Supporting Information for

NHC-Iron catalysed Aerobic Oxidative Aromatic Esterification of Aldehydes using Boronic Acids

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General Remarks

Dioxane was freshly distilled over sodium. All reactions were performed in oven-dried glassware under air. Preparative thin layer chromatography plates were prepared with silica gel 60 GF_{254} MercK (Ref. 1.07730.1000). Reaction mixtures were analysed by TLC using ALUGRAM® SIL G/UV_{254} from MN (Ref. 818133, silica gel 60), and visualisation of TLC spots was effected using UV and $KMnO_4$ solution. NMR spectra were recorded in a Bruker AMX 400 using $CDCl_3$ as solvent and $(CH_3)_4Si$ (^1H) as internal standard. All coupling constants are expressed in Hz. Mass spectrometer (Micromass Quattro Micro API, Waters, Milford, USA) with a Triple Quadrupole (TQ) and an electrospray ion source (ESI) operating in positive mode was used. Iron sources: $Fe(TfO)_2$ (Solchemar, >99.5 %); $Fe(NO_3)_3.9H_2O$ (Merck, 99 %); $FeCl_3$ (Aldrich, 97 %); TPPFeCl (Aldrich, 95 %); $FeCl_3.6H_2O$ and $FeCl_2.4H_2O$ (Aldrich, 97 %, 99 %, 99 %); $Fe(acac)_2$ (Aldrich, 99.95 %). NHC ligands used were prepared following reported procedures: 1,3-bis(*t*-butyl) imidazolium chloride, [1] 1,3-bis(2,6-di*iso*propylphenyl) imidazolium chloride and 1,3-bis(2,6-di*iso*propylphenyl) imidazolinium chloride, [2] were prepared according to literature procedures, except 1,3-bis(2, 4, 6-trimethy-phenyl) imidazolinium chloride which was purchased from Aldrich. The aldehydes and boronic acids were purchased from Aldrich and used without further purification.

General procedure:
Typically the reactions were performed as follows: To a round bottom flask under N_2 were added freshly dried dioxane over sodium (1.5 mL), NHC ligand precursor (20 mol%) and sublimed KO^{t}Bu (0.247 mmol). The mixture was allowed to react at room temperature for 20 min. after which the iron source (20 mol%) was also added. The mixture was left reacting 5 min. at room temperature and then the boronic acid (0.247 mmol) and the aldehyde (0.247 mmol) were sequentially added. The N_2

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[9] Zhang L.; Zhang J. Y. *J. Comb. Chem.* **2006,** *8,* 361-367.
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[11] Coulthard; Charles E.; Marshall, Joseph; Payman, Frank L. J. Chem. Soc. **1930**, 280-291.
[12] Qian C.; Zhang X.; Li J.; Xu F.; Zhang Y.; Shen Q. Organometallics **2009**, 28, 3856–3862.

atmosphere was removed and the mixture was heated at 90 ºC. Typically, after a reaction time of 24 h the volatiles were removed under reduced pressure and the product isolated by preparative thin layer chromatography (Hexanes:AcOEt).
(**10**, **15**, **21**, **22**, **24**)[3]; **12**[4]; **13**[5]; **14**[6]; **16**[7]; (**17**, **23**)[8]; (**18, 19**)[9]; **26**[10]; **11**[11]; (**30**, **31**)[12]

4-fluorophenyl benzoate (10)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (2H, d, *J* = 7.6 Hz), 7.68 (1H, t, *J* = 7.6 Hz), 7.55 (2H, t, *J* = 7.6 Hz), 7.24-7.19 (2H, m), 7.17-7.12 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 160.3 (d, J_{CF} = 244.4 Hz), 146.8 (d, J_{CF} = 2.8 Hz), 133.8, 130.2, 129.3, 128.7, 123.1 (d, J_{CF} = 8.5 Hz), 116.2 (d, J_{CF} = 23.6 Hz).

4-(*n*-butyl)-phenyl benzoate (11)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (2H, d, *J* = 7.6 Hz), 7.67 (1H, t, *J* = 7.6 Hz), 7.55 (2H, t, *J* = 7.6 Hz), 7.27 (2H, d, *J* = 8.6 Hz), 7.16 (2H, d, *J* = 8.6 Hz), 2.67 (2H, t, *J* = 7.8 Hz), 1.66 (2H, quint, *J* = 7.6 Hz), 1.42 (2H, sext, *J* = 7.4 Hz), 0.98 (3H, t, *J* = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 148.9, 140.6, 133.5, 130.2, 129.8, 129.4, 128.6, 121.4, 35.1, 33.7, 22.4, 14.0.

4-methoxyphenyl benzoate (12)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (2H, d, *J* = 7.6 Hz), 7.66 (1H, t, *J* = 7.6 Hz), 7.54 (2H, t, *J* = 7.6 Hz), 7.16 (2H, d, *J* = 9.0 Hz), 6.97 (2H, d, *J* = 9.0 Hz), 3.85 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 157.3, 144.4, 133.5, 130.2, 129.7, 128.6, 122.5, 114.5, 55.6.

2-naphtyl benzoate (13)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (2H, d, *J* = 8.2 Hz), 7.96 (1H, d, *J* = 9.0 Hz), 7.91 (2H, m), 7.76 (1H, d, *J* = 2.3 Hz), 7.70 (1H, t, *J* = 7.5 Hz), 7.59 (2H, d, *J* = 7.9 Hz), 7.57-7.53 (2H, m), 7.43 (1H, dd, J_1 = 8.8 Hz, J_2 = 2.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 148.7, 133.9, 133.7, 131.6, 130.3, 129.6, 129.5, 128.7, 127.9, 127.8, 126.7, 125.8, 121.3, 118.8.

phenyl 2-naphthenate (14)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.8 (1H, s), 8.24 (1H, d, *J* = 8.6 Hz), 8.04 (1H, d, *J* = 8.1 Hz), 7.98 (1H, d, *J* = 8.8 Hz), 7.95 (1H, d, *J* = 8.6 Hz), 7.64 (2H, m), 7.50 (2H, t, *J* = 7.4 Hz), 7.32 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 151.1, 135.8, 132.5, 132.0, 129.6, 129.5, 128.7, 128.4, 127.9, 126.9, 126.8, 126.0, 125.5, 121.8.

phenyl 4-methylbenzoate (15)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (2H, d, *J* = 8.1 Hz), 7.47 (2H, t, *J* = 7.8 Hz), 7.35 (2H, d, *J* = 8.1 Hz), 7.31 (1H, t, *J* = 7.8 Hz), 7.26 (2H, d, *J* = 7.8 Hz), 1.55 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 151.1, 144.5, 130.3, 129.5, 129.3, 126.8, 125.8, 121.8, 21.8.

phenyl 4-chlorobenzoate (16)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (2H, d, *J* = 8.4 Hz), 7.52 (2H, d, *J* = 8.4 Hz), 7.47 (2H, t, *J* = 7.8 Hz), 7.32 (1H, t, *J* = 7.8 Hz), 7.24 (2H, d, *J* = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.8, 140.2, 131.6, 129.6, 129.0, 128.0, 126.1, 121.7.

phenyl 4-bromobenzoate (17)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (2H, d, *J* = 8.4 Hz), 7.68 (2H, d, *J* = 8.4 Hz), 7.46 (2H, t, *J* = 7.8 Hz), 7.31 (1H, t, *J* = 7.8 Hz), 7.23 (2H, d, *J* = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 150.8, 132.0, 131.7, 129.6, 128.9, 128.5, 126.1, 121.6.

4-methylphenyl 4-bromobenzoate (18)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (2H, d, *J* = 8.3 Hz), 7.68 (2H, d, *J* = 8.3 Hz), 7.26 (2H, d, *J* = 8.2 Hz), 7.12 (2H, d, *J* = 8.2 Hz), 2.41 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 148.5, 135.7, 131.9, 131.7, 130.1, 128.8, 128.6, 121.3, 21.0.

4-methoxyphenyl 4-bromobenzoate (19)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (2H, d, *J* = 8.4 Hz), 7.67 (2H, d, *J* = 8.4 Hz), 7.15 (2H, d, *J* = 9.1 Hz), 6.97 (2H, d, *J* = 9.1 Hz), 3.85 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 157.4, 144.2, 131.9, 131.6, 128.8, 128.5, 122.4, 114.6, 55.6.

4-fluorophenyl 4-bromobenzoate (20)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (2H, d, *J* = 8.5 Hz), 7.68 (2H, d, *J* = 8.5 Hz), 7.20 (2H, dd, J_{HH} = 9.2 Hz, J_{HF} = 4.8 Hz), 7.14 (2H, dd, J_{HH} = 9.2 Hz, J_{HF} = 9.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 160.4 (d, J_{CF} = 244.5 Hz), 146.5 (d, J_{CF} = 3.0 Hz), 132.0, 131.7, 129.0, 128.2, 123.1 (d, J_{CF} = 8.5 Hz), 116.2 (d, J_{CF} = 23.4 Hz).

phenyl 4-cyanobenzoate (21)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (2H, d, *J* = 7.8 Hz), 7.84 (2H, d, *J* = 7.8 Hz), 7.48 (2H, t, *J* = 7.8 Hz), 7.33 (1H, t, *J* = 7.8 Hz), 7.25 (2H, d, *J* = 7.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 150.5, 133.4, 132.4, 130.7, 129.7, 126.4, 121.5, 117.9, 117.0.

phenyl 4-fluorobenzoate (22)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (2H, dd, J_{HH} = 8.7 Hz, J_{HF} = 5.6 Hz), 7.47 (2H, t, *J* = 7.8 Hz), 7.32 (1H, t, *J* = 7.8 Hz), 7.24 (2H, d, *J* = 7.8 Hz), 7.22 (2H, t, J_{HH} = J_{HF} = 8.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2 (d, J_{CF} = 255.4 Hz), 164.3, 150.8, 132.8 (d, J_{CF} = 9.7 Hz), 129.6, 126.0, 125.8 (d, J_{CF} = 2.8 Hz), 121.7, 115.8 (d, J_{CF} = 22.1 Hz).

2-naphtyl 4-methoxybenzoate (23)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (2H, d, J = 8.8 Hz), 7.93 (1H, d, J = 8.9 Hz), 7.89 (2H, m), 7.72 (1H, d, J = 2.3 Hz), 7.53 (2H, m), 7.40 (1H, dd, J_1 = 8.9 Hz, J_2 = 2.3 Hz), 7.04 (2H, d, J = 8.8 Hz), 3.92 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 164.0, 148.8, 133.9, 132.4, 131.5, 129.4, 127.8, 127.7, 126.6, 127.7, 121.9, 121.5, 118.8, 113.9, 55.6.

phenyl 3,4-methylenedioxybenzoate (24)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (1H, dd, J_1 = 8.2 Hz, J_2 = 1.5 Hz), 7.65 (1H, d, J = 1.5 Hz), 7.45 (2H, t, J = 7.8 Hz), 7.29 (1H, t, J = 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz), 6.93 (1H, d, J = 8.2 Hz), 6.10 (2H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 152.2, 151.0, 147.9, 129.5, 126.2, 125.8, 123.4, 121.8, 110.0, 108.2, 102.0.

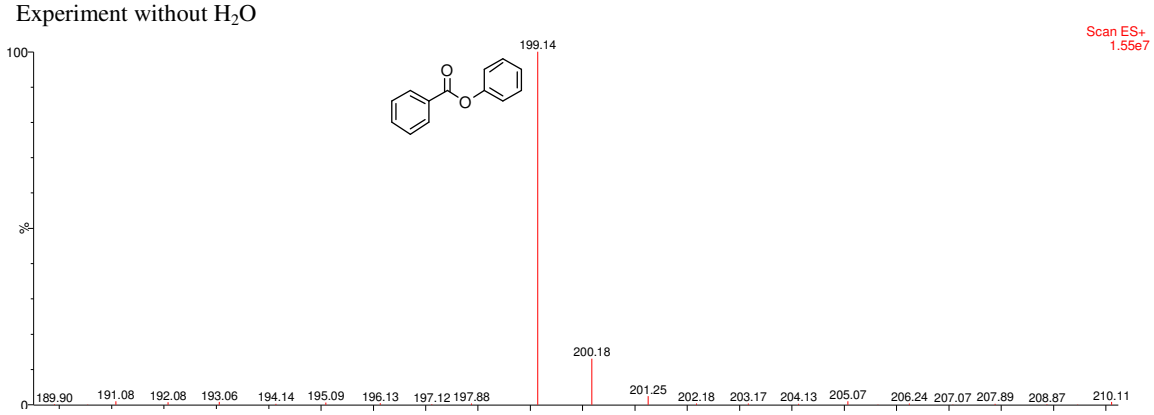
4-fluorophenyl cyclohexanecarboxylate (26)
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10-7.01 (4H, m), 2.57 (1H, tt, J_1 = 11.3 Hz, J_2 = 3.7 Hz), 2.07 (2H, br d, J = 13.0 Hz), 1.88-1.81 (2H, m), 1.74-1.68 (1H, m), 1.60 (2H, q of d, J_1 = 11.9 Hz, J_2 = 3.3 Hz), 1.44-1.27 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 160.1 (d, J_{CF} = 246.0 Hz), 146.7 (d, J_{CF} = 2.7 Hz), 122.9 (d, J_{CF} = 8.2 Hz), 116.0 (d, J_{CF} = 23.5 Hz), 43.1, 28.9, 25.7, 25.4.

General procedure for the synthesis of 30 and 31:
Typically the reactions were performed as follows: To a round bottom flask under N_2 were added freshly dried dioxane over sodium (1.5 mL), NHC ligand precursor (20 mol%) and sublimed KO^{t}Bu (0.247 mmol). The mixture was allowed to react at room temperature for 20 min. after which the iron source (20 mol%) was also added. The mixture was left reacting 5 min. at room temperature and then the boronic acid (0.247 mmol), the aldehyde (0.247 mmol) and the amine (2 eq,) were sequentially added. The N_2 atmosphere was removed and the mixture was heated at 90 ºC. Typically, after a reaction time of 24 h the volatiles were removed under reduced pressure and the product isolated by preparative thin layer chromatography (Hexanes:AcOEt). The ^{1}H and ^{13}C of the synthesised products are in agreement with the literature.

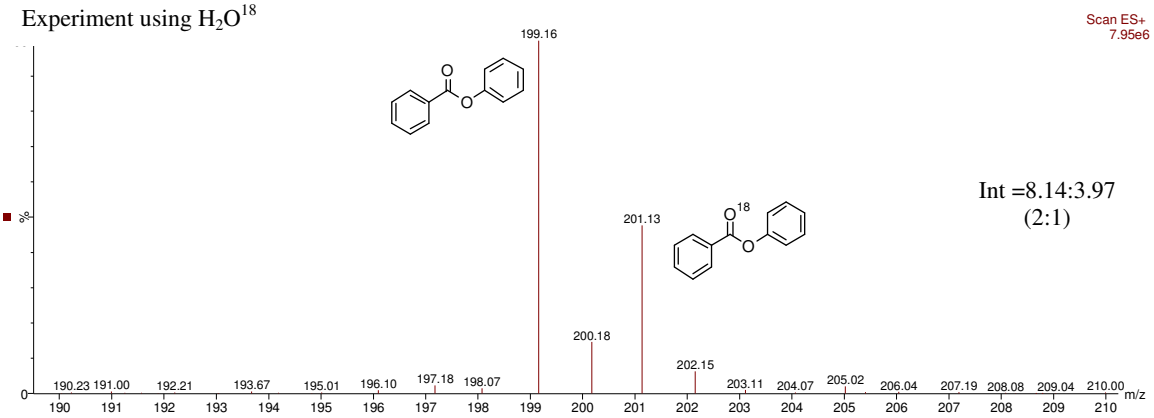
Amide **30**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.82-1.88 (2H, m), 1.91-1.98 (2H, m), 3.61-3.65 (2H, t, J = 6.8 Hz), 7.34-7.41 (3H, m), 7.47-7.51 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.71, 26.64, 46.43, 49.88, 127.32, 128.50, 137.43, 170.00.

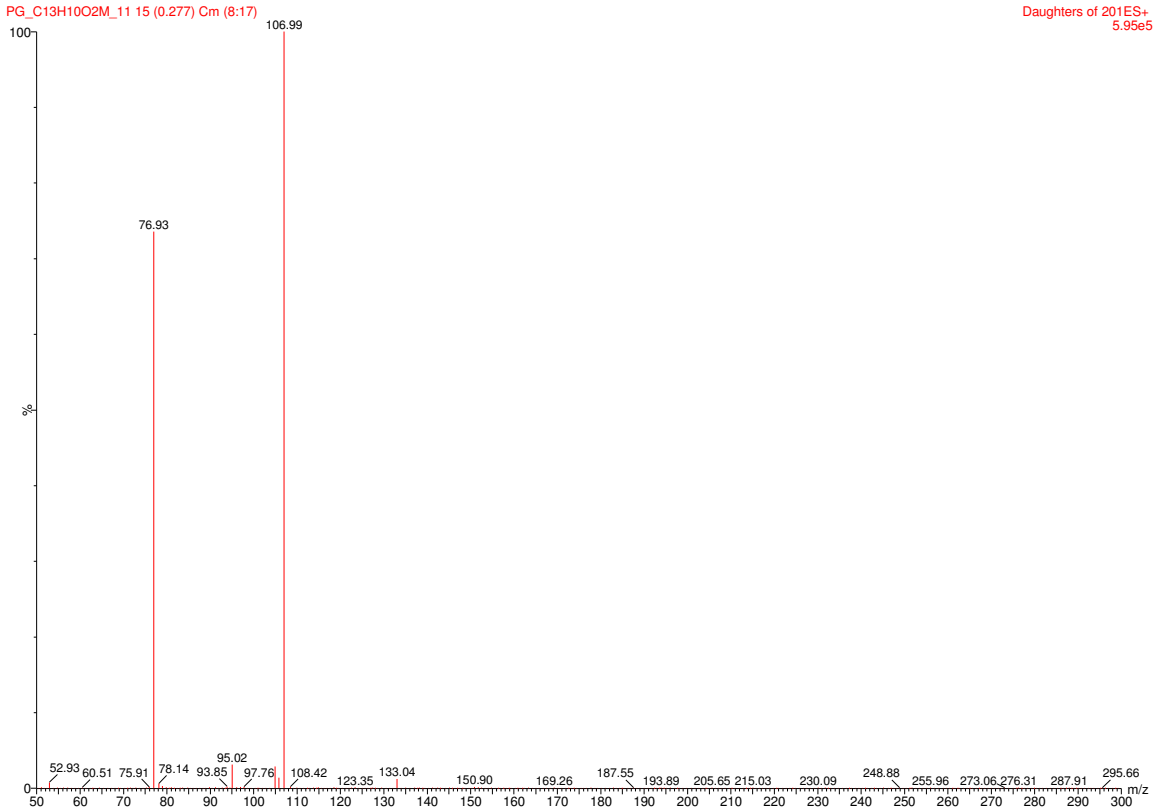
Amide **31**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.49 (2H, m), 1.65 (4H, m), 3.31 (2H, m), 3.69 (2H, m), 7.34-7.38 (5H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.83, 25.86, 26.79, 43.36, 49.01, 127.02, 128.65, 129.61, 136.71, 170.58.

