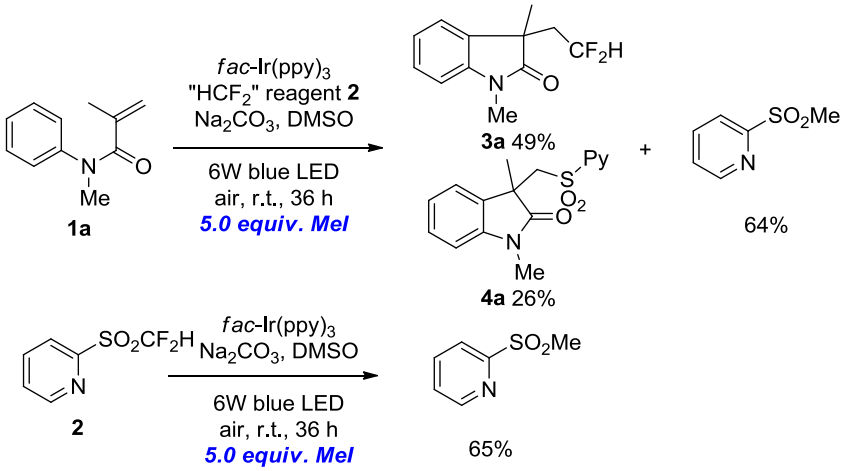
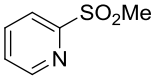
Mechanistic study

1. Sulfinate anion capture experiment



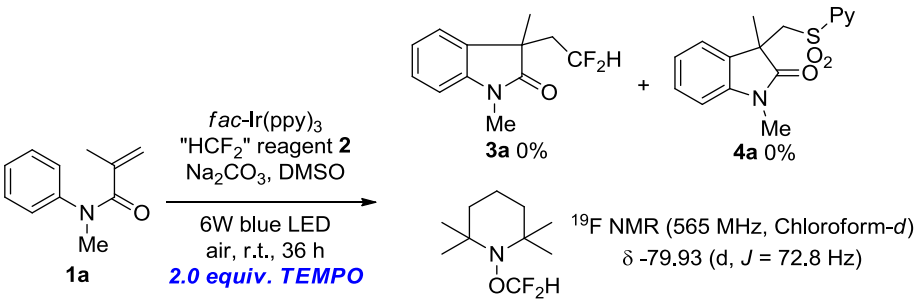
Typical procedures:

fac-Ir(ppy)$_3$ (0.001 mmol, 1 mol%), *N*-arylacrylamide **1a** (0.2 mmol, 2.0 equiv.), difluoromethyl 2-pyridyl sulfone **2** (0.1 mmol, 1.0 eq.), Na_2CO_3 (0.2 mmol, 2.0 eq.) and MeI (0.5 mmol, 5.0 eq.) were sequentially weighed into a tube. DMSO (1.0 mL) were added by using a syringe. The mixture was irradiated by a 6W blue LED at room temperature under air atmosphere for 36h. Then the volatile solvent and reagents were removed by rotary evaporation and the residue was purified by silica gel flash chromatography using petroleum ether/EtOAc to provide **3a** as colourless liquid (49% yield), **4a** as colourless liquid (26% yield) and 2-(methylsulfonyl)pyridine as white solid (64% yield). The trapping product 2-(methylsulfonyl)pyridine could also be observed with 65% yield if removing *N*-arylacrylamide **1a** from the reaction system.



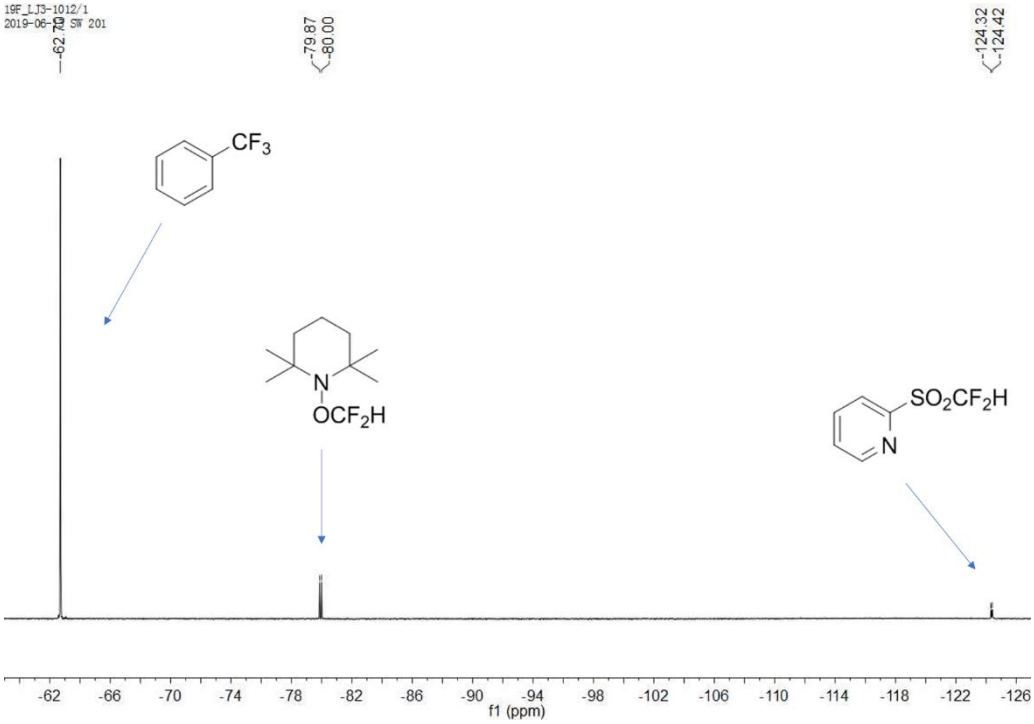
2-(methylsulfonyl)pyridine:^{1}HNMR (600 MHz, Chloroform-*d*) δ 8.74 (d, *J* = 4.6 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 7.98 (td, *J* = 7.7, 1.7 Hz, 1H), 7.57 (dd, *J* = 6.6, 4.7 Hz, 0H), 3.24 (s, 3H).^{13}C NMR (151 MHz, Chloroform-*d*) δ 158.04, 150.11, 138.31, 127.48, 121.13, 40.04. HRMS (ESI): m/z = 158.0270, calcd. For $C_6H_8NO_2S$ ([M+H$^+$]) 158.0276.

2. Radical Inhibition Experiments



Typical procedures:

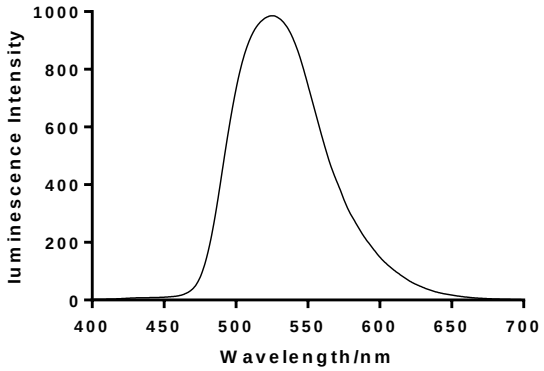
fac-Ir(ppy)$_3$ (0.001 mmol, 1 mol%), *N*-arylacrylamide **1a** (0.2 mmol, 2.0 equiv.), difluoromethyl 2-pyridyl sulfone **2** (0.1 mmol, 1.0 eq.), Na_2CO_3 (0.2 mmol, 2.0 eq.) and TEMPO (0.2 mmol, 2.0 eq.) were sequentially weighed into a tube. DMSO (1.0 mL) were added by using a syringe. The mixture was irradiated by a 6W blue LED at room temperature under air atmosphere for 36h (monitored by ^{19}F NMR using $PhCF_3$ as the internal standard).



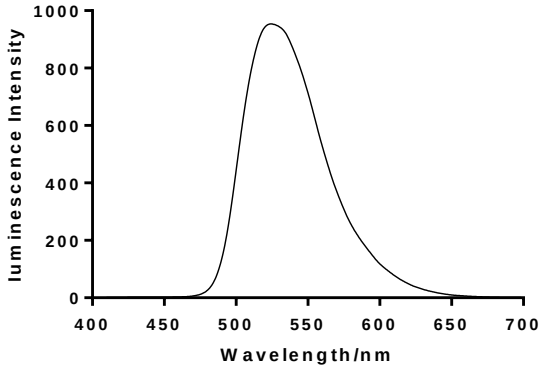
3. Luminescence Quenching Experiments

To verify the oxidative quenching cycle, we conducted the luminescence quenching experiments.

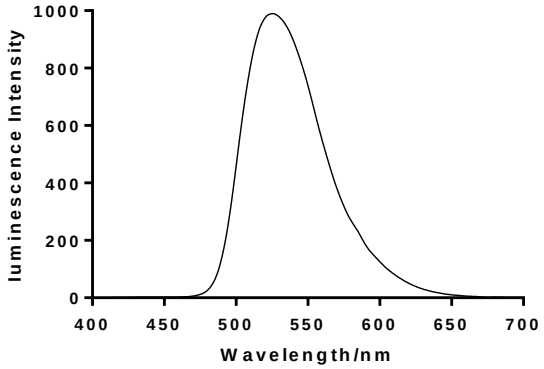
PerkinElmer LS55 fluorescence spectrophotometer was used for the luminescence quenching experiment. Samples with *fac*-Ir(ppy)$_3$ were irradiated at 380 nm and emission was detected at 540 nm. Sample with Na_2CO_3 were stirred for 10 min and filtrated with a syringe filter (pore size = 0.22 μm) before the luminescence measurement. I_0 is the luminescence intensity without the quencher, I is the intensity with the quencher.



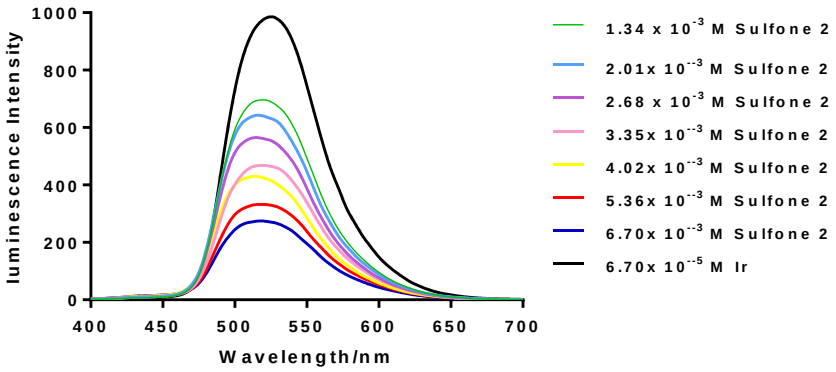
Fluorescence-emission of a 6.7×10^{-5} M solution of *fac*-Ir(ppy)$_3$ (without the quencher) in DMSO, $I_0 = 985.70$.



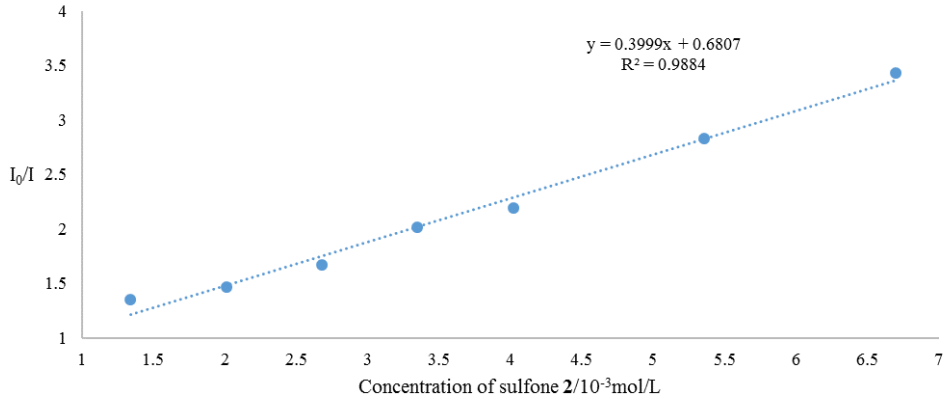
Fluorescence-emission of a 6.7×10^{-5} M solution of *fac*-Ir(ppy)$_3$ with *N*-arylacrylamide **1a** (6.7×10^{-3} M) in DMSO, I = 953.88.



Fluorescence-emission of a 6.7×10^{-5} M solution of *fac*-Ir(ppy)$_3$ with Na_2CO_3 (1.3×10^{-2} M) in DMSO/H_2O (4:1), I = 989.78.



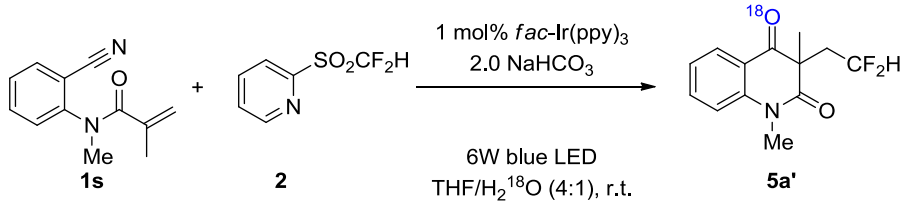
Fluorescence-emission of a 6.7×10^{-5} M solution of *fac*-Ir(ppy)$_3$ with difluoromethyl 2-pyridyl sulfone **2** in DMSO.

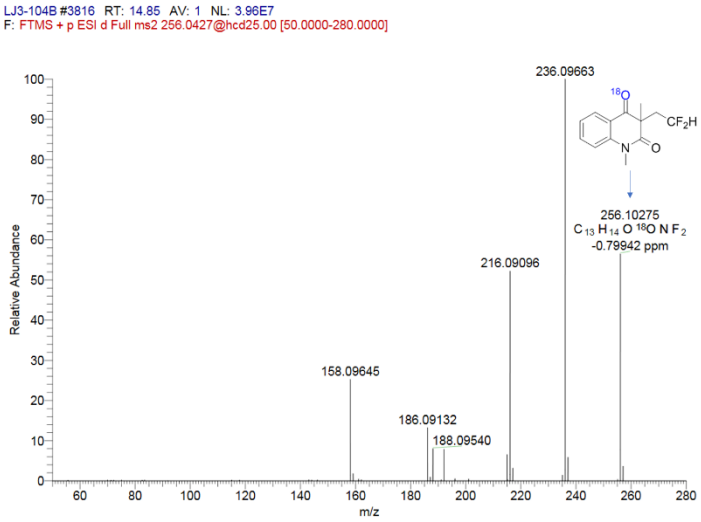


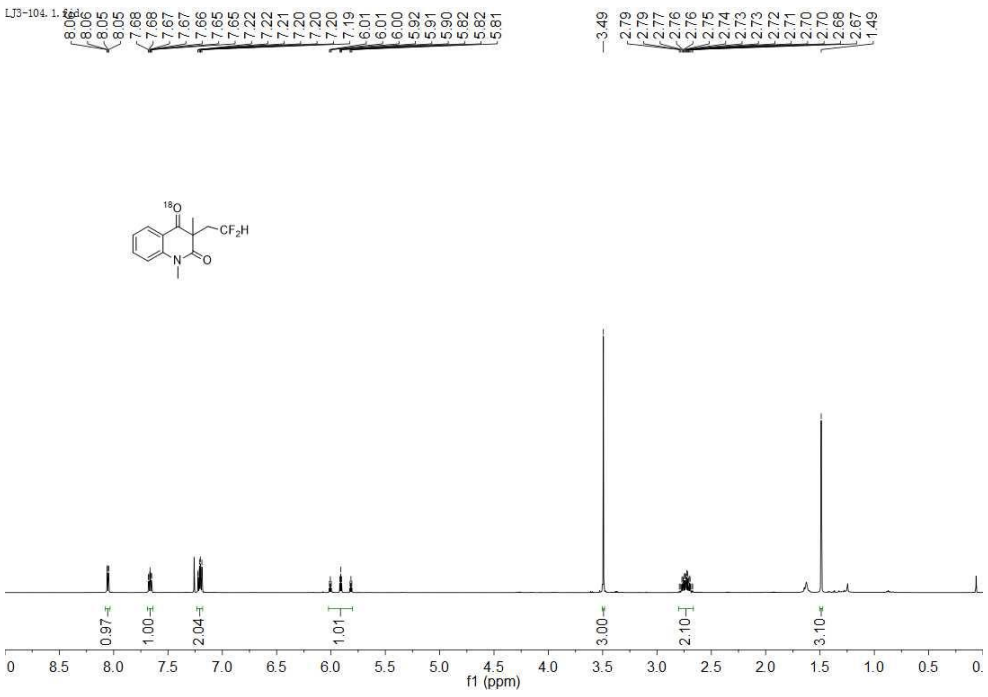
These results suggested difluoromethyl 2-pyridyl sulfone **2** could be used as an efficient quencher to $[Ir]^{III*}$, and the reaction proceeds through an oxidative quenching cycle, which is consistent with the reduction potential of difluoromethyl 2-pyridyl sulfone **2** (the first reduction potential: -1.50 V vs. SCE) and *fac*-Ir(ppy)$_3$ ($E_{1/2}^{IV/*III}$=-1.73 V Vs SCE in CH_3CN).

4. $H_2{}^{18}O$-labeling experiment

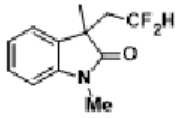
In order to verify H_2O providing the new oxygen of quinoline-2,4-diones in this reaction, an $H_2{}^{18}O$-labeling experiment was performed using THF (anhydrous)/$H_2{}^{18}O$ (v/v, 4:1) as the solvent. The mixture was irradiated by a 6W blue LED at room temperature under air atmosphere for 12h. Then the volatile solvent and reagents were removed by rotary evaporation and the residue was purified by silica gel flash chromatography using petroleum ether/EtOAc to afford the desired product **5a'** with 60% yield.





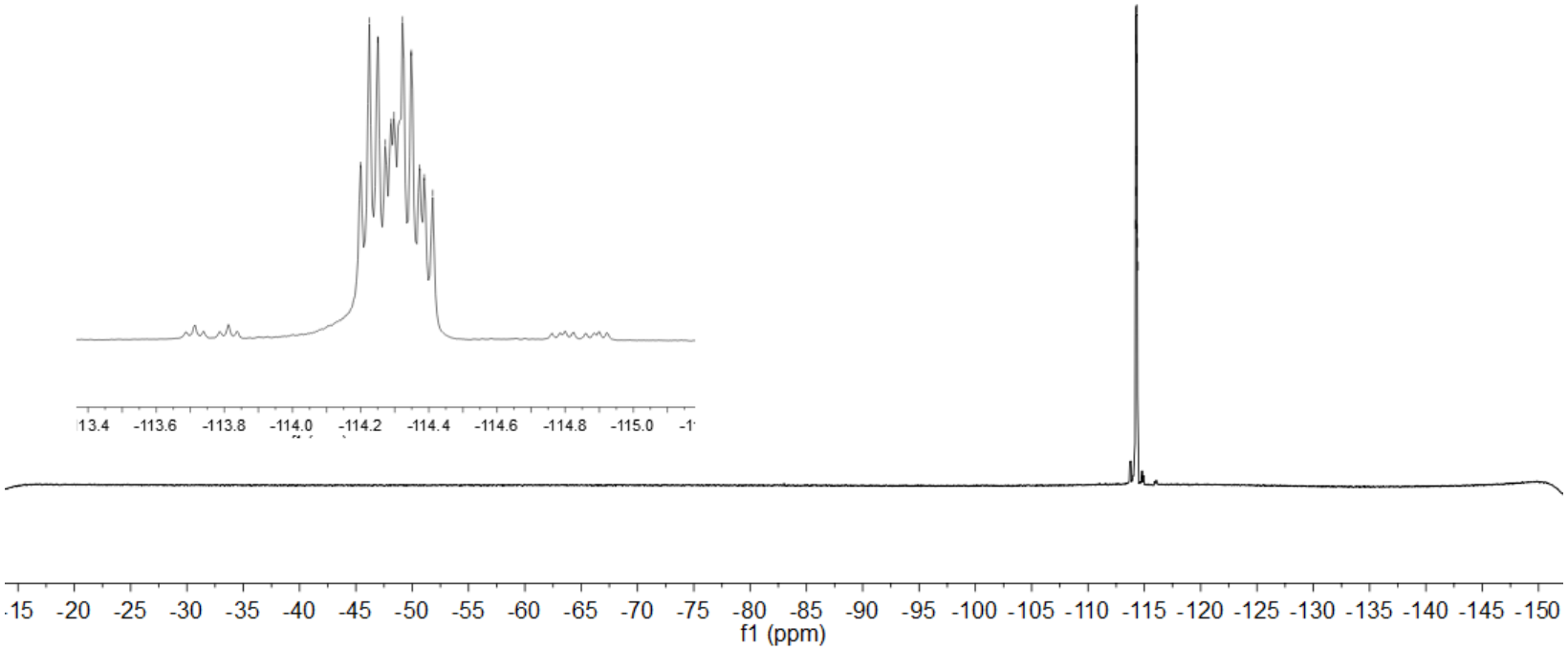

LJ3-104.1.fid
8.06
8.06
8.05
8.05
7.68
7.68
7.67
7.67
7.66
7.65
7.65
7.22
7.22
7.21
7.20
7.20
7.20
7.19
6.01
6.01
6.00
5.92
5.91
5.90
5.82
5.82
5.81
3.49
2.79
2.79
2.77
2.76
2.76
2.75
2.74
2.73
2.73
2.72
2.71
2.70
2.70
2.68
2.67
1.49
18O
CF2H
N
O
0.97
1.00
2.04
1.01
3.00
2.10
3.10
0
8.5
8.0
7.5
7.0
6.5
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.
f1 (ppm)

19F_LYS-31C/2
2018-12-13

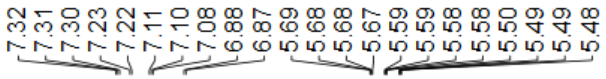


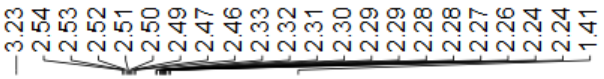
114.20
114.23
114.25
114.27
114.29
114.30
114.32
114.35
114.37
114.39
114.41

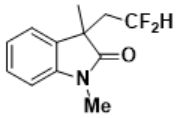
3a $CDCl_3$



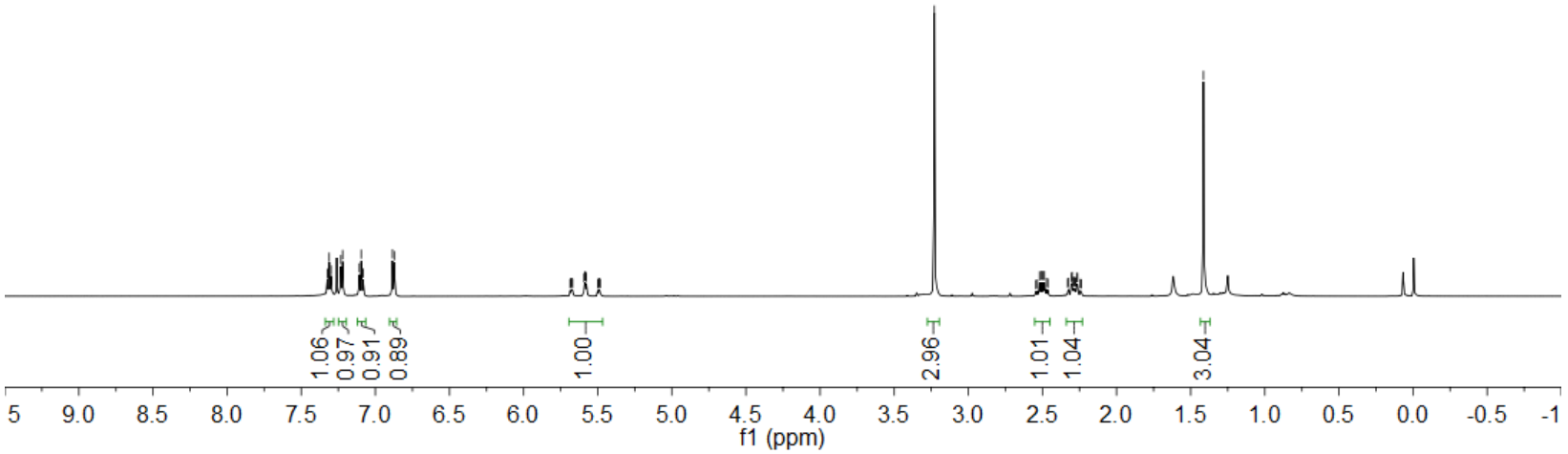
LYS-31c. 1. fid





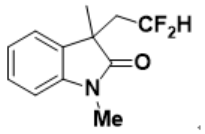


3a $CDCl_3$

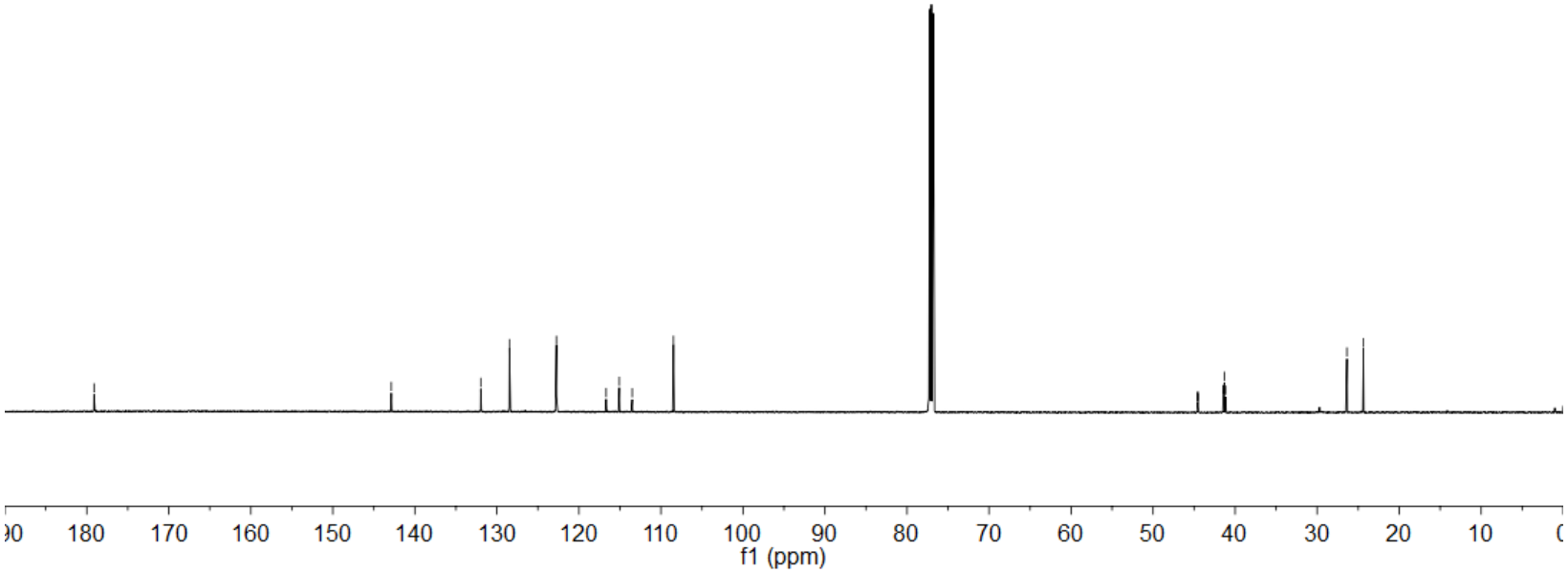


LYS-31c.2.fid

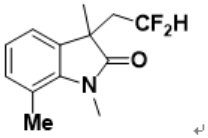
179.11
142.87
131.97
128.47
122.74
116.68
115.09
113.50
108.47
44.59
44.56
44.55
44.52
41.46
41.31
41.17
26.37
24.35



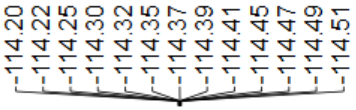
3a $CDCl_3$

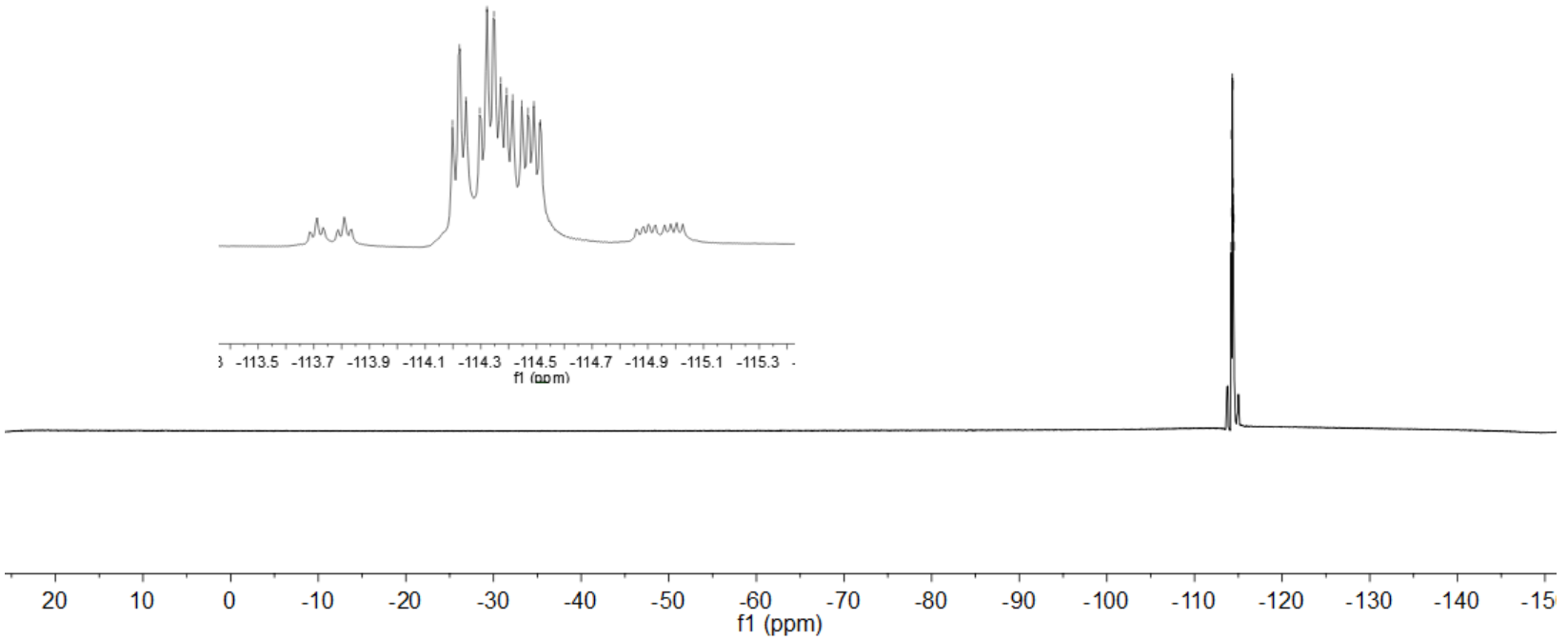


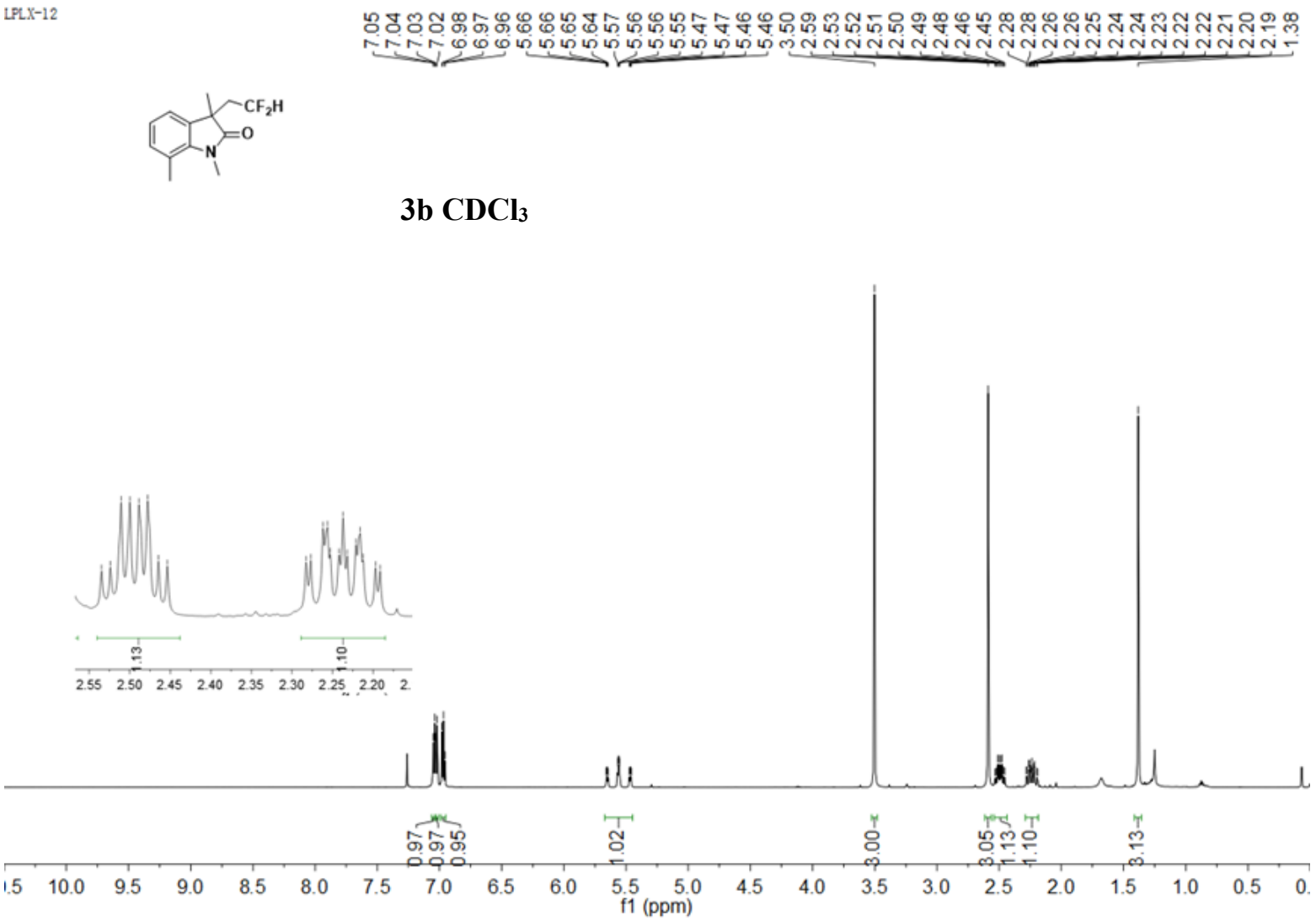
19F_LPZX-12/1
2018-10-12



3b CDCl₃






LPLX-12
7.05 7.04 7.03 7.02 6.98 6.97 6.96 5.66 5.66 5.65 5.64 5.57 5.56 5.56 5.55 5.47 5.47 5.46 5.46 3.50 2.59 2.53 2.52 2.51 2.50 2.49 2.48 2.46 2.45 2.28 2.28 2.26 2.26 2.25 2.24 2.24 2.23 2.22 2.22 2.21 2.20 2.19 1.38
CF2H
O
N
1.13
1.10
2.55 2.50 2.45 2.40 2.35 2.30 2.25 2.20
0.97 0.97 0.95 1.02 3.00 3.05 1.13 1.10 3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

3b $CDCl_3$

LPZX-12

179.8561
140.6060
132.5505
132.1257
122.6357
120.5986
120.1463
116.6990
115.1108
113.5237
43.8908
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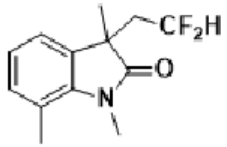
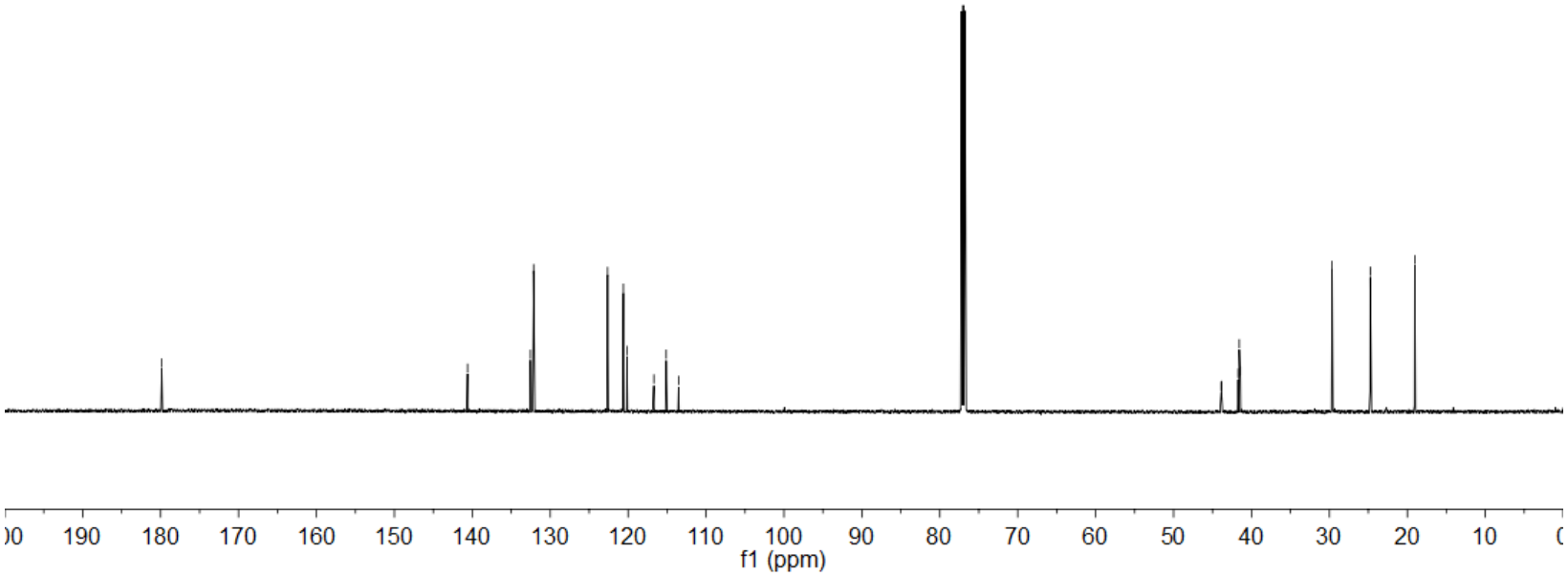
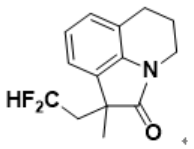
43.8454
43.8208
41.7106
41.5656
41.4213
29.6646
24.7546
19.0429

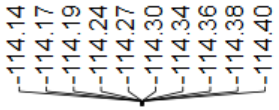


3bCDCl$_3$




HF2C
N
O

3c $CDCl_3$


-114.14
-114.17
-114.19
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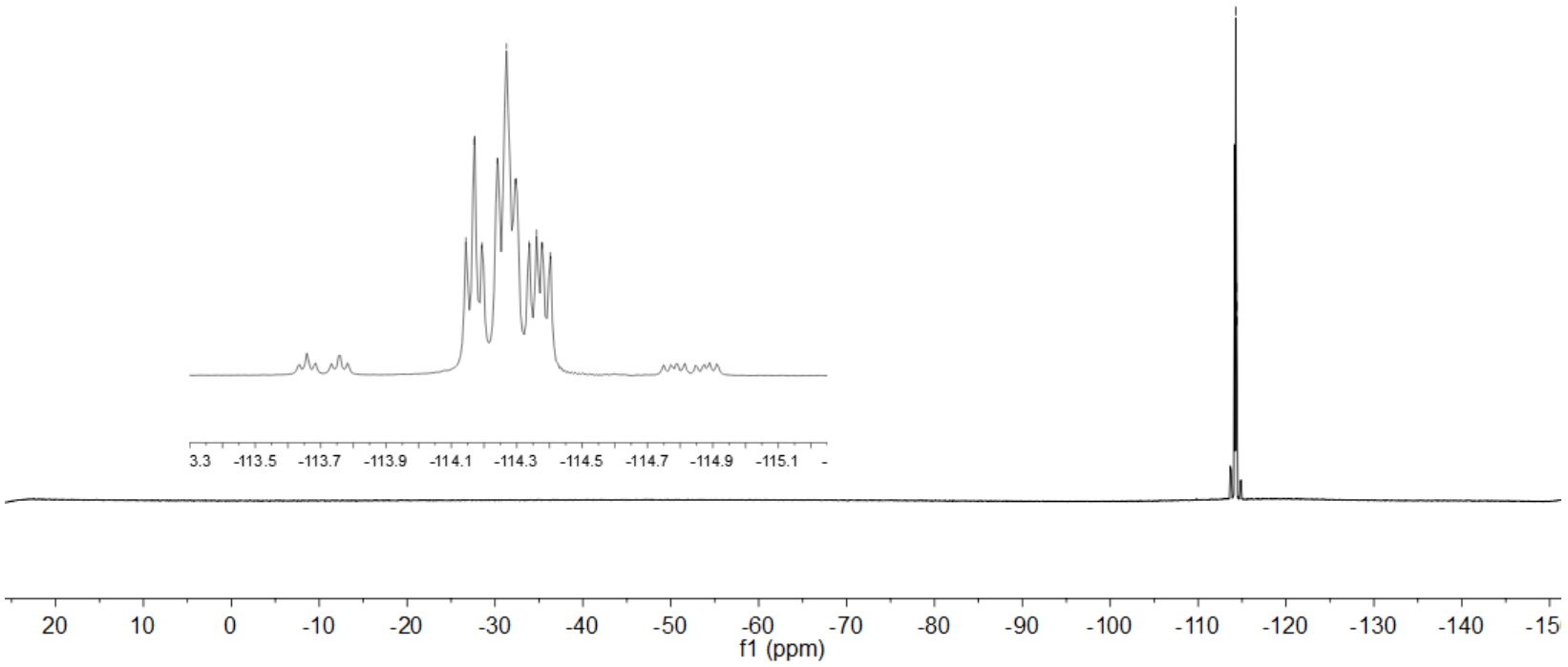
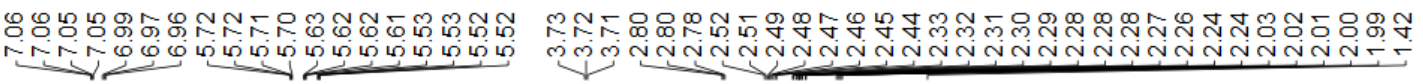
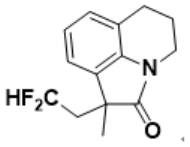
-114.27
-114.30
-114.34
-114.36
-114.38
-114.40

