Organocatalytic Asymmetric Strecker Reaction of Di- and Trifluoromethyl Ketoimines. Remarkable Fluorine Effect

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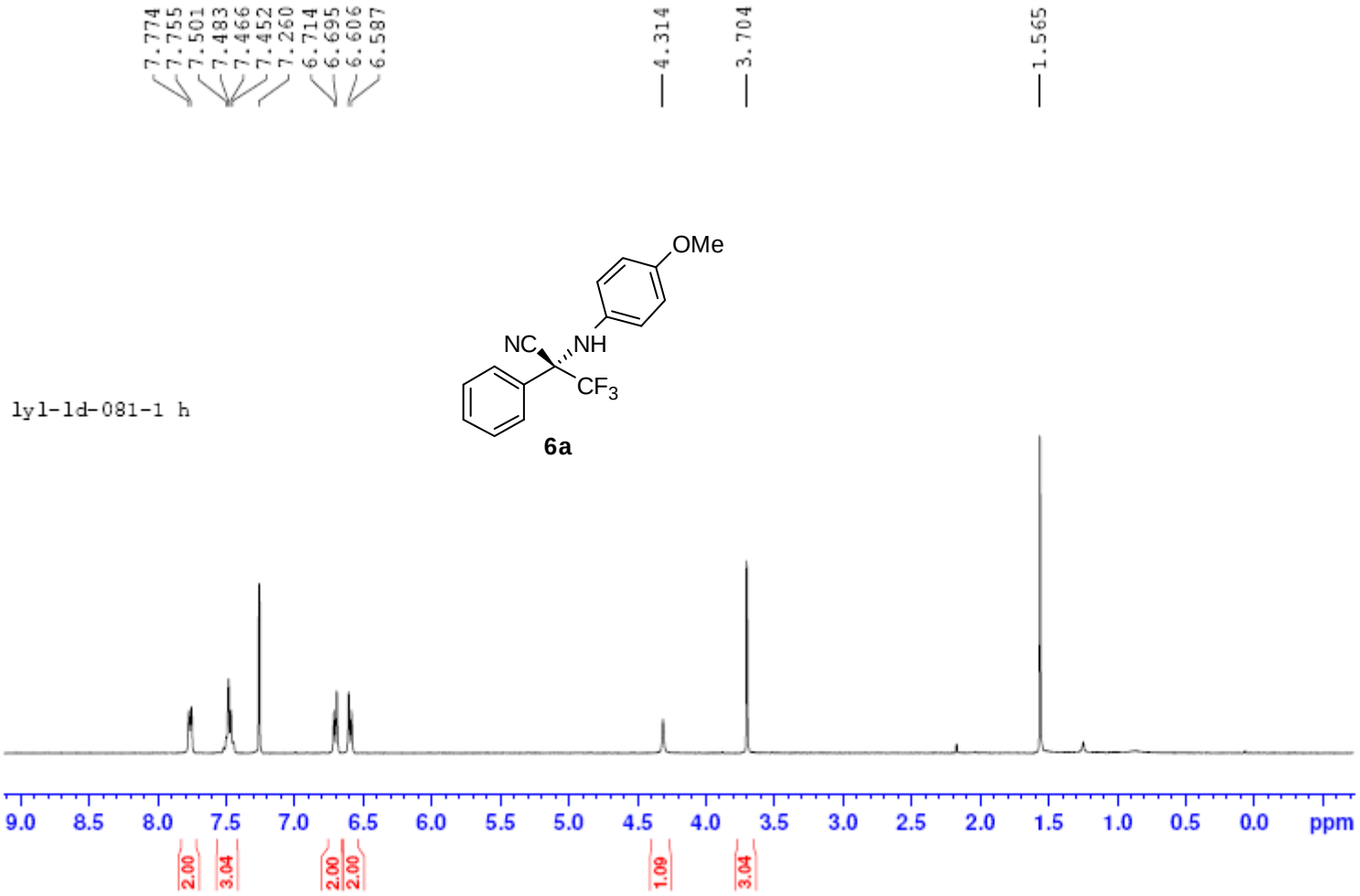
Supporting Information

(Part III)

Content **Page**

^{1}H, ^{13}C NMR and ^{19}F NMR spectra were recorded on 400 MHz. Chemical shifts are reported in ppm from $CDCl_3$, $(CD_3)_2SO$ or D_2O with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad. Coupling constants, *J*, are reported in Hertz.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3.704
1.565
OMe
NC
NH
CF3
6a
lyl-ld-081-1 h
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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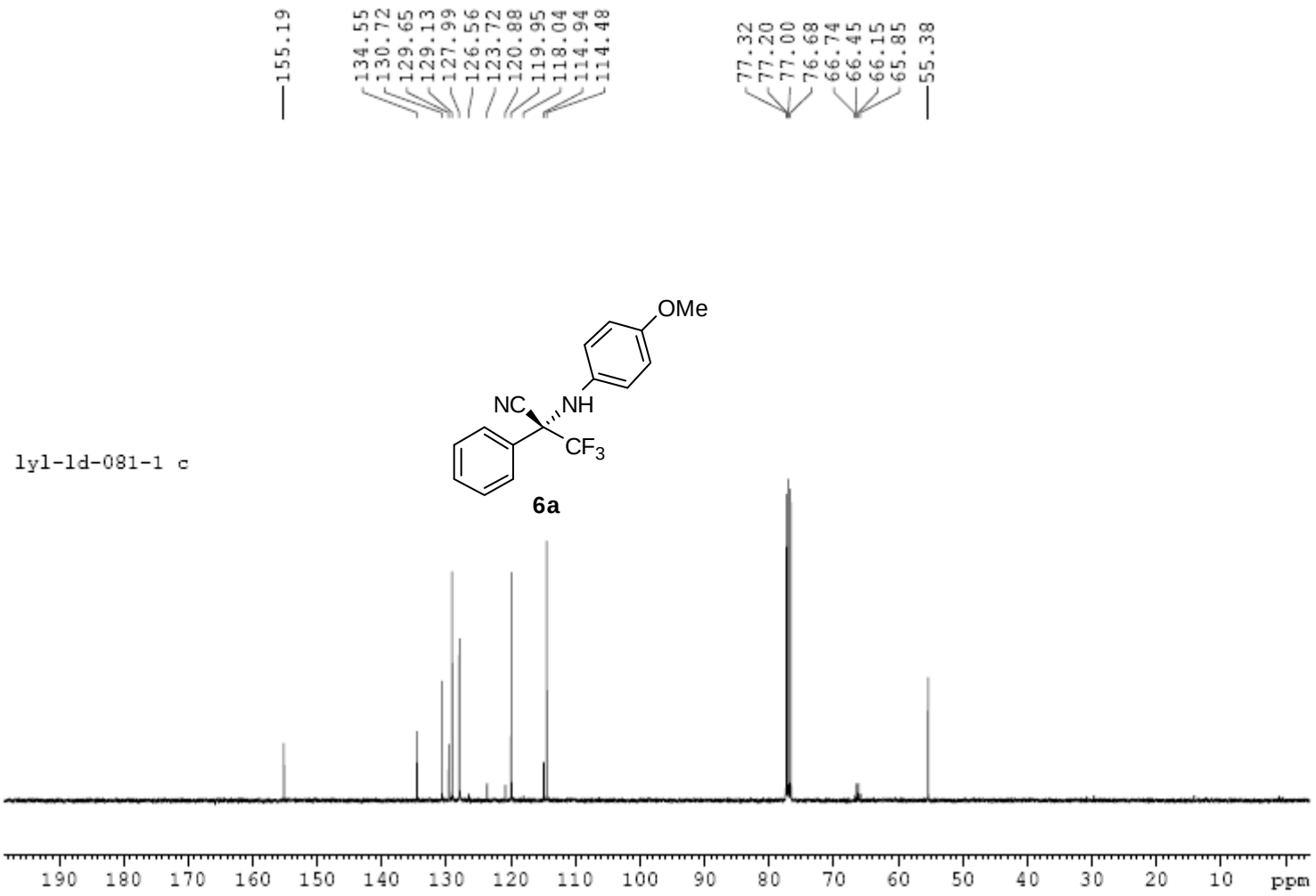
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77.00
76.68
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65.85
55.38
OMe
NC
NH
CF3
6a
lyl-ld-081-1 c
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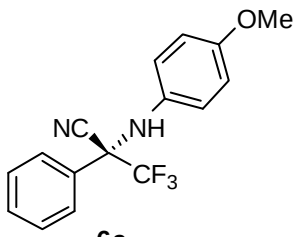

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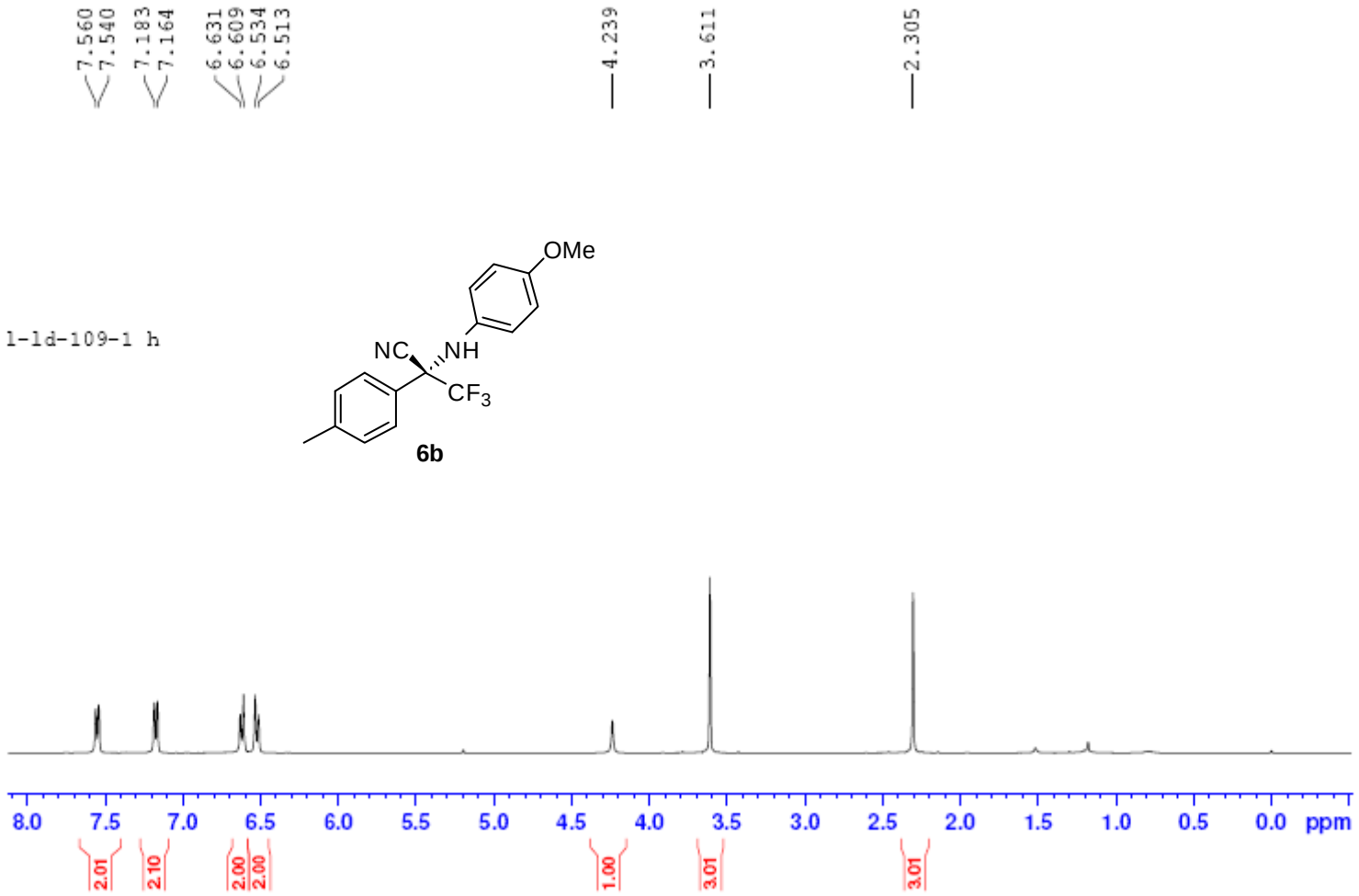
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OMe
NC
NH
CF3
6b
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7.0
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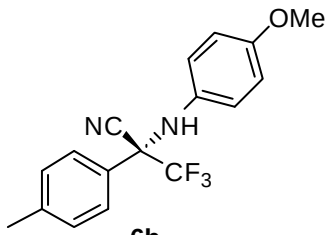

6b

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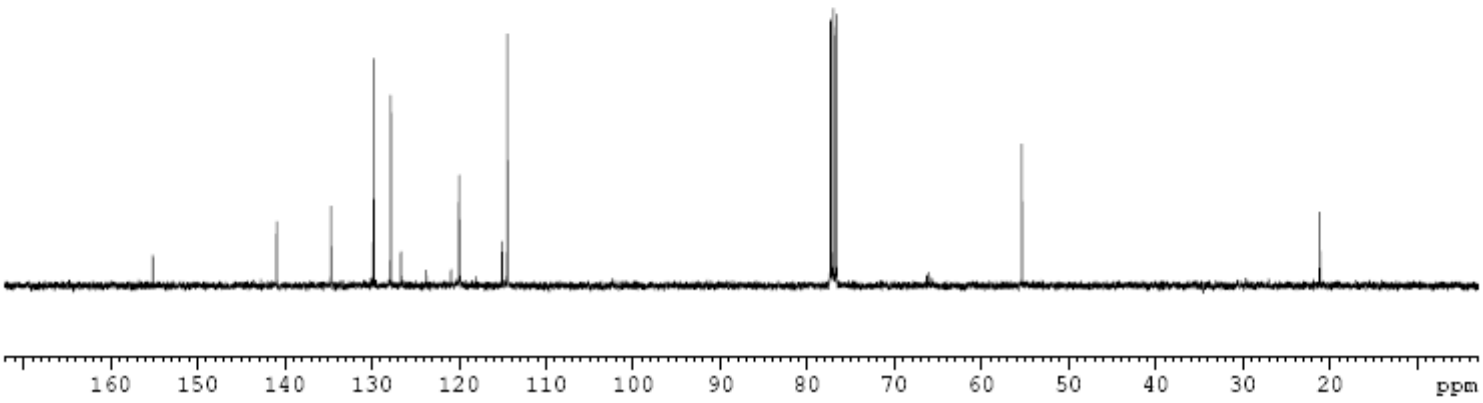

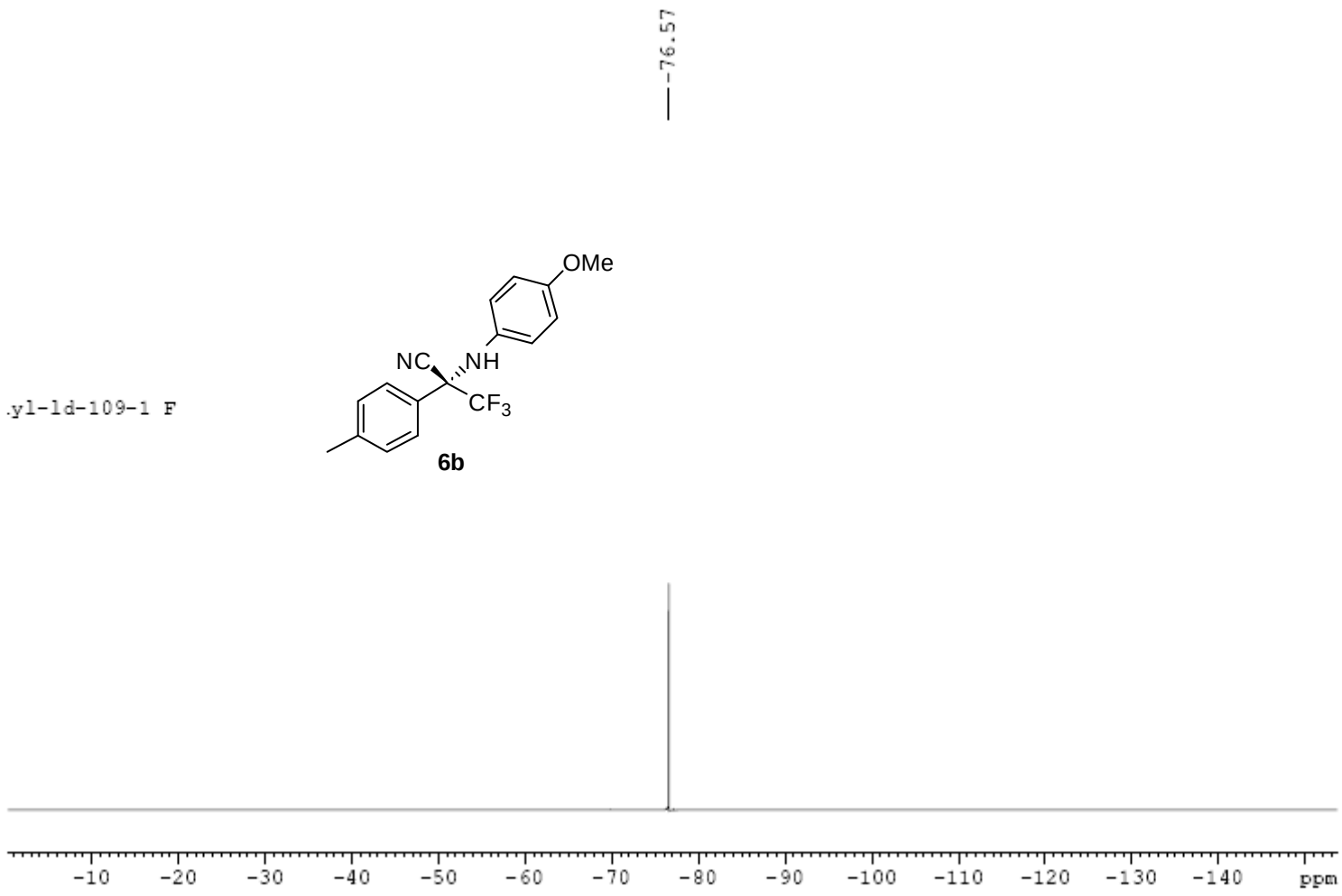
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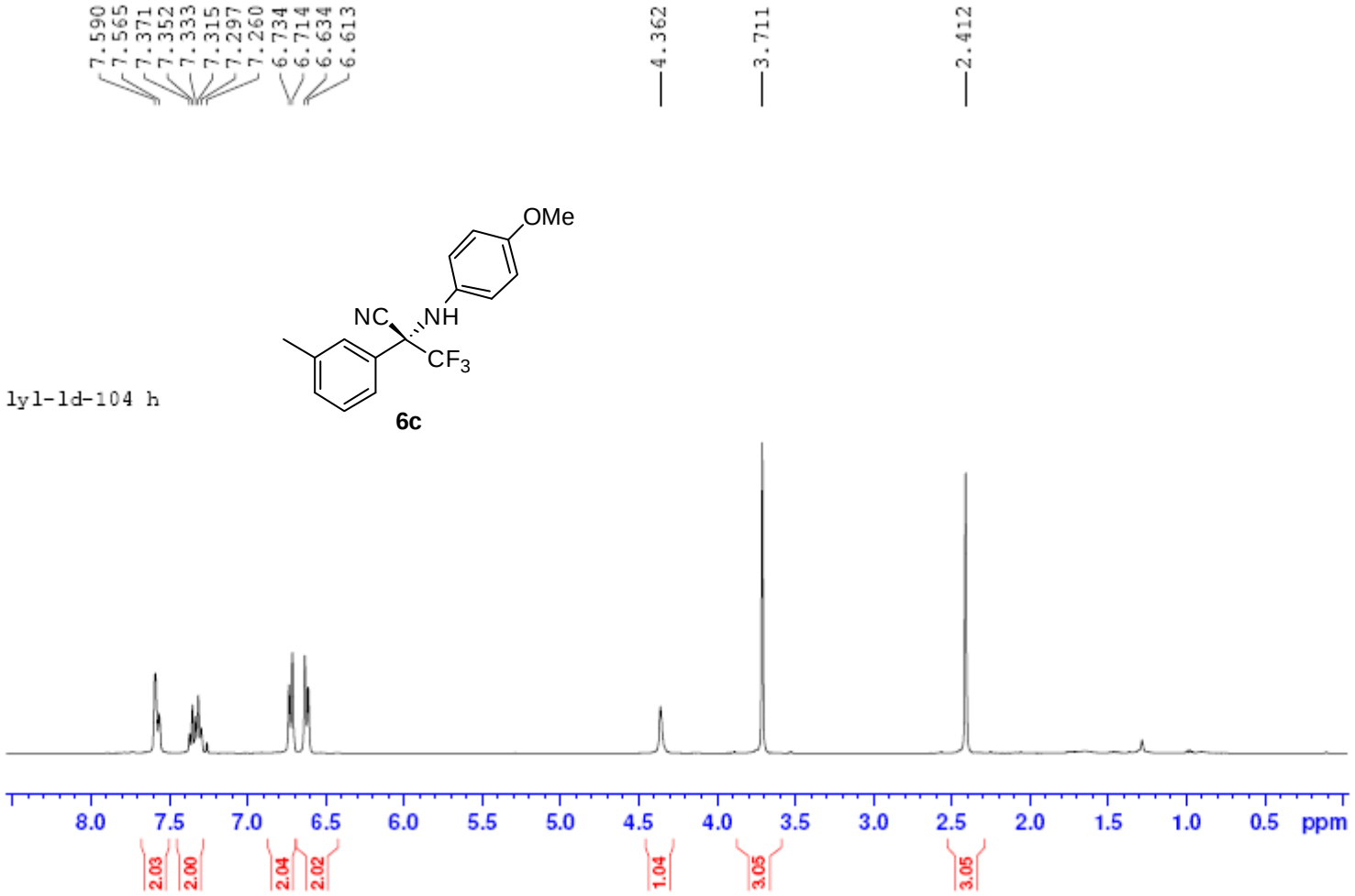
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NH
CF3
6c
lyl-1d-104 h
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2.02
1.04
3.05
3.05


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131.48
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128.43
125.04
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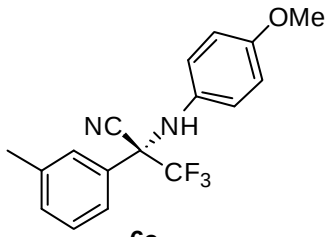
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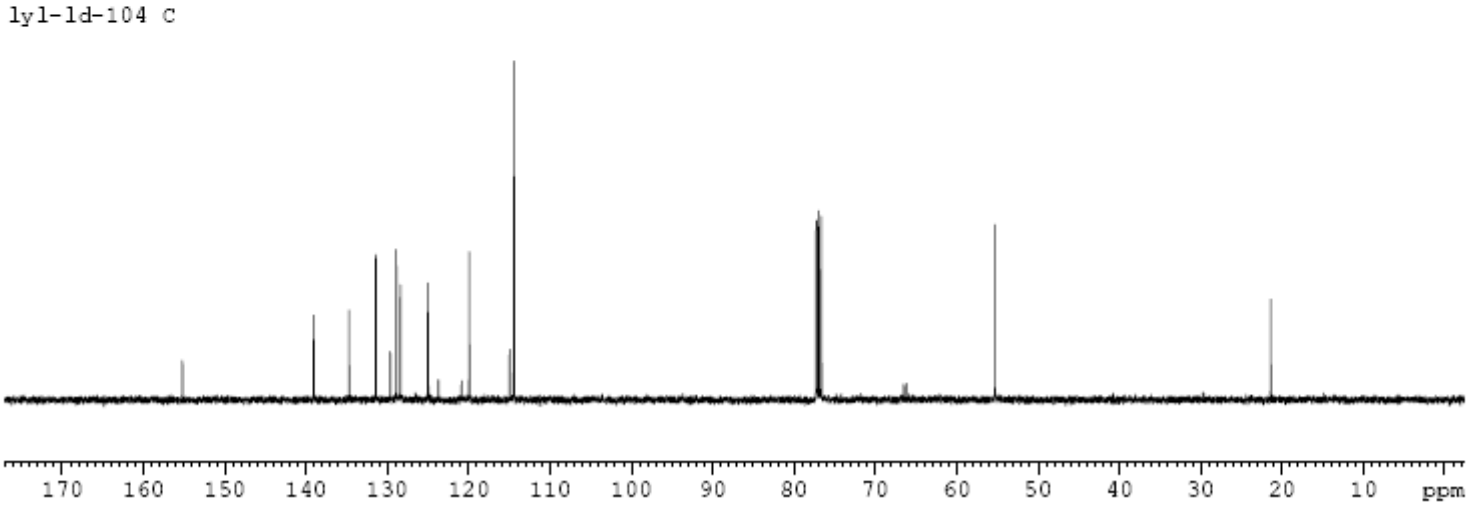
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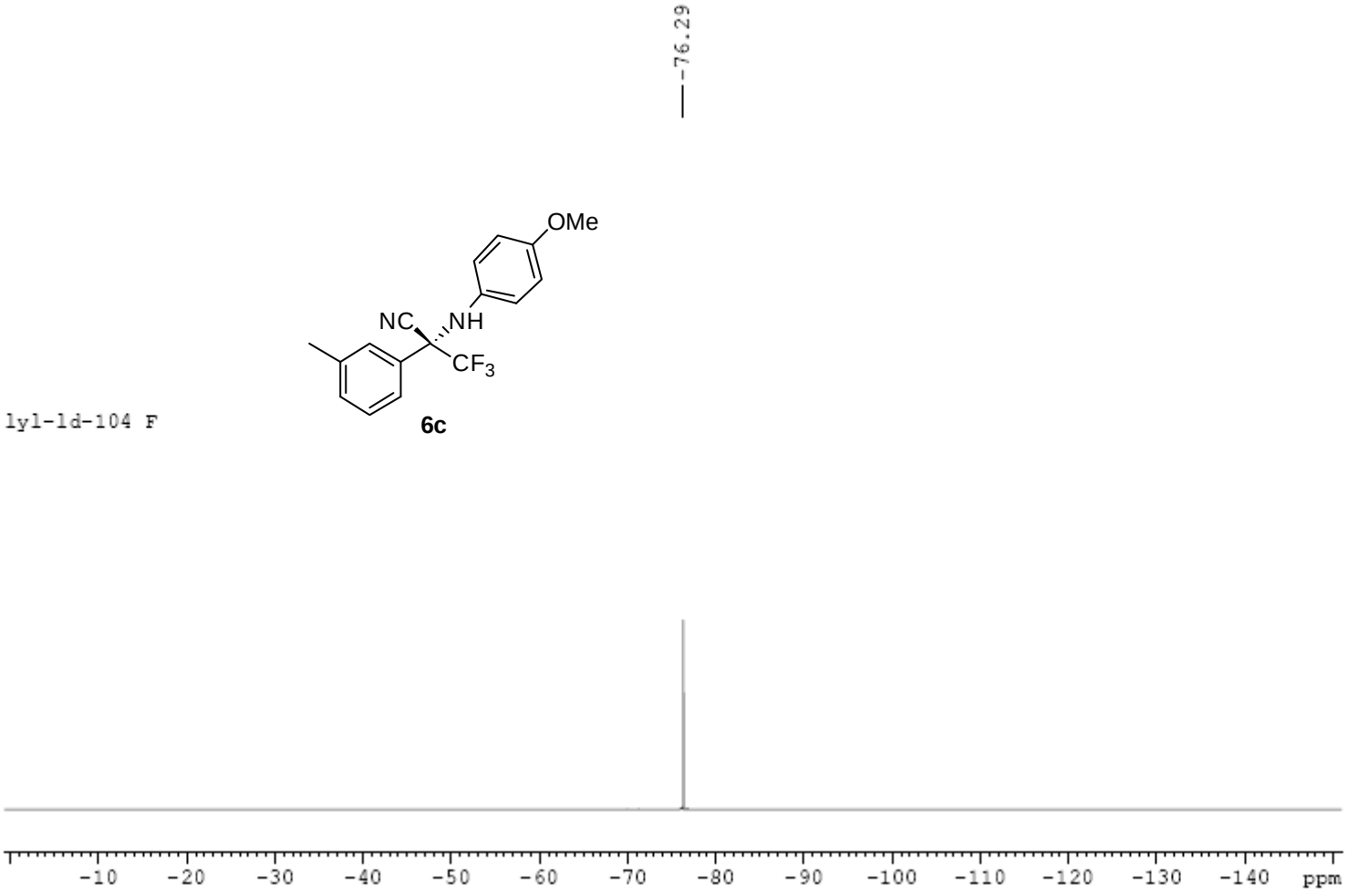
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ppm