Experiment without H_2O

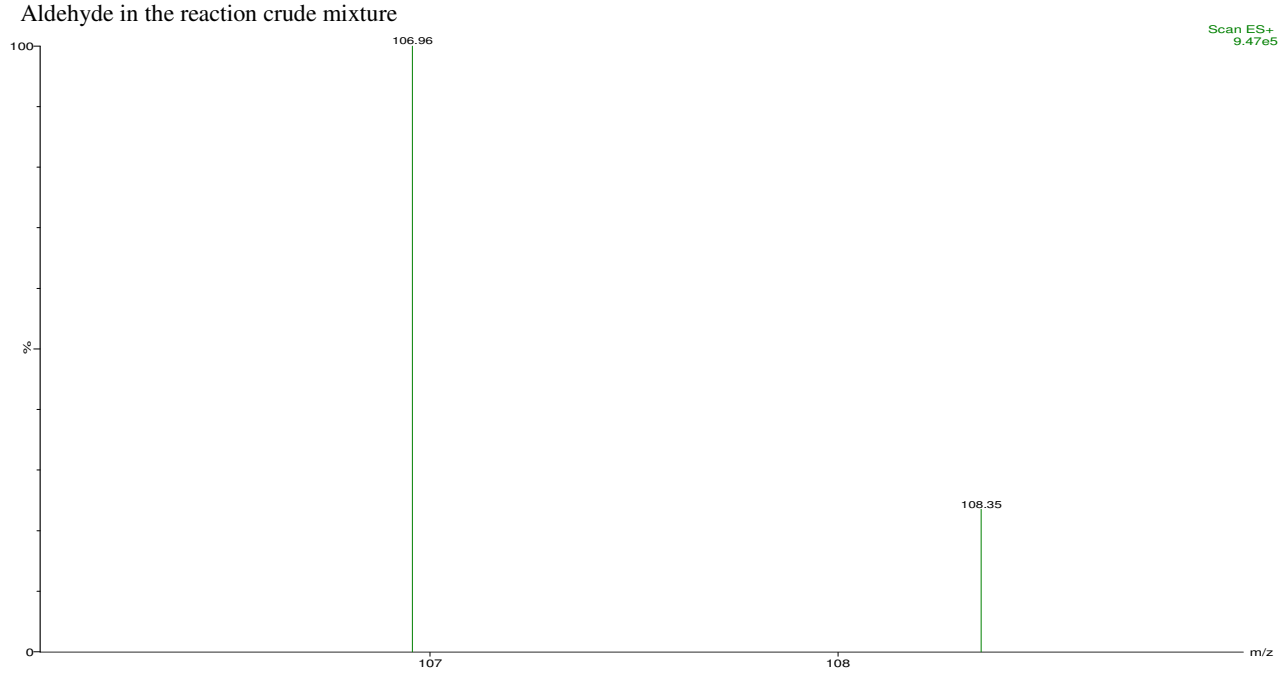


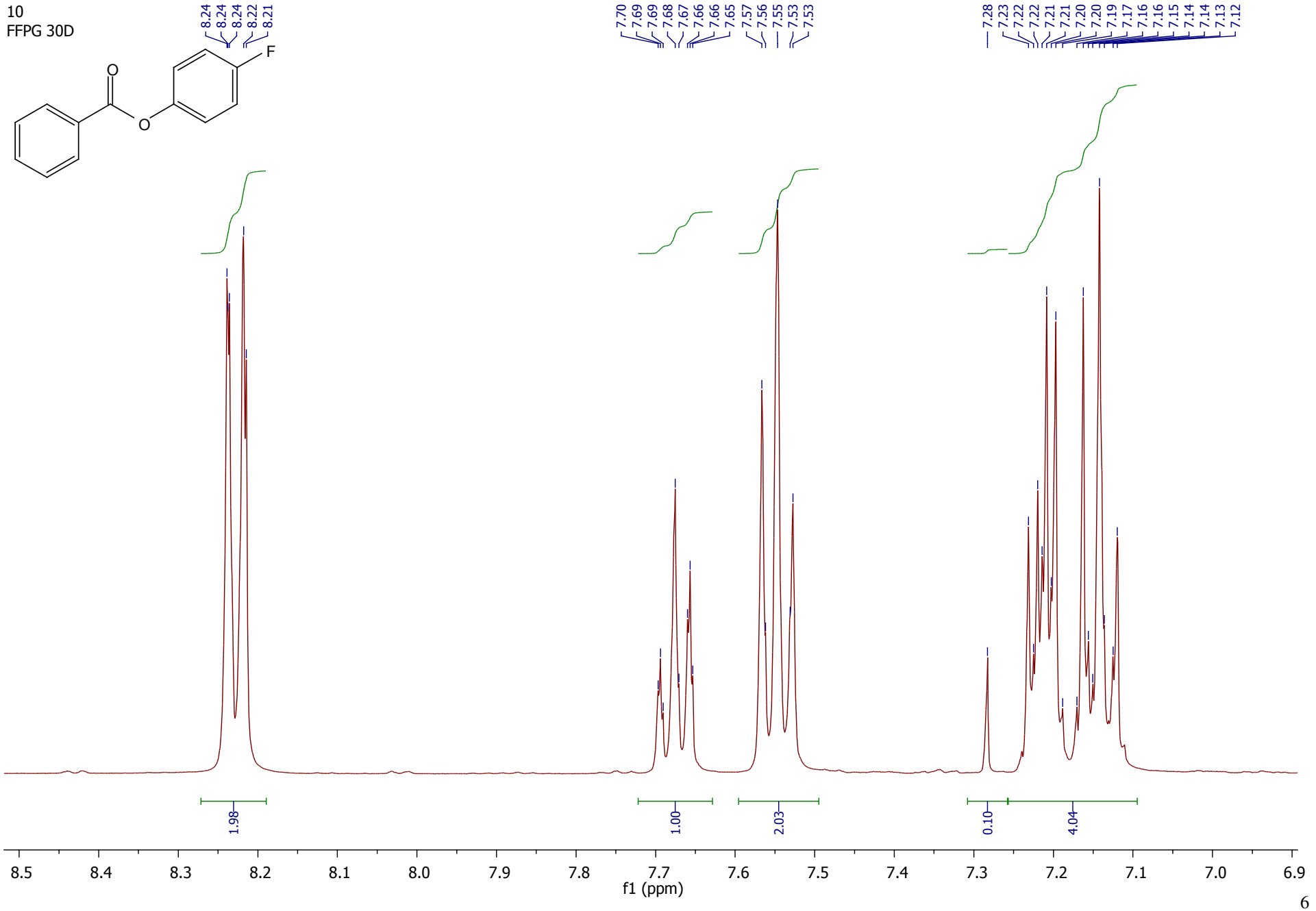
Experiment using H_2O^{18}





Aldehyde in the reaction crude mixture

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O
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7.57
7.56
7.55
7.53
7.53
7.28
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.17
7.16
7.16
7.15
7.14
7.14
7.13
7.12
1.98
1.00
2.03
0.10
4.04
8.5
8.4
8.3
8.2
8.1
8.0
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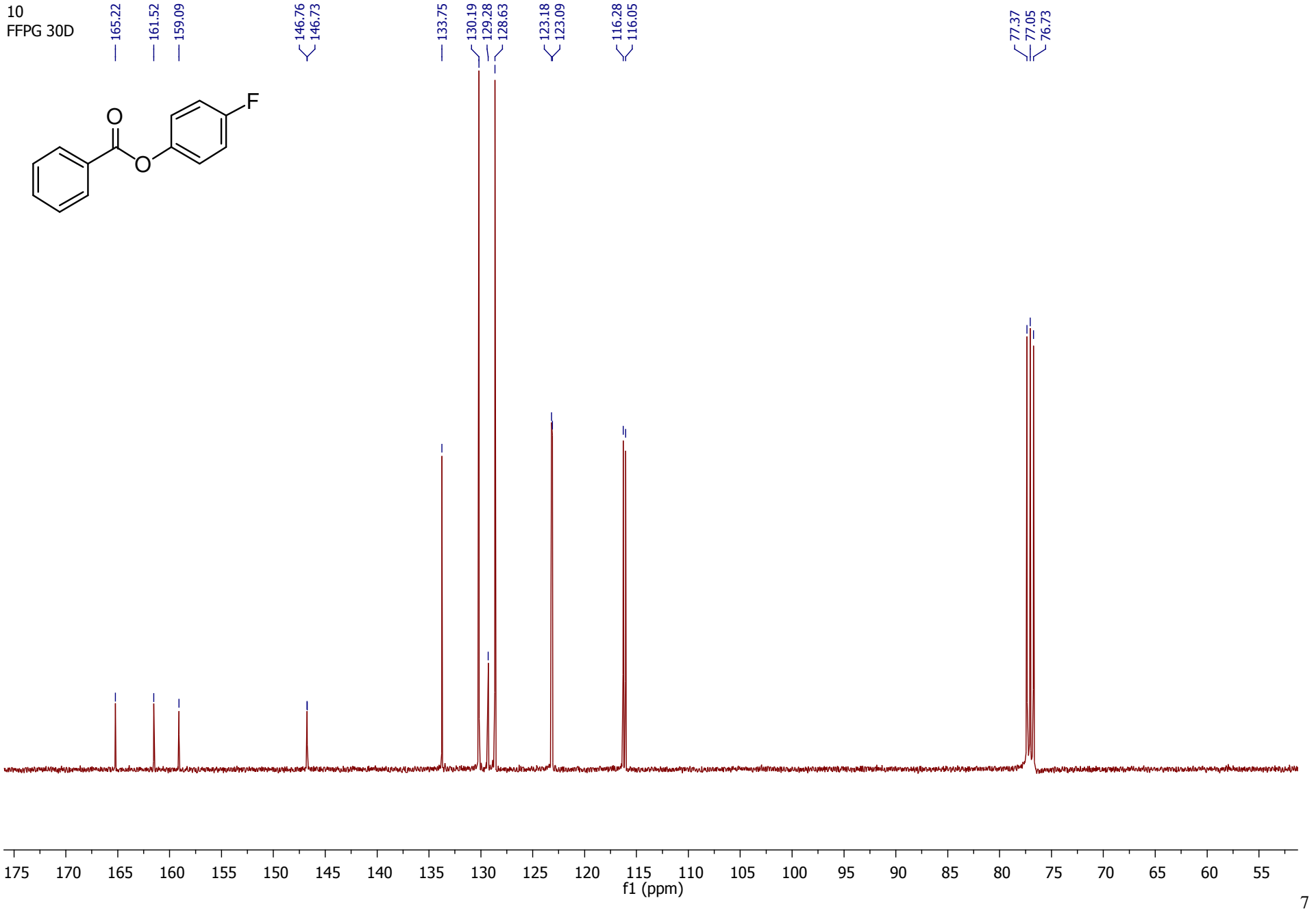
f1 (ppm)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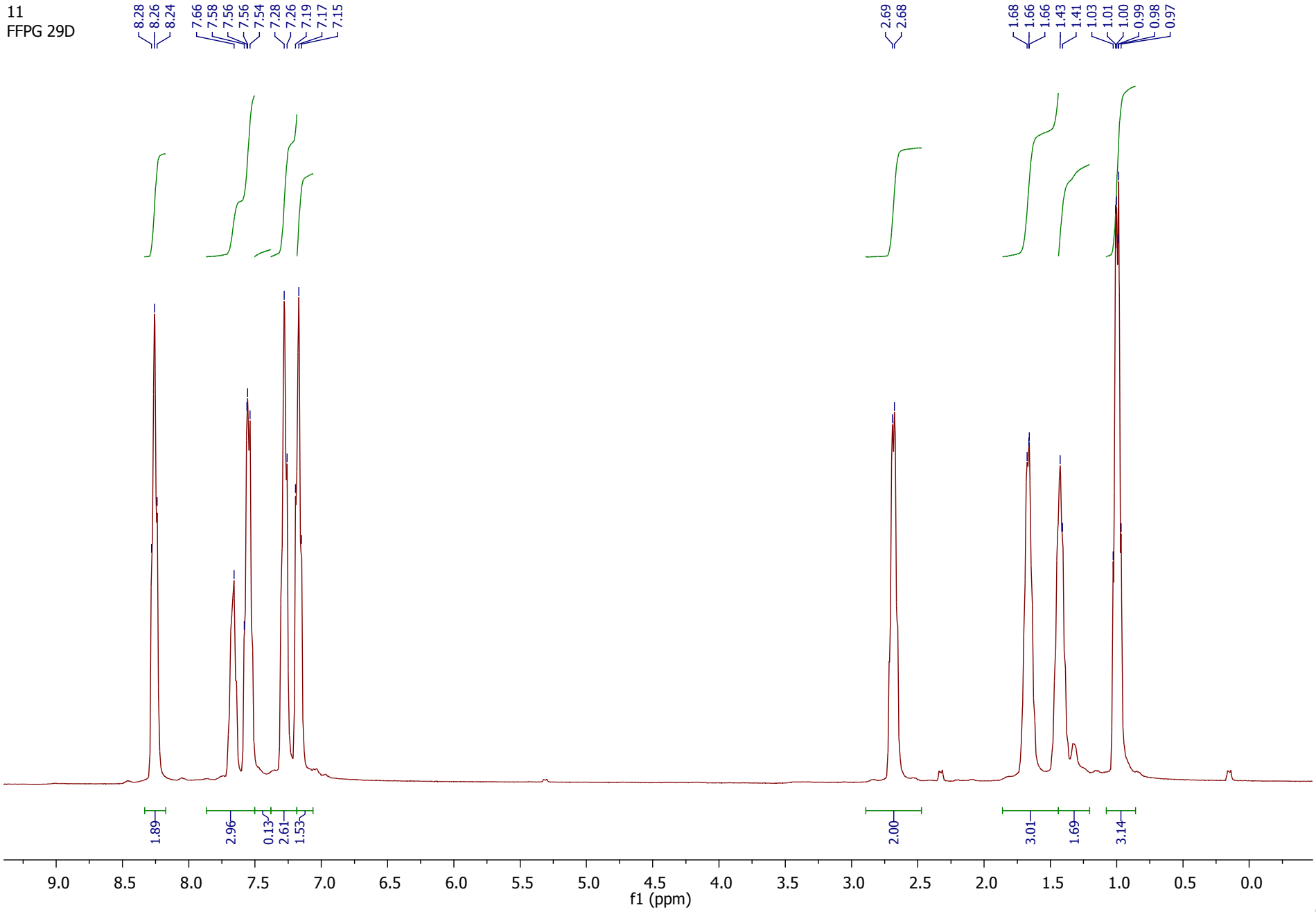
f1 (ppm)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2.00
3.01
1.69
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4.5
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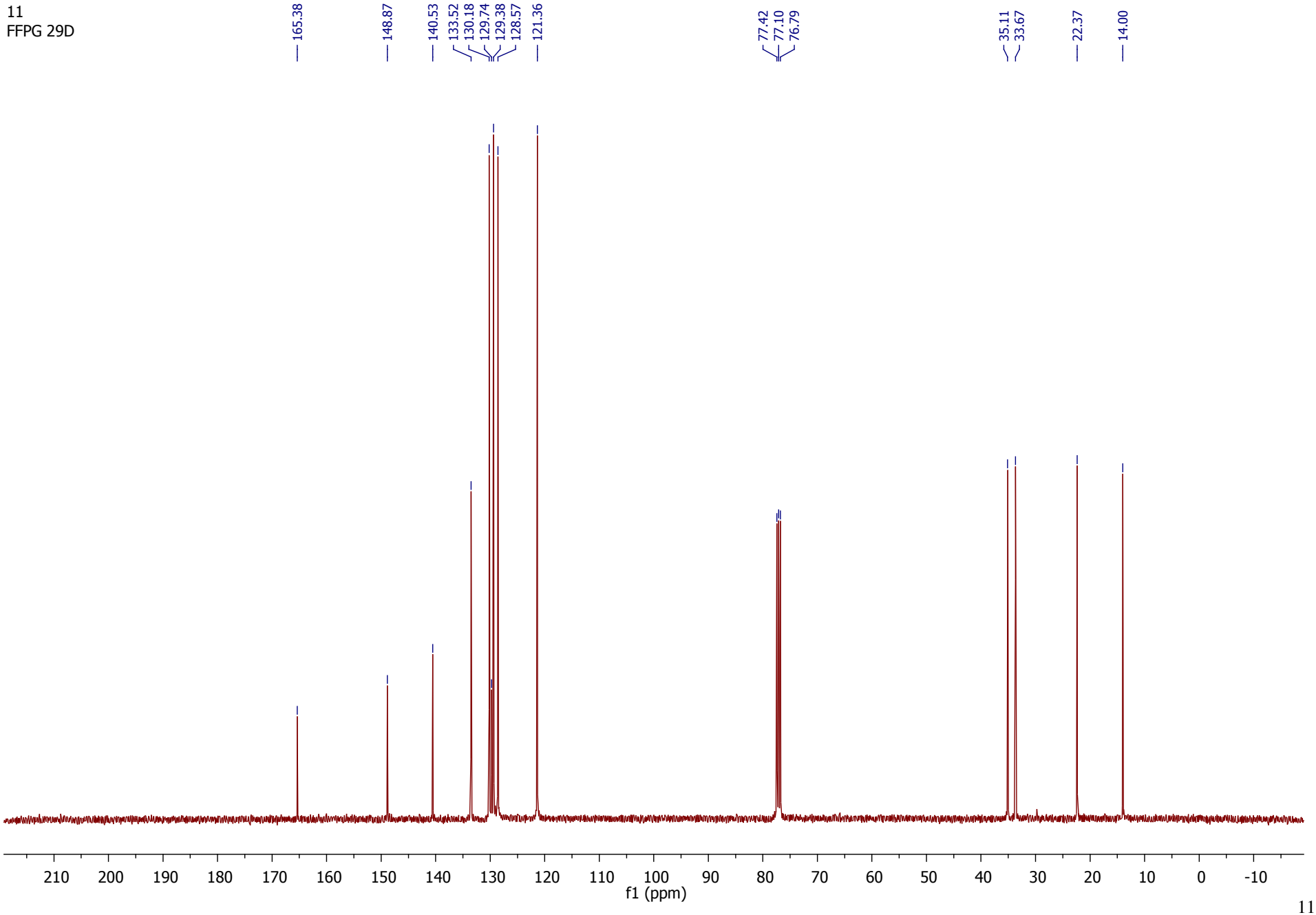
0.5
0.0
f1 (ppm)

