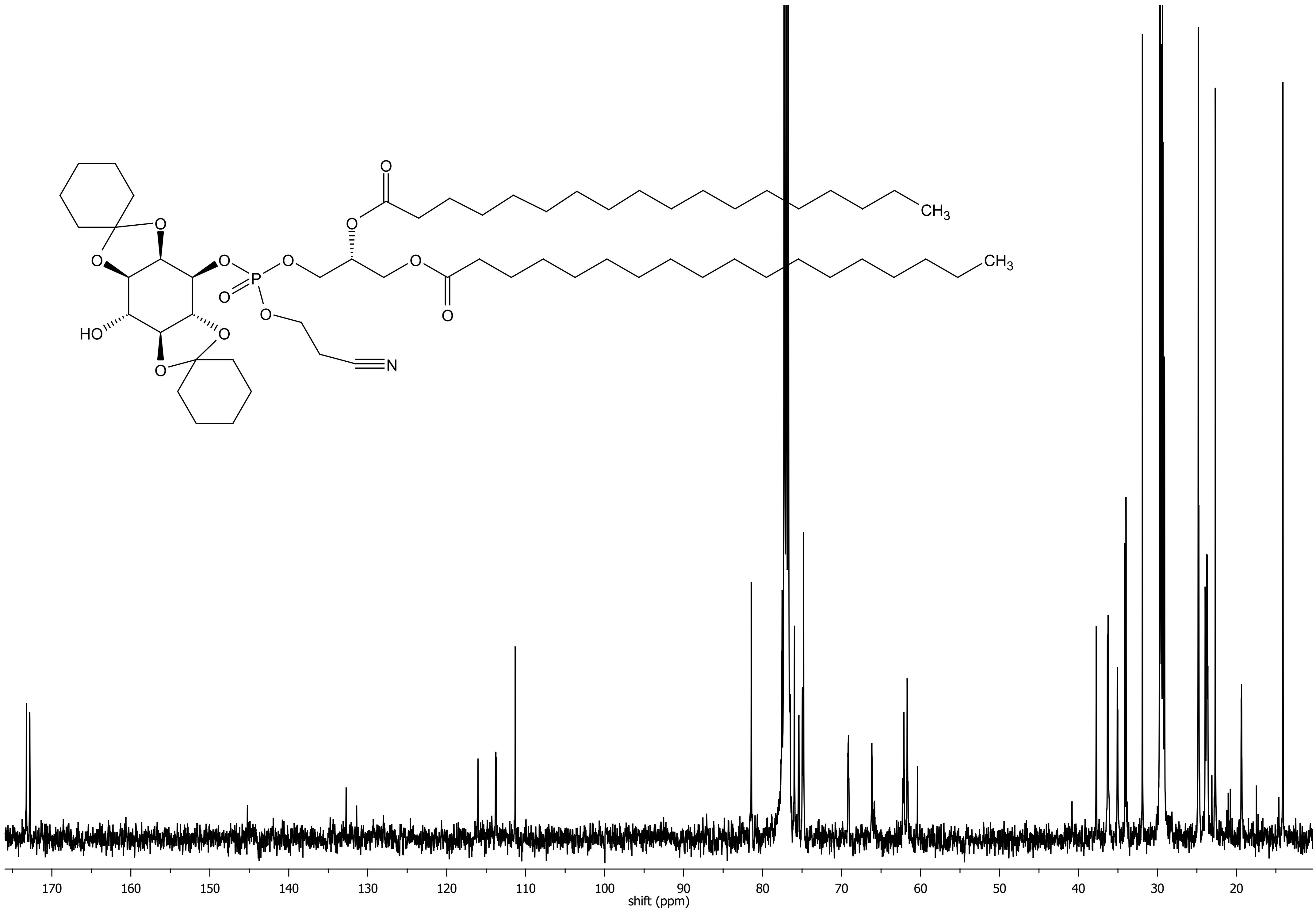
1-*O*-[(Cyanoethyloxy)(*sn*-1,2-*O*-distearoylglyceryloxy) phosphoryl]-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 23a.

HRMS (ESI+) *m/z* found $[M+H]^+$ 1,080·7462, $C_{60}H_{107}NO_{13}P$ requires 1,080·7480.

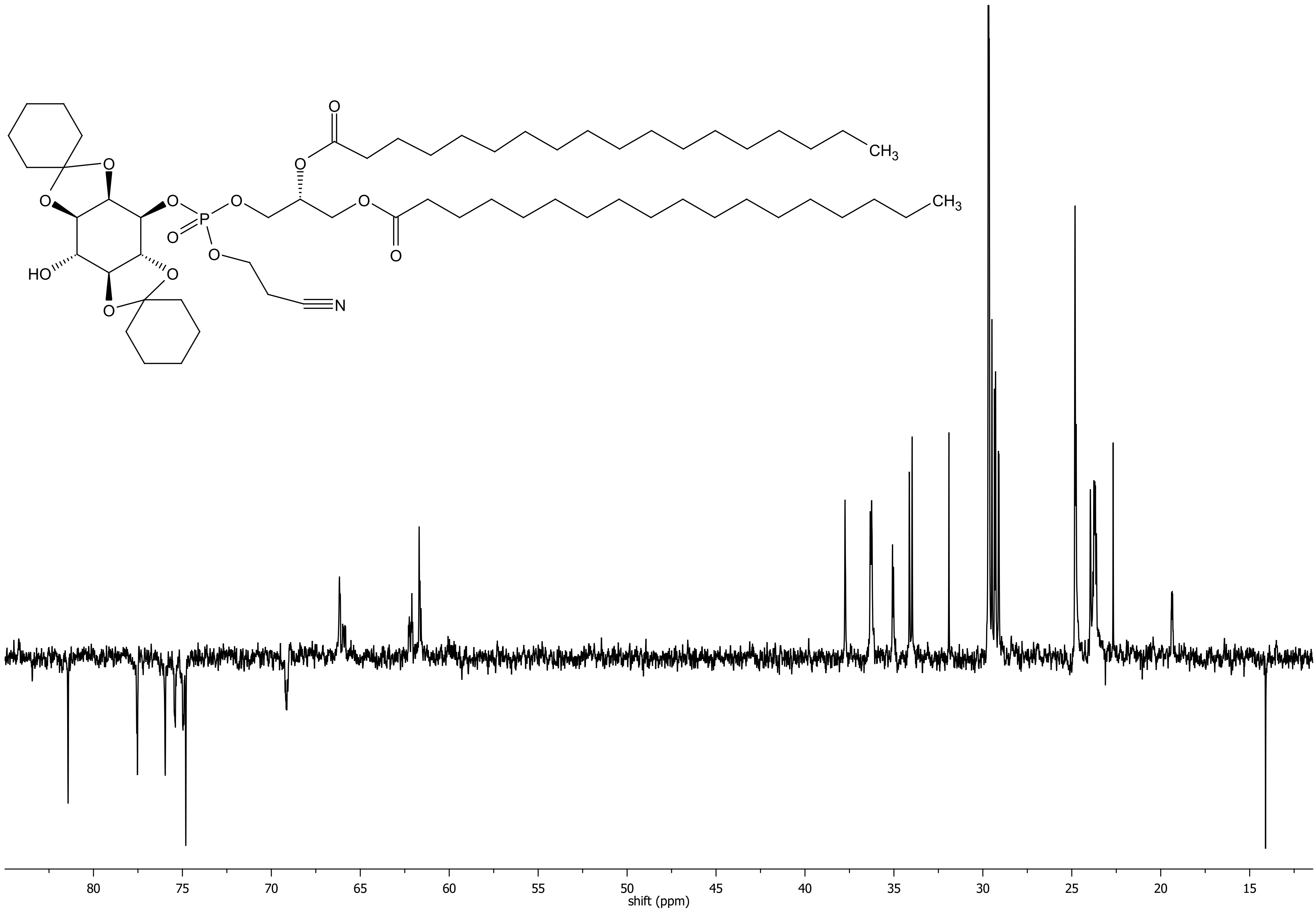

HO
O
P
N
CH3
CH3
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
shift (ppm)



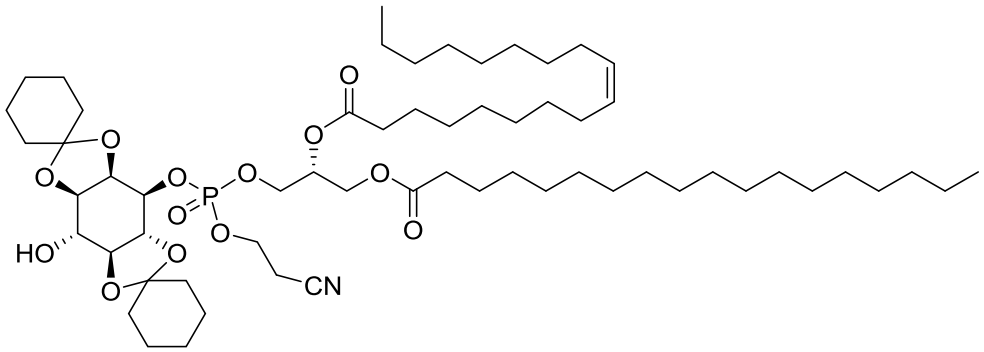
shift (ppm)



O
O
O
O
P
O
O
O
O
O
O
HO
O
O
O
N
CH3
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
shift (ppm)

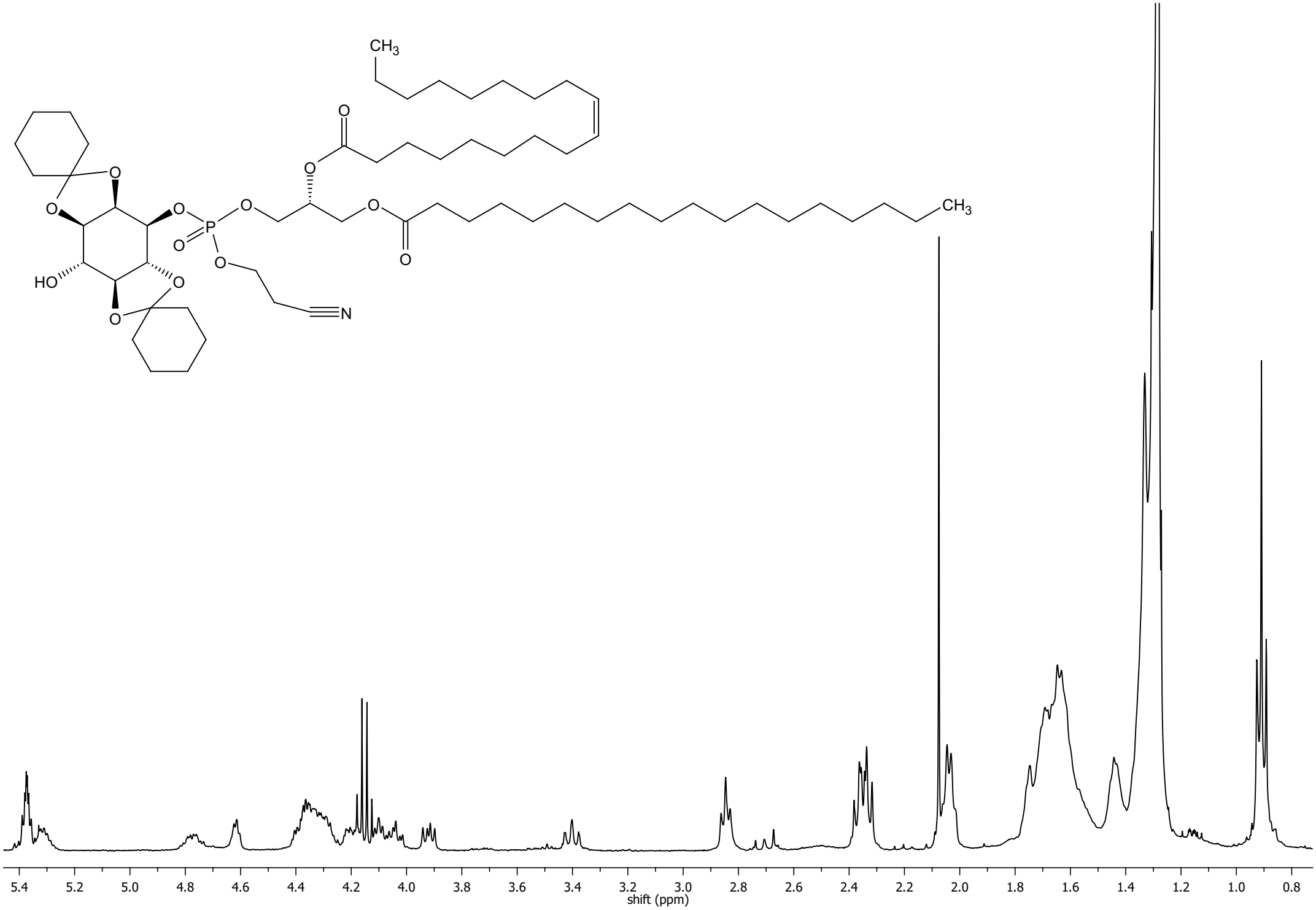


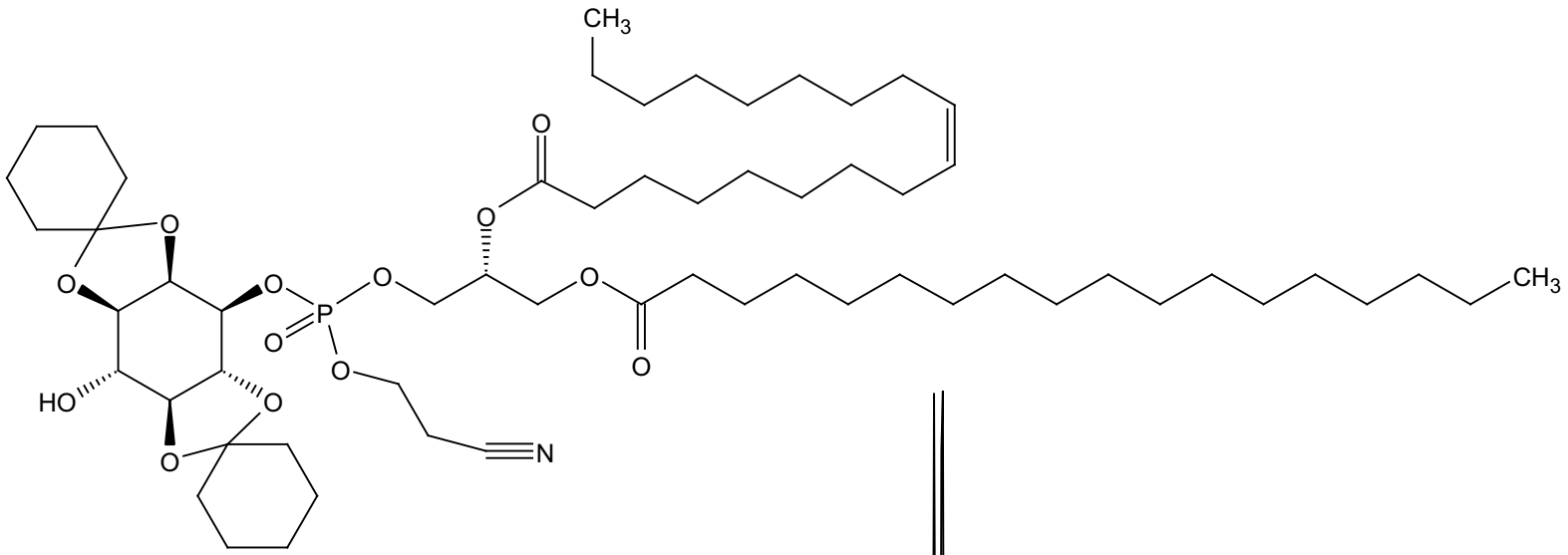
O
O
O
O
O
O
P
O
O
O
O
HO
O
O
O
N
CH3
CH3
80
75
70
65
60
55
50
45
40
35
30
25
20
15
shift (ppm)

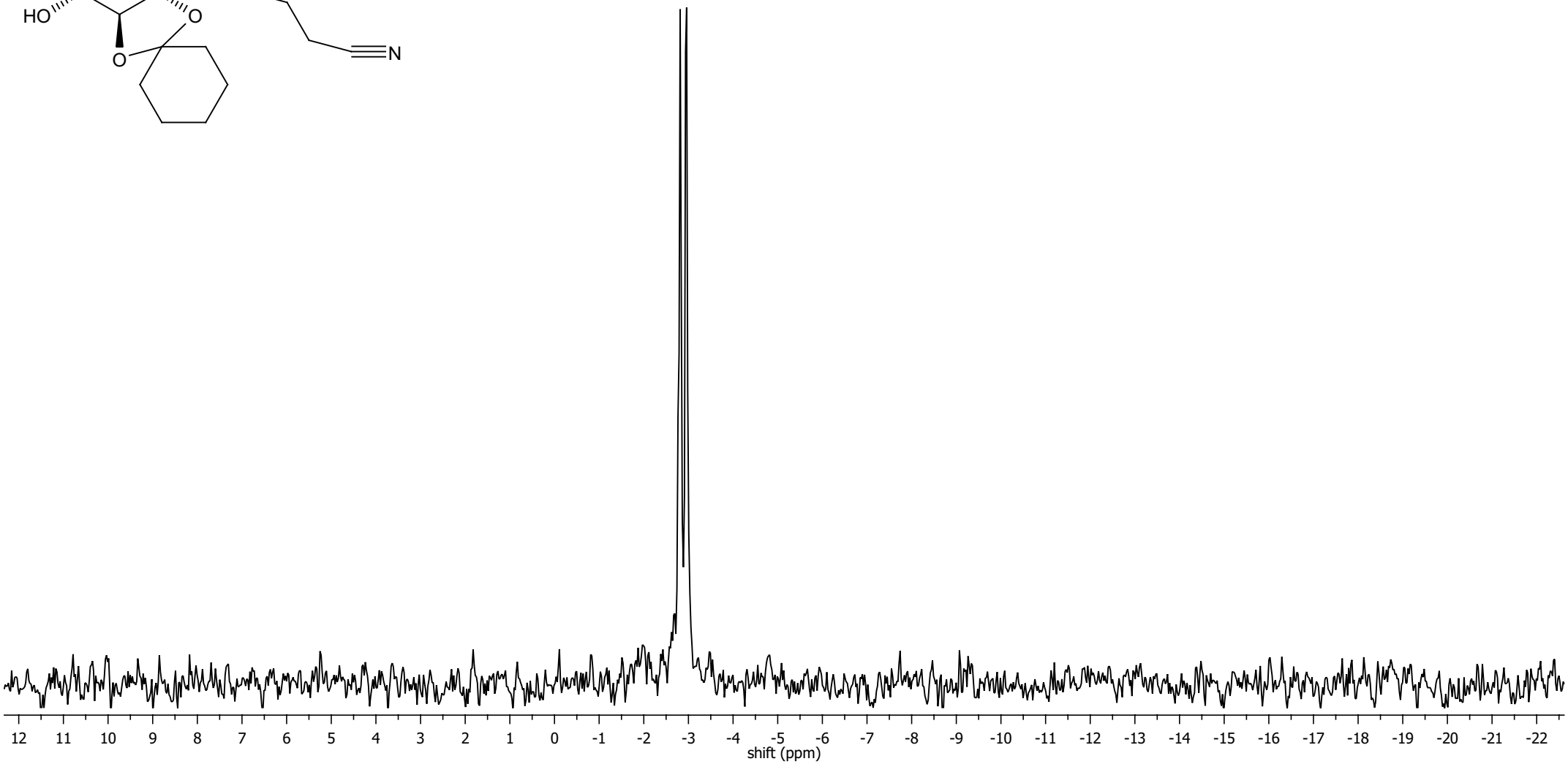


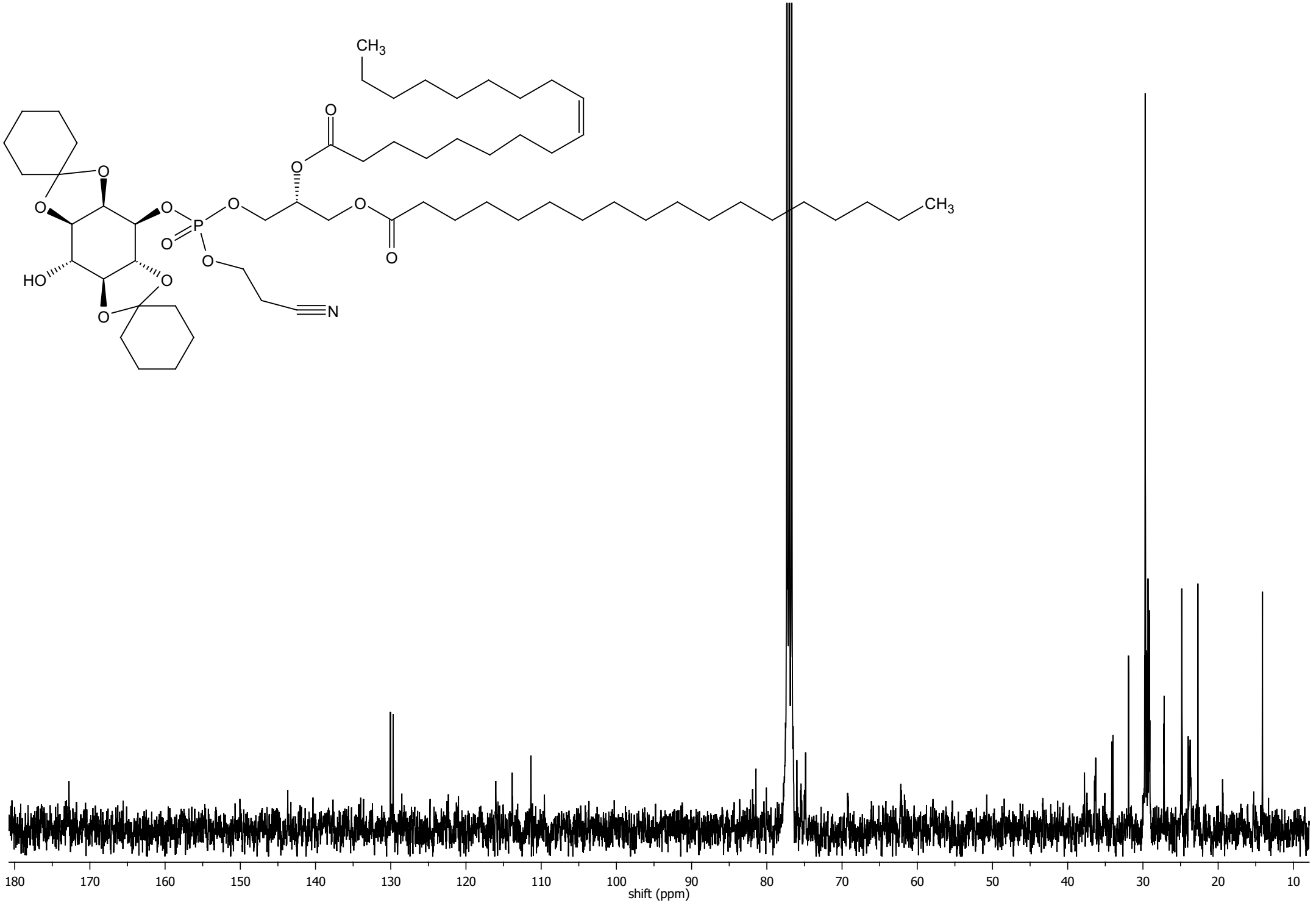
1-*O*-[(Cyanoethyloxy)(*sn*-1-*O*-stearoyl-2-oleoylglyceryloxy) phosphoryl]-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 23b.

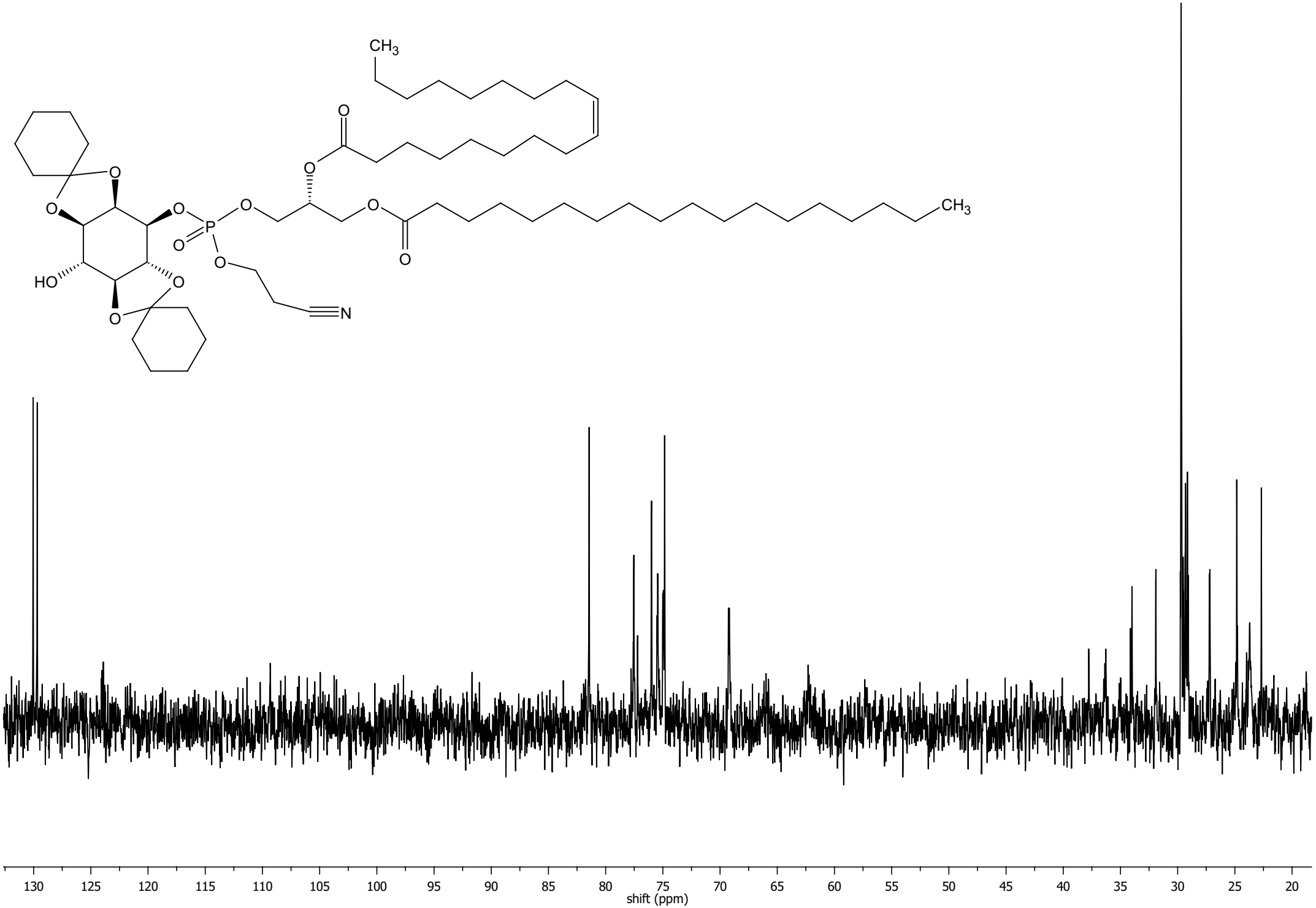
HRMS (ESI+) *m/z* found $[M+H]^+$ = 1,078·7323, $C_{60}H_{105}NO_{13}P$ requires 1,078·7324.