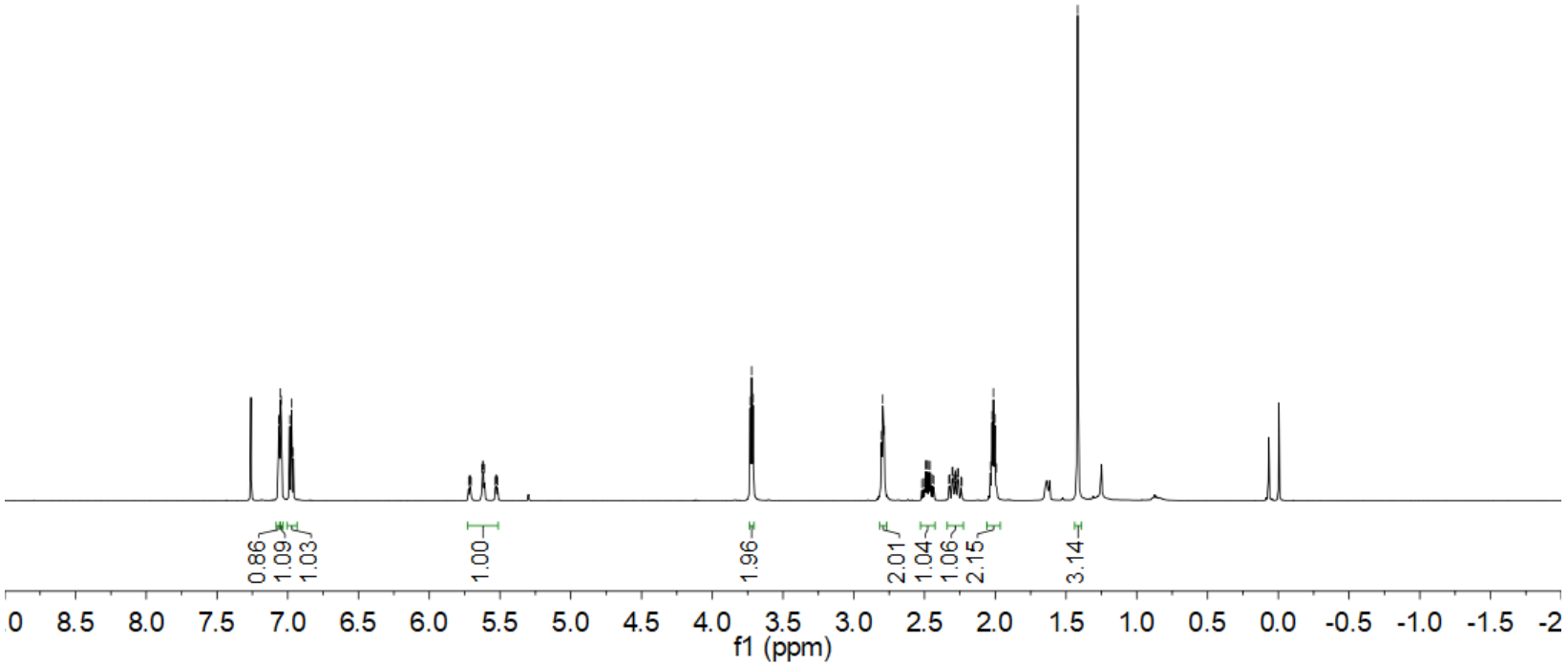

3.3
-113.5
-113.7
-113.9
-114.1
-114.3
-114.5
-114.7
-114.9
-115.1
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

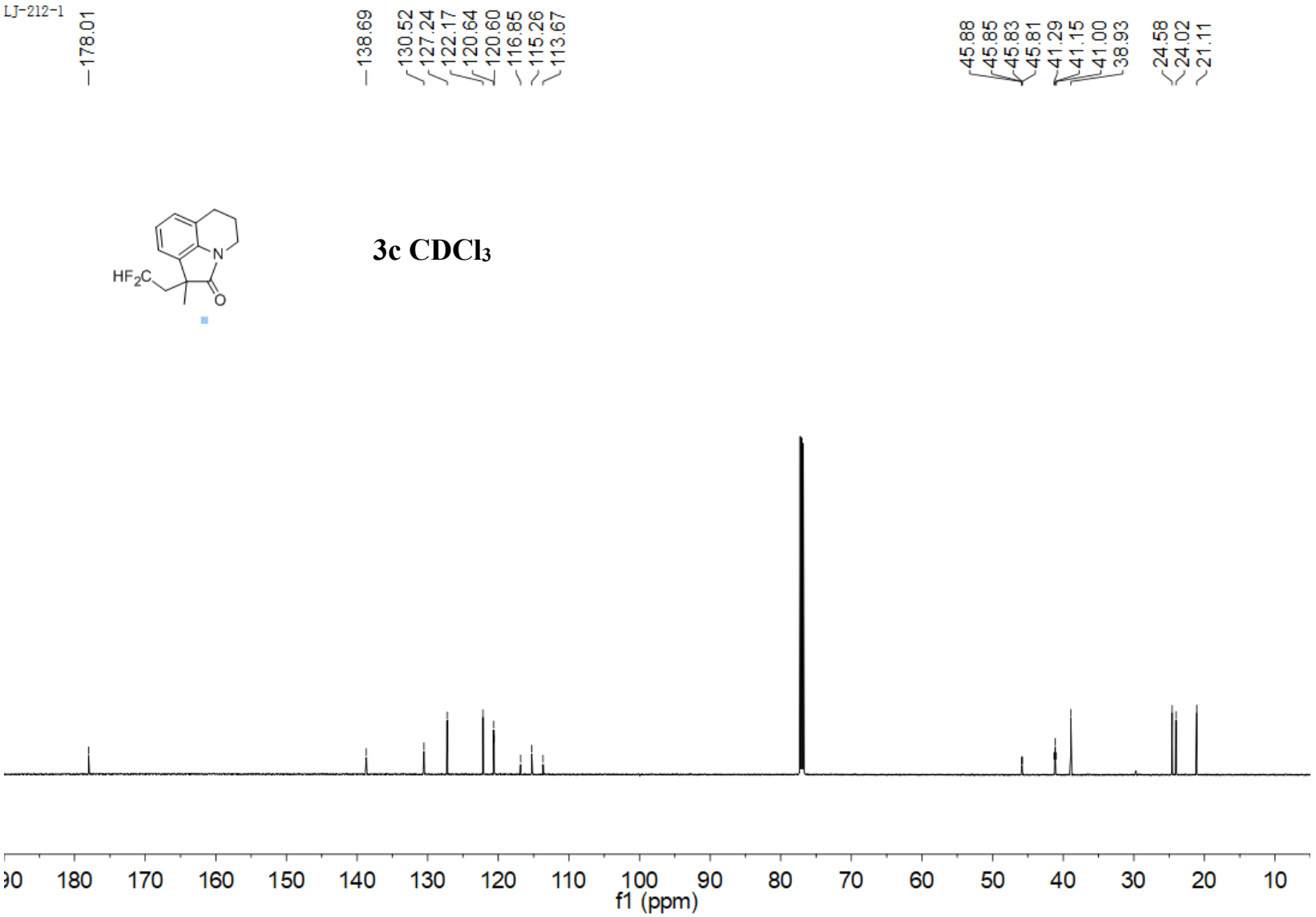
LJ-212-1

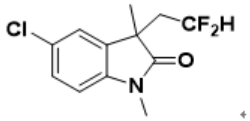




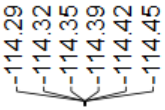
3c $CDCl_3$

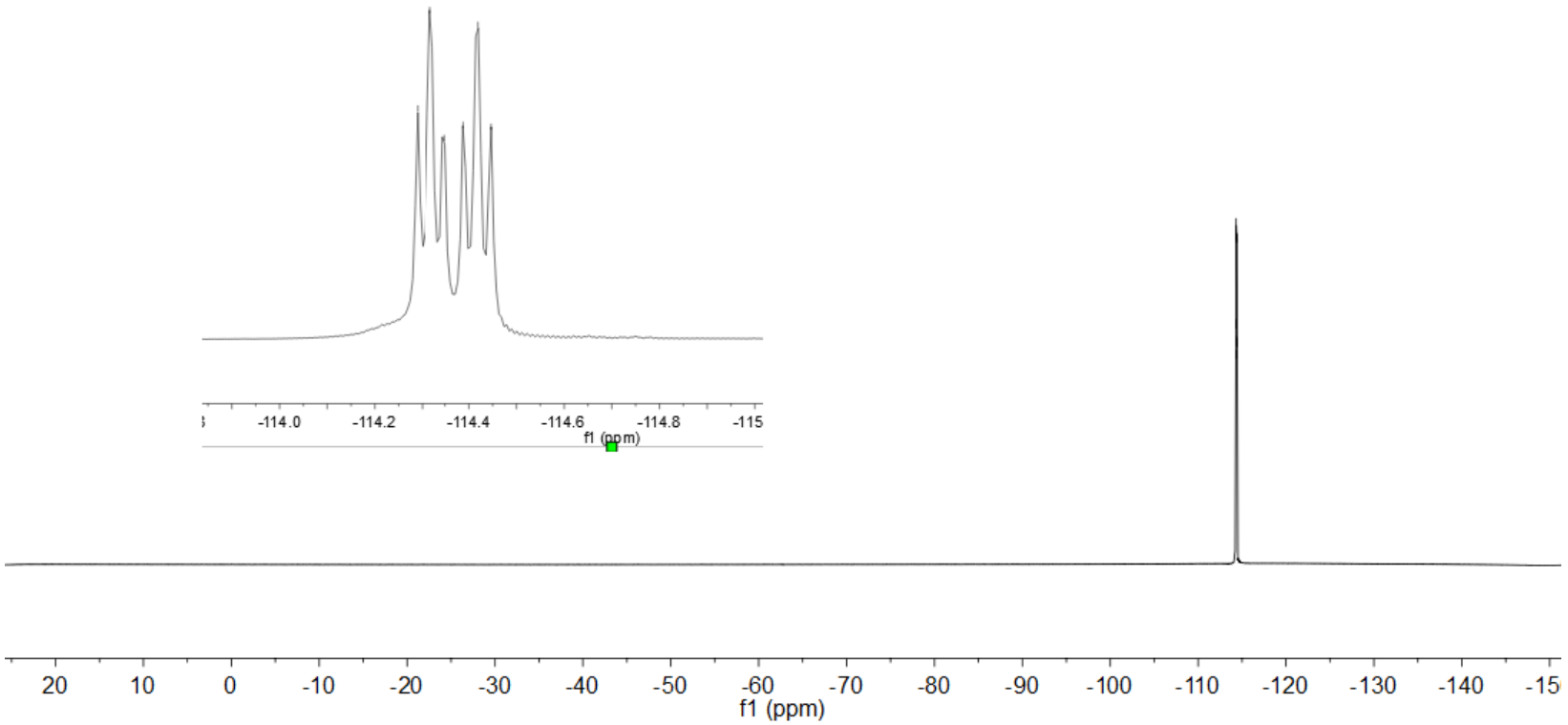



LJ-212-1
178.01
138.69
130.52
127.24
122.17
120.64
120.60
116.85
115.26
113.67
45.88
45.85
45.83
45.81
41.29
41.15
41.00
38.93
24.58
24.02
21.11
HF2C
N
O
3c CDCl3
f1 (ppm)

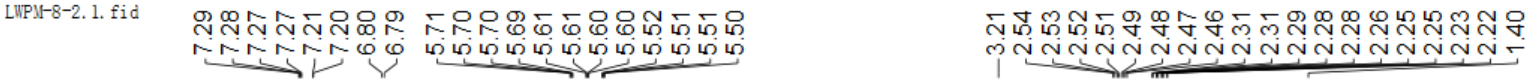

Cl
CF2H
O
N

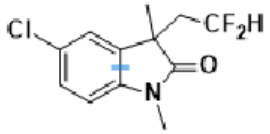
3d $CDCl_3$


-114.29
-114.32
-114.35
-114.39
-114.42
-114.45

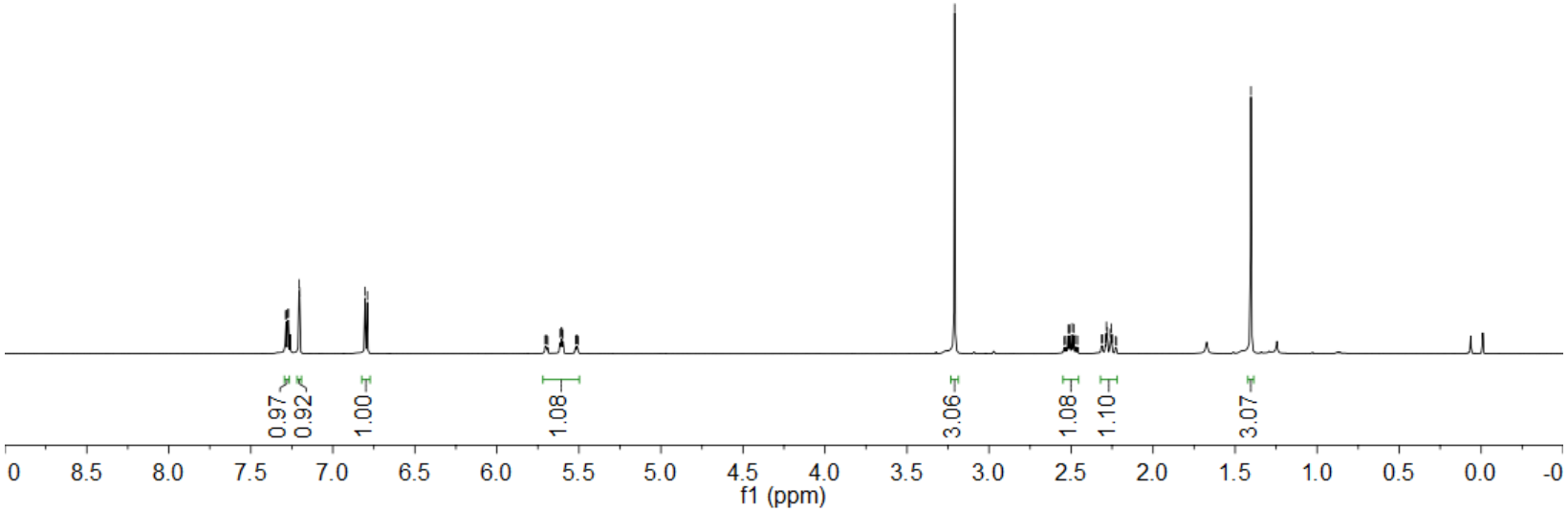

-114.0
-114.2
-114.4
-114.6
-114.8
-115
f1 (ppm)
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

LWPM-8-2.1.fid



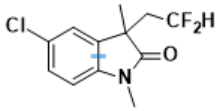


3d $CDCl_3$

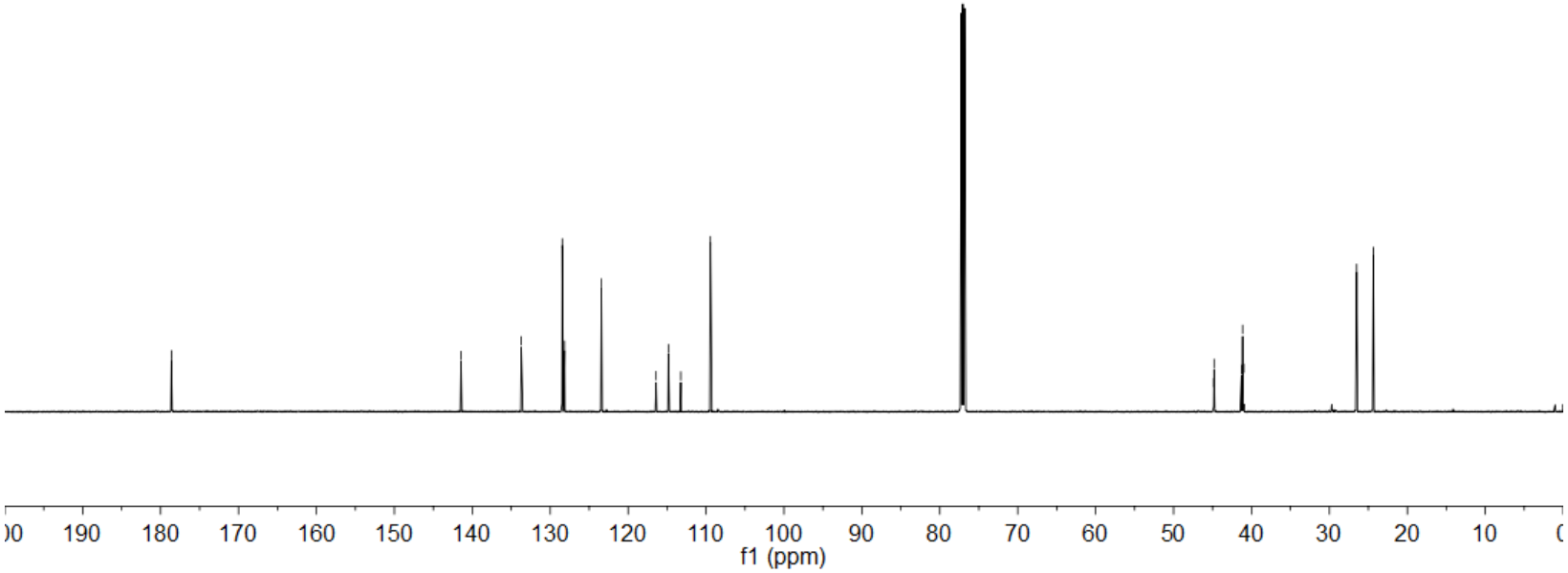


LWPM-8-2

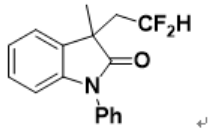
178.61
141.45
133.72
128.45
128.16
123.43
116.42
114.83
113.24
109.44
44.83
44.80
44.76
41.29
41.14
41.00
26.50
24.36



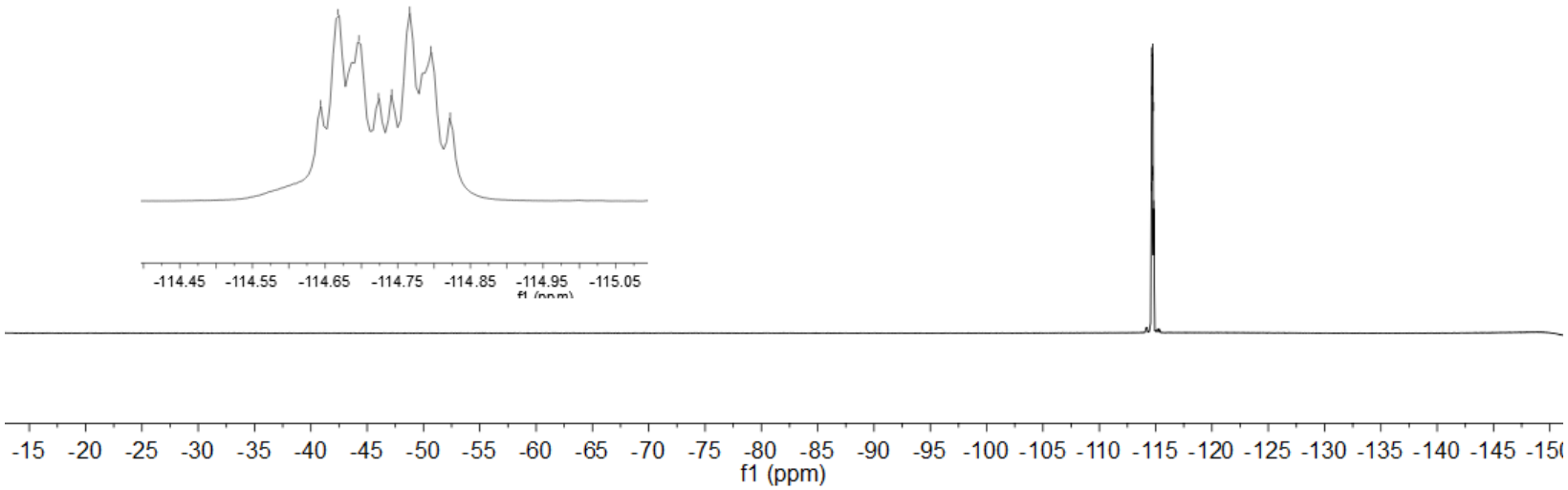
3d $CDCl_3$

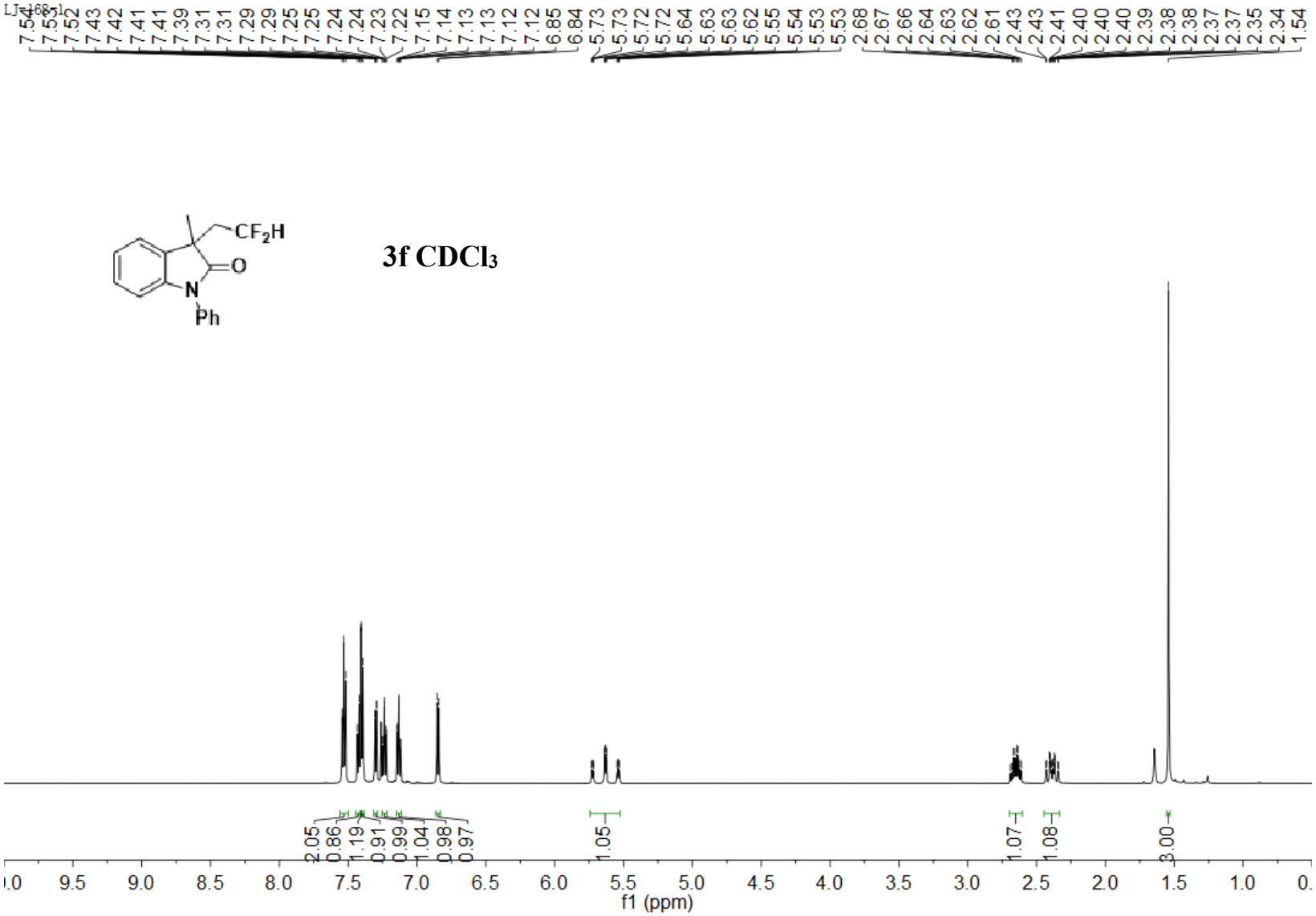


19F_LJ-168-1/2
2018-12-13



3f $CDCl_3$




LJ-168-1
7.54 7.53 7.52 7.43 7.42 7.41 7.41 7.39 7.31 7.31 7.29 7.29 7.25 7.25 7.24 7.24 7.23 7.22 7.15 7.14 7.13 7.13 7.12 7.12 6.85 6.84
5.73 5.73 5.72 5.72 5.64 5.63 5.63 5.62 5.55 5.54 5.53 5.53
2.68 2.67 2.66 2.64 2.63 2.62 2.61 2.43 2.43 2.41 2.40 2.40 2.40 2.39 2.38 2.38 2.37 2.37 2.35 2.34 1.54
CF2H
O
N
Ph
3f CDCl3
2.05 0.86 1.19 0.91 0.99 1.04 0.98 0.97 1.05 1.07 1.08 3.00
f1 (ppm)

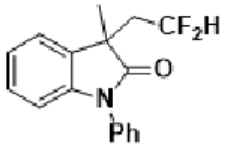
LJ-168-1

178.58

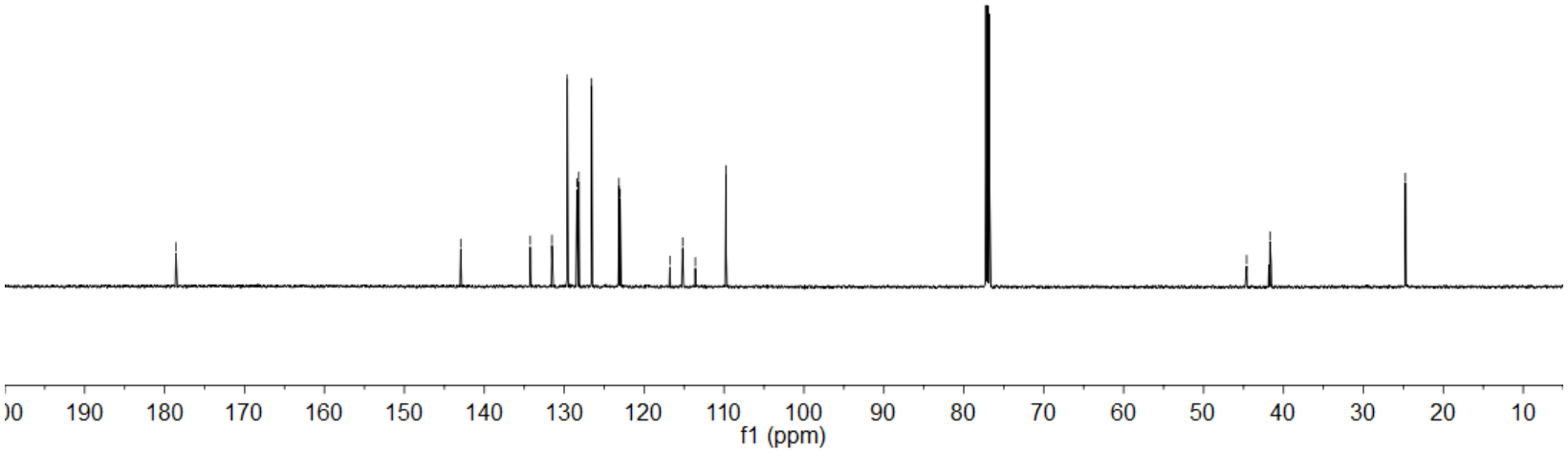
142.95
134.25
131.53
129.62
128.40
128.17
126.57
123.15
123.00
116.77
115.18
113.59
109.76

44.61
41.69

24.74

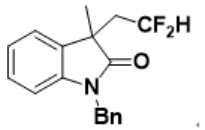


3f $CDCl_3$

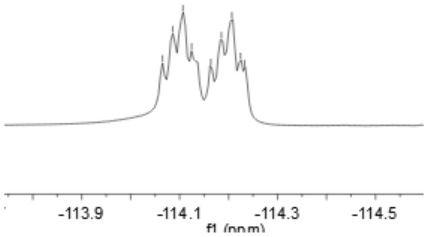


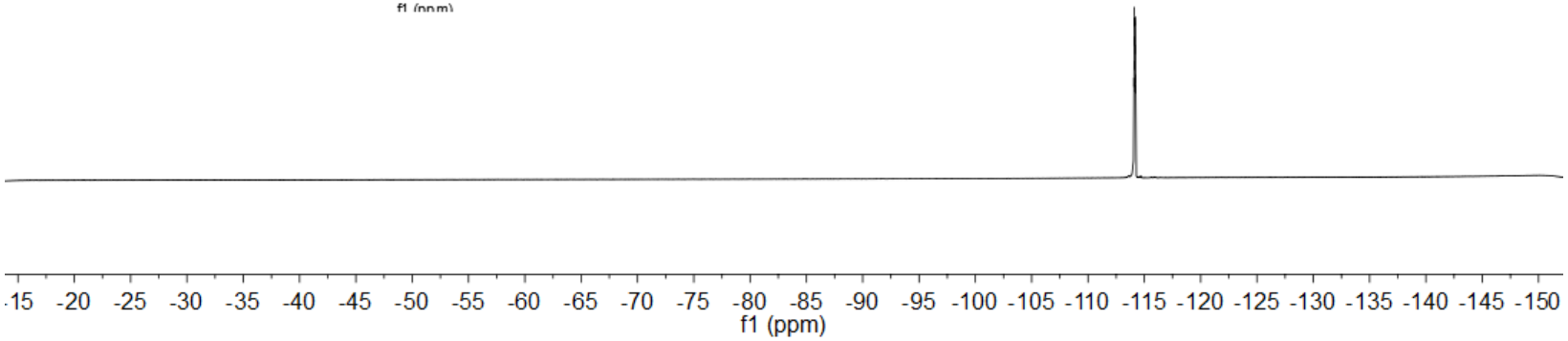
19F_LJ-168-2/2
2018-12-13

114.06
114.09
114.11
114.12
114.16
114.19
114.21
114.22
114.23



3g $CDCl_3$

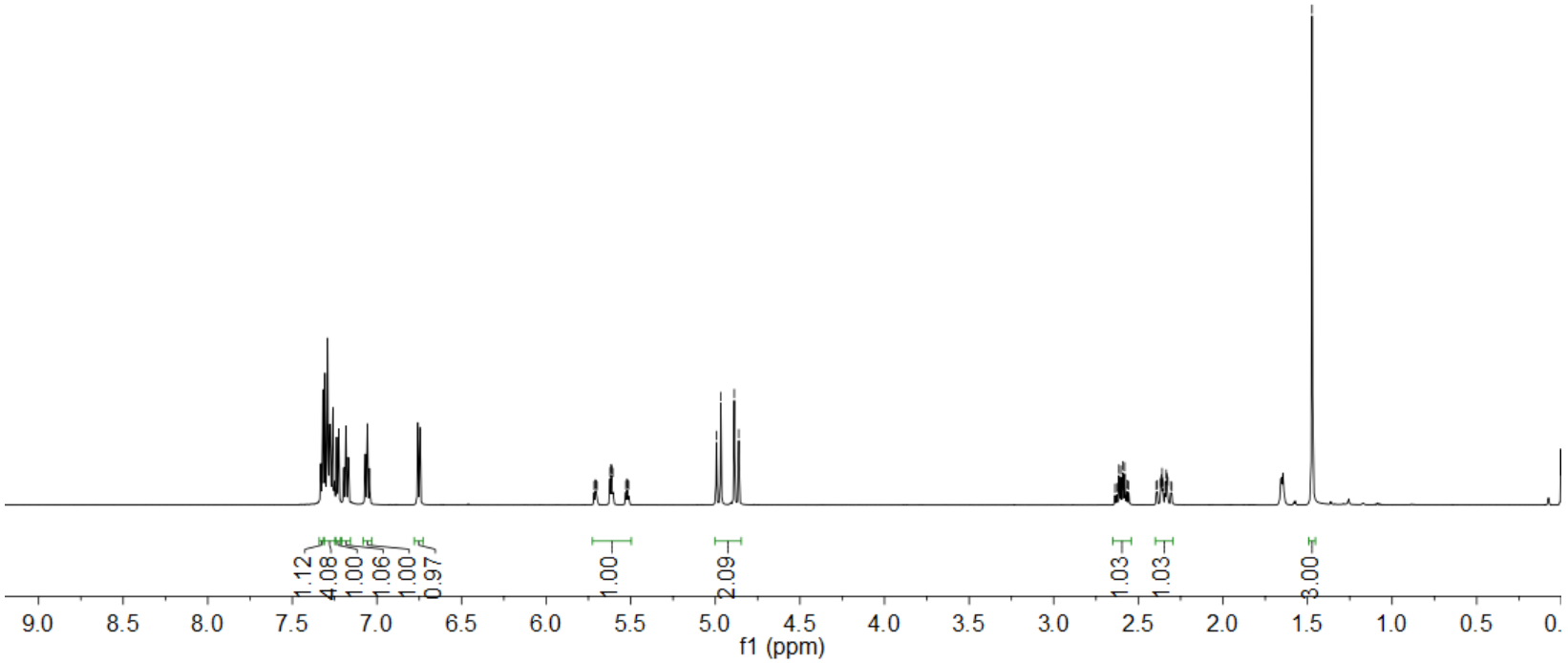




LJ-168-2

5.72 5.71 5.71 5.70 5.62 5.62 5.61 5.61 5.53 5.52 5.52 5.51 4.99 4.97 4.89 4.86 2.64 2.63 2.61 2.60 2.59 2.58 2.57 2.56 2.39 2.39 2.37 2.37 2.36 2.36 2.35 2.34 2.34 2.33 2.33 2.33 2.31 2.30 1.47

3g $CDCl_3$



LJ-168-2

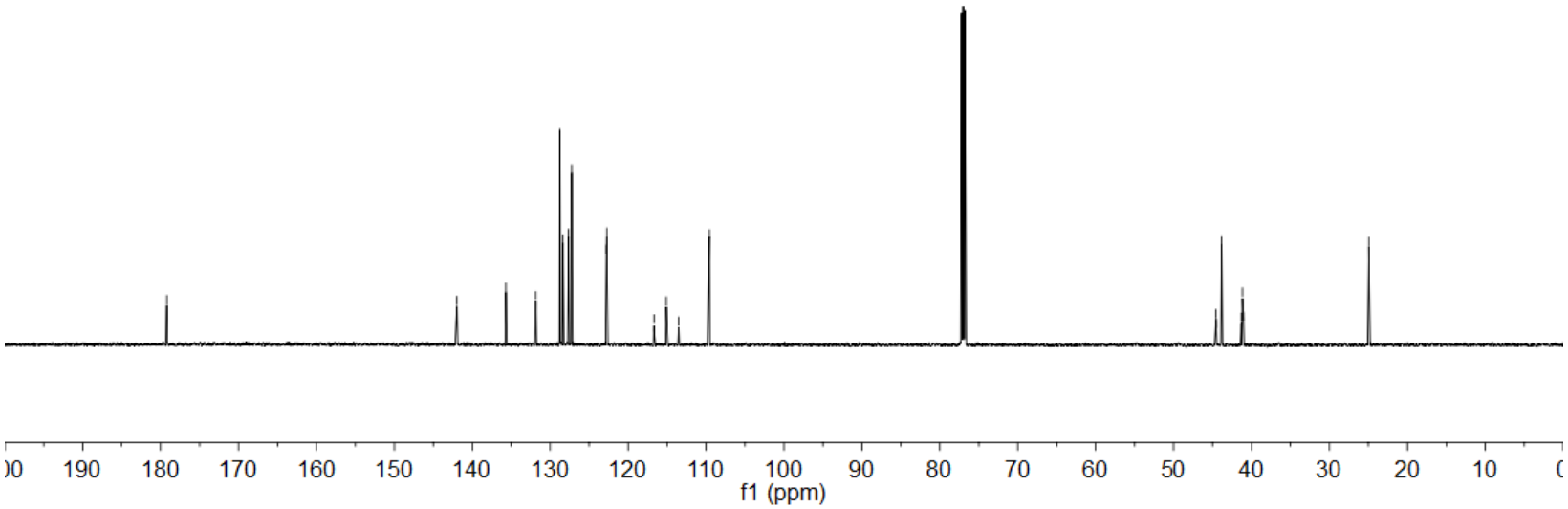
179.20

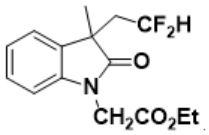
141.97
135.68
131.84
128.77
128.37
127.63
127.22
122.79
122.74
116.68
115.09
113.50
109.57

44.59
44.55
44.51
43.83
41.31
41.17
41.02

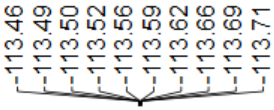
24.95

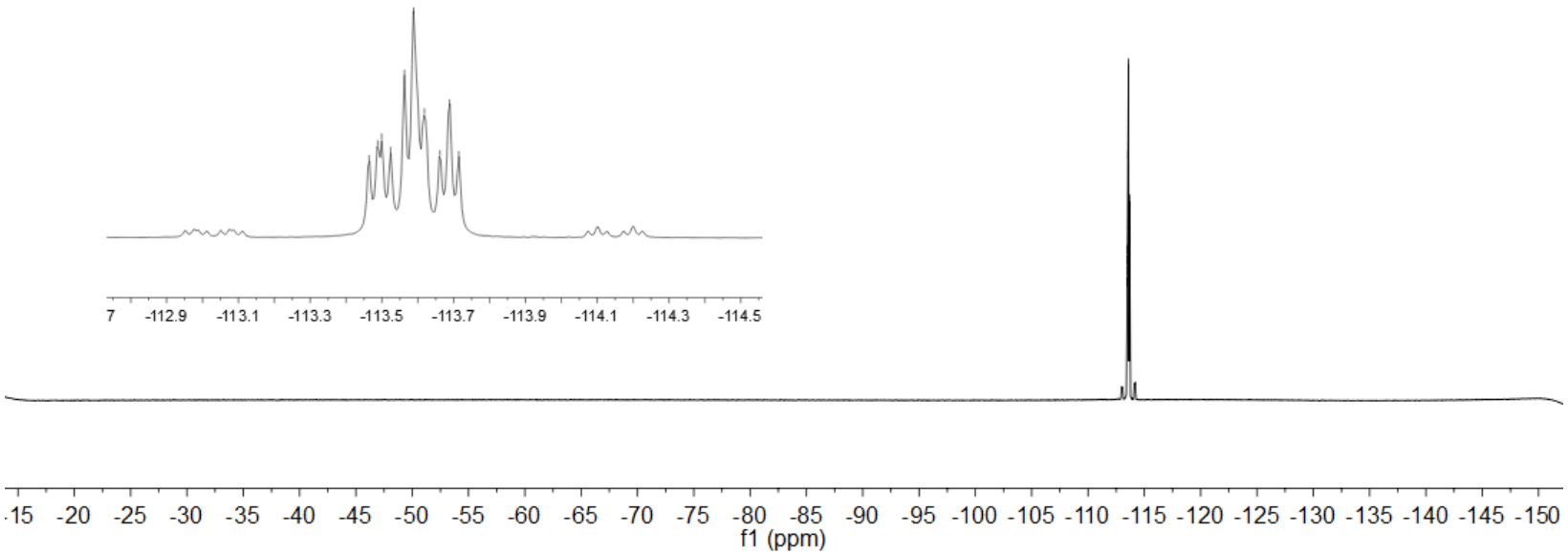
3g $CDCl_3$

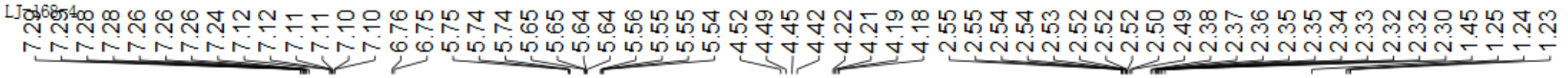


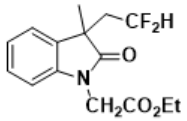

CF2H
O
N
CH2CO2Et

3h $CDCl_3$

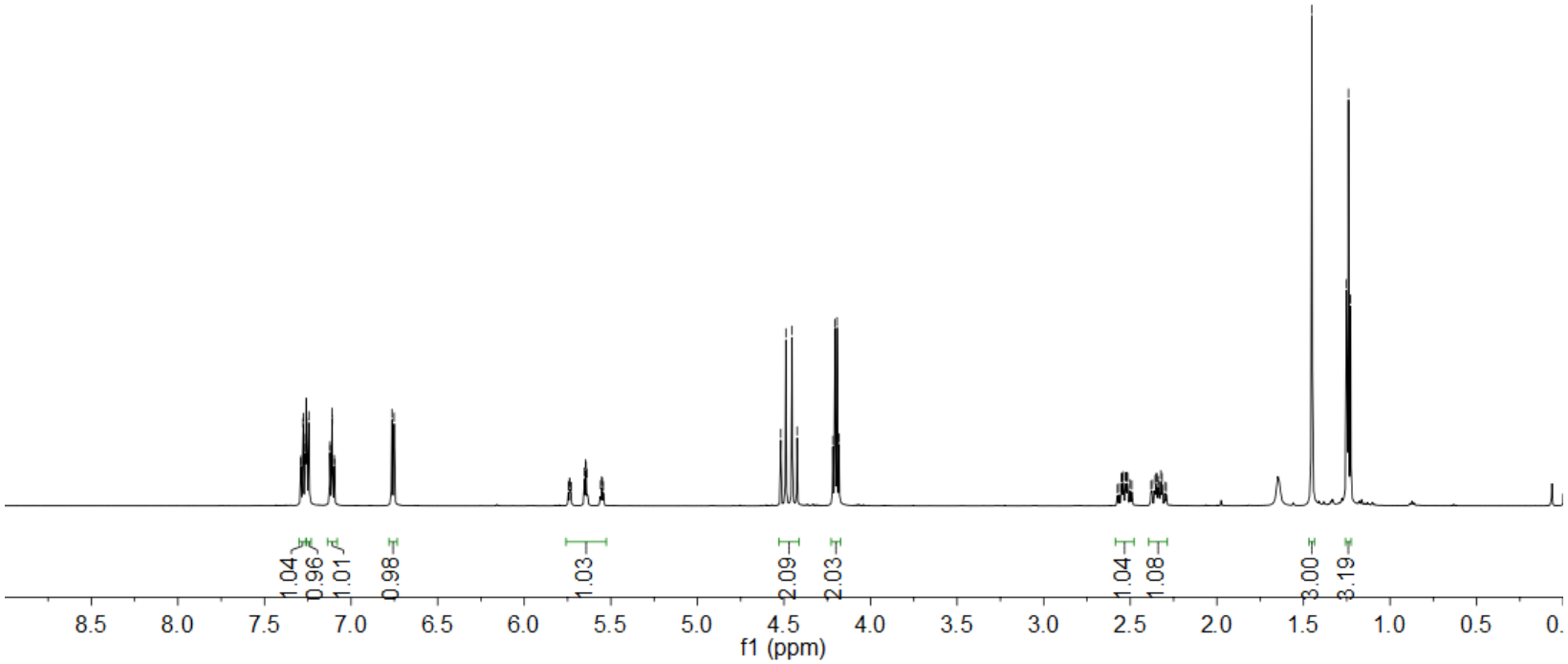

-113.46
-113.49
-113.50
-113.52
-113.56
-113.59
-113.62
-113.66
-113.69
-113.71

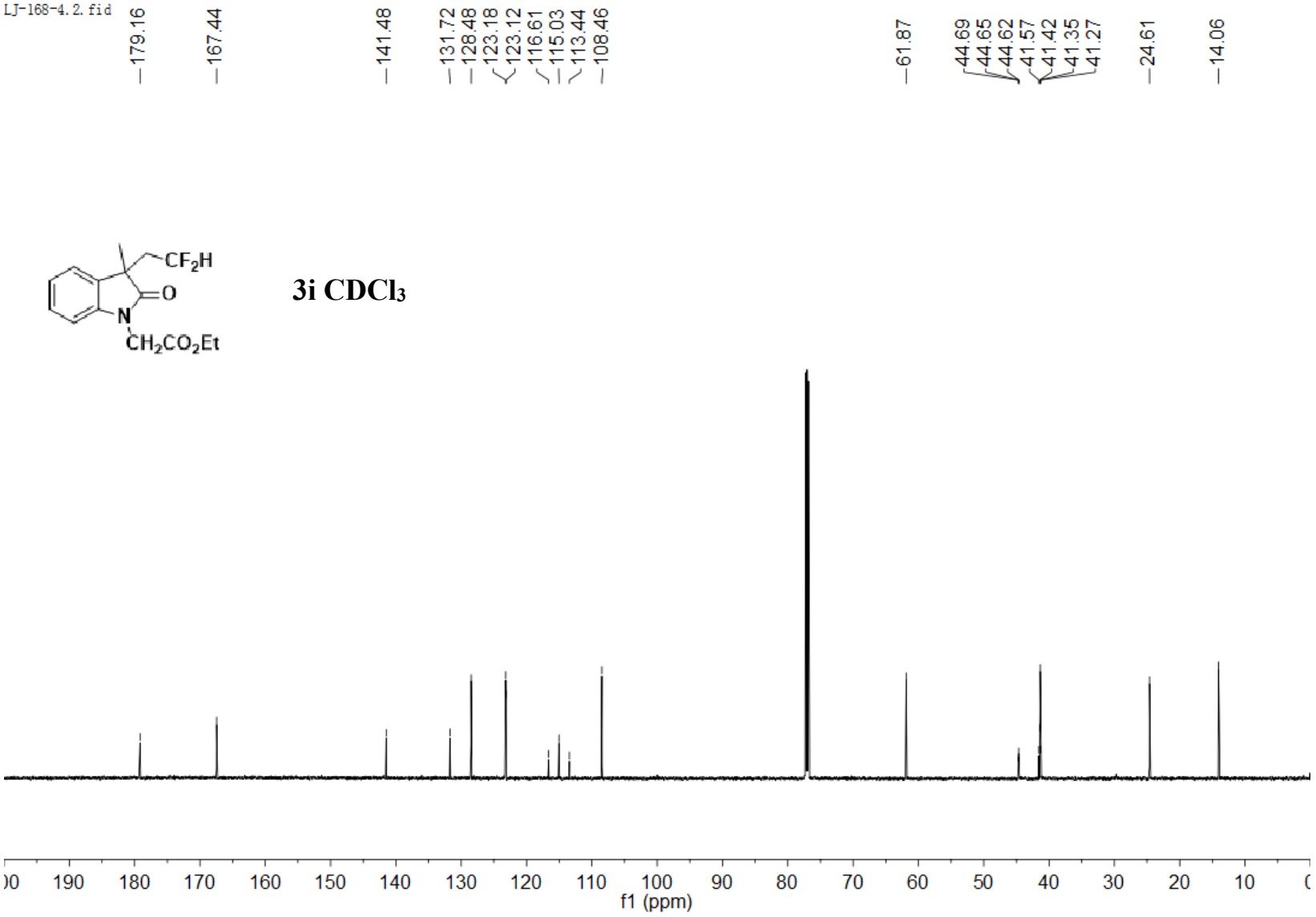

7 -112.9 -113.1 -113.3 -113.5 -113.7 -113.9 -114.1 -114.3 -114.5
15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