11
FFPG 29D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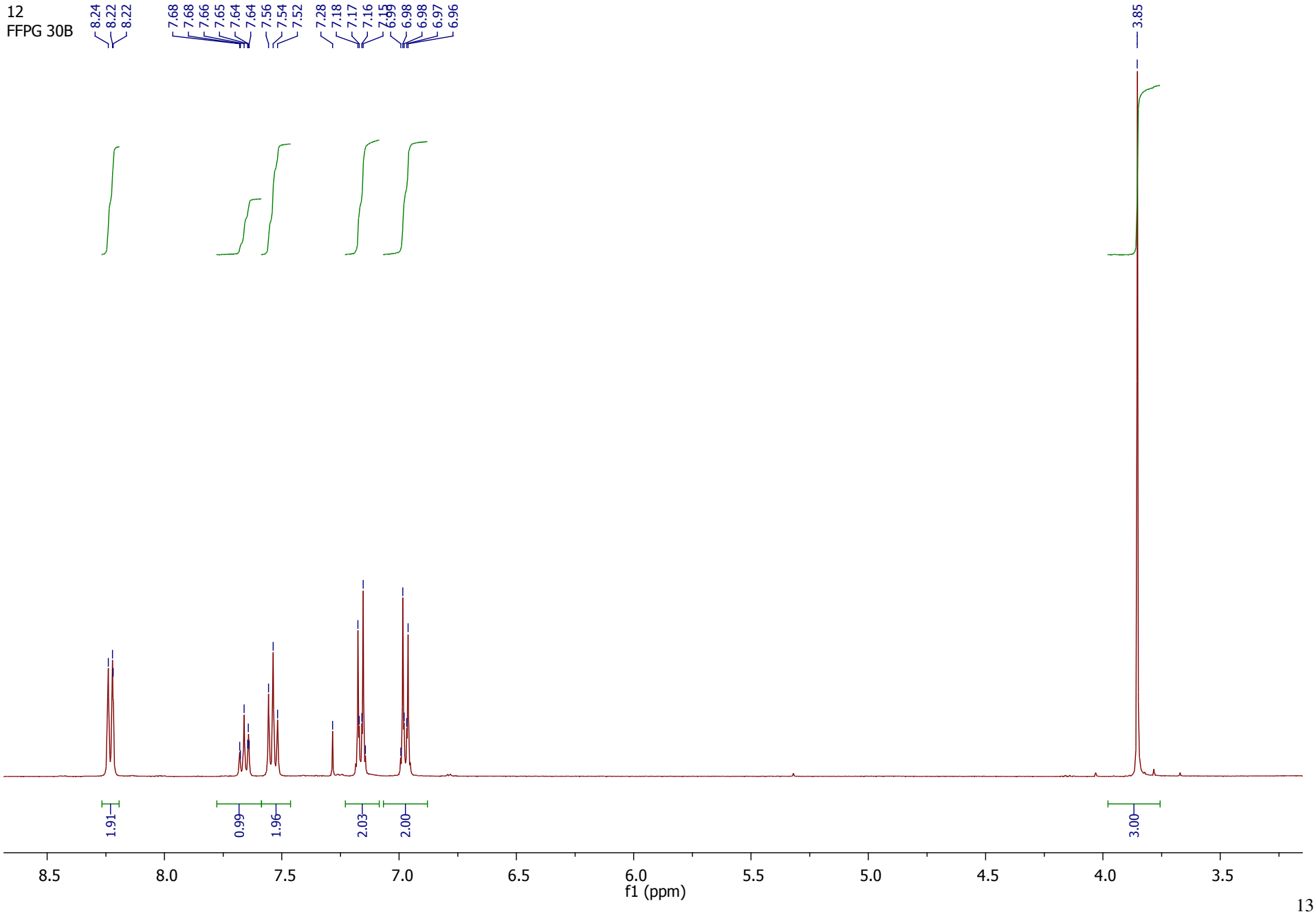
f1 (ppm)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7.28
7.18
7.17
7.16
7.15
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6.98
6.98
6.97
6.96
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8.0
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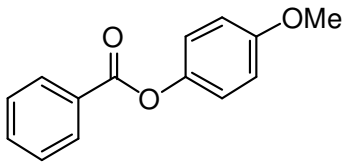
4.5
4.0
3.5
f1 (ppm)

12
FFPG 30B


O
O
OMe

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157.31
144.41
133.53
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129.63
128.56
122.47
114.53
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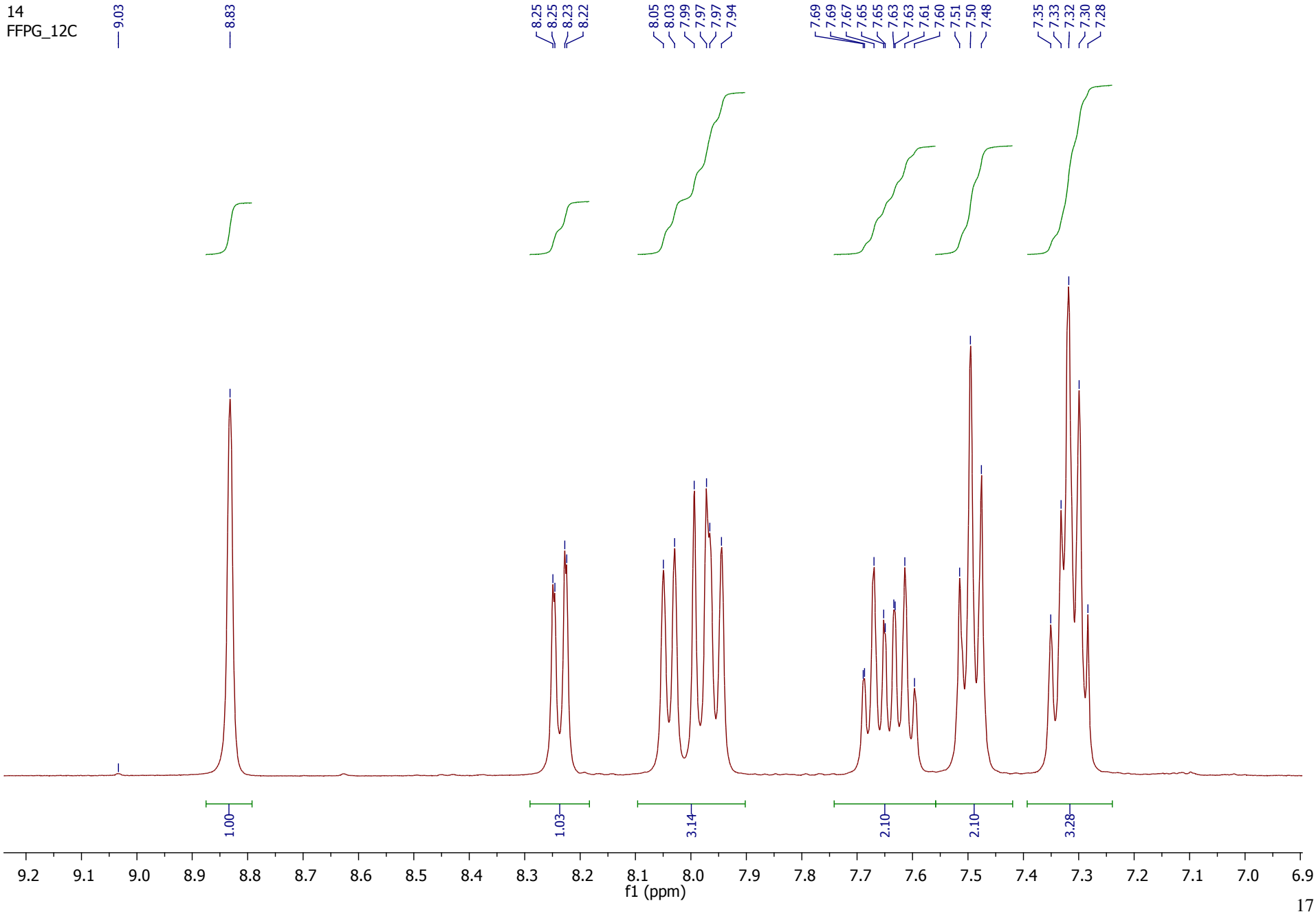
76.74
55.64
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)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8.03
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7.63
7.63
7.61
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7.50
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7.35
7.33
7.32
7.30
7.28
1.00
1.03
3.14
2.10
2.10
3.28
9.2
9.1
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
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7.8
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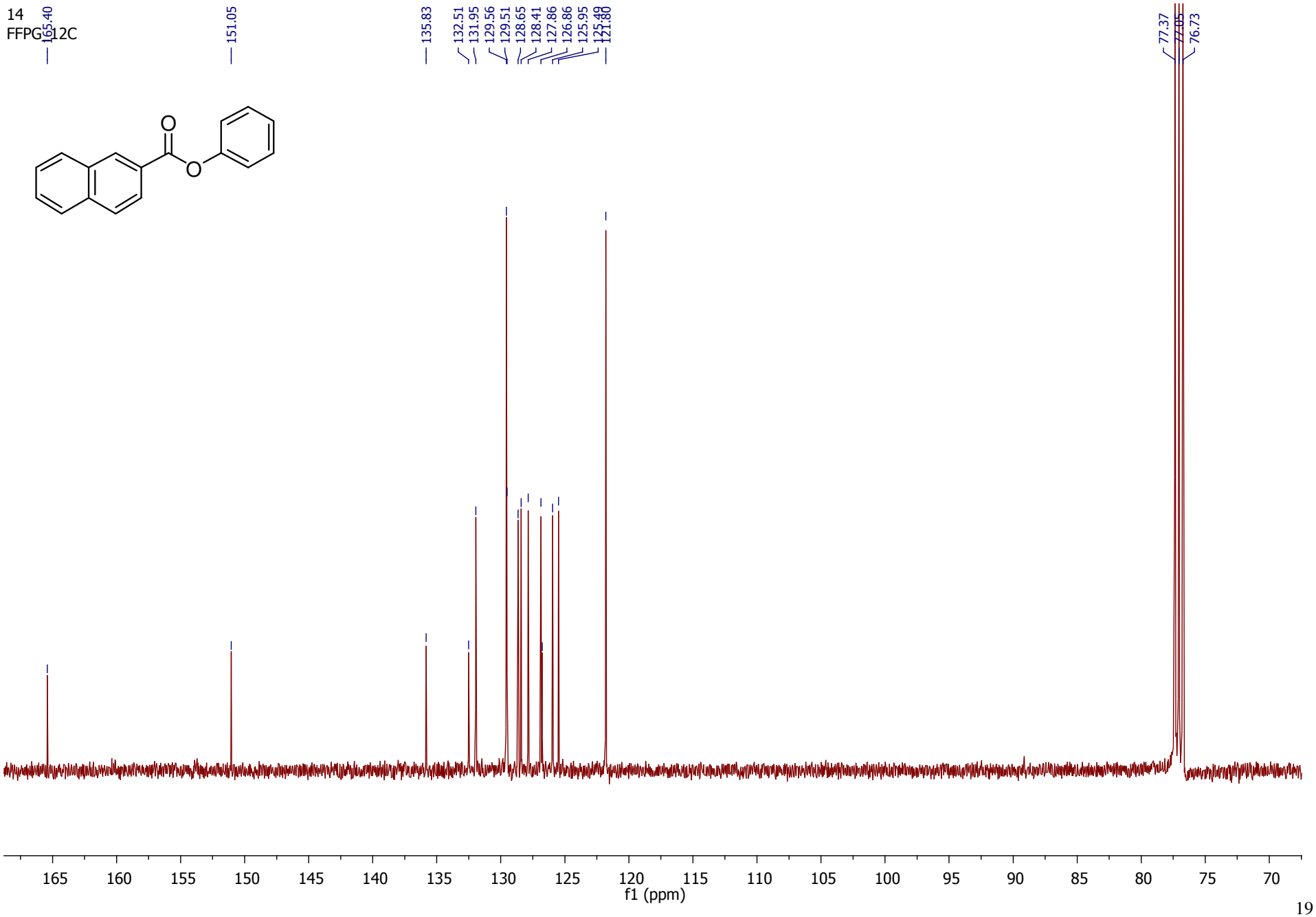
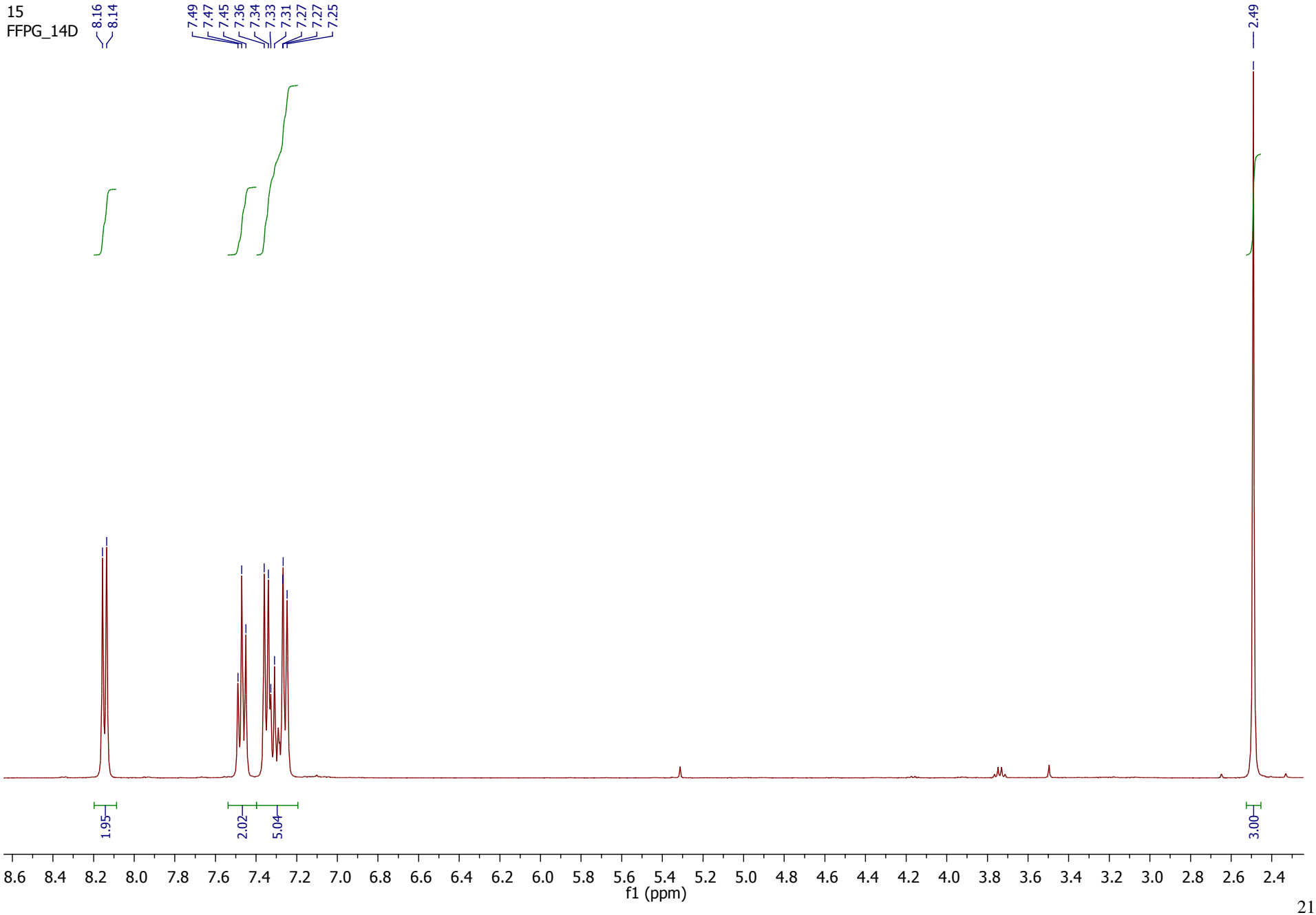
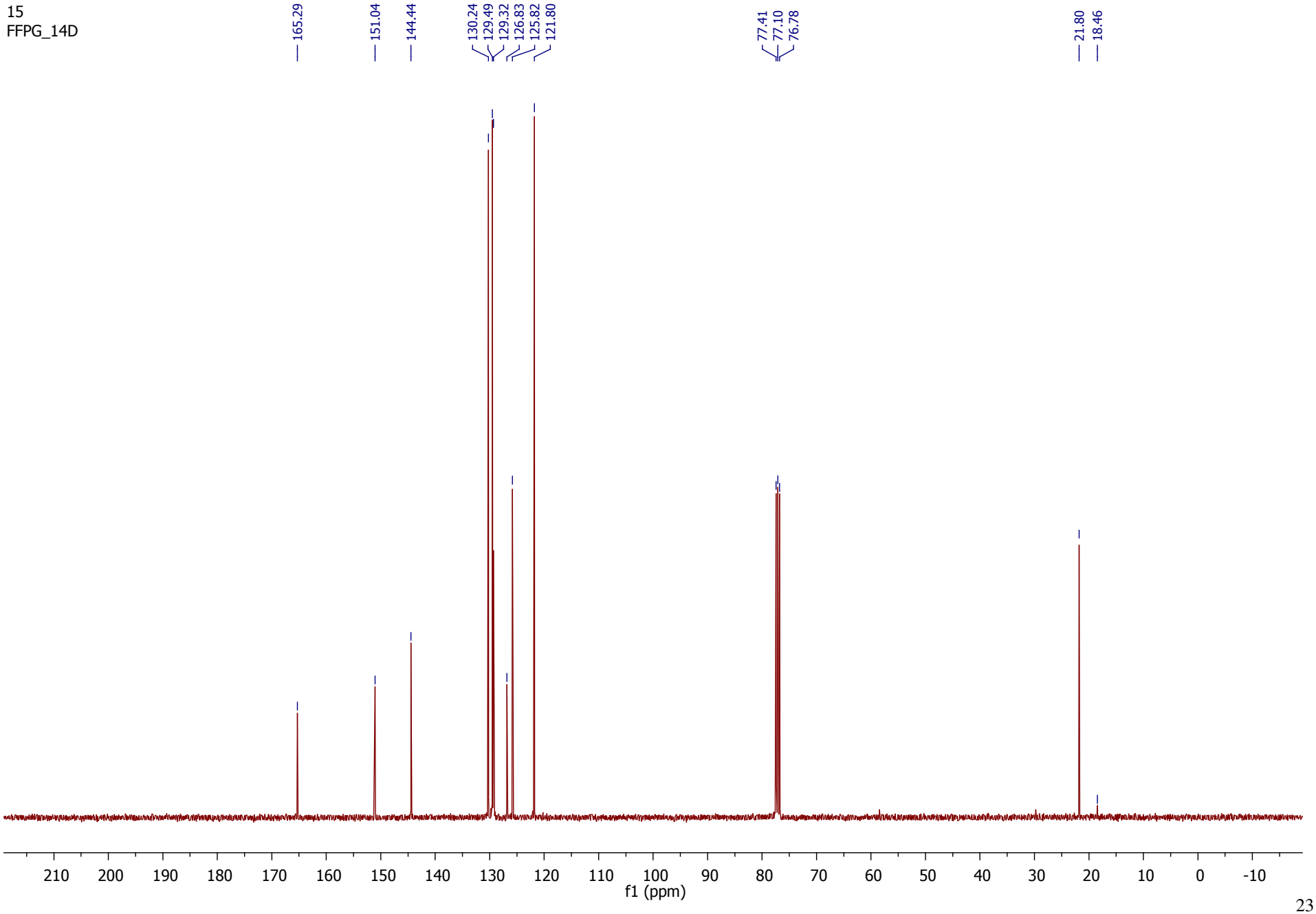
7.2
7.1
7.0
6.9
f1 (ppm)

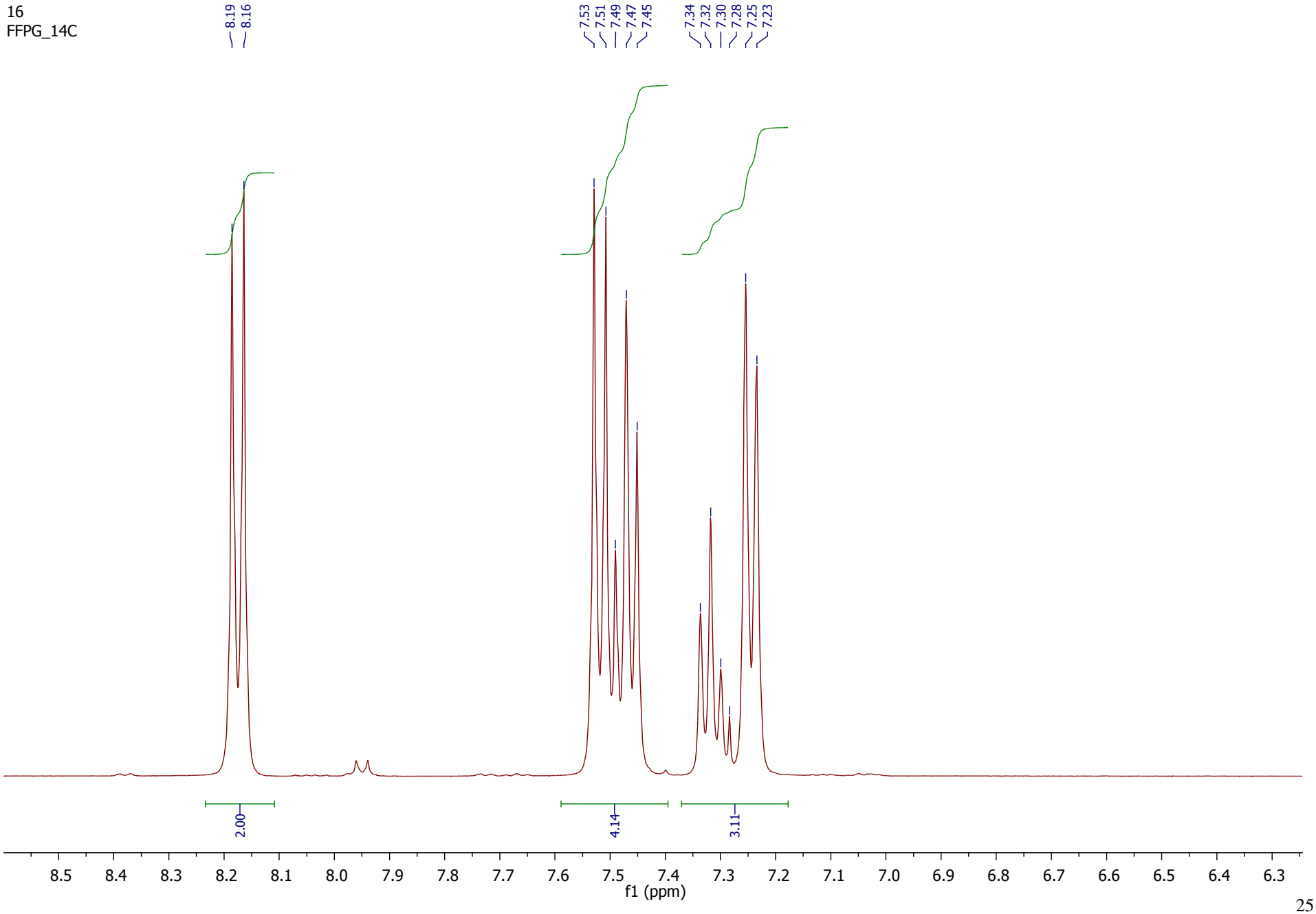

14
FFPG-12C
165.40
151.05
135.83
132.51
131.95
129.56
129.51
128.65
128.41
127.86
126.86
125.95
125.49
121.80
77.37
77.05
76.73
O
O
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
f1 (ppm)

