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

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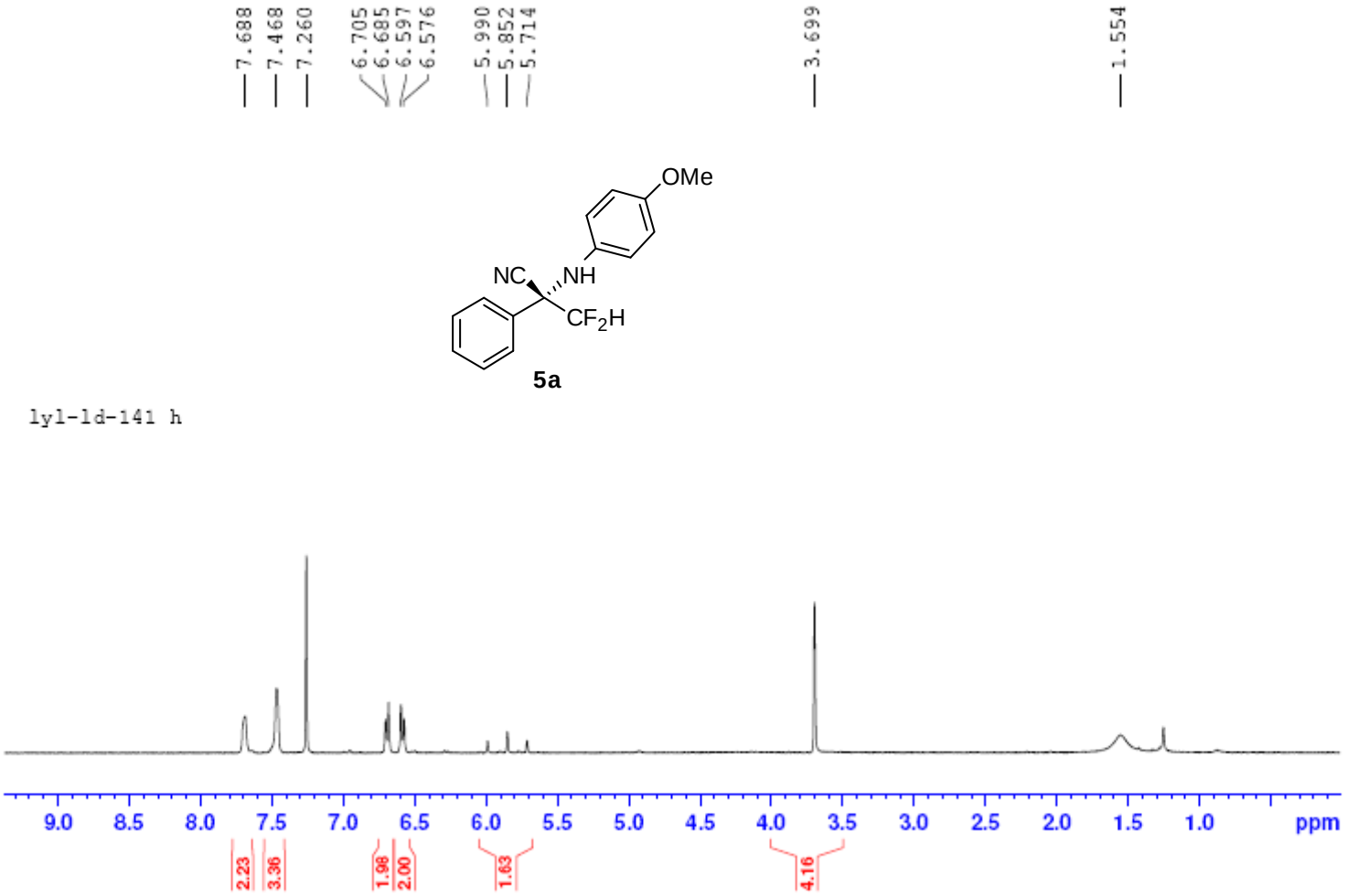
Supporting Information

(Part II)

^{1}H, ^{13}C NMR and ^{19}F NMR spectra of α-CF_2H α-tetrasubstituted α-aminonitriles 5a-p

^{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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OMe
NC
NH
CF2H
5a
lyl-ld-141 h
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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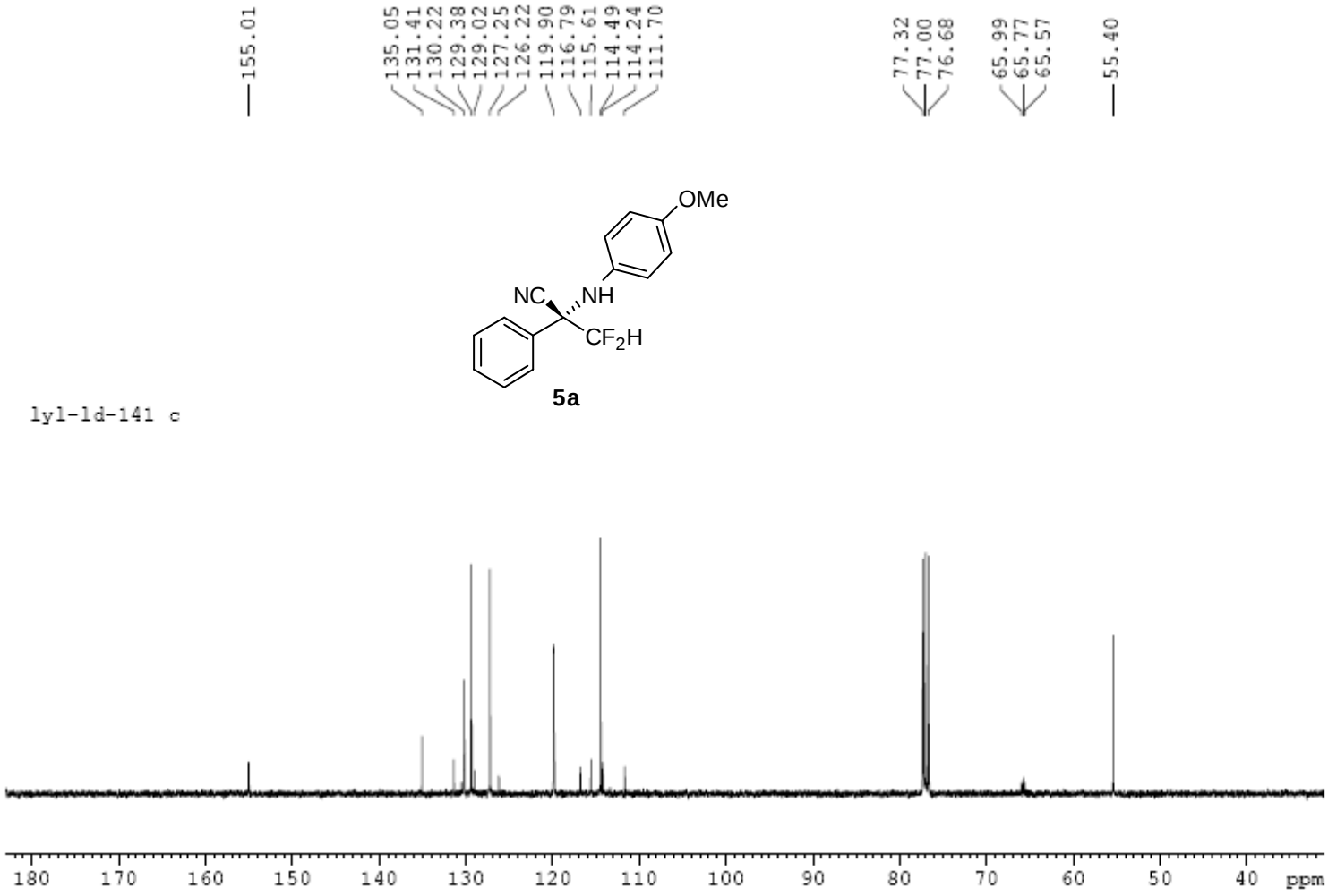
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111.70
77.32
77.00
76.68
65.99
65.77
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55.40
OMe
NC
NH
CF2H
5a
lyl-ld-141 c
180
170
160
150
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40
ppm

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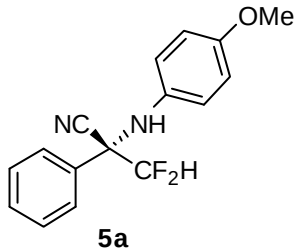
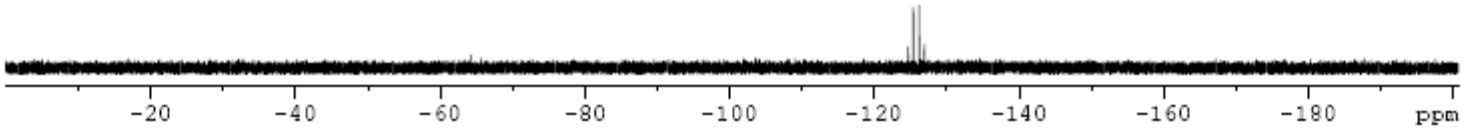
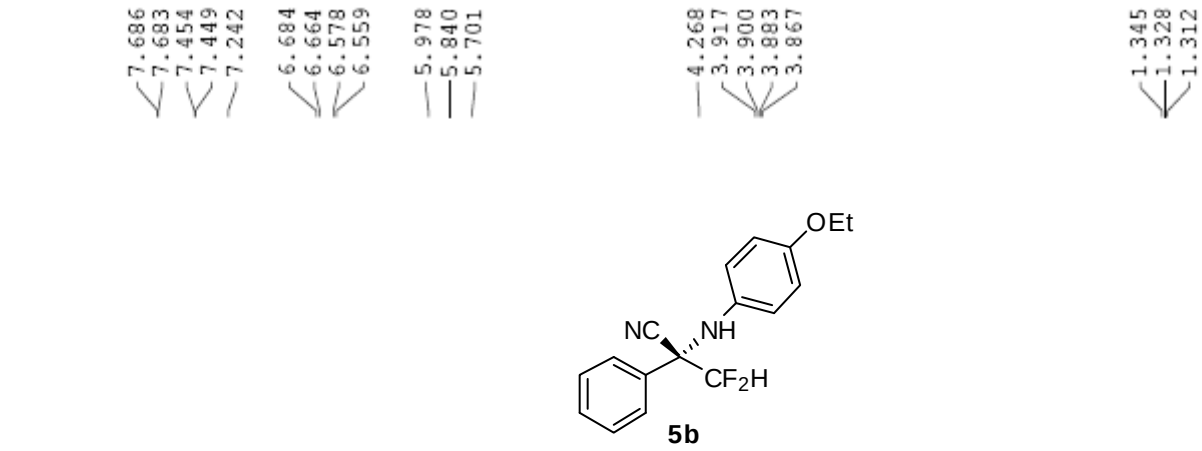
-126.96