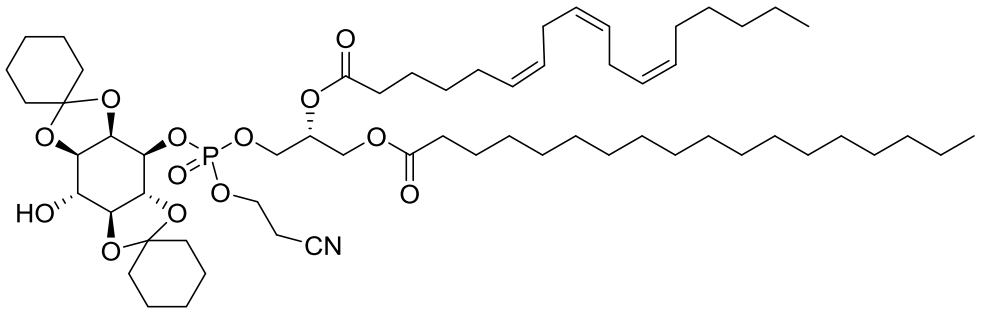

CH3
O
O
O
O
O
O
P
O
O
O
O
HO
O
O
N
CH3
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
shift (ppm)


CH3
O
O
O
O
O
O
O
P
O
O
O
O
HO
O
O
N
CH3


12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7 -8 -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19 -20 -21 -22
shift (ppm)

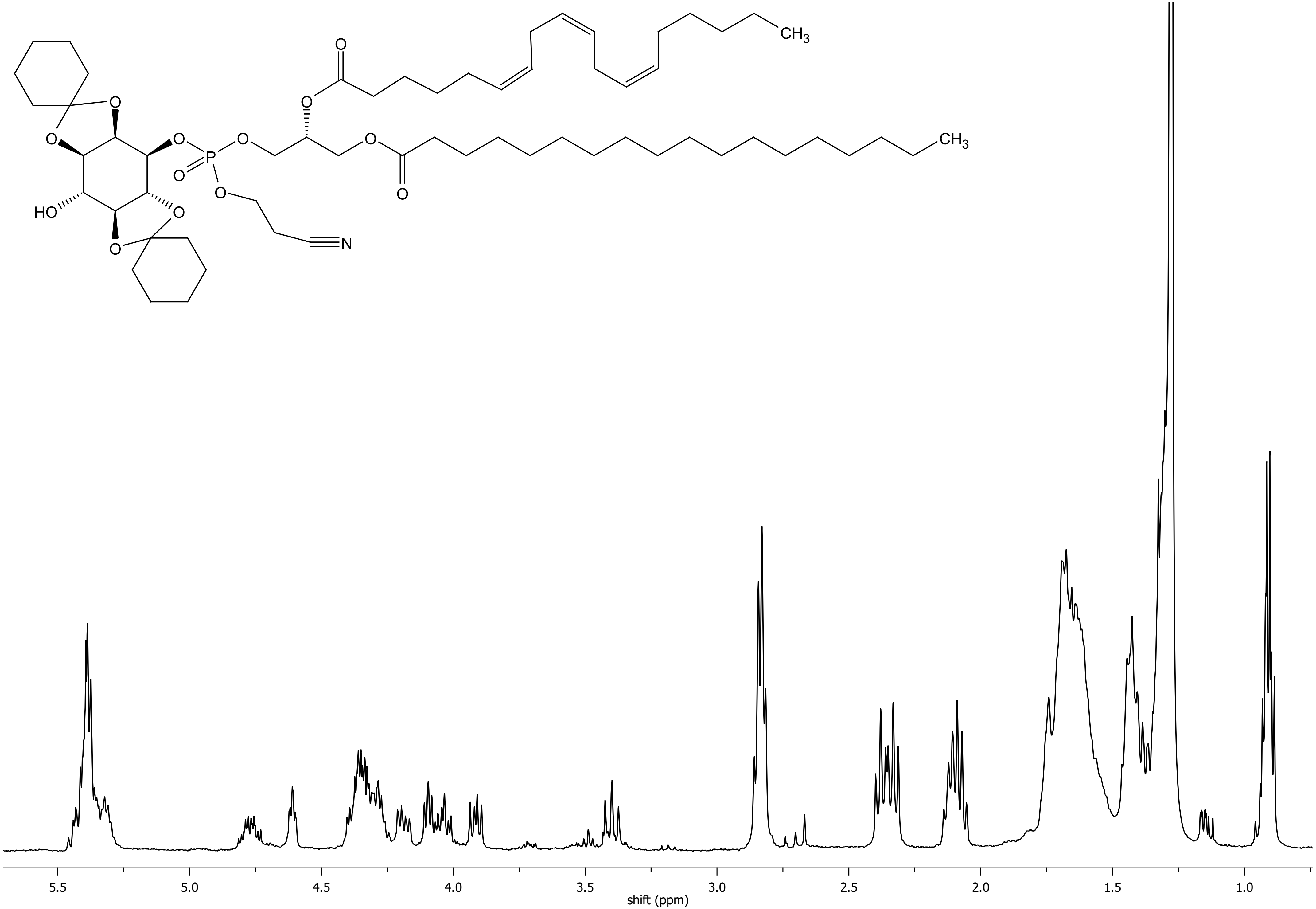

CH3
O
O
O
O
O
P
O
O
O
O
O
O
HO
O
O
N
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)

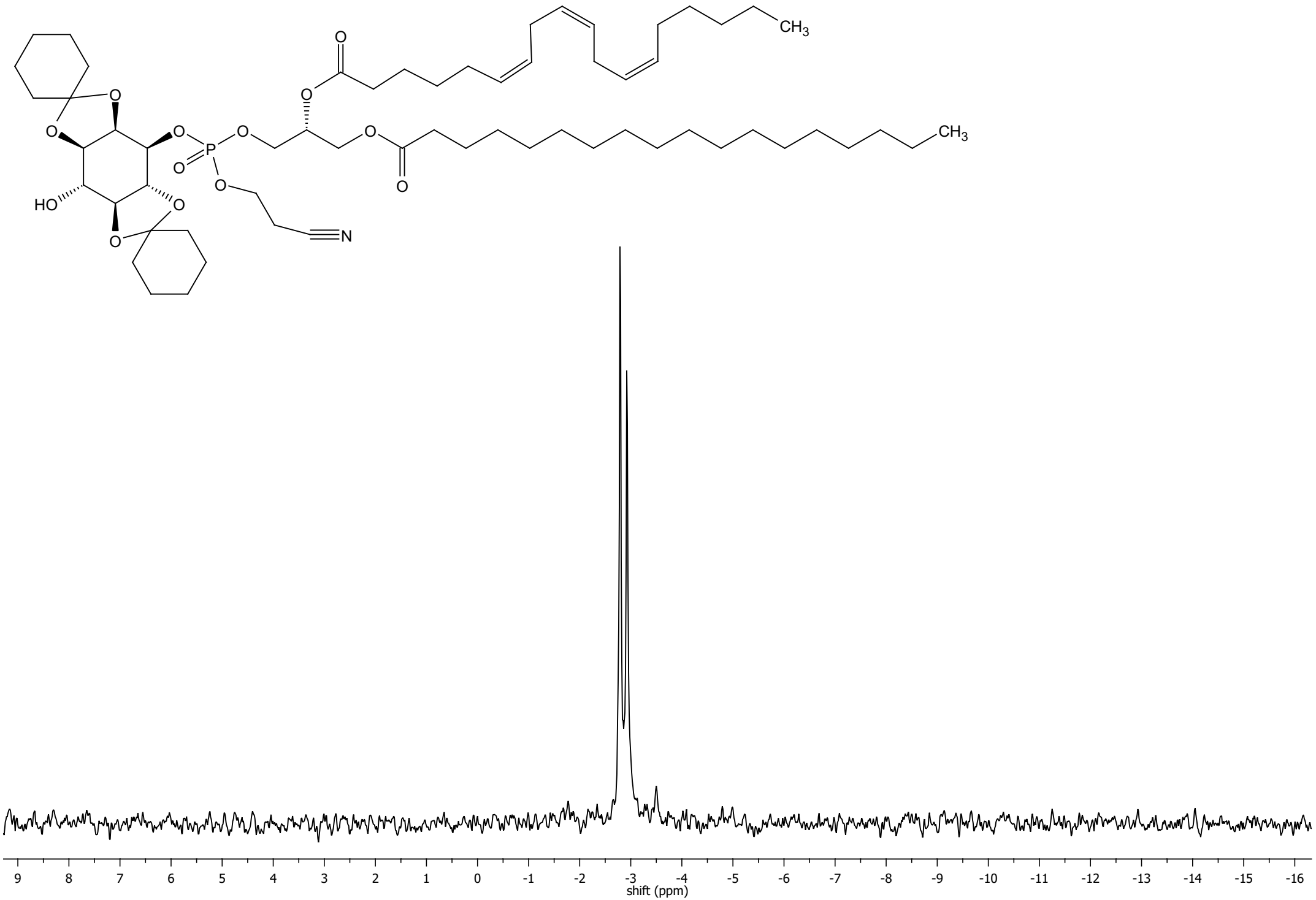

CH3
O
O
O
O
O
O
P
O
O
O
O
HO
O
O
N
CH3
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
shift (ppm)

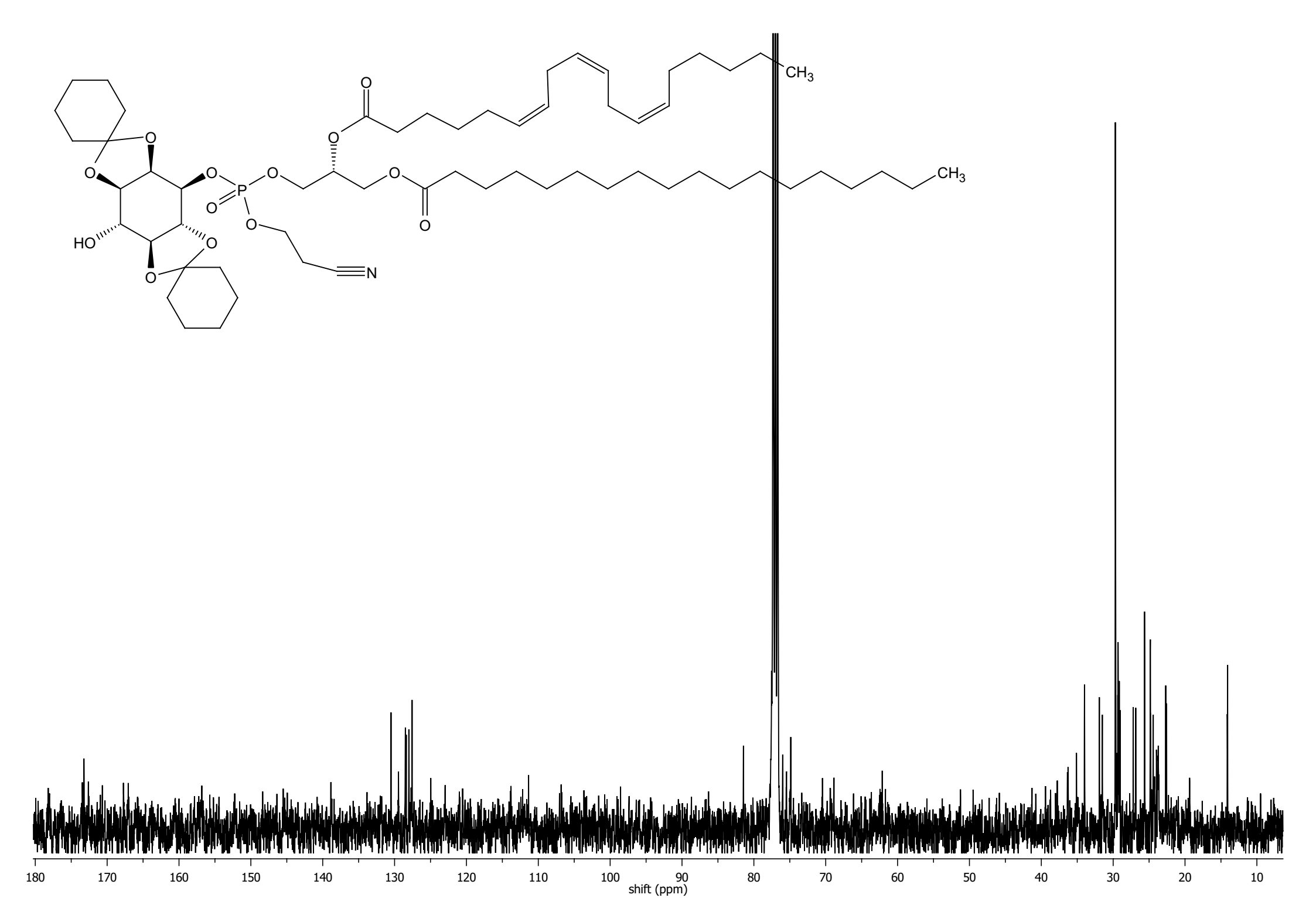


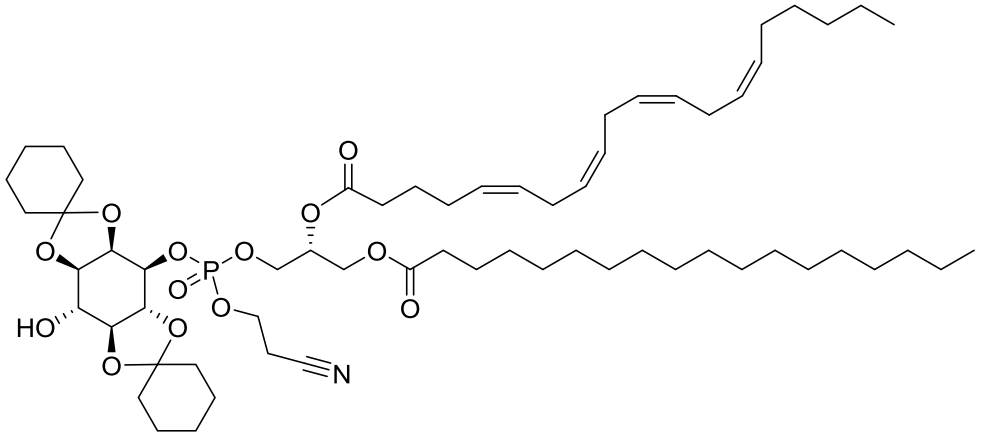
1-*O*-[(Cyanoethyloxy)(*sn*-1-*O*-stearoyl-2-*O*-γ-linolenoylglyceryloxy)phosphoryl]-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 23c.

HRMS (ESI+) *m/z* found $[M+H]^+$ = 1,074·7007, $C_{60}H_{101}NO_{13}P$ requires 1,074·7011.


CH3
CH3
O
O
O
O
O
O
P
O
O
O
O
O
HO
O
O
N
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
shift (ppm)

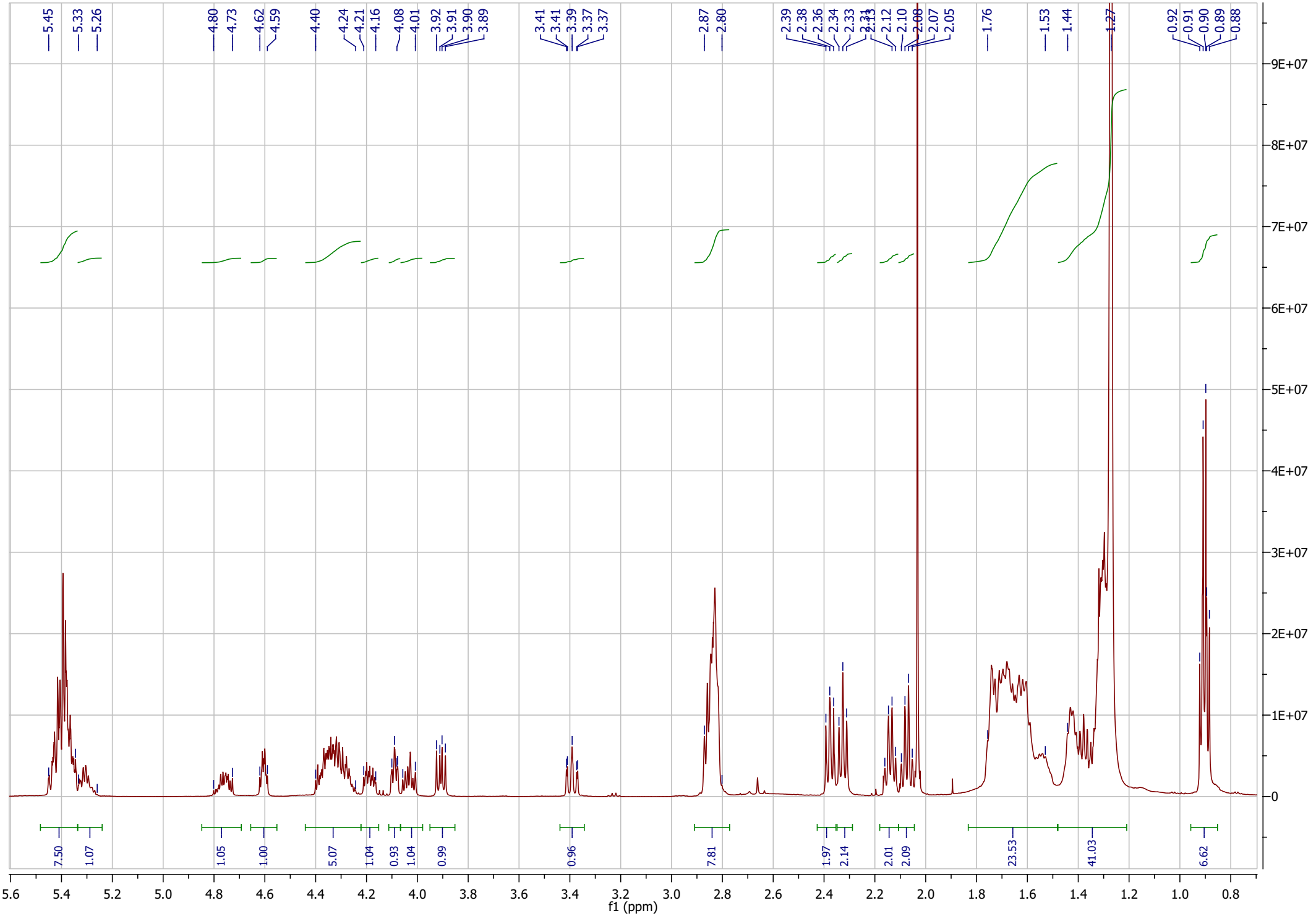

CH3
CH3
HO
N
9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7 -8 -9 -10 -11 -12 -13 -14 -15 -16
shift (ppm)

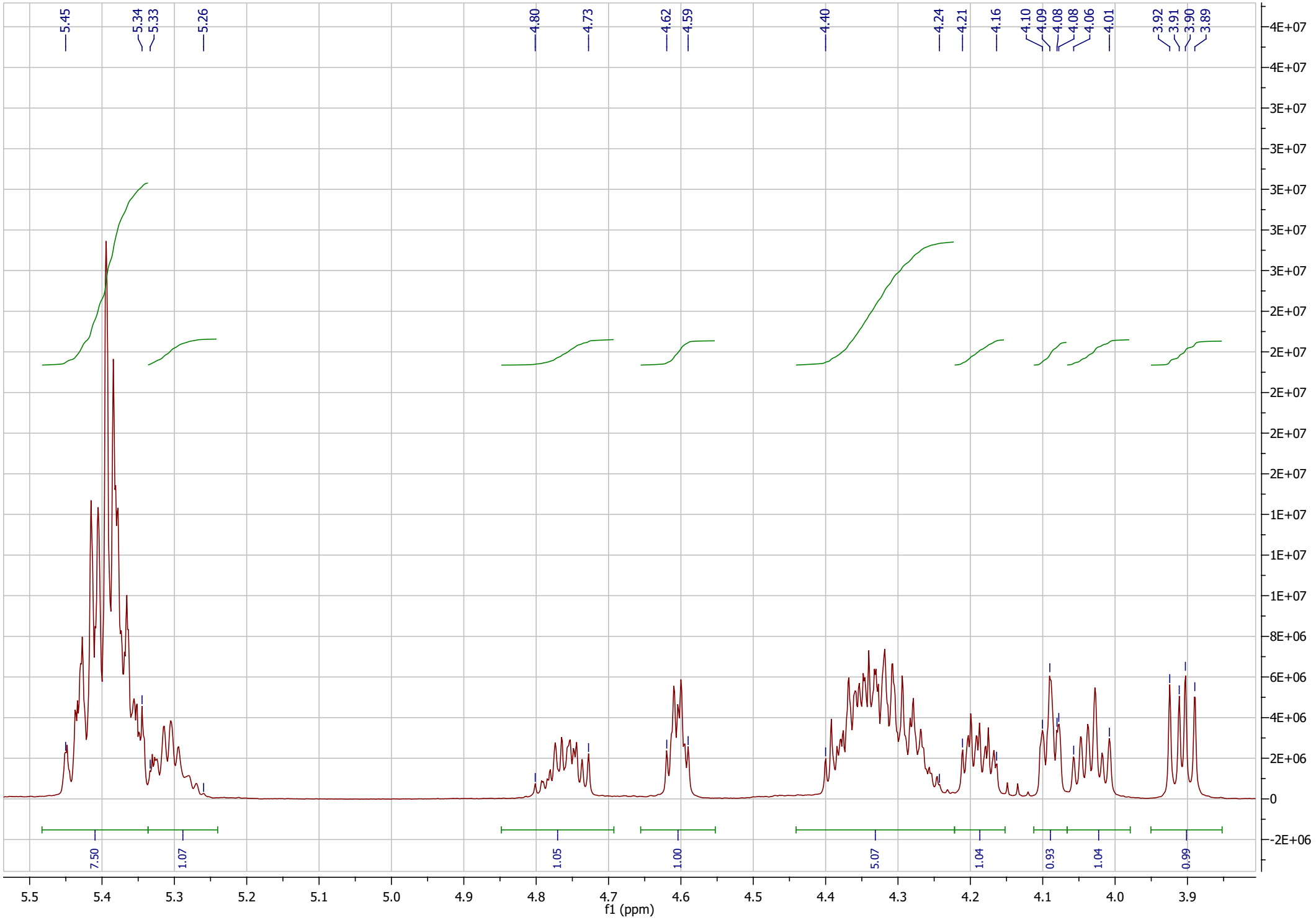

CH3
CH3
HO
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)

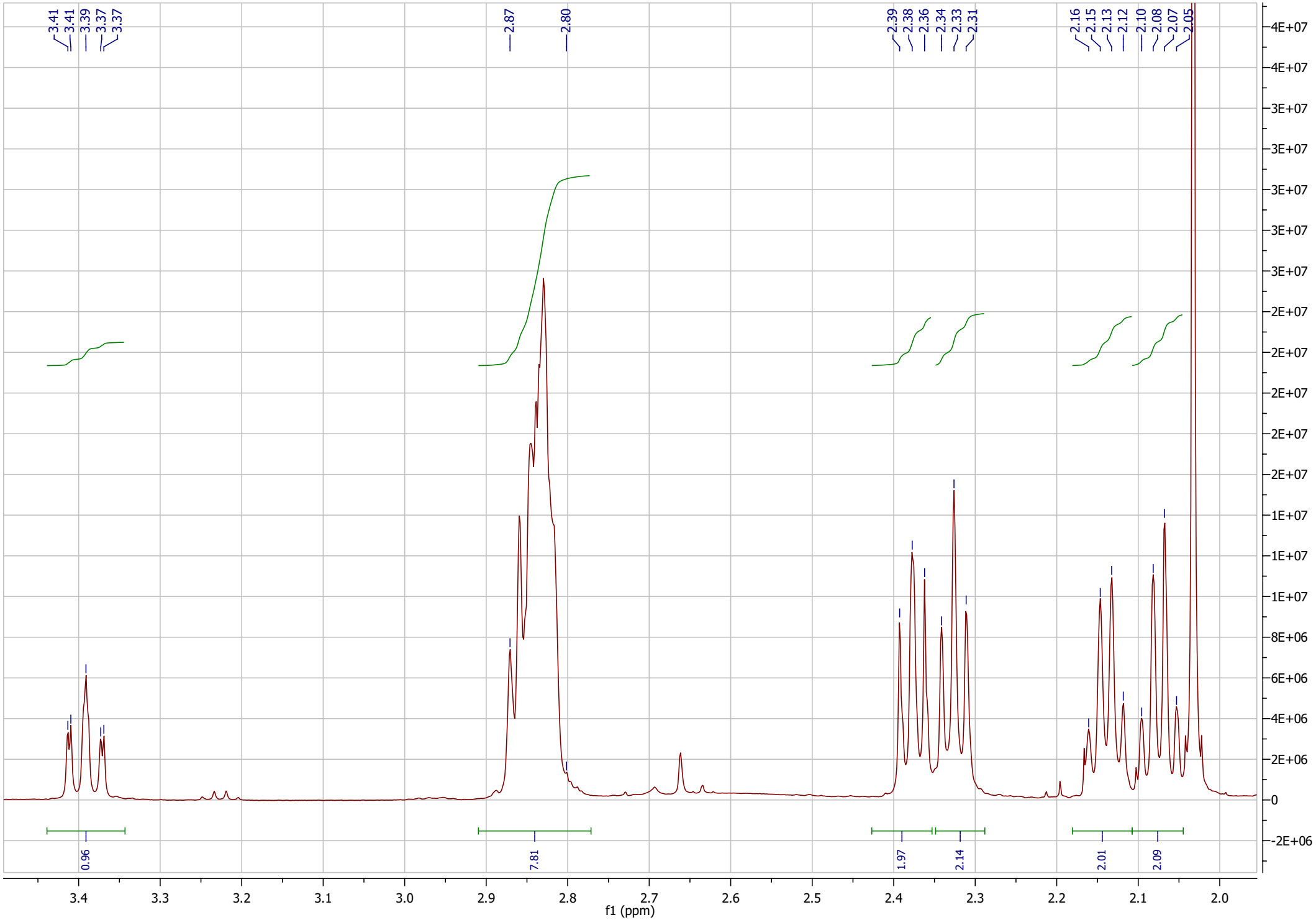


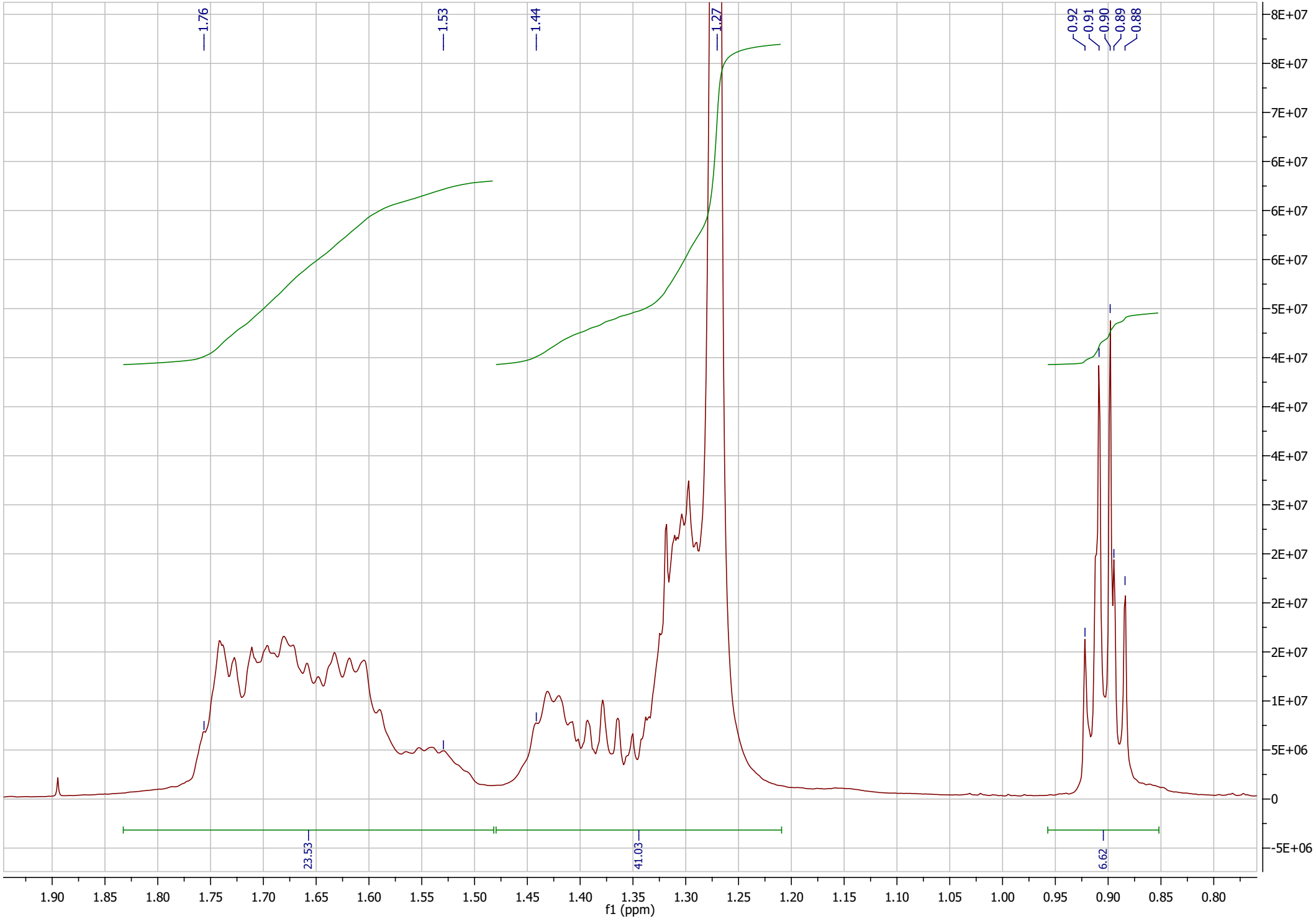
1-*O*-[(Cyanoethyloxy)(*sn*-1-*O*-stearoyl-2-*O*-arachidonoylglycer-3-yloxy)phosphoryl]-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 23d.

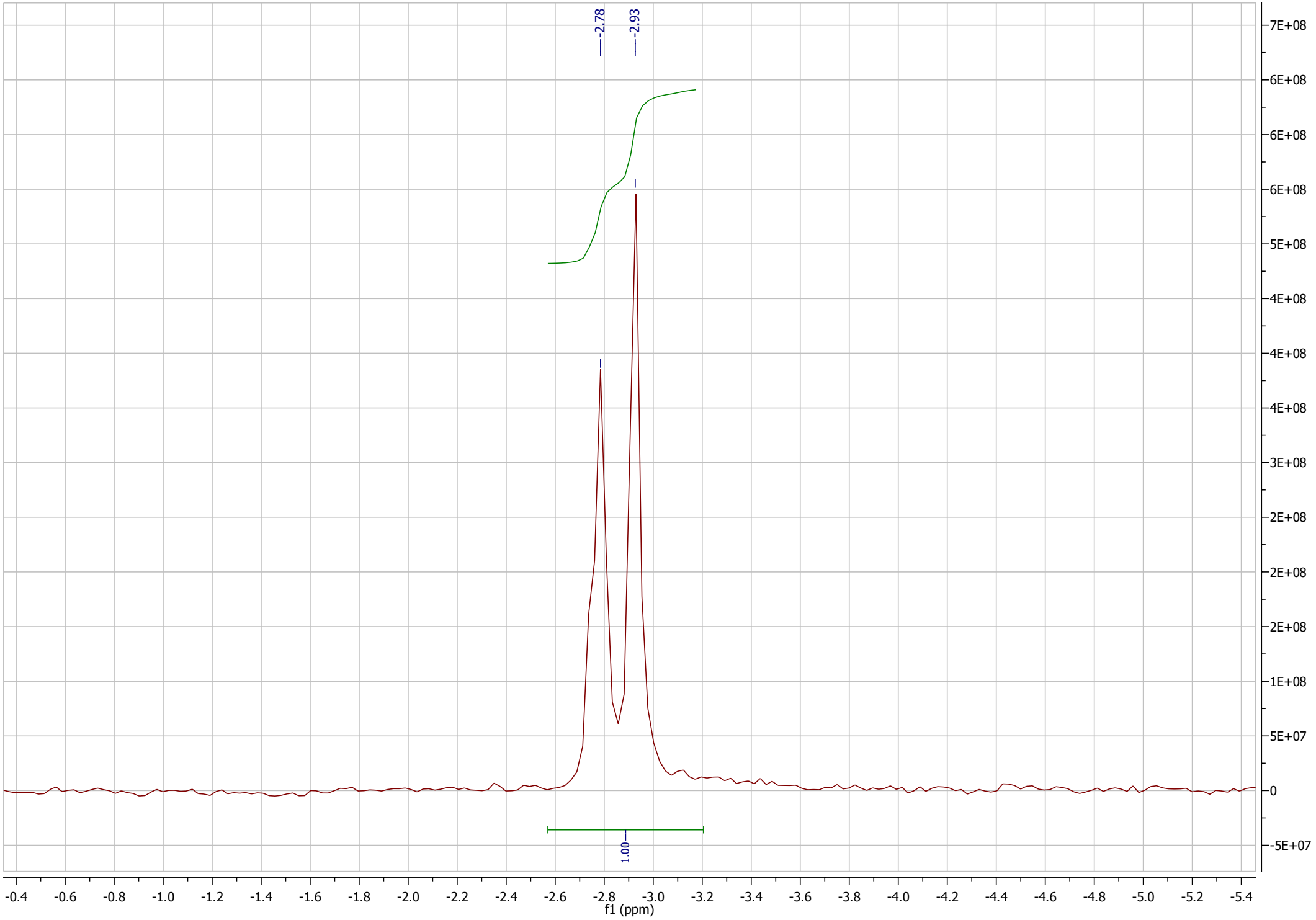
HRMS (ESI+) *m/z* found $[M+Na]^+$ = 1,122·7013, $C_{62}H_{102}NO_{13}PNa^+$ requires 1,122·6987.

