Supporting Information

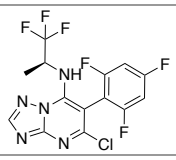
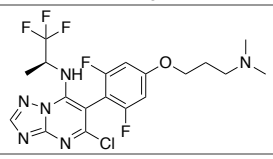
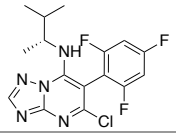
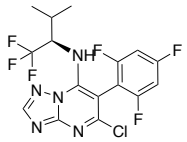
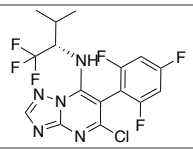
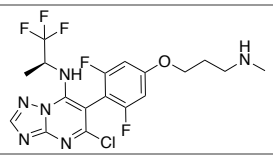
Evaluation of Structure-Activity Relationship of Microtubule (MT)-Targeting 1,2,4-Triazolo[1,5-*a*]pyrimidines Identifies New Candidates for Neurodegenerative Tauopathies.

Killian Oukoloff,[a] Goodwell Nzou,[b] Carmine Varricchio,[c] Bobby Lucero,[d] Thibault Alle,[a] Jane Kovalevich,[b] Ludovica Monti,[a] Anne-Sophie Cornec,[c] Yuemang Yao,[b] Michael J. James,[b] John Q. Trojanowski,[b] Virginia M.-Y. Lee,[b] Amos B. Smith III,[c] Andrea Brancale,[c] Kurt R. Brunden[b,*] and Carlo Ballatore[a,*]

[a]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093; [b]Center for Neurodegenerative Disease Research, Perelman School of Medicine, University of Pennsylvania, 3600 Spruce St., Philadelphia, PA 19104; [c]Cardiff School of Pharmacy and Pharmaceutical Sciences, Cardiff, King Edward VII Avenue, Cardiff CF103NB, UK; [d]Department of Chemistry & Biochemistry, University of California San Diego, 9500 Gilman Drive, La Jolla, CA, 92093, USA;[e]Department of Chemistry, School of Arts and Sciences, University of Pennsylvania, 231 South 34th St., Philadelphia, PA 19104-6323.

Table of contents

Table S-1: HeLa/QBI293 cell cytotoxicity assay of selected compounds

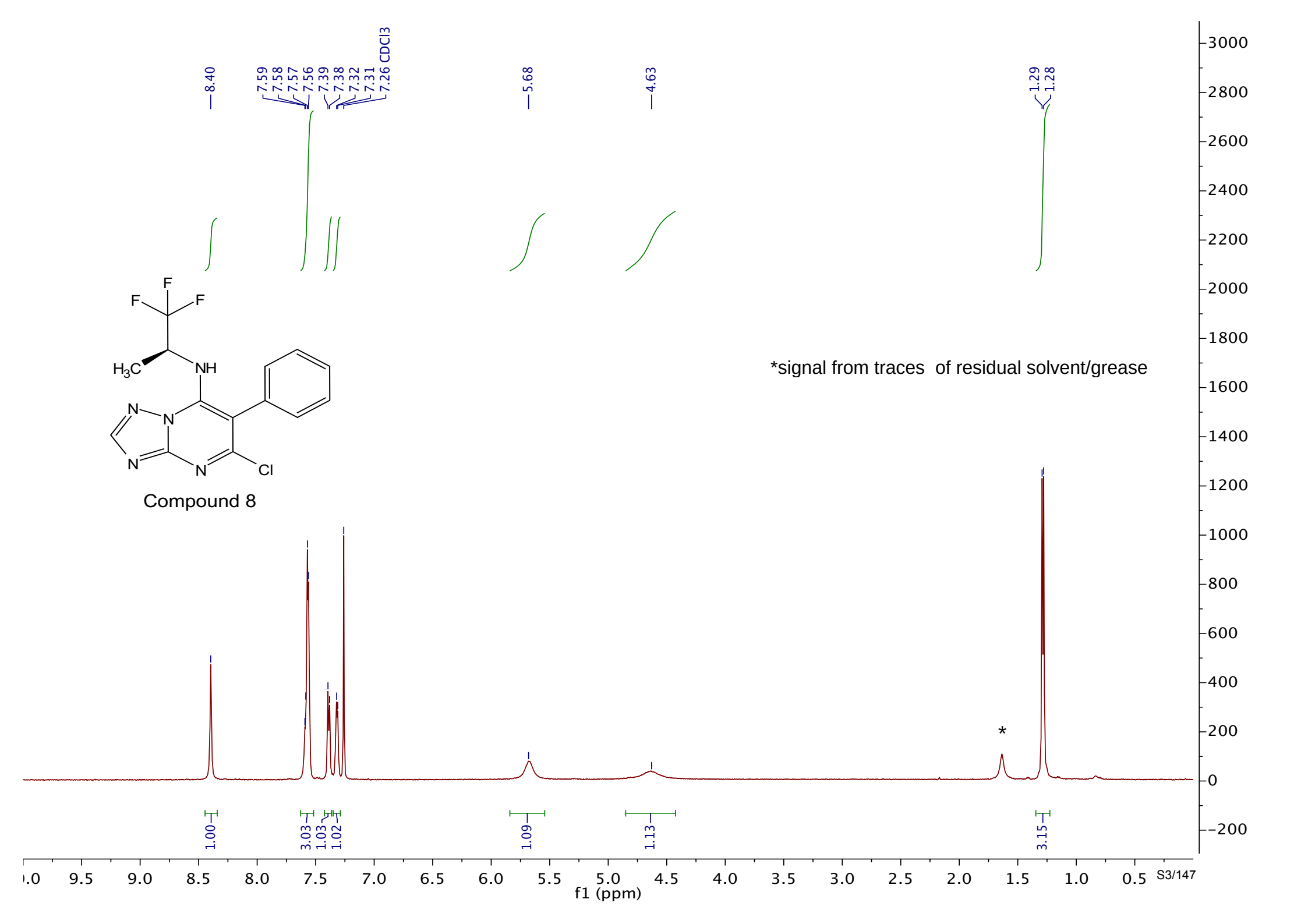
Cpd#	Structure	HeLa IC_{50} (nM)	QBI293 IC_{50} (nM)
Taxol	-	1.45 ± 0.083	1.40 ± 0.129
Vinblastine	-	3.11 ± 0.252	1.93 ± 0.286
7		50.8 ± 0.051	102 ± 0.120
6		10.1 ± 0.066	21.2 ± 0.101
3		51.9 ± 0.081	84.0 ± 0.141
46		80.7 ± 0.080	186 ± 0.142
47		75.4 ± 0.077	236 ± 0.138
5 (Cevipabulin)		12.8 ± 0.117	28.0 ± 0.168

Experimental section

HeLa/QBI293 cells cytotoxicity assay

The CellTiter-Glo® luminescent cell viability assay (G7572; Promega) was employed to measure the ability of test compounds to inhibit cancer cell proliferation. Compounds in 100% DMSO stocks were diluted in 50 µL medium in 96-well plates (Corning 3903) such that the final DMSO

concentration was 1%. Eight-point dose response assays were set up. HeLa or QBI293 cells were then diluted to $1x10^5$ cells/mL in medium and dispensed into the previously prepared 96-well plates at 50 µL per well. After 48 h incubation at 37°C and 5% CO_2, cells were lysed by the addition of 100 µL/well of Cell-titer Glo®. Plates were read on the 2104 EnVision® multilabel plate reader (PerkinElmer). The activity of test compounds was normalized against controls from the same plate. ED_{50} values, *i.e.*, the concentration of drug required to inhibit cell growth by 50%, were calculated using GraphPad Prism software, version 8.3.0 for macOS. Each assay was performed as three experimental replicates and means ± SD values are shown.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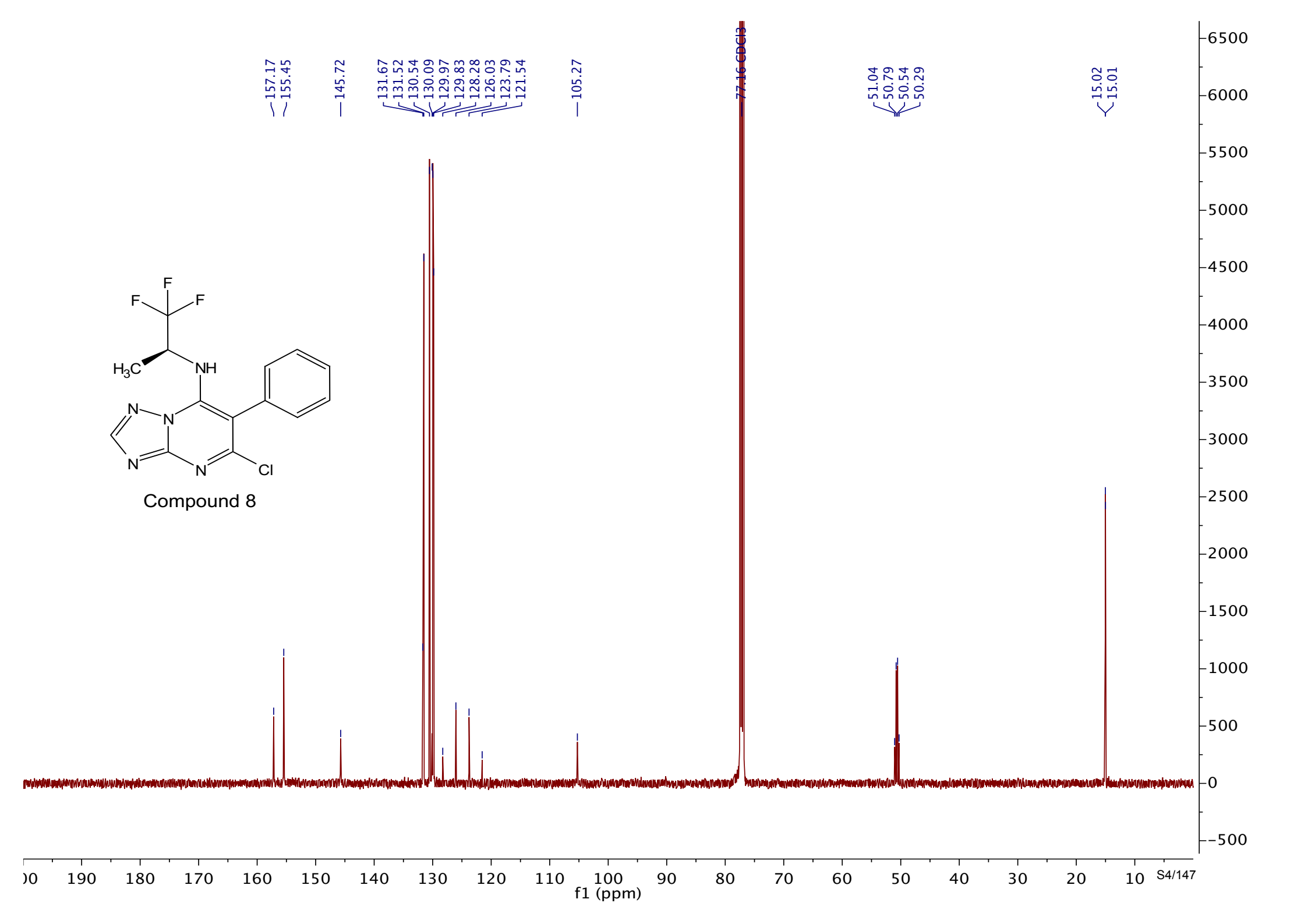
7.58
7.57
7.56
7.39
7.38
7.32
7.31
7.26 CDCl3
5.68
4.63
1.29
1.28
F
F
F
H3C
NH
N
N
N
N
Cl
Compound 8
*signal from traces of residual solvent/grease
*
1.00
3.03
1.03
1.02
1.09
1.13
3.15
f1 (ppm)
S3/147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129.97
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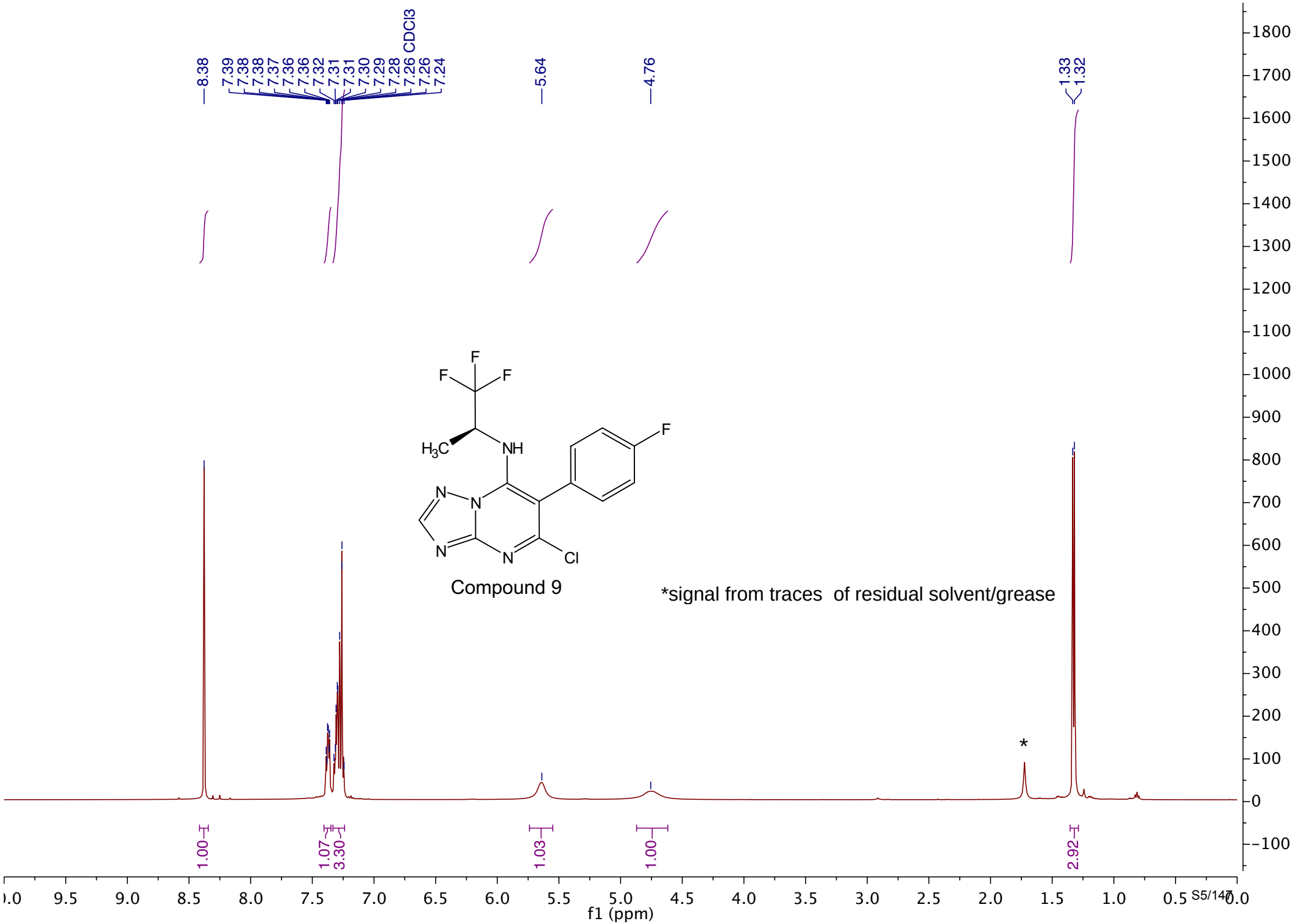
123.79
121.54
105.27
77.16 CDCl3
51.04
50.79
50.54
50.29
15.02
15.01
F
F
F
H3C
NH
N
N
N
N
Cl
Compound 8
f1 (ppm)
S4/147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7.38
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7.32
7.31
7.31
7.30
7.29
7.28
CDCl3
7.26
7.26
7.24
5.64
4.76
1.33
1.32
F
F
F
H3C
NH
N
N
N
N
Cl
F
Compound 9
*signal from traces of residual solvent/grease
*
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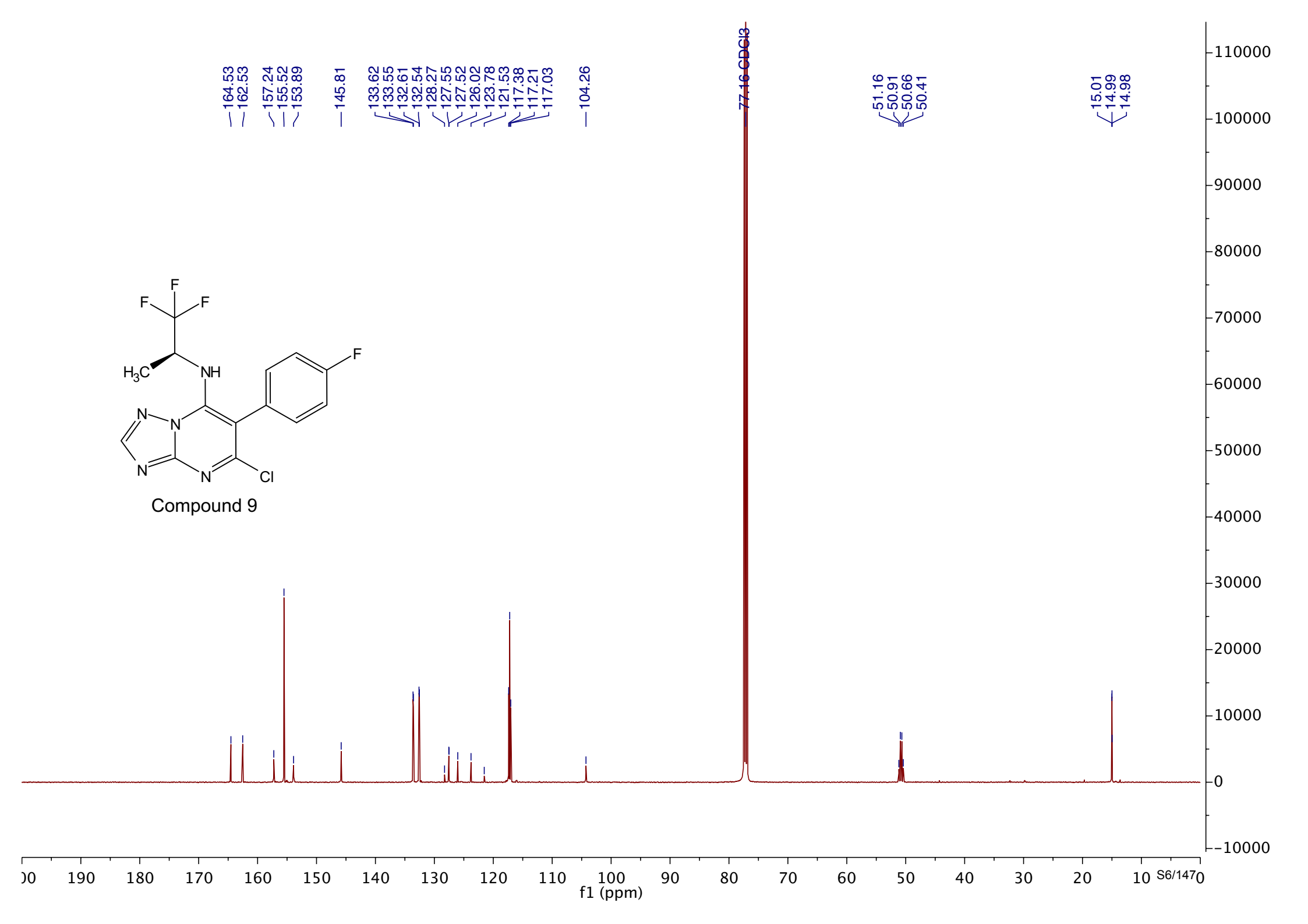
1.07
3.30
1.03
1.00
2.92
f1 (ppm)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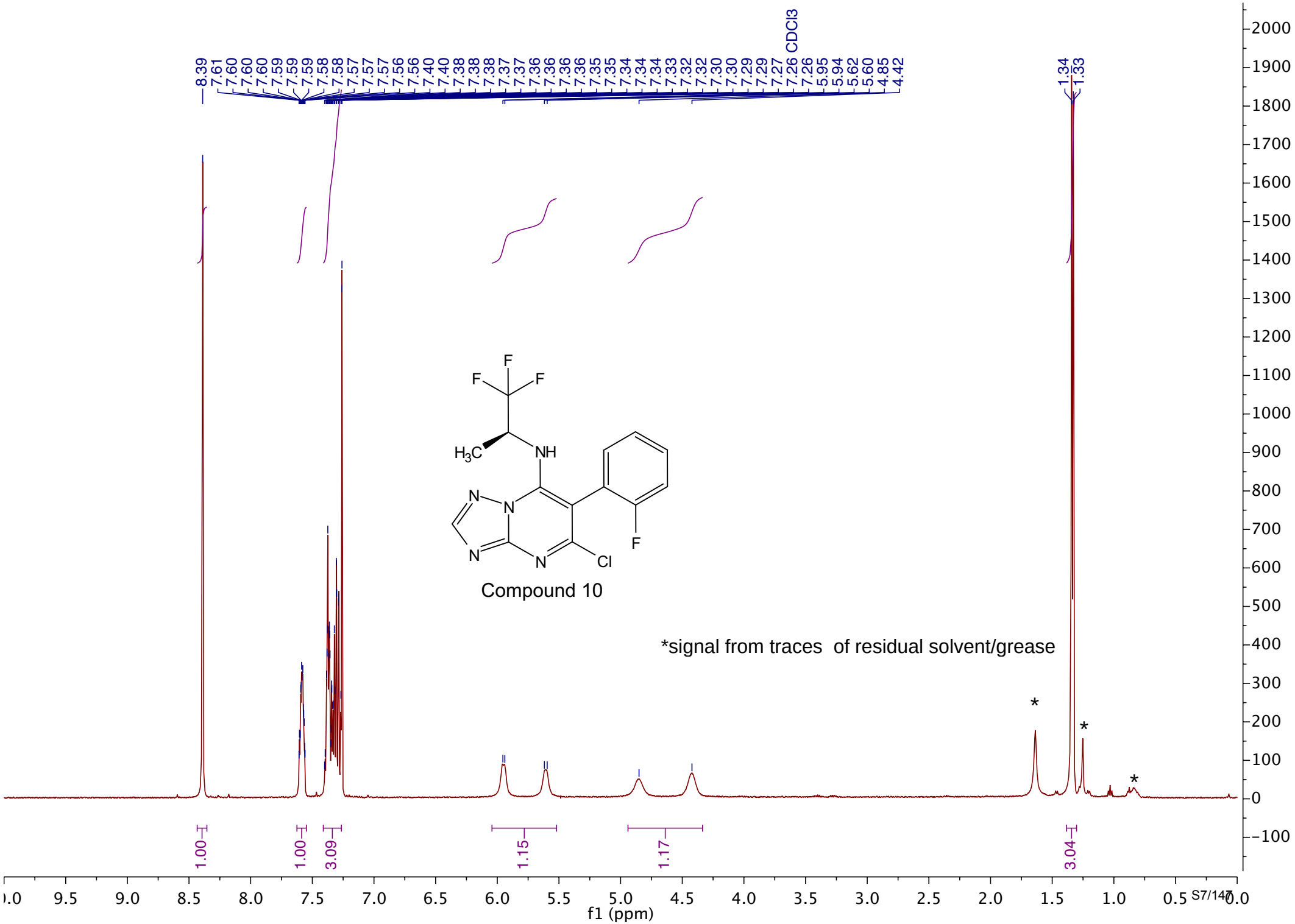
162.53
157.24
155.52
153.89
145.81
133.62
133.55
132.61
132.54
128.27
127.55
127.52
126.02
123.78
121.53
117.38
117.21
117.03
104.26
77.16 CDCl3
51.16
50.91
50.66
50.41
15.01
14.99
14.98
F
F
F
H3C
NH
F
N
N
N
N
Cl
Compound 9
f1 (ppm)
S6/147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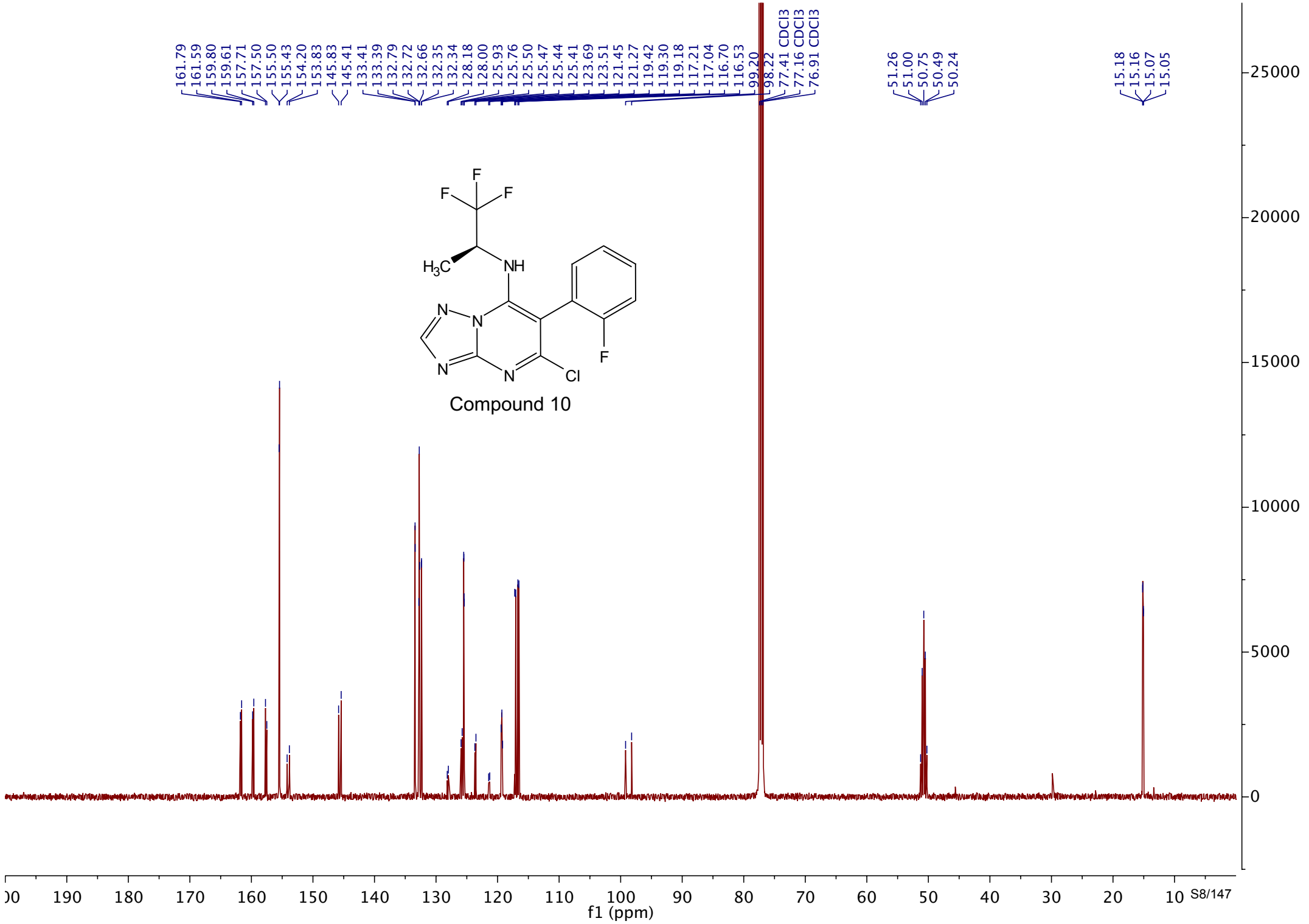
7.61
7.60
7.60
7.60
7.59
7.59
7.59
7.58
7.58
7.58
7.57
7.57
7.57
7.56
7.56
7.40
7.40
7.38
7.38
7.38
7.37
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.34
7.34
7.33
7.32
7.30
7.30
7.29
7.29
7.27
7.26
7.26
5.95
5.94
5.62
5.60
4.85
4.42
1.34
1.33
F
F
F
H3C
NH
N
N
N
N
Cl
F
Compound 10
*signal from traces of residual solvent/grease
*
*
*
1.00
1.00
3.09
1.15
1.17
3.04
f1 (ppm)
S7/147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155.50
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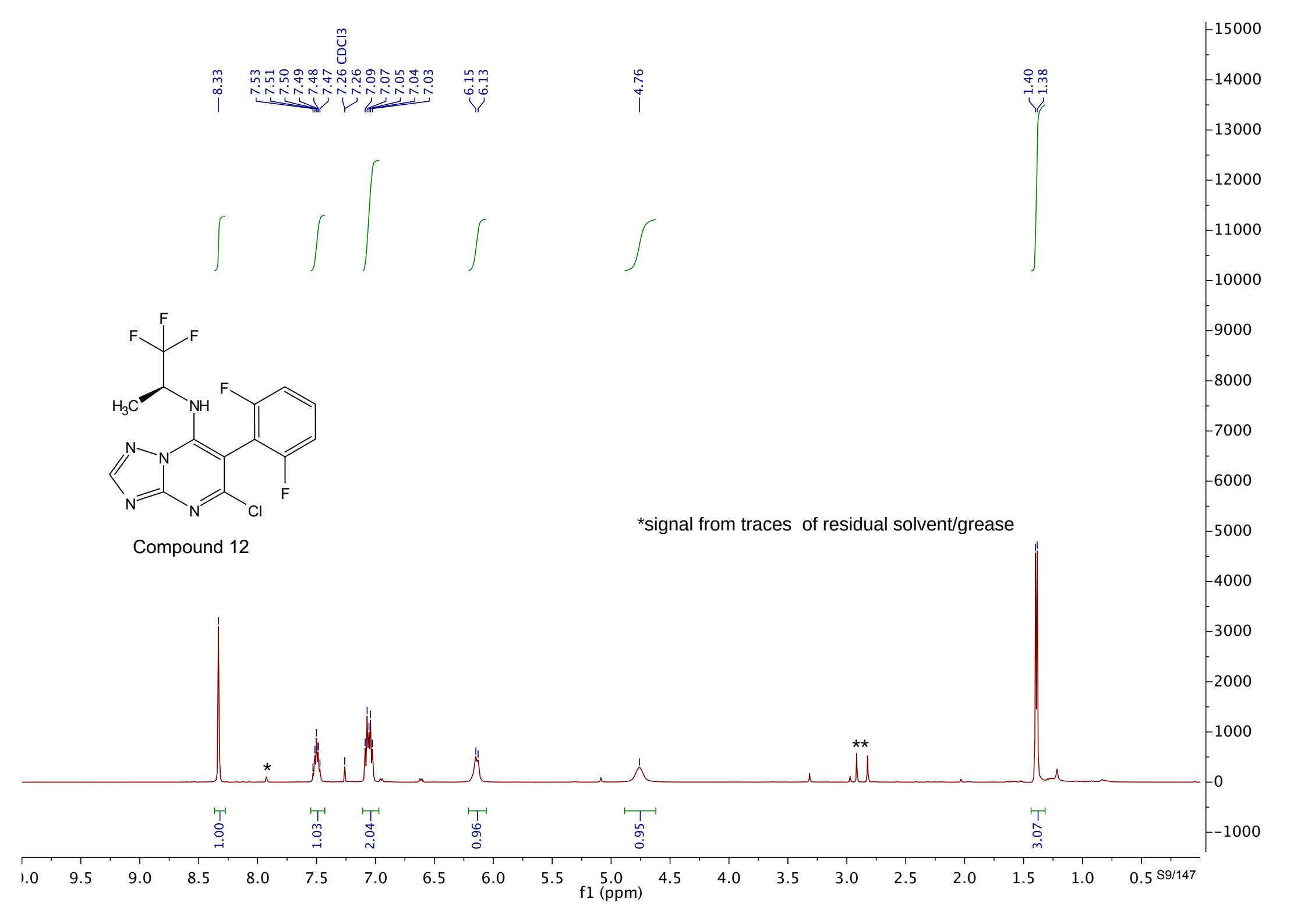
153.83
145.83
145.41
133.41
133.39
132.79
132.72
132.66
132.35
132.34
128.18
128.00
125.93
125.76
125.50
125.47
125.44
125.41
123.69
123.51
121.45
121.27
119.42
119.30
119.18
117.21
117.04
116.70
116.53
99.20
98.22
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
51.26
51.00
50.75
50.49
50.24
15.18
15.16
15.07
15.05
F
F
F
H3C
NH
N
N
N
N
Cl
F
Compound 10
25000
20000
15000
10000
5000
0
f1 (ppm)
S8/147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7.50
7.49
7.48
7.47
7.26 CDCl3
7.26
7.09
7.07
7.05
7.04
7.03
6.15
6.13
4.76
1.40
1.38
F
F
F
H3C
NH
F
N
N
N
N
Cl
Compound 12
*signal from traces of residual solvent/grease
*
**
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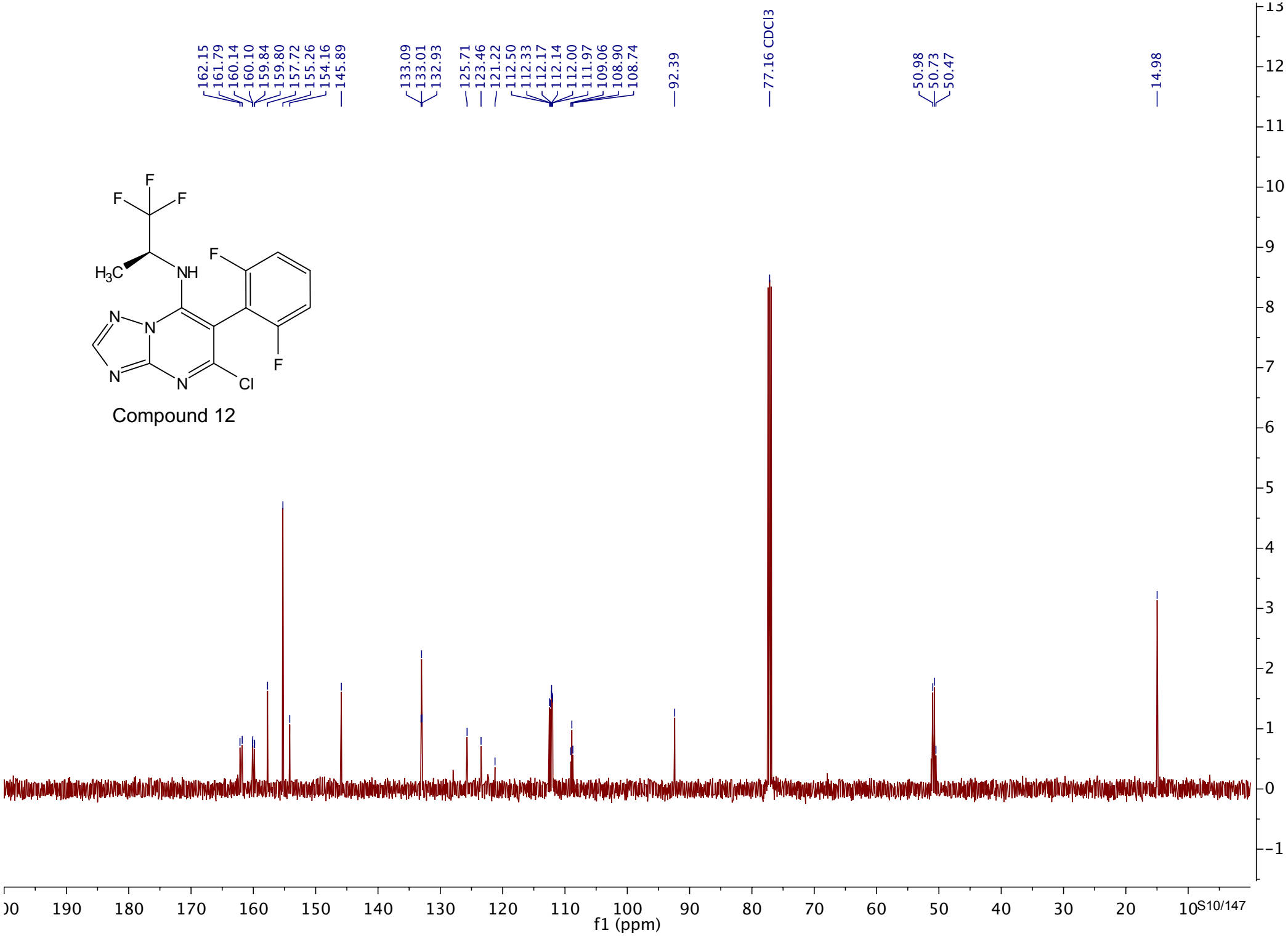
1.03
2.04
0.96
0.95
3.07
f1 (ppm)
S9/147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133.01
132.93
125.71
123.46
121.22
112.50
112.33
112.17
112.14
112.00
111.97
109.06
108.90
108.74
92.39
77.16 CDCl3
50.98
50.73
50.47
14.98
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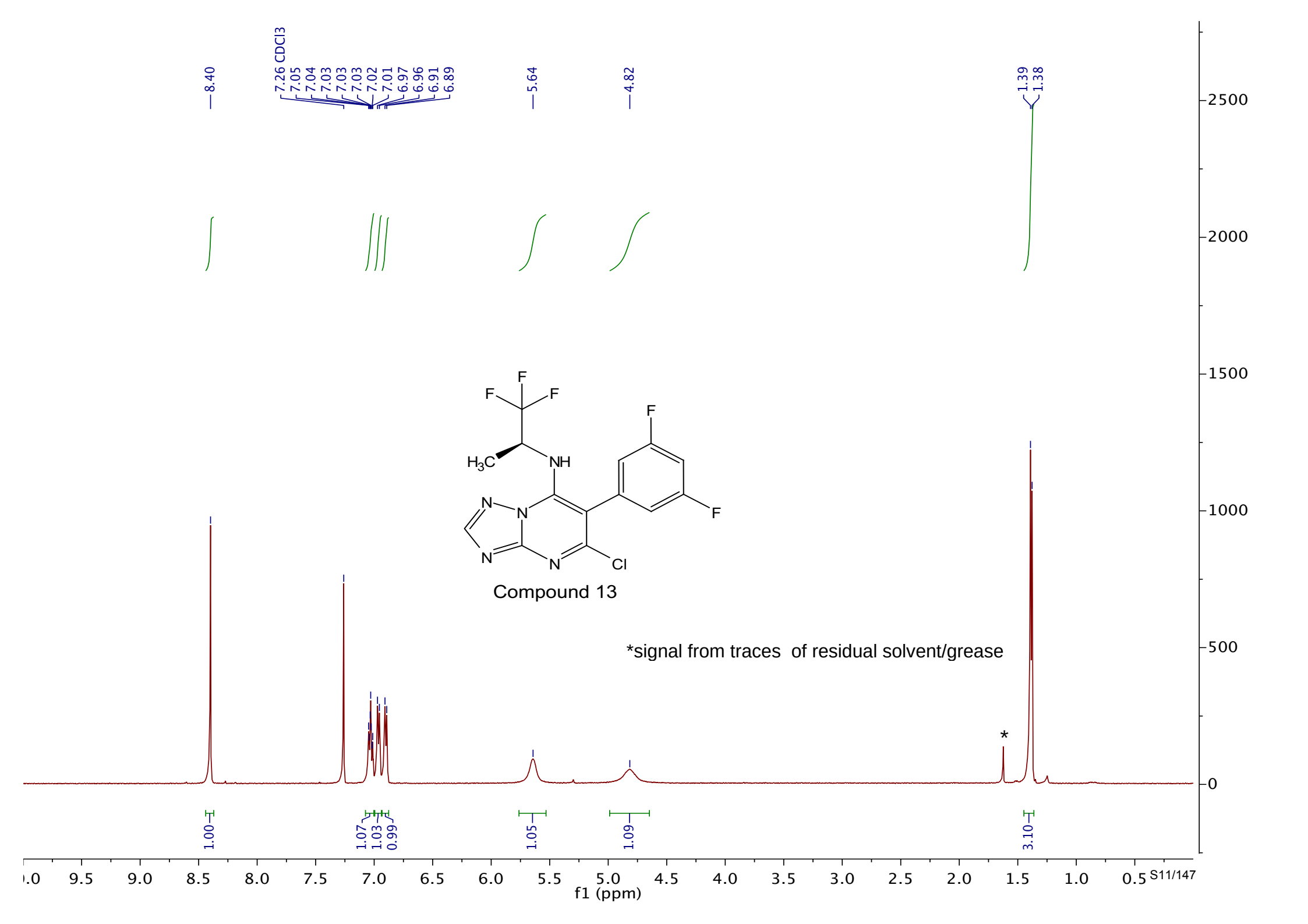
F
F
H3C
NH
F
N
N
N
N
Cl
F
Compound 12
f1 (ppm)
S10/147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7.26 CDCl3
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7.04
7.03
7.03
7.03
7.02
7.01
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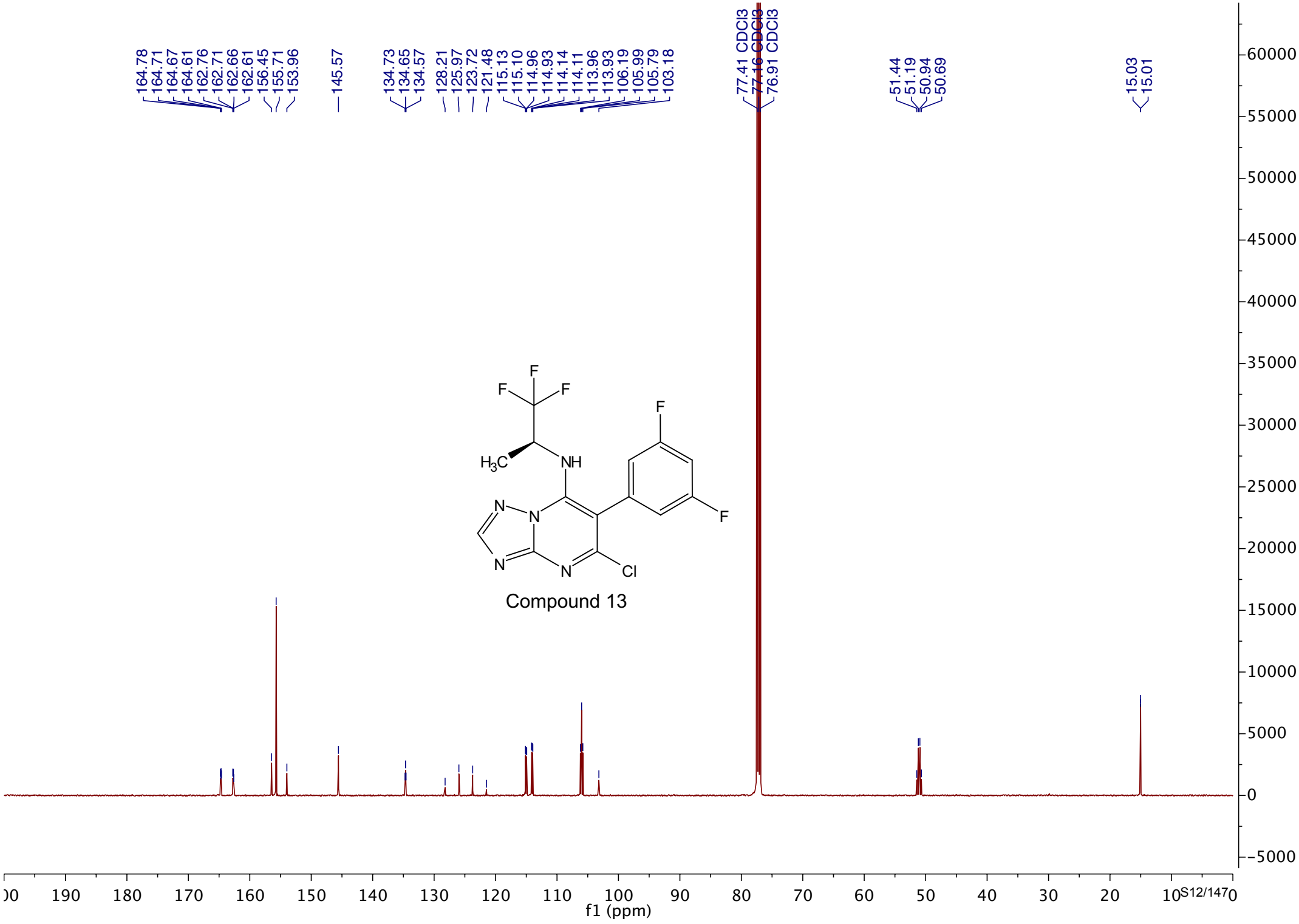
6.89
5.64
4.82
1.39
1.38
F
F
F
H3C
NH
N
N
N
N
Cl
F
F
Compound 13
*signal from traces of residual solvent/grease
*
1.00
1.07
1.03
0.99
1.05
1.09
3.10
2500
2000
1500
1000
500
0
f1 (ppm)
S11/147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162.61
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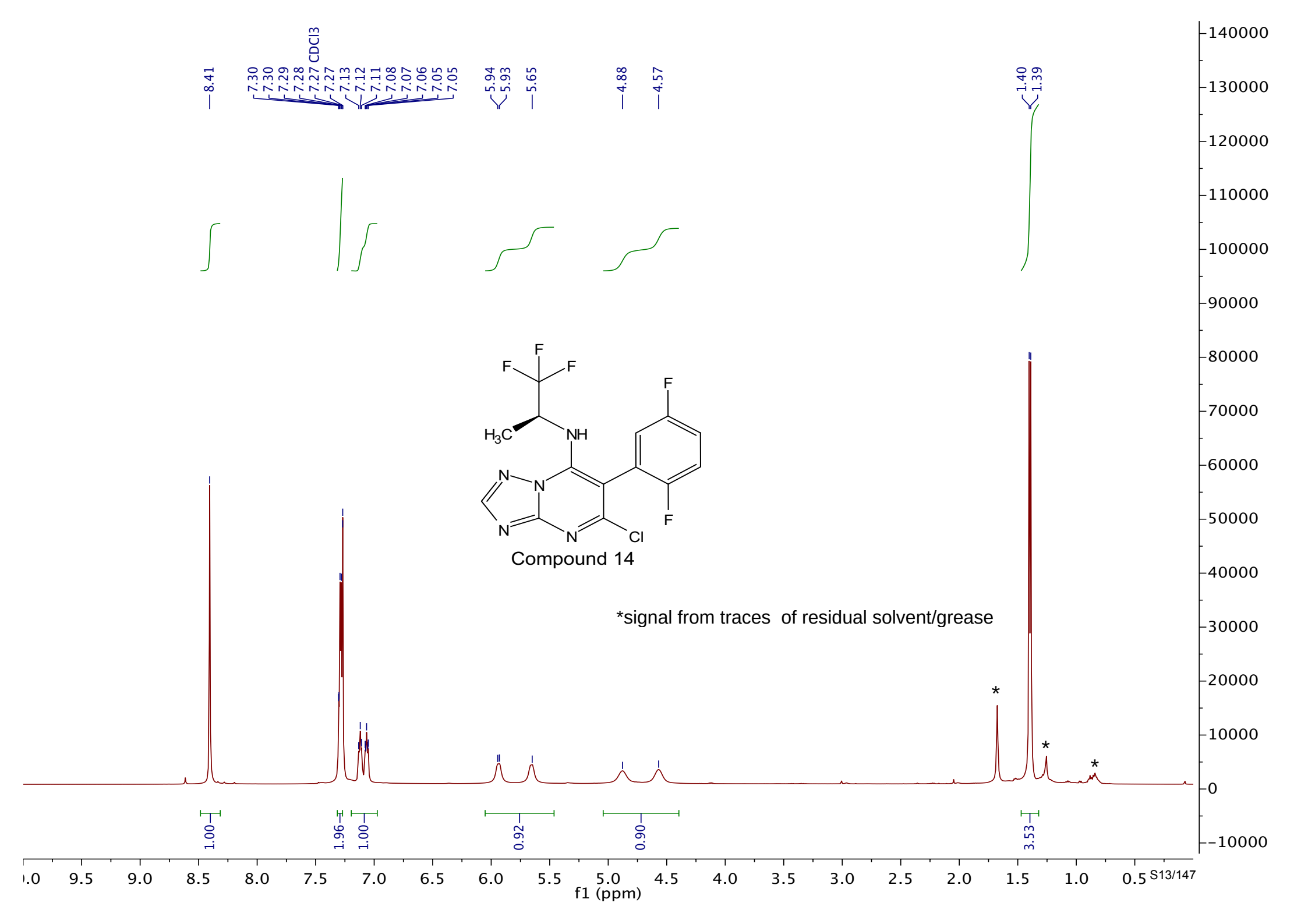
134.73
134.65
134.57
128.21
125.97
123.72
121.48
115.13
115.10
114.96
114.93
114.14
114.11
113.96
113.93
106.19
105.99
105.79
103.18
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
51.44
51.19
50.94
50.69
15.03
15.01
F
F
F
H3C
NH
N
N
N
N
F
F
Cl
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Compound 13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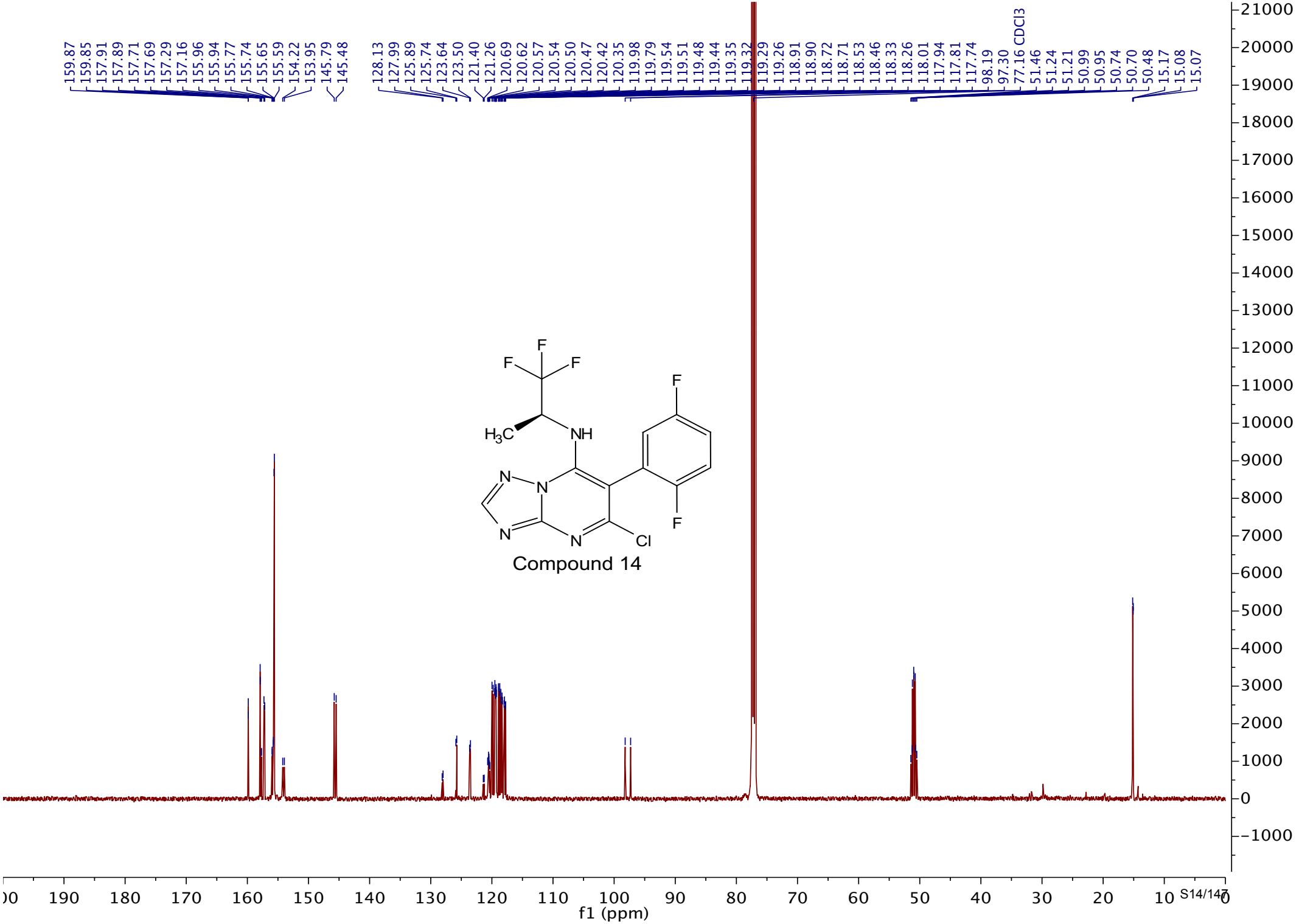
7.13
7.12
7.11
7.08
7.07
7.06
7.05
7.05
5.94
5.93
5.65
4.88
4.57
1.40
1.39
F
F
F
H3C
NH
F
N
N
N
N
Cl
F
Compound 14
*signal from traces of residual solvent/grease
*
*
*
1.00
1.96
1.00
0.92
0.90
3.53
f1 (ppm)
S13/147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155.59
154.22
153.95
145.79
145.48
128.13
127.99
125.89
125.74
123.64
123.50
121.40
121.26
120.69
120.62
120.57
120.54
120.50
120.47
120.42
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119.98
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119.26
118.91
118.90
118.72
118.71
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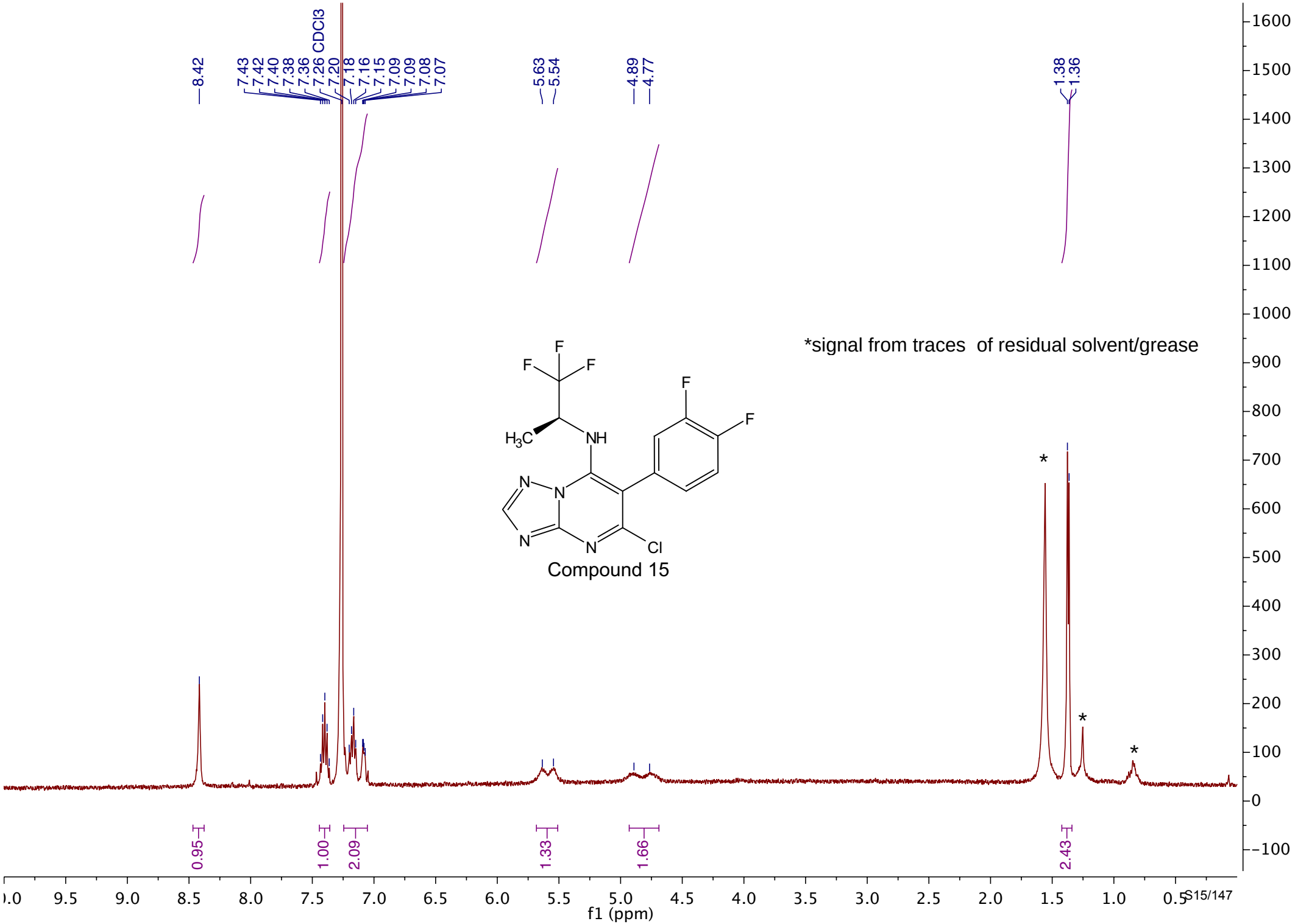
118.46
118.33
118.26
118.01
117.94
117.81
117.74
98.19
97.30
77.16 CDCl3
51.46
51.24
51.21
50.99
50.95
50.74
50.70
50.48
15.17
15.08
15.07
F
F
F
F
H3C
NH
N
N
N
N
Cl
F
Compound 14
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
S14/147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7.36
CDCl3
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7.20
7.18
7.16
7.15
7.09
7.09
7.08
7.07
5.63
5.54
4.89
4.77
1.38
1.36
*signal from traces of residual solvent/grease
Compound 15
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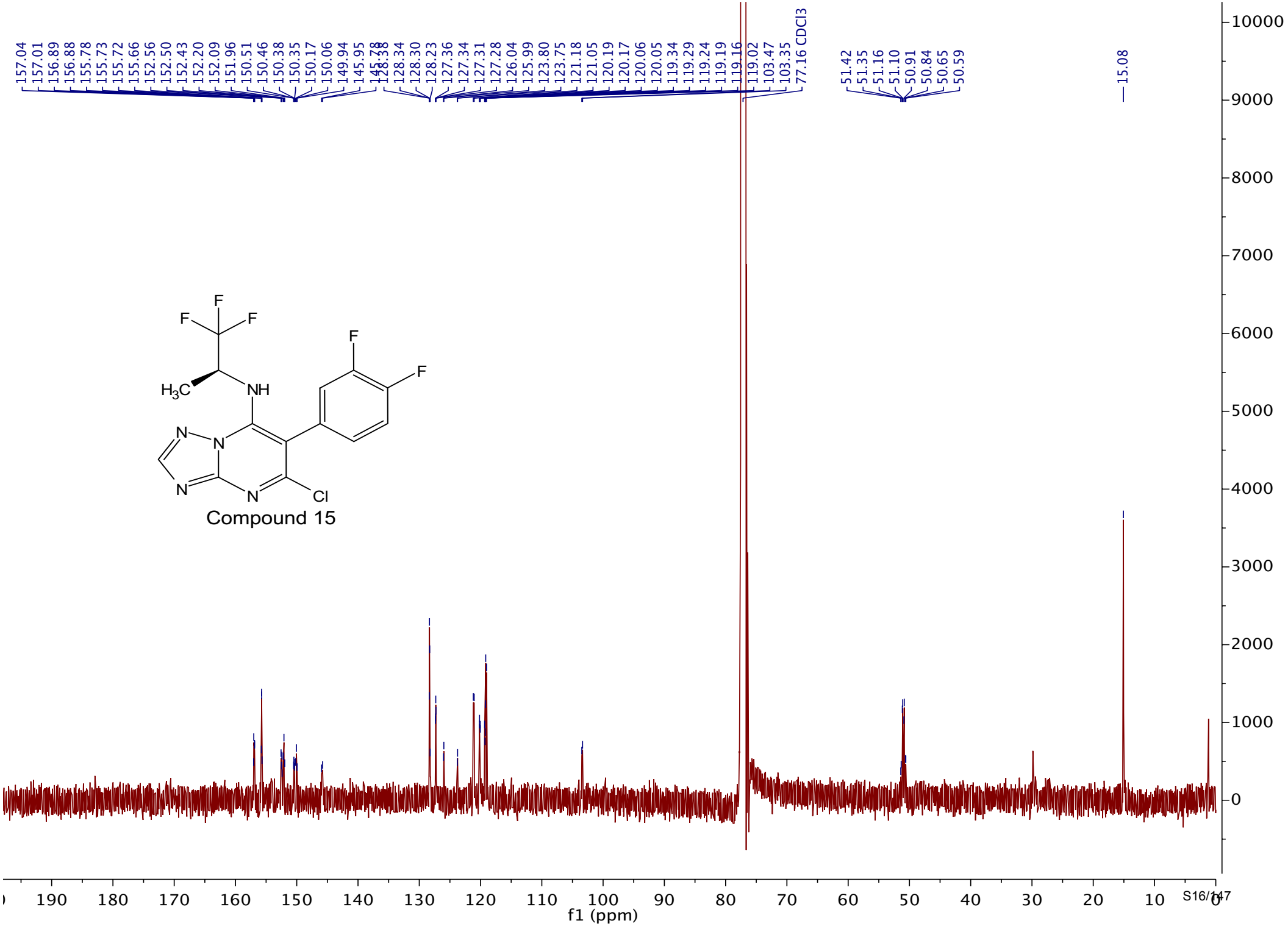
1.00
2.09
1.33
1.66
2.43
f1 (ppm)
S15/147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151.96
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145.95
128.34
128.30
128.23
127.36
127.34
127.31
127.28
126.04
125.99
123.80
123.75
121.18
121.05
120.19
120.17
120.06
120.05
119.34
119.29
119.24
119.19
119.16
119.02
103.47
103.35
77.16 CDCl3
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51.35
51.16
51.10
50.91
50.84
50.65
50.59
15.08
F
F
F
F
F
H3C
NH
N
N
N
N
Cl
Compound 15
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
190
180
170
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130
120
110
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70
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50
40
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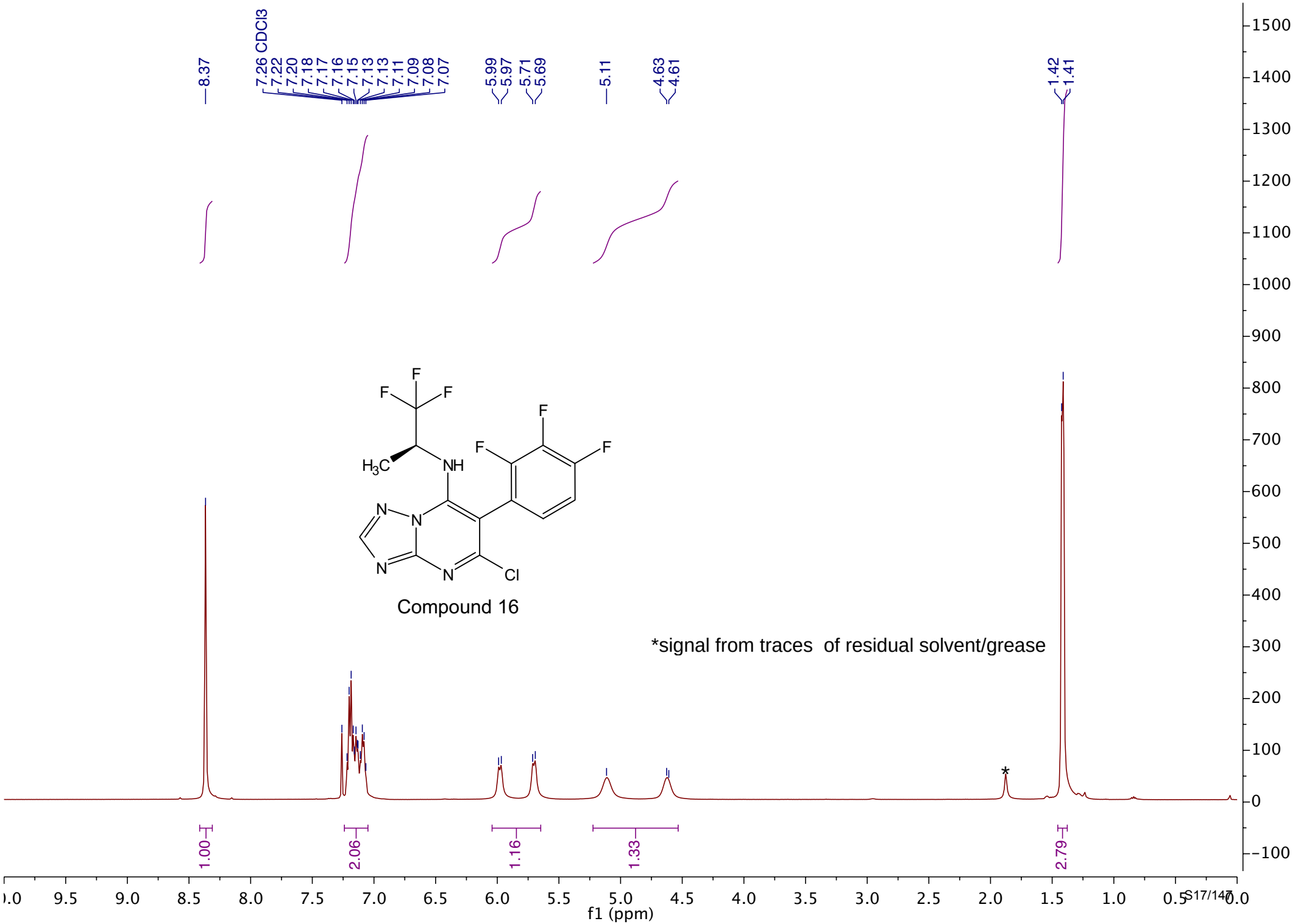
20
10
0
f1 (ppm)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7.11
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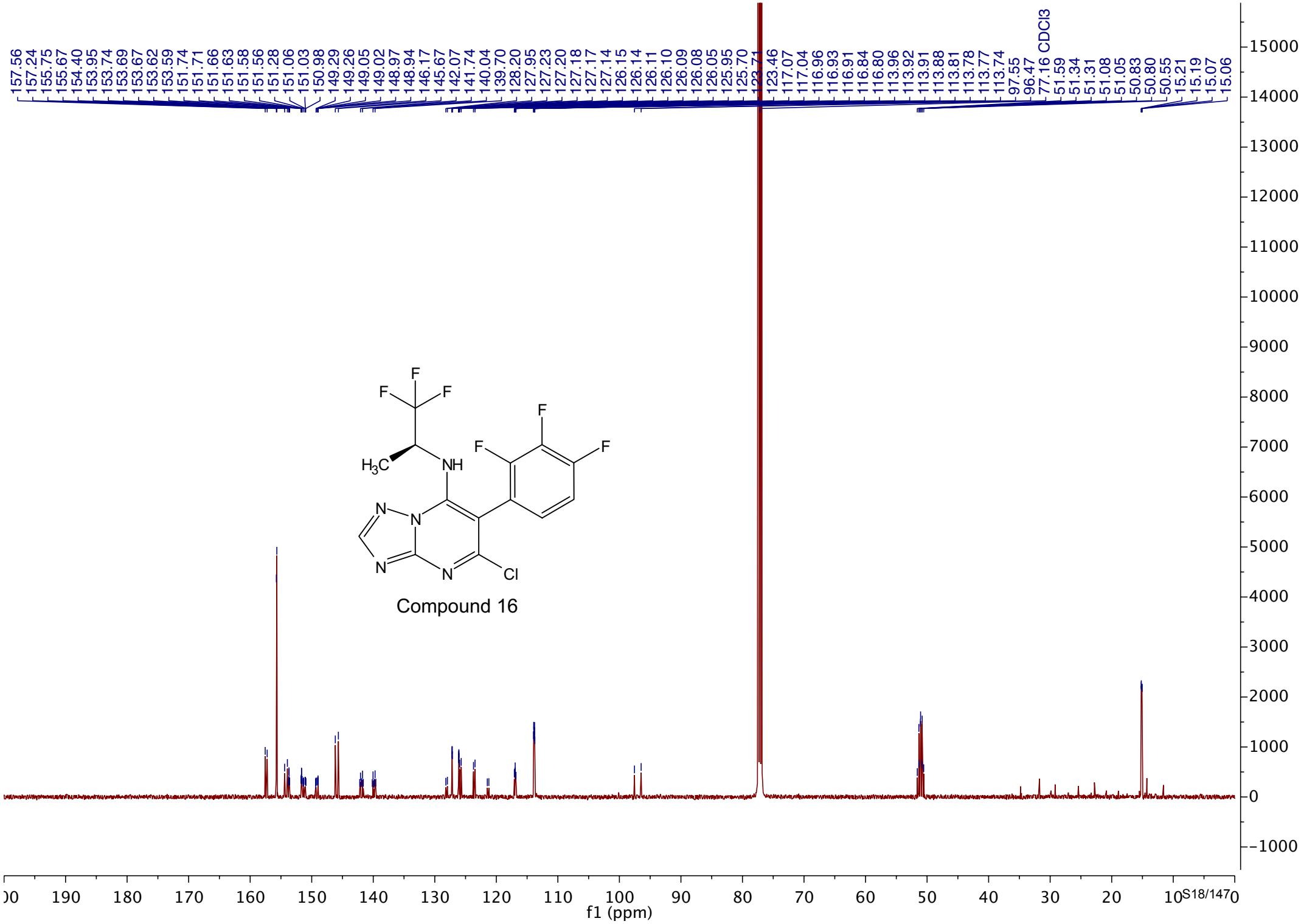
7.08
7.07
5.99
5.97
5.71
5.69
5.11
4.63
4.61
1.42
1.41
F
F
F
F
F
F
H3C
NH
N
N
N
N
Cl
Compound 16
*signal from traces of residual solvent/grease
1.00
2.06
1.16
1.33
2.79
f1 (ppm)
S17/147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153.95
153.74
153.69
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153.62
153.59
151.74
151.71
151.66
151.63
151.58
151.56
151.28
151.06
151.03
150.98
149.29
149.26
149.05
149.02
148.97
148.94
146.17
145.67
142.07
141.74
140.04
139.70
128.20
127.95
127.23
127.20
127.18
127.17
127.14
126.15
126.14
126.11
126.10
126.09
126.08
126.05
125.95
125.70
123.71
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117.07
117.04
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15.21
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15.06
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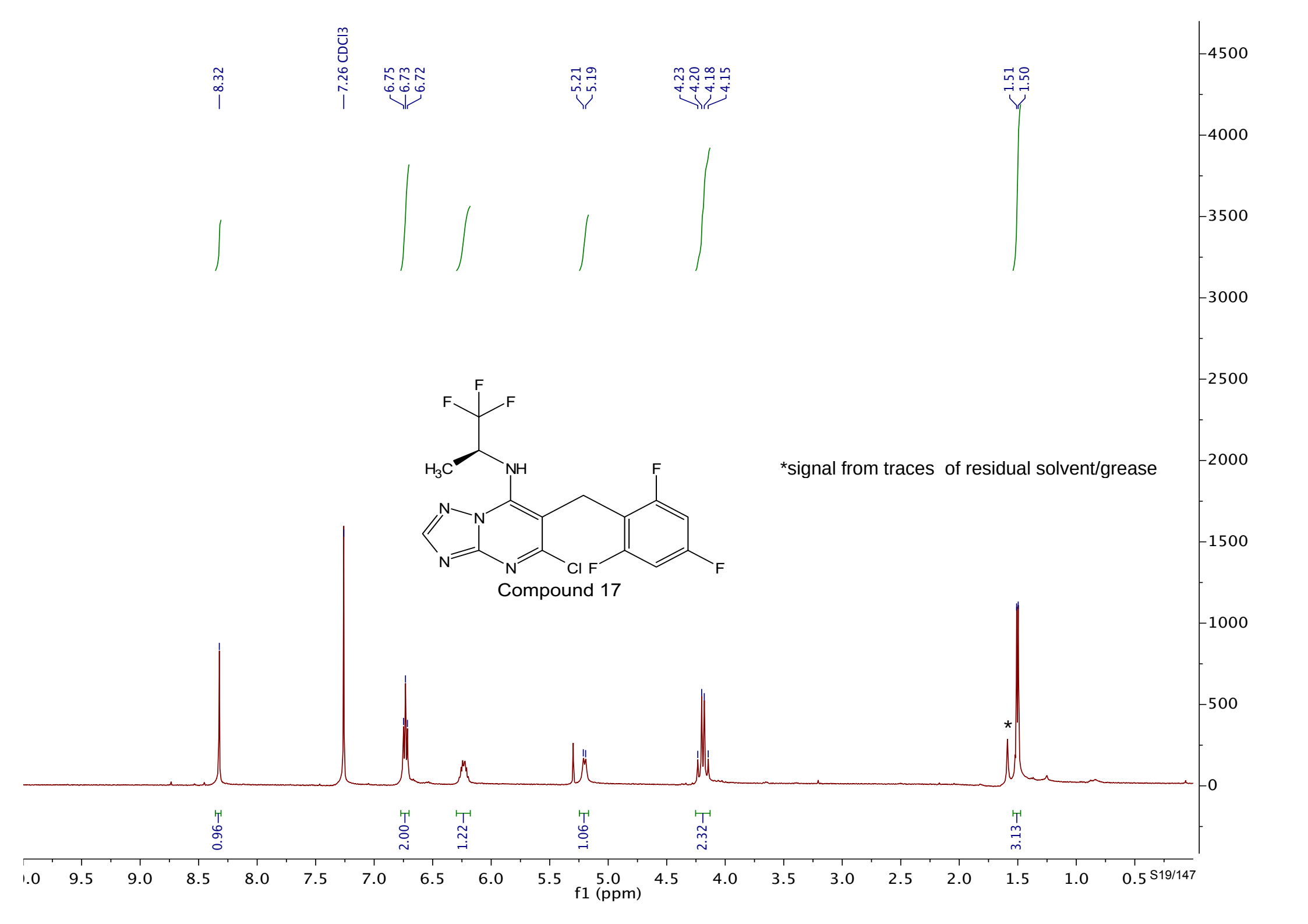
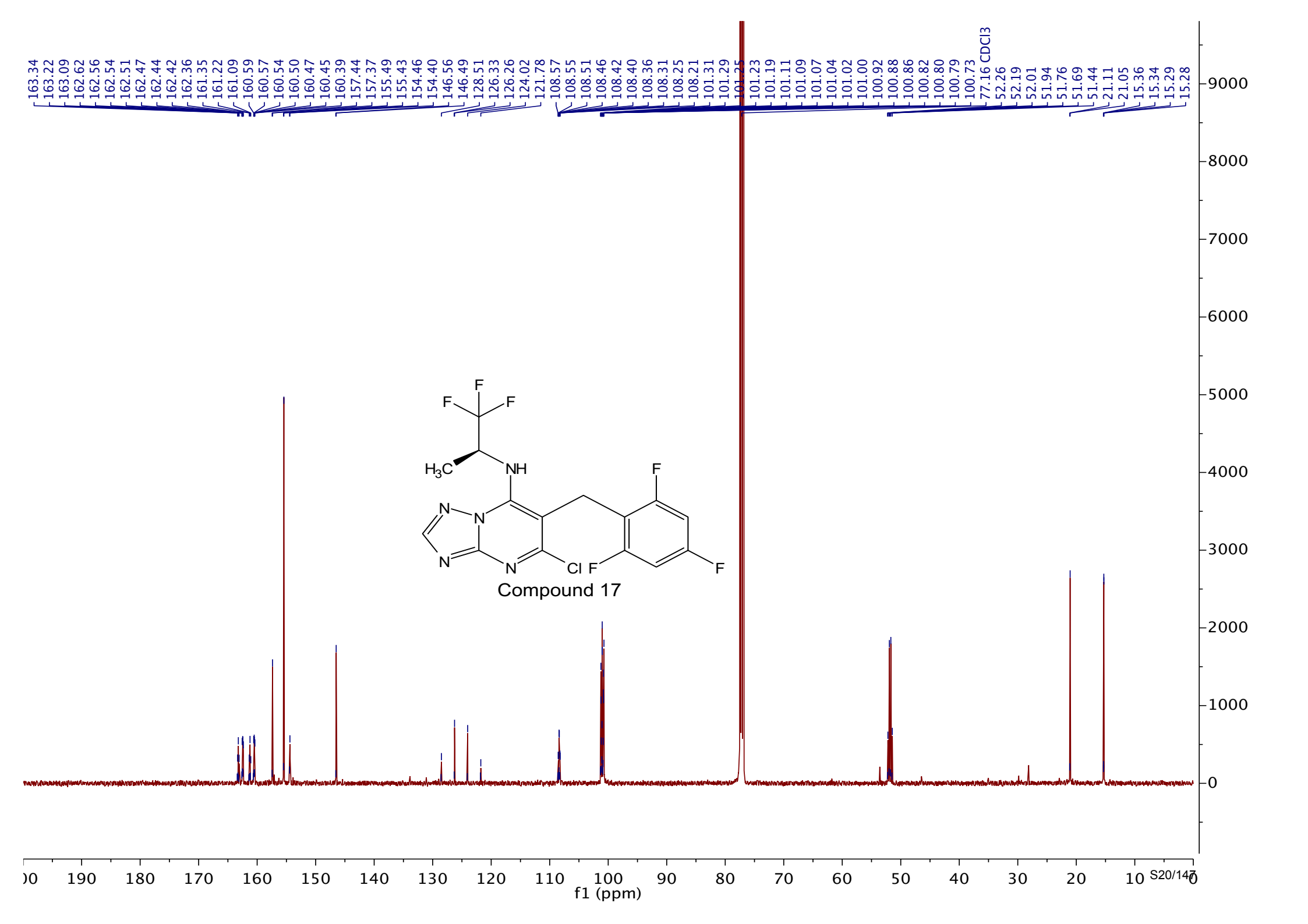
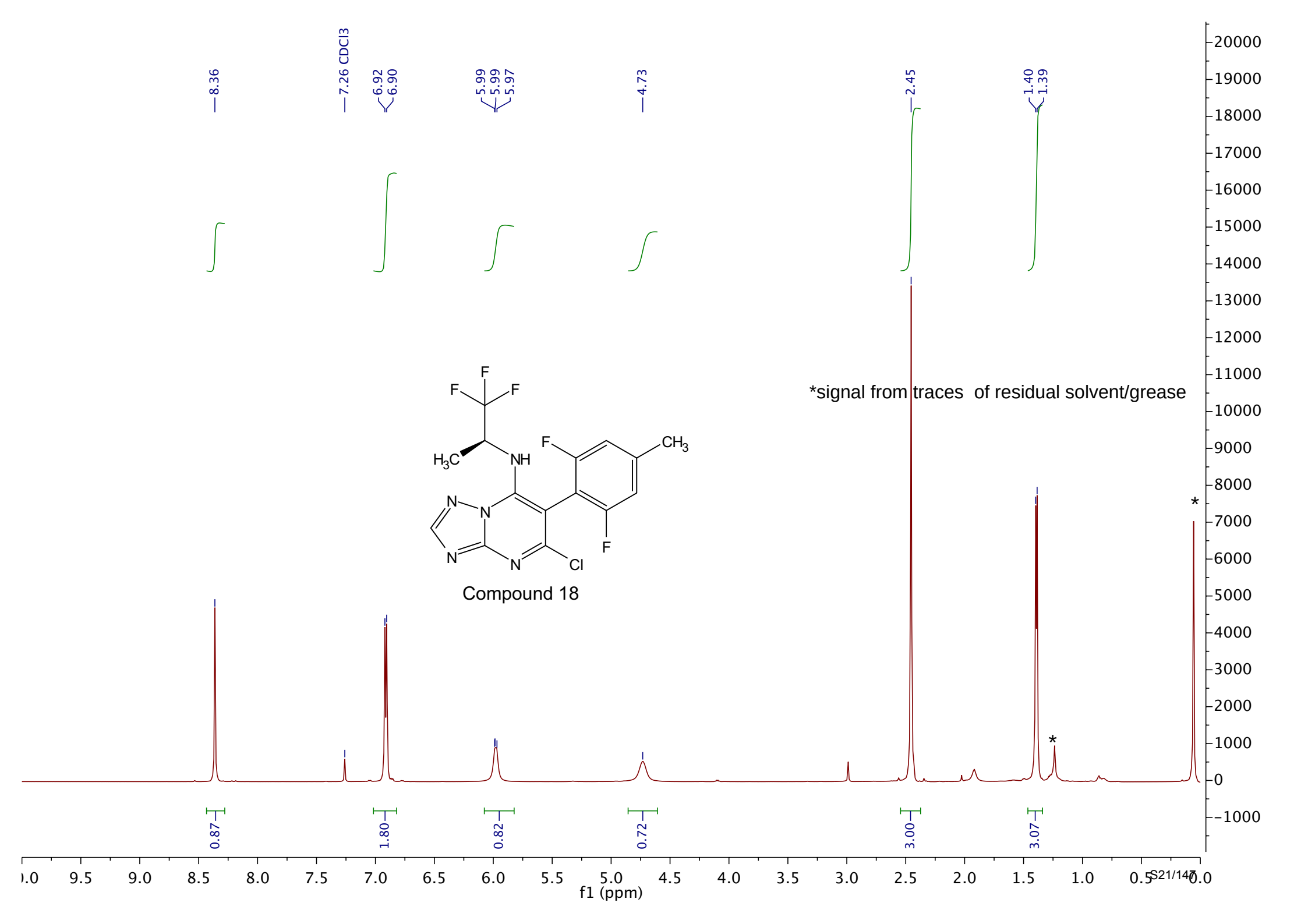
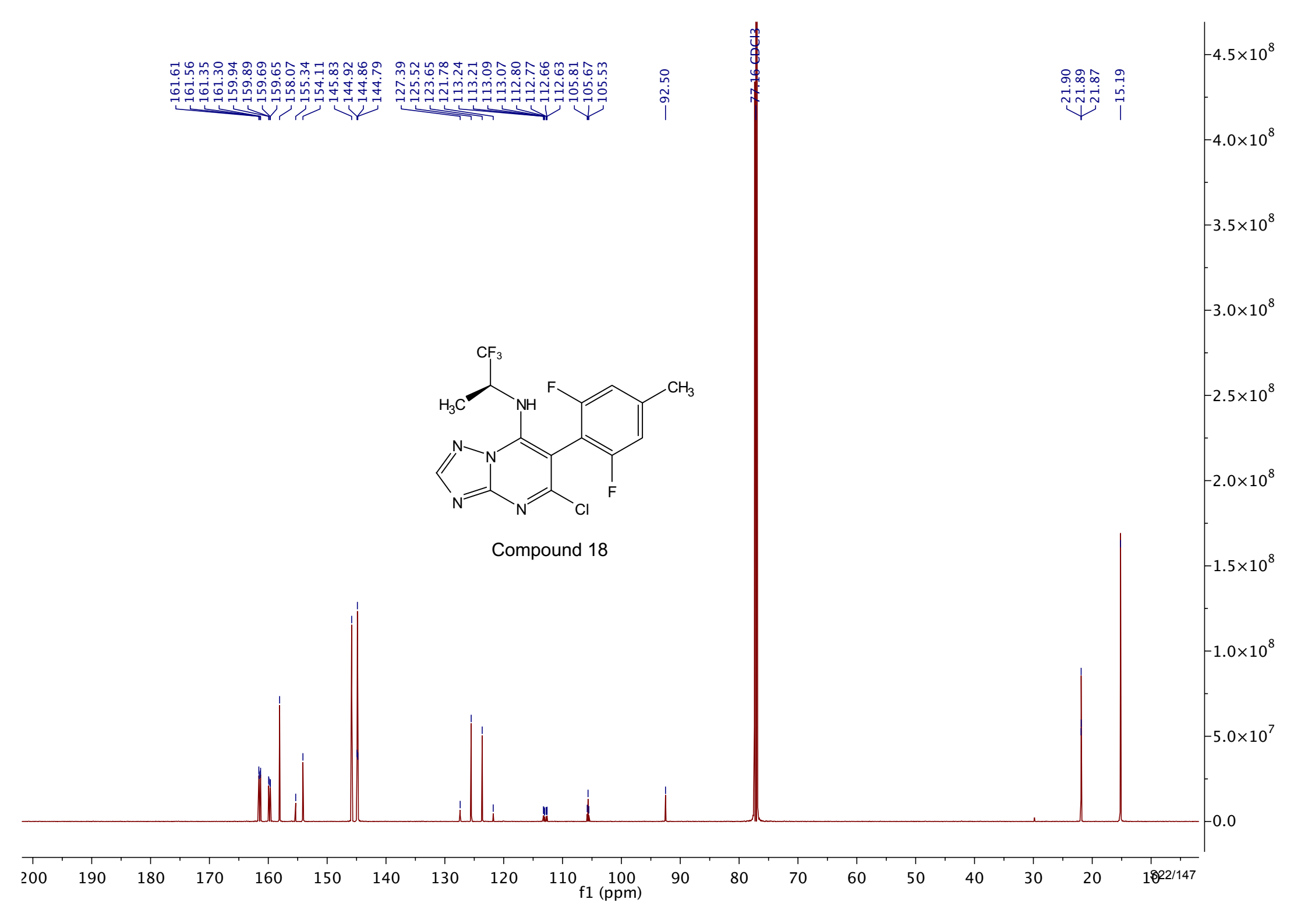
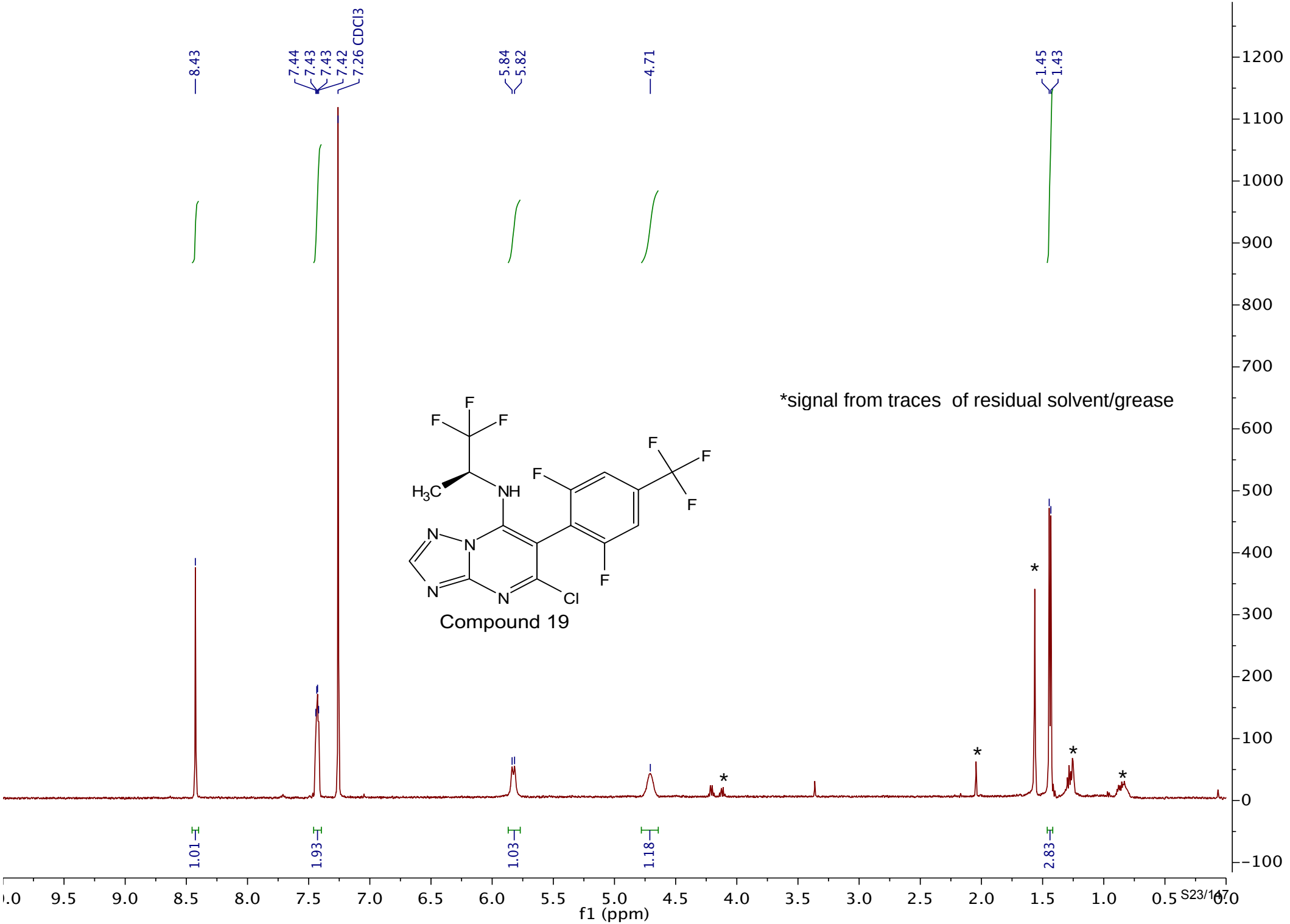
H3C
NH
F
F
N
N
N
N
Cl
Compound 16
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