5a

lyl-le-048-3 f

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CF2H
5b
lyl-le-076-2 h
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7.0
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6.0
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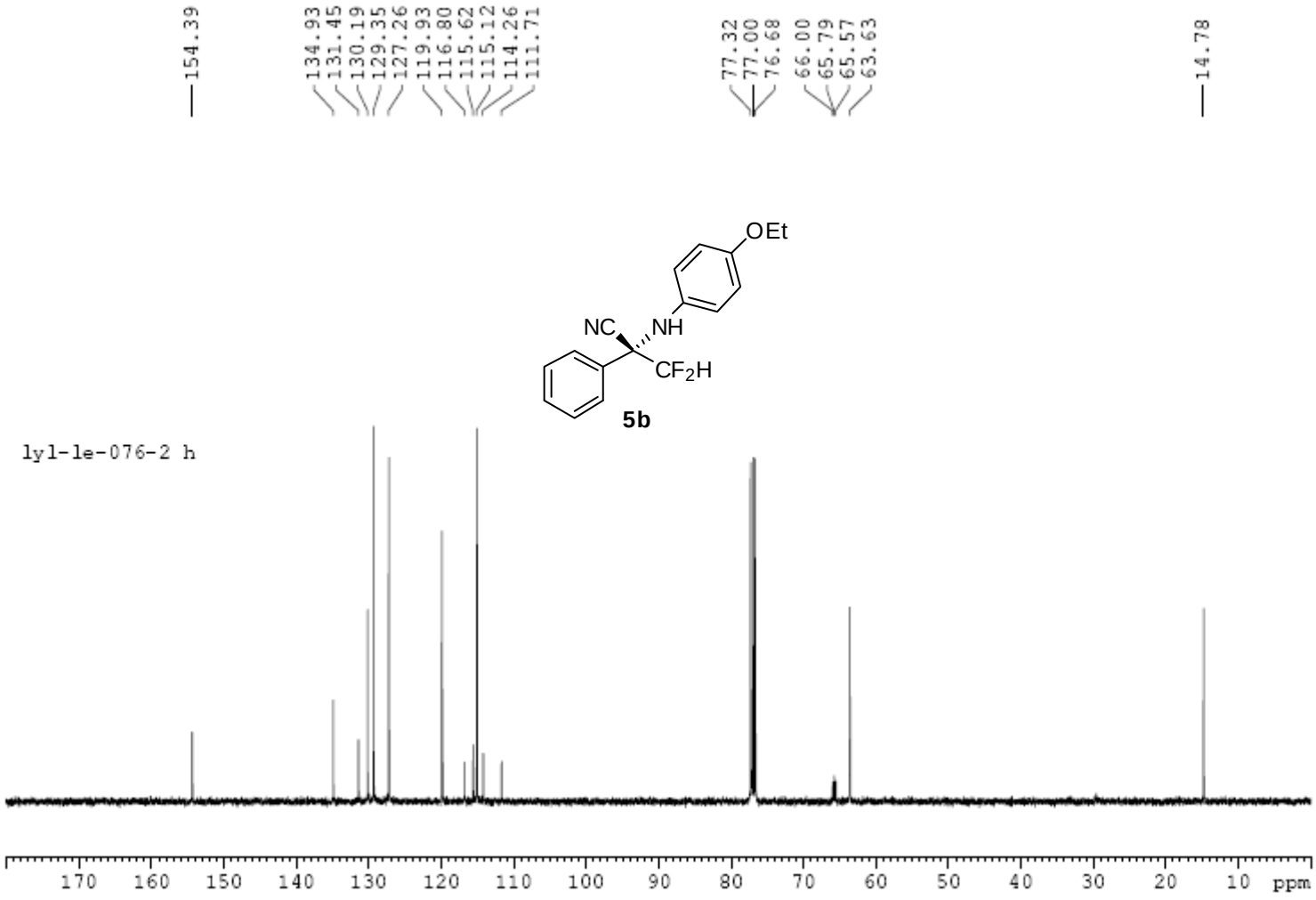
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76.68
66.00
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14.78
OEt
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NH
CF2H
5b
lyl-le-076-2 h
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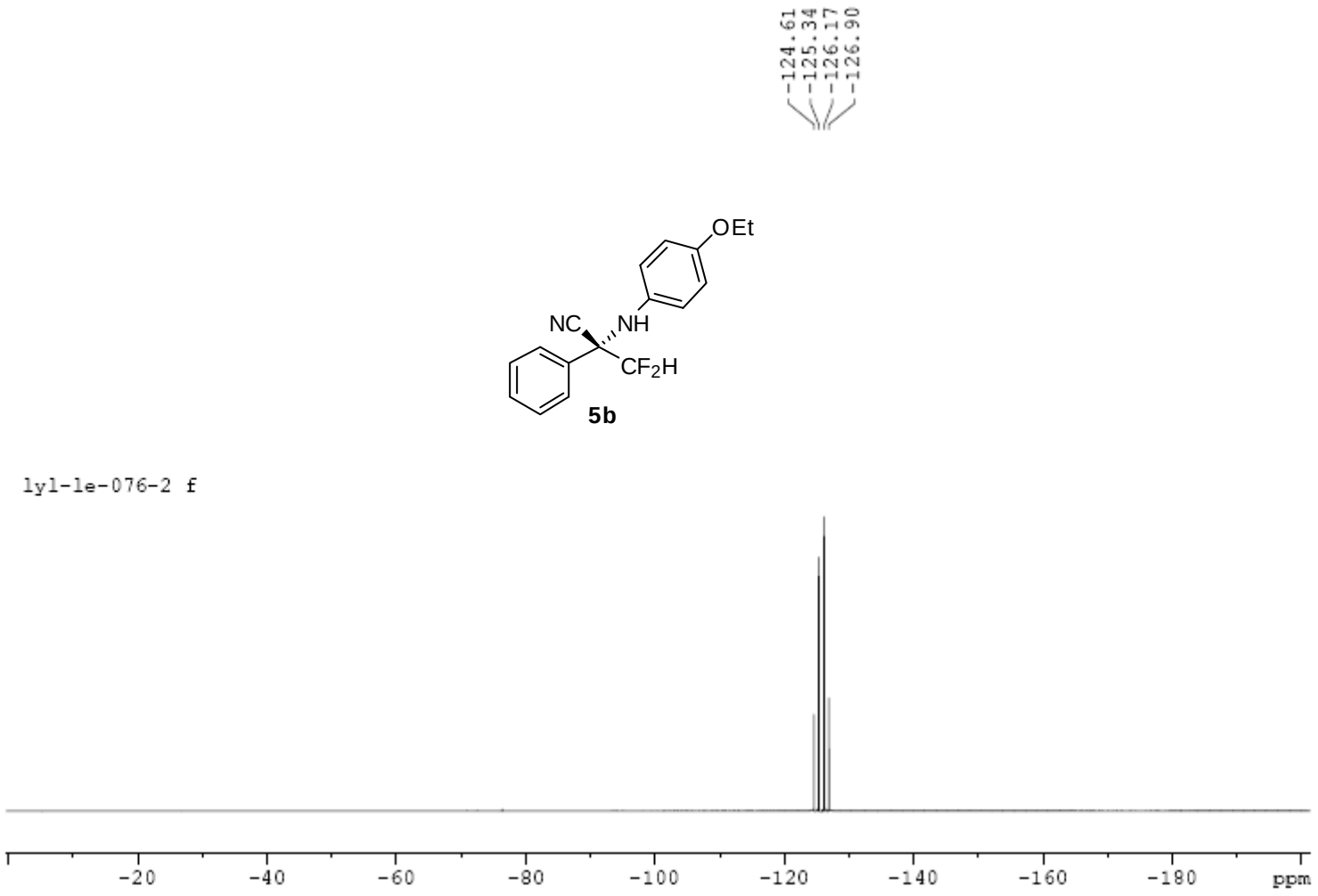
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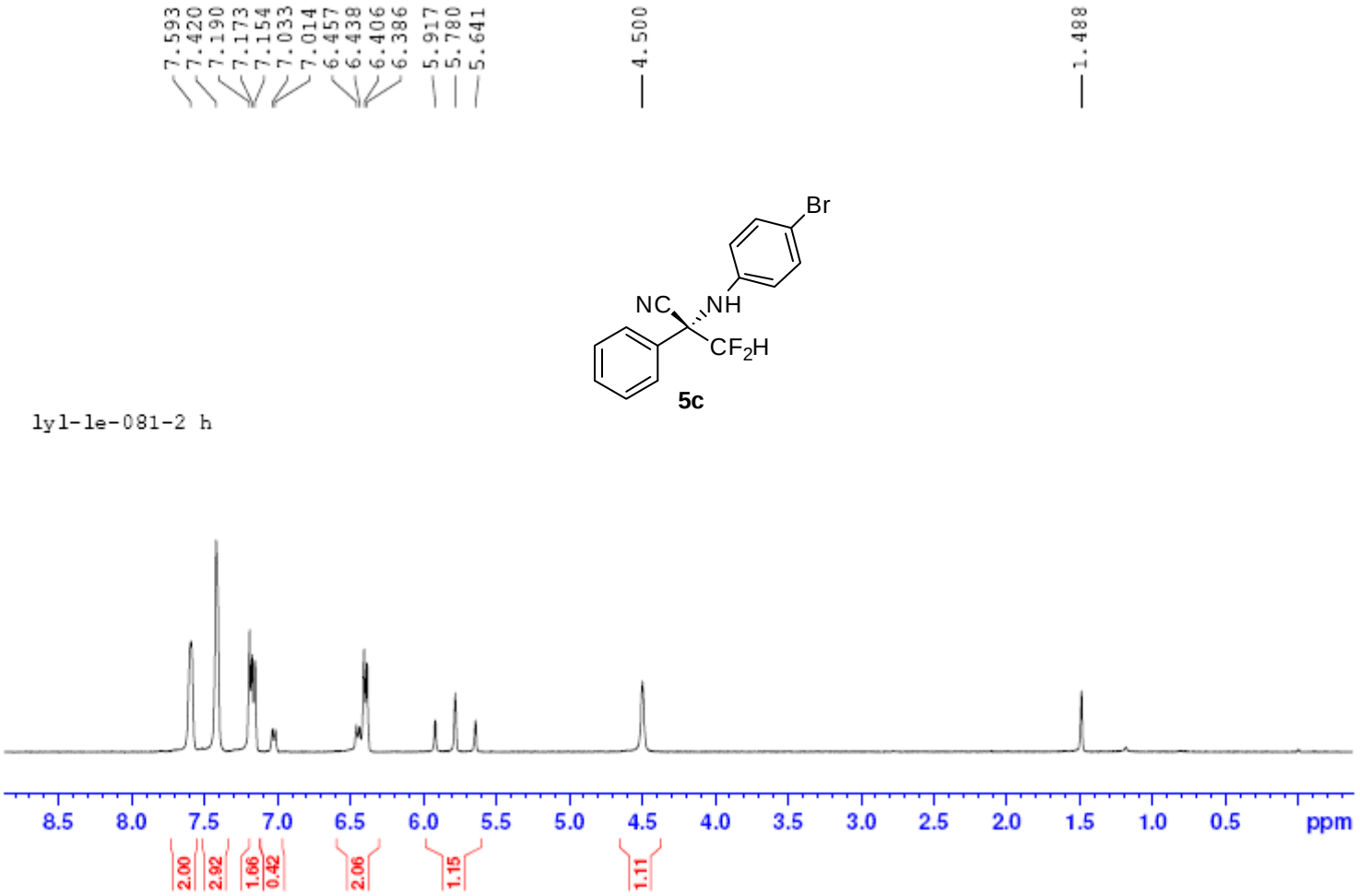
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5c
lyl-le-081-2 h
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7.5
7.0
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6.0
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5.0
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4.0
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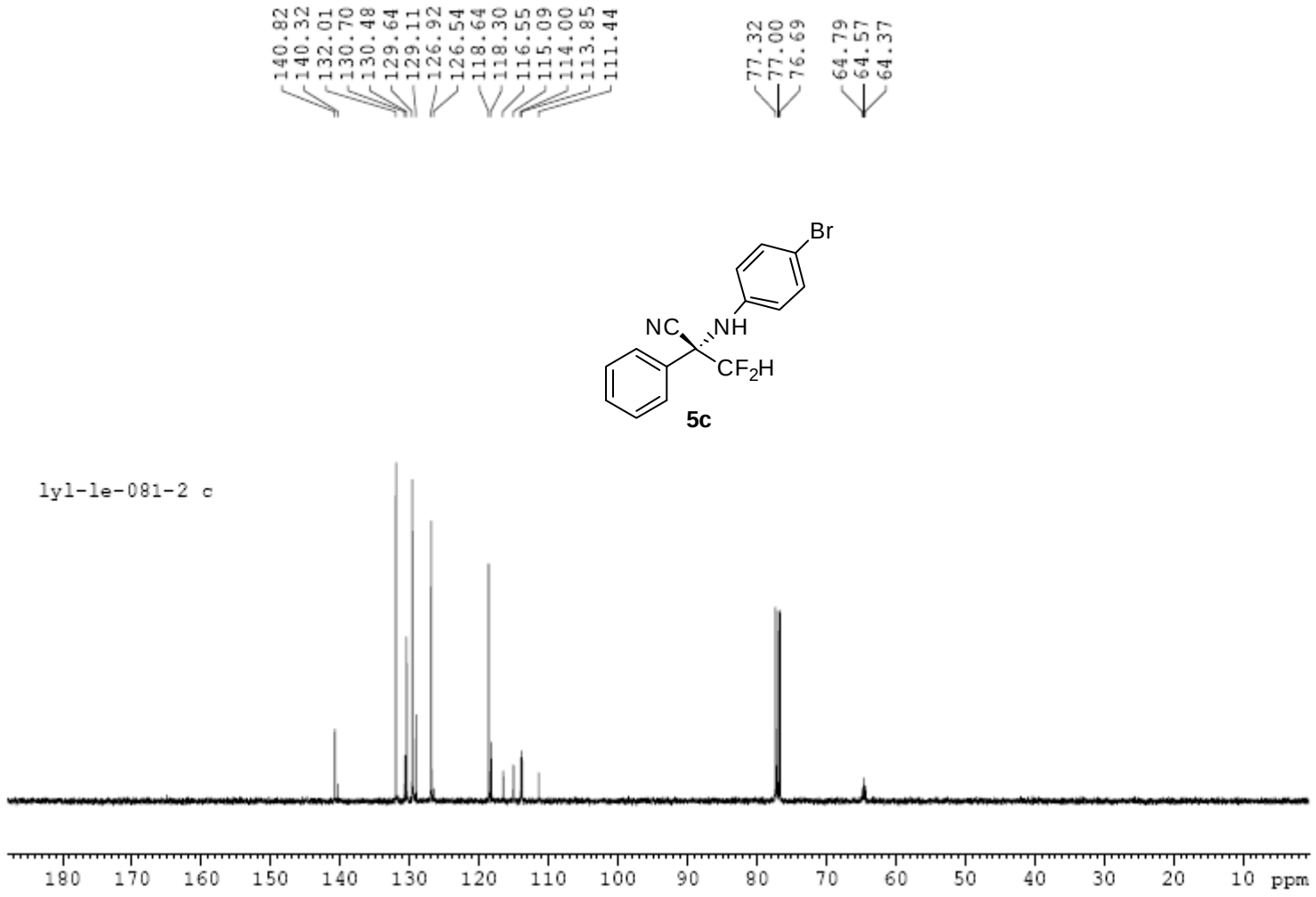
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CF2H
5c
lyl-le-081-2 c
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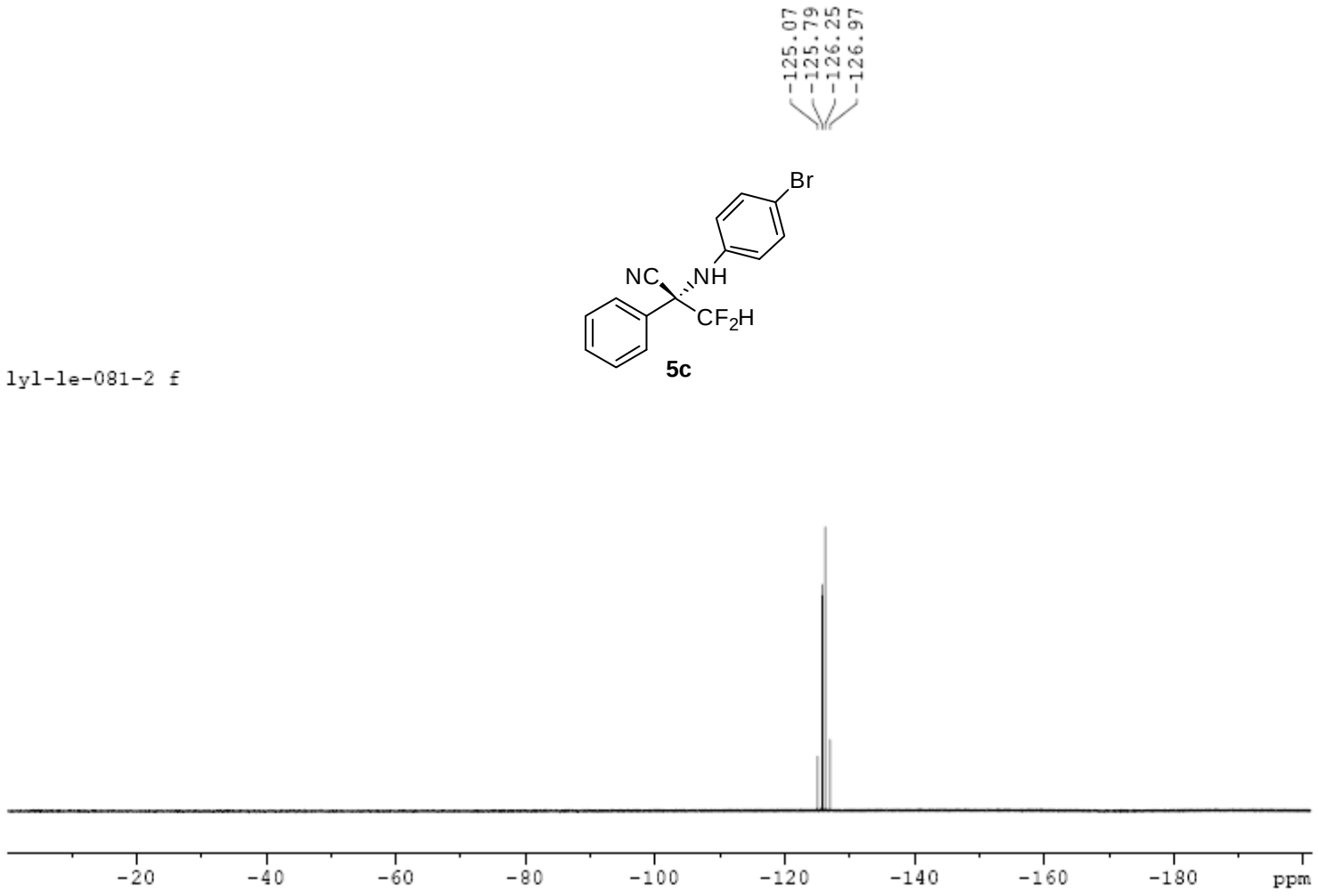
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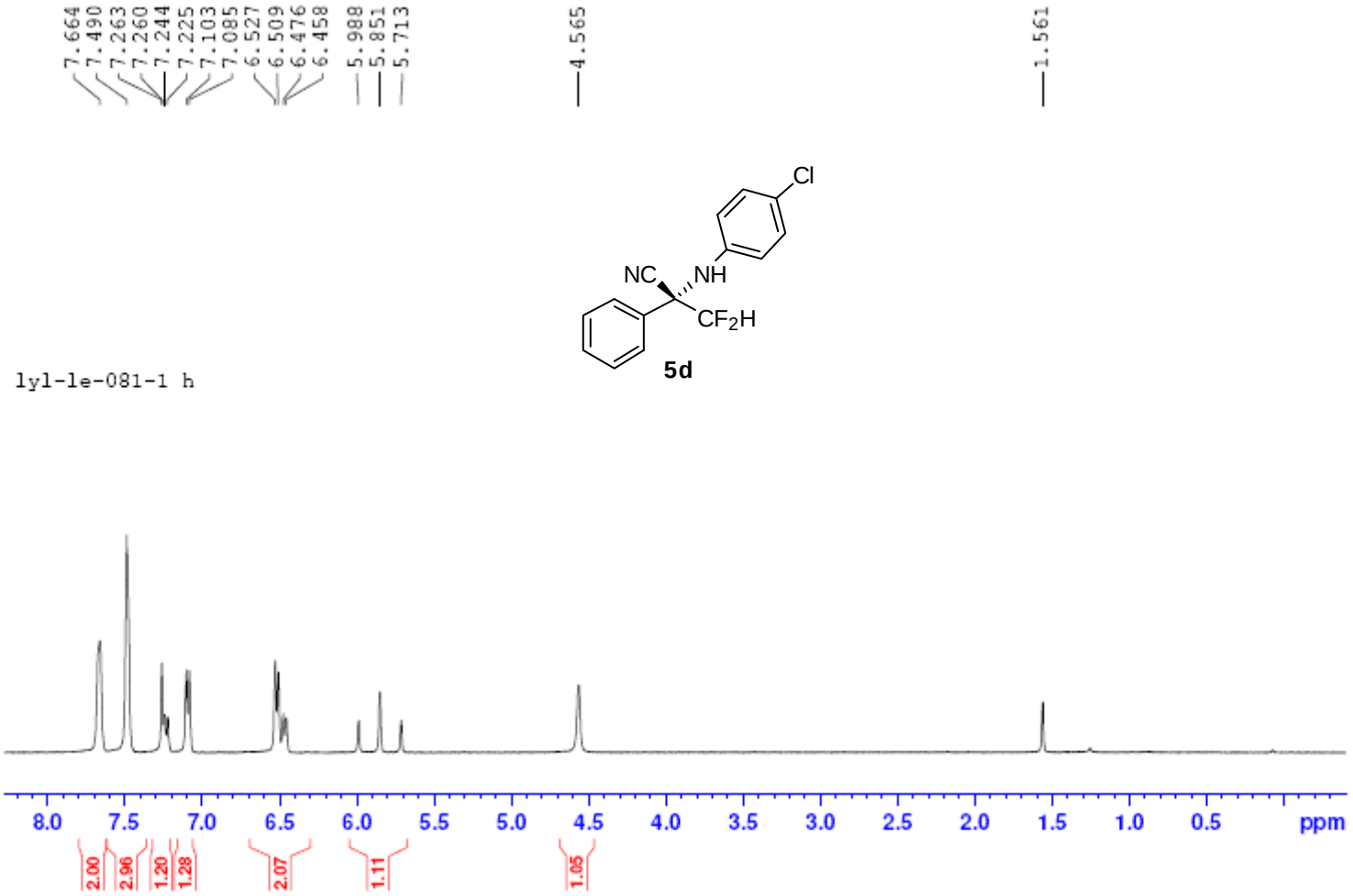
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lyl-le-081-1 h
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6.0
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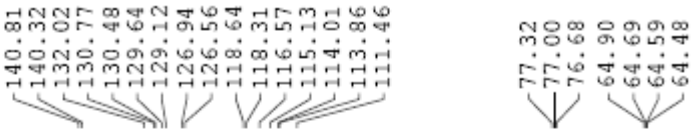