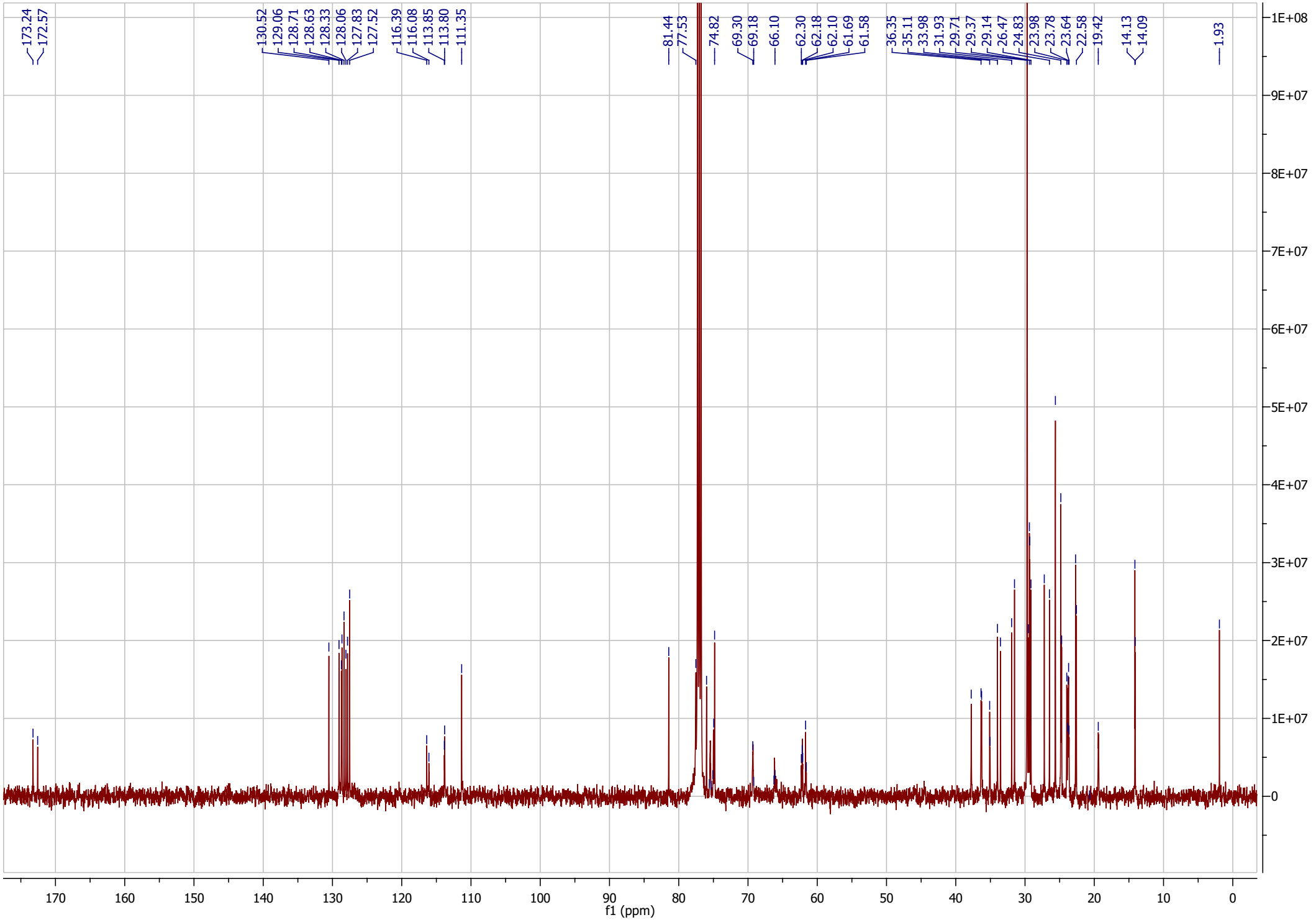

5.45
5.33
5.26
4.80
4.73
4.62
4.59
4.40
4.24
4.21
4.16
4.08
4.01
3.92
3.91
3.90
3.89
3.41
3.41
3.39
3.37
3.37
2.87
2.80
2.39
2.38
2.36
2.34
2.33
2.31
2.12
2.10
2.08
2.07
2.05
1.76
1.53
1.44
1.27
0.92
0.91
0.90
0.89
0.88
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
7.50
1.07
1.05
1.00
5.07
1.04
0.93
1.04
0.99
0.96
7.81
1.97
2.14
2.01
2.09
23.53
41.03
6.62
5.6
5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
f1 (ppm)

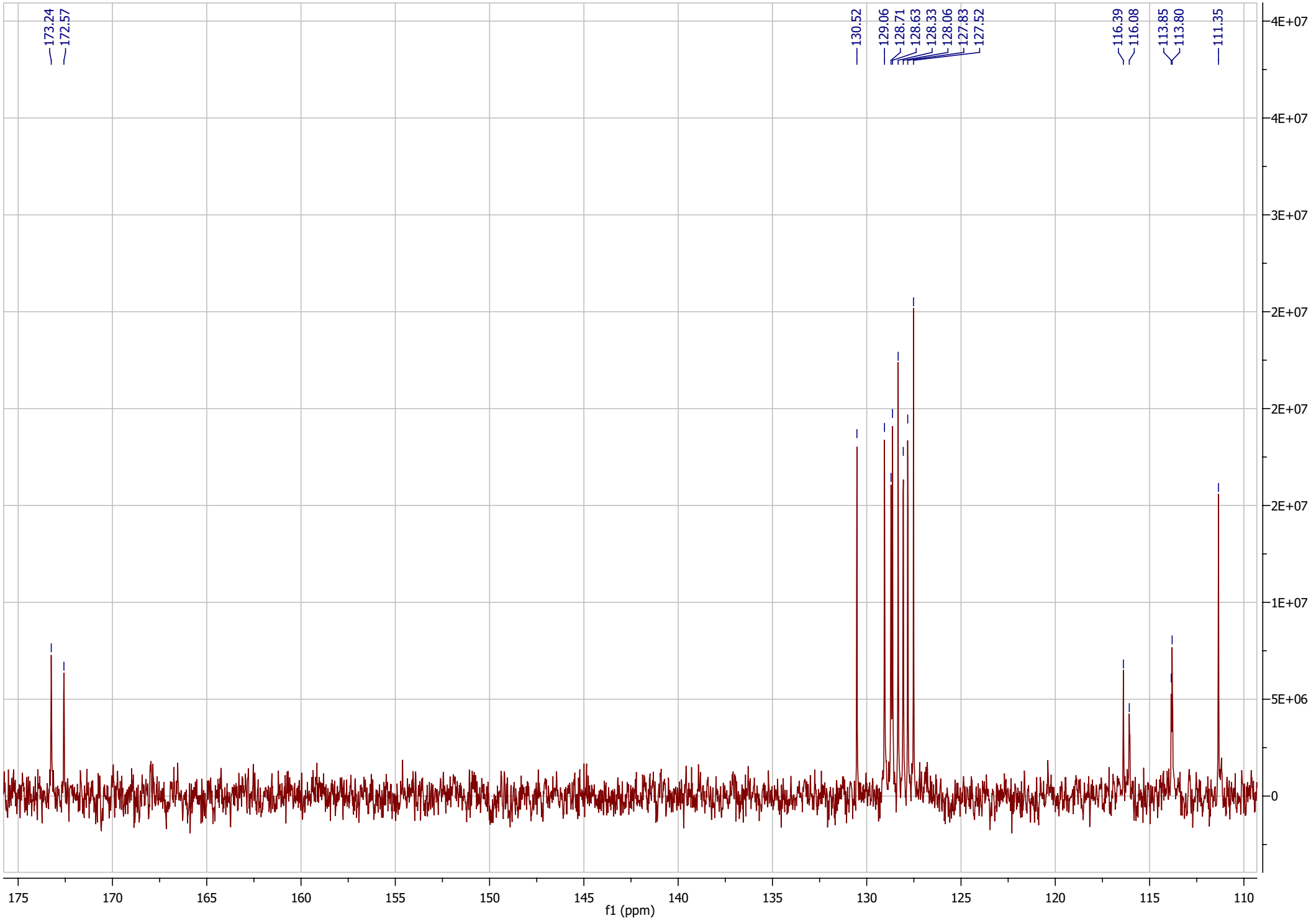

5.45
5.34
5.33
5.26
4.80
4.73
4.62
4.59
4.40
4.24
4.21
4.16
4.10
4.09
4.08
4.08
4.06
4.01
3.92
3.91
3.90
3.89
7.50
1.07
1.05
1.00
5.07
1.04
0.93
1.04
0.99
f1 (ppm)

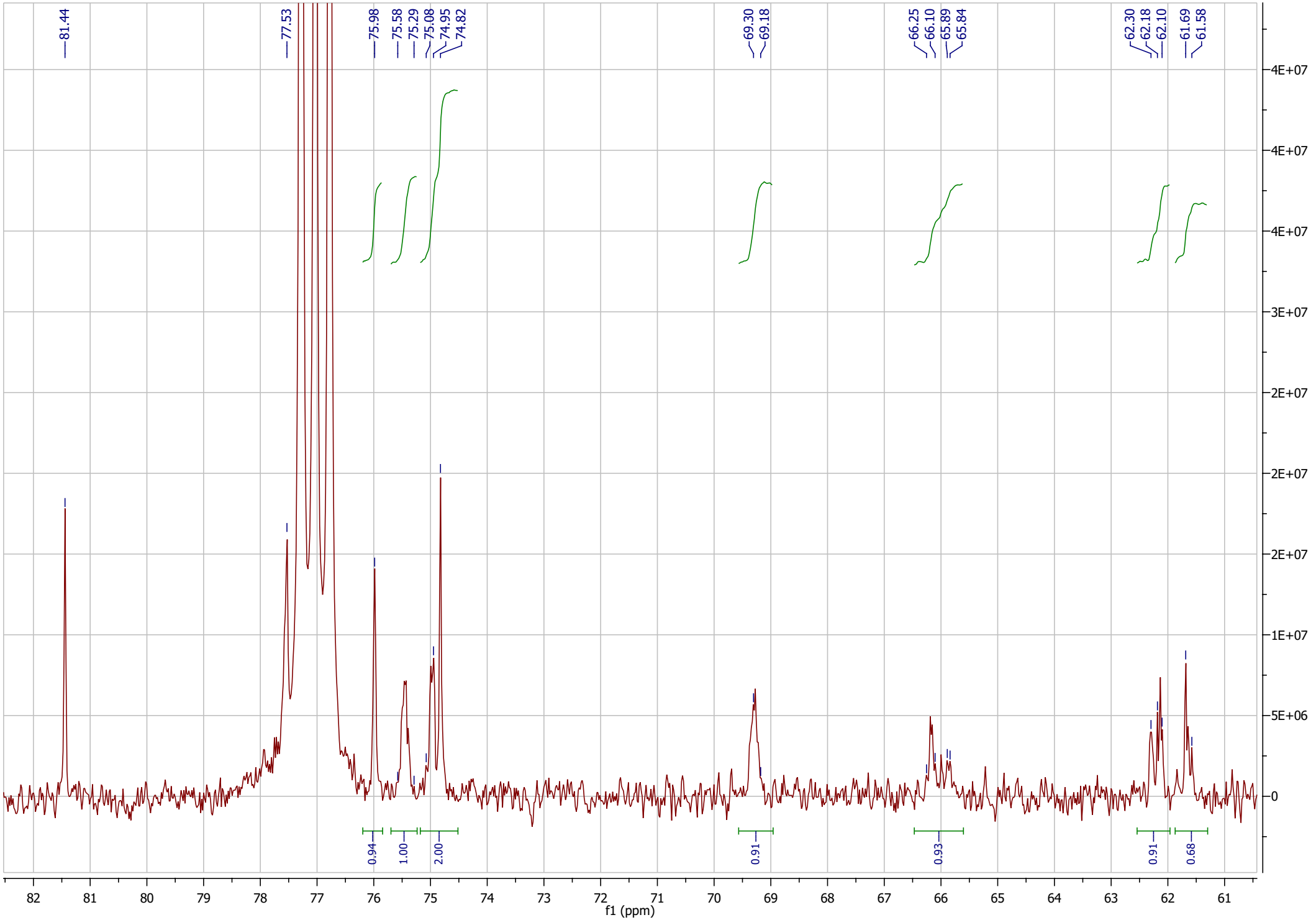

3.41
3.41
3.39
3.37
3.37
2.87
2.80
2.39
2.38
2.36
2.34
2.33
2.31
2.16
2.15
2.13
2.12
2.10
2.08
2.07
2.05
0.96
7.81
1.97
2.14
2.01
2.09
f1 (ppm)

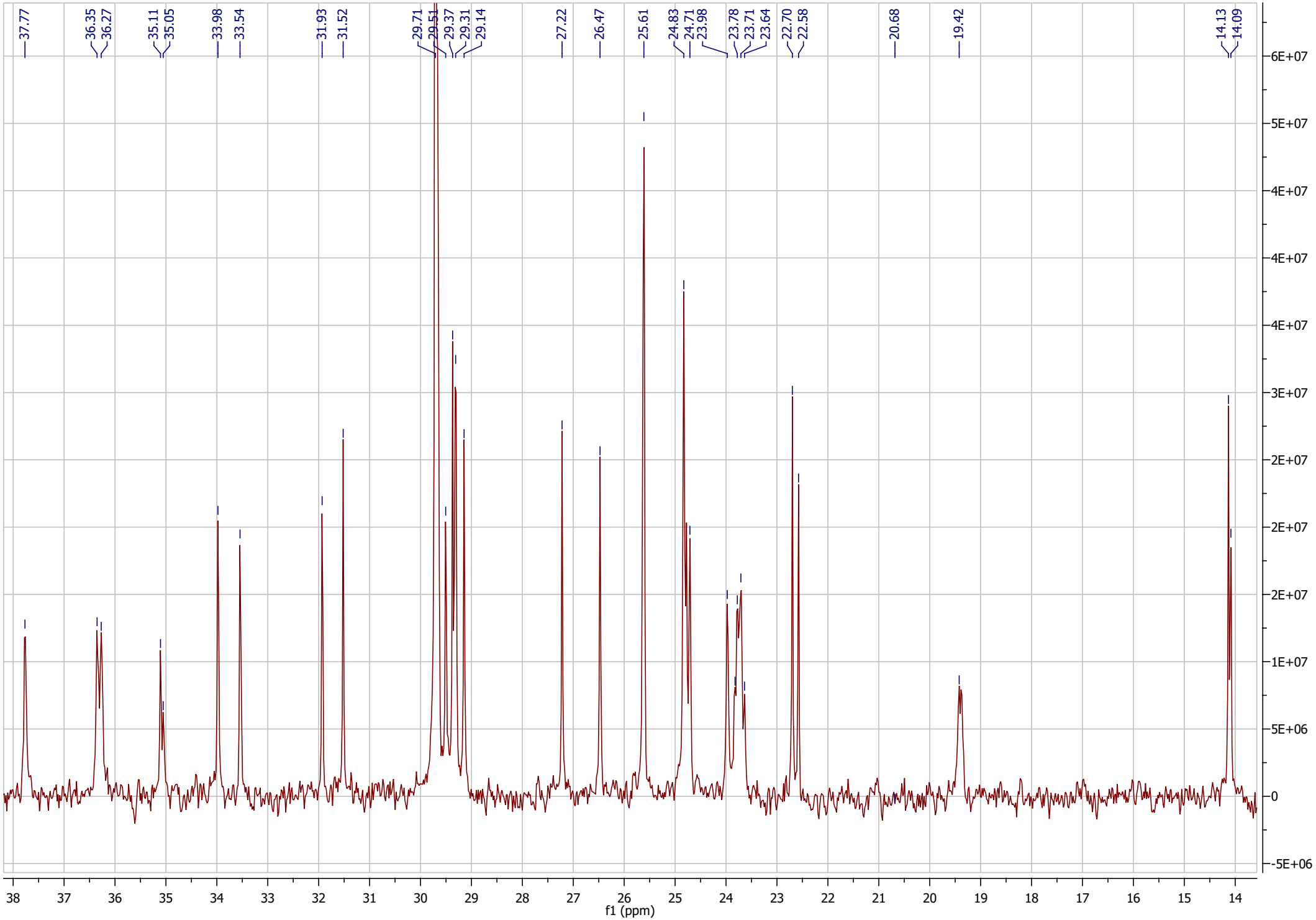

1.76
1.53
1.44
1.27
0.92
0.91
0.90
0.89
0.88
23.53
41.03
6.62
8E+07
8E+07
7E+07
6E+07
6E+07
6E+07
5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
-5E+06
1.90
1.85
1.80
1.75
1.70
1.65
1.60
1.55
1.50
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
f1 (ppm)

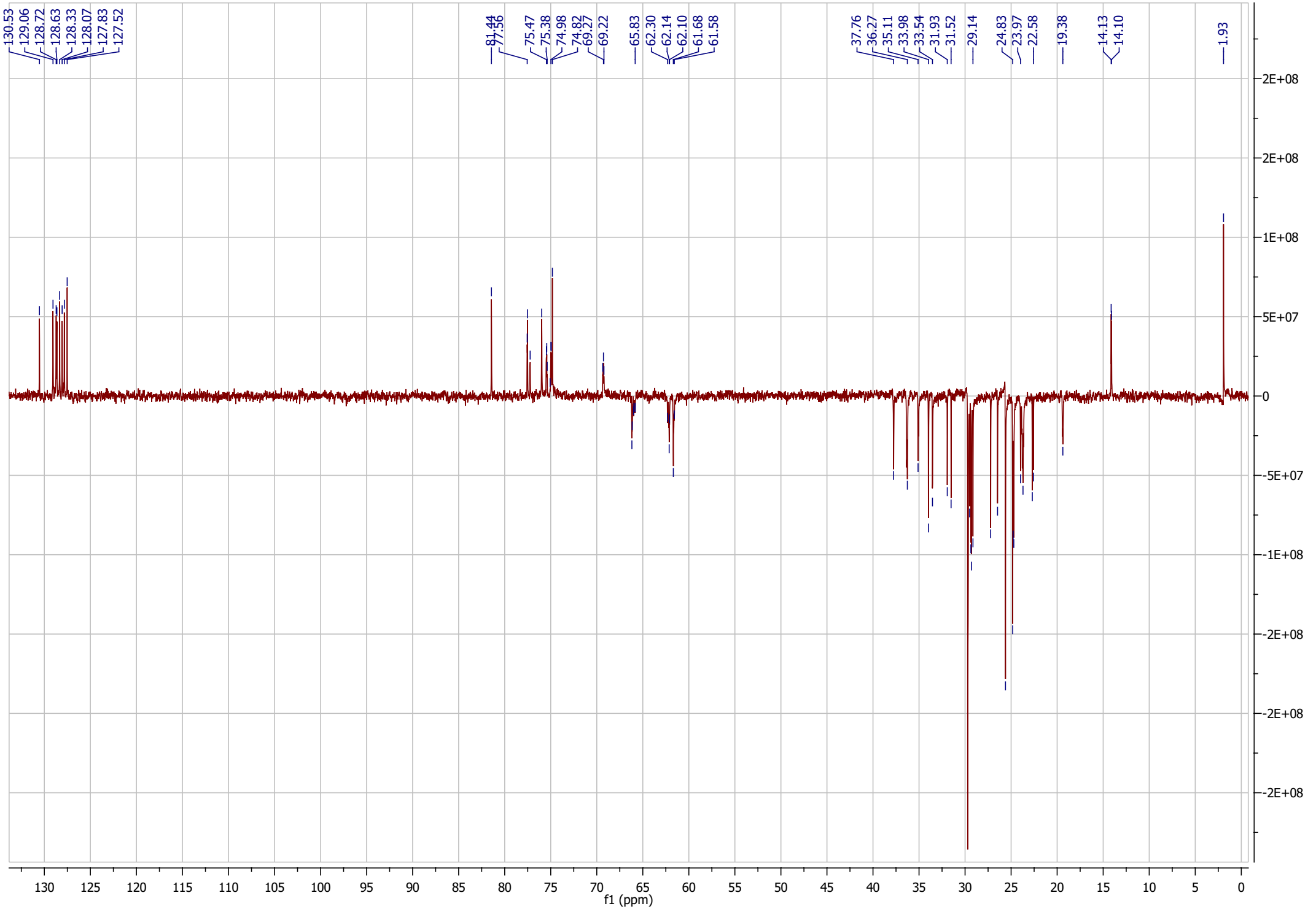

-2.78
-2.93
1.00
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-0.4 -0.6 -0.8 -1.0 -1.2 -1.4 -1.6 -1.8 -2.0 -2.2 -2.4 -2.6 -2.8 -3.0 -3.2 -3.4 -3.6 -3.8 -4.0 -4.2 -4.4 -4.6 -4.8 -5.0 -5.2 -5.4
f1 (ppm)

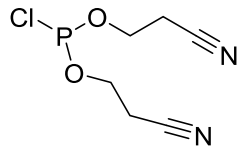

173.24
172.57
130.52
129.06
128.71
128.63
128.33
128.06
127.83
127.52
116.39
116.08
113.85
113.80
111.35
81.44
77.53
74.82
69.30
69.18
66.10
62.30
62.18
62.10
61.69
61.58
36.35
35.11
33.98
31.93
29.71
29.37
29.14
26.47
24.83
23.98
23.78
23.64
22.58
19.42
14.13
14.09
1.93
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


173.24
172.57
130.52
129.06
128.71
128.63
128.33
128.06
127.83
127.52
116.39
116.08
113.85
113.80
111.35
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)


81.44
77.53
75.98
75.58
75.29
75.08
74.95
74.82
69.30
69.18
66.25
66.10
65.89
65.84
62.30
62.18
62.10
61.69
61.58
0.94
1.00
2.00
0.91
0.93
0.91
0.68
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
82
81
80
79
78
77
76
75
74
73
72
71
70
69
68
67
66
65
64
63
62
61
f1 (ppm)


37.77
36.35
36.27
35.11
35.05
33.98
33.54
31.93
31.52
29.71
29.51
29.37
29.31
29.14
27.22
26.47
25.61
24.83
24.71
23.98
23.78
23.71
23.64
22.70
22.58
20.68
19.42
14.13
14.09
6E+07
5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
-5E+06
38
37
36
35
34
33
32
31
30
29
28
27
26
25
24
23
22
21
20
19
18
17
16
15
14
f1 (ppm)

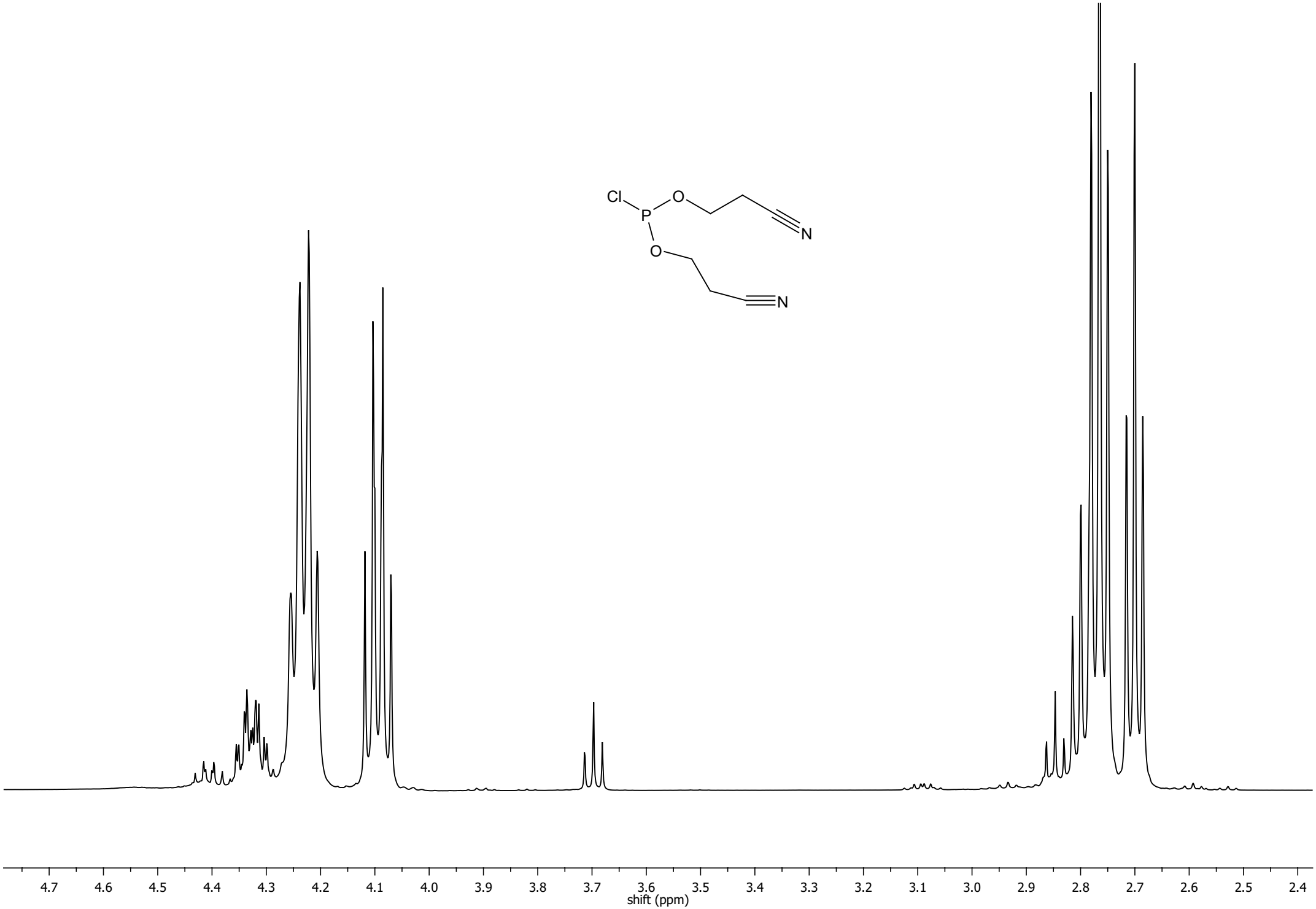

130.53
129.06
128.72
128.63
128.33
128.07
127.83
127.52
81.44
77.56
75.47
75.38
74.98
74.82
69.27
69.22
65.83
62.30
62.14
62.10
61.68
61.58
37.76
36.27
35.11
33.98
33.54
31.93
31.52
29.14
24.83
23.97
22.58
19.38
14.13
14.10
1.93
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
-2E+08
-2E+08
130
125
120
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)

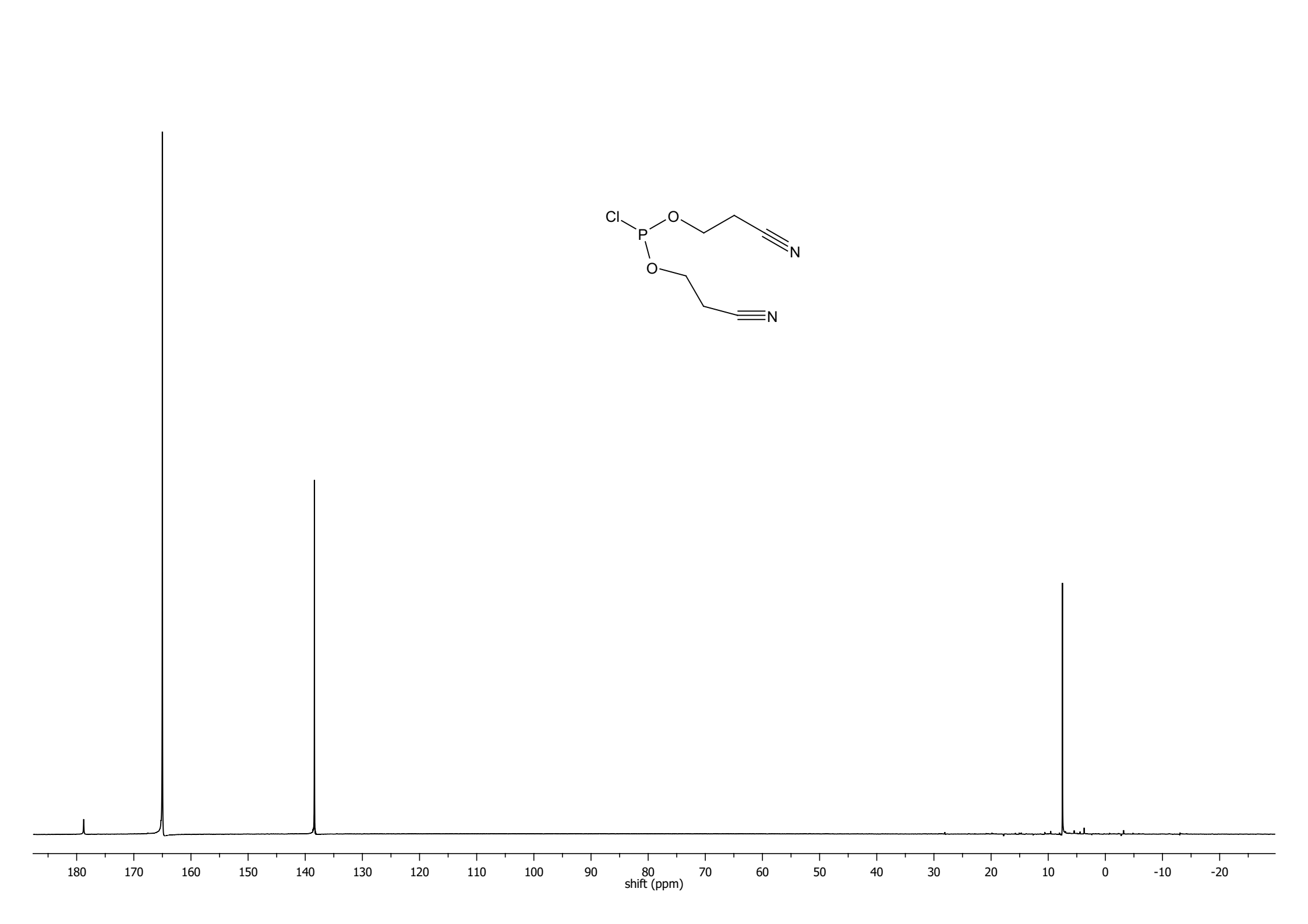


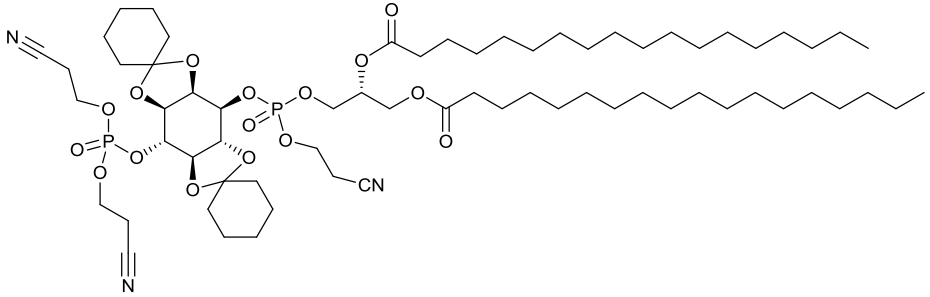
Di(2-cyanoethyl) phosphorochloridite, 15.

No Mass Spectrometry data available.

NB. Due to this compound's sensitivity to air and water, there is contamination with the *H*-phosphonate derivative. The reactivity of this reacgent and the material isolated after phosphorylation reactions suggest that this contaminant was not present in the stocks made.