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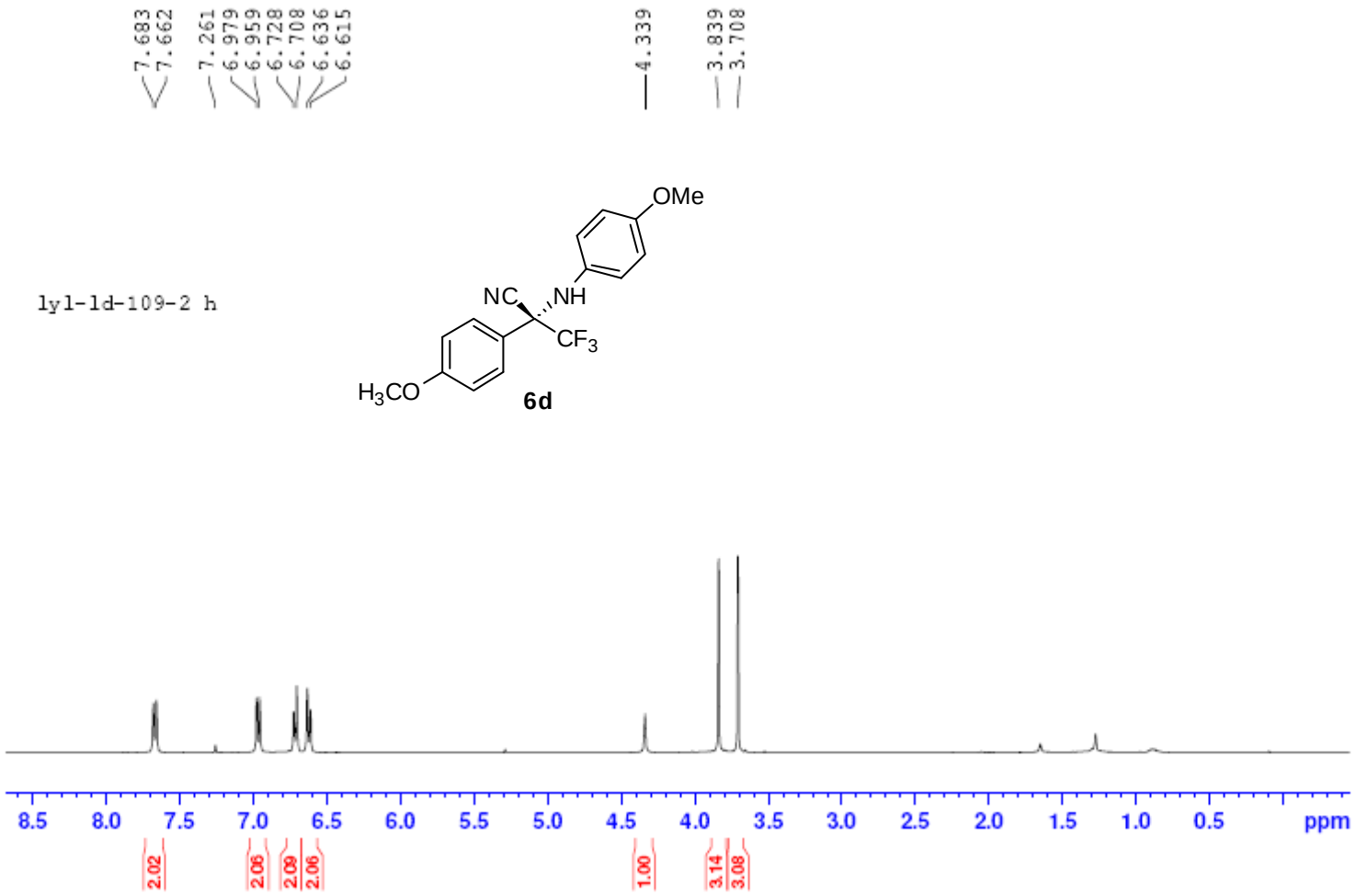
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CF3
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6d
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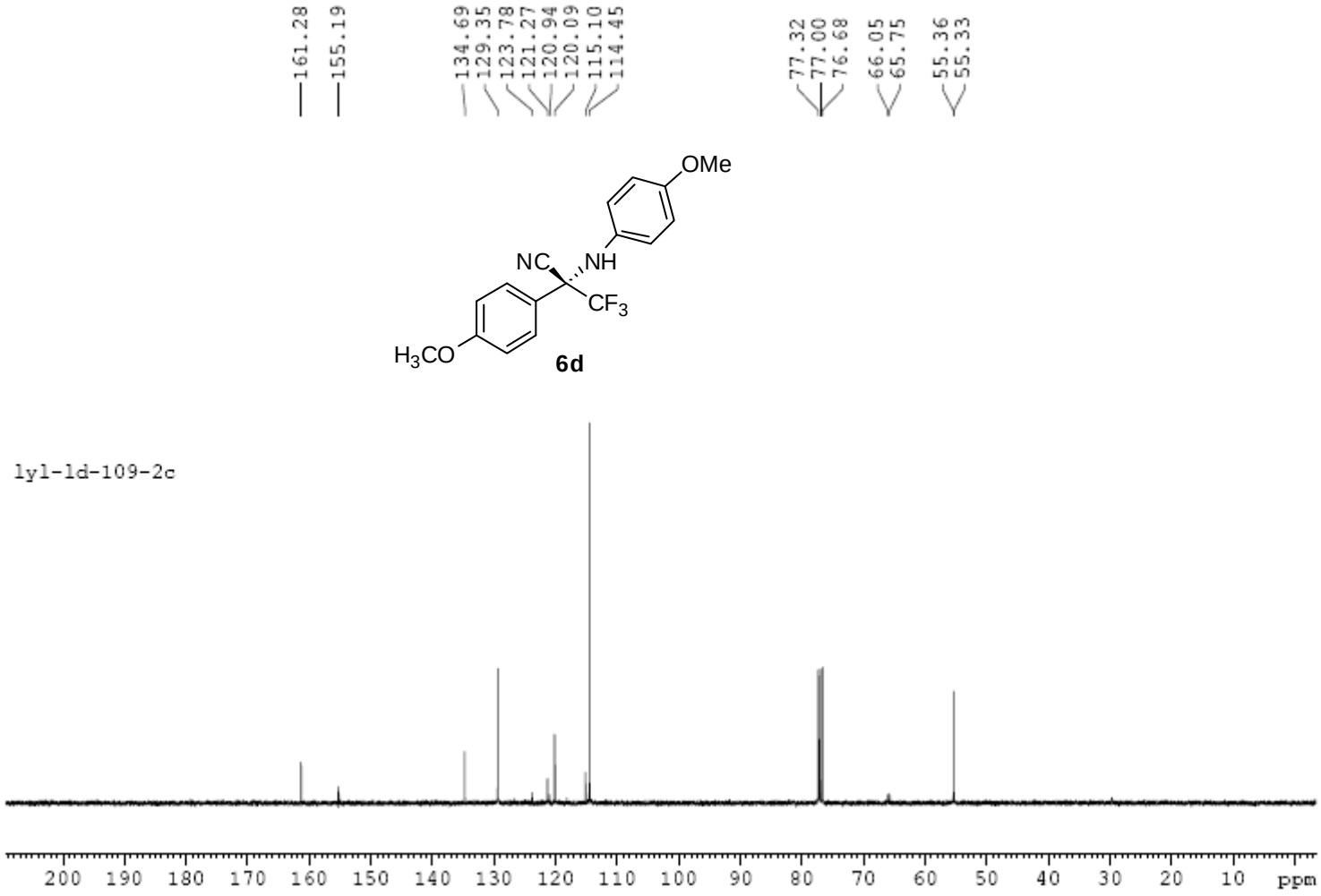
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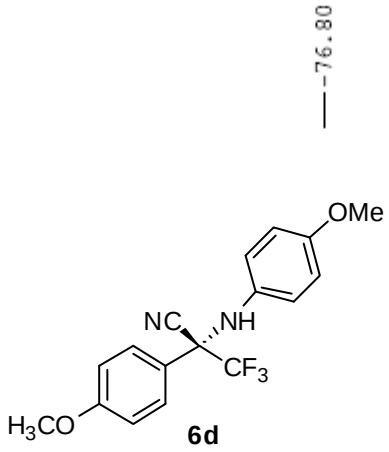
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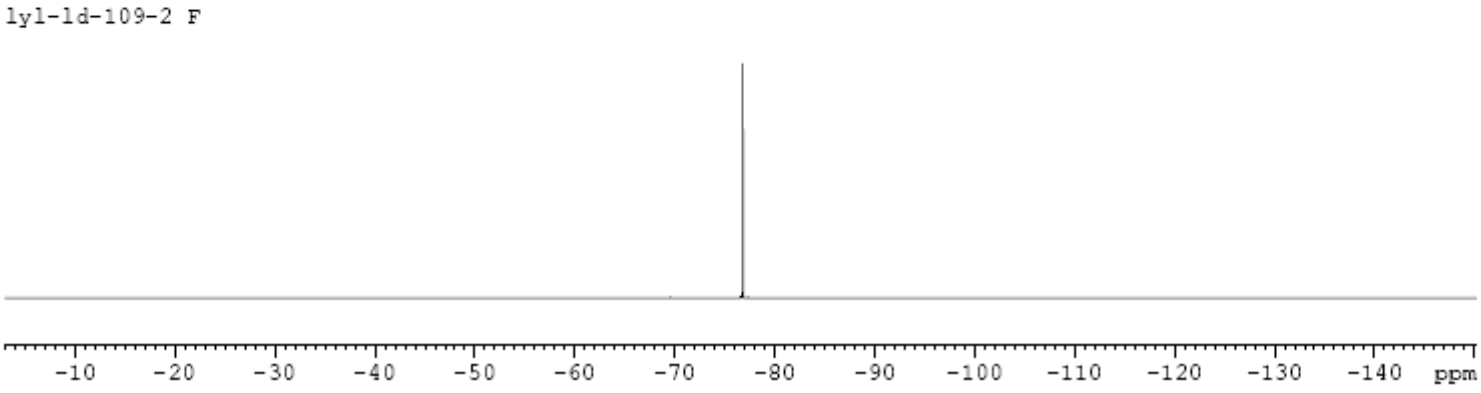
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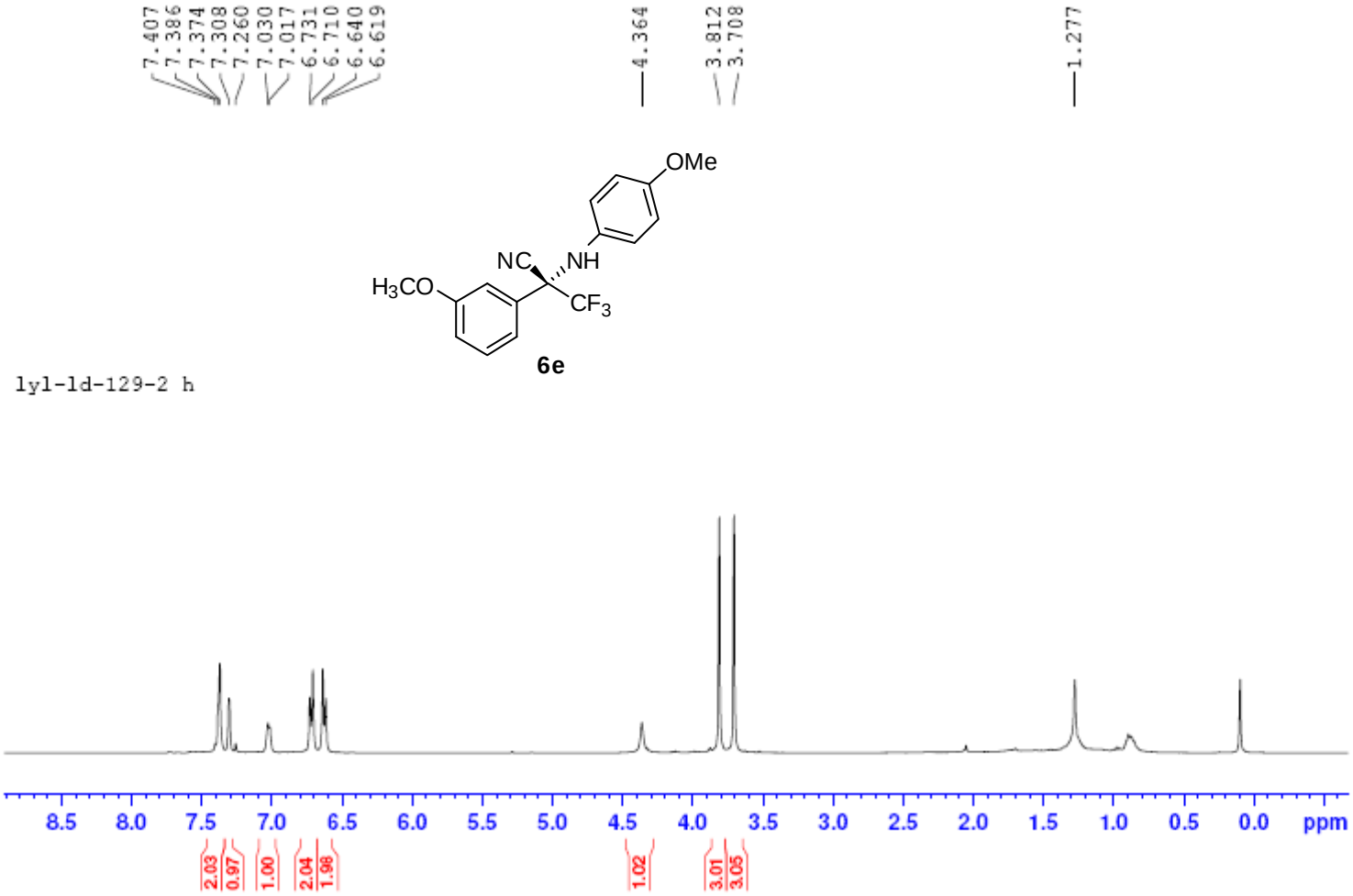
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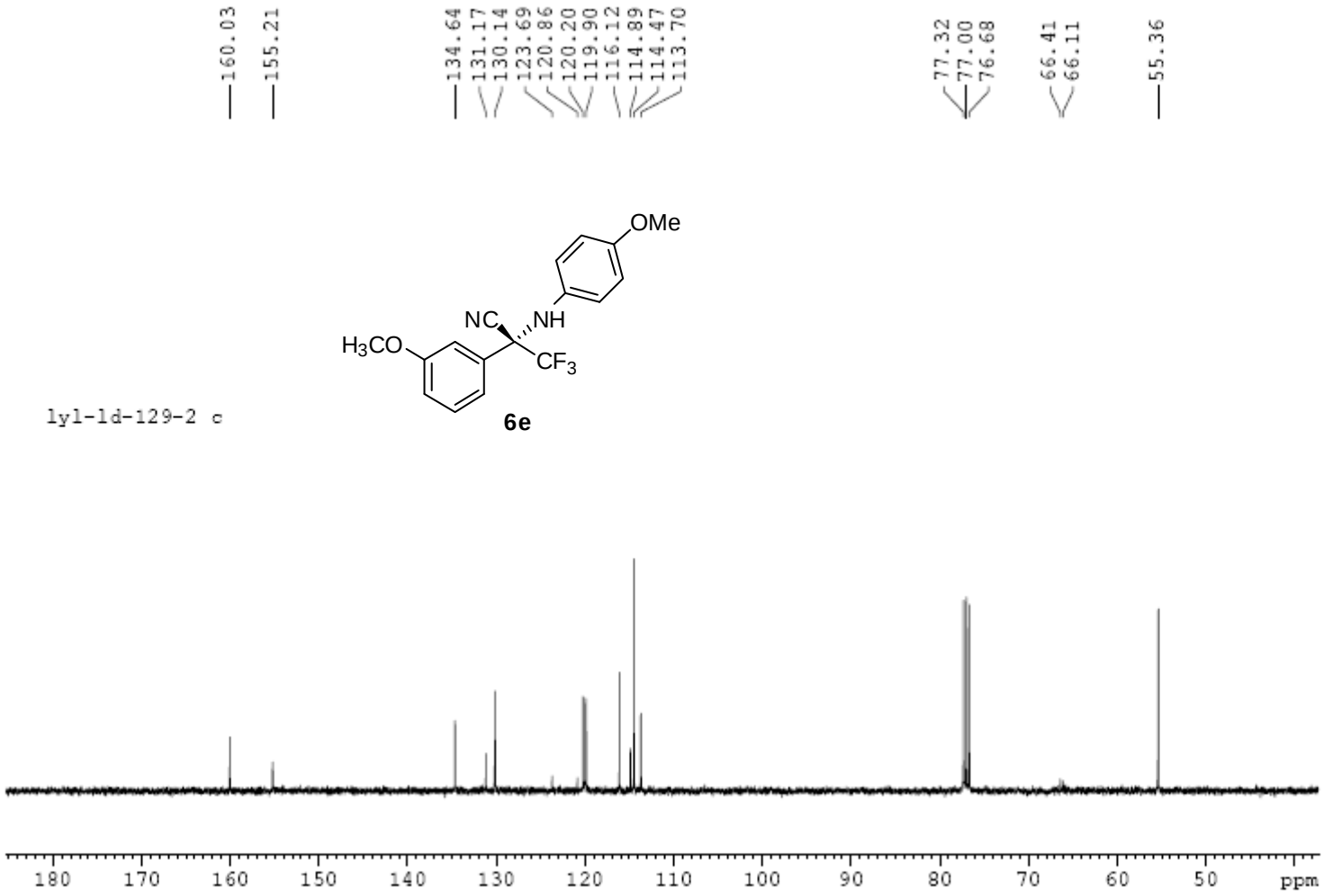
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55.36
OMe
NC
NH
H3CO
CF3
6e
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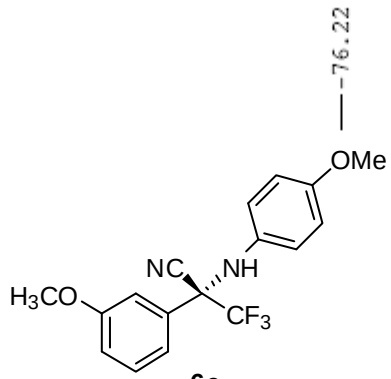
ppm

lyl-1d-129-2 f



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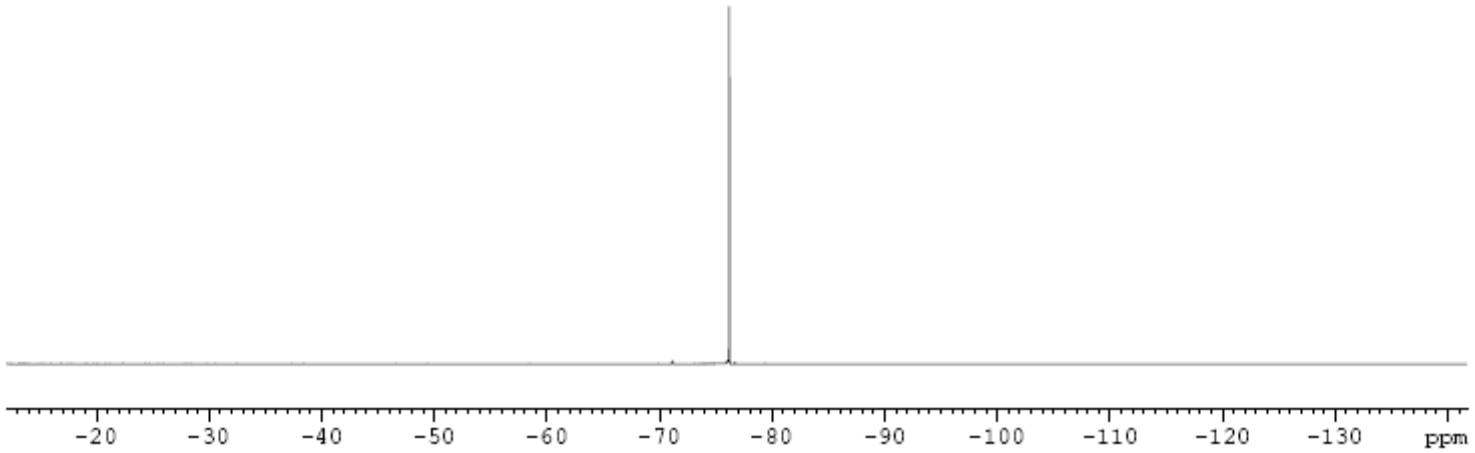