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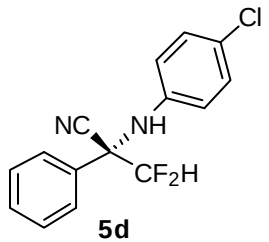
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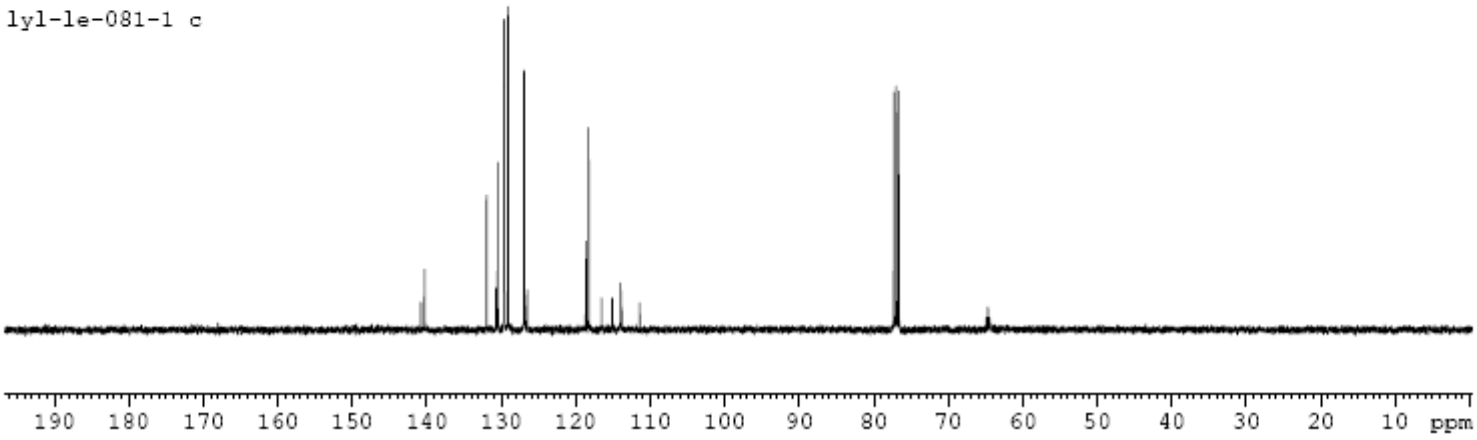
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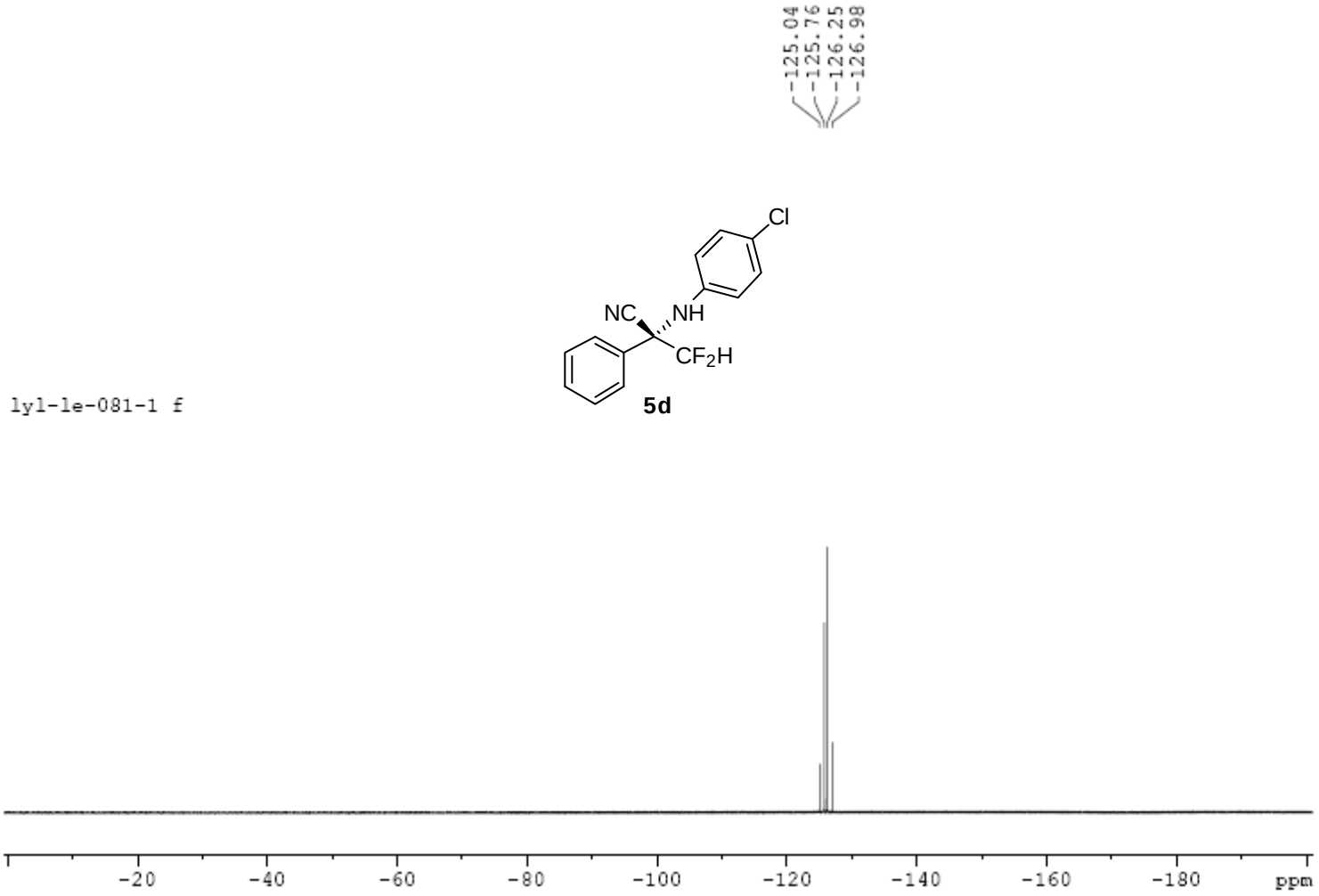
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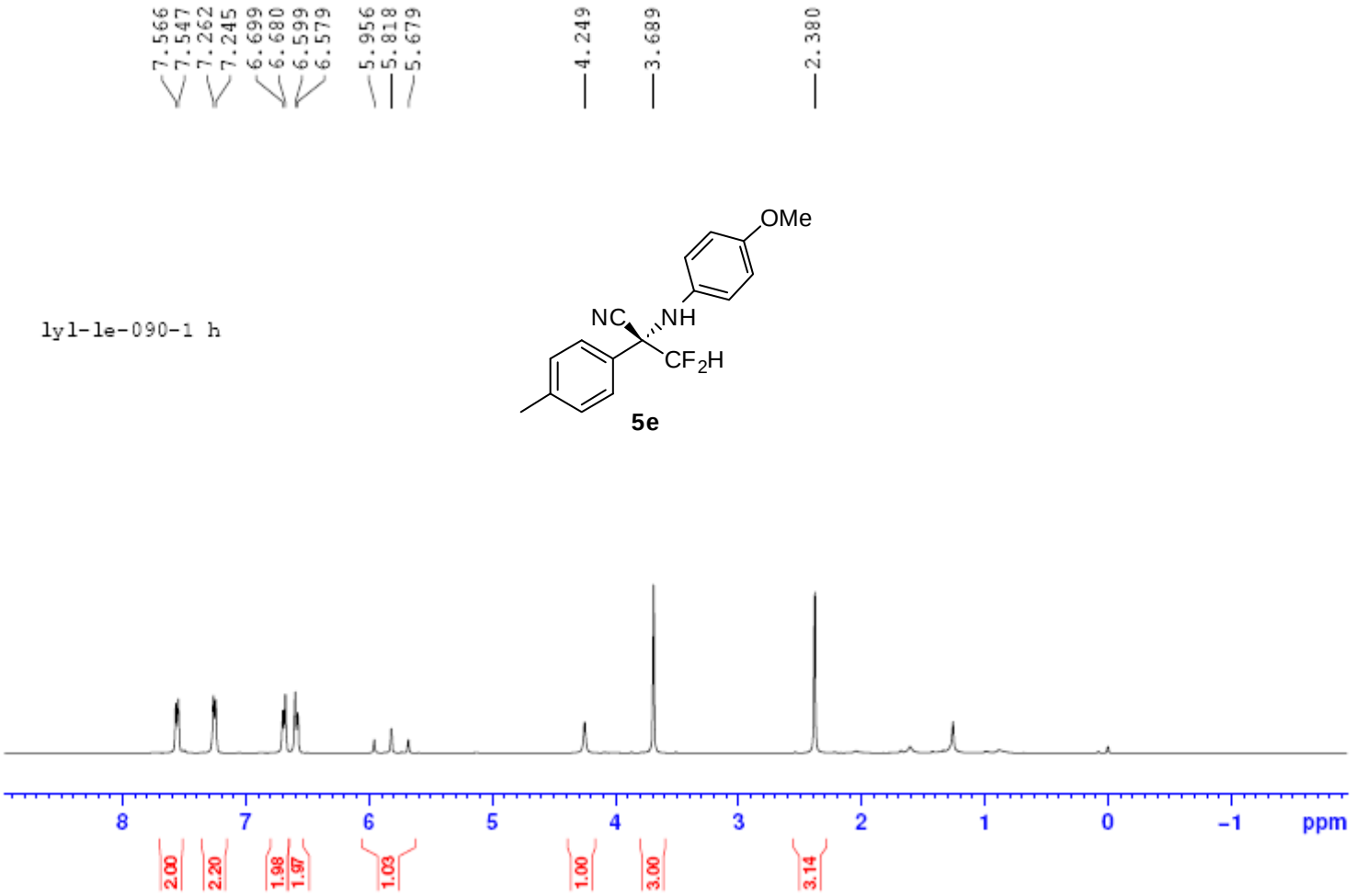
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lyl-le-090-1 h
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NH
CF2H
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7
6
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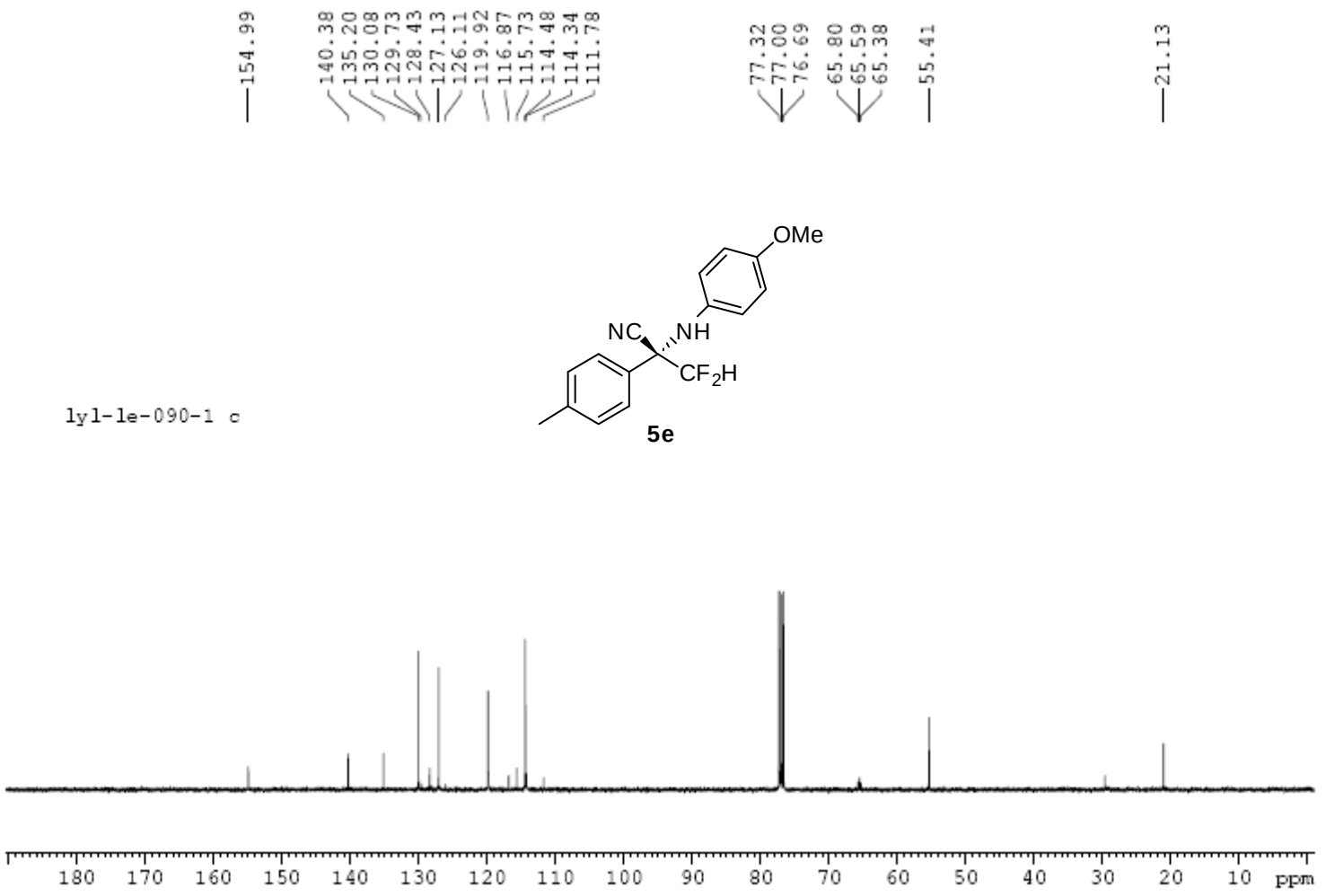
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lyl-le-090-1 c
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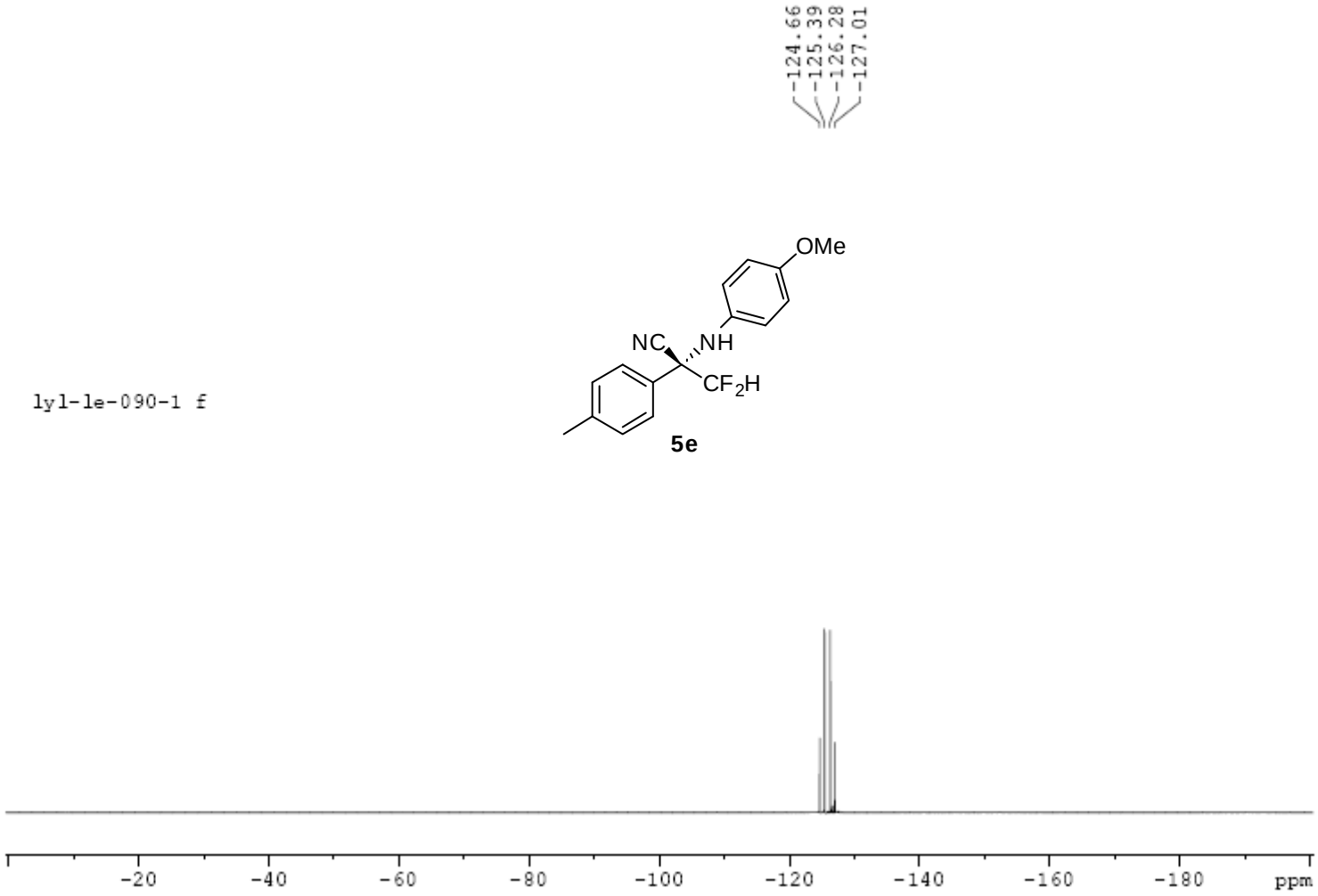
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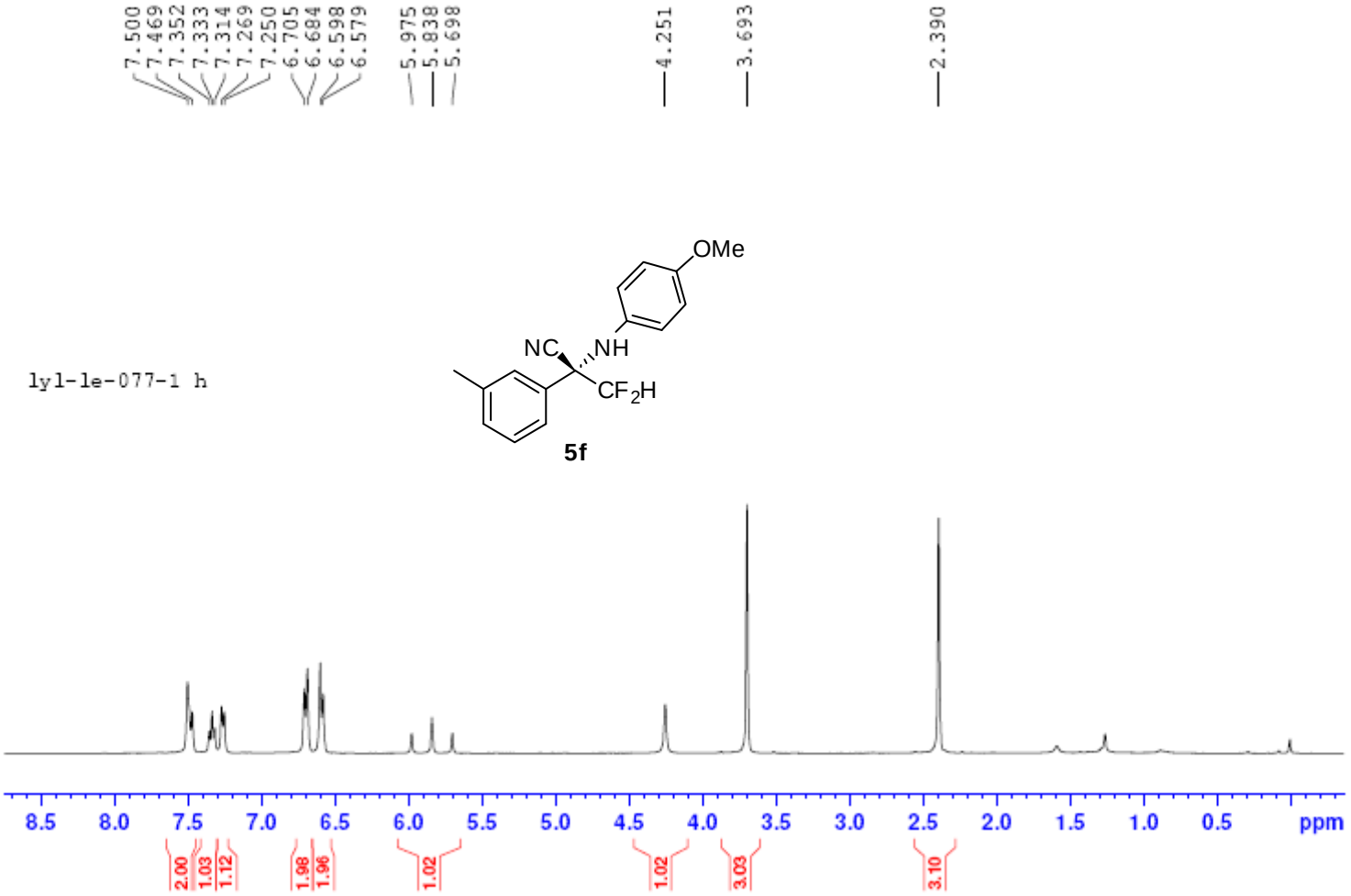
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lyl-le-077-1 h
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CF2H
5f
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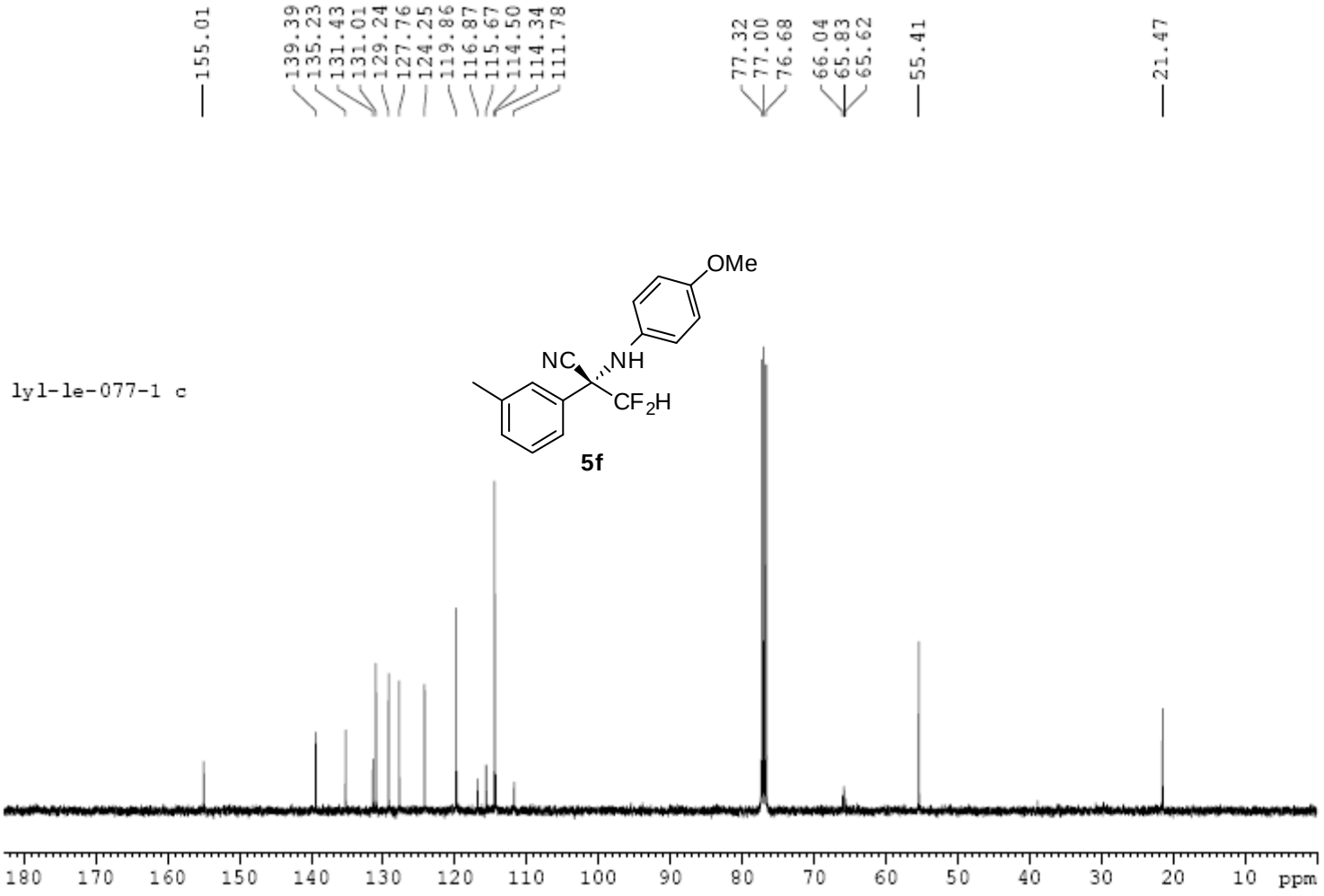
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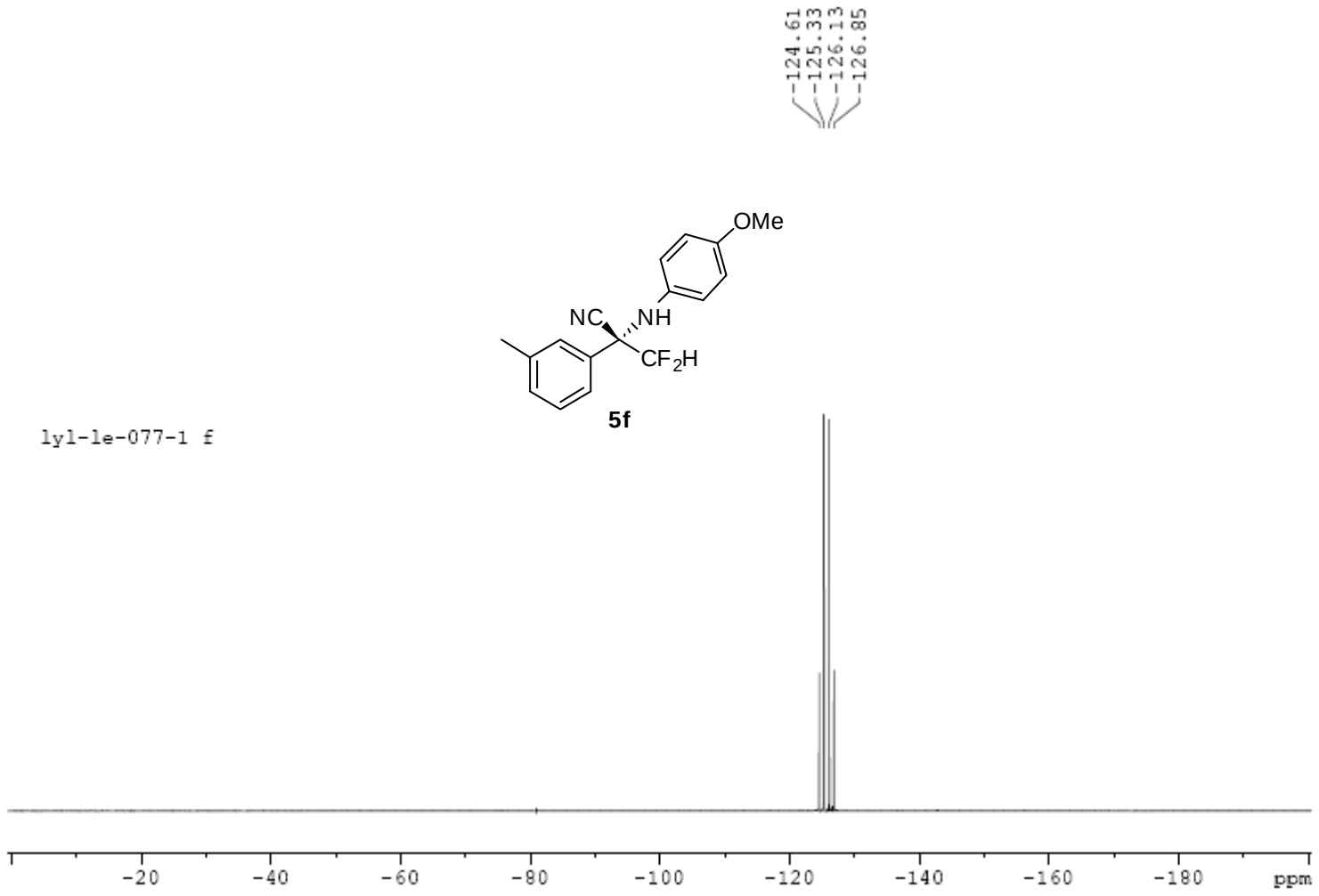
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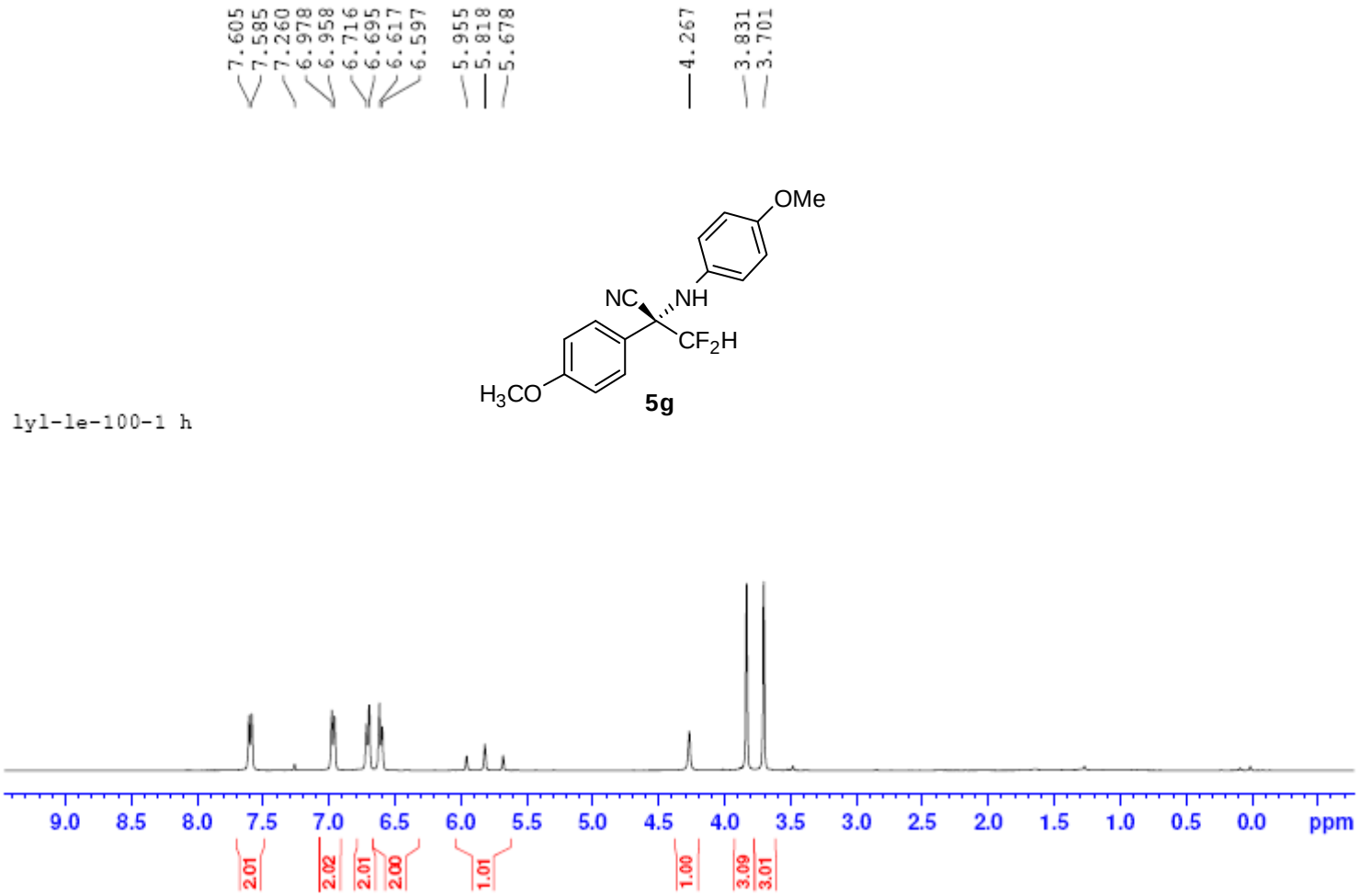
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CF2H
H3CO
5g
lyl-le-100-1 h
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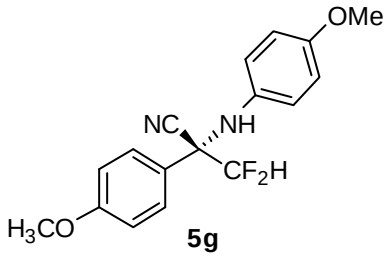