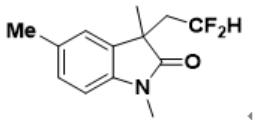

7.29
7.28
7.28
7.28
7.26
7.26
7.26
7.24
7.12
7.12
7.11
7.11
7.10
7.10
6.76
6.75
5.75
5.74
5.74
5.65
5.65
5.64
5.64
5.56
5.55
5.55
5.54
4.52
4.49
4.45
4.42
4.22
4.21
4.19
4.18
2.55
2.55
2.54
2.54
2.53
2.52
2.52
2.52
2.50
2.49
2.38
2.37
2.36
2.35
2.35
2.34
2.33
2.32
2.32
2.30
1.45
1.25
1.24
1.23


CF2H
O
N
CH2CO2Et

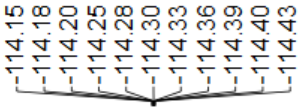
3h $CDCl_3$

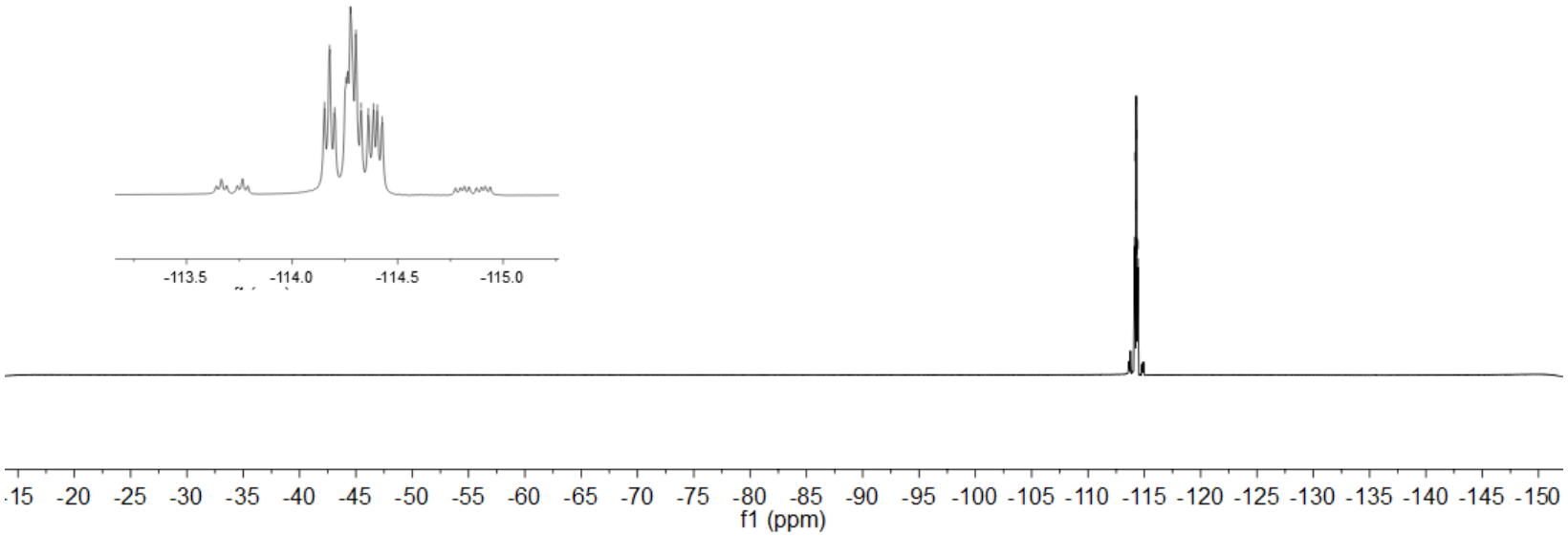

1.04
0.96
1.01
0.98
1.03
2.09
2.03
1.04
1.08
3.00
3.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)


LJ-168-4.2.fid
179.16
167.44
141.48
131.72
128.48
123.18
123.12
116.61
115.03
113.44
108.46
61.87
44.69
44.65
44.62
41.57
41.42
41.35
41.27
24.61
14.06
CF2H
O
N
CH2CO2Et
3i CDCl3
f1 (ppm)


Me
CF2H
O
N

3i $CDCl_3$

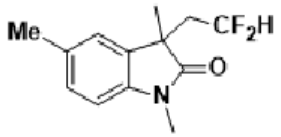

-114.15
-114.18
-114.20
-114.25
-114.28
-114.30
-114.33
-114.36
-114.39
-114.40
-114.43


-113.5
-114.0
-114.5
-115.0
-15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

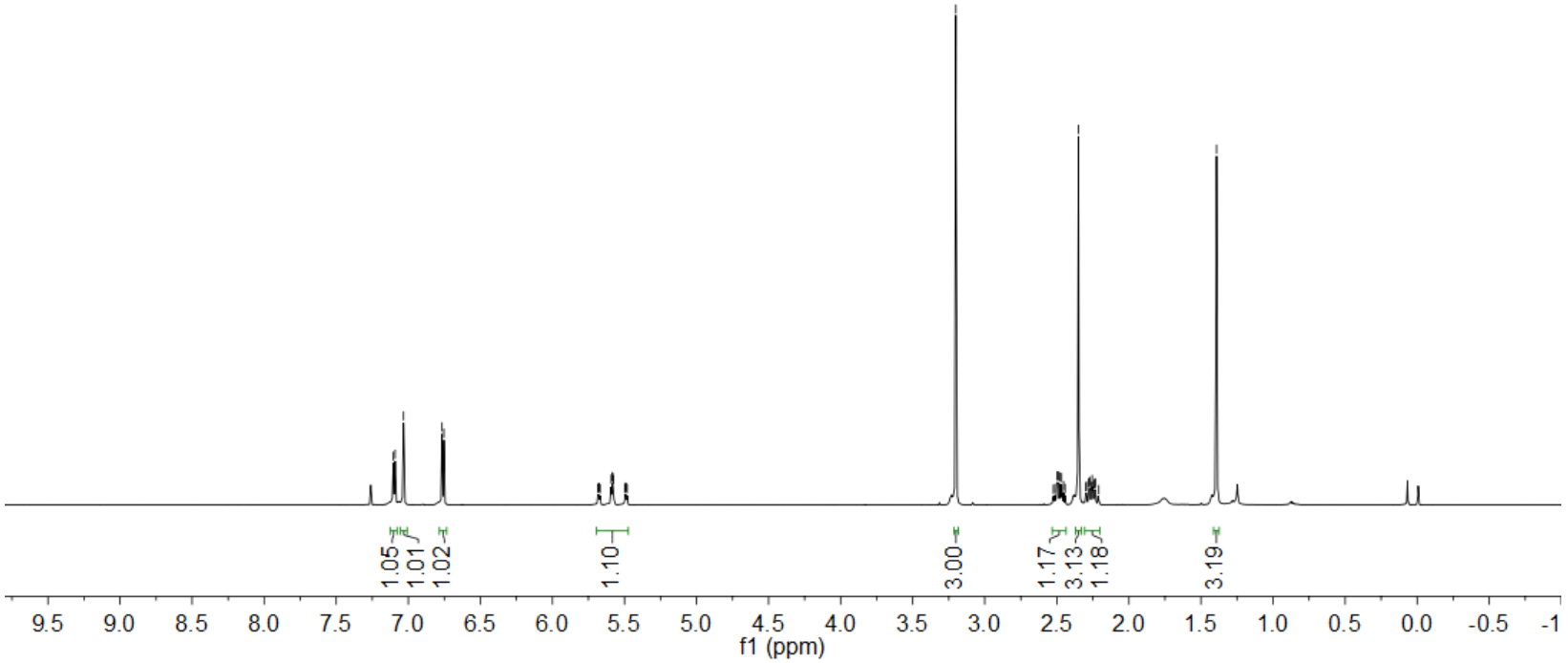
LPZX-14.1.fid

7.10 7.09 7.03 6.77 6.75 5.69 5.68 5.67 5.67 5.59 5.59 5.58 5.58 5.50 5.49 5.49 5.48

3.20 2.52 2.51 2.50 2.49 2.48 2.47 2.45 2.44 2.35 2.30 2.29 2.28 2.28 2.27 2.26 2.25 2.25 2.24 2.24 2.23 2.21 1.39

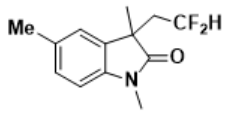


3i $CDCl_3$

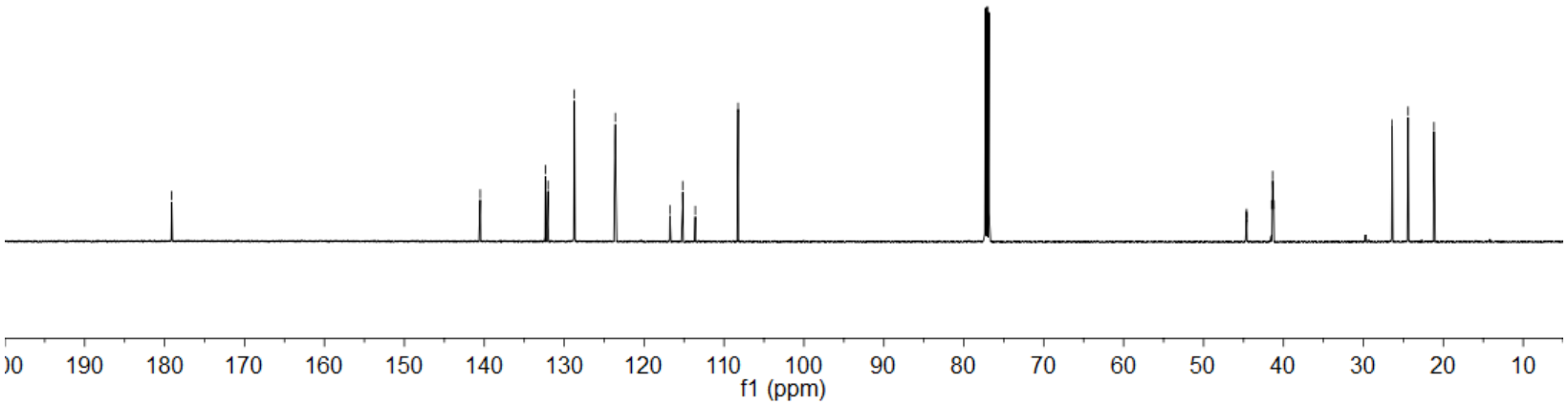


LPZX-14.2.fid

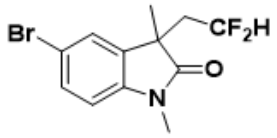
179.10
140.51
132.36
132.04
128.73
123.61
116.77
115.18
113.59
108.23
44.67
44.64
44.62
44.60
41.51
41.36
41.22
26.40
24.40
21.16



3i $CDCl_3$



19F_LPZX-9/1
2018-



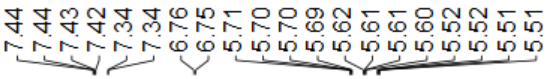
3j $CDCl_3$

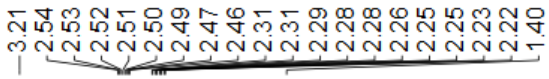
-114.32
-114.35
-114.38
-114.42
-114.45
-114.48

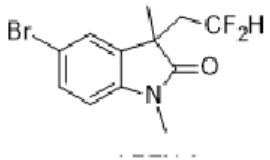
-113.9 -114.1 -114.3 -114.5 -114.7 -114.9 -115.1

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -15
f1 (ppm)

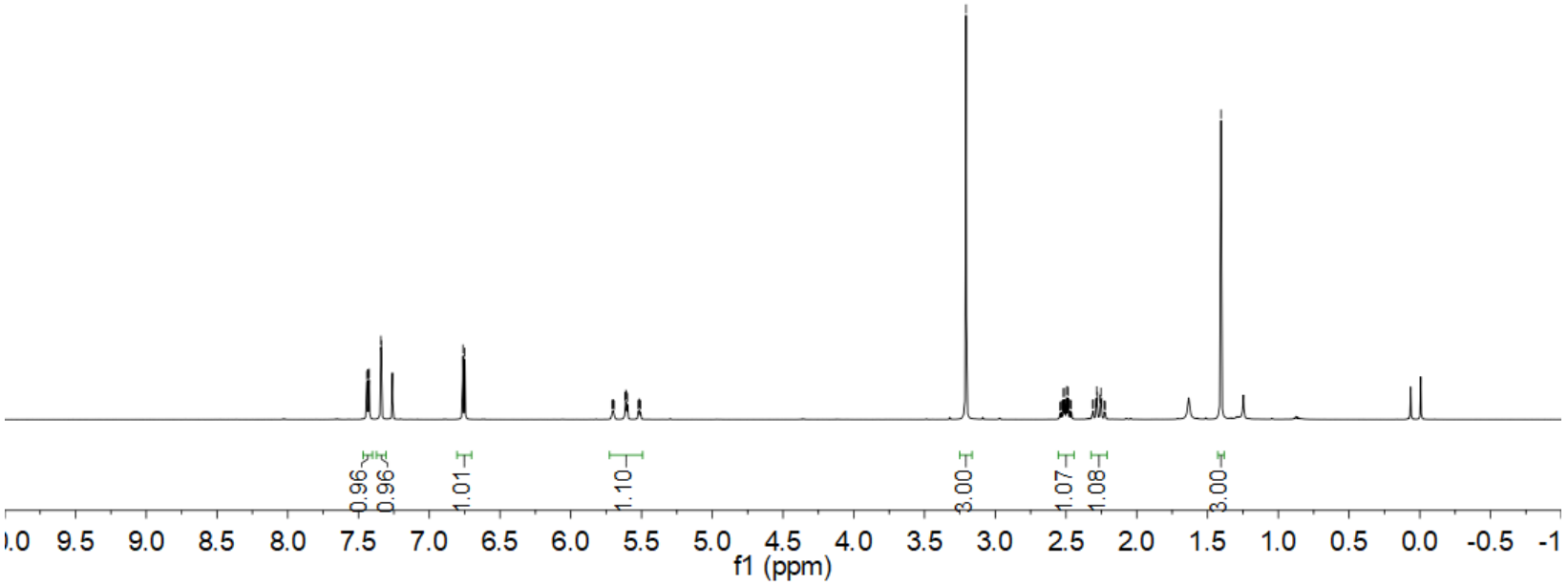
LP2X-9

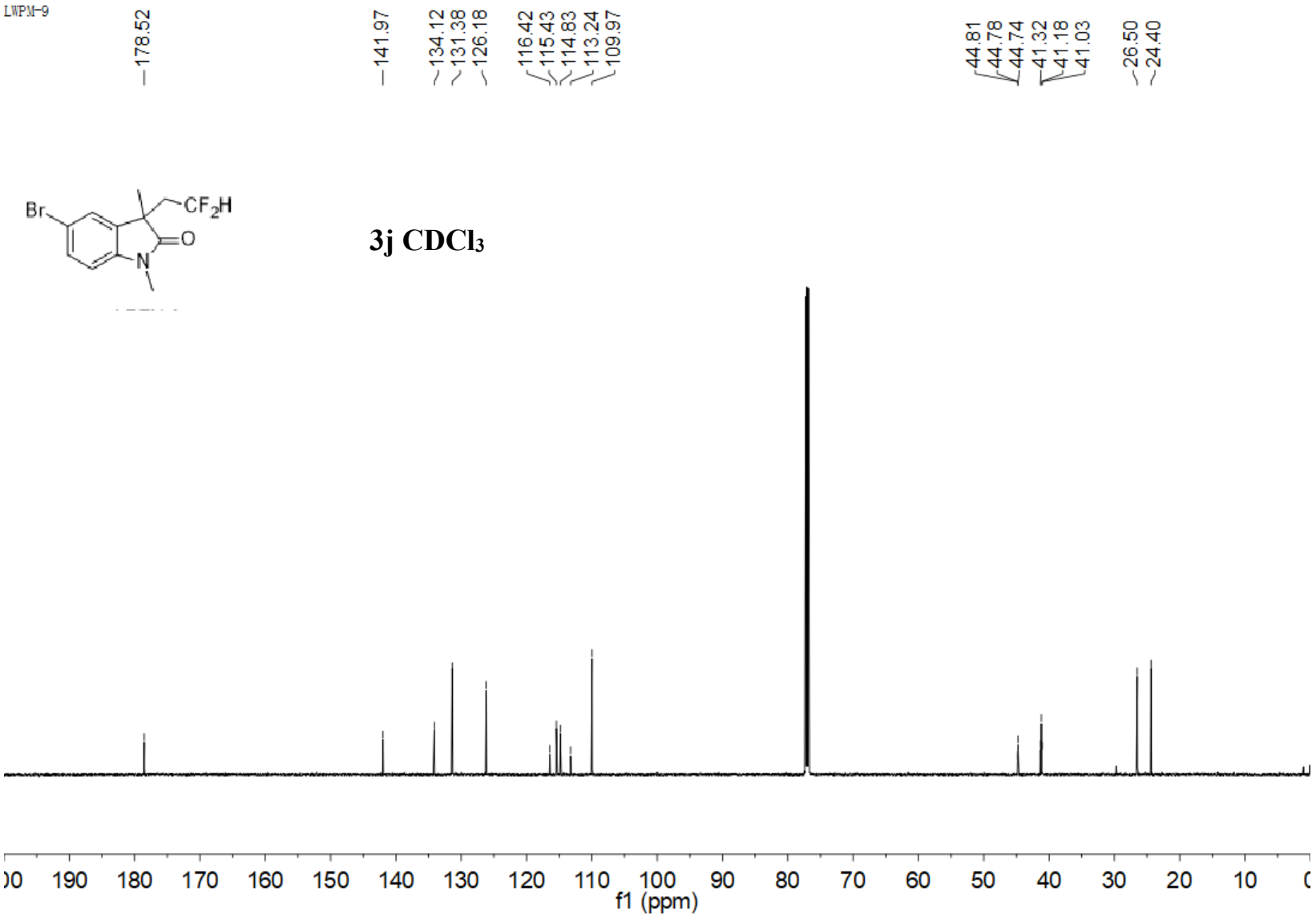


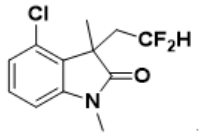


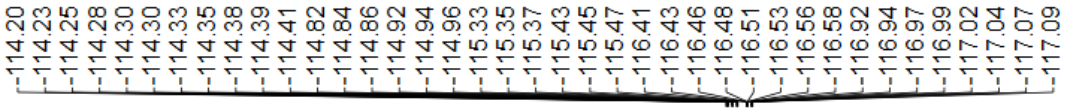


3j $CDCl_3$

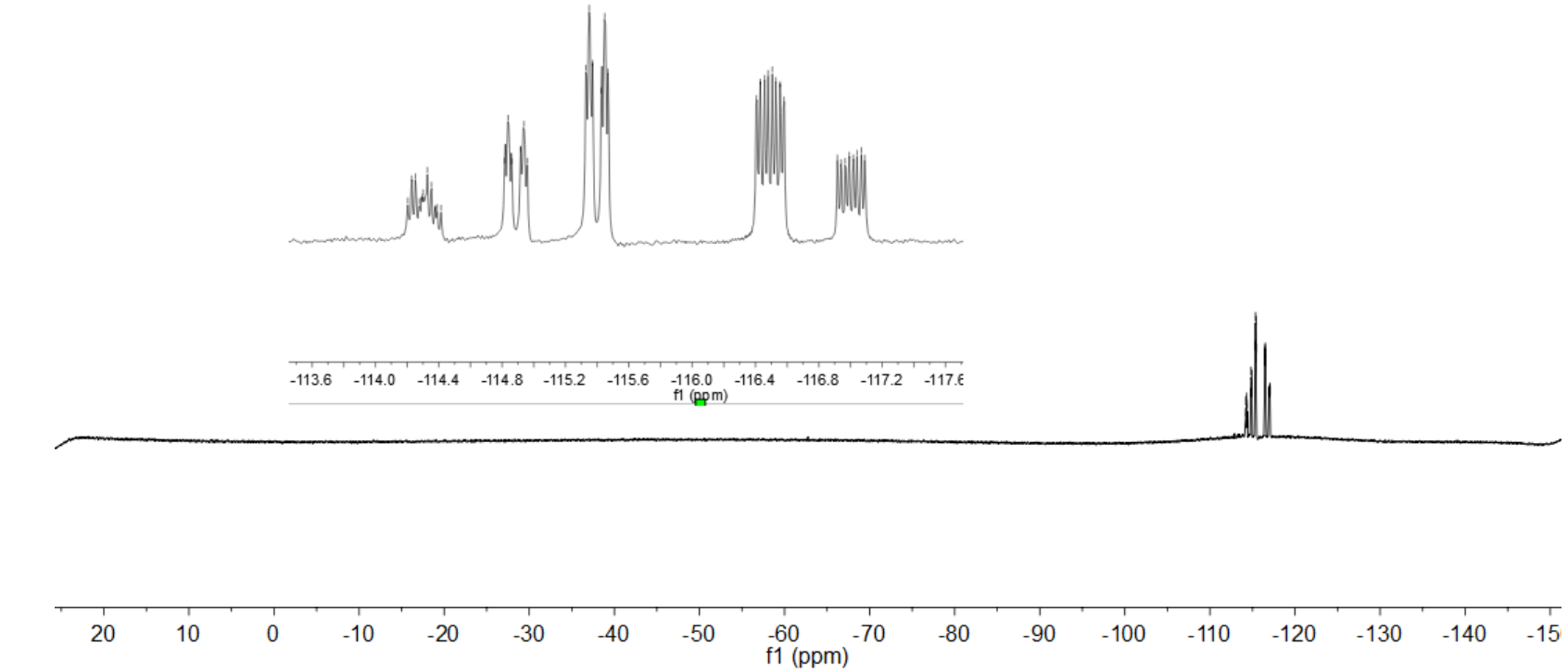



LWPM-9
178.52
141.97
134.12
131.38
126.18
116.42
115.43
114.83
113.24
109.97
44.81
44.78
44.74
41.32
41.18
41.03
26.50
24.40
Br
CF2H
O
N
3j CDCl3
f1 (ppm)

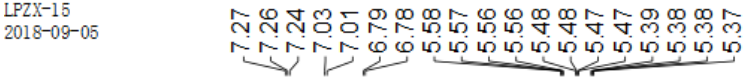

Cl
CF2H
O
N

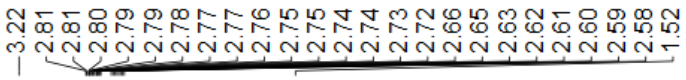

-114.20
-114.23
-114.25
-114.28
-114.30
-114.30
-114.33
-114.35
-114.38
-114.39
-114.41
-114.82
-114.84
-114.86
-114.92
-114.94
-114.96
-115.33
-115.35
-115.37
-115.43
-115.45
-115.47
-116.41
-116.43
-116.46
-116.48
-116.51
-116.53
-116.56
-116.58
-116.92
-116.94
-116.97
-116.99
-117.02
-117.04
-117.07
-117.09

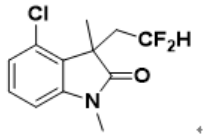
3k $CDCl_3$


-113.6
-114.0
-114.4
-114.8
-115.2
-115.6
-116.0
-116.4
-116.8
-117.2
f1 (ppm)
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

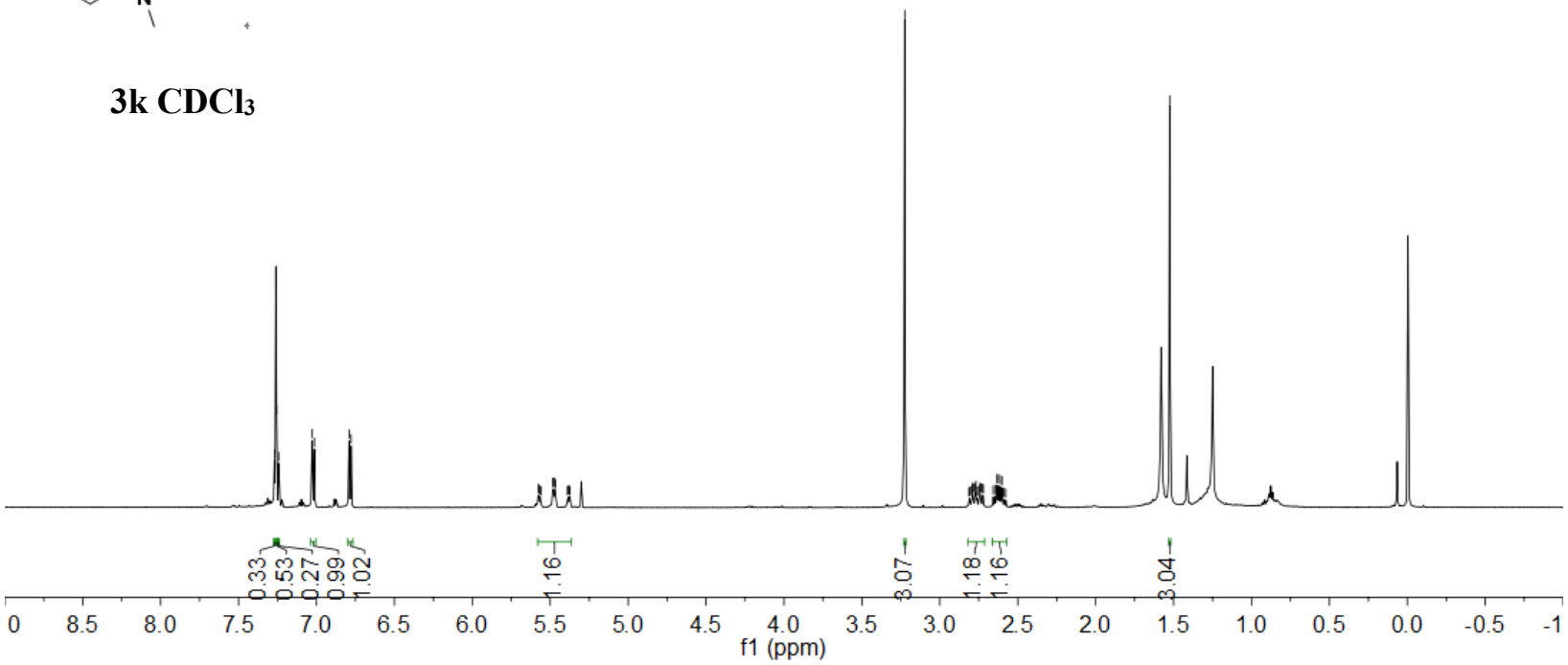
LPZX-15
2018-09-05

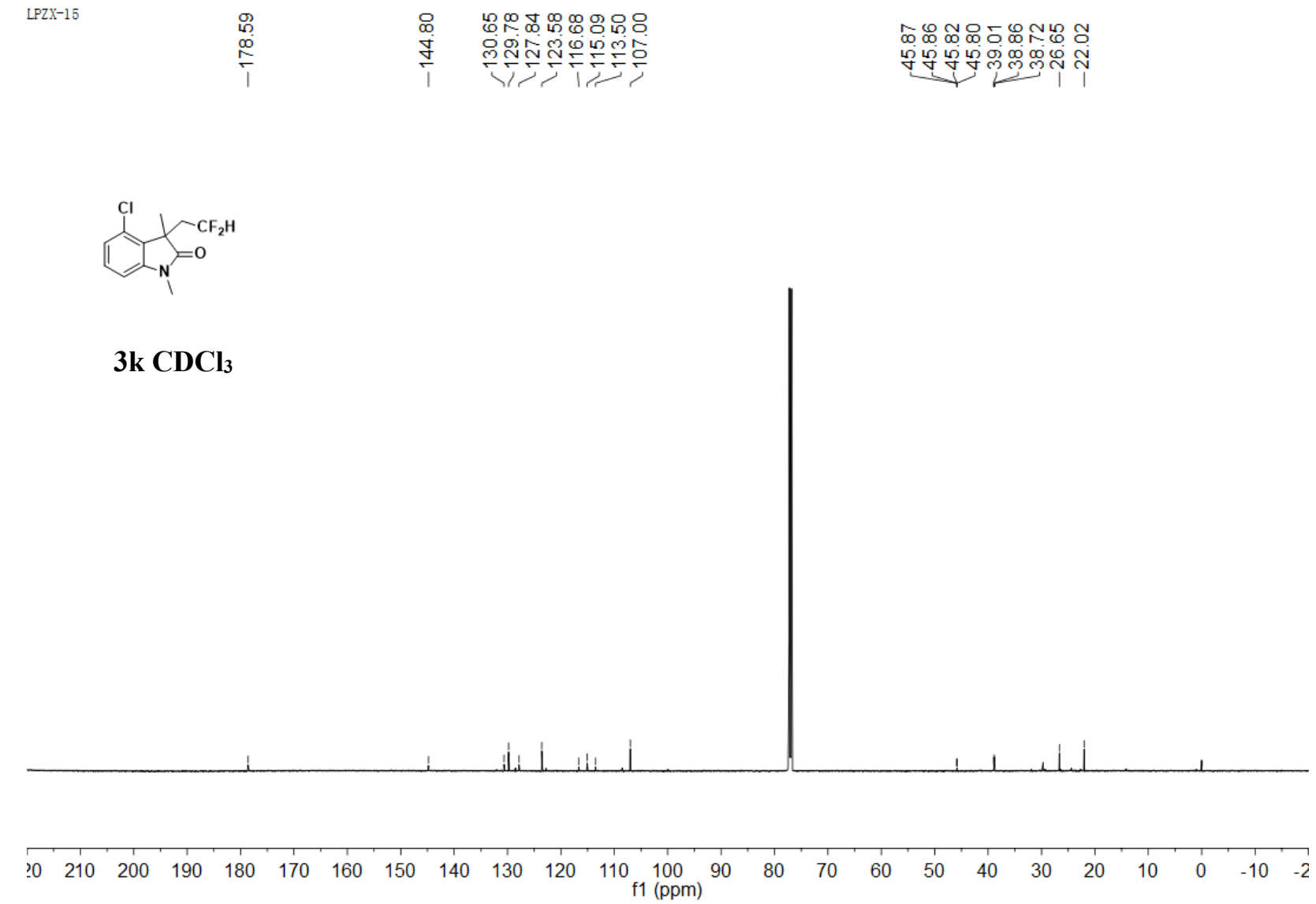




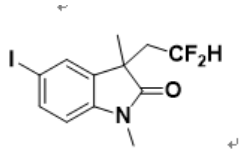


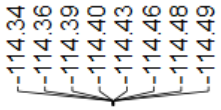
3k $CDCl_3$



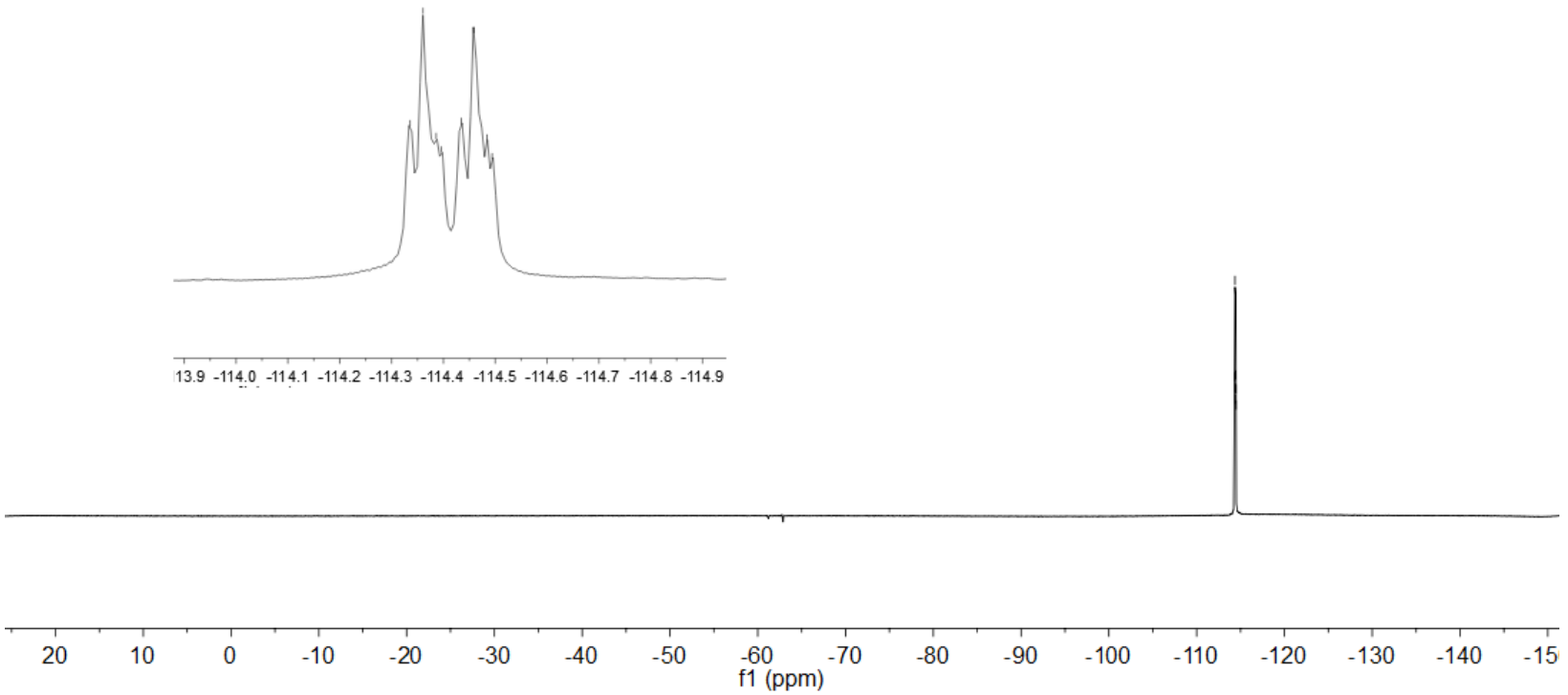

LPZX-15
178.59
144.80
130.65
129.78
127.84
123.58
116.68
115.09
113.50
107.00
45.87
45.86
45.82
45.80
39.01
38.86
38.72
26.65
22.02
Cl
CF2H
O
N
f1 (ppm)

3k $CDCl_3$


I
CF2H
O
N

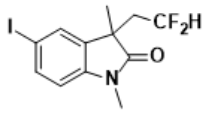

-114.34
-114.36
-114.39
-114.40
-114.43
-114.46
-114.48
-114.49

3l $CDCl_3$

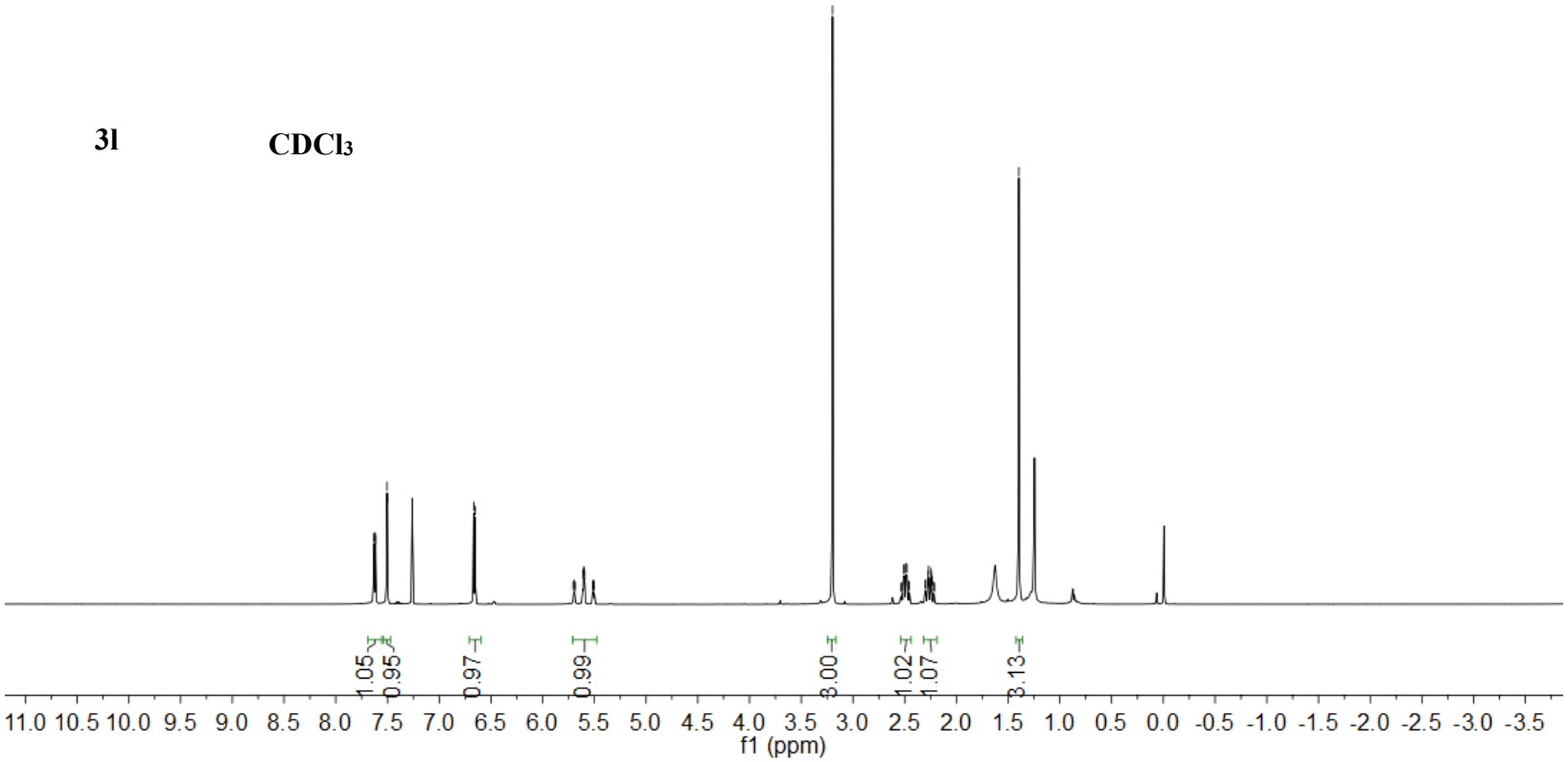

13.9 -114.0 -114.1 -114.2 -114.3 -114.4 -114.5 -114.6 -114.7 -114.8 -114.9
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -15
f1 (ppm)