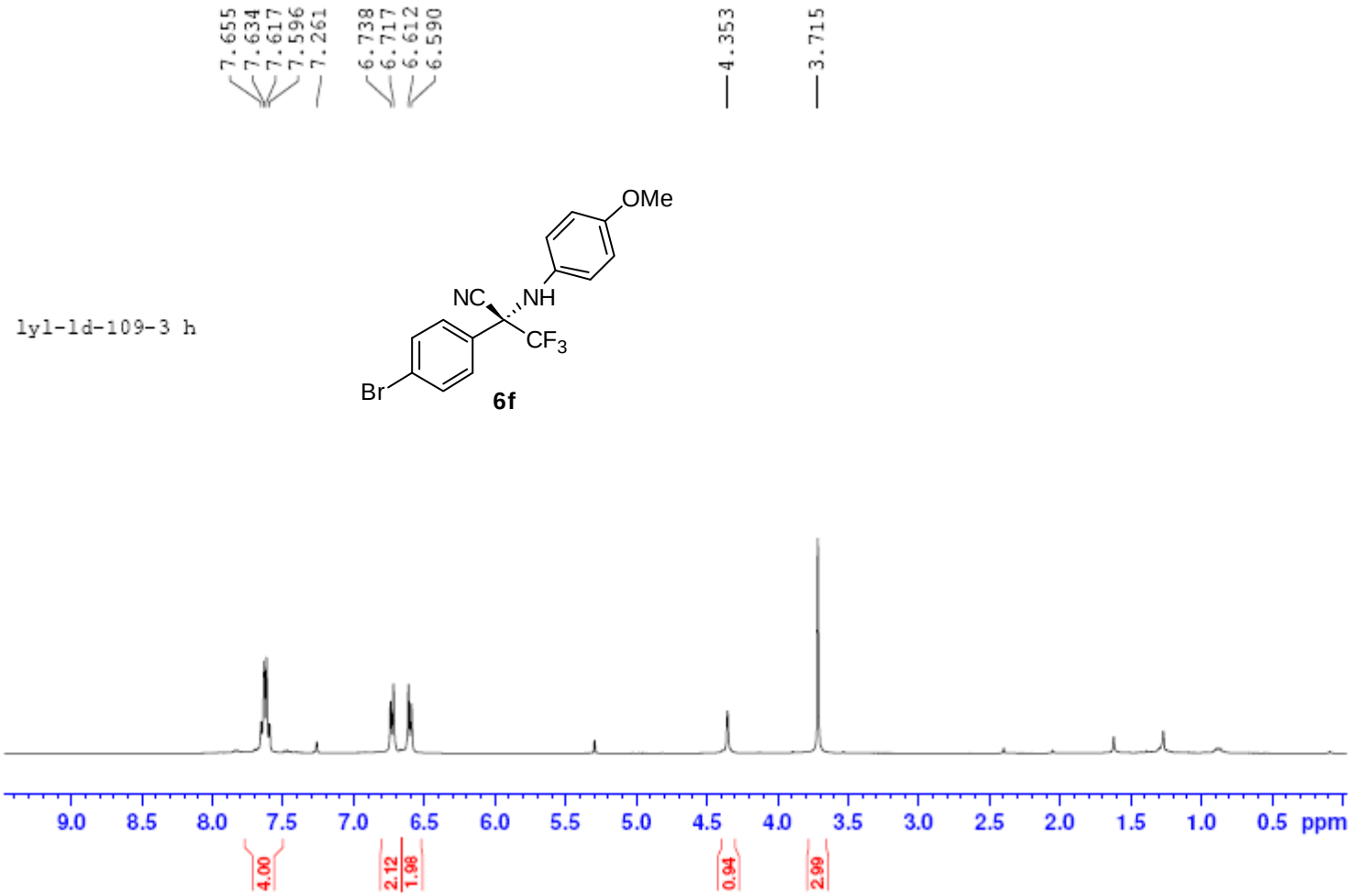
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NC
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CF3
Br
6f
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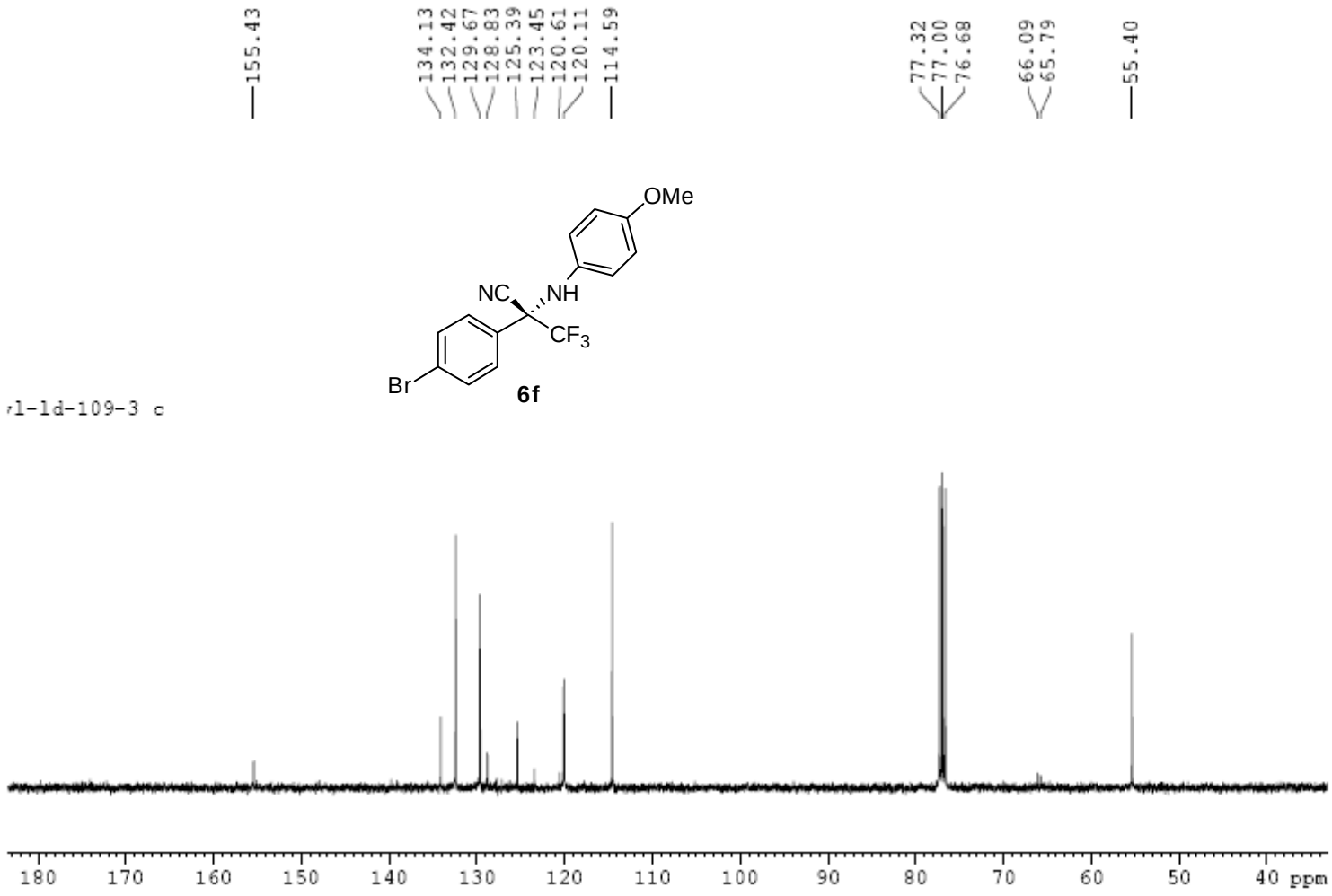
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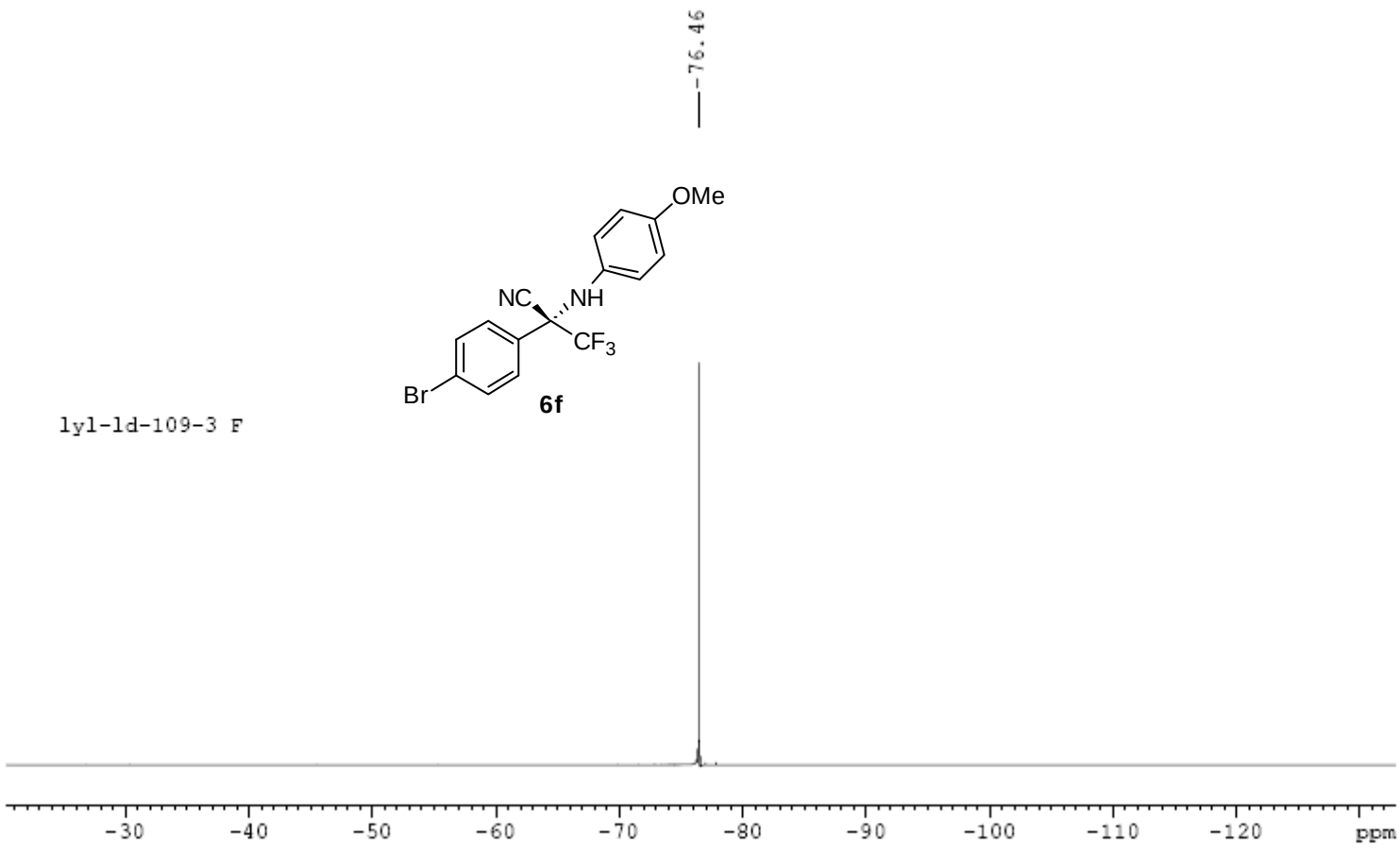
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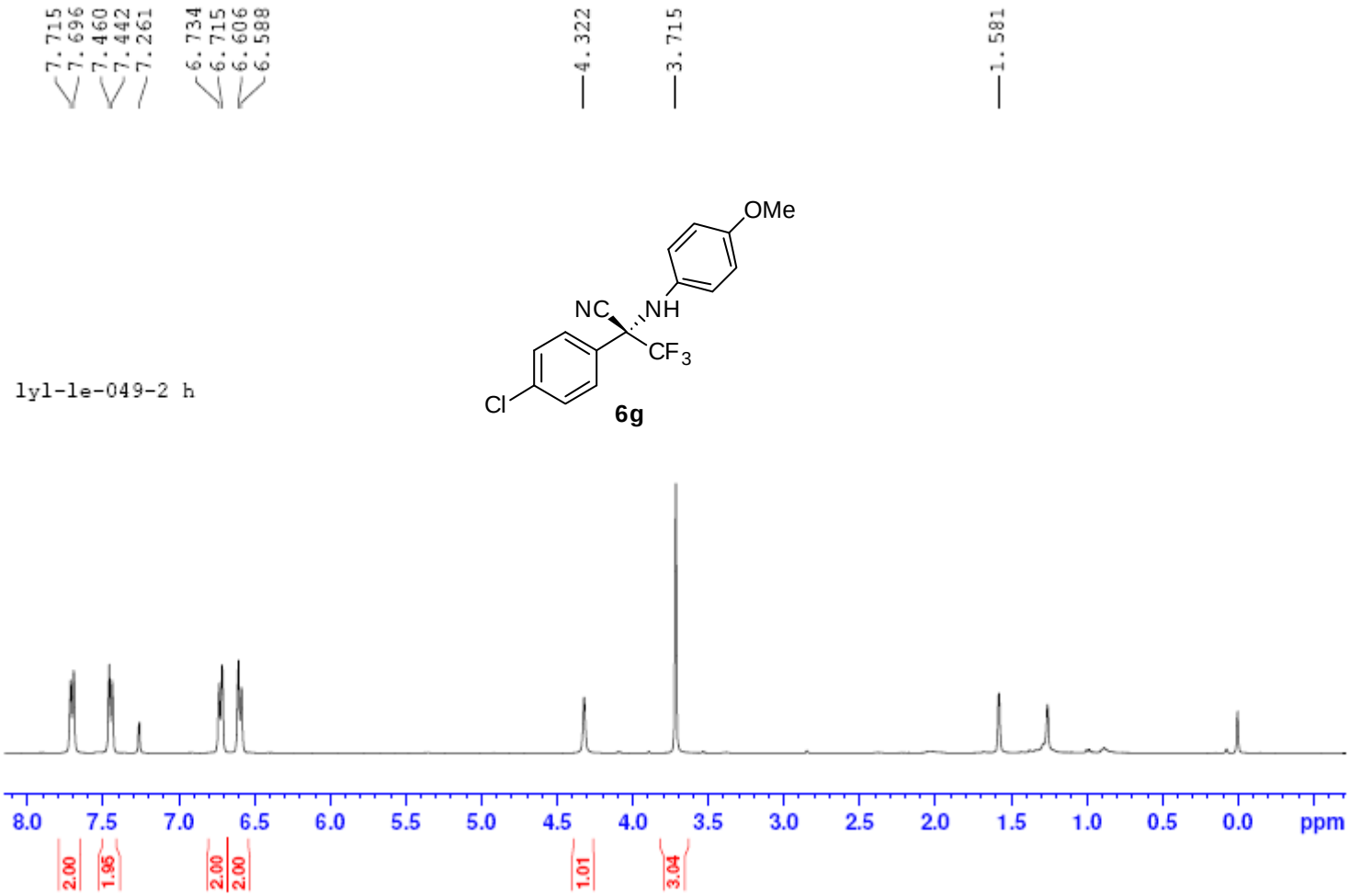
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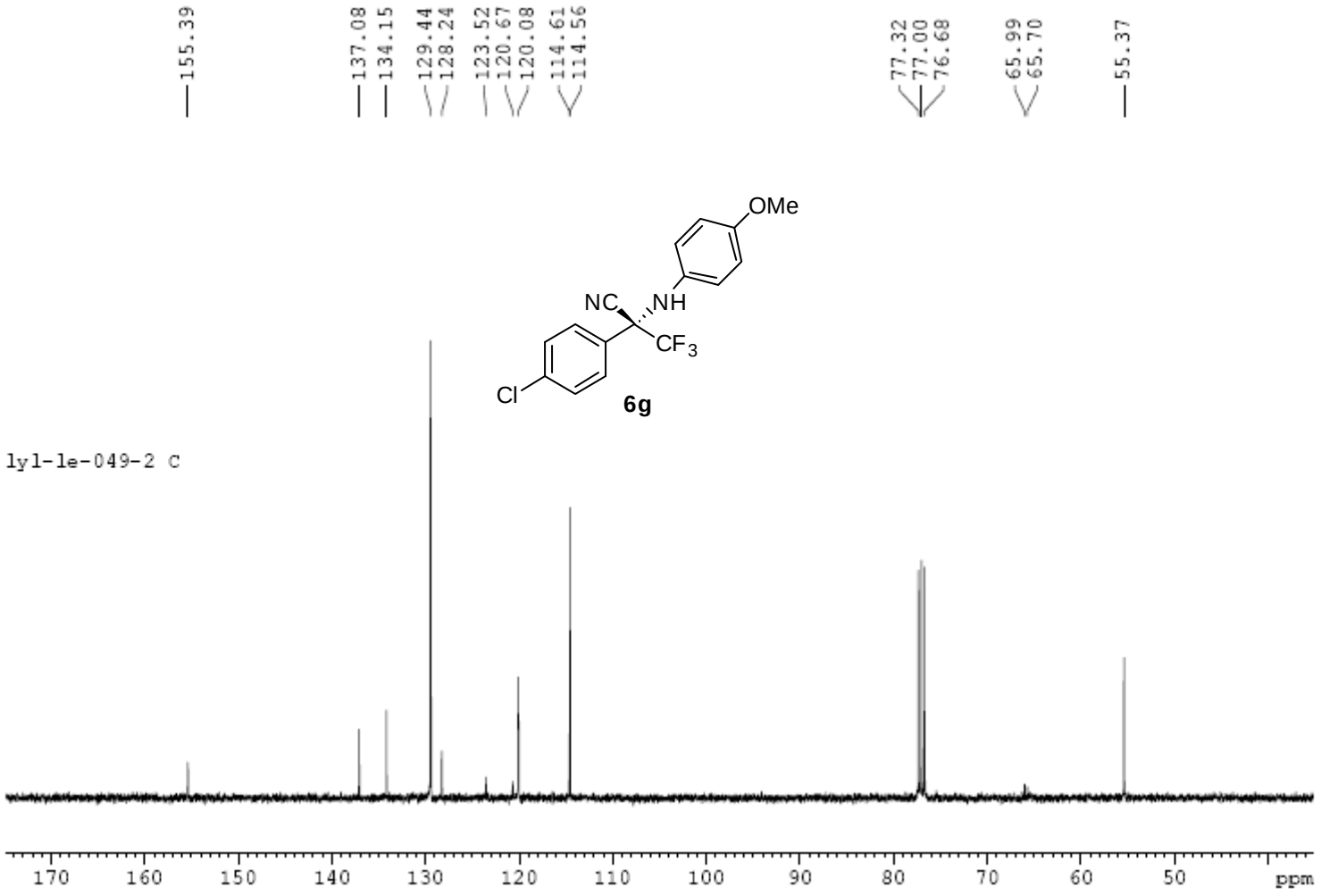
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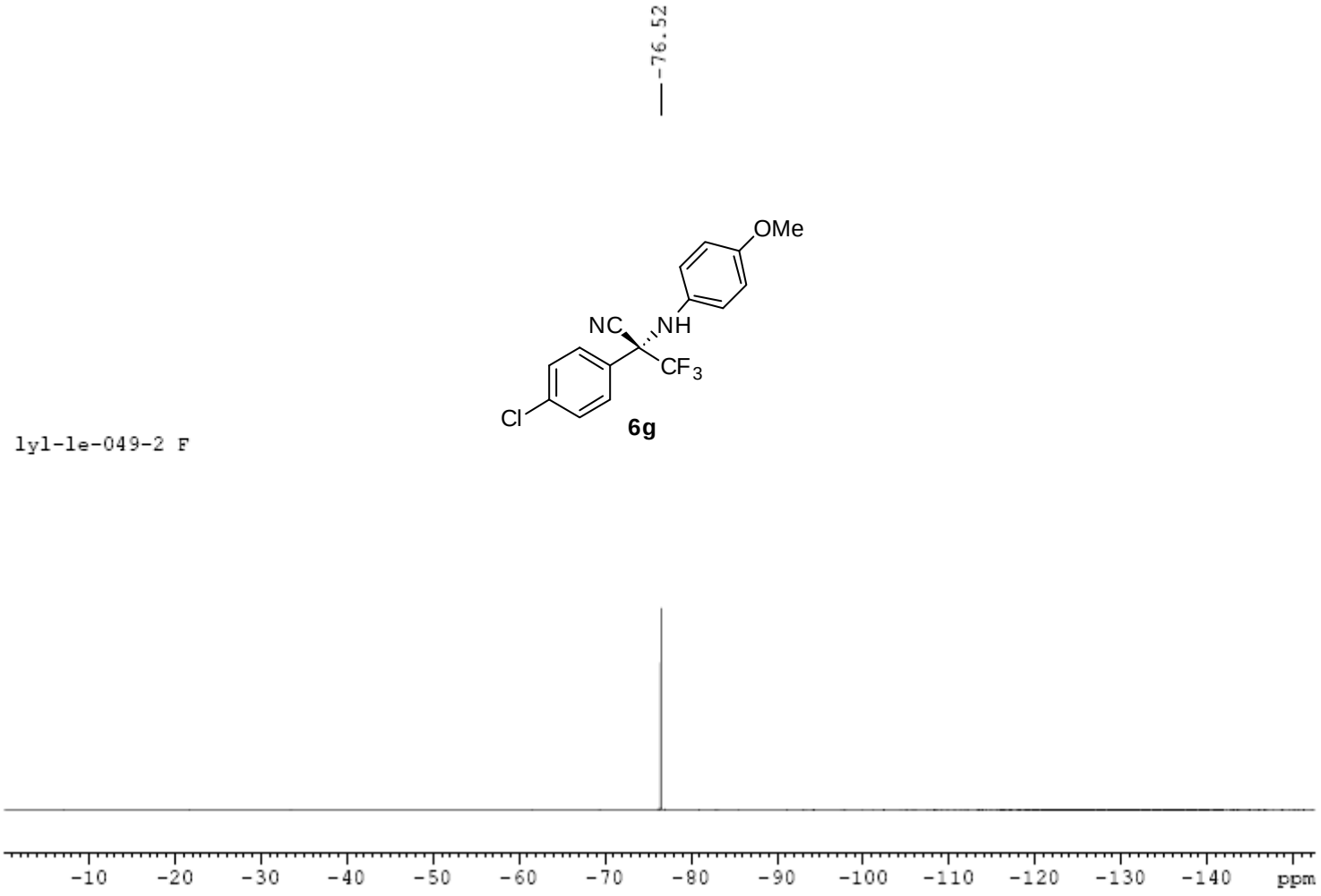
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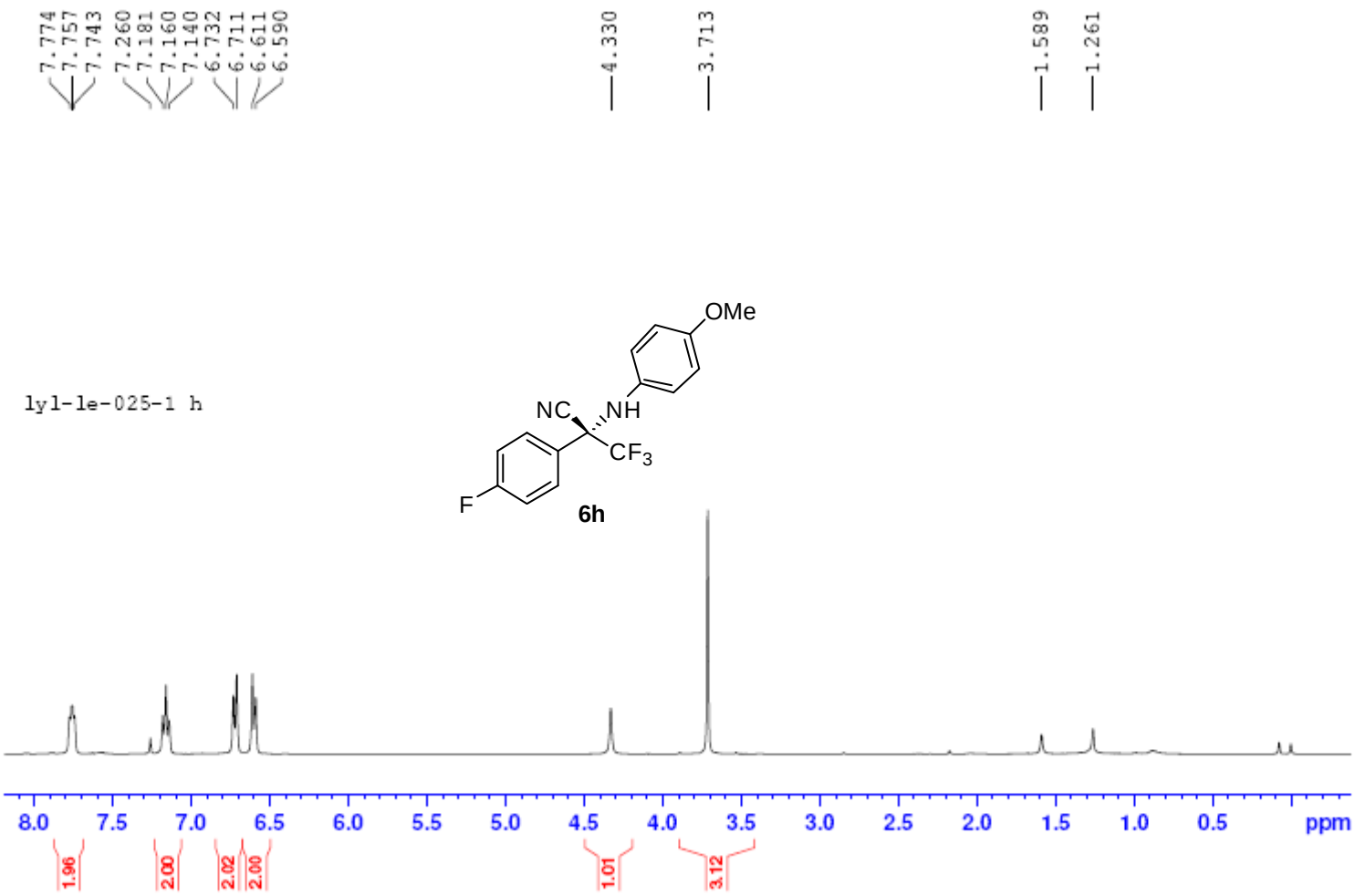
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lyl-le-025-1 h
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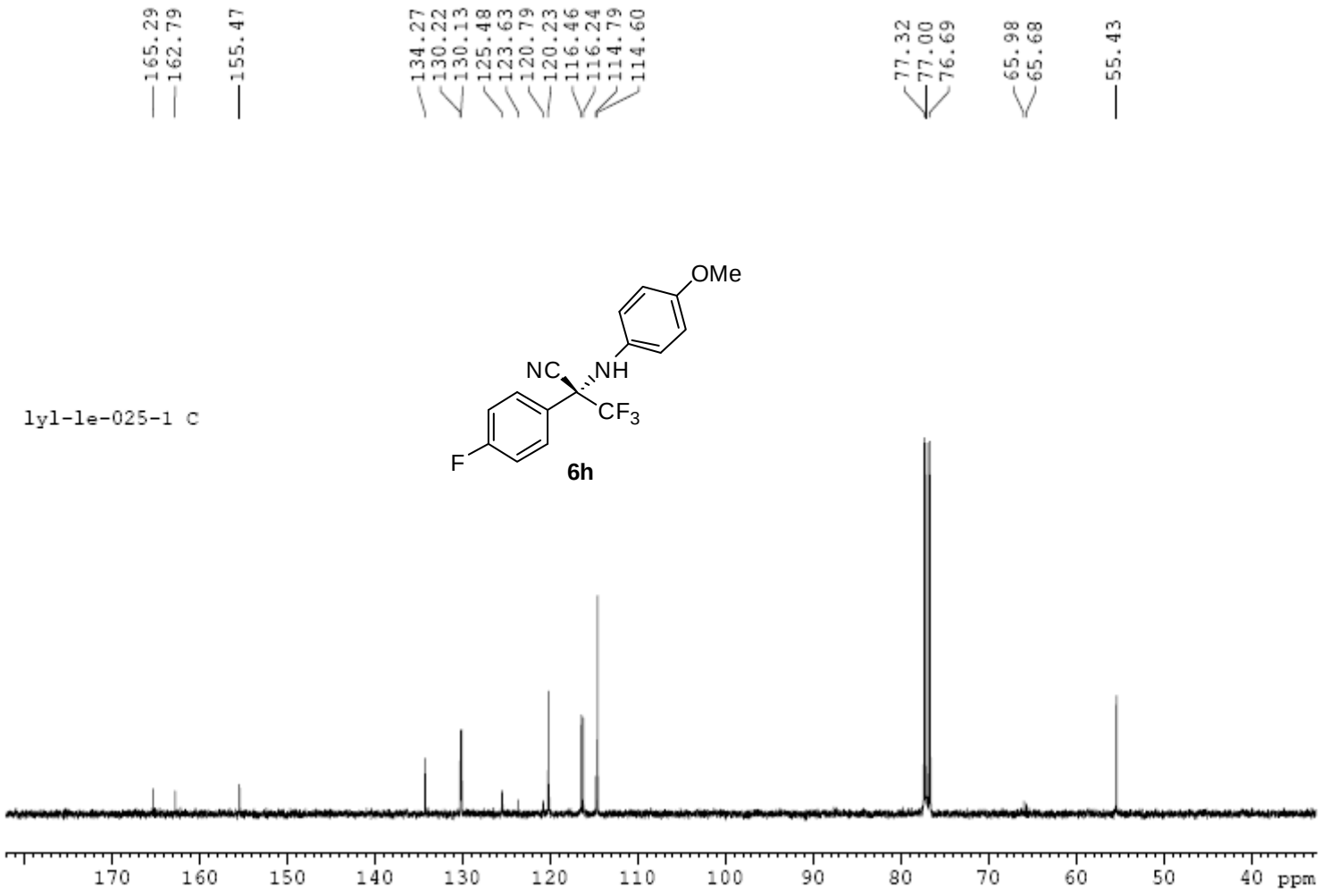
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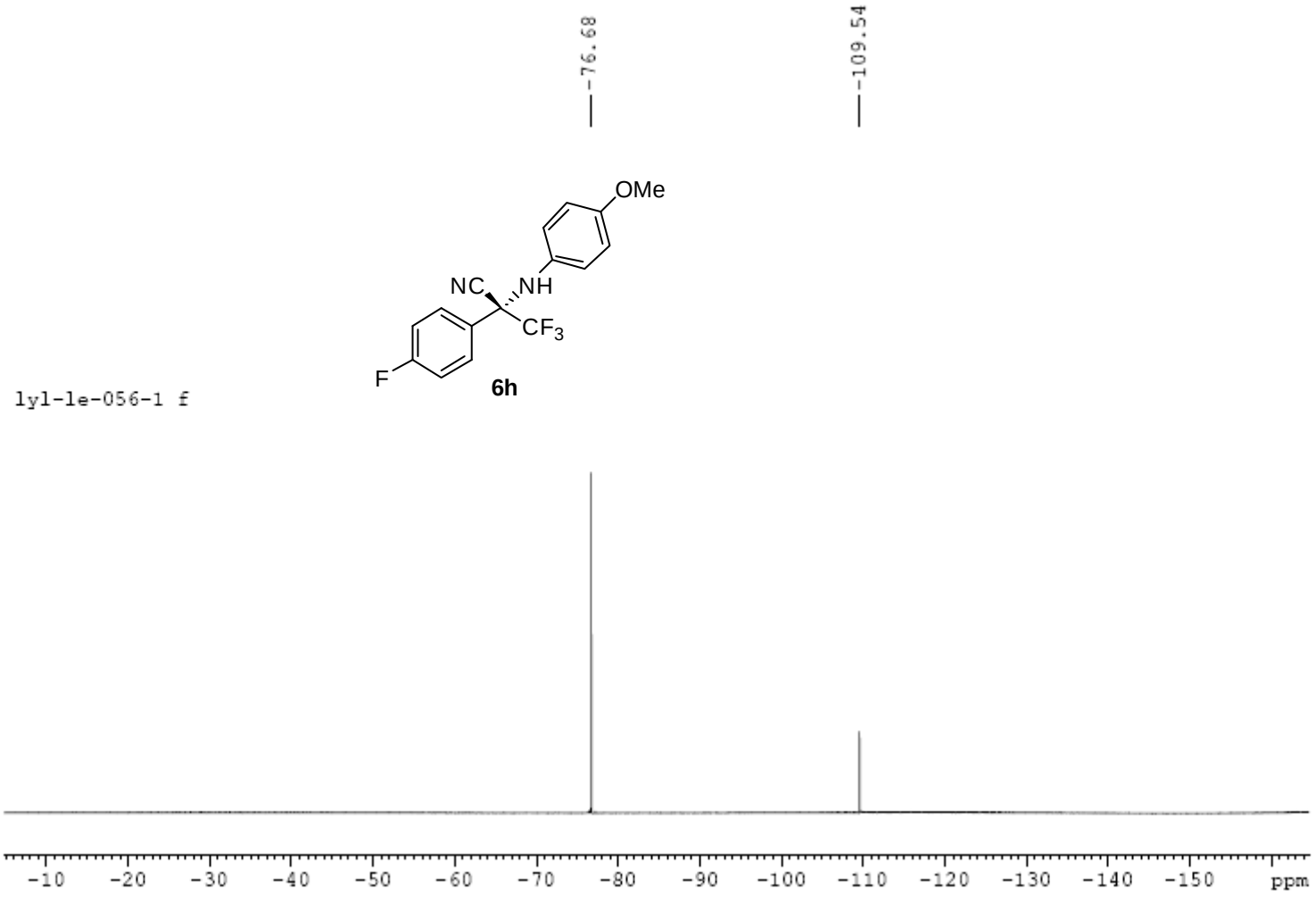
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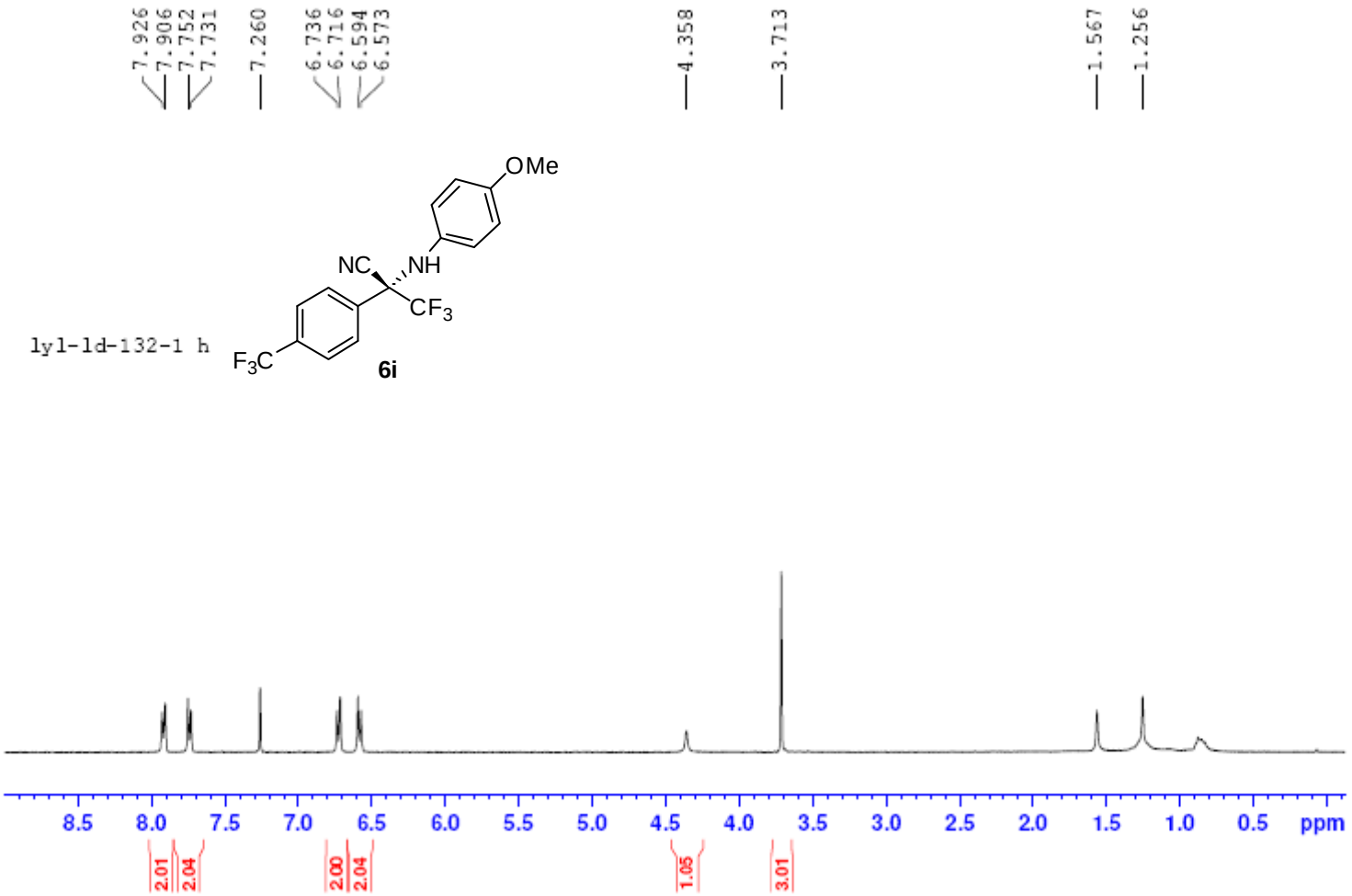
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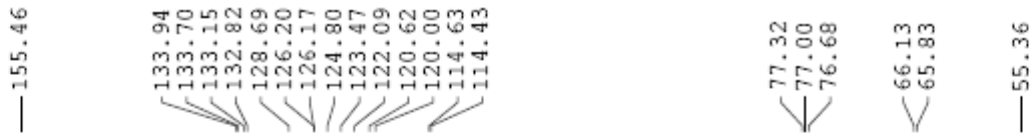
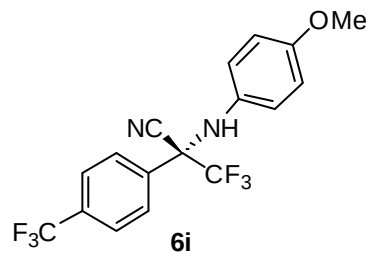
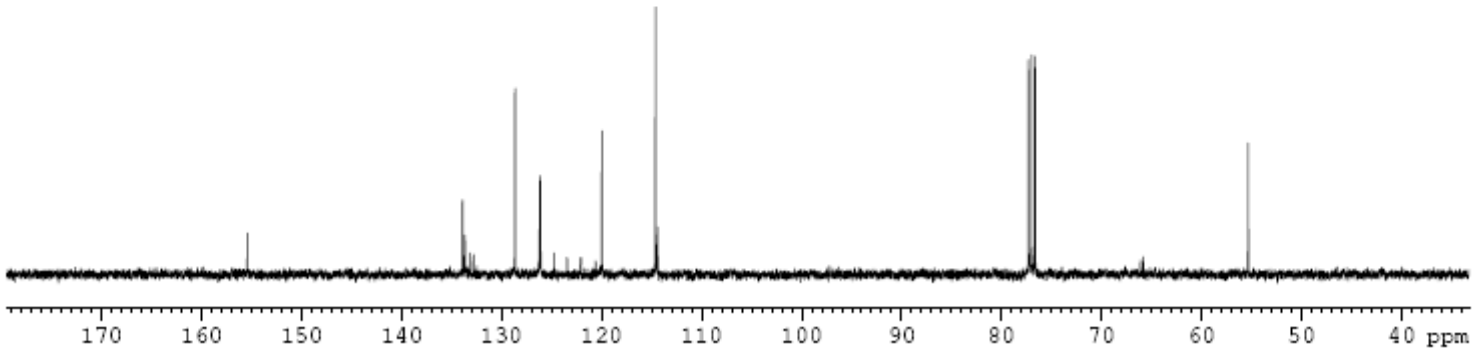
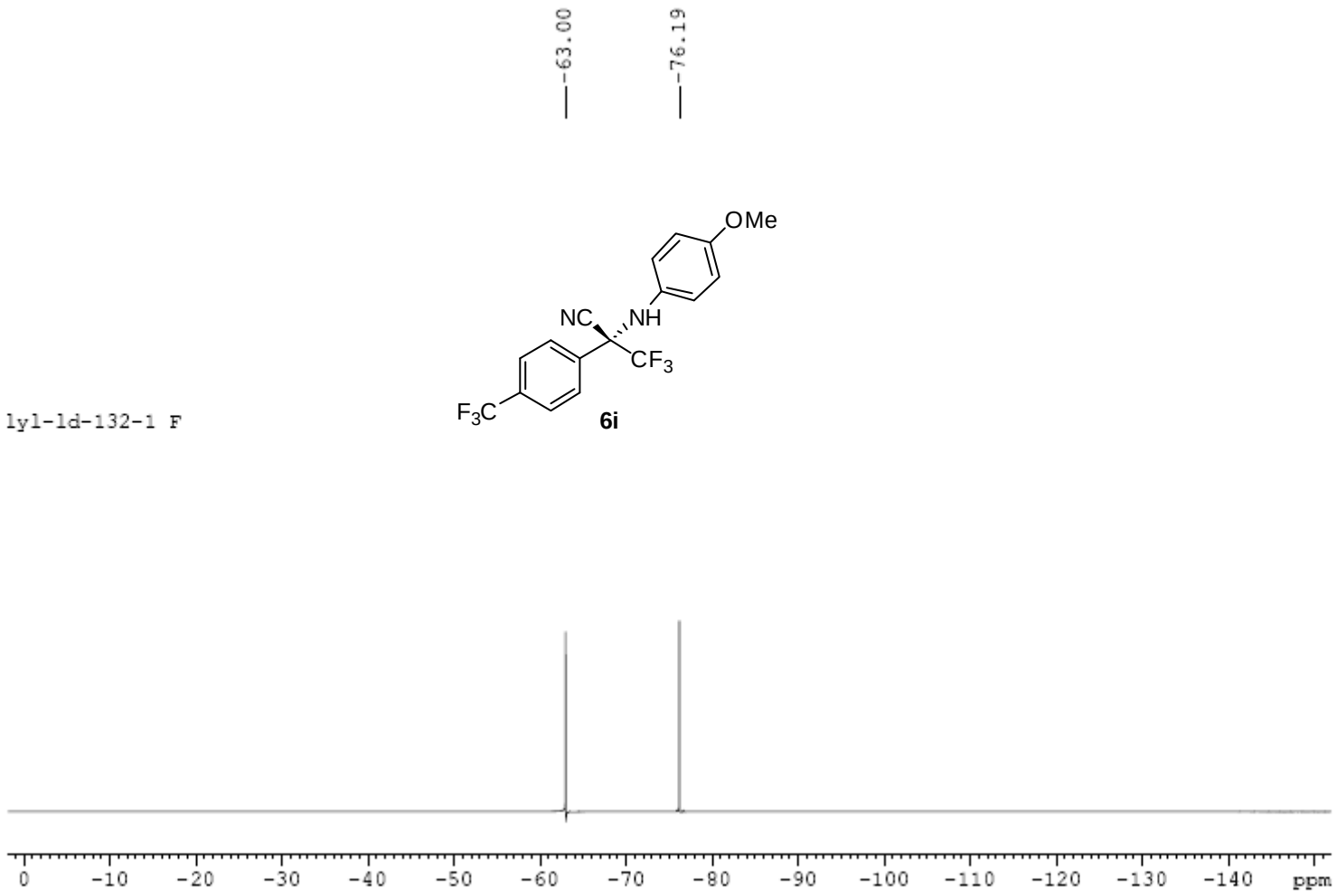