5g

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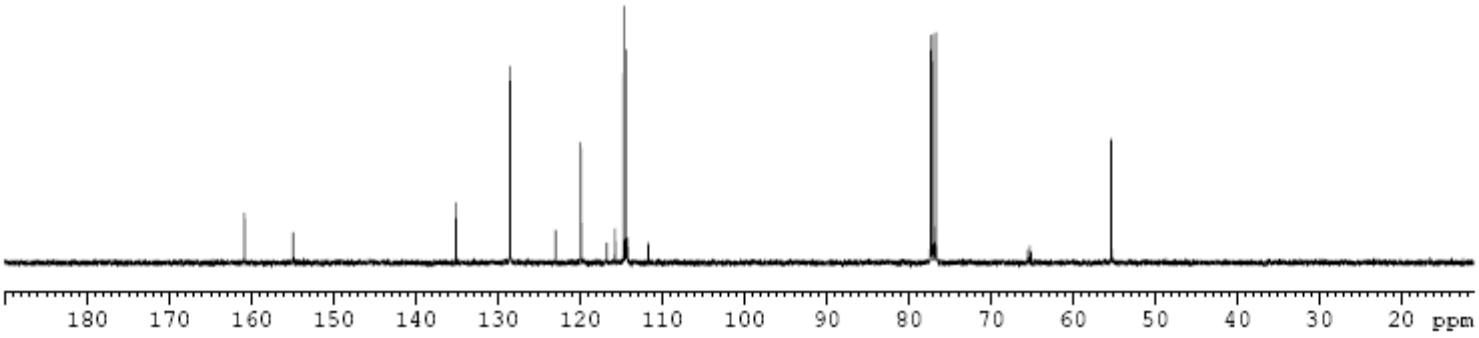

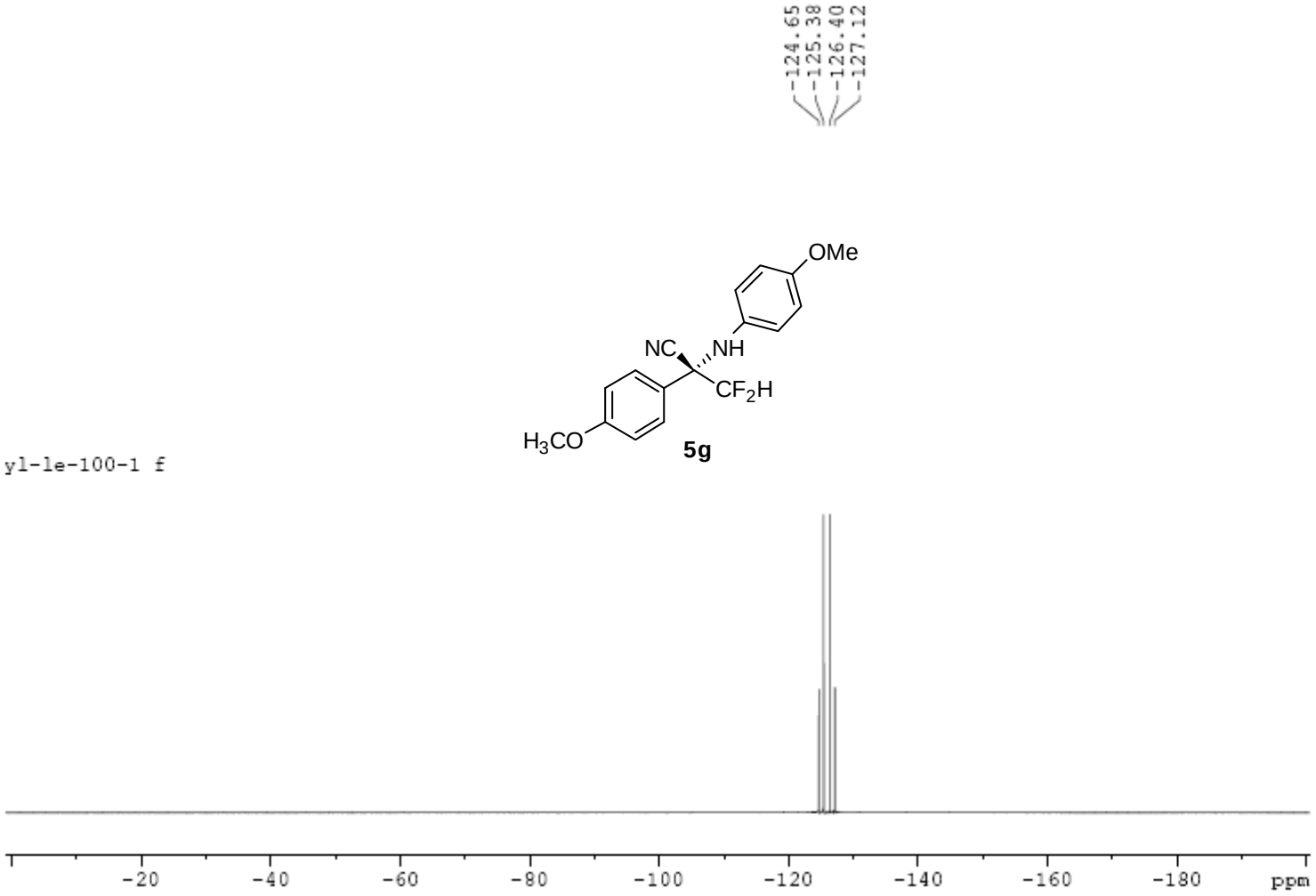
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yl-le-100-1 f
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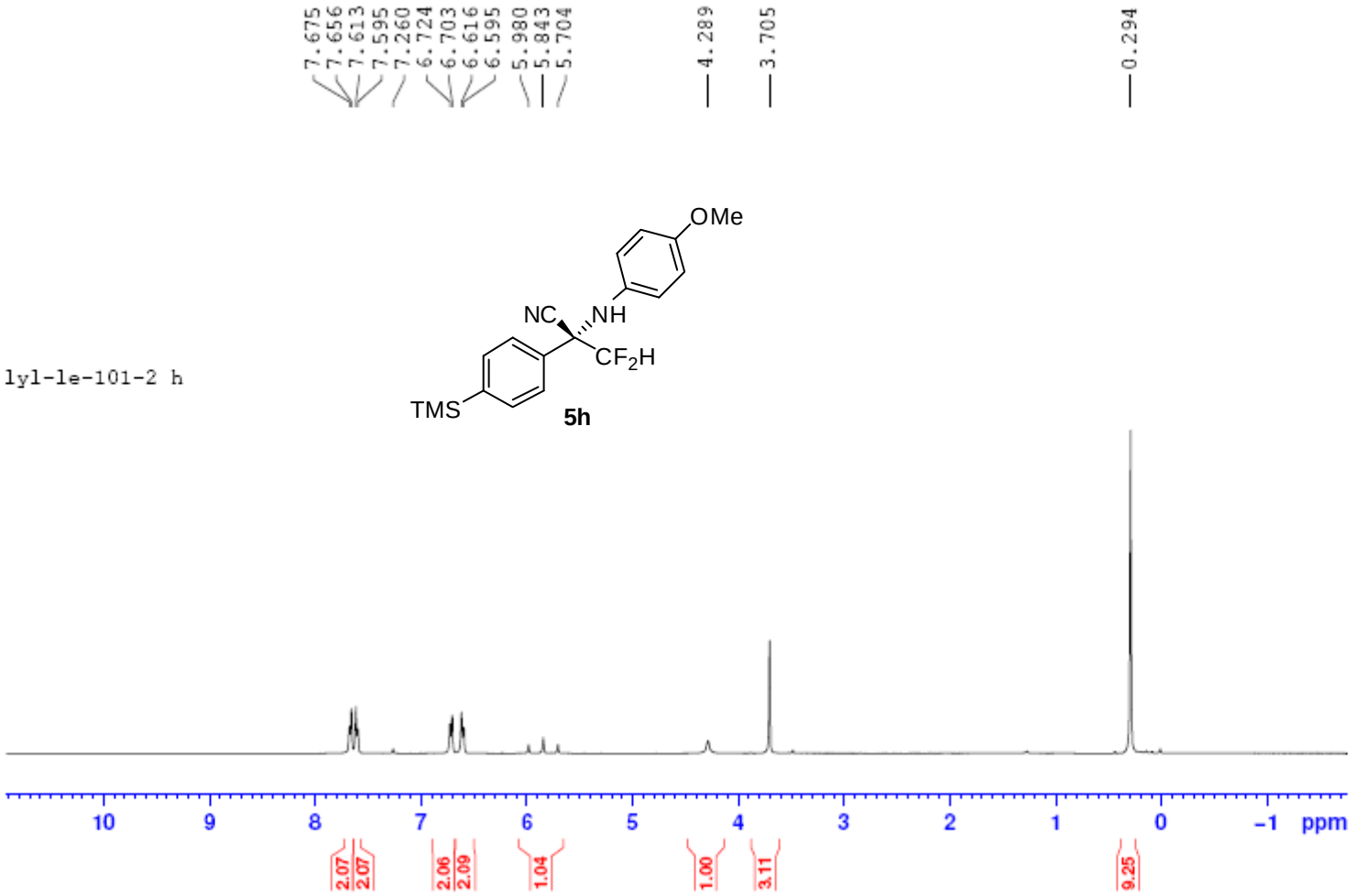
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TMS
5h
lyl-le-101-2 h
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8
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6
5
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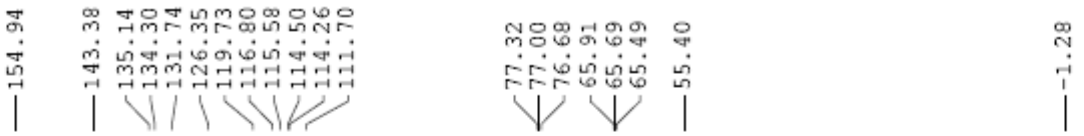
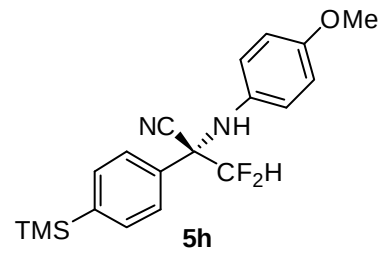
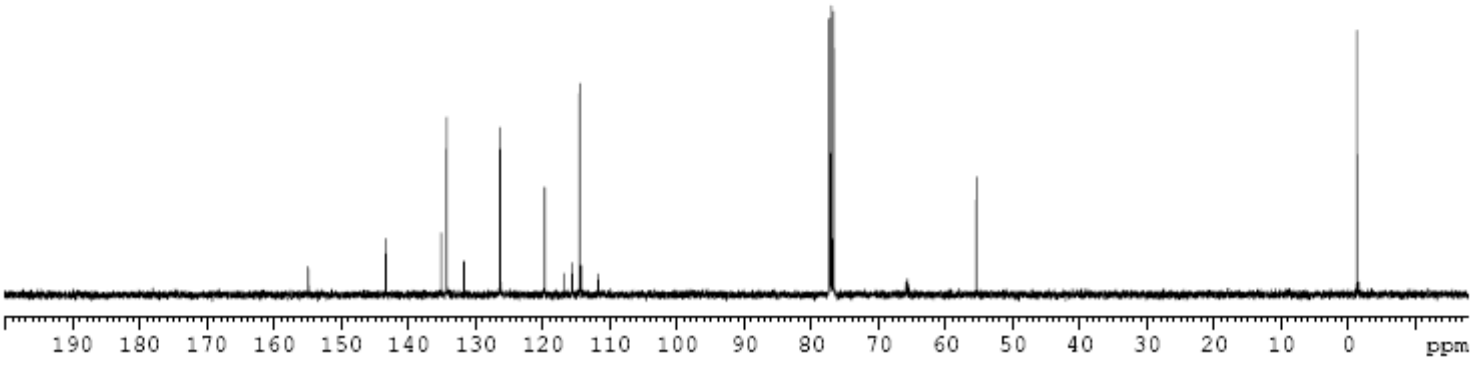
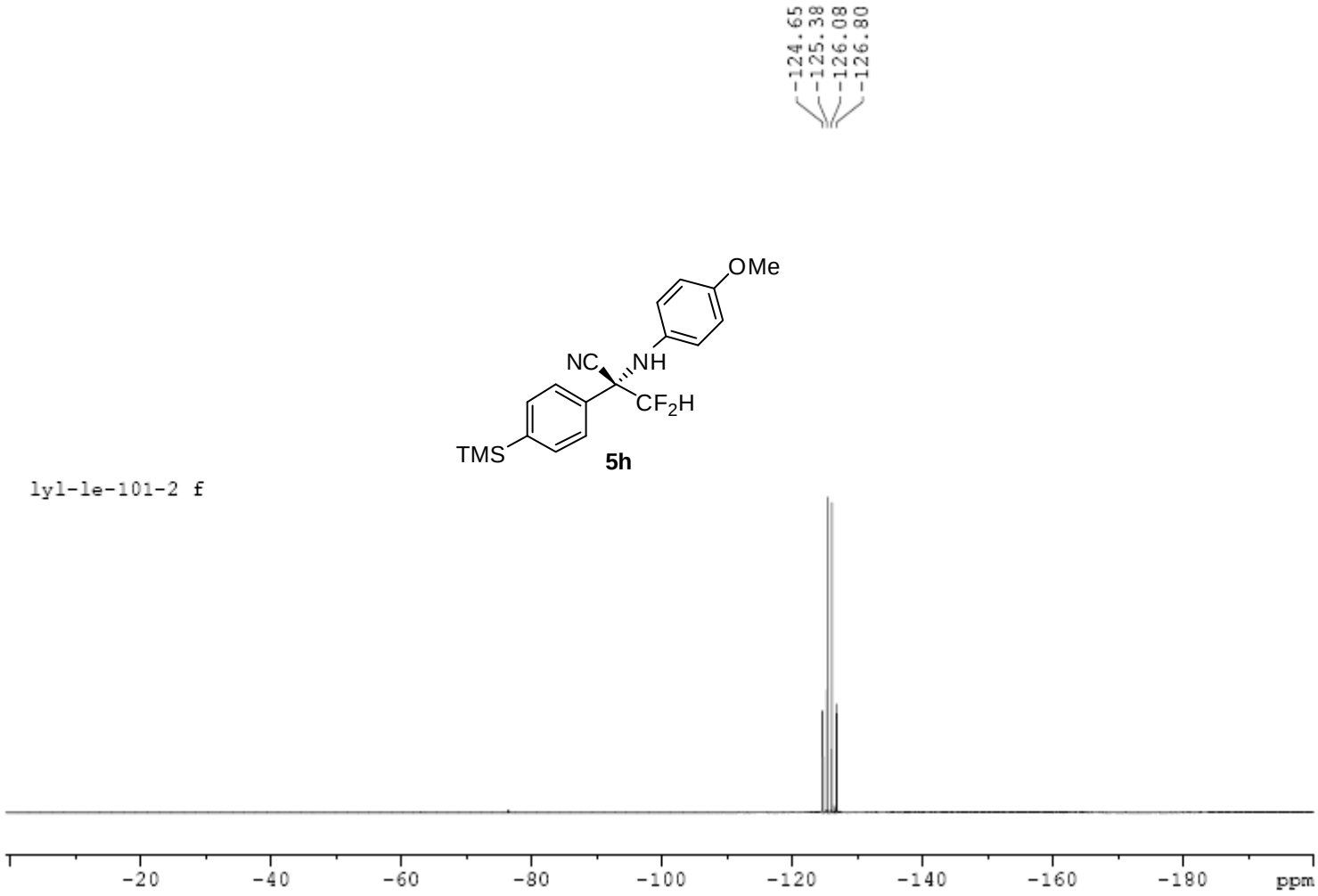