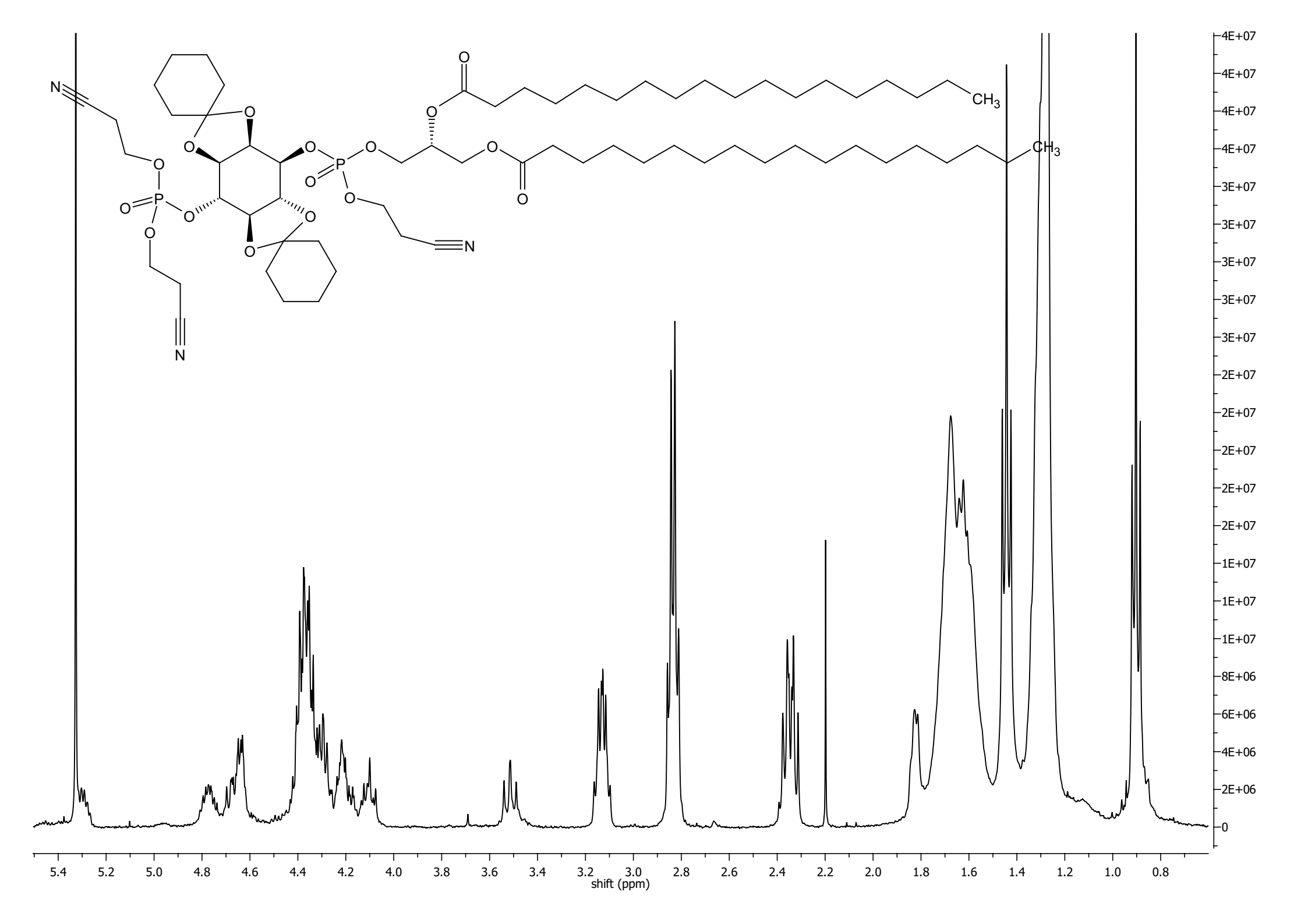

Cl
P
O
O
N
O
N
4.7
4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
shift (ppm)

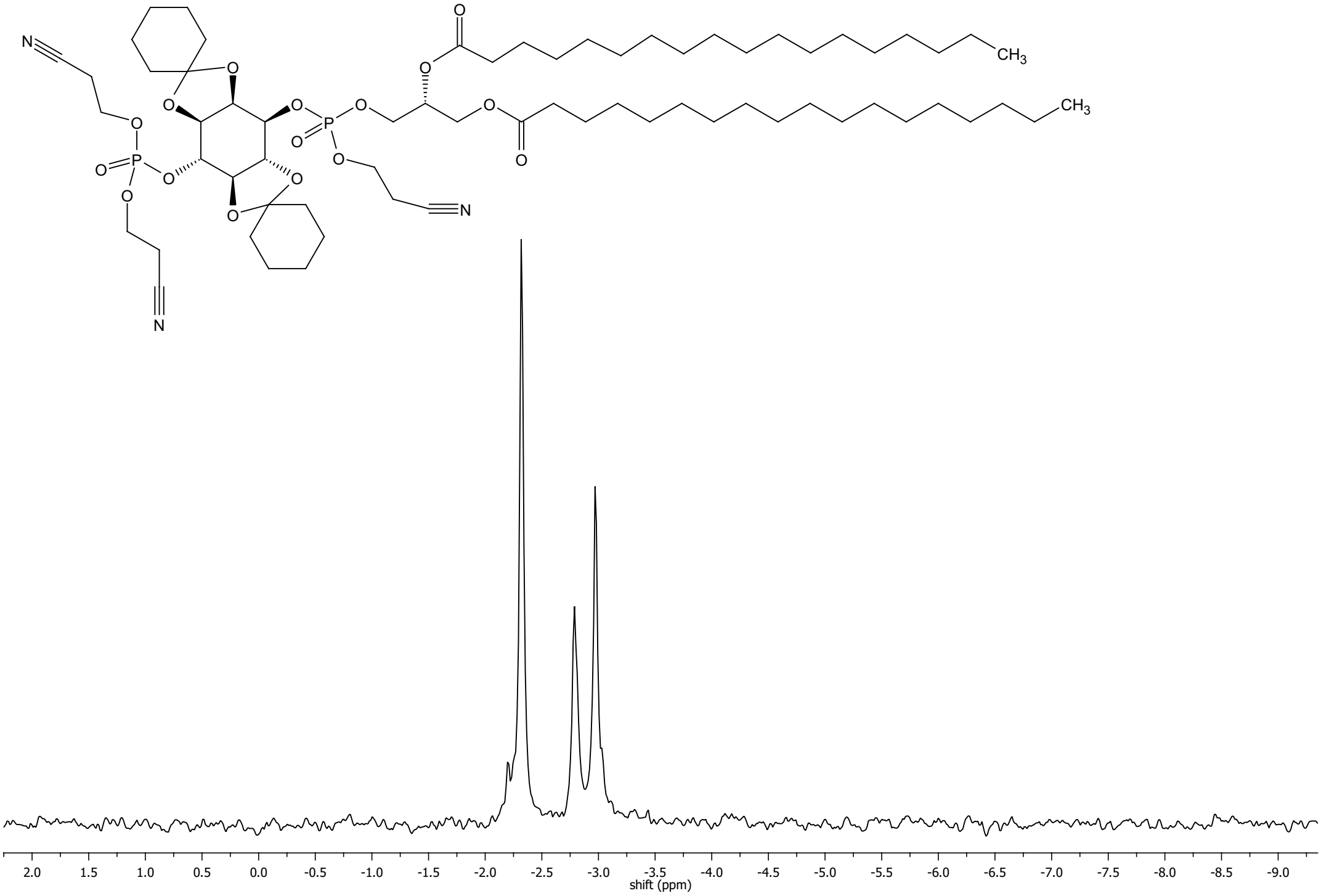

Cl
P
O
O
N
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
shift (ppm)

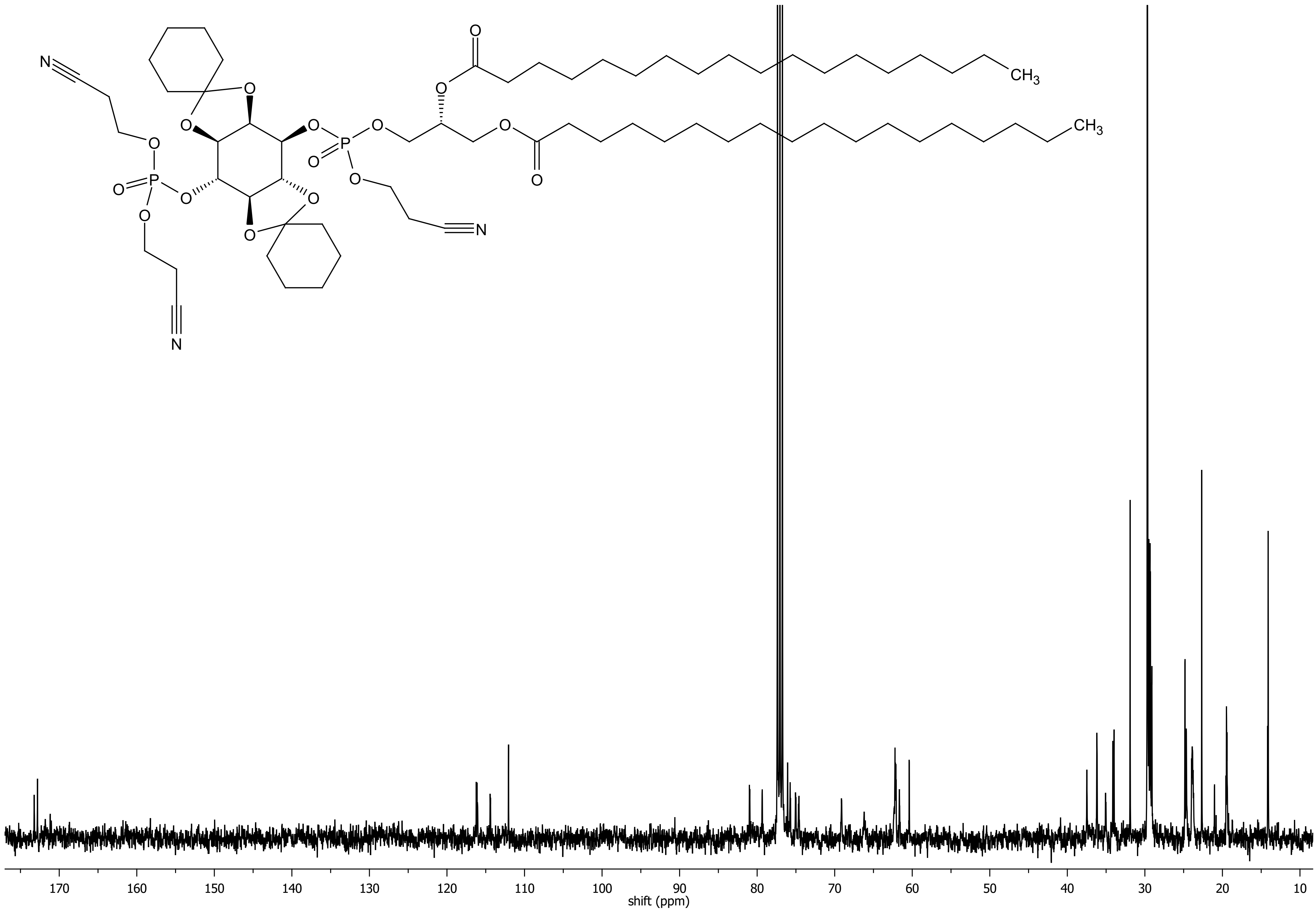


1-*O*-[(Cyanoethyloxy)(*sn*-1,2-*O*-distearoylglyceryloxy) phosphoryl]-4-*O*-(dicyanoethyloxyphosphoryl)-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 24a.

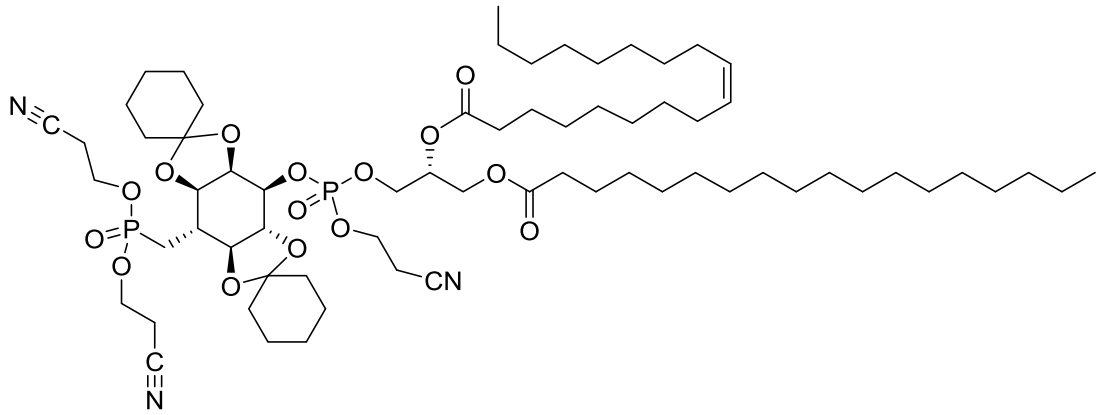
HRMS (ES+) *m/z*, calcd for $C_{66}H_{113}N_3O_{16}P_2Na$ = 1,288·7, found $[M+Na]^+$ 1,288·7 (62%), $[M+NH_4]^+$ 1,283·7 (40%), $[M-C_6H_9]^+$ 1186.6 (78%), $[DAG]^+$ 607.5 (25%).


shift (ppm)


2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
-4.0
-4.5
-5.0
-5.5
-6.0
-6.5
-7.0
-7.5
-8.0
-8.5
-9.0
shift (ppm)

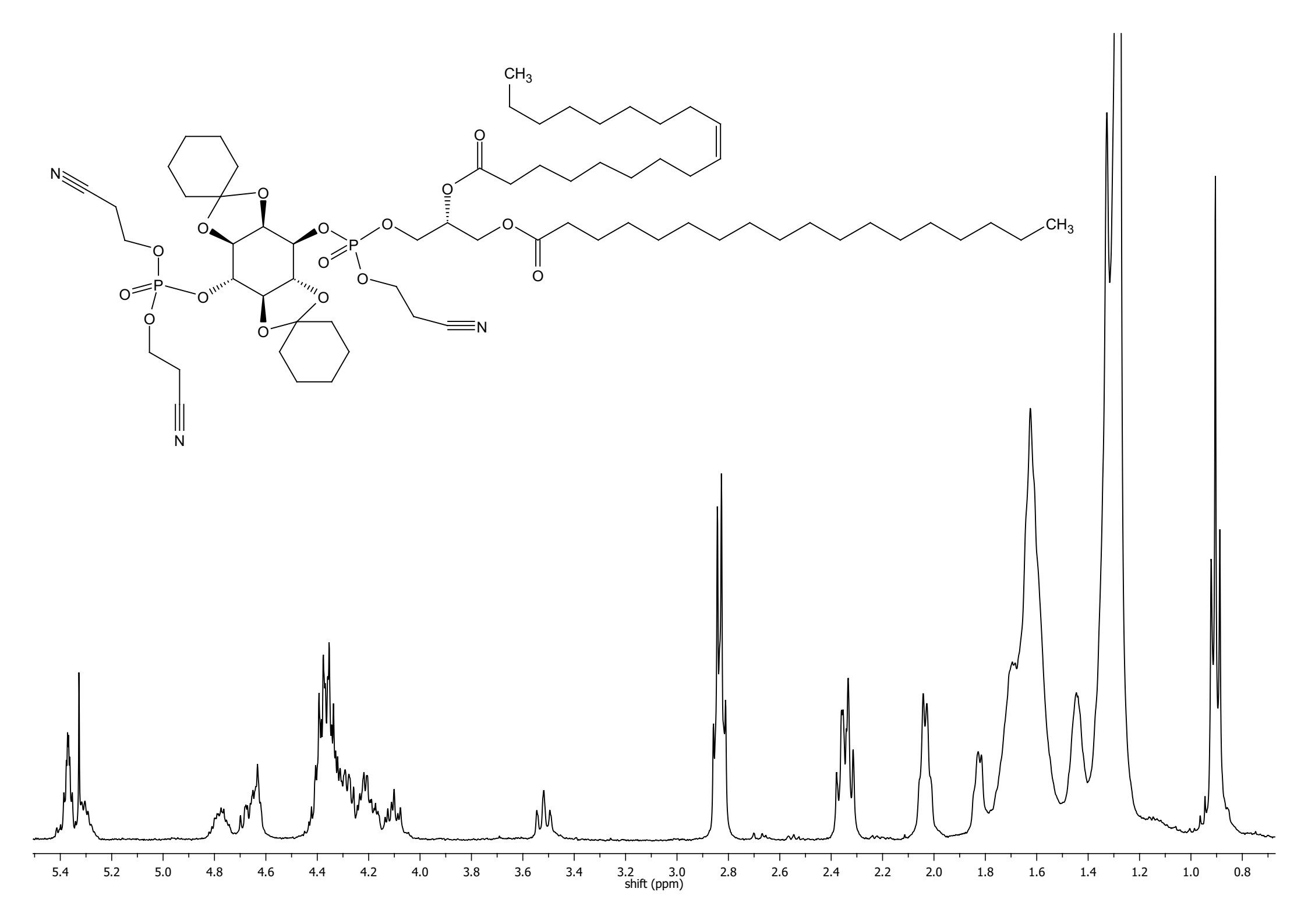


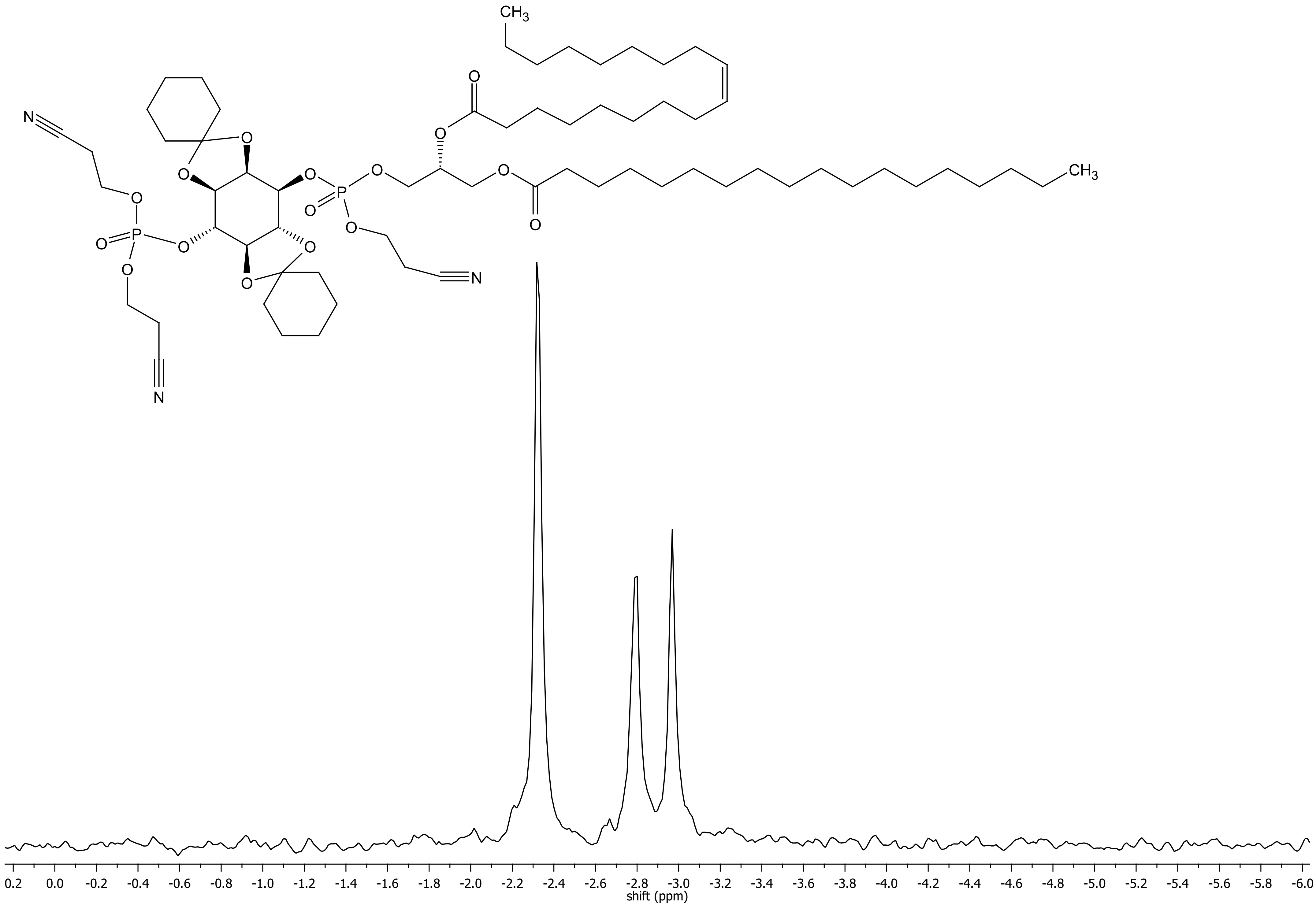
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)



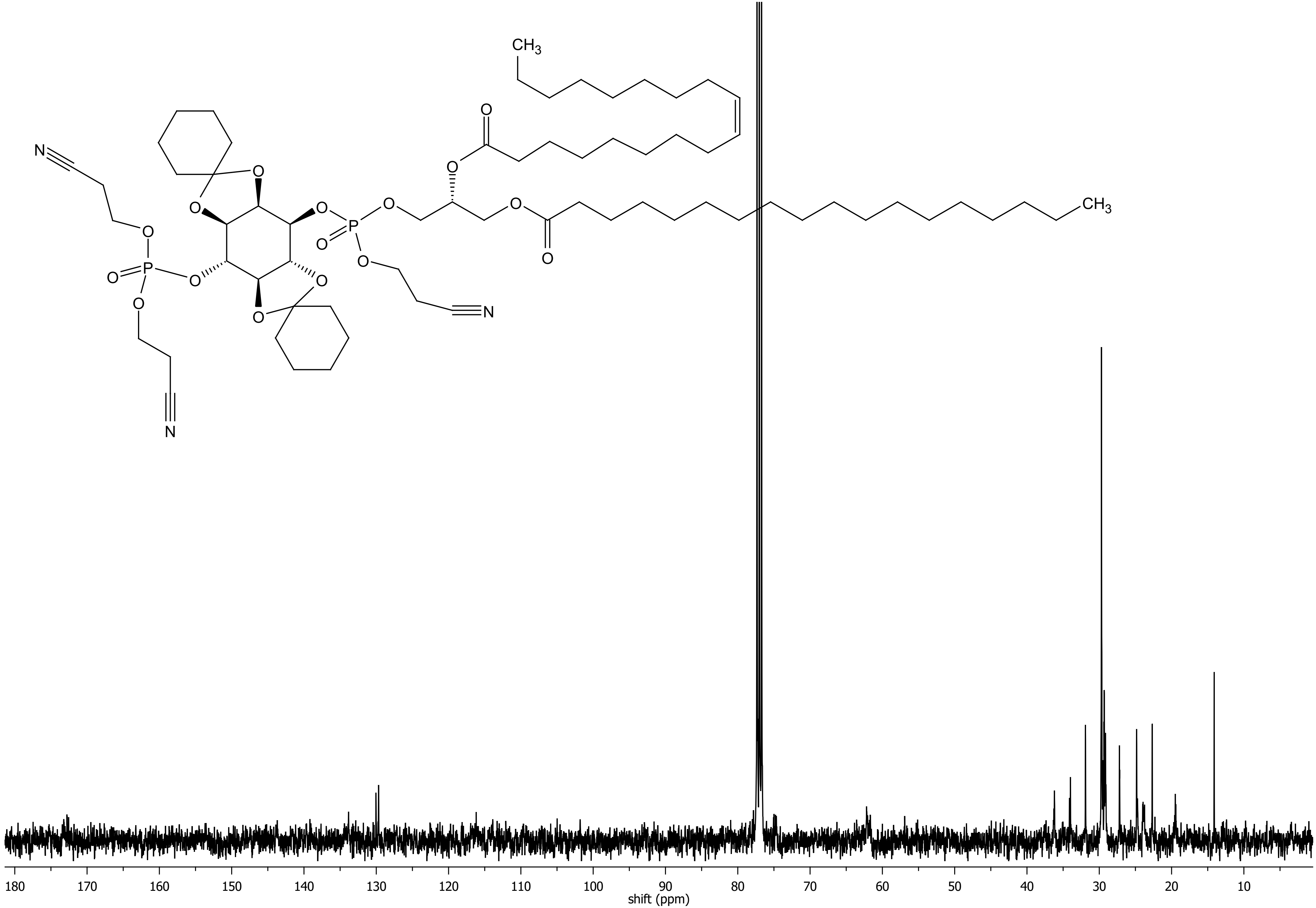
1-*O*-(1-*O*-stearoyl-*sn*-2-oleoyl glycer-3-yloxy)(2-cyanoethyloxy) phosphoryl-4-*O*-di(2-cyanoethyloxy)phosphoryl-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, **24b**.

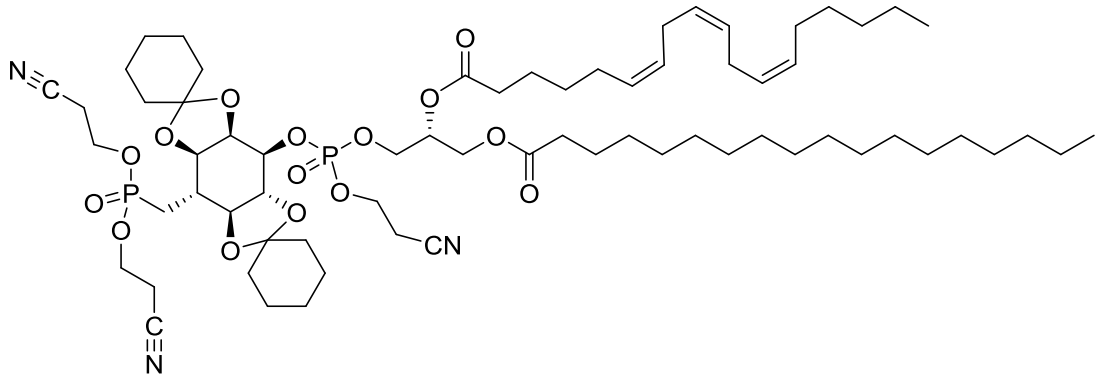
MS (ESI+) *m/z* $[M+Na]^+$ = 1,286·7 (85%), $C_{66}H_{111}N_3O_{16}P_2Na$ requires 1,286·7, also observed $[M-C_6H_7]^+$ = 1184.6 (100%), $[DAG+Na]^+$ = 651·8 (22%), $[Dag-OH]^+$ = 605·5 (40%).