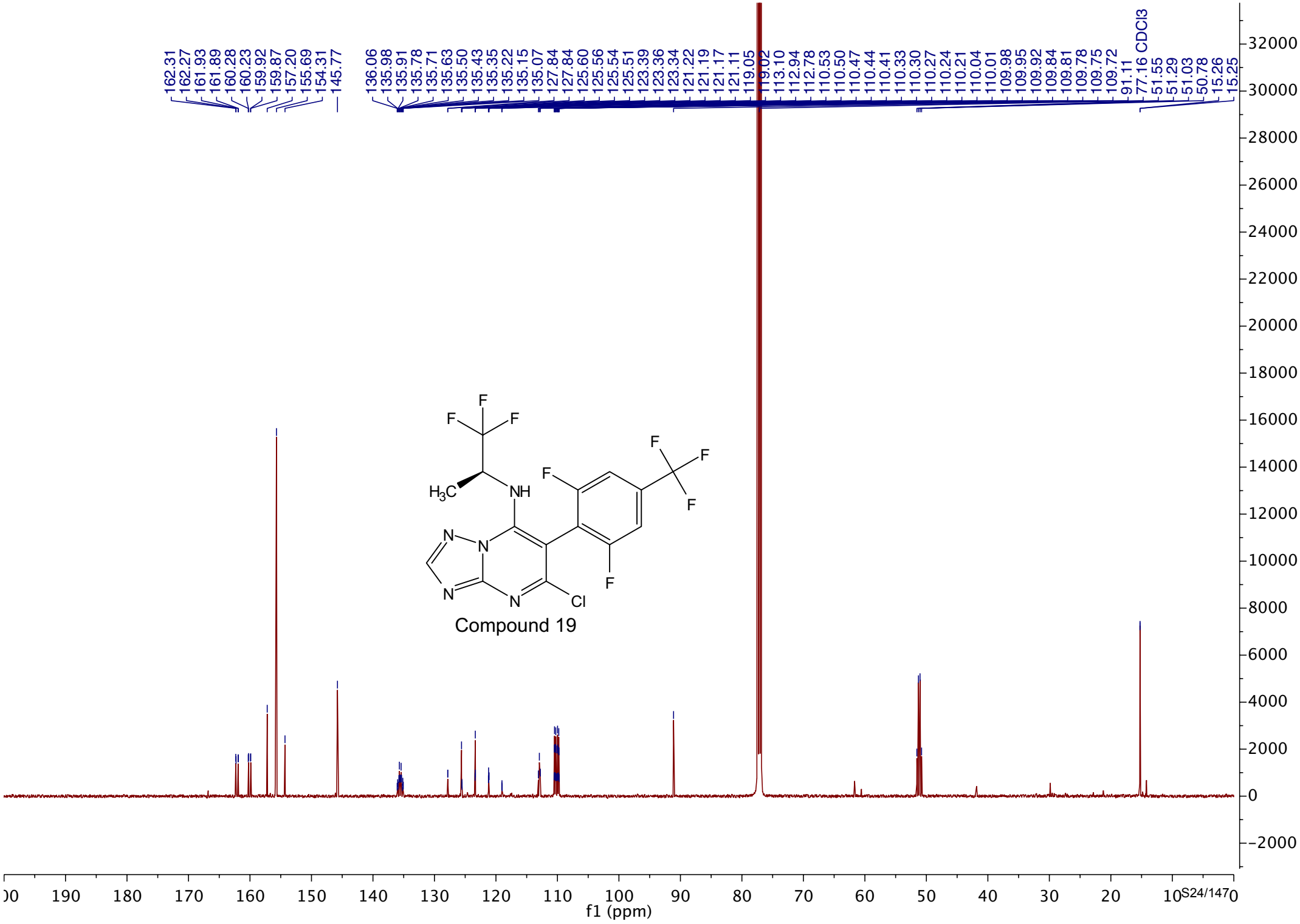

8.32
7.26 CDCl3
6.75
6.73
6.72
5.21
5.19
4.23
4.20
4.18
4.15
1.51
1.50
F
F
F
H3C
NH
F
N
N
N
N
Cl F
F
Compound 17
*signal from traces of residual solvent/grease
*
0.96
2.00
1.22
1.06
2.32
3.13
f1 (ppm)
S19/147

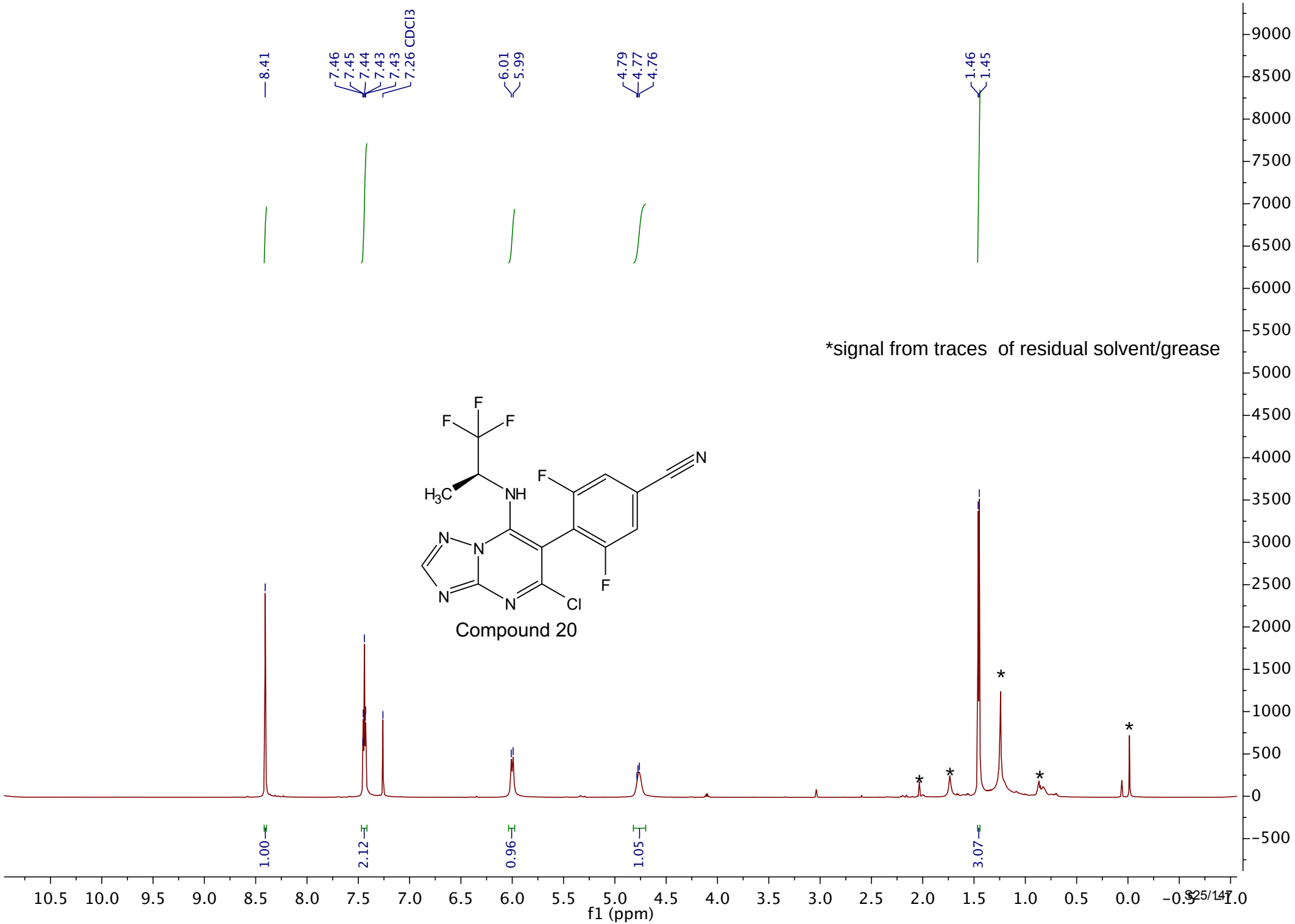

163.34
163.22
163.09
162.62
162.56
162.54
162.51
162.47
162.44
162.42
162.36
161.35
161.22
161.09
160.59
160.57
160.54
160.50
160.47
160.45
160.39
157.44
157.37
155.49
155.43
154.46
154.40
146.56
146.49
128.51
126.33
126.26
124.02
121.78
108.57
108.55
108.51
108.46
108.42
108.40
108.36
108.31
108.25
108.21
101.31
101.29
101.25
101.23
101.19
101.11
101.09
101.07
101.04
101.02
101.00
100.92
100.88
100.86
100.82
100.80
100.79
100.73
77.16 CDCl3
52.26
52.19
52.01
51.94
51.76
51.69
51.44
21.11
21.05
15.36
15.34
15.29
15.28
F
F
F
H3C
NH
F
N
N
N
N
Cl
F
F
Compound 17
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
S20/147

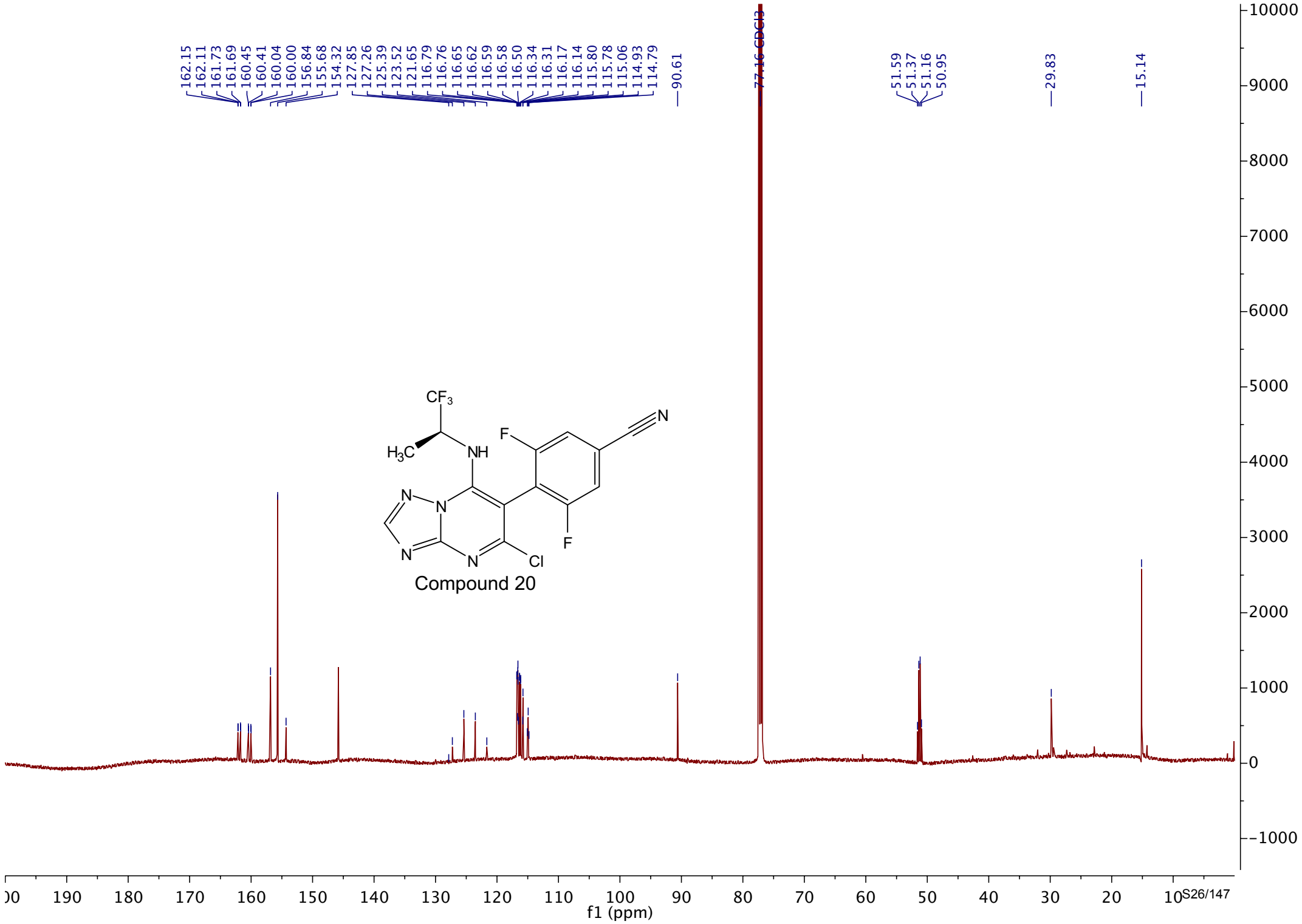

8.36
7.26 CDCl3
6.92
6.90
5.99
5.99
5.97
4.73
2.45
1.40
1.39
F
F
F
H3C
NH
F
CH3
N
N
N
N
Cl
F
Compound 18
*signal from traces of residual solvent/grease
*
*
0.87
1.80
0.82
0.72
3.00
3.07
f1 (ppm)
S21/147

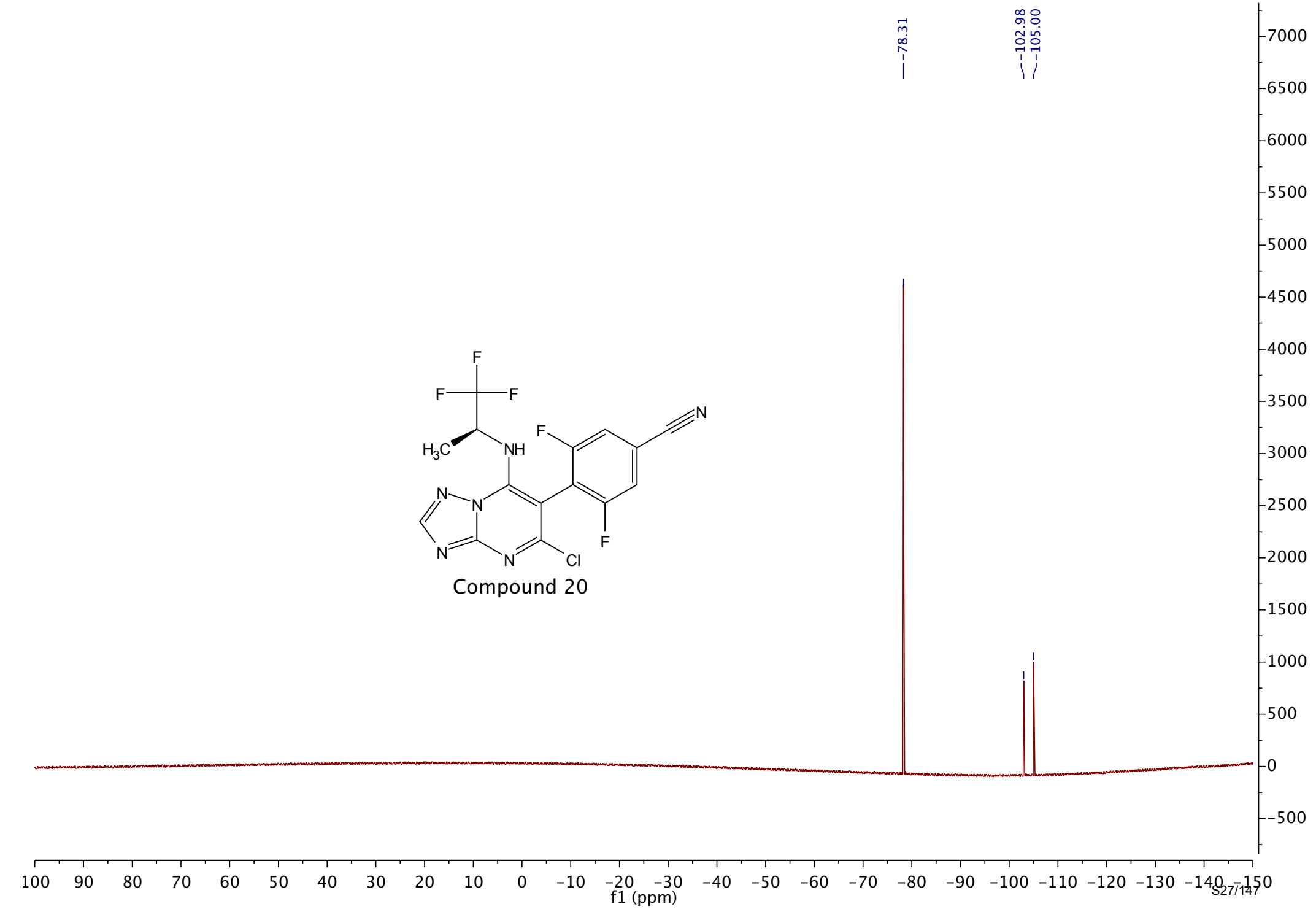

161.61
161.56
161.35
161.30
159.94
159.89
159.69
159.65
158.07
155.34
154.11
145.83
144.92
144.86
144.79
127.39
125.52
123.65
121.78
113.24
113.21
113.09
113.07
112.80
112.77
112.66
112.63
105.81
105.67
105.53
92.50
77.16 CDCl3
21.90
21.89
21.87
15.19
CF3
H3C
NH
F
CH3
N
N
N
N
Cl
F
Compound 18
4.5×10^8
4.0×10^8
3.5×10^8
3.0×10^8
2.5×10^8
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0.0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.43
7.44
7.43
7.43
7.42
7.26 CDCl3
5.84
5.82
4.71
1.45
1.43
1.01
1.93
1.03
1.18
2.83
f1 (ppm)
*signal from traces of residual solvent/grease
Compound 19

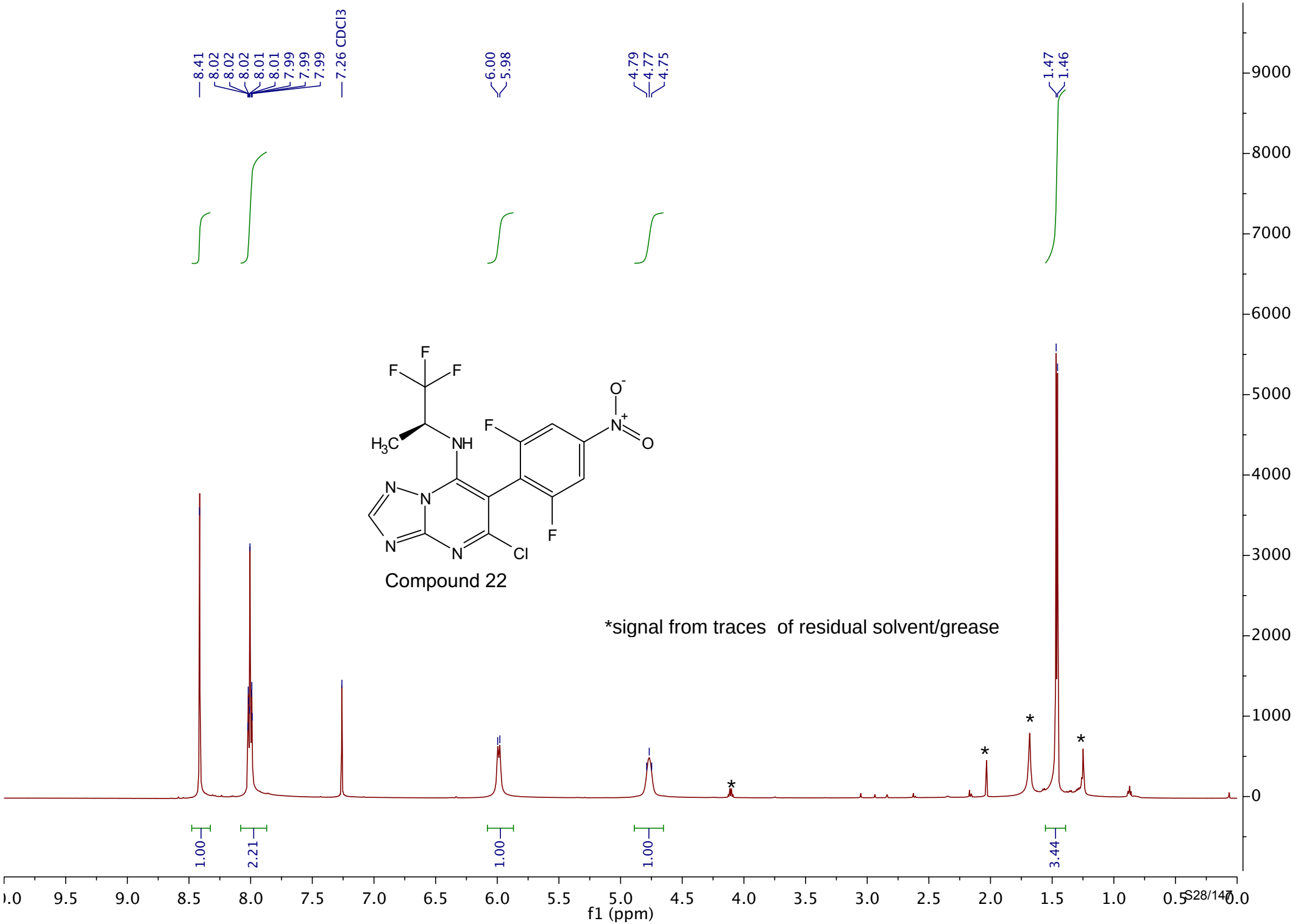

162.31
162.27
161.93
161.89
160.28
160.23
159.92
159.87
157.20
155.69
154.31
145.77
136.06
135.98
135.91
135.78
135.71
135.63
135.50
135.43
135.35
135.22
135.15
135.07
127.84
127.84
125.60
125.56
125.54
125.51
123.39
123.36
123.34
121.22
121.19
121.17
121.11
119.05
119.02
113.10
112.94
112.78
110.53
110.50
110.47
110.44
110.41
110.33
110.30
110.27
110.24
110.21
110.04
110.01
109.98
109.95
109.92
109.84
109.81
109.78
109.75
109.72
91.11
77.16 CDCl3
51.55
51.29
51.03
50.78
15.26
15.25
F
F
F
H3C
NH
F
F
F
F
N
N
N
N
Cl
Compound 19
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

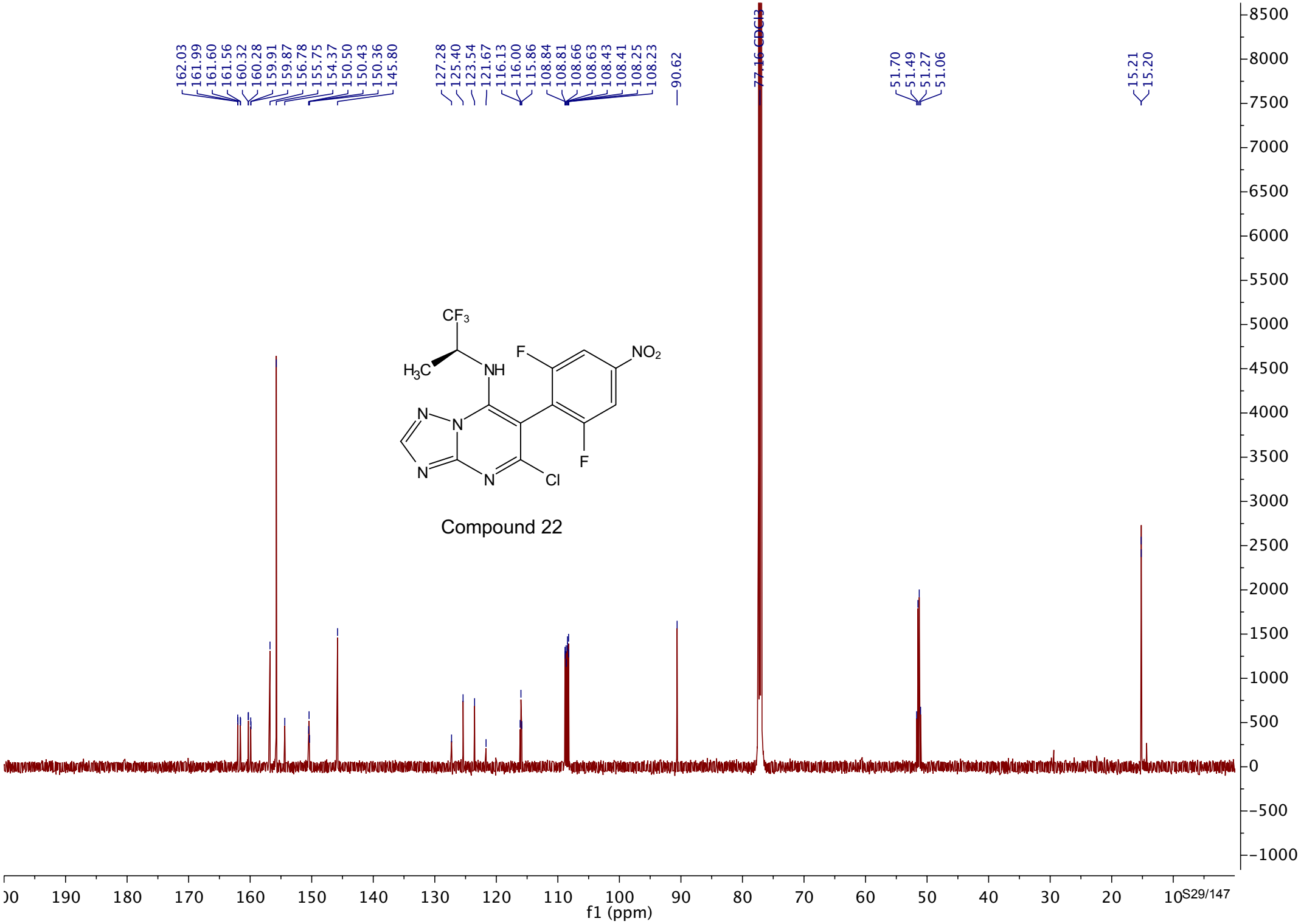

8.41
7.46
7.45
7.44
7.43
7.43
7.26 CDCl3
6.01
5.99
4.79
4.77
4.76
1.46
1.45
*signal from traces of residual solvent/grease
F
F
F
H3C
NH
F
N
N
N
N
N
Cl
F
Compound 20
1.00
2.12
0.96
1.05
3.07
f1 (ppm)

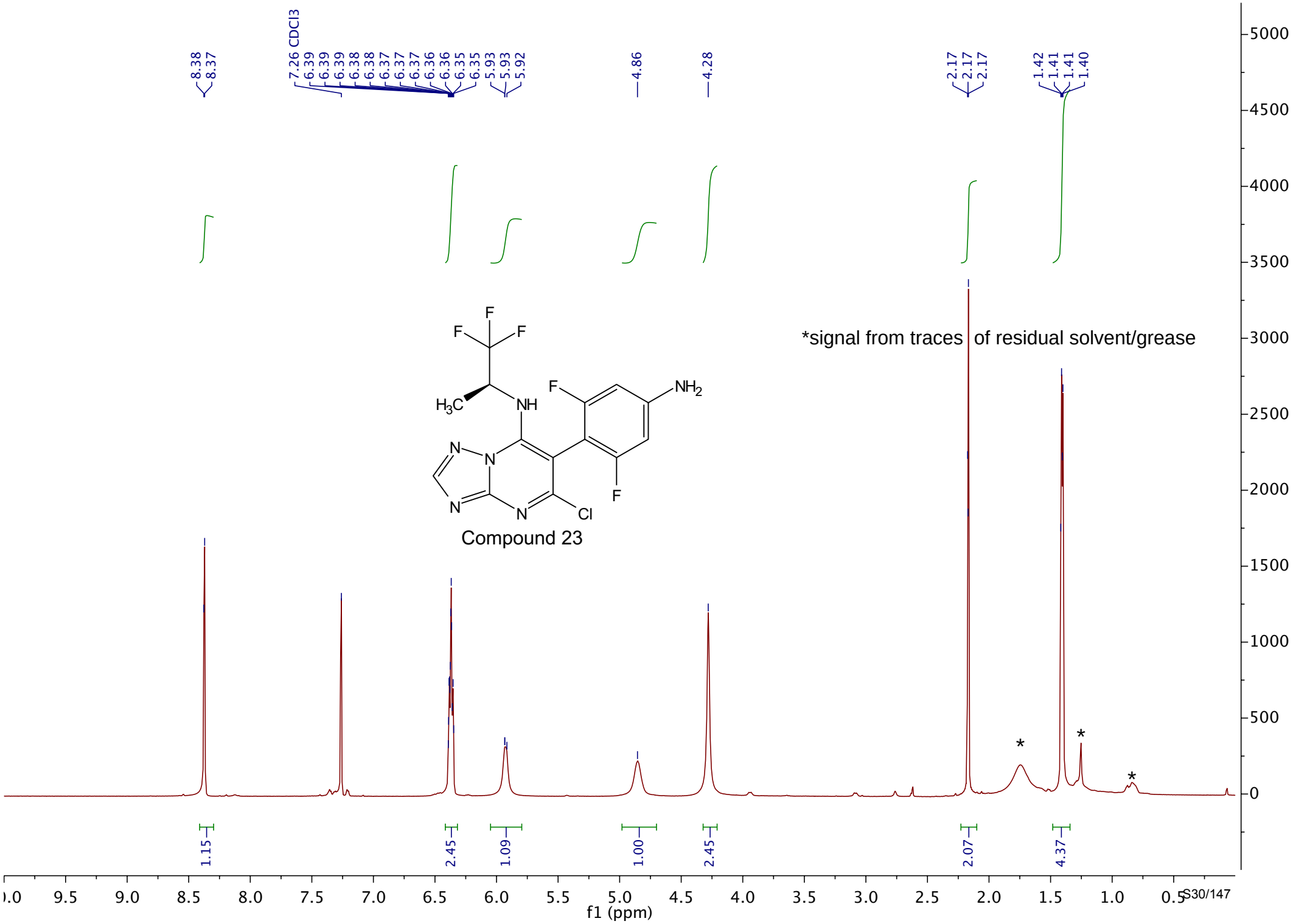

162.15
162.11
161.73
161.69
160.45
160.41
160.04
160.00
156.84
155.68
154.32
127.85
127.26
125.39
123.52
121.65
116.79
116.76
116.65
116.62
116.59
116.58
116.50
116.34
116.31
116.17
116.14
115.80
115.78
115.06
114.93
114.79
90.61
77.16 CDCl3
51.59
51.37
51.16
50.95
29.83
15.14
CF3
H3C
NH
F
N
N
N
N
Cl
F
N
Compound 20
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
f1 (ppm)
S26/147

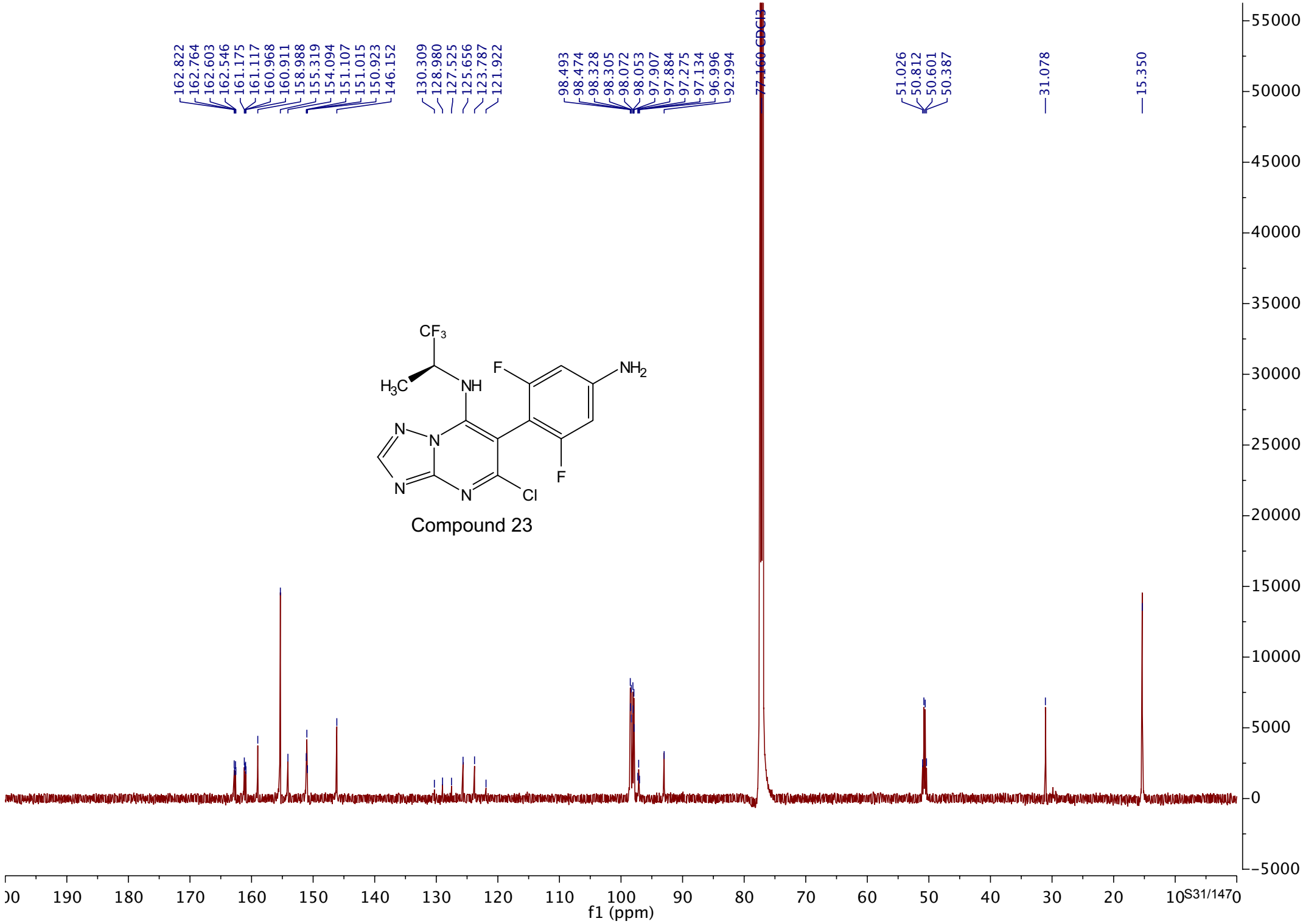

-78.31
-102.98
-105.00
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)
F
F
F
H3C
NH
N
N
N
N
Cl
F
F
N

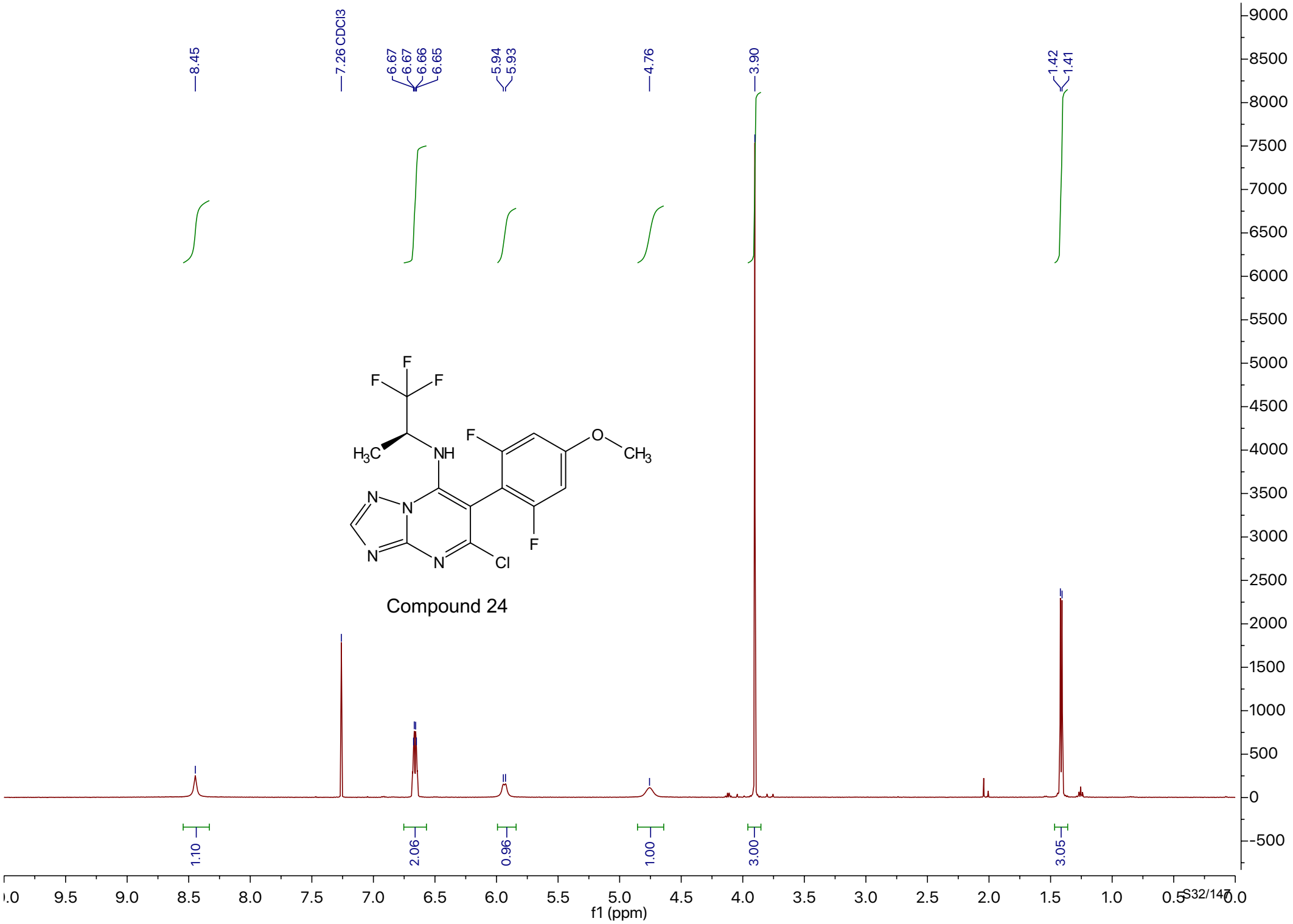
Compound 20

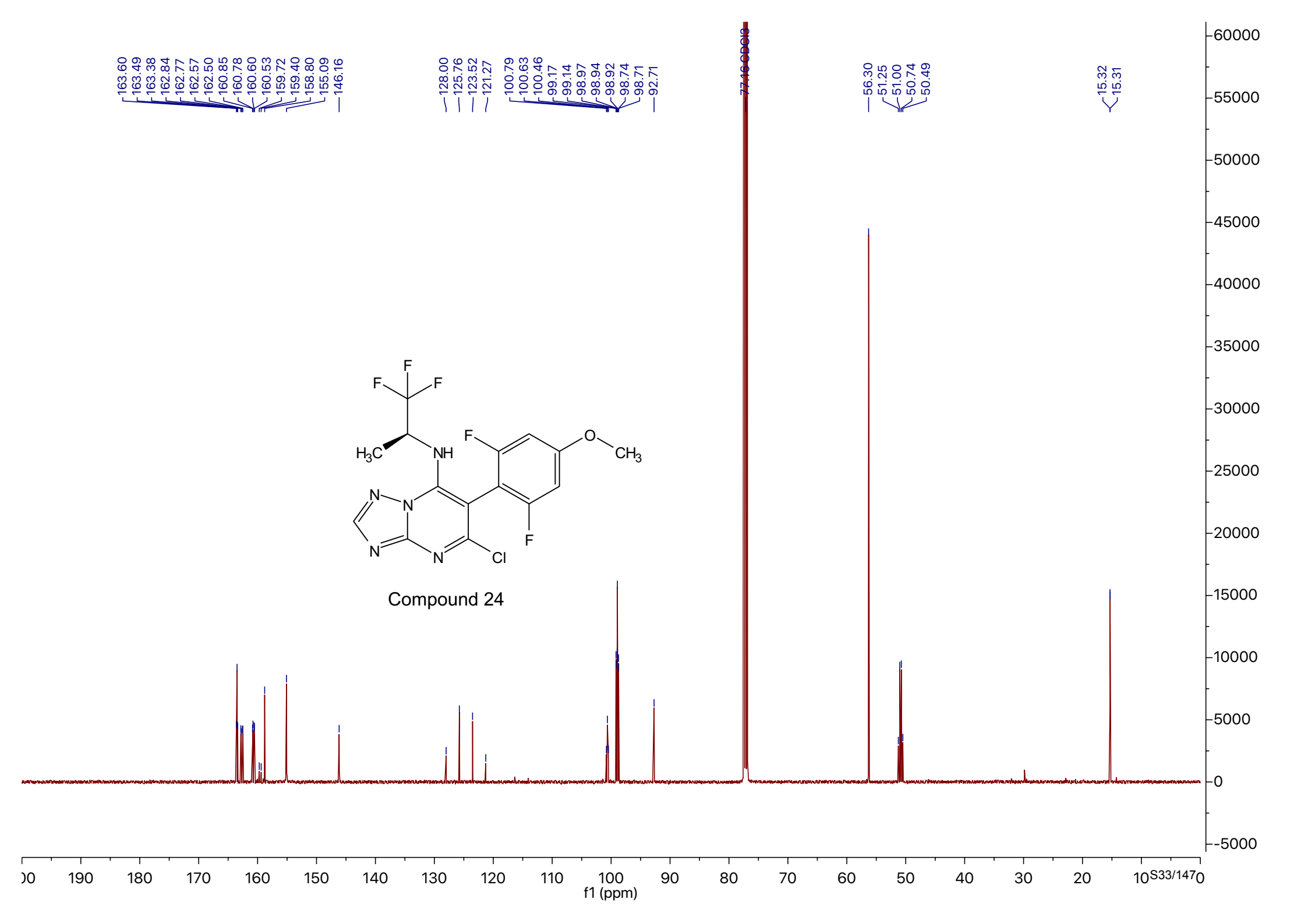

8.41
8.02
8.02
8.02
8.01
8.01
7.99
7.99
7.99
7.26 CDCl3
6.00
5.98
4.79
4.77
4.75
1.47
1.46
F
F
F
H3C
NH
F
O-
N+
O
N
N
N
N
Cl
F
Compound 22
*signal from traces of residual solvent/grease
1.00
2.21
1.00
1.00
3.44
f1 (ppm)

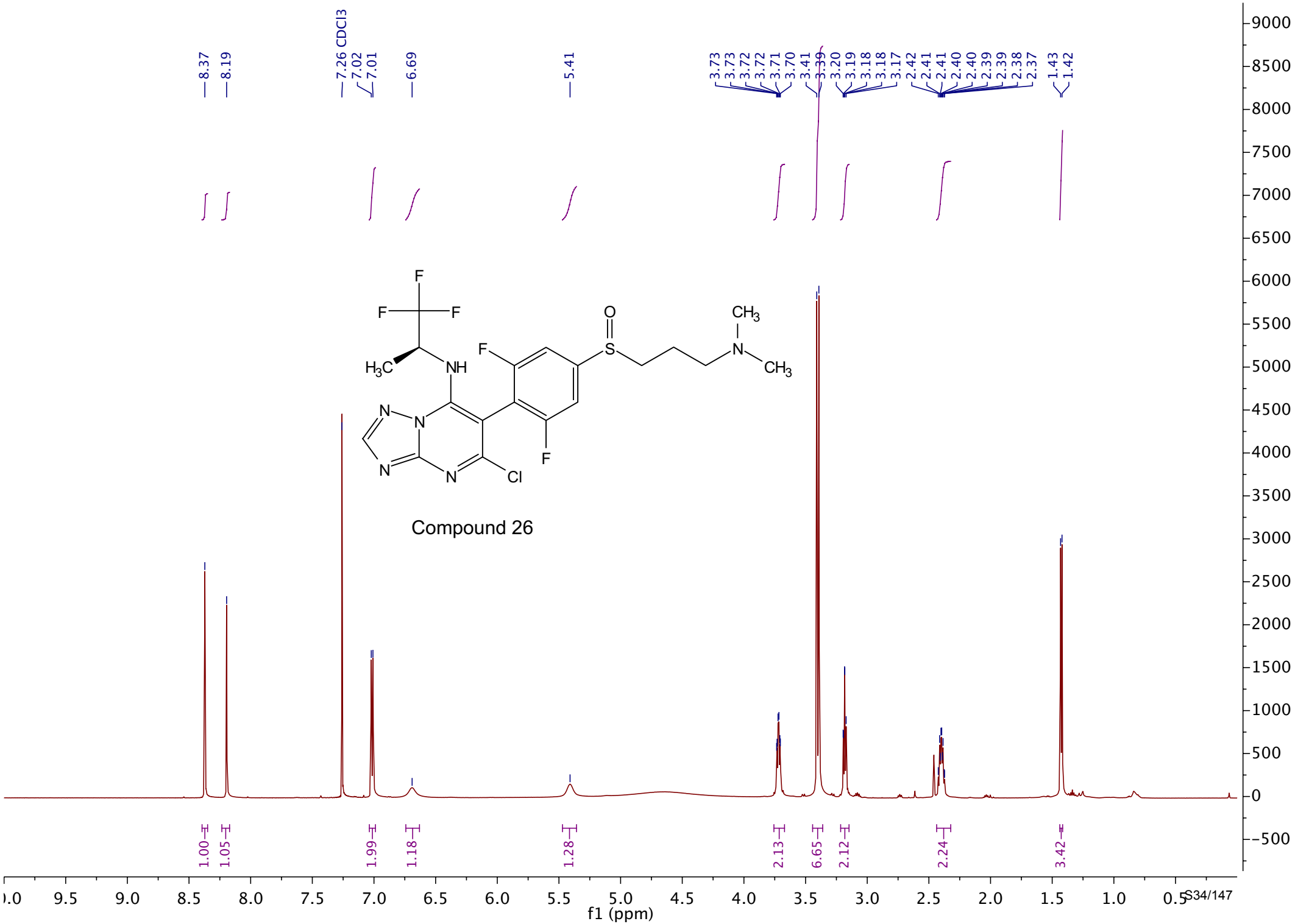

162.03
161.99
161.60
161.56
160.32
160.28
159.91
159.87
156.78
155.75
154.37
150.50
150.43
150.36
145.80
127.28
125.40
123.54
121.67
116.13
116.00
115.86
108.84
108.81
108.66
108.63
108.43
108.41
108.25
108.23
90.62
77.16 CDCl3
51.70
51.49
51.27
51.06
15.21
15.20
CF3
H3C
NH
F
NO2
N
N
N
N
Cl
F
Compound 22
f1 (ppm)
S29/147

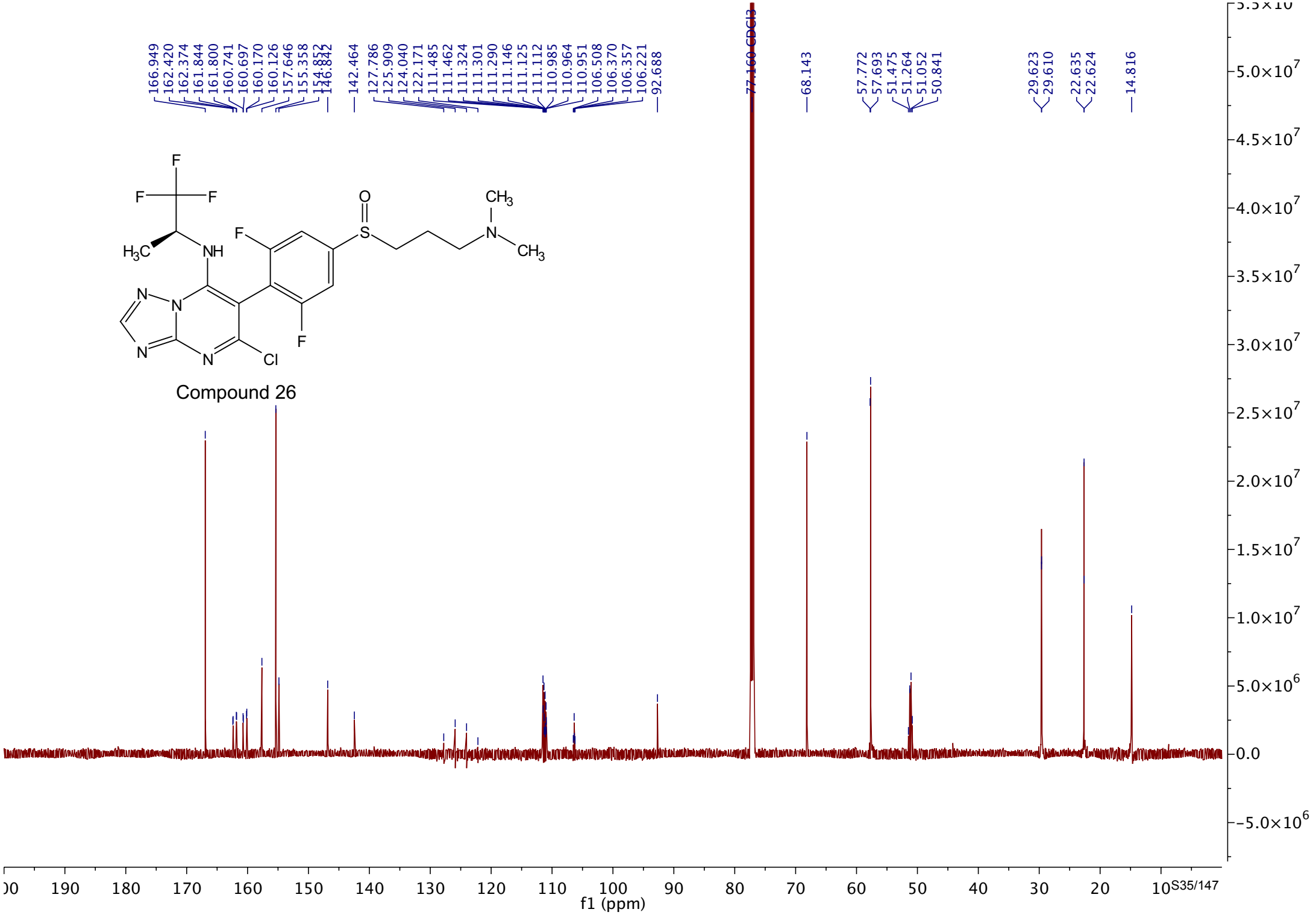

7.26 CDCl3
8.38
8.37
6.39
6.39
6.39
6.38
6.38
6.37
6.37
6.37
6.36
6.36
6.35
6.35
5.93
5.93
5.92
4.86
4.28
2.17
2.17
2.17
1.42
1.41
1.41
1.40
F
F
F
H3C
NH
F
NH2
N
N
N
N
Cl
F
Compound 23
*signal from traces of residual solvent/grease
1.15
2.45
1.09
1.00
2.45
2.07
4.37
f1 (ppm)