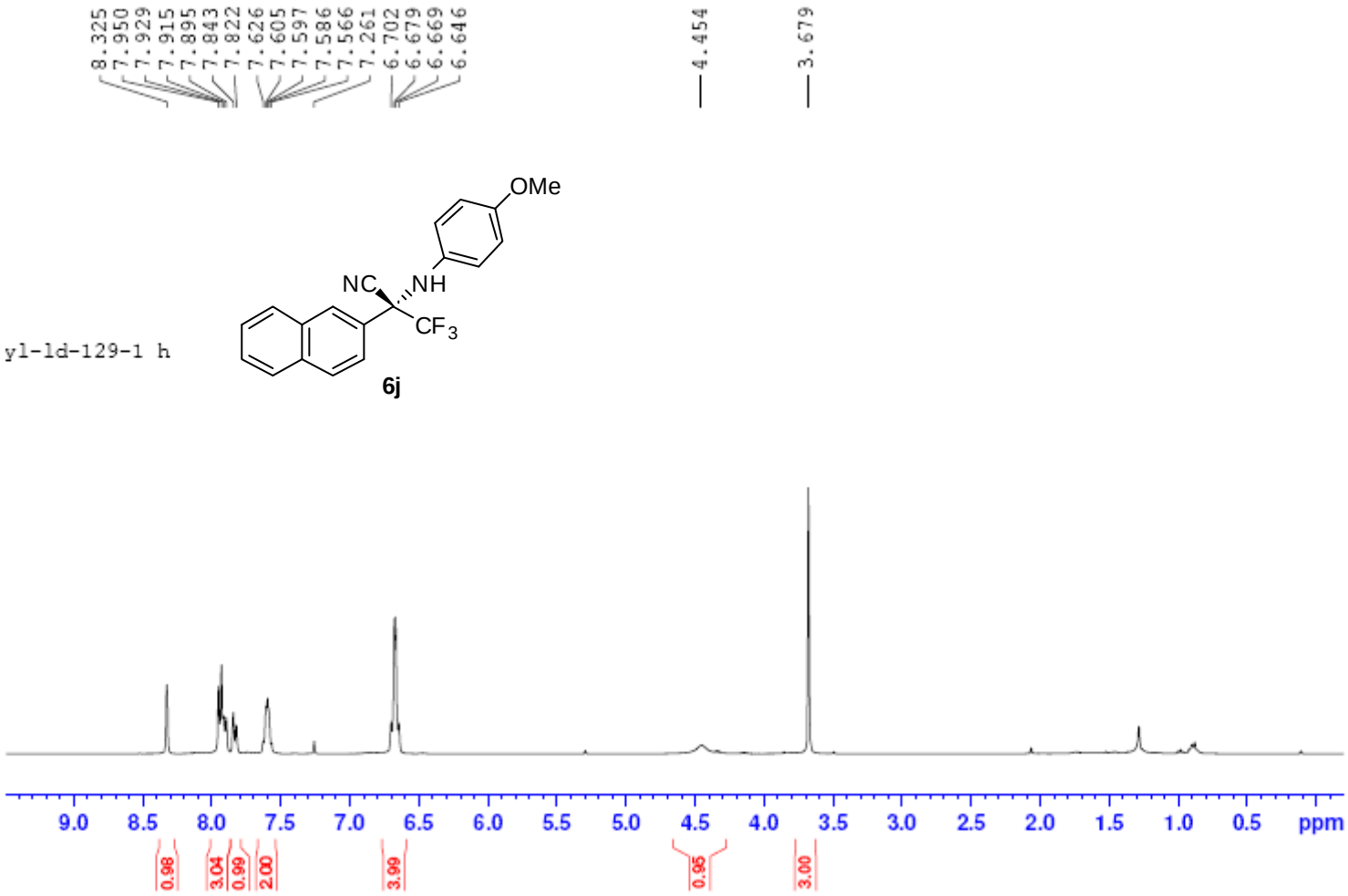


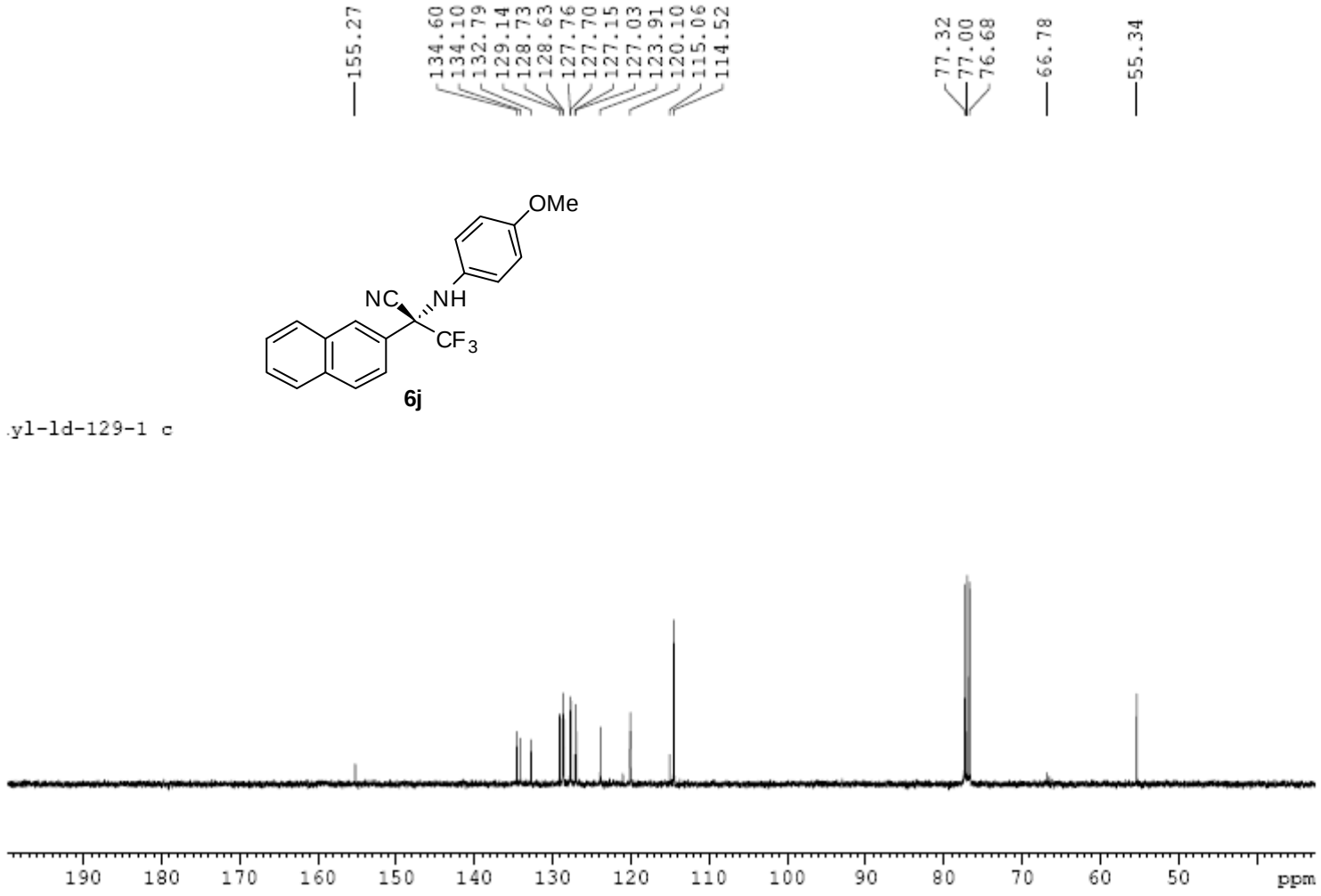
6i

lyl-le-056-2 c




-63.00
-76.19
OMe
NC
NH
CF3
F3C
6i
lyl-ld-132-1 F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm


8.325
7.950
7.929
7.915
7.895
7.843
7.822
7.626
7.605
7.597
7.586
7.566
7.261
6.702
6.679
6.669
6.646
4.454
3.679
OMe
NC
NH
CF3
yl-ld-129-1 h
6j
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.98
3.04
0.99
2.00
3.99
0.95
3.00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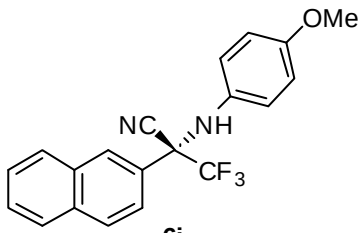
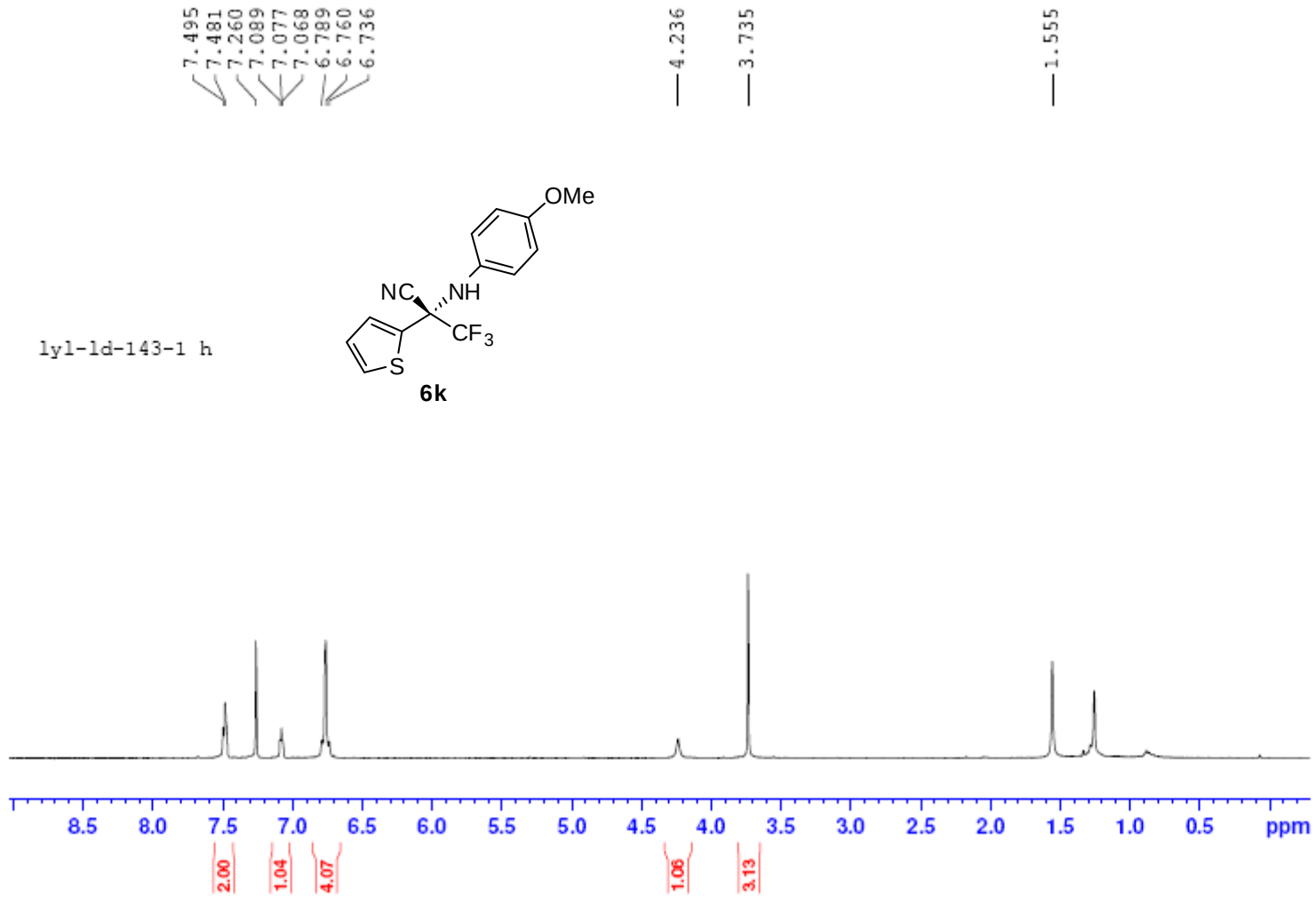
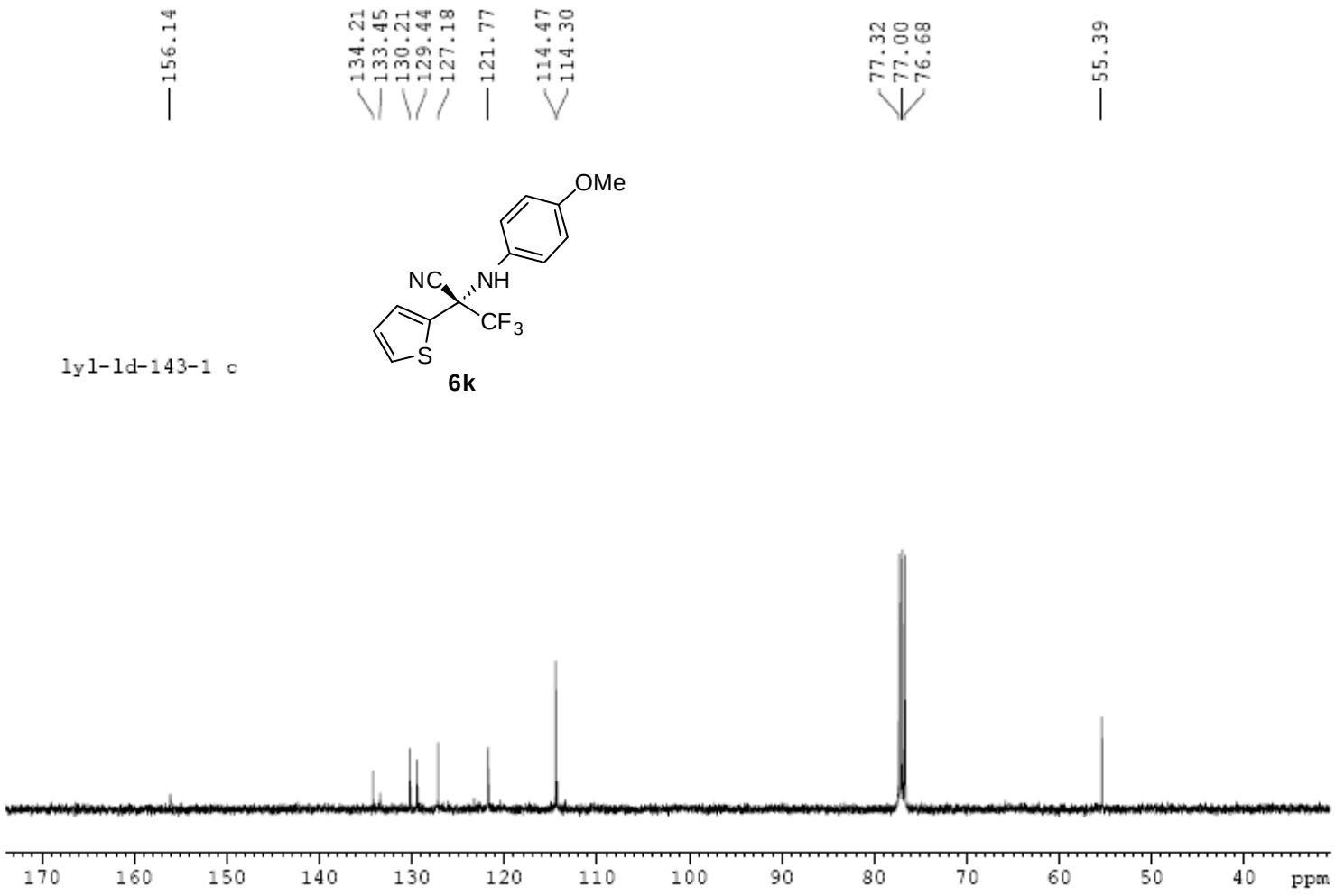
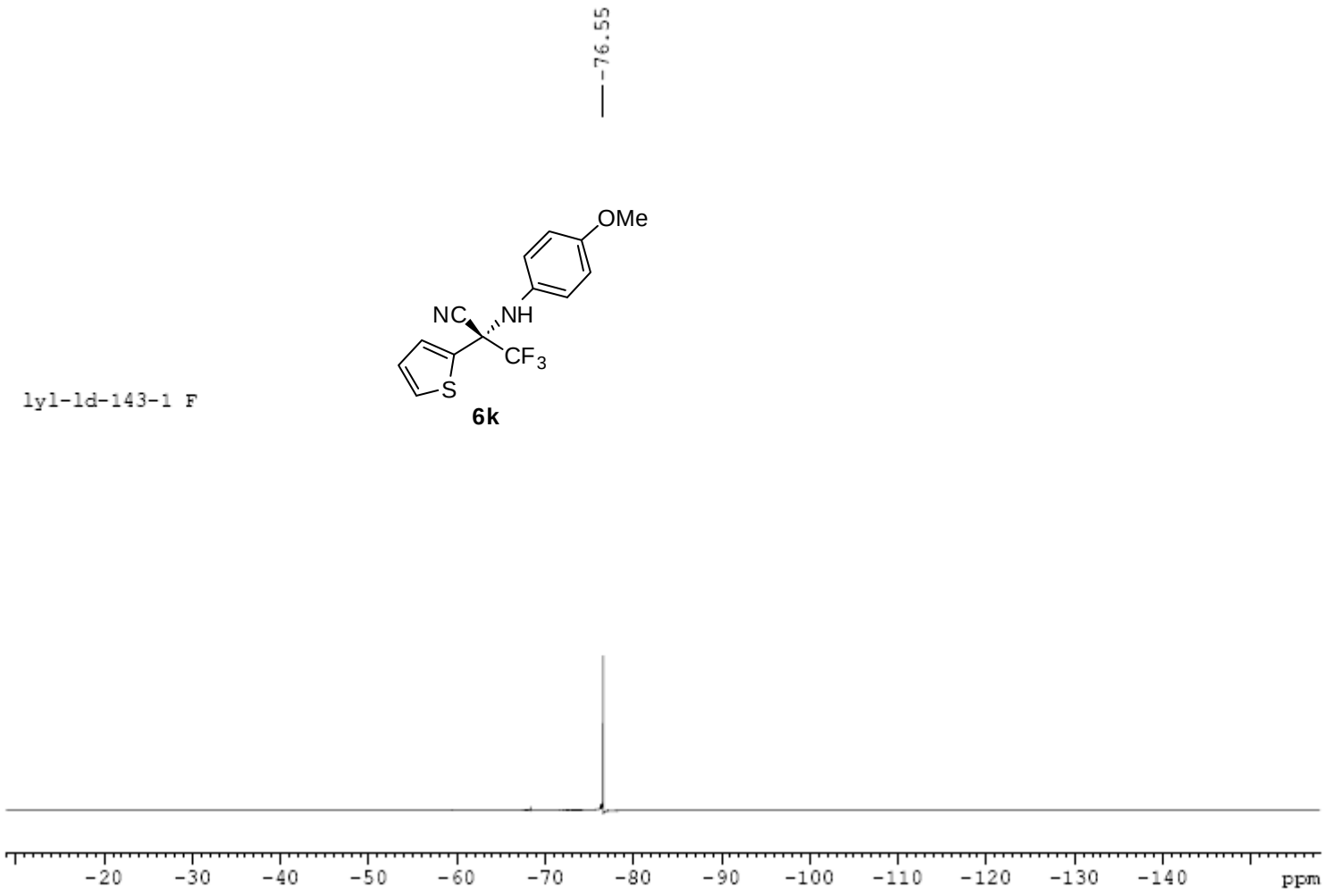
134.60
134.10
132.79
129.14
128.73
128.63
127.76
127.70
127.15
127.03
123.91
120.10
115.06
114.52
77.32
77.00
76.68
66.78
55.34
OMe
NC
NH
CF3
6j
yl-ld-129-1 c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm

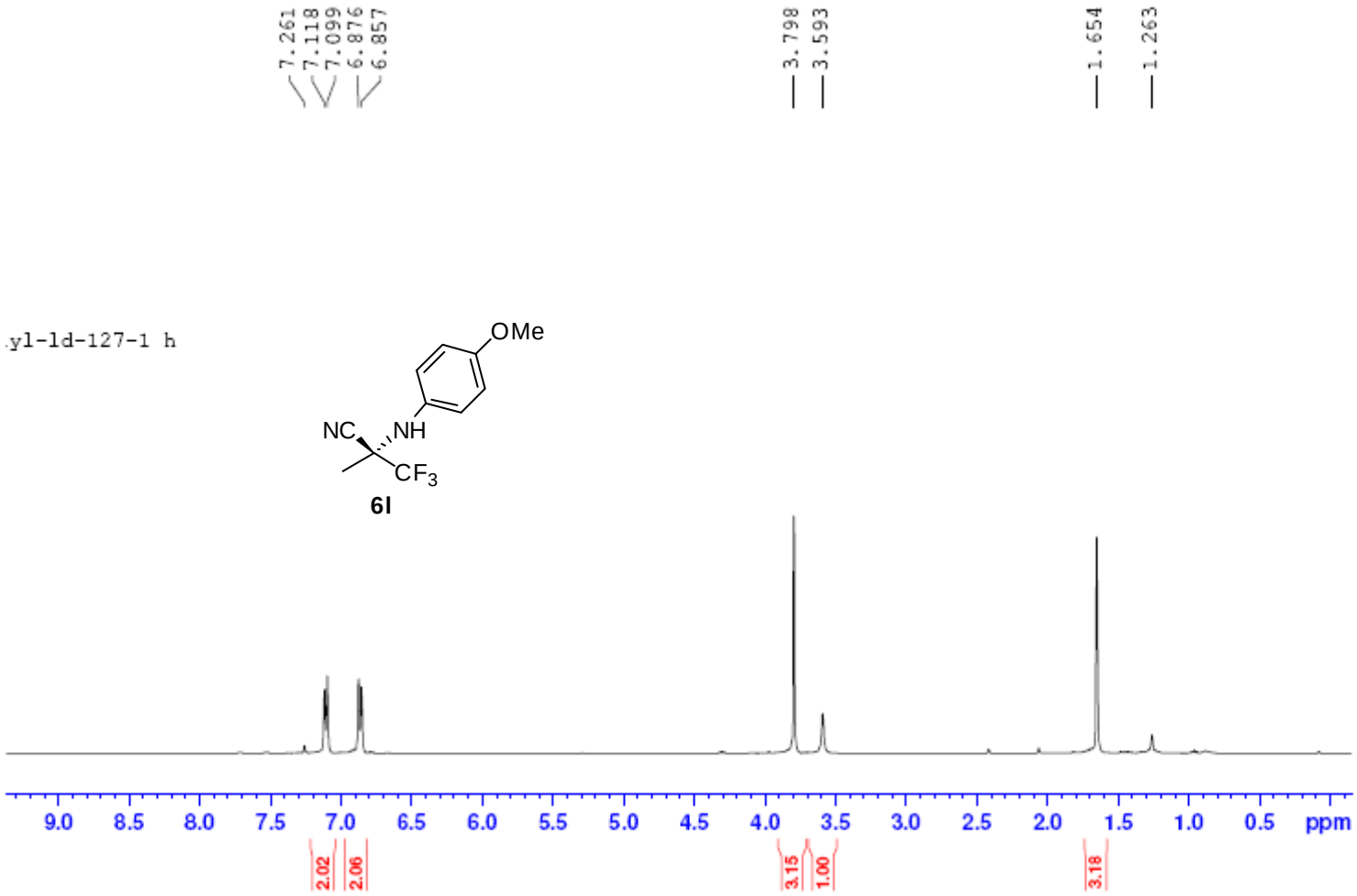


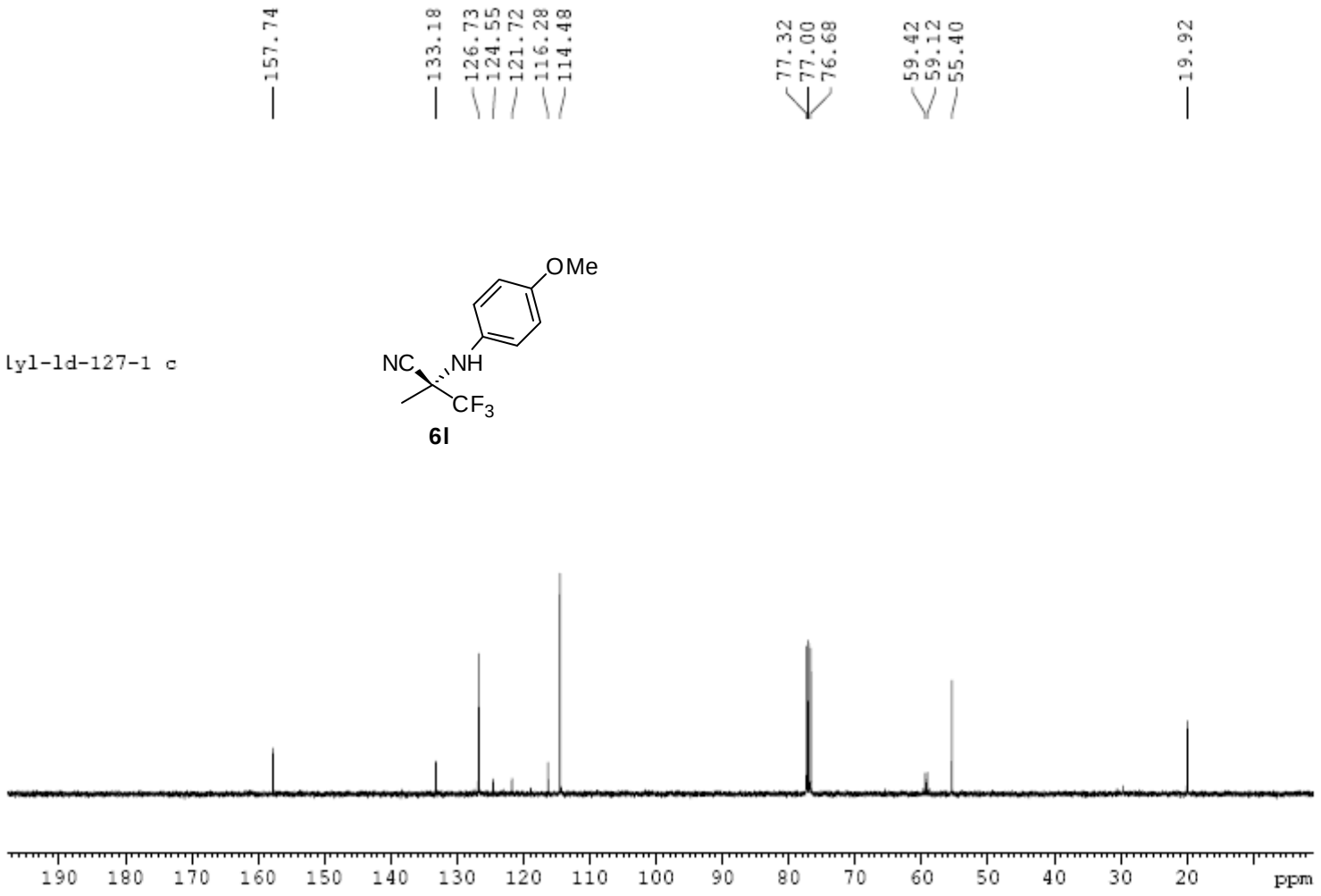
6j


7.495
7.481
7.260
7.089
7.077
7.068
6.789
6.760
6.736
4.236
3.735
1.555
lyl-ld-143-1 h
OMe
NC
NH
CF3
S
6k
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
1.04
4.07
1.06
3.13


156.14
134.21
133.45
130.21
129.44
127.18
121.77
114.47
114.30
77.32
77.00
76.68
55.39
OMe
NC
NH
CF3
S
6k
lyl-ld-143-1 c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm


-76.55
OMe
NC
NH
CF3
S
6k
lyl-ld-143-1 F
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm


7.261
7.118
7.099
6.876
6.857
3.798
3.593
1.654
1.263
yl-ld-127-1 h
OMe
NC
NH
CF3
6l
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.02
2.06
3.15
1.00
3.18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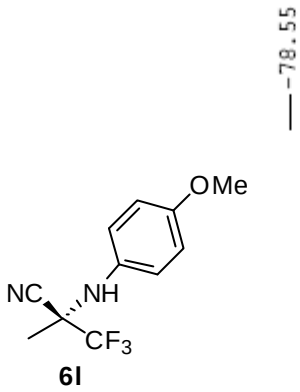
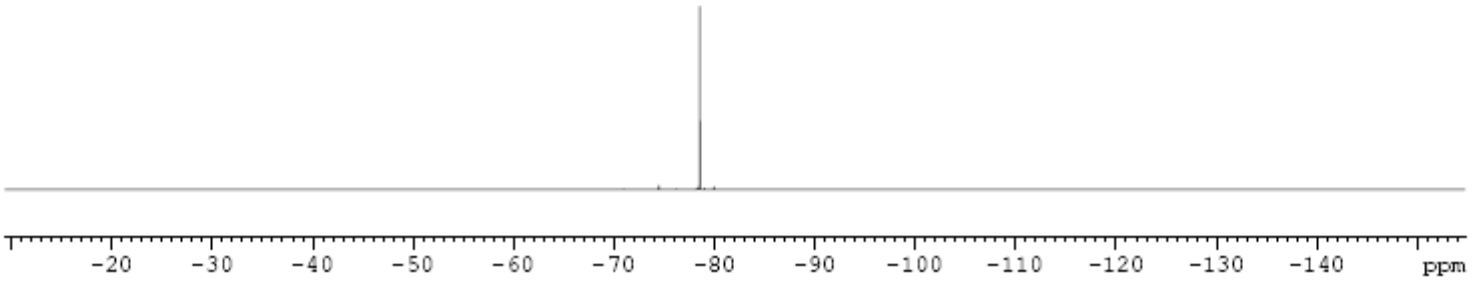
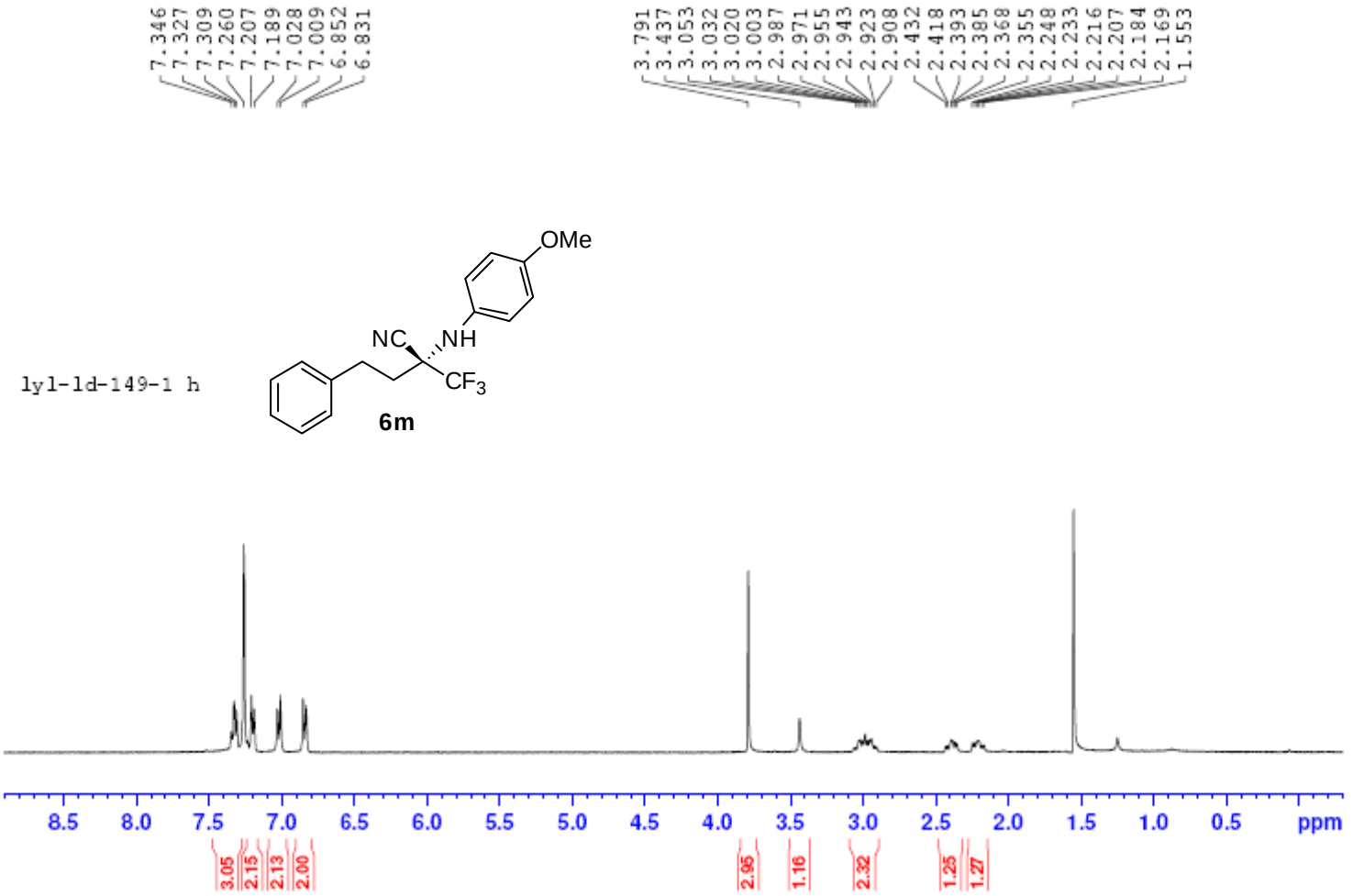
133.18
126.73
124.55
121.72
116.28
114.48
77.32
77.00
76.68
59.42
59.12
55.40
19.92
lyl-ld-127-1 c
OMe
NC
NH
CF3
6l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm



6l

lyl-ld-127-1 f

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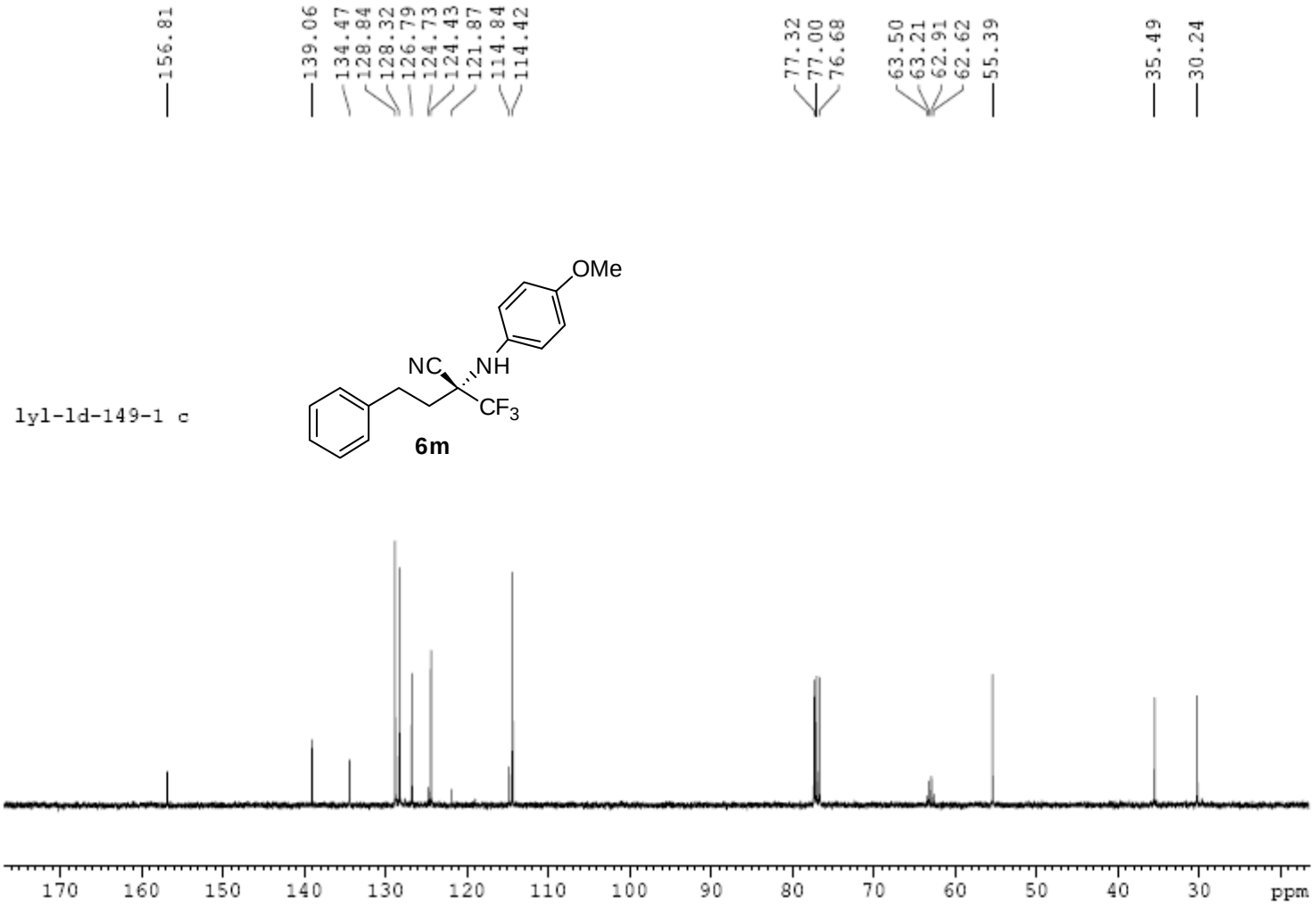
7.327
7.309
7.260
7.207
7.189
7.028
7.009
6.852
6.831
3.791
3.437
3.053
3.032
3.020
3.003
2.987
2.971
2.955
2.943
2.923
2.908
2.432
2.418
2.393
2.385
2.368
2.355
2.248
2.233
2.216
2.207
2.184
2.169
1.553
lyl-ld-149-1 h
OMe
NC
NH
CF3
6m
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.05
2.15
2.13
2.00
2.95
1.16
2.32
1.25
1.27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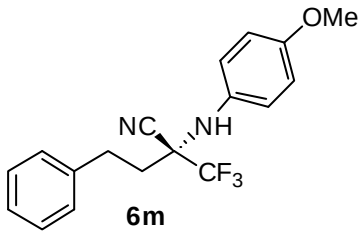
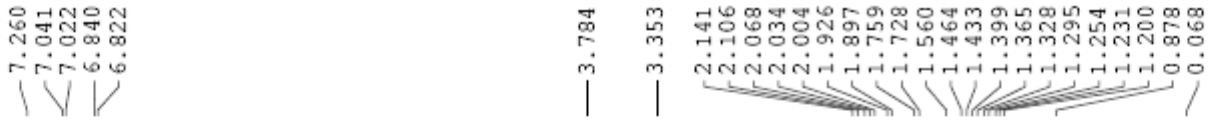
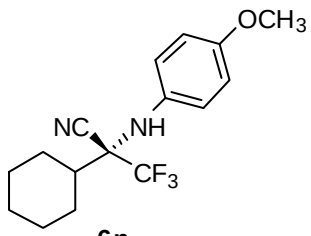
134.47
128.84
128.32
126.79
124.73
124.43
121.87
114.84
114.42
77.32
77.00
76.68
63.50
63.21
62.91
62.62
55.39
35.49
30.24
lyl-ld-149-1 c
OMe
NC
NH
CF3
6m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm



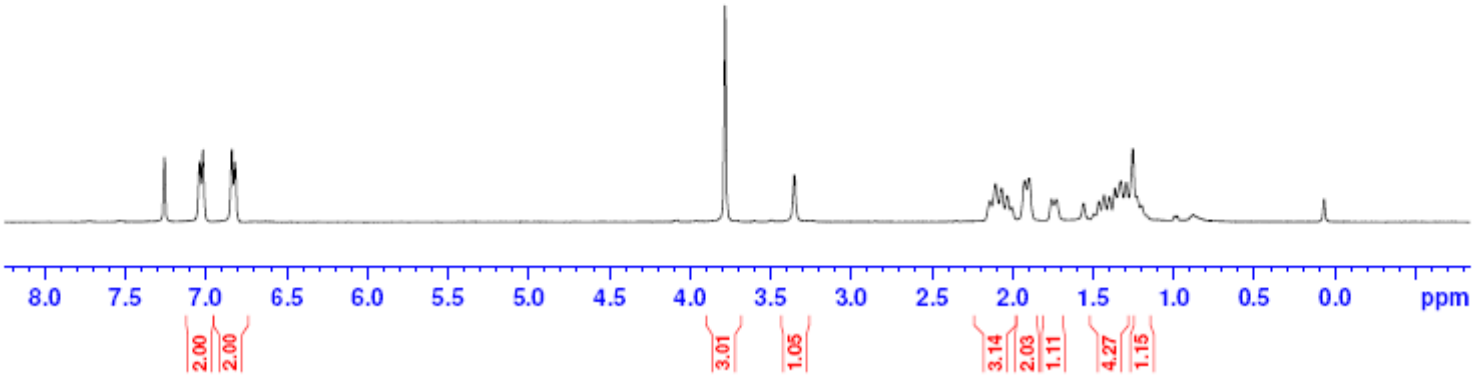
6m

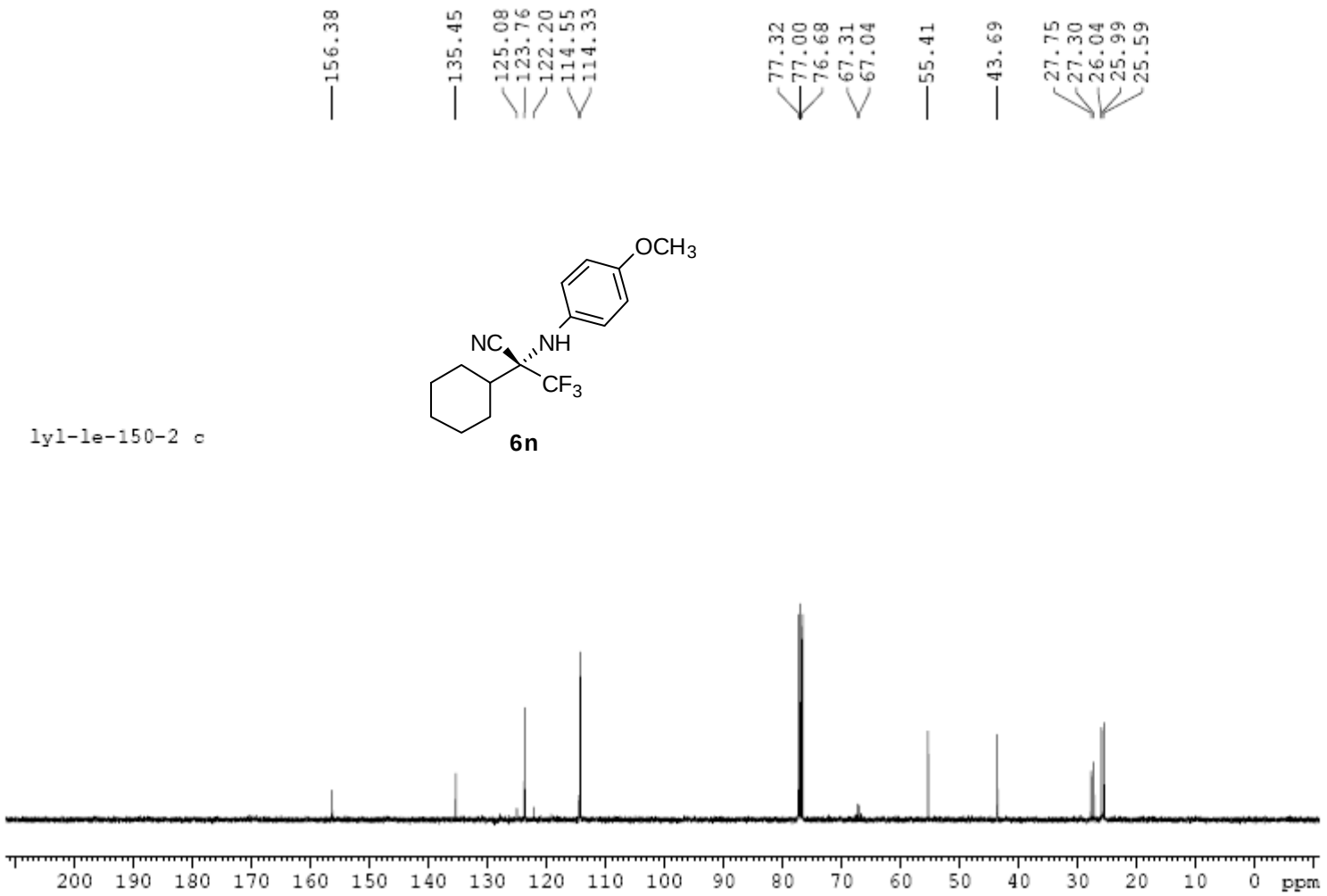




6n

lyl-le-129 h

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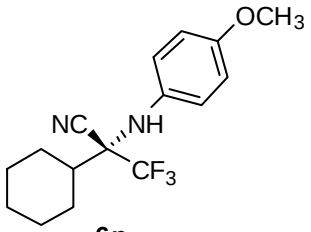
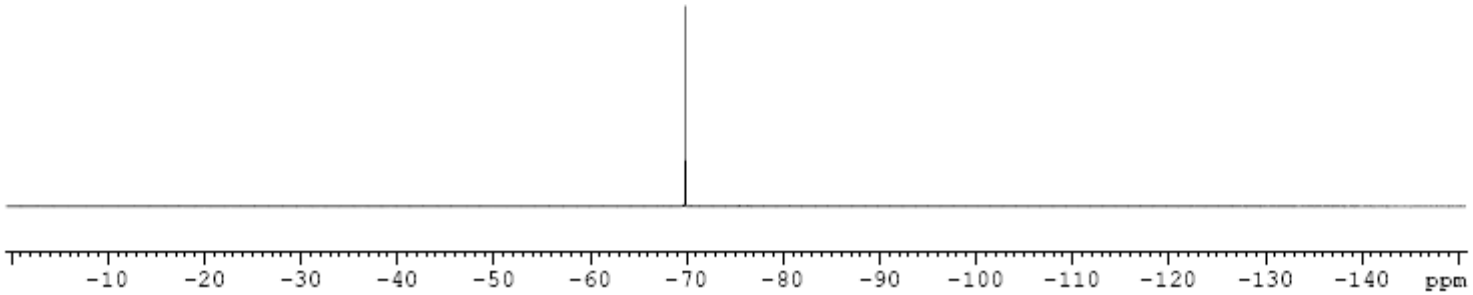
135.45
125.08
123.76
122.20
114.55
114.33
77.32
77.00
76.68
67.31
67.04
55.41
43.69
27.75
27.30
26.04
25.99
25.59
OCH3
NC
NH
CF3
lyl-le-150-2 c
6n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

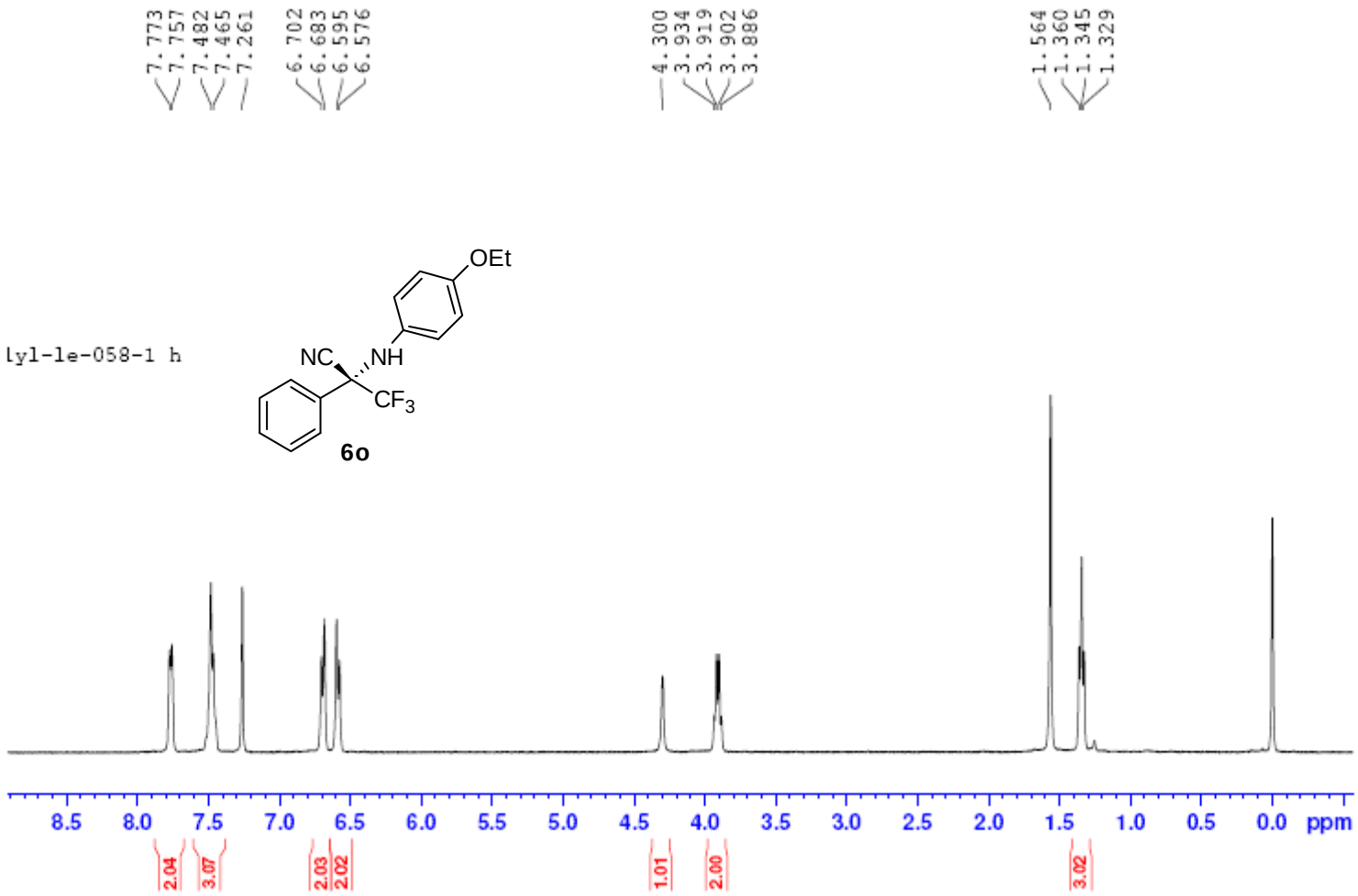


6n

-69.90

lyl-le-129 f

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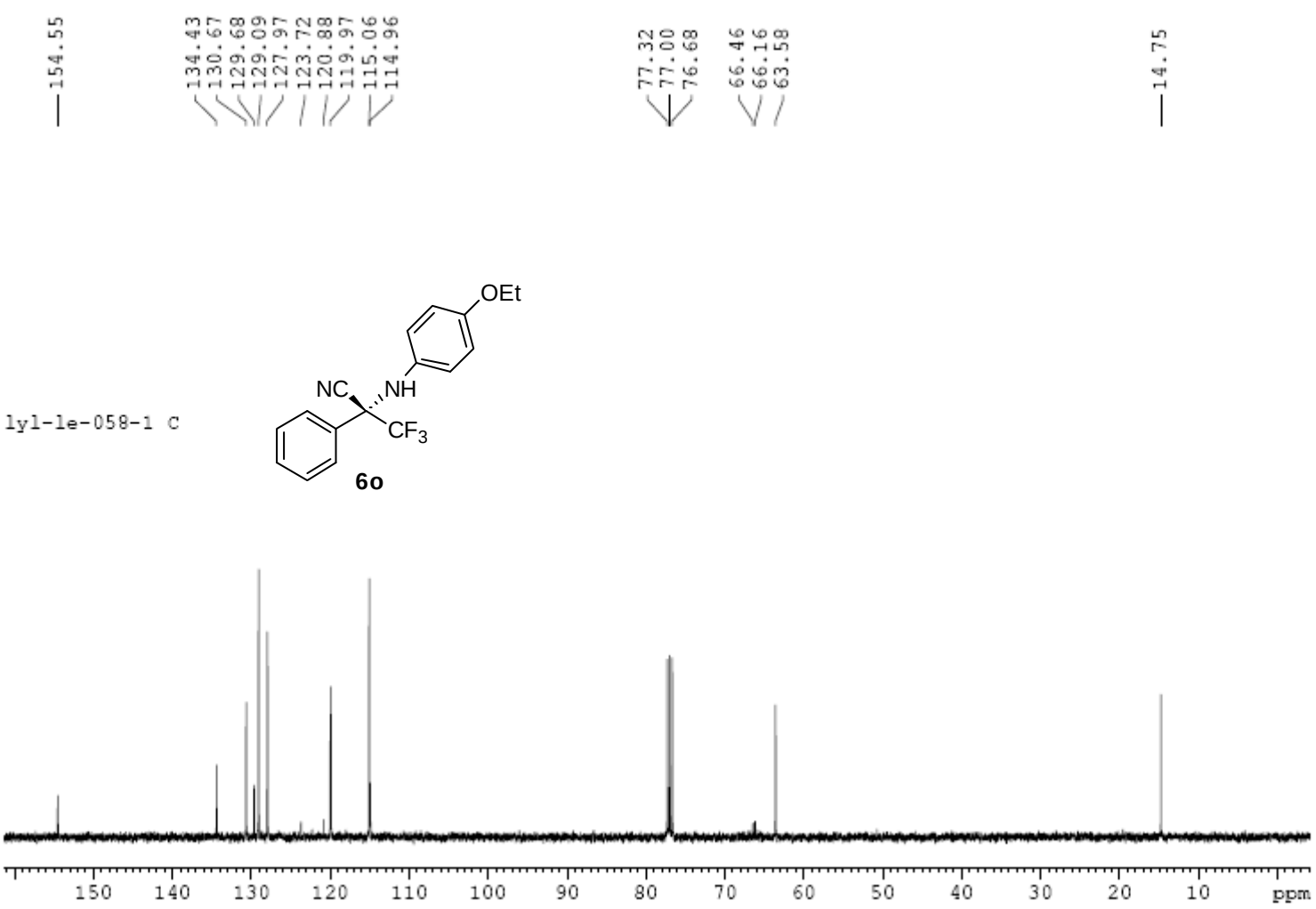
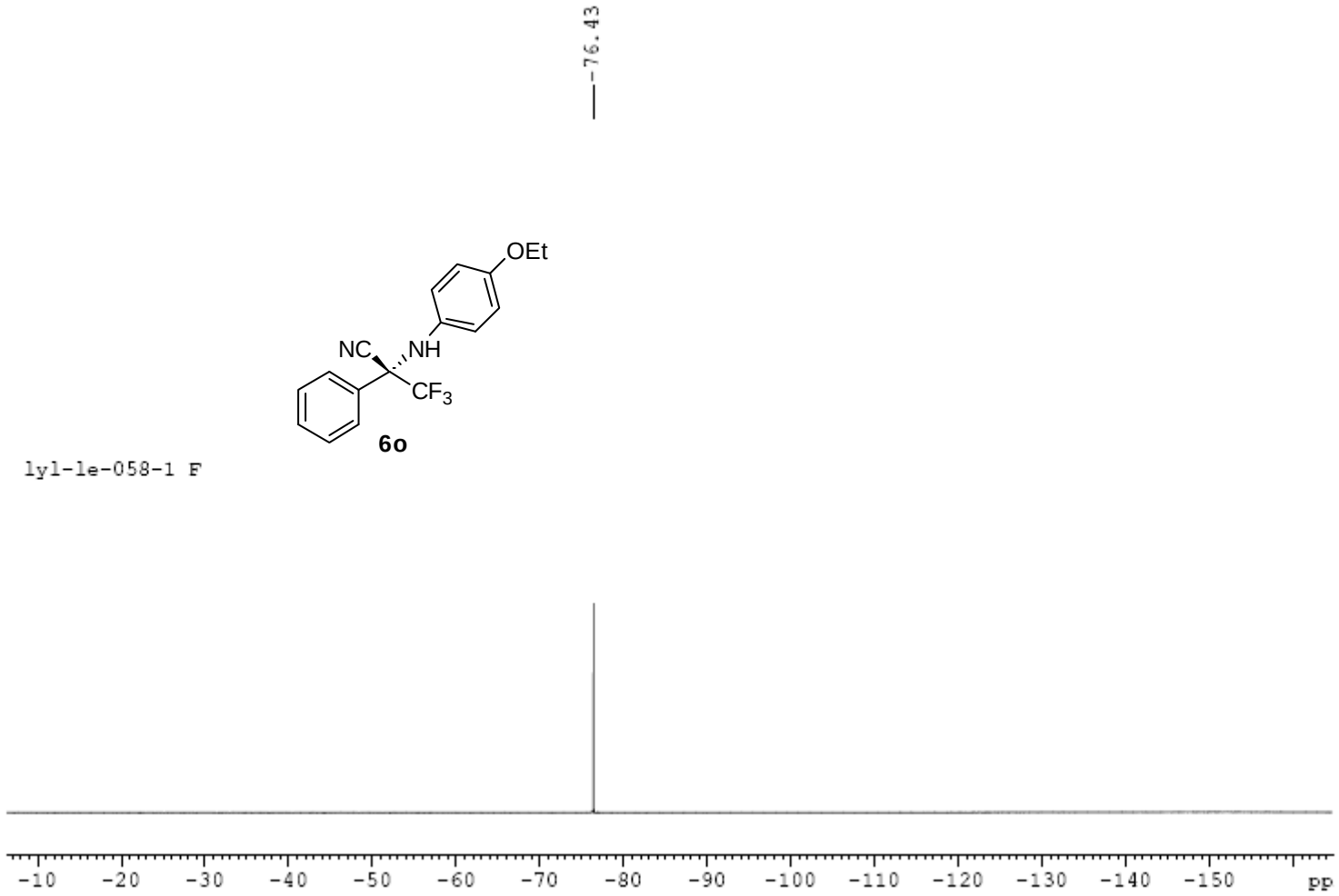
7.482
7.465
7.261
6.702
6.683
6.595
6.576
4.300
3.934
3.919
3.902
3.886
1.564
1.360
1.345
1.329
lyl-1e-058-1 h
OEt
NC
NH
CF3
6o
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.04
3.07
2.03
2.02
1.01
2.00
3.02


154.55
134.43
130.67
129.68
129.09
127.97
123.72
120.88
119.97
115.06
114.96
77.32
77.00
76.68
66.46
66.16
63.58
14.75
lyl-le-058-1 C
OEt
NC
NH
CF3
6o
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-76.43
OEt
NC
NH
CF3
6o
lyl-le-058-1 F
-10
-20
-30
-40
-50
-60
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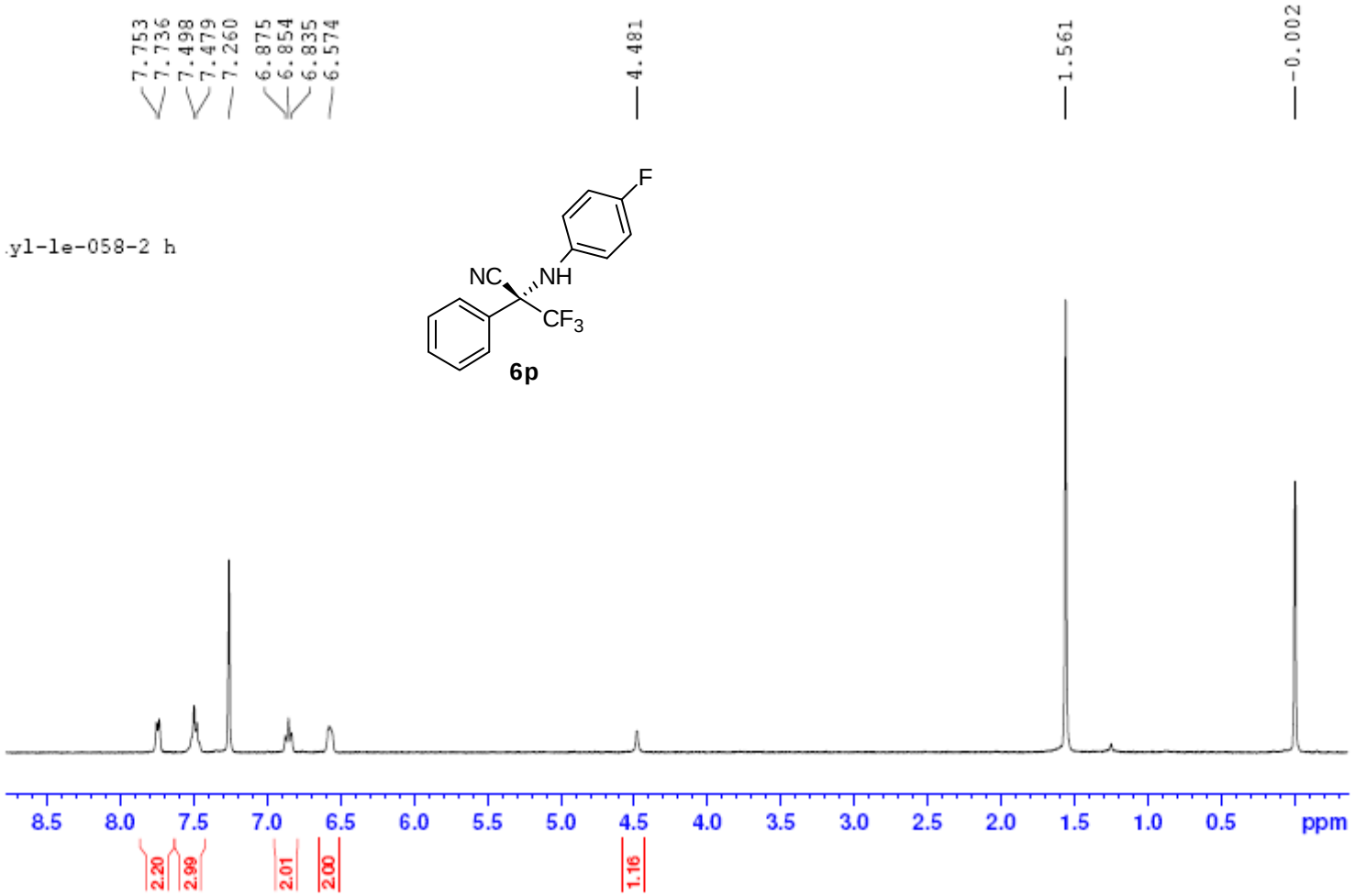
-100
-110
-120
-130
-140
-150
pp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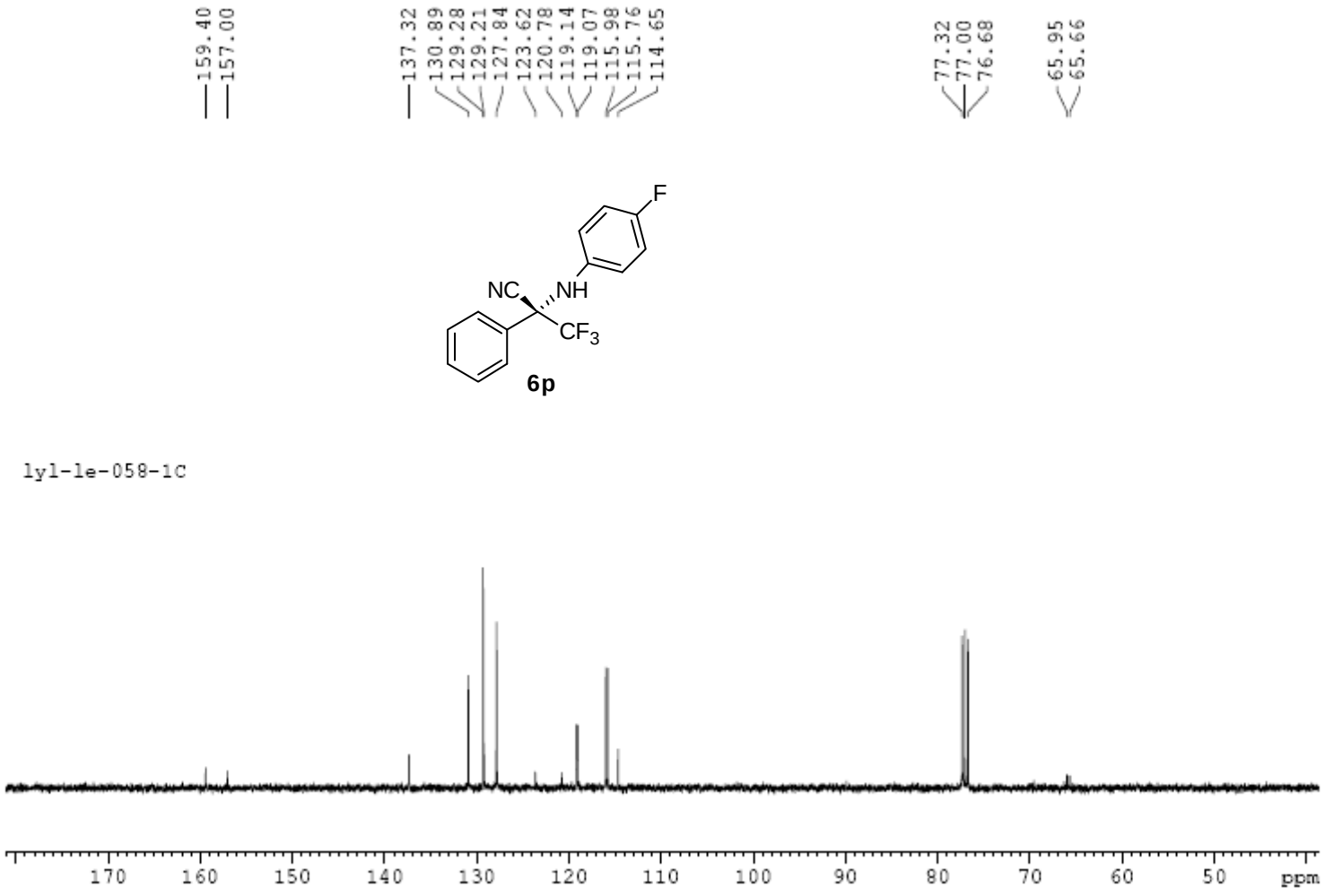
7.736
7.498
7.479
7.260
6.875
6.854
6.835
6.574
4.481
1.561
-0.002
yl-le-058-2 h
F
NC
NH
CF3
6p
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.20
2.99
2.01
2.00
1.16


159.40
157.00
137.32
130.89
129.28
129.21
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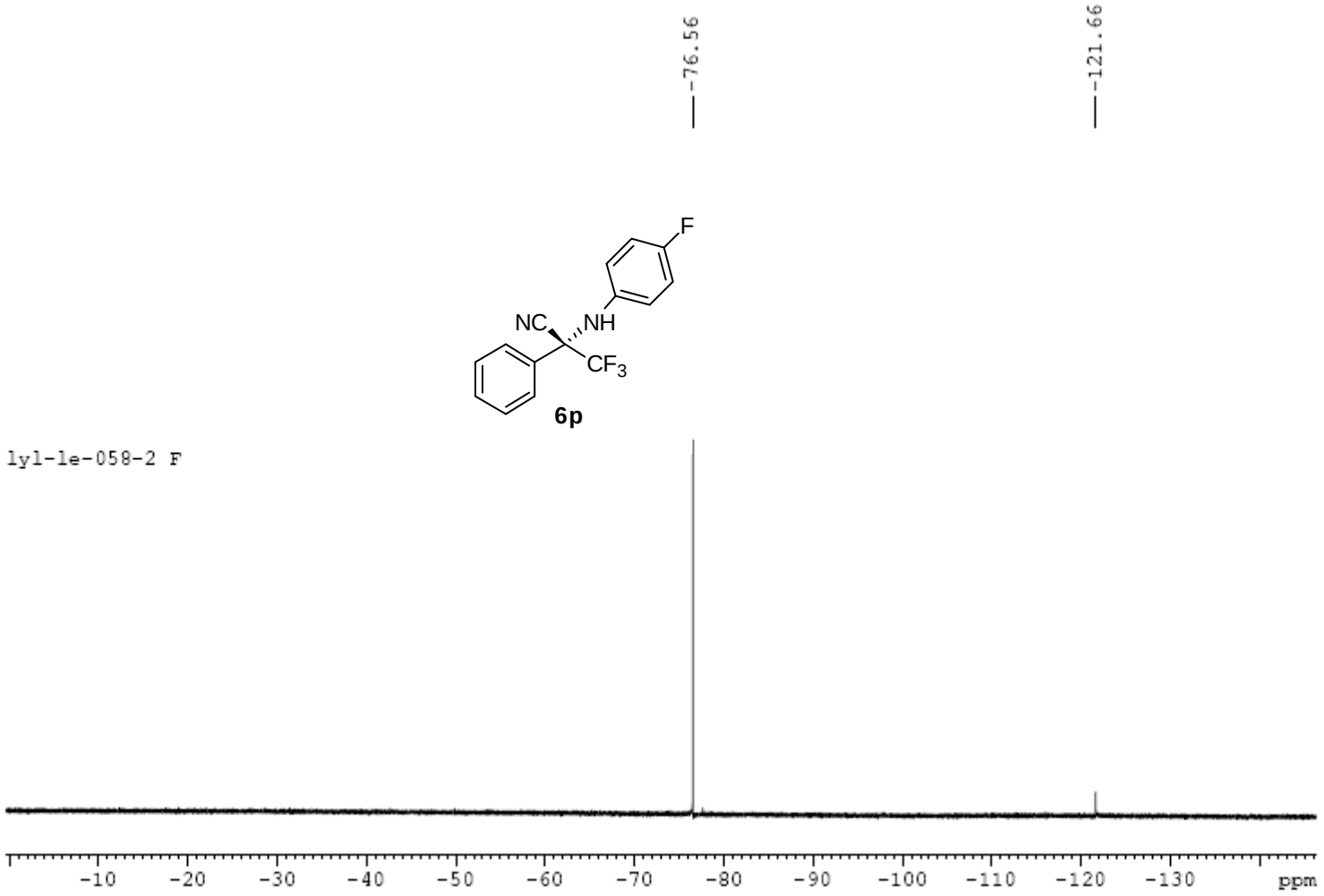
123.62
120.78
119.14
119.07
115.98
115.76
114.65
77.32
77.00
76.68
65.95
65.66
F
NC
NH
CF3
6p
lyl-le-058-1C
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm


-76.56
-121.66
F
NC
NH
CF3
6p
lyl-le-058-2 F
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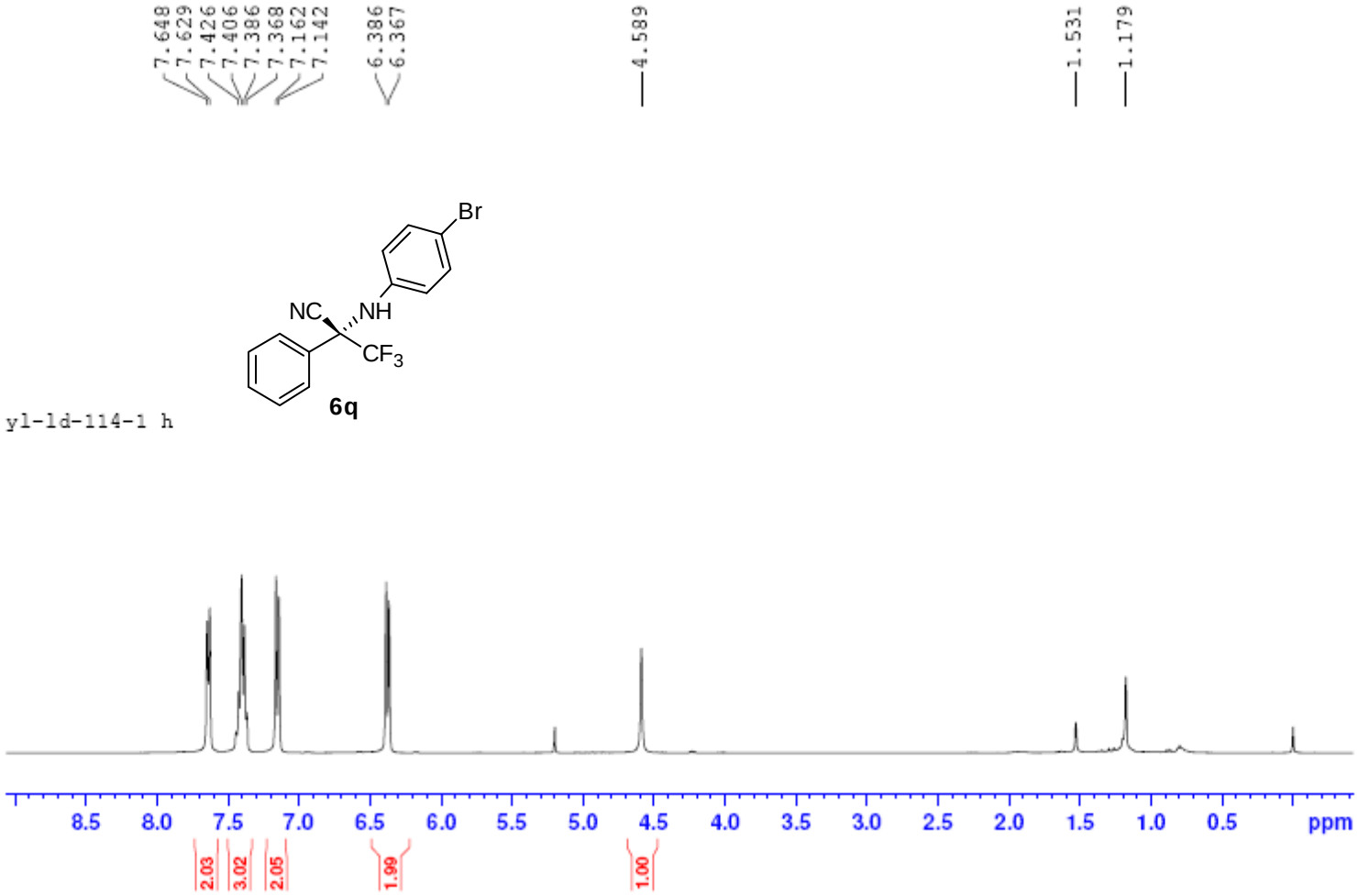
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
ppm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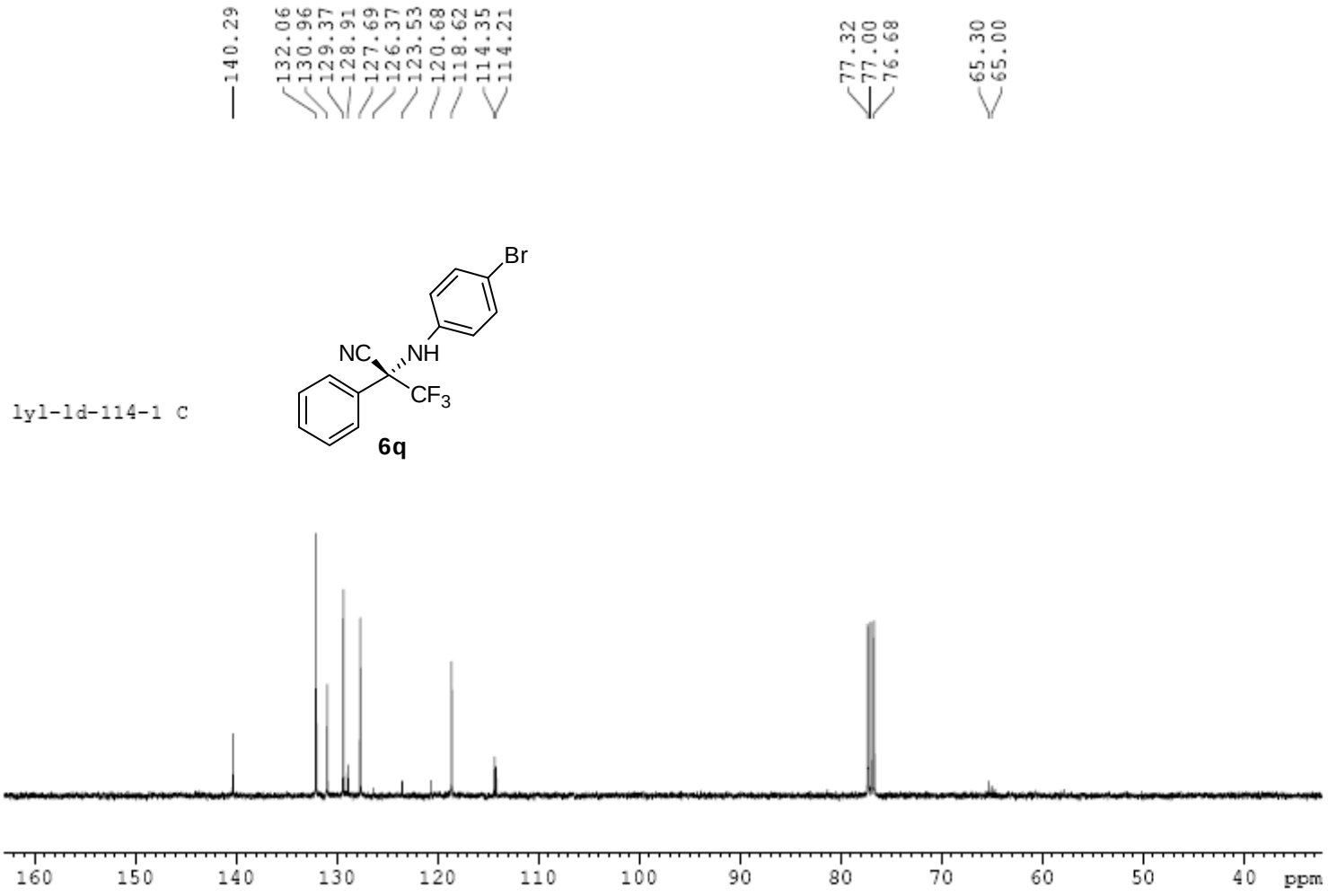
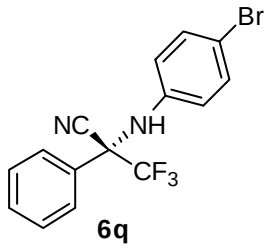
7.629
7.426
7.406
7.386
7.368
7.162
7.142
6.386
6.367
4.589
1.531
1.179
Br
NC
NH
CF3
6q
yl-ld-114-1 h
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.03
3.02
2.05
1.99
1.00

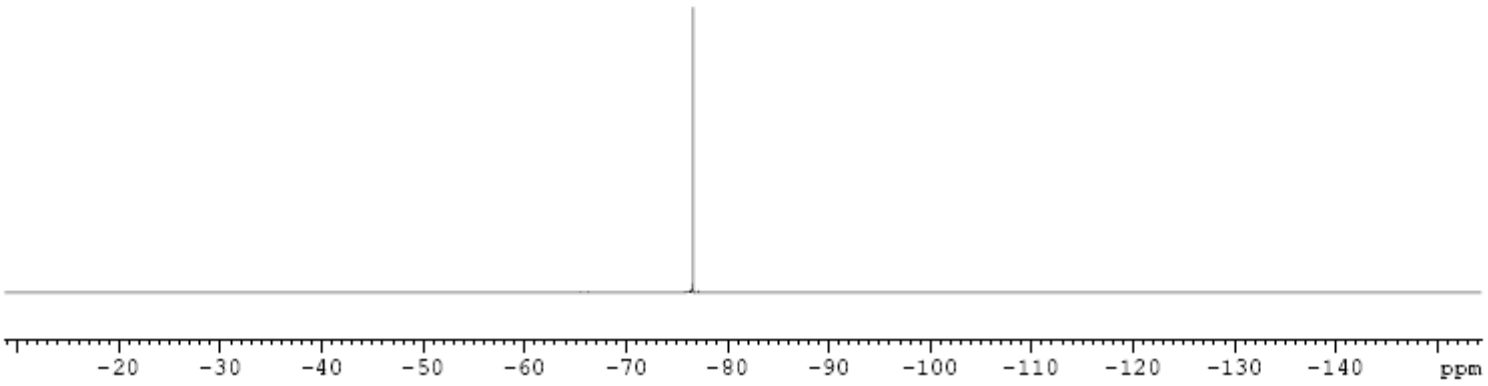

140.29
132.06
130.96
129.37
128.91
127.69
126.37
123.53
120.68
118.62
114.35
114.21
77.32
77.00
76.68
65.30
65.00
Br
NC
NH
CF3
6q
lyl-1d-114-1 C
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

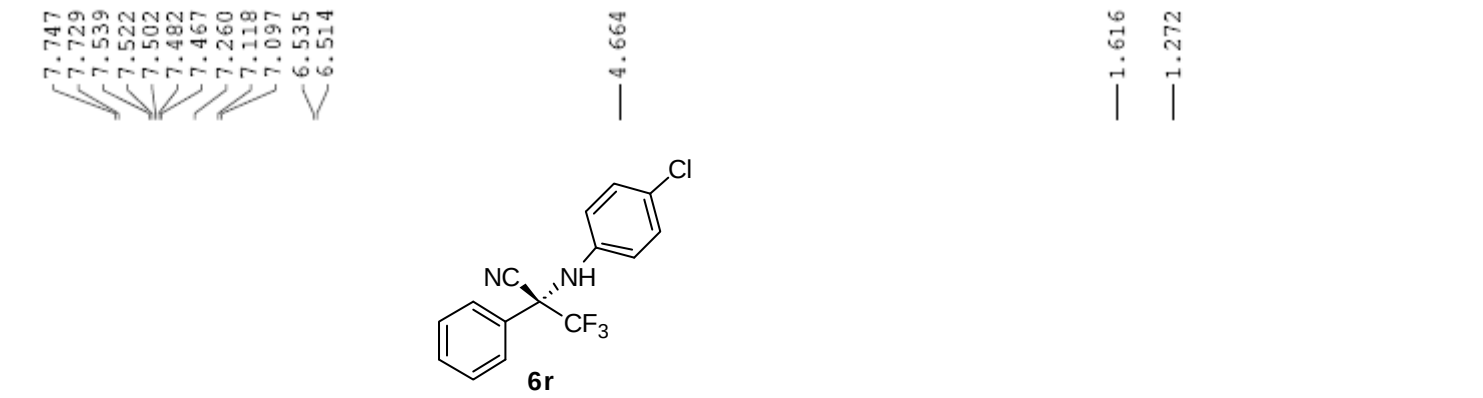


6q

-76.59

lyl-ld-114-1 F

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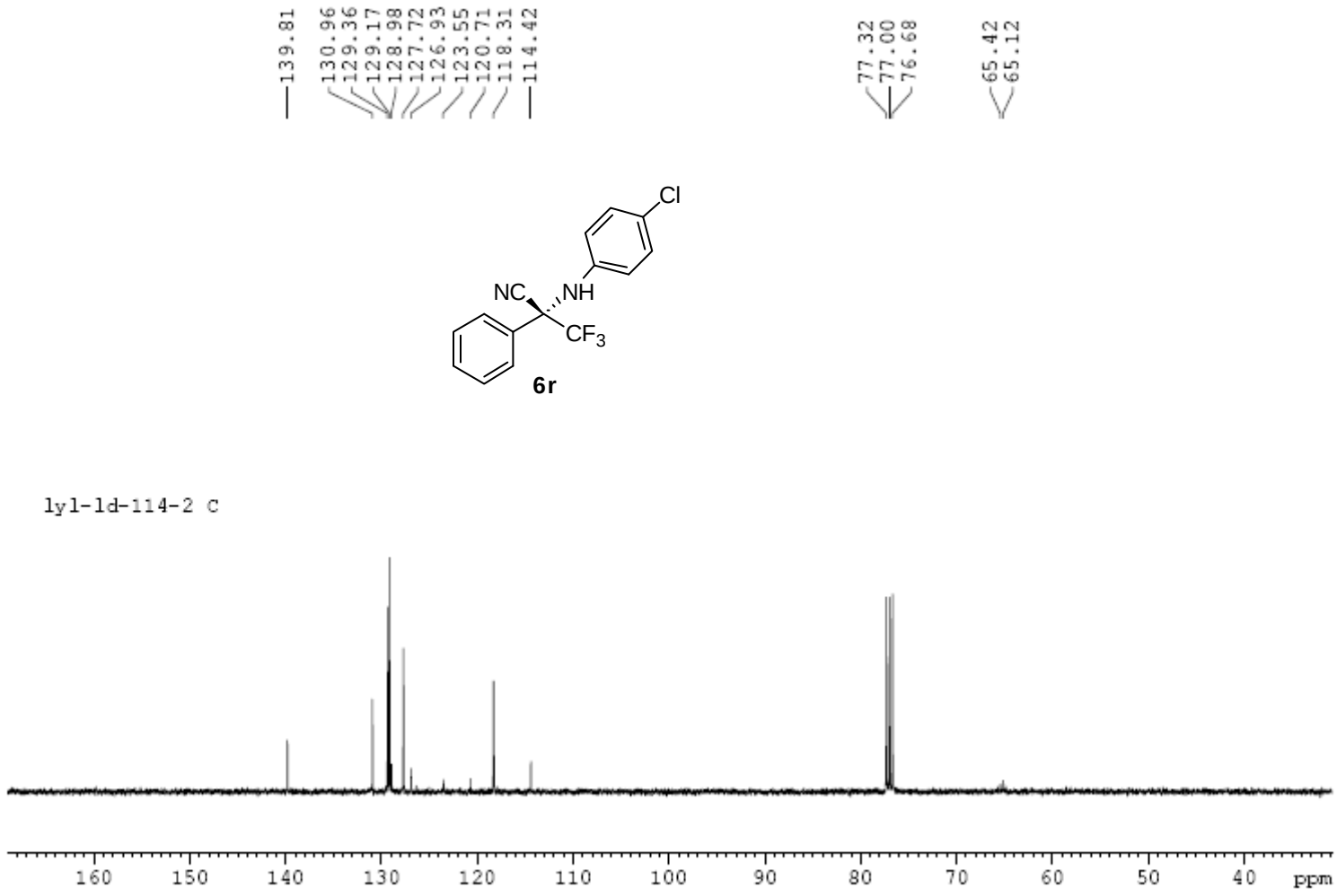
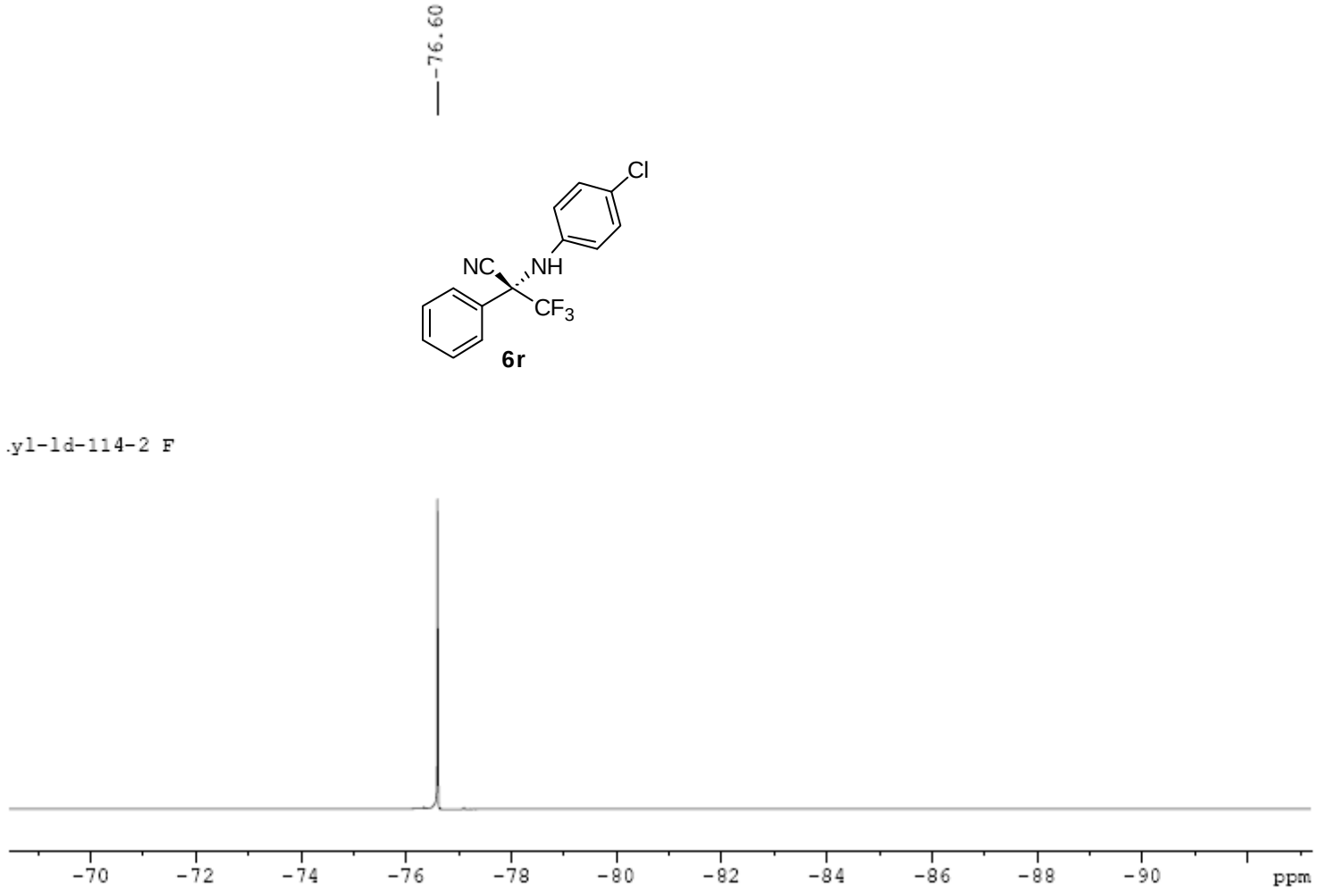
7.729
7.539
7.522
7.502
7.482
7.467
7.260
7.118
7.097
6.535
6.514
4.664
1.616
1.272
Cl
NC
NH
CF3
6r
lyl-1d-114-2 h
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.05
3.07
2.00
1.99
1.02


139.81
130.96
129.36
129.17
128.98
127.72
126.93
123.55
120.71
118.31
114.42
77.32
77.00
76.68
65.42
65.12
Cl
NC
NH
CF3
6r
lyl-1d-114-2 C
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

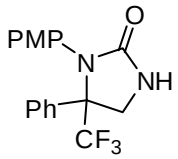

-76.60
Cl
NC
NH
CF3
6r
.yl-ld-114-2 F
-70
-72
-74
-76
-78
-80
-82
-84
-86
-88
-90
ppm

7.601
7.585
7.430
7.415
7.260
6.912
6.855
6.835
6.731
6.711

4.106
4.080
3.825
3.800
3.717

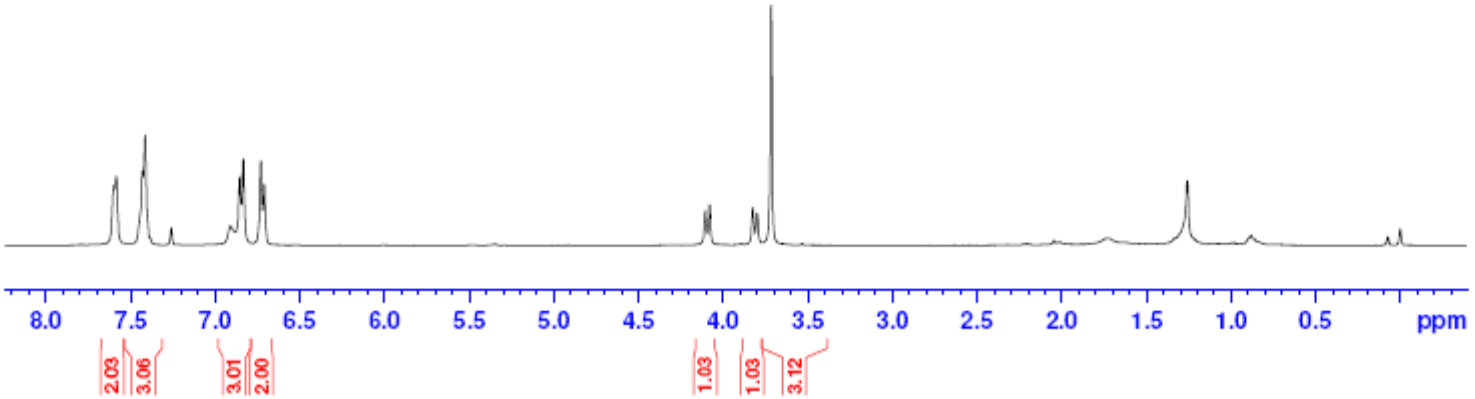
1.725

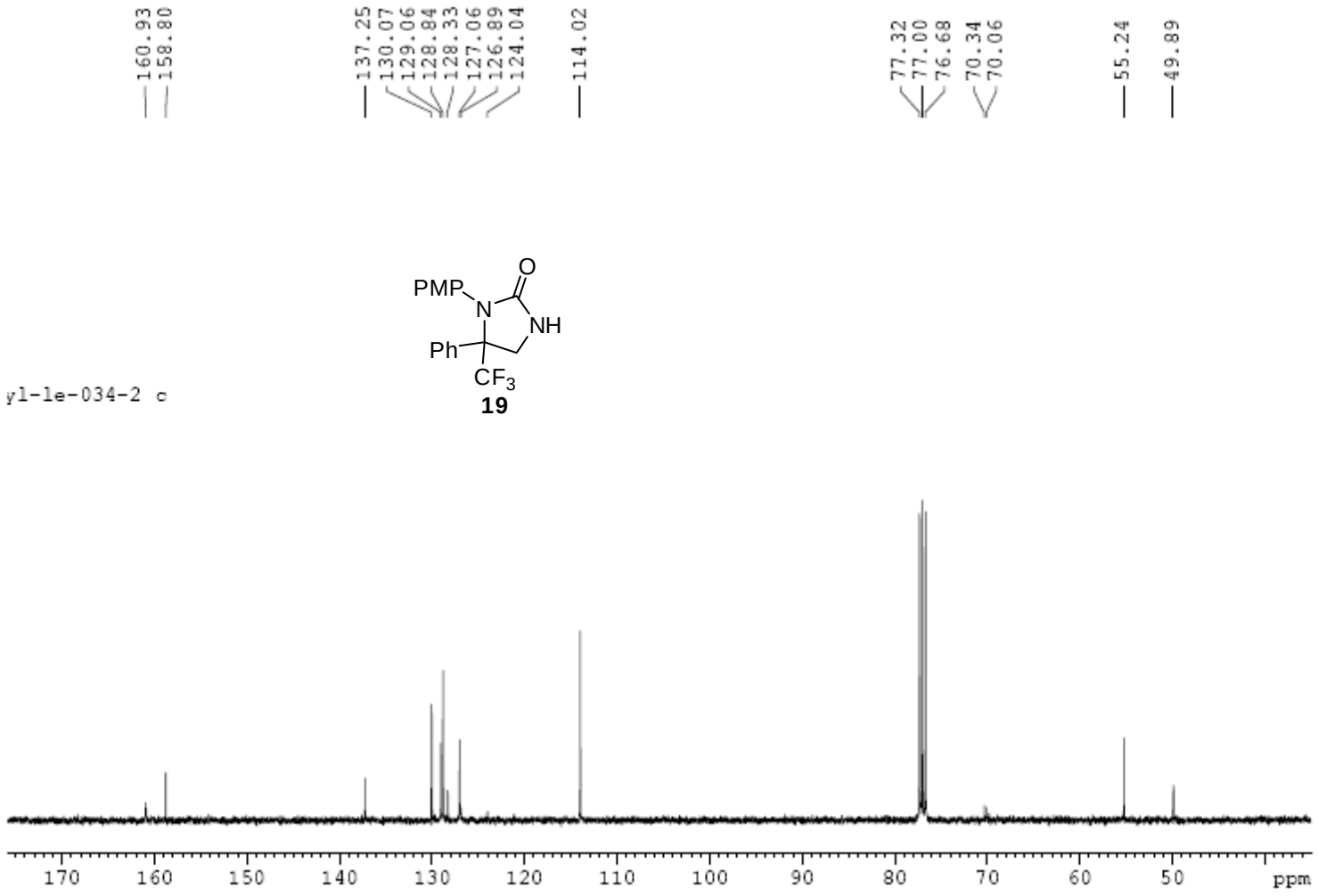
1.259

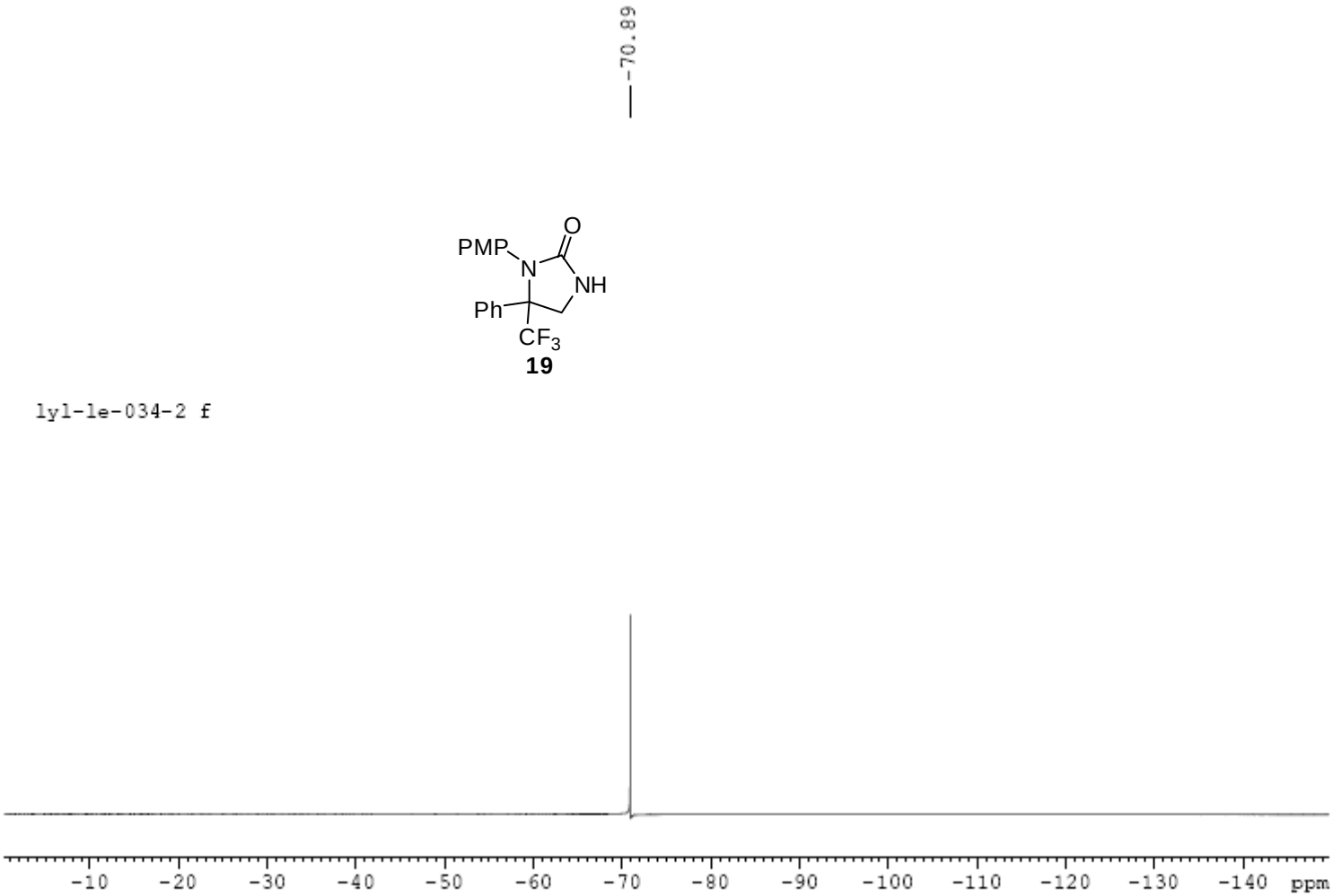


19

lyl-le-034-2 h

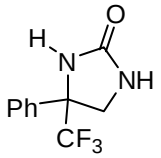



160.93
158.80
137.25
130.07
129.06
128.84
128.33
127.06
126.89
124.04
114.02
77.32
77.00
76.68
70.34
70.06
55.24
49.89
PMP
N
O
NH
Ph
CF3
19
yl-le-034-2 c
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm

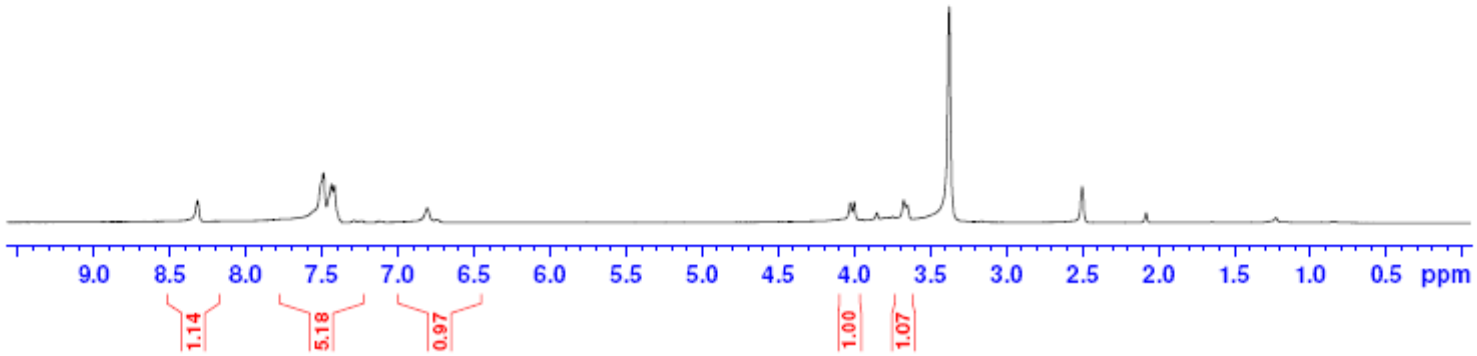

-70.89
PMP
N
O
NH
Ph
CF3
19
lyl-le-034-2 f
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm

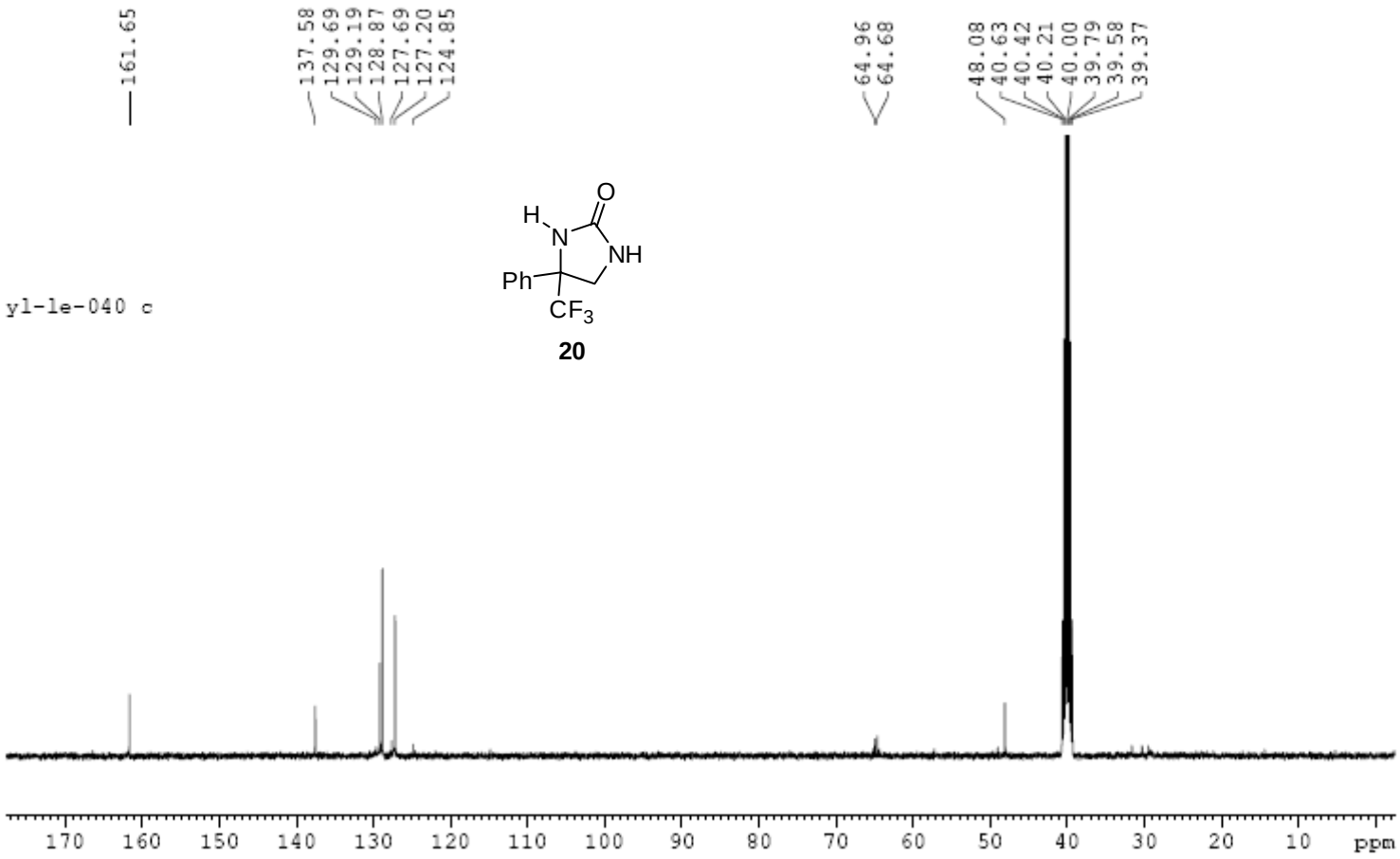
8.318
7.490
7.438
7.419
6.807
4.025
3.999
3.674
3.649
3.375
2.501

lyl-le-040-3 h

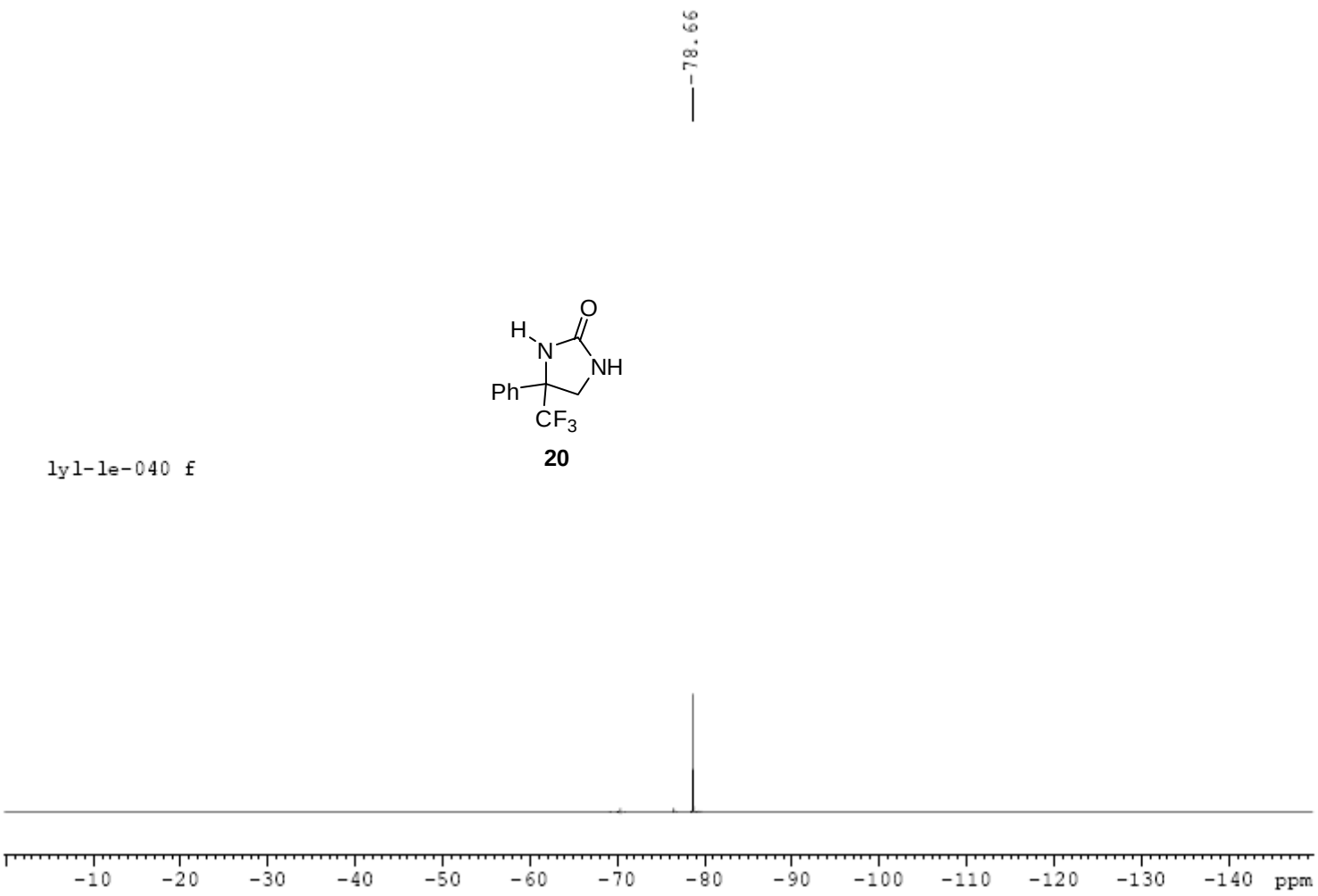


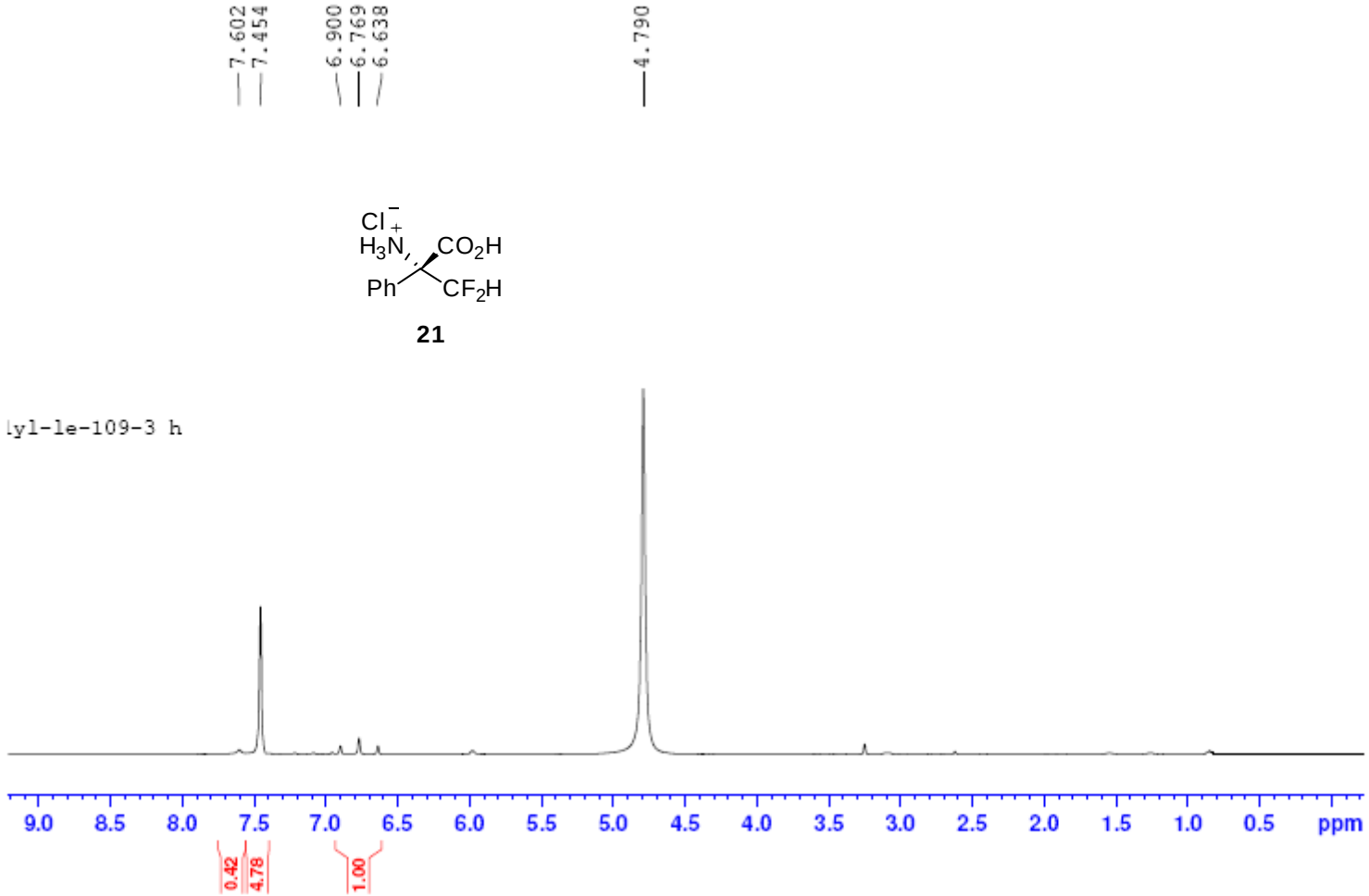
20

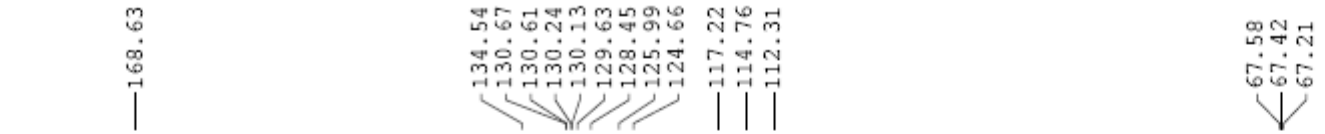


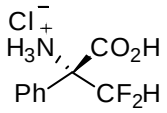

161.65
137.58
129.69
129.19
128.87
127.69
127.20
124.85
64.96
64.68
48.08
40.63
40.42
40.21
40.00
39.79
39.58
39.37
yl-le-040 c
H
N
O
NH
Ph
CF3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

20

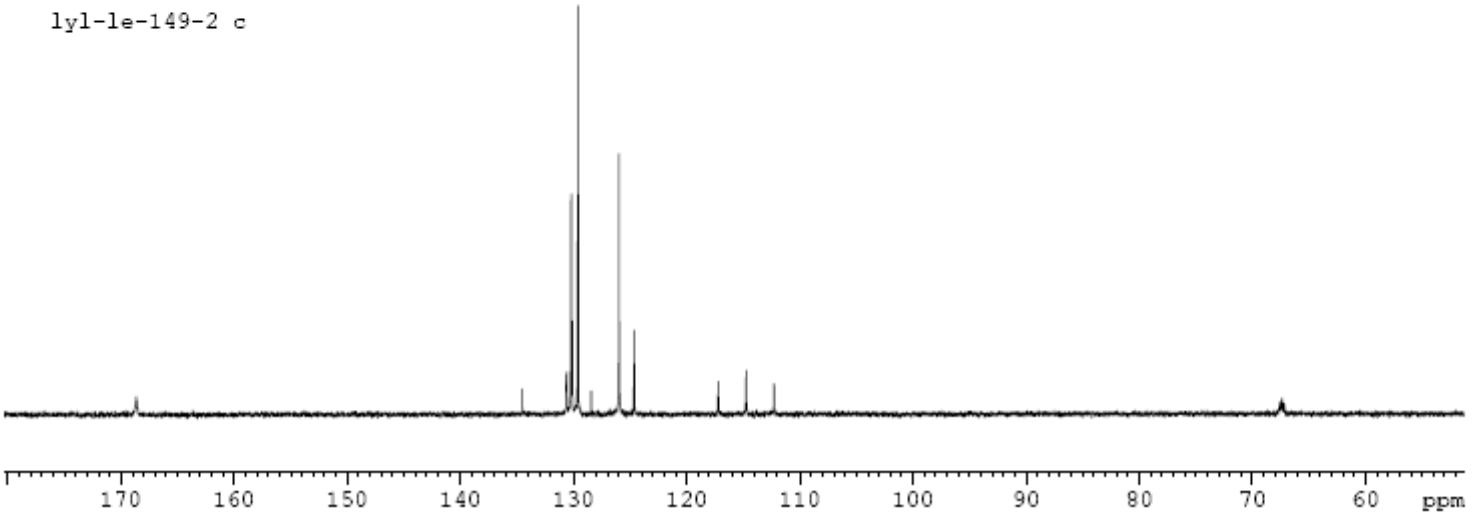

-78.99
H
N
O
NH
Ph
CF3
20
lyl-le-040 f
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm

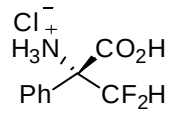

7.602
7.454
6.900
6.769
6.638
4.790
Cl⁻
H3N+
CO2H
Ph
CF2H
21
lyl-le-109-3 h
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.42
4.78
1.00


168.63
134.54
130.67
130.61
130.24
130.13
129.63
128.45
125.99
124.66
117.22
114.76
112.31
67.58
67.42
67.21


Cl⁻
H3N+
CO2H
Ph
CF2H

21


lyl-le-149-2 c
170
160
150
140
130
120
110
100
90
80
70
60
ppm



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lyl-le-109-3 f