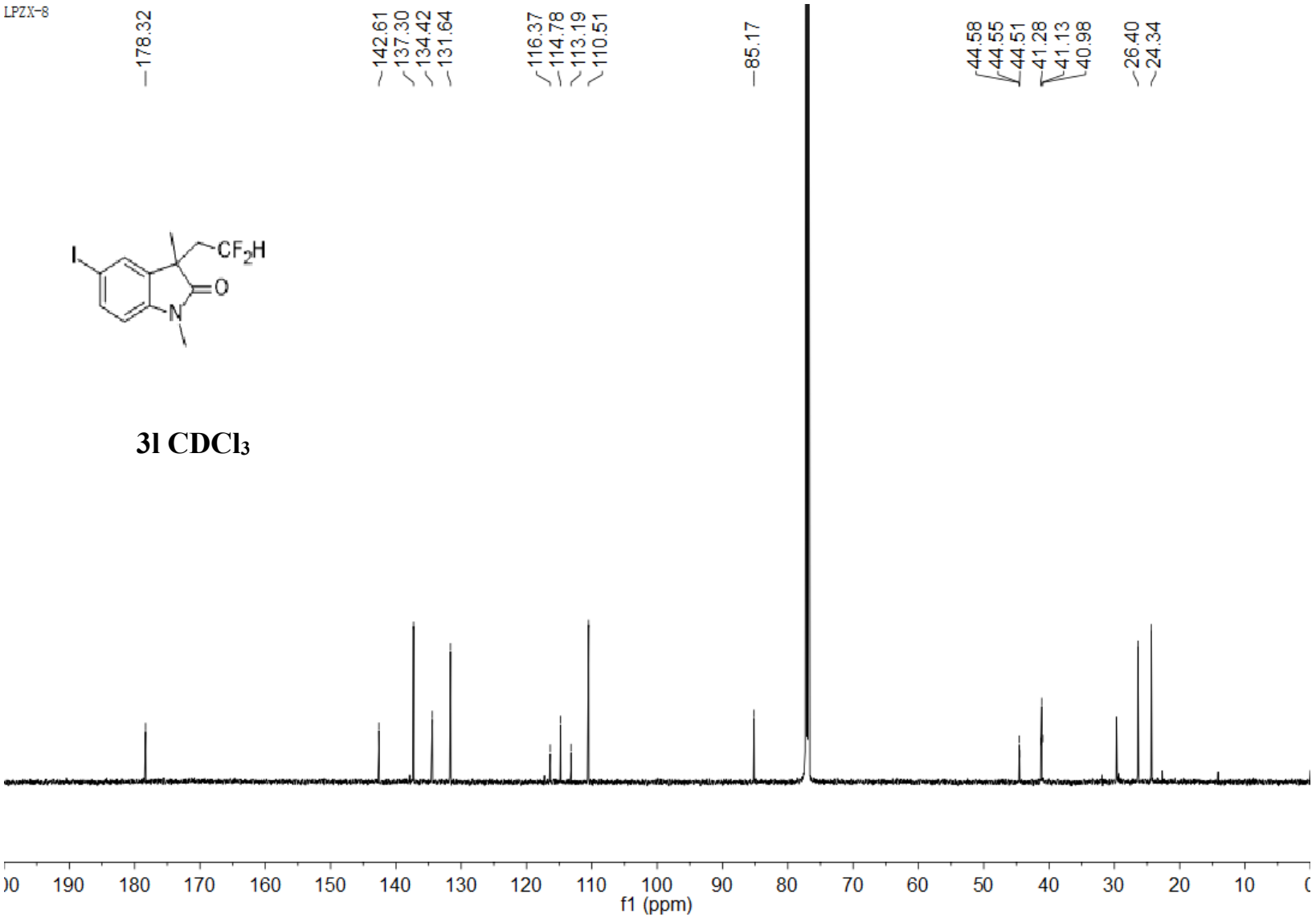
LPZX-8
2018-09-04

7.63 7.63 7.62 7.61 7.50 7.50 6.67 6.65 5.70 5.70 5.69 5.69 5.61 5.60 5.60 5.59 5.52 5.51 5.51 5.50 3.20 2.54 2.53 2.51 2.50 2.49 2.48 2.46 2.45 2.30 2.30 2.28 2.27 2.26 2.25 2.25 2.24 2.24 2.24 2.22 2.21 1.40



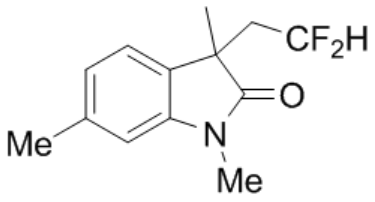
3l **$CDCl_3$**

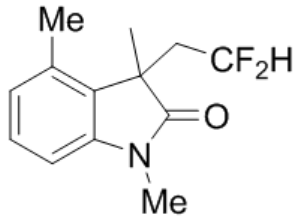



LPZX-8
178.32
142.61
137.30
134.42
131.64
116.37
114.78
113.19
110.51
85.17
44.58
44.55
44.51
41.28
41.13
40.98
26.40
24.34
I
CF2H
O
N
f1 (ppm)

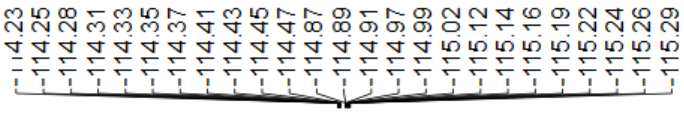
3l $CDCl_3$

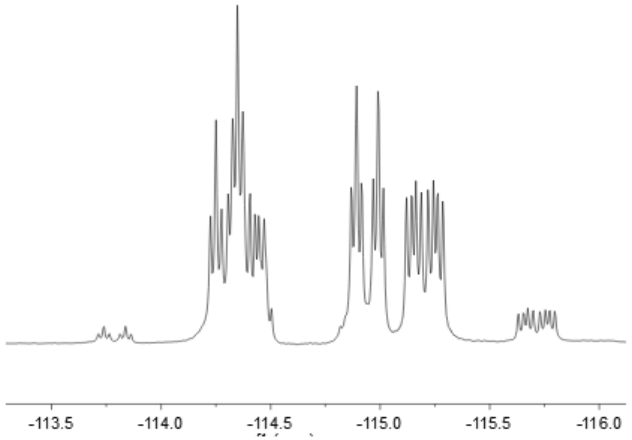
19F_LYS-30/2
2018-12-13

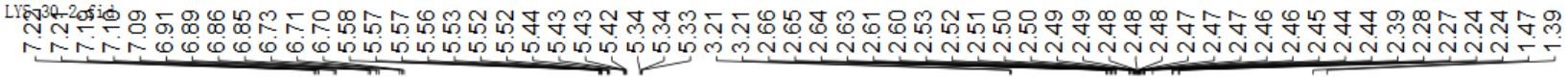


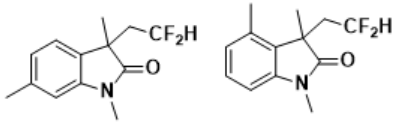


3m **$CDCl_3$**



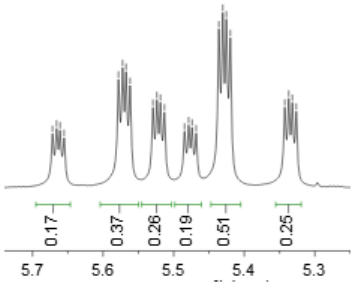


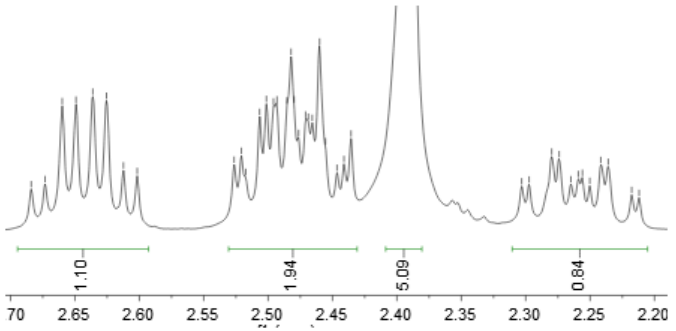

LYS-30-2.fid
7.22
7.21
7.16
7.09
6.91
6.89
6.86
6.85
6.73
6.71
6.70
5.58
5.57
5.57
5.56
5.53
5.52
5.52
5.44
5.43
5.43
5.42
5.34
5.34
5.33
3.21
3.21
2.66
2.65
2.64
2.63
2.61
2.60
2.53
2.52
2.51
2.50
2.50
2.49
2.49
2.48
2.48
2.48
2.47
2.47
2.47
2.46
2.46
2.45
2.44
2.44
2.39
2.28
2.27
2.24
2.24
1.47
1.39

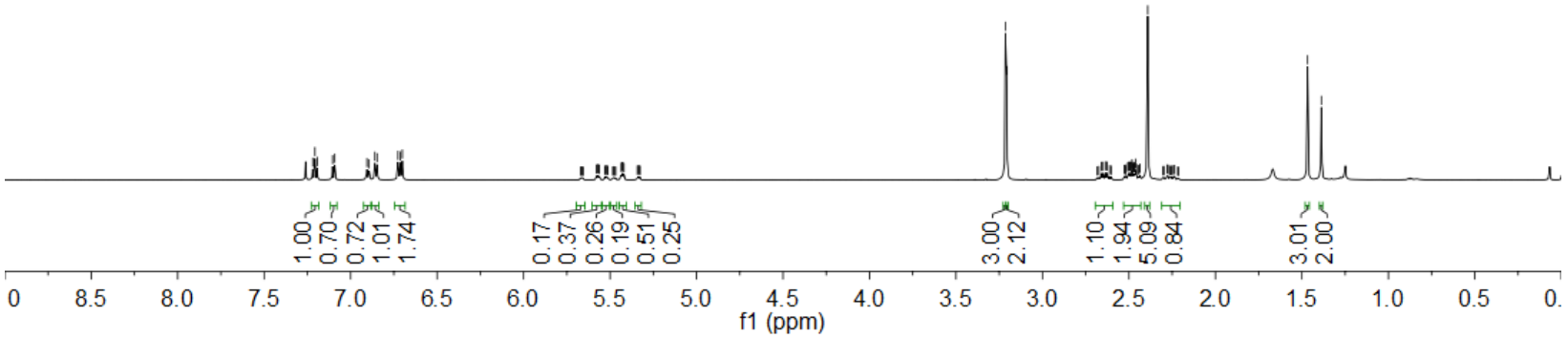

CF2H
O
N

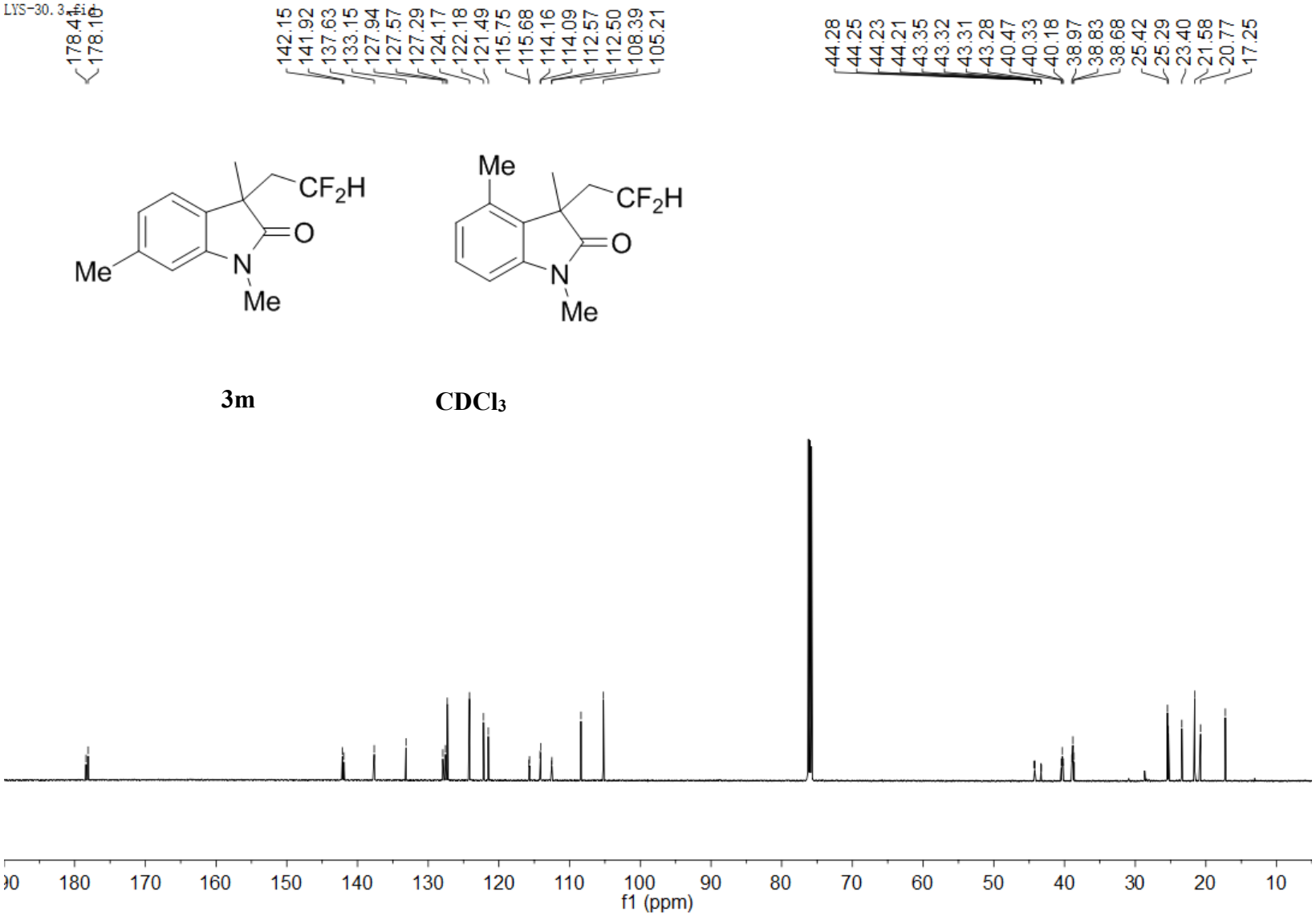
CF2H
O
N

3m $CDCl_3$

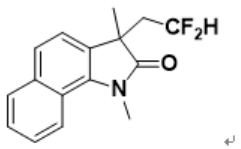

0.17
0.37
0.26
0.19
0.51
0.25
5.7
5.6
5.5
5.4
5.3

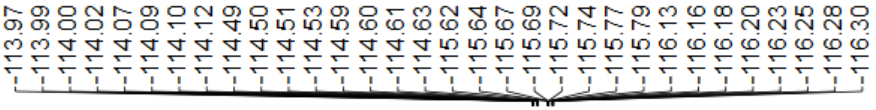

1.10
1.94
5.09
0.84
70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
2.20


1.00
0.70
0.72
1.01
1.74
0.17
0.37
0.26
0.19
0.51
0.25
3.00
2.12
1.10
1.94
5.09
0.84
3.01
2.00
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.
f1 (ppm)

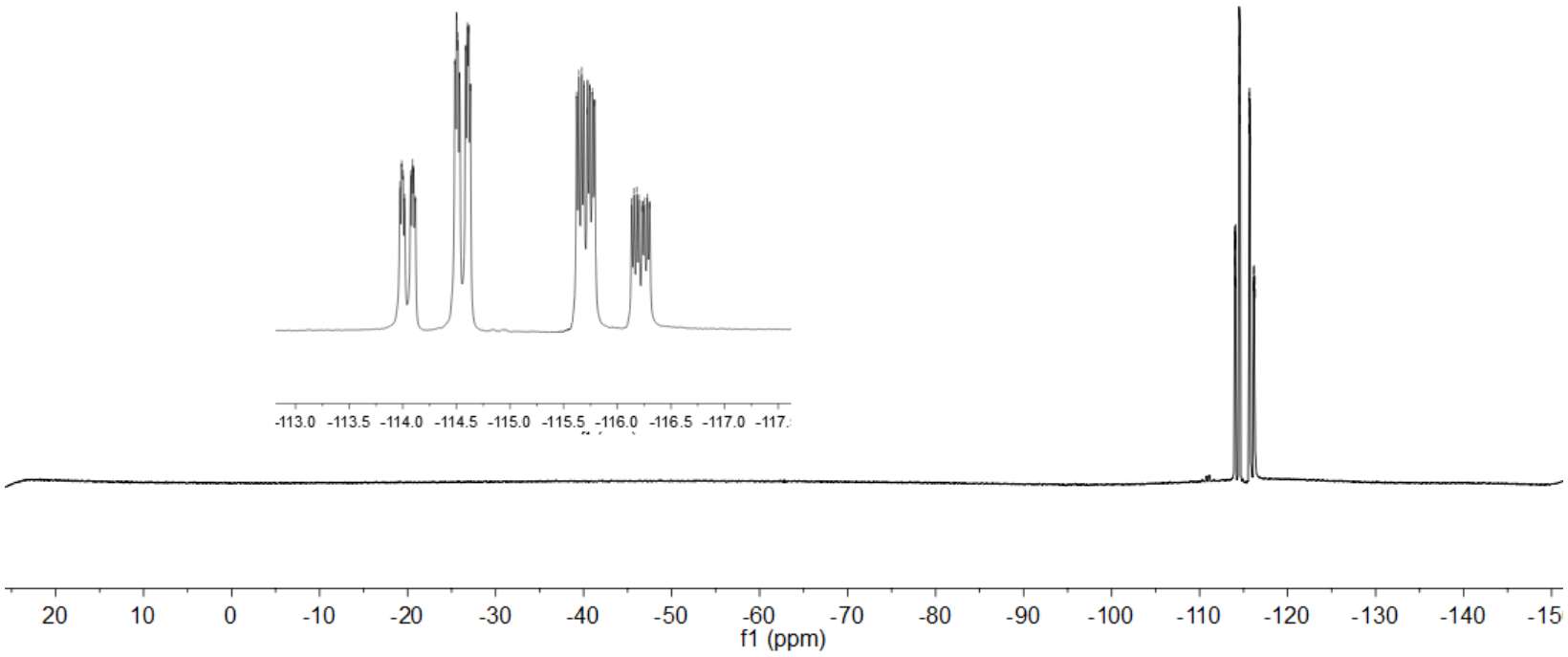

LYS-30.3.fid
178.41
178.10
142.15
141.92
137.63
133.15
127.94
127.57
127.29
124.17
122.18
121.49
115.75
115.68
114.16
114.09
112.57
112.50
108.39
105.21
44.28
44.25
44.23
44.21
43.35
43.32
43.31
43.28
40.47
40.33
40.18
38.97
38.83
38.68
25.42
25.29
23.40
21.58
20.77
17.25
CF2H
O
N
Me
Me
Me
CF2H
O
N
Me
f1 (ppm)

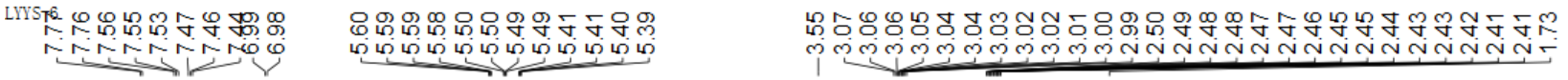
3m **$CDCl_3$**

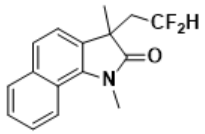

CF2H
O
N


-113.97
-113.99
-114.00
-114.02
-114.07
-114.09
-114.10
-114.12
-114.49
-114.50
-114.51
-114.53
-114.59
-114.60
-114.61
-114.63
-115.62
-115.64
-115.67
-115.69
-115.72
-115.74
-115.77
-115.79
-116.13
-116.16
-116.18
-116.20
-116.23
-116.25
-116.28
-116.30

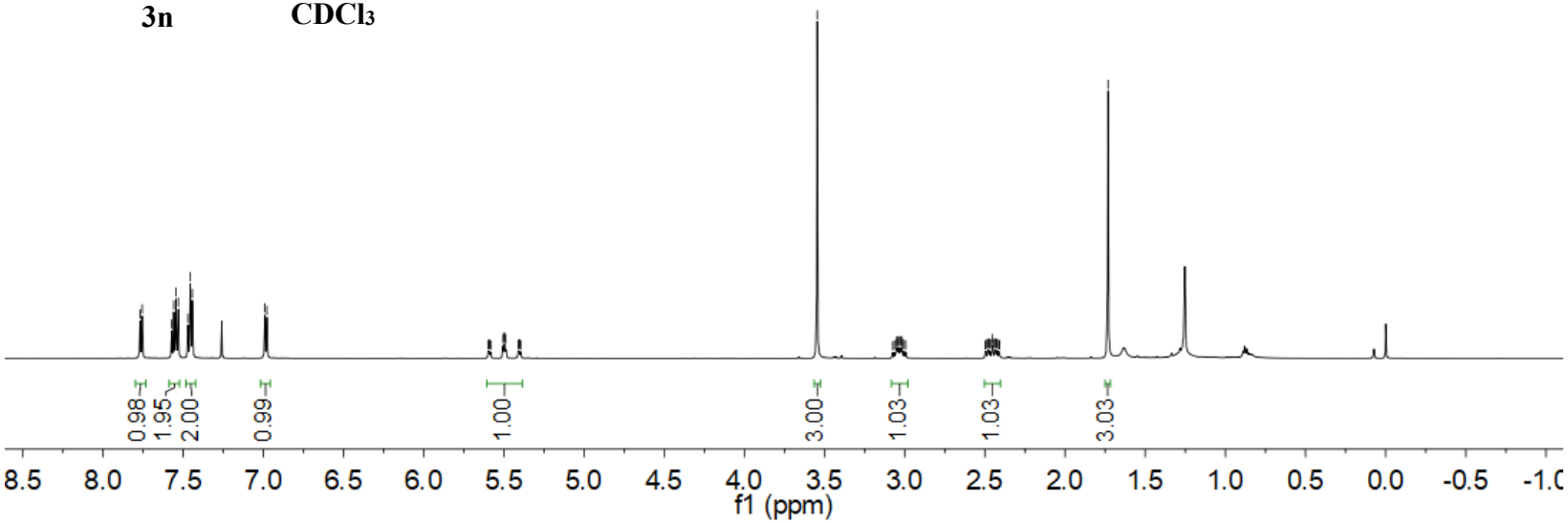
3n $CDCl_3$

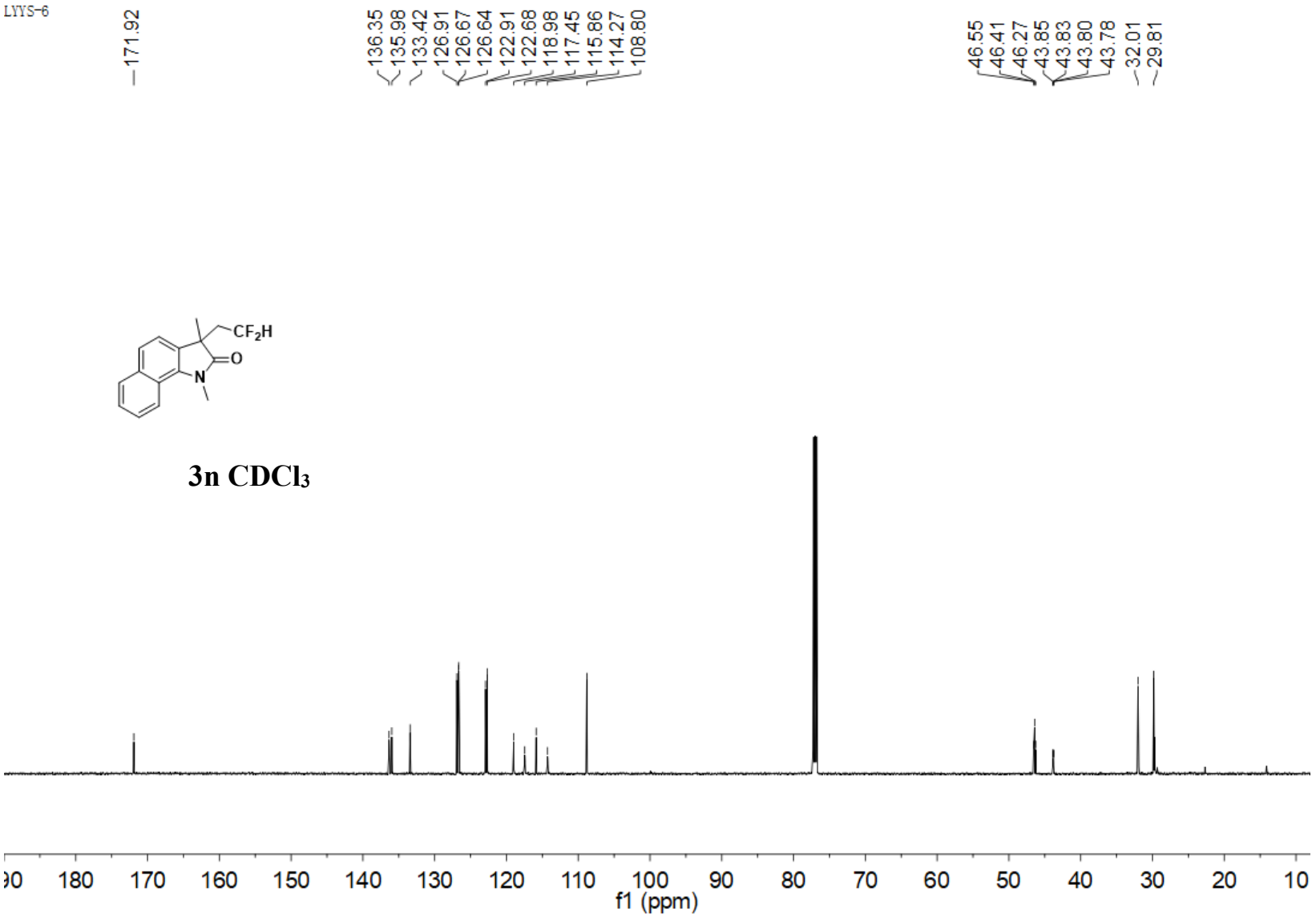

-113.0
-113.5
-114.0
-114.5
-115.0
-115.5
-116.0
-116.5
-117.0
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


LYYS-6
7.78
7.76
7.56
7.55
7.53
7.47
7.46
7.44
6.99
6.98
5.60
5.59
5.59
5.58
5.50
5.50
5.49
5.49
5.41
5.41
5.40
5.39
3.55
3.07
3.06
3.06
3.05
3.04
3.04
3.03
3.02
3.02
3.01
3.00
2.99
2.50
2.49
2.48
2.48
2.47
2.47
2.46
2.45
2.45
2.44
2.43
2.43
2.42
2.41
2.41
1.73


CF2H
O
N

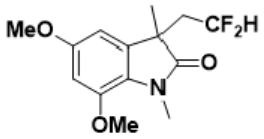
3n **$CDCl_3$**

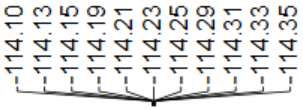

0.98
1.95
2.00
0.99
1.00
3.00
1.03
1.03
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


LYYS-6
171.92
136.35
135.98
133.42
126.91
126.67
126.64
122.91
122.68
118.98
117.45
115.86
114.27
108.80
46.55
46.41
46.27
43.85
43.83
43.80
43.78
32.01
29.81
CF2H
O
N
f1 (ppm)

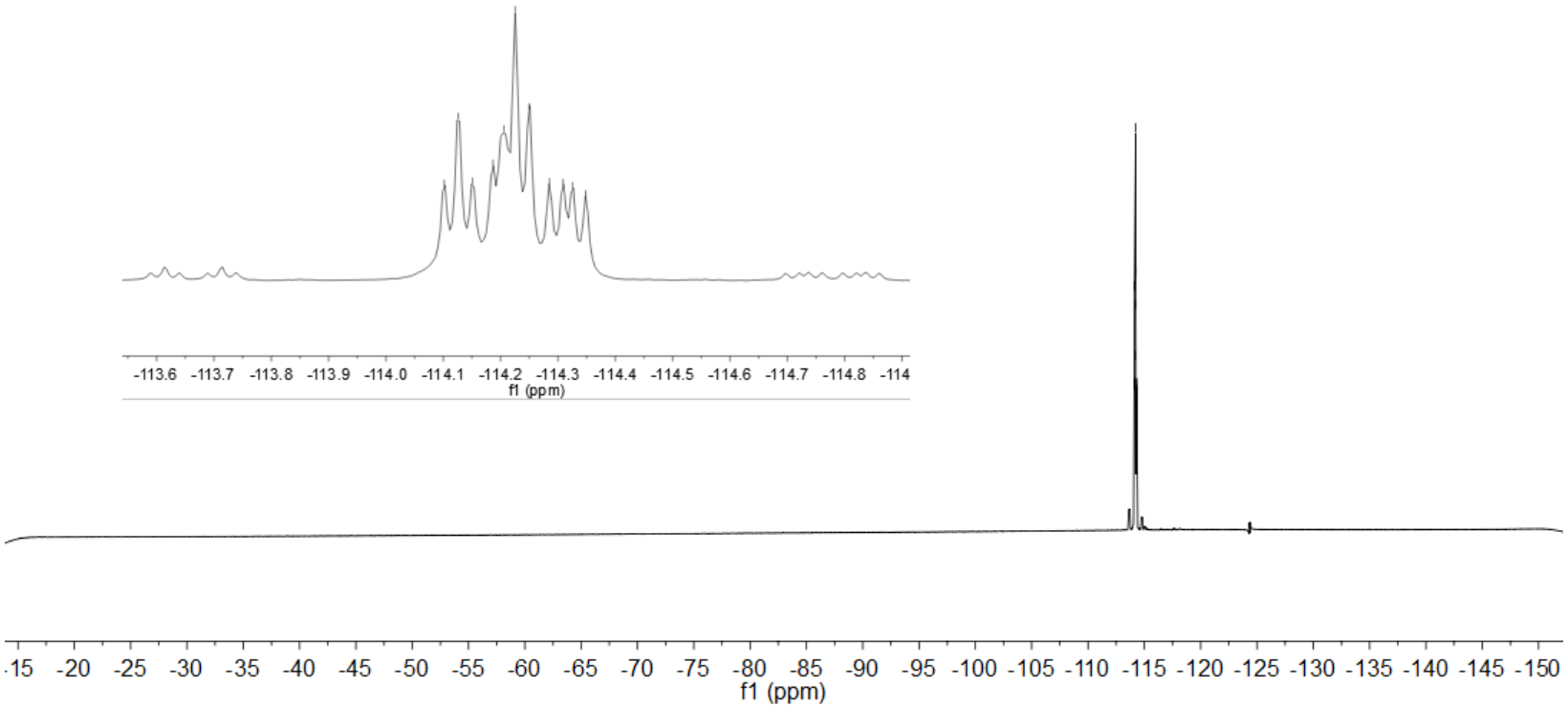
3n $CDCl_3$

19F_LJ-243/2
2018-12-13

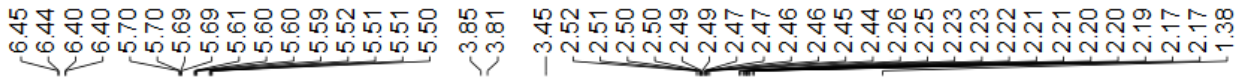


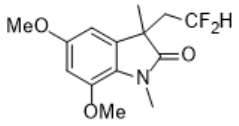


3o **$CDCl_3$**

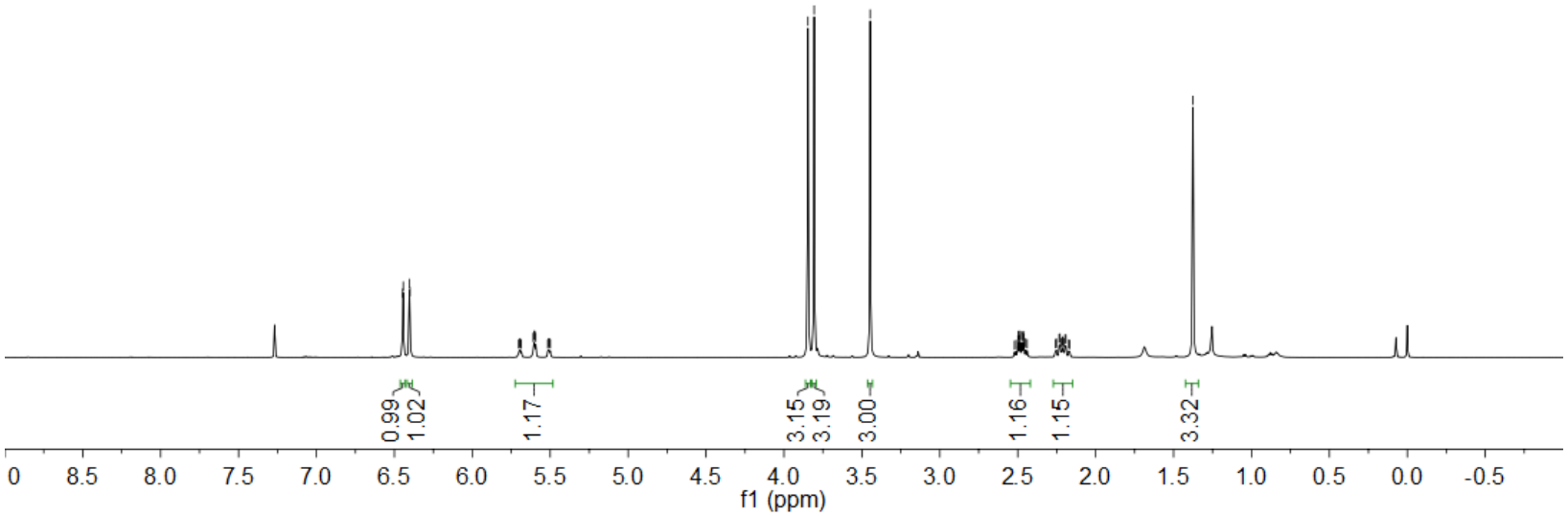


LJ-243.1.fid



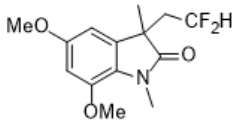


3o $CDCl_3$

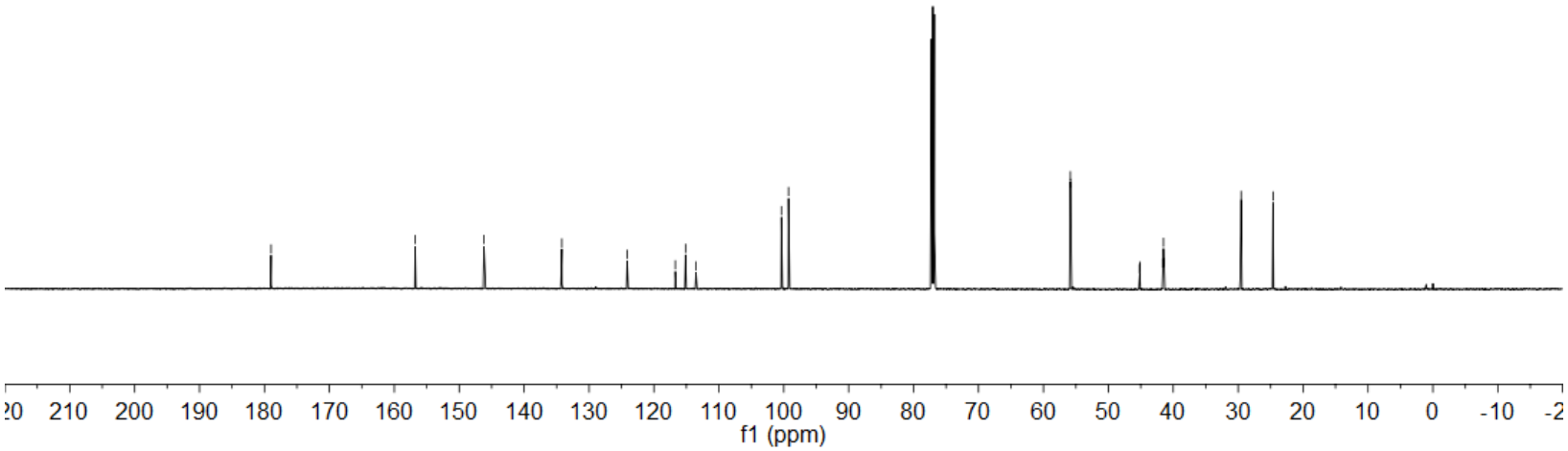


LJ-243.2.fid

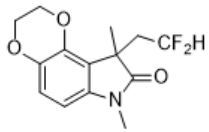
178.98
156.79
146.19
134.19
124.13
116.71
115.12
113.53
100.35
99.27
55.85
55.82
45.20
45.17
45.15
45.13
41.65
41.50
41.36
29.54
24.63



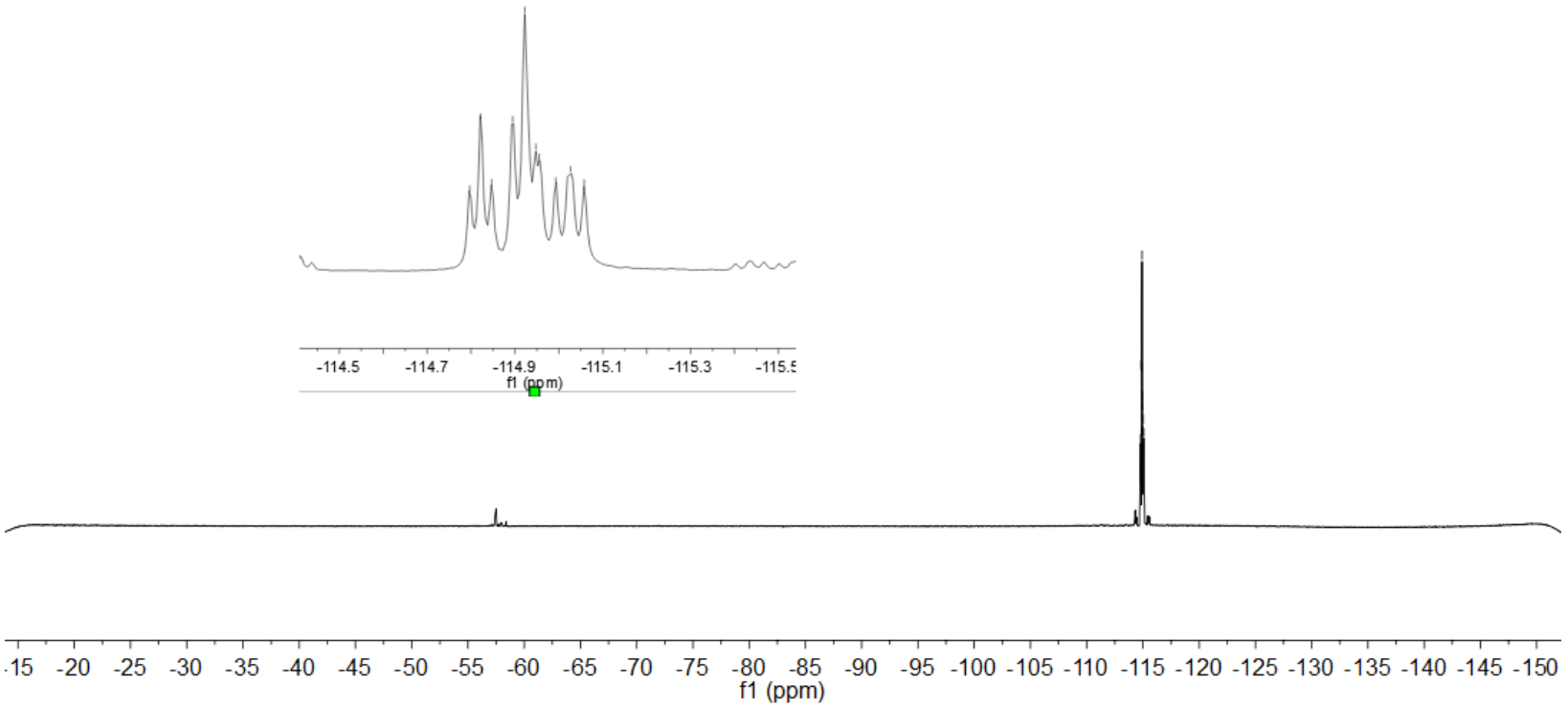
3o **$CDCl_3$**



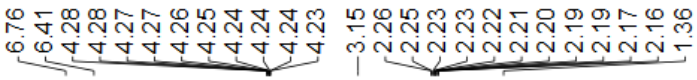
19F_LYYS-23/1
2018-12-11

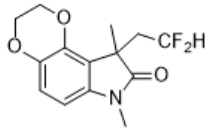


3p $CDCl_3$

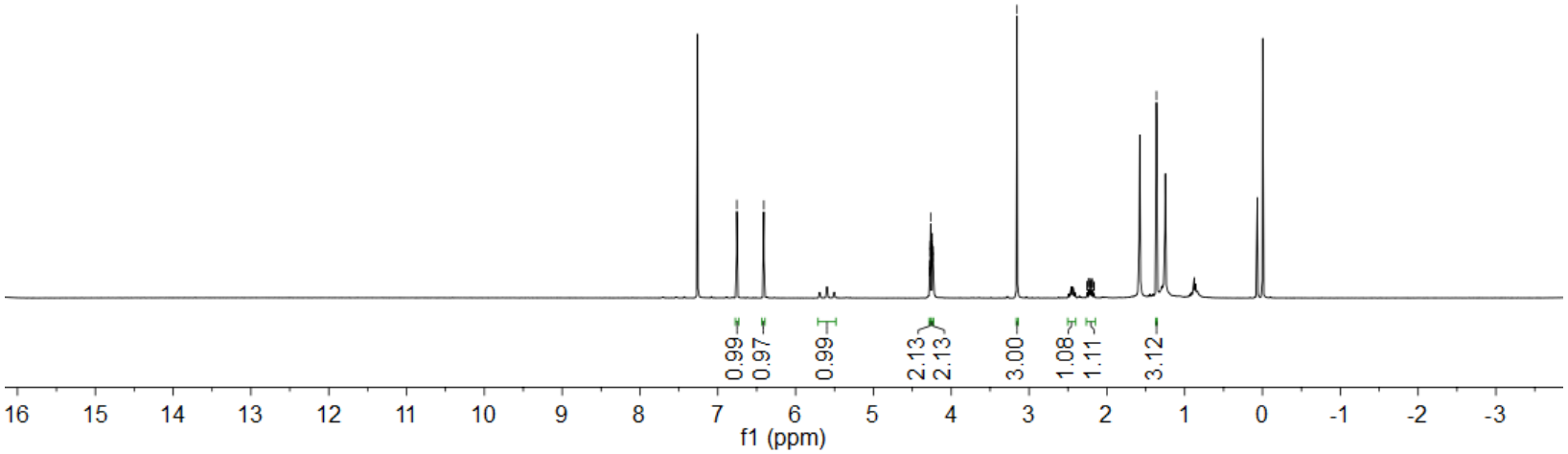


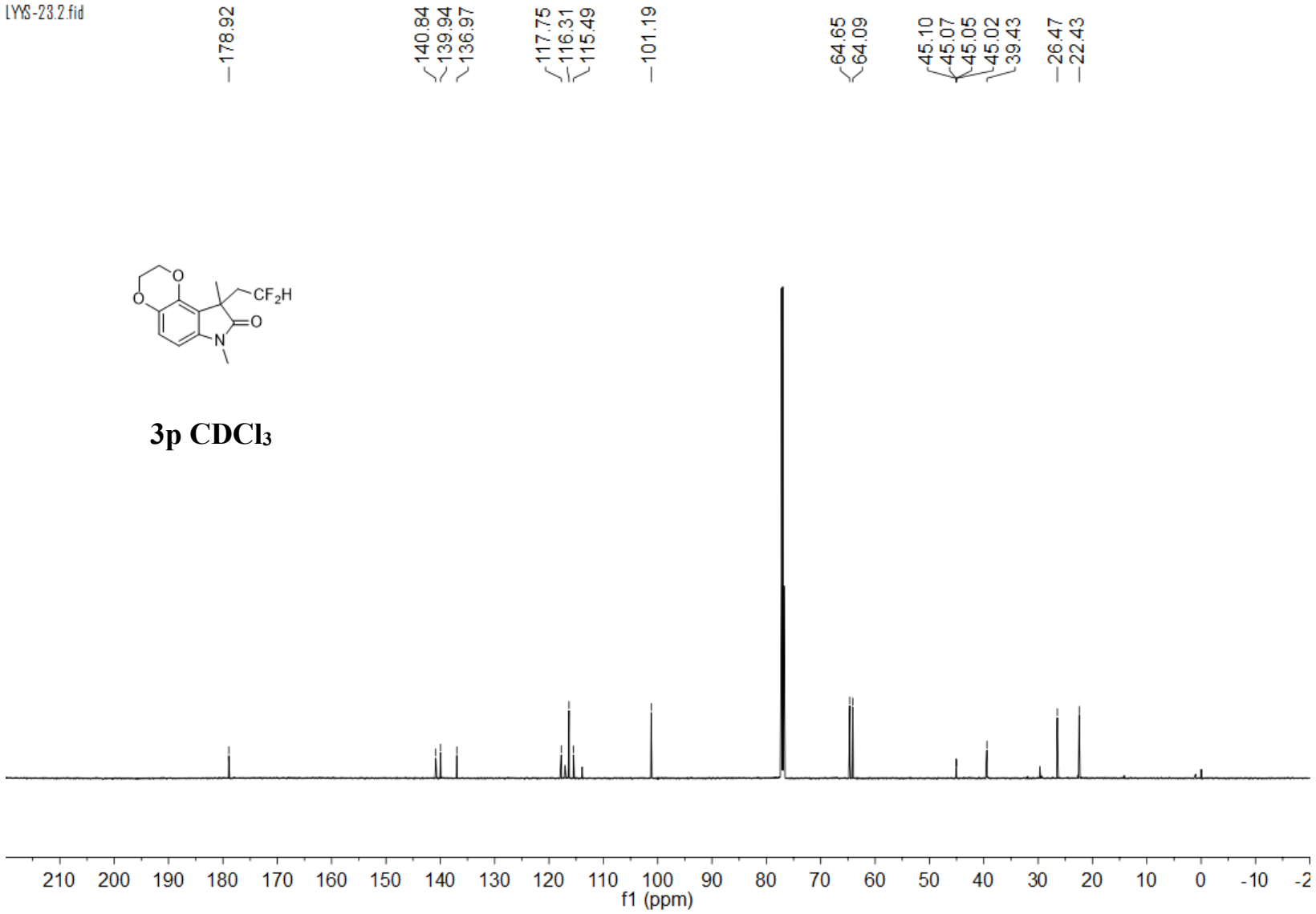
LYS-232.1.fid





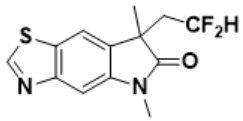
3p **$CDCl_3$**



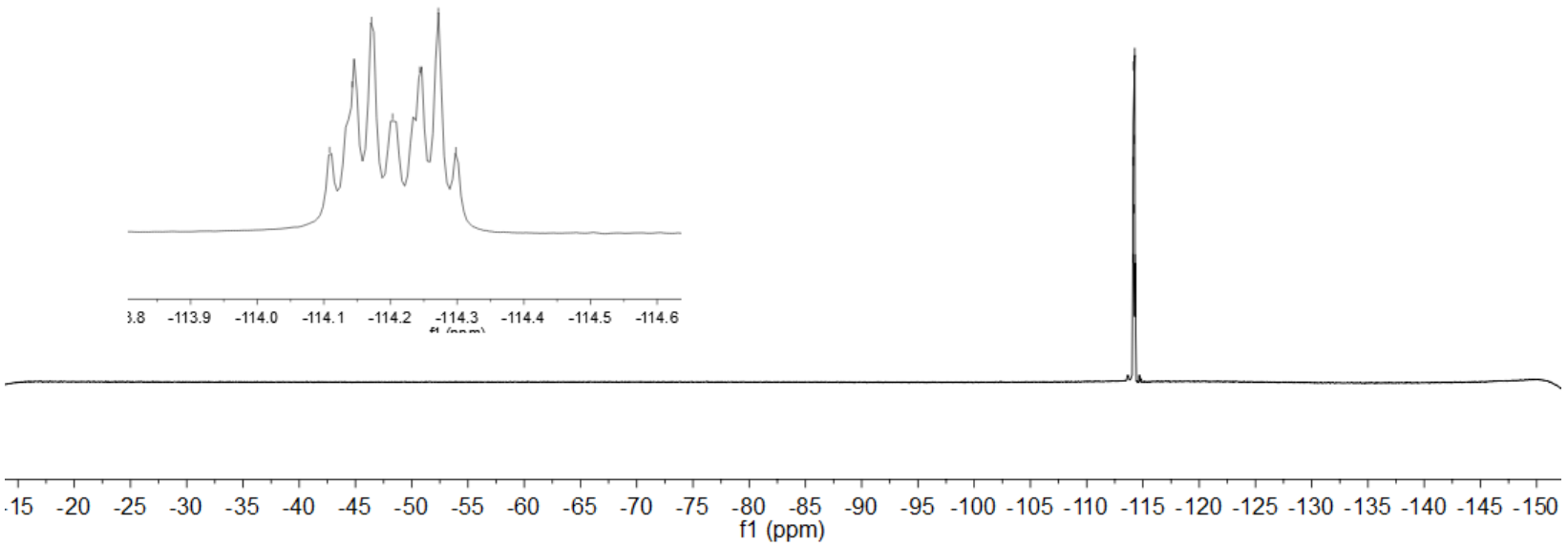

LYYS-23.2.fid
178.92
140.84
139.94
136.97
117.75
116.31
115.49
101.19
64.65
64.09
45.10
45.07
45.05
45.02
39.43
26.47
22.43
O
O
CF2H
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