162.822
162.764
162.603
162.546
161.175
161.117
160.968
160.911
158.988
155.319
154.094
151.107
151.015
150.923
146.152
130.309
128.980
127.525
125.656
123.787
121.922
98.493
98.474
98.328
98.305
98.072
98.053
97.907
97.884
97.275
97.134
96.996
92.994
77.160 CDCl3
51.026
50.812
50.601
50.387
31.078
15.350
CF3
H3C
NH
F
NH2
N
N
N
N
Cl
F
Compound 23
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

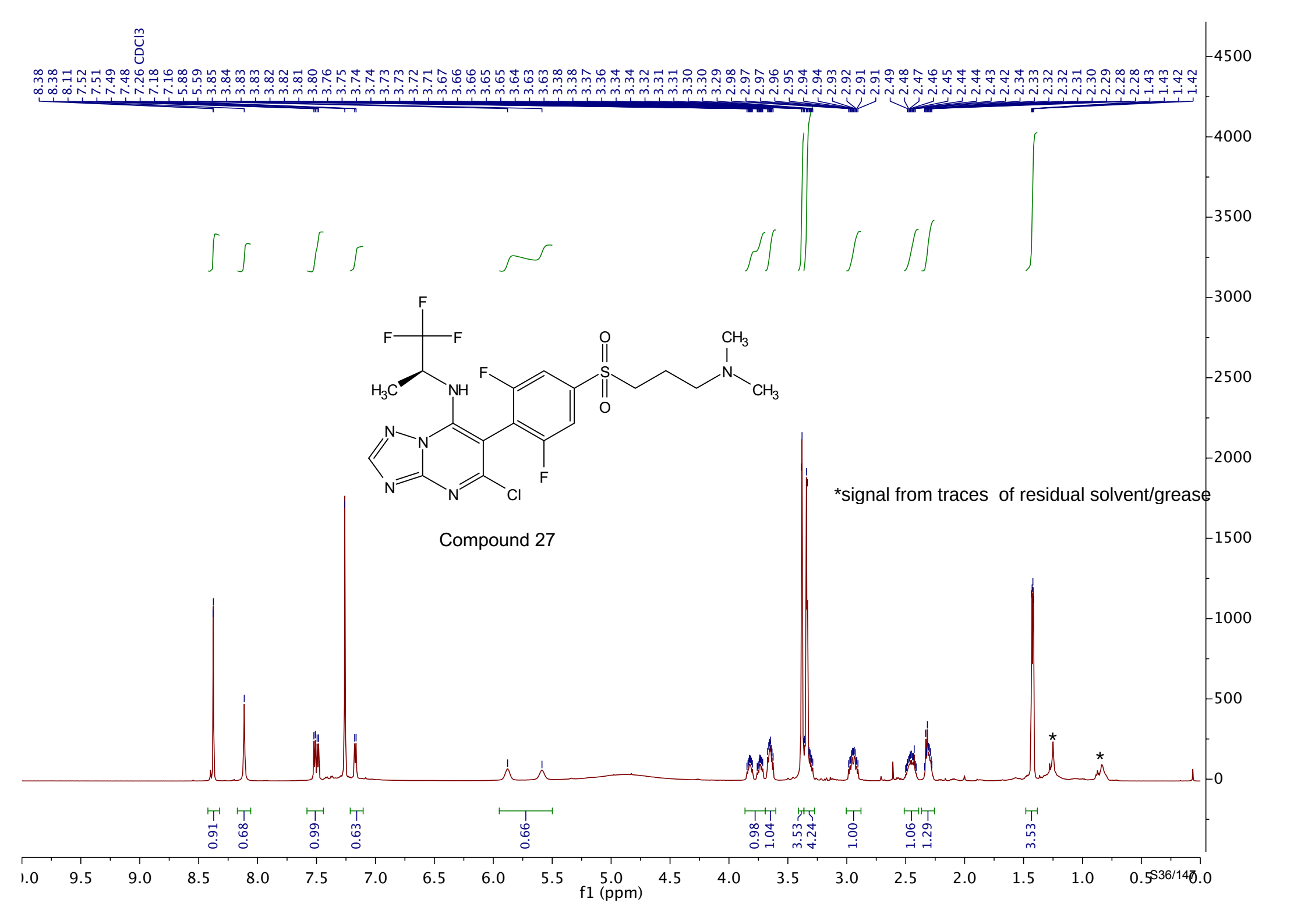

8.45
7.26 CDCl3
6.67
6.67
6.66
6.65
5.94
5.93
4.76
3.90
1.42
1.41
F
F
F
H3C
NH
F
O
CH3
N
N
N
N
Cl
F
Compound 24
1.10
2.06
0.96
1.00
3.00
3.05
f1 (ppm)

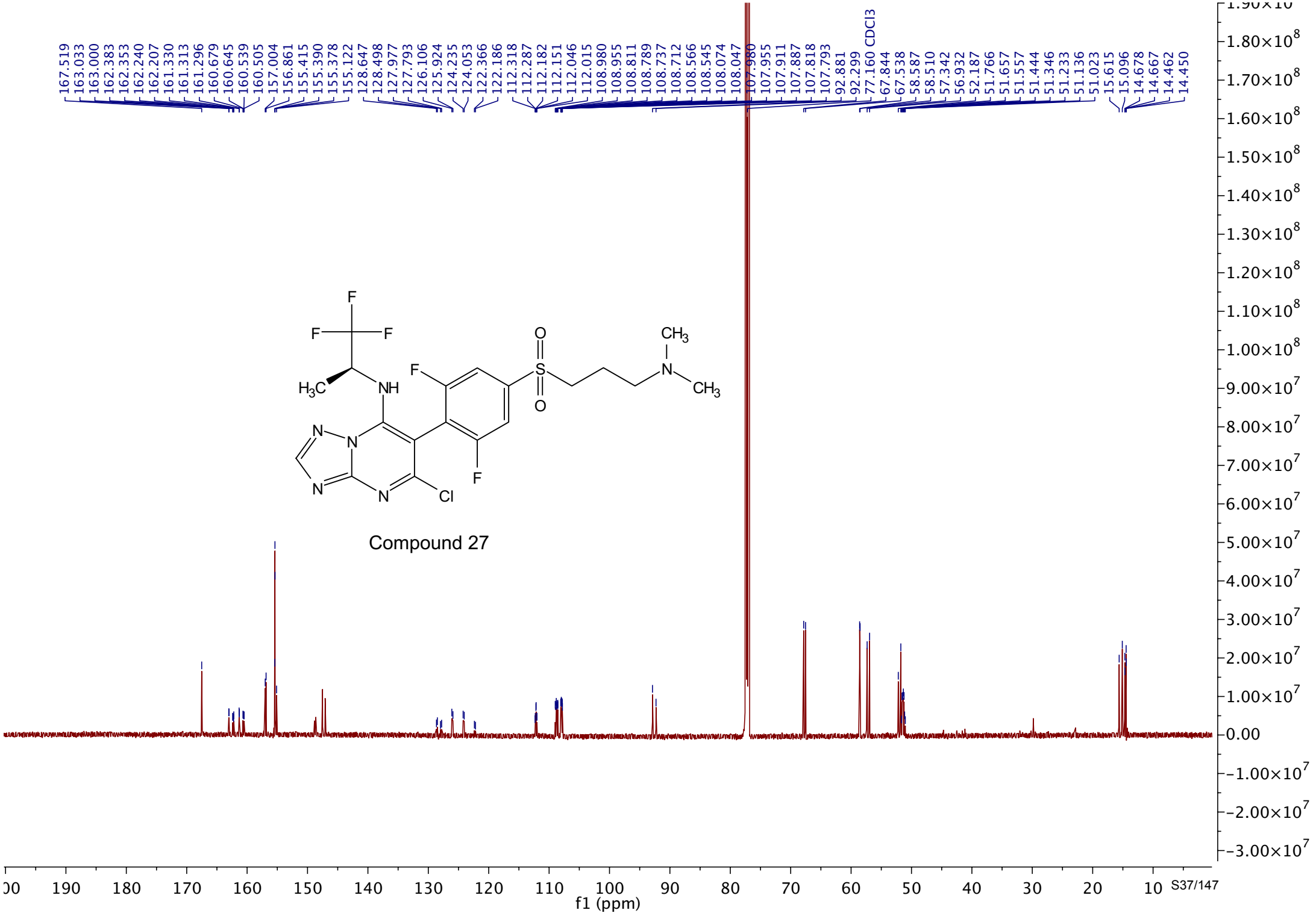

163.60
163.49
163.38
162.84
162.77
162.57
162.50
160.85
160.78
160.60
160.53
159.72
159.40
158.80
155.09
146.16
128.00
125.76
123.52
121.27
100.79
100.63
100.46
99.17
99.14
98.97
98.94
98.92
98.74
98.71
92.71
77.16 CDCl3
56.30
51.25
51.00
50.74
50.49
15.32
15.31
F
F
F
H3C
NH
F
O
CH3
N
N
N
N
Cl
F
Compound 24
f1 (ppm)
S33/147

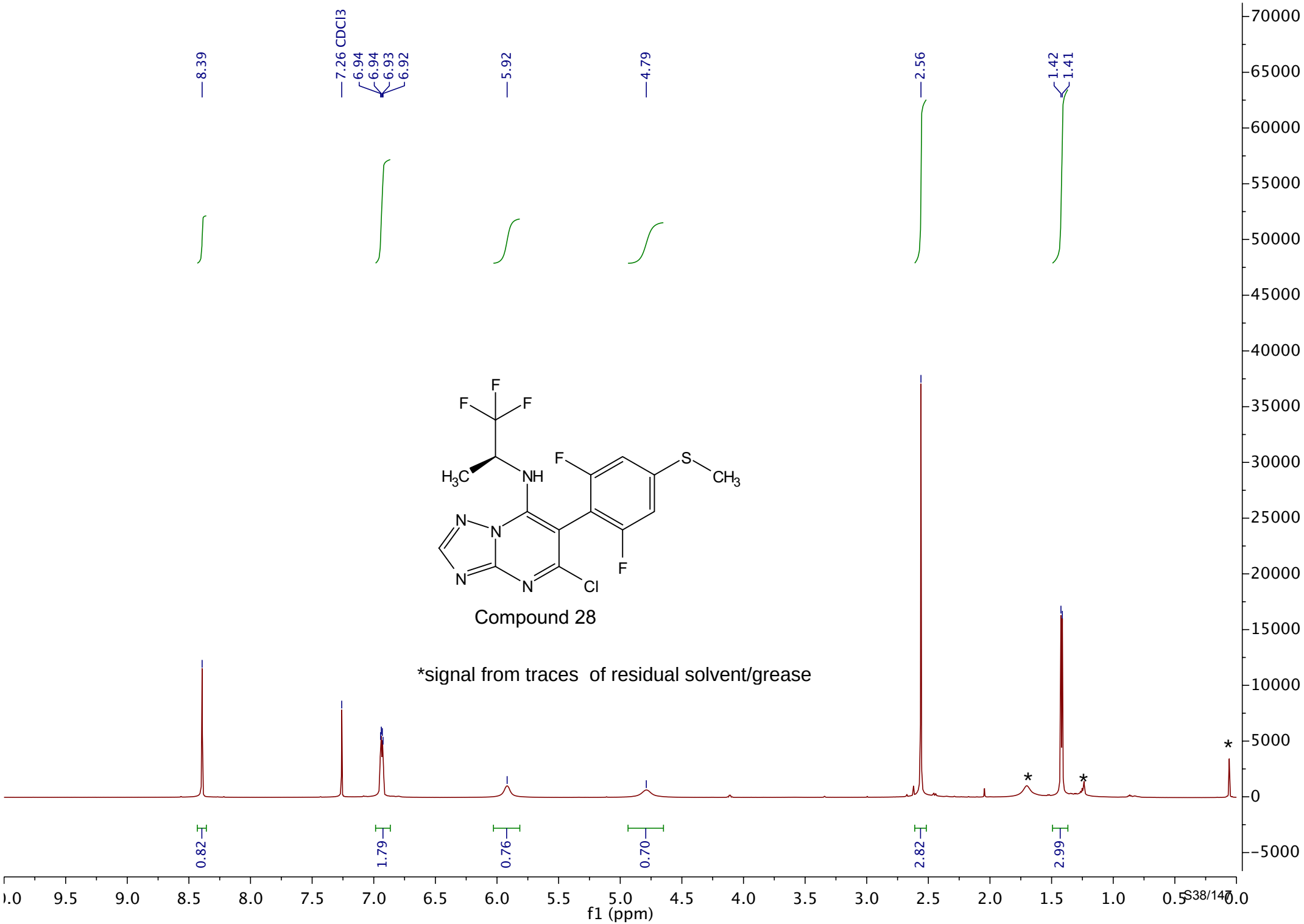

8.37
8.19
7.26 CDCl3
7.02
7.01
6.69
5.41
3.73
3.73
3.72
3.72
3.71
3.70
3.41
3.39
3.20
3.19
3.18
3.18
3.17
2.42
2.41
2.41
2.40
2.40
2.39
2.39
2.38
2.37
1.43
1.42
F
F
F
H3C
NH
F
O
S
CH3
N
CH3
N
N
N
N
Cl
F
Compound 26
1.00
1.05
1.99
1.18
1.28
2.13
6.65
2.12
2.24
3.42
f1 (ppm)
S34/147


166.949
162.420
162.374
161.844
161.800
160.741
160.697
160.170
160.126
157.646
155.358
154.852
154.842
146.842
142.464
127.786
125.909
124.040
122.171
111.485
111.462
111.324
111.301
111.290
111.146
111.125
111.112
110.985
110.964
110.951
106.508
106.370
106.357
106.221
92.688
77.160 CDCl3
68.143
57.772
57.693
51.475
51.264
51.052
50.841
29.623
29.610
22.635
22.624
14.816
F
F
F
H3C
NH
N
N
N
N
Cl
F
F
O
S
CH3
N
CH3
5.0×10^7
4.5×10^7
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Compound 26

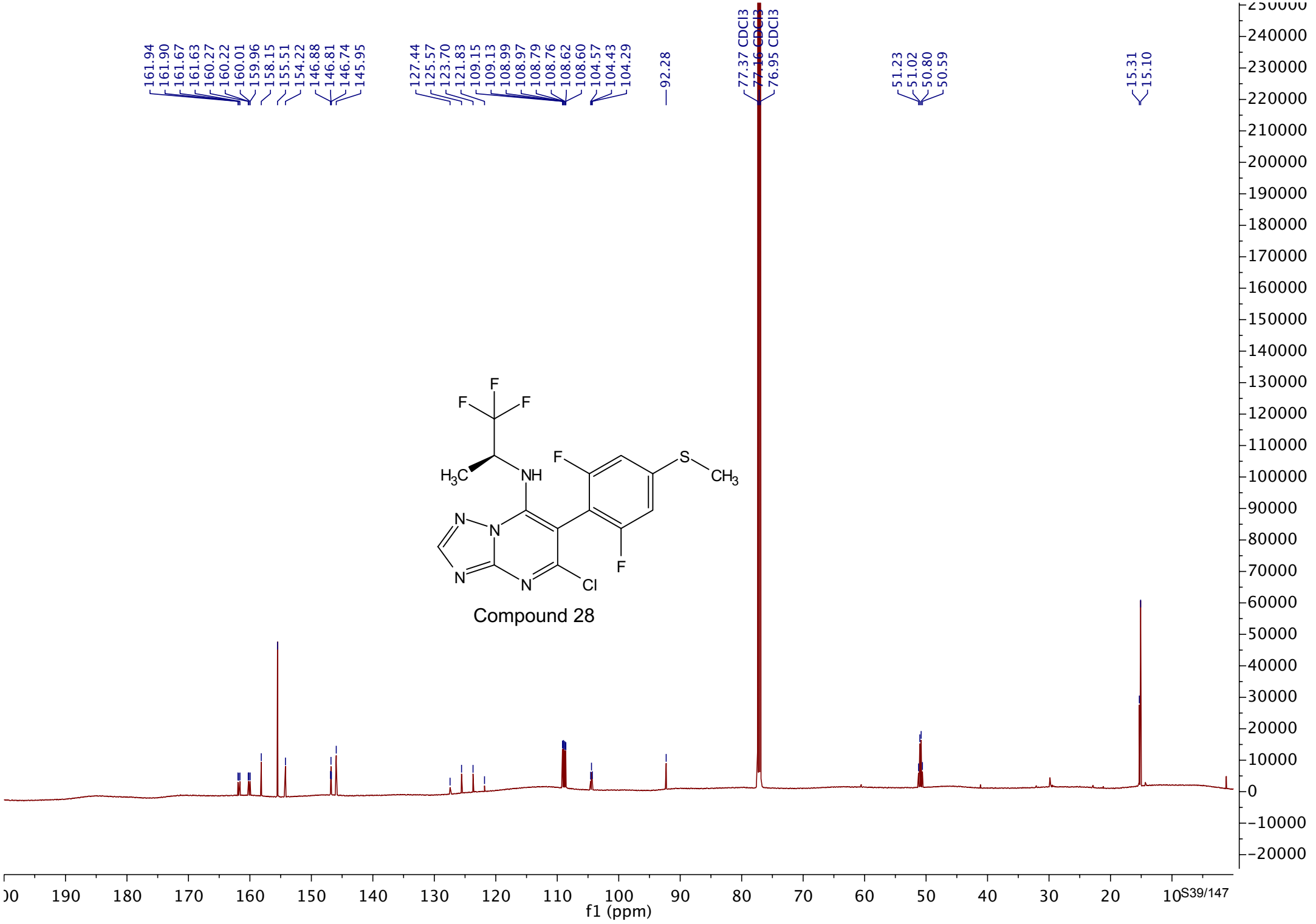

CDCl3
8.38 8.38 8.11 7.52 7.51 7.49 7.48 7.26 7.18 7.16 5.88 5.59 3.85 3.84 3.83 3.83 3.82 3.82 3.81 3.80 3.76 3.75 3.74 3.74 3.73 3.73 3.72 3.71 3.67 3.66 3.66 3.65 3.65 3.64 3.63 3.63 3.38 3.38 3.37 3.36 3.34 3.34 3.32 3.31 3.31 3.30 3.30 3.29 2.98 2.97 2.97 2.96 2.95 2.94 2.94 2.93 2.92 2.91 2.91 2.49 2.48 2.47 2.46 2.45 2.44 2.44 2.43 2.42 2.34 2.33 2.32 2.32 2.31 2.30 2.29 2.28 2.28 1.43 1.43 1.42 1.42
F
F
F
H3C
NH
N
N
N
N
Cl
F
F
O
S
O
N
CH3
CH3
Compound 27
*signal from traces of residual solvent/grease
0.91
0.68
0.99
0.63
0.66
0.98
1.04
3.53
4.24
1.00
1.06
1.29
3.53
f1 (ppm)
S36/147

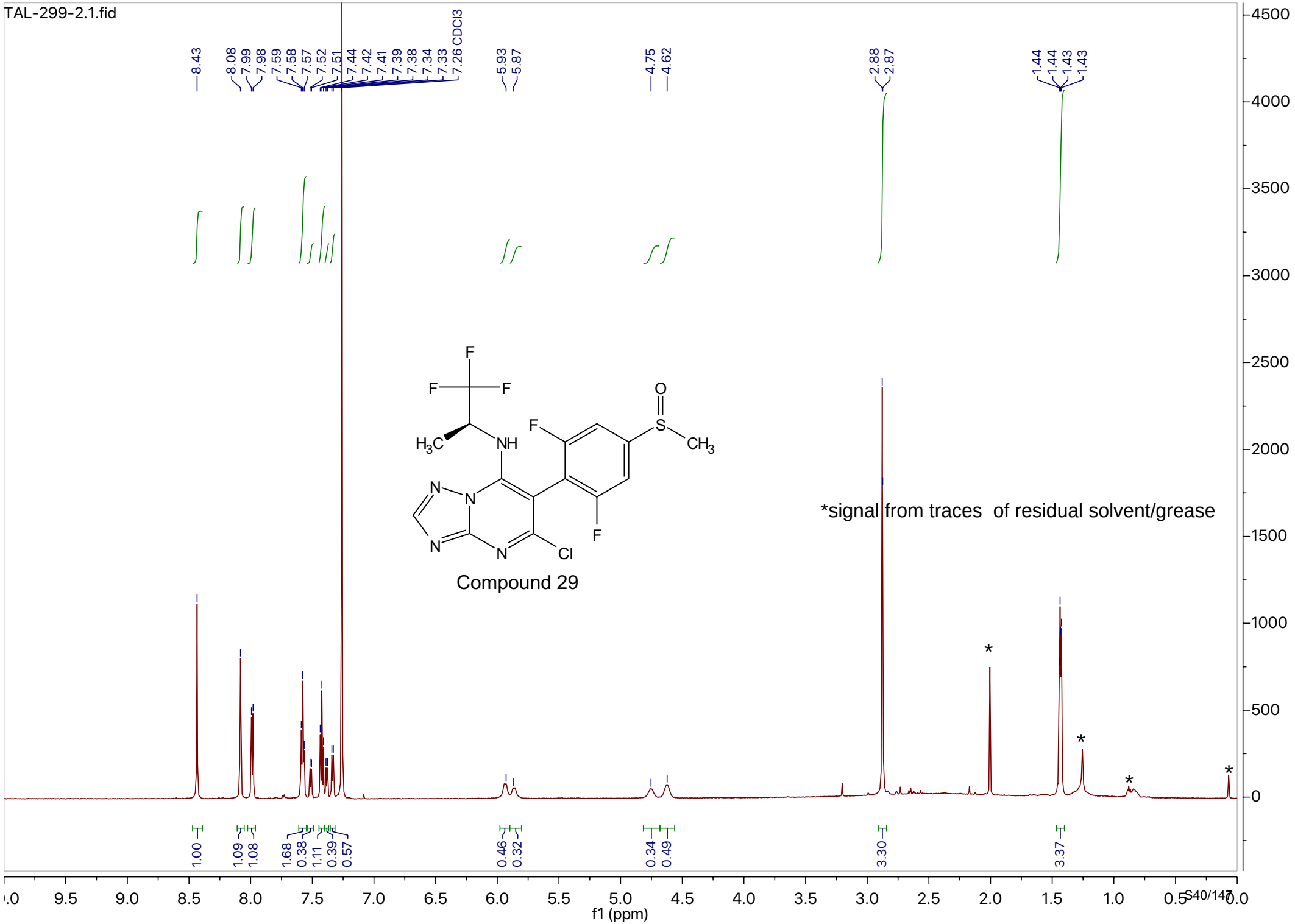

167.519
163.033
163.000
162.383
162.353
162.240
162.207
161.330
161.313
161.296
160.679
160.645
160.539
160.505
157.004
156.861
155.415
155.390
155.378
155.122
128.647
128.498
127.977
127.793
126.106
125.924
124.235
124.053
122.366
122.186
112.318
112.287
112.182
112.151
112.046
112.015
108.980
108.955
108.811
108.789
108.737
108.712
108.566
108.545
108.074
108.047
107.980
107.955
107.911
107.887
107.818
107.793
92.881
92.299
77.160 CDCl3
67.844
67.538
58.587
58.510
57.342
56.932
52.187
51.766
51.657
51.557
51.444
51.346
51.233
51.136
51.023
15.615
15.096
14.678
14.667
14.462
14.450
1.90×10
1.80×10^8
1.70×10^8
1.60×10^8
1.50×10^8
1.40×10^8
1.30×10^8
1.20×10^8
1.10×10^8
1.00×10^8
9.00×10^7
8.00×10^7
7.00×10^7
6.00×10^7
5.00×10^7
4.00×10^7
3.00×10^7
2.00×10^7
1.00×10^7
0.00
-1.00×10^7
-2.00×10^7
-3.00×10^7
F
F
F
H3C
NH
F
O
S
O
CH3
N
CH3
N
N
N
N
Cl
F
Compound 27
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
S37/147

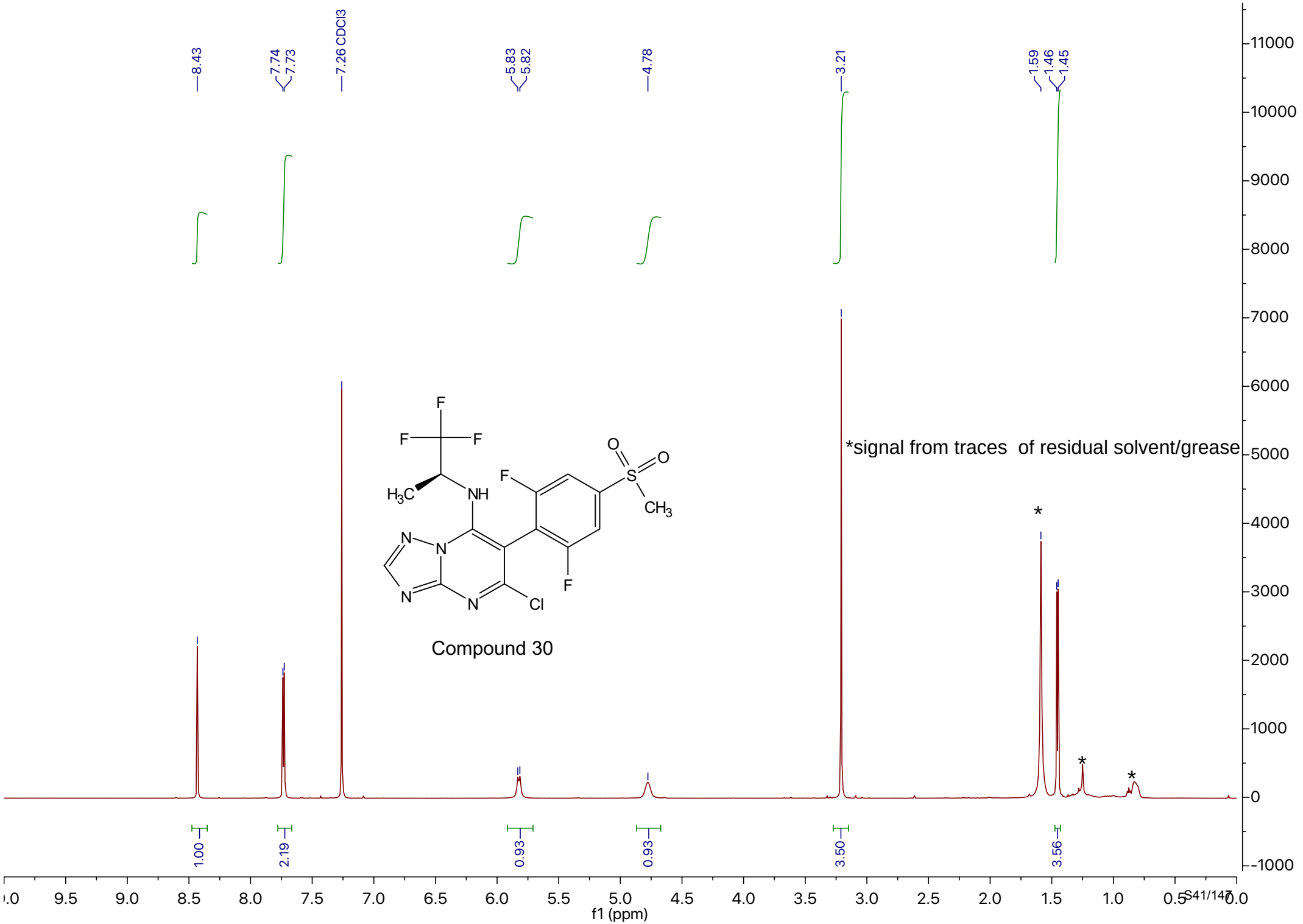


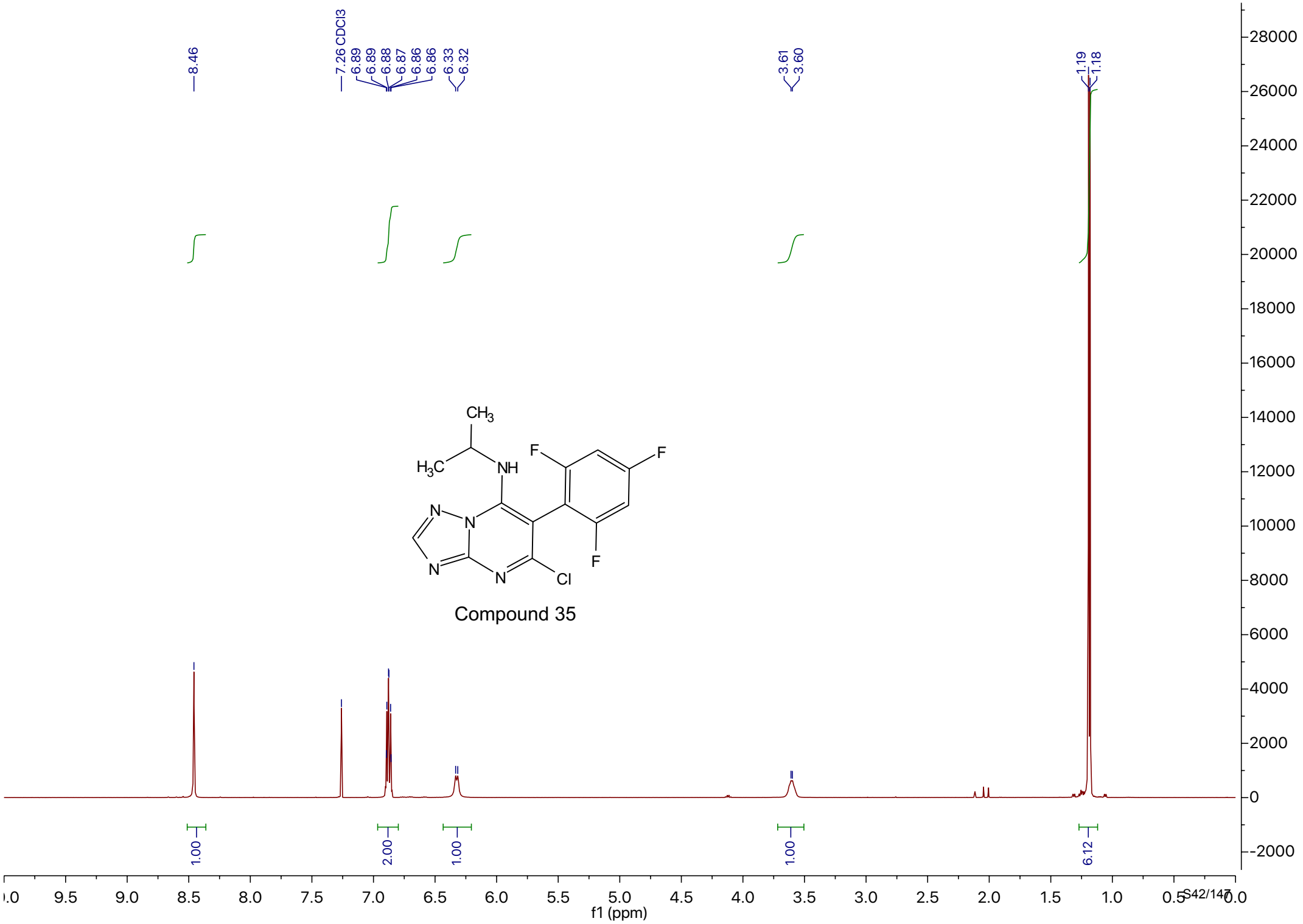
Compound 28

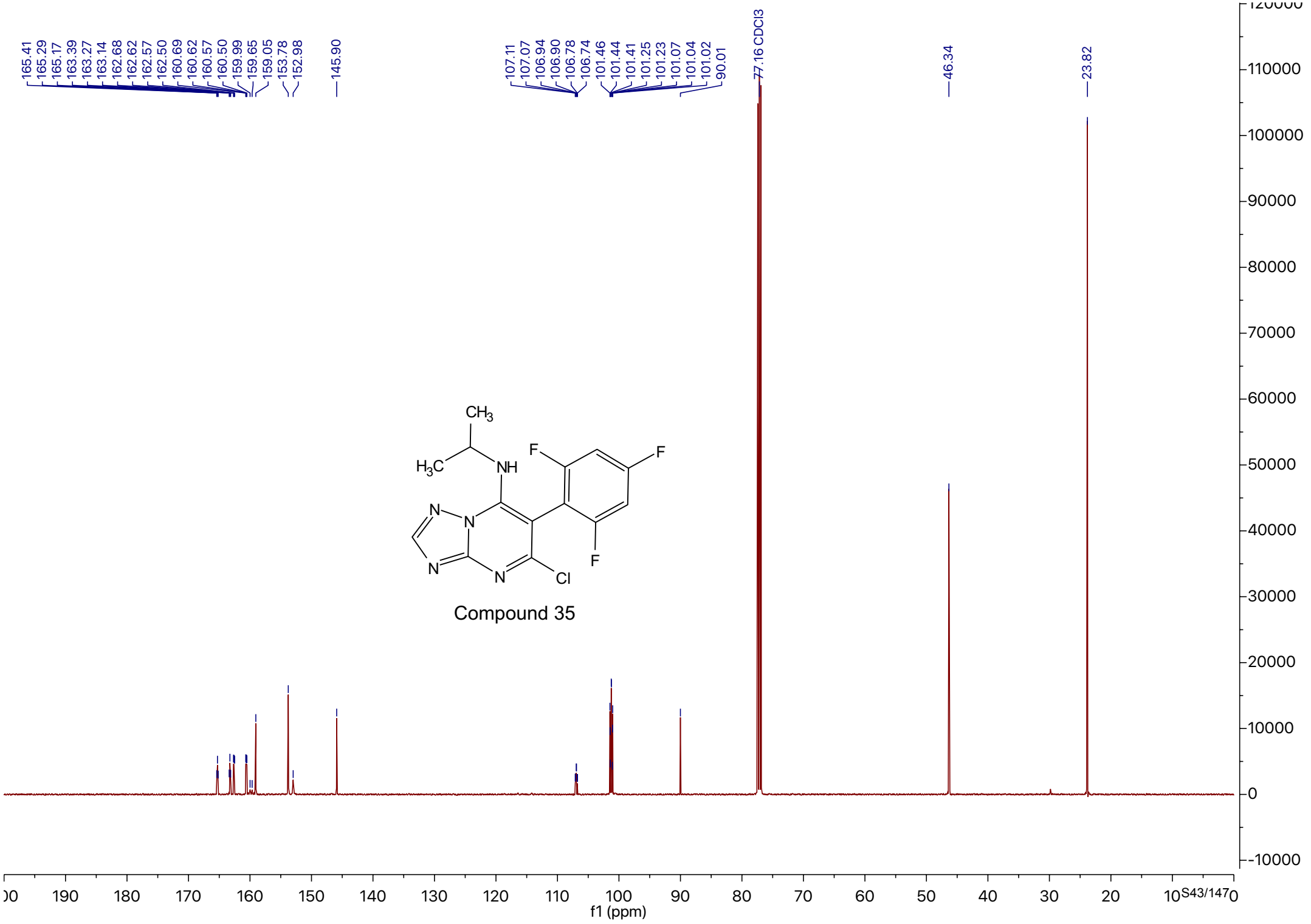
*signal from traces of residual solvent/grease

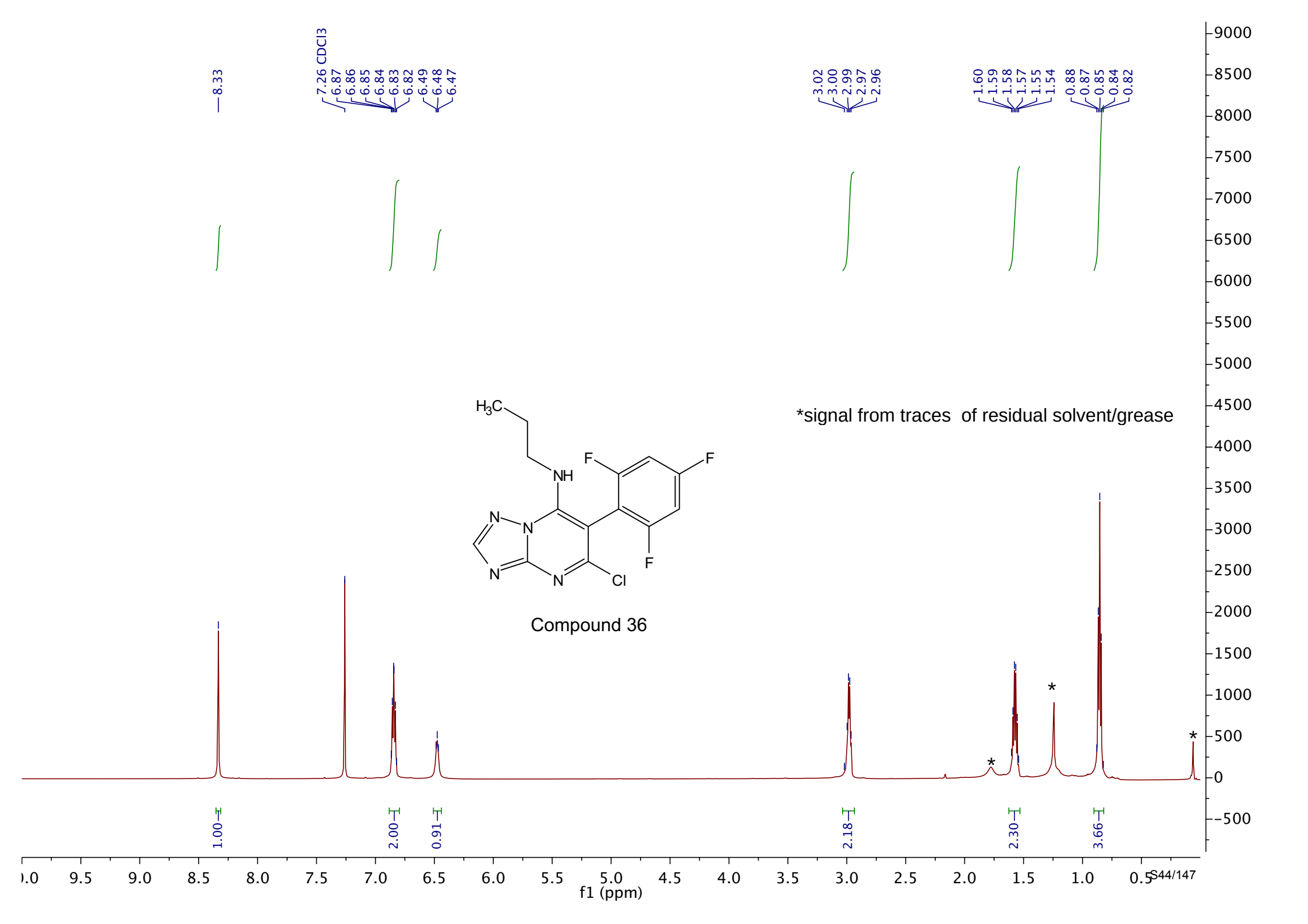

161.94
161.90
161.67
161.63
160.27
160.22
160.01
159.96
158.15
155.51
154.22
146.88
146.81
146.74
145.95
127.44
125.57
123.70
121.83
109.15
109.13
108.99
108.97
108.79
108.76
108.62
108.60
104.57
104.43
104.29
92.28
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
51.23
51.02
50.80
50.59
15.31
15.10
F
F
F
H3C
NH
F
S
CH3
N
N
N
N
Cl
F
Compound 28
f1 (ppm)

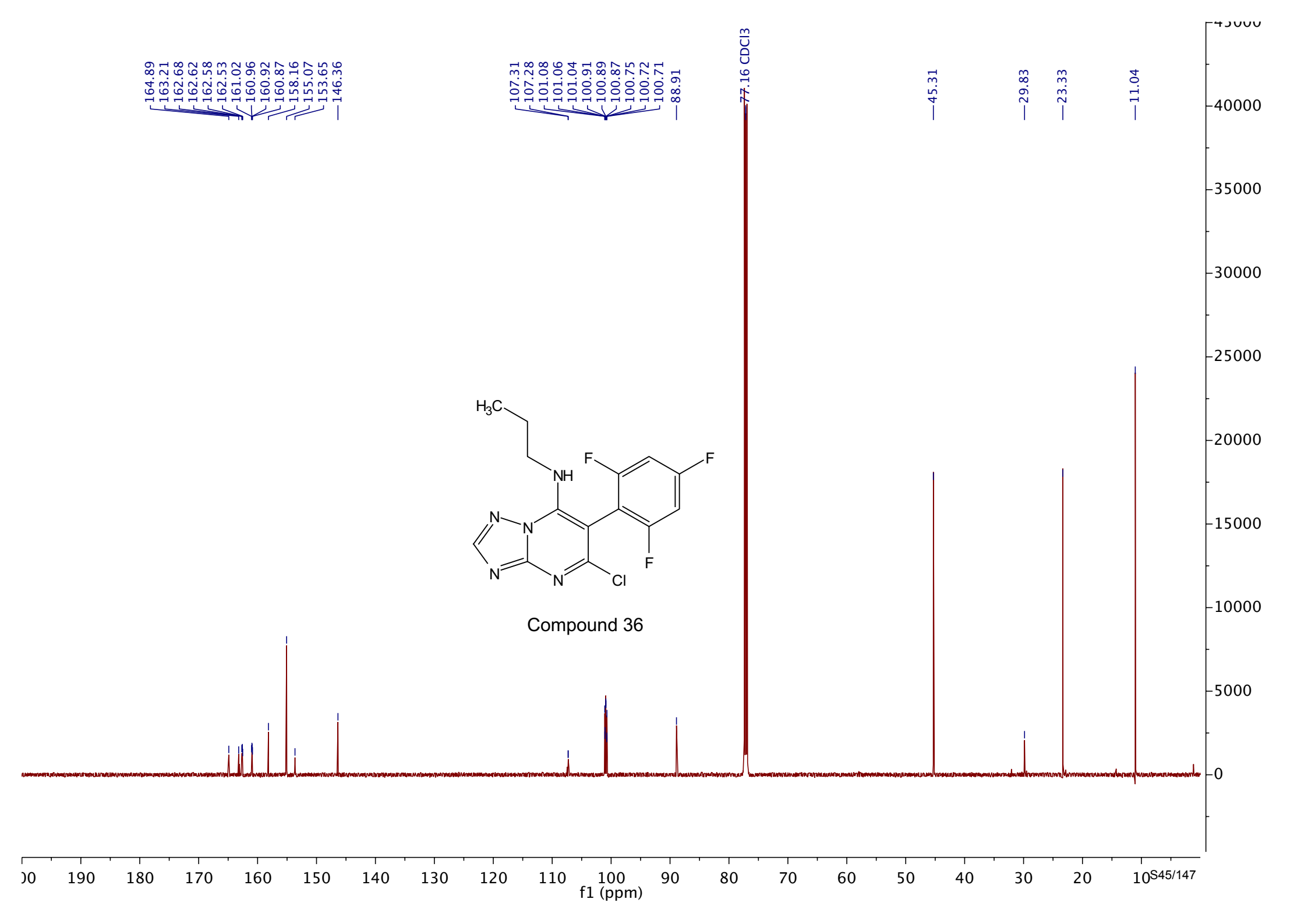

TAL-299-2.1.fid
8.43
8.08
7.99
7.98
7.59
7.58
7.57
7.52
7.51
7.44
7.42
7.41
7.39
7.38
7.34
7.33
7.26 CDCl3
5.93
5.87
4.75
4.62
2.88
2.87
1.44
1.44
1.43
1.43
F
F
F
H3C
NH
F
O
S
CH3
N
N
N
N
Cl
F
Compound 29
*signal from traces of residual solvent/grease
1.00
1.09
1.08
1.68
0.38
1.11
0.39
0.57
0.46
0.32
0.34
0.49
3.30
3.37
f1 (ppm)

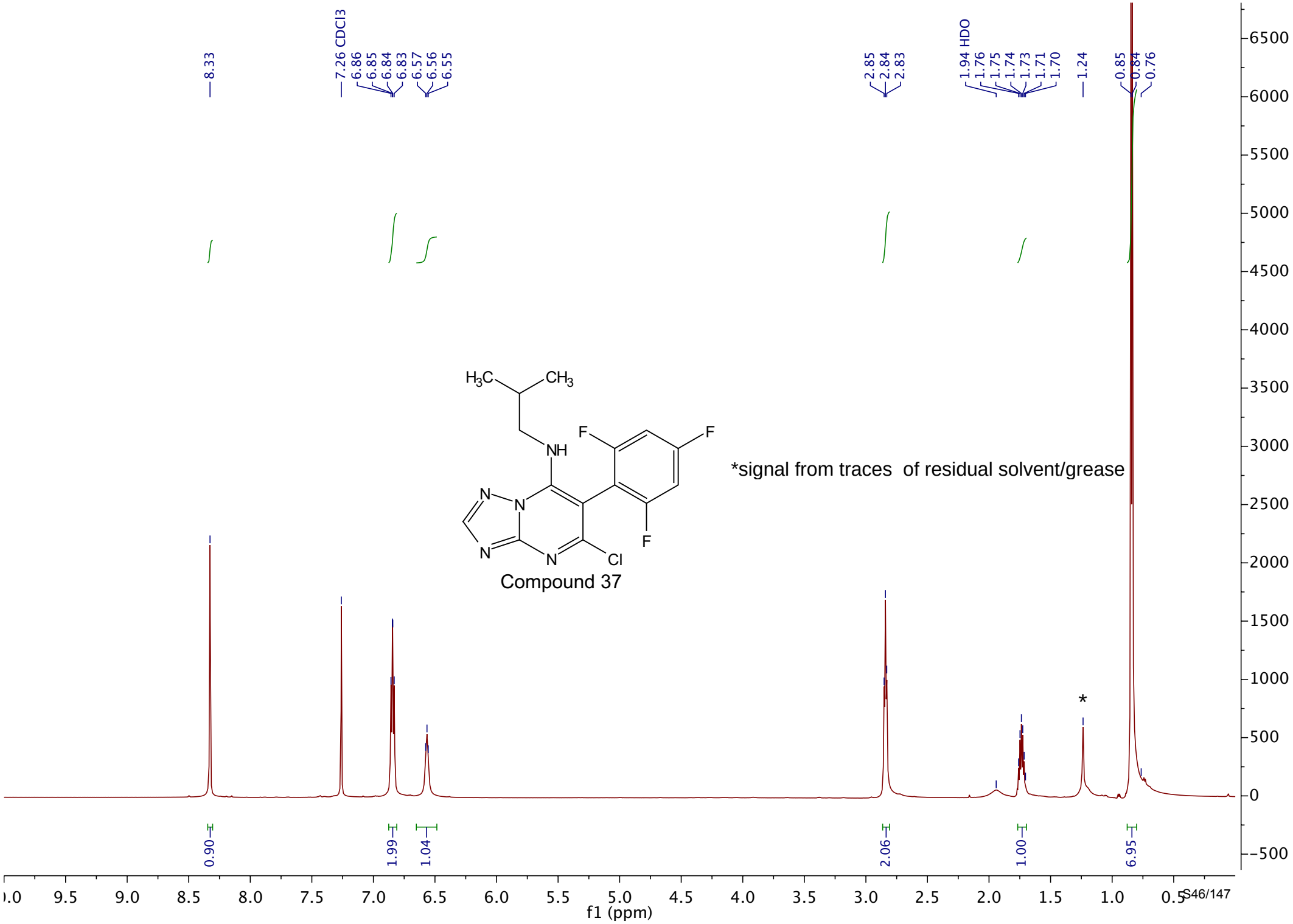

8.43
7.74
7.73
7.26 CDCl3
5.83
5.82
4.78
3.21
1.59
1.46
1.45
*signal from traces of residual solvent/grease
Compound 30
1.00
2.19
0.93
0.93
3.50
3.56
f1 (ppm)

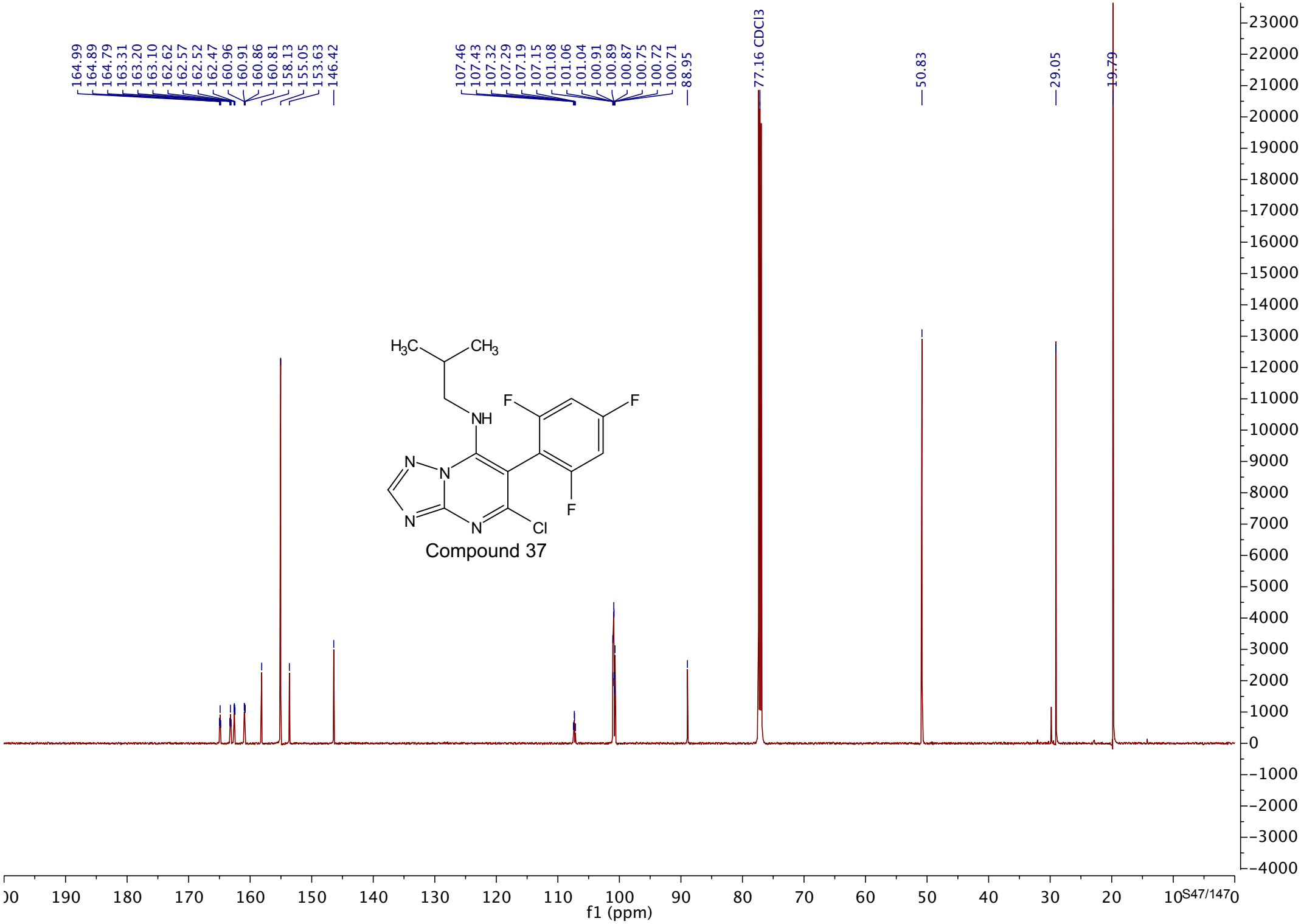

8.46
7.26 CDCl3
6.89
6.89
6.88
6.87
6.86
6.86
6.33
6.32
3.61
3.60
1.19
1.18
CH3
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 35
1.00
2.00
1.00
1.00
6.12
f1 (ppm)

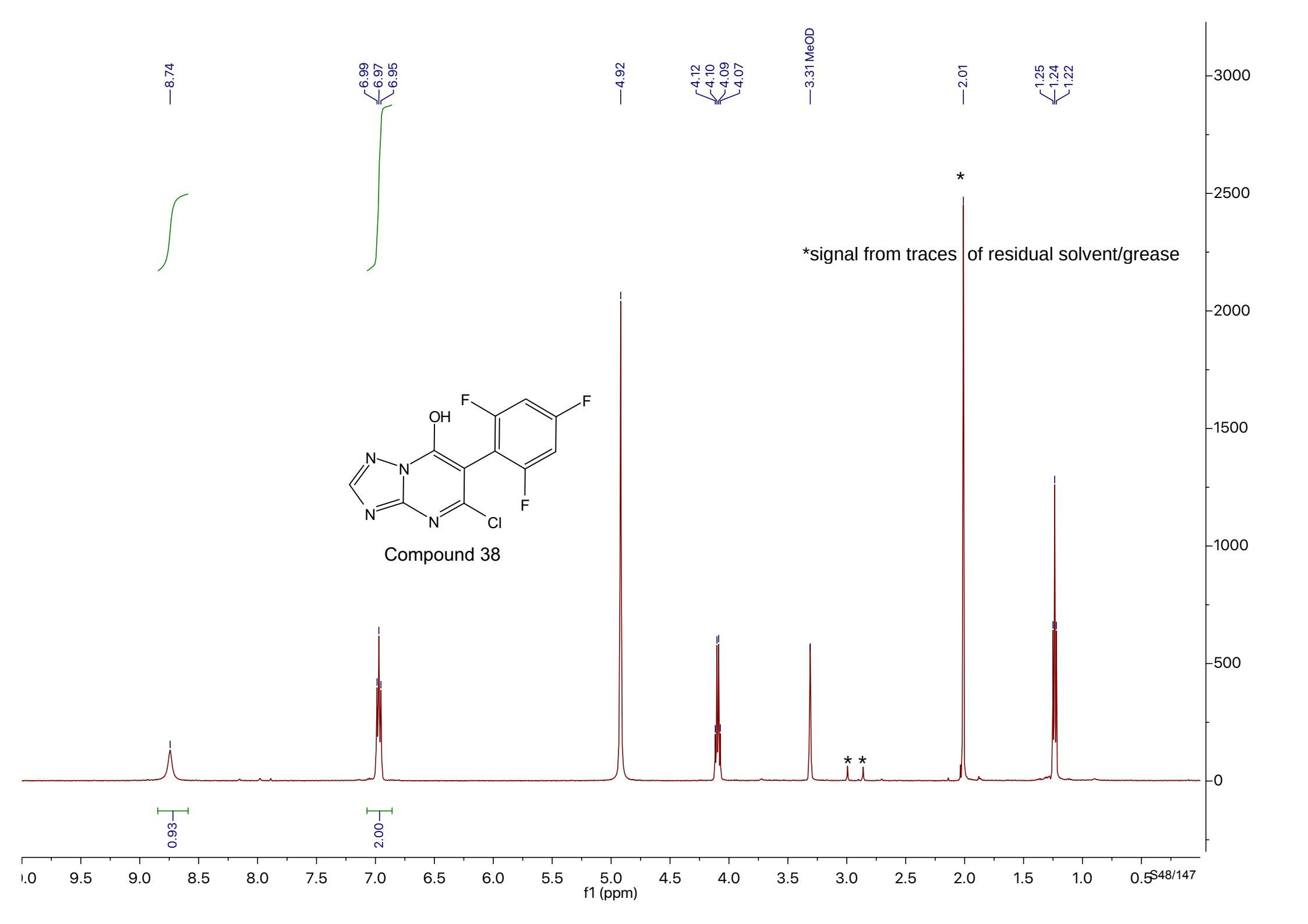

165.41
165.29
165.17
163.39
163.27
163.14
162.68
162.62
162.57
162.50
160.69
160.62
160.57
160.50
159.99
159.65
159.05
153.78
152.98
145.90
107.11
107.07
106.94
106.90
106.78
106.74
101.46
101.44
101.41
101.25
101.23
101.07
101.04
101.02
90.01
77.16 CDCl3
46.34
23.82
CH3
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 35
f1 (ppm)

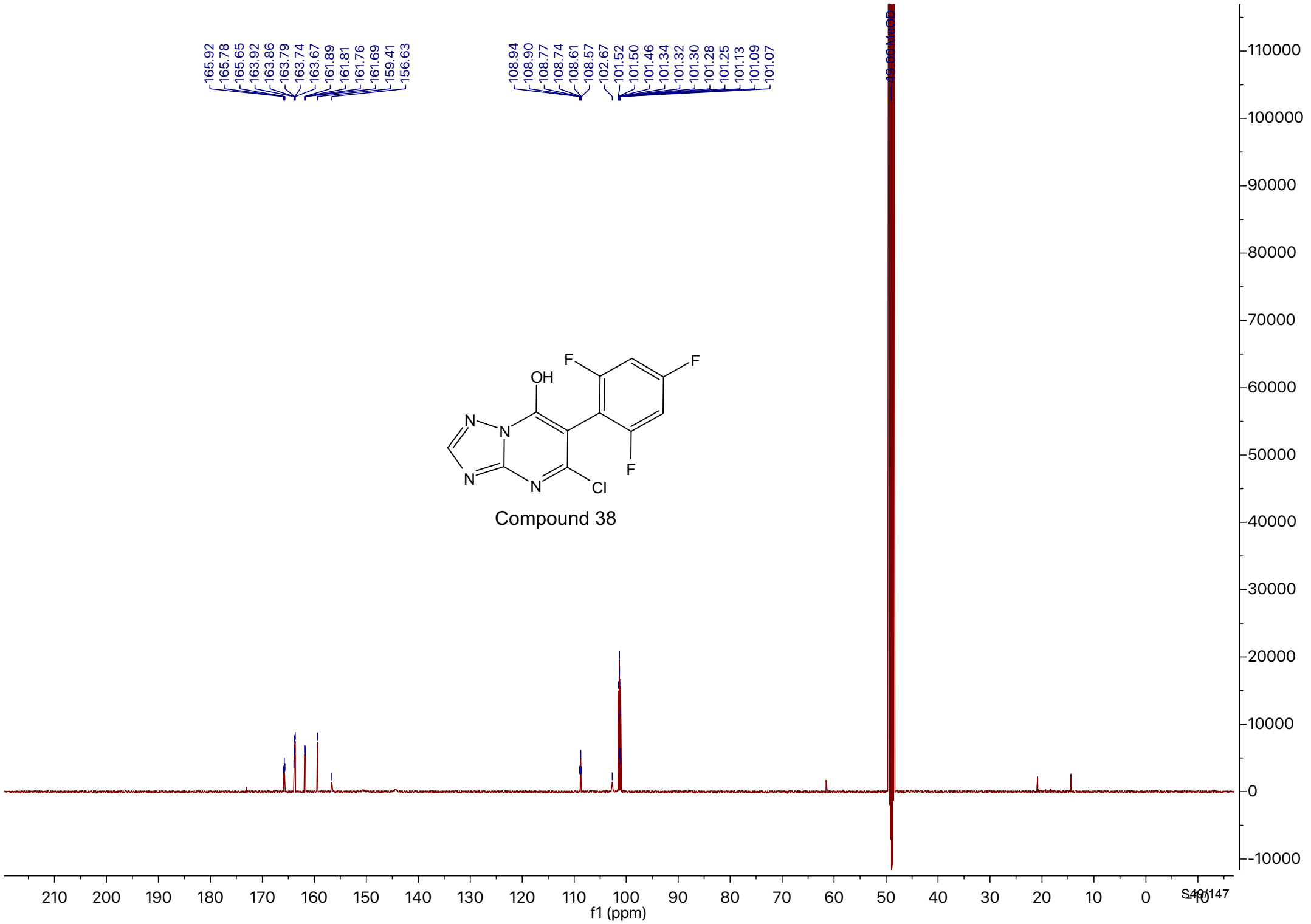

8.33
7.26 CDCl3
6.87
6.86
6.85
6.84
6.83
6.82
6.49
6.48
6.47
3.02
3.00
2.99
2.97
2.96
1.60
1.59
1.58
1.57
1.55
1.54
0.88
0.87
0.85
0.84
0.82
H3C
NH
F
F
F
N
N
N
N
Cl
*signal from traces of residual solvent/grease
Compound 36
1.00
2.00
0.91
2.18
2.30
3.66
f1 (ppm)
S44/147


164.89
163.21
162.68
162.62
162.58
162.53
161.02
160.96
160.92
160.87
158.16
155.07
153.65
146.36
107.31
107.28
101.08
101.06
101.04
100.91
100.89
100.87
100.75
100.72
100.71
88.91
77.16 CDCl3
45.31
29.83
23.33
11.04
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 36
40000
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

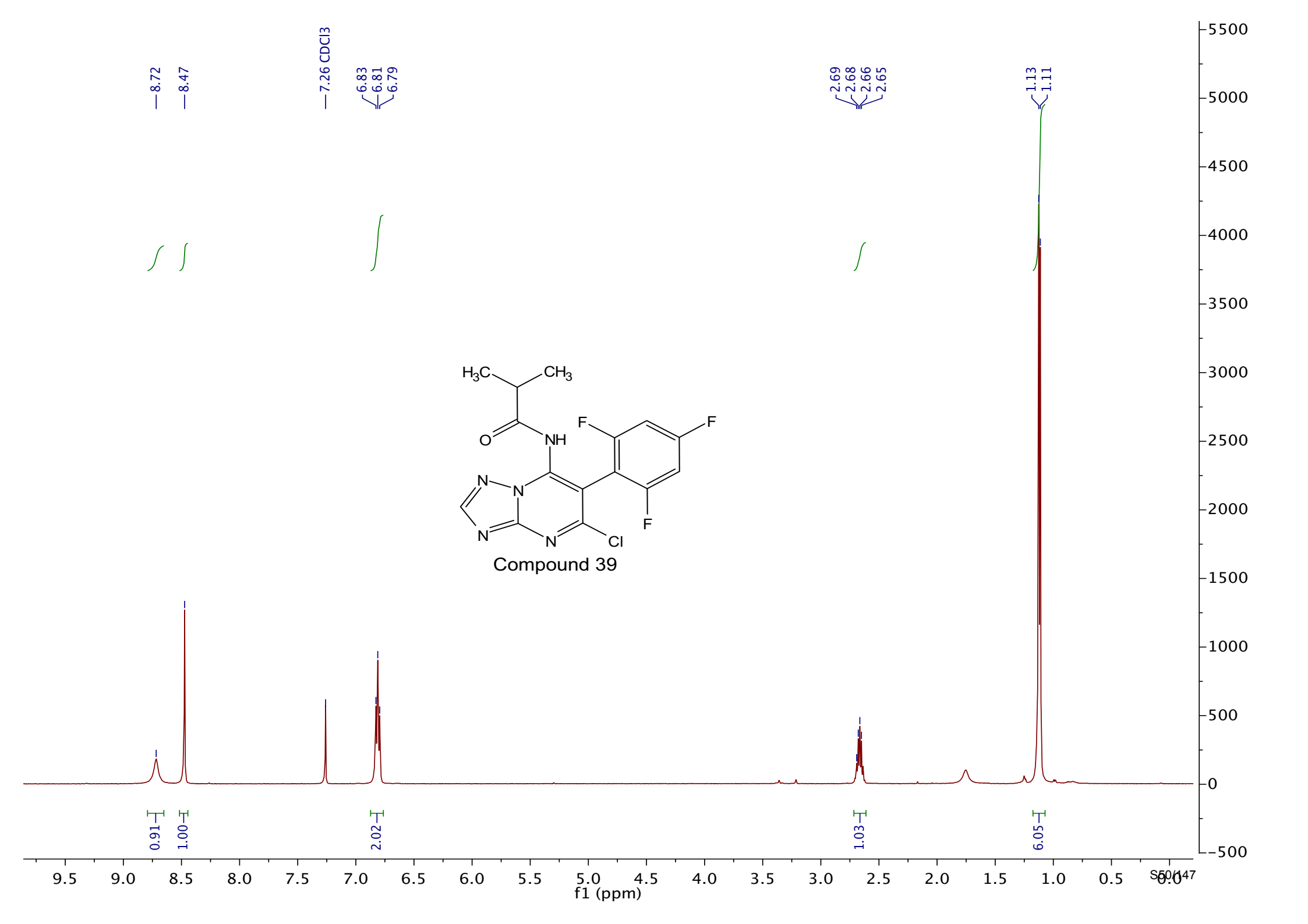

8.33
7.26 CDCl3
6.86
6.85
6.84
6.83
6.57
6.56
6.55
2.85
2.84
2.83
1.94 HDO
1.76
1.75
1.74
1.73
1.71
1.70
1.24
0.85
0.84
0.76
H3C
CH3
NH
F
F
F
N
N
N
N
Cl
*signal from traces of residual solvent/grease
Compound 37
0.90
1.99
1.04
2.06
1.00
6.95
f1 (ppm)
S46/147

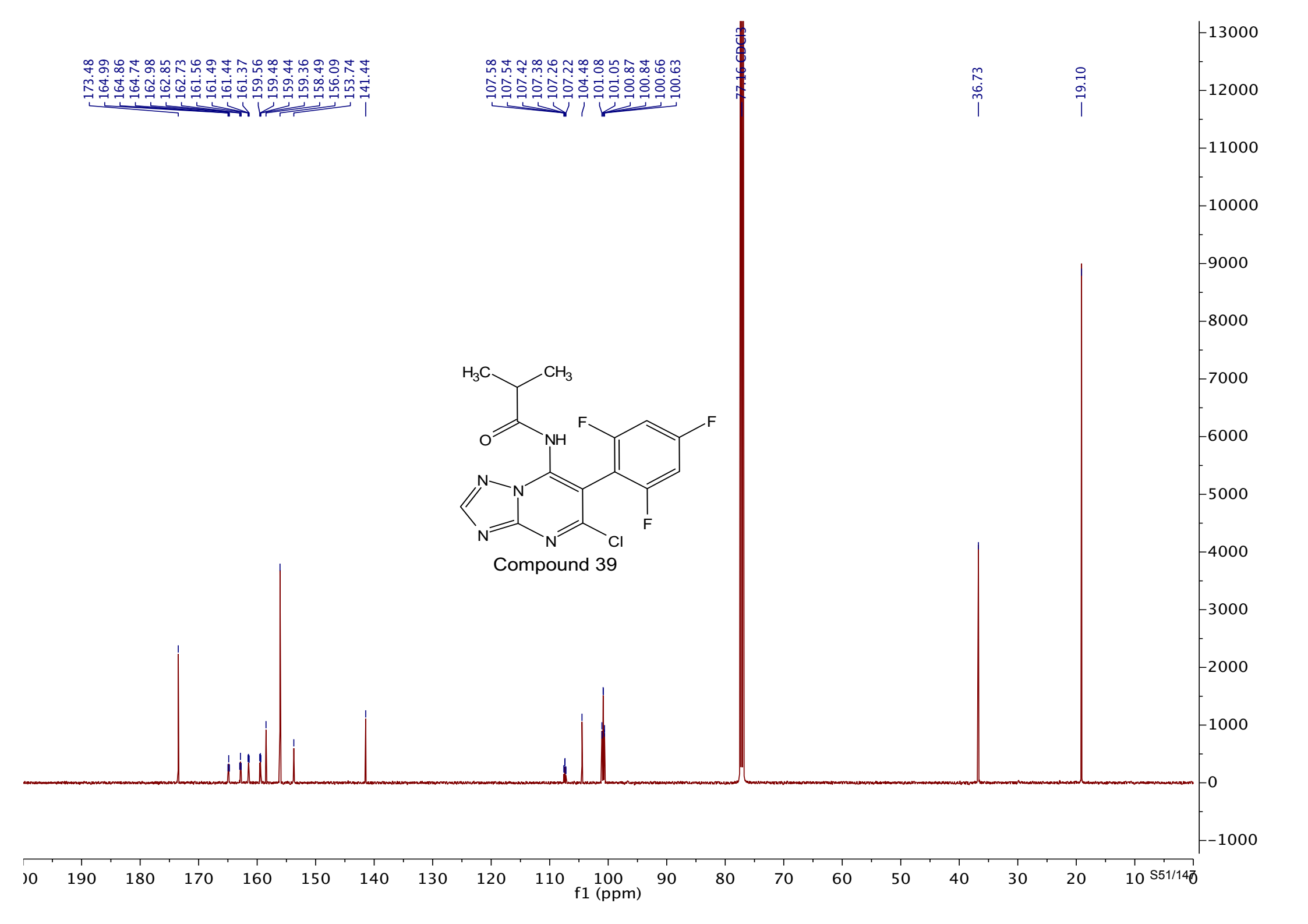

164.99
164.89
164.79
163.31
163.20
163.10
162.62
162.57
162.52
162.47
160.96
160.91
160.86
160.81
158.13
155.05
153.63
146.42
107.46
107.43
107.32
107.29
107.19
107.15
101.08
101.06
101.04
100.91
100.89
100.87
100.75
100.72
100.71
88.95
77.16 CDCl3
50.83
29.05
19.79
H3C
CH3
NH
F
F
F
N
N
N
N
Cl
Compound 37
f1 (ppm)