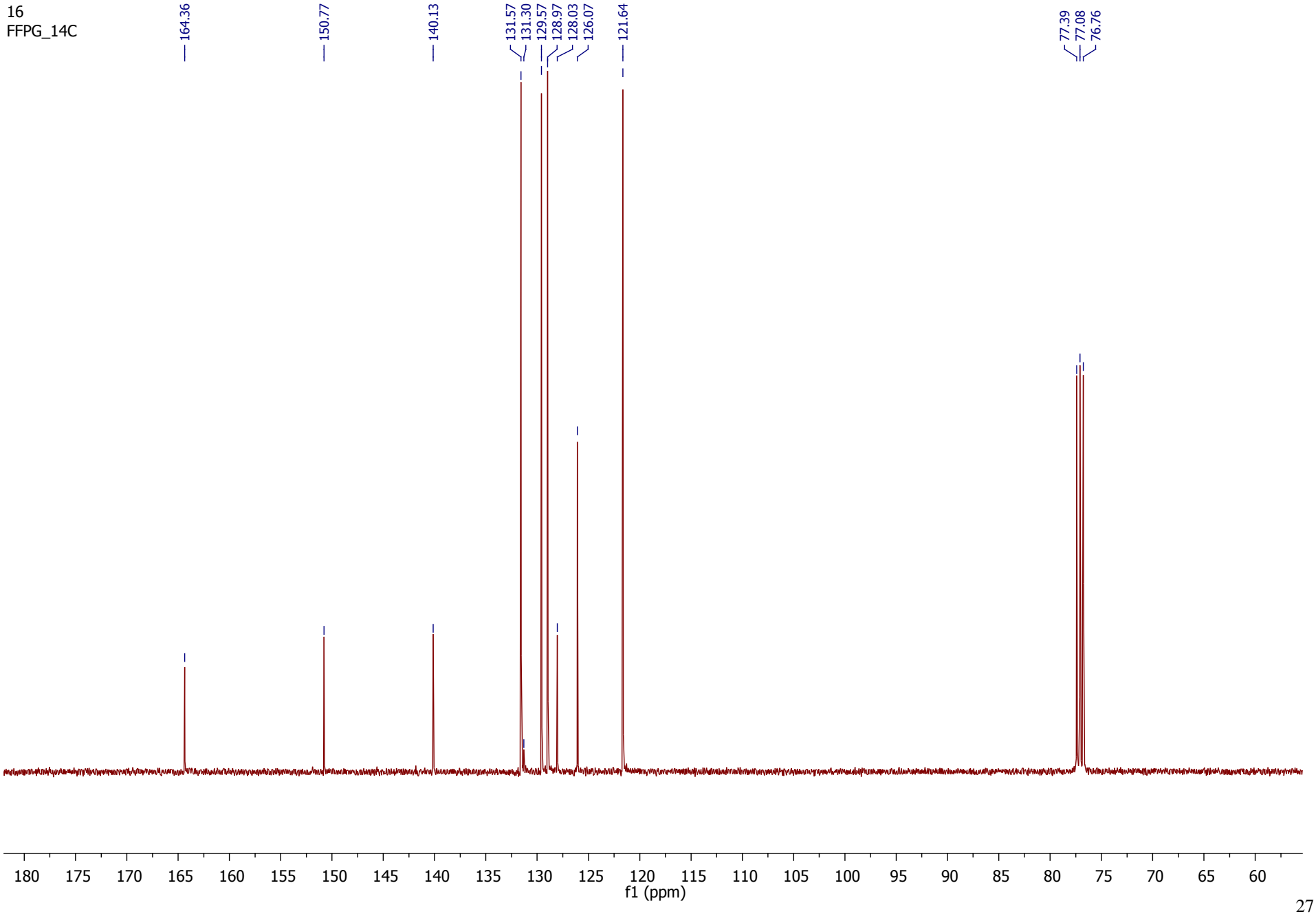

15
FFPG_14D
8.16
8.14
7.49
7.47
7.45
7.36
7.34
7.33
7.31
7.27
7.27
7.25
2.49
1.95
2.02
5.04
3.00
8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4
f1 (ppm)

15
FFPG_14D

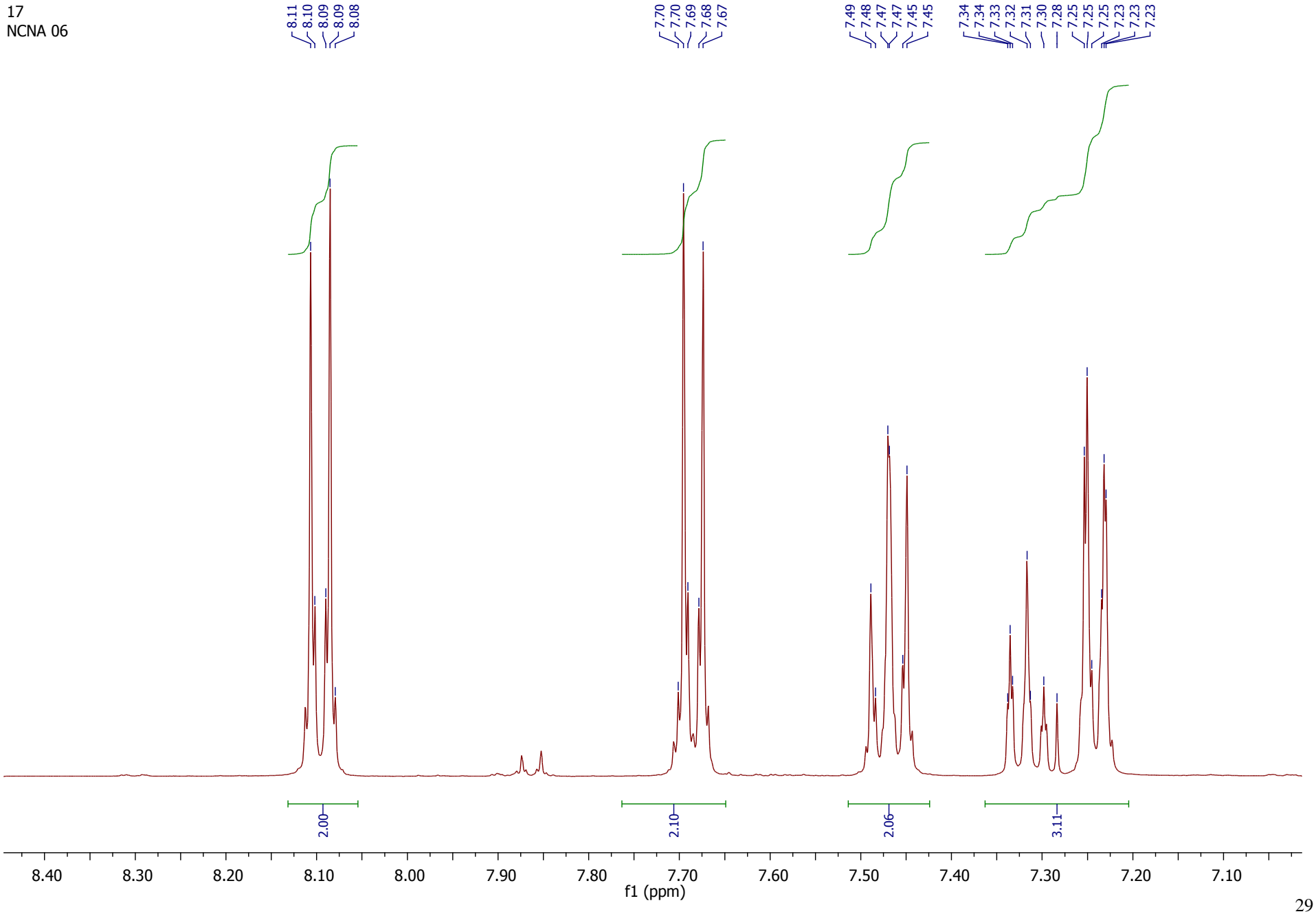

165.29
151.04
144.44
130.24
129.49
129.32
126.83
125.82
121.80
77.41
77.10
76.78
21.80
18.46
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

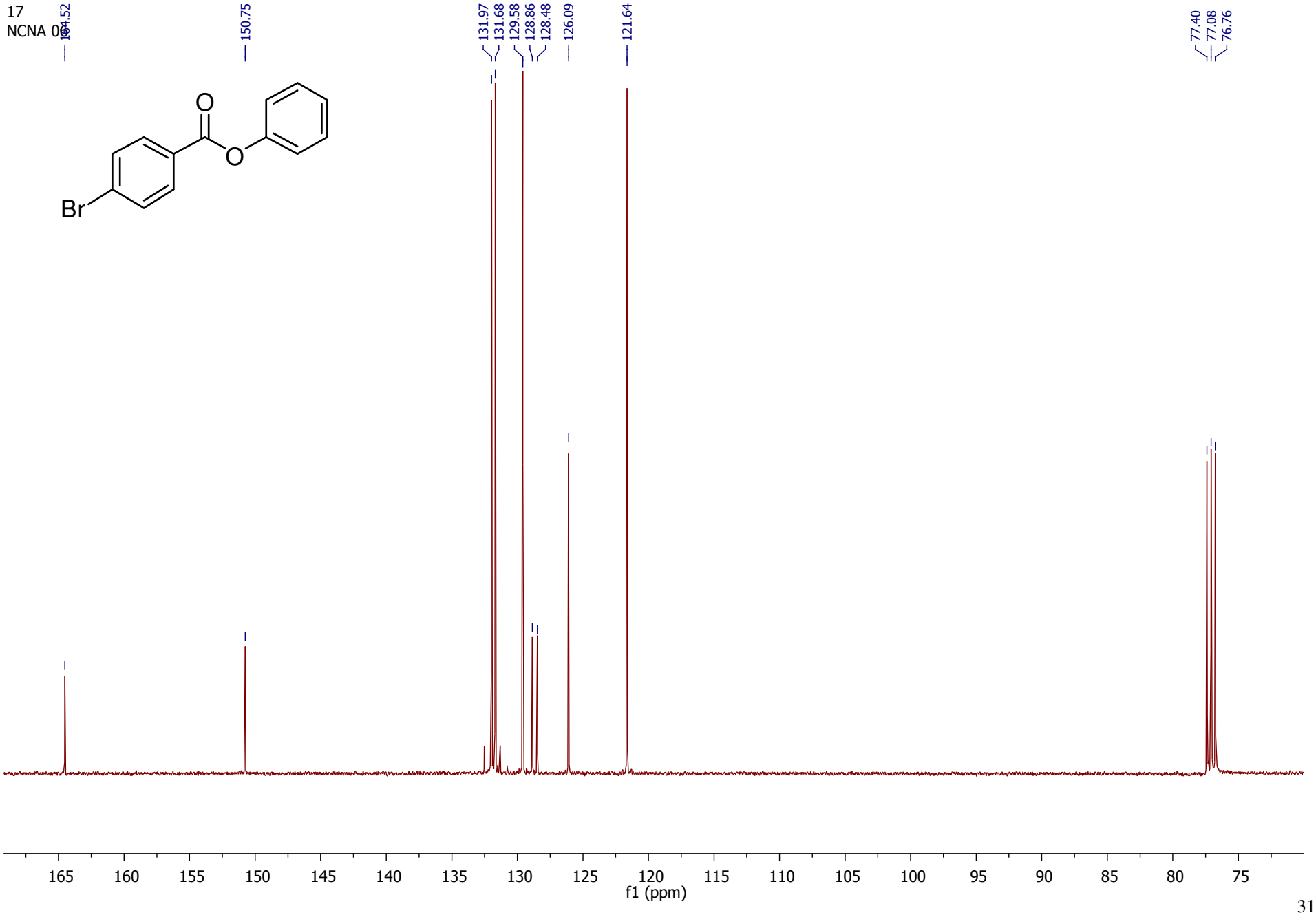
16
FFPG_14C

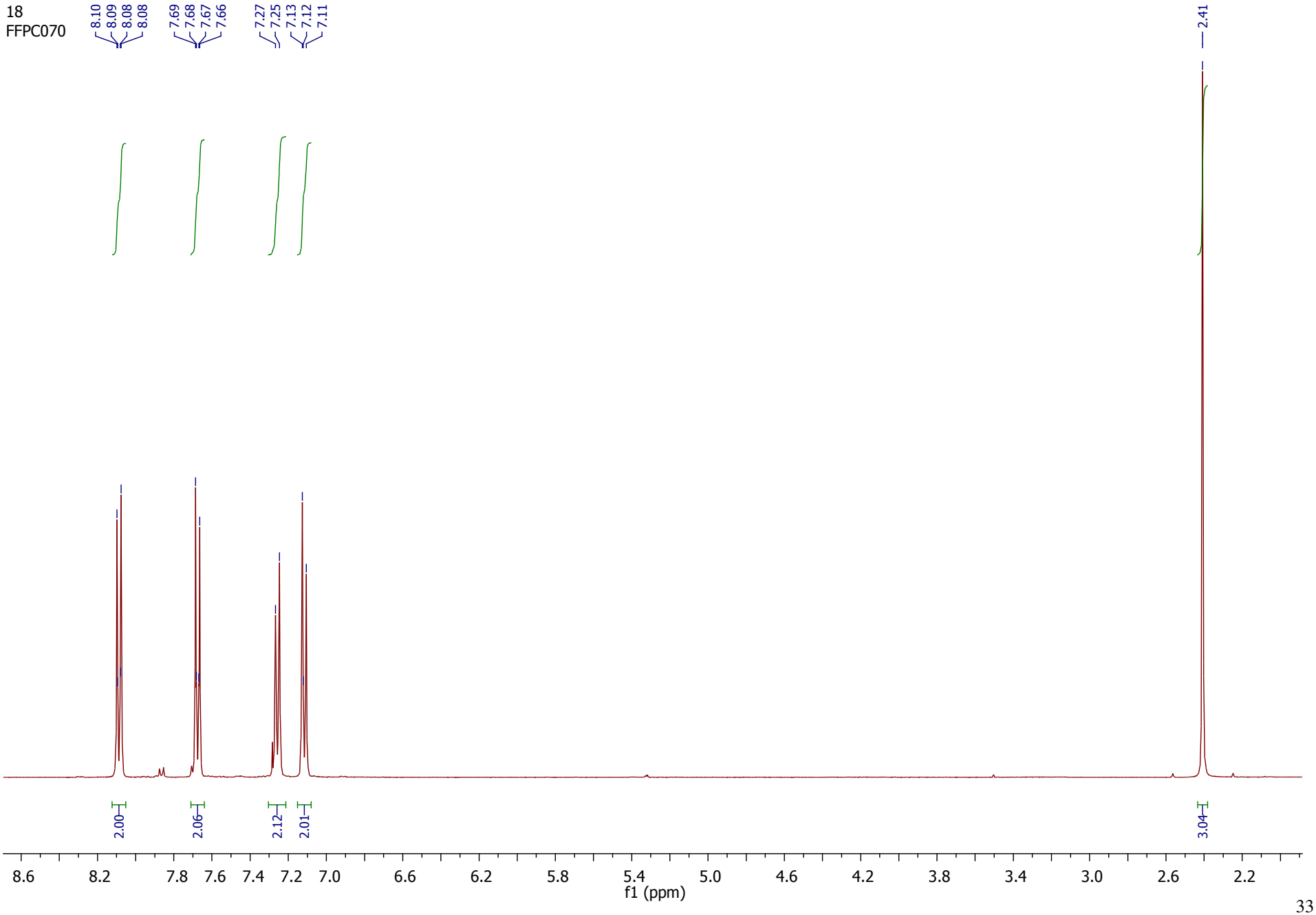

8.19
8.16
7.53
7.51
7.49
7.47
7.45
7.34
7.32
7.30
7.28
7.25
7.23
2.00
4.14
3.11
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
f1 (ppm)

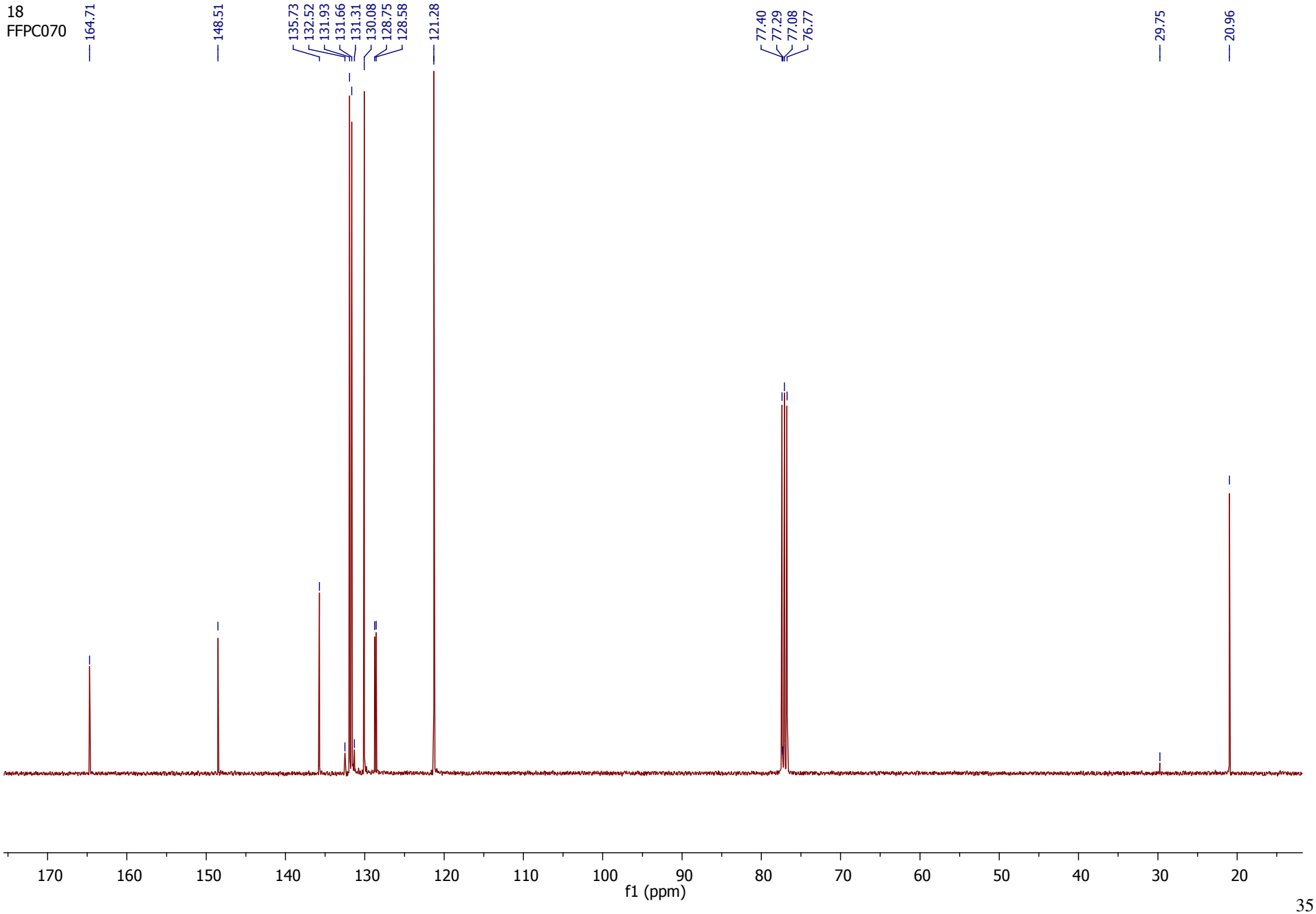

16
FFPG_14C
164.36
150.77
140.13
131.57
131.30
129.57
128.97
128.03
126.07
121.64
77.39
77.08
76.76
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60
f1 (ppm)