5h

lyl-le-101-2 c

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CF2H
TMS
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lyl-le-101-2 f
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-60
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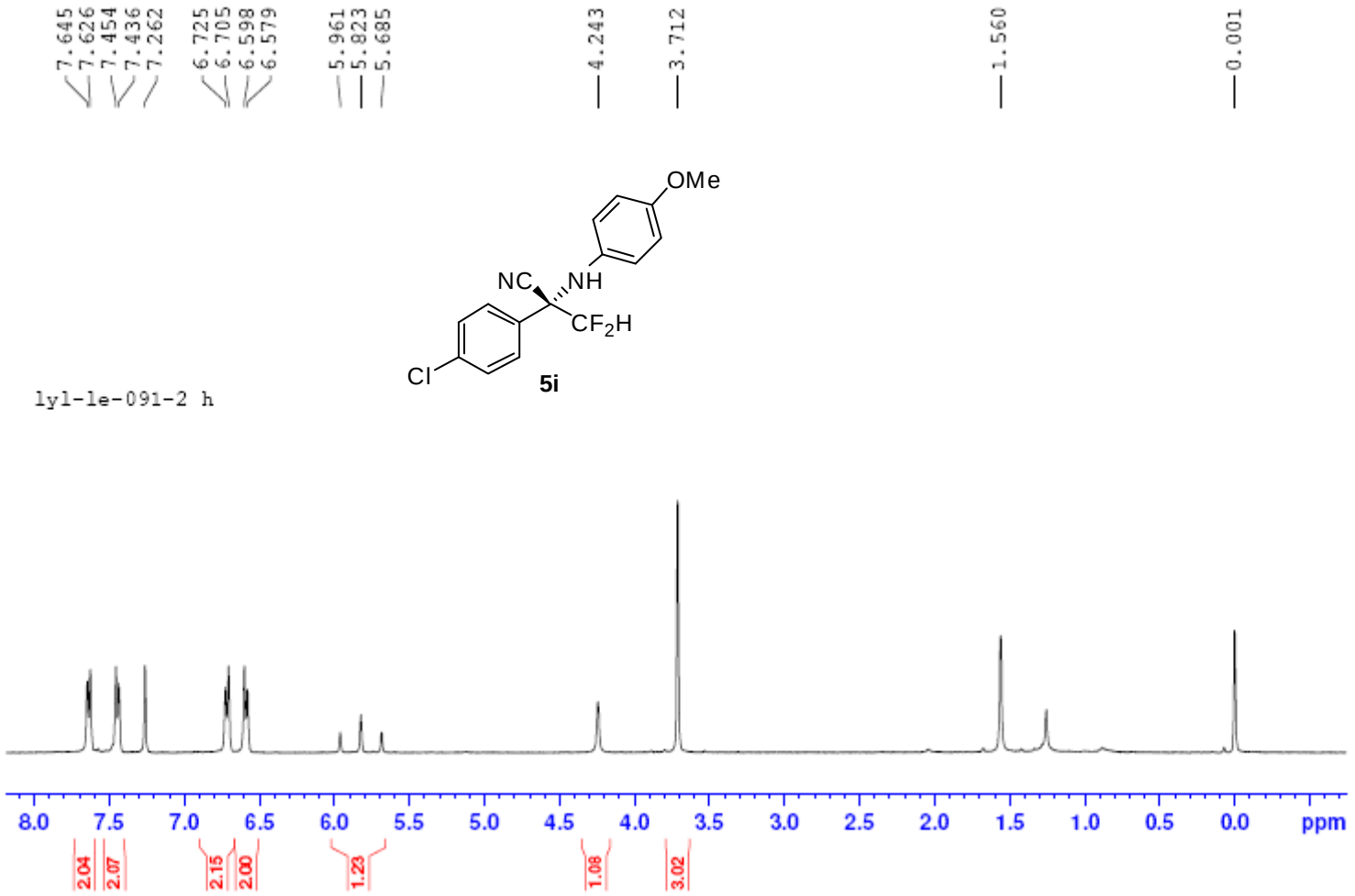
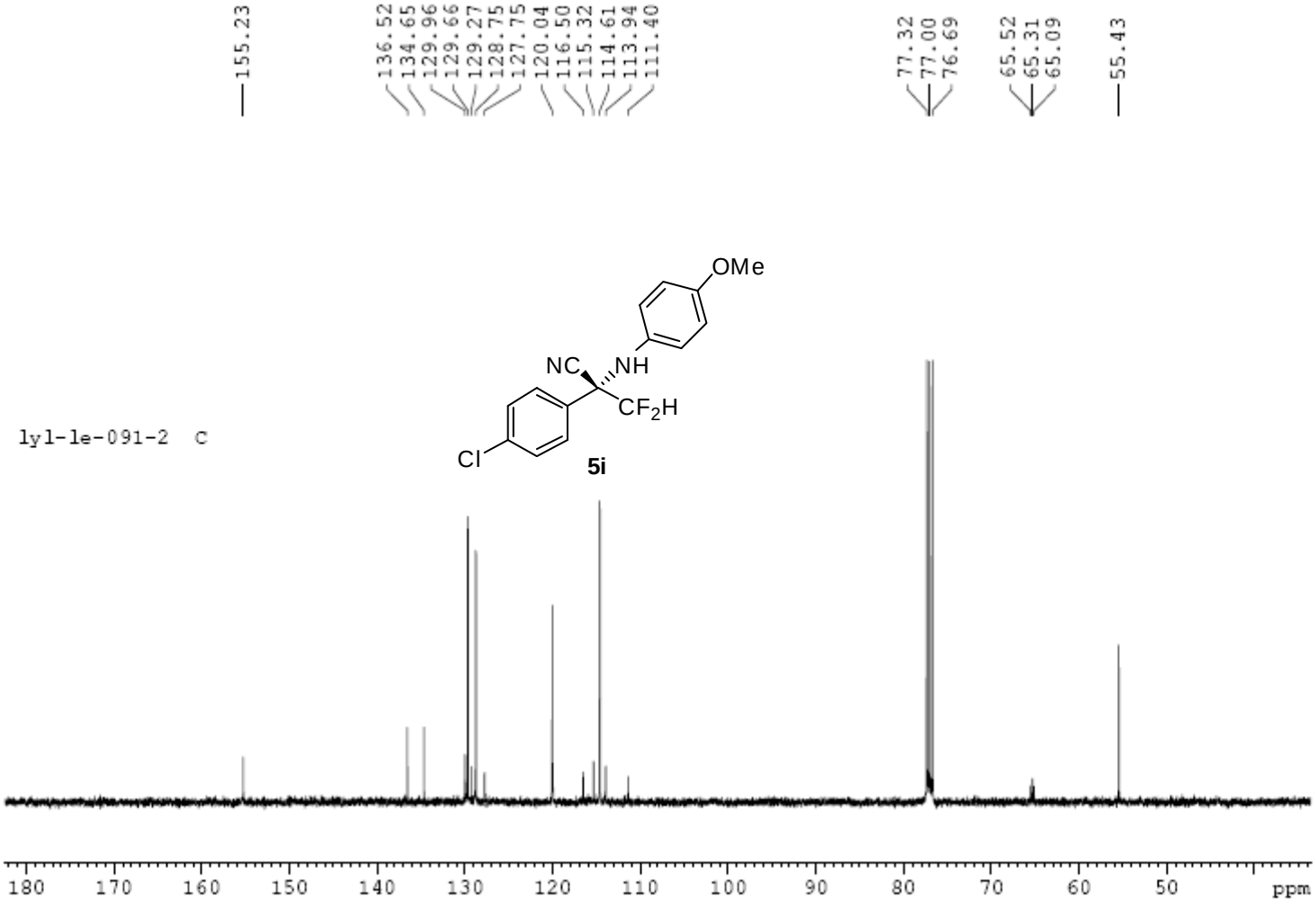
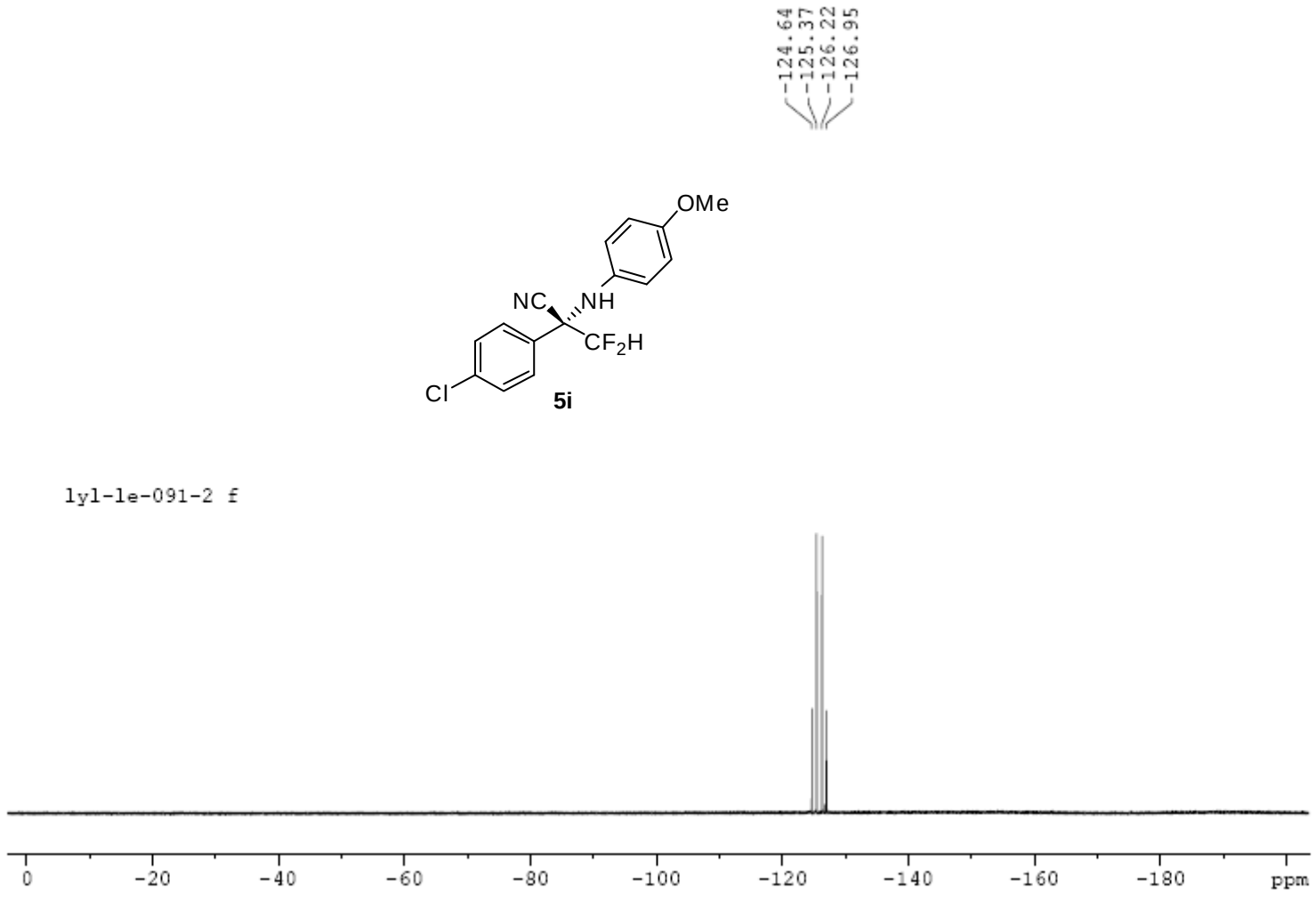
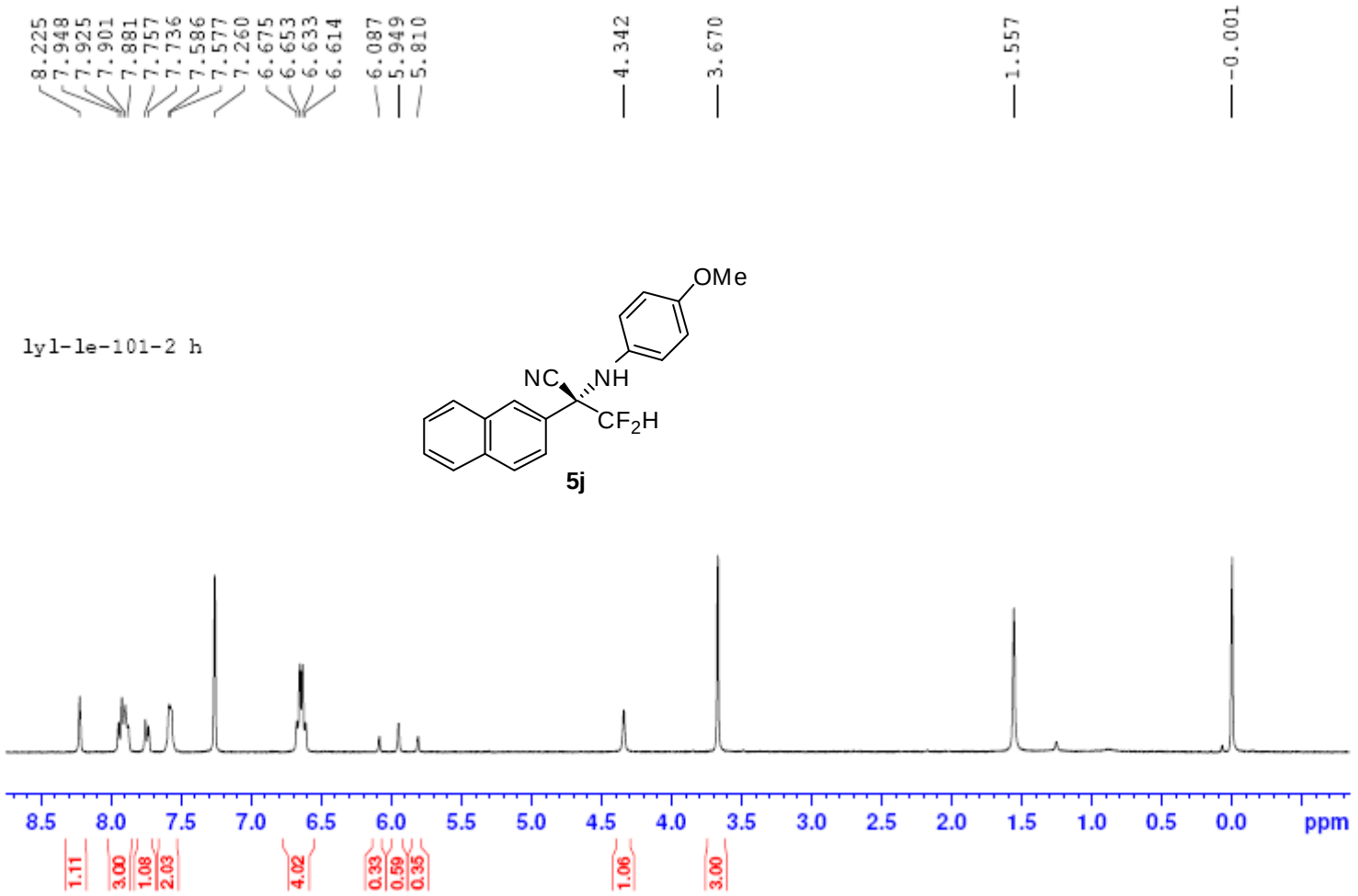
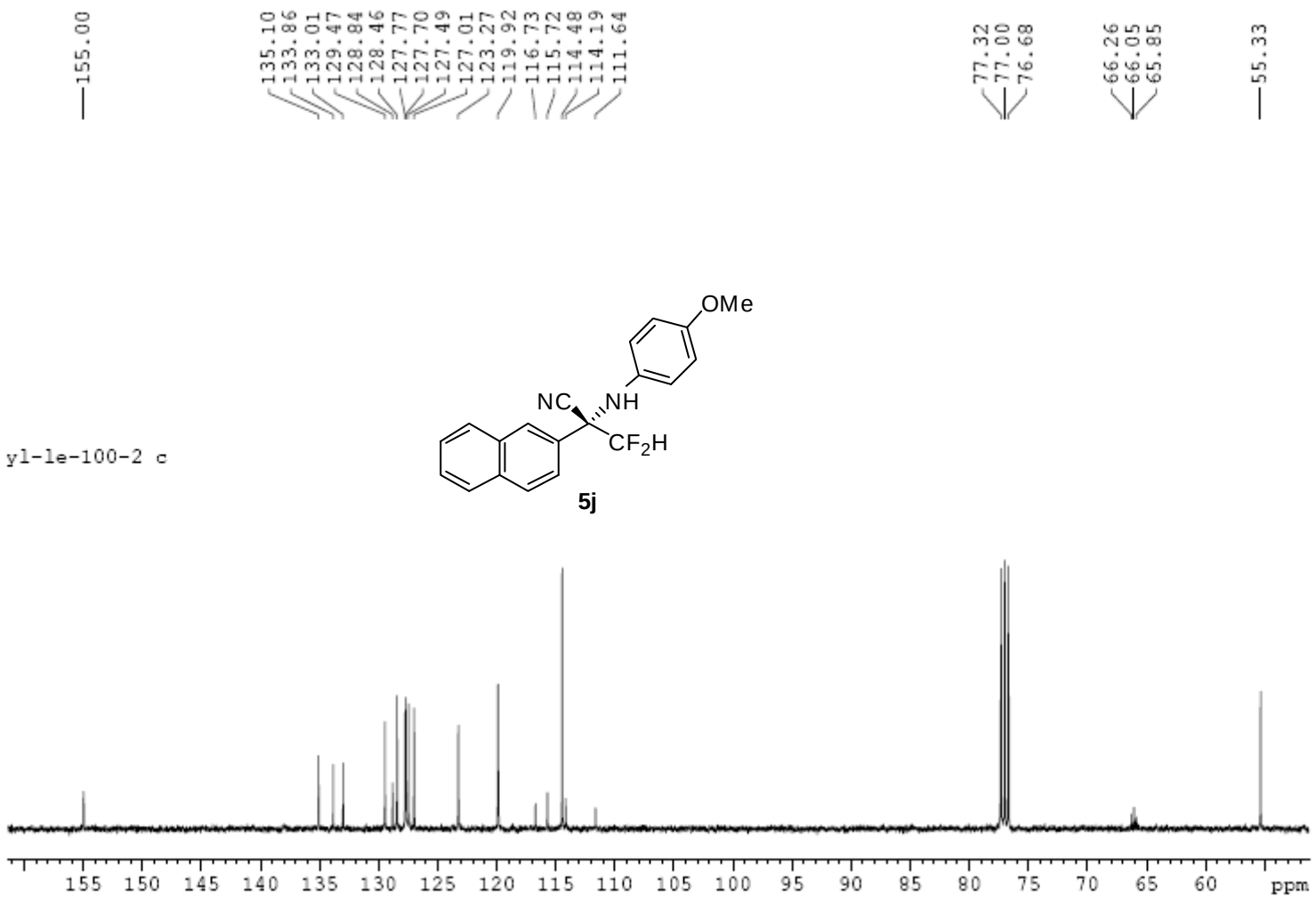
-140
-160
-180
ppm

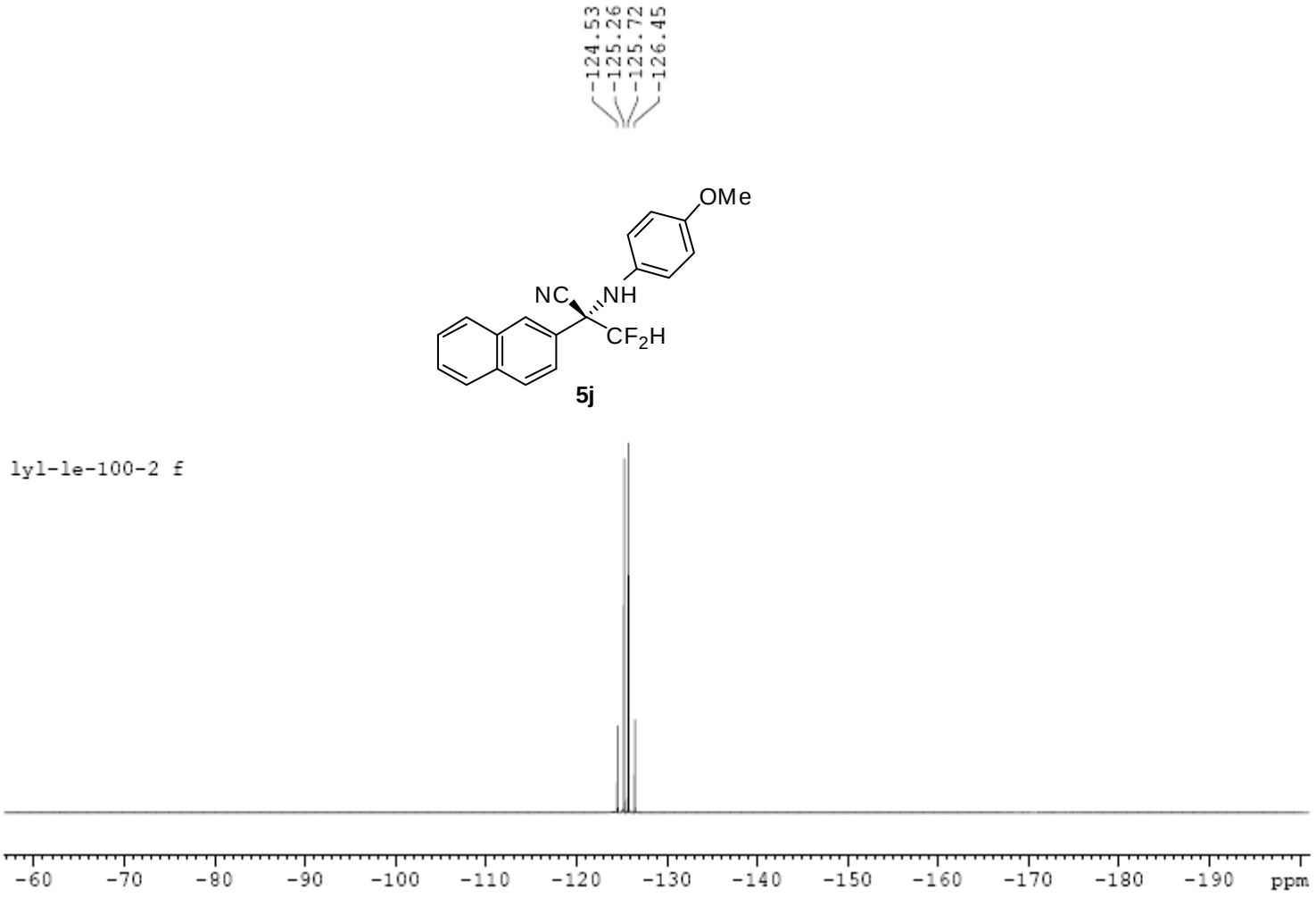

7.645
7.626
7.454
7.436
7.262
6.725
6.705
6.598
6.579
5.961
5.823
5.685
4.243
3.712
1.560
0.001
OMe
NC
NH
CF2H
Cl
5i
lyl-le-091-2 h
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.04
2.07
2.15
2.00
1.23
1.08
3.02