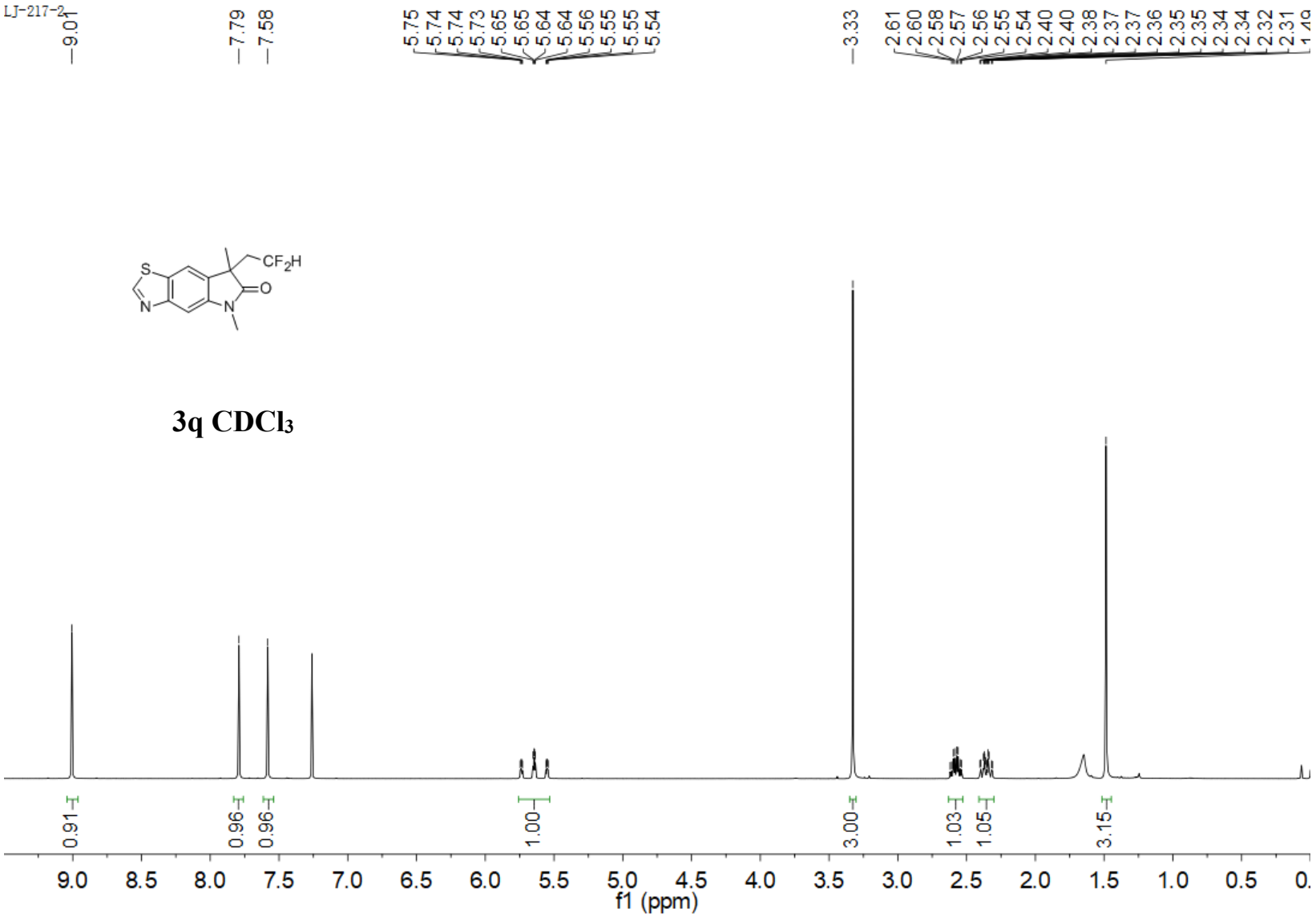
3p $CDCl_3$

19F_LJ-217-2/2
2018-12-13

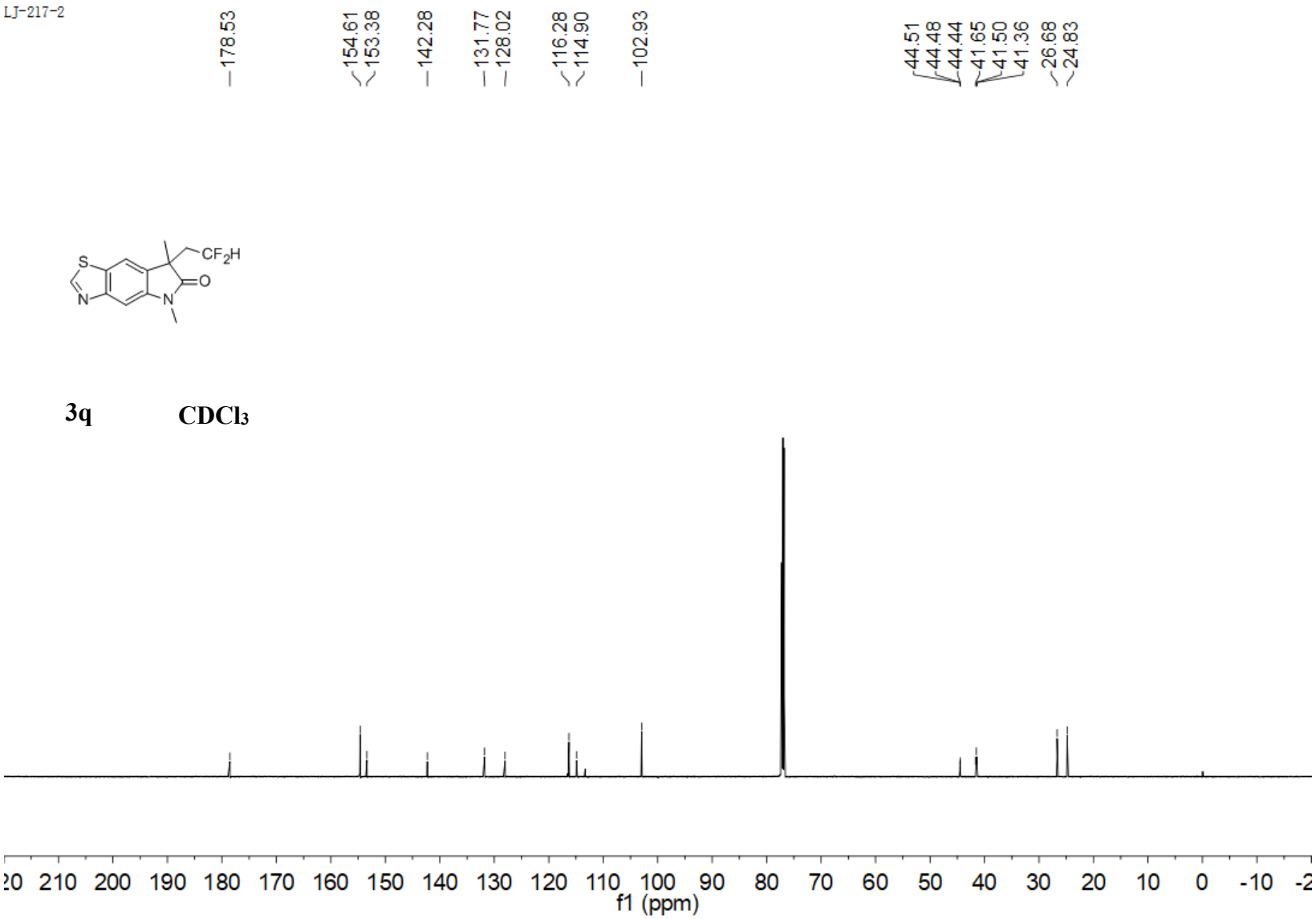


3q **$CDCl_3$**



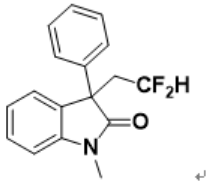

LJ-217-2
9.01
7.79
7.58
5.75
5.74
5.74
5.73
5.65
5.65
5.64
5.64
5.56
5.55
5.55
5.54
3.33
2.61
2.60
2.58
2.57
2.56
2.55
2.54
2.40
2.40
2.38
2.37
2.37
2.36
2.35
2.35
2.34
2.34
2.32
2.31
S
N
CF2H
O
N
0.91
0.96
0.96
1.00
3.00
1.03
1.05
3.15
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

3q $CDCl_3$

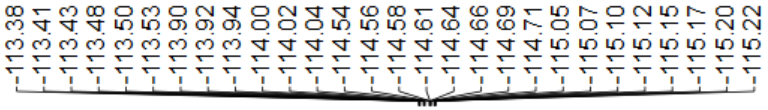

LJ-217-2
178.53
154.61
153.38
142.28
131.77
128.02
116.28
114.90
102.93
44.51
44.48
44.44
41.65
41.50
41.36
26.68
24.83
S
N
CF2H
O
N
f1 (ppm)

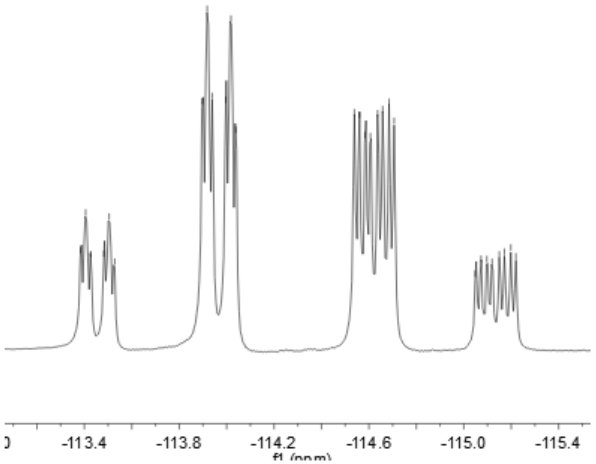
3q **$CDCl_3$**

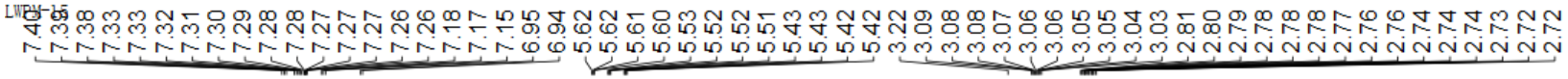
19F_LWPM-15/1
2018-10-12

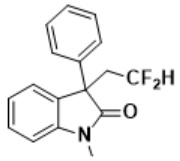


3r $CDCl_3$

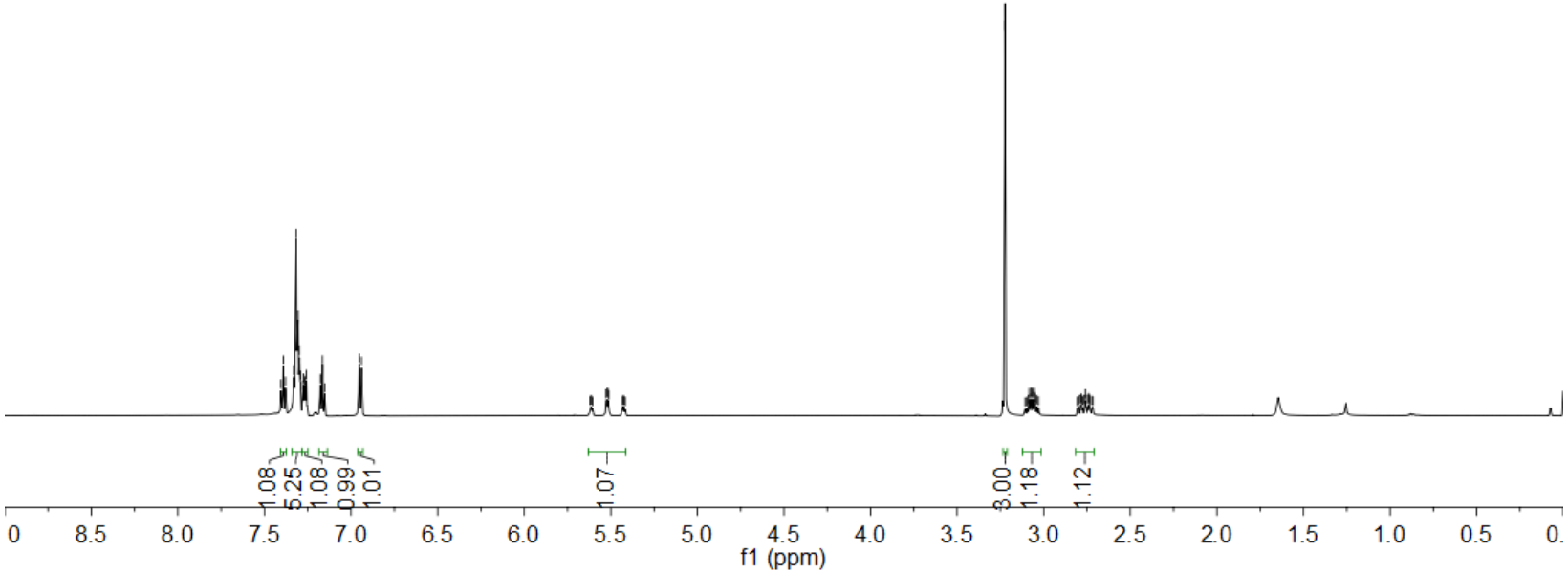





LWPW-15
7.40
7.39
7.38
7.33
7.33
7.32
7.31
7.30
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.26
7.18
7.17
7.15
6.95
6.94
5.62
5.62
5.61
5.60
5.53
5.52
5.52
5.51
5.43
5.43
5.42
5.42
3.22
3.09
3.08
3.08
3.07
3.06
3.06
3.05
3.05
3.04
3.03
2.81
2.80
2.79
2.78
2.78
2.78
2.77
2.76
2.76
2.74
2.74
2.74
2.73
2.72
2.72

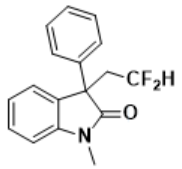

CF2H
O
N

3r **$CDCl_3$**

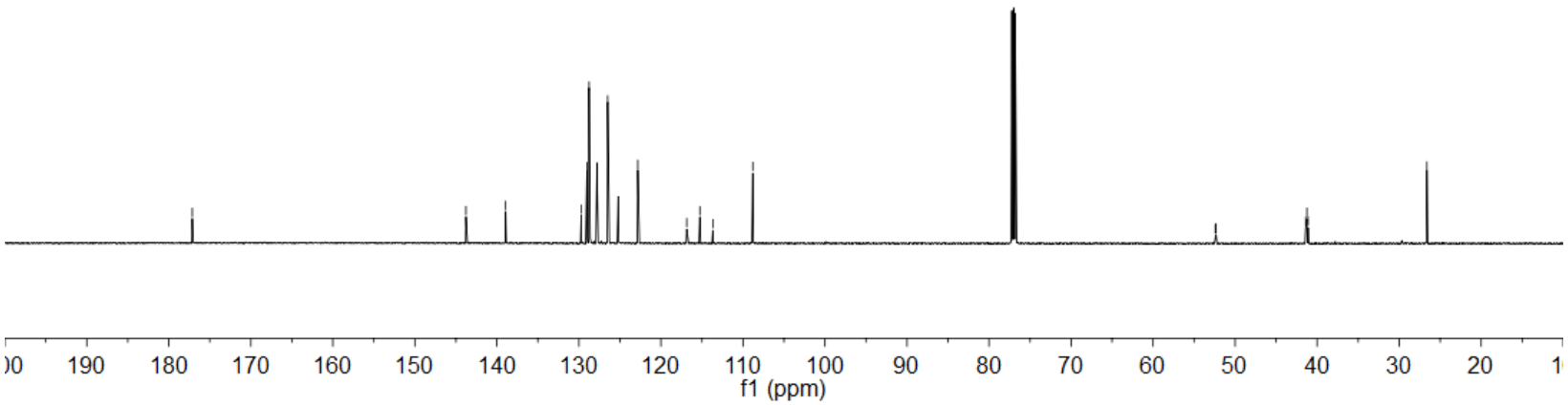

1.08
5.25
1.08
0.99
1.01
1.07
3.00
1.18
1.12
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

LWPM-15

177.13
143.77
138.94
129.72
129.02
128.76
126.50
122.81
116.85
115.26
113.67
108.80
52.40
52.38
52.34
52.32
41.39
41.24
41.10
26.62

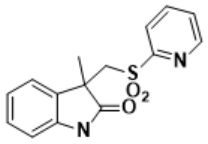


3r $CDCl_3$

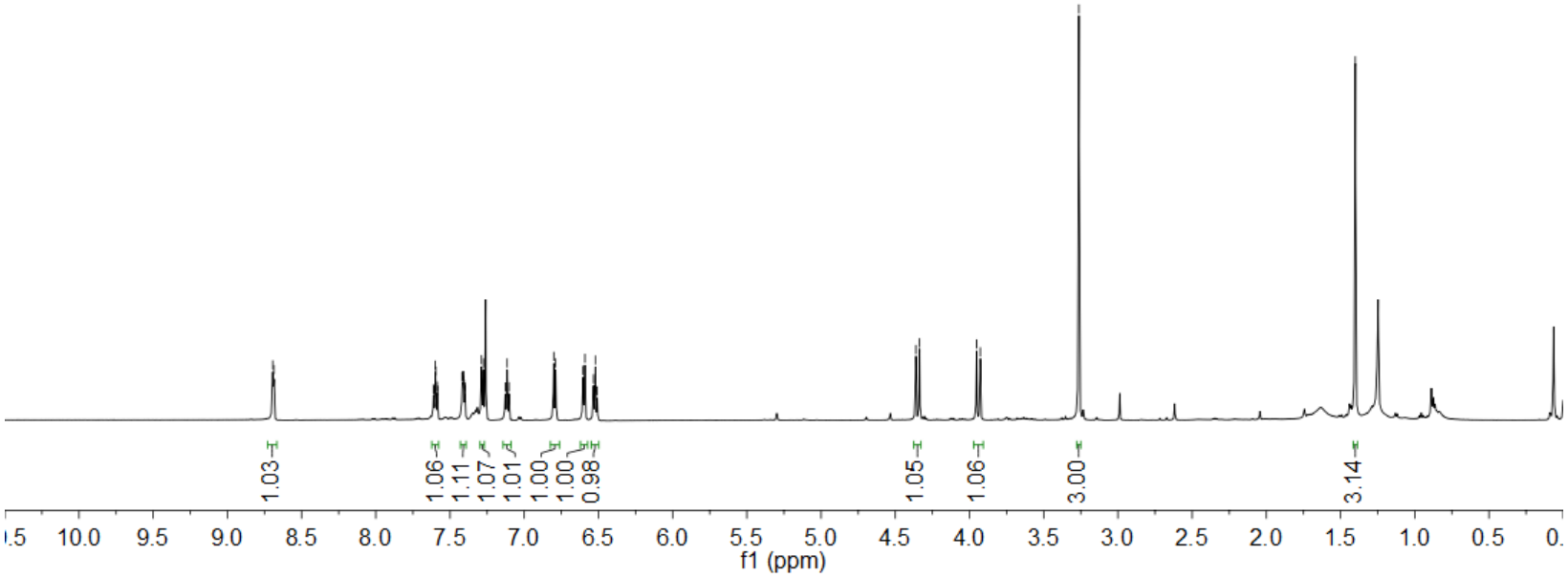


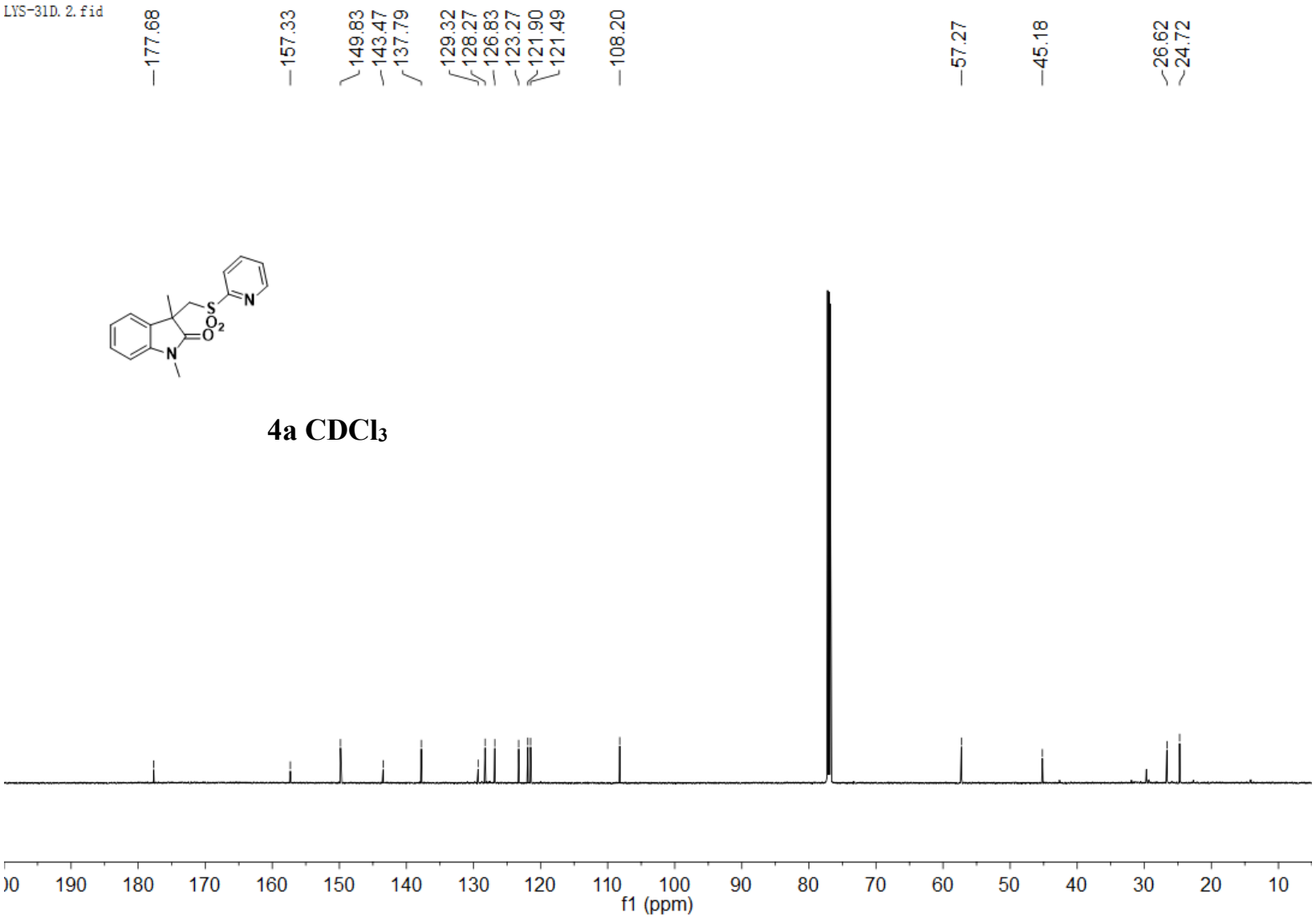
LYS-31D.1.fid

8.69 8.69 7.61 7.61 7.60 7.60 7.59 7.58 7.42 7.42 7.41 7.41 7.41 7.40 7.40 7.40 7.29 7.28 7.13 7.12 7.10 6.80 6.79 6.60 6.59 6.53 6.52 6.51 4.36 4.34 3.95 3.93 3.26 1.40

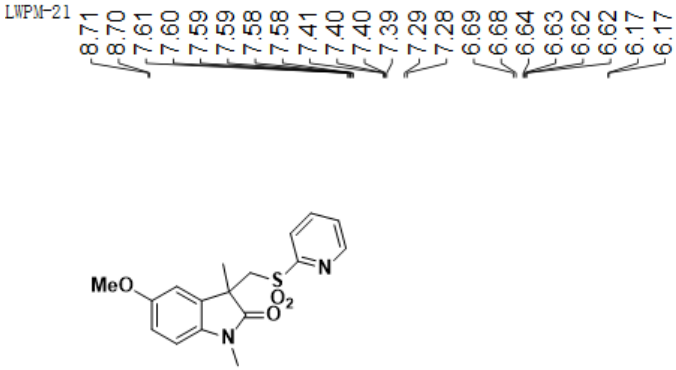


4a **$CDCl_3$**

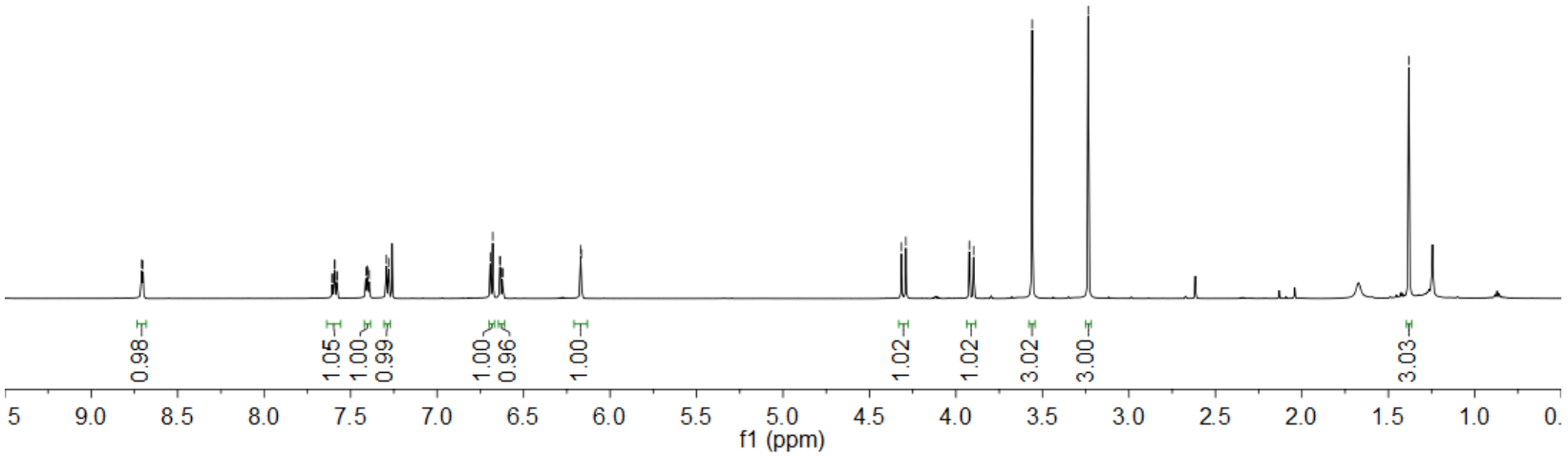


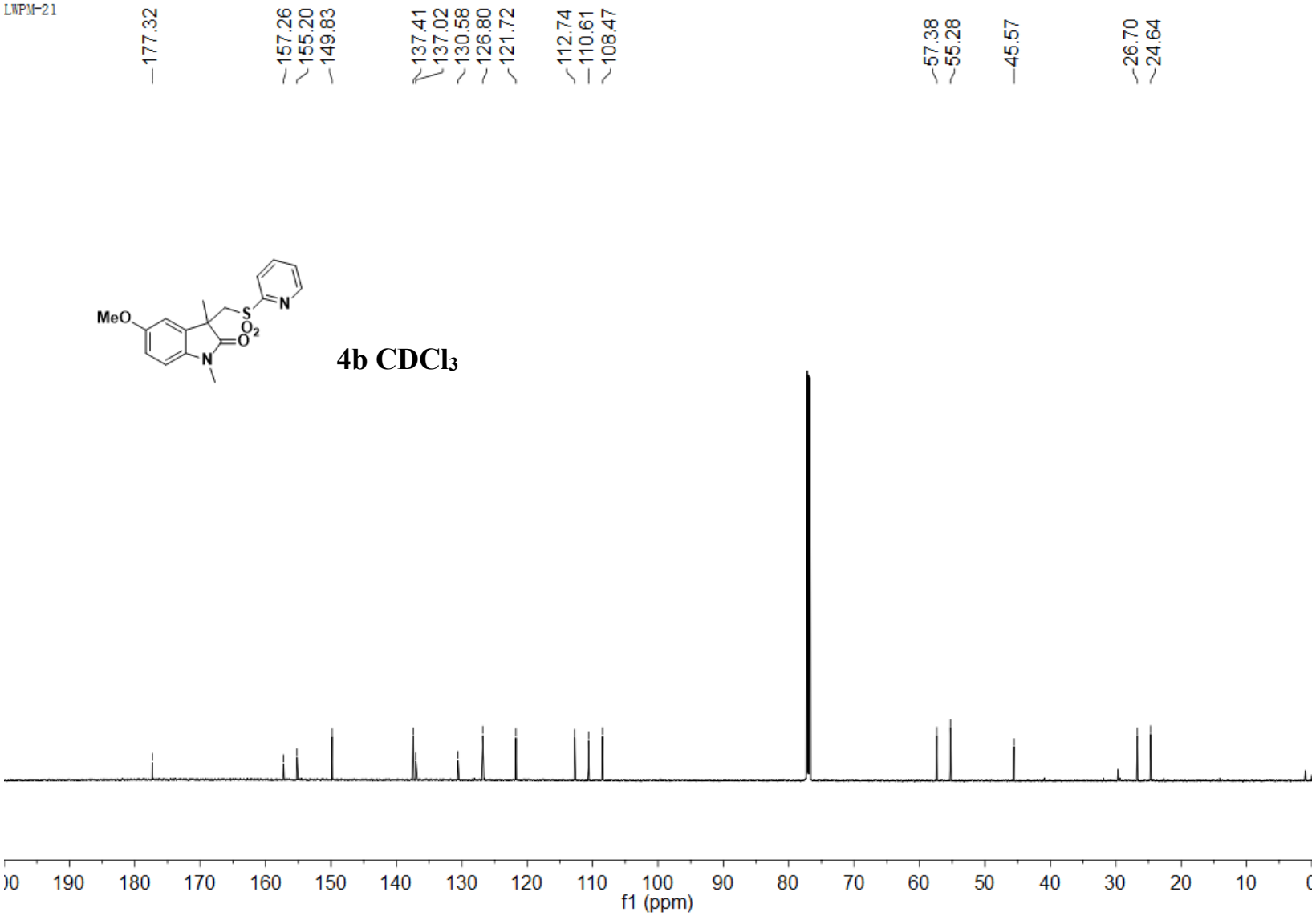

LYS-31D. 2. fid
177.68
157.33
149.83
143.47
137.79
129.32
128.27
126.83
123.27
121.90
121.49
108.20
57.27
45.18
26.62
24.72
S
O2
O
N
N
f1 (ppm)

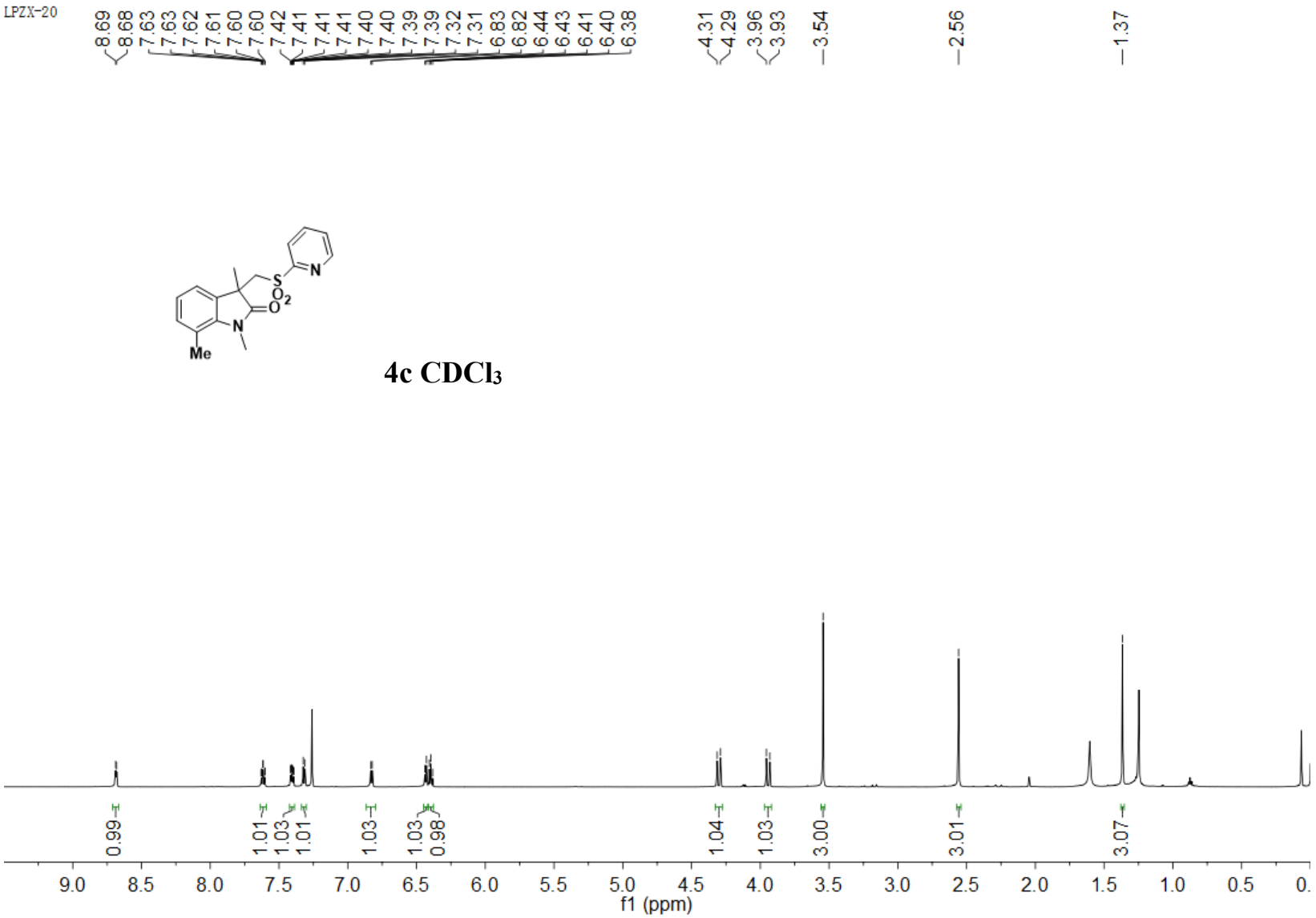
4a $CDCl_3$


LWPM-21
8.71
8.70
7.61
7.60
7.59
7.59
7.58
7.58
7.41
7.40
7.40
7.39
7.29
7.28
6.69
6.68
6.64
6.63
6.62
6.62
6.17
6.17
4.31
4.29
3.92
3.90
3.56
3.24
1.38
MeO
S
O2
O
N
N

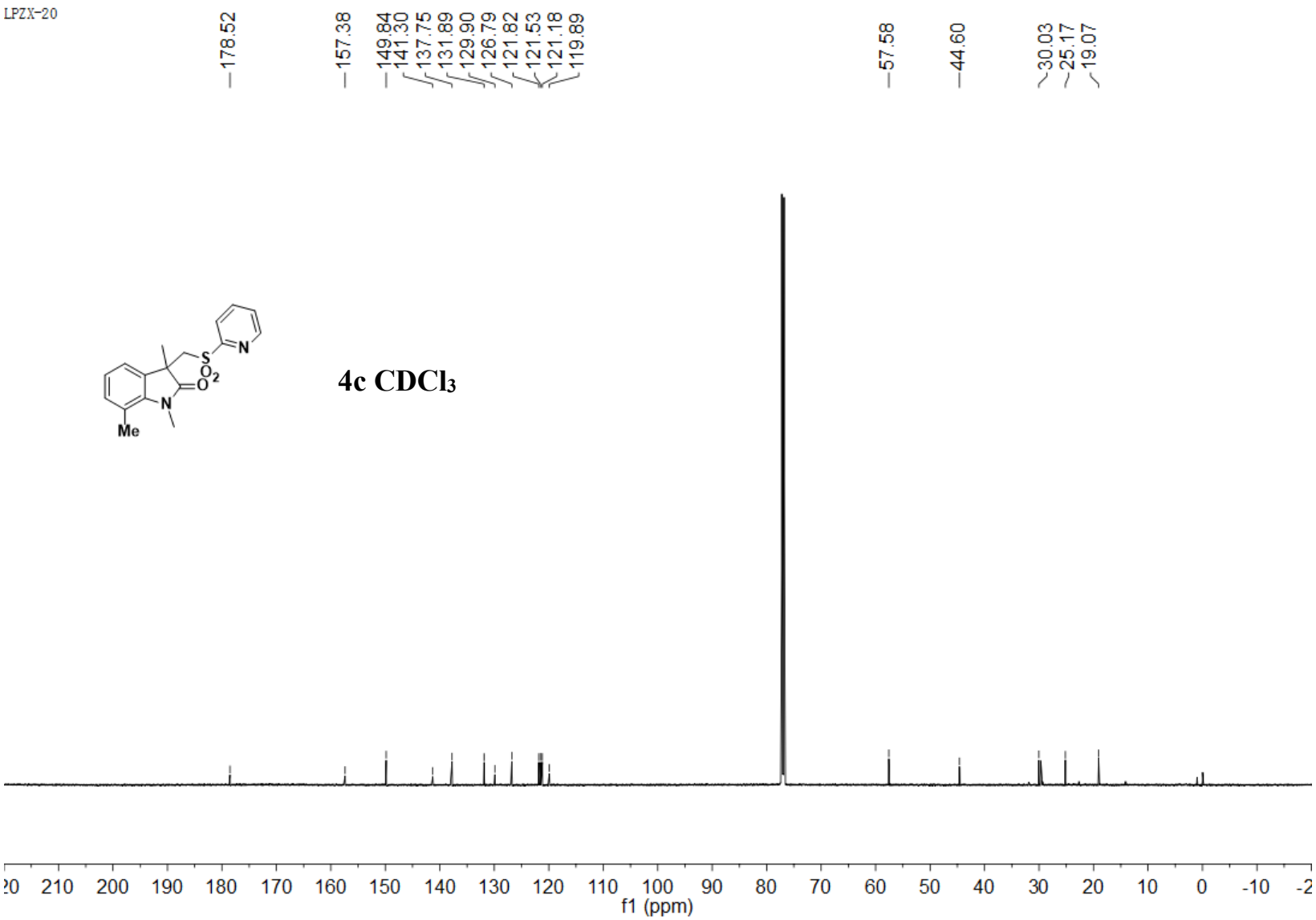
4b **$CDCl_3$**

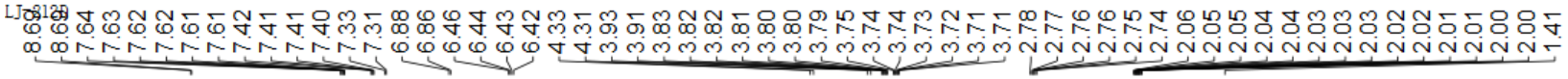

0.98
1.05
1.00
0.99
1.00
0.96
1.00
1.02
1.02
3.02
3.00
3.03
5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.
f1 (ppm)