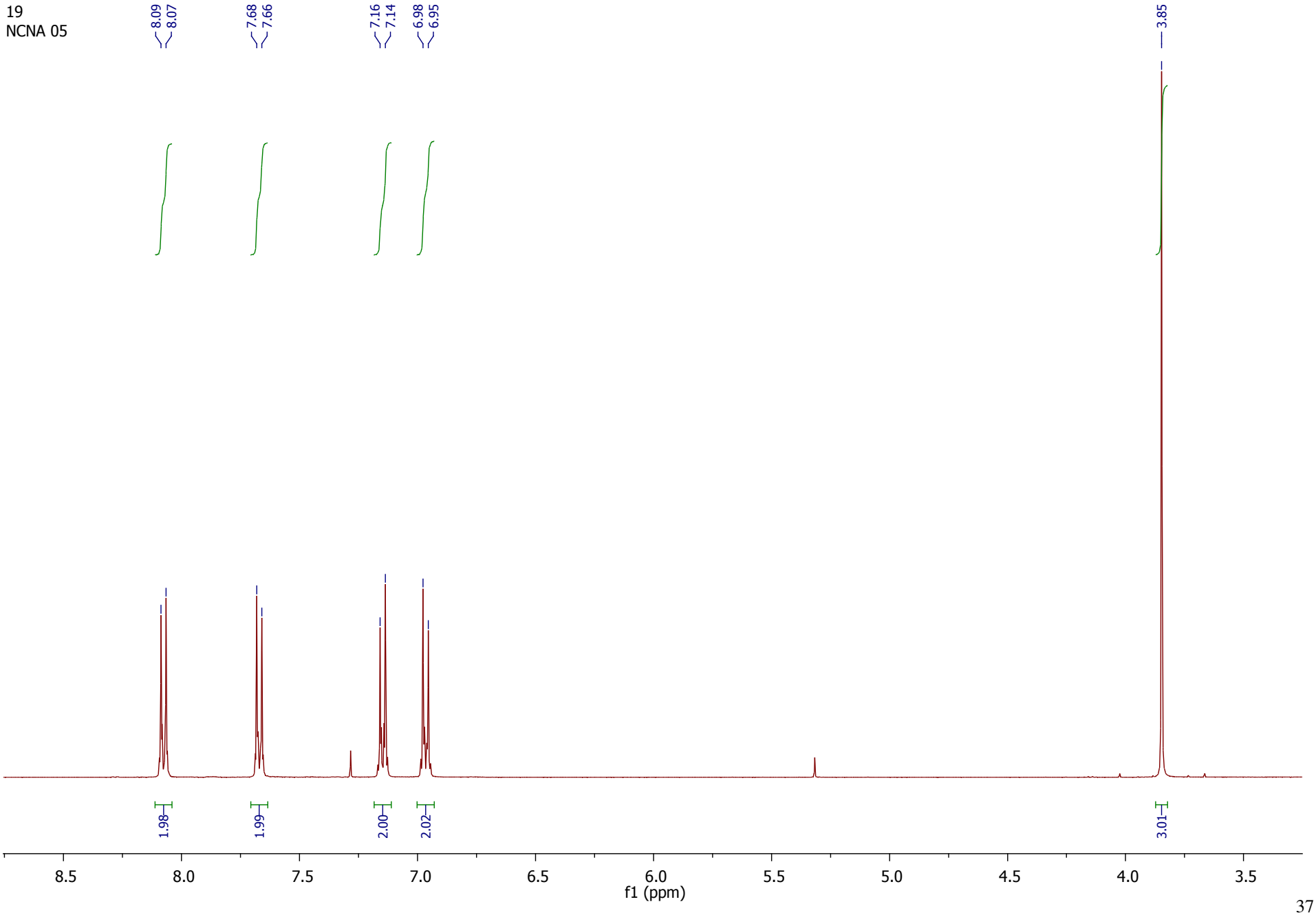
17
NCNA 06

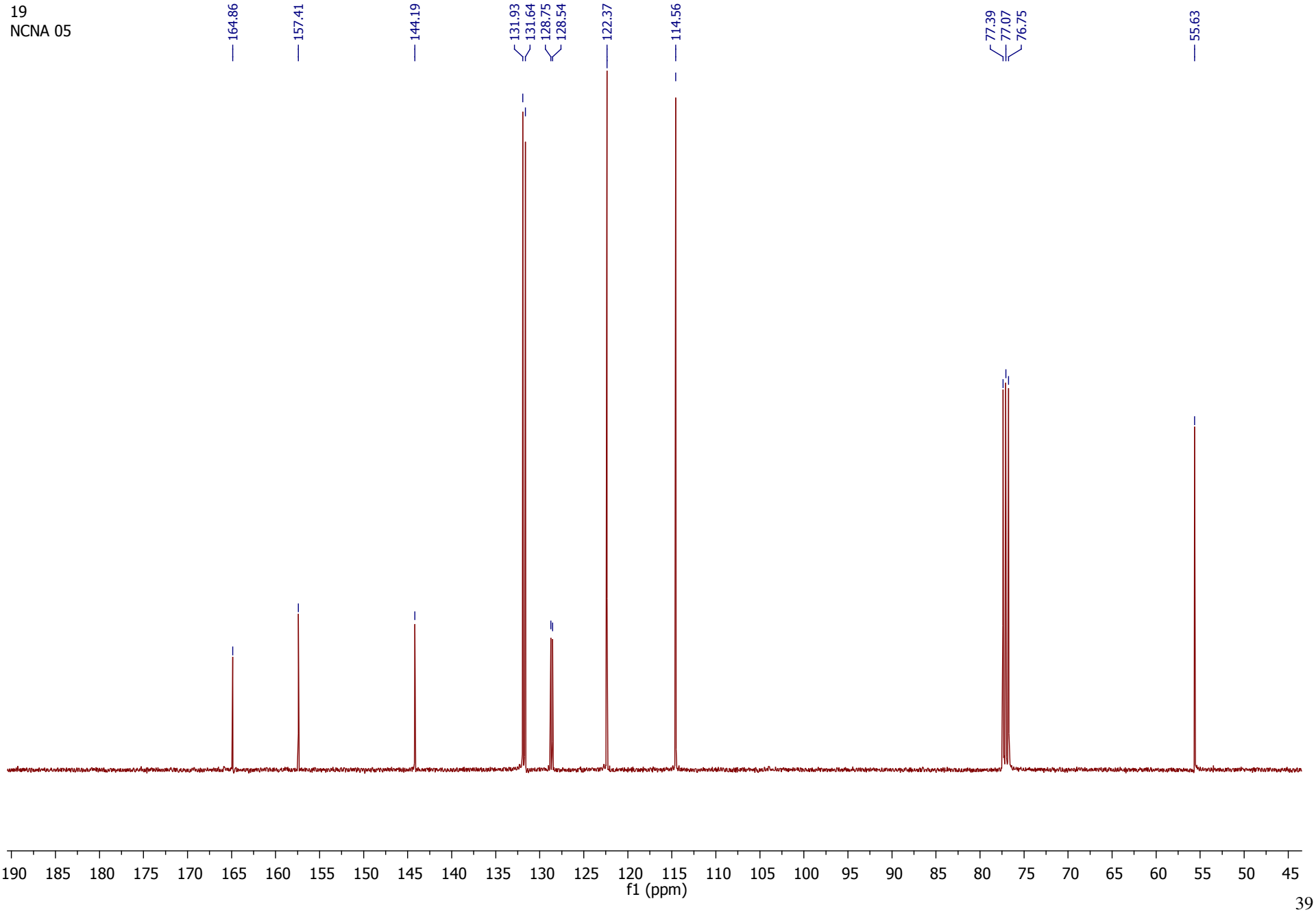

8.11
8.10
8.09
8.09
8.08
7.70
7.70
7.69
7.68
7.67
7.49
7.48
7.47
7.47
7.45
7.45
7.34
7.34
7.33
7.32
7.31
7.30
7.28
7.25
7.25
7.25
7.23
7.23
7.23
2.00
2.10
2.06
3.11
8.40
8.30
8.20
8.10
8.00
7.90
7.80
7.70
7.60
7.50
7.40
7.30
7.20
7.10
f1 (ppm)

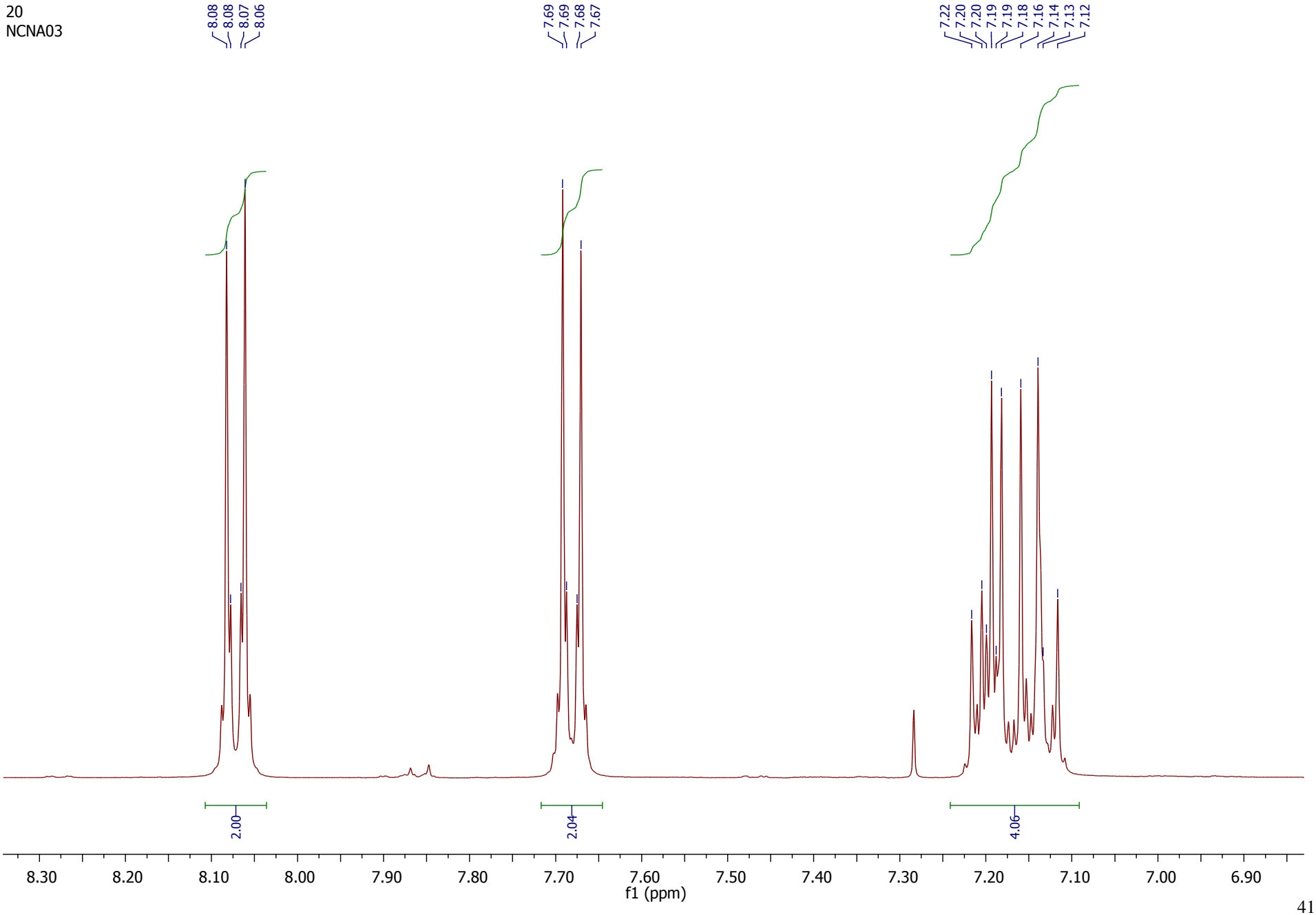

17
NCNA 06
164.52
150.75
131.97
131.68
129.58
128.86
128.48
126.09
121.64
77.40
77.08
76.76
O
O
Br
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
f1 (ppm)

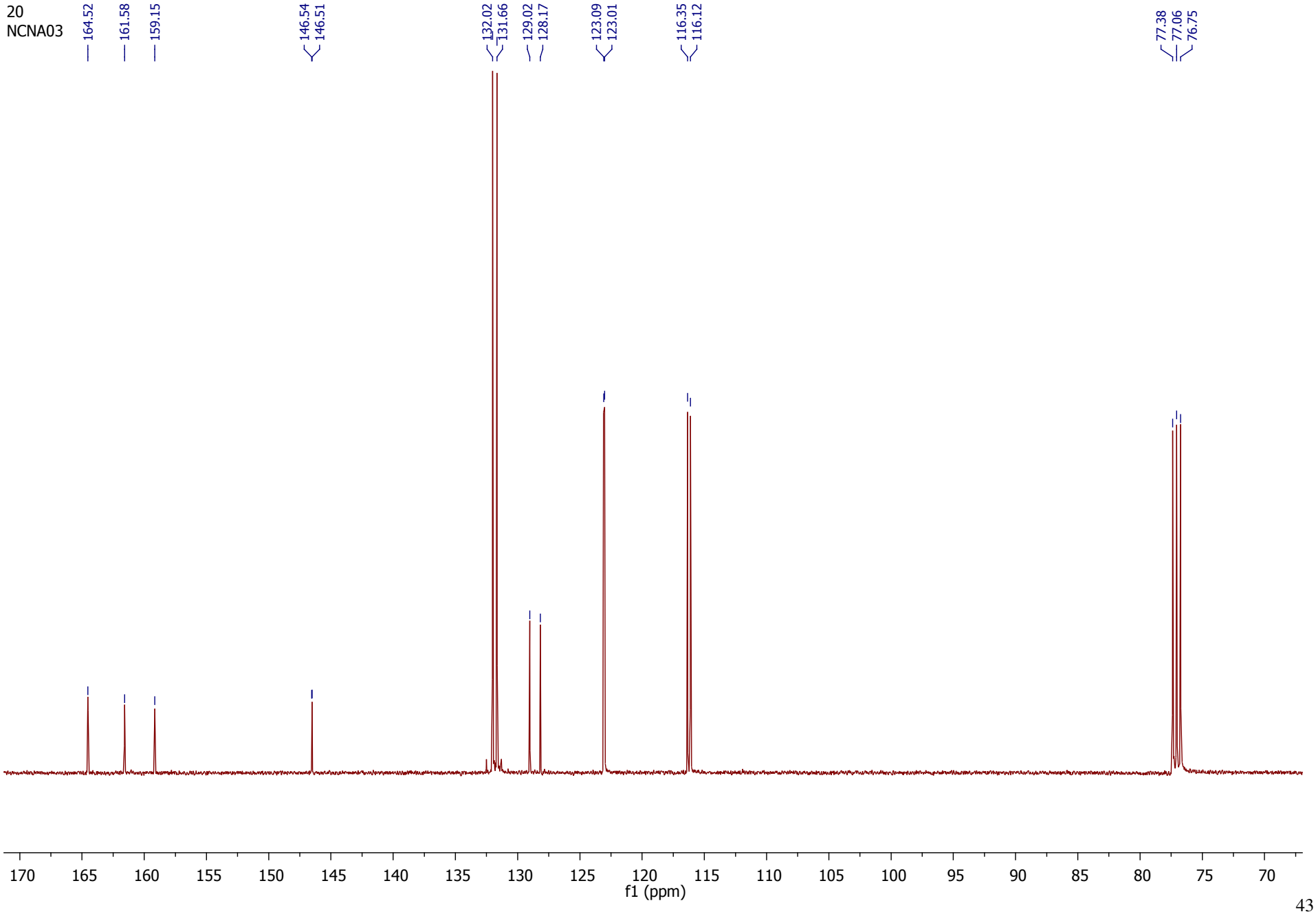

18
FFPC070
8.10
8.09
8.08
8.08
7.69
7.68
7.67
7.66
7.27
7.25
7.13
7.12
7.11
2.41
2.00
2.06
2.12
2.01
3.04
8.6
8.2
7.8
7.6
7.4
7.2
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
3.0
2.6
2.2
f1 (ppm)


18
FFPC070
164.71
148.51
135.73
132.52
131.93
131.66
131.31
130.08
128.75
128.58
121.28
77.40
77.29
77.08
76.77
29.75
20.96
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