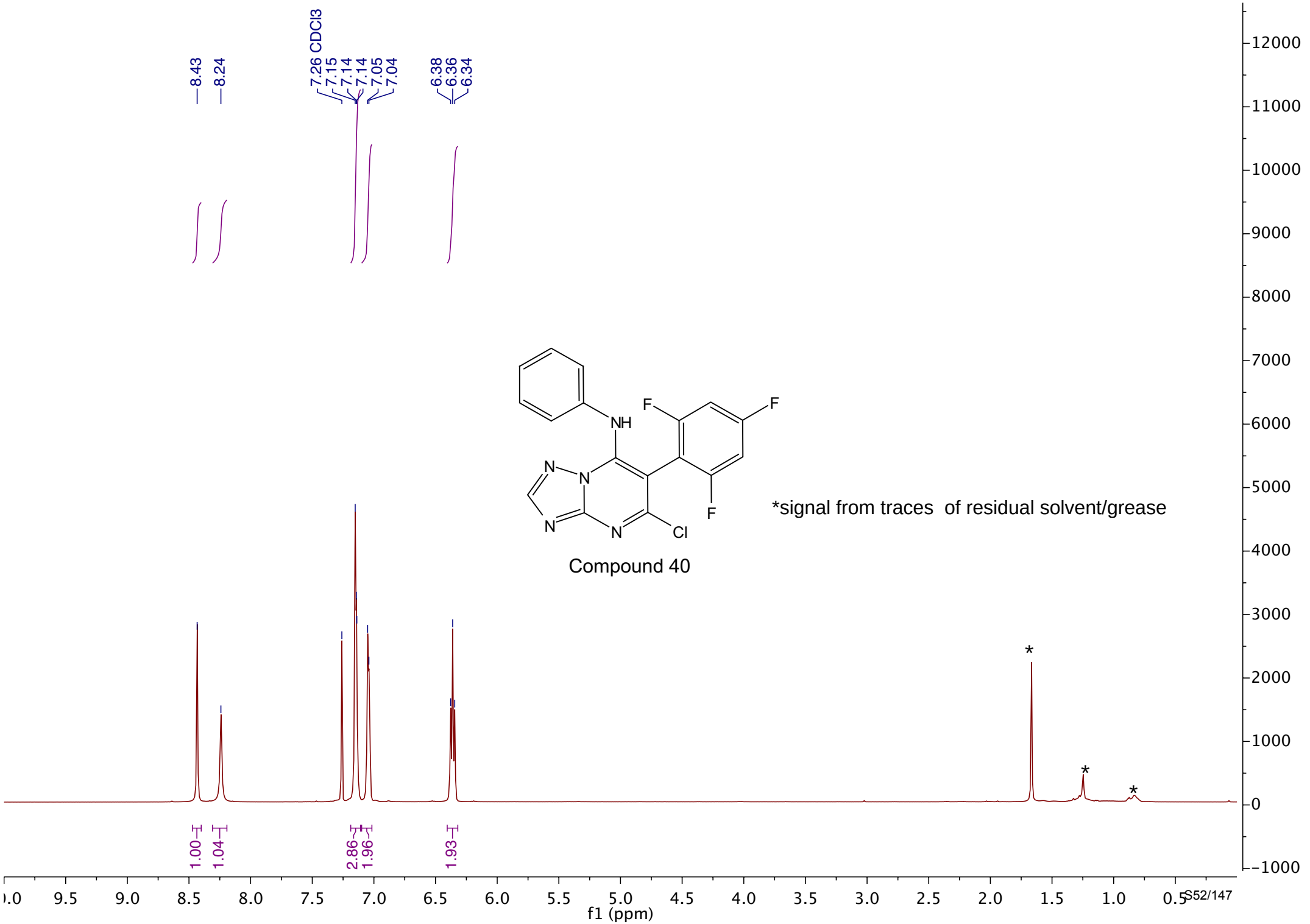

8.74
6.99
6.97
6.95
4.92
4.12
4.10
4.09
4.07
3.31 MeOD
2.01
1.25
1.24
1.22
*signal from traces of residual solvent/grease
Compound 38
0.93
2.00
f1 (ppm)
S48/147


165.92
165.78
165.65
163.92
163.86
163.79
163.74
163.67
161.89
161.81
161.76
161.69
159.41
156.63
108.94
108.90
108.77
108.74
108.61
108.57
102.67
101.52
101.50
101.46
101.34
101.32
101.30
101.28
101.25
101.13
101.09
101.07
49.00
F
F
OH
N
N
N
N
Cl
F
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
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)

Compound 38

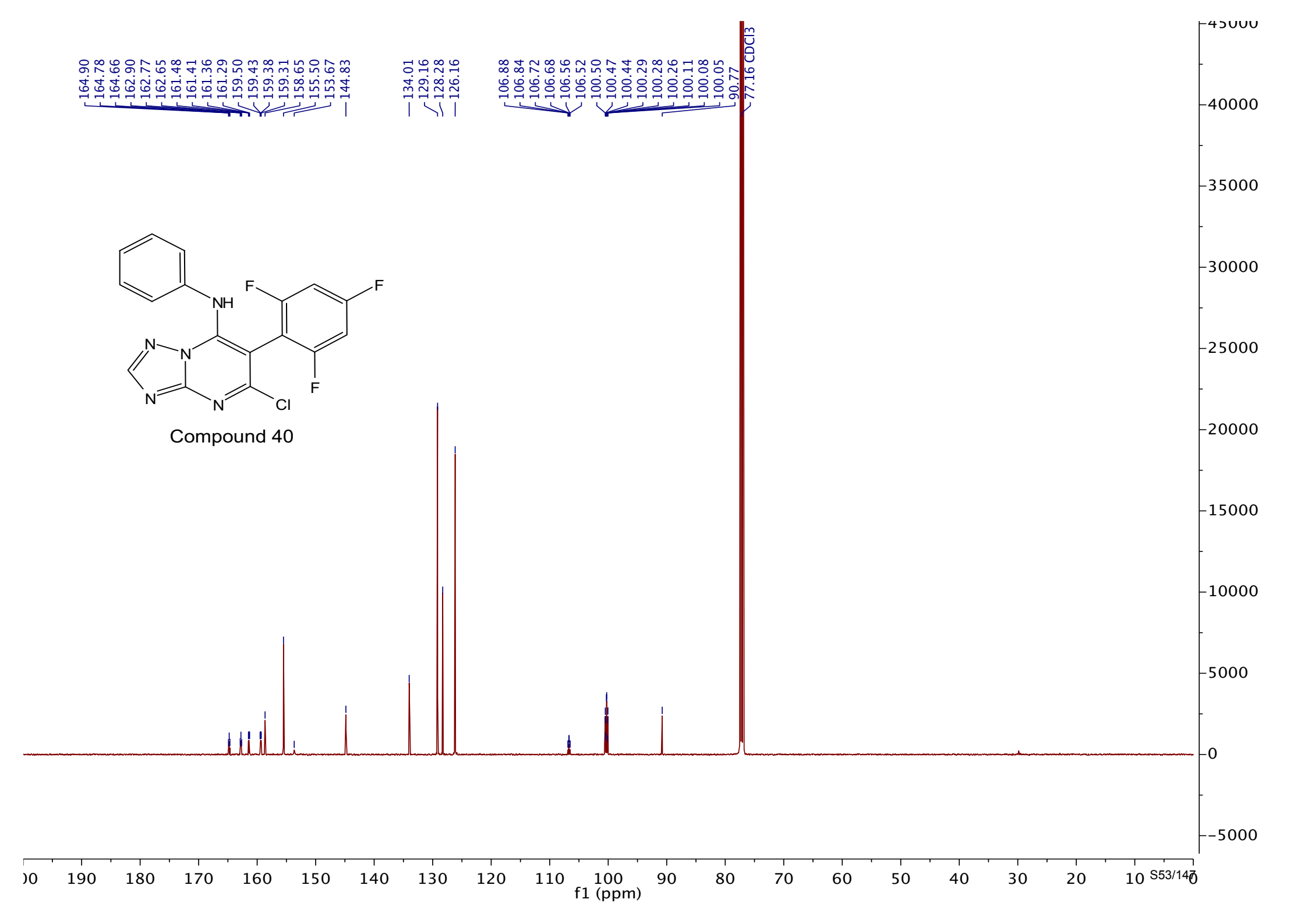

8.72
8.47
7.26 CDCl3
6.83
6.81
6.79
2.69
2.68
2.66
2.65
1.13
1.11
0.91
1.00
2.02
1.03
6.05
f1 (ppm)
Compound 39

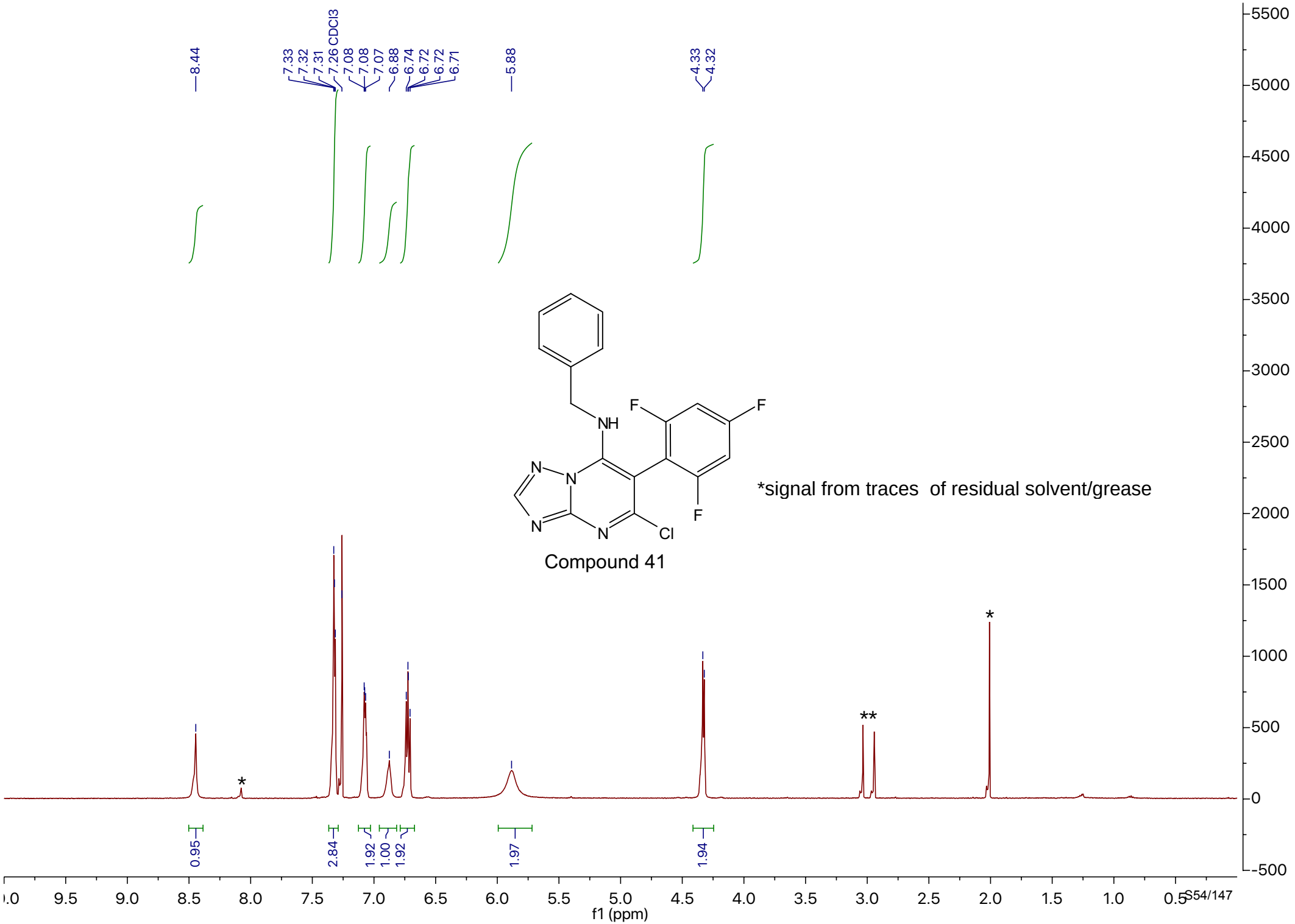

173.48
164.99
164.86
164.74
162.98
162.85
162.73
161.56
161.49
161.44
161.37
159.56
159.48
159.44
159.36
158.49
156.09
153.74
141.44
107.58
107.54
107.42
107.38
107.26
107.22
104.48
101.08
101.05
100.87
100.84
100.66
100.63
77.16 CDCl3
36.73
19.10
H3C
CH3
O
NH
F
F
F
N
N
N
N
Cl
Compound 39
f1 (ppm)
S51/147



Compound 40

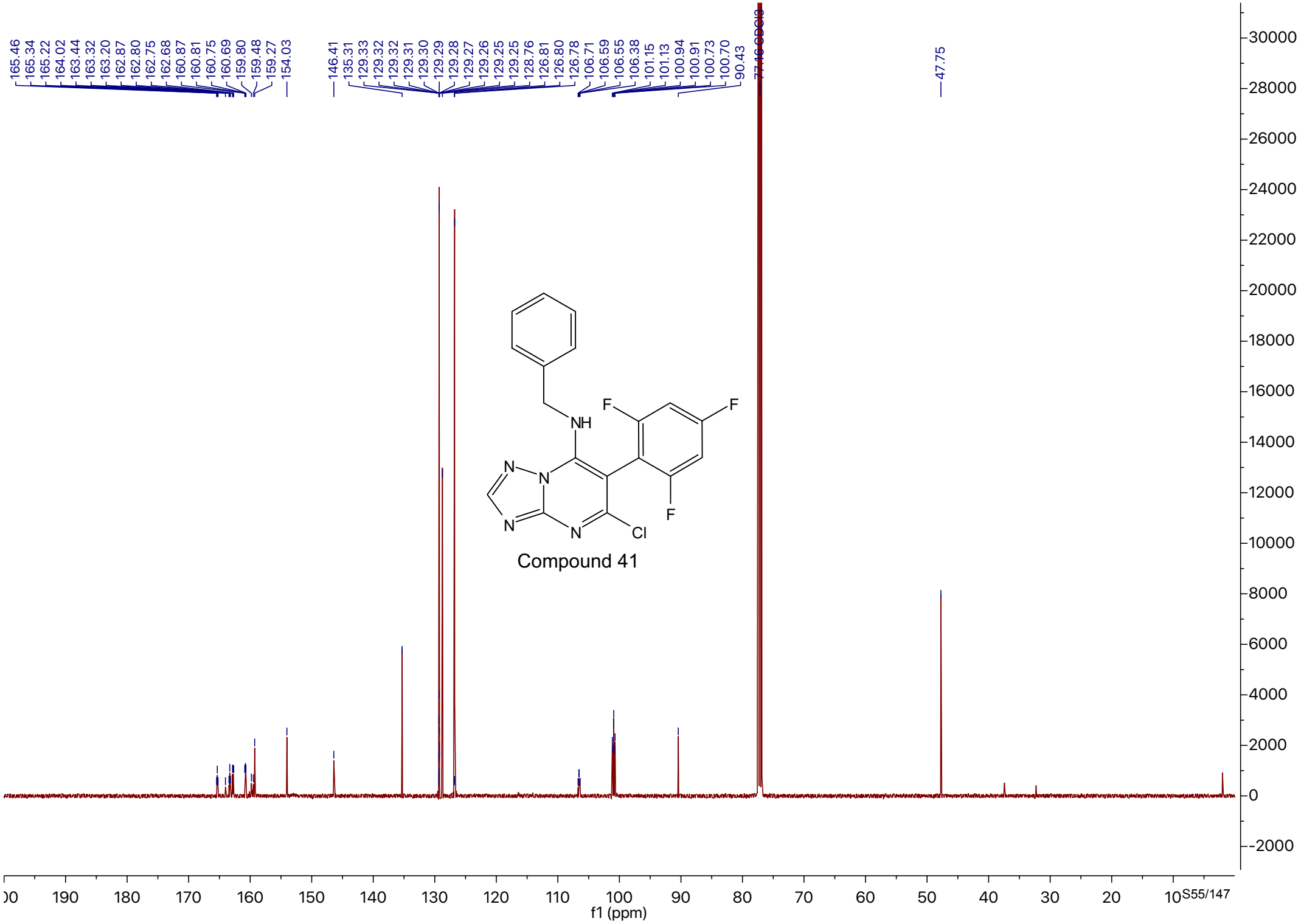
*signal from traces of residual solvent/grease

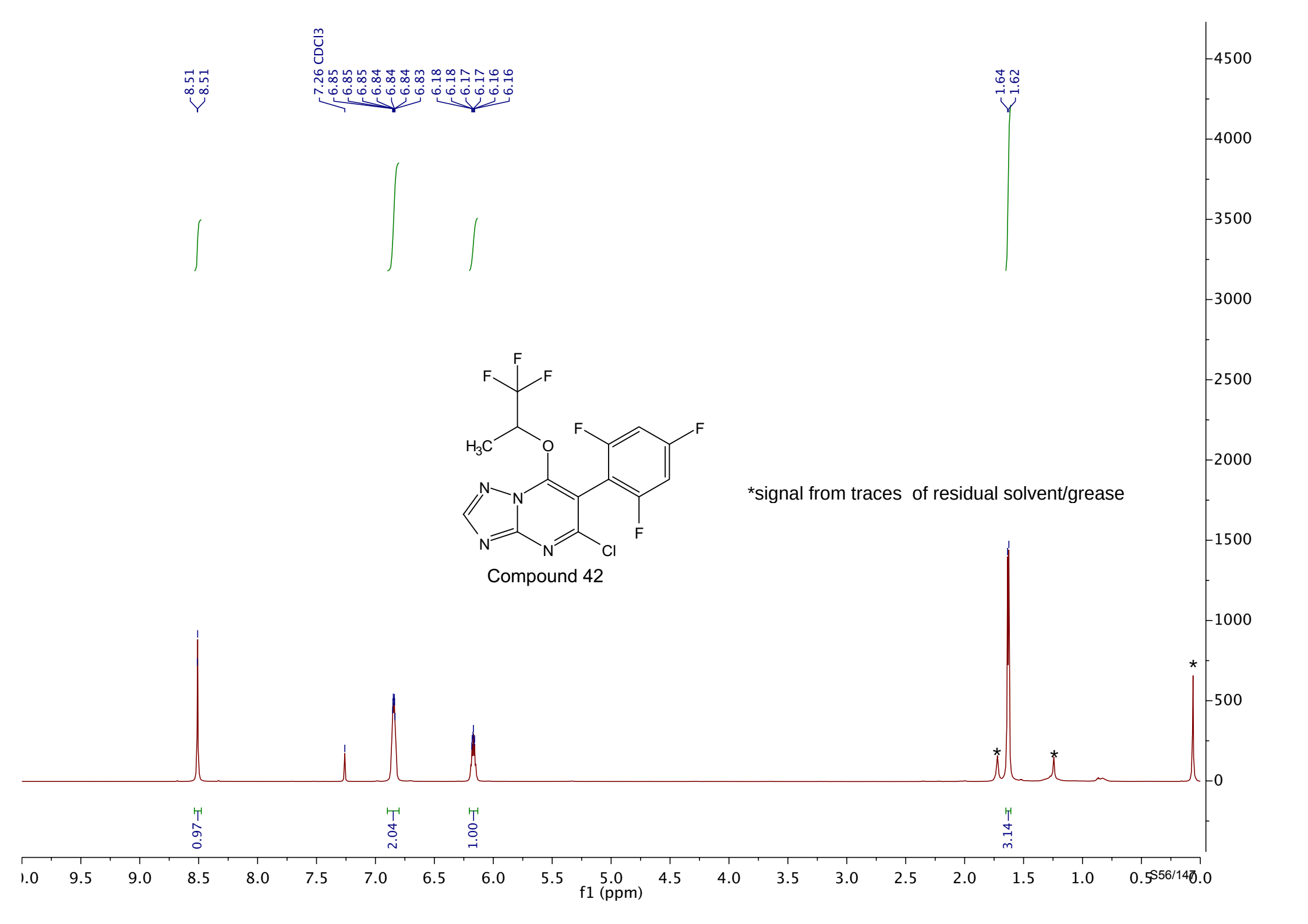

164.90
164.78
164.66
162.90
162.77
162.65
161.48
161.41
161.36
161.29
159.50
159.43
159.38
159.31
158.65
155.50
153.67
144.83
134.01
129.16
128.28
126.16
106.88
106.84
106.72
106.68
106.56
106.52
100.50
100.47
100.44
100.29
100.28
100.26
100.11
100.08
100.05
90.77
77.16 CDCl3
NH
F
F
F
N
N
N
N
Cl
Compound 40
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

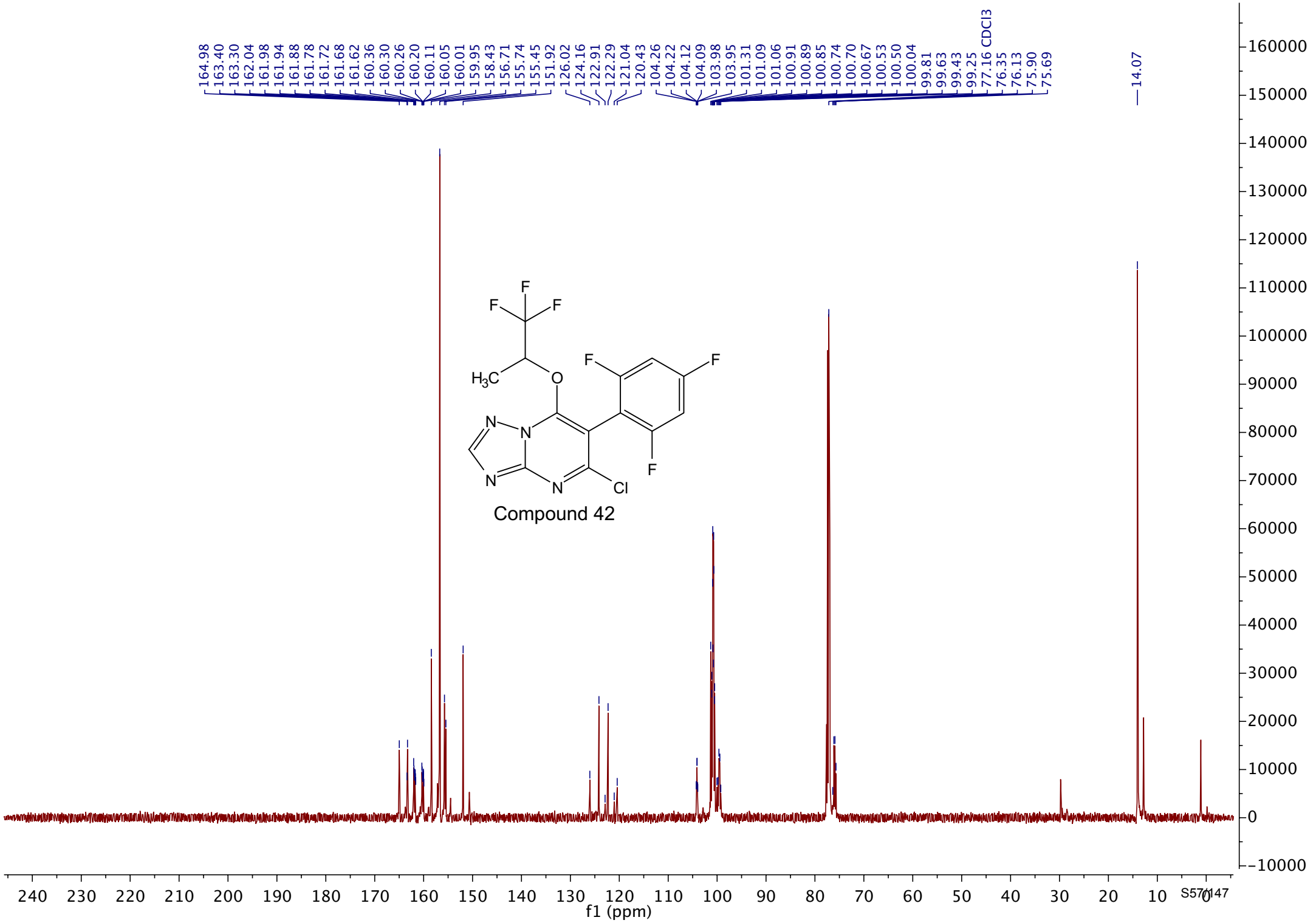


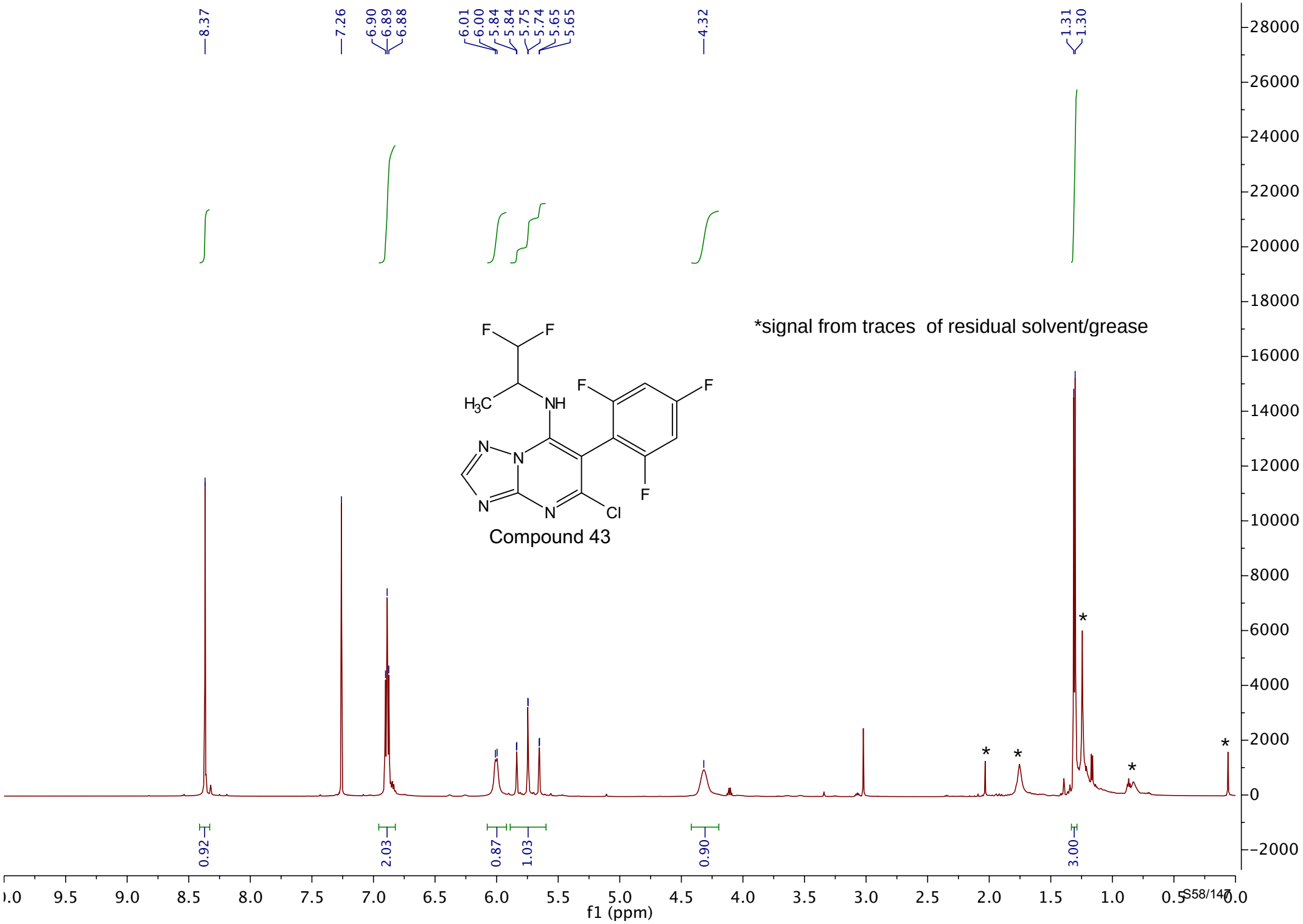
*signal from traces of residual solvent/grease

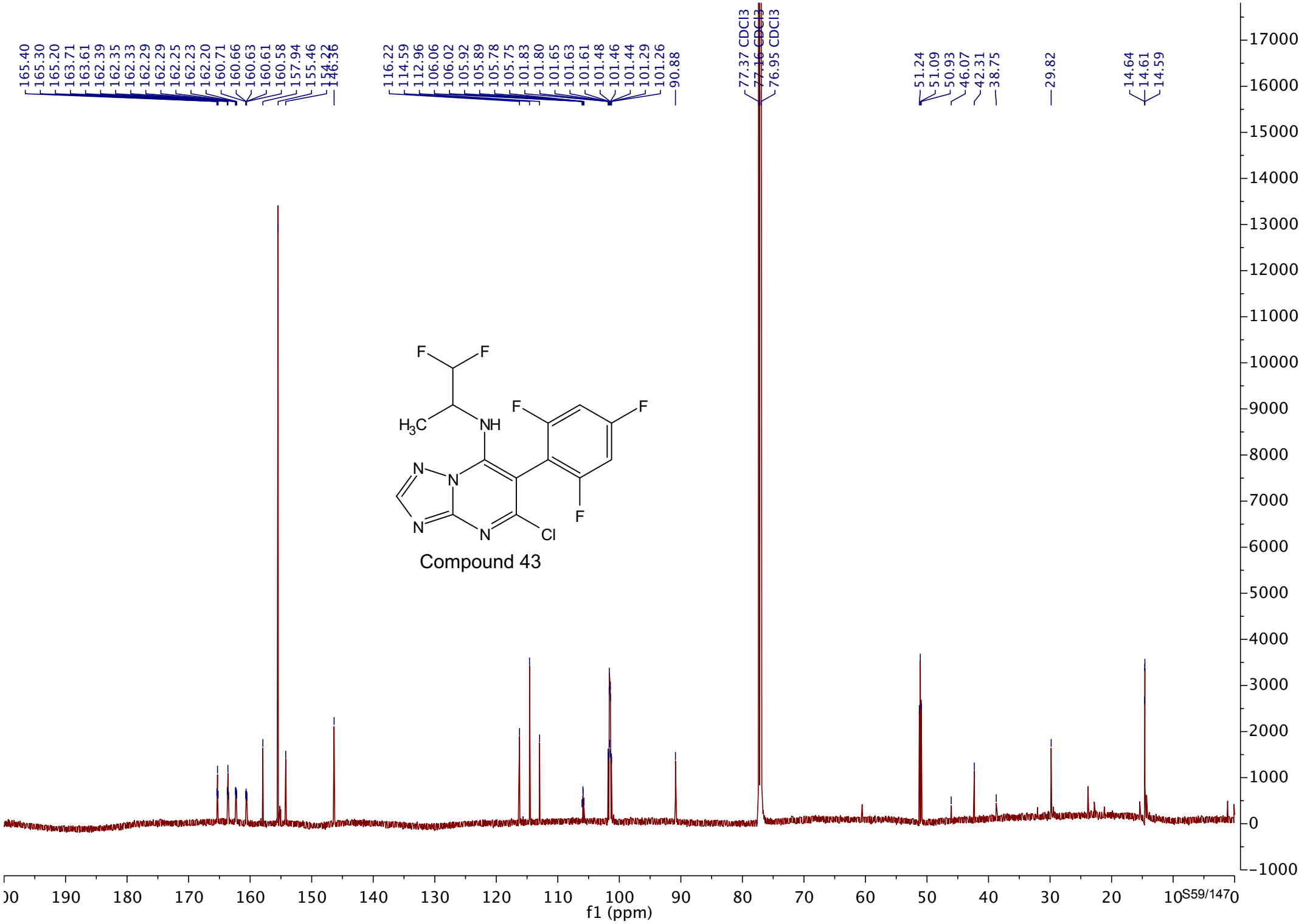
Compound 41

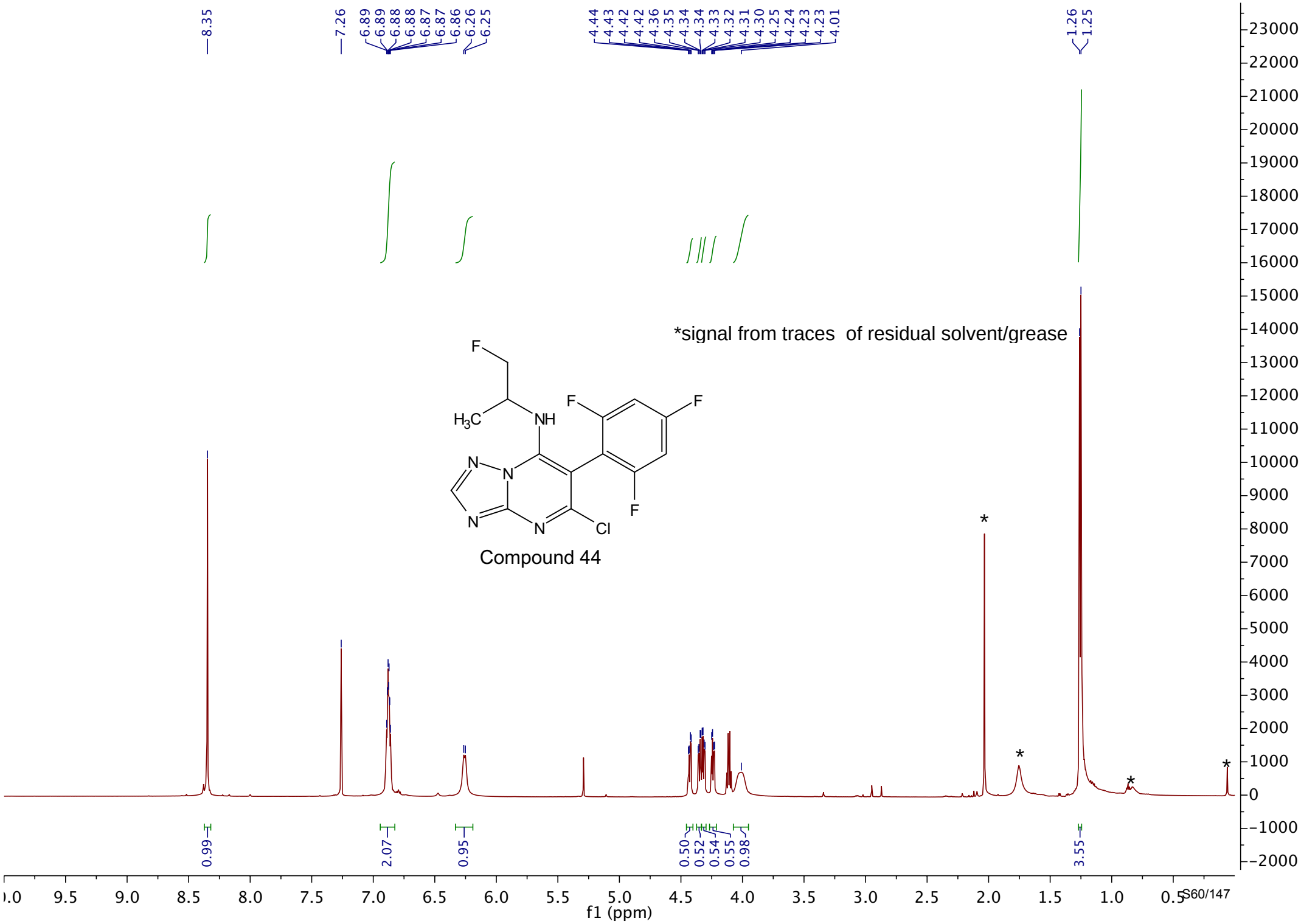

165.46
165.34
165.22
164.02
163.44
163.32
163.20
162.87
162.80
162.75
162.68
160.87
160.81
160.75
160.69
159.80
159.48
159.27
154.03
146.41
135.31
129.33
129.32
129.32
129.31
129.30
129.29
129.28
129.27
129.26
129.25
129.25
128.76
126.81
126.80
126.78
106.71
106.59
106.55
106.38
101.15
101.13
100.94
100.91
100.73
100.70
90.43
77.16 CDCl3
47.75
NH
F
F
F
N
N
N
N
Cl
Compound 41
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

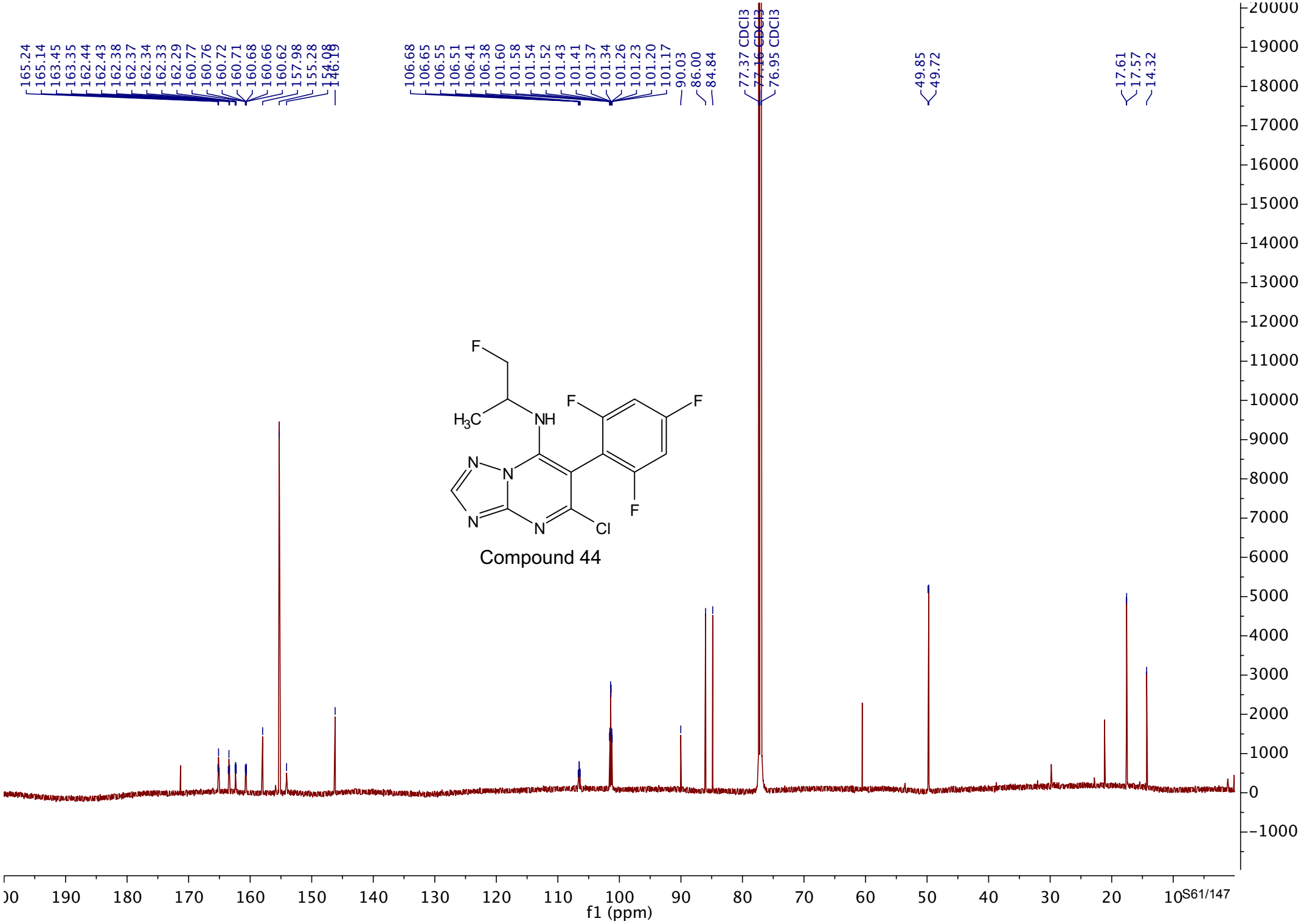

8.51
8.51
7.26 CDCl3
6.85
6.85
6.84
6.84
6.84
6.83
6.18
6.18
6.17
6.17
6.16
6.16
1.64
1.62
F
F
F
H3C
O
F
F
N
N
N
N
Cl
F
Compound 42
*signal from traces of residual solvent/grease
0.97
2.04
1.00
3.14
f1 (ppm)
S56/147

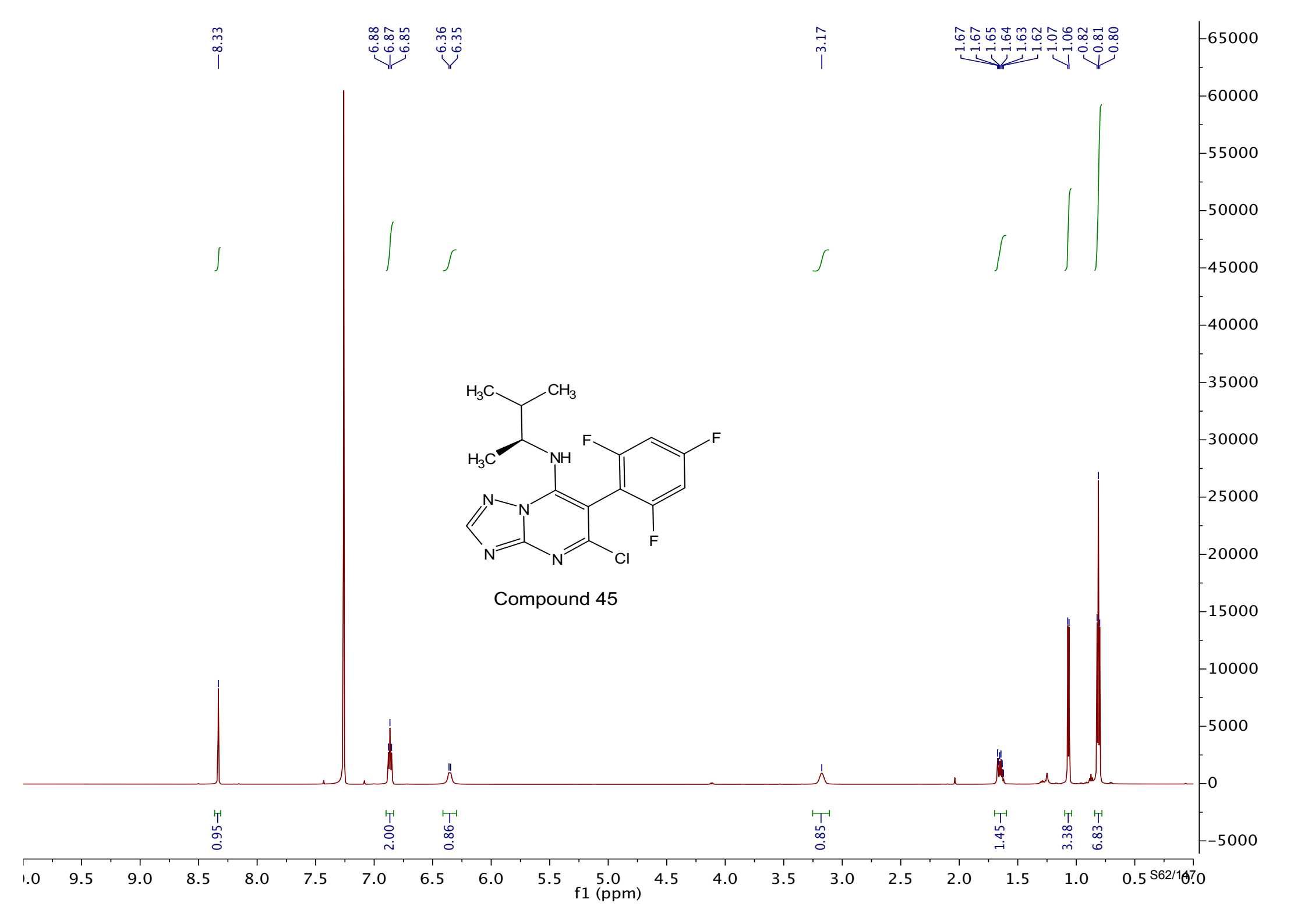

164.98
163.40
163.30
162.04
161.98
161.94
161.88
161.78
161.72
161.68
161.62
160.36
160.30
160.26
160.20
160.11
160.05
160.01
159.95
158.43
156.71
155.74
155.45
151.92
126.02
124.16
122.91
122.29
121.04
120.43
104.26
104.22
104.12
104.09
103.98
103.95
101.31
101.09
101.06
100.91
100.89
100.85
100.74
100.70
100.67
100.53
100.50
100.04
99.81
99.63
99.43
99.25
77.16 CDCl3
76.35
76.13
75.90
75.69
14.07
F
F
F
H3C
O
F
F
N
N
N
N
Cl
Compound 42
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
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
f1 (ppm)
S57/147

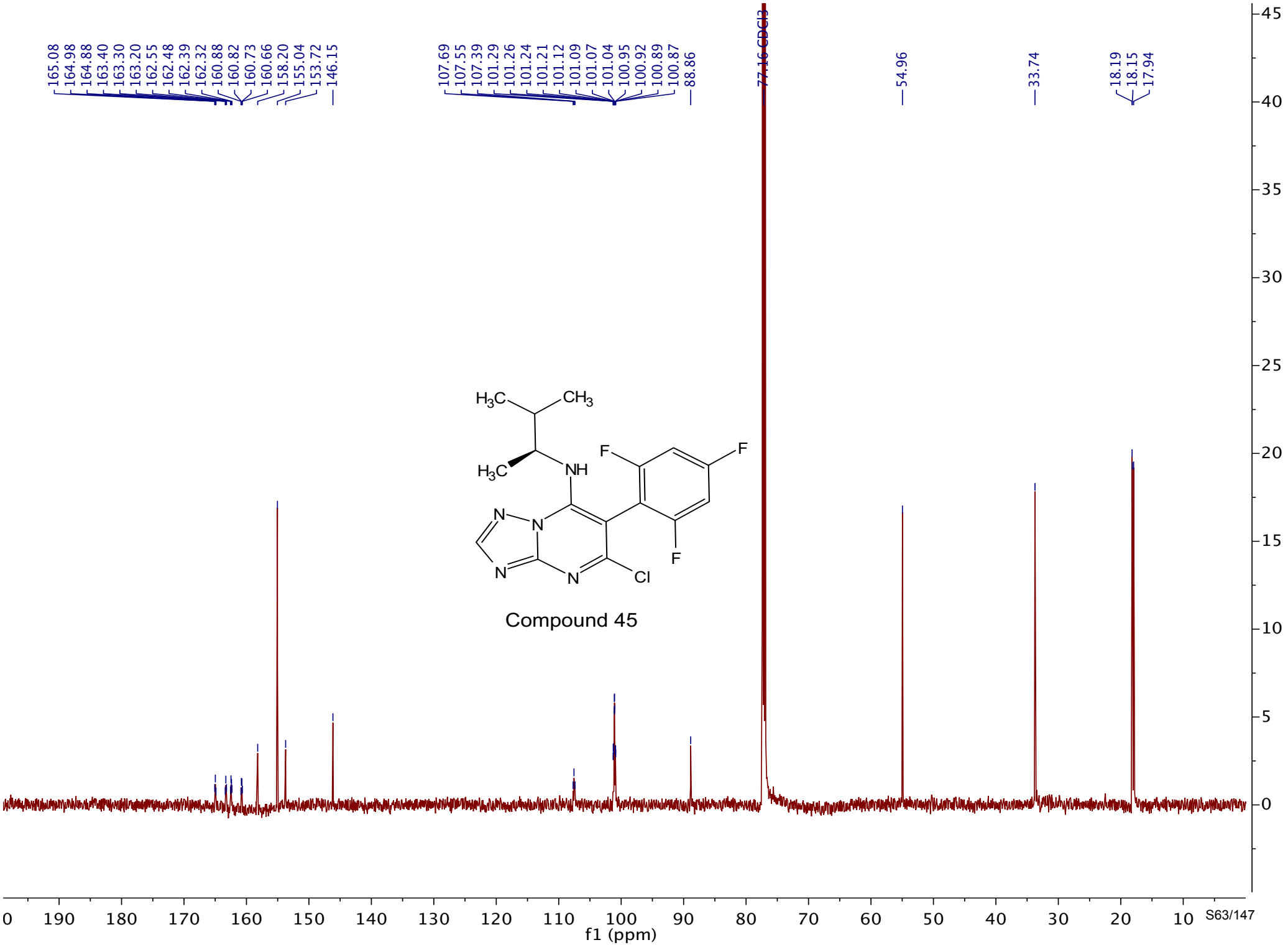

8.37
7.26
6.90
6.89
6.88
6.01
6.00
5.84
5.84
5.75
5.74
5.65
5.65
4.32
1.31
1.30
F
F
H3C
NH
F
F
N
N
N
N
Cl
F
Compound 43
*signal from traces of residual solvent/grease
0.92
2.03
0.87
1.03
0.90
3.00
f1 (ppm)

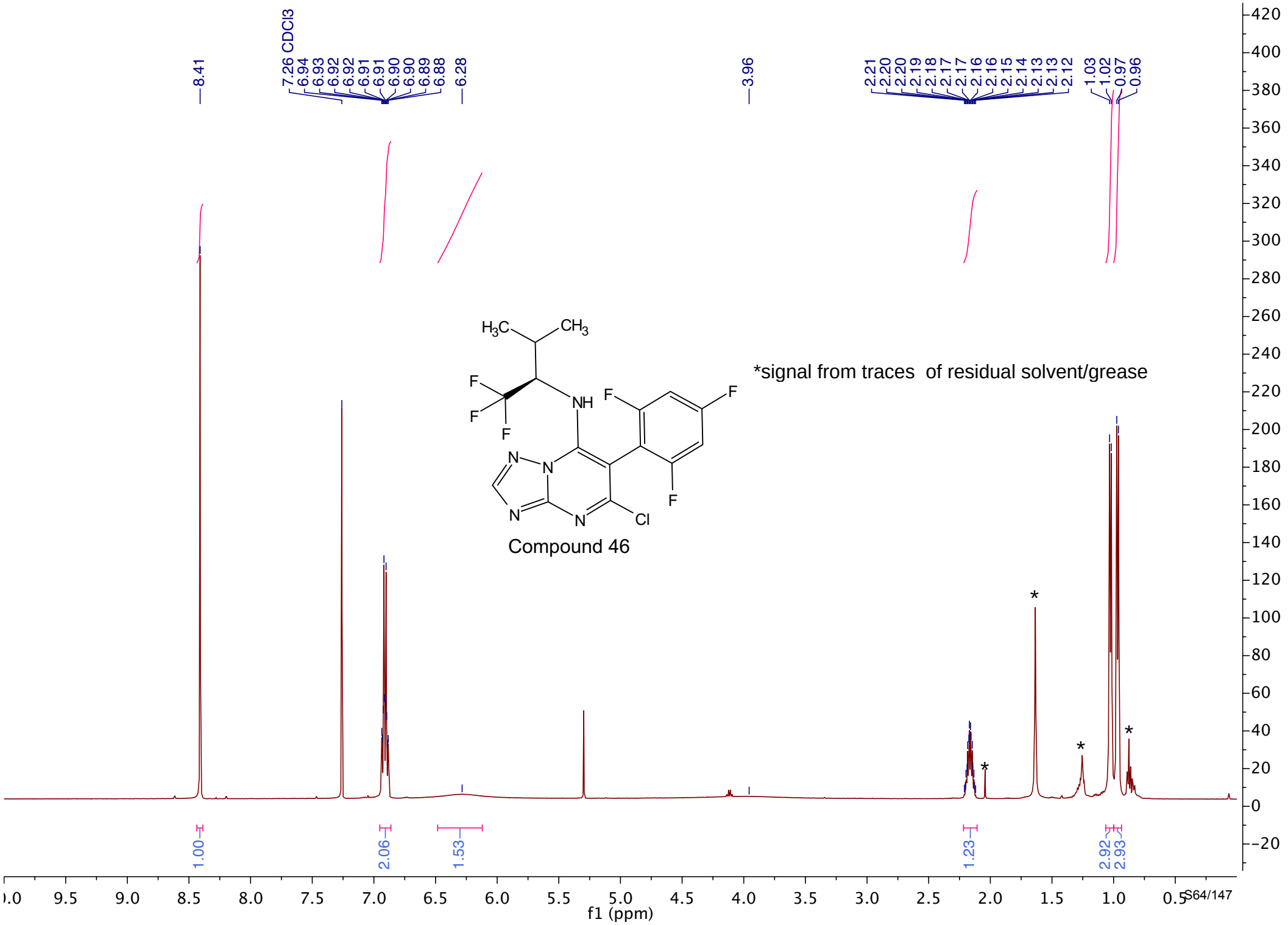

165.40
165.30
165.20
163.71
163.61
162.39
162.35
162.33
162.29
162.29
162.25
162.23
162.20
160.71
160.66
160.63
160.61
160.58
157.94
155.46
116.22
114.59
112.96
106.06
106.02
105.92
105.89
105.78
105.75
101.83
101.80
101.65
101.63
101.61
101.48
101.46
101.44
101.29
101.26
90.88
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
51.24
51.09
50.93
46.07
42.31
38.75
29.82
14.64
14.61
14.59
F
F
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 43
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

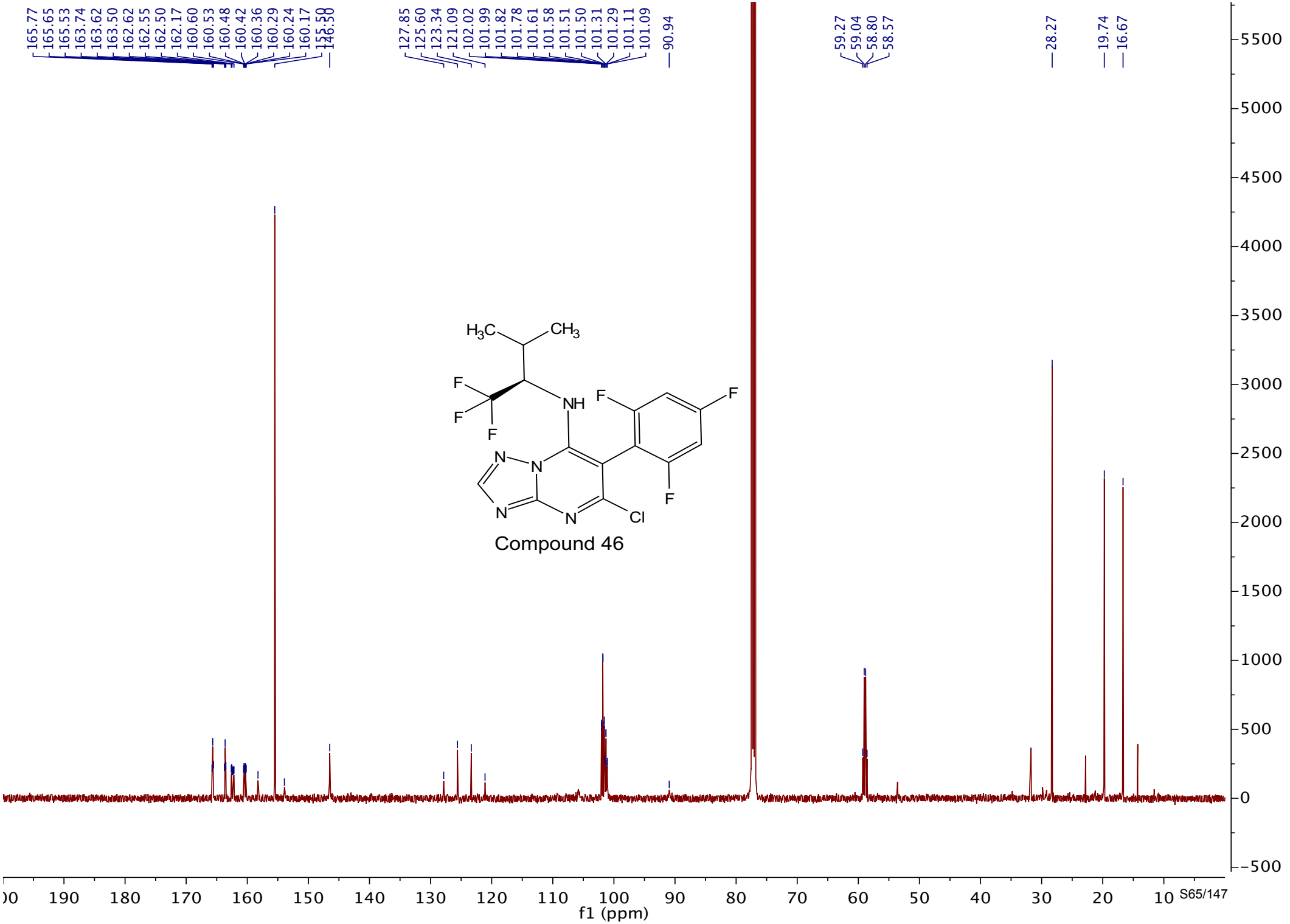

8.35
7.26
6.89
6.89
6.88
6.88
6.87
6.87
6.86
6.26
6.25
4.44
4.43
4.42
4.42
4.36
4.35
4.34
4.34
4.33
4.32
4.31
4.30
4.25
4.24
4.23
4.23
4.01
1.26
1.25
*signal from traces of residual solvent/grease
F
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 44
*
*
*
*
0.99
2.07
0.95
0.50
0.52
0.54
0.55
0.98
3.55
f1 (ppm)
S60/147


165.24
165.14
163.45
163.35
162.44
162.43
162.38
162.37
162.34
162.33
162.29
160.77
160.76
160.72
160.71
160.68
160.66
160.62
157.98
155.28
154.08
146.19
106.68
106.65
106.55
106.51
106.41
106.38
101.60
101.58
101.54
101.52
101.43
101.41
101.37
101.34
101.26
101.23
101.20
101.17
90.03
86.00
84.84
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
49.85
49.72
17.61
17.57
14.32
F
H3C
NH
F
F
N
N
N
N
Cl
F
Compound 44
f1 (ppm)
S61/147

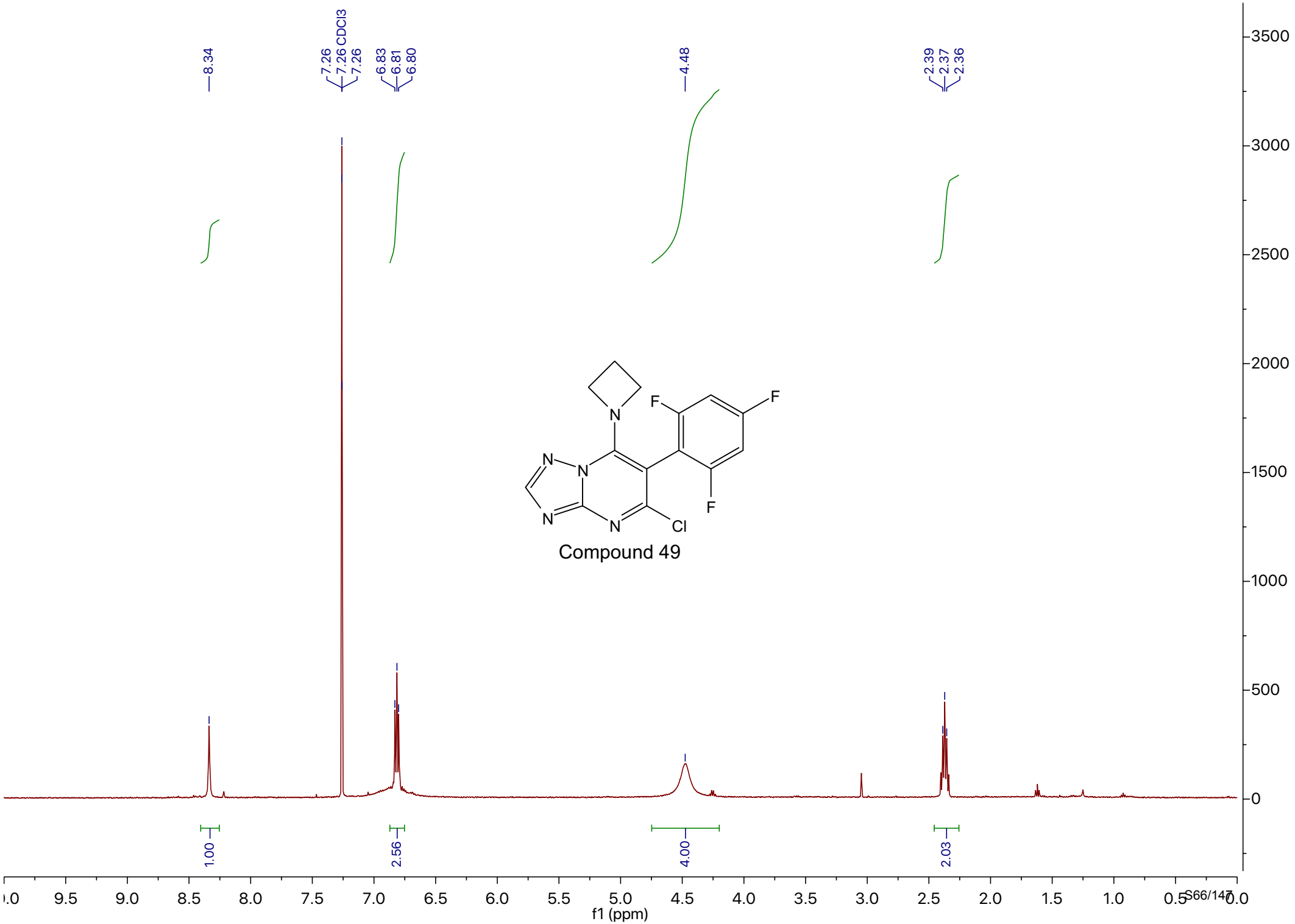

8.33
6.88
6.87
6.85
6.36
6.35
3.17
1.67
1.67
1.65
1.64
1.63
1.62
1.07
1.06
0.82
0.81
0.80
H3C
CH3
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 45
0.95
2.00
0.86
0.85
1.45
3.38
6.83
f1 (ppm)
S62/147


165.08
164.98
164.88
163.40
163.30
163.20
162.55
162.48
162.39
162.32
160.88
160.82
160.73
160.66
158.20
155.04
153.72
146.15
107.69
107.55
107.39
101.29
101.26
101.24
101.21
101.12
101.09
101.07
101.04
100.95
100.92
100.89
100.87
88.86
77.16 CDCl3
54.96
33.74
18.19
18.15
17.94
H3C
CH3
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 45
45
40
35
30
25
20
15
10
5
0
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
S63/147

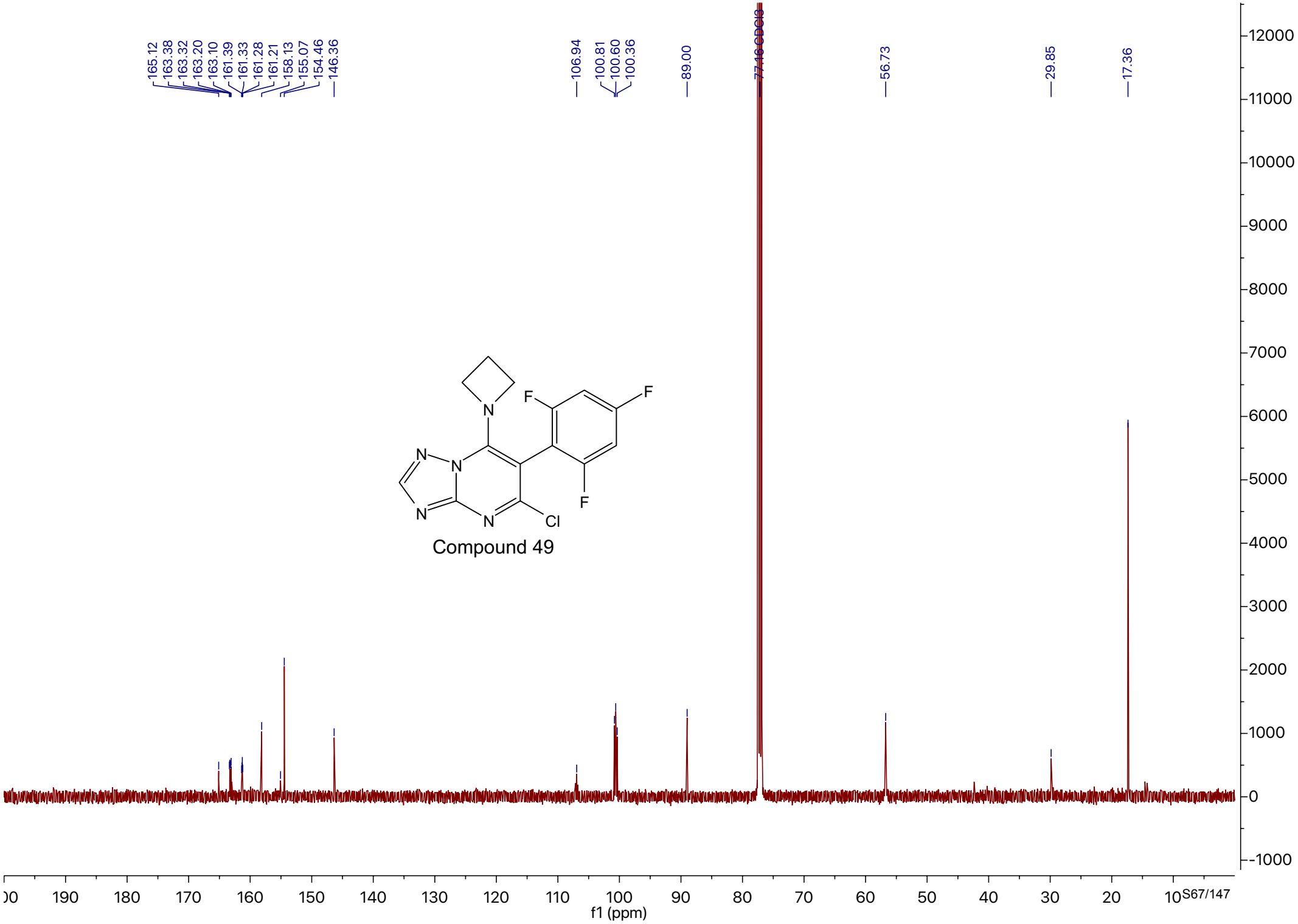

7.26 CDCl3
8.41
6.94
6.93
6.92
6.92
6.91
6.91
6.90
6.90
6.89
6.88
6.28
3.96
2.21
2.20
2.20
2.19
2.18
2.17
2.17
2.16
2.16
2.15
2.14
2.13
2.13
2.12
1.03
1.02
0.97
0.96
H3C
CH3
F
F
F
NH
F
F
N
N
N
N
Cl
F
*signal from traces of residual solvent/grease
Compound 46
1.00
2.06
1.53
1.23
2.92
2.93
f1 (ppm)

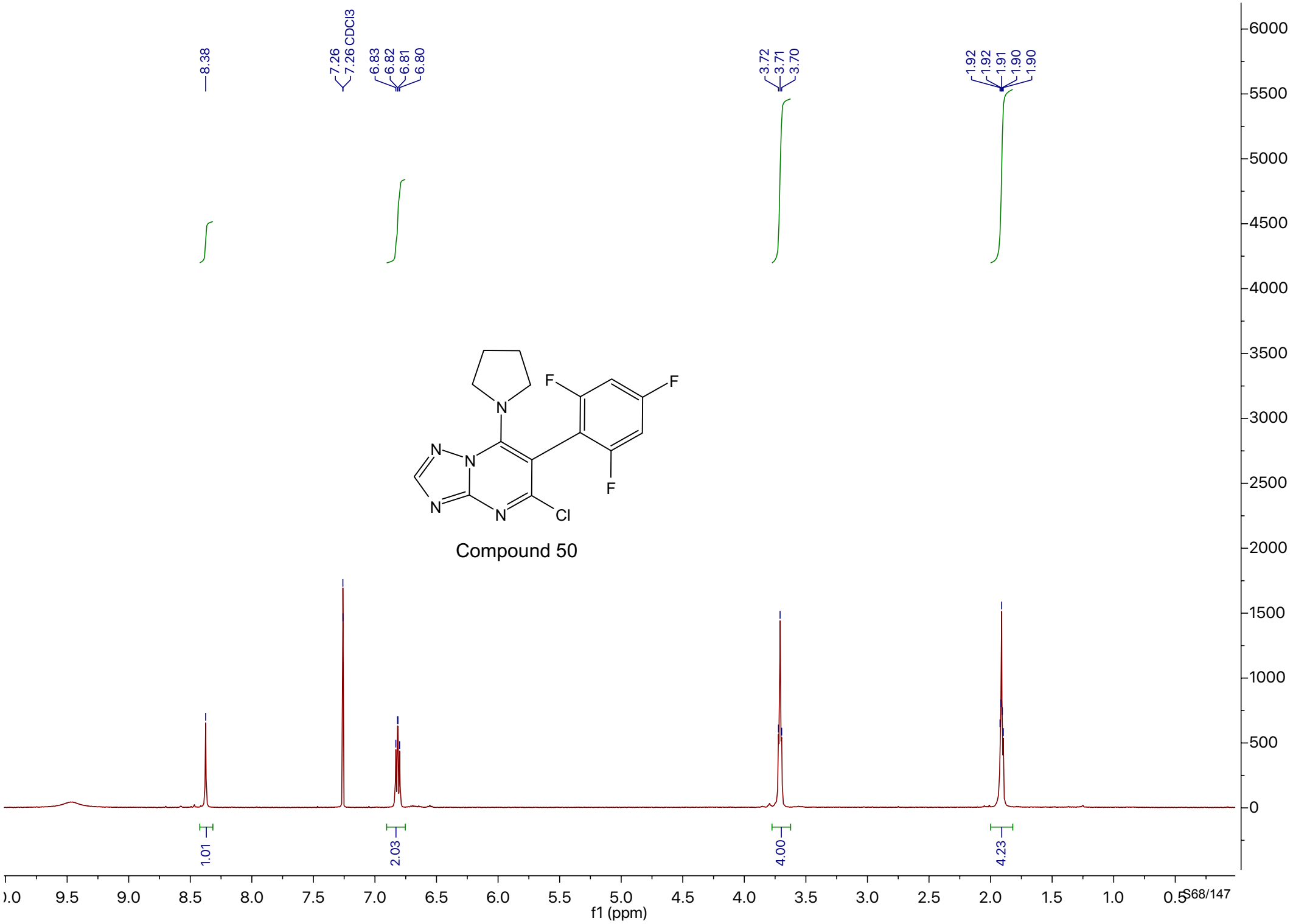

165.77
165.65
165.53
163.74
163.62
163.50
162.62
162.55
162.50
162.17
160.60
160.53
160.48
160.42
160.36
160.29
160.24
160.17
155.50
146.30
127.85
125.60
123.34
121.09
102.02
101.99
101.82
101.78
101.61
101.58
101.51
101.50
101.31
101.29
101.11
101.09
90.94
59.27
59.04
58.80
58.57
28.27
19.74
16.67
H3C
CH3
F
F
F
NH
F
F
F
N
N
N
N
Cl
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