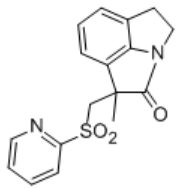

LWPM-21
177.32
157.26
155.20
149.83
137.41
137.02
130.58
126.80
121.72
112.74
110.61
108.47
57.38
55.28
45.57
26.70
24.64
MeO
S
O2
O
N
N
4b CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


LPZX-20
8.69
8.68
7.63
7.63
7.62
7.61
7.60
7.60
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.39
7.32
7.31
6.83
6.82
6.44
6.43
6.41
6.40
6.38
4.31
4.29
3.96
3.93
3.54
2.56
1.37
S
O2
O
N
N
Me
0.99
1.01
1.03
1.01
1.03
1.03
0.98
1.04
1.03
3.00
3.01
3.07
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.
f1 (ppm)

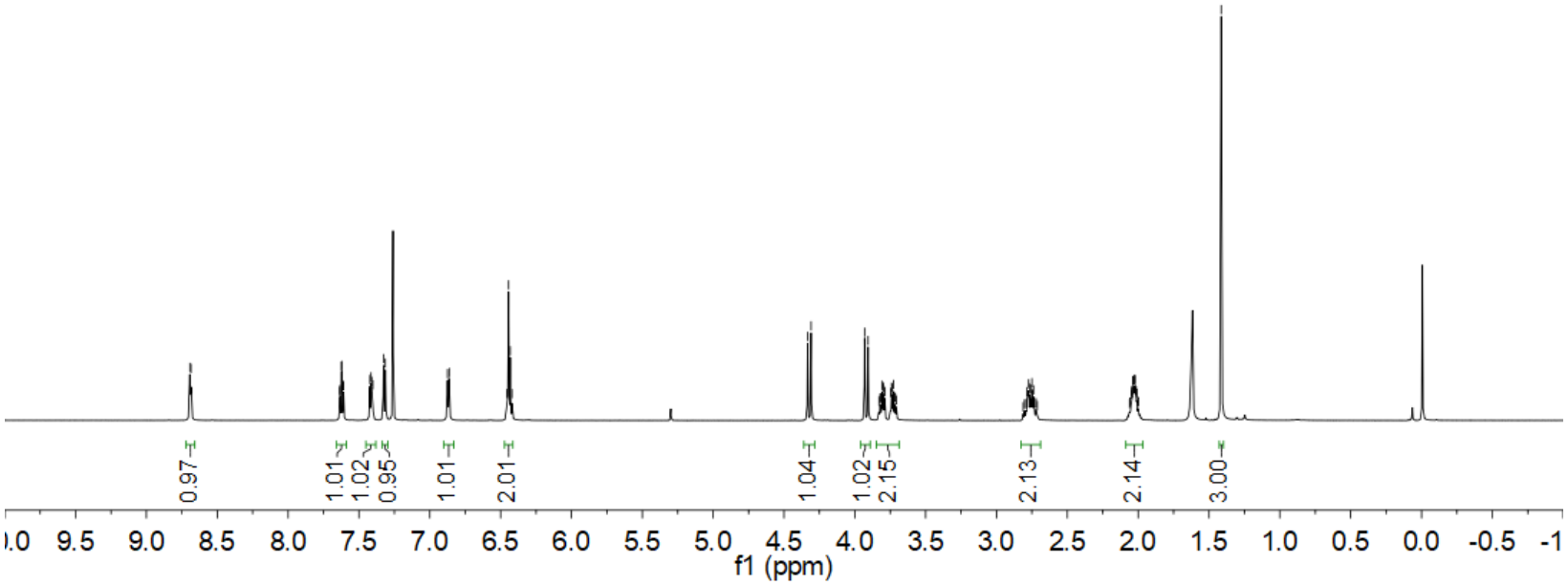
4c $CDCl_3$


LPZX-20
178.52
157.38
149.84
141.30
137.75
131.89
129.90
126.79
121.82
121.53
121.18
119.89
57.58
44.60
30.03
25.17
19.07
4c CDCl3
f1 (ppm)


8.69
8.69
7.64
7.63
7.62
7.62
7.61
7.61
7.42
7.41
7.41
7.40
7.33
7.31
6.88
6.86
6.46
6.44
6.43
6.42
4.33
4.31
3.93
3.91
3.83
3.82
3.82
3.81
3.80
3.80
3.79
3.75
3.74
3.74
3.73
3.72
3.71
3.71
2.78
2.77
2.76
2.76
2.75
2.74
2.06
2.05
2.05
2.04
2.04
2.03
2.03
2.02
2.02
2.01
2.01
2.00
2.00
1.41

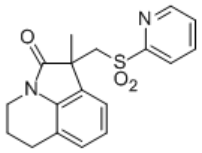

N
O
N
SO2

4d $CDCl_3$

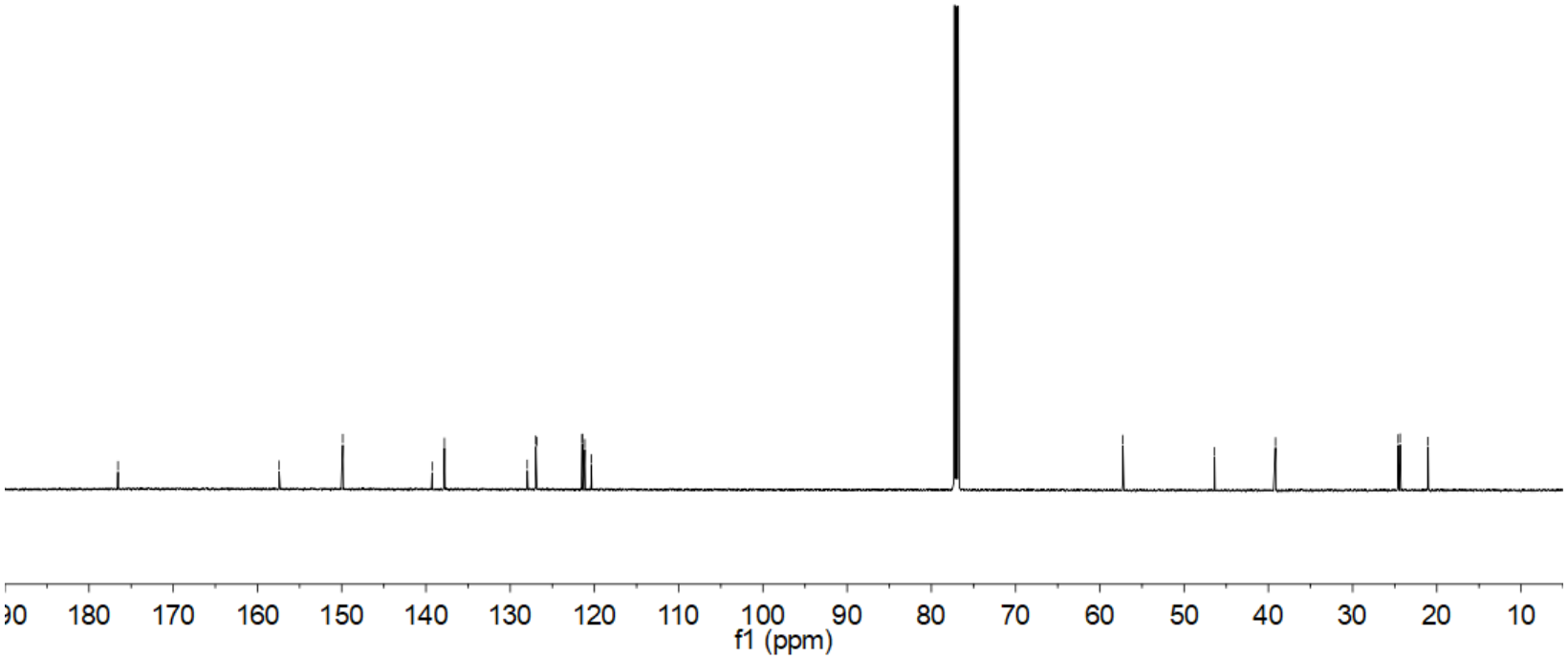

0.97
1.01
1.02
0.95
1.01
2.01
1.04
1.02
2.15
2.13
2.14
3.00
f1 (ppm)

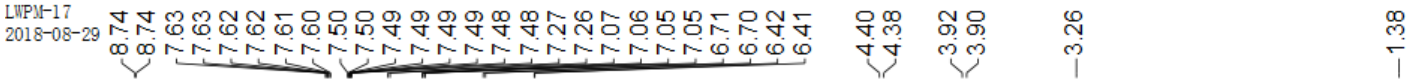
LJ-212D

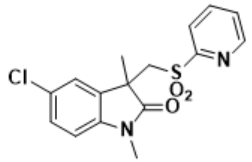
176.55
157.43
149.87
139.26
137.81
127.98
126.97
126.86
121.47
121.44
121.14
120.37
57.28
46.39
39.16
24.59
24.36
21.04



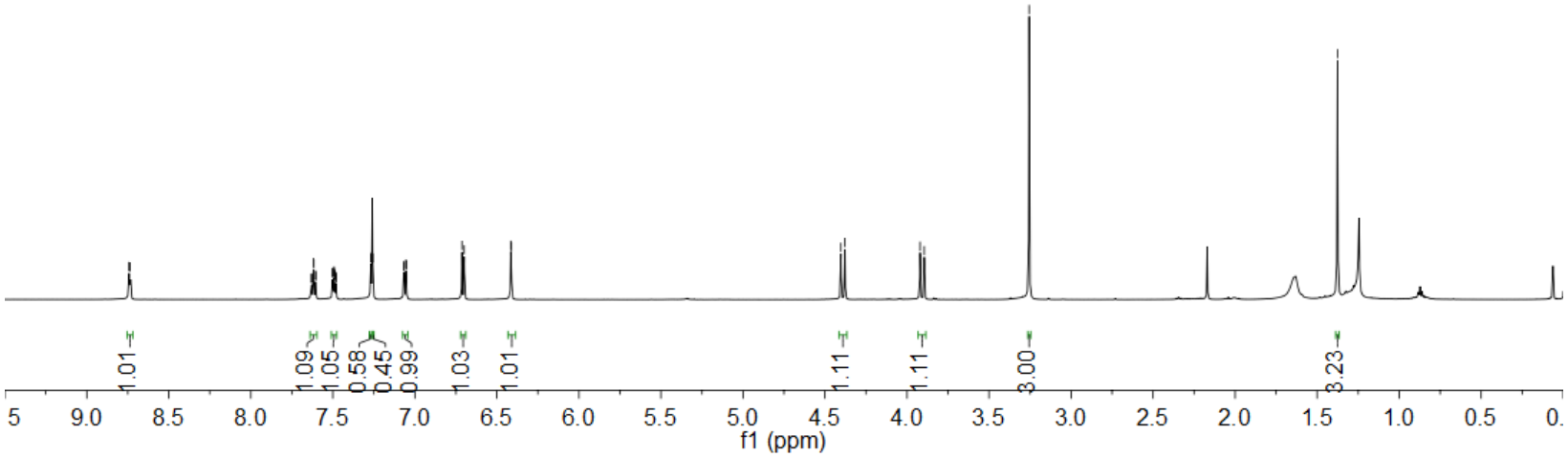
4d $CDCl_3$




LWPM-17
2018-08-29
8.74
8.74
7.63
7.63
7.62
7.62
7.61
7.60
7.50
7.50
7.49
7.49
7.49
7.49
7.48
7.48
7.27
7.26
7.07
7.06
7.05
7.05
6.71
6.70
6.42
6.41
4.40
4.38
3.92
3.90
3.26
1.38

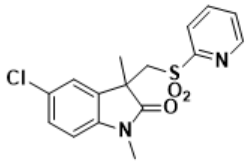

Cl
S
O2
O
N
N

4e $CDCl_3$

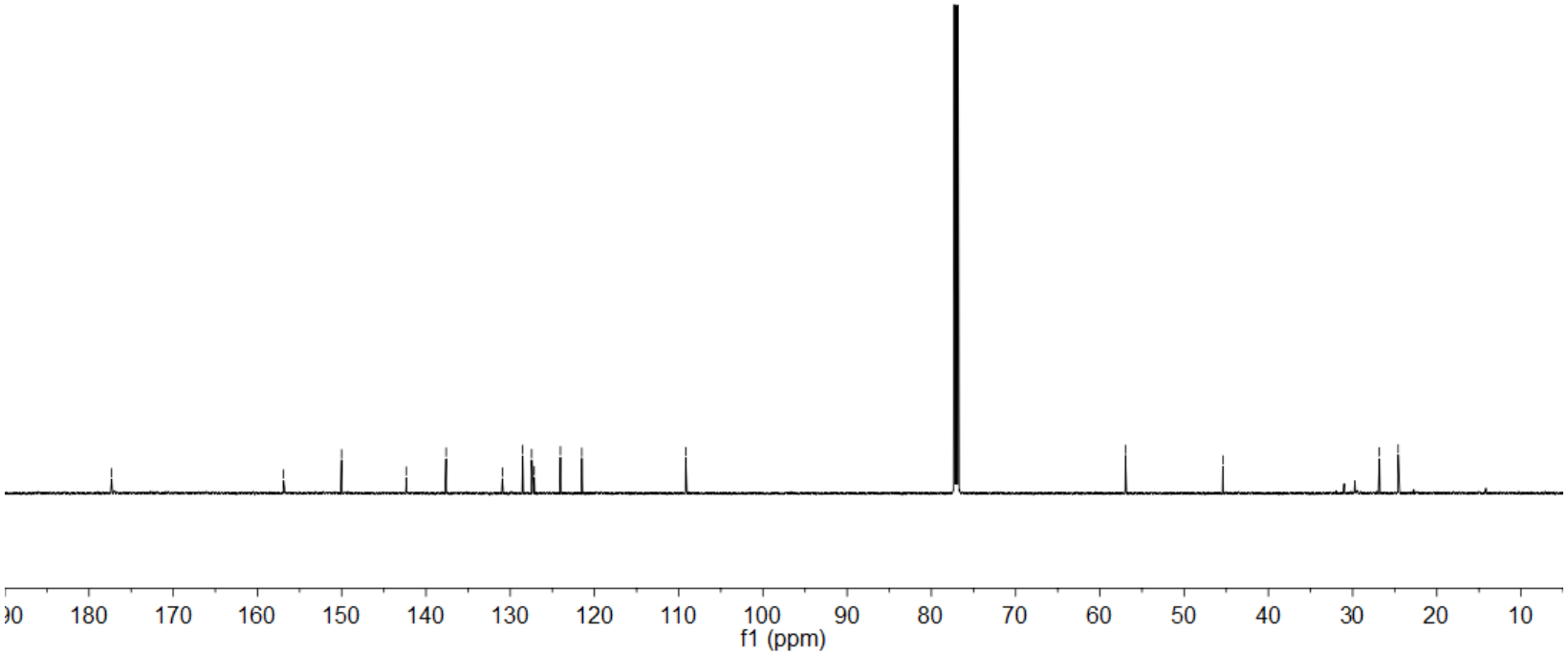

1.01
1.09
1.05
0.58
0.45
0.99
1.03
1.01
1.11
1.11
3.00
3.23
5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

LWPM-17

177.31
156.90
150.01
142.34
137.61
130.93
128.51
127.45
127.14
124.03
121.50
109.17
56.96
45.40
26.82
24.59



4e $CDCl_3$



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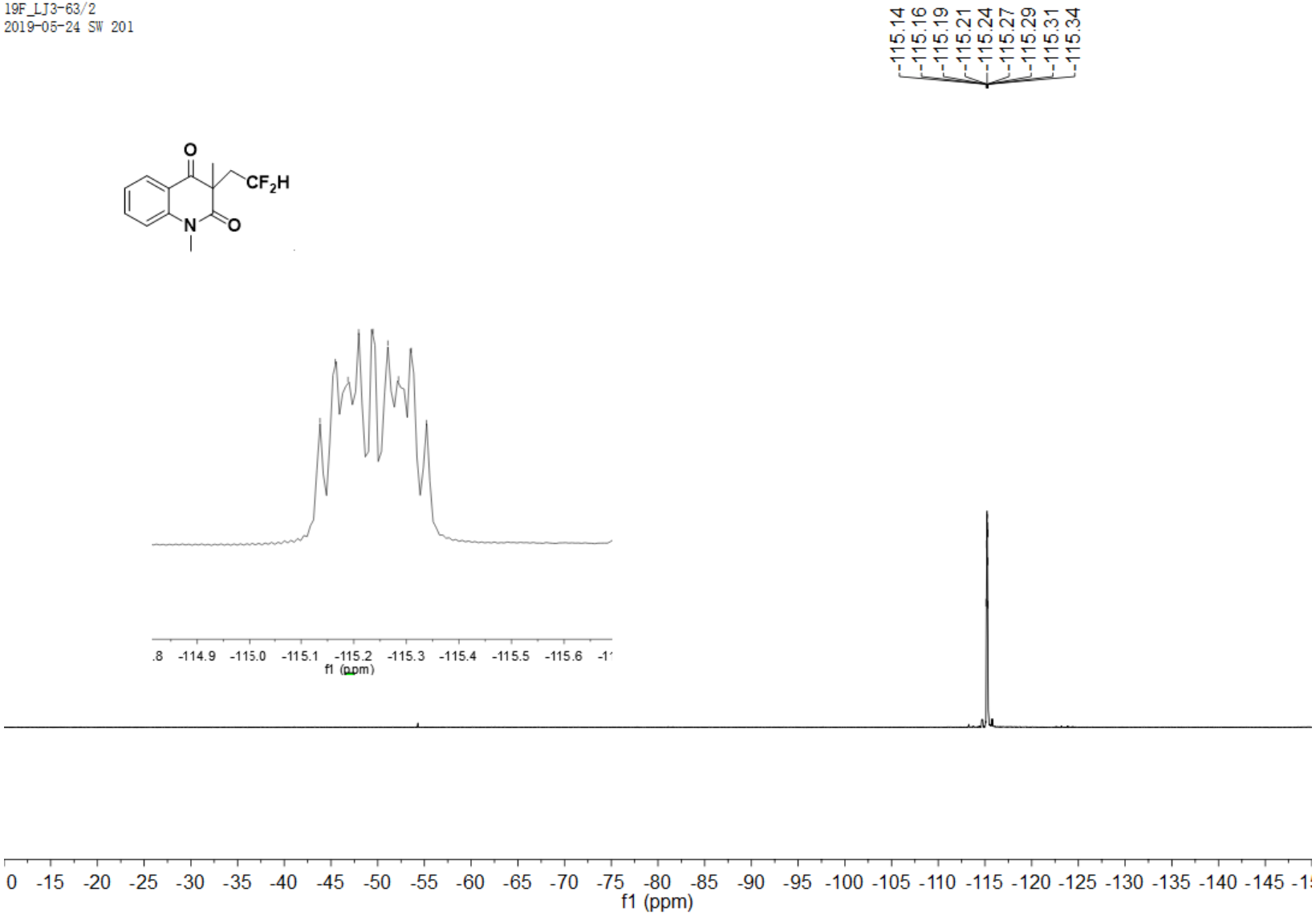
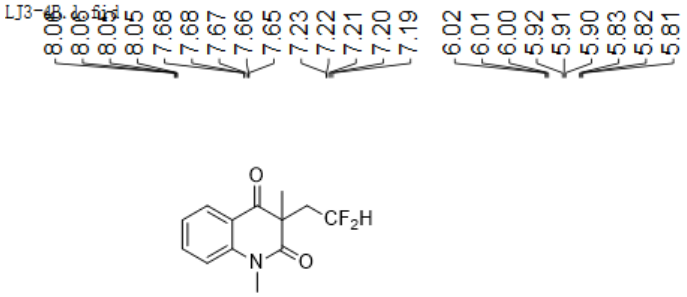
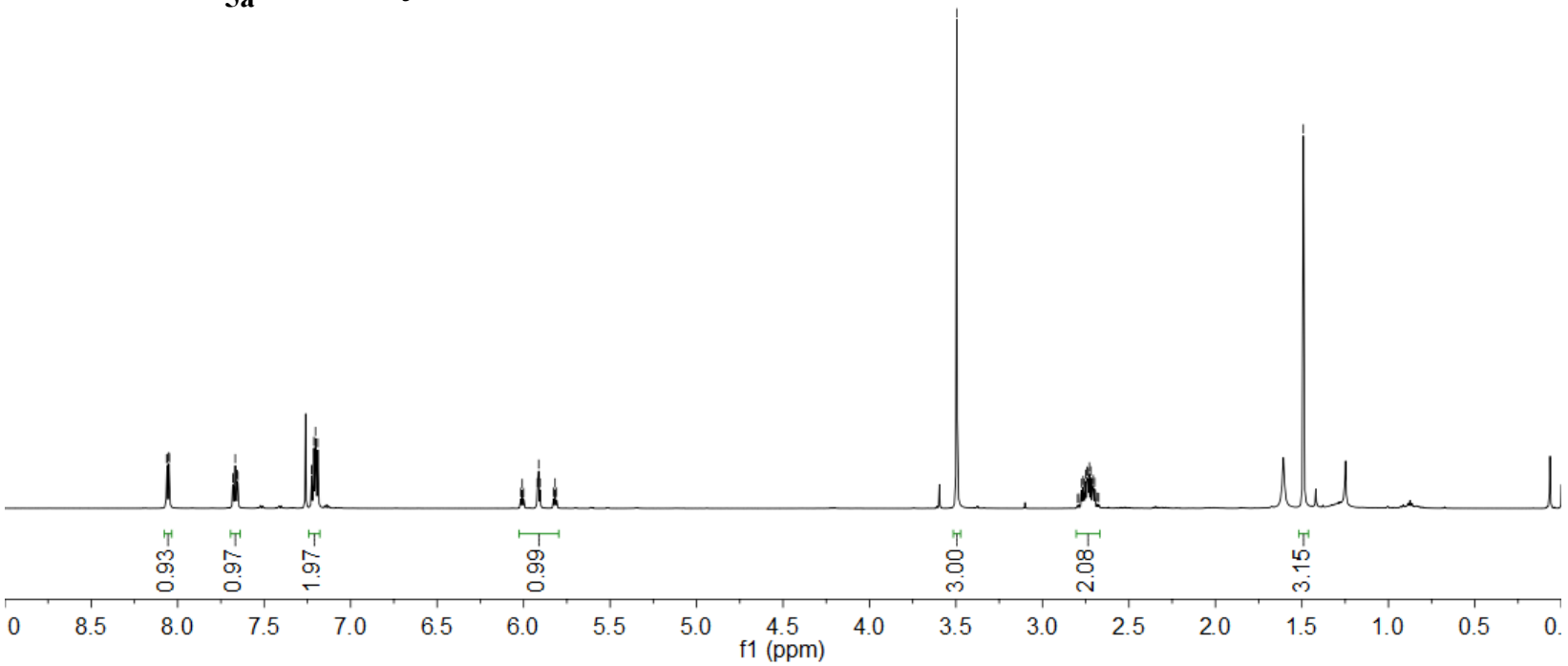
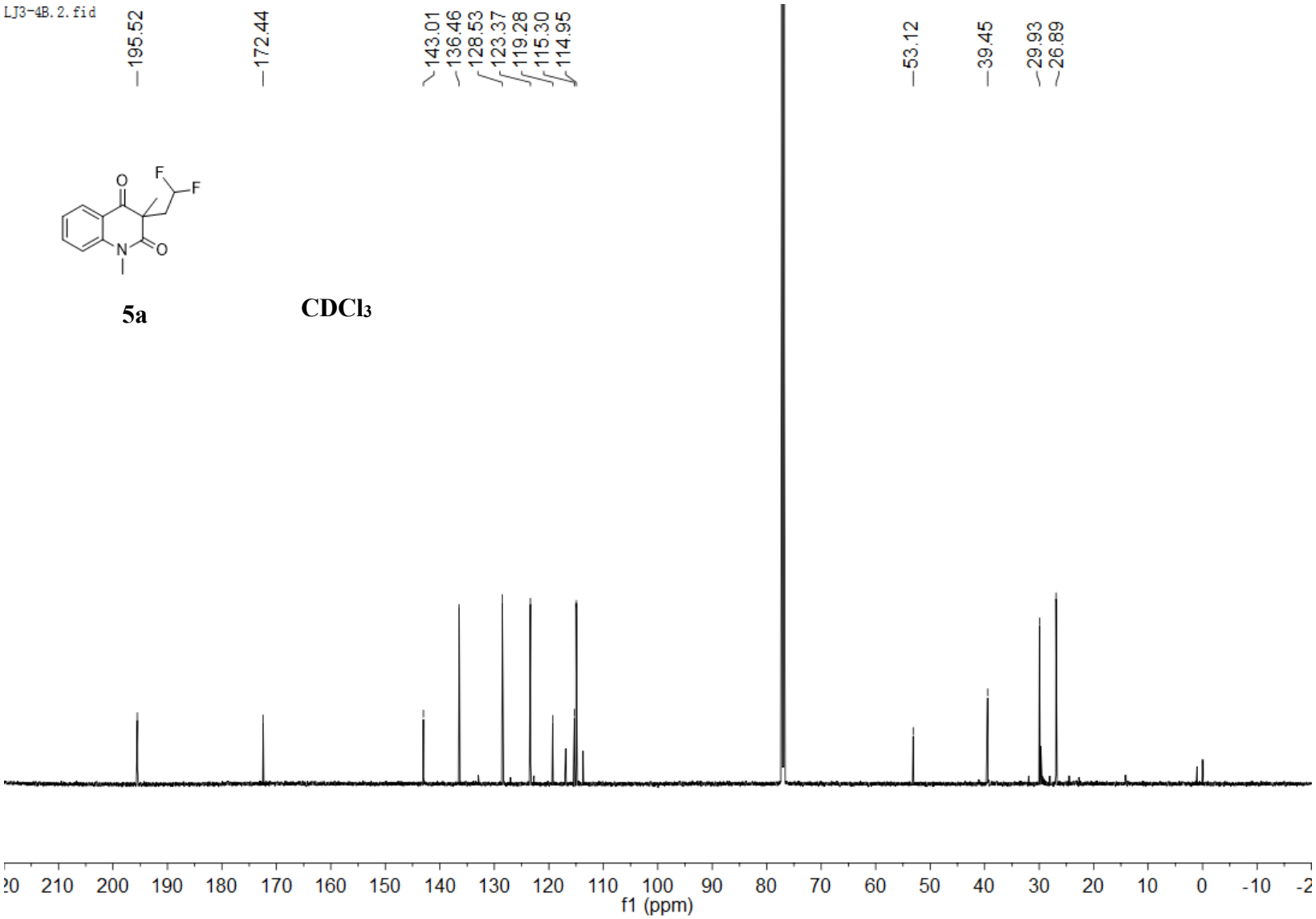



8.06
8.05
8.05
8.05
7.68
7.68
7.67
7.66
7.65
7.23
7.22
7.21
7.20
7.19
6.02
6.01
6.00
5.92
5.91
5.90
5.83
5.82
5.81
3.50
2.80
2.79
2.77
2.76
2.76
2.75
2.74
2.74
2.73
2.72
2.71
2.71
2.70
2.68
2.67
1.49
O
CF2H
N
O

5a **$CDCl_3$**


0.93
0.97
1.97
0.99
3.00
2.08
3.15
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.
f1 (ppm)


LJ3-4B.2.fid
195.52
172.44
143.01
136.46
128.53
123.37
119.28
115.30
114.95
53.12
39.45
29.93
26.89
O
F
F
O
N
O
5a
CDCl3
f1 (ppm)

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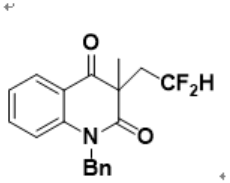
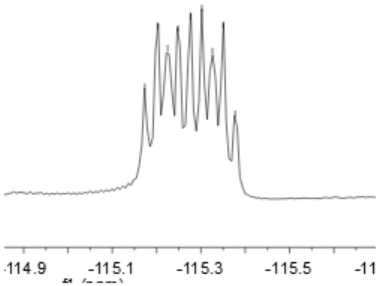
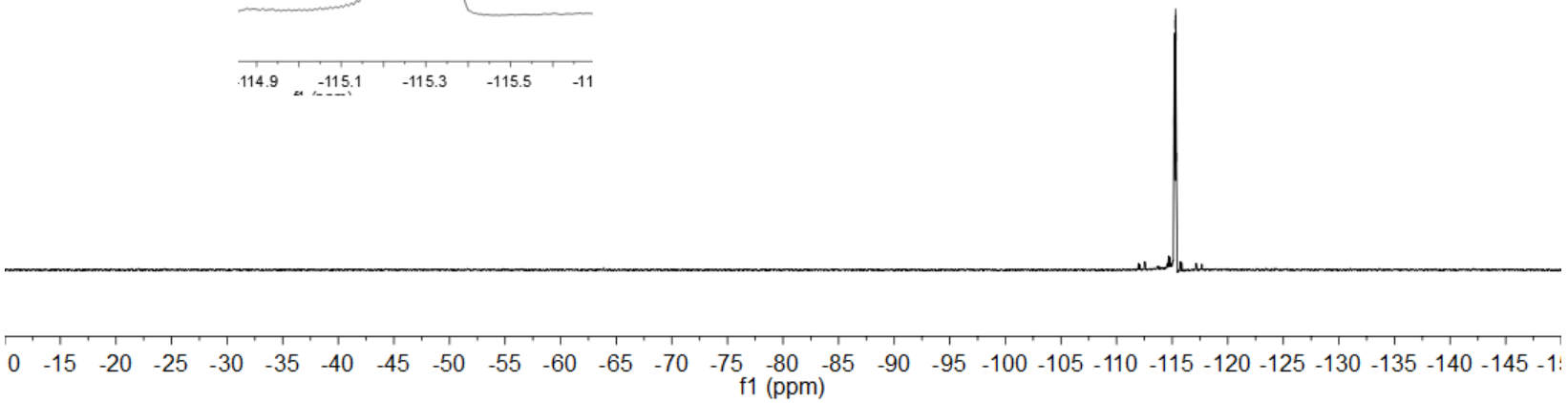
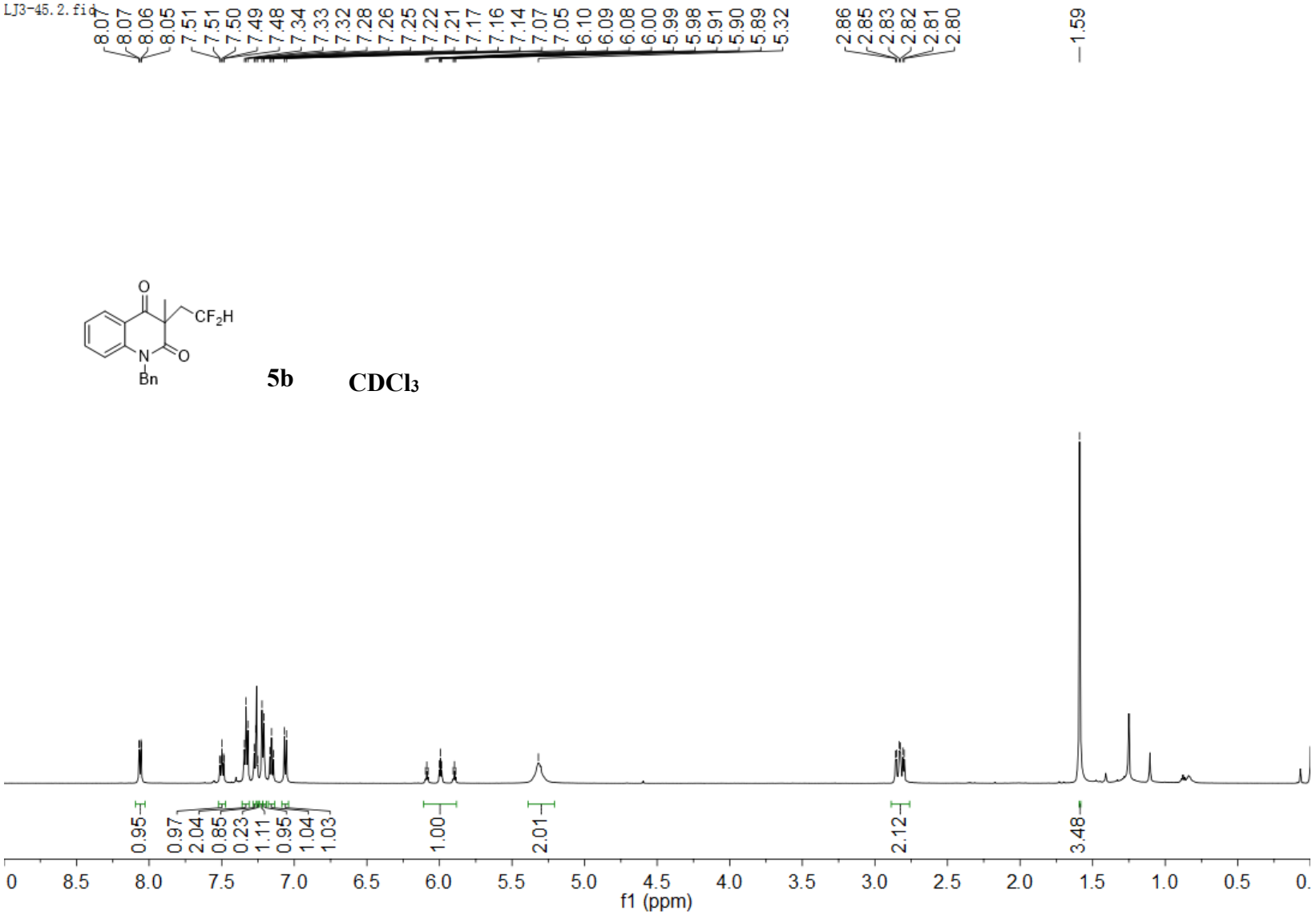
115.17
115.20
115.22
115.25
115.28
115.30
115.33
115.35
115.38



5b **$CDCl_3$**

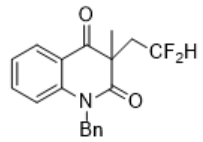





LJ3-45.2.fid
8.07
8.07
8.06
8.05
7.51
7.51
7.50
7.49
7.48
7.34
7.33
7.32
7.28
7.26
7.25
7.22
7.21
7.17
7.16
7.14
7.07
7.05
6.10
6.09
6.08
6.00
5.99
5.98
5.91
5.90
5.89
5.32
2.86
2.85
2.83
2.82
2.81
2.80
1.59
O
CF2H
N
O
Bn
5b
CDCl3
0.95
0.97
2.04
0.85
0.23
1.11
0.95
1.04
1.03
1.00
2.01
2.12
3.48
0
8.5
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.
f1 (ppm)

LJ3-45.3.fid

195.37
172.84
142.23
136.36
135.67
129.00
128.62
127.50
126.14
123.44
119.45
116.97
115.92
115.38
113.79
53.32
46.18
39.29
39.14
38.99
27.27



5b **$CDCl_3$**

19F_LJ3-46/1
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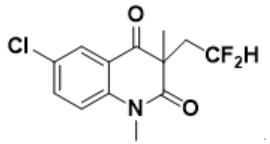
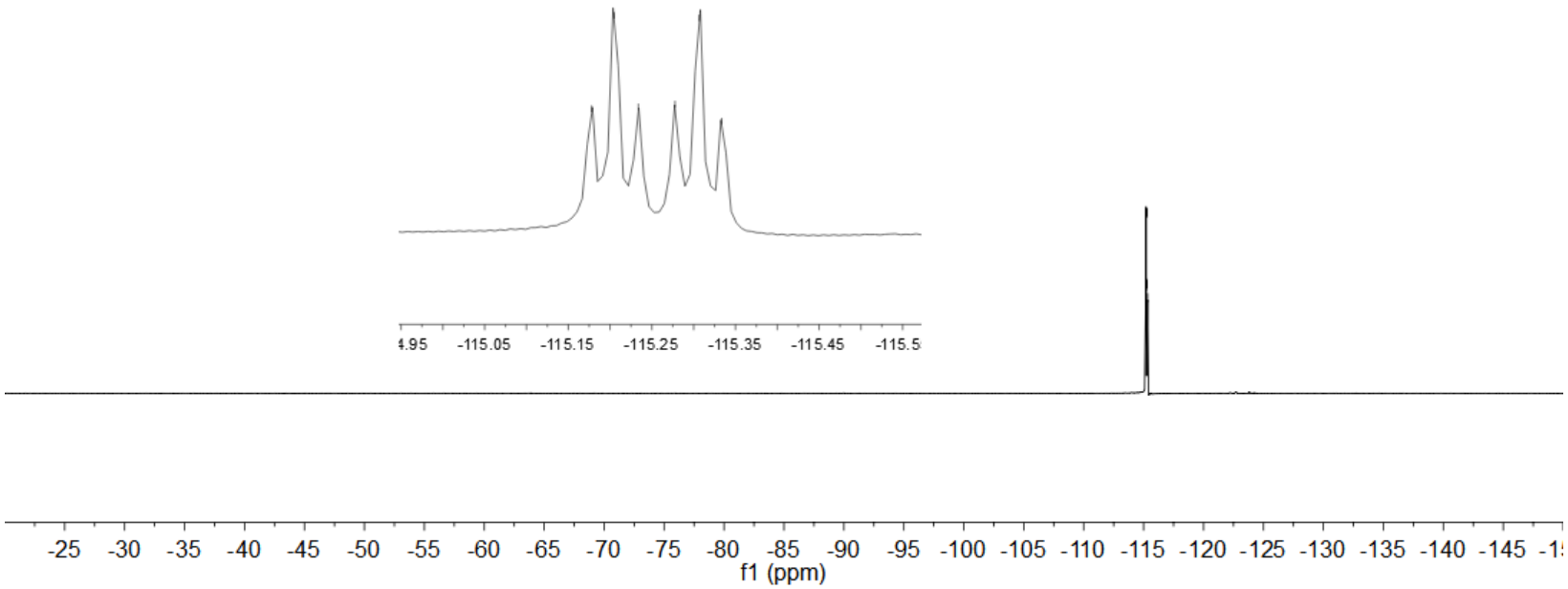
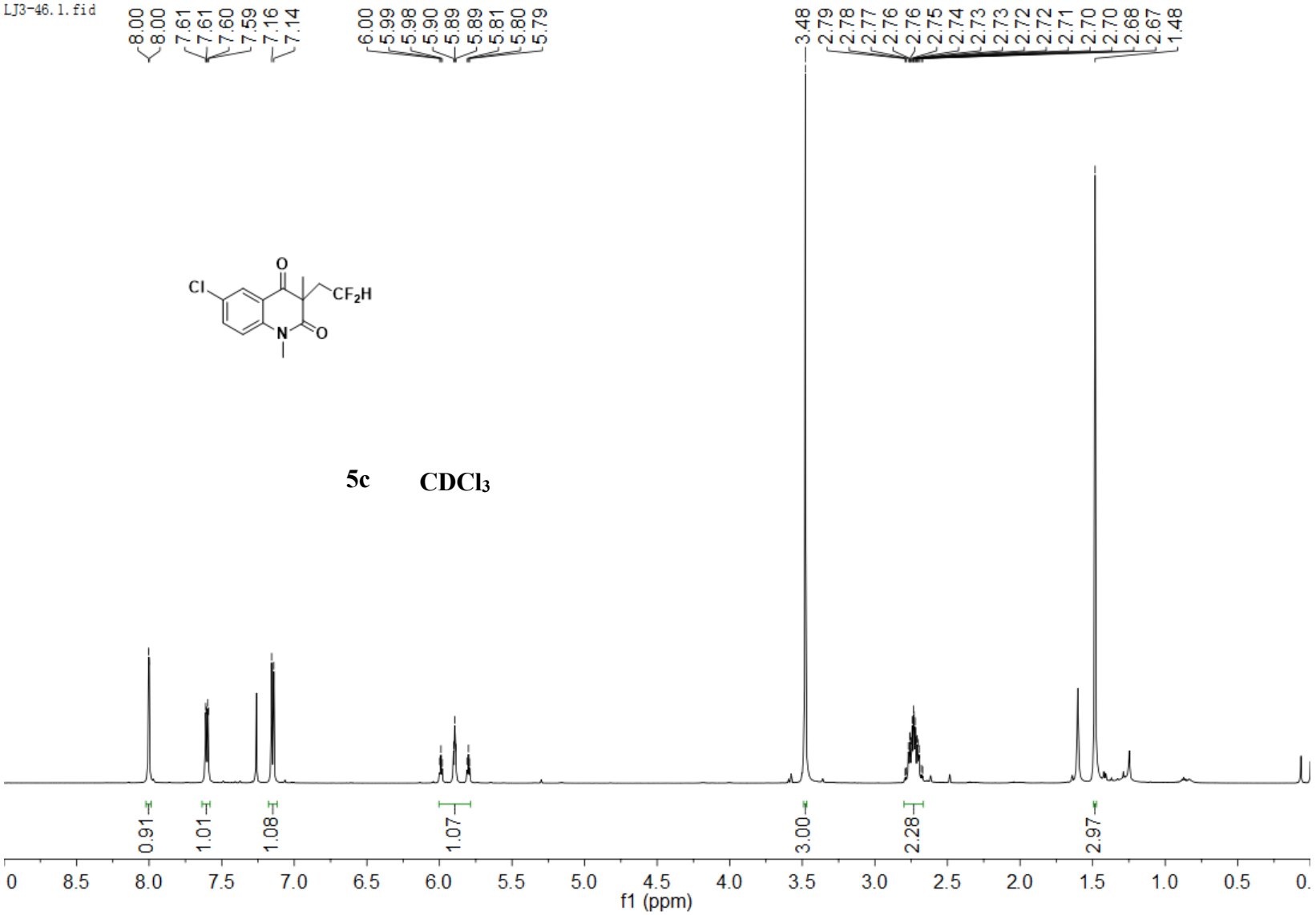
-115.18
-115.20
-115.23
-115.28
-115.31
-115.33