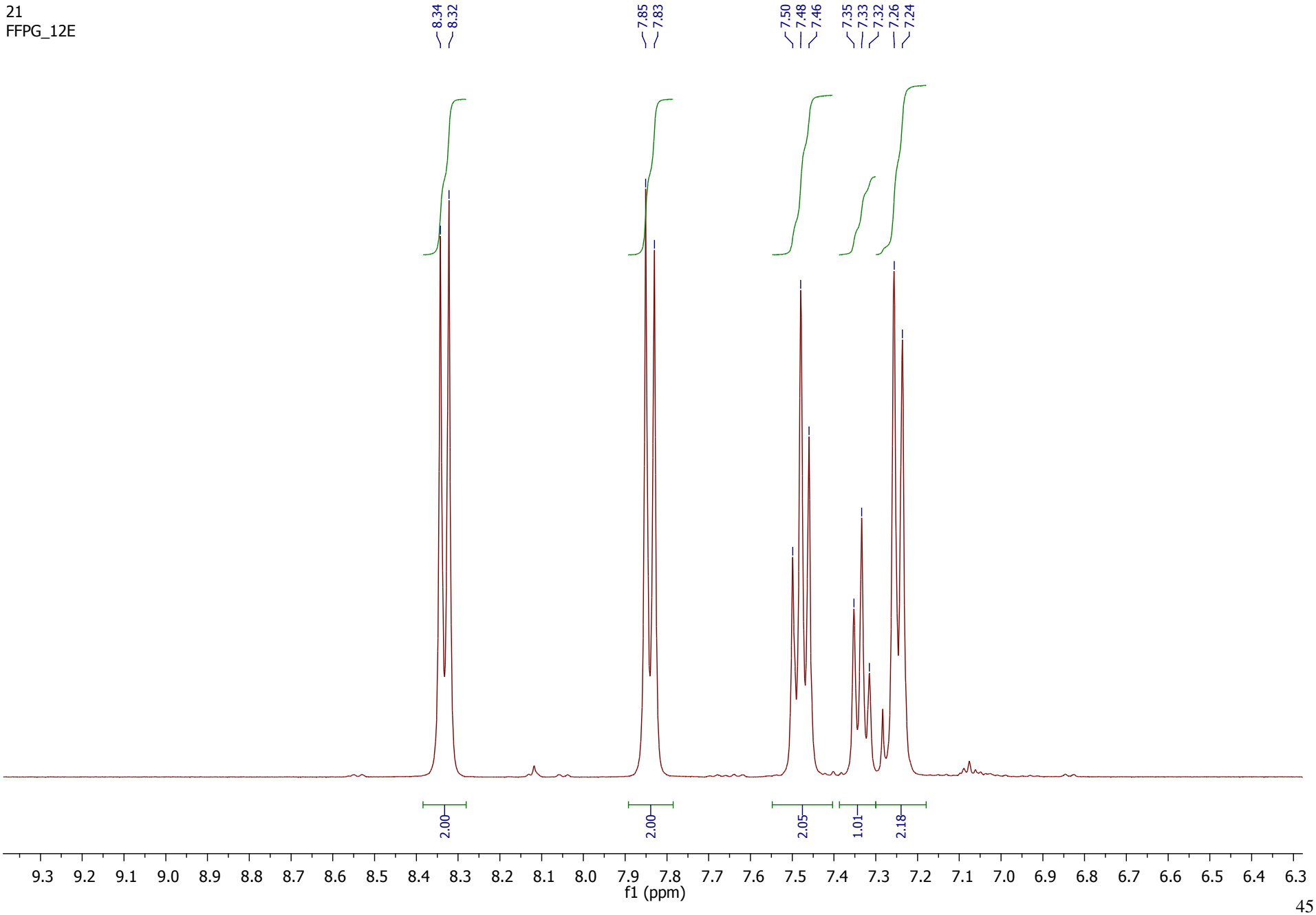

19
NCNA 05
8.09
8.07
7.68
7.66
7.16
7.14
6.98
6.95
3.85
1.98
1.99
2.00
2.02
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)

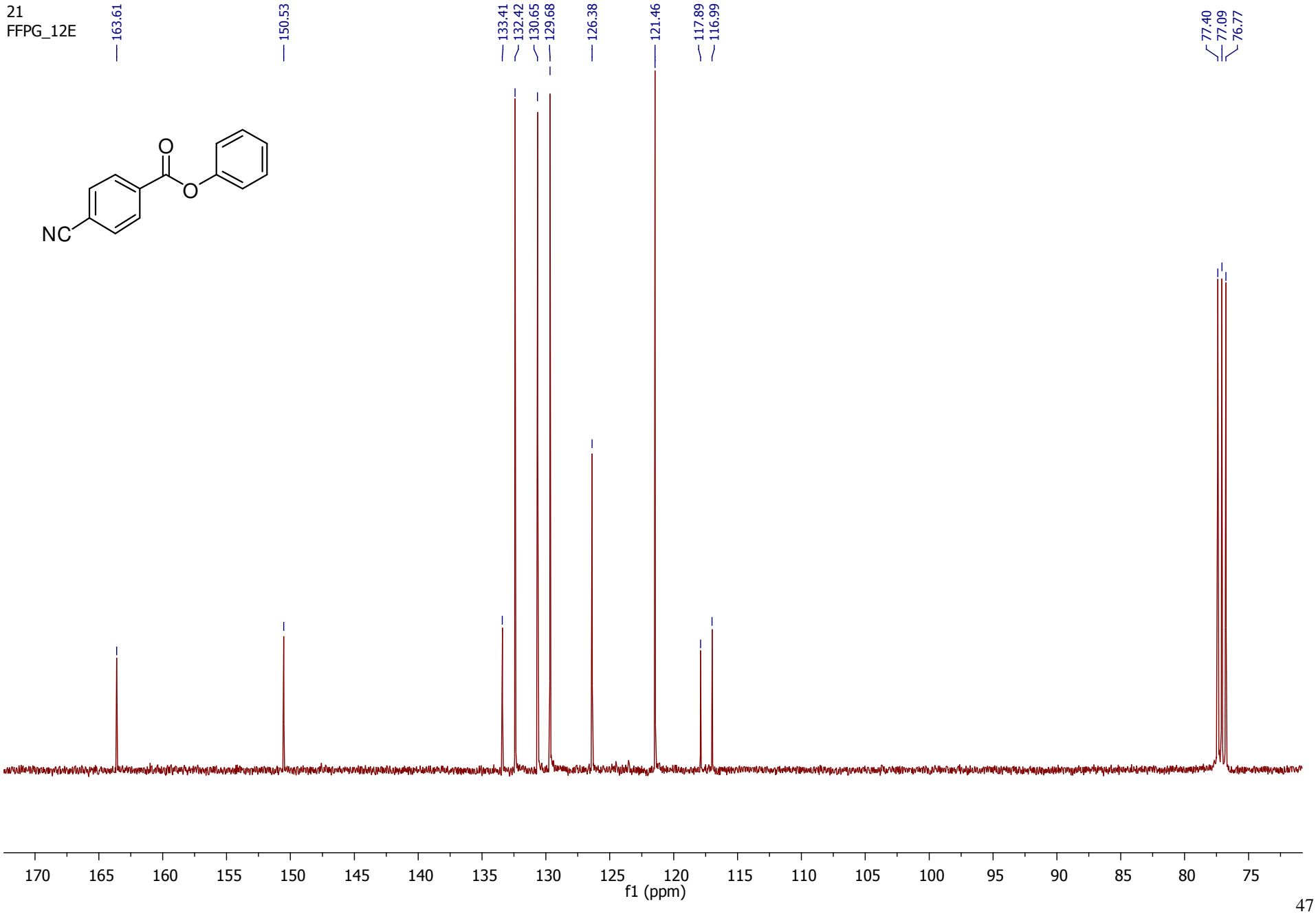

19
NCNA 05
164.86
157.41
144.19
131.93
131.64
128.75
128.54
122.37
114.56
77.39
77.07
76.75
55.63
190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)

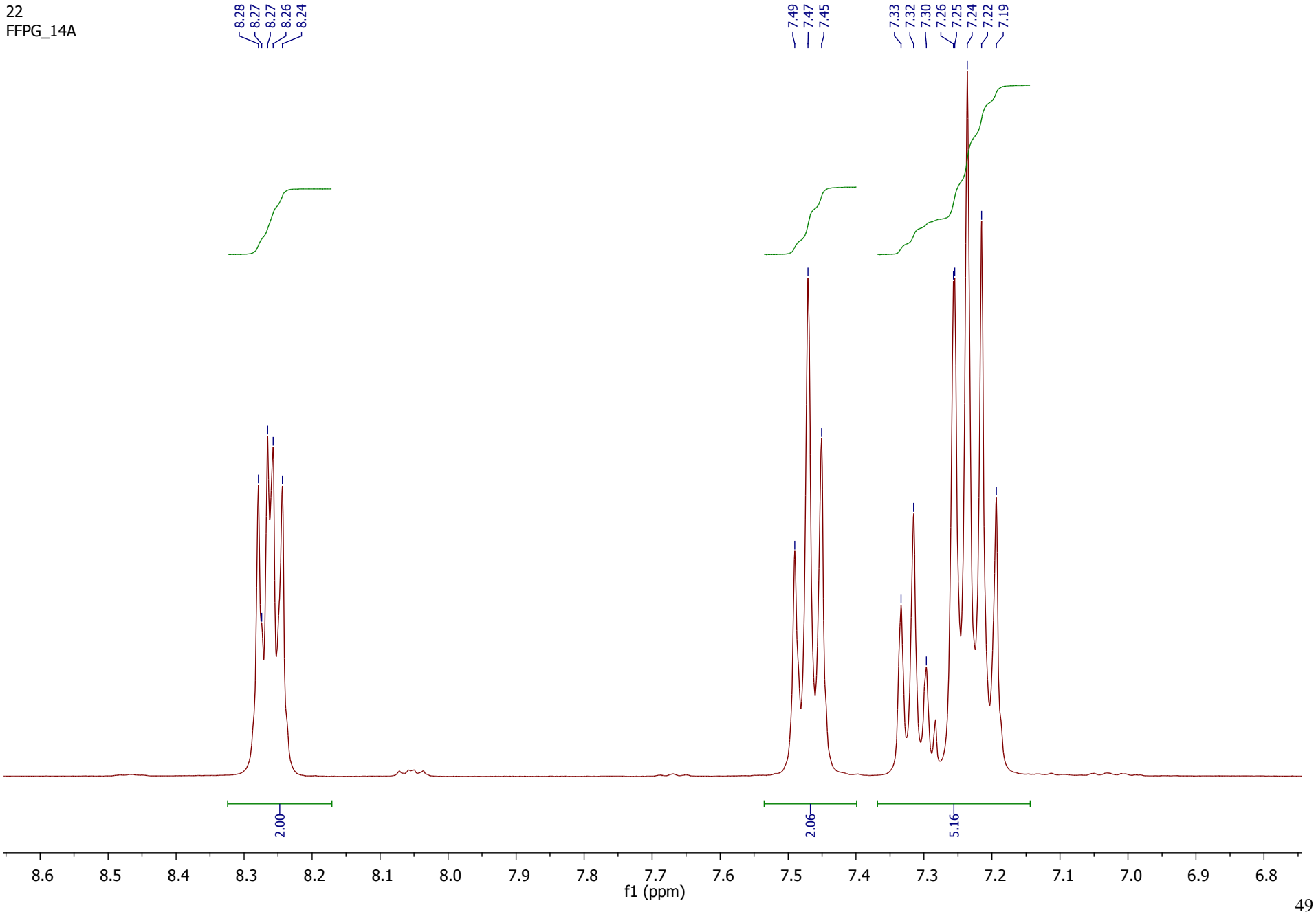

20
NCNA03
8.08
8.08
8.07
8.06
7.69
7.69
7.68
7.67
7.22
7.20
7.20
7.19
7.19
7.18
7.16
7.14
7.13
7.12
2.00
2.04
4.06
8.30
8.20
8.10
8.00
7.90
7.80
7.70
7.60
7.50
7.40
7.30
7.20
7.10
7.00
6.90
f1 (ppm)

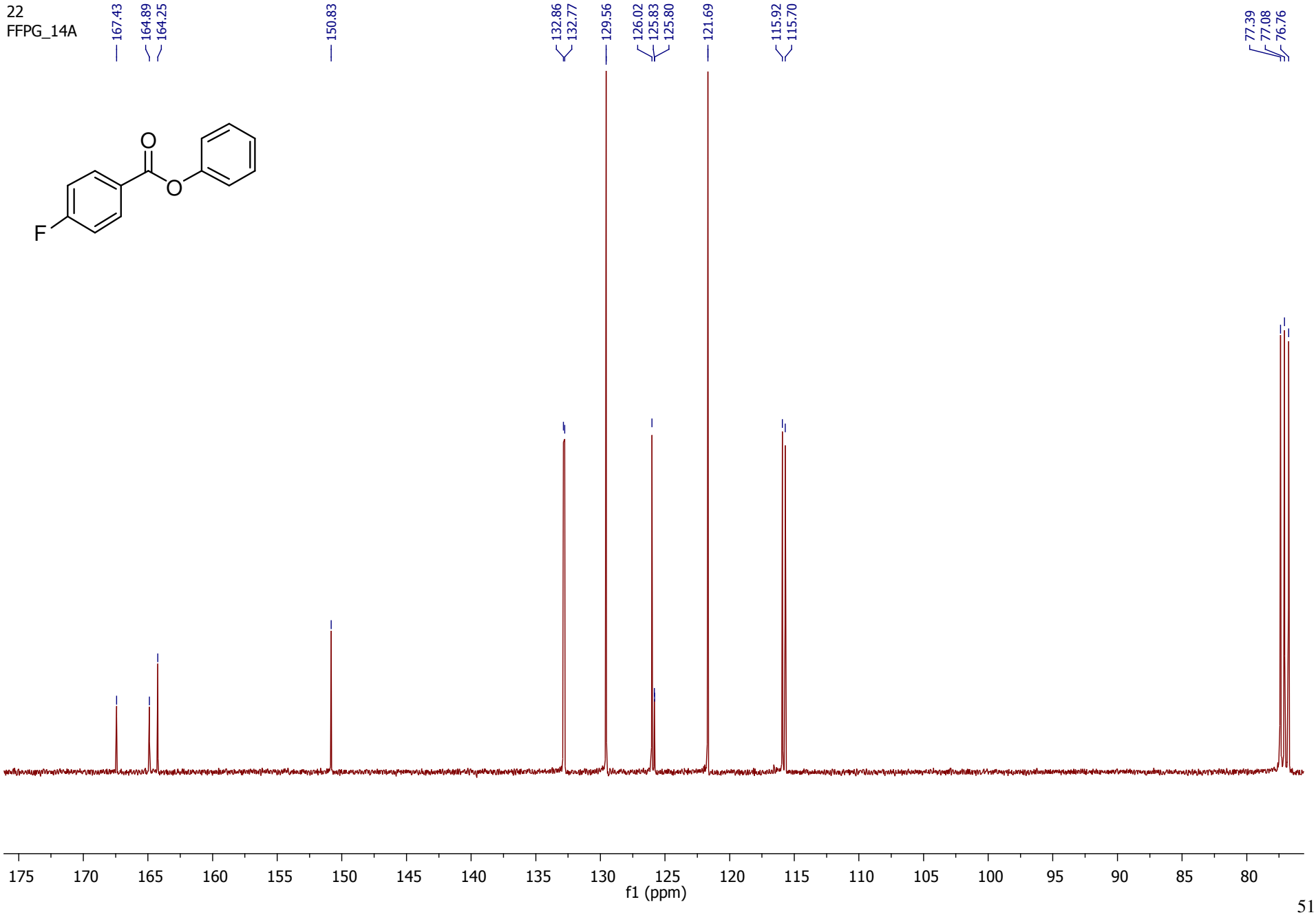

20
NCNA03
164.52
161.58
159.15
146.54
146.51
132.02
131.66
129.02
128.17
123.09
123.01
116.35
116.12
77.38
77.06
76.75
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
f1 (ppm)

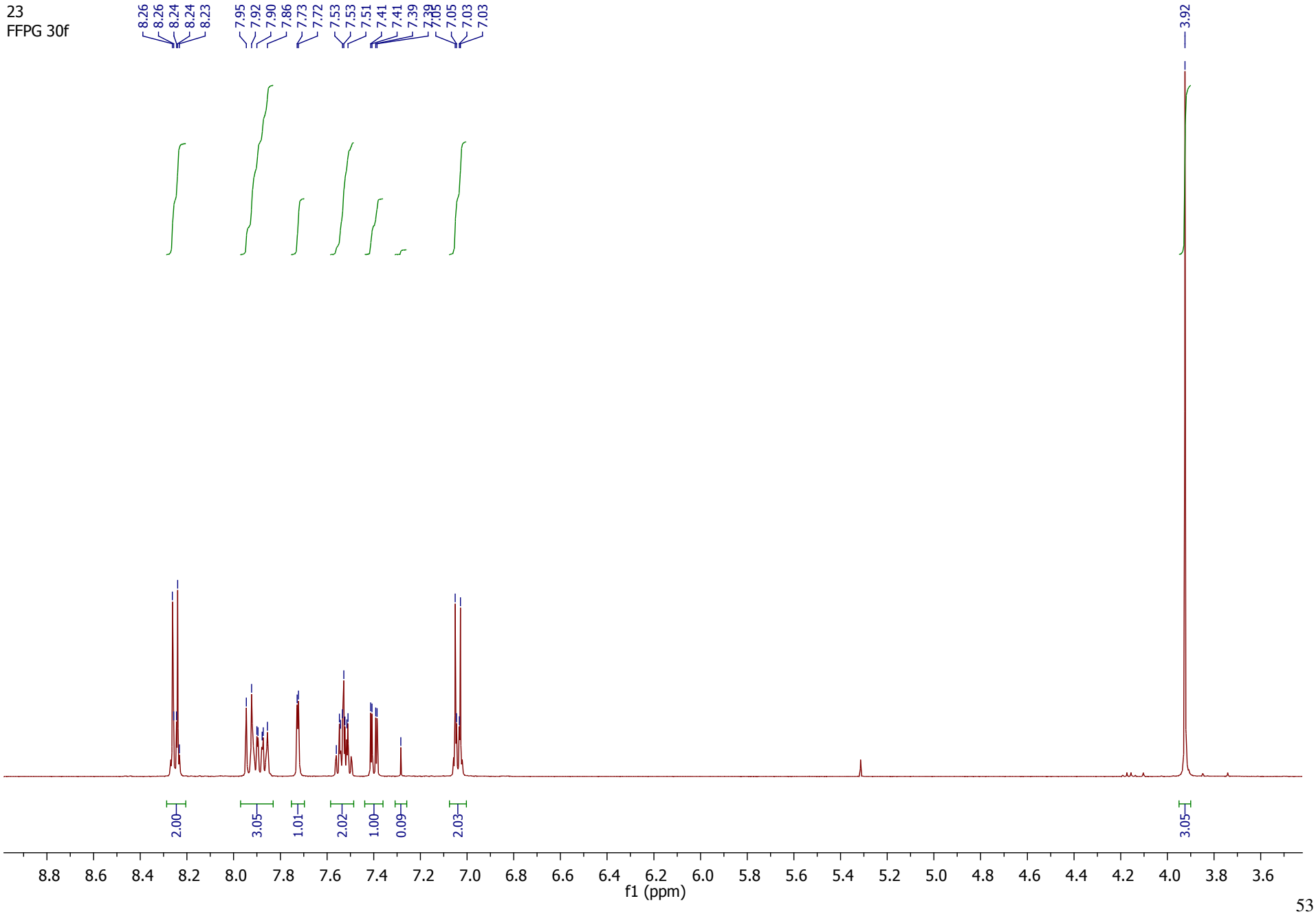
21
FFPG_12E

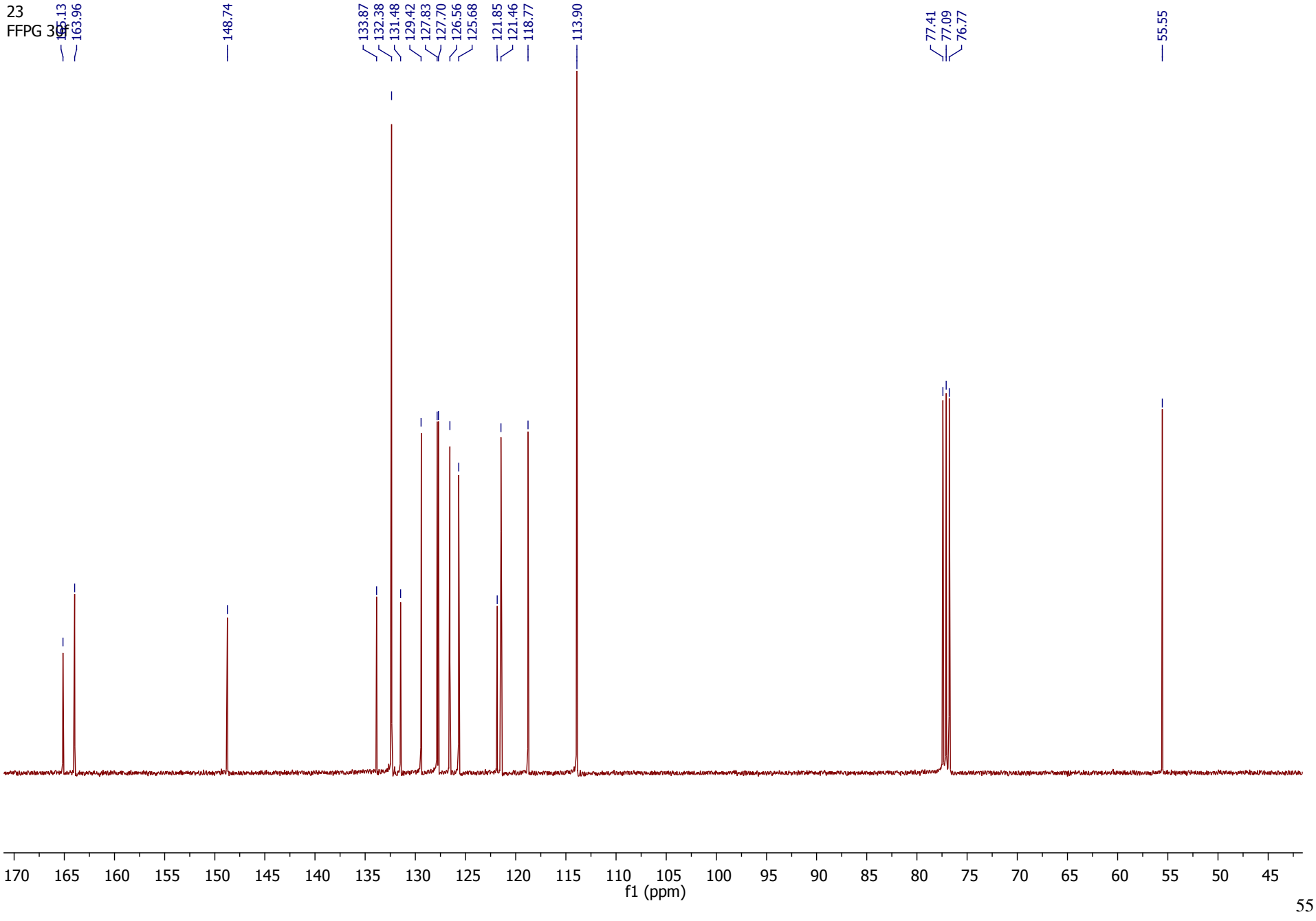

8.34
8.32
7.85
7.83
7.50
7.48
7.46
7.35
7.33
7.32
7.26
7.24
2.00
2.00
2.05
1.01
2.18
9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3
f1 (ppm)