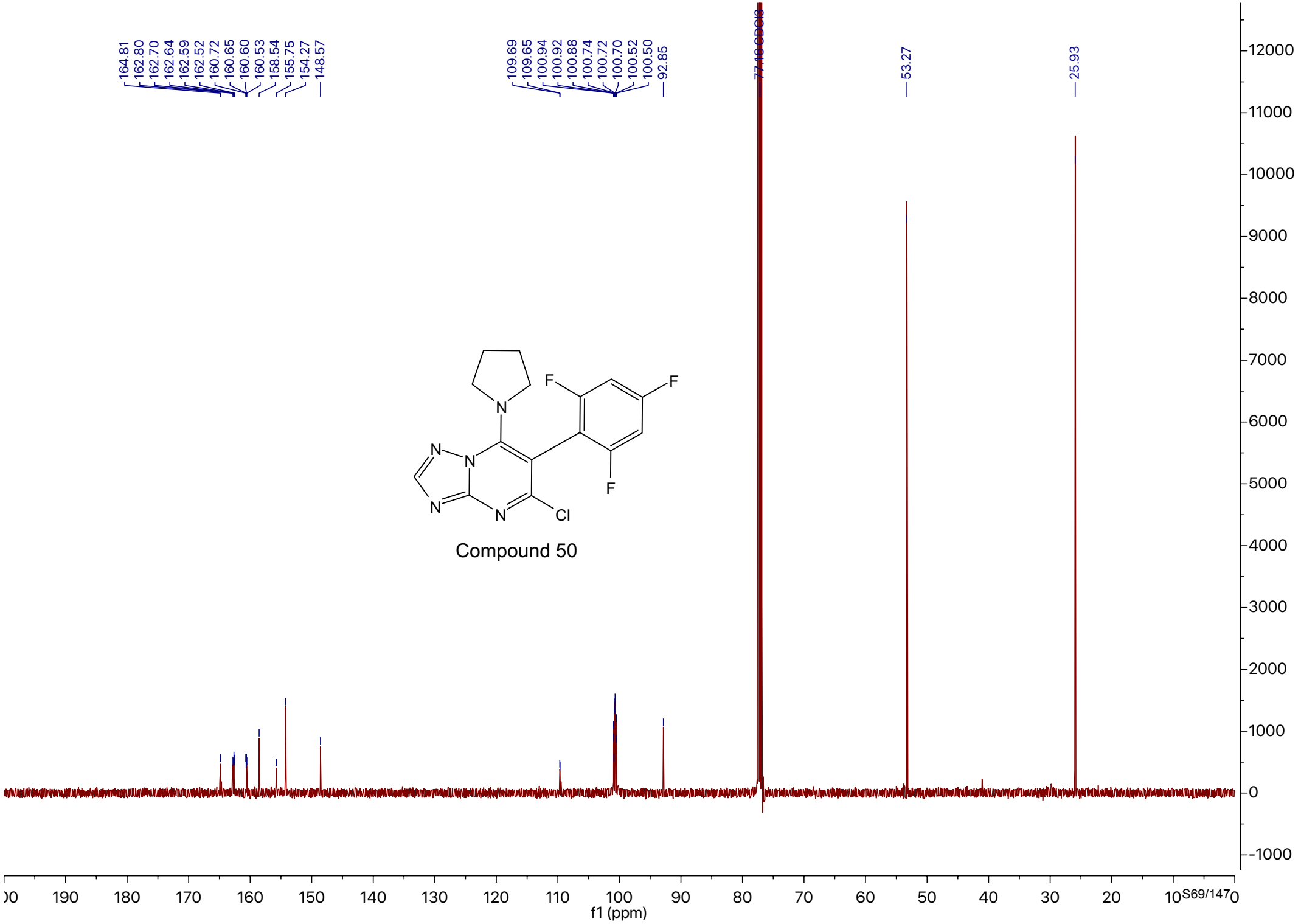
Compound 46


8.34
7.26
7.26 CDCl3
7.26
6.83
6.81
6.80
4.48
2.39
2.37
2.36
F
F
F
N
N
N
N
N
Cl
1.00
2.56
4.00
2.03
3500
3000
2500
2000
1500
1000
500
0
f1 (ppm)

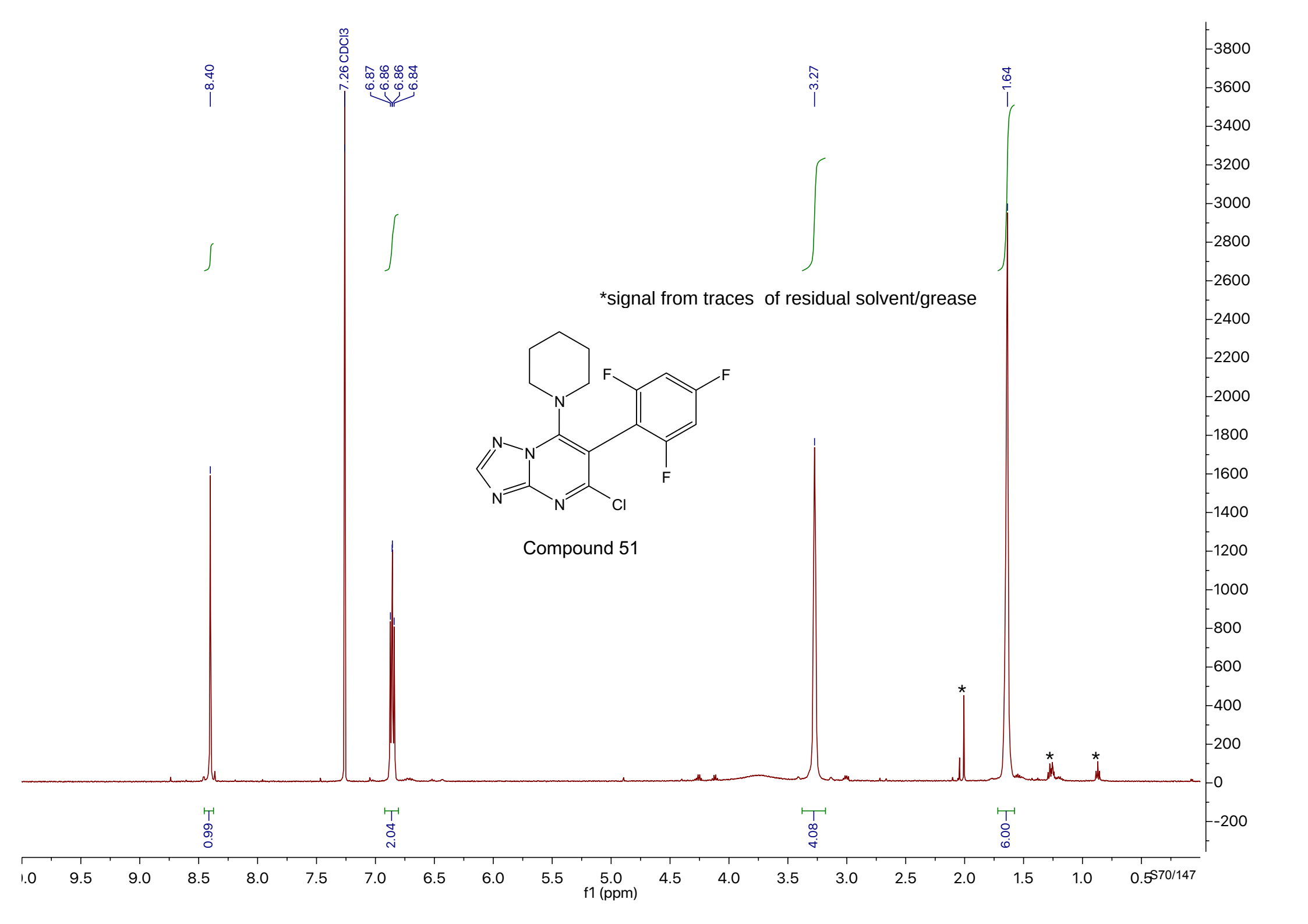
Compound 49

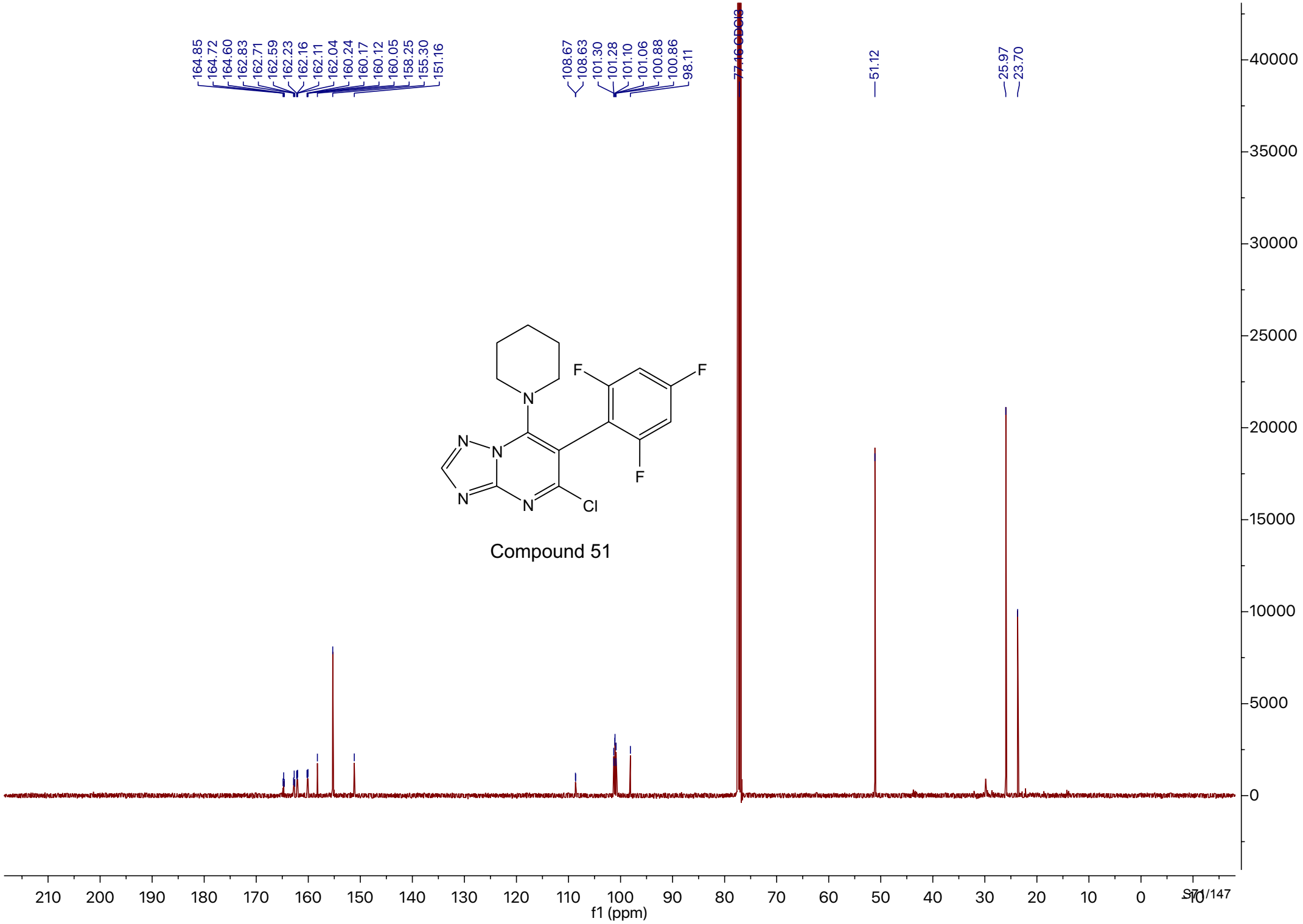

165.12
163.38
163.32
163.20
163.10
161.39
161.33
161.28
161.21
158.13
155.07
154.46
146.36
106.94
100.81
100.60
100.36
89.00
77.16 CDCl3
56.73
29.85
17.36
F
F
F
N
N
N
N
N
Cl
Compound 49
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.38
7.26
7.26 CDCl3
6.83
6.82
6.81
6.80
3.72
3.71
3.70
1.92
1.92
1.91
1.90
1.90
F
F
F
N
N
N
N
N
Cl
Compound 50
1.01
2.03
4.00
4.23
f1 (ppm)

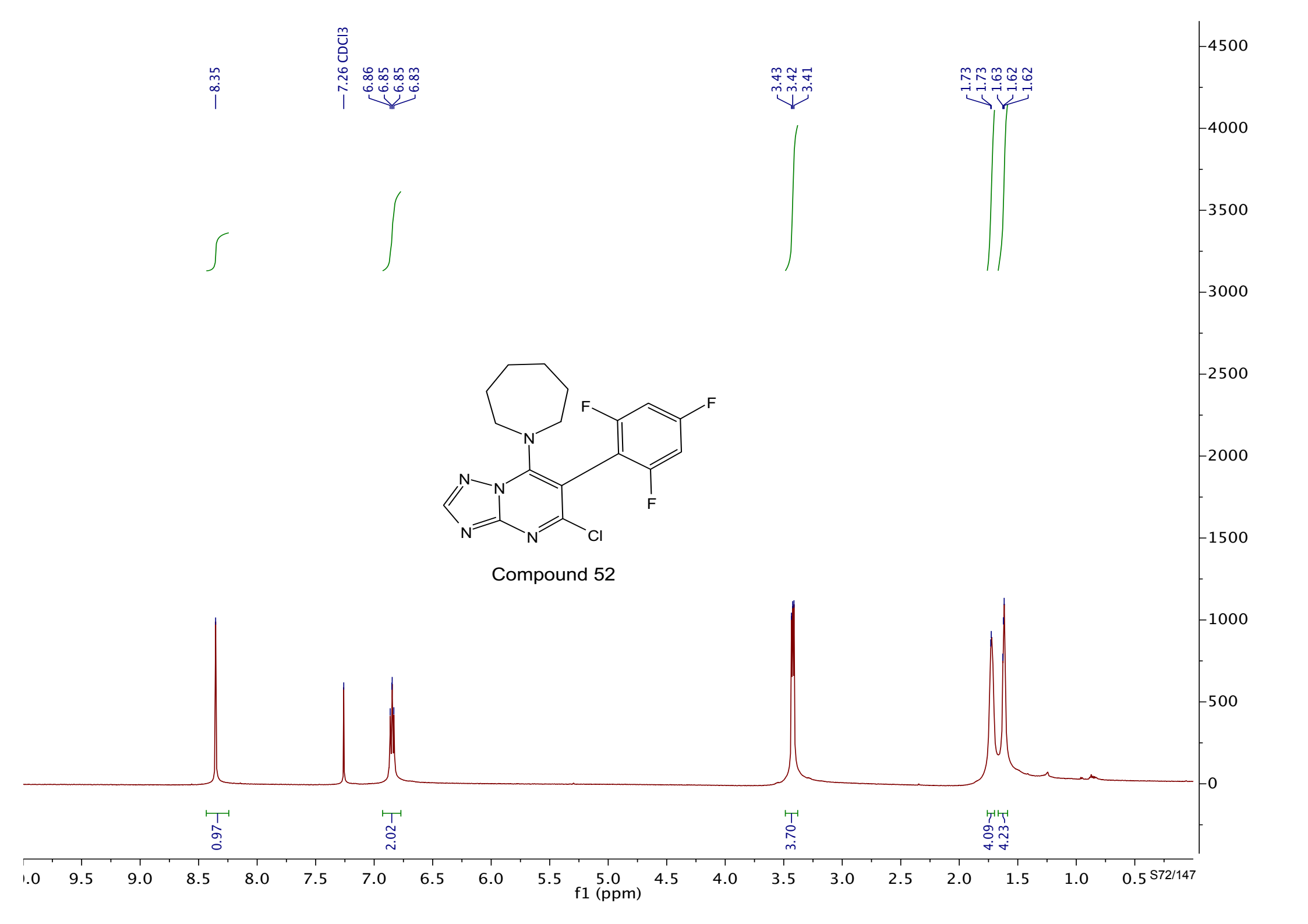

164.81
162.80
162.70
162.64
162.59
162.52
160.72
160.65
160.60
160.53
158.54
155.75
154.27
148.57
109.69
109.65
100.94
100.92
100.88
100.74
100.72
100.70
100.52
100.50
92.85
77.16 CDCl3
53.27
25.93
F
F
F
N
N
N
N
N
Cl
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Compound 50

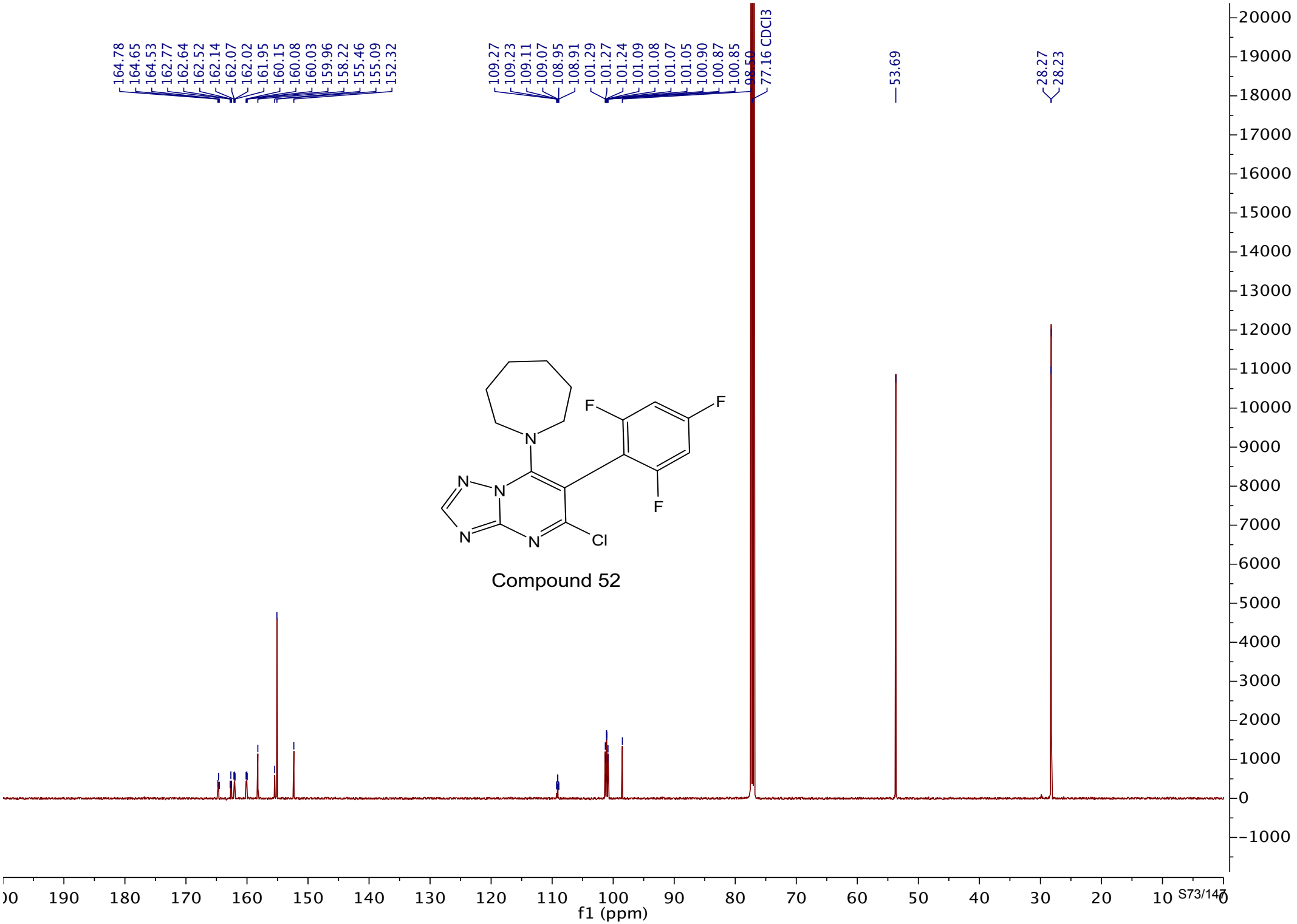

8.40
7.26 CDCl3
6.87
6.86
6.86
6.84
3.27
1.64
*signal from traces of residual solvent/grease
F
F
F
N
N
N
N
N
Cl
Compound 51
0.99
2.04
4.08
6.00
f1 (ppm)
S70/147

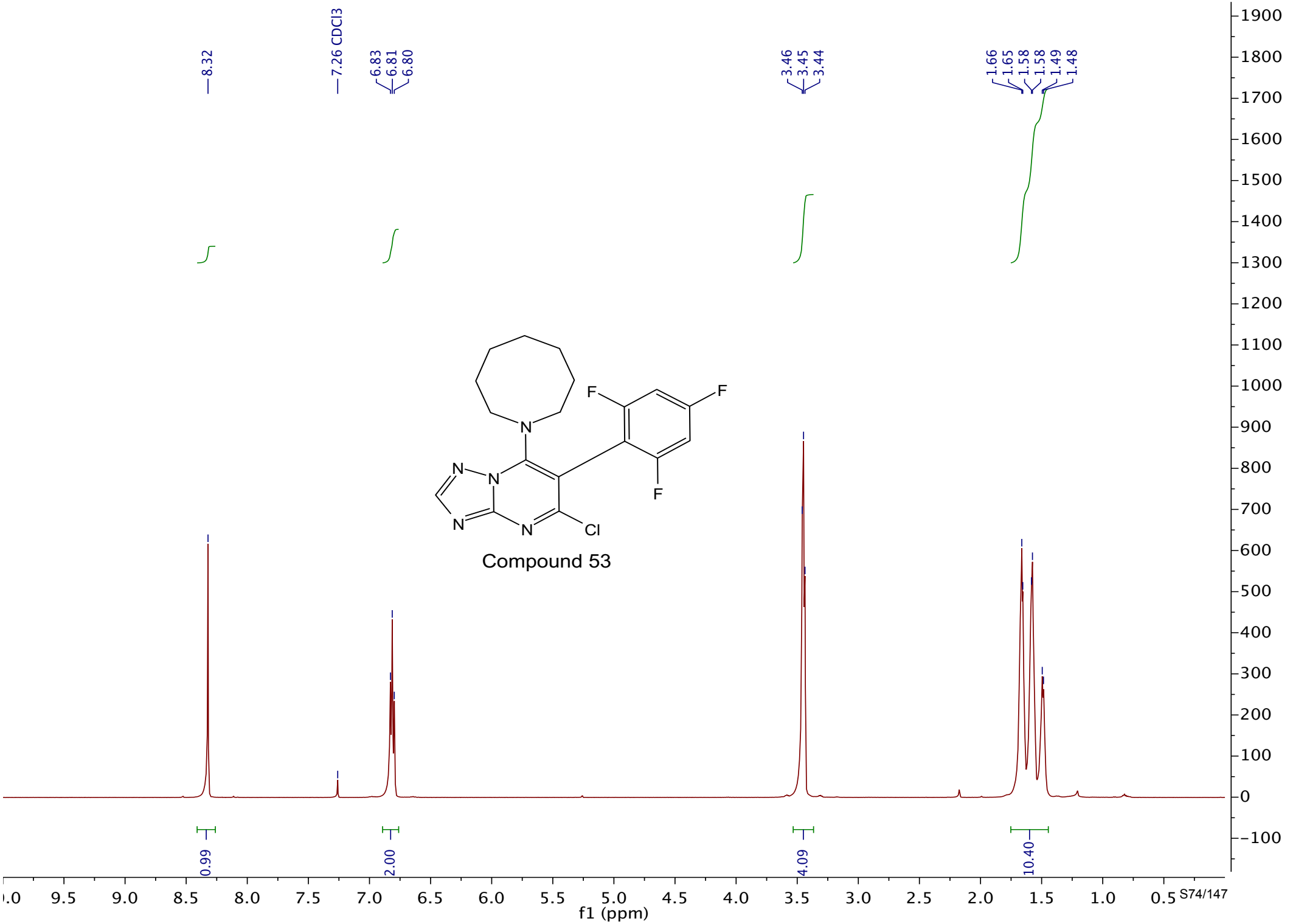

164.85
164.72
164.60
162.83
162.71
162.59
162.23
162.16
162.11
162.04
160.24
160.17
160.12
160.05
158.25
155.30
151.16
108.67
108.63
101.30
101.28
101.10
101.06
100.88
100.86
98.11
77.16 CDCl3
51.12
25.97
23.70
F
F
F
N
N
N
N
N
Cl
40000
35000
30000
25000
20000
15000
10000
5000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Compound 51

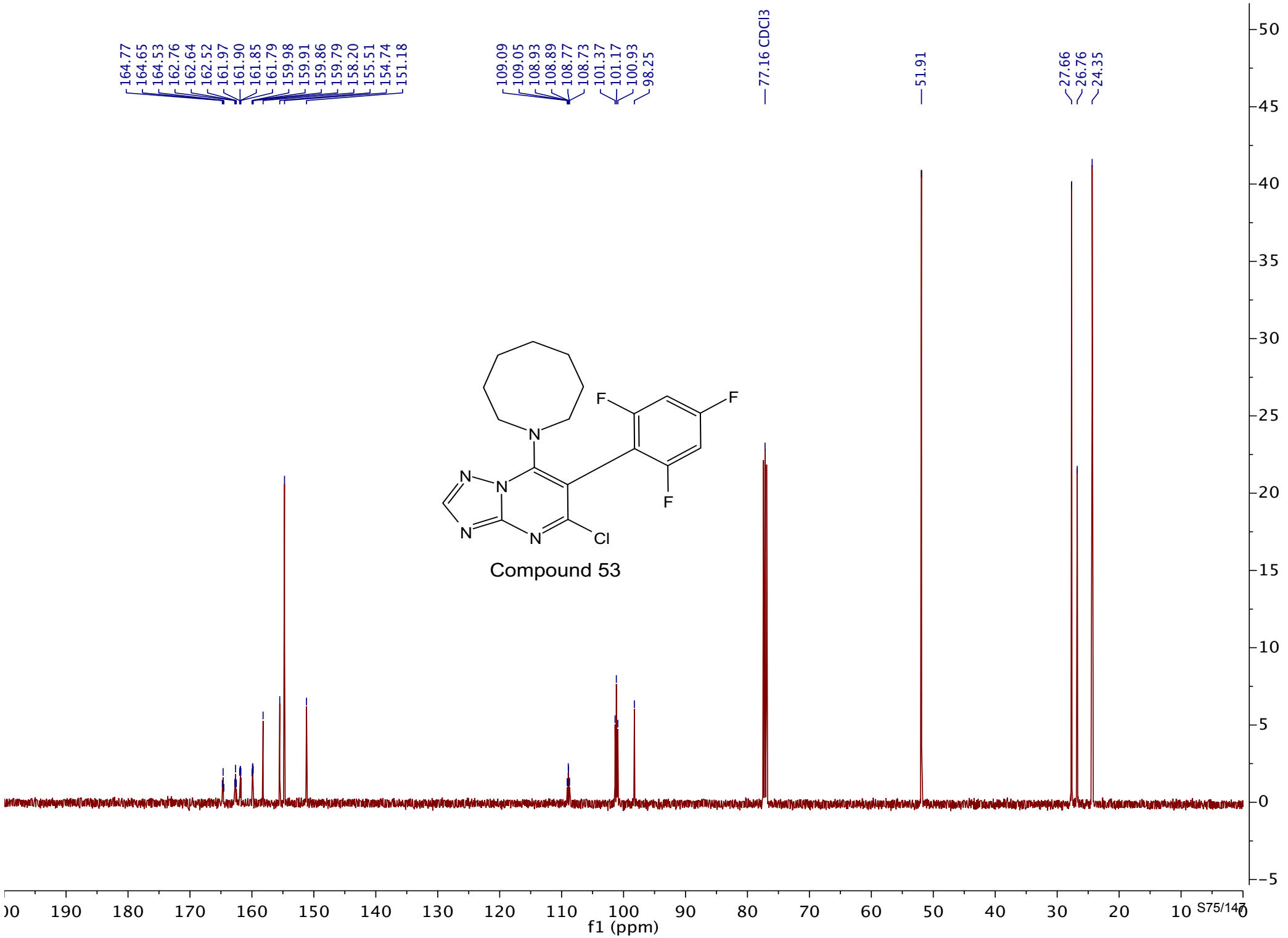

8.35
7.26 CDCl3
6.86
6.85
6.85
6.83
3.43
3.42
3.41
1.73
1.73
1.63
1.62
1.62
F
F
F
N
N
N
N
N
Cl
0.97
2.02
3.70
4.09
4.23
f1 (ppm)

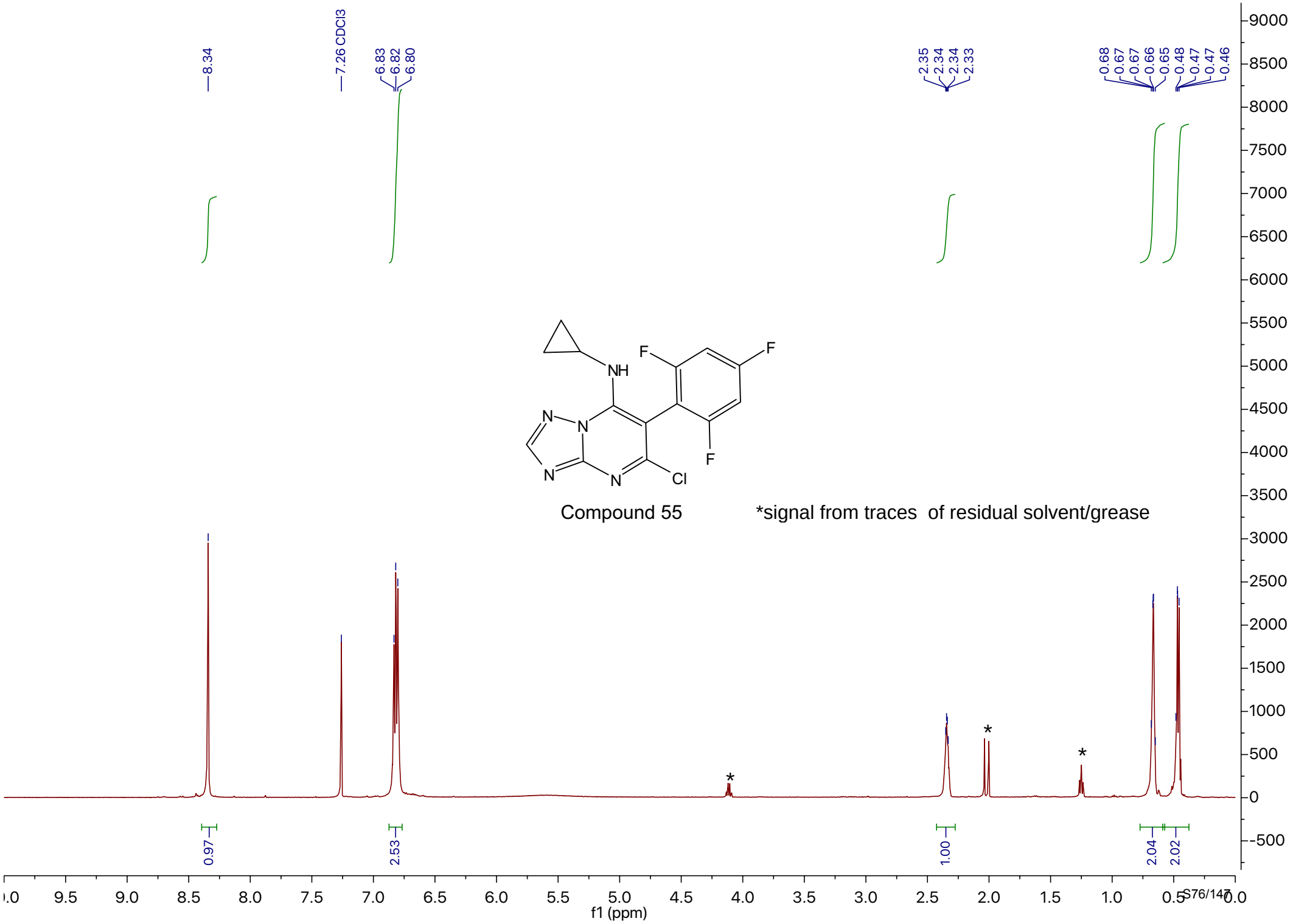
Compound 52


164.78
164.65
164.53
162.77
162.64
162.52
162.14
162.07
162.02
161.95
160.15
160.08
160.03
159.96
158.22
155.46
155.09
152.32
109.27
109.23
109.11
109.07
108.95
108.91
101.29
101.27
101.24
101.09
101.08
101.07
101.05
100.90
100.87
100.85
98.50
77.16 CDCl3
53.69
28.27
28.23
F
F
F
N
N
N
N
N
Cl
Compound 52
f1 (ppm)
S73/147


8.32
7.26 CDCl3
6.83
6.81
6.80
3.46
3.45
3.44
1.66
1.65
1.58
1.58
1.49
1.48
F
F
F
N
N
N
N
N
Cl
0.99
2.00
4.09
10.40
f1 (ppm)
S74/147

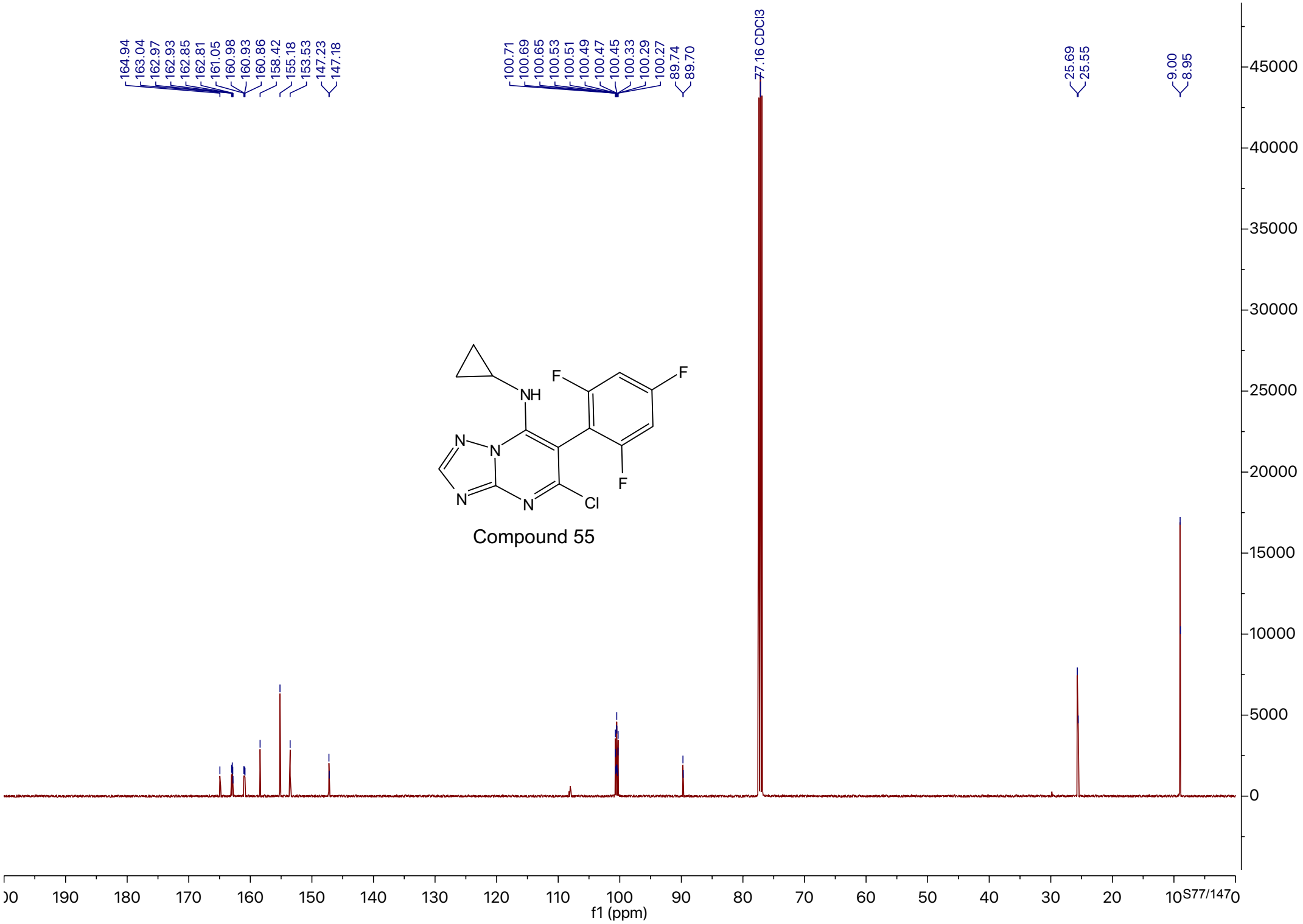
Compound 53


164.77
164.65
164.53
162.76
162.64
162.52
161.97
161.90
161.85
161.79
159.98
159.91
159.86
159.79
158.20
155.51
154.74
151.18
109.09
109.05
108.93
108.89
108.77
108.73
101.37
101.17
100.93
98.25
77.16 CDCl3
51.91
27.66
26.76
24.35
F
F
F
N
N
N
N
N
Cl
Compound 53
f1 (ppm)
S75/147

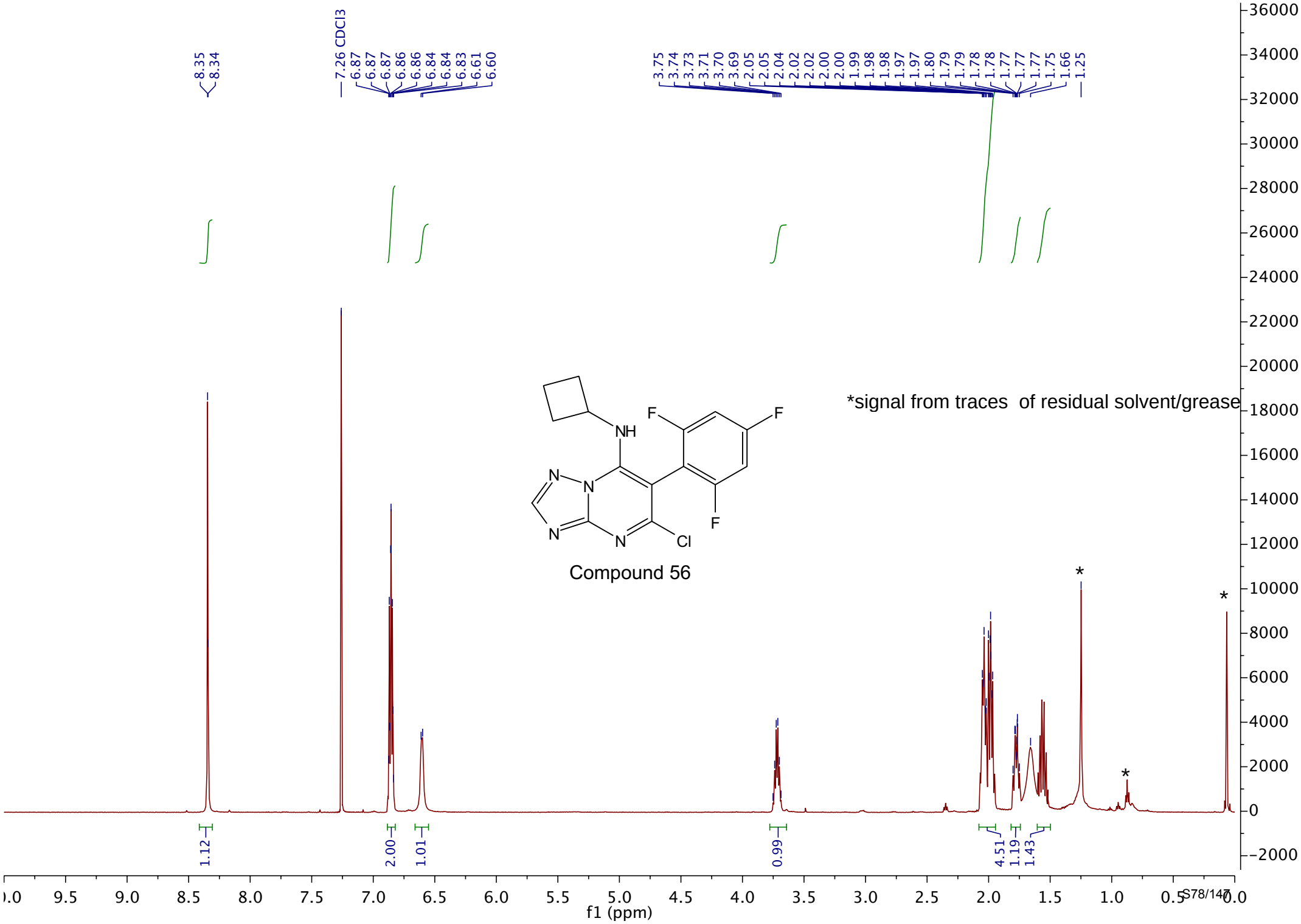


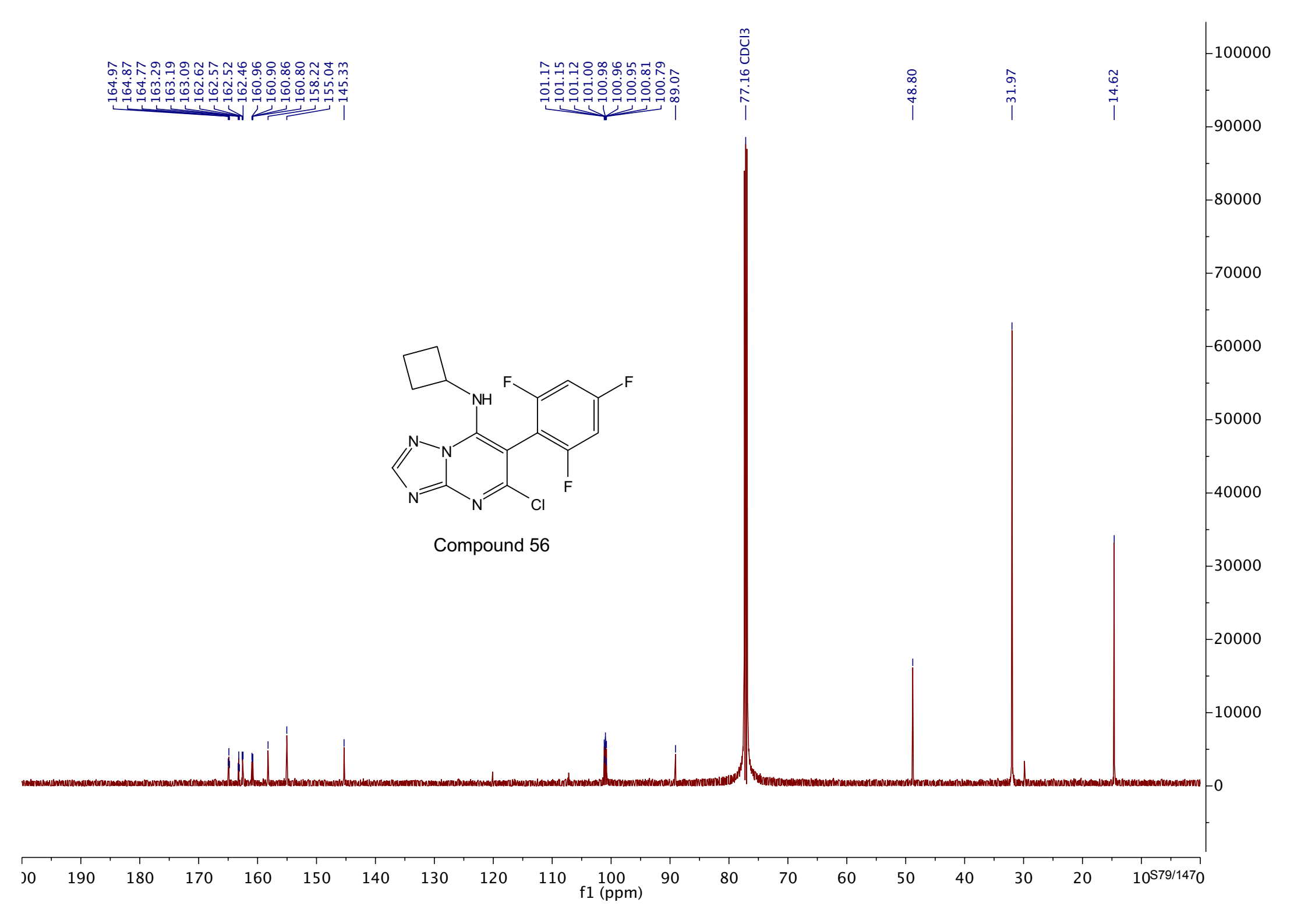
Compound 55

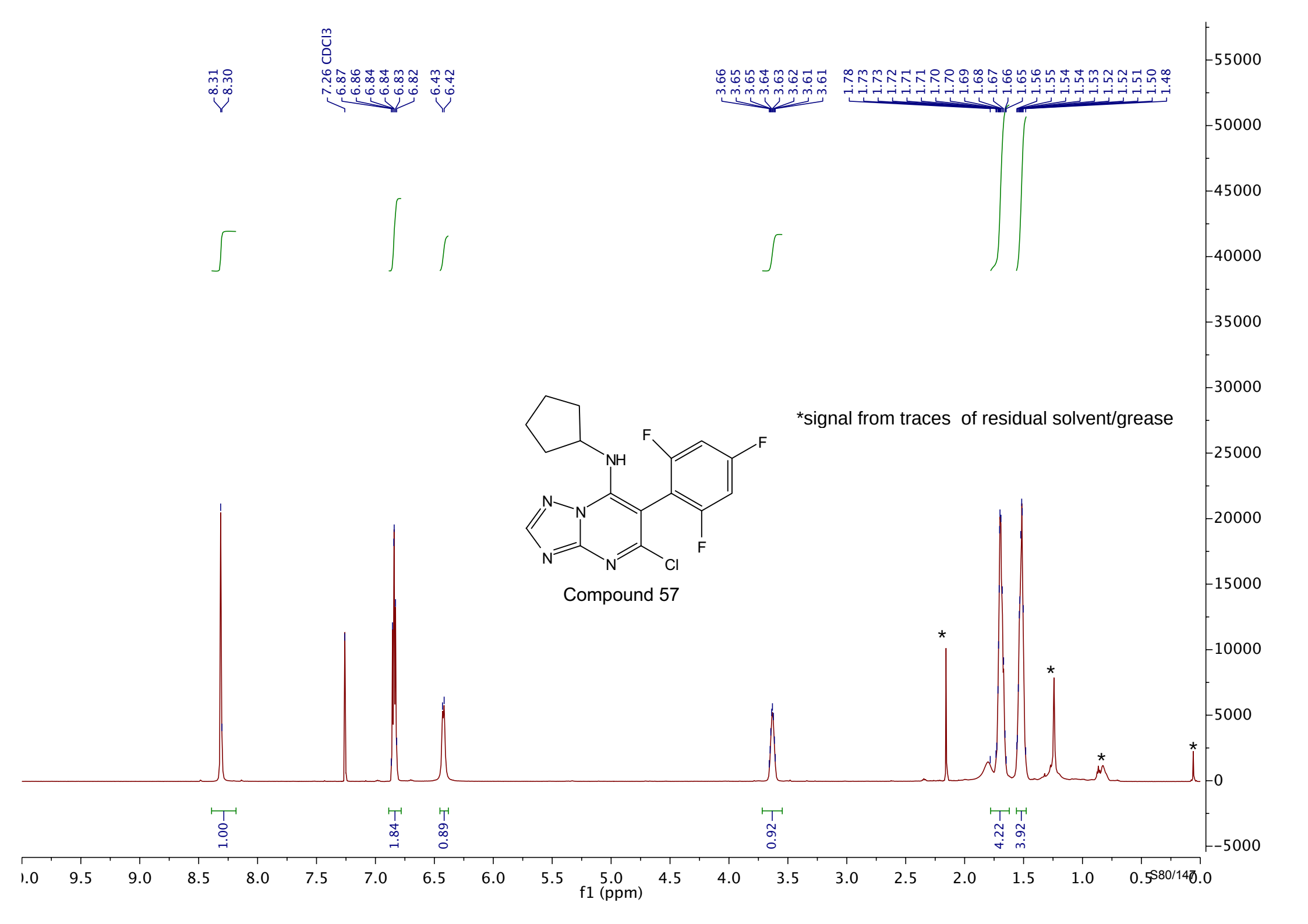
*signal from traces of residual solvent/grease

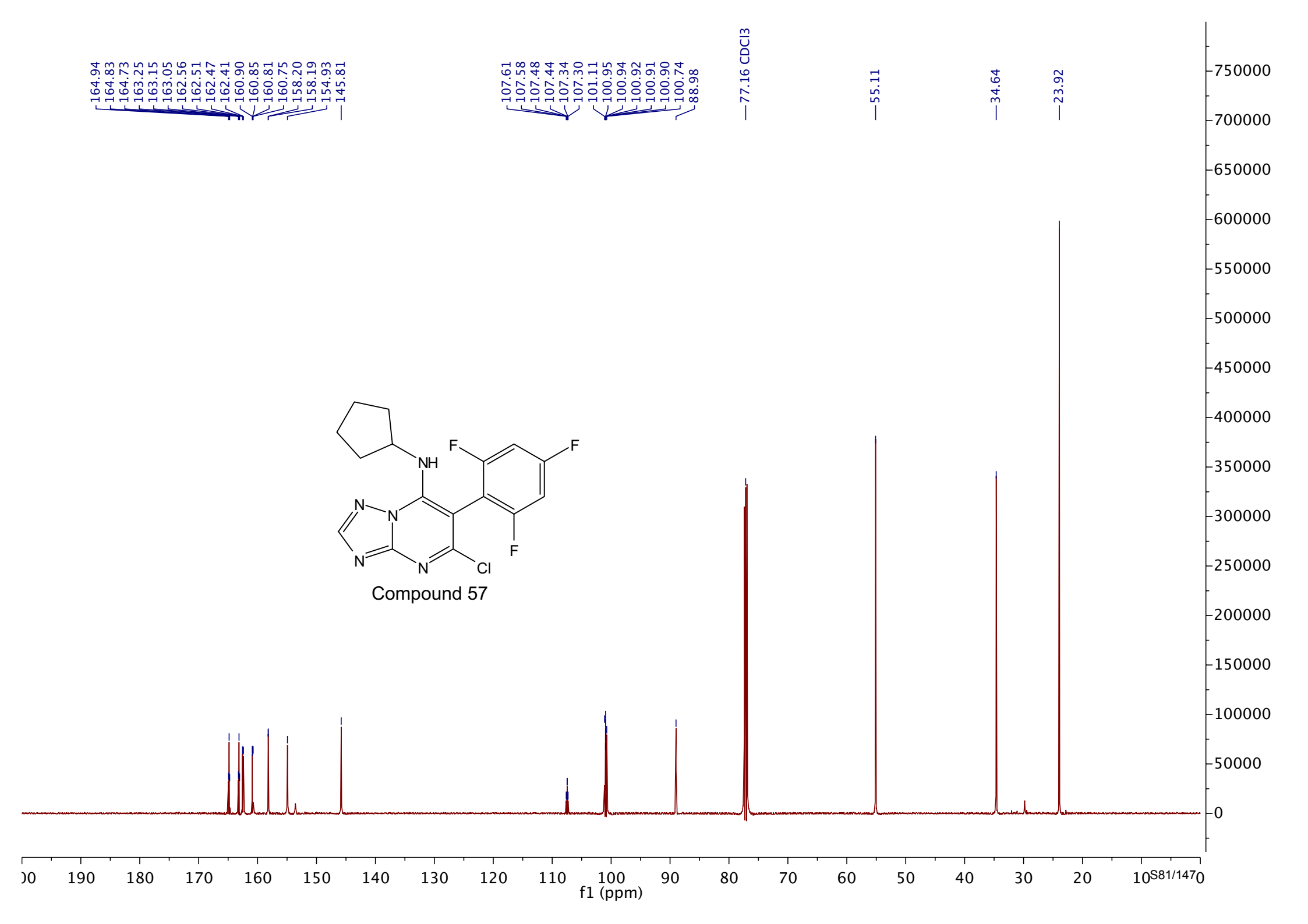

164.94
163.04
162.97
162.93
162.85
162.81
161.05
160.98
160.93
160.86
158.42
155.18
153.53
147.23
147.18
100.71
100.69
100.65
100.53
100.51
100.49
100.47
100.45
100.33
100.29
100.27
89.74
89.70
77.16 CDCl3
25.69
25.55
9.00
8.95
NH
F
F
F
N
N
N
N
Cl
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

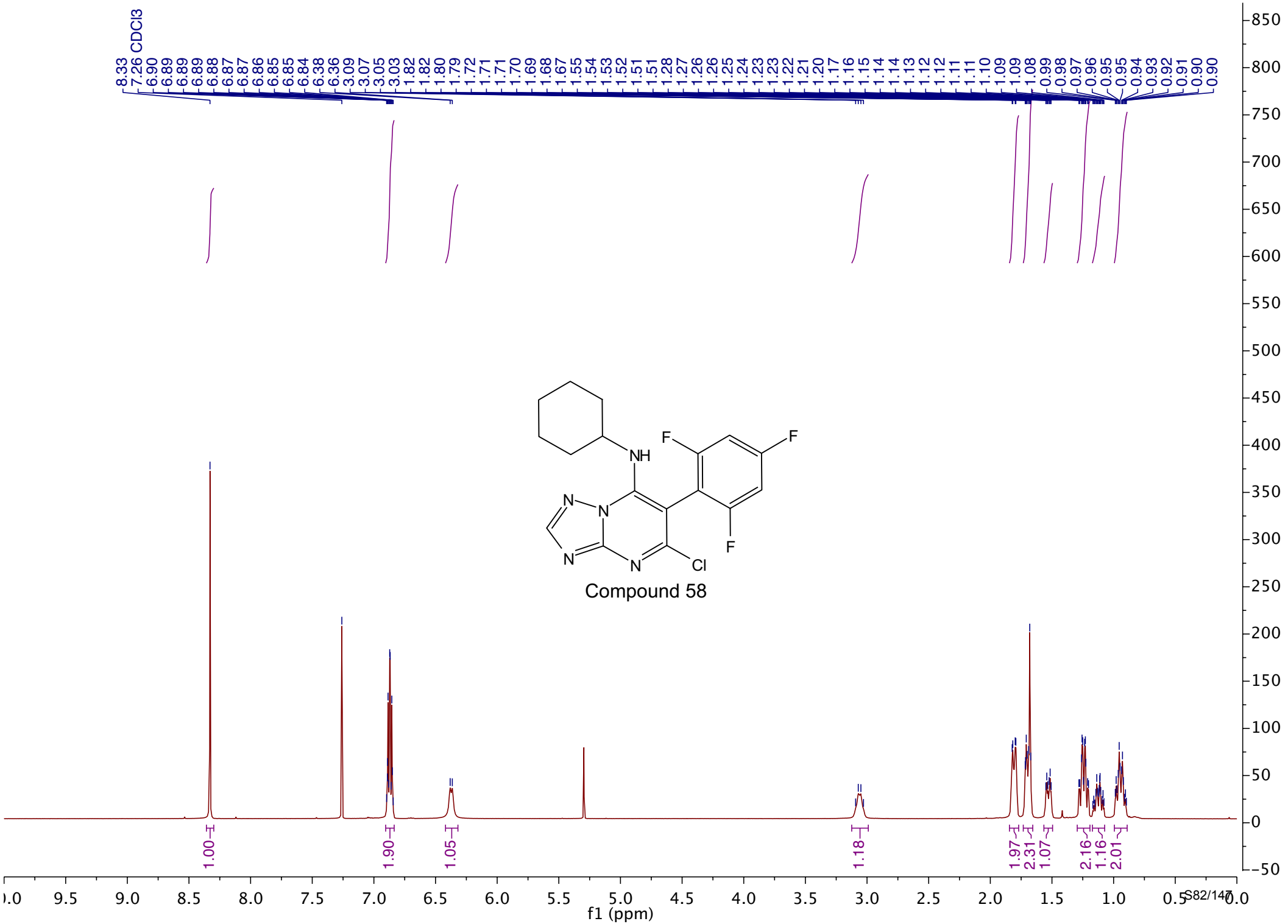
Compound 55


8.35
8.34
7.26 CDCl3
6.87
6.87
6.87
6.86
6.86
6.84
6.84
6.83
6.61
6.60
3.75
3.74
3.73
3.71
3.70
3.69
2.05
2.05
2.04
2.02
2.02
2.00
2.00
1.99
1.98
1.98
1.97
1.97
1.80
1.79
1.79
1.78
1.78
1.77
1.77
1.77
1.75
1.66
1.25
NH
F
F
F
N
N
N
N
Cl
Compound 56
*signal from traces of residual solvent/grease
1.12
2.00
1.01
0.99
4.51
1.19
1.43
f1 (ppm)

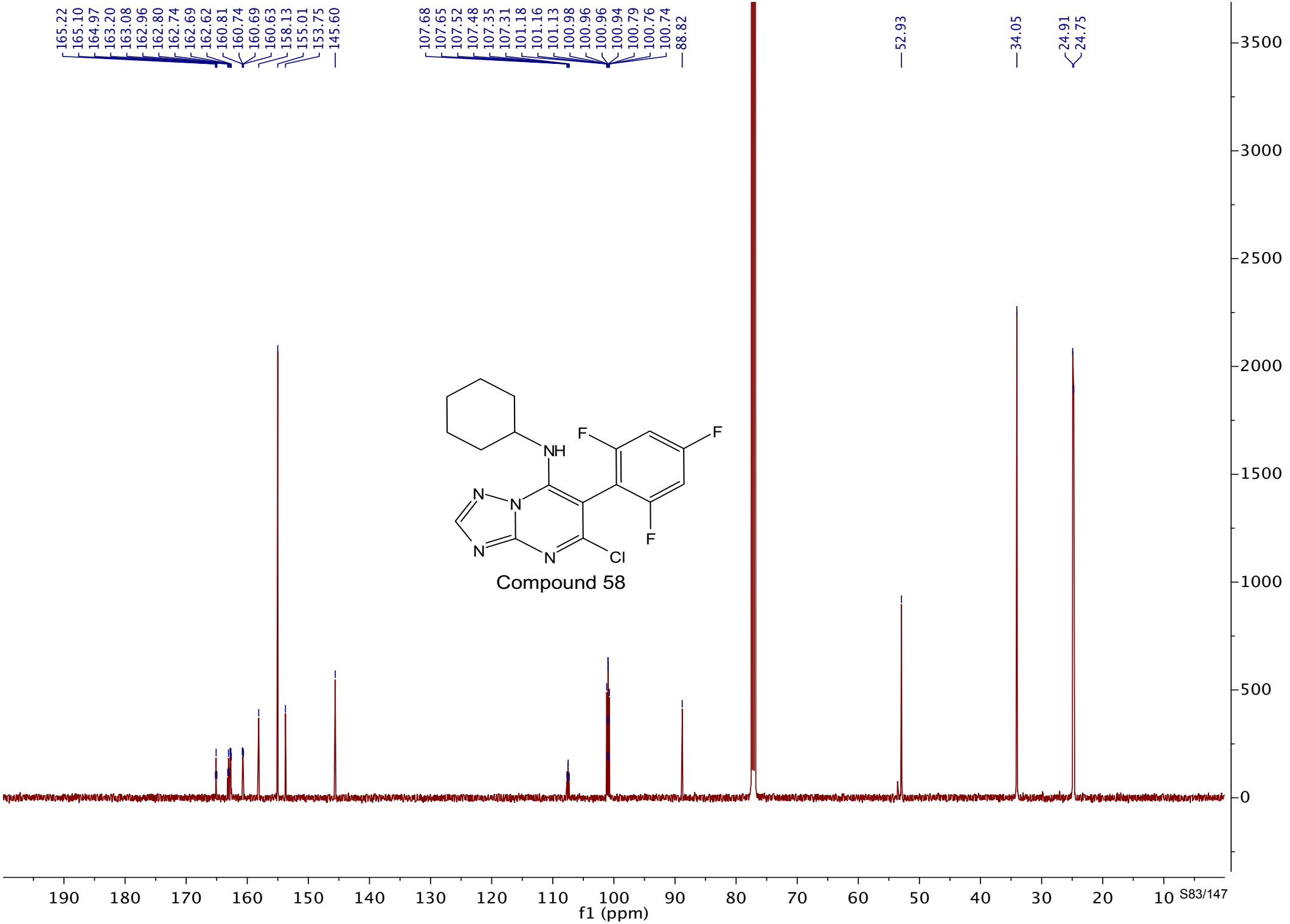

164.97
164.87
164.77
163.29
163.19
163.09
162.62
162.57
162.52
162.46
160.96
160.90
160.86
160.80
158.22
155.04
145.33
101.17
101.15
101.12
101.00
100.98
100.96
100.95
100.81
100.79
89.07
77.16 CDCl3
48.80
31.97
14.62
NH
F
F
F
N
N
N
N
Cl
Compound 56
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

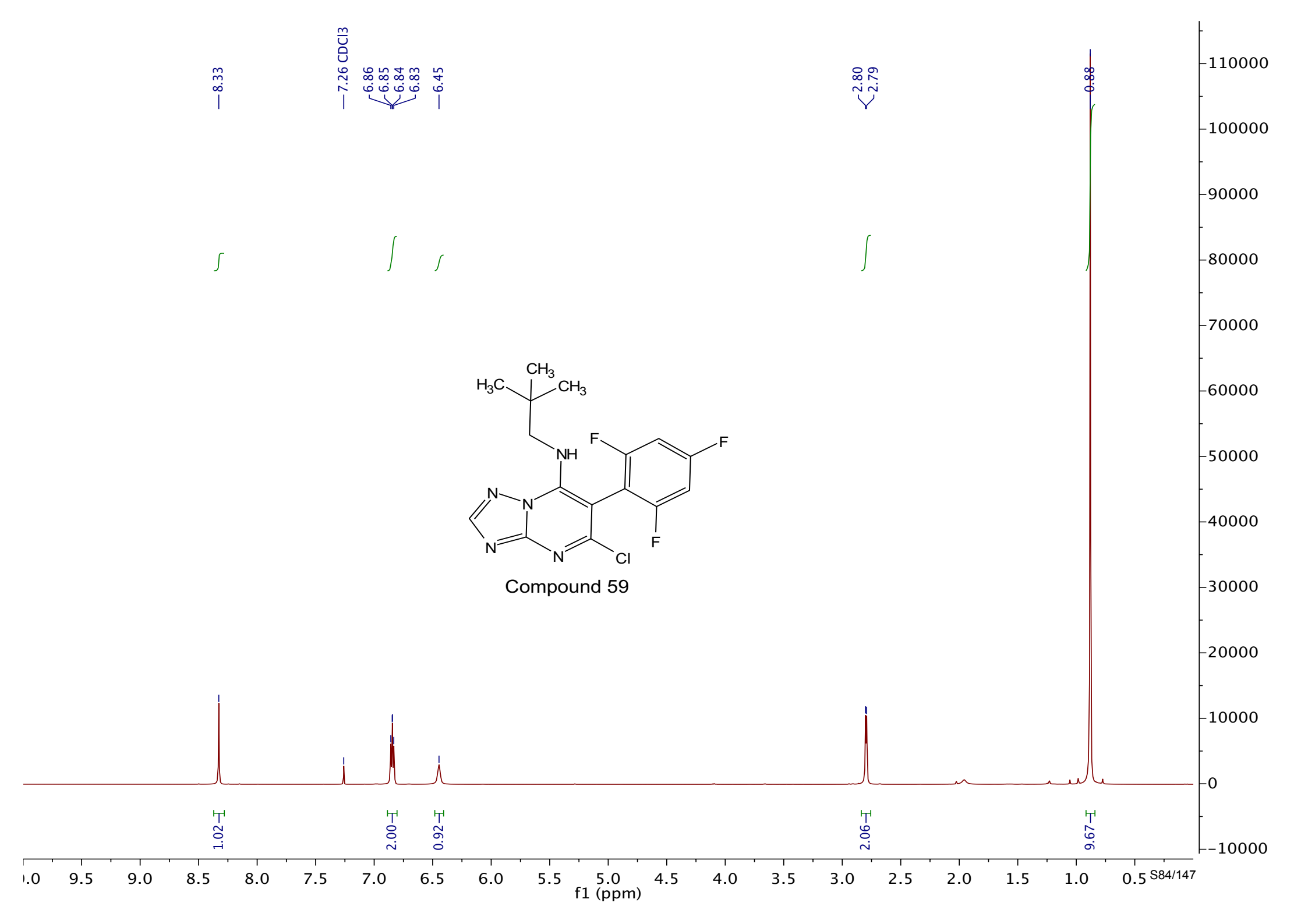

8.31
8.30
7.26 CDCl3
6.87
6.86
6.84
6.84
6.83
6.82
6.43
6.42
3.66
3.65
3.65
3.64
3.63
3.62
3.61
3.61
1.78
1.73
1.73
1.72
1.71
1.71
1.70
1.70
1.69
1.68
1.67
1.66
1.65
1.56
1.55
1.54
1.54
1.53
1.52
1.52
1.51
1.50
1.48
NH
F
F
F
N
N
N
N
Cl
Compound 57
*signal from traces of residual solvent/grease
1.00
1.84
0.89
0.92
4.22
3.92
f1 (ppm)
S80/147


164.94
164.83
164.73
163.25
163.15
163.05
162.56
162.51
162.47
162.41
160.90
160.85
160.81
160.75
158.20
158.19
154.93
145.81
107.61
107.58
107.48
107.44
107.34
107.30
101.11
100.95
100.94
100.92
100.91
100.90
100.74
88.98
77.16 CDCl3
55.11
34.64
23.92
NH
F
F
F
N
N
N
N
Cl
Compound 57
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


CDCl3
8.33 7.26 6.90 6.89 6.89 6.89 6.88 6.87 6.87 6.86 6.85 6.85 6.84 6.38 6.36 3.09 3.07 3.05 3.03 1.82 1.82 1.80 1.79 1.72 1.71 1.71 1.70 1.69 1.68 1.67 1.55 1.54 1.53 1.52 1.51 1.51 1.28 1.27 1.26 1.26 1.25 1.24 1.23 1.23 1.22 1.21 1.20 1.17 1.16 1.15 1.14 1.14 1.13 1.12 1.12 1.11 1.11 1.10 1.09 1.09 1.08 0.99 0.98 0.97 0.96 0.95 0.95 0.94 0.93 0.92 0.91 0.90 0.90
NH
F
F
F
N
N
N
N
Cl
1.00
1.90
1.05
1.18
1.97
2.31
1.07
2.16
1.16
2.01
f1 (ppm)