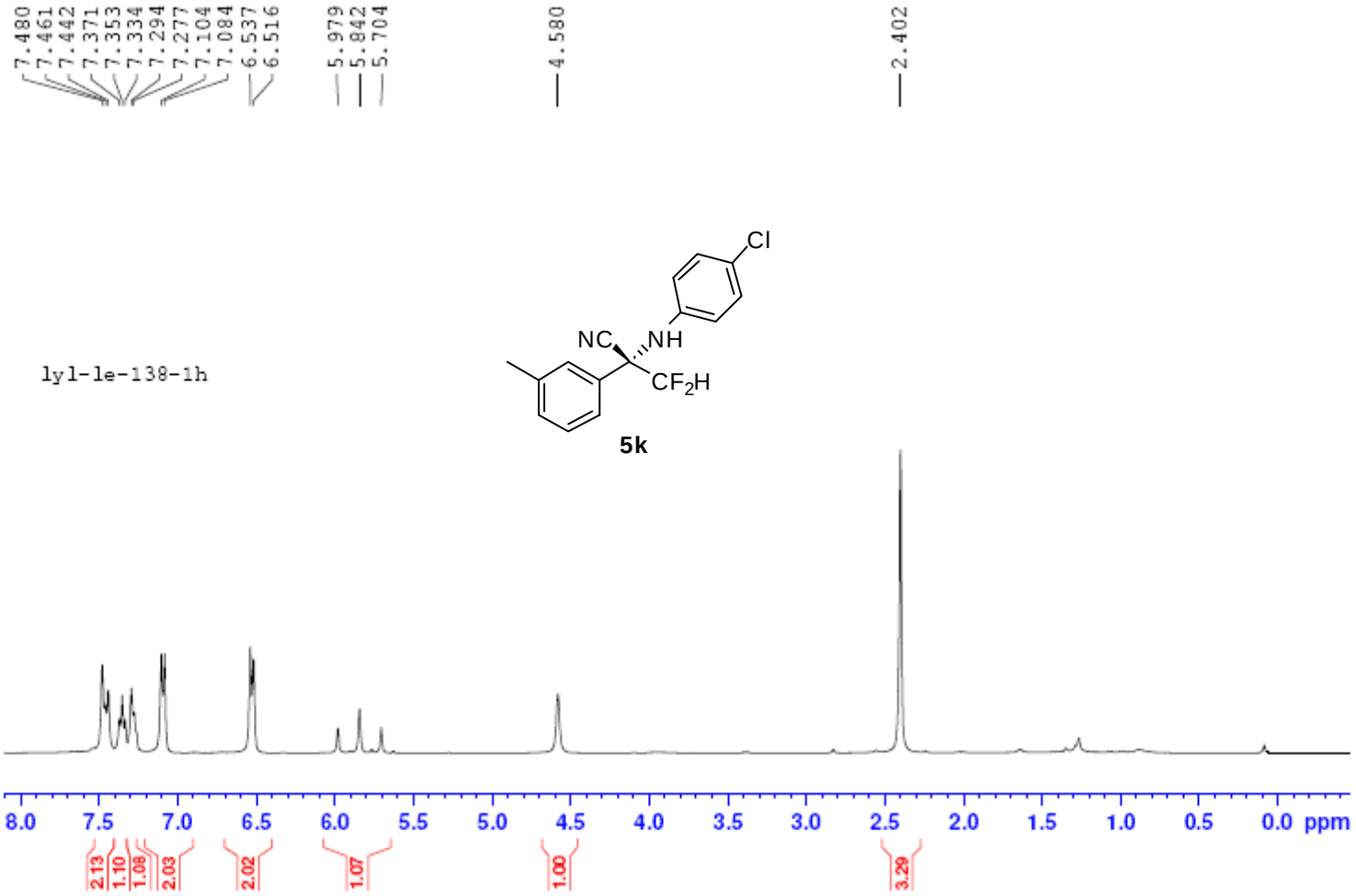

155.23
136.52
134.65
129.96
129.66
129.27
128.75
127.75
120.04
116.50
115.32
114.61
113.94
111.40
77.32
77.00
76.69
65.52
65.31
65.09
55.43
OMe
NC
NH
CF2H
Cl
5i
lyl-le-091-2 C
180
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm

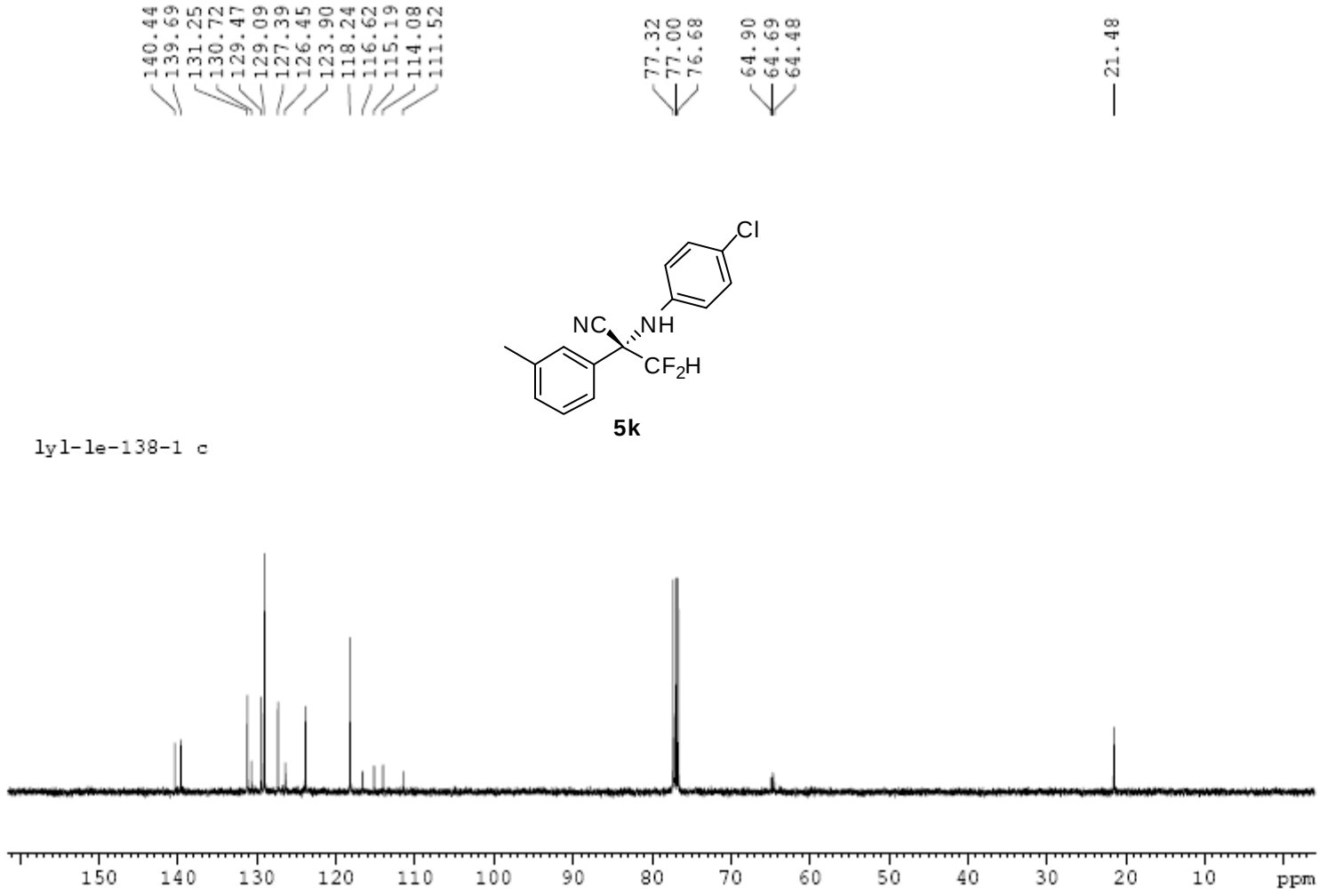

-124.64
-125.37
-126.22
-126.95
OMe
NC
NH
CF2H
Cl
5i
lyl-le-091-2 f
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

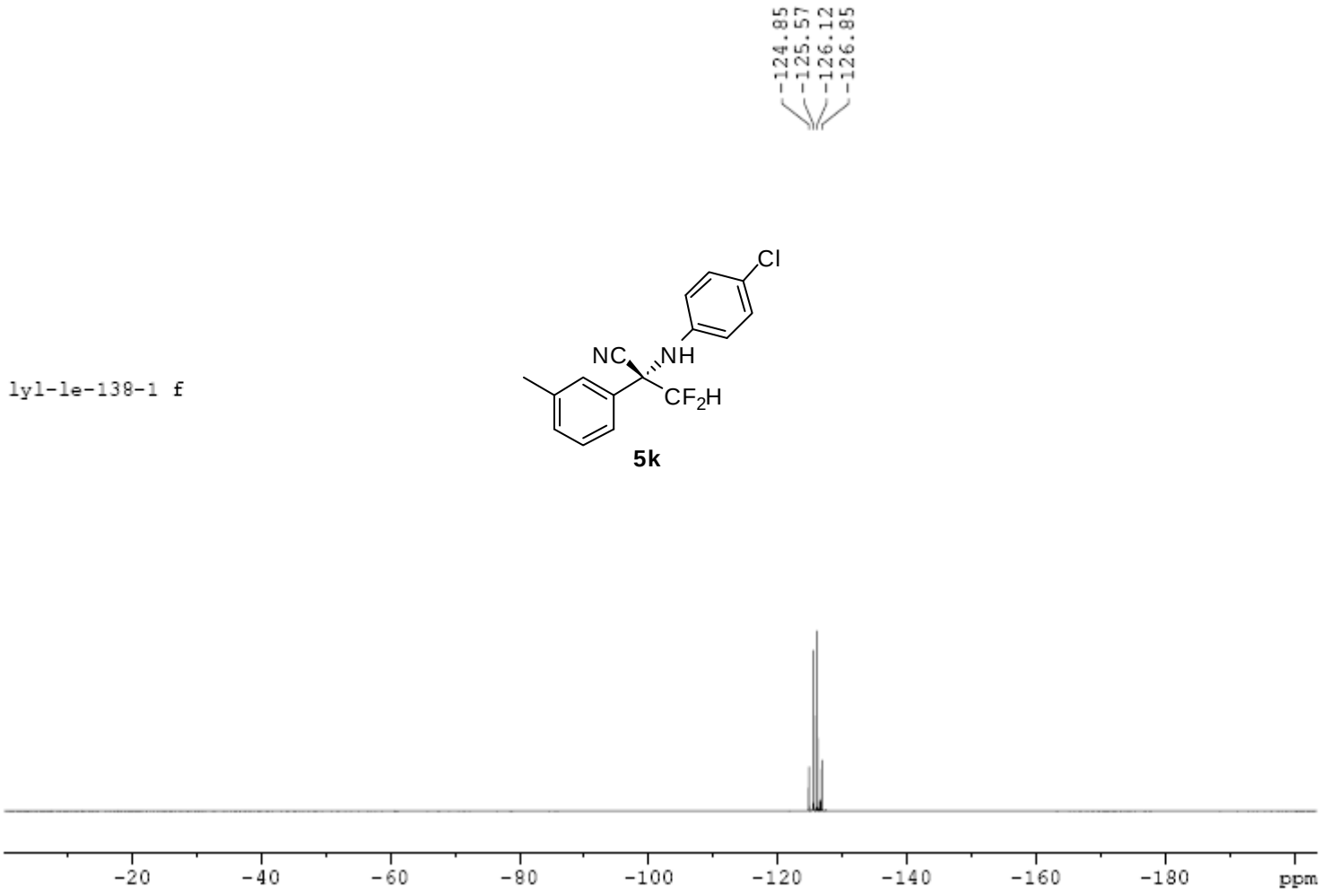

8.225
7.948
7.925
7.901
7.881
7.757
7.736
7.586
7.577
7.260
6.675
6.653
6.633
6.614
6.087
5.949
5.810
4.342
3.670
1.557
-0.001
lyl-le-101-2 h
OMe
NC
NH
CF2H
5j
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.11
3.00
1.08
2.03
4.02
0.33
0.59
0.35
1.06
3.00

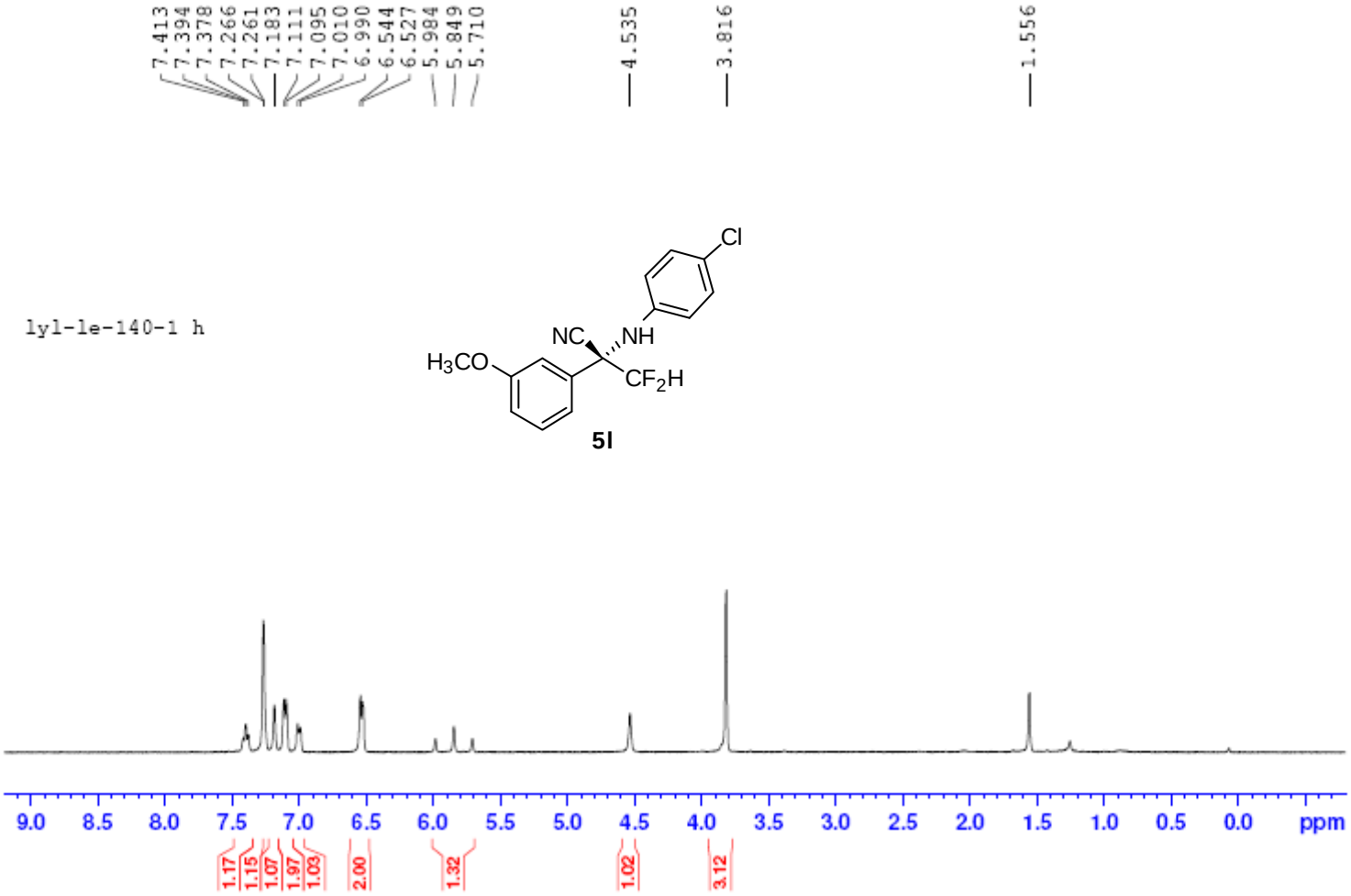

155.00
135.10
133.86
133.01
129.47
128.84
128.46
127.77
127.70
127.49
127.01
123.27
119.92
116.73
115.72
114.48
114.19
111.64
77.32
77.00
76.68
66.26
66.05
65.85
55.33
OMe
NC
NH
CF2H
5j
yl-le-100-2 c
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 ppm

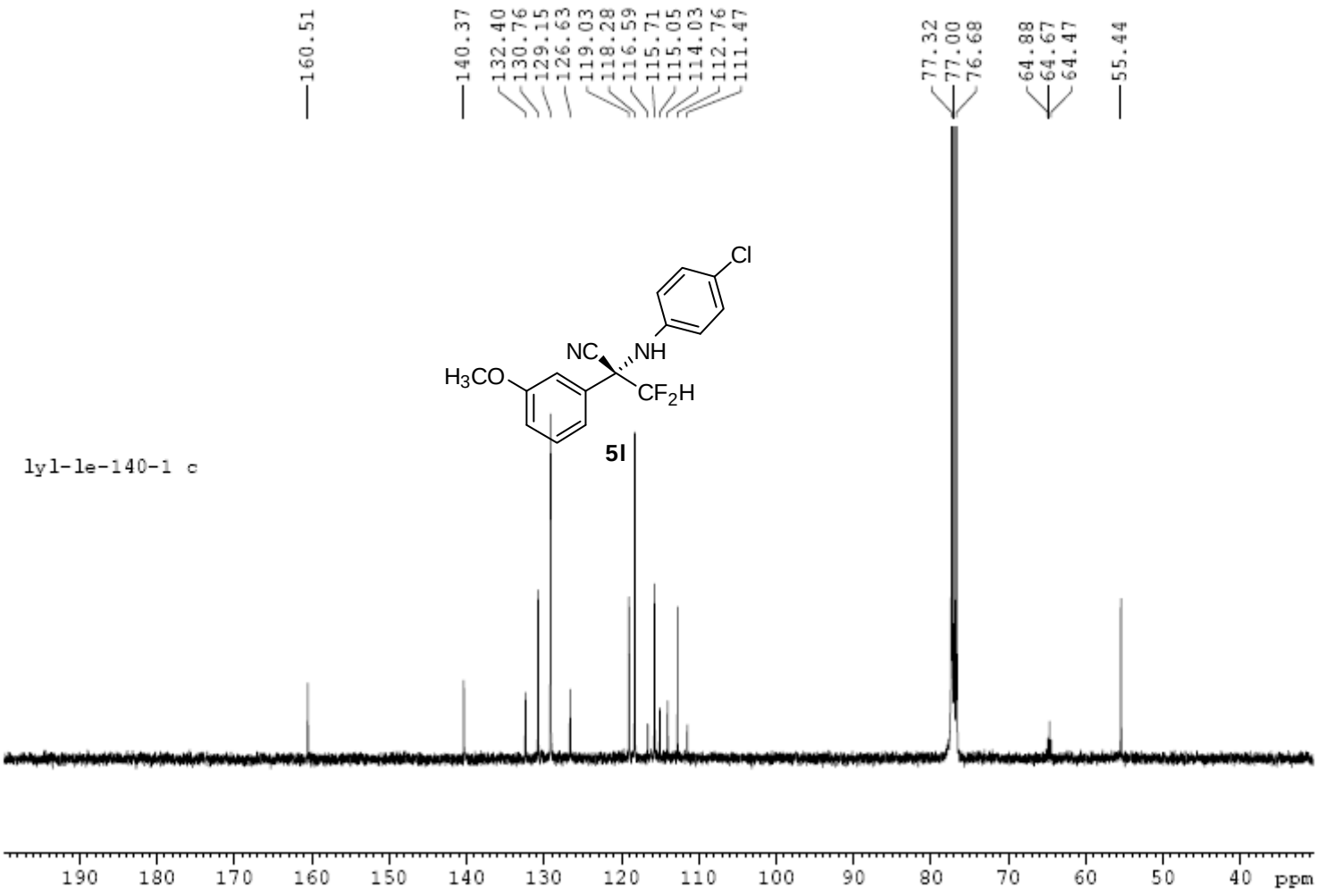

-124.53
-125.26
-125.72
-126.45
OMe
NC
NH
CF2H
5j
lyl-le-100-2 f
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
ppm

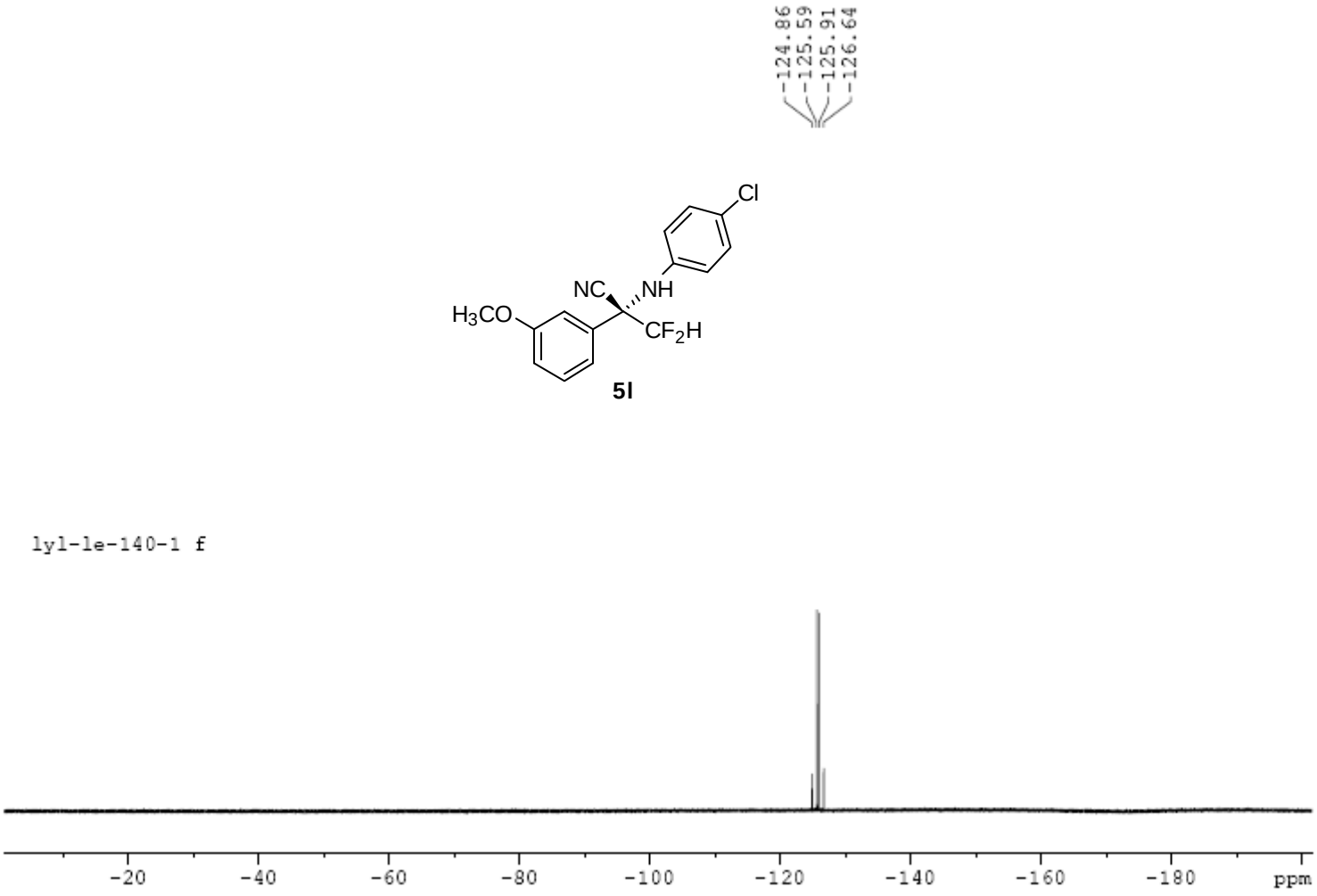

7.480
7.461
7.442
7.371
7.353
7.334
7.294
7.277
7.104
7.084
6.537
6.516
5.979
5.842
5.704
4.580
2.402
lyl-le-138-1h
Cl
NC
NH
CF2H
5k
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
2.13
1.10
1.06
2.03
2.02
1.07
1.00
3.29