21
FFPG_12E
163.61
150.53
133.41
132.42
130.65
129.68
126.38
121.46
117.89
116.99
77.40
77.09
76.77
O
O
NC
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
f1 (ppm)

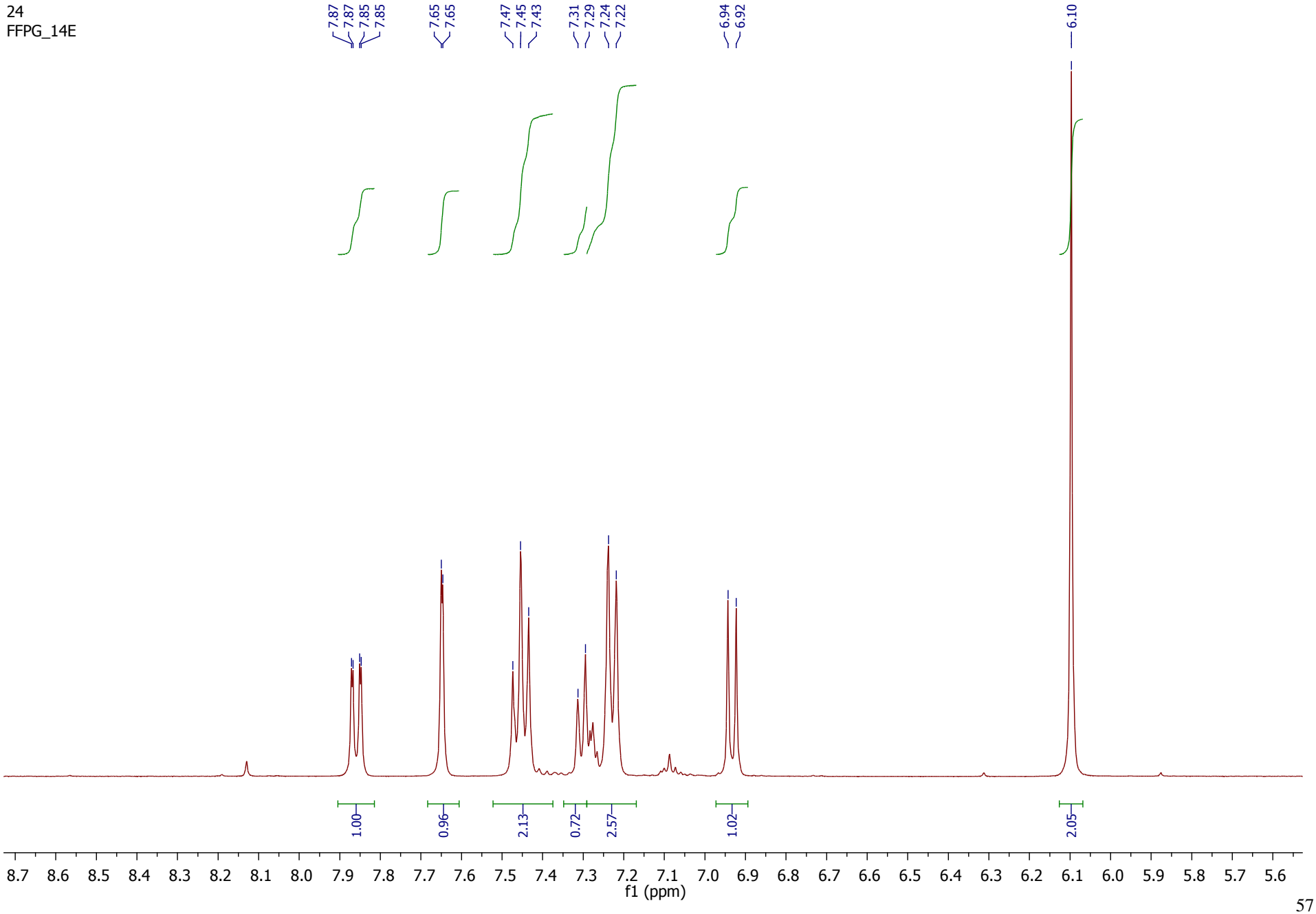

22
FFPG_14A
8.28
8.27
8.27
8.26
8.24
7.49
7.47
7.45
7.33
7.32
7.30
7.26
7.25
7.24
7.22
7.19
2.00
2.06
5.16
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)

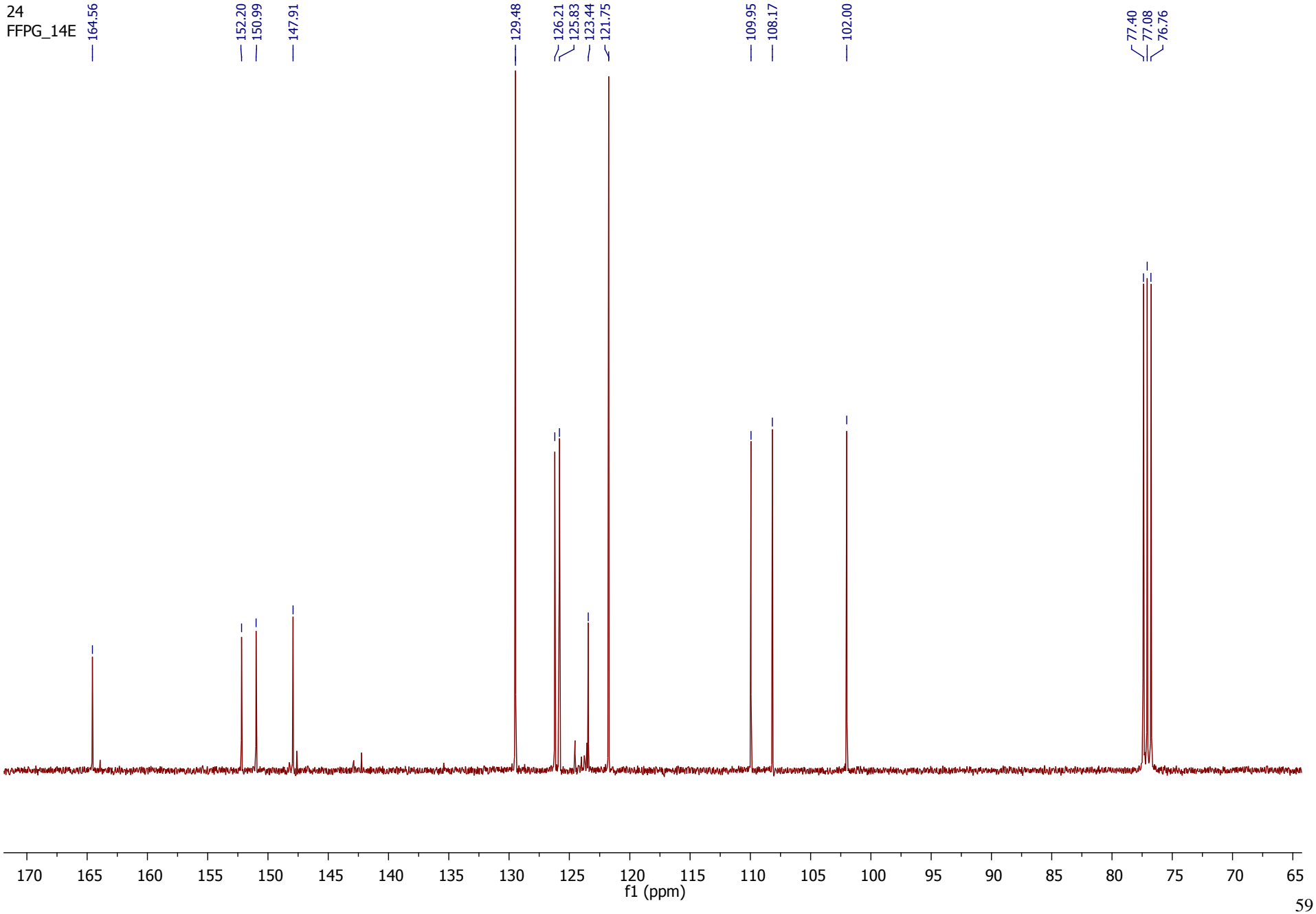

22
FFPG_14A
167.43
164.89
164.25
150.83
132.86
132.77
129.56
126.02
125.83
125.80
121.69
115.92
115.70
77.39
77.08
76.76
O
O
F
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
f1 (ppm)

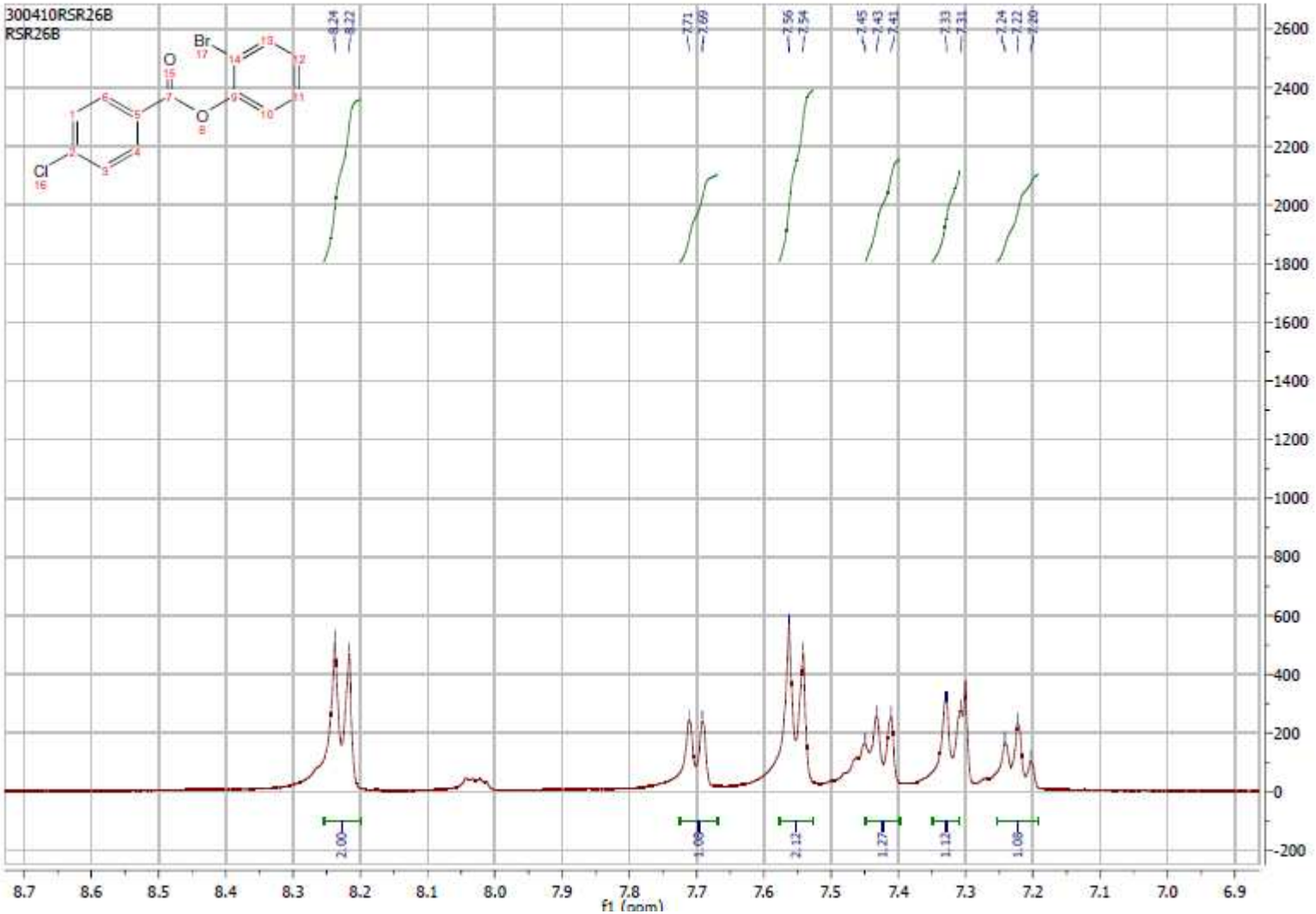

23
FFPG 30f
8.26
8.26
8.24
8.24
8.23
7.95
7.92
7.90
7.86
7.73
7.72
7.53
7.53
7.51
7.41
7.41
7.39
7.38
7.05
7.05
7.03
7.03
3.92
2.00
3.05
1.01
2.02
1.00
0.09
2.03
3.05
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
f1 (ppm)

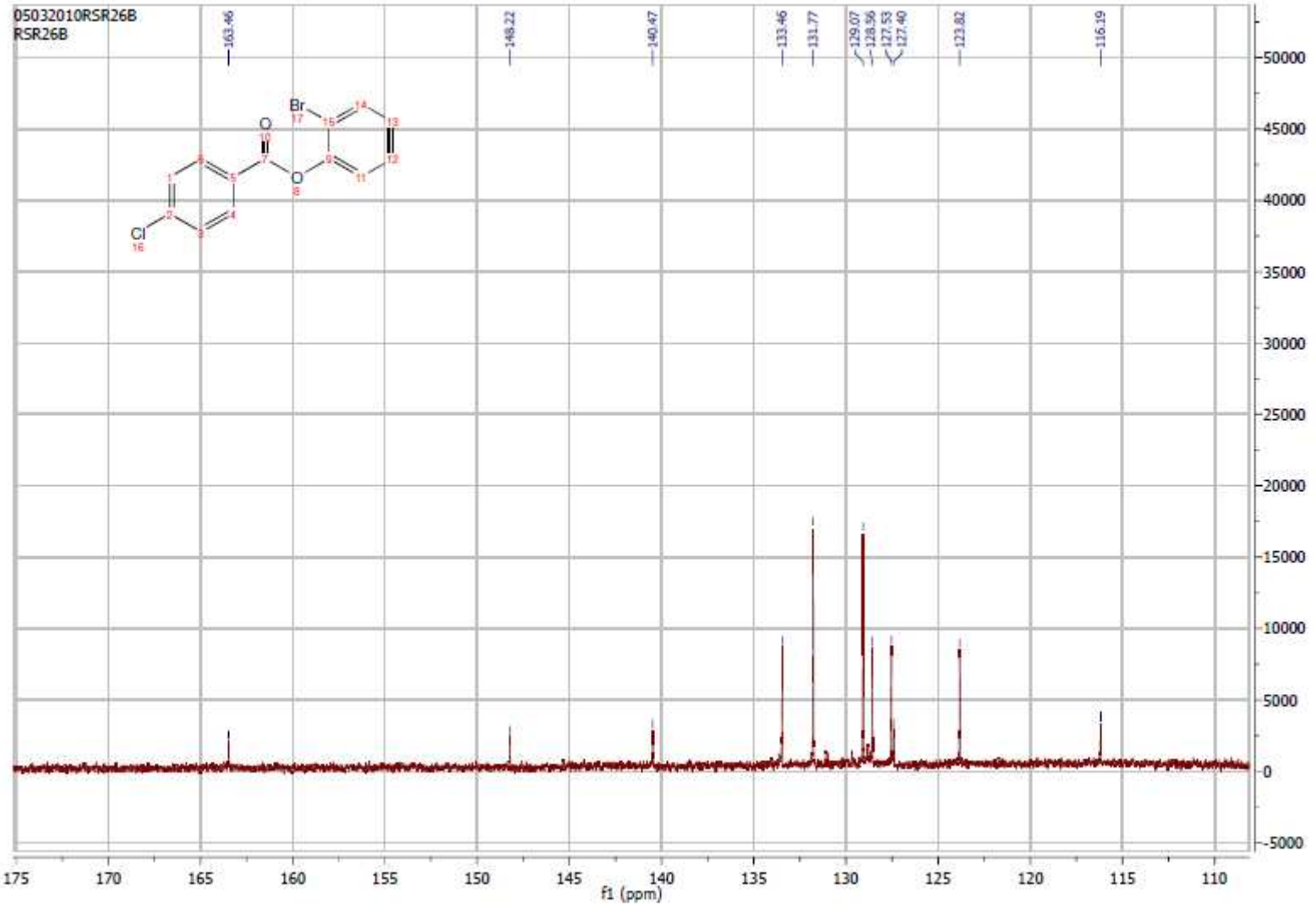

23
FFPG 39F
165.13
163.96
148.74
133.87
132.38
131.48
129.42
127.83
127.70
126.56
125.68
121.85
121.46
118.77
113.90
77.41
77.09
76.77
55.55
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)