CH3
CH3
N
N
N
O
P
shift (ppm)
5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8



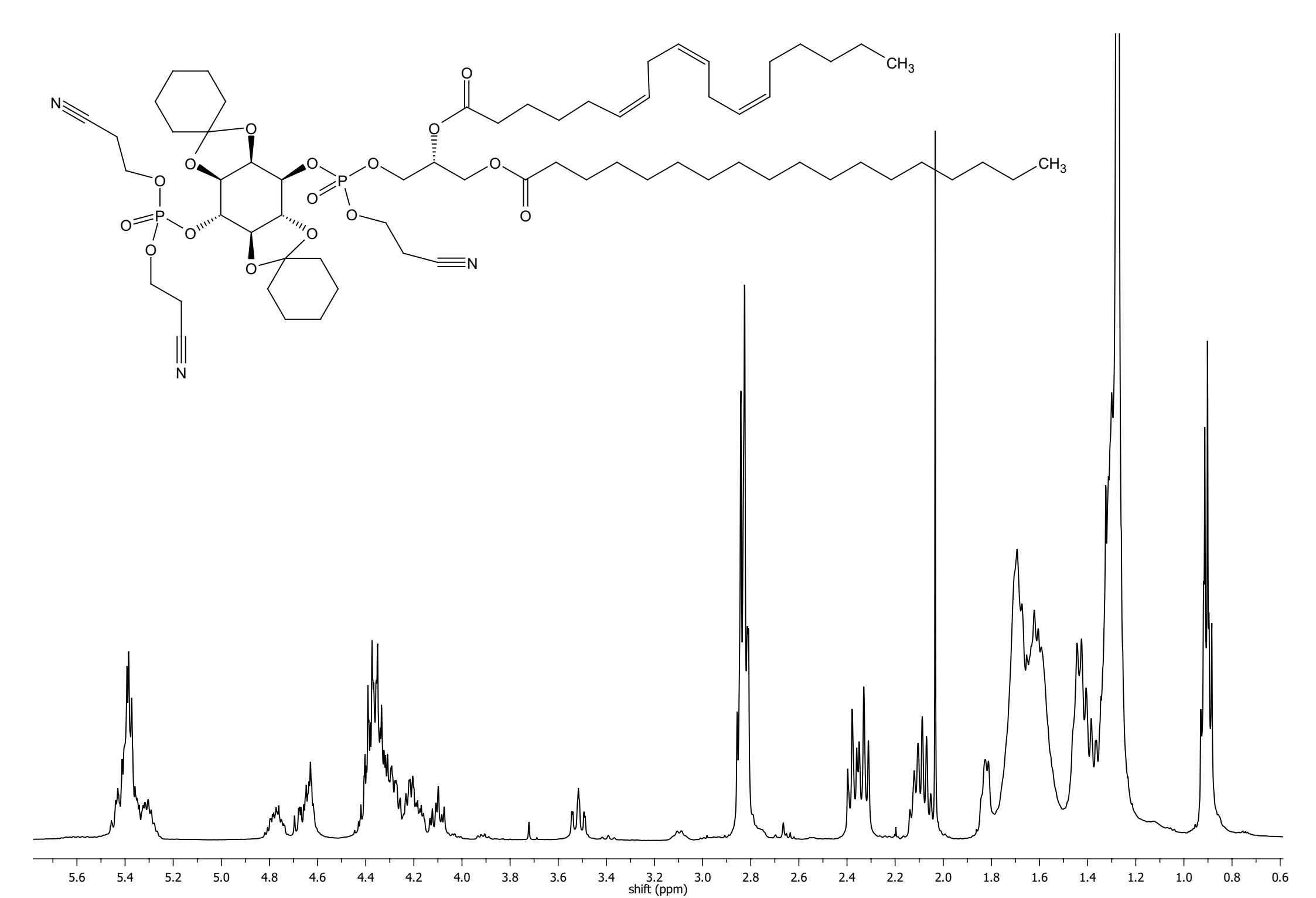
CH3
O
N
O
O
O
O
P
O
O
O
N
O
P
O
O
O
O
O
O
N
O
O
CH3
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-1.4
-1.6
-1.8
-2.0
-2.2
-2.4
-2.6
-2.8
-3.0
-3.2
-3.4
-3.6
-3.8
-4.0
-4.2
-4.4
-4.6
-4.8
-5.0
-5.2
-5.4
-5.6
-5.8
-6.0
shift (ppm)

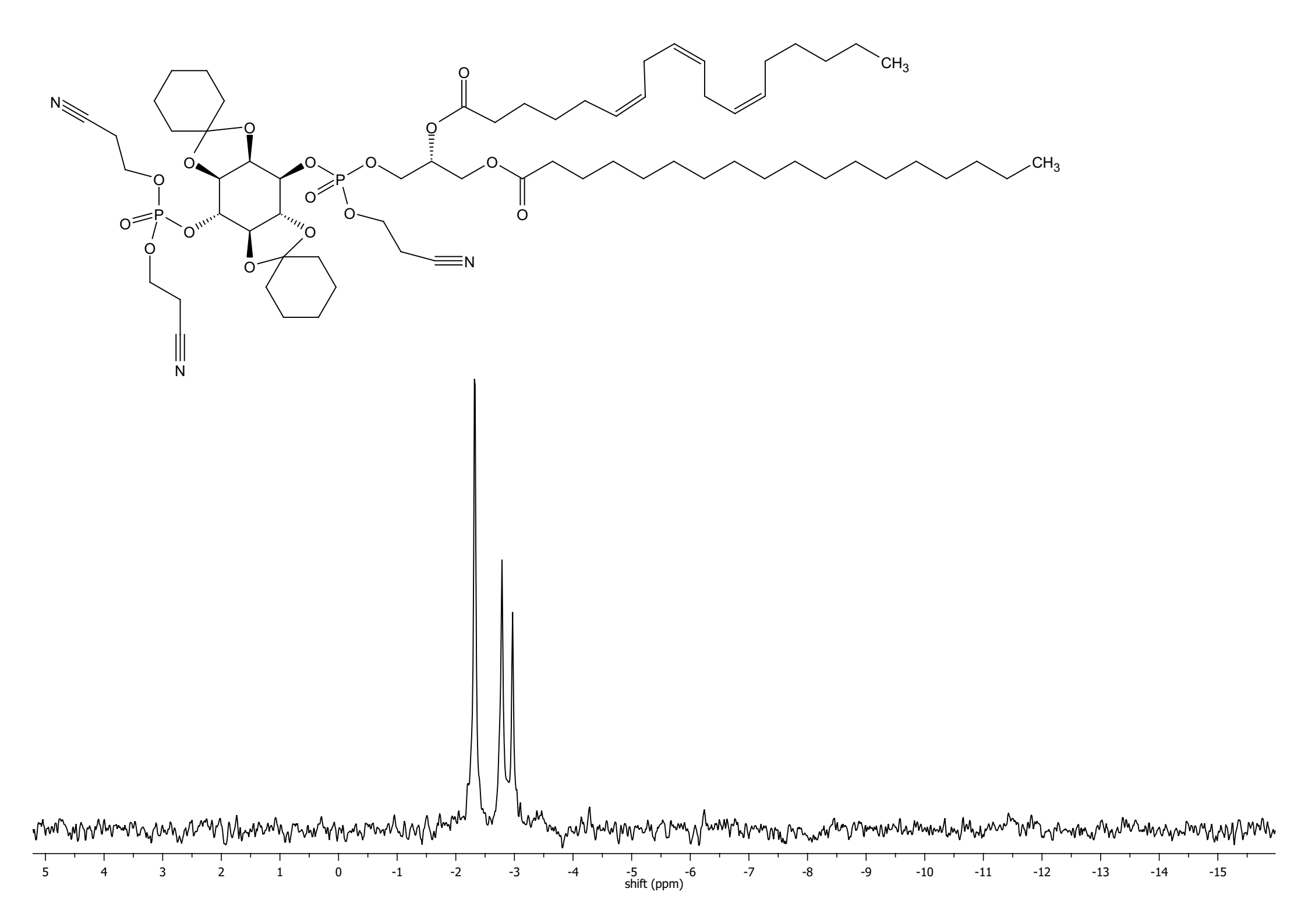

CH3
O
N
P
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
shift (ppm)

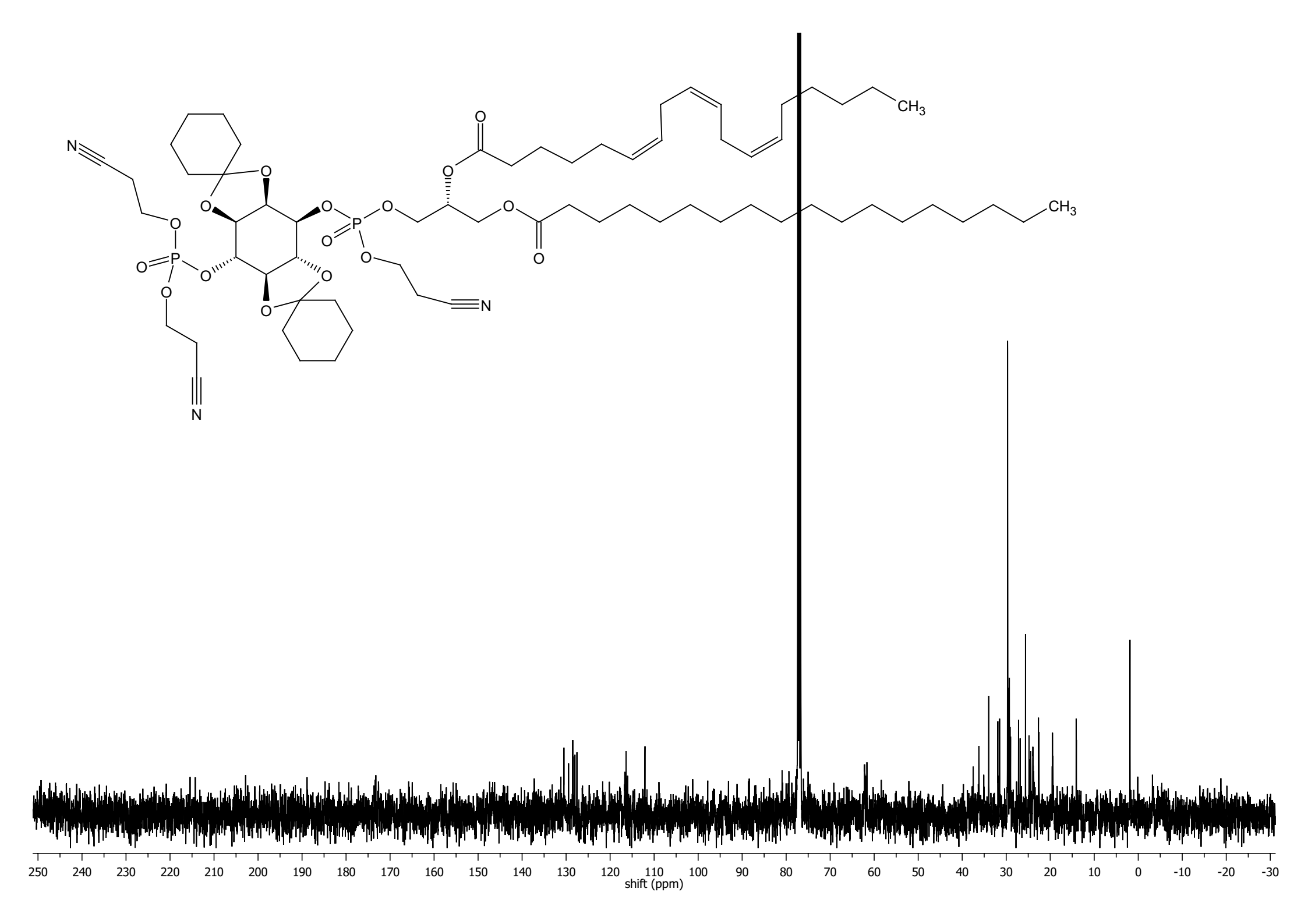


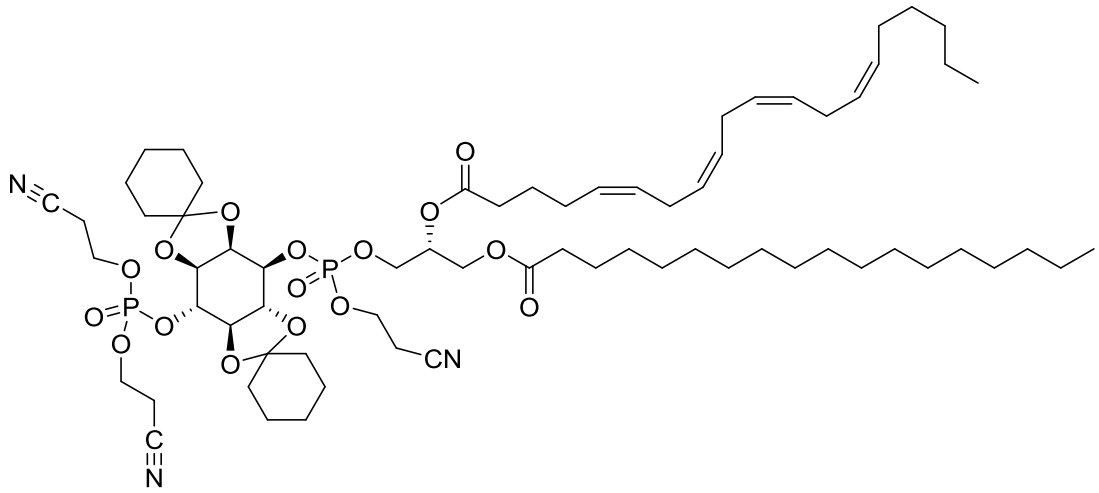
1-*O*-[(Cyanoethyloxy)(*sn*-1-*O*-stearoyl-2-*O*-γ-linolenoylglyceryloxy)phosphoryl]-4-*O*-(dicyanoethyloxyphosphoryl)-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 24c.

HRMS (ESI+) *m/z,* calcd for $C_{66}H_{107}N_3O_{16}P_2Na$ = 1,282·6, found $[M+Na]^+$ 1,282·6 (48%), $[M+NH_4]^+$ 1,277·7 (30%), $[M-C_6H_9]^+$ 1180.6 (53%), $[DAG]^+$ 601·5 (22%).


CH3
CH3
N
N
N
O
P
shift (ppm)
5.6
5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
0.6

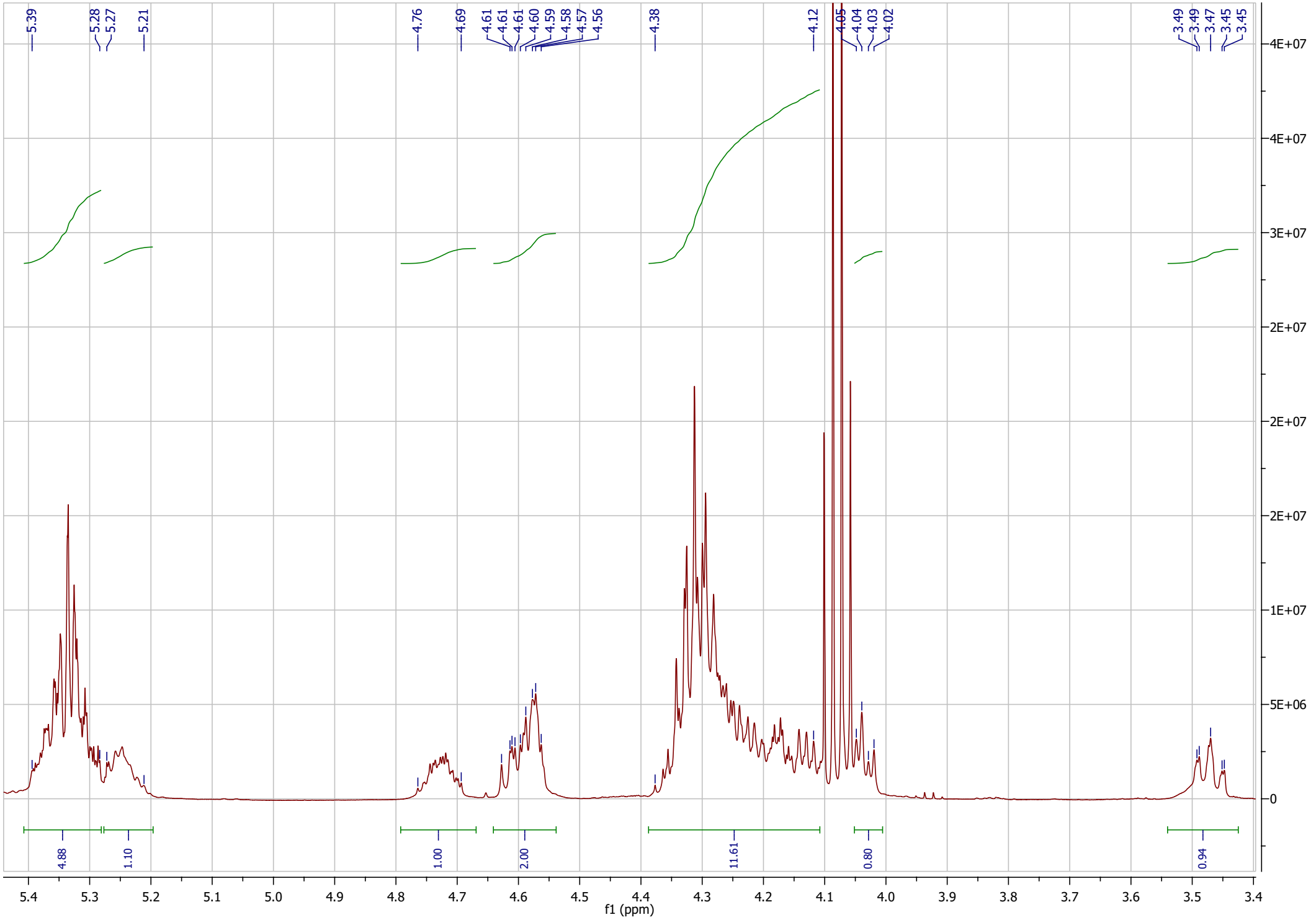

CH3
CH3
shift (ppm)
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15

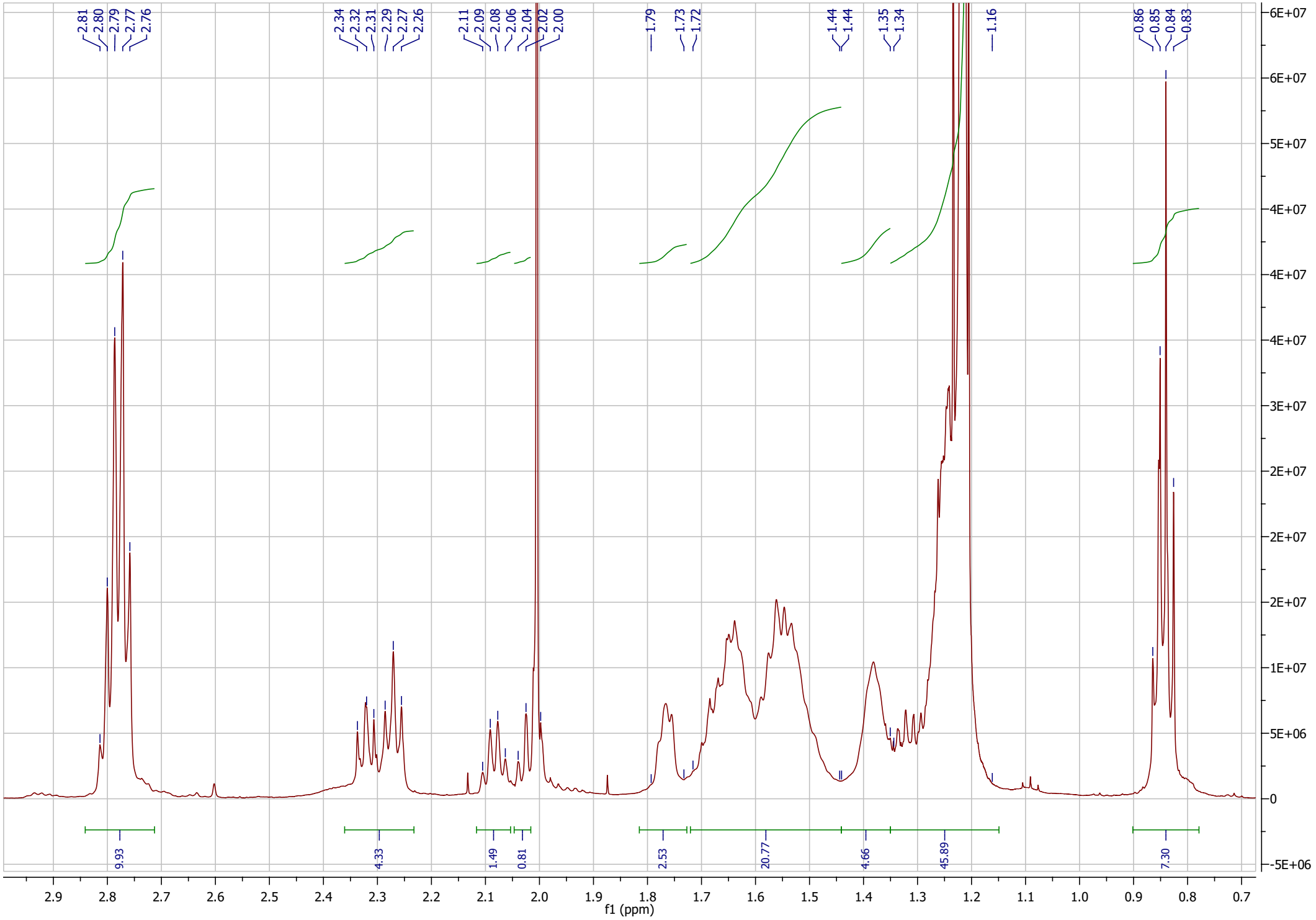

CH3
CH3
N
N
N
O
P
shift (ppm)
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30

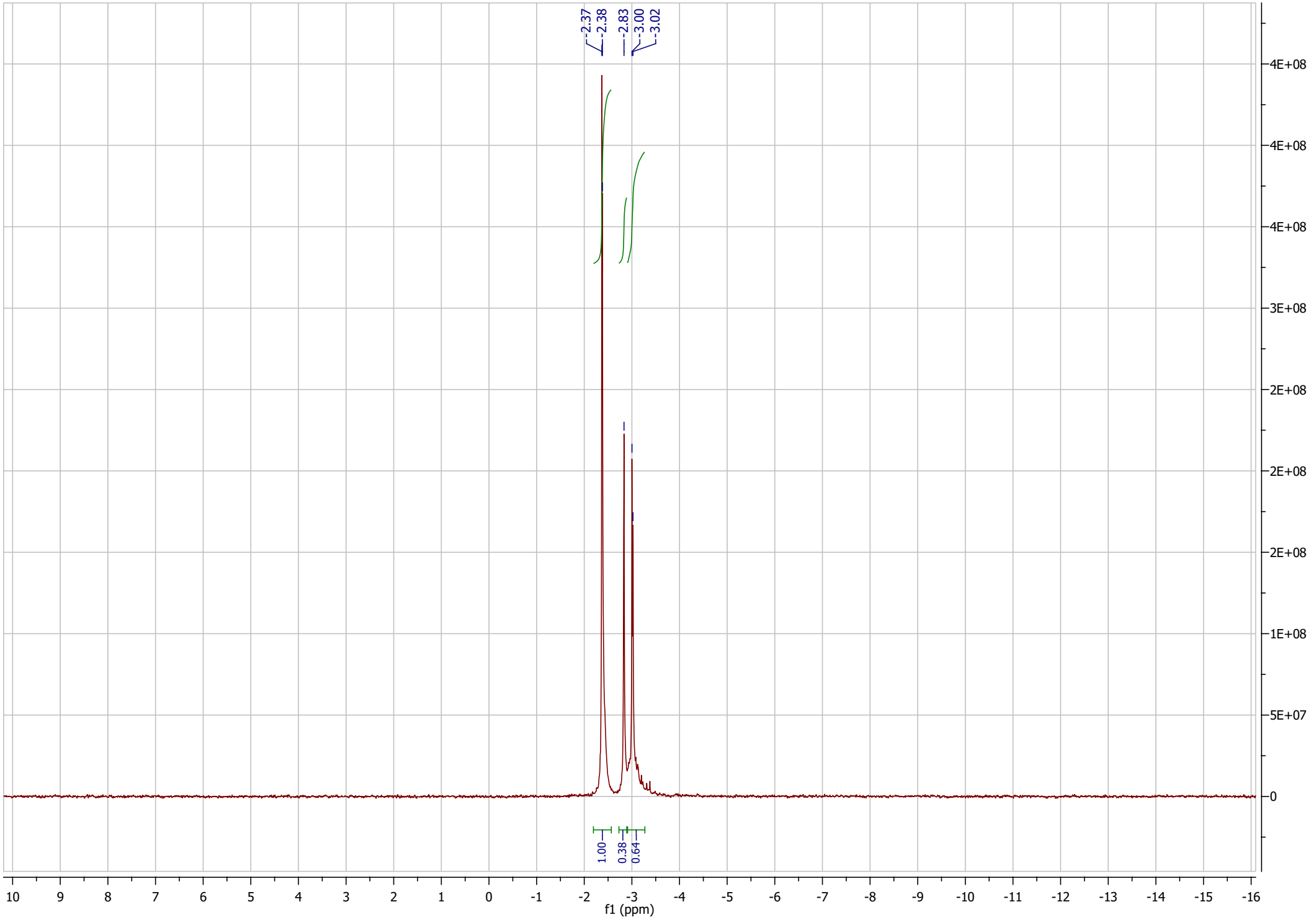


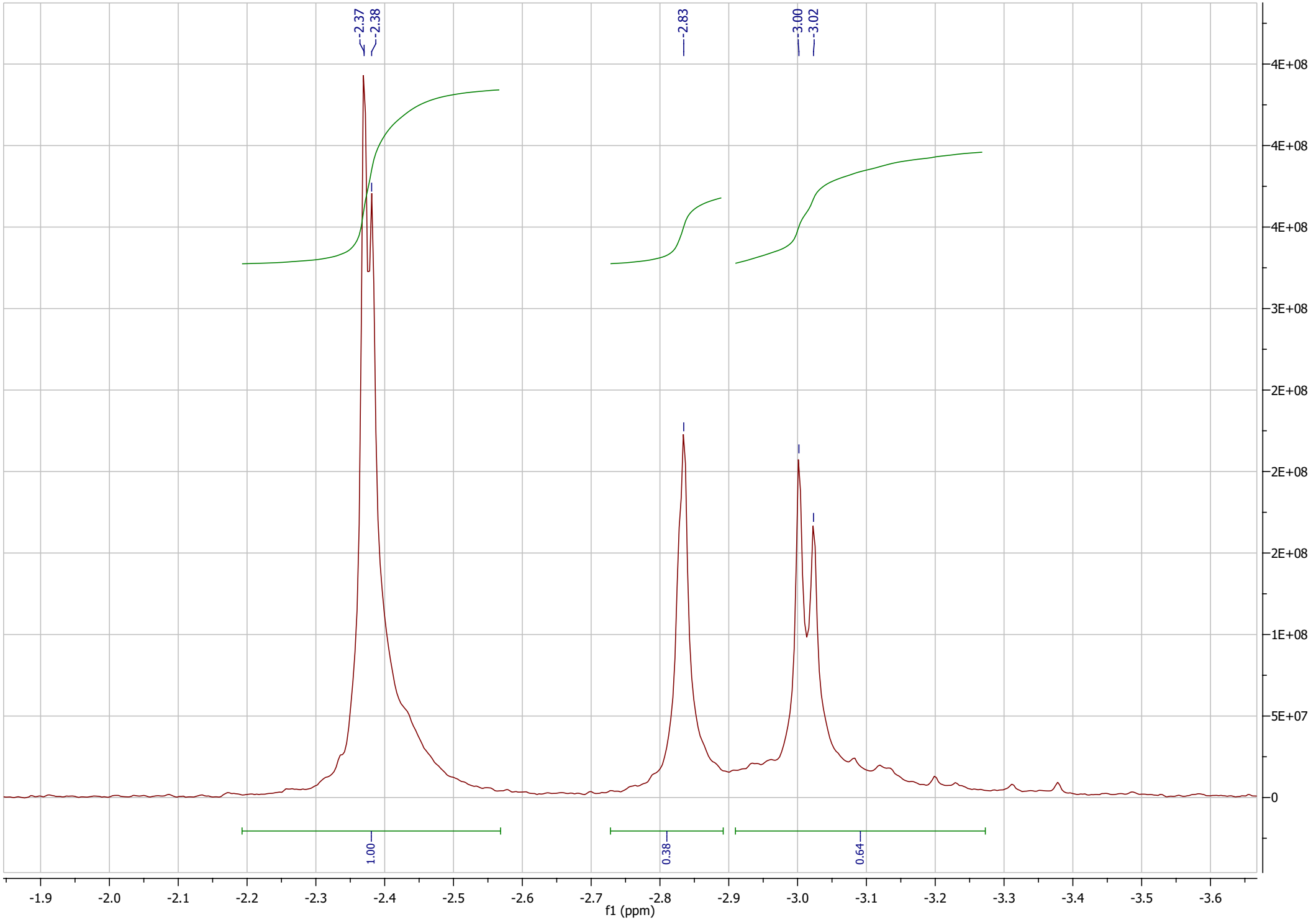
1-*O*-[(Cyanoethyloxy)(*sn*-1-*O*-stearoyl-2-*O*-arachidonoylglyceryloxy)phosphoryl]-4-*O*-(dicyanoethyloxyphosphoryl)-(2,3)(5,6)-*O*-dicyclohexylidene-*myo*-inositol, 24d.

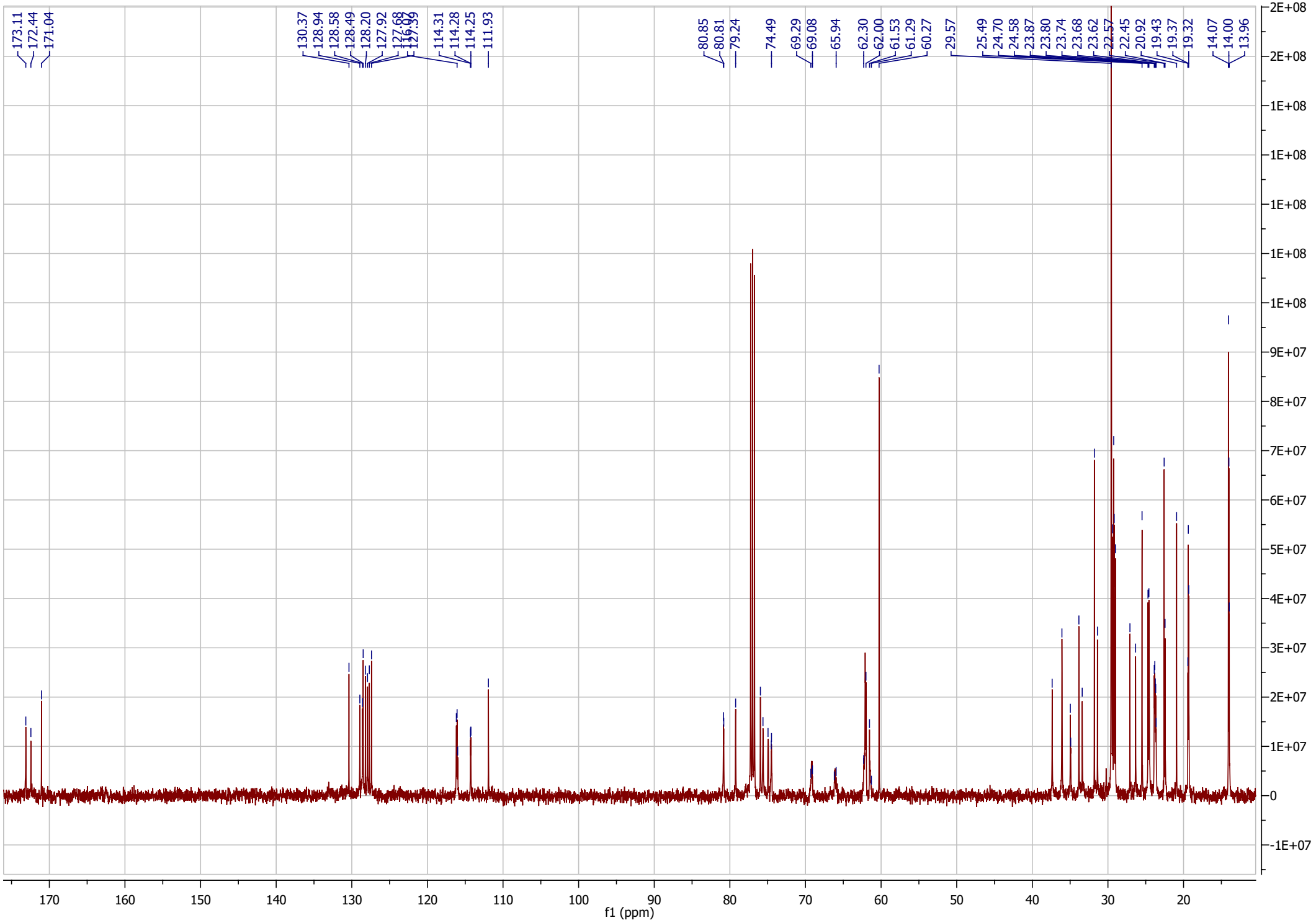
HRMS (ESI+) *m/z* found $[M+H]^+$ = 1,286·7357, $C_{68}H_{110}N_3O_{16}P_2$ requires 1,286·7361.