5c **$CDCl_3$**

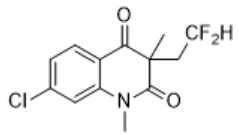



LJ3-46.1.fid
8.00
8.00
7.61
7.61
7.60
7.59
7.16
7.14
6.00
5.99
5.98
5.90
5.89
5.89
5.81
5.80
5.79
3.48
2.79
2.78
2.77
2.76
2.76
2.75
2.74
2.73
2.73
2.72
2.72
2.71
2.70
2.70
2.68
2.67
1.48
Cl
O
CF2H
N
O
0.91
1.01
1.08
1.07
3.00
2.28
2.97
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

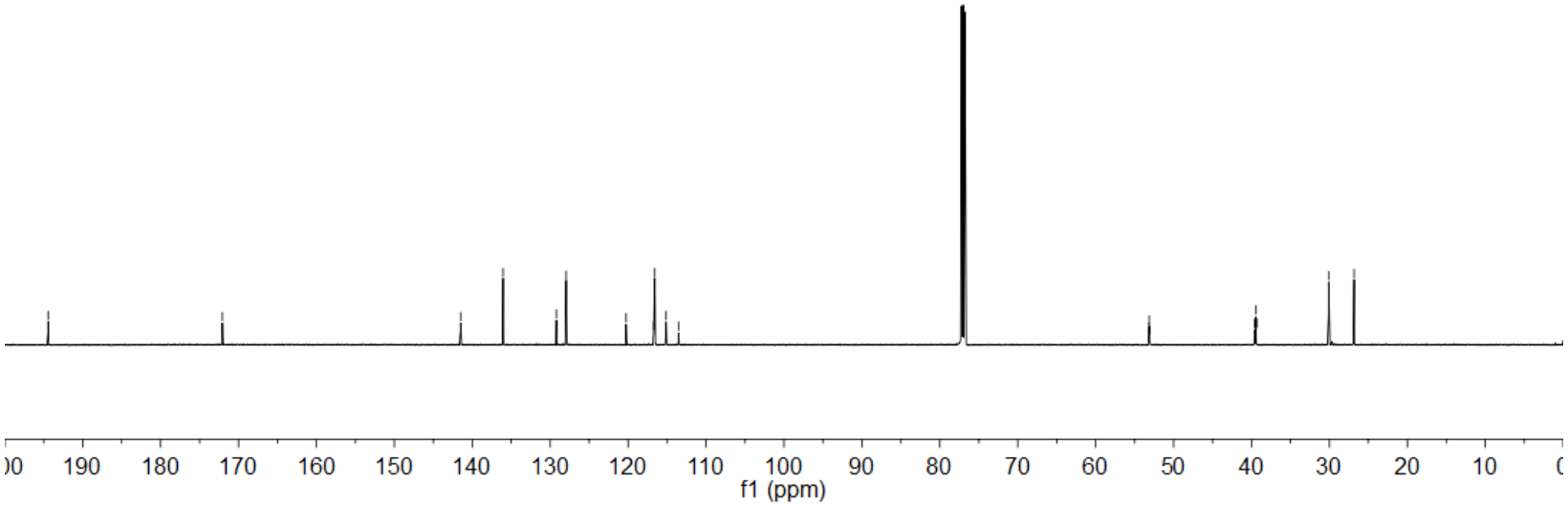
5c **$CDCl_3$**

LJ3-48.2.fid

194.44
172.08
141.49
136.04
129.21
127.95
120.26
116.72
116.59
115.13
113.54
53.15
53.12
53.08
39.61
39.46
39.31
30.09
26.83



5c **$CDCl_3$**



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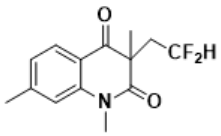
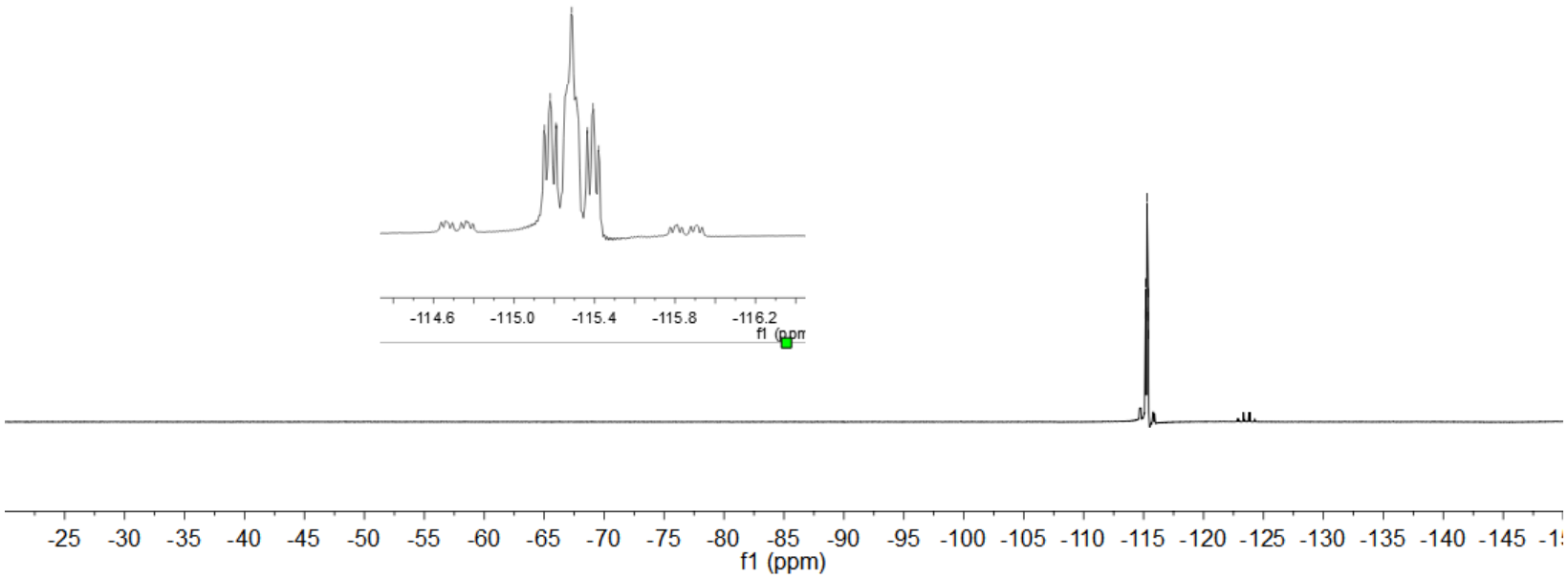
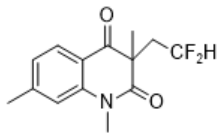


5d **$CDCl_3$**

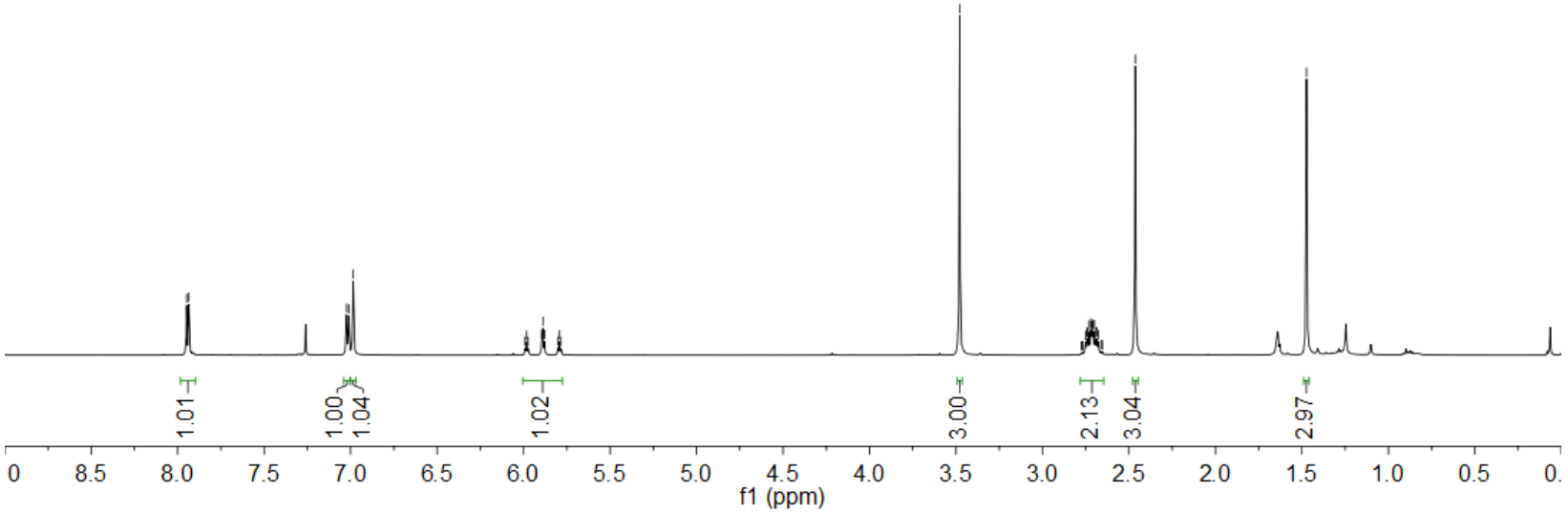


LJ3-49.1.fid

7.95 7.94 7.02 7.01 6.98 5.99 5.98 5.97 5.90 5.89 5.88 5.80 5.79 5.78 3.48 2.77 2.77 2.75 2.74 2.74 2.73 2.72 2.72 2.71 2.71 2.70 2.69 2.69 2.68 2.66 2.65 2.46 1.47

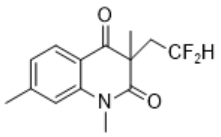


5d **$CDCl_3$**

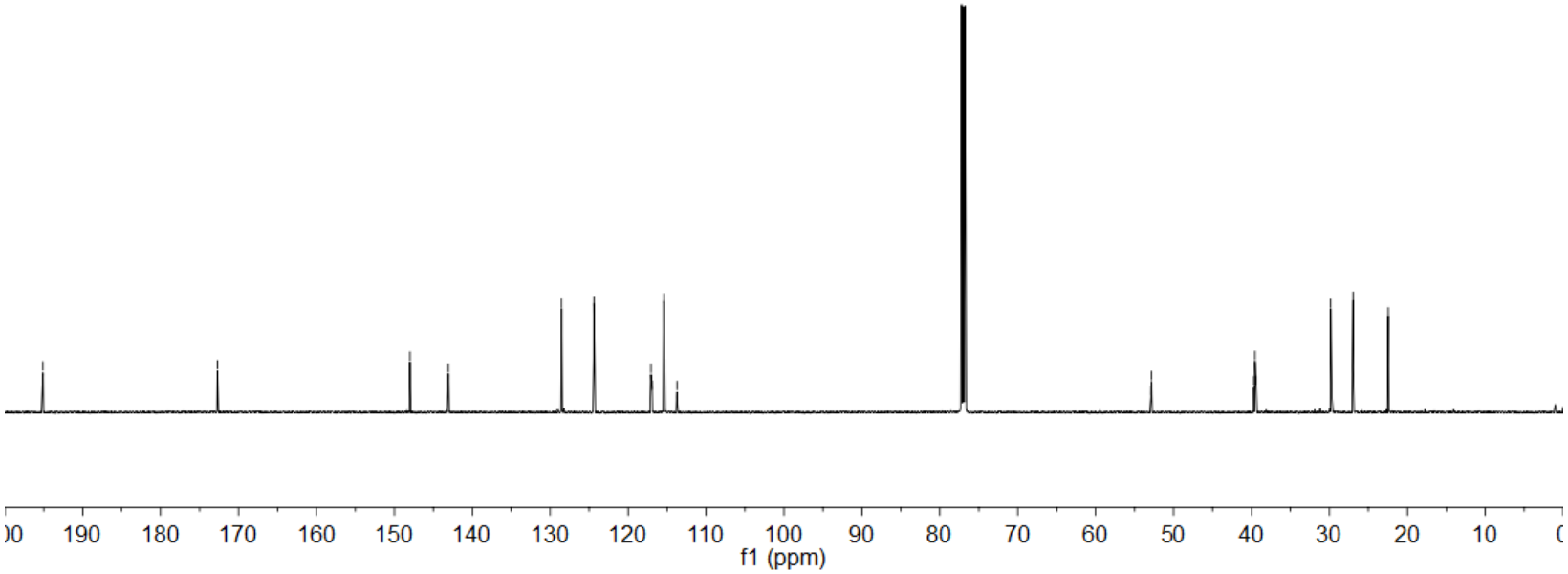


LJ3-49.2.fid

195.09
172.71
147.99
143.06
128.54
124.39
117.08
116.91
115.40
115.32
113.74
52.89
52.86
52.82
39.70
39.55
39.40
29.84
26.98
22.44



5d **$CDCl_3$**



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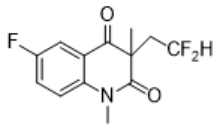
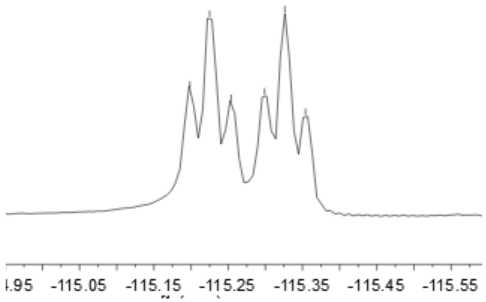
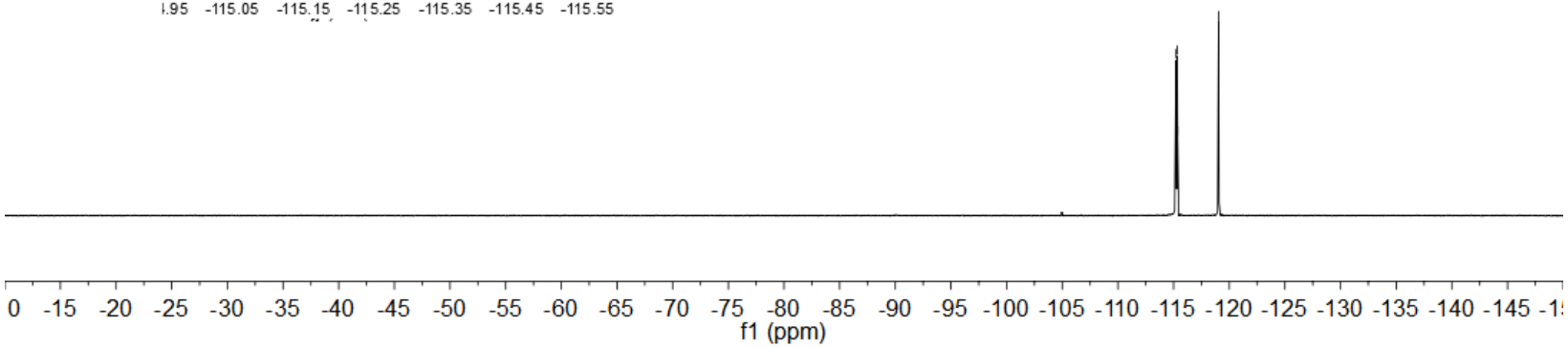
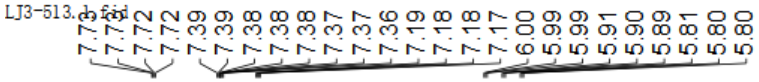
-115.20
-115.22
-115.25
-115.30
-115.33
-115.35
-119.05

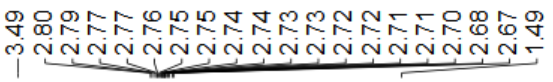


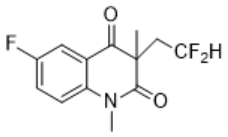
5e **$CDCl_3$**



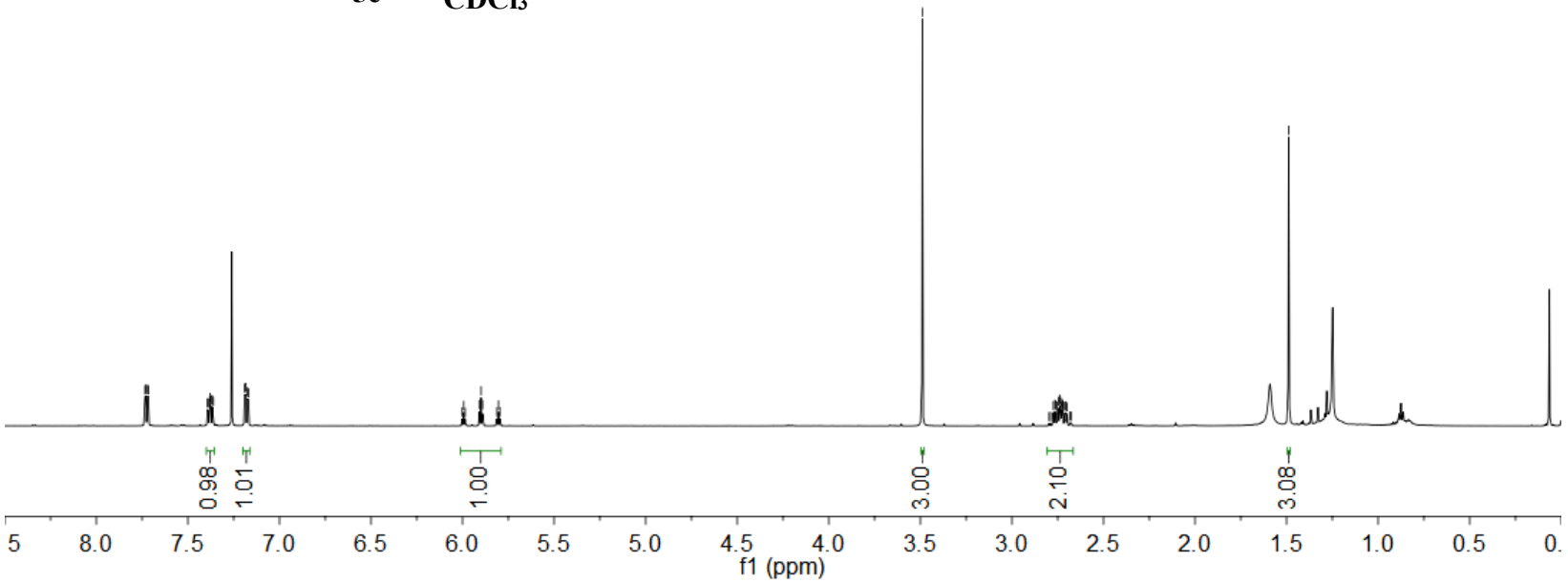


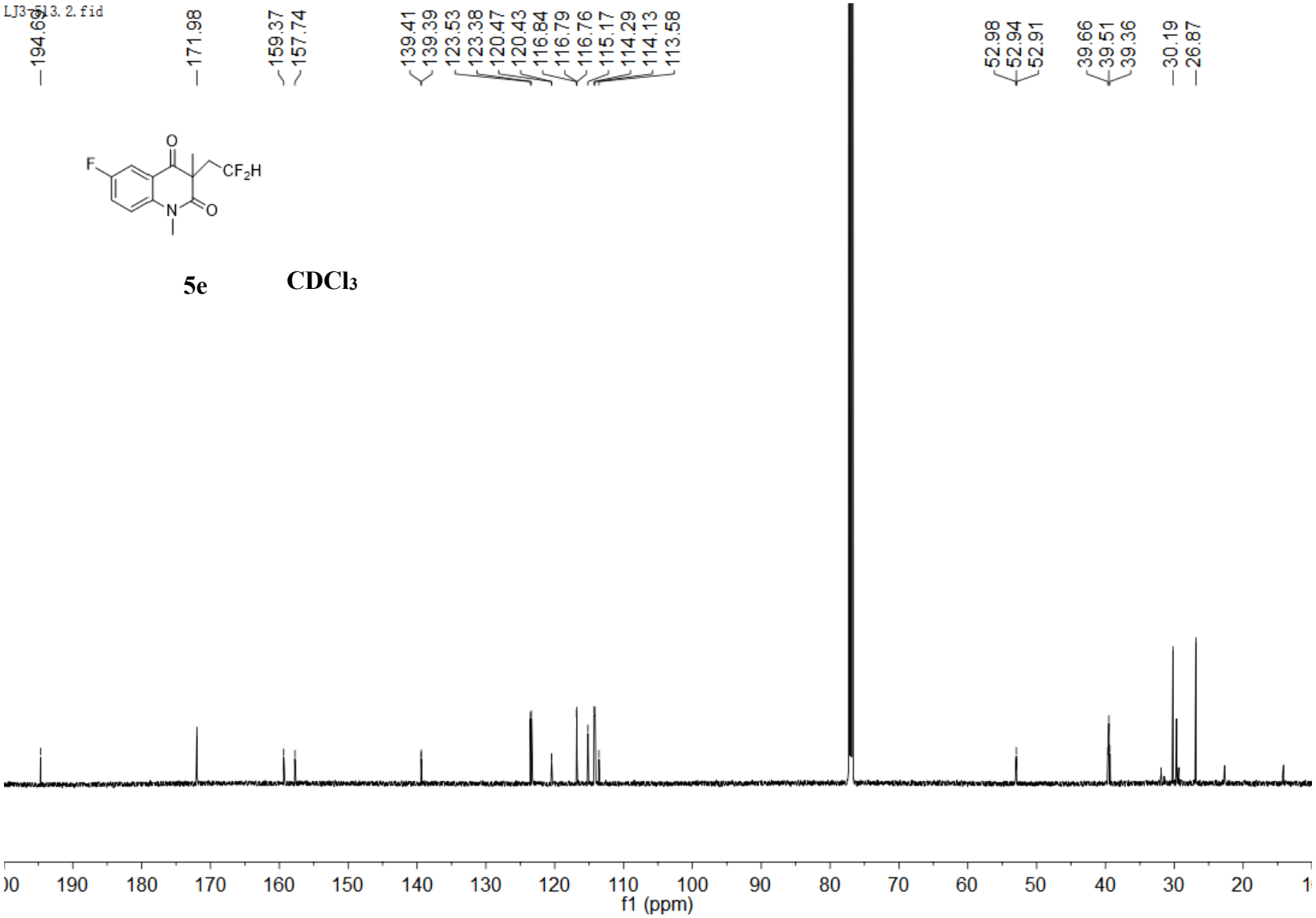

LJ3-513.1.fid
7.73
7.72
7.72
7.39
7.39
7.38
7.38
7.38
7.37
7.37
7.36
7.19
7.18
7.18
7.17
6.00
5.99
5.99
5.91
5.90
5.89
5.81
5.80
5.80


3.49
2.80
2.79
2.77
2.77
2.76
2.75
2.75
2.74
2.74
2.73
2.73
2.72
2.72
2.71
2.71
2.70
2.68
2.67
1.49


O
F
CF2H
N
O

5e **$CDCl_3$**


0.98
1.01
1.00
3.00
2.10
3.08
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.
f1 (ppm)


LJ3-513.2.fid
194.69
171.98
159.37
157.74
139.41
139.39
123.53
123.38
120.47
120.43
116.84
116.79
116.76
115.17
114.29
114.13
113.58
52.98
52.94
52.91
39.66
39.51
39.36
30.19
26.87
F
O
CF2H
N
O
f1 (ppm)

5e **$CDCl_3$**

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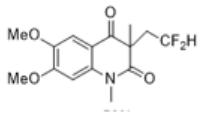
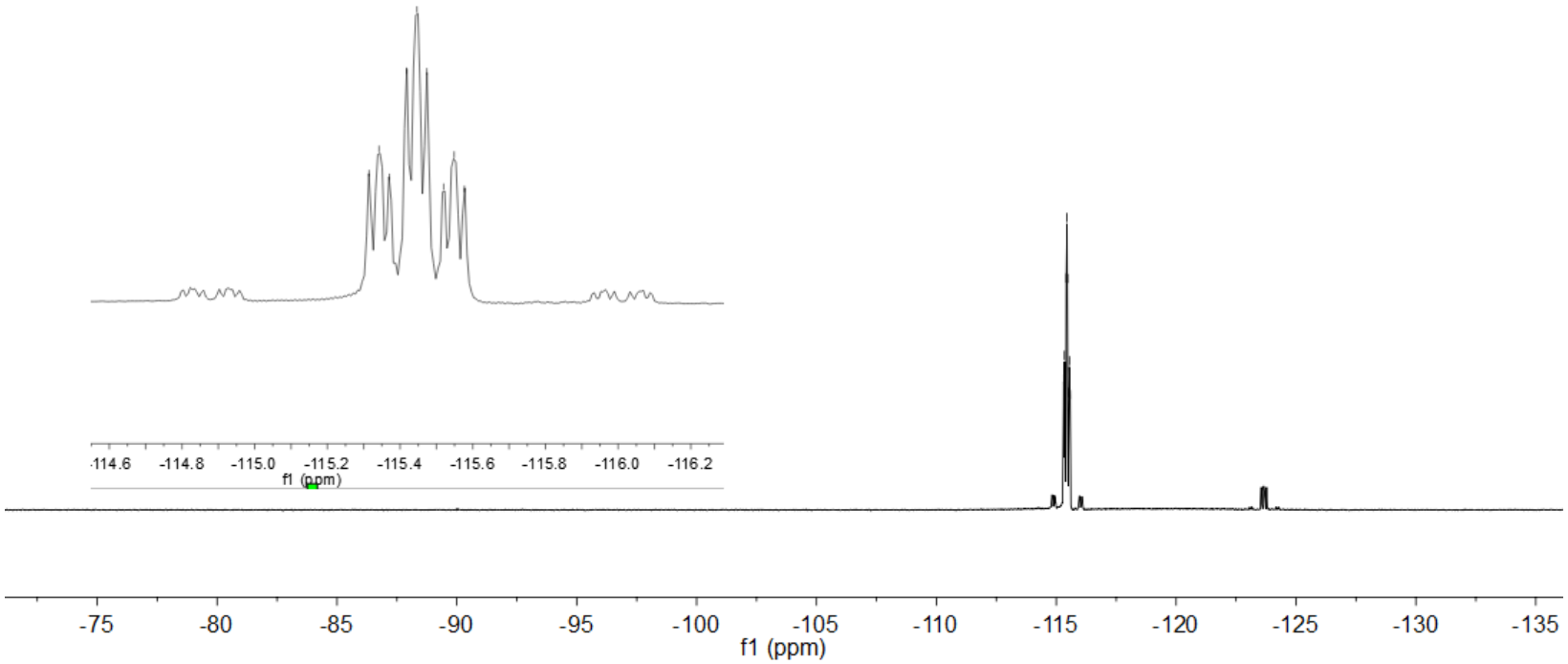
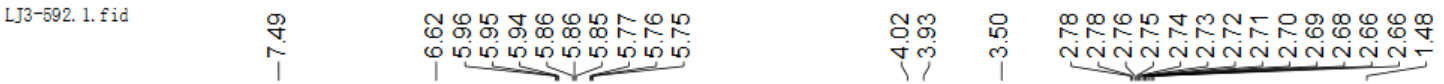
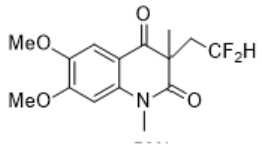
-115.31
-115.34
-115.37
-115.42
-115.45
-115.47
-115.52
-115.55
-115.58



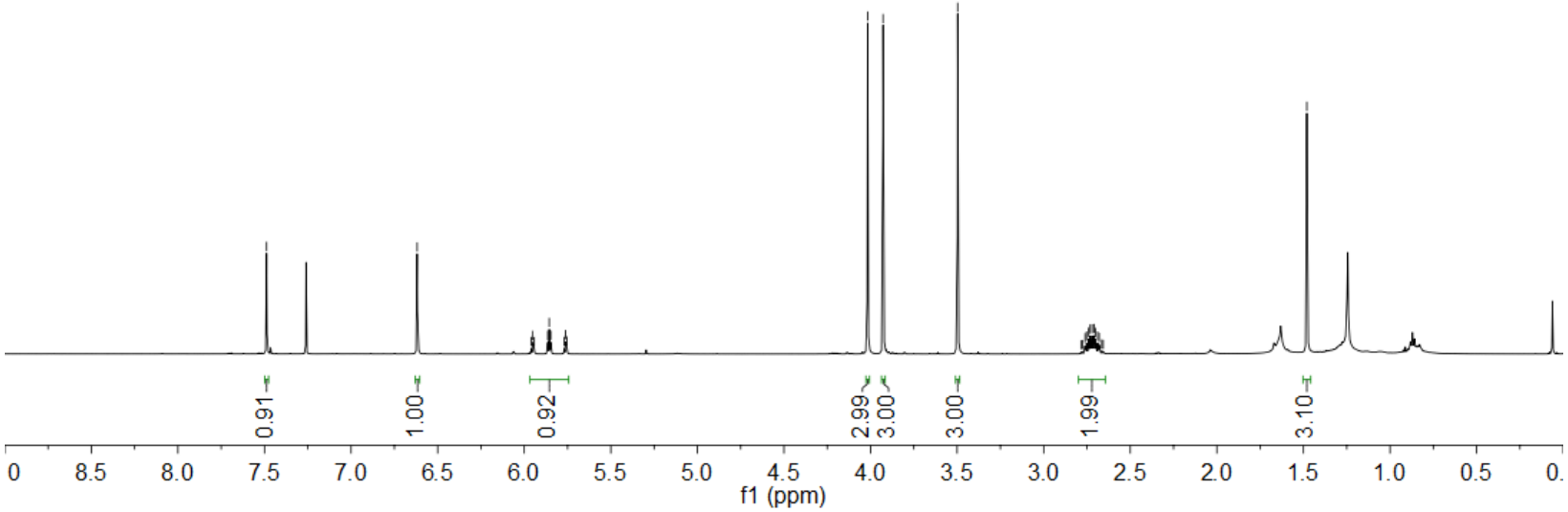
5f **$CDCl_3$**




LJ3-592.1.fid
7.49
6.62
5.96
5.95
5.94
5.86
5.86
5.85
5.77
5.76
5.75
4.02
3.93
3.50
2.78
2.78
2.76
2.75
2.74
2.73
2.72
2.71
2.70
2.69
2.68
2.66
2.66
1.48

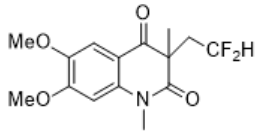

O
MeO
MeO
CF2H
N
O

5f **$CDCl_3$**

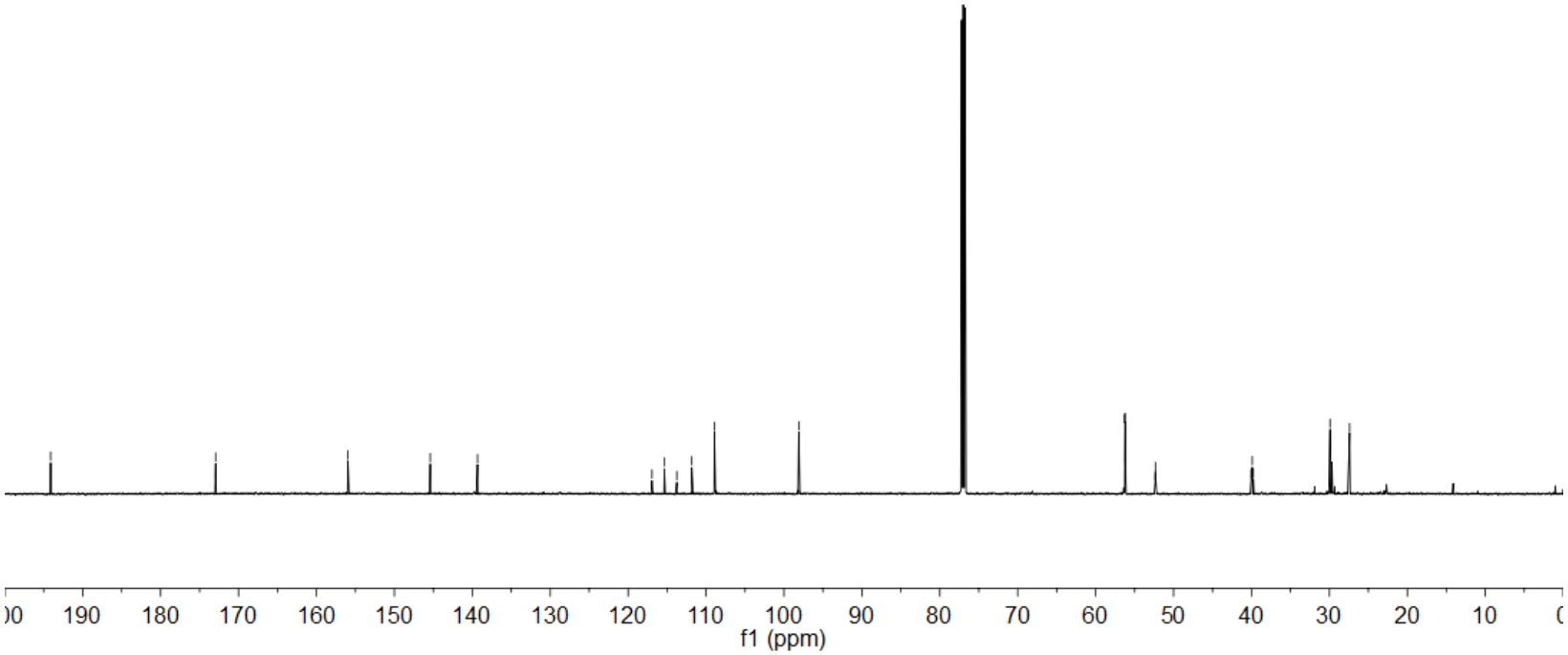

0.91
1.00
0.92
2.99
3.00
3.00
1.99
3.10
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

LJ3-592.2.fid

194.11
172.93
155.95
145.39
139.32
116.94
115.35
113.76
111.83
108.92
98.09
56.35
56.20
52.36
52.33
52.30
40.05
39.91
39.76
29.92
27.41



5f **$CDCl_3$**



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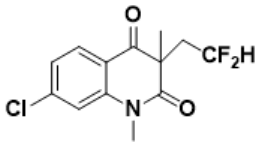
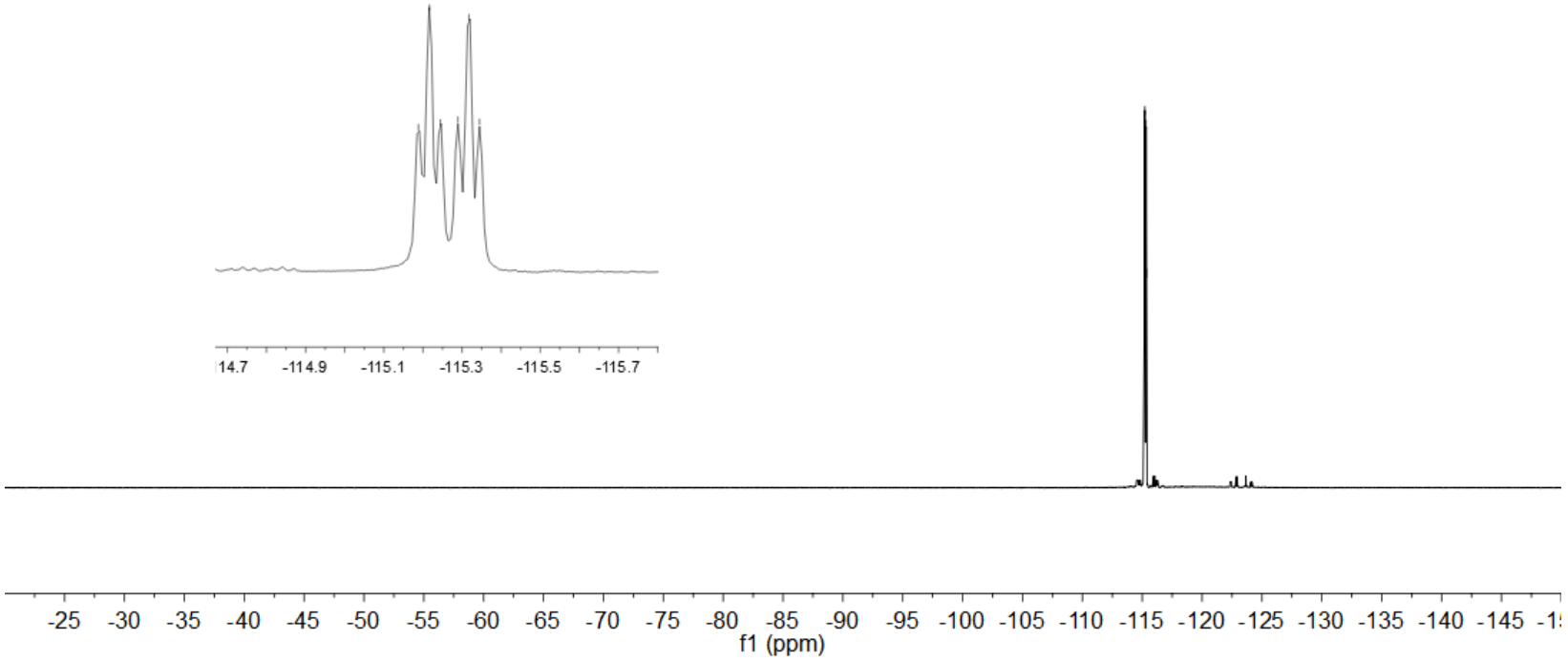


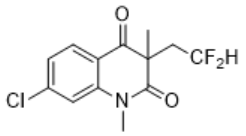
5g **$CDCl_3$**



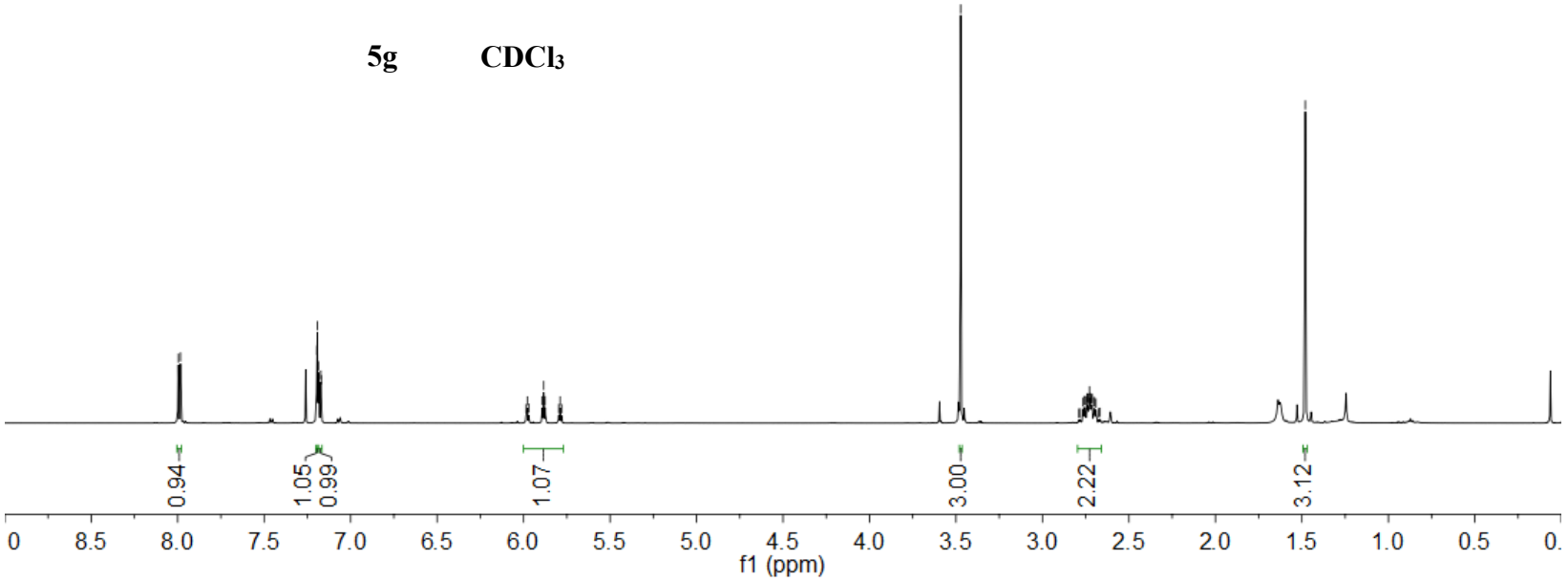
LJ3-61.3.fid

8.00 7.98 7.20 7.19 7.19 7.18 7.17 7.17 5.99 5.98 5.97 5.89 5.88 5.88 5.80 5.79 5.78

3.47 2.79 2.78 2.77 2.76 2.75 2.74 2.74 2.74 2.73 2.73 2.72 2.72 2.72 2.71 2.70 2.70 2.69 2.67 2.67 1.48

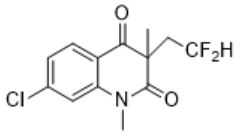


5g **$CDCl_3$**

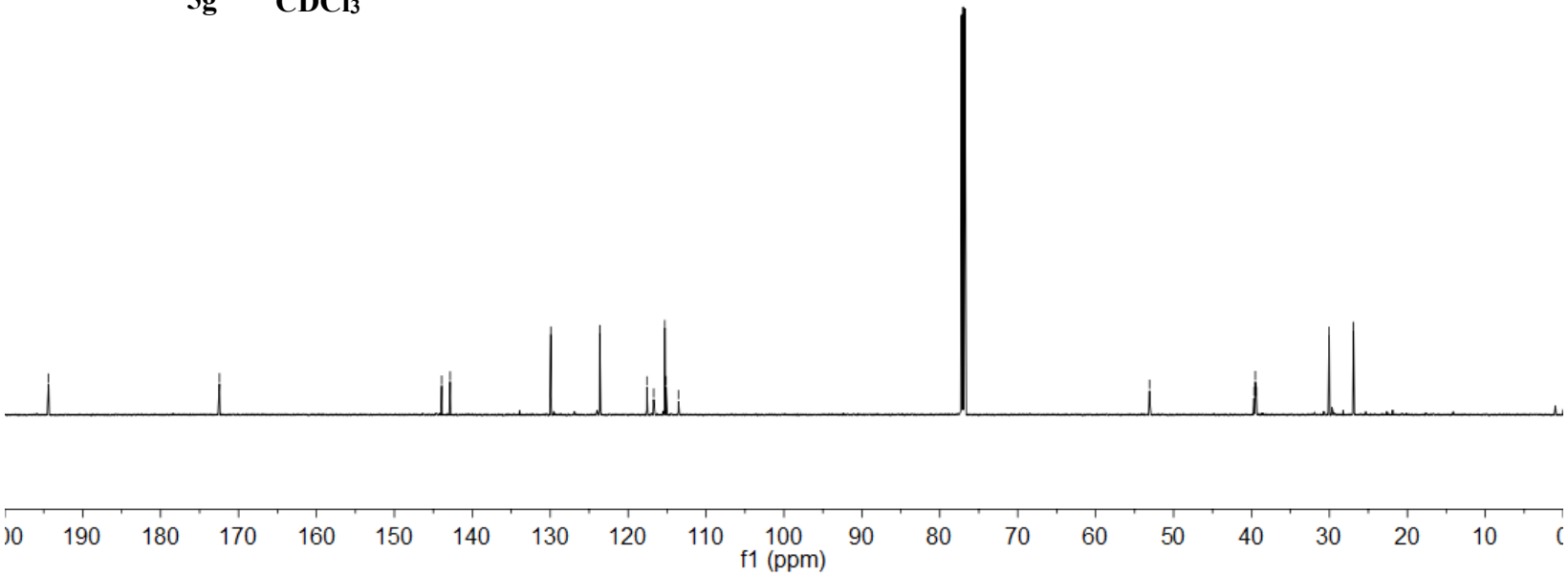


LJ3761.4.fid

194.37
172.45
143.93
142.85
129.92
123.64
117.59
116.72
115.29
115.13
113.54
53.08
39.66
39.52
39.37
30.04
26.91