24
FFPG_14E

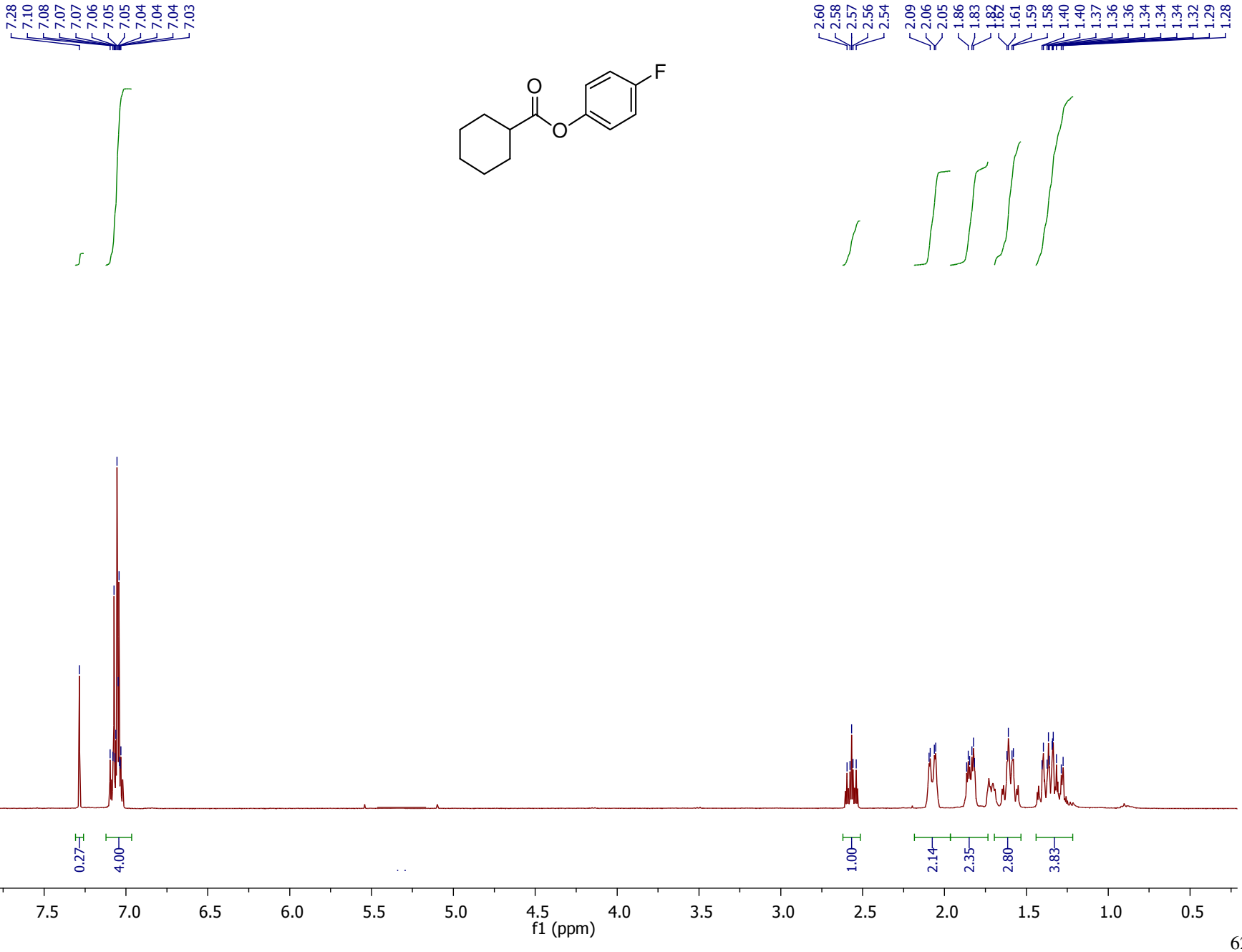

7.87
7.87
7.85
7.85
7.65
7.65
7.47
7.45
7.43
7.31
7.29
7.24
7.22
6.94
6.92
6.10
1.00
0.96
2.13
0.72
2.57
1.02
2.05
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6
f1 (ppm)

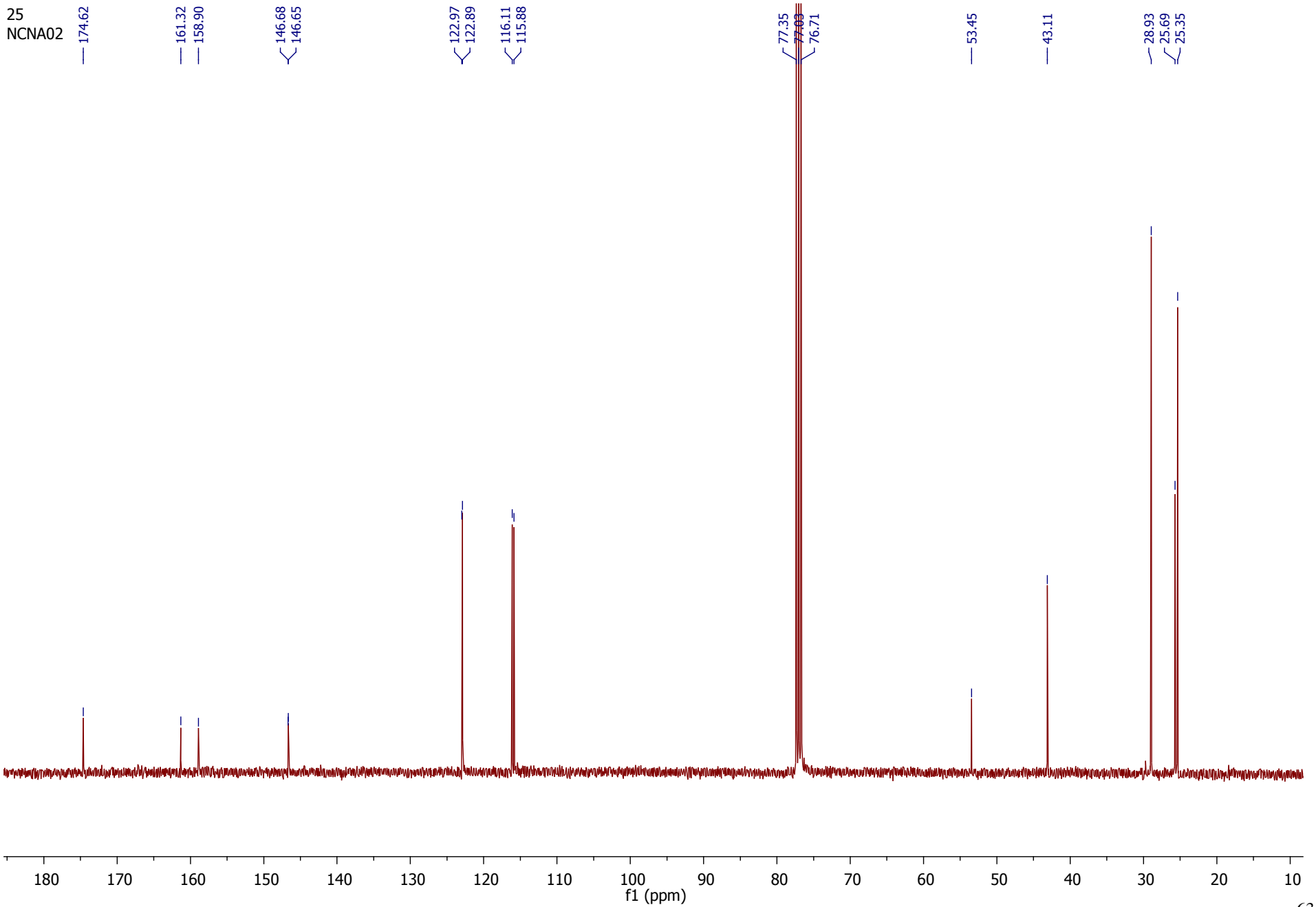

24
FFPG_14E
164.56
152.20
150.99
147.91
129.48
126.21
125.83
123.44
121.75
109.95
108.17
102.00
77.40
77.08
76.76
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
f1 (ppm)

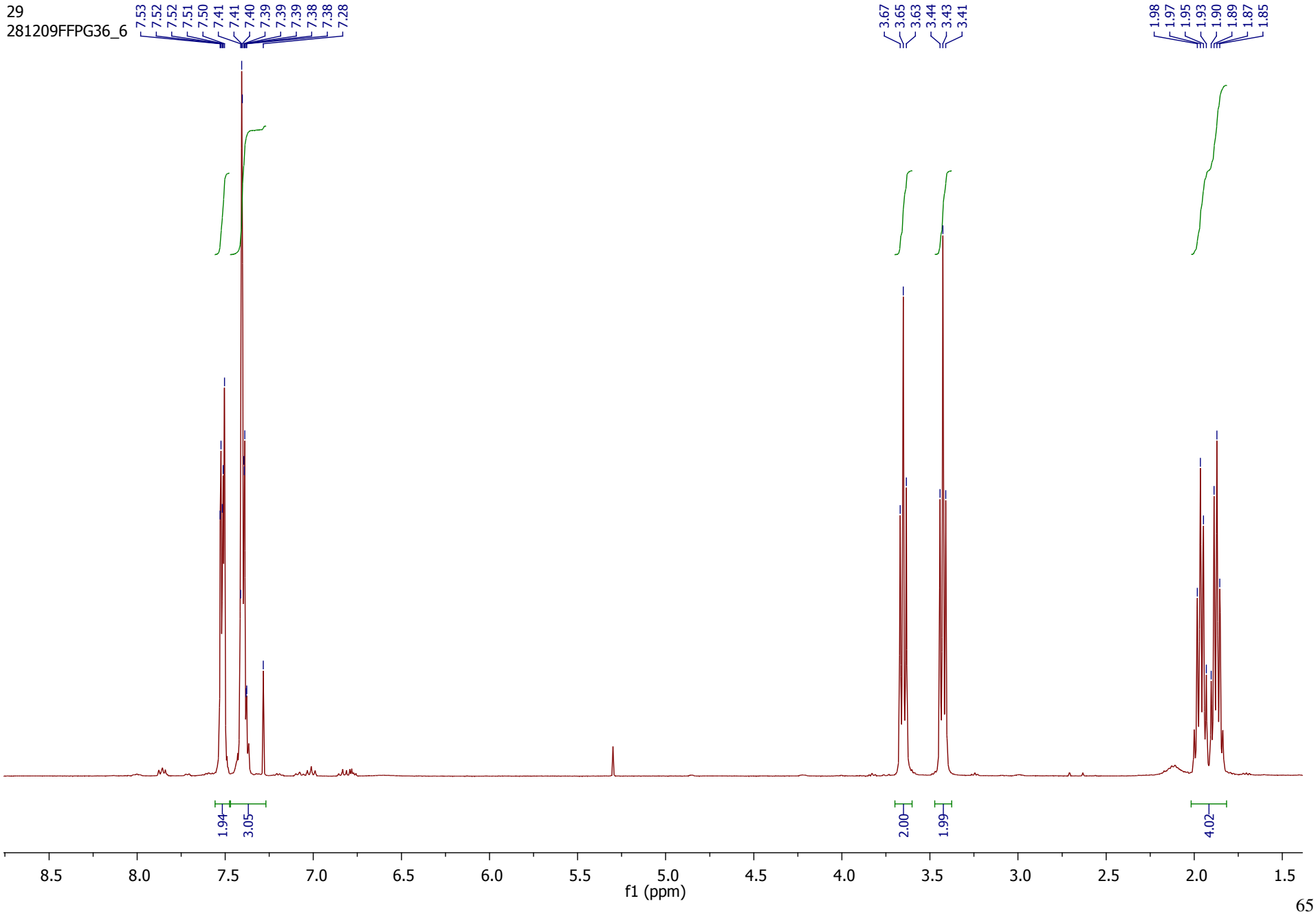

300410RSR26B
RSR26B
Br
O
O
Cl
8.24
8.22
7.71
7.69
7.56
7.54
7.45
7.43
7.41
7.33
7.31
7.24
7.22
7.20
2.00
1.09
2.12
1.27
1.13
1.08
f1 (ppm)

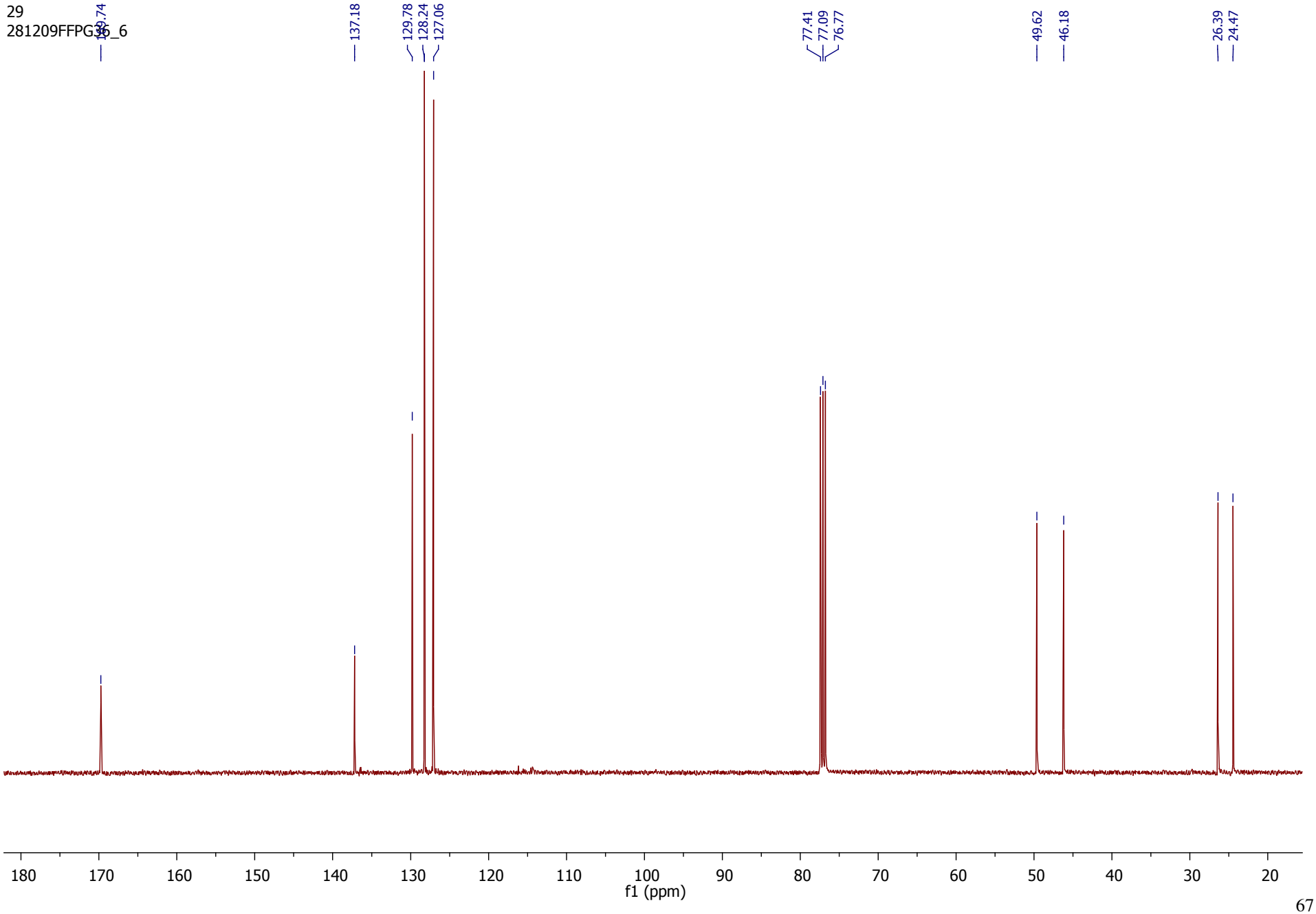

05032010RSR26B
RSR26B
163.46
148.22
140.47
133.46
131.77
129.07
128.56
127.53
127.40
123.82
116.19
Br
O
O
Cl
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)

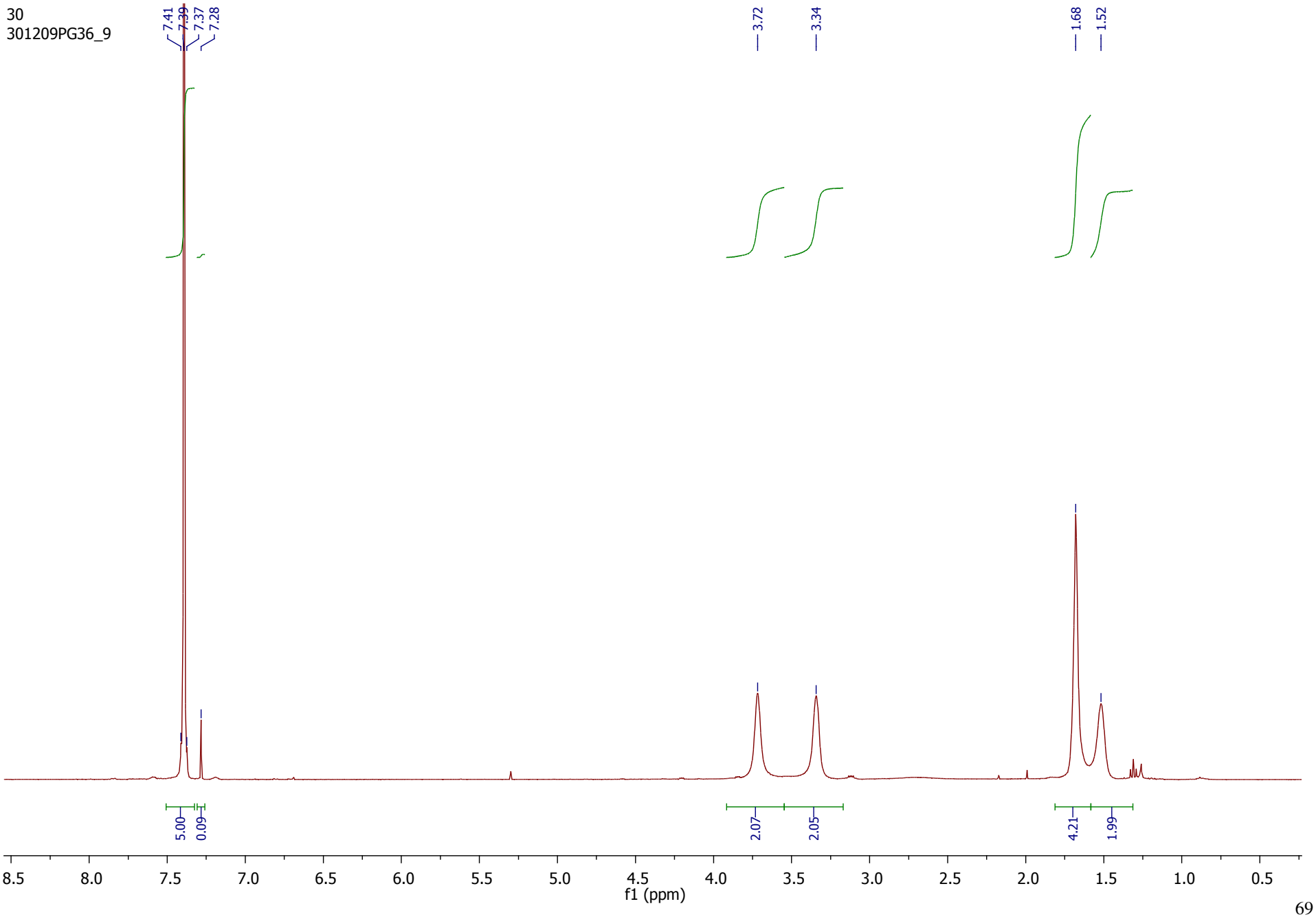
25
NCNA02


7.28
7.10
7.08
7.07
7.07
7.06
7.05
7.05
7.04
7.04
7.04
7.03
2.60
2.58
2.57
2.56
2.54
2.09
2.06
2.05
1.86
1.83
1.82
1.82
1.61
1.59
1.58
1.40
1.40
1.37
1.36
1.36
1.34
1.34
1.34
1.32
1.29
1.28
O
O
F
0.27
4.00
1.00
2.14
2.35
2.80
3.83
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


25
NCNA02
174.62
161.32
158.90
146.68
146.65
122.97
122.89
116.11
115.88
77.35
77.03
76.71
53.45
43.11
28.93
25.69
25.35
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


29
281209FFPG36_6
7.53
7.52
7.52
7.51
7.50
7.41
7.41
7.40
7.39
7.39
7.39
7.38
7.38
7.28
3.67
3.65
3.63
3.44
3.43
3.41
1.98
1.97
1.95
1.93
1.90
1.89
1.87
1.85
1.94
3.05
2.00
1.99
4.02
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
f1 (ppm)


29
281209FFPG36_6
169.74
137.18
129.78
128.24
127.06
77.41
77.09
76.77
49.62
46.18
26.39
24.47
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


30
301209PG36_9
7.41
7.39
7.37
7.28
3.72
3.34
1.68
1.52
5.00
0.09
2.07
2.05
4.21
1.99
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
f1 (ppm)

30
301209PG36_9