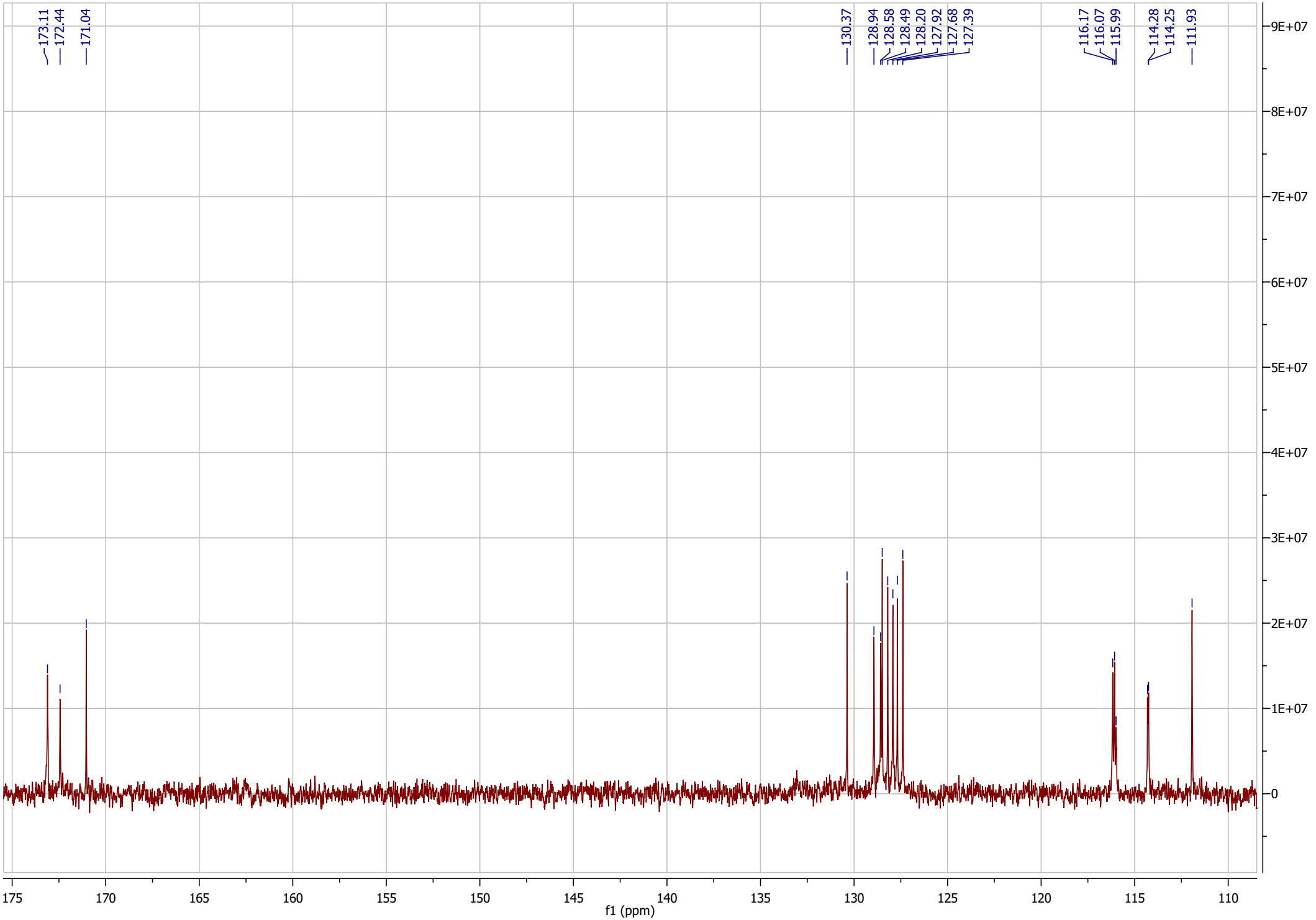

5.39
5.28
5.27
5.21
4.76
4.69
4.61
4.61
4.61
4.60
4.59
4.58
4.57
4.56
4.38
4.12
4.05
4.04
4.03
4.02
3.49
3.49
3.47
3.45
3.45
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
4.88
1.10
1.00
2.00
11.61
0.80
0.94
5.4
5.3
5.2
5.1
5.0
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
f1 (ppm)

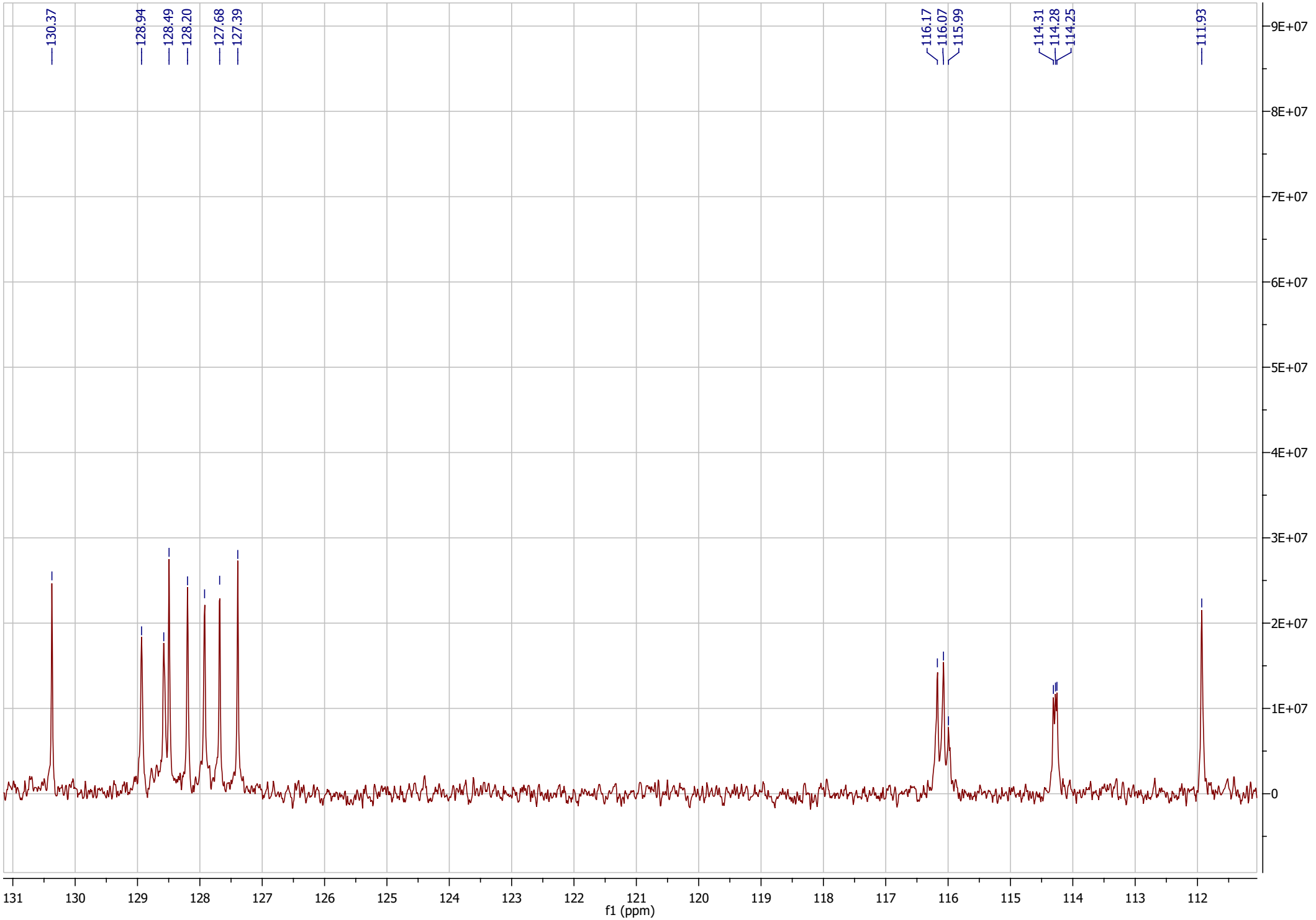

2.81
2.80
2.79
2.77
2.76
2.34
2.32
2.31
2.29
2.27
2.26
2.11
2.09
2.08
2.06
2.04
2.02
2.00
1.79
1.73
1.72
1.44
1.44
1.35
1.34
1.16
0.86
0.85
0.84
0.83
9.93
4.33
1.49
0.81
2.53
20.77
4.66
45.89
7.30
f1 (ppm)

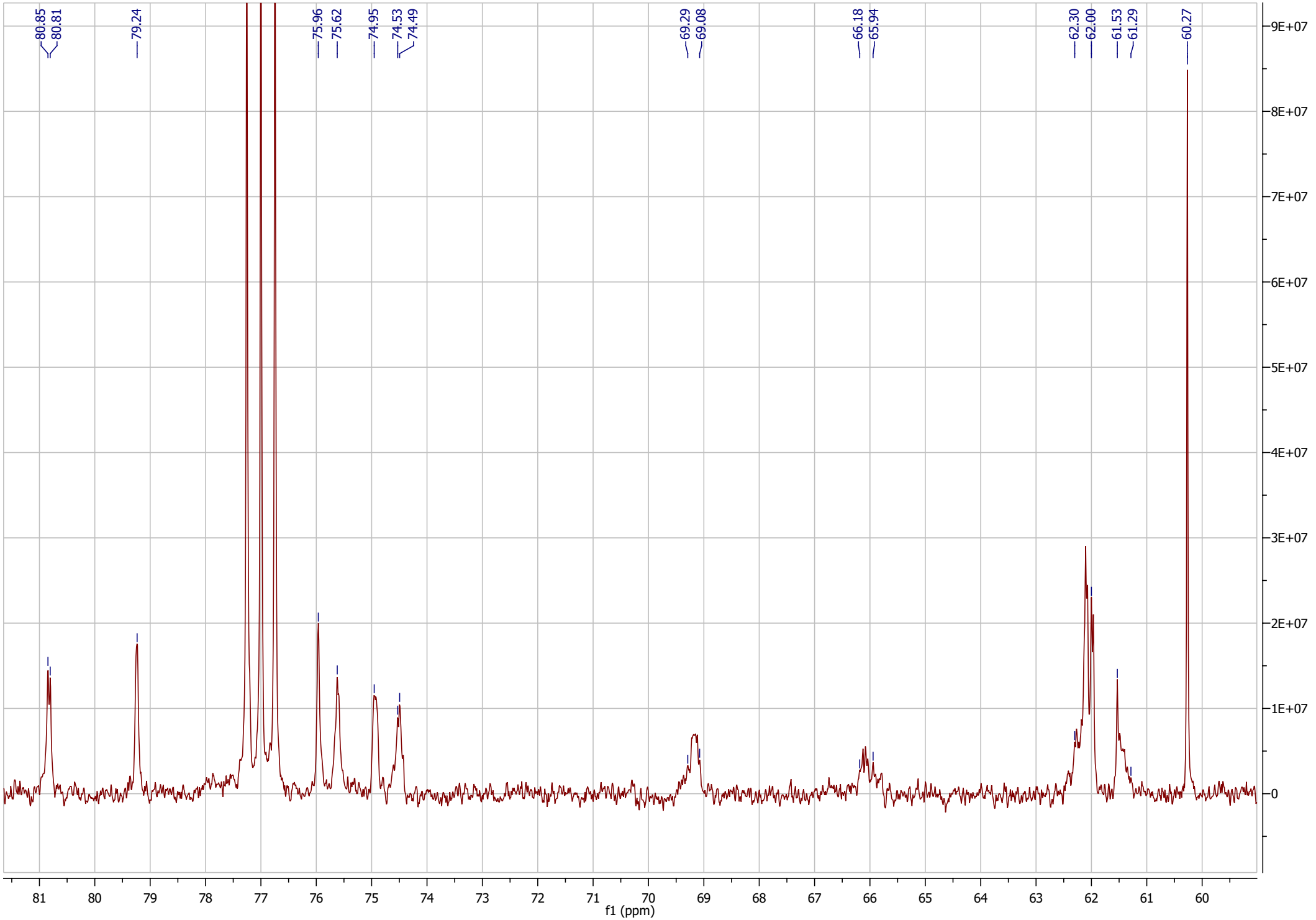

-2.37
-2.38
-2.83
-3.00
-3.02
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
0.38
0.64
10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7 -8 -9 -10 -11 -12 -13 -14 -15 -16
f1 (ppm)

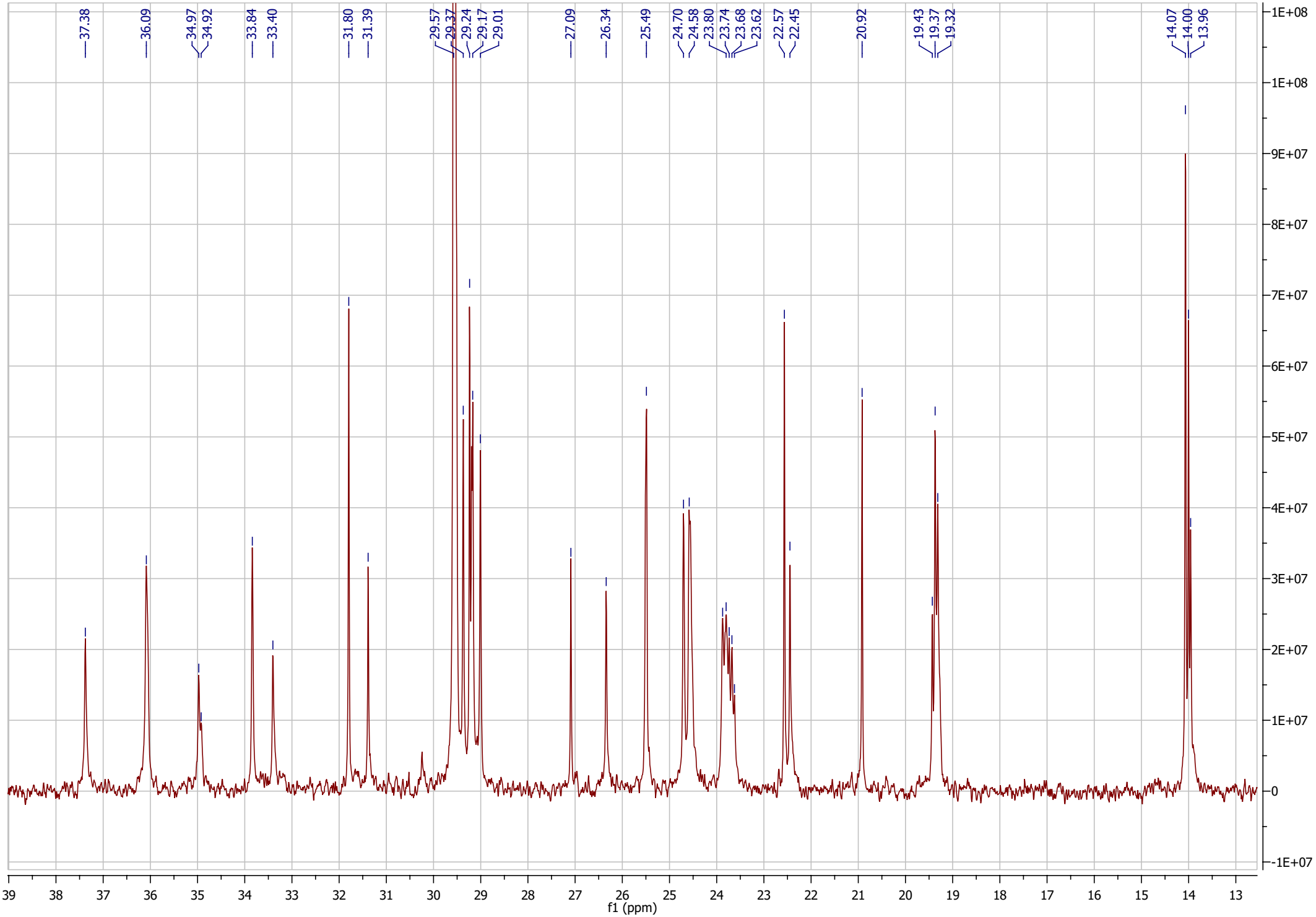

-2.37
-2.38
-2.83
-3.00
-3.02
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
0.38
0.64
-1.9
-2.0
-2.1
-2.2
-2.3
-2.4
-2.5
-2.6
-2.7
-2.8
-2.9
-3.0
-3.1
-3.2
-3.3
-3.4
-3.5
-3.6
f1 (ppm)

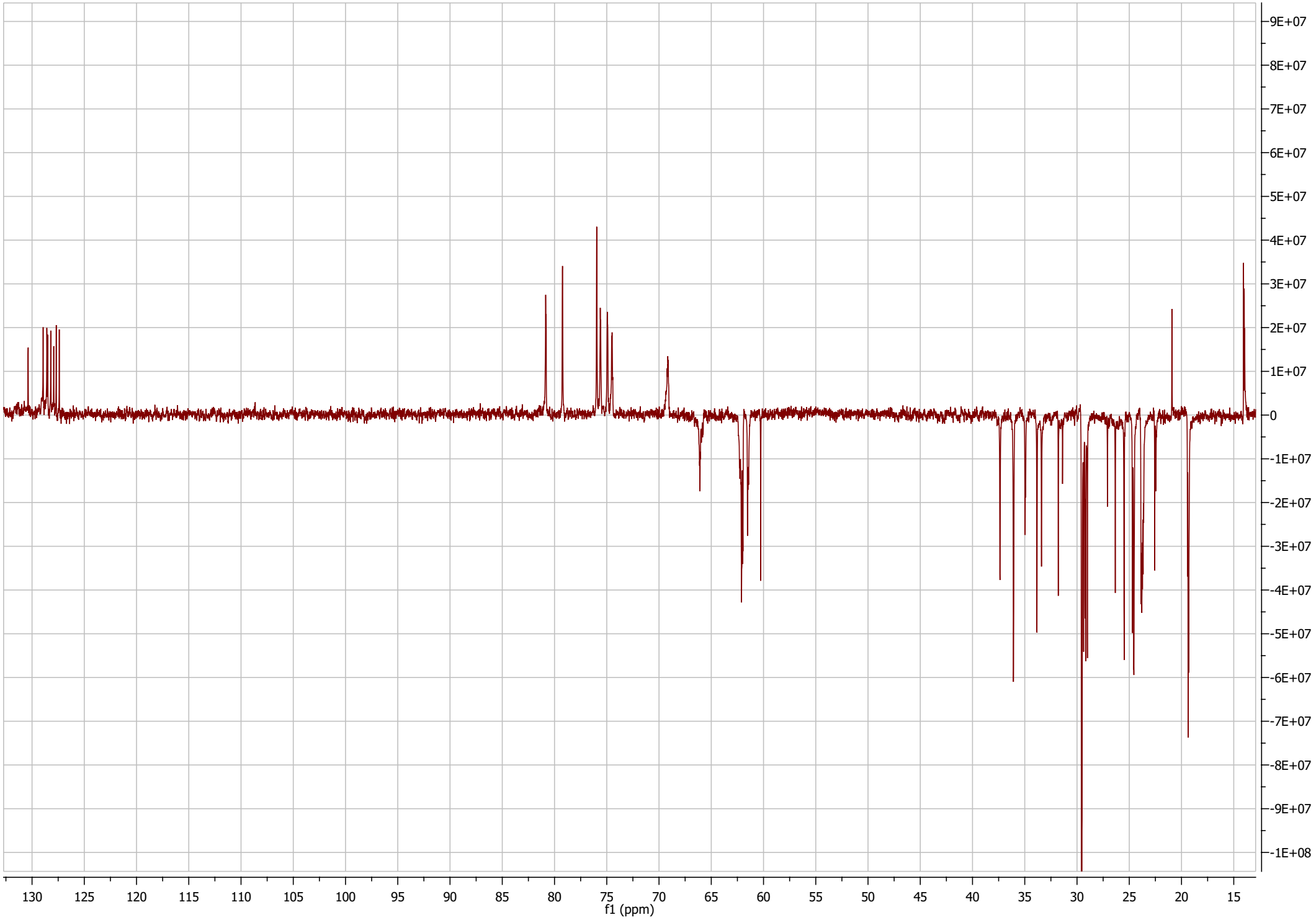

173.11
172.44
171.04
130.37
128.94
128.58
128.49
128.20
127.92
114.31
114.28
114.25
111.93
80.85
80.81
79.24
74.49
69.29
69.08
65.94
62.30
62.00
61.53
61.29
60.27
29.57
25.49
24.70
24.58
23.87
23.80
23.74
23.68
23.62
22.57
22.45
20.92
19.43
19.37
19.32
14.07
14.00
13.96
2E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

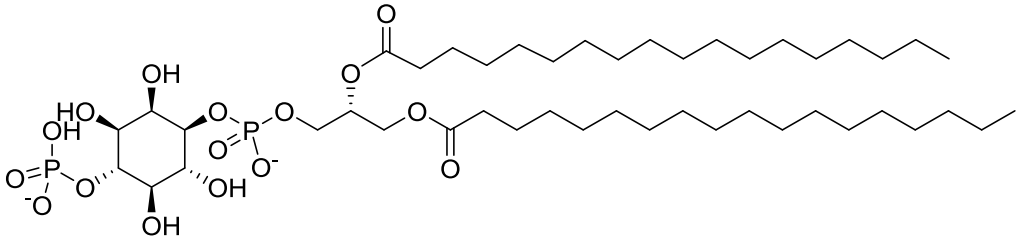

173.11
172.44
171.04
130.37
128.94
128.58
128.49
128.20
127.92
127.68
127.39
116.17
116.07
115.99
114.28
114.25
111.93
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)


130.37
128.94
128.49
128.20
127.68
127.39
116.17
116.07
115.99
114.31
114.28
114.25
111.93
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
131
130
129
128
127
126
125
124
123
122
121
120
119
118
117
116
115
114
113
112
f1 (ppm)


80.85
80.81
79.24
75.96
75.62
74.95
74.53
74.49
69.29
69.08
66.18
65.94
62.30
62.00
61.53
61.29
60.27
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
81
80
79
78
77
76
75
74
73
72
71
70
69
68
67
66
65
64
63
62
61
60
f1 (ppm)

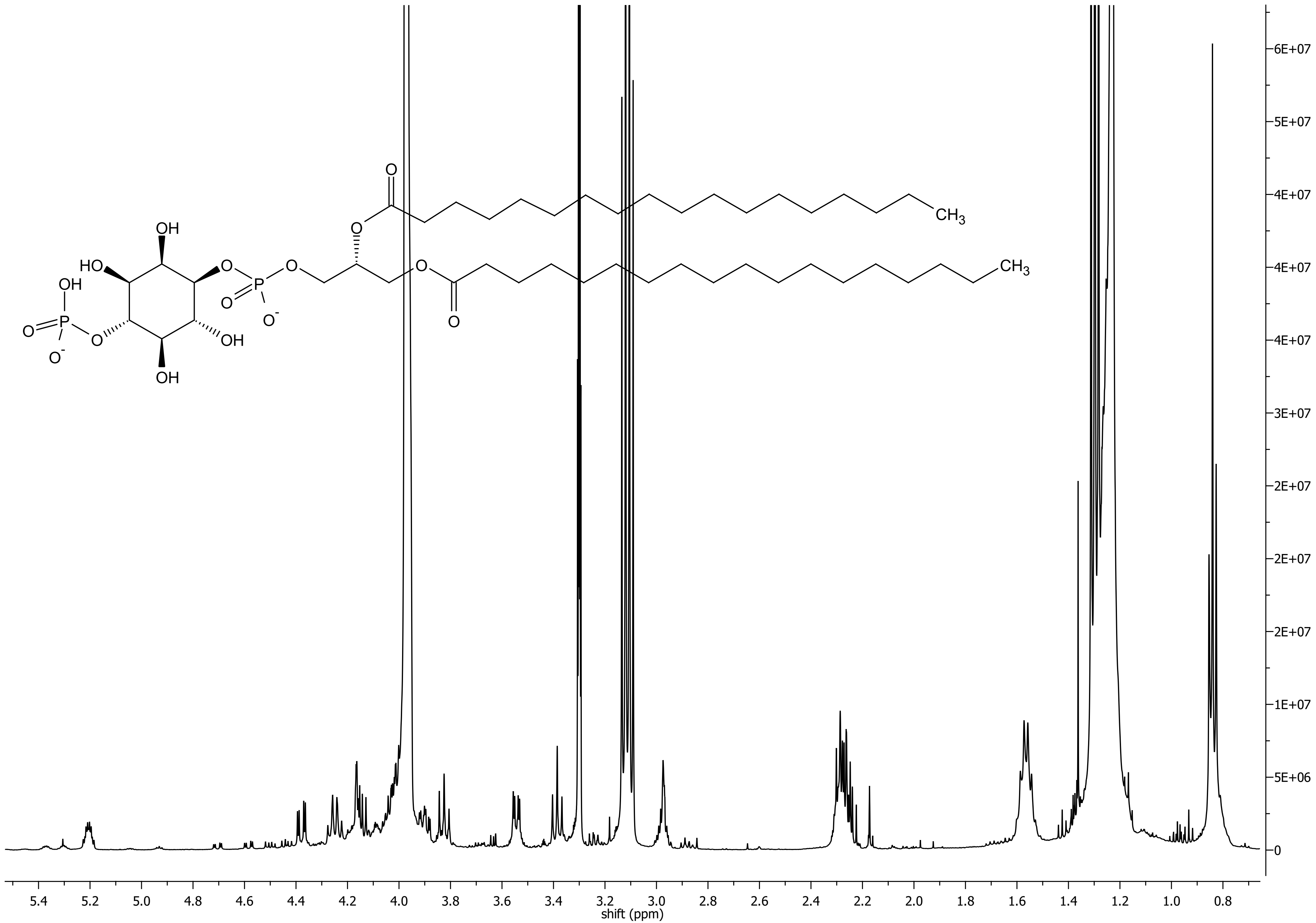

37.38
36.09
34.97
34.92
33.84
33.40
31.80
31.39
29.57
29.37
29.24
29.17
29.01
27.09
26.34
25.49
24.70
24.58
23.80
23.74
23.68
23.62
22.57
22.45
20.92
19.43
19.37
19.32
14.07
14.00
13.96
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
39
38
37
36
35
34
33
32
31
30
29
28
27
26
25
24
23
22
21
20
19
18
17
16
15
14
13
f1 (ppm)


9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
-2E+07
-3E+07
-4E+07
-5E+07
-6E+07
-7E+07
-8E+07
-9E+07
-1E+08
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)

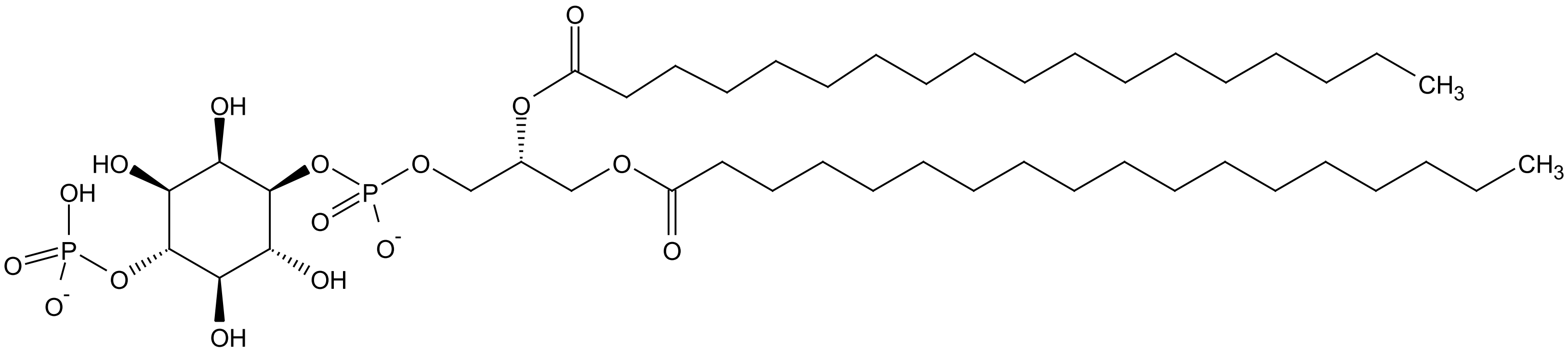


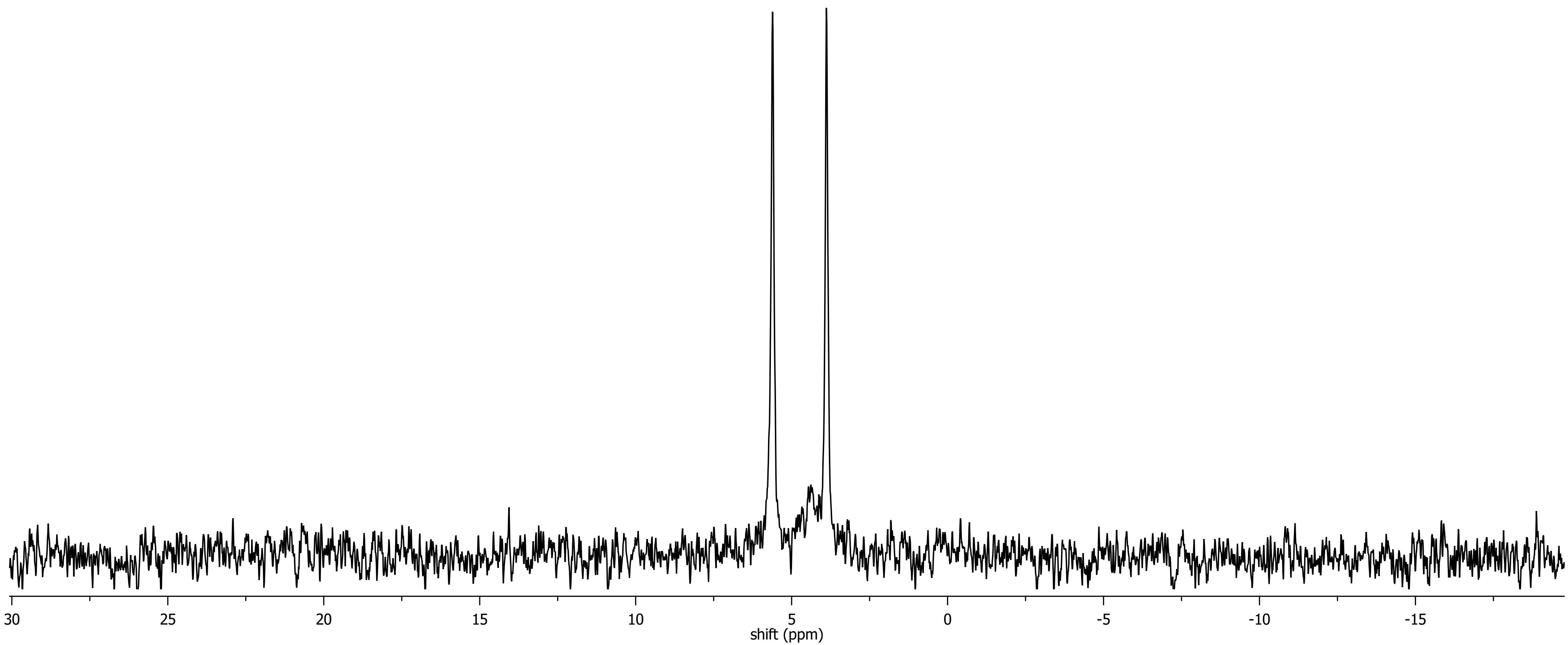
Distearoylphosphatidylinositol 4-*P*hosphate, triethylammonium salt, 2a.

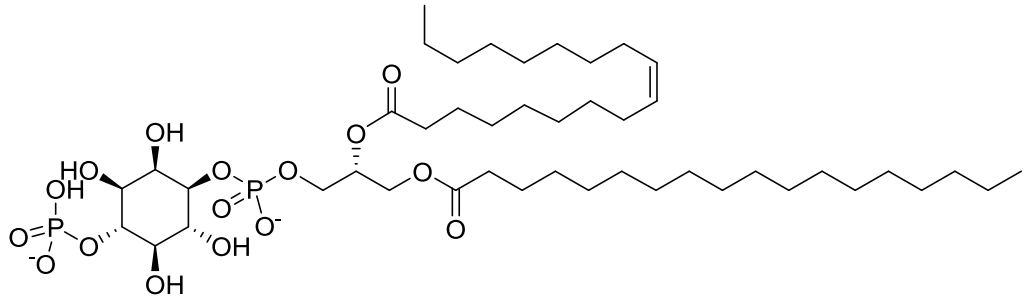
HRMS (ESI-) *m/z*, [M+H]+ = $C_{45}H_{87}O_{16}P_2^{=}$ calculated 945·5469, found 945·5505.