5g **$CDCl_3$**



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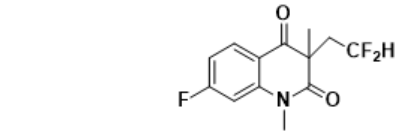
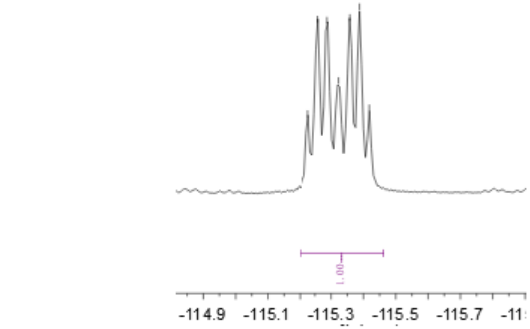
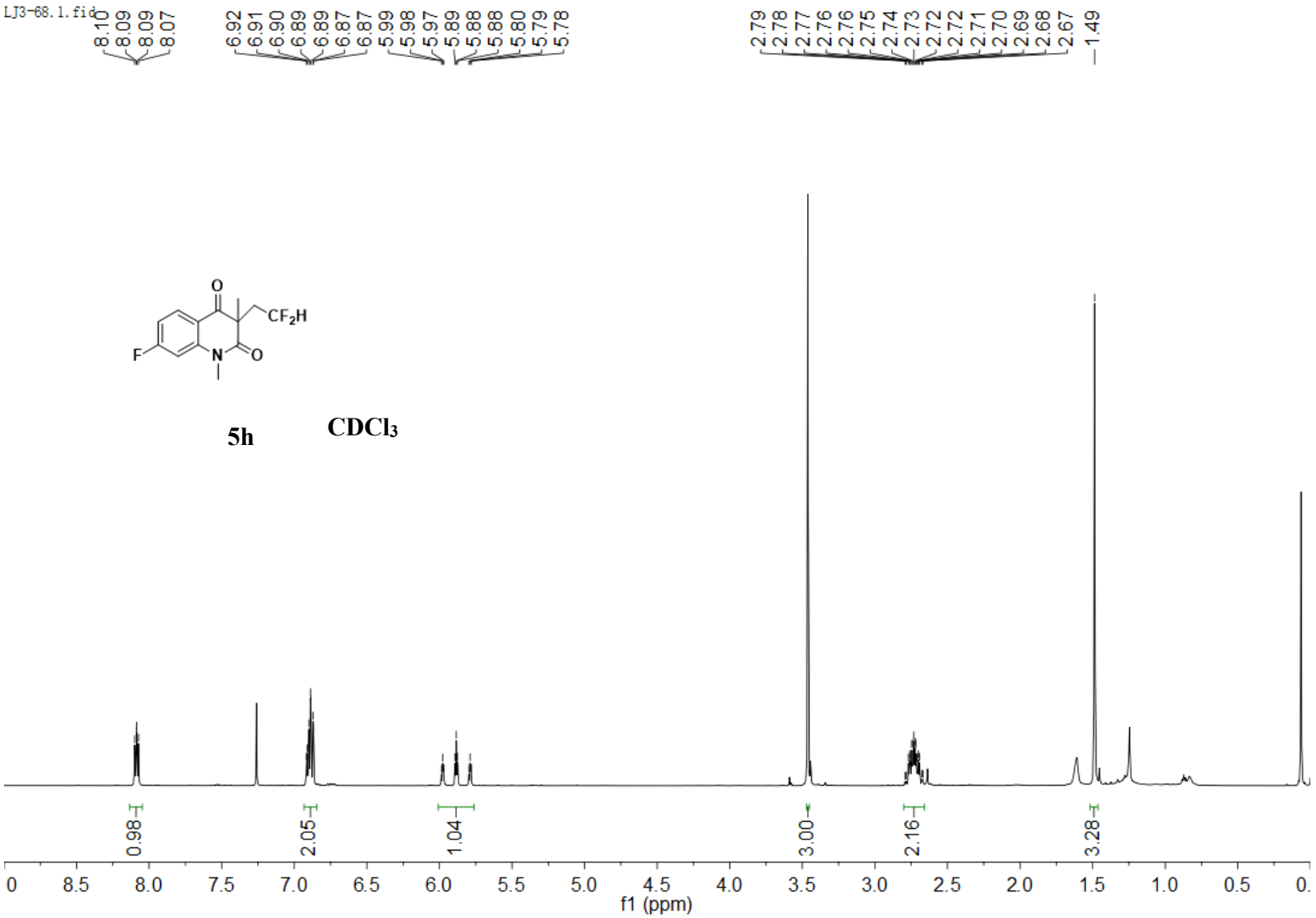


5h **$CDCl_3$**

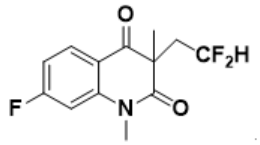



LJ3-68.1.fid
8.10
8.09
8.09
8.07
6.92
6.91
6.90
6.89
6.89
6.87
6.87
5.99
5.98
5.97
5.89
5.88
5.88
5.80
5.79
5.78
2.79
2.78
2.77
2.76
2.76
2.75
2.74
2.73
2.72
2.72
2.71
2.70
2.69
2.68
2.67
1.49
O
CF2H
F
N
O
0.98
2.05
1.04
3.00
2.16
3.28
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

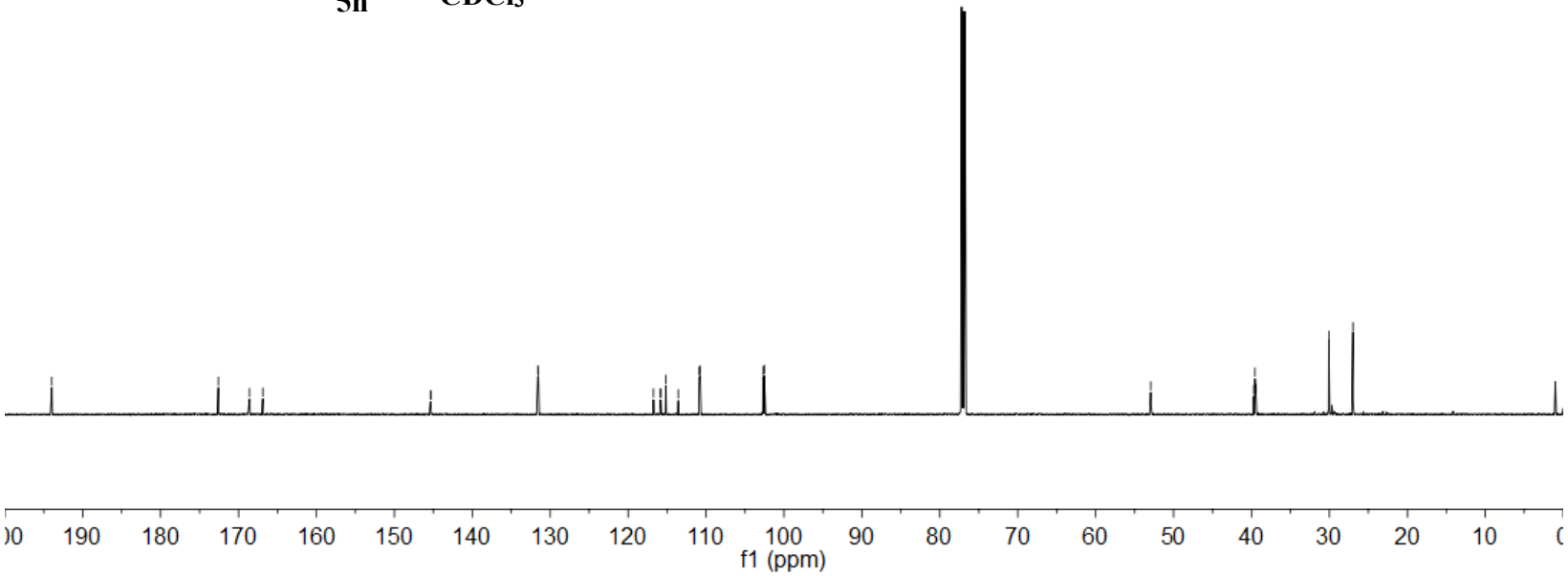
5h **$CDCl_3$**

LJ3-68.2.fid

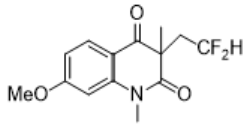
193.97
172.59
168.58
166.88
145.36
145.28
131.58
131.51
116.75
115.84
115.82
115.16
113.57
110.89
110.74
102.70
102.51
52.93
39.70
39.56
39.41
30.08
26.99



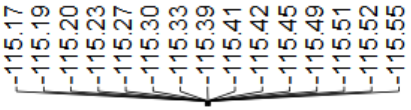
5h **$CDCl_3$**

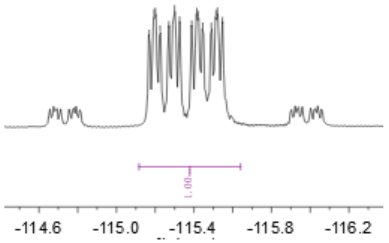


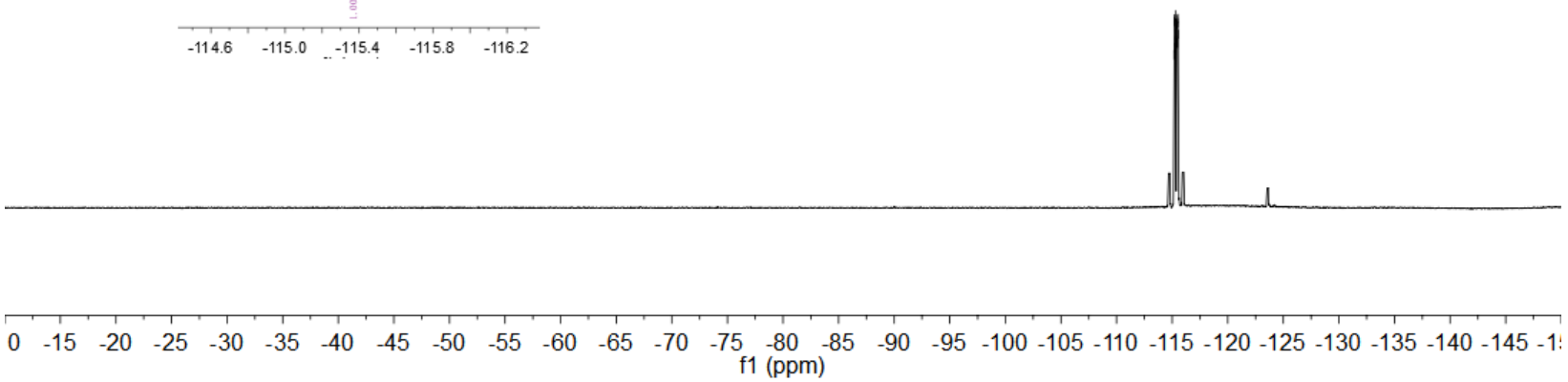
19F_LJ3-722/1
2019-05-23 SW 201



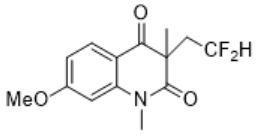
5j CDCl3



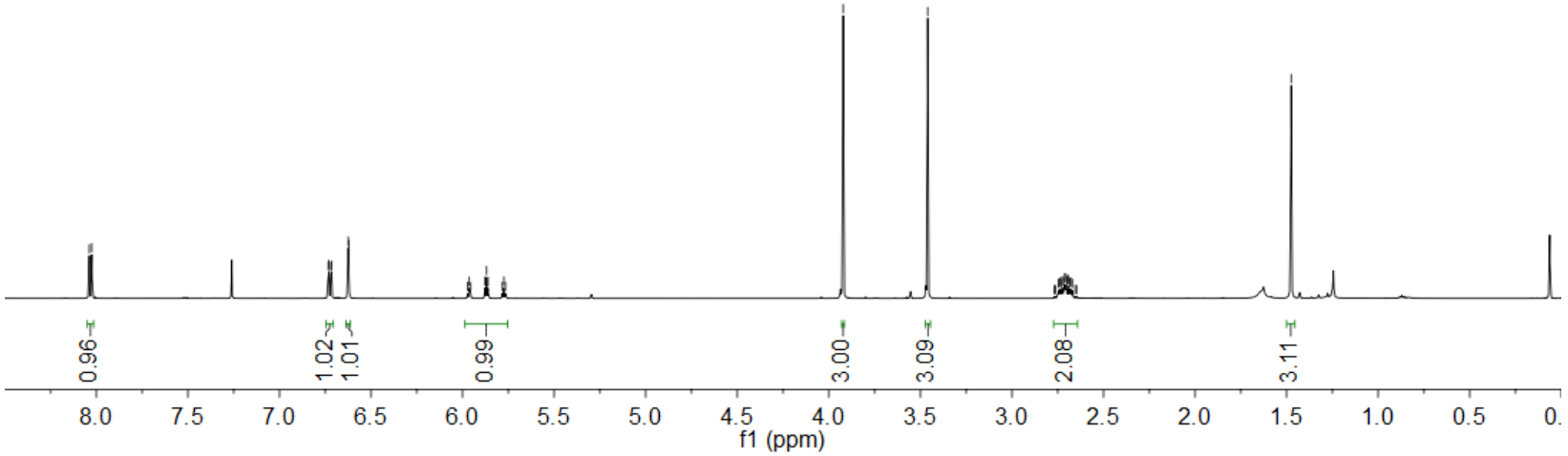


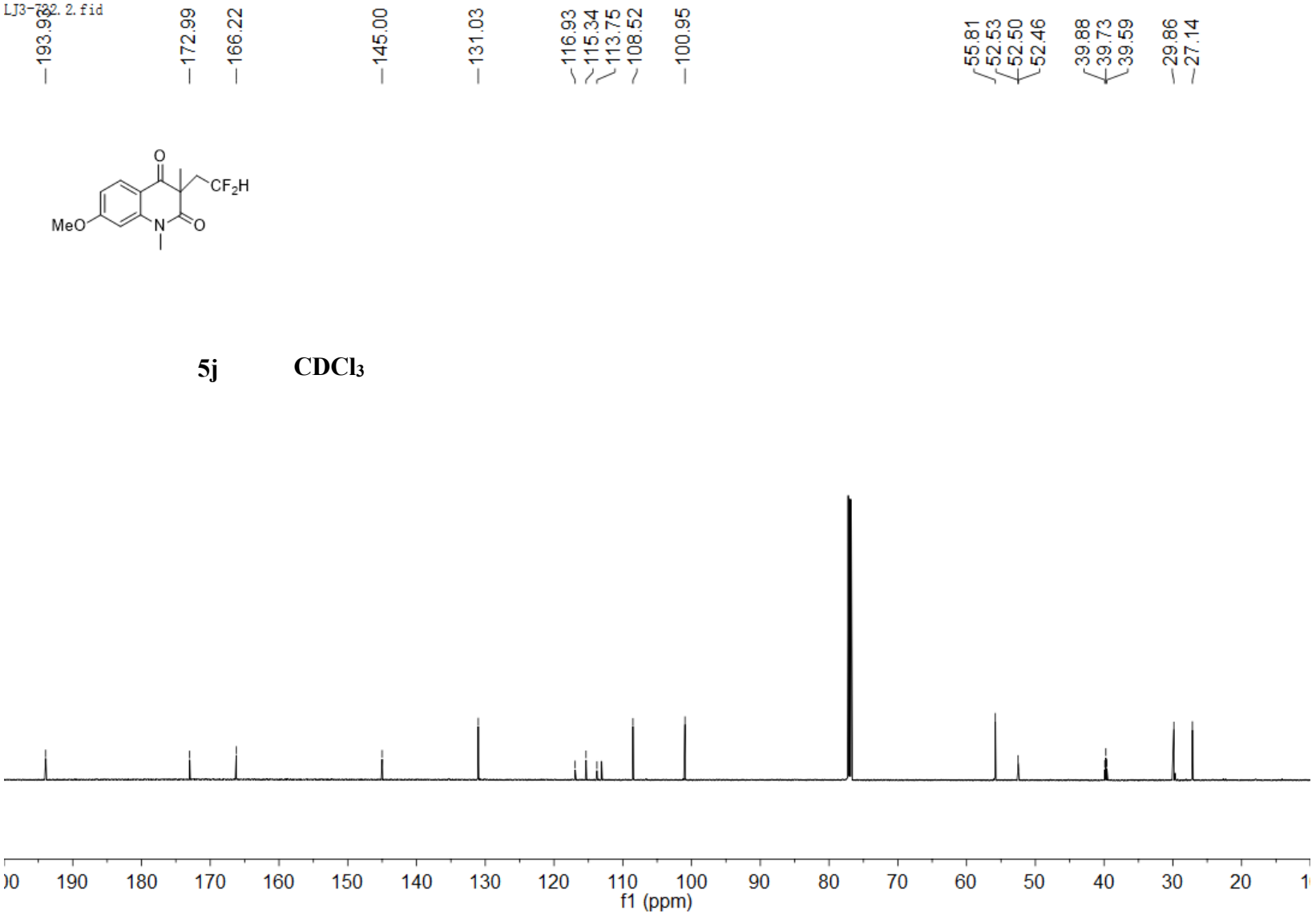



LJ3-722-1.fid
8.04
8.02
6.73
6.73
6.72
6.71
6.62
6.62
5.97
5.96
5.96
5.88
5.87
5.86
5.78
5.77
5.77
3.92
3.46
2.77
2.76
2.75
2.74
2.73
2.73
2.72
2.71
2.70
2.70
2.69
2.68
2.68
2.67
2.66
2.65
1.47

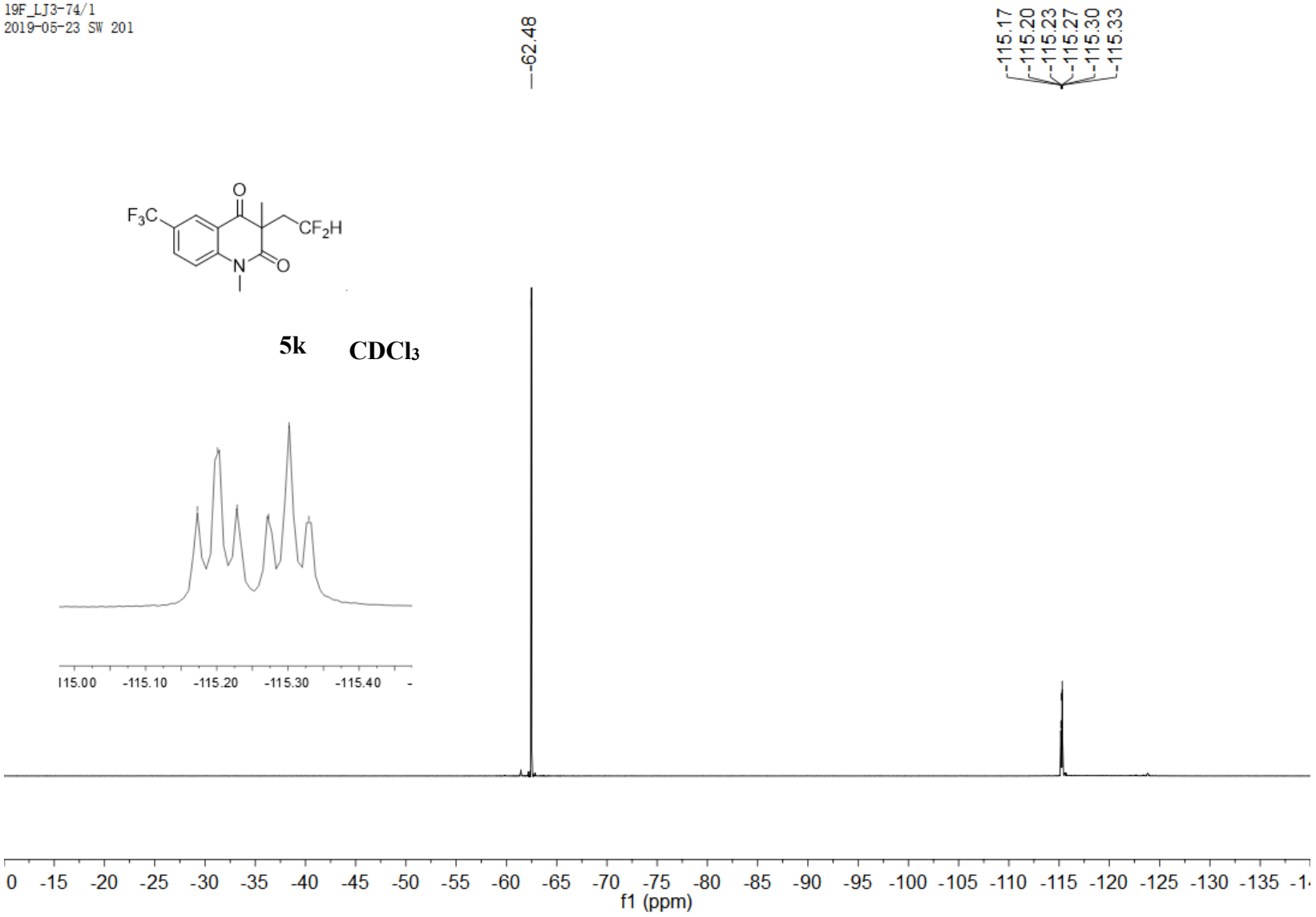

O
CF2H
MeO
N
O

5j **$CDCl_3$**

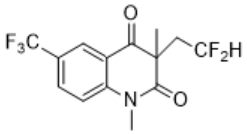

0.96
1.02
1.01
0.99
3.00
3.09
2.08
3.11
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)


LJ3-732.2.fid
193.98
172.99
166.22
145.00
131.03
116.93
115.34
113.75
108.52
100.95
55.81
52.53
52.50
52.46
39.88
39.73
39.59
29.86
27.14
O
CF2H
MeO
N
O
f1 (ppm)

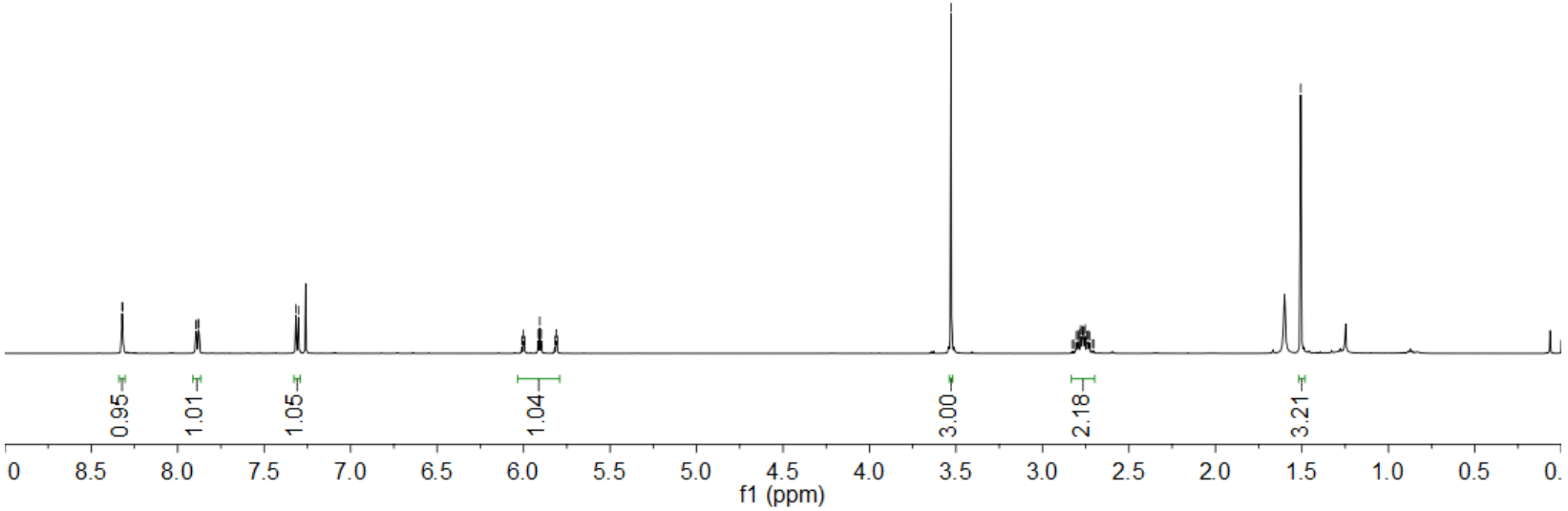
5j **$CDCl_3$**

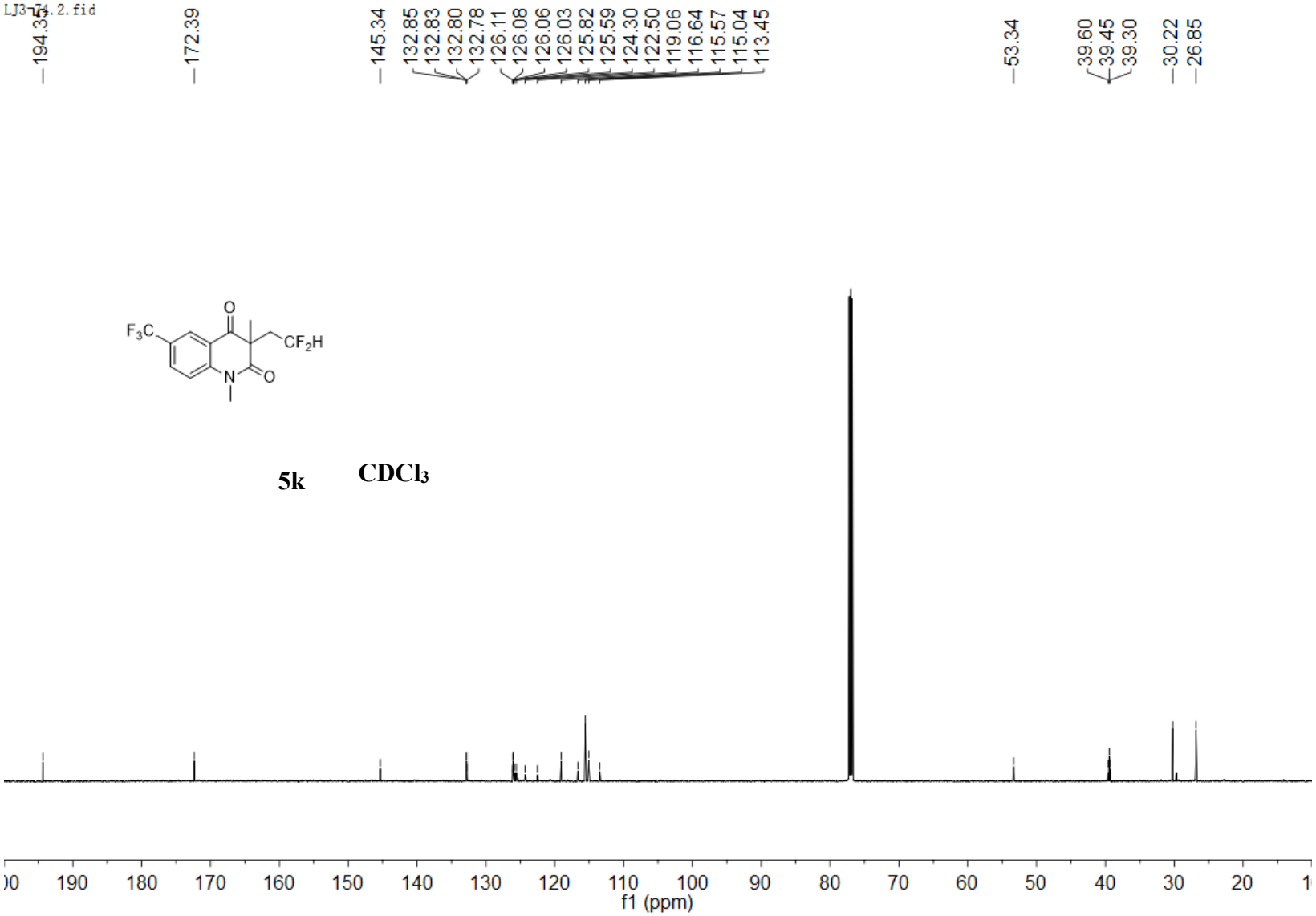

19F_LJ3-74/1
2019-05-23 SW 201
-62.48
-115.17
-115.20
-115.23
-115.27
-115.30
-115.33
F3C
CF2H
O
N
O
5k
CDCl3
115.00
-115.10
-115.20
-115.30
-115.40
0
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
f1 (ppm)


LJ3-74.1.fid
8.32
8.32
7.90
7.89
7.88
7.88
7.32
7.30
6.01
6.00
5.99
5.91
5.91
5.90
5.82
5.81
5.80
3.53
2.83
2.82
2.80
2.80
2.79
2.78
2.78
2.77
2.77
2.76
2.76
2.75
2.74
2.74
2.73
2.71
2.70
1.51

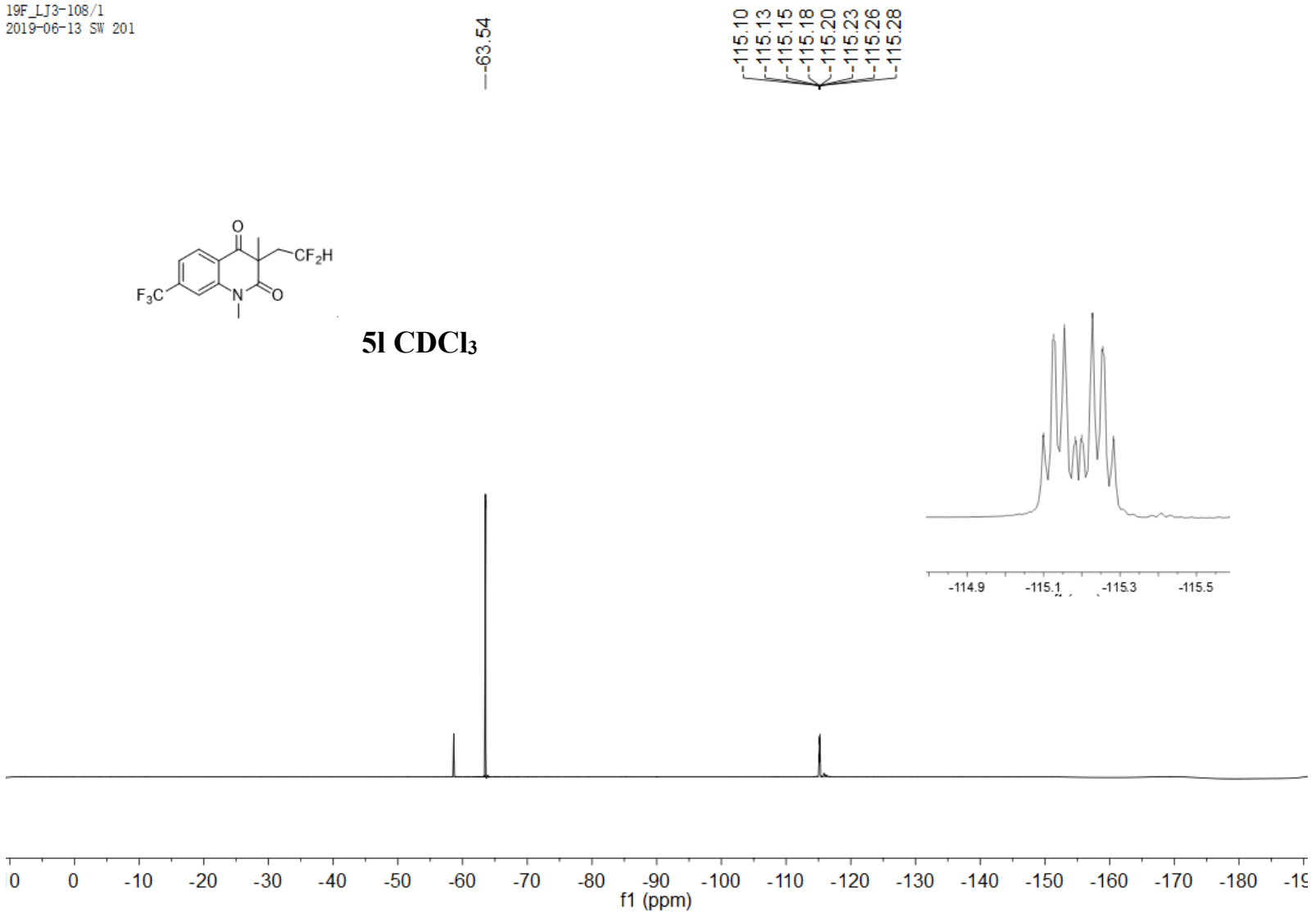

O
F3C
CF2H
N
O

5k **$CDCl_3$**

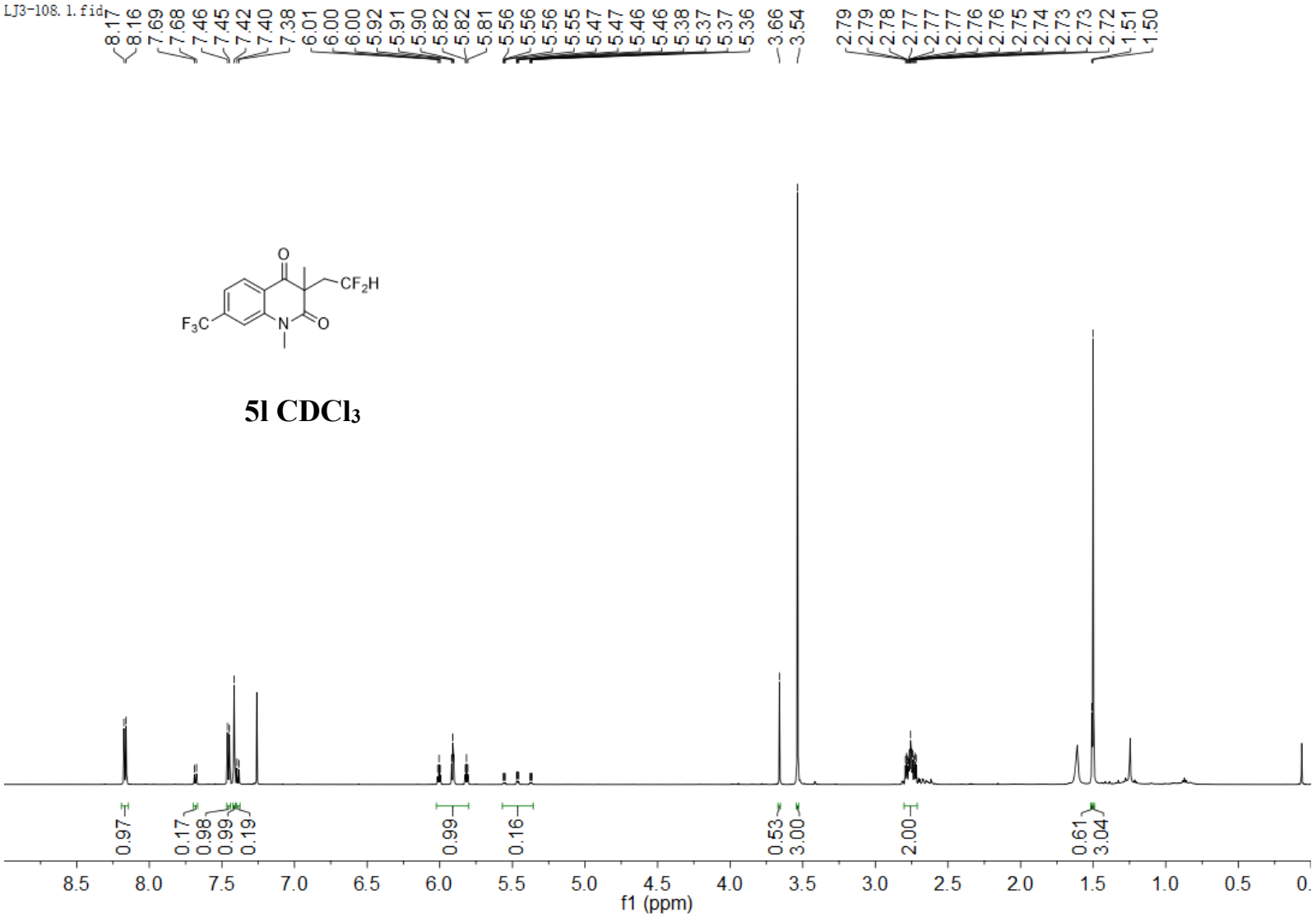

0.95
1.01
1.05
1.04
3.00
2.18
3.21
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)


LJ3-74.2.fid
194.35
172.39
145.34
132.85
132.83
132.80
132.78
126.11
126.08
126.06
126.03
125.82
125.59
124.30
122.50
119.06
116.64
115.57
115.04
113.45
53.34
39.60
39.45
39.30
30.22
26.85
O
F3C
CF2H
N
O
f1 (ppm)

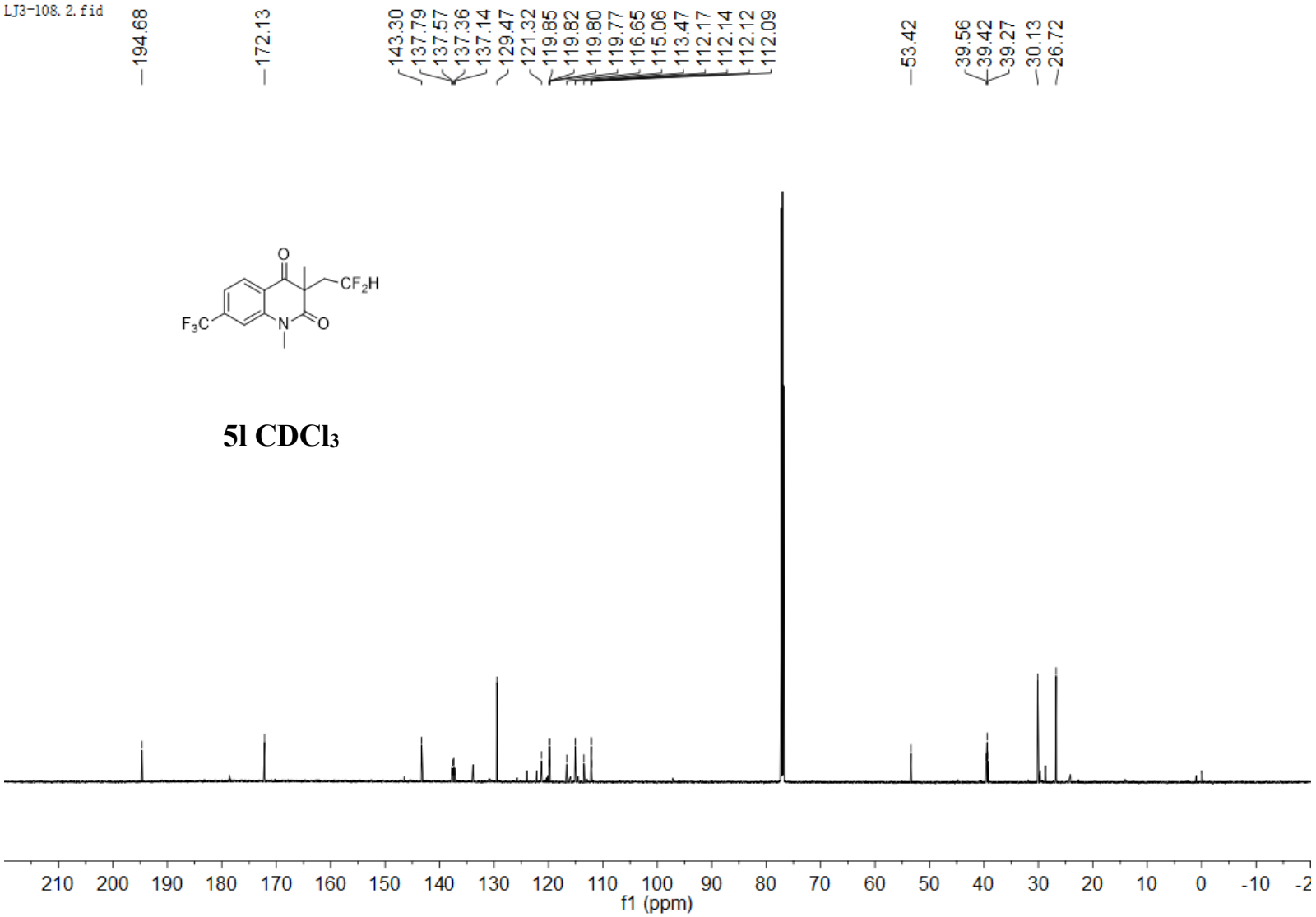
5k **$CDCl_3$**


19F_LJ3-108/1
2019-06-13 SW 201
-63.54
-115.10
-115.13
-115.15
-115.18
-115.20
-115.23
-115.26
-115.28
O
CF2H
F3C
N
O
-114.9
-115.1
-115.3
-115.5
0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

5l $CDCl_3$


LJ3-108.1.fid
8.17 8.16 7.69 7.68 7.46 7.45 7.42 7.40 7.38 6.01 6.00 6.00 5.92 5.91 5.90 5.82 5.82 5.81 5.56 5.56 5.56 5.55 5.47 5.47 5.46 5.46 5.38 5.37 5.37 5.36 3.66 3.54 2.79 2.79 2.78 2.77 2.77 2.77 2.76 2.76 2.75 2.74 2.73 2.73 2.72 1.51 1.50
O
CF2H
F3C
N
O
0.97 0.17 0.98 0.99 0.19 0.99 0.16 0.53 3.00 2.00 0.61 3.04
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.
f1 (ppm)

5l $CDCl_3$


LJ3-108.2.fid
194.68
172.13
143.30
137.79
137.57
137.36
137.14
129.47
121.32
119.85
119.82
119.80
119.77
116.65
115.06
113.47
112.17
112.14
112.12
112.09
53.42
39.56
39.42
39.27
30.13
26.72
O
CF2H
F3C
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

5l $CDCl_3$