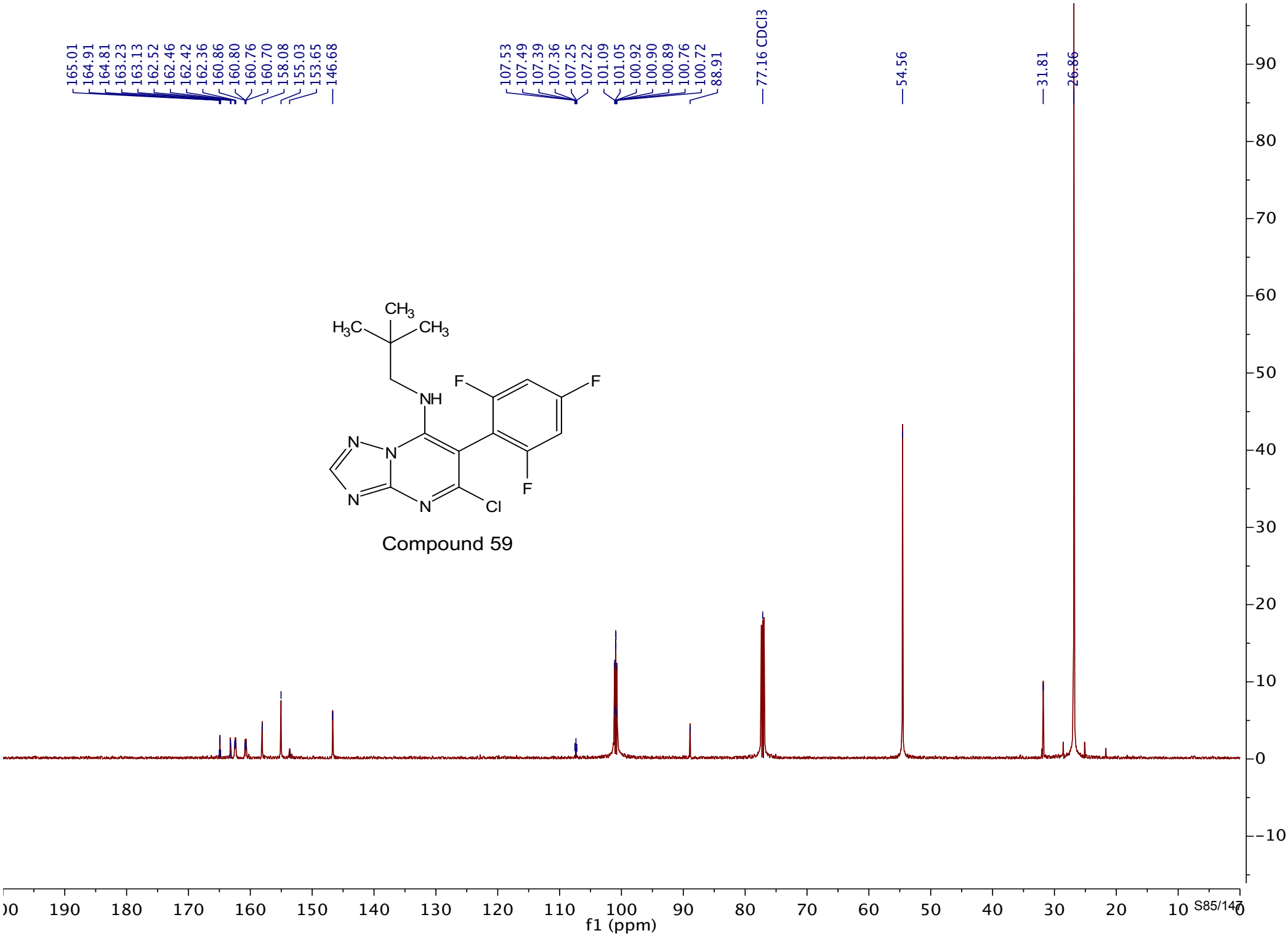
Compound 58

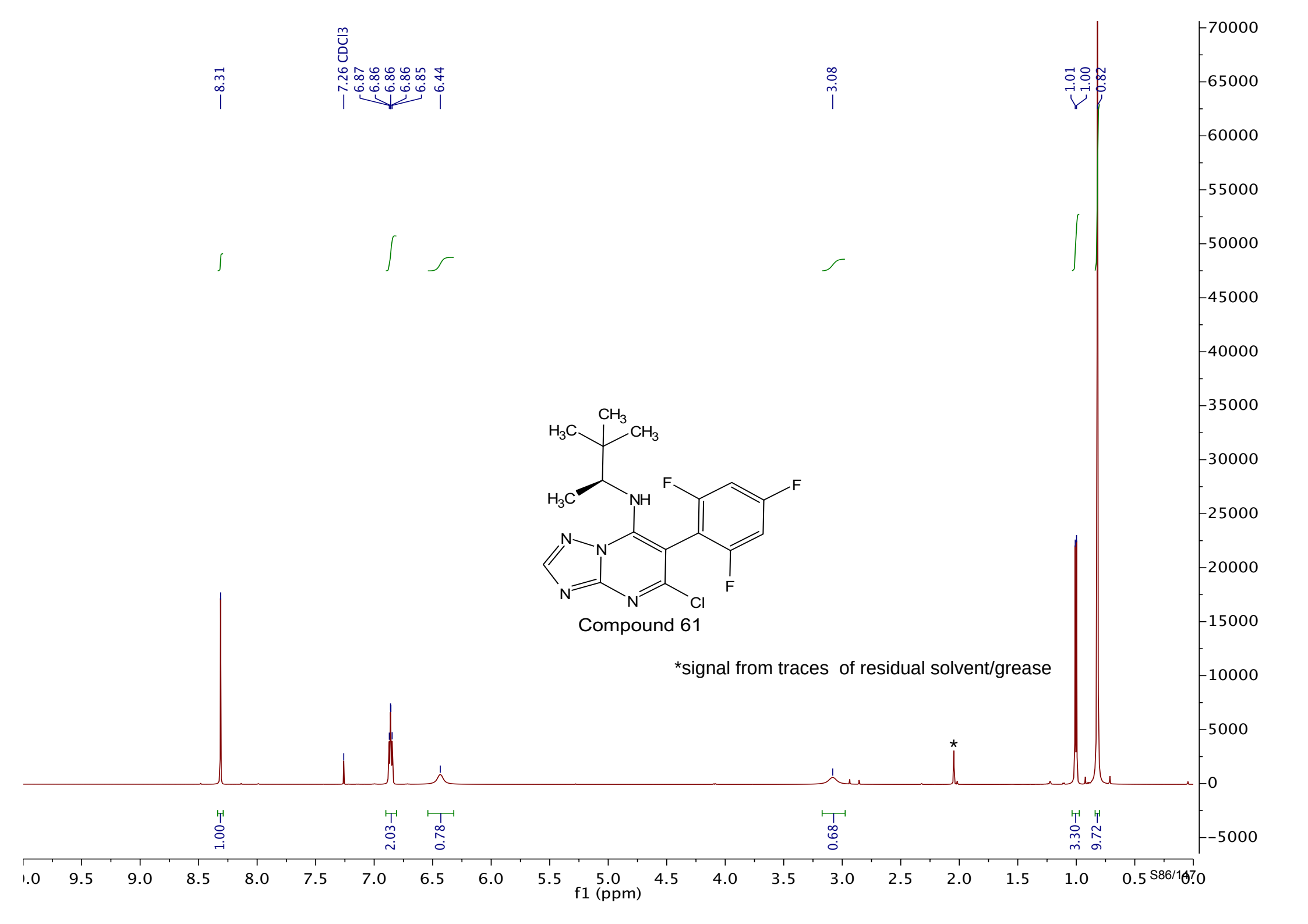

165.22
165.10
164.97
163.20
163.08
162.96
162.80
162.74
162.69
162.62
160.81
160.74
160.69
160.63
158.13
155.01
153.75
145.60
107.68
107.65
107.52
107.48
107.35
107.31
101.18
101.16
101.13
100.98
100.96
100.96
100.94
100.79
100.76
100.74
88.82
52.93
34.05
24.91
24.75
NH
F
F
F
N
N
N
N
Cl
Compound 58
3500
3000
2500
2000
1500
1000
500
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
S83/147

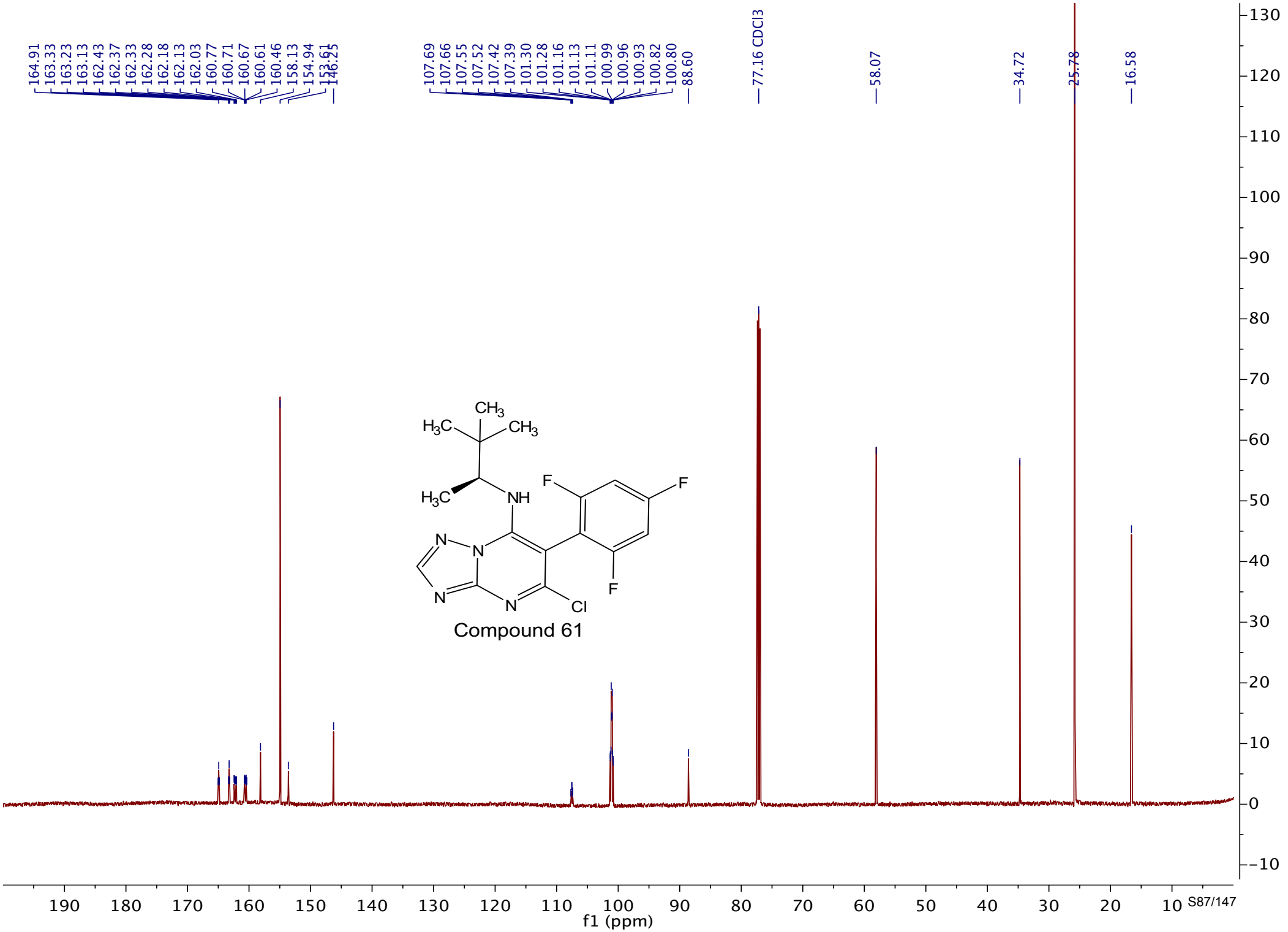

8.33
7.26 CDCl3
6.86
6.85
6.84
6.83
6.45
2.80
2.79
0.88
1.02
2.00
0.92
2.06
9.67
f1 (ppm)
S84/147

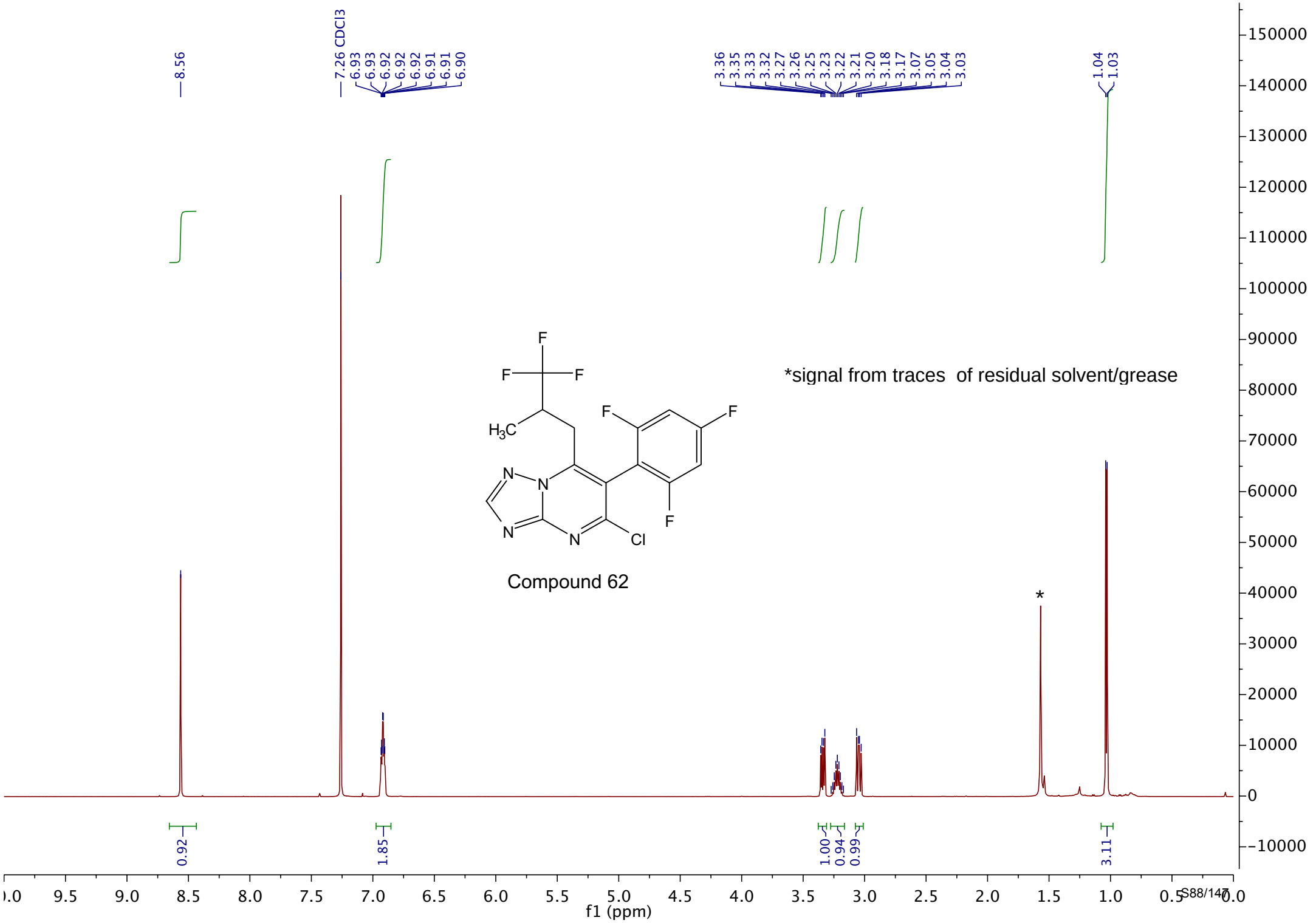
CH3
H3C
CH3
NH
F
F
F
N
N
N
N
Cl

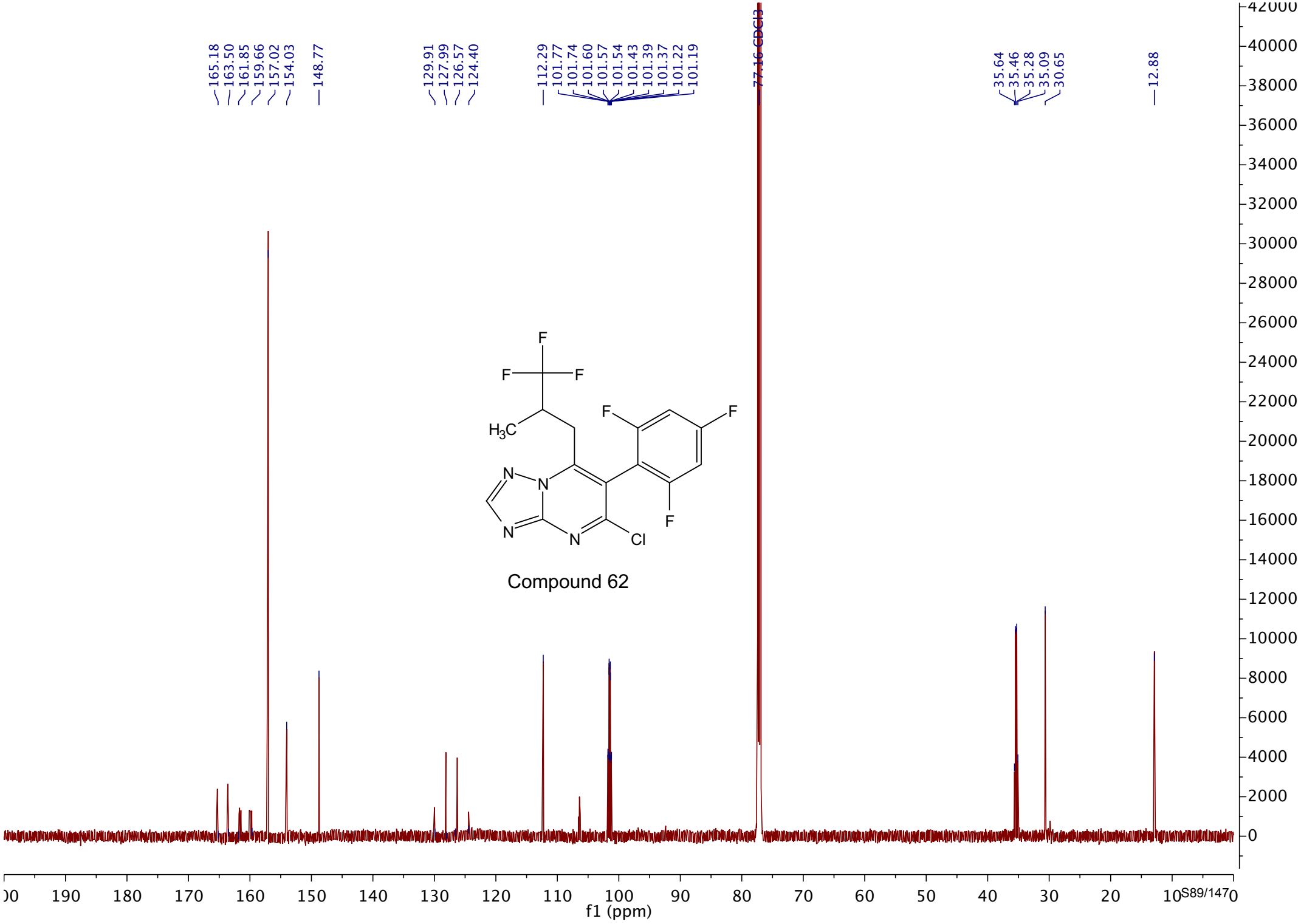
Compound 59

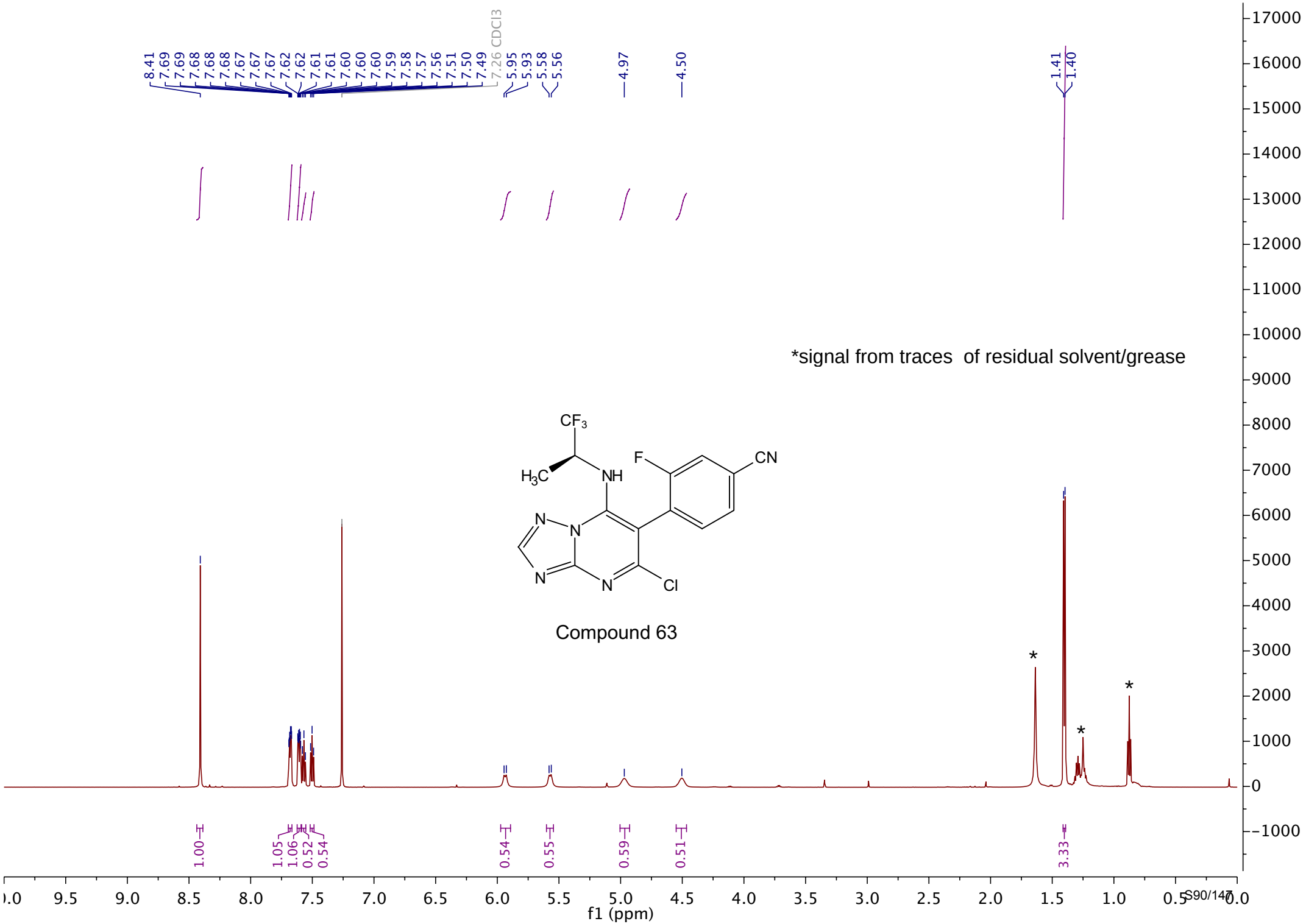

165.01
164.91
164.81
163.23
163.13
162.52
162.46
162.42
162.36
160.86
160.80
160.76
160.70
158.08
155.03
153.65
146.68
107.53
107.49
107.39
107.36
107.25
107.22
101.09
101.05
100.92
100.90
100.89
100.76
100.72
88.91
77.16 CDCl3
54.56
31.81
26.86
CH3
H3C
CH3
NH
F
F
F
N
N
N
N
Cl
Compound 59
f1 (ppm)
S85/147

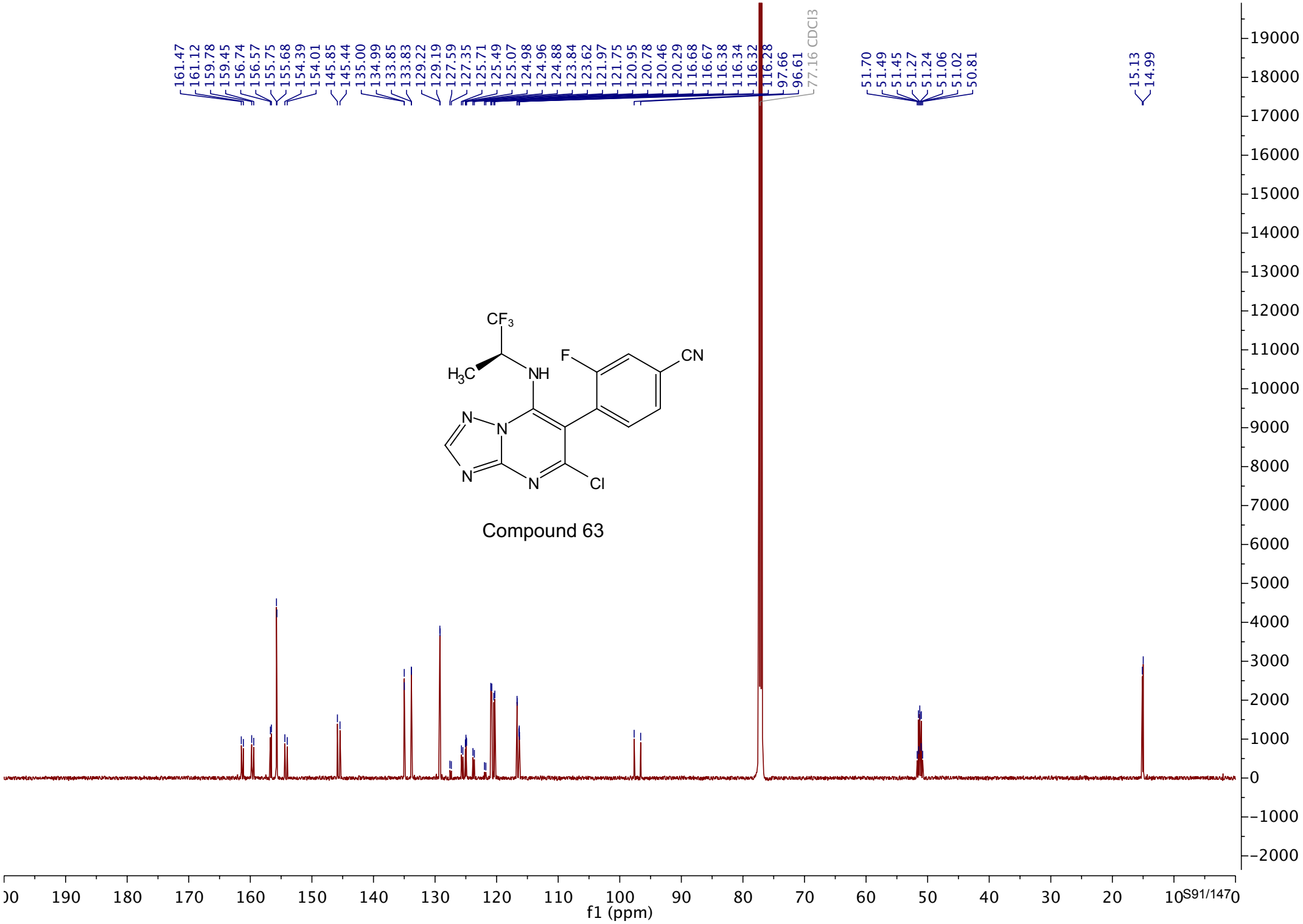

8.31
7.26 CDCl3
6.87
6.86
6.86
6.86
6.85
6.44
3.08
1.01
1.00
0.82
1.00
2.03
0.78
0.68
3.30
9.72
*
f1 (ppm)
Compound 61
*signal from traces of residual solvent/grease

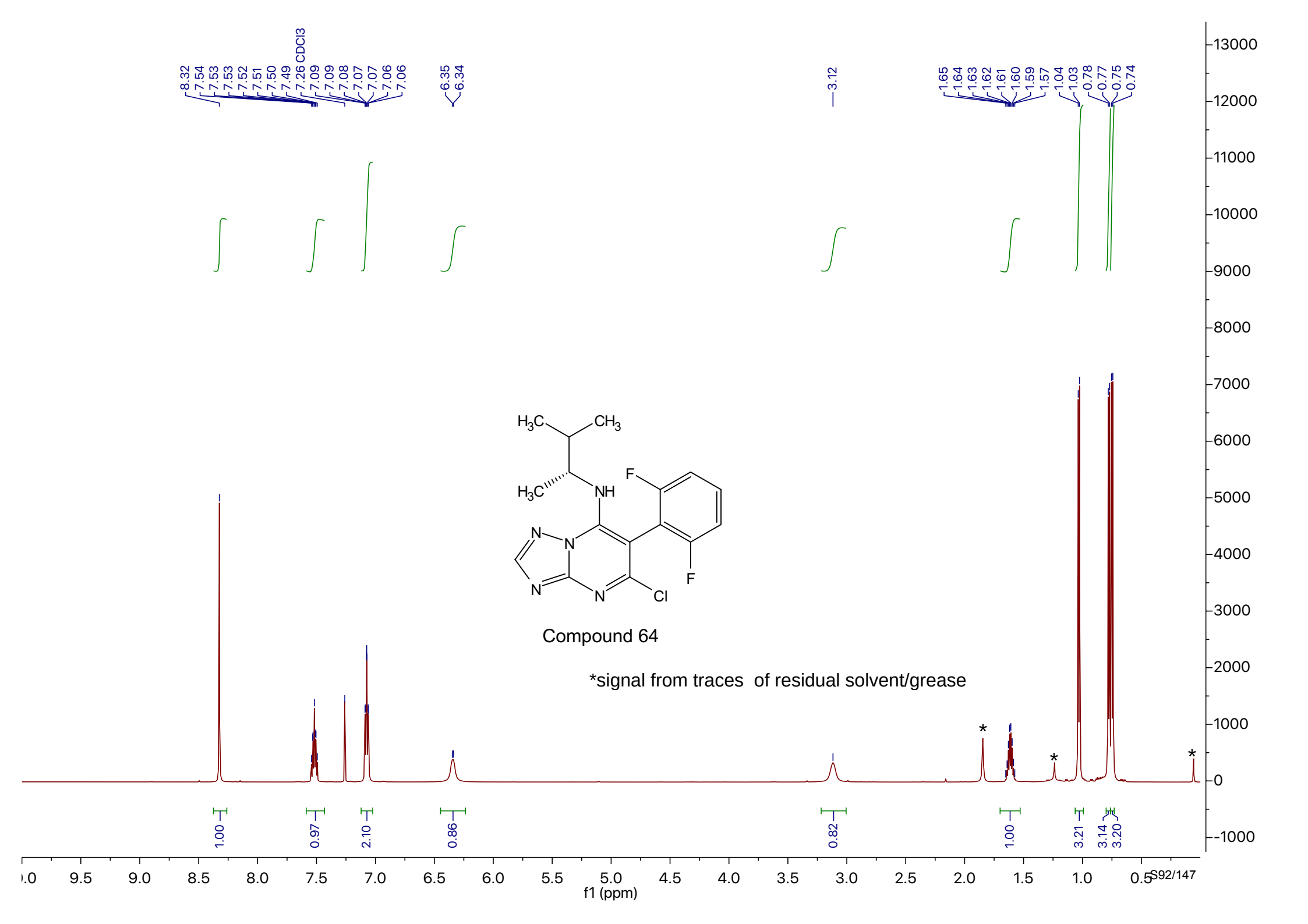

164.91
163.33
163.23
163.13
162.43
162.37
162.33
162.28
162.18
162.13
162.03
160.77
160.71
160.67
160.61
160.46
158.13
154.94
153.61
146.25
107.69
107.66
107.55
107.52
107.42
107.39
101.30
101.28
101.16
101.13
101.11
100.99
100.96
100.93
100.82
100.80
88.60
77.16 CDCl3
58.07
34.72
25.78
16.58
CH3
H3C
CH3
H3C
NH
F
F
F
N
N
N
N
Cl
Compound 61
f1 (ppm)
S87/147

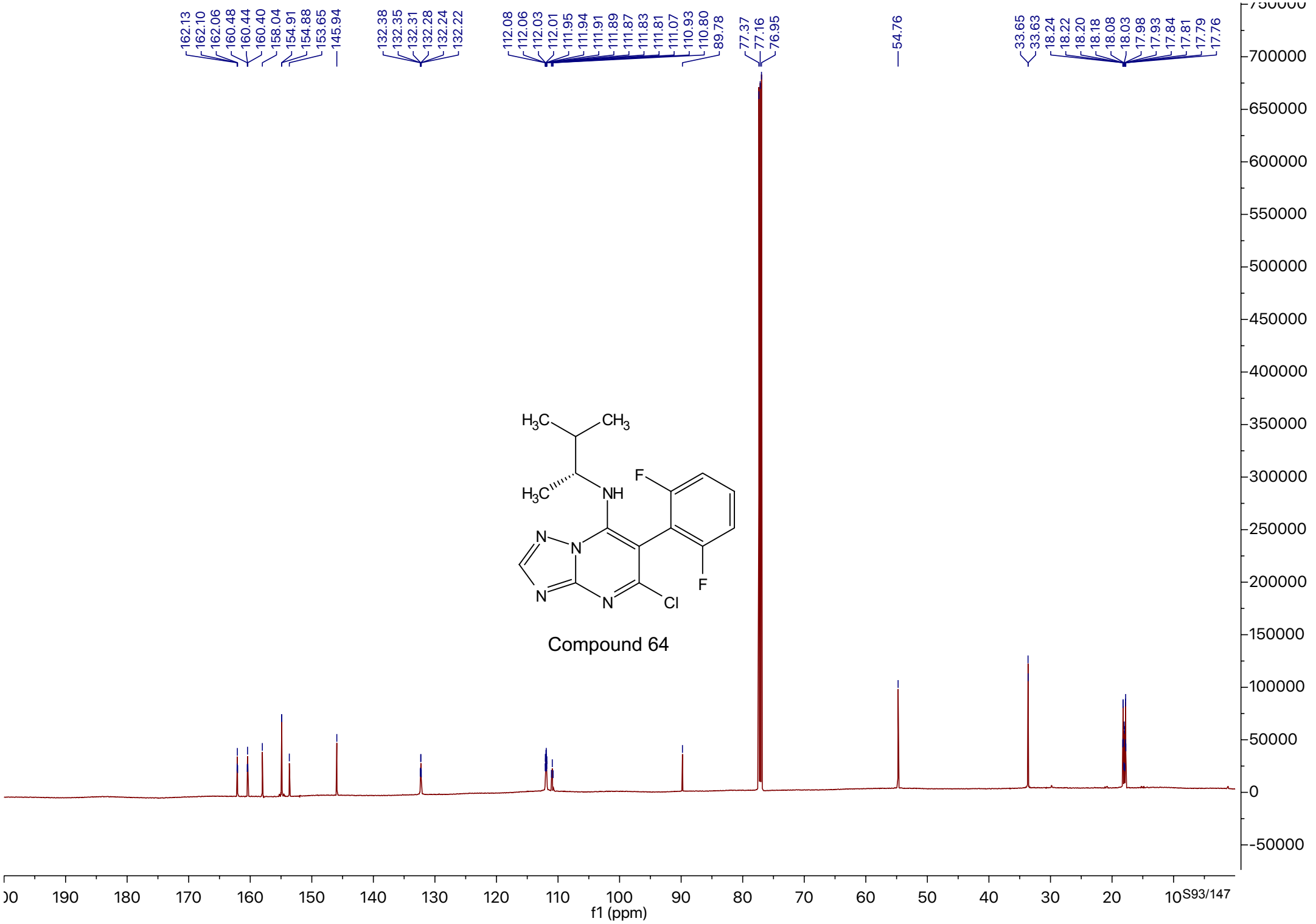

8.56
7.26 CDCl3
6.93
6.93
6.92
6.92
6.92
6.91
6.91
6.90
3.36
3.35
3.33
3.32
3.27
3.26
3.25
3.23
3.22
3.21
3.20
3.18
3.17
3.07
3.05
3.04
3.03
1.04
1.03
F
F
F
H3C
F
F
N
N
N
N
Cl
*signal from traces of residual solvent/grease
Compound 62
*
0.92
1.85
1.00
0.94
0.99
3.11
f1 (ppm)
S88/147

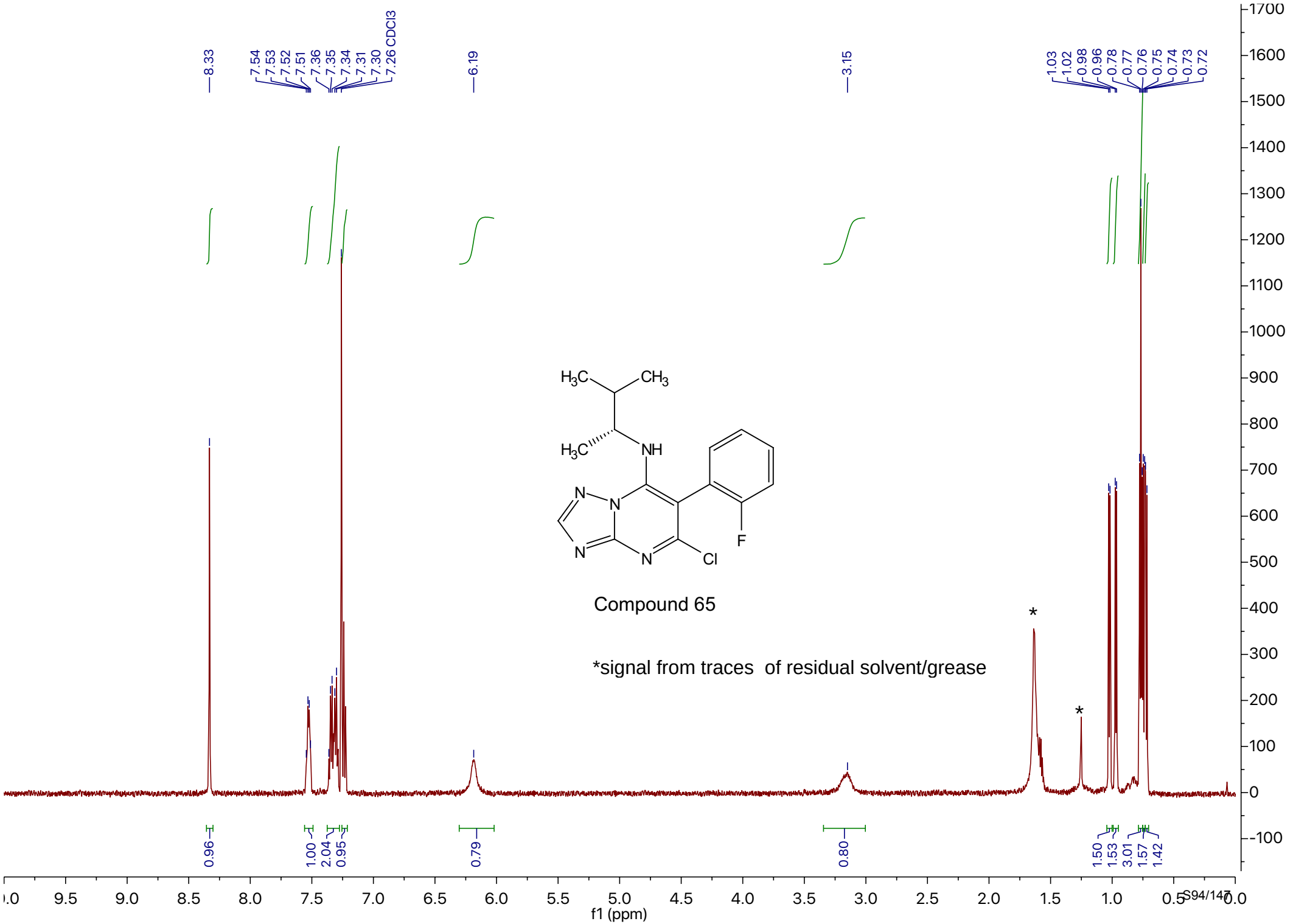

165.18
163.50
161.85
159.66
157.02
154.03
148.77
129.91
127.99
126.57
124.40
112.29
101.77
101.74
101.60
101.57
101.54
101.43
101.39
101.37
101.22
101.19
77.16 CDCl3
35.64
35.46
35.28
35.09
30.65
12.88
F
F
F
H3C
F
F
N
N
N
N
Cl
Compound 62
f1 (ppm)

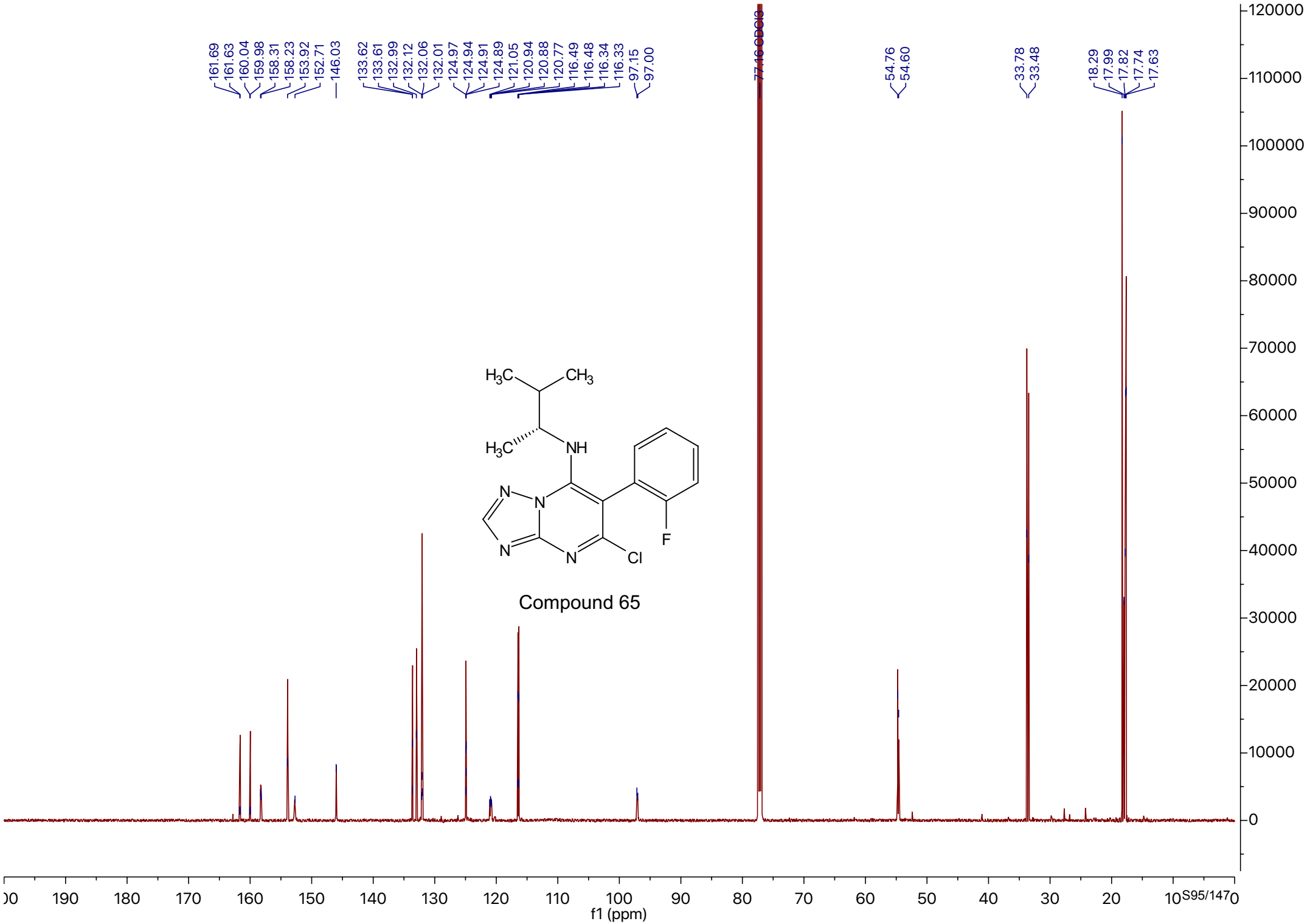

8.41
7.69
7.69
7.68
7.68
7.68
7.67
7.67
7.67
7.62
7.62
7.61
7.61
7.60
7.60
7.60
7.59
7.58
7.57
7.56
7.51
7.50
7.49
7.26 CDCl3
5.95
5.93
5.58
5.56
4.97
4.50
1.41
1.40
*signal from traces of residual solvent/grease
CF3
H3C
NH
F
CN
N
N
N
N
Cl
Compound 63
1.00
1.05
1.06
0.52
0.54
0.54
0.55
0.59
0.51
3.33
f1 (ppm)
S90/147

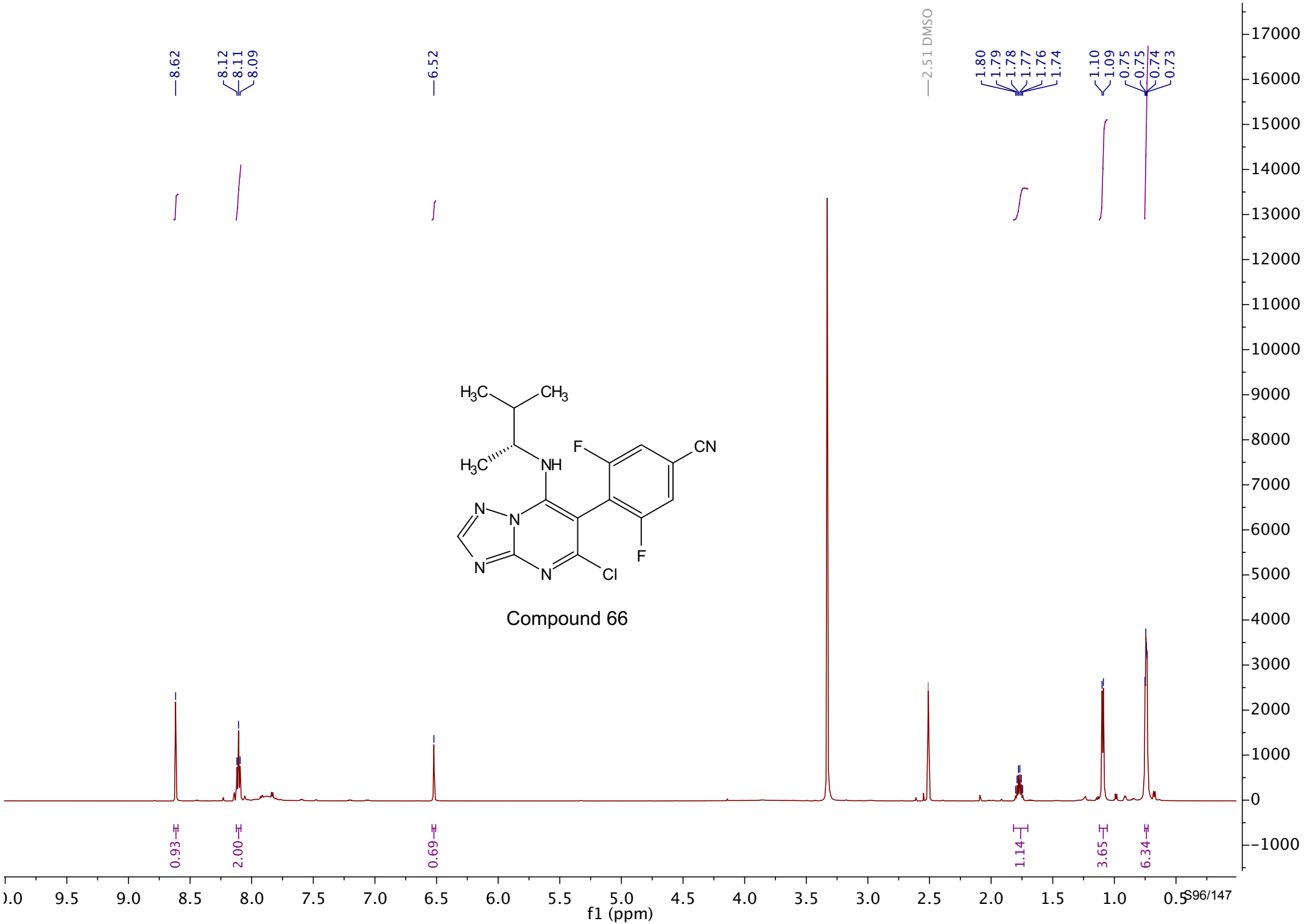

161.47
161.12
159.78
159.45
156.74
156.57
155.75
155.68
154.39
154.01
145.85
145.44
135.00
134.99
133.85
133.83
129.22
129.19
127.59
127.35
125.71
125.49
125.07
124.98
124.96
124.88
123.84
123.62
121.97
121.75
120.95
120.78
120.46
120.29
116.68
116.67
116.38
116.34
116.32
116.28
97.66
96.61
77.16 CDCl3
51.70
51.49
51.45
51.27
51.24
51.06
51.02
50.81
15.13
14.99
CF3
H3C
NH
F
CN
N
N
N
N
Cl
Compound 63
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.32
7.54
7.53
7.53
7.52
7.51
7.50
7.49
7.26 CDCl3
7.09
7.09
7.08
7.07
7.07
7.06
7.06
6.35
6.34
3.12
1.65
1.64
1.63
1.62
1.61
1.60
1.59
1.57
1.04
1.03
0.78
0.77
0.75
0.74
H3C
CH3
H3C
NH
F
F
N
N
N
N
Cl
Compound 64
*signal from traces of residual solvent/grease
1.00
0.97
2.10
0.86
0.82
1.00
3.21
3.14
3.20
f1 (ppm)
S92/147

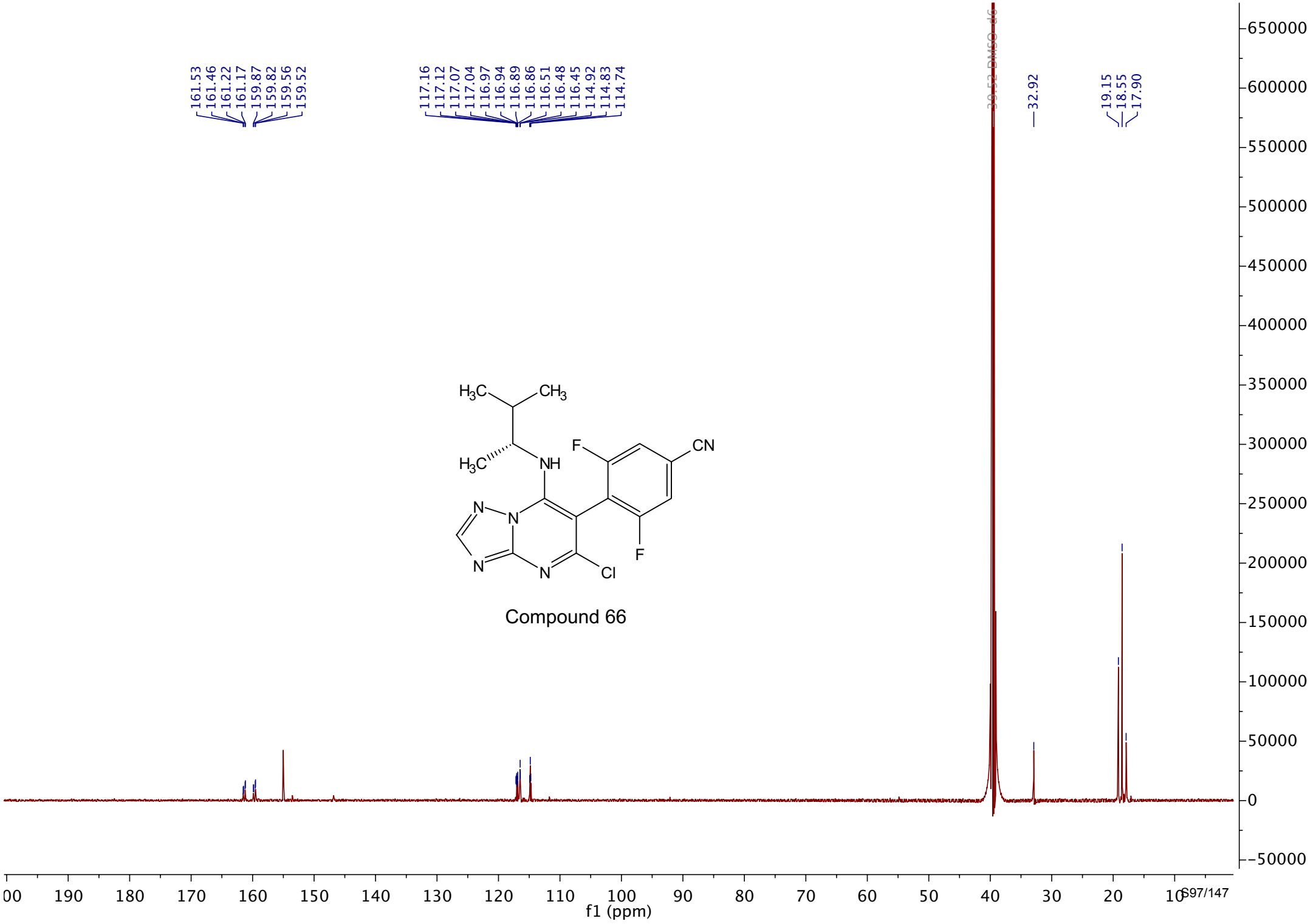

162.13
162.10
162.06
160.48
160.44
160.40
158.04
154.91
154.88
153.65
145.94
132.38
132.35
132.31
132.28
132.24
132.22
112.08
112.06
112.03
112.01
111.95
111.94
111.91
111.89
111.87
111.83
111.81
111.07
110.93
110.80
89.78
77.37
77.16
76.95
54.76
33.65
33.63
18.24
18.22
18.20
18.18
18.08
18.03
17.98
17.93
17.84
17.81
17.79
17.76
H3C
CH3
H3C
NH
F
F
N
N
N
N
Cl
Compound 64
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.33
7.54
7.53
7.52
7.51
7.36
7.35
7.34
7.31
7.30
7.26 CDCl3
6.19
3.15
1.03
1.02
0.98
0.96
0.78
0.77
0.76
0.75
0.74
0.73
0.72
H3C
CH3
H3C
NH
N
N
N
N
Cl
F
Compound 65
*signal from traces of residual solvent/grease
*
*
0.96
1.00
2.04
0.95
0.79
0.80
1.50
1.53
3.01
1.57
1.42
f1 (ppm)
S94/147

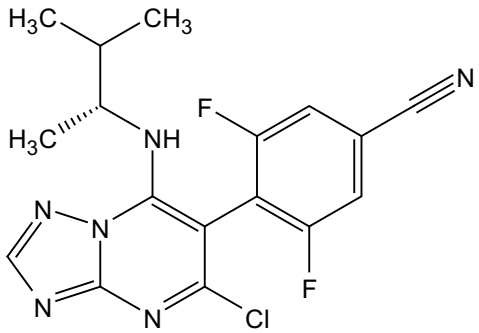

161.69
161.63
160.04
159.98
158.31
158.23
153.92
152.71
146.03
133.62
133.61
132.99
132.12
132.06
132.01
124.97
124.94
124.91
124.89
121.05
120.94
120.88
120.77
116.49
116.48
116.34
116.33
97.15
97.00
77.16 CDCl3
54.76
54.60
33.78
33.48
18.29
17.99
17.82
17.74
17.63
H3C
CH3
H3C
NH
N
N
N
N
Cl
F
Compound 65
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.62
8.12
8.11
8.09
6.52
2.51 DMSO
1.80
1.79
1.78
1.77
1.76
1.74
1.10
1.09
0.75
0.75
0.74
0.73
H3C
CH3
H3C
NH
F
CN
N
N
N
N
F
Cl
0.93
2.00
0.69
1.14
3.65
6.34
f1 (ppm)
S96/147

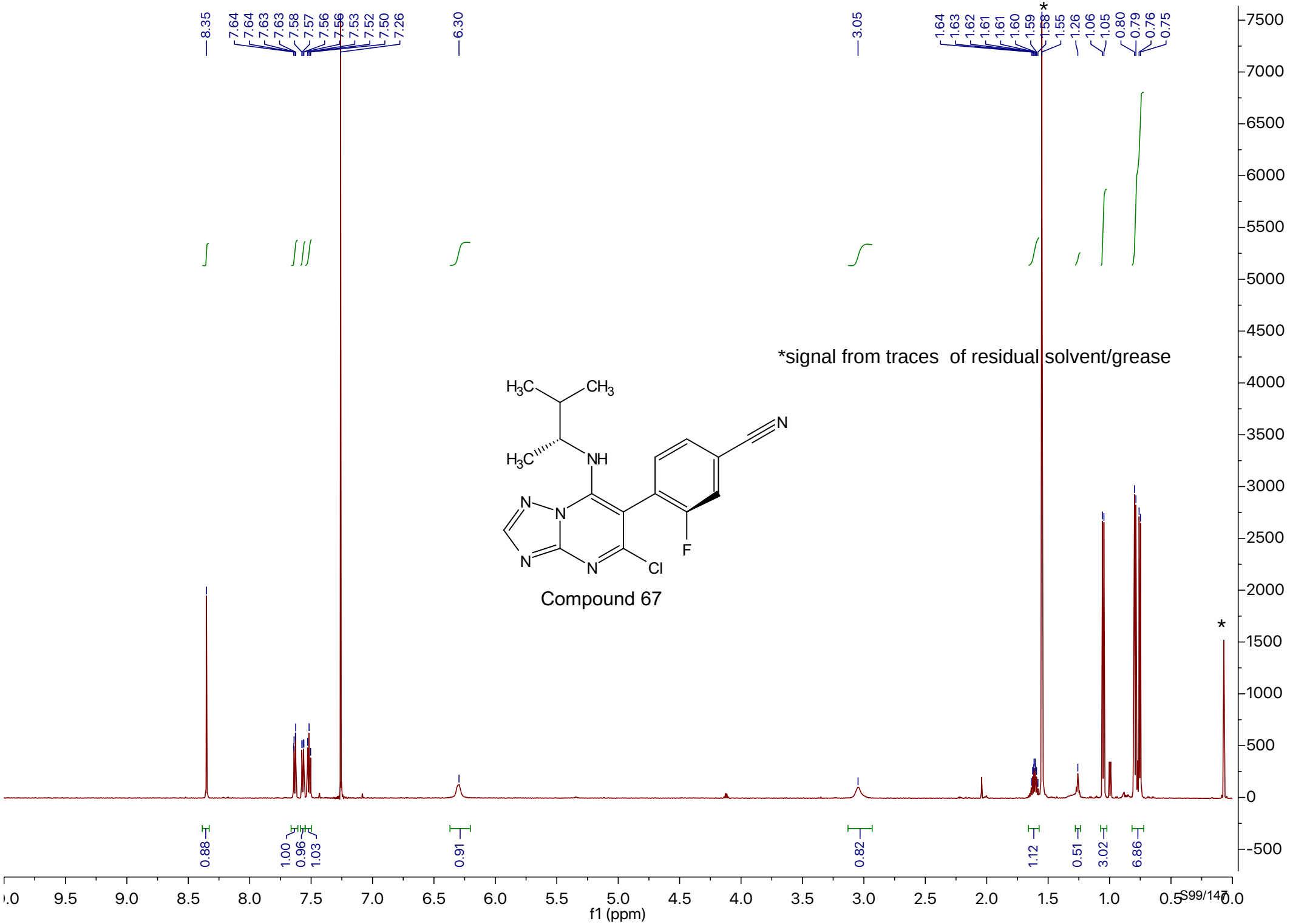
Compound 66

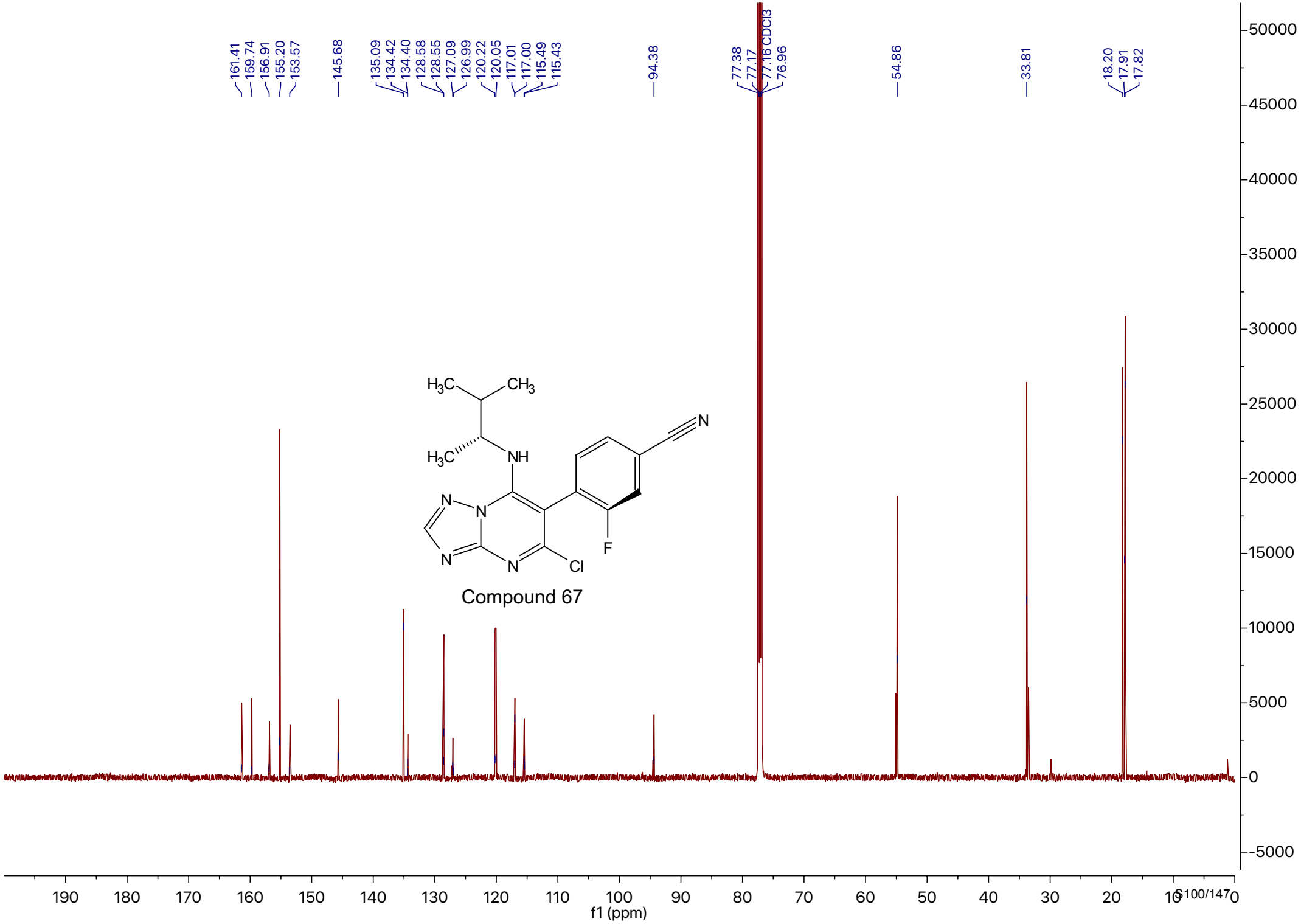

161.53
161.46
161.22
161.17
159.87
159.82
159.56
159.52
117.16
117.12
117.07
117.04
116.97
116.94
116.89
116.86
116.51
116.48
116.45
114.92
114.83
114.74
39.52 DMSO-d6
32.92
19.15
18.55
17.90
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
f1 (ppm)
S97/147

Compound 66

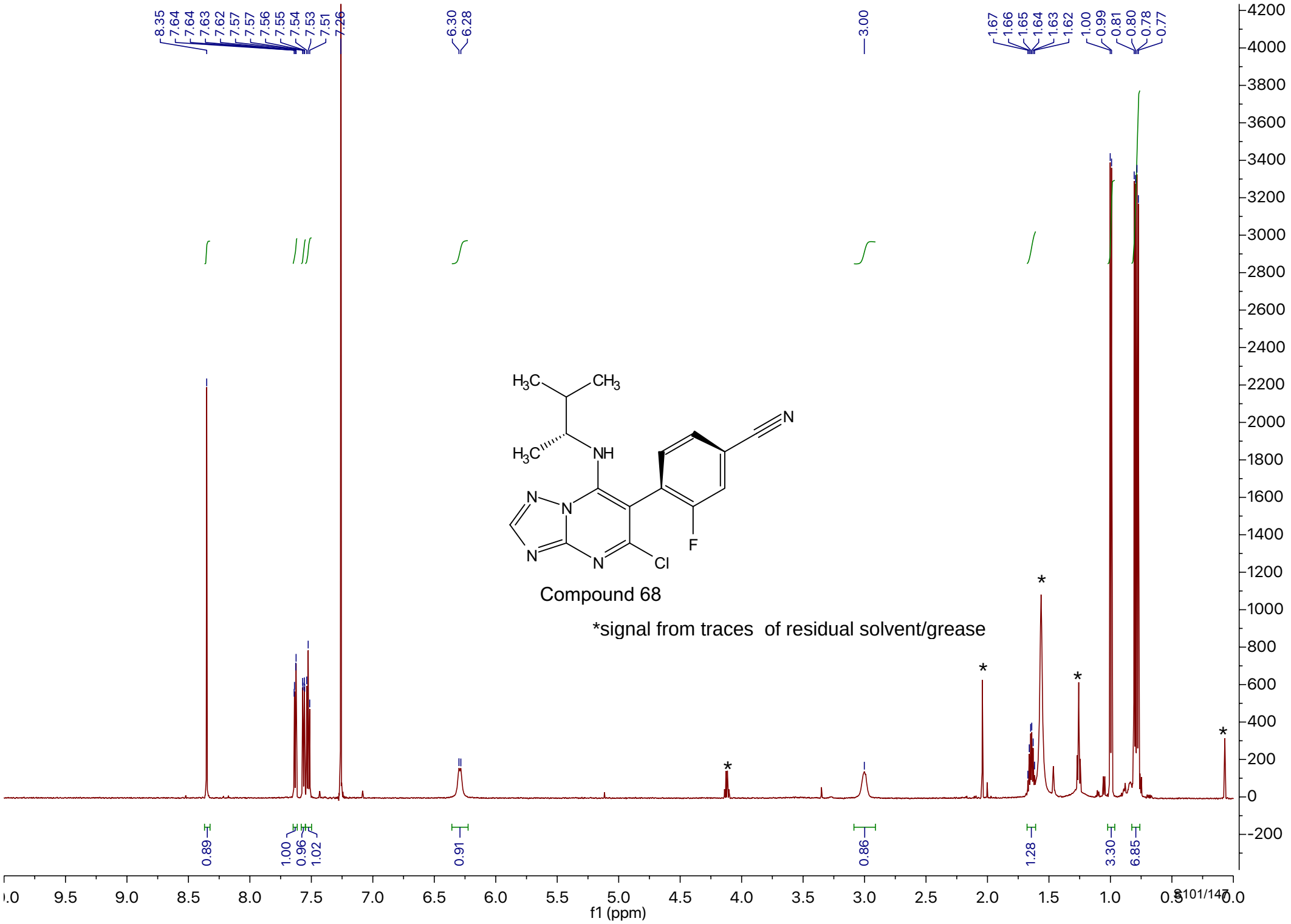


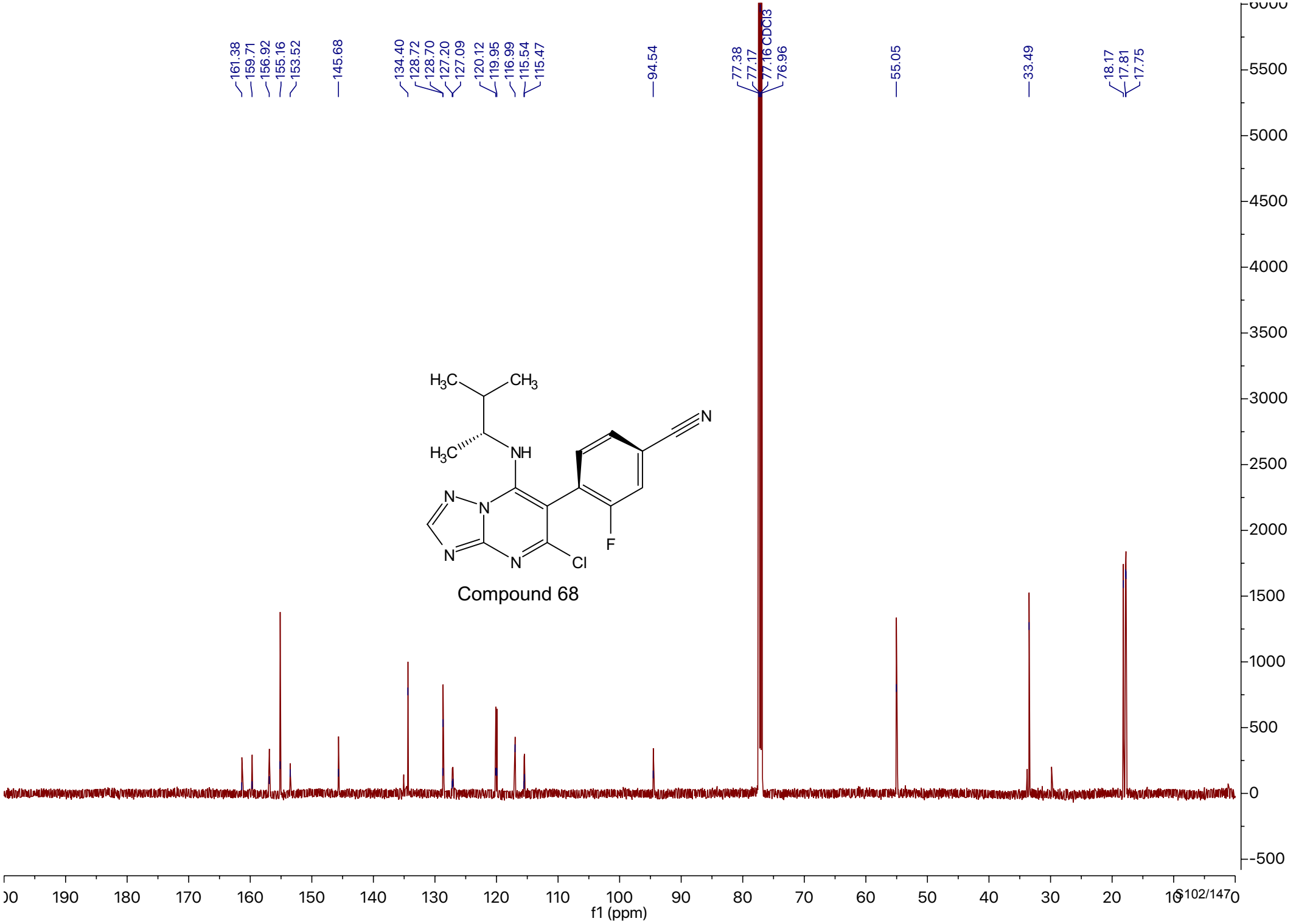
Compound 66

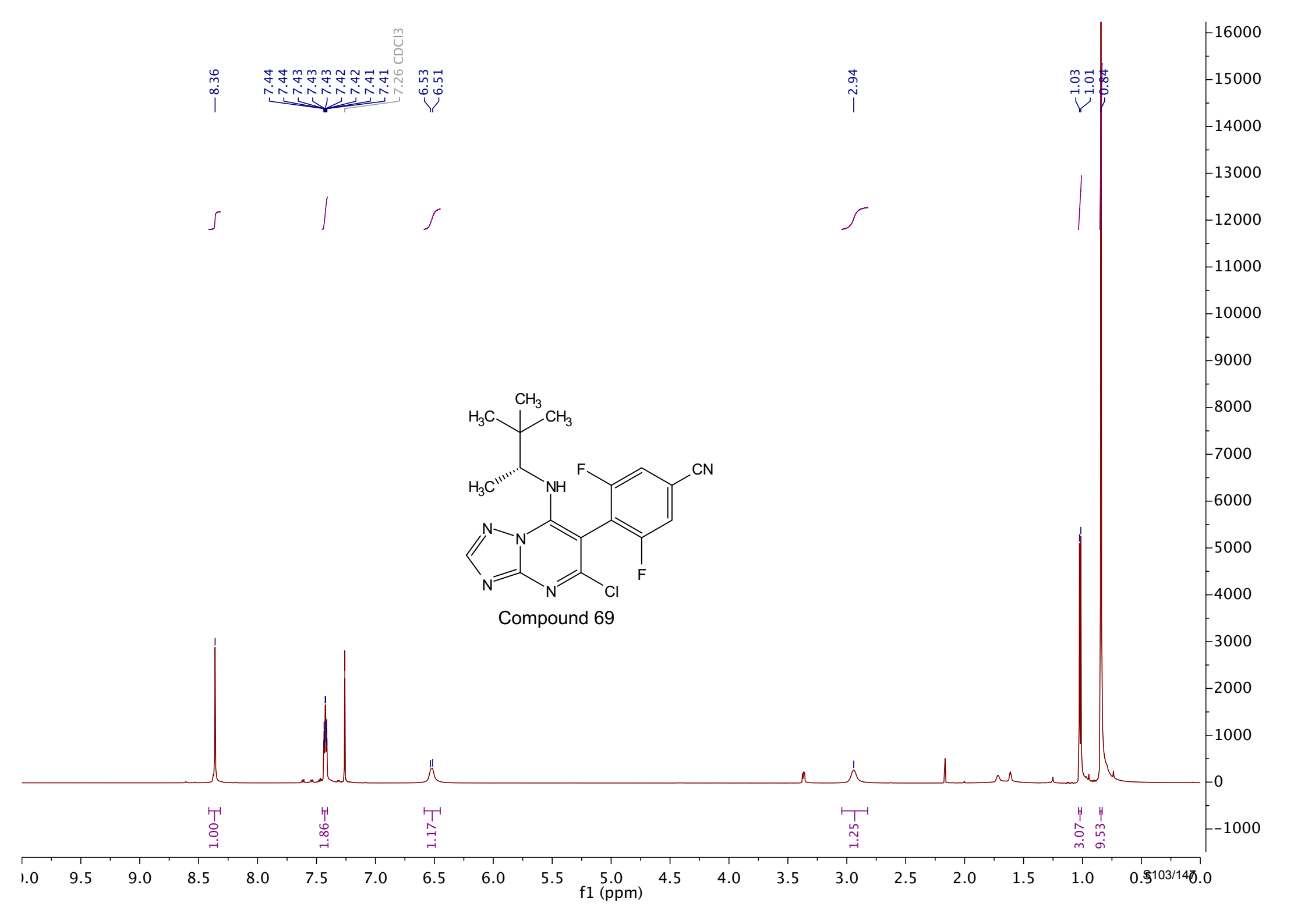

8.35
7.64
7.64
7.63
7.63
7.58
7.57
7.56
7.56
7.53
7.52
7.50
7.26
6.30
3.05
1.64
1.63
1.62
1.61
1.61
1.60
1.59
1.58
1.55
1.26
1.06
1.05
0.80
0.79
0.76
0.75
*
*signal from traces of residual solvent/grease
H3C
CH3
H3C
NH
N
N
N
N
Cl
F
N
Compound 67
0.88
1.00
0.96
1.03
0.91
0.82
1.12
0.51
3.02
6.86
f1 (ppm)
S99/147

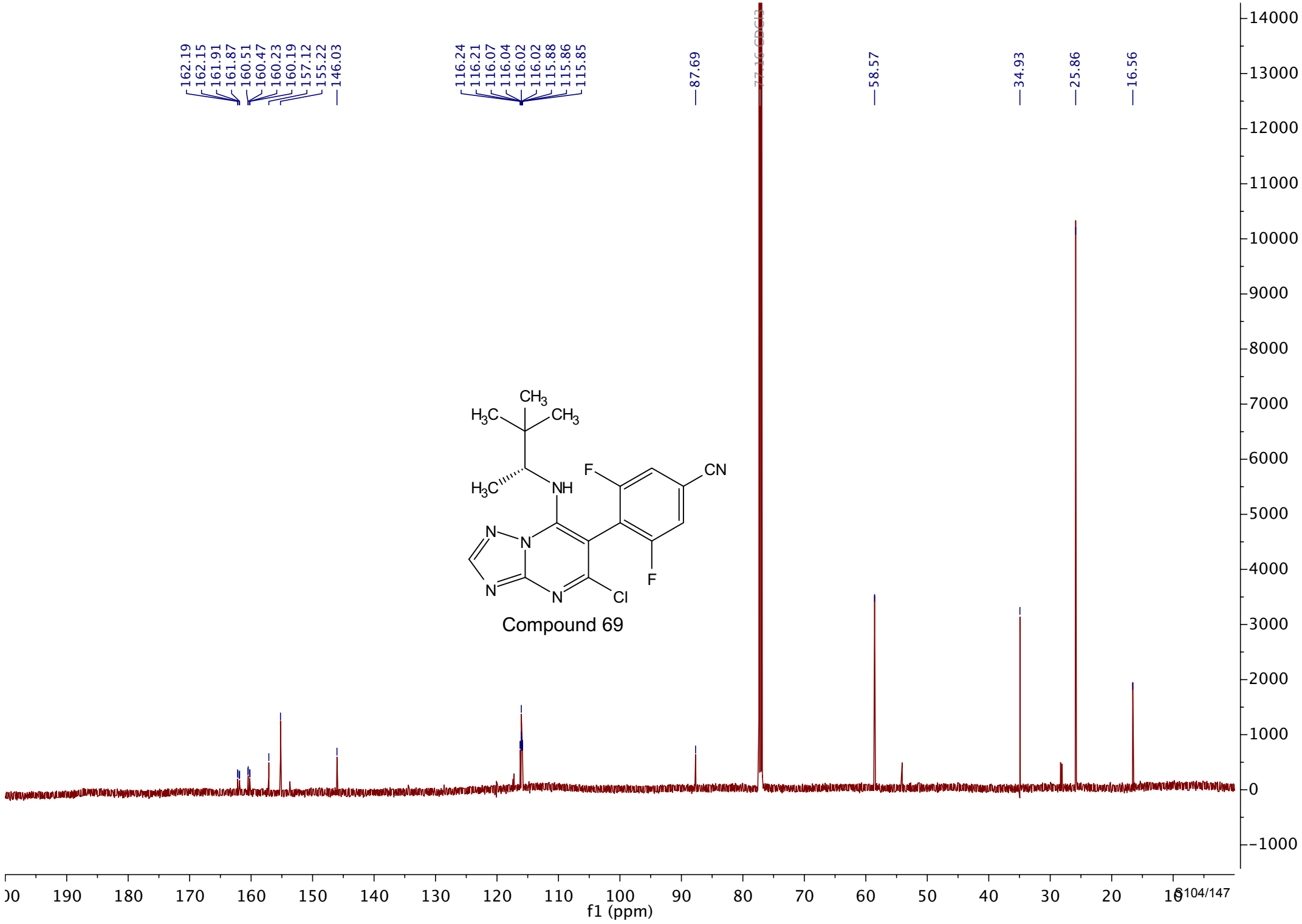

161.41
159.74
156.91
155.20
153.57
145.68
135.09
134.42
134.40
128.58
128.55
127.09
126.99
120.22
120.05
117.01
117.00
115.49
115.43
94.38
77.38
77.17
77.16 CDCl3
76.96
54.86
33.81
18.20
17.91
17.82
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
S100/147
H3C
CH3
H3C
NH
N
N
N
N
N
Cl
F
N

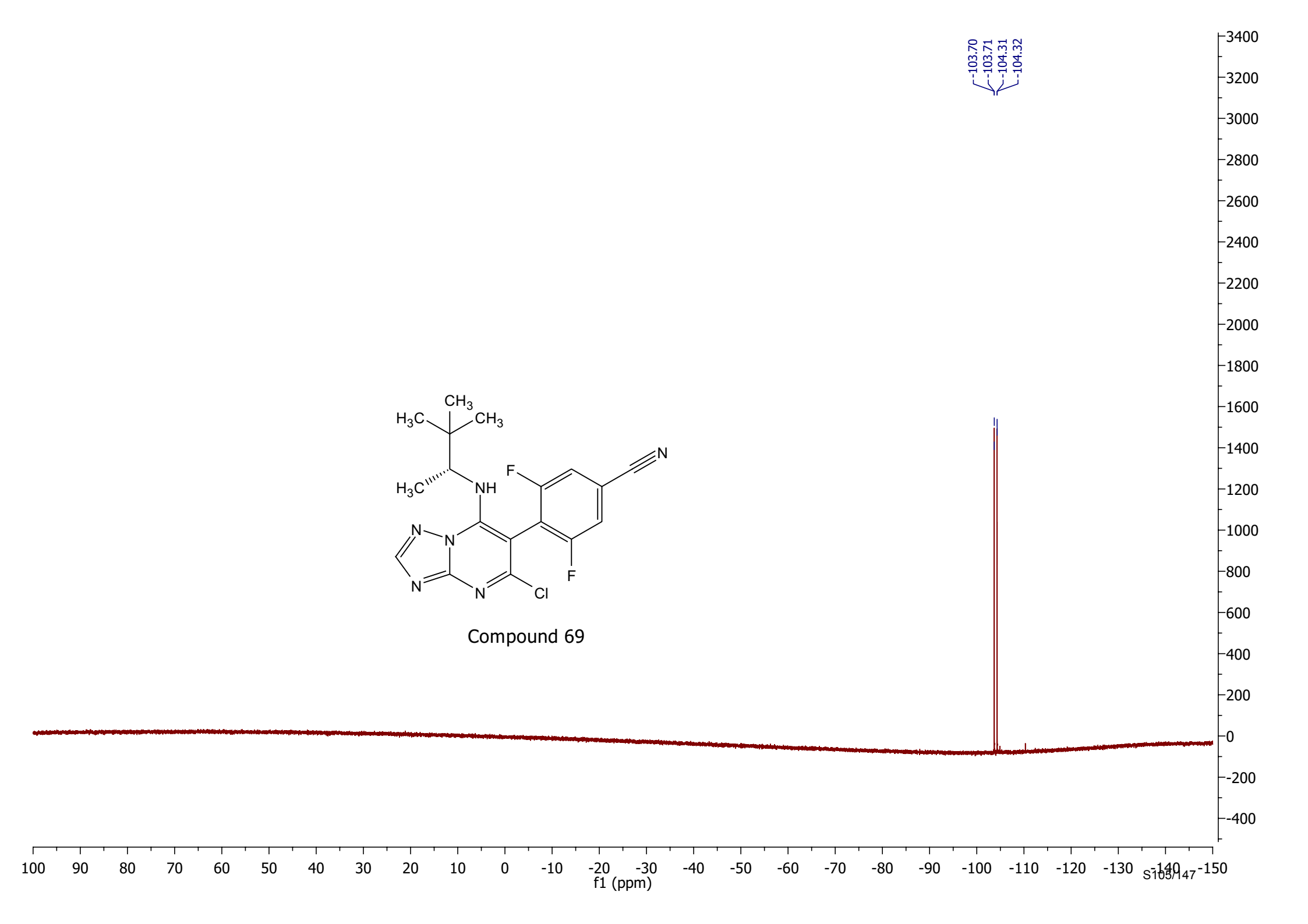
Compound 67

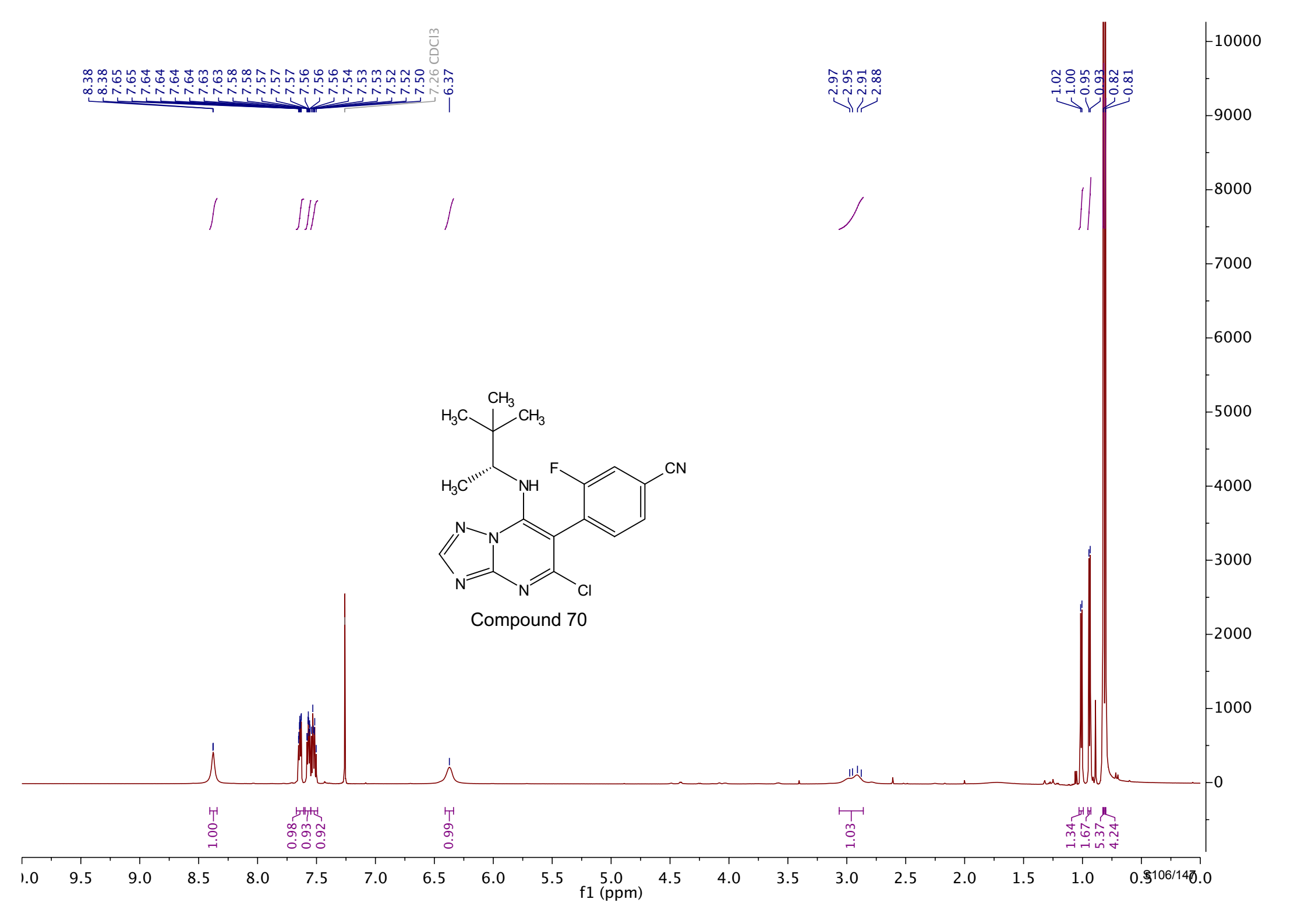

8.35
7.64
7.64
7.63
7.62
7.57
7.57
7.56
7.55
7.54
7.53
7.51
7.26
6.30
6.28
3.00
1.67
1.66
1.65
1.64
1.63
1.62
1.00
0.99
0.81
0.80
0.78
0.77
0.89
1.00
0.96
1.02
0.91
0.86
1.28
3.30
6.85
f1 (ppm)
Compound 68
*signal from traces of residual solvent/grease

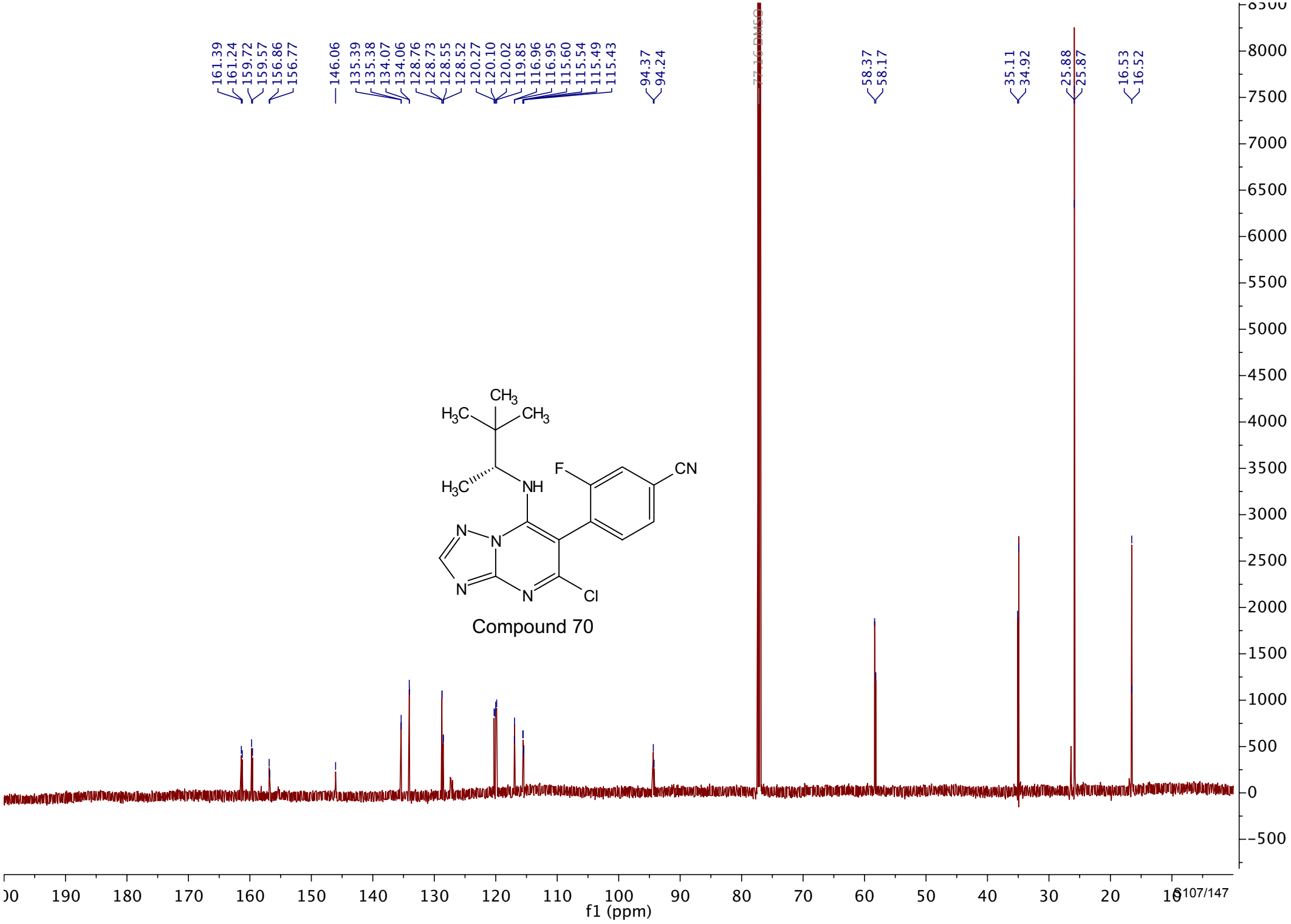

161.38
159.71
156.92
155.16
153.52
145.68
134.40
128.72
128.70
127.20
127.09
120.12
119.95
116.99
115.54
115.47
94.54
77.38
77.17
77.16 CDCl3
76.96
55.05
33.49
18.17
17.81
17.75
H3C
CH3
H3C
NH
N
N
N
N
Cl
F
N
Compound 68
f1 (ppm)

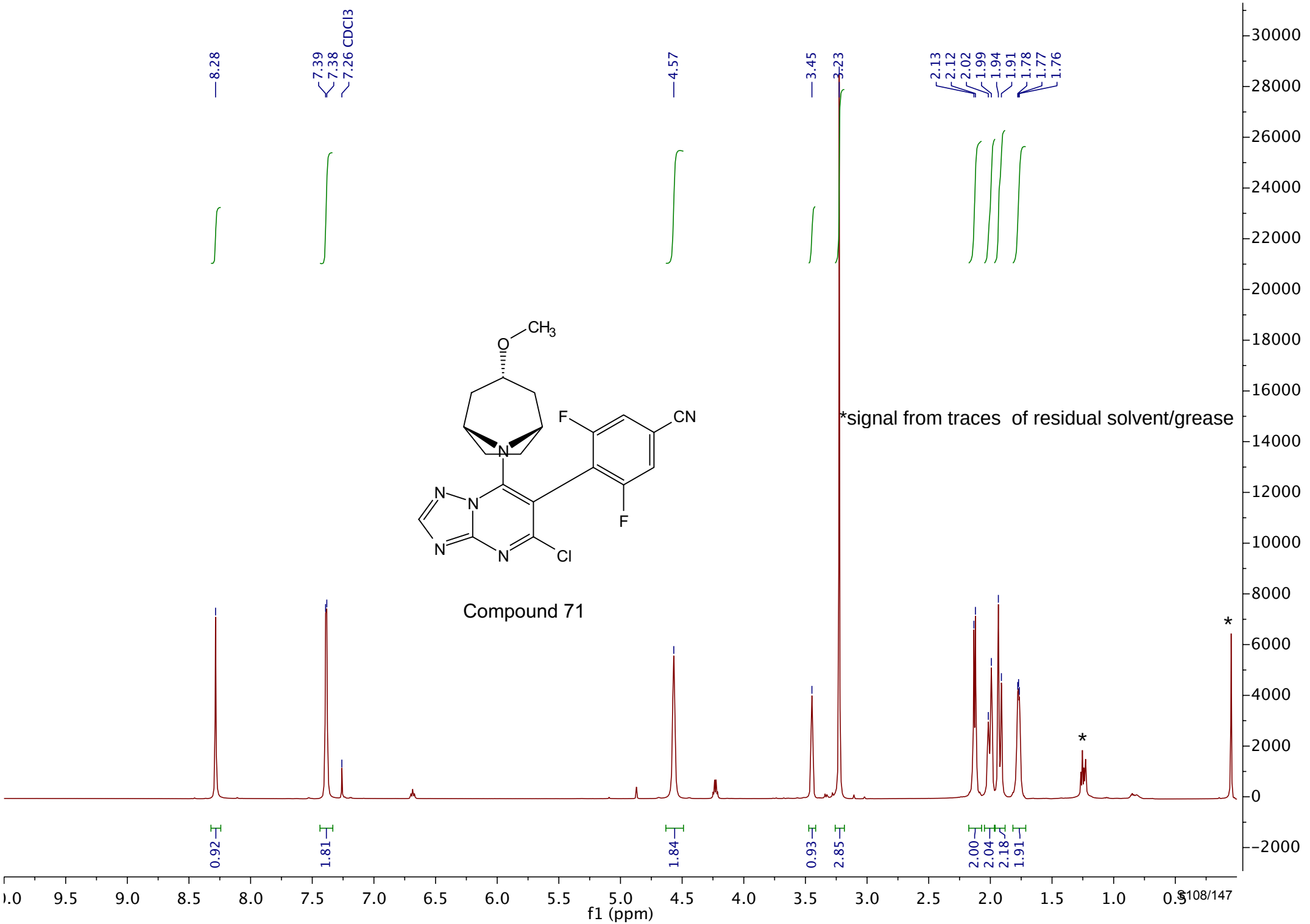

8.36
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.26 CDCl3
6.53
6.51
2.94
1.03
1.01
0.84
CH3
H3C
CH3
H3C
NH
F
CN
N
N
N
N
Cl
F
Compound 69
1.00
1.86
1.17
1.25
3.07
9.53
f1 (ppm)
S103/147

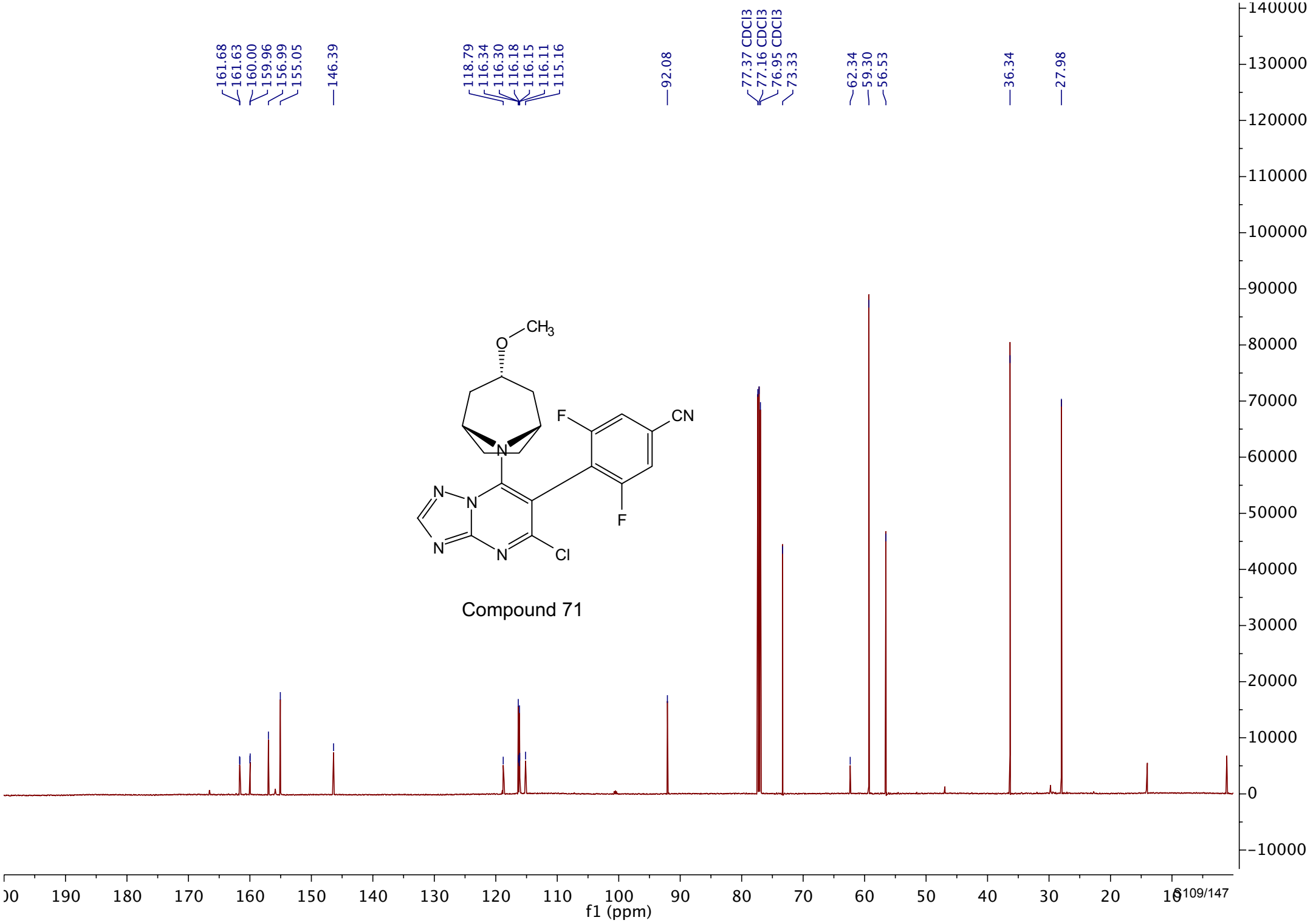

162.19
162.15
161.91
161.87
160.51
160.47
160.23
160.19
157.12
155.22
146.03
116.24
116.21
116.07
116.04
116.02
116.02
115.88
115.86
115.85
87.69
77.16 CDCl3
58.57
34.93
25.86
16.56
CH3
H3C
CH3
H3C
NH
F
CN
N
N
N
N
Cl
F
Compound 69
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

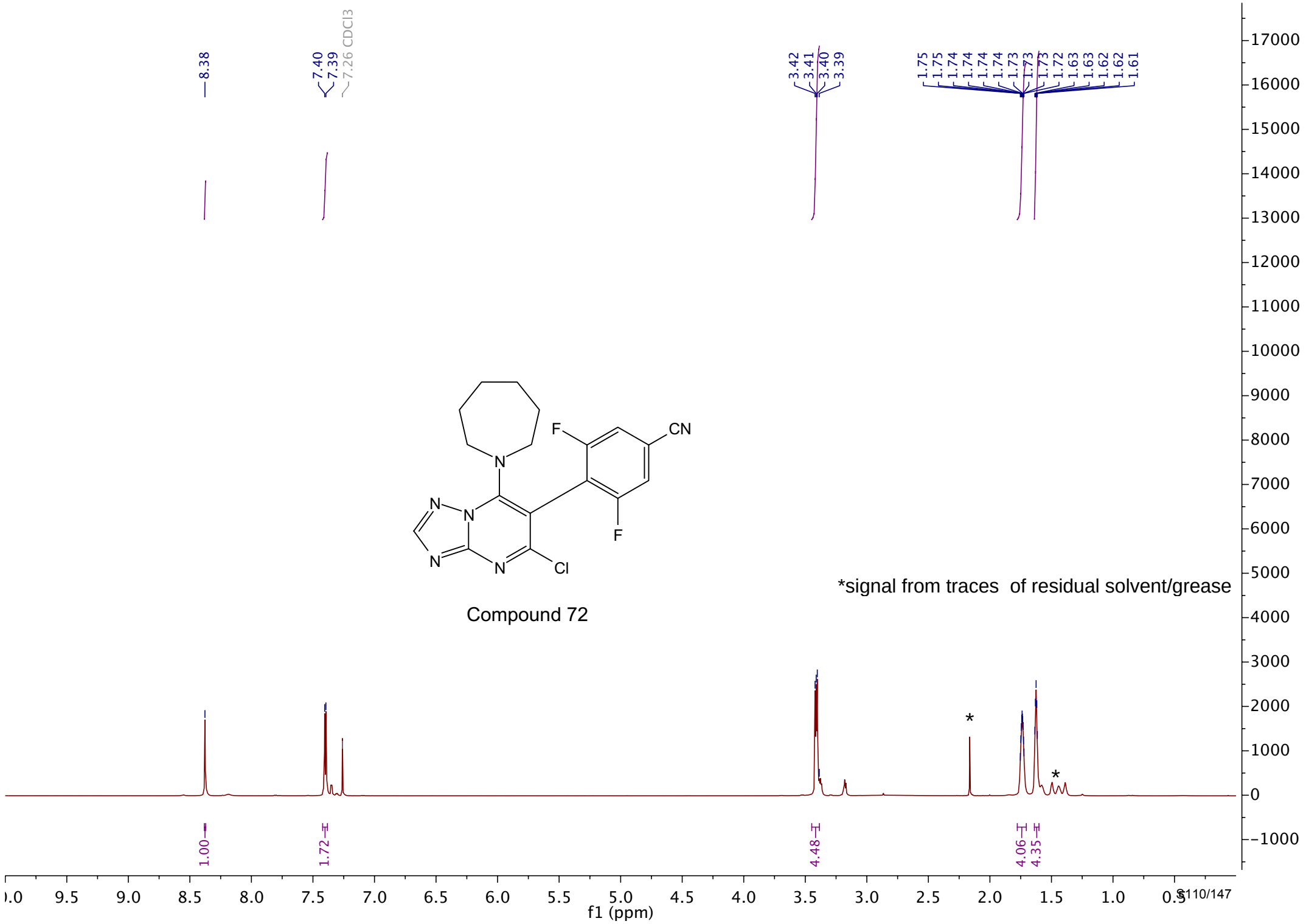

-103.70
-103.71
-104.31
-104.32
CH3
H3C
CH3
H3C
NH
F
N
N
N
N
N
Cl
F
Compound 69
f1 (ppm)
S105/147

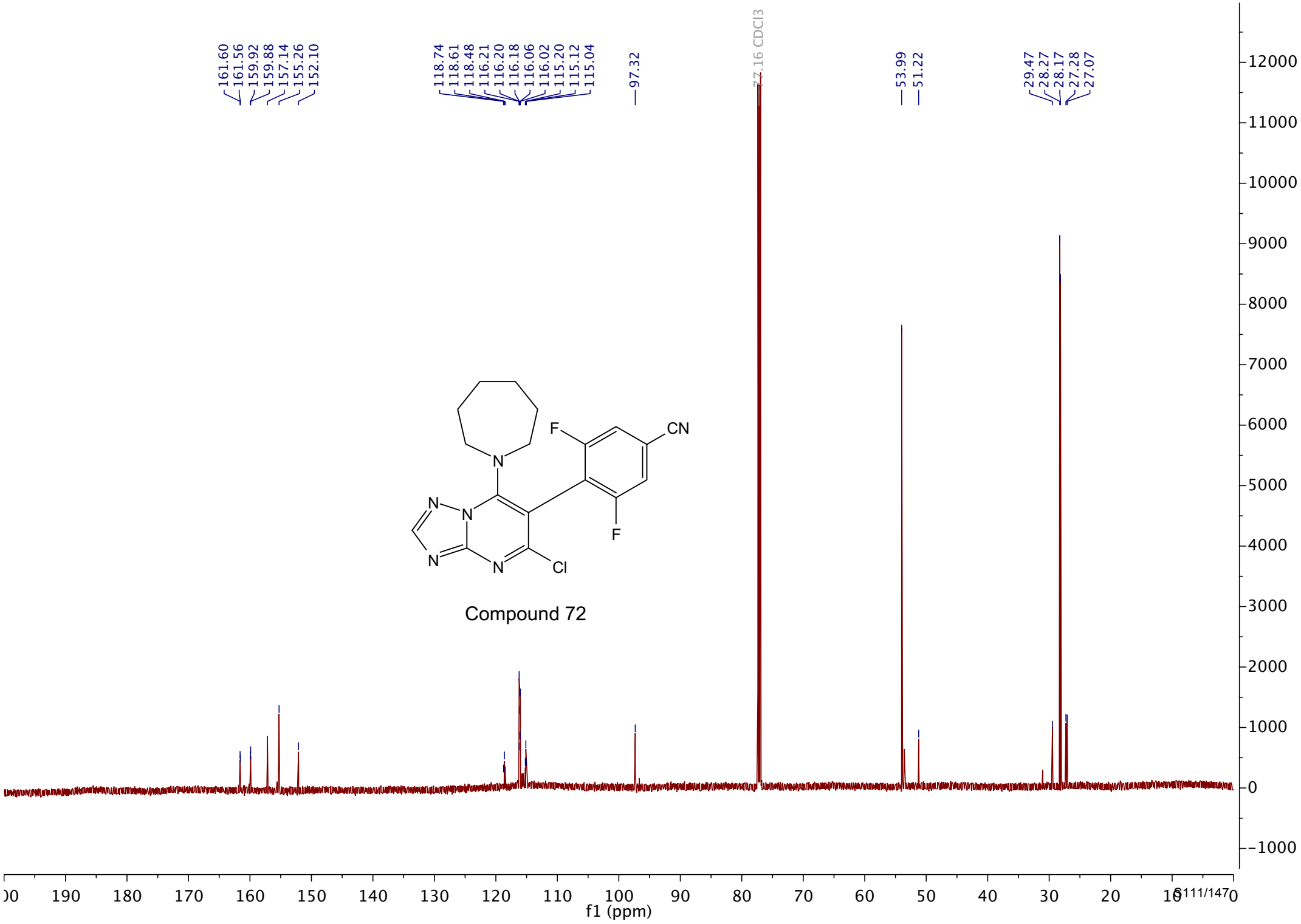

8.38
8.38
7.65
7.65
7.64
7.64
7.64
7.64
7.63
7.63
7.58
7.58
7.57
7.57
7.57
7.56
7.56
7.56
7.54
7.53
7.53
7.52
7.52
7.50
7.26 CDCl3
6.37
2.97
2.95
2.91
2.88
1.02
1.00
0.95
0.93
0.82
0.81
CH3
H3C
CH3
H3C
NH
F
CN
N
N
N
N
Cl
Compound 70
1.00
0.98
0.93
0.92
0.99
1.03
1.34
1.67
5.37
4.24
f1 (ppm)
S106/147


161.39
161.24
159.72
159.57
156.86
156.77
146.06
135.39
135.38
134.07
134.06
128.76
128.73
128.55
128.52
120.27
120.10
120.02
119.85
116.96
116.95
115.60
115.54
115.49
115.43
94.37
94.24
77.16 DMSO
58.37
58.17
35.11
34.92
25.88
25.87
16.53
16.52
CH3
H3C
CH3
H3C
NH
F
CN
N
N
N
N
Cl
Compound 70
f1 (ppm)

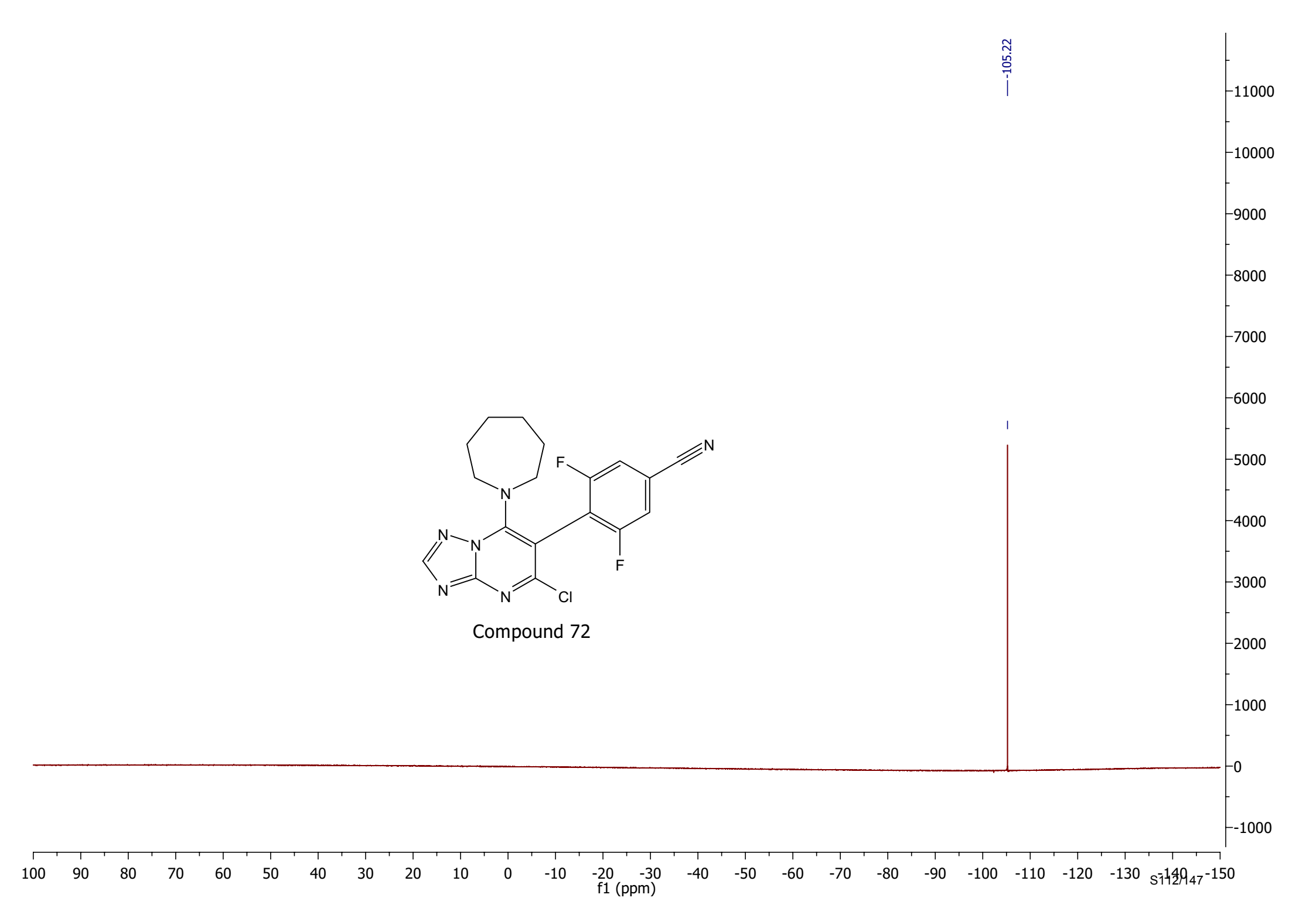

8.28
7.39
7.38
7.26 CDCl3
4.57
3.45
3.23
2.13
2.12
2.02
1.99
1.94
1.91
1.78
1.77
1.76
CH3
O
N
F
CN
F
N
N
N
N
Cl
Compound 71
*signal from traces of residual solvent/grease
0.92
1.81
1.84
0.93
2.85
2.00
2.04
2.18
1.91
f1 (ppm)


161.68
161.63
160.00
159.96
156.99
155.05
146.39
118.79
116.34
116.30
116.18
116.15
116.11
115.16
92.08
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
73.33
62.34
59.30
56.53
36.34
27.98
O
CH3
N
F
CN
F
N
N
N
N
Cl
Compound 71
f1 (ppm)
S109/147

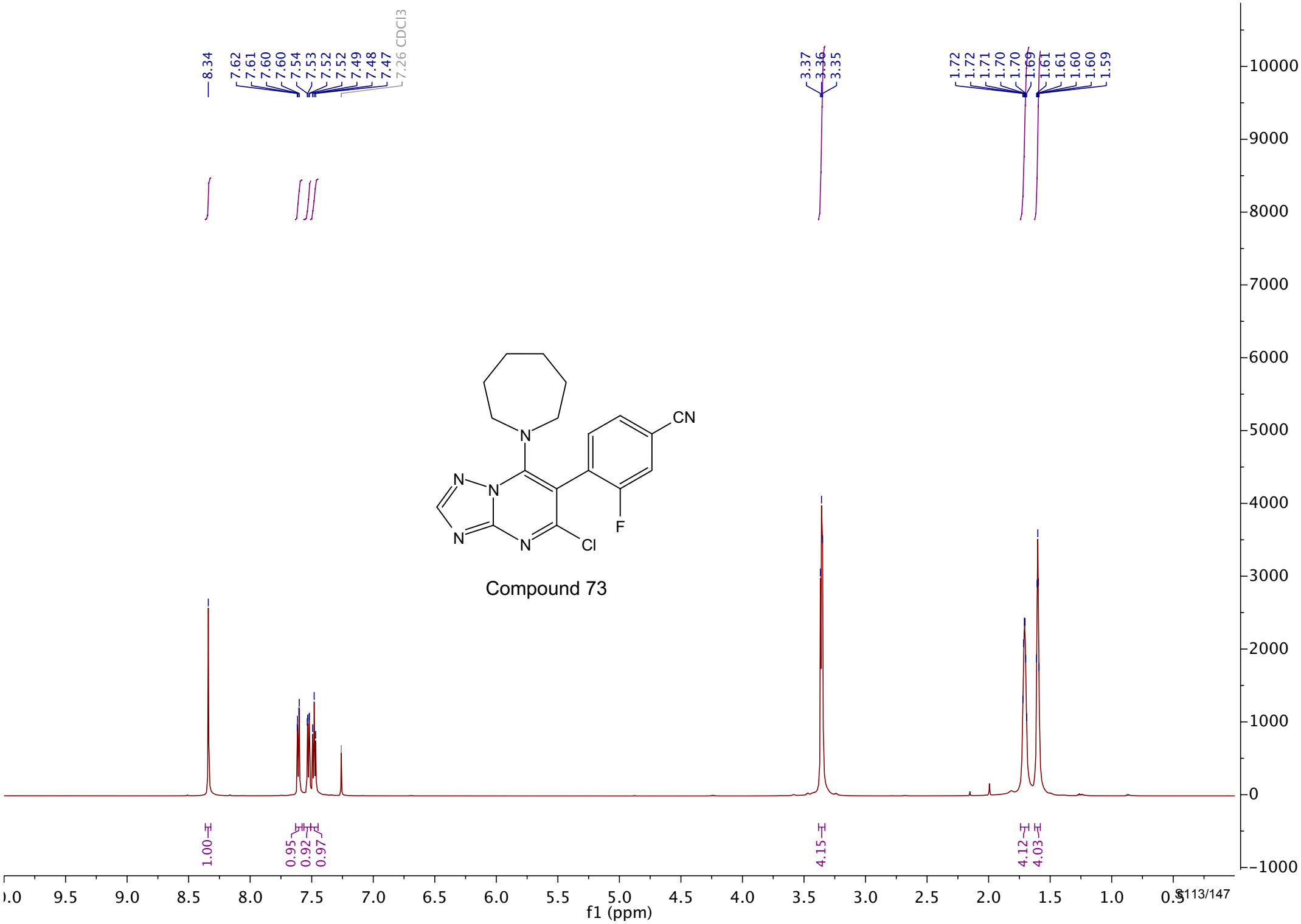

8.38
7.40
7.39
7.26 CDCl3
3.42
3.41
3.40
3.39
1.75
1.75
1.74
1.74
1.74
1.74
1.73
1.73
1.73
1.72
1.63
1.63
1.62
1.62
1.61
F
CN
N
N
N
N
N
F
Cl
Compound 72
*signal from traces of residual solvent/grease
*
*
1.00
1.72
4.48
4.06
4.35
f1 (ppm)
S110/147

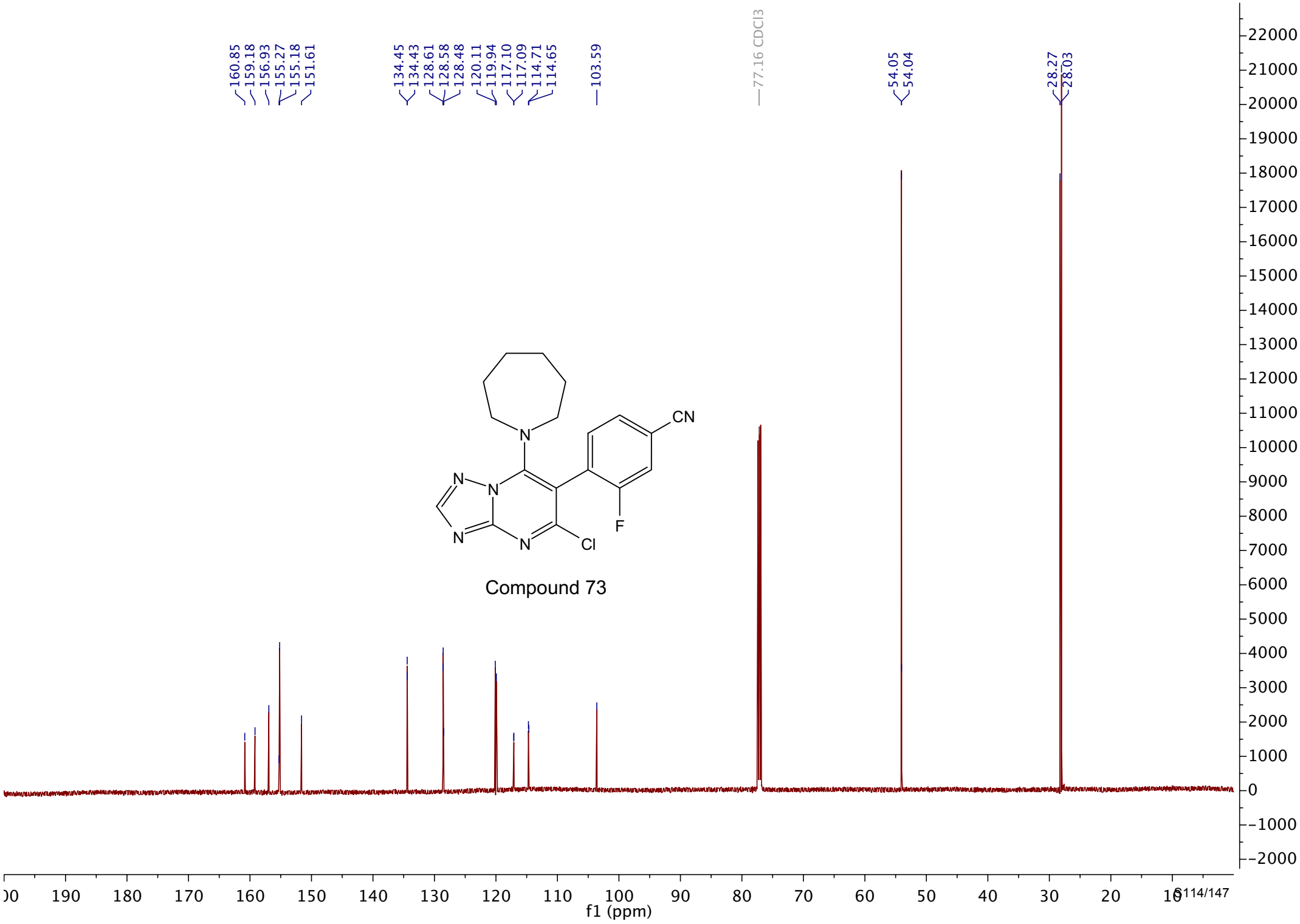

161.60
161.56
159.92
159.88
157.14
155.26
152.10
118.74
118.61
118.48
116.21
116.20
116.18
116.06
116.02
115.20
115.12
115.04
97.32
77.16 CDCl3
53.99
51.22
29.47
28.27
28.17
27.28
27.07
F
CN
F
N
N
N
N
N
Cl
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

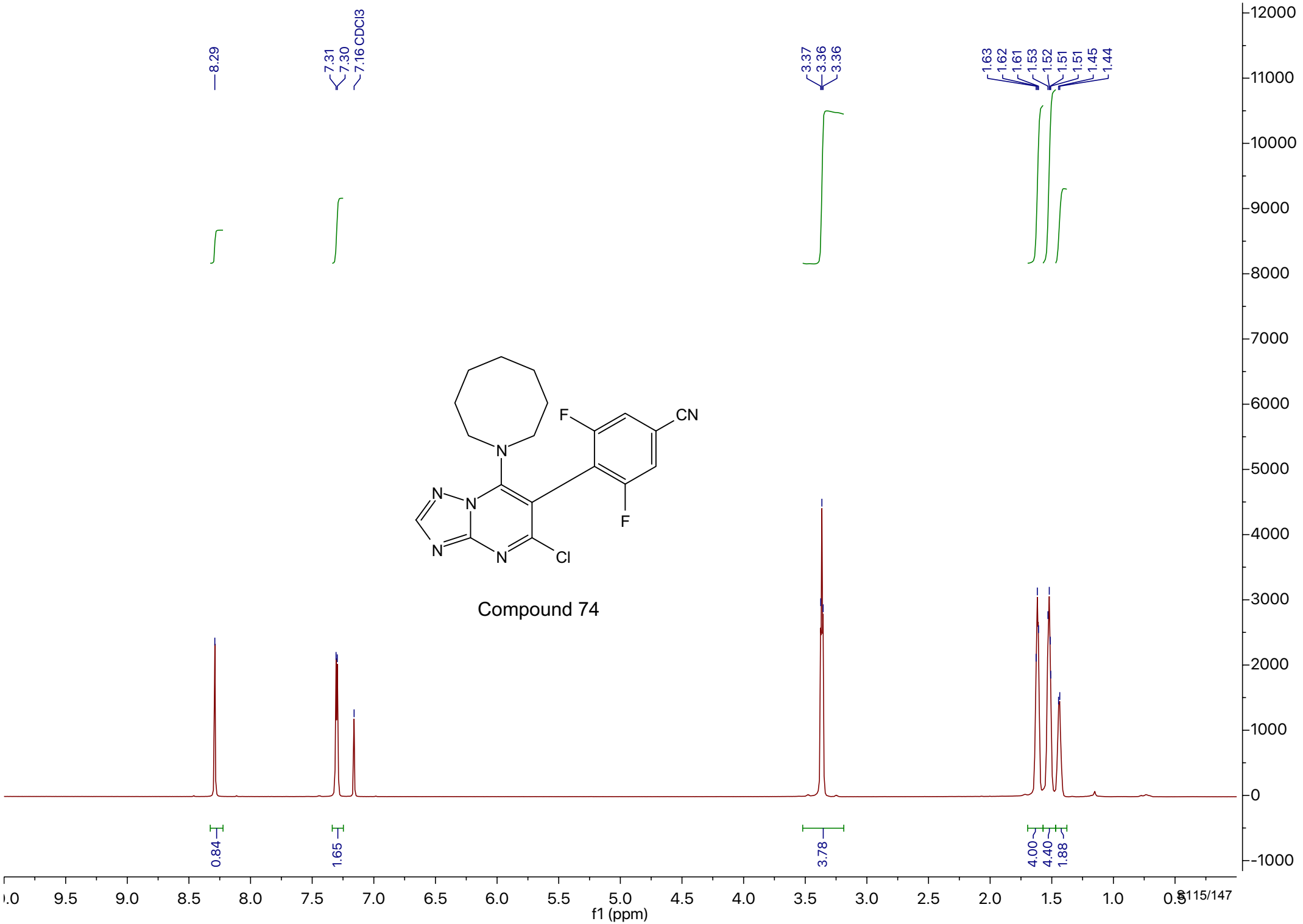
Compound 72


-105.22
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)
F
N
N
N
N
N
Cl
F
N

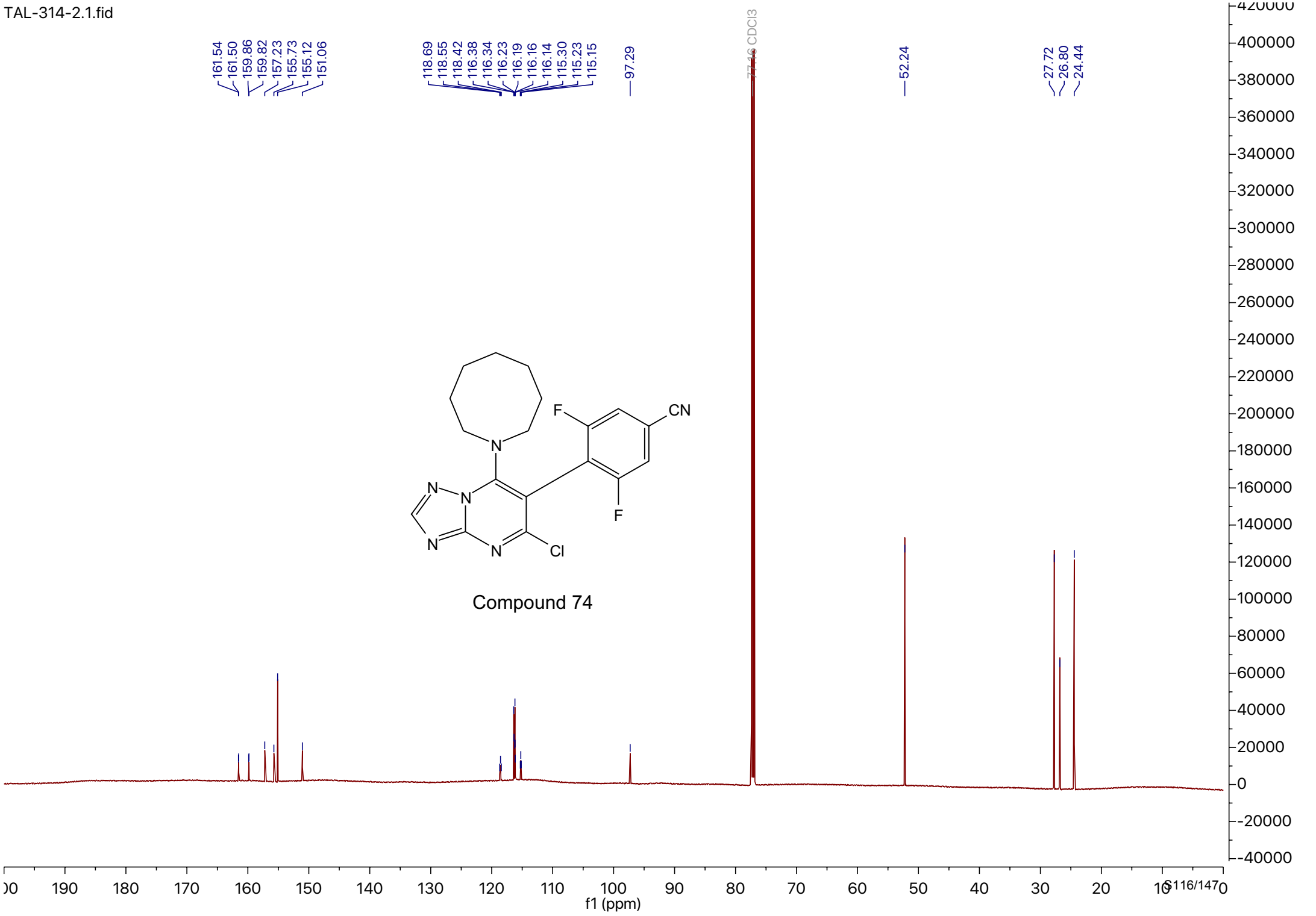
Compound 72


8.34
7.62
7.61
7.60
7.60
7.54
7.53
7.52
7.52
7.49
7.48
7.47
7.26 CDCl3
3.37
3.36
3.35
1.72
1.72
1.71
1.70
1.70
1.69
1.61
1.61
1.60
1.60
1.59
CN
F
Cl
N
Compound 73
1.00
0.95
0.92
0.97
4.15
4.12
4.03
f1 (ppm)
S113/147


160.85
159.18
156.93
155.27
155.18
151.61
134.45
134.43
128.61
128.58
128.48
120.11
119.94
117.10
117.09
114.71
114.65
103.59
77.16 CDCl3
54.05
54.04
28.27
28.03
CN
F
Cl
N
N
N
N
N
Compound 73
f1 (ppm)
S114/147

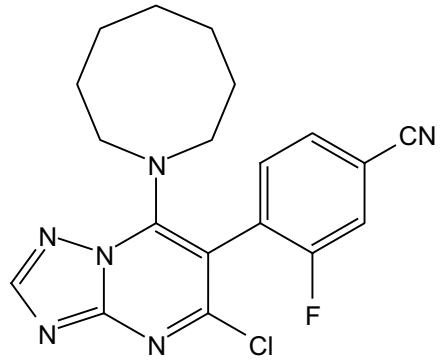

8.29
7.31
7.30
7.16 CDCl3
3.37
3.36
3.36
1.63
1.62
1.61
1.53
1.52
1.51
1.51
1.45
1.44
F
CN
N
N
N
N
N
F
Cl
Compound 74
0.84
1.65
3.78
4.00
4.40
1.88
f1 (ppm)
S115/147

TAL-314-2.1.fid



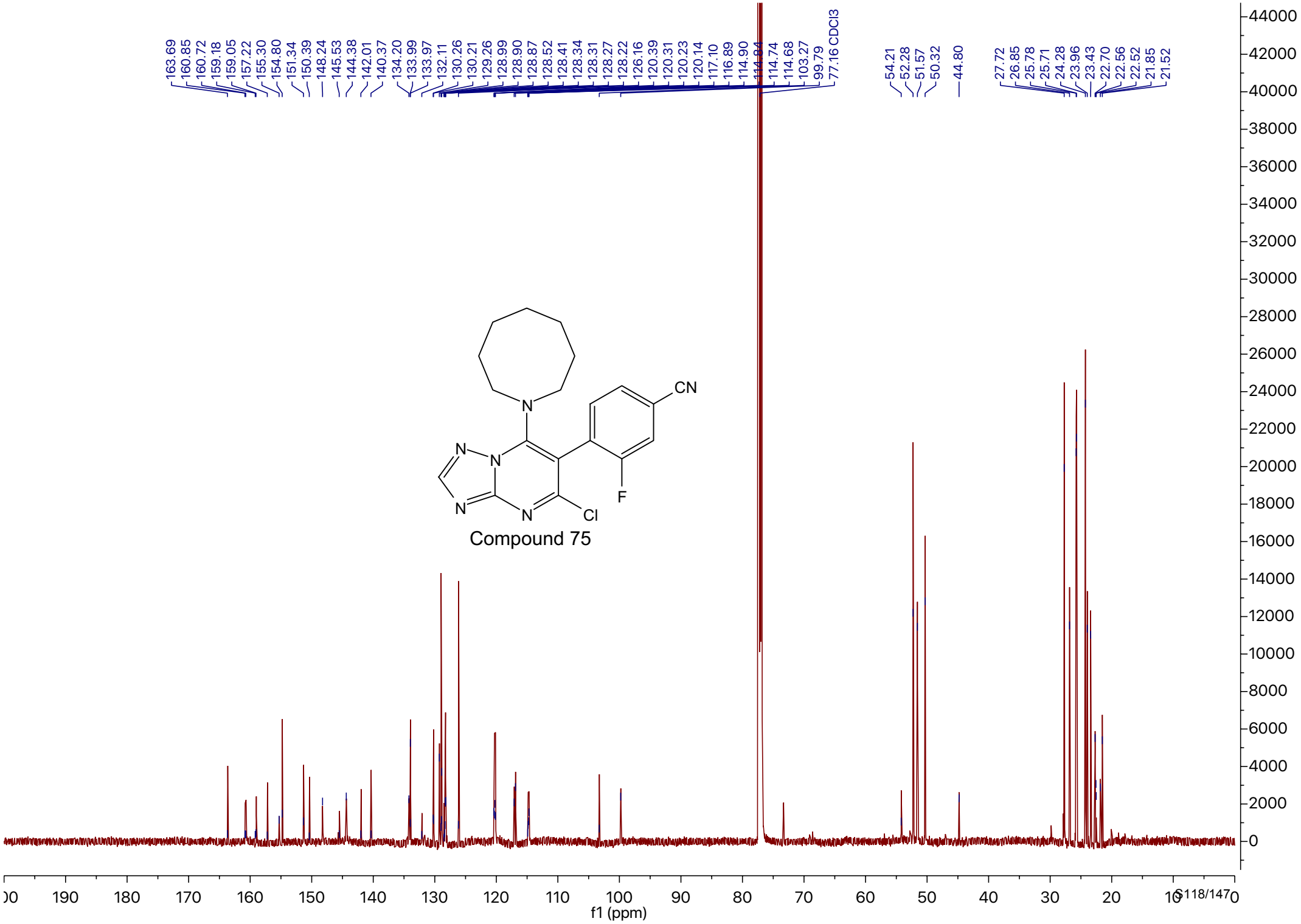
Compound 74

TAL-345-2.1.fid



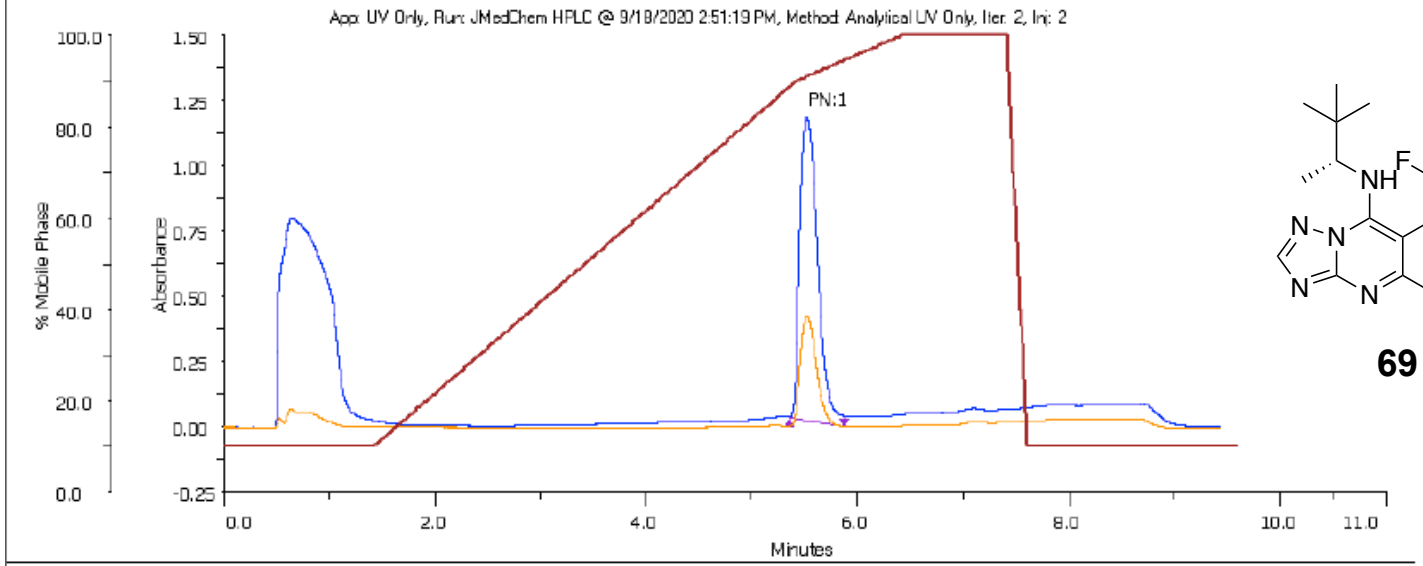
Compound 75

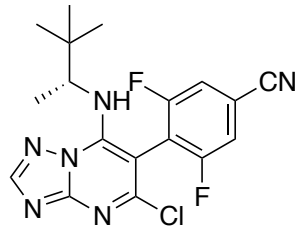
f1 (ppm)


163.69
160.85
160.72
159.18
159.05
157.22
155.30
154.80
151.34
150.39
148.24
145.53
144.38
142.01
140.37
134.20
133.99
133.97
132.11
130.26
130.21
129.26
128.99
128.90
128.87
128.52
128.41
128.34
128.31
128.27
128.22
126.16
120.39
120.31
120.23
120.14
117.10
116.89
114.90
114.84
114.74
114.68
103.27
99.79
77.16 CDCl3
54.21
52.28
51.57
50.32
44.80
27.72
26.85
25.78
25.71
24.28
23.96
23.43
22.70
22.56
22.52
21.85
21.52
N
N
N
N
N
Cl
F
CN
Compound 75
f1 (ppm)
S118/147

Graph

Sample Name	69
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	2





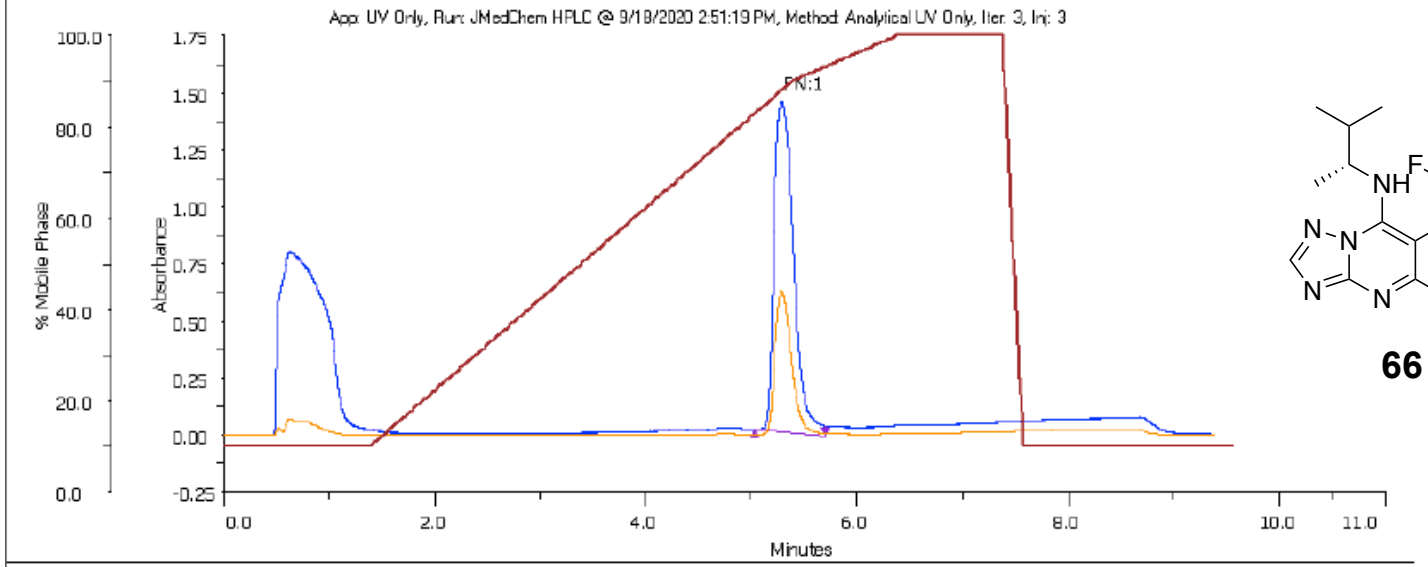
69

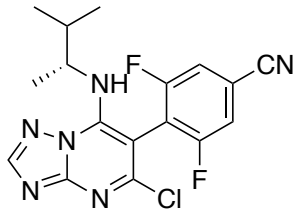
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
69	5.529	23132.6158	100	1.166					