OH
HO
OH
O
P
O
O
OH
OH
O
O
P
O
O
O
O
O
CH3
O
O
CH3
6E+07
5E+07
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
shift (ppm)

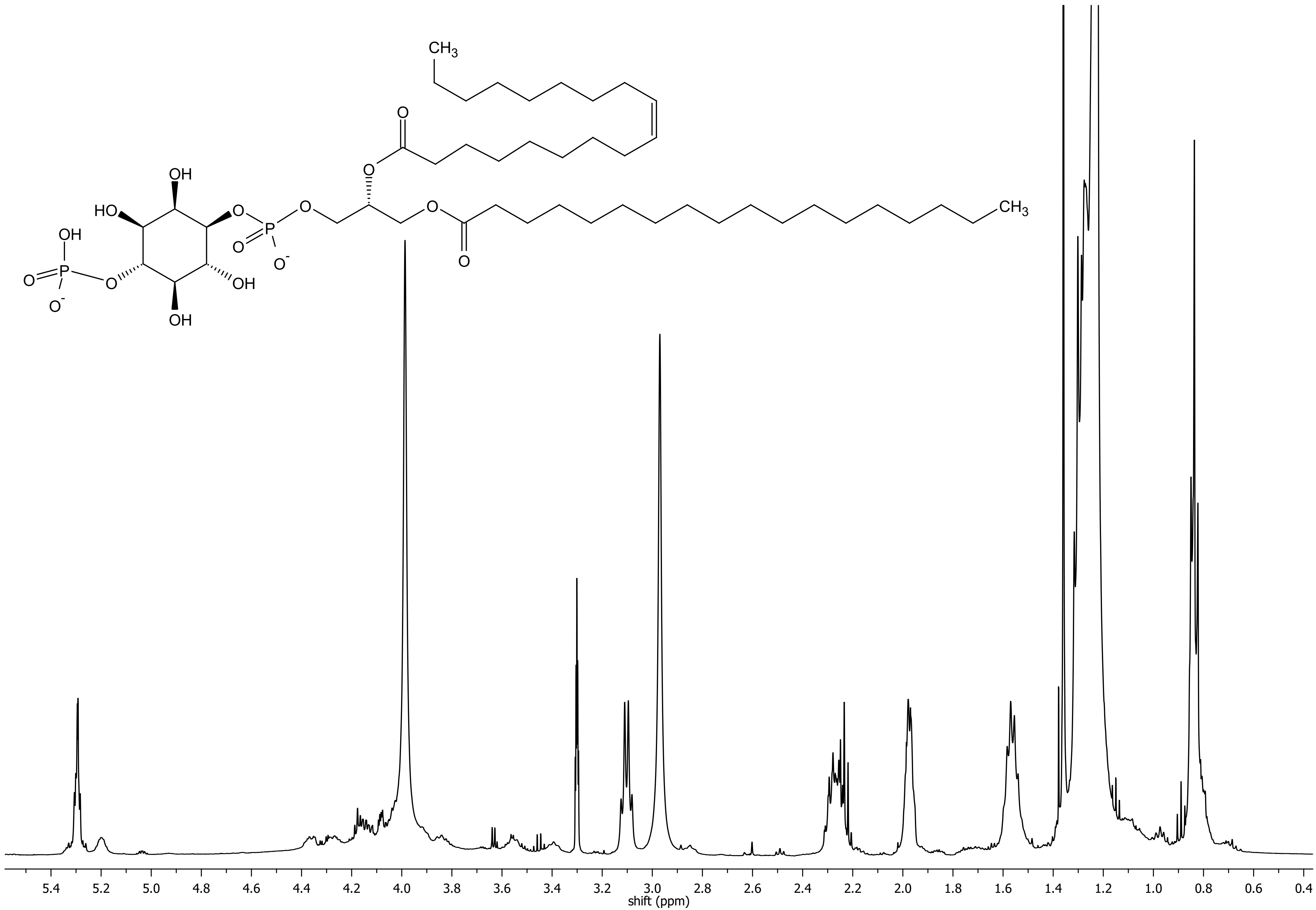

OH
HO
OH
O
P
O
O
OH
OH
O
O
P
O
O
O
O
O
O
CH3
CH3


30
25
20
15
10
5
0
-5
-10
-15
shift (ppm)

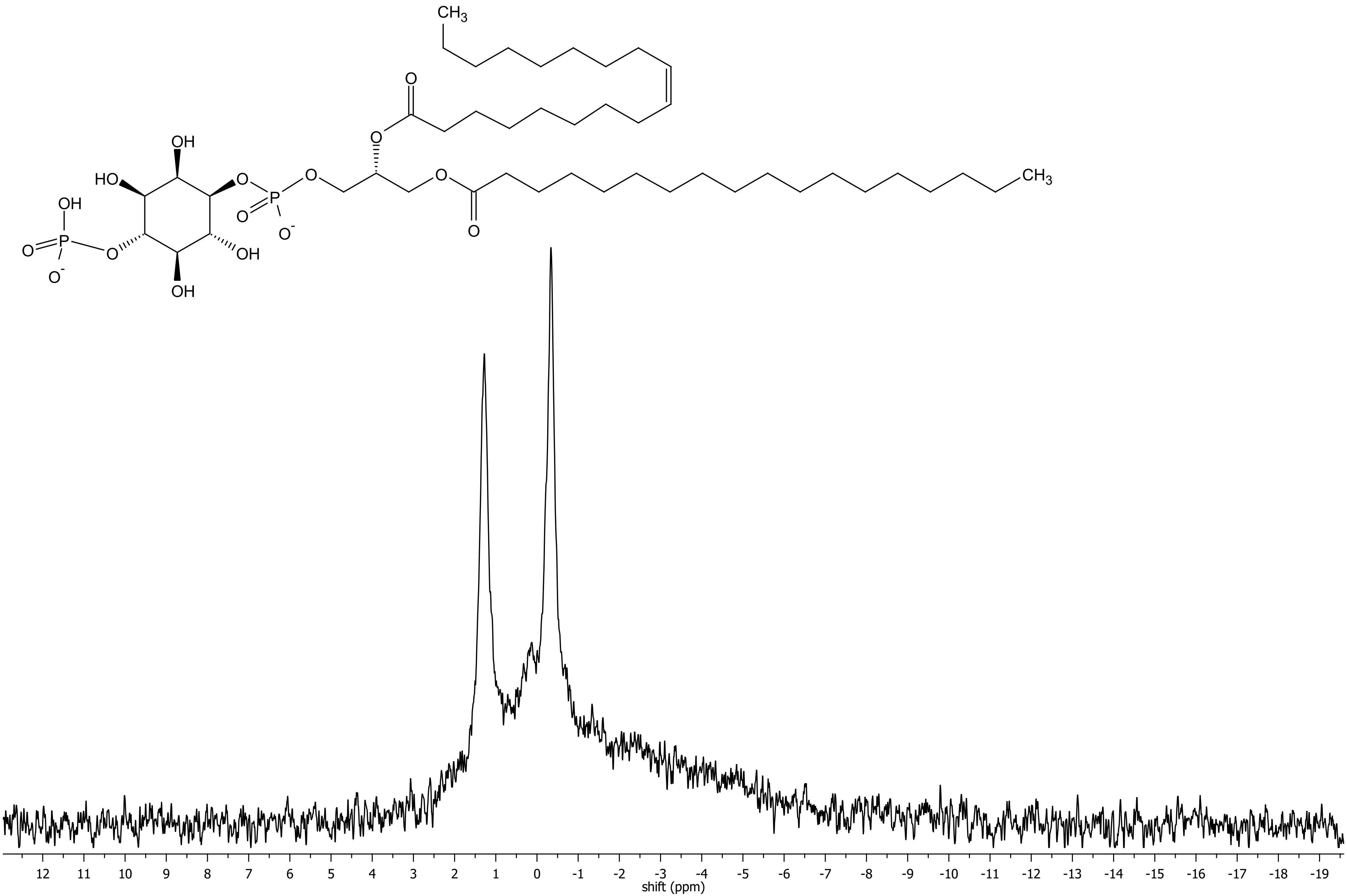


Stearoyl-oleoyl-phospatidylinositol-4-phosphate, triethylammonium salt, **2b.**

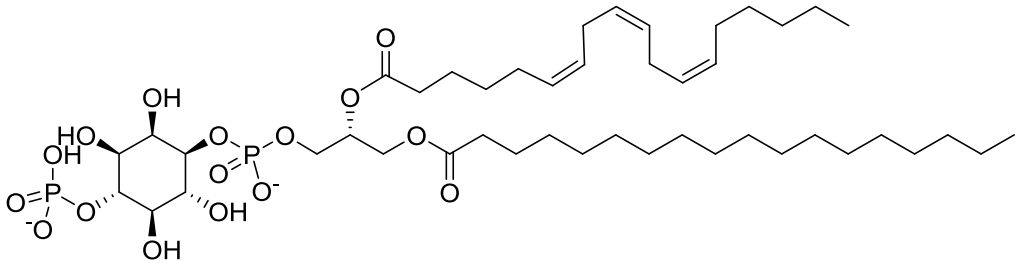
m/z (HR-ESI-) for **2b**, [M+H]+ = $C_{45}H_{85}O_{16}P_2^{=}$ calculated 943·5313, found 943·5346.



5.4
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
0.6
0.4
shift (ppm)

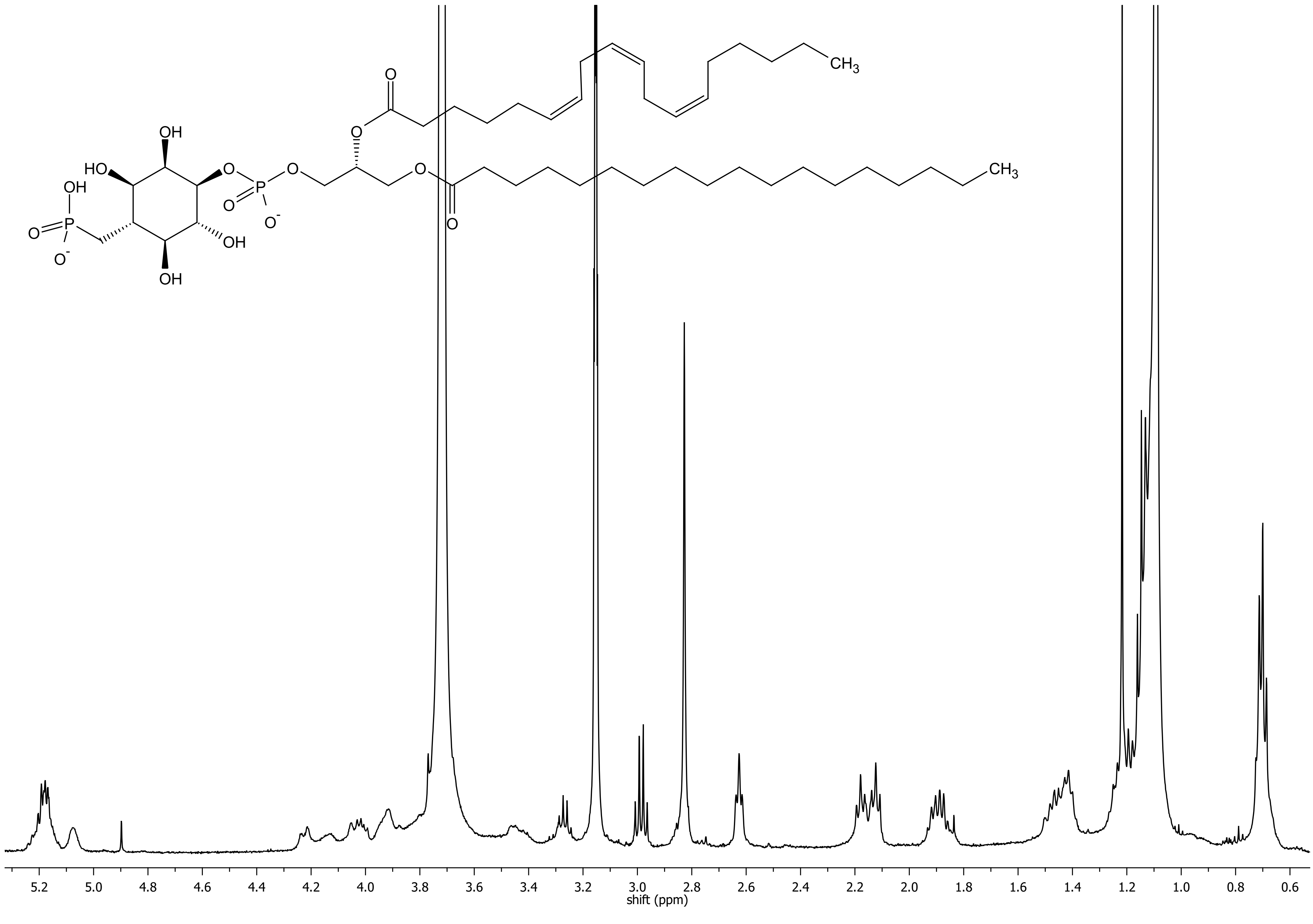


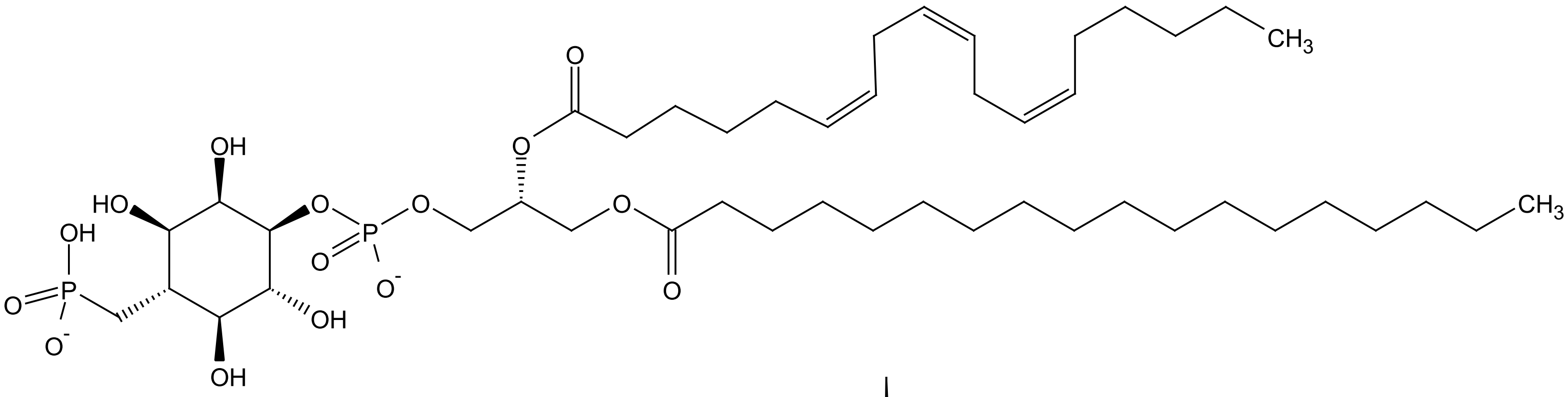
CH3
O
O
OH
HO
O
O
OH
O
P
O
P
O
O
OH
O
OH
OH
O
O
CH3
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
-18
-19
shift (ppm)

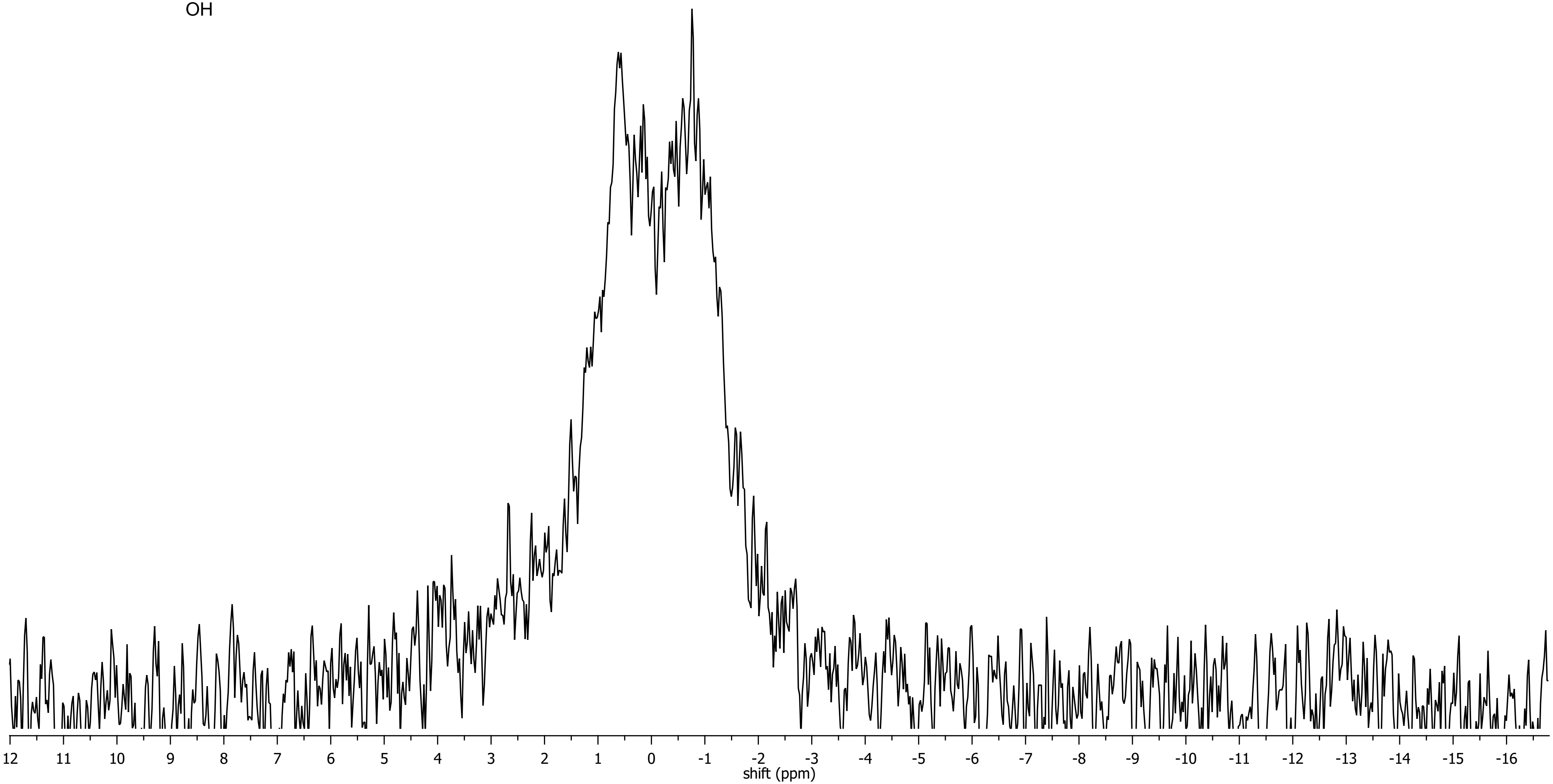


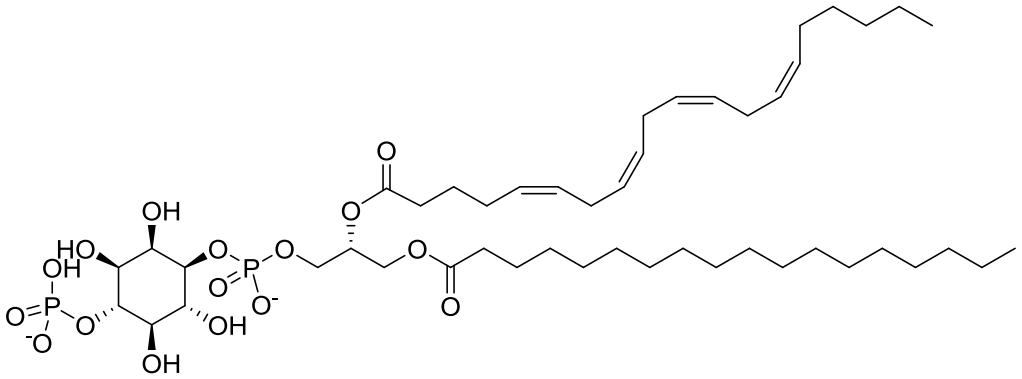
Stearoyl-γ-linolenoyl-phospatidylinositol-4-phosphate triethylammonium salt, 2c.

HRMS (ESI-) *m/z,* calcd for $C_{45}H_{87}O_{16}P_2^-$ = 945·5474, found $[M-H]^-$ 945·5505.


CH3
O
OH
HO
O
O
O
CH3
OH
P
O
O-
O
P
O
O-
OH
OH
O
5.2
5.0
4.8
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
1.6
1.4
1.2
1.0
0.8
0.6
shift (ppm)

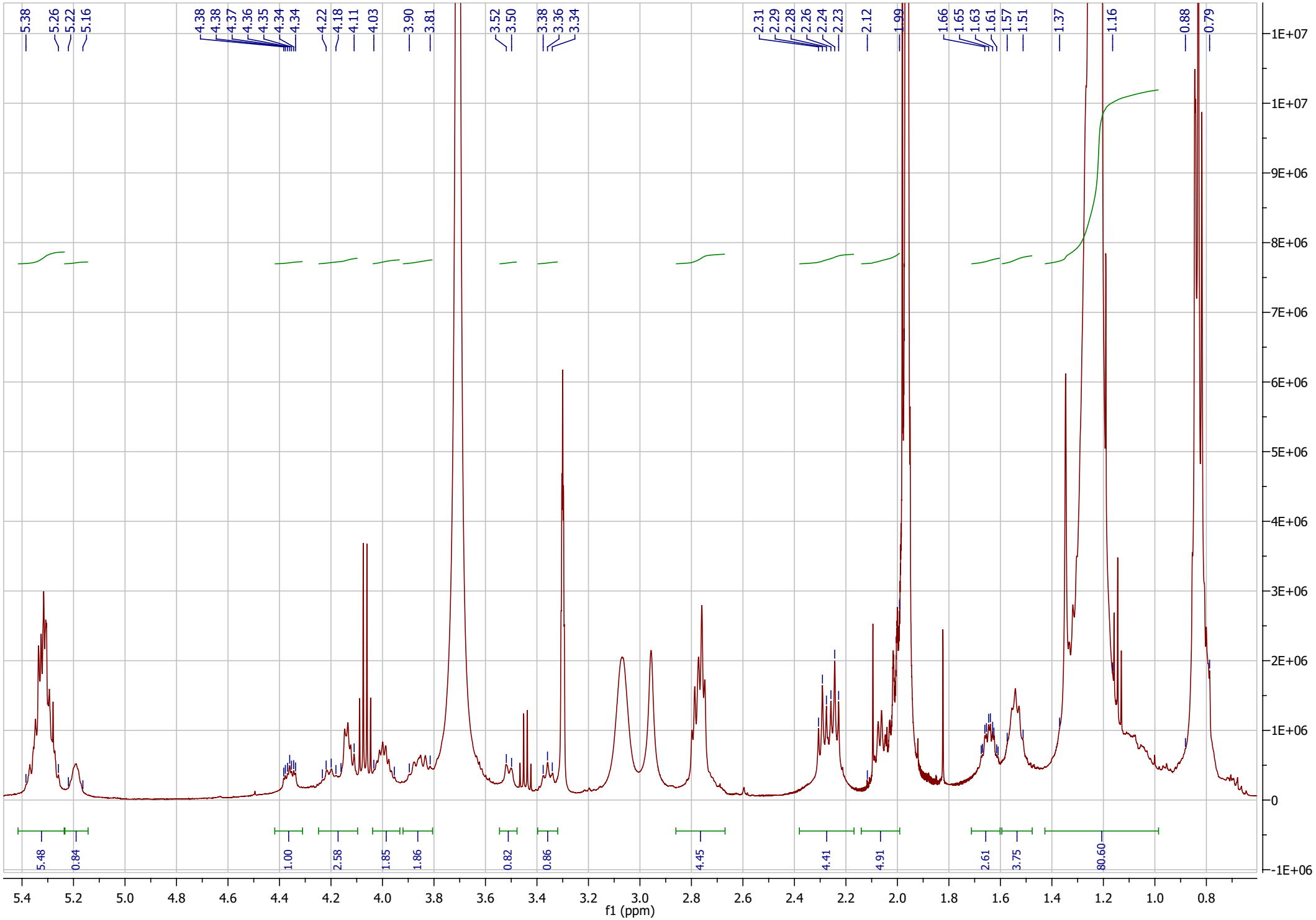



12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7 -8 -9 -10 -11 -12 -13 -14 -15 -16
shift (ppm)



Stearoyl-arachidonoyl-phospatidylinositol-4-phosphate, triethylammonium salt, 2d.

HRMS (ESI+) *m/z* found $[M+Na]^+$ = 989·5085, $C_{47}H_{85}O_{16}P_2Na$ requires 989·5143.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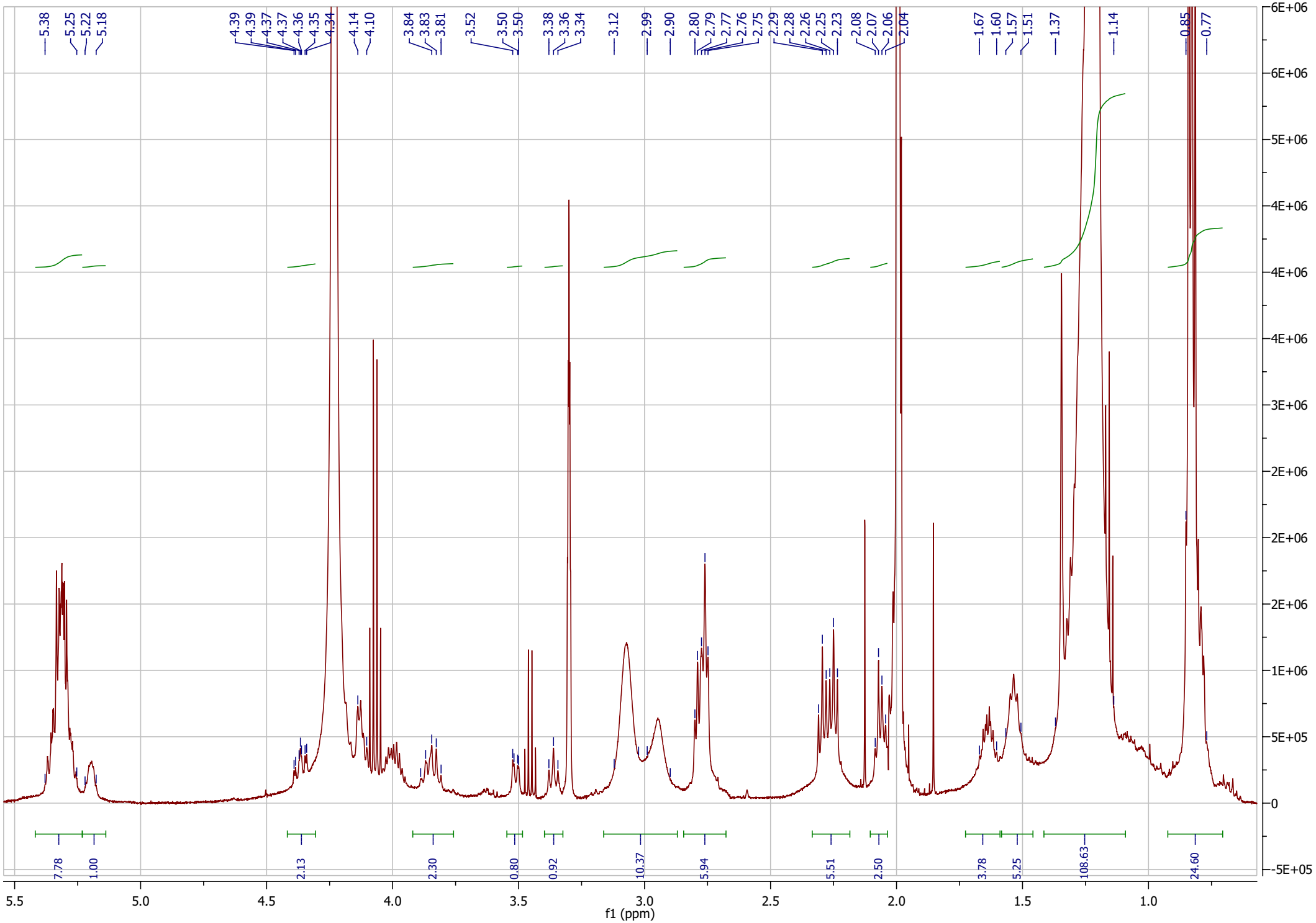
5.26
5.22
5.16
4.38
4.38
4.37
4.36
4.35
4.34
4.34
4.22
4.18
4.11
4.03
3.90
3.81
3.52
3.50
3.38
3.36
3.34
2.31
2.29
2.28
2.26
2.24
2.23
2.12
1.99
1.66
1.65
1.63
1.61
1.57
1.51
1.37
1.16
0.88
0.79
5.48
0.84
1.00
2.58
1.85
1.86
0.82
0.86
4.45
4.41
4.91
2.61
3.75
80.60
f1 (ppm)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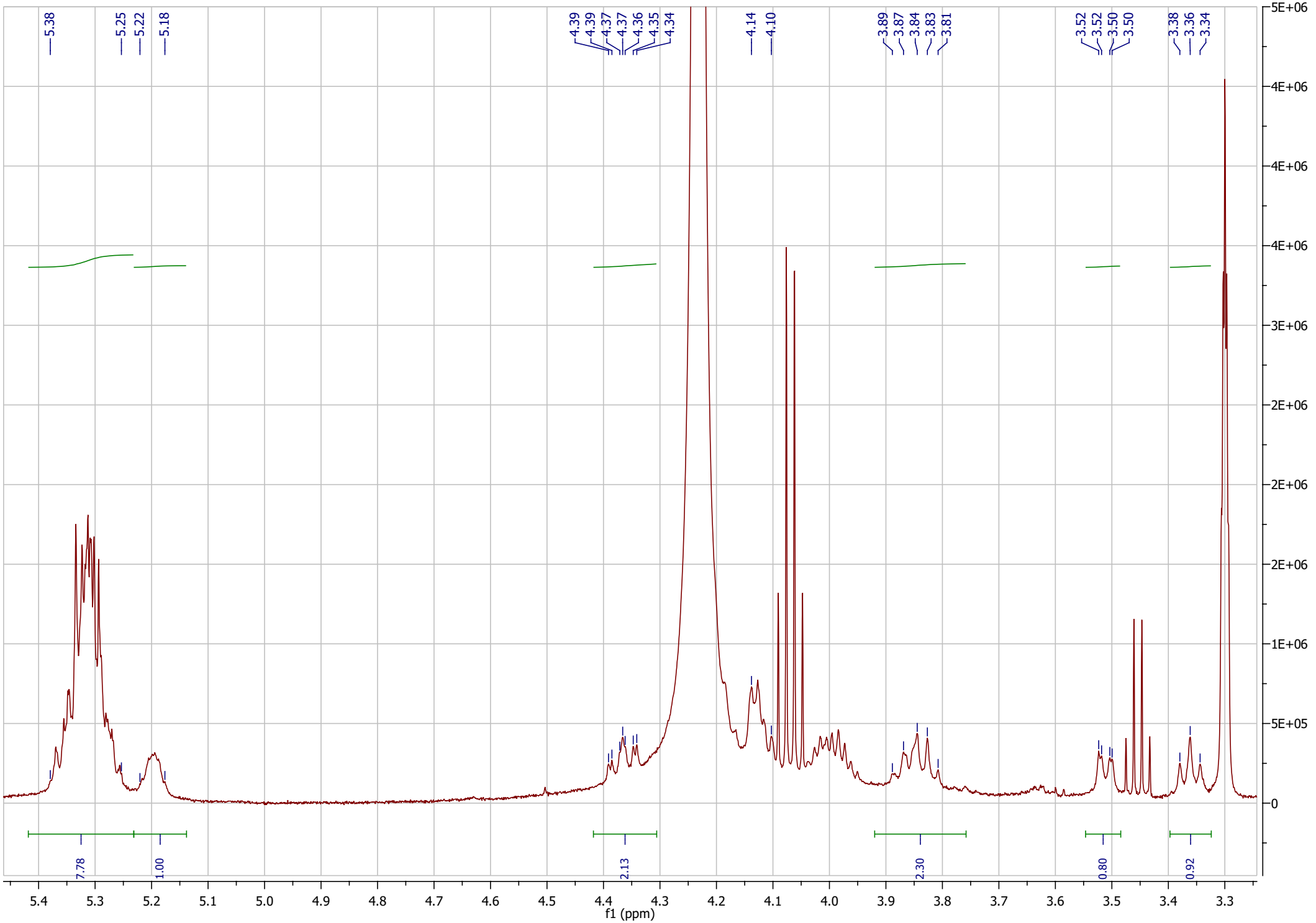
5.25
5.22
5.18
4.39
4.39
4.37
4.37
4.36
4.35
4.34
4.14
4.10
3.84
3.83
3.81
3.52
3.50
3.50
3.38
3.36
3.34
3.12
2.99
2.90
2.80
2.79
2.77
2.76
2.75
2.29
2.28
2.26
2.25
2.23
2.08
2.07
2.06
2.04
1.67
1.60
1.57
1.51
1.37
1.14
0.85
0.77
7.78
1.00
2.13
2.30
0.80
0.92
10.37
5.94
5.51
2.50
3.78
5.25
108.63
24.60
6E+06
6E+06
5E+06
4E+06
4E+06
4E+06
3E+06
2E+06
2E+06
2E+06
1E+06
5E+05
0
-5E+05
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)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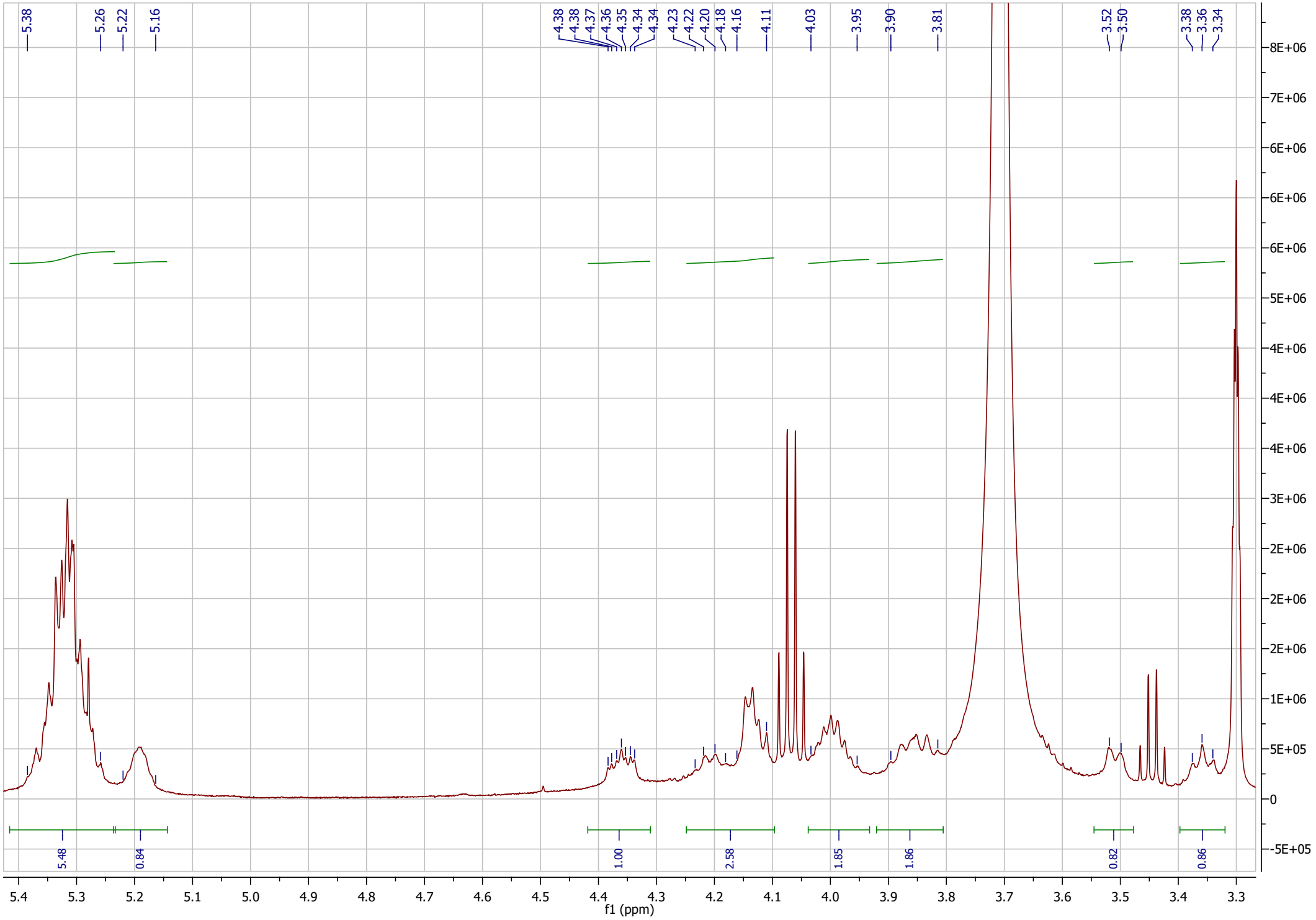
5.25
5.22
5.18
4.39
4.39
4.37
4.37
4.36
4.35
4.34
4.14
4.10
3.89
3.87
3.84
3.83
3.81
3.52
3.52
3.50
3.50
3.38
3.36
3.34
7.78
1.00
2.13
2.30
0.80
0.92
5E+06
4E+06
4E+06
4E+06
3E+06
2E+06
2E+06
2E+06
1E+06
5E+05
0
5.4
5.3
5.2
5.1
5.0
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
f1 (ppm)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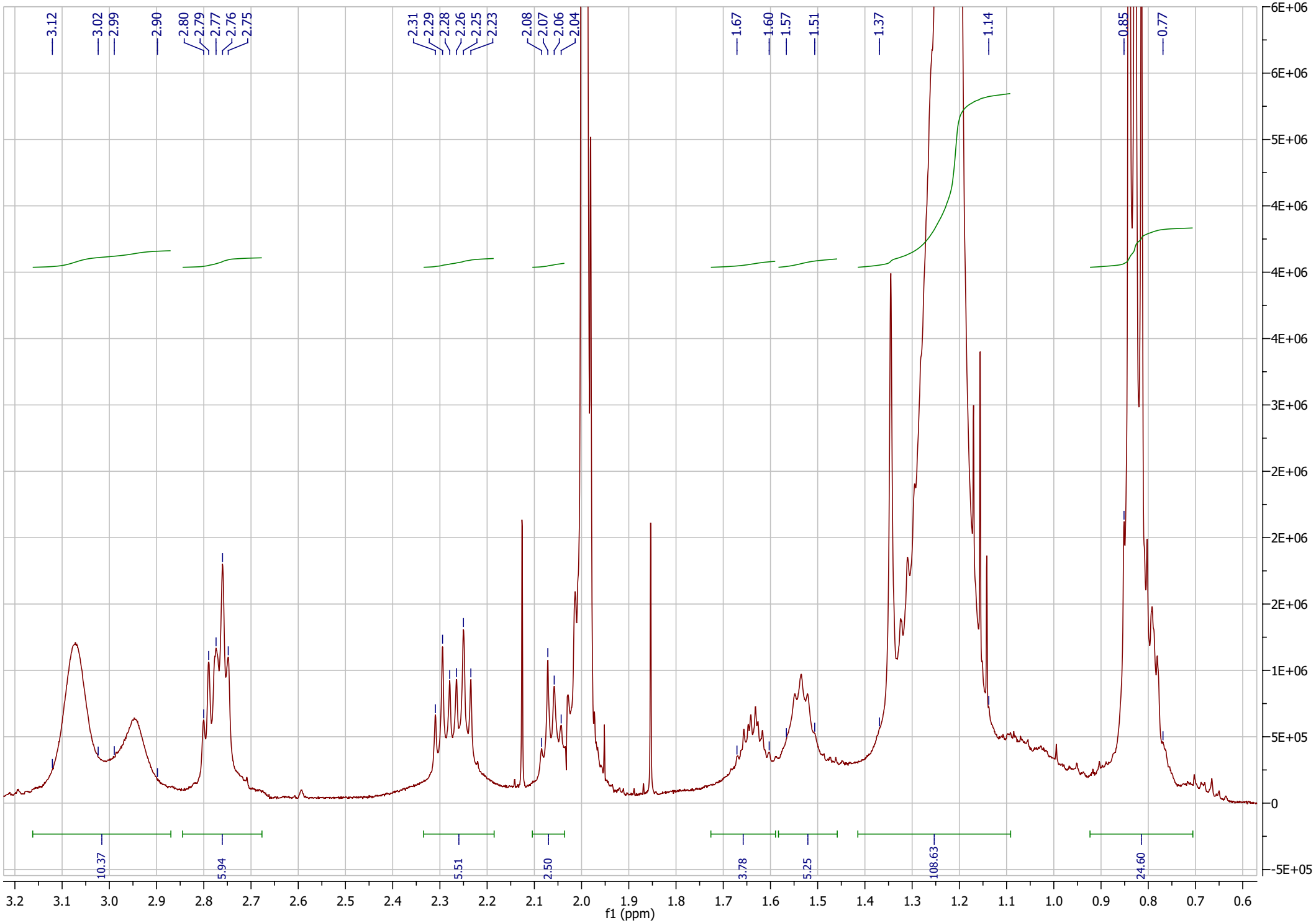
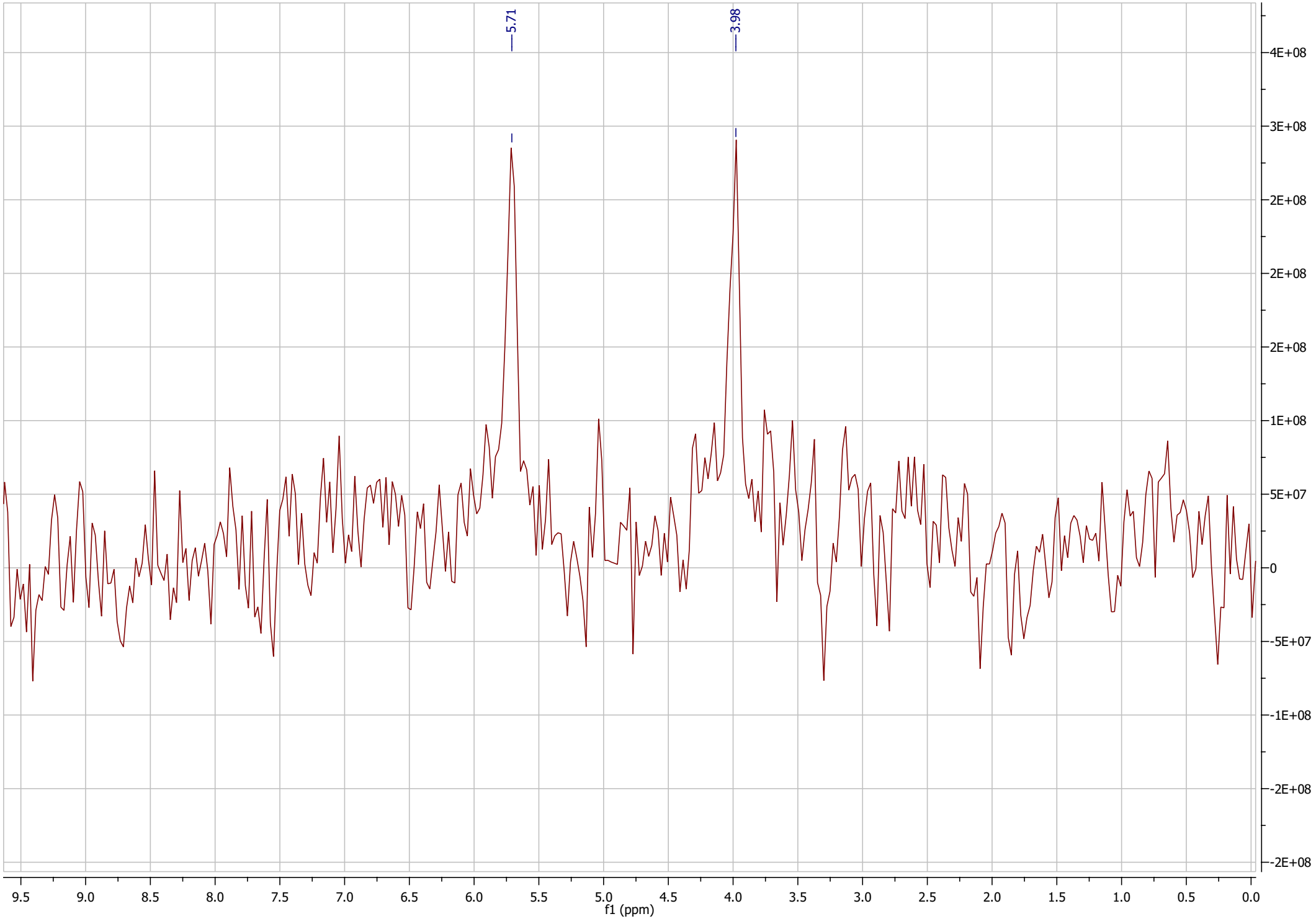
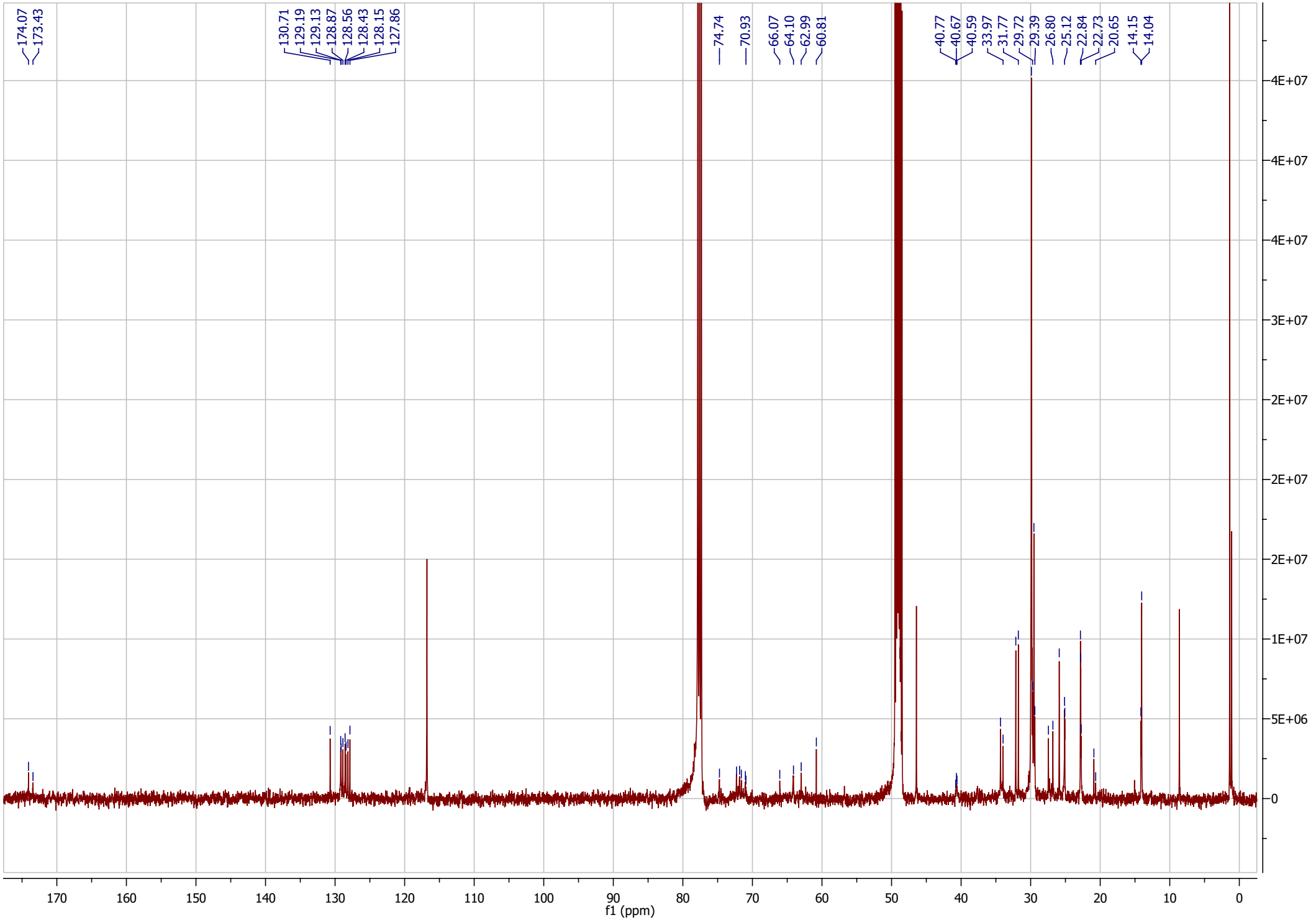
5.26
5.22
5.16
4.38
4.38
4.37
4.36
4.35
4.34
4.34
4.23
4.22
4.20
4.18
4.16
4.11
4.03
3.95
3.90
3.81
3.52
3.50
3.38
3.36
3.34
5.48
0.84
1.00
2.58
1.85
1.86
0.82
0.86
f1 (ppm)


3.12
3.02
2.99
2.90
2.80
2.79
2.77
2.76
2.75
2.31
2.29
2.28
2.26
2.25
2.23
2.08
2.07
2.06
2.04
1.67
1.60
1.57
1.51
1.37
1.14
0.85
0.77
10.37
5.94
5.51
2.50
3.78
5.25
108.63
24.60
f1 (ppm)


5.71
3.98
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
-2E+08
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)


174.07
173.43
130.71
129.19
129.13
128.87
128.56
128.43
128.15
127.86
74.74
70.93
66.07
64.10
62.99
60.81
40.77
40.67
40.59
33.97
31.77
29.72
29.39
26.80
25.12
22.84
22.73
20.65
14.15
14.04
4E+07
4E+07
4E+07
3E+07
2E+07
2E+07
2E+07
1E+07
5E+06
0
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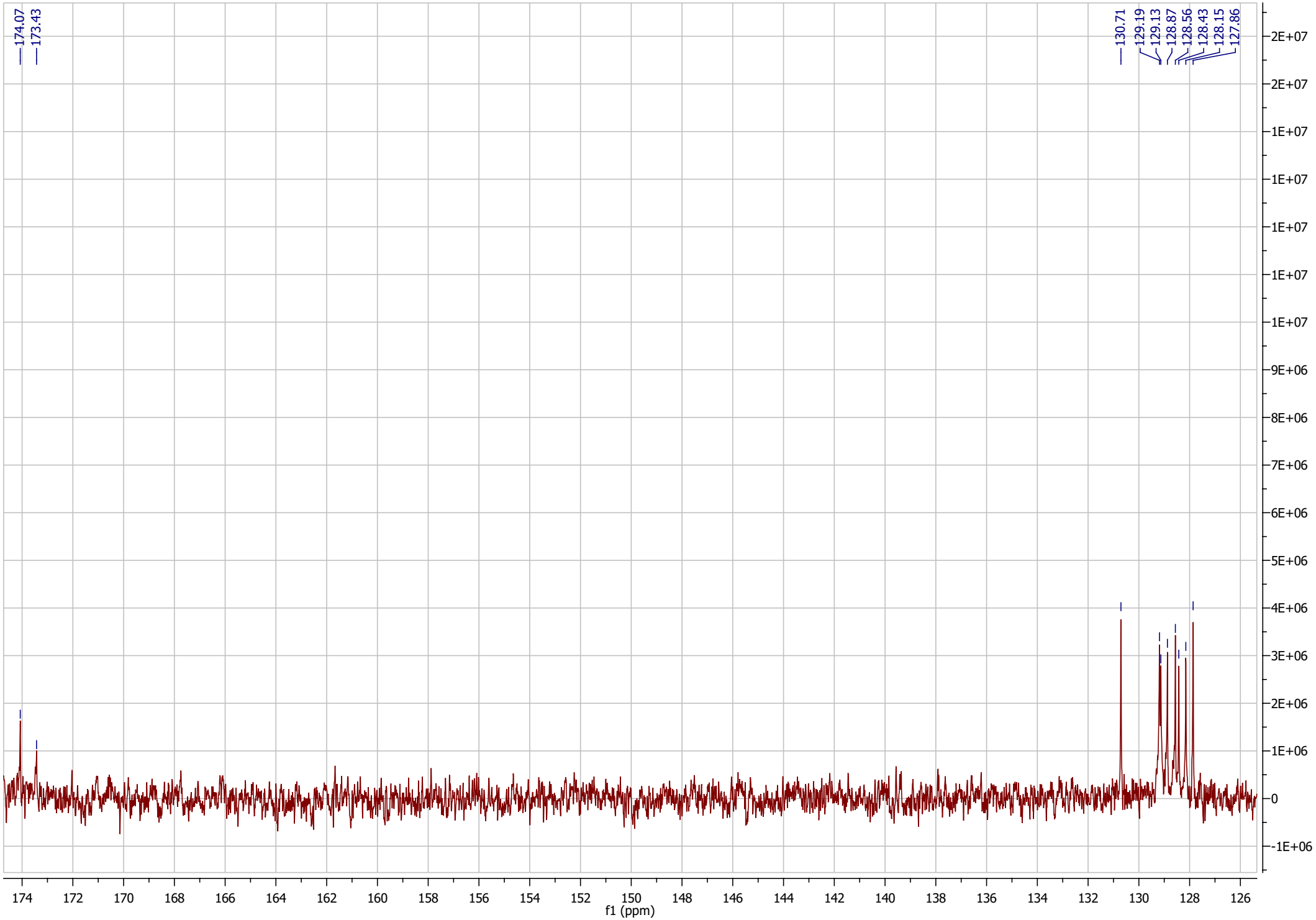
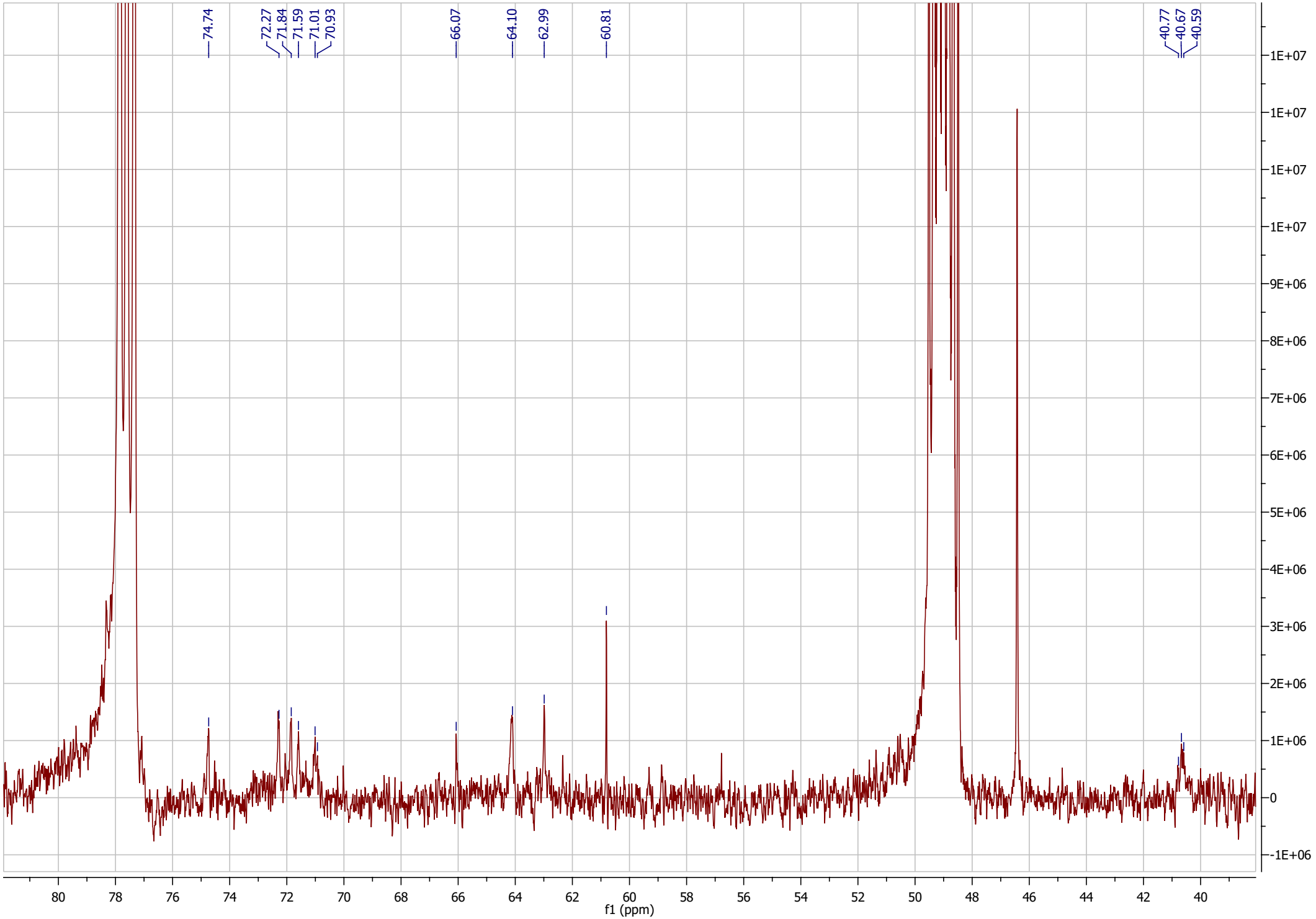
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


174.07
173.43
130.71
129.19
129.13
128.87
128.56
128.43
128.15
127.86
2E+07
2E+07
1E+07
1E+07
1E+07
1E+07
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
174
172
170
168
166
164
162
160
158
156
154
152
150
148
146
144
142
140
138
136
134
132
130
128
126
f1 (ppm)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72.27
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71.59
71.01
70.93
66.07
64.10
62.99
60.81
40.77
40.67
40.59
1E+07
1E+07
1E+07
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
80
78
76
74
72
70
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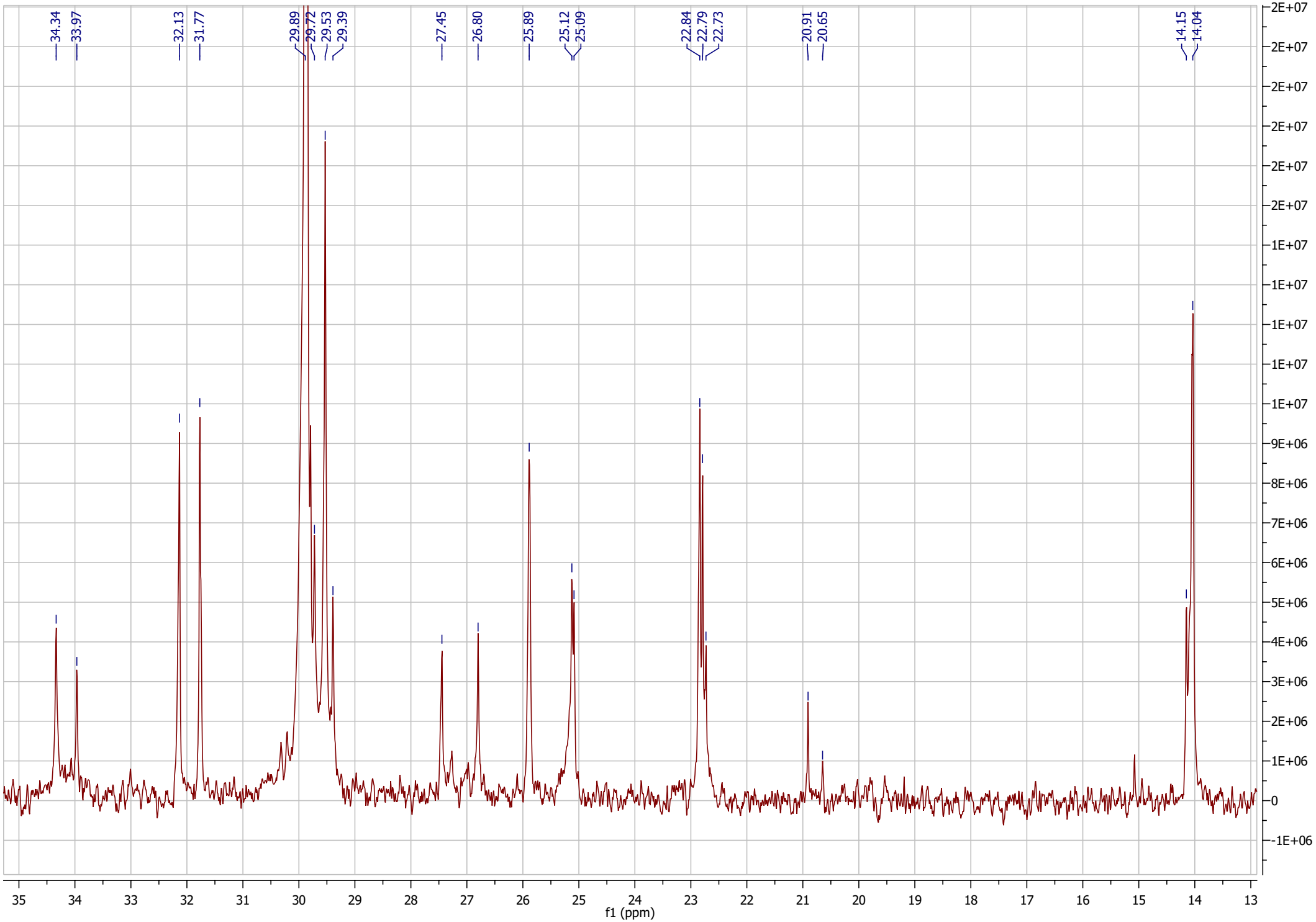
66
64
62
60
58
56
54
52
50
48
46
44
42
40
f1 (ppm)


34.34
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29.72
29.53
29.39
27.45
26.80
25.89
25.12
25.09
22.84
22.79
22.73
20.91
20.65
14.15
14.04
2E+07
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
35
34
33
32
31
30
29
28
27
26
25
24
23
22
21
20
19
18
17
16
15
14
13
f1 (ppm)