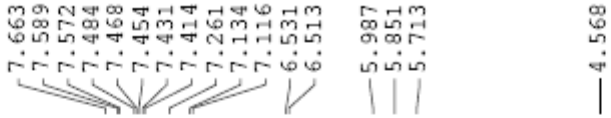

140.44
139.69
131.25
130.72
129.47
129.09
127.39
126.45
123.90
118.24
116.62
115.19
114.08
111.52
77.32
77.00
76.68
64.90
64.69
64.48
21.48
Cl
NC
NH
CF2H
5k
lyl-le-138-1 c
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-124.85
-125.57
-126.12
-126.85
Cl
NC
NH
CF2H
5k
lyl-le-138-1 f
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

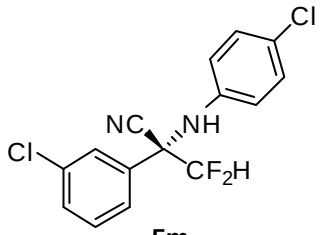

7.413
7.394
7.378
7.266
7.261
7.183
7.111
7.095
7.010
6.990
6.544
6.527
5.984
5.849
5.710
4.535
3.816
1.556
lyl-le-140-1 h
Cl
NC
NH
H3CO
CF2H
5l
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.17
1.15
1.07
1.97
1.03
2.00
1.32
1.02
3.12


160.51
140.37
132.40
130.76
129.15
126.63
119.03
118.28
116.59
115.71
115.05
114.03
112.76
111.47
77.32
77.00
76.68
64.88
64.67
64.47
55.44
Cl
NC
NH
H3CO
CF2H
5l
lyl-le-140-1 c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

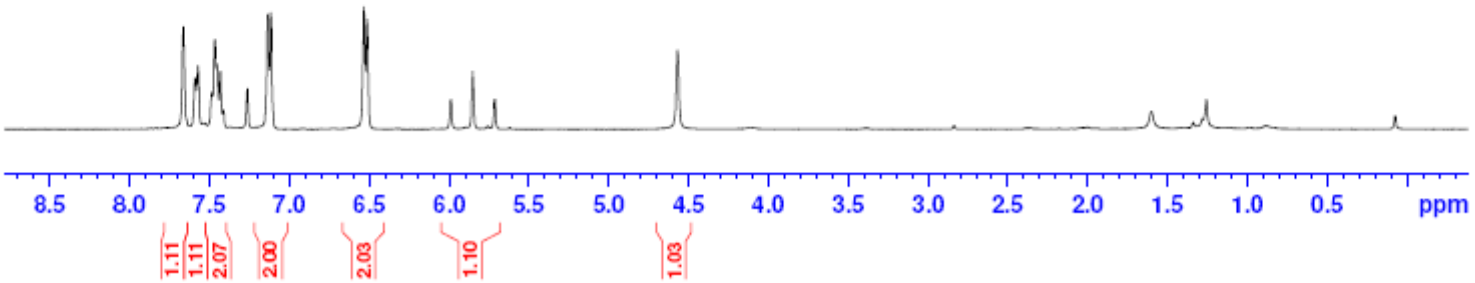

-124.86
-125.59
-125.91
-126.64
Cl
NC
NH
H3CO
CF2H
5l
lyl-le-140-1 f
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

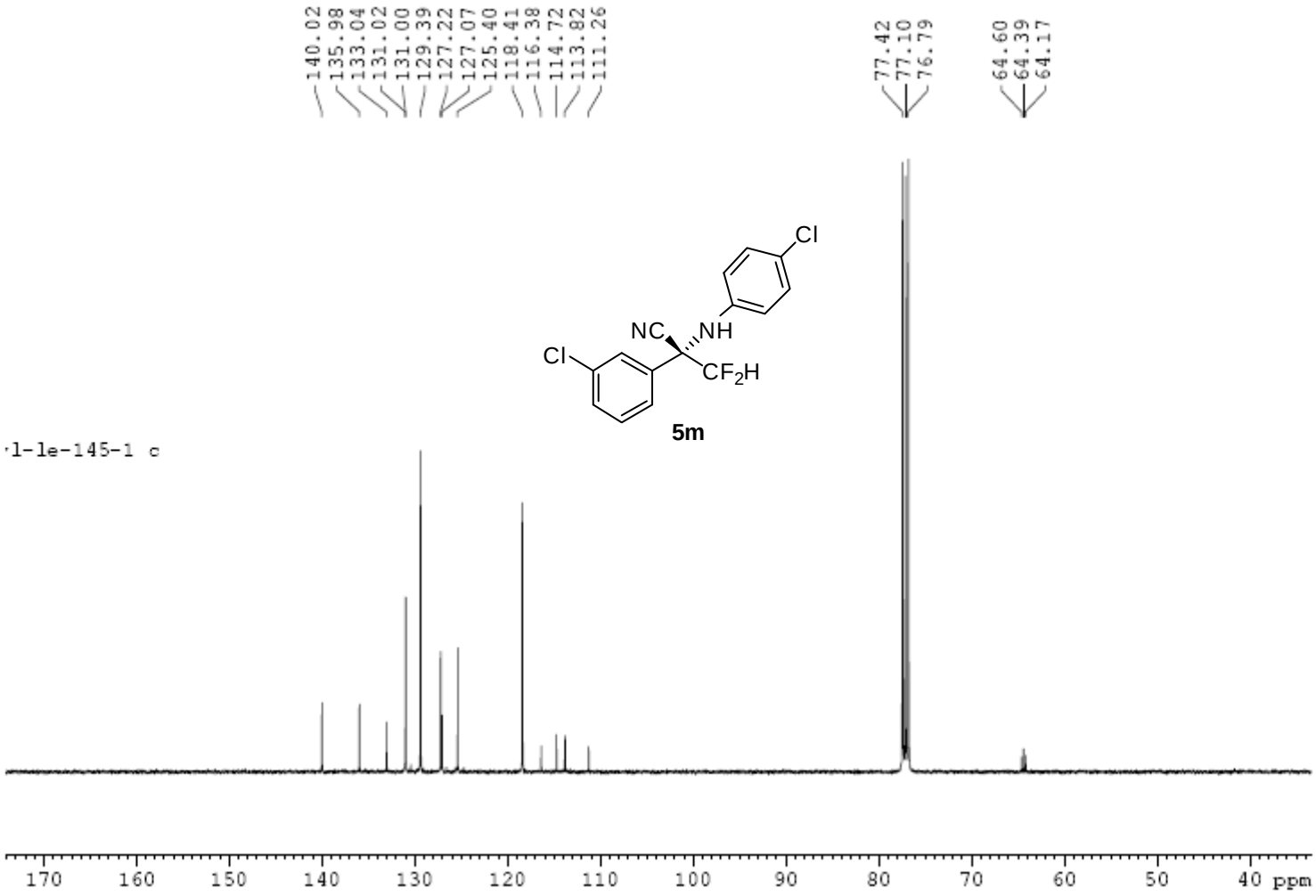


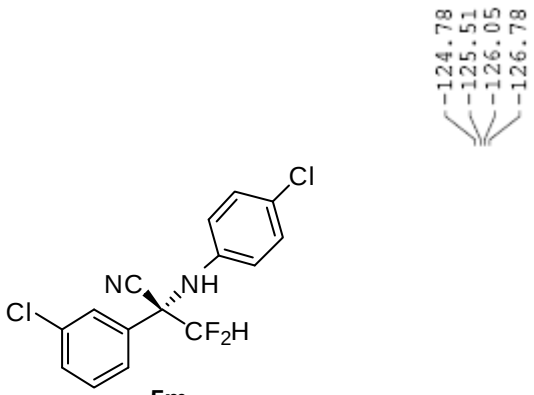
lyl-le-145-1 h



5m

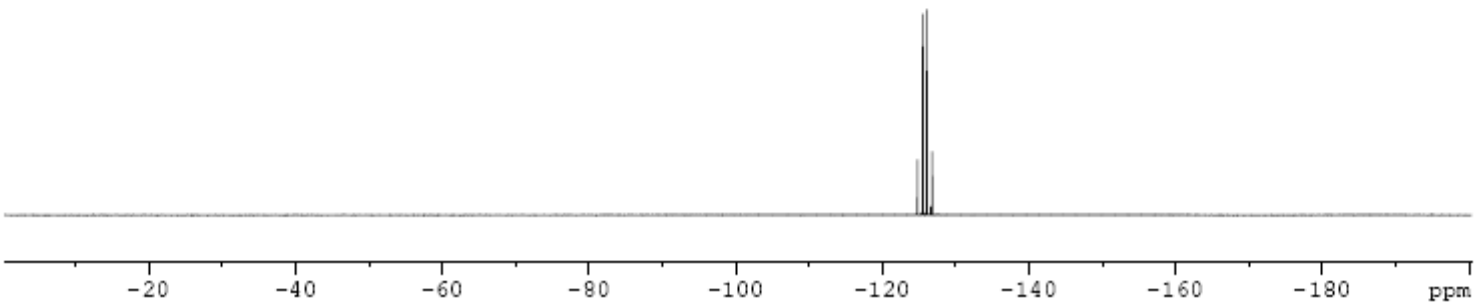


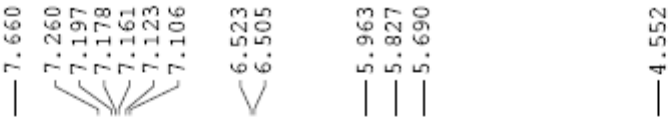

140.02
135.98
133.04
131.02
131.00
129.39
127.22
127.07
125.40
118.41
116.38
114.72
113.82
111.26
77.42
77.10
76.79
64.60
64.39
64.17
Cl
NC
NH
Cl
CF2H
5m
l-le-145-1 c
170
160
150
140
130
120
110
100
90
80
70
60
50
40 ppm