Graph

Sample Name	66
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	3





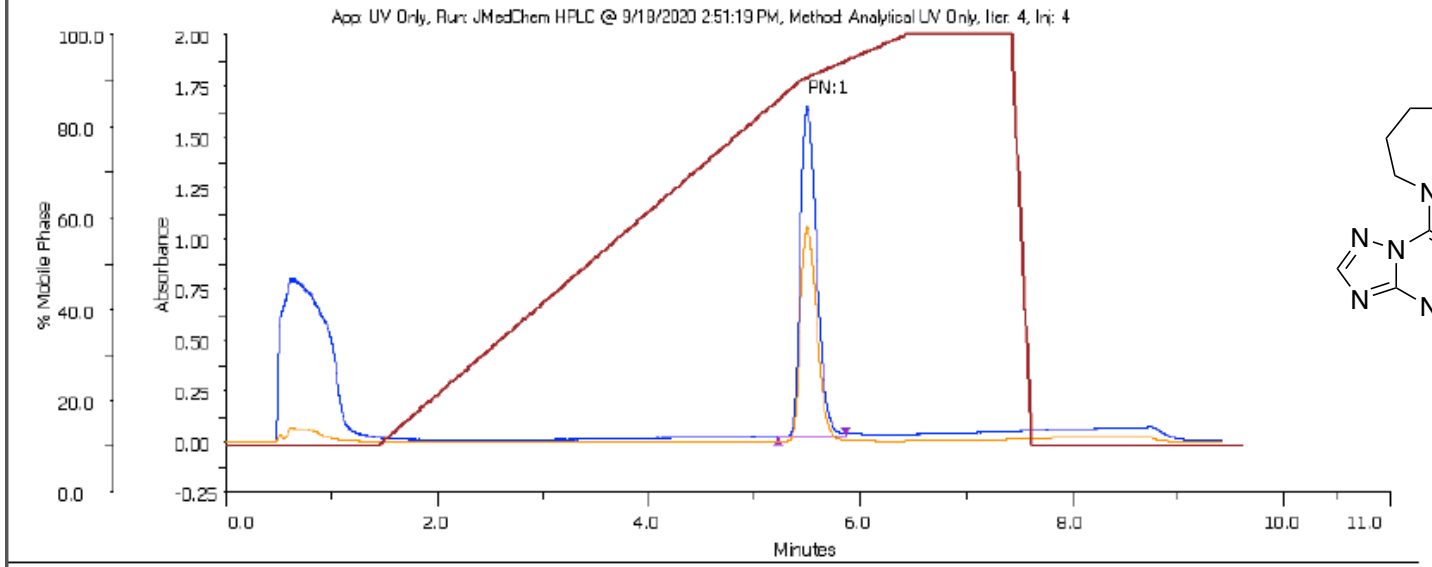
66

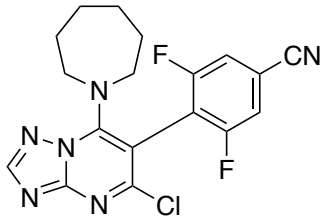
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
66	5.299	31371.6585	100	1.45					

Graph

Sample Name	72
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	4





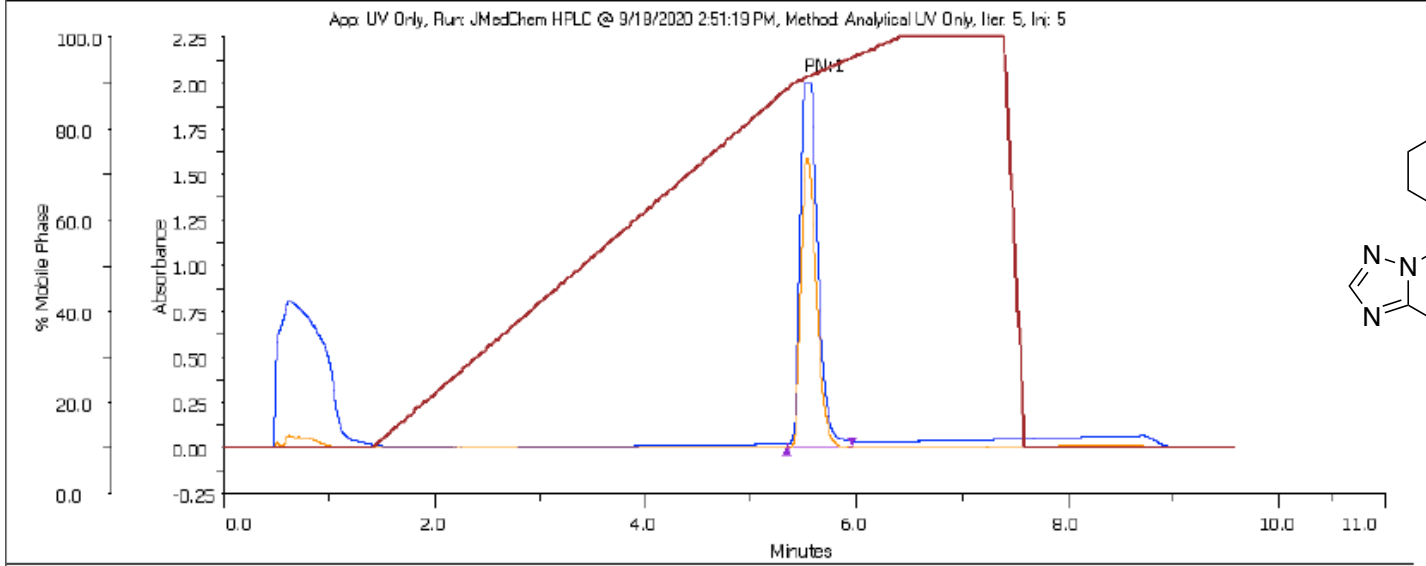
72

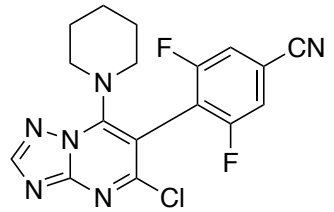
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
72	5.504	28724.2049	100	1.627					

Graph

Sample Name	51
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	5





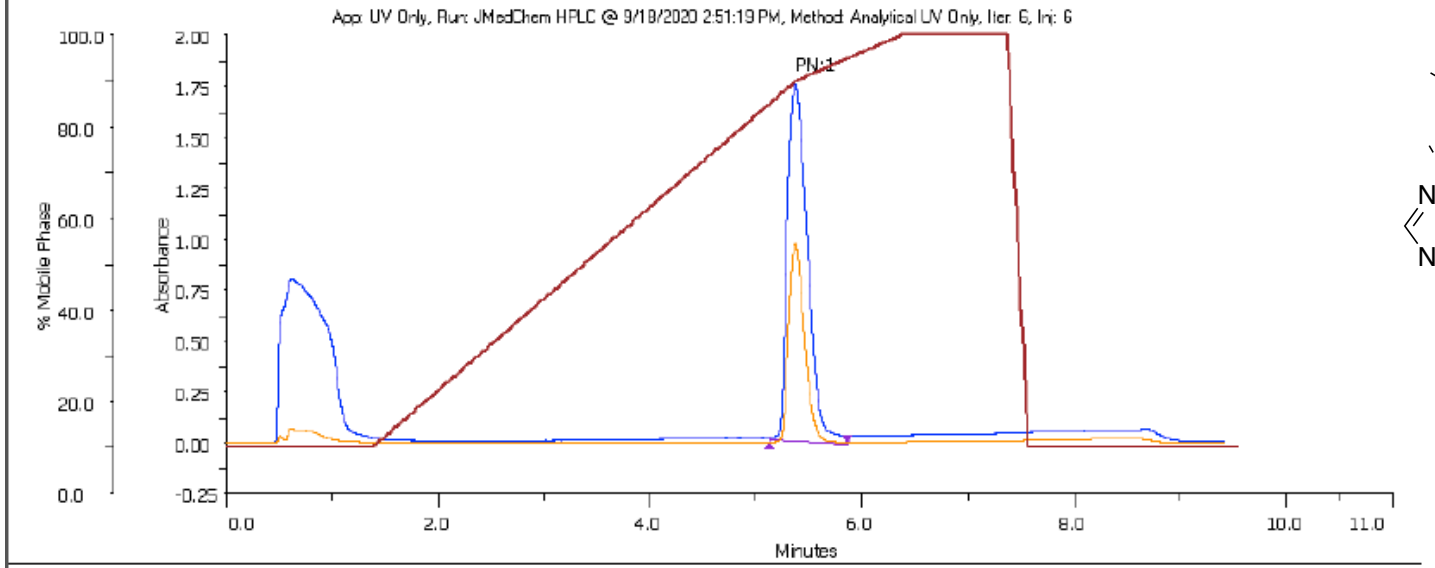
51

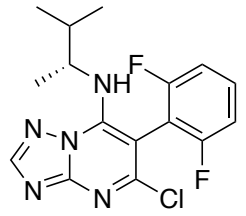
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
51	5.517	38736.4657	100	1.987					

Graph

Sample Name	64
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	6





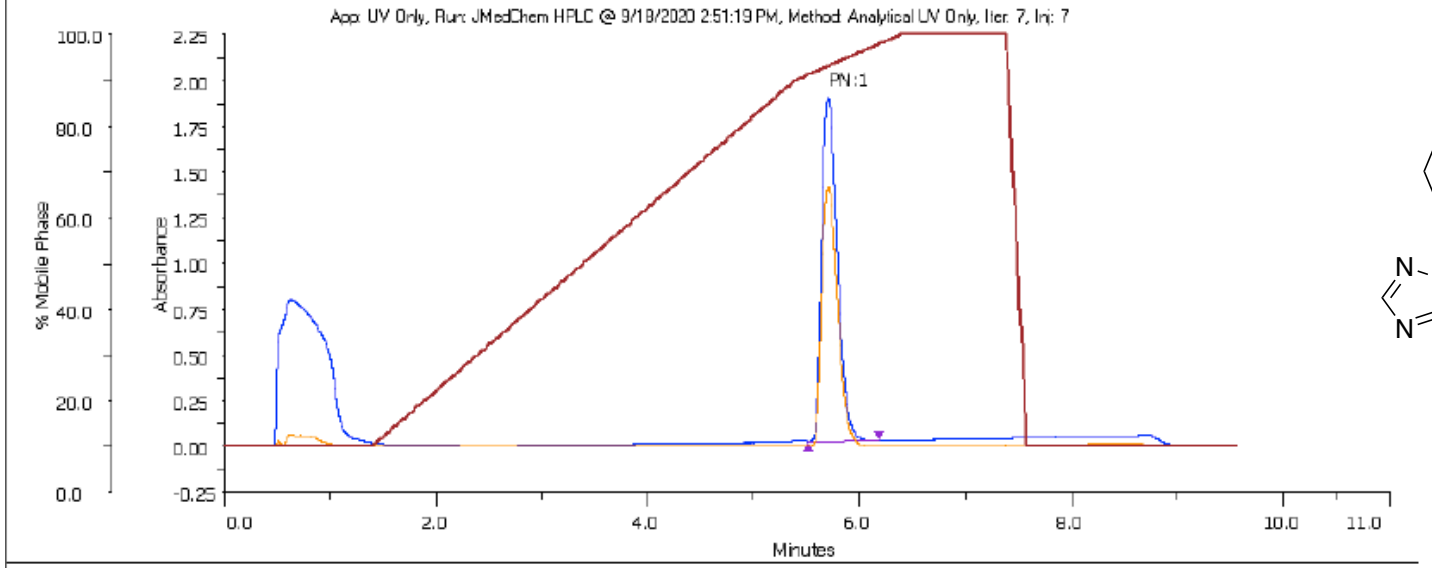
64

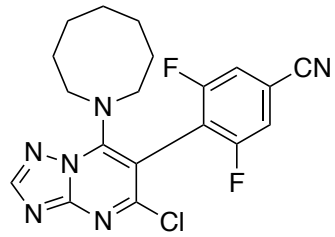
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
64	5.373	39104.2447	100	1.761					

Graph

Sample Name	74
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	7





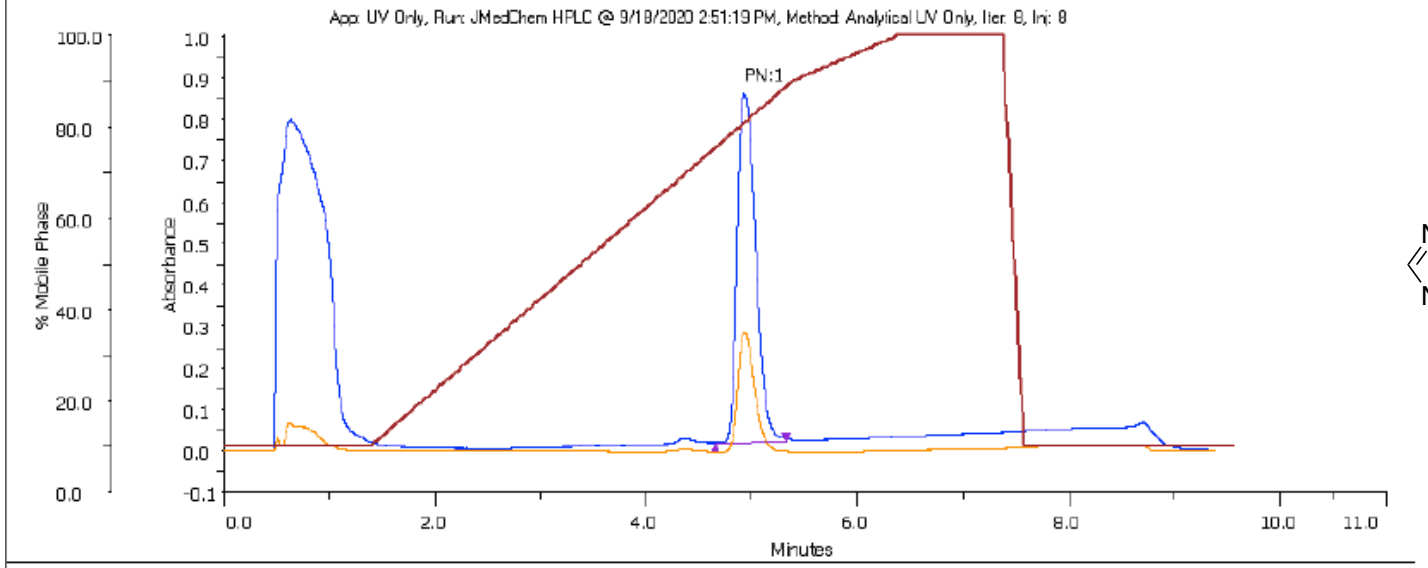
74

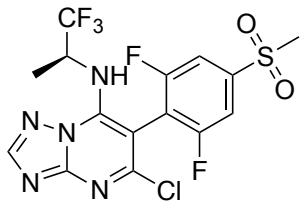
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
74	5.712	32280.4836	100	1.874					

Graph

Sample Name	30
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	8





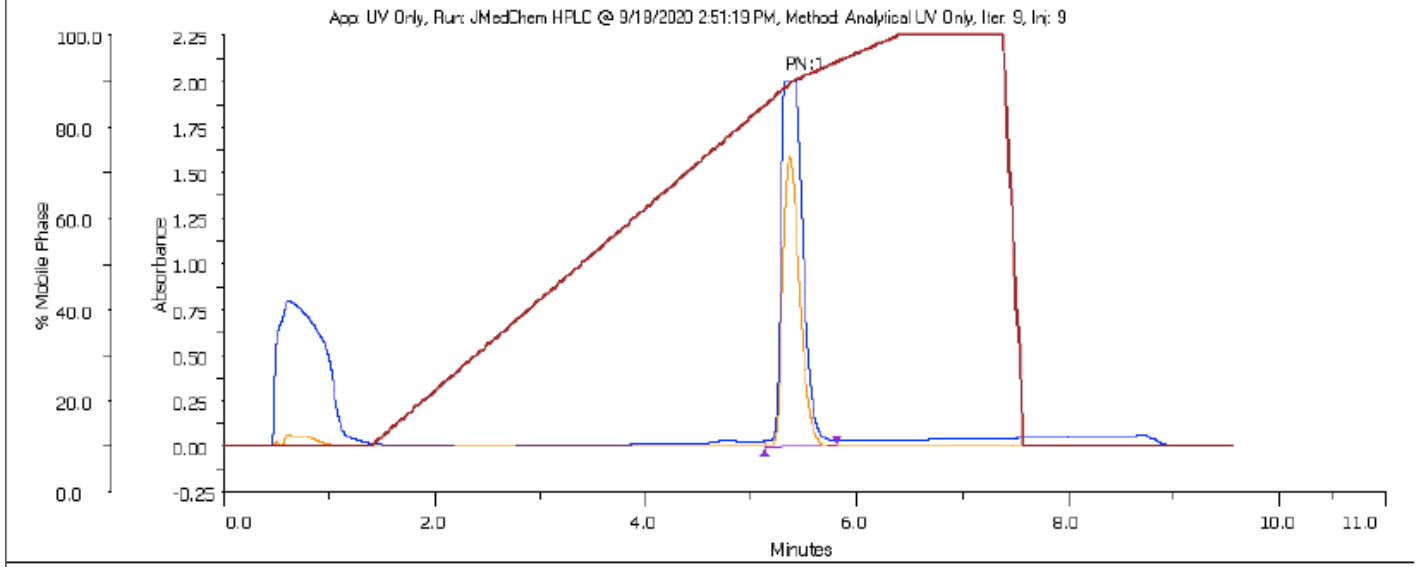
30

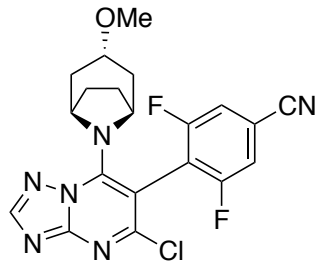
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
30	4.933	17037.6122	100	0.84					

Graph

Sample Name	71
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	9





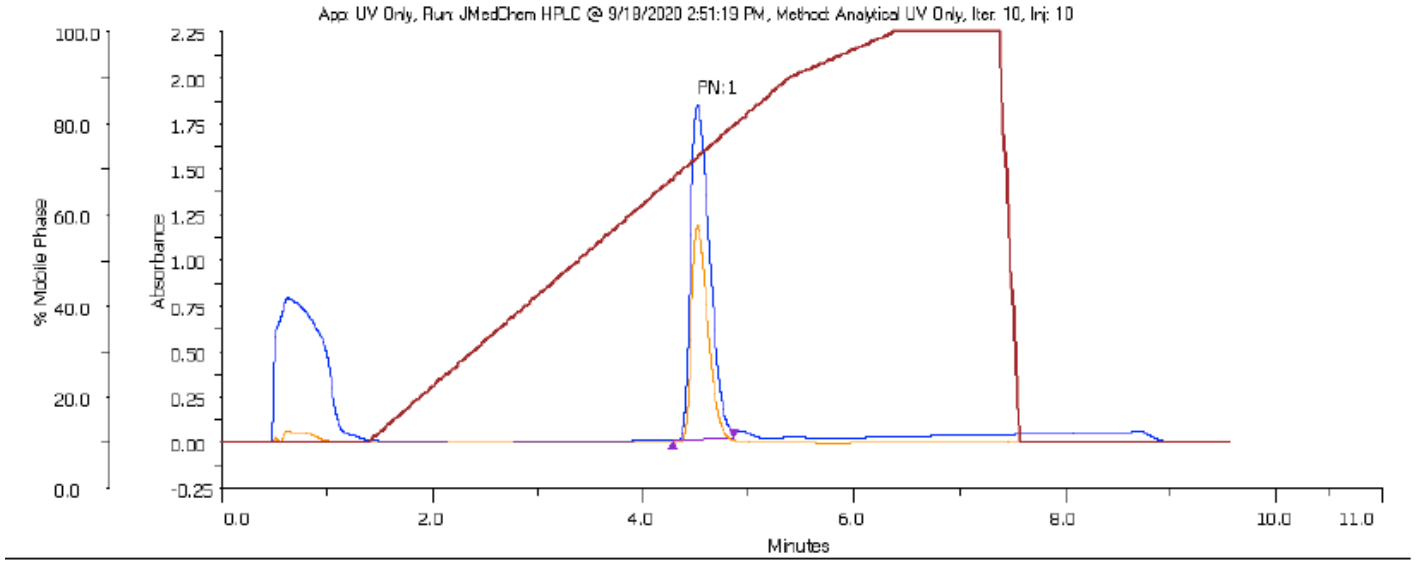
71

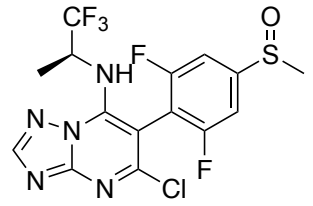
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
71	5.326	47603.6358	100	2.001					

Graph

Sample Name	29
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	10





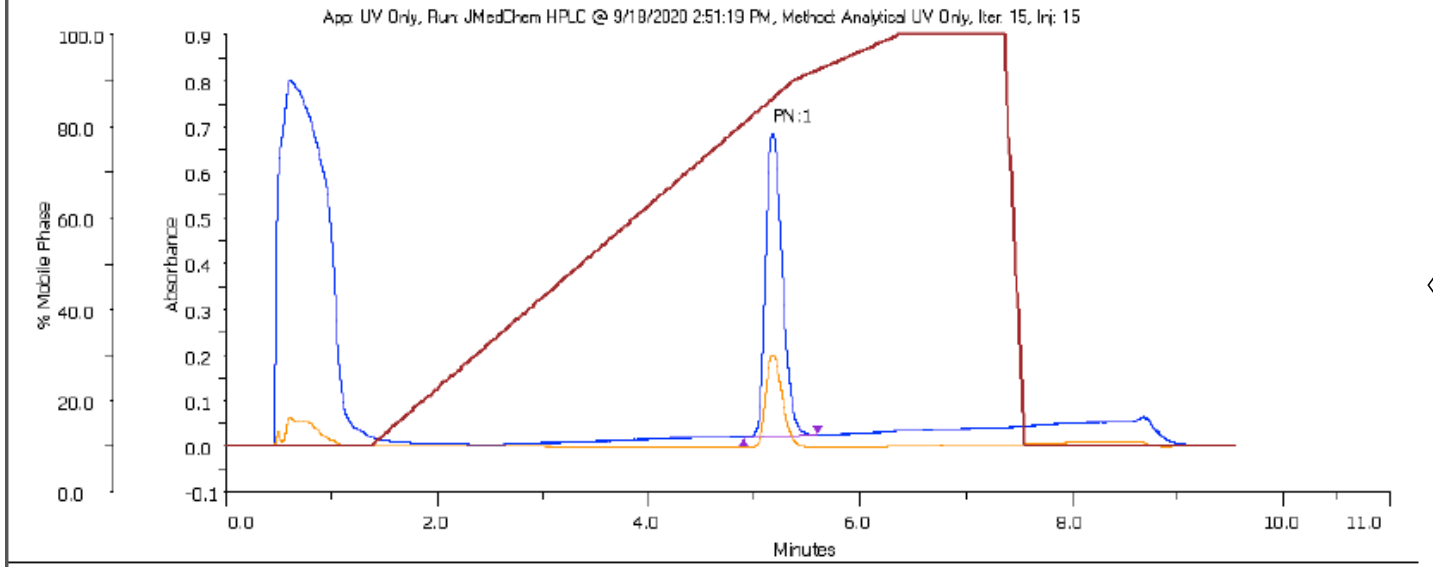
29

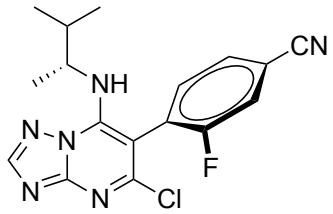
Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)
29	4.519	38639.9498	100	1.834

Graph

Sample Name	67
Application Name	UV Only (Administrator)
Method Name	Analytical UV Only
Configuration Name	UV Only Config
Version	17
Data Instrument Name	Detector
Data Channel Name	159 Channel 1
Notes	
Injection Number	15





67

Sample Table

Sample Name	Retention Time (min)	Area (mAUmin x100)	Area %	Height (AU)					
67	5.176	12156.9832	100	0.662					

Crystal Structure Report

For The Ballatore Lab @ UCSD

Maximilian Bernbeck
UCSD Crystallography Lab
5128 Urey Hall
9500 Gilman Dr
La Jolla, CA 92093-0358
Tel: (858) 822-3871
Fax: (858) 822-3872
mbernbec@ucsd.edu

Experimental Summary

The single crystal X-ray diffraction studies were carried out on a Bruker APEX II Ultra CCD diffractometer equipped with Mo K_α radiation (λ = 0.71073). Crystals of the subject compound were recrystallized from evaporating dichloromethane. A 0.346 x 0.209 x 0.068 mm colorless plate crystal was mounted on a Cryoloop with Paratone oil.

Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 40 mm using exposure time 4 seconds with a scan width of 0.8°. Data collection was 100.0 complete to 25.242° in θ. A total of 30086 reflections were collected. 3902 reflections were found to be symmetry independent, with a R_{int} of 0.0438. Indexing and unit cell refinement indicated a **Primitive Monoclinic** lattice. The space group was found to be ***P*2$_1$.** The data were integrated using the Bruker SAINT Software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model consistent with the proposed structure.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

Notes: Excellent data and refinement

Compound 68 (CCDC : 1995770)

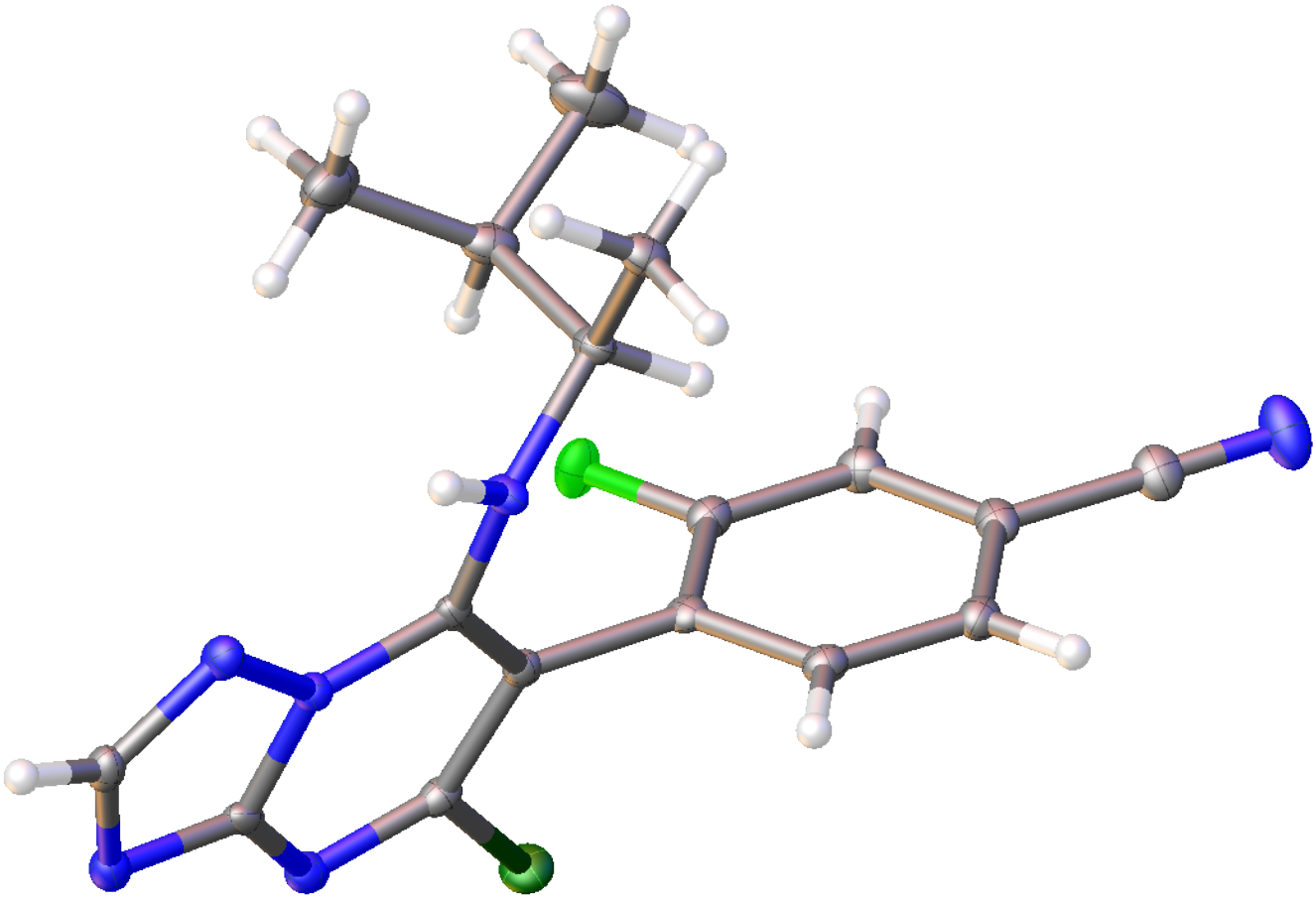


Table S-2. Crystal data and structure refinement for Ballatore_TAL_374_2.

Identification code	ballatore_tal_374_2_0m	
Empirical formula	C17 H16 Cl F N6	
Formula weight	358.81	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 10.0763(6) Å	α= 90°.
	b = 6.6106(4) Å	β= 105.610(2)°.
	c = 13.2029(9) Å	γ = 90°.
Volume	847.01(9) $Å^3$	
Z	2	
Density (calculated)	1.407 Mg/m^3	
Absorption coefficient	0.249 mm^{-1}	
F(000)	372	
Crystal size	0.346 x 0.209 x 0.068 mm^3	
Theta range for data collection	1.601 to 27.517°.	
Index ranges	-13<=h<=13, -8<=k<=8, -17<=l<=17	
Reflections collected	30086	
Independent reflections	3902 [R(int) = 0.0438]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5946	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3902 / 2 / 232	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0607	
R indices (all data)	R1 = 0.0275, wR2 = 0.0620	
Absolute structure parameter	0.000(19)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.280 and -0.188 $e.Å^{-3}$	

Table S-3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Ballatore_TAL_374_2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6697(1)	4428(1)	5611(1)	18(1)
F(1)	5512(1)	7291(2)	3510(1)	19(1)
N(1)	852(2)	2407(3)	1238(1)	26(1)
N(2)	9255(2)	4468(3)	5609(1)	14(1)
N(3)	11621(2)	4436(3)	5522(1)	15(1)
N(4)	11164(1)	4330(3)	3726(1)	14(1)
N(5)	9971(1)	4325(3)	4031(1)	11(1)
N(6)	8576(2)	4128(3)	2334(1)	12(1)
C(1)	1969(2)	2736(3)	1692(2)	18(1)
C(2)	3391(2)	3139(3)	2239(2)	15(1)
C(3)	3770(2)	5080(3)	2625(2)	16(1)
C(4)	5137(2)	5415(3)	3138(1)	14(1)
C(5)	6144(2)	3921(3)	3287(1)	12(1)
C(6)	5728(2)	1988(3)	2896(1)	14(1)
C(7)	4367(2)	1599(3)	2374(1)	15(1)
C(8)	7603(2)	4295(3)	3868(1)	12(1)
C(9)	8008(2)	4416(3)	4976(1)	13(1)
C(10)	8662(2)	4255(3)	3364(1)	11(1)
C(11)	10257(2)	4404(3)	5111(1)	13(1)
C(12)	12094(2)	4387(4)	4655(1)	15(1)
C(13)	7465(2)	4991(3)	1478(1)	13(1)
C(14)	7392(2)	7304(3)	1609(2)	18(1)
C(15)	8702(3)	8395(3)	1566(2)	28(1)
C(16)	6128(3)	8165(4)	808(2)	30(1)
C(17)	7708(2)	4322(4)	438(1)	17(1)

Table S-4. Bond lengths [Å] and angles [°] for Ballatore_TAL_374_2.

Cl(1)-C(9)	1.7443(16)	C(10)-N(6)-C(13)	125.51(16)
F(1)-C(4)	1.350(2)	N(1)-C(1)-C(2)	178.4(2)
N(1)-C(1)	1.144(3)	C(3)-C(2)-C(1)	119.29(19)
N(2)-C(9)	1.309(2)	C(7)-C(2)-C(1)	119.98(18)
N(2)-C(11)	1.345(2)	C(7)-C(2)-C(3)	120.73(18)
N(3)-C(11)	1.335(2)	C(4)-C(3)-C(2)	117.77(18)
N(3)-C(12)	1.354(2)	F(1)-C(4)-C(3)	118.09(17)
N(4)-N(5)	1.3662(19)	F(1)-C(4)-C(5)	118.59(17)
N(4)-C(12)	1.328(2)	C(3)-C(4)-C(5)	123.33(18)
N(5)-C(10)	1.376(2)	C(4)-C(5)-C(6)	117.44(17)
N(5)-C(11)	1.378(2)	C(4)-C(5)-C(8)	122.55(17)
N(6)-C(10)	1.342(2)	C(6)-C(5)-C(8)	119.98(17)
N(6)-C(13)	1.475(2)	C(7)-C(6)-C(5)	120.83(18)
C(1)-C(2)	1.445(3)	C(6)-C(7)-C(2)	119.90(18)
C(2)-C(3)	1.395(3)	C(9)-C(8)-C(5)	120.98(14)
C(2)-C(7)	1.393(3)	C(10)-C(8)-C(5)	121.78(15)
C(3)-C(4)	1.379(3)	C(10)-C(8)-C(9)	116.63(15)
C(4)-C(5)	1.392(3)	N(2)-C(9)-Cl(1)	114.51(12)
C(5)-C(6)	1.399(3)	N(2)-C(9)-C(8)	128.50(15)
C(5)-C(8)	1.484(2)	C(8)-C(9)-Cl(1)	116.96(13)
C(6)-C(7)	1.383(3)	N(5)-C(10)-C(8)	114.68(14)
C(8)-C(9)	1.412(2)	N(6)-C(10)-N(5)	116.10(14)
C(8)-C(10)	1.401(2)	N(6)-C(10)-C(8)	129.21(16)
C(13)-C(14)	1.542(3)	N(2)-C(11)-N(5)	122.09(15)
C(13)-C(17)	1.524(2)	N(3)-C(11)-N(2)	128.83(15)
C(14)-C(15)	1.518(3)	N(3)-C(11)-N(5)	109.07(14)
C(14)-C(16)	1.530(3)	N(4)-C(12)-N(3)	117.39(15)
		N(6)-C(13)-C(14)	110.28(16)
C(9)-N(2)-C(11)	113.96(13)	N(6)-C(13)-C(17)	107.78(15)
C(11)-N(3)-C(12)	102.35(13)	C(17)-C(13)-C(14)	114.38(17)
C(12)-N(4)-N(5)	100.71(13)	C(15)-C(14)-C(13)	113.51(18)
N(4)-N(5)-C(10)	125.41(13)	C(15)-C(14)-C(16)	111.58(19)
N(4)-N(5)-C(11)	110.47(13)	C(16)-C(14)-C(13)	110.30(18)
C(10)-N(5)-C(11)	124.12(14)		

Table S-5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Ballatore_TAL_374_2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	19(1)	24(1)	15(1)	0(1)	11(1)	0(1)
F(1)	16(1)	13(1)	29(1)	-4(1)	7(1)	0(1)
N(1)	15(1)	38(1)	25(1)	-11(1)	5(1)	0(1)
N(2)	18(1)	13(1)	12(1)	-1(1)	4(1)	-1(1)
N(3)	14(1)	14(1)	16(1)	0(1)	2(1)	0(1)
N(4)	11(1)	14(1)	17(1)	1(1)	5(1)	1(1)
N(5)	11(1)	12(1)	12(1)	0(1)	4(1)	1(1)
N(6)	11(1)	17(1)	10(1)	1(1)	4(1)	2(1)
C(1)	17(1)	23(1)	17(1)	-4(1)	8(1)	1(1)
C(2)	13(1)	21(1)	12(1)	-1(1)	6(1)	-1(1)
C(3)	13(1)	18(1)	18(1)	1(1)	7(1)	3(1)
C(4)	16(1)	13(1)	14(1)	-1(1)	7(1)	0(1)
C(5)	13(1)	15(1)	11(1)	2(1)	6(1)	-1(1)
C(6)	16(1)	13(1)	13(1)	1(1)	6(1)	1(1)
C(7)	17(1)	15(1)	13(1)	-1(1)	5(1)	-2(1)
C(8)	13(1)	10(1)	12(1)	0(1)	4(1)	0(1)
C(9)	16(1)	11(1)	14(1)	0(1)	8(1)	-1(1)
C(10)	12(1)	8(1)	12(1)	0(1)	2(1)	1(1)
C(11)	16(1)	10(1)	11(1)	2(1)	1(1)	0(1)
C(12)	11(1)	13(1)	18(1)	0(1)	3(1)	0(1)
C(13)	12(1)	16(1)	12(1)	2(1)	3(1)	1(1)
C(14)	24(1)	18(1)	13(1)	2(1)	6(1)	6(1)
C(15)	38(1)	18(1)	27(1)	1(1)	9(1)	-6(1)
C(16)	35(1)	30(1)	22(1)	4(1)	5(1)	17(1)
C(17)	19(1)	18(1)	12(1)	0(1)	3(1)	3(1)

Table S-6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Ballatore_TAL_374_2.

	x	y	z	U(eq)
H(6)	9382(19)	4050(40)	2228(16)	15
H(3)	3109	6135	2537	19
H(6A)	6388	930	2990	16
H(7)	4098	283	2107	18
H(12)	13053	4393	4709	17
H(13)	6571	4399	1527	16
H(14)	7261	7555	2323	22
H(15A)	9492	7790	2078	41
H(15B)	8631	9828	1735	41
H(15C)	8828	8272	858	41
H(16A)	6246	8027	99	45
H(16B)	6023	9598	961	45
H(16C)	5304	7421	853	45
H(17A)	8584	4877	376	25
H(17B)	6955	4817	-145	25
H(17C)	7739	2842	414	25

Compound 111 (CCDC: 2003391)

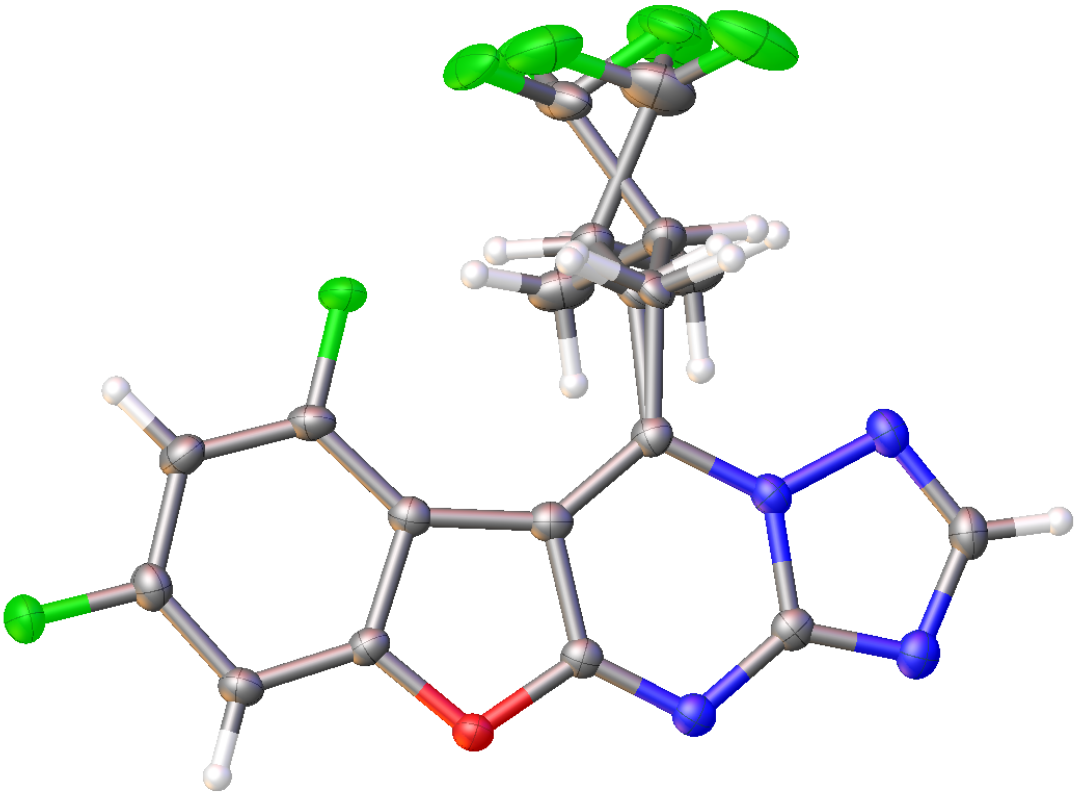


Table S-7. Crystal data and structure refinement for Ballatore_BRL_I_205.

Identification code	ballatore_brl_i_205_redo_0m_a	
Empirical formula	C15 H9 F5 N4 O	
Formula weight	356.26	
Temperature	100.0 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.71530(10) Å	α= 94.8510(10)°.
	b = 10.56760(10) Å	β= 92.2480(10)°.
	c = 14.1191(2) Å	γ = 98.7440(10)°.
Volume	1425.59(3) $Å^3$	
Z	4	
Density (calculated)	1.660 Mg/m^3	
Absorption coefficient	1.358 mm^{-1}	
F(000)	720	
Crystal size	0.22 x 0.18 x 0.08 mm^3	
Theta range for data collection	3.146 to 66.663°.	
Index ranges	-11<=h<=11, -12<=k<=12, -16<=l<=16	
Reflections collected	40759	
Independent reflections	4785 [R(int) = 0.0301]	
Completeness to theta = 66.663°	94.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5201 and 0.4391	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4785 / 54 / 541	
Goodness-of-fit on F^2	1.136	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1157	
R indices (all data)	R1 = 0.0479, wR2 = 0.1169	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.554 and -0.309 $e.Å^{-3}$	

Table S-8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Ballatore_BRL_I_205. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1A)	-4692(1)	7745(1)	2031(1)	30(1)
F(2A)	-417(1)	6403(1)	1393(1)	27(1)
O(1A)	-1541(2)	7147(1)	4558(1)	19(1)
N(1A)	2472(2)	5921(2)	5918(1)	23(1)
N(2A)	351(2)	6604(2)	5362(1)	20(1)
N(3A)	2089(2)	5926(2)	4356(1)	19(1)
N(4A)	3341(2)	5483(2)	4462(2)	23(1)
C(1A)	3490(2)	5510(2)	5397(2)	24(1)
C(2A)	1587(2)	6176(2)	5251(2)	19(1)
C(3A)	-272(2)	6739(2)	4558(2)	18(1)
C(4A)	-1975(2)	7152(2)	3611(2)	18(1)
C(5A)	-3243(2)	7473(2)	3331(2)	21(1)
C(6A)	-3482(2)	7413(2)	2360(2)	23(1)
C(7A)	-2563(2)	7055(2)	1698(2)	24(1)
C(8A)	-1323(2)	6746(2)	2031(2)	21(1)
C(9A)	-975(2)	6779(2)	3000(2)	19(1)
C(10A)	156(2)	6500(2)	3612(2)	19(1)
C(11A)	1423(2)	6088(2)	3512(2)	19(1)
F(3A)	1637(5)	5153(4)	545(3)	43(1)
F(4A)	3352(6)	4316(5)	1114(4)	41(1)
F(5A)	1453(4)	3108(3)	646(2)	45(1)
C(12A)	2240(20)	5877(9)	2644(11)	19(2)
C(13A)	2108(6)	4429(5)	2357(4)	23(1)
C(14A)	636(6)	3728(5)	2225(4)	33(1)
C(15A)	1938(8)	4231(6)	1113(5)	32(1)
F(3B)	2266(6)	4818(6)	737(3)	61(1)
F(4B)	2850(4)	3043(4)	1147(3)	64(1)
F(5B)	4193(5)	4820(4)	1545(4)	68(1)
C(12B)	2010(20)	5748(8)	2569(10)	19(2)
C(13B)	1423(5)	4404(5)	2089(4)	23(1)
C(14B)	1753(6)	3326(4)	2660(4)	33(1)

C(15B)	2868(11)	4281(7)	1432(7)	48(2)
F(1C)	12809(1)	-954(1)	2253(1)	31(1)
F(2C)	8755(2)	158(2)	866(1)	33(1)
O(1B)	9263(2)	313(1)	4181(1)	20(1)
N(1B)	4954(2)	1600(2)	4798(1)	23(1)
N(2B)	7197(2)	920(2)	4637(1)	20(1)
N(3B)	5672(2)	1252(2)	3343(1)	19(1)
N(4B)	4399(2)	1644(2)	3211(1)	24(1)
C(1C)	4048(2)	1830(2)	4106(2)	25(1)
C(2C)	5988(2)	1242(2)	4309(2)	19(1)
C(3C)	7998(2)	651(2)	3957(2)	18(1)
C(4C)	9867(2)	72(2)	3328(2)	19(1)
C(5C)	11161(2)	-314(2)	3276(2)	21(1)
C(6C)	11577(2)	-534(2)	2361(2)	24(1)
C(7C)	10802(3)	-377(2)	1551(2)	26(1)
C(8C)	9524(2)	12(2)	1659(2)	23(1)
C(9C)	9004(2)	245(2)	2552(2)	19(1)
C(10C)	7754(2)	635(2)	2952(2)	18(1)
C(11C)	6509(2)	939(2)	2628(2)	18(1)
F(3D)	6369(2)	1651(3)	-287(2)	46(1)
F(4D)	4247(3)	1488(2)	108(2)	48(1)
F(5D)	5411(2)	3354(2)	-26(1)	45(1)
C(12D)	5958(7)	954(9)	1629(2)	19(1)
C(13D)	5995(3)	2309(3)	1313(2)	26(1)
C(14D)	7430(4)	3131(3)	1465(2)	39(1)
C(15D)	5523(5)	2210(4)	286(3)	33(1)
F(3C)	6509(18)	926(19)	-329(11)	46(4)
F(4C)	4890(30)	2060(30)	88(18)	54(5)
F(5C)	6850(20)	3040(16)	-297(11)	66(4)
C(12C)	6170(70)	860(80)	1583(11)	19(1)
C(13C)	6720(30)	2190(18)	1174(13)	26(1)
C(14C)	6440(30)	3435(18)	1689(17)	39(1)
C(15C)	6230(40)	2010(30)	150(16)	33(1)

Table S-9. Bond lengths [Å] and angles [°] for Ballatore_BRL_I_205.

F(1A)-C(6A)	1.353(3)	C(13A)-C(15A)	1.748(7)
F(2A)-C(8A)	1.350(2)	C(14A)-H(14G)	0.9800
O(1A)-C(3A)	1.367(3)	C(14A)-H(14I)	0.9800
O(1A)-C(4A)	1.386(3)	C(14A)-H(14H)	0.9800
N(1A)-C(1A)	1.356(3)	F(3B)-C(15B)	1.334(12)
N(1A)-C(2A)	1.322(3)	F(4B)-C(15B)	1.333(8)
N(2A)-C(2A)	1.356(3)	F(5B)-C(15B)	1.324(11)
N(2A)-C(3A)	1.294(3)	C(12B)-H(12C)	0.9900
N(3A)-N(4A)	1.375(3)	C(12B)-H(12D)	0.9900
N(3A)-C(2A)	1.392(3)	C(12B)-C(13B)	1.536(7)
N(3A)-C(11A)	1.369(3)	C(13B)-H(13B)	1.0000
N(4A)-C(1A)	1.320(3)	C(13B)-C(14B)	1.515(7)
C(1A)-H(1A)	0.9500	C(13B)-C(15B)	1.728(8)
C(3A)-C(10A)	1.428(3)	C(14B)-H(14D)	0.9800
C(4A)-C(5A)	1.378(3)	C(14B)-H(14E)	0.9800
C(4A)-C(9A)	1.403(3)	C(14B)-H(14F)	0.9800
C(5A)-H(5A)	0.9500	F(1C)-C(6C)	1.348(3)
C(5A)-C(6A)	1.376(4)	F(2C)-C(8C)	1.354(3)
C(6A)-C(7A)	1.386(3)	O(1B)-C(3C)	1.364(3)
C(7A)-H(7A)	0.9500	O(1B)-C(4C)	1.382(3)
C(7A)-C(8A)	1.372(3)	N(1B)-C(1C)	1.352(3)
C(8A)-C(9A)	1.392(3)	N(1B)-C(2C)	1.325(3)
C(9A)-C(10A)	1.452(3)	N(2B)-C(2C)	1.348(3)
C(10A)-C(11A)	1.375(3)	N(2B)-C(3C)	1.299(3)
C(11A)-C(12A)	1.502(7)	N(3B)-N(4B)	1.374(3)
C(11A)-C(12B)	1.504(6)	N(3B)-C(2C)	1.387(3)
F(3A)-C(15A)	1.371(8)	N(3B)-C(11C)	1.372(3)
F(4A)-C(15A)	1.363(9)	N(4B)-C(1C)	1.328(3)
F(5A)-C(15A)	1.318(7)	C(1C)-H(1C)	0.9500
C(12A)-H(12F)	0.9900	C(3C)-C(10C)	1.427(3)
C(12A)-H(12E)	0.9900	C(4C)-C(5C)	1.383(3)
C(12A)-C(13A)	1.535(8)	C(4C)-C(9C)	1.394(3)
C(13A)-H(13A)	1.0000	C(5C)-H(5C)	0.9500
C(13A)-C(14A)	1.505(8)	C(5C)-C(6C)	1.380(3)

C(6C)-C(7C)	1.380(4)	C(11A)-N(3A)-N(4A)	126.20(19)
C(7C)-H(7C)	0.9500	C(11A)-N(3A)-C(2A)	124.84(19)
C(7C)-C(8C)	1.376(3)	C(1A)-N(4A)-N(3A)	101.24(18)
C(8C)-C(9C)	1.393(3)	N(1A)-C(1A)-H(1A)	121.2
C(9C)-C(10C)	1.459(3)	N(4A)-C(1A)-N(1A)	117.7(2)
C(10C)-C(11C)	1.370(3)	N(4A)-C(1A)-H(1A)	121.2
C(11C)-C(12D)	1.490(4)	N(1A)-C(2A)-N(2A)	128.2(2)
C(11C)-C(12C)	1.491(10)	N(1A)-C(2A)-N(3A)	109.93(19)
F(3D)-C(15D)	1.340(4)	N(2A)-C(2A)-N(3A)	121.8(2)
F(4D)-C(15D)	1.356(5)	O(1A)-C(3A)-C(10A)	111.39(19)
F(5D)-C(15D)	1.340(4)	N(2A)-C(3A)-O(1A)	119.16(19)
C(12D)-H(12A)	0.9900	N(2A)-C(3A)-C(10A)	129.4(2)
C(12D)-H(12B)	0.9900	O(1A)-C(4A)-C(9A)	111.37(19)
C(12D)-C(13D)	1.531(9)	C(5A)-C(4A)-O(1A)	122.94(19)
C(13D)-H(13D)	1.0000	C(5A)-C(4A)-C(9A)	125.7(2)
C(13D)-C(14D)	1.523(4)	C(4A)-C(5A)-H(5A)	123.0
C(13D)-C(15D)	1.494(5)	C(6A)-C(5A)-C(4A)	114.1(2)
C(14D)-H(14A)	0.9800	C(6A)-C(5A)-H(5A)	123.0
C(14D)-H(14B)	0.9800	F(1A)-C(6A)-C(5A)	117.6(2)
C(14D)-H(14C)	0.9800	F(1A)-C(6A)-C(7A)	117.8(2)
F(3C)-C(15C)	1.35(3)	C(5A)-C(6A)-C(7A)	124.6(2)
F(4C)-C(15C)	1.31(4)	C(6A)-C(7A)-H(7A)	121.0
F(5C)-C(15C)	1.37(3)	C(8A)-C(7A)-C(6A)	117.9(2)
C(12C)-H(12G)	0.9900	C(8A)-C(7A)-H(7A)	121.0
C(12C)-H(12H)	0.9900	F(2A)-C(8A)-C(7A)	118.4(2)
C(12C)-C(13C)	1.59(9)	F(2A)-C(8A)-C(9A)	119.5(2)
C(13C)-H(13C)	1.0000	C(7A)-C(8A)-C(9A)	122.1(2)
C(13C)-C(14C)	1.517(11)	C(4A)-C(9A)-C(10A)	105.91(19)
C(13C)-C(15C)	1.492(11)	C(8A)-C(9A)-C(4A)	115.6(2)
C(14C)-H(14J)	0.9800	C(8A)-C(9A)-C(10A)	138.5(2)
C(14C)-H(14K)	0.9800	C(3A)-C(10A)-C(9A)	104.91(19)
C(14C)-H(14L)	0.9800	C(11A)-C(10A)-C(3A)	117.3(2)
C(3A)-O(1A)-C(4A)	106.40(16)	C(11A)-C(10A)-C(9A)	137.8(2)
C(2A)-N(1A)-C(1A)	102.18(19)	N(3A)-C(11A)-C(10A)	114.0(2)
C(3A)-N(2A)-C(2A)	112.59(19)	N(3A)-C(11A)-C(12A)	115.0(11)
N(4A)-N(3A)-C(2A)	108.96(19)	N(3A)-C(11A)-C(12B)	121.8(9)

C(10A)-C(11A)-C(12A)	130.8(11)	C(14B)-C(13B)-C(15B)	90.3(4)
C(10A)-C(11A)-C(12B)	124.1(9)	C(15B)-C(13B)-H(13B)	117.8
C(11A)-C(12A)-H(12F)	109.8	C(13B)-C(14B)-H(14D)	109.5
C(11A)-C(12A)-H(12E)	109.8	C(13B)-C(14B)-H(14E)	109.5
C(11A)-C(12A)-C(13A)	109.3(6)	C(13B)-C(14B)-H(14F)	109.5
H(12F)-C(12A)-H(12E)	108.3	H(14D)-C(14B)-H(14E)	109.5
C(13A)-C(12A)-H(12F)	109.8	H(14D)-C(14B)-H(14F)	109.5
C(13A)-C(12A)-H(12E)	109.8	H(14E)-C(14B)-H(14F)	109.5
C(12A)-C(13A)-H(13A)	116.5	F(3B)-C(15B)-C(13B)	88.8(6)
C(12A)-C(13A)-C(15A)	106.6(8)	F(4B)-C(15B)-F(3B)	108.0(8)
C(14A)-C(13A)-C(12A)	114.7(9)	F(4B)-C(15B)-C(13B)	108.0(6)
C(14A)-C(13A)-H(13A)	116.5	F(5B)-C(15B)-F(3B)	108.3(7)
C(14A)-C(13A)-C(15A)	80.3(4)	F(5B)-C(15B)-F(4B)	107.0(7)
C(15A)-C(13A)-H(13A)	116.5	F(5B)-C(15B)-C(13B)	133.5(6)
C(13A)-C(14A)-H(14G)	109.5	C(3C)-O(1B)-C(4C)	106.34(17)
C(13A)-C(14A)-H(14I)	109.5	C(2C)-N(1B)-C(1C)	102.62(19)
C(13A)-C(14A)-H(14H)	109.5	C(3C)-N(2B)-C(2C)	112.48(19)
H(14G)-C(14A)-H(14I)	109.5	N(4B)-N(3B)-C(2C)	109.63(18)
H(14G)-C(14A)-H(14H)	109.5	C(11C)-N(3B)-N(4B)	125.0(2)
H(14I)-C(14A)-H(14H)	109.5	C(11C)-N(3B)-C(2C)	125.37(19)
F(3A)-C(15A)-C(13A)	124.9(5)	C(1C)-N(4B)-N(3B)	100.83(19)
F(4A)-C(15A)-F(3A)	104.4(6)	N(1B)-C(1C)-H(1C)	121.3
F(4A)-C(15A)-C(13A)	87.7(5)	N(4B)-C(1C)-N(1B)	117.5(2)
F(5A)-C(15A)-F(3A)	106.7(6)	N(4B)-C(1C)-H(1C)	121.3
F(5A)-C(15A)-F(4A)	104.9(5)	N(1B)-C(2C)-N(2B)	128.7(2)
F(5A)-C(15A)-C(13A)	121.8(5)	N(1B)-C(2C)-N(3B)	109.5(2)
C(11A)-C(12B)-H(12C)	108.4	N(2B)-C(2C)-N(3B)	121.81(19)
C(11A)-C(12B)-H(12D)	108.4	O(1B)-C(3C)-C(10C)	111.55(18)
C(11A)-C(12B)-C(13B)	115.3(5)	N(2B)-C(3C)-O(1B)	119.1(2)
H(12C)-C(12B)-H(12D)	107.5	N(2B)-C(3C)-C(10C)	129.3(2)
C(13B)-C(12B)-H(12C)	108.4	O(1B)-C(4C)-C(5C)	122.7(2)
C(13B)-C(12B)-H(12D)	108.4	O(1B)-C(4C)-C(9C)	111.73(19)
C(12B)-C(13B)-H(13B)	117.8	C(5C)-C(4C)-C(9C)	125.5(2)
C(12B)-C(13B)-C(15B)	94.5(6)	C(4C)-C(5C)-H(5C)	122.8
C(14B)-C(13B)-C(12B)	113.3(9)	C(6C)-C(5C)-C(4C)	114.4(2)
C(14B)-C(13B)-H(13B)	117.8	C(6C)-C(5C)-H(5C)	122.8

F(1C)-C(6C)-C(5C)	117.7(2)	C(13D)-C(14D)-H(14C)	109.5
F(1C)-C(6C)-C(7C)	118.0(2)	H(14A)-C(14D)-H(14B)	109.5
C(7C)-C(6C)-C(5C)	124.3(2)	H(14A)-C(14D)-H(14C)	109.5
C(6C)-C(7C)-H(7C)	121.0	H(14B)-C(14D)-H(14C)	109.5
C(8C)-C(7C)-C(6C)	118.1(2)	F(3D)-C(15D)-F(4D)	105.3(3)
C(8C)-C(7C)-H(7C)	121.0	F(3D)-C(15D)-C(13D)	113.0(4)
F(2C)-C(8C)-C(7C)	118.3(2)	F(4D)-C(15D)-C(13D)	112.3(3)
F(2C)-C(8C)-C(9C)	119.7(2)	F(5D)-C(15D)-F(3D)	107.5(3)
C(7C)-C(8C)-C(9C)	122.0(2)	F(5D)-C(15D)-F(4D)	105.5(4)
C(4C)-C(9C)-C(10C)	105.87(19)	F(5D)-C(15D)-C(13D)	112.8(3)
C(8C)-C(9C)-C(4C)	115.7(2)	C(11C)-C(12C)-H(12G)	109.5
C(8C)-C(9C)-C(10C)	138.4(2)	C(11C)-C(12C)-H(12H)	109.5
C(3C)-C(10C)-C(9C)	104.51(19)	C(11C)-C(12C)-C(13C)	111(5)
C(11C)-C(10C)-C(3C)	117.6(2)	H(12G)-C(12C)-H(12H)	108.1
C(11C)-C(10C)-C(9C)	137.9(2)	C(13C)-C(12C)-H(12G)	109.5
N(3B)-C(11C)-C(12D)	117.4(3)	C(13C)-C(12C)-H(12H)	109.5
N(3B)-C(11C)-C(12C)	127(2)	C(12C)-C(13C)-H(13C)	106.0
C(10C)-C(11C)-N(3B)	113.4(2)	C(14C)-C(13C)-C(12C)	119(2)
C(10C)-C(11C)-C(12D)	129.2(3)	C(14C)-C(13C)-H(13C)	106.0
C(10C)-C(11C)-C(12C)	120(2)	C(15C)-C(13C)-C(12C)	105(2)
C(11C)-C(12D)-H(12A)	108.8	C(15C)-C(13C)-H(13C)	106.0
C(11C)-C(12D)-H(12B)	108.8	C(15C)-C(13C)-C(14C)	114(2)
C(11C)-C(12D)-C(13D)	113.6(5)	C(13C)-C(14C)-H(14J)	109.5
H(12A)-C(12D)-H(12B)	107.7	C(13C)-C(14C)-H(14K)	109.5
C(13D)-C(12D)-H(12A)	108.8	C(13C)-C(14C)-H(14L)	109.5
C(13D)-C(12D)-H(12B)	108.8	H(14J)-C(14C)-H(14K)	109.5
C(12D)-C(13D)-H(13D)	108.2	H(14J)-C(14C)-H(14L)	109.5
C(14D)-C(13D)-C(12D)	113.2(3)	H(14K)-C(14C)-H(14L)	109.5
C(14D)-C(13D)-H(13D)	108.2	F(3C)-C(15C)-F(5C)	108(3)
C(15D)-C(13D)-C(12D)	109.1(3)	F(3C)-C(15C)-C(13C)	114(2)
C(15D)-C(13D)-H(13D)	108.2	F(4C)-C(15C)-F(3C)	111(2)
C(15D)-C(13D)-C(14D)	109.7(3)	F(4C)-C(15C)-F(5C)	106(3)
C(13D)-C(14D)-H(14A)	109.5	F(4C)-C(15C)-C(13C)	109(3)
C(13D)-C(14D)-H(14B)	109.5	F(5C)-C(15C)-C(13C)	109(2)

Symmetry transformations used to generate equivalent atoms:

Table S-10. Anisotropic displacement parameters ($Å^2$x 10^3) for Ballatore_BRL_I_205. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1A)	26(1)	42(1)	26(1)	3(1)	-1(1)	16(1)
F(2A)	30(1)	37(1)	18(1)	0(1)	6(1)	16(1)
O(1A)	20(1)	21(1)	18(1)	0(1)	2(1)	6(1)
N(1A)	24(1)	20(1)	24(1)	1(1)	-2(1)	2(1)
N(2A)	21(1)	18(1)	22(1)	0(1)	1(1)	2(1)
N(3A)	18(1)	18(1)	23(1)	2(1)	2(1)	4(1)
N(4A)	20(1)	21(1)	29(1)	3(1)	1(1)	5(1)
C(1A)	21(1)	21(1)	29(2)	4(1)	-4(1)	3(1)
C(2A)	22(1)	14(1)	20(1)	0(1)	0(1)	1(1)
C(3A)	20(1)	14(1)	20(1)	0(1)	2(1)	2(1)
C(4A)	23(1)	16(1)	16(1)	1(1)	2(1)	3(1)
C(5A)	22(1)	20(1)	21(1)	1(1)	4(1)	5(1)
C(6A)	22(1)	22(1)	27(1)	3(1)	-1(1)	6(1)
C(7A)	31(1)	24(1)	17(1)	2(1)	1(1)	7(1)
C(8A)	26(1)	20(1)	19(1)	1(1)	7(1)	6(1)
C(9A)	20(1)	15(1)	21(1)	2(1)	3(1)	3(1)
C(10A)	21(1)	16(1)	20(1)	1(1)	3(1)	2(1)
C(11A)	21(1)	17(1)	19(1)	4(1)	1(1)	3(1)
F(3A)	65(3)	58(2)	18(2)	12(2)	6(2)	43(2)
F(4A)	37(3)	56(3)	38(3)	12(2)	23(2)	28(2)
F(5A)	81(3)	41(2)	17(2)	-14(1)	0(2)	27(2)
C(12A)	12(5)	21(2)	22(2)	4(1)	4(3)	2(2)
C(13A)	25(3)	26(2)	20(3)	-2(2)	0(2)	8(2)
C(14A)	46(2)	26(2)	25(2)	-3(1)	11(2)	2(2)
C(15A)	39(4)	36(4)	28(4)	11(3)	15(3)	22(3)
F(3B)	75(4)	82(4)	29(3)	-3(2)	14(3)	22(3)
F(4B)	72(3)	56(2)	64(3)	-22(2)	16(2)	24(2)
F(5B)	52(3)	64(3)	88(3)	-14(2)	34(2)	16(2)
C(12B)	12(5)	21(2)	22(2)	4(1)	4(3)	2(2)
C(13B)	25(3)	26(2)	20(3)	-2(2)	0(2)	8(2)
C(14B)	46(2)	26(2)	25(2)	-3(1)	11(2)	2(2)
C(15B)	52(6)	40(4)	54(6)	-7(3)	19(5)	16(4)

F(1C)	22(1)	33(1)	40(1)	0(1)	5(1)	11(1)
F(2C)	33(1)	53(1)	16(1)	1(1)	2(1)	18(1)
O(1B)	22(1)	22(1)	16(1)	2(1)	-1(1)	4(1)
N(1B)	23(1)	21(1)	23(1)	-2(1)	6(1)	1(1)
N(2B)	23(1)	19(1)	16(1)	2(1)	3(1)	0(1)
N(3B)	18(1)	20(1)	19(1)	-1(1)	1(1)	2(1)
N(4B)	19(1)	27(1)	25(1)	-2(1)	2(1)	6(1)
C(1C)	20(1)	25(1)	28(1)	-5(1)	7(1)	2(1)
C(2C)	24(1)	17(1)	16(1)	0(1)	4(1)	-1(1)
C(3C)	20(1)	14(1)	18(1)	1(1)	-1(1)	1(1)
C(4C)	23(1)	16(1)	18(1)	1(1)	3(1)	1(1)
C(5C)	21(1)	20(1)	24(1)	3(1)	-3(1)	3(1)
C(6C)	18(1)	21(1)	34(2)	1(1)	4(1)	5(1)
C(7C)	27(1)	28(1)	24(1)	-1(1)	8(1)	5(1)
C(8C)	24(1)	27(1)	17(1)	2(1)	0(1)	6(1)
C(9C)	19(1)	17(1)	18(1)	1(1)	1(1)	2(1)
C(10C)	22(1)	16(1)	16(1)	1(1)	3(1)	1(1)
C(11C)	21(1)	16(1)	18(1)	1(1)	3(1)	1(1)
F(3D)	66(1)	59(2)	19(1)	-2(1)	3(1)	34(1)
F(4D)	50(1)	58(1)	36(1)	6(1)	-17(1)	11(1)
F(5D)	66(1)	47(1)	28(1)	12(1)	3(1)	27(1)
C(12D)	19(3)	23(2)	17(1)	-3(1)	0(1)	7(2)
C(13D)	37(2)	28(1)	17(1)	4(1)	1(1)	12(1)
C(14D)	57(2)	27(2)	31(2)	6(1)	1(2)	-1(1)
C(15D)	42(2)	35(2)	26(2)	3(1)	-2(2)	19(2)
F(3C)	63(9)	45(5)	32(7)	-7(5)	4(6)	17(6)
F(4C)	47(5)	71(13)	48(10)	0(10)	-13(5)	25(7)
F(5C)	107(10)	55(6)	28(7)	15(6)	-9(8)	-12(7)
C(12C)	19(3)	23(2)	17(1)	-3(1)	0(1)	7(2)
C(13C)	37(2)	28(1)	17(1)	4(1)	1(1)	12(1)
C(14C)	57(2)	27(2)	31(2)	6(1)	1(2)	-1(1)
C(15C)	42(2)	35(2)	26(2)	3(1)	-2(2)	19(2)

Table S-11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Ballatore_BRL_I_205.

	x	y	z	U(eq)
H(1A)	4283	5252	5694	28
H(5A)	-3894	7714	3770	25
H(7A)	-2786	7024	1035	28
H(12F)	3228	6251	2782	22
H(12E)	1868	6309	2115	22
H(13A)	2807	3968	2665	28
H(14G)	202	3732	2840	49
H(14I)	643	2838	1967	49
H(14H)	103	4157	1781	49
H(12C)	3030	5814	2663	22
H(12D)	1819	6393	2131	22
H(13B)	492	4288	1737	28
H(14D)	2765	3408	2779	49
H(14E)	1404	2497	2303	49
H(14F)	1304	3378	3269	49
H(1C)	3192	2113	4254	30
H(5C)	11717	-420	3823	26
H(7C)	11142	-532	937	31
H(12A)	4984	504	1566	23
H(12B)	6514	471	1197	23
H(13D)	5323	2745	1690	32
H(14A)	7405	3960	1207	58
H(14B)	8117	2688	1139	58
H(14C)	7690	3275	2148	58
H(12G)	5148	649	1457	23
H(12H)	6606	169	1256	23
H(13C)	7762	2254	1179	32
H(14J)	6881	4164	1366	58
H(14K)	6824	3509	2347	58
H(14L)	5432	3437	1688	58