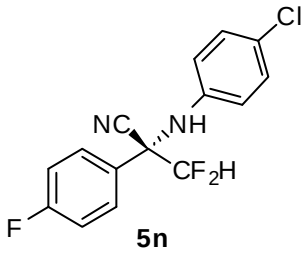


5m

lyl-le-145-1 f

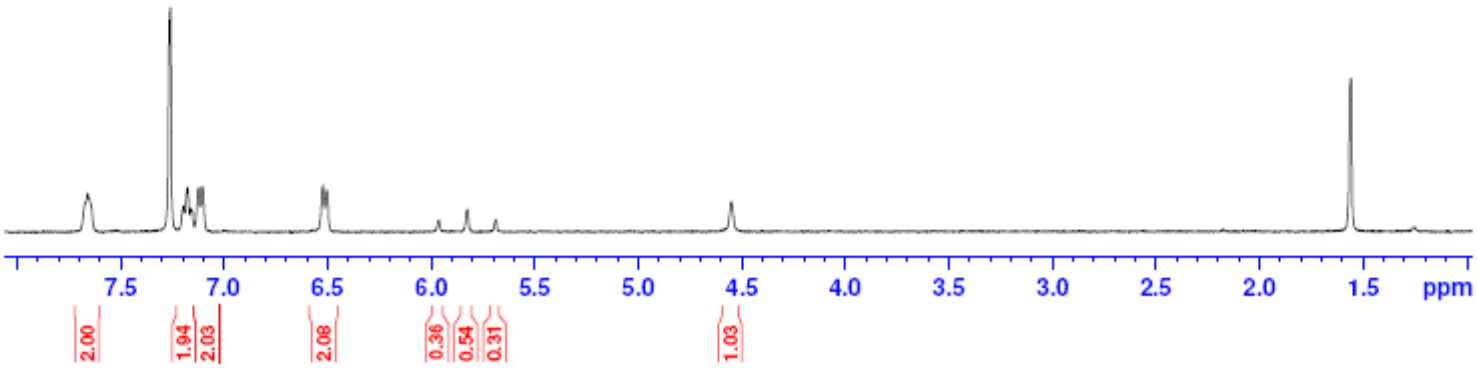


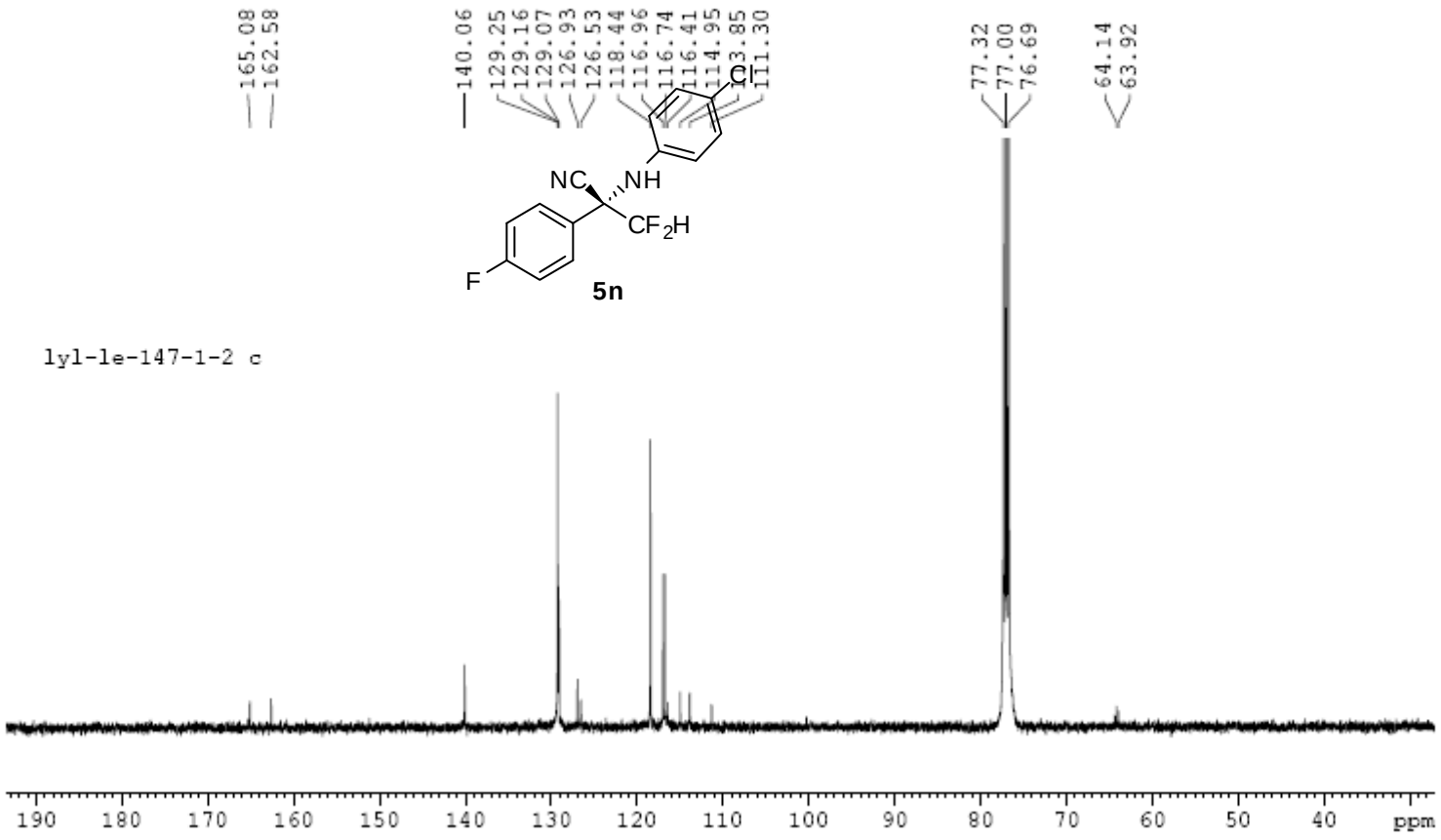


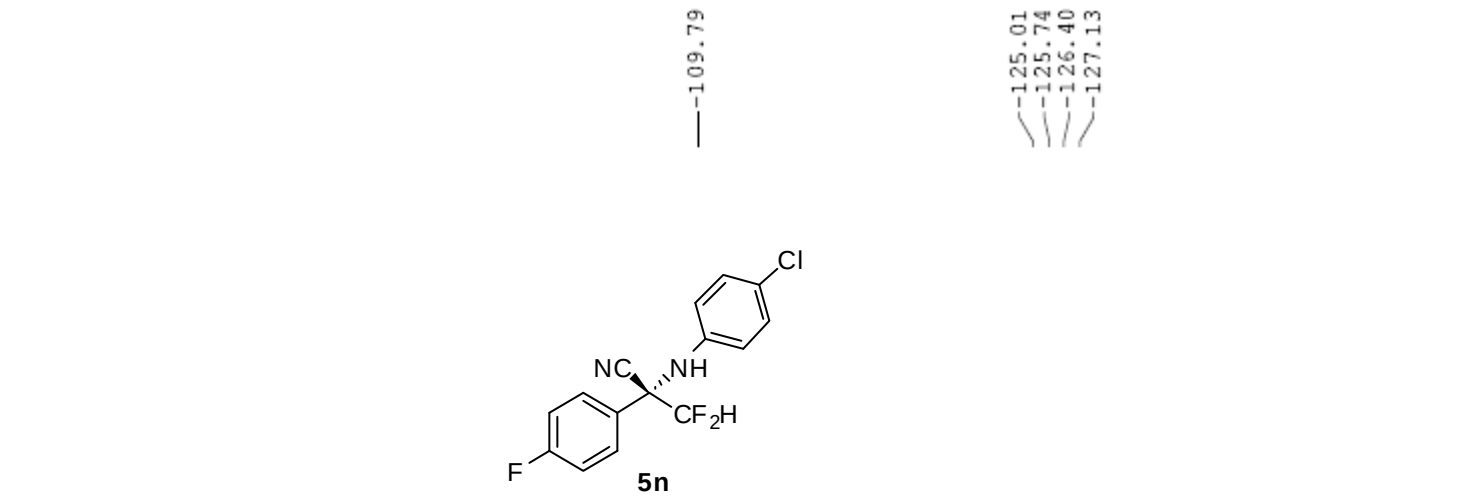


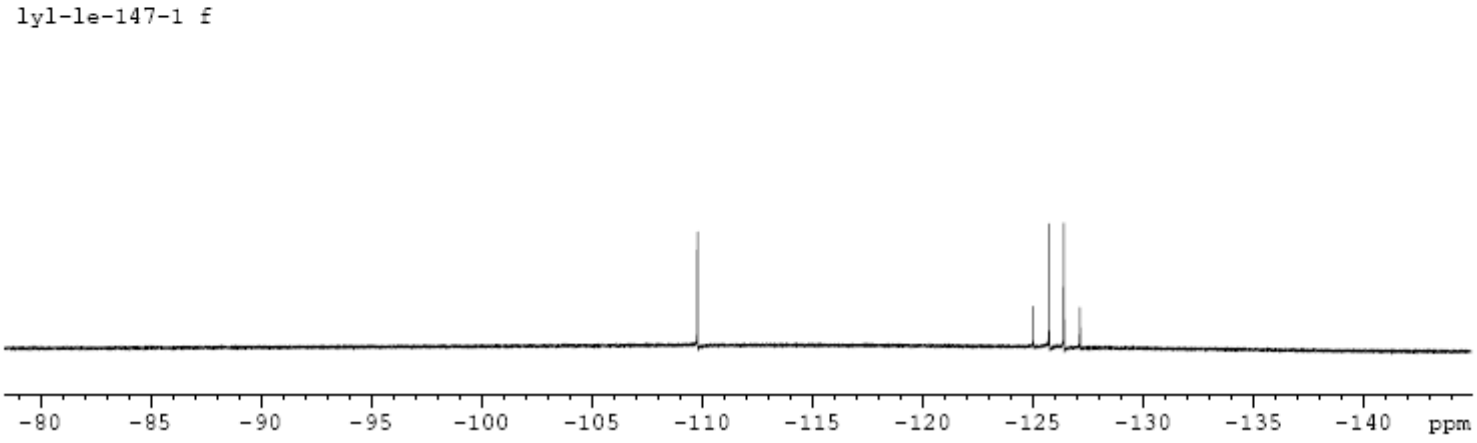
5n

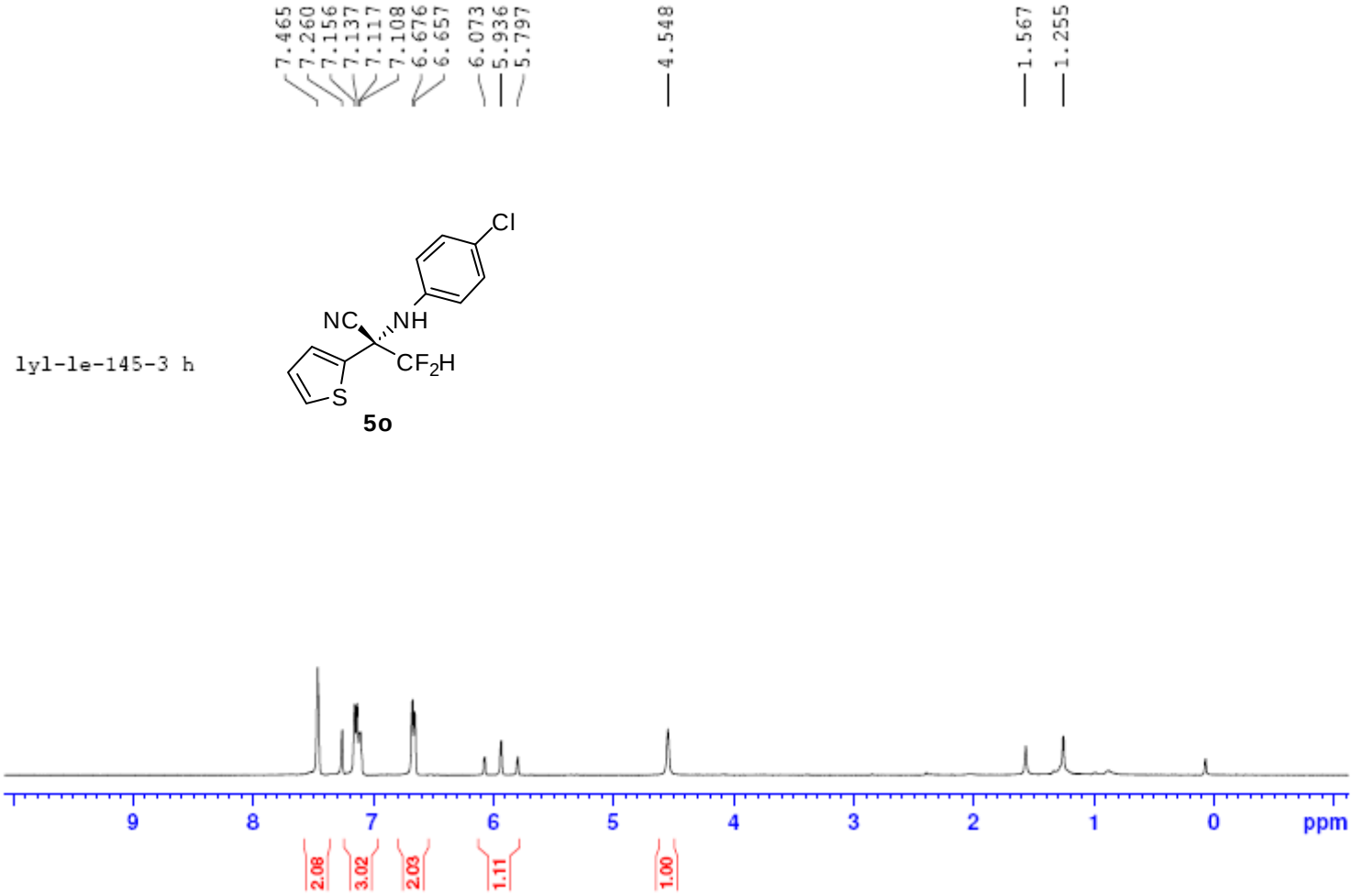
lyl-le-147-1 h

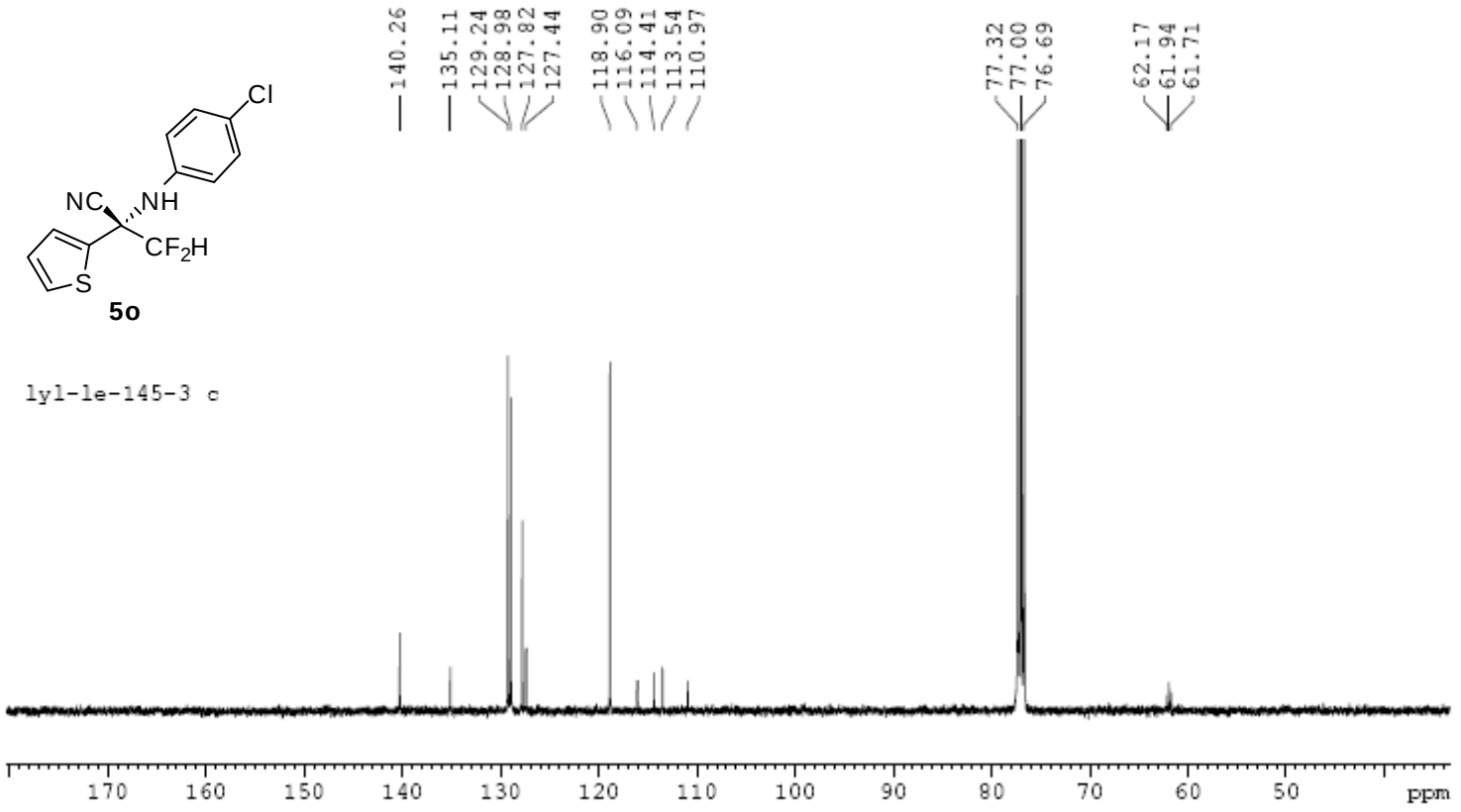


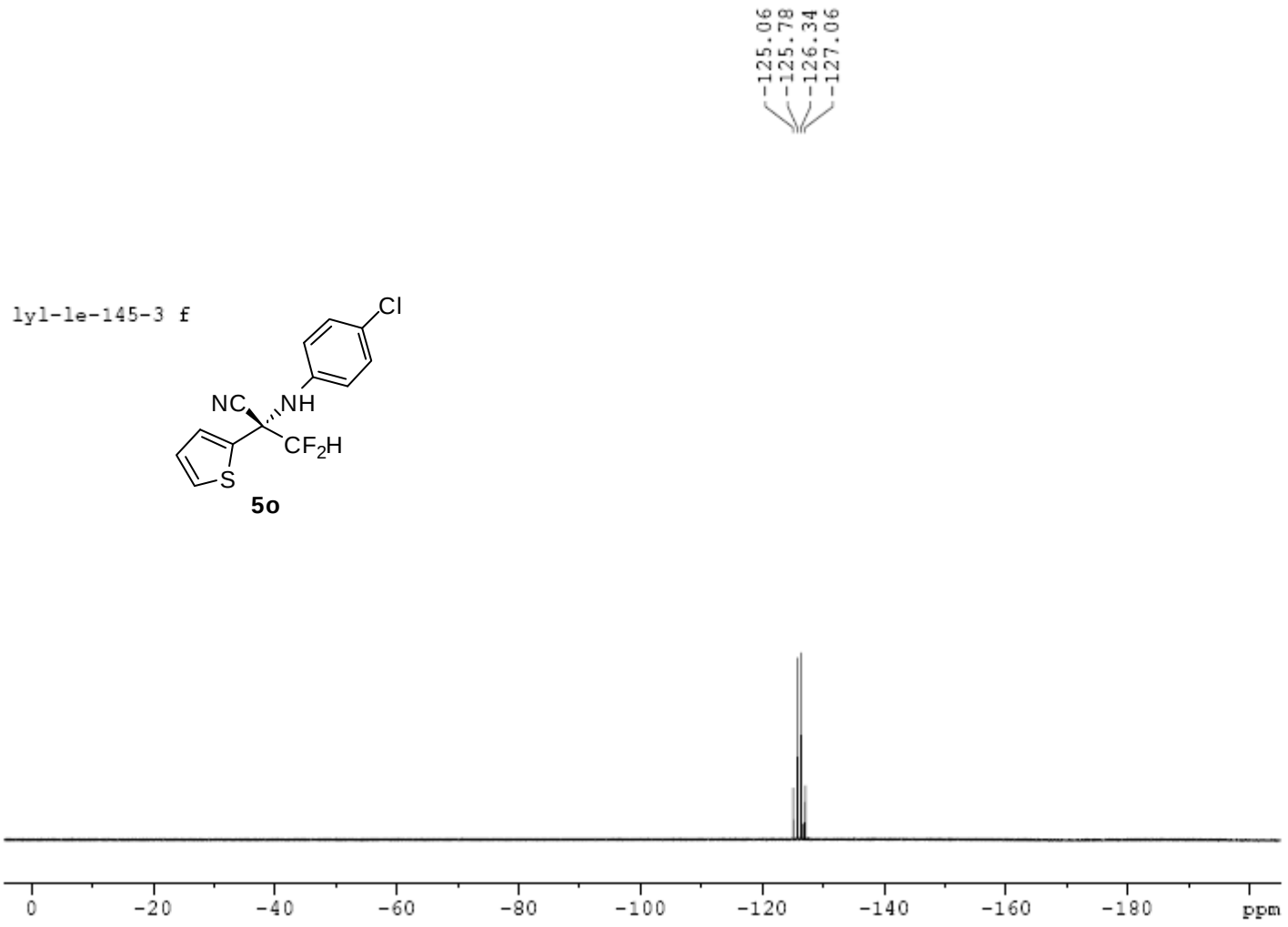

165.08
162.58
140.06
129.25
129.16
129.07
126.93
126.53
118.44
116.96
116.74
116.41
114.95
113.85
111.30
77.32
77.00
76.69
64.14
63.92
NC
NH
CF2H
F
Cl
5n
lyl-le-147-1-2 c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm


-109.79
-125.01
-125.74
-126.40
-127.13
Cl
NC
NH
CF2H
F
5n

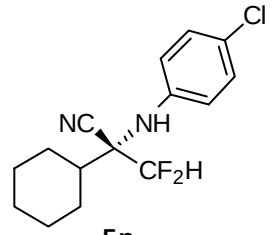

lyl-le-147-1 f
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
ppm


7.465
7.260
7.156
7.137
7.117
7.108
6.676
6.657
6.073
5.936
5.797
4.548
1.567
1.255
lyl-le-145-3 h
Cl
NC
NH
CF2H
S
5o
9
8
7
6
5
4
3
2
1
0
ppm
2.08
3.02
2.03
1.11
1.00

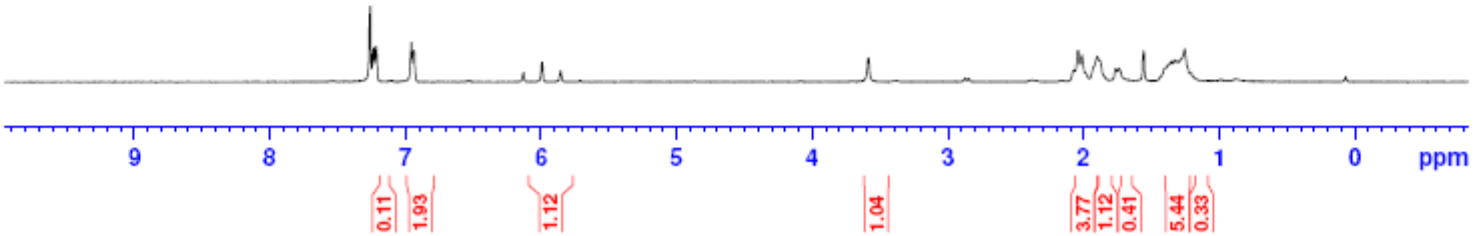

140.26
135.11
129.24
128.98
127.82
127.44
118.90
116.09
114.41
113.54
110.97
77.32
77.00
76.69
62.17
61.94
61.71
Cl
NC
NH
CF2H
S
5o
lyl-le-145-3 c
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm

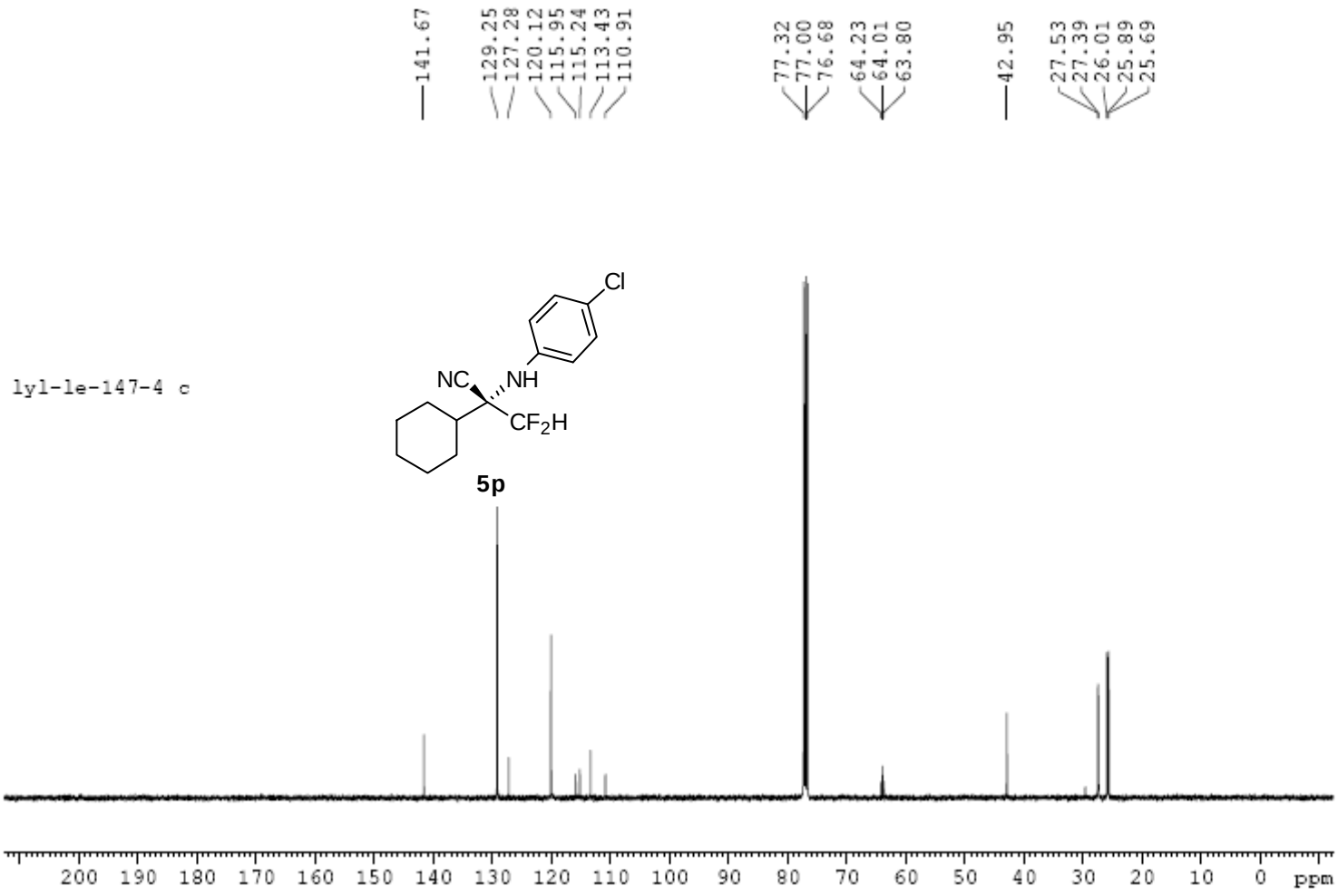

-125.06
-125.78
-126.34
-127.06
lyl-le-145-3 f
Cl
NC
NH
CF2H
S
5o
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

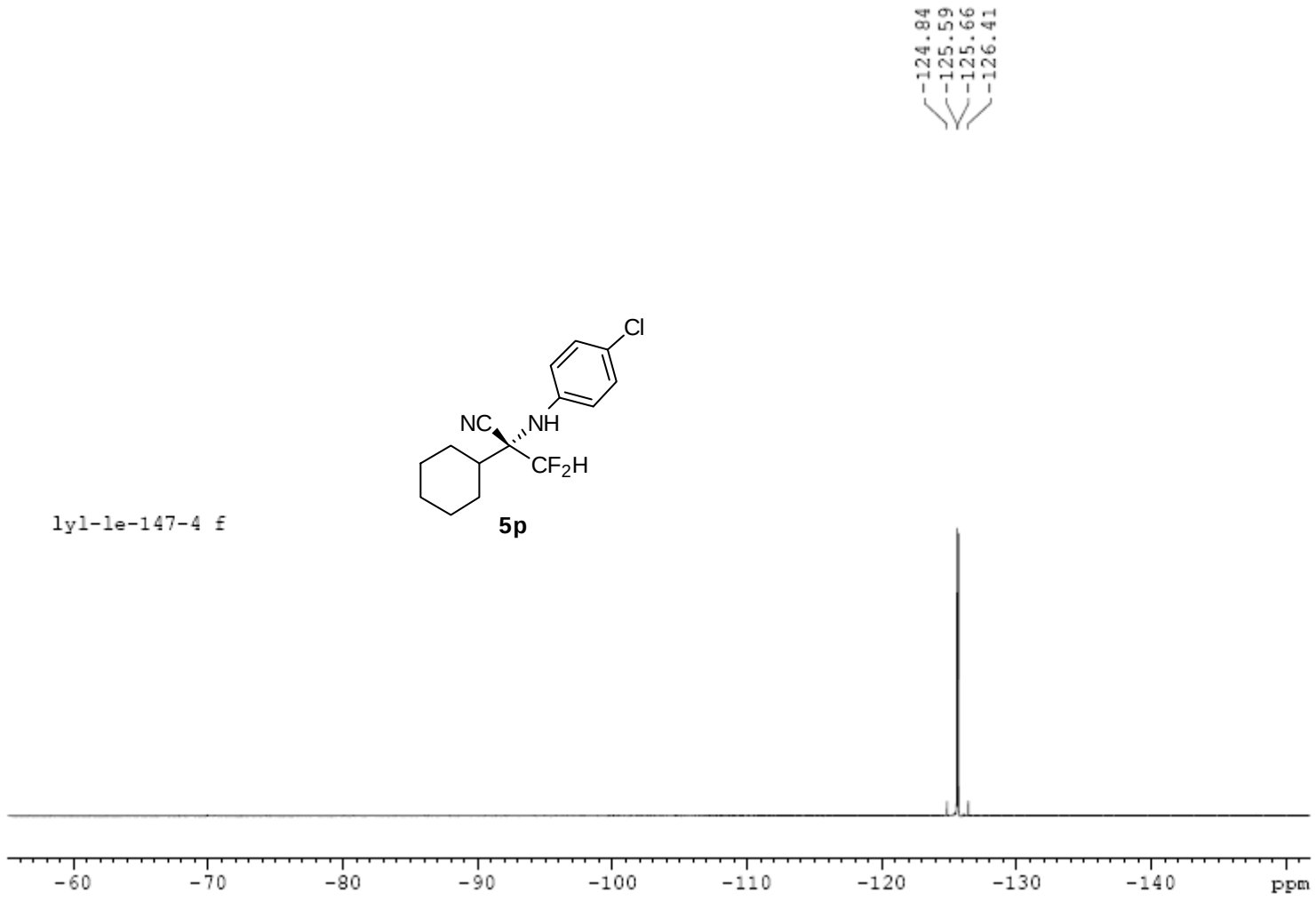
lyl-le-142-2 h



5p




141.67
129.25
127.28
120.12
115.95
115.24
113.43
110.91
77.32
77.00
76.68
64.23
64.01
63.80
42.95
27.53
27.39
26.01
25.89
25.69
lyl-le-147-4 c
Cl
NC
NH
CF2H
5p
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-124.84
-125.59
-125.66
-126.41
Cl
NC
NH
CF2H
5p
lyl-le-147-4 f
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm