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SUPPORTING INFORMATION

Synthesis and Biological Evaluation of Fluoro-Substituted Spiro-Isoxazolines as Potential Anti-Viral and Anti-Cancer Agents

Prasanta Das,*[a] Sarah Boone,[b] Dipanwita Mitra,[b] Lindsay Turner,[c] Ritesh Tandon,[b] Drazen Raucher,[c] and Ashton T. Hamme II*[a]

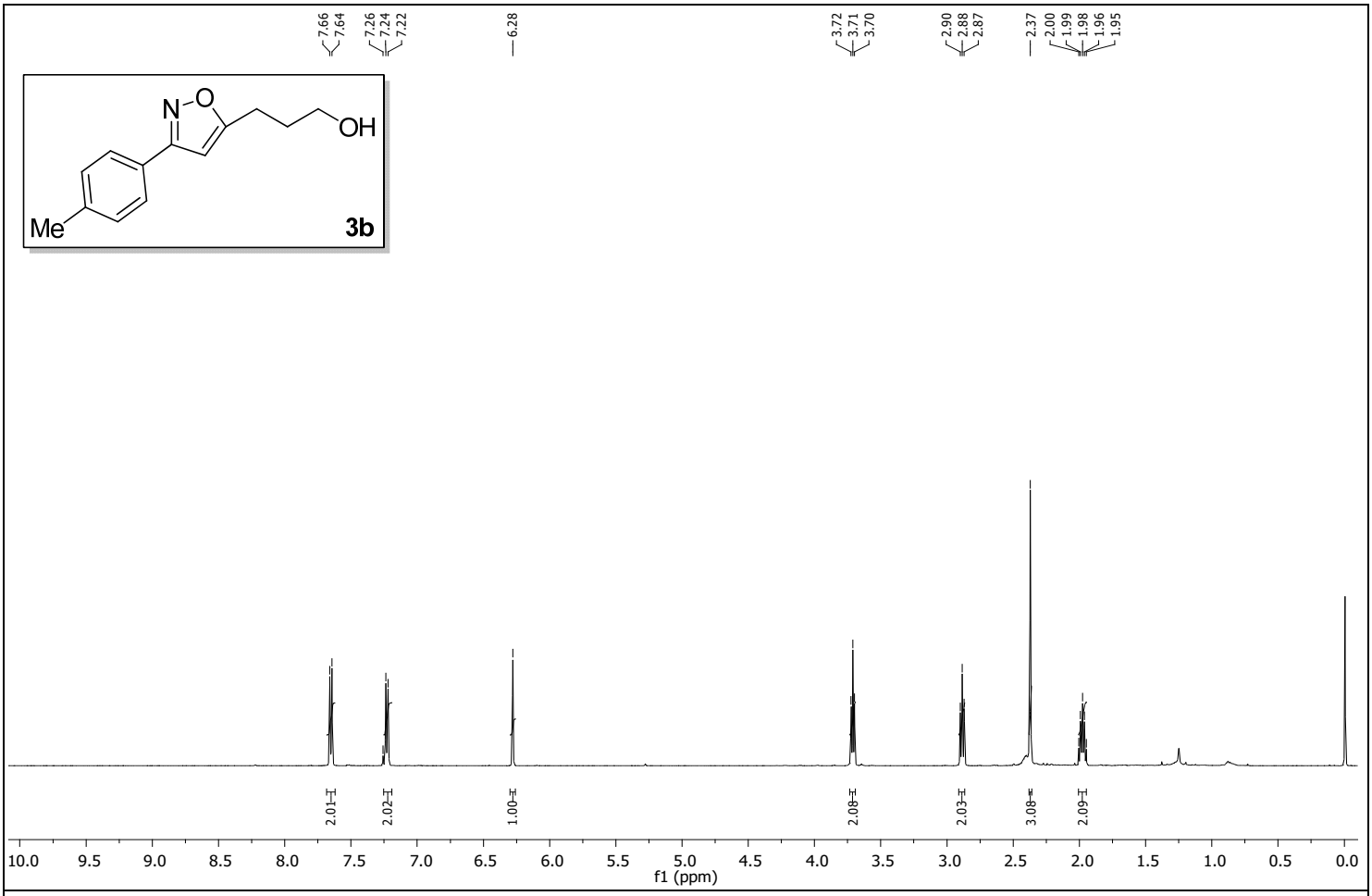
[a.]Department of Chemistry and Biochemistry, Jackson State University, Jackson, Mississippi 39217, United States

[b.]Department of Microbiology and Immunology and [c.]Department of Cellular and Molecular Biology, University of Mississippi Medical Center, Jackson, Mississippi 39216, United States

Email: prasanta.das@jsums.edu, and ashton.t.hamme@jsums.edu

Table of Contents **Page**

^{1}H and ^{13}C Spectra of **3b**....S2
^{1}H and ^{13}C Spectra of **3c**....S3
^{1}H and ^{13}C Spectra of **3e**....S4
^{1}H and ^{13}C Spectra of **3g**....S5
^{1}H and ^{13}C Spectra of **3h**....S6
^{1}H and ^{13}C Spectra of **3j**....S7
^{1}H and ^{13}C Spectra of **3l**....S8
^{1}H and ^{13}C Spectra of **3n**....S9
^{1}H and ^{13}C Spectra of **3o**....S10
^{1}H and ^{13}C Spectra of **3q**....S11
^{1}H and ^{13}C Spectra of **3r**....S12
^{1}H and ^{13}C Spectra of **3t**....S13
^{1}H and ^{13}C Spectra of **3v**....S14
^{1}H and ^{13}C Spectra of **3w**....S15
^{1}H and ^{13}C Spectra of **3x**....S16
^{1}H and ^{13}C Spectra of **4a/4a'**....S17
^{19}F spectra of **4a/4a'** S18
^{1}H and ^{13}C Spectra of **4b/4b'**....S19
^{19}F spectra of **4b/4b'**....S20
^{1}H and ^{13}C Spectra of **4c**....S21
^{1}H and ^{13}C Spectra of **4c'**....S22
^{19}F spectra of **4c/4c'**....S23
^{1}H and ^{13}C Spectra of **4d**....S24
^{1}H and ^{13}C Spectra of **4d'**....S25
^{19}F spectra of **4d/4d'**....S26
^{1}H and ^{13}C Spectra of **4e**....S27
^{1}H Spectra of **4e'**....S28
^{19}F spectra of **4e/4e'**....S29
^{1}H and ^{13}C Spectra of **4f/4f'**....S30
^{19}F spectra of **4f/4f'**....S31
^{1}H and ^{13}C Spectra of **4g**....S32
^{1}H and ^{19}F Spectra of **4g'**....S33
^{1}H and ^{13}C Spectra of **4h/4h'**....S34
^{19}F spectra of **4h** S35
^{1}H and ^{13}C Spectra of **4i**....S36
^{19}F spectra of **4i/4i'**....S37
^{1}H and ^{13}C Spectra of **4j/4j'**....S38
^{19}F spectra of **4j/4j'**....S39
^{1}H and ^{13}C Spectra of **4k/4k'**....S40
^{19}F spectra of **4k/4k'**....S41
^{1}H and ^{13}C Spectra of **4l/4l'**....S42
^{19}F spectra of **4l/4l'**....S43
^{1}H and ^{13}C Spectra of **4m/4m'**....S44
^{19}F spectra of **4m/4m'**....S45
^{1}H and ^{13}C Spectra of **4n/4n'**....S46
^{19}F spectra of **4n'**....S47
^{1}H and ^{13}C Spectra of **4o/4o'**....S48
^{19}F spectra of **4o'**....S49
^{1}H and ^{13}C Spectra of **5a**....S50
^{1}H and ^{13}C Spectra of **5a'**....S51
^{19}F spectra of **5a/5a'**....S52
^{1}H and ^{13}C Spectra of **5b**....S53
^{1}H and ^{13}C Spectra of **5b'**....S54
^{19}F spectra of **5a/5a'**....S55
^{1}H and ^{13}C Spectra of **5c**....S56
^{1}H and ^{13}C Spectra of **5c'**....S57
^{19}F spectra of **5c/5c'**....S58
^{1}H and ^{13}C Spectra of **5d**....S59
^{1}H and ^{13}C Spectra of **5d'**....S60
^{19}F spectra of **5d/5d'**....S61
^{1}H and ^{13}C Spectra of **5e**....S62
^{1}H and ^{13}C Spectra of **5e'**....S63
^{19}F spectra of **5e/5e'**....S64
^{1}H and ^{13}C Spectra of **5f**....S65
^{1}H and ^{13}C Spectra of **5f'**....S66
^{19}F spectra of **5f/5f'**....S67
^{1}H and ^{13}C Spectra of **5g**....S68
^{1}H and ^{13}C Spectra of **5g'**....S69
^{19}F spectra of **5g/5g'**....S70
^{1}H and ^{13}C Spectra of **5h**....S71
^{1}H and ^{13}C Spectra of **5h'**....S72
^{19}F spectra of **5h/5h'**....S73
^{1}H and ^{13}C Spectra of **5i**....S74
^{1}Hspectra of **5i'**....S75
^{19}F spectra of **5i/5i'**....S76
^{1}H and ^{13}C Spectra of **5j/5j'**....S77
^{19}F spectra of **5j/5j'**....S78
^{1}H and ^{13}C Spectra of **5k/5k'**....S79
^{19}F spectra of **5k/5k'**....S80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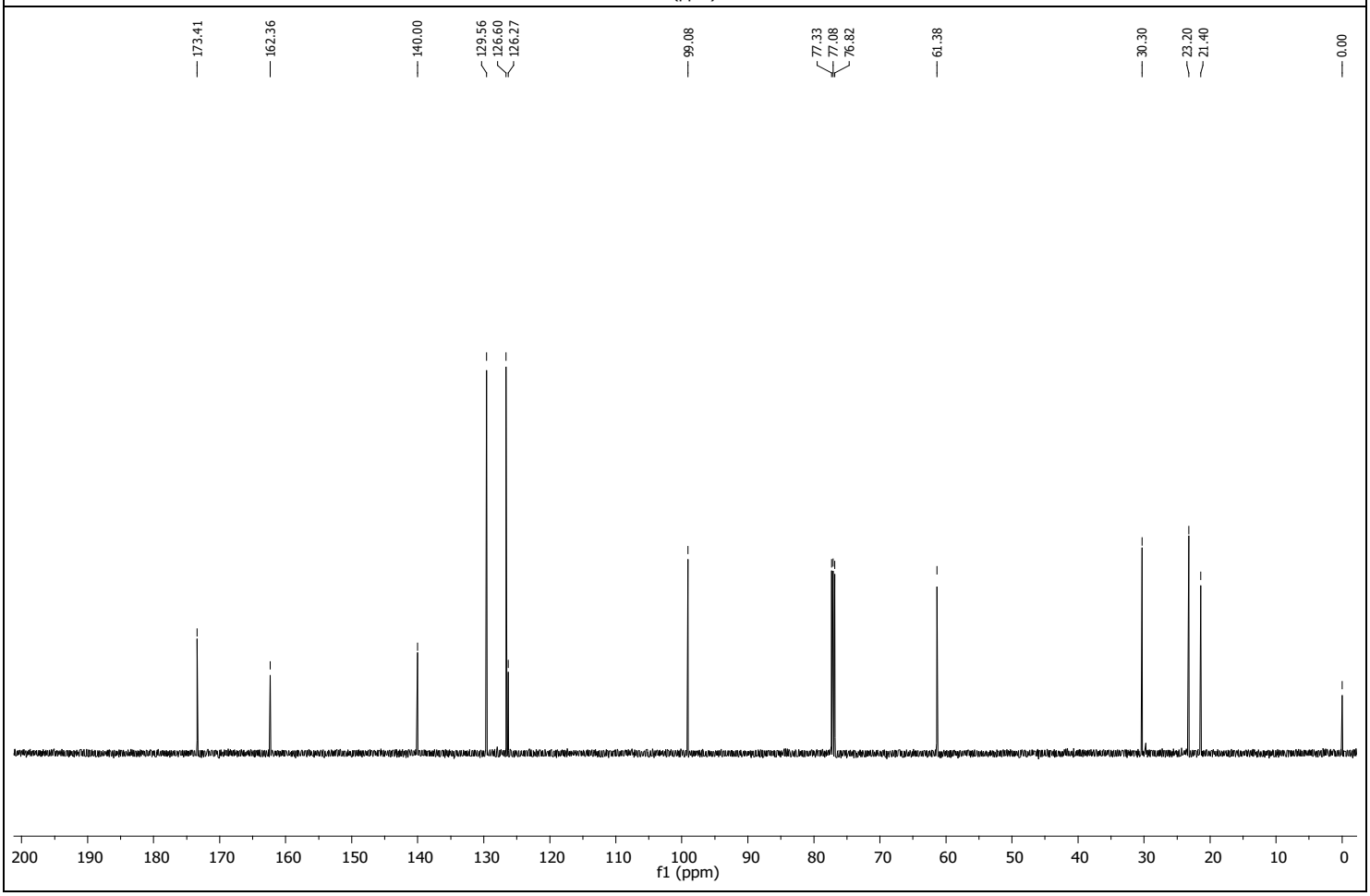
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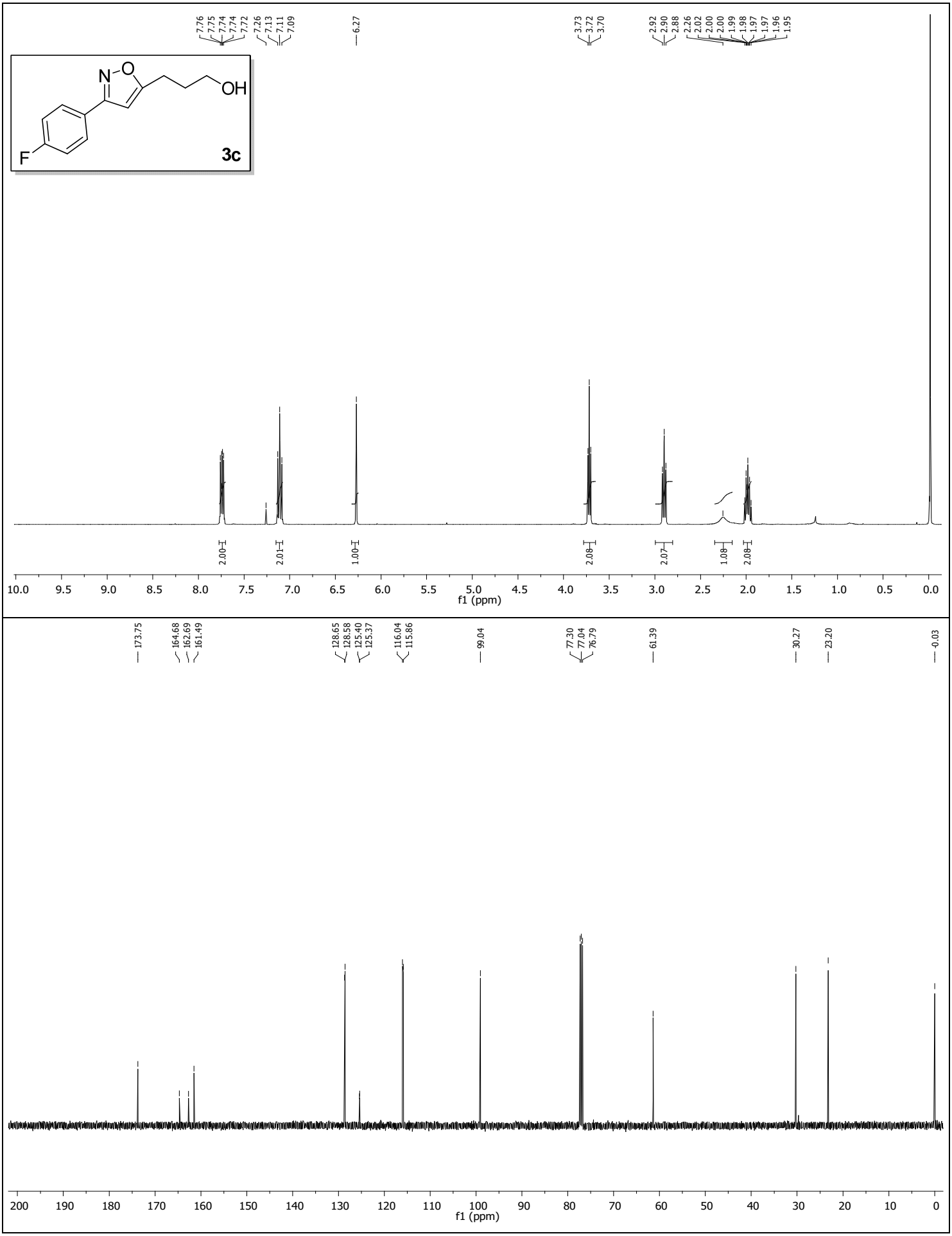
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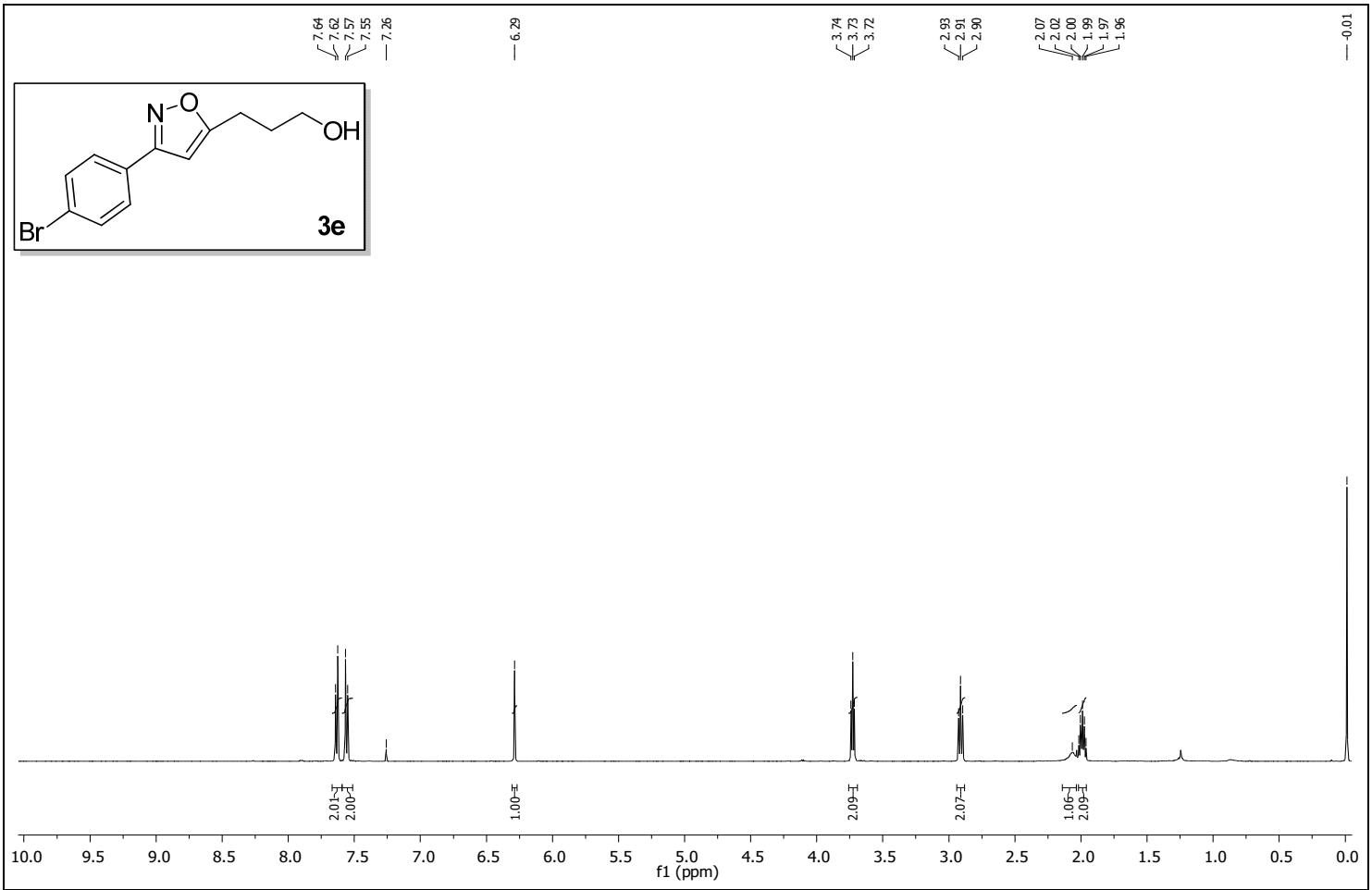
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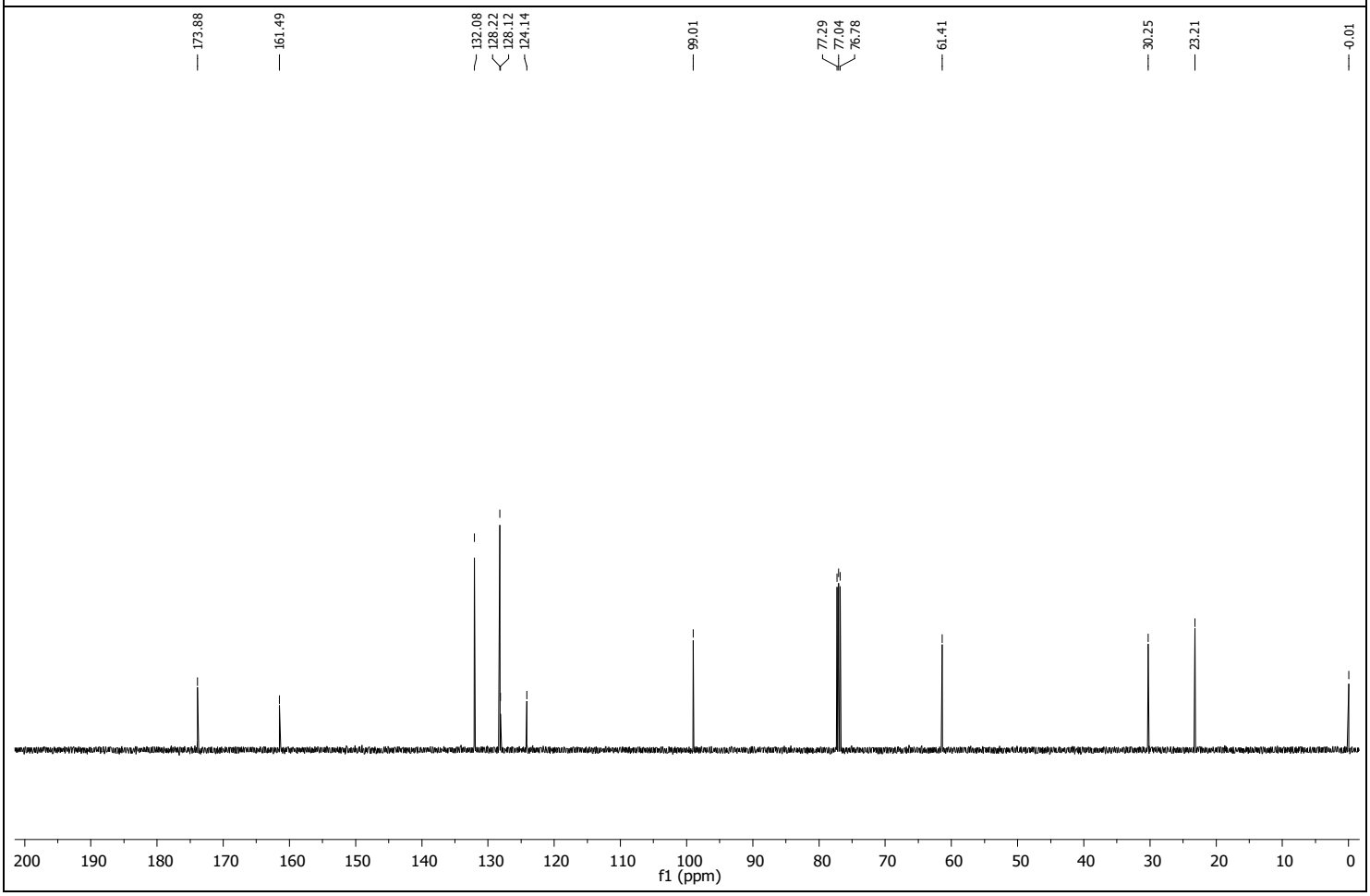
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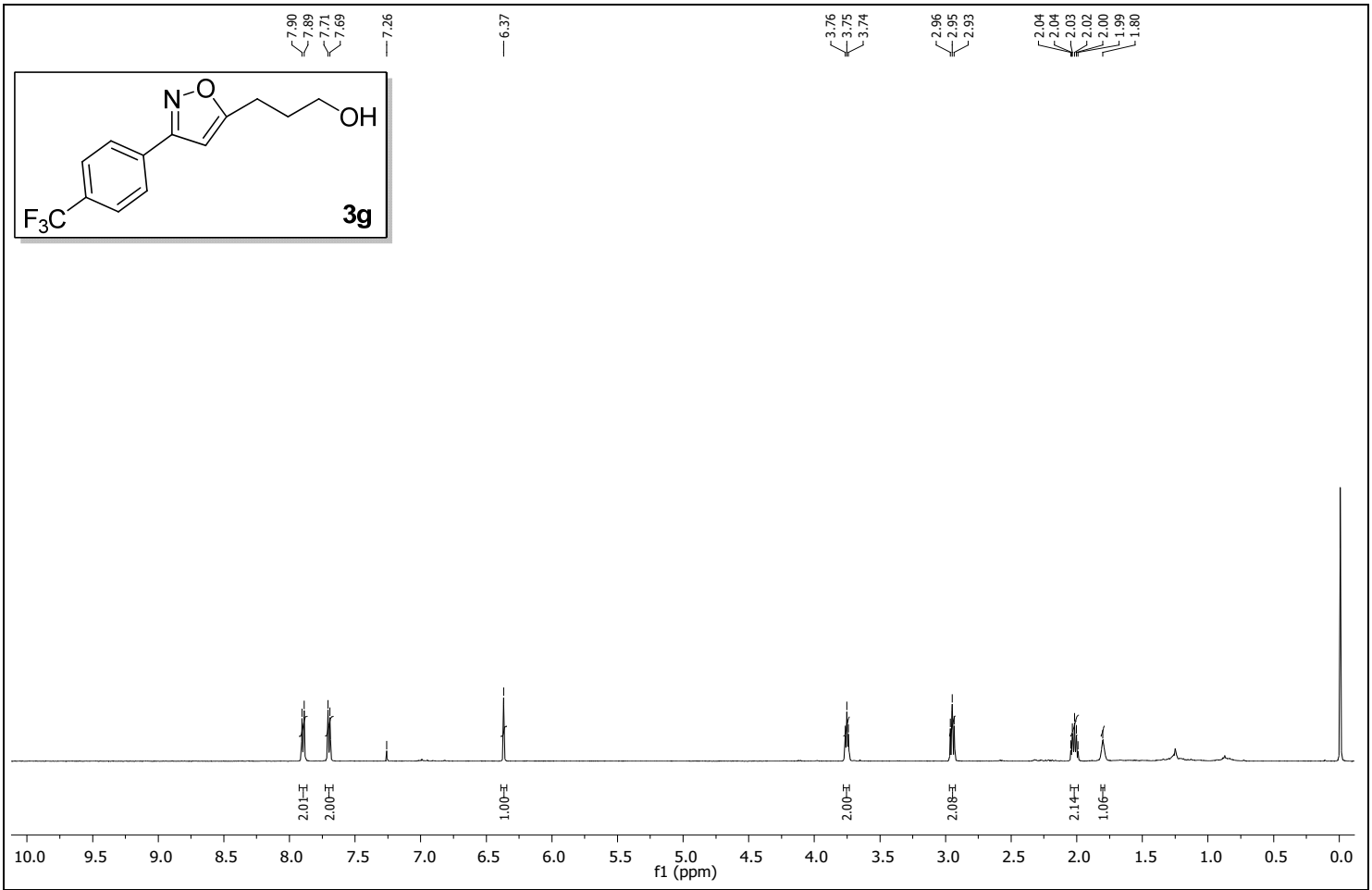
F3C
3g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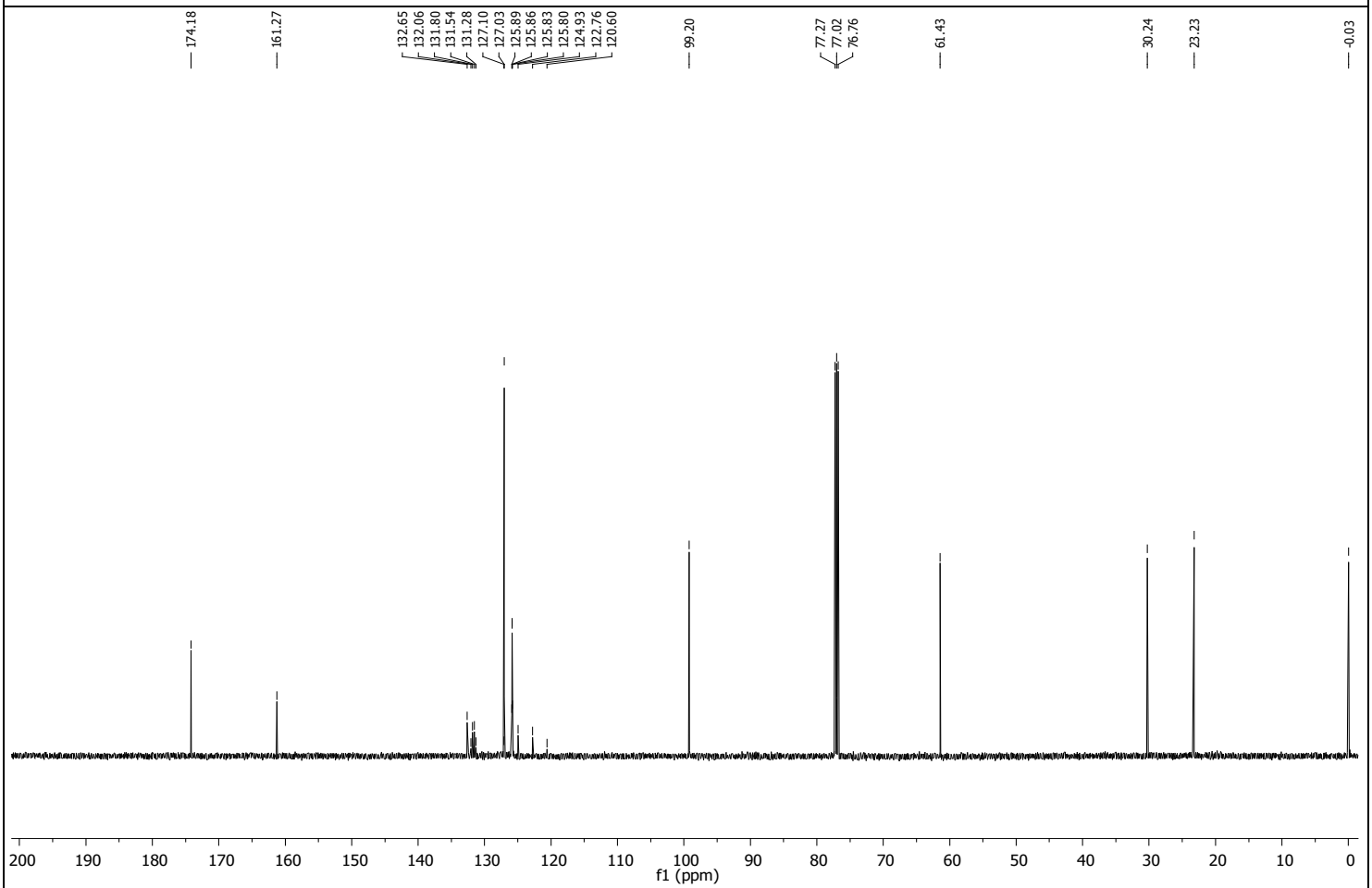
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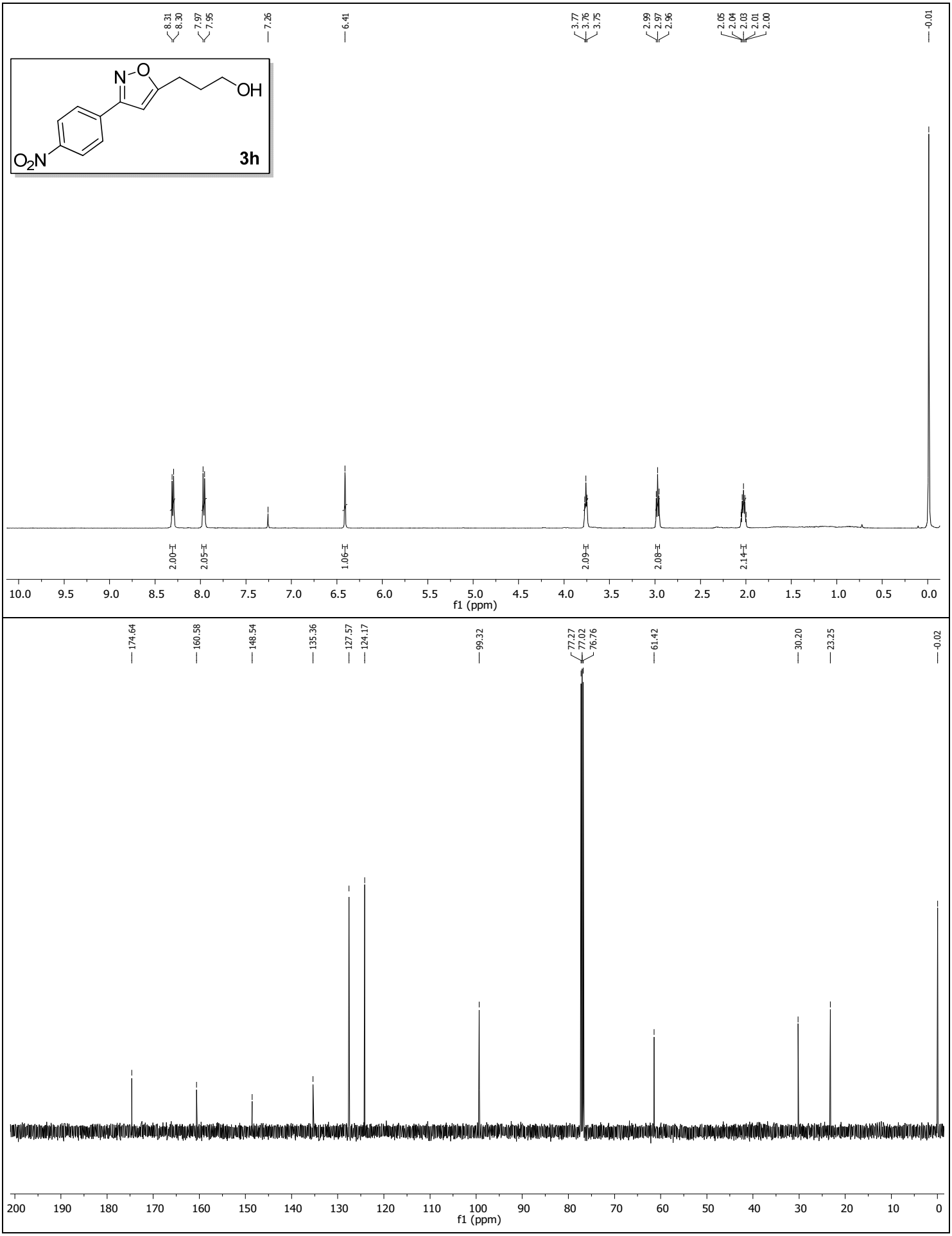
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f1 (ppm)
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f1 (ppm)

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F
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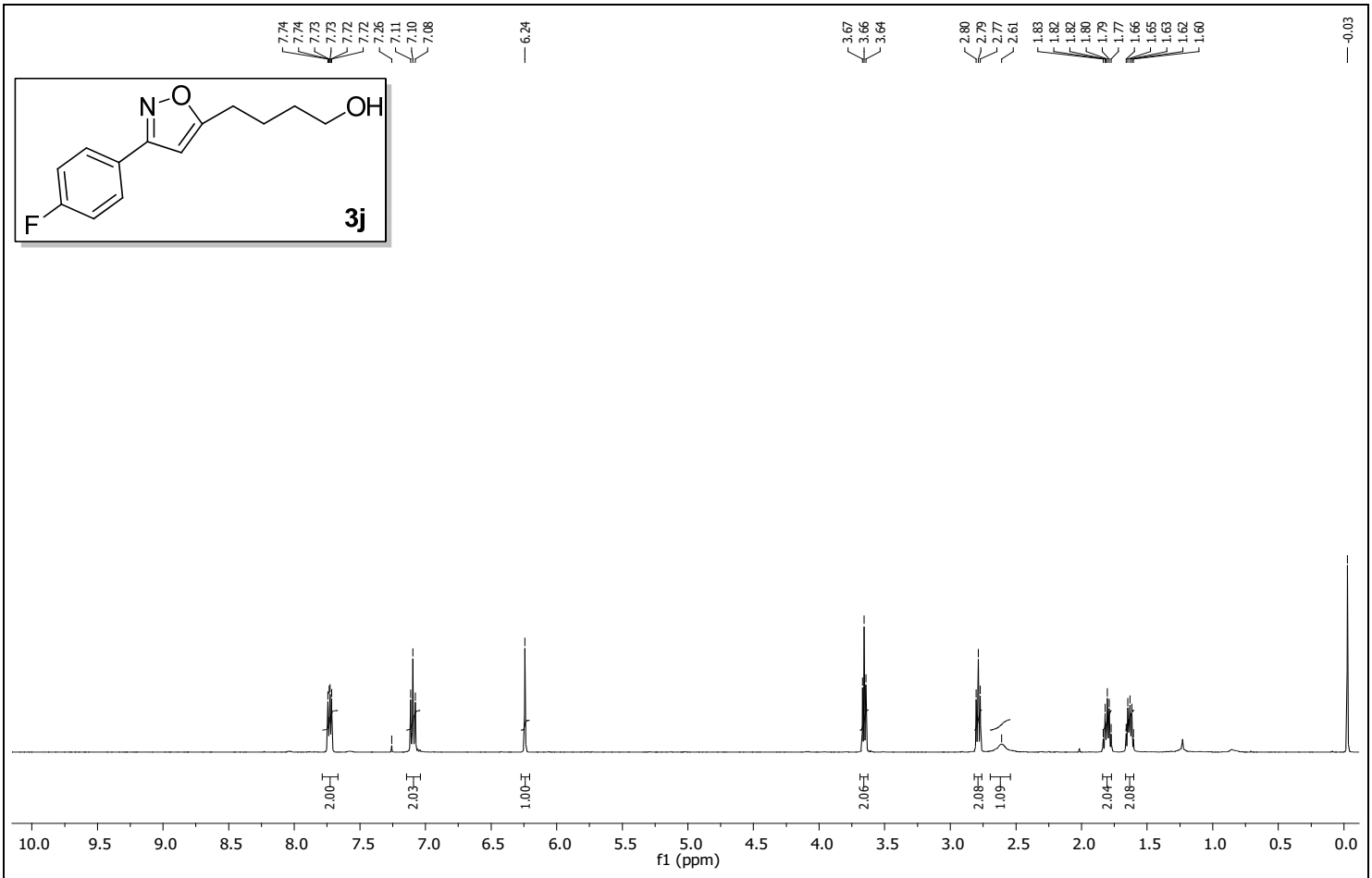
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1.82
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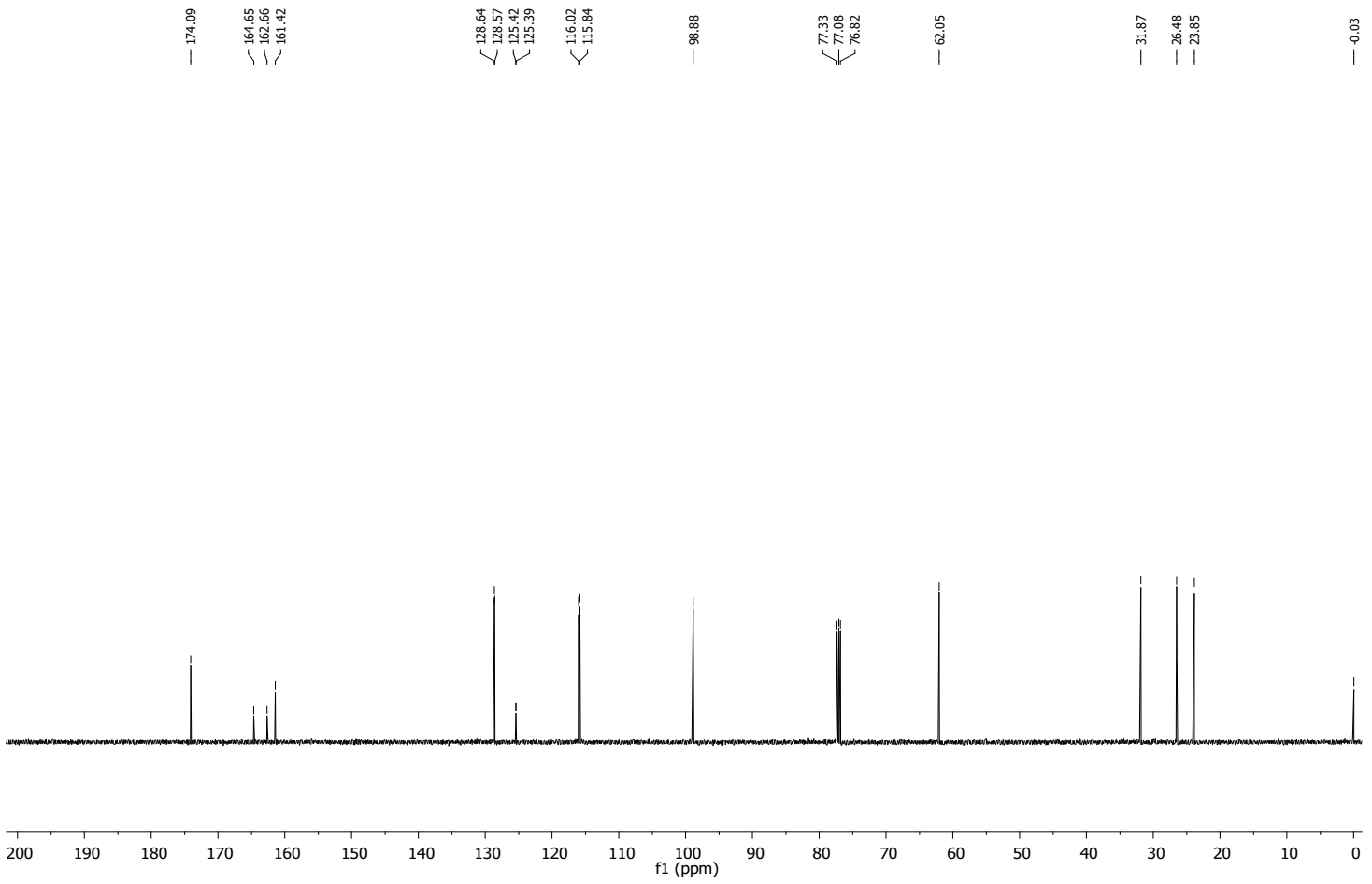
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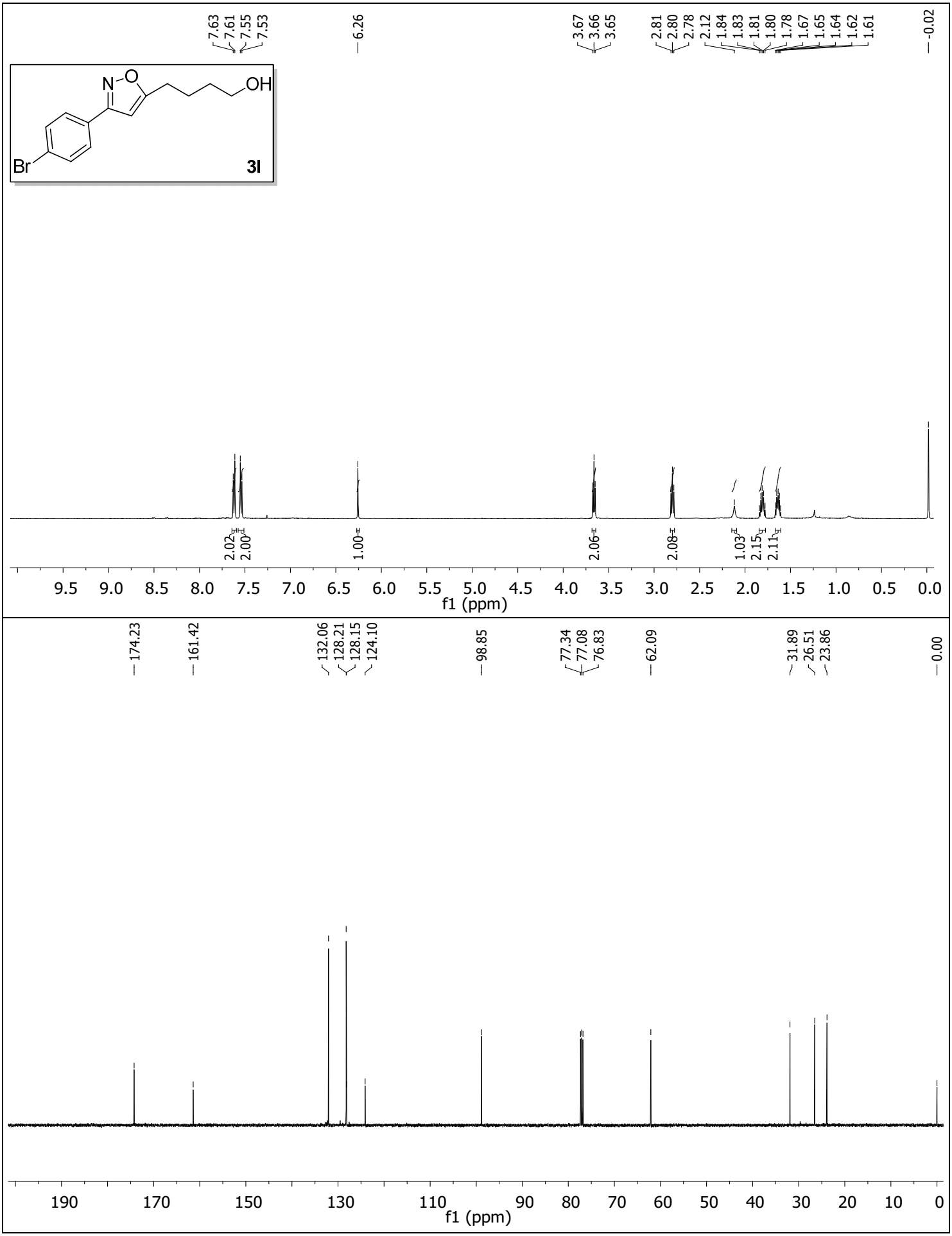
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1.00
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1.03
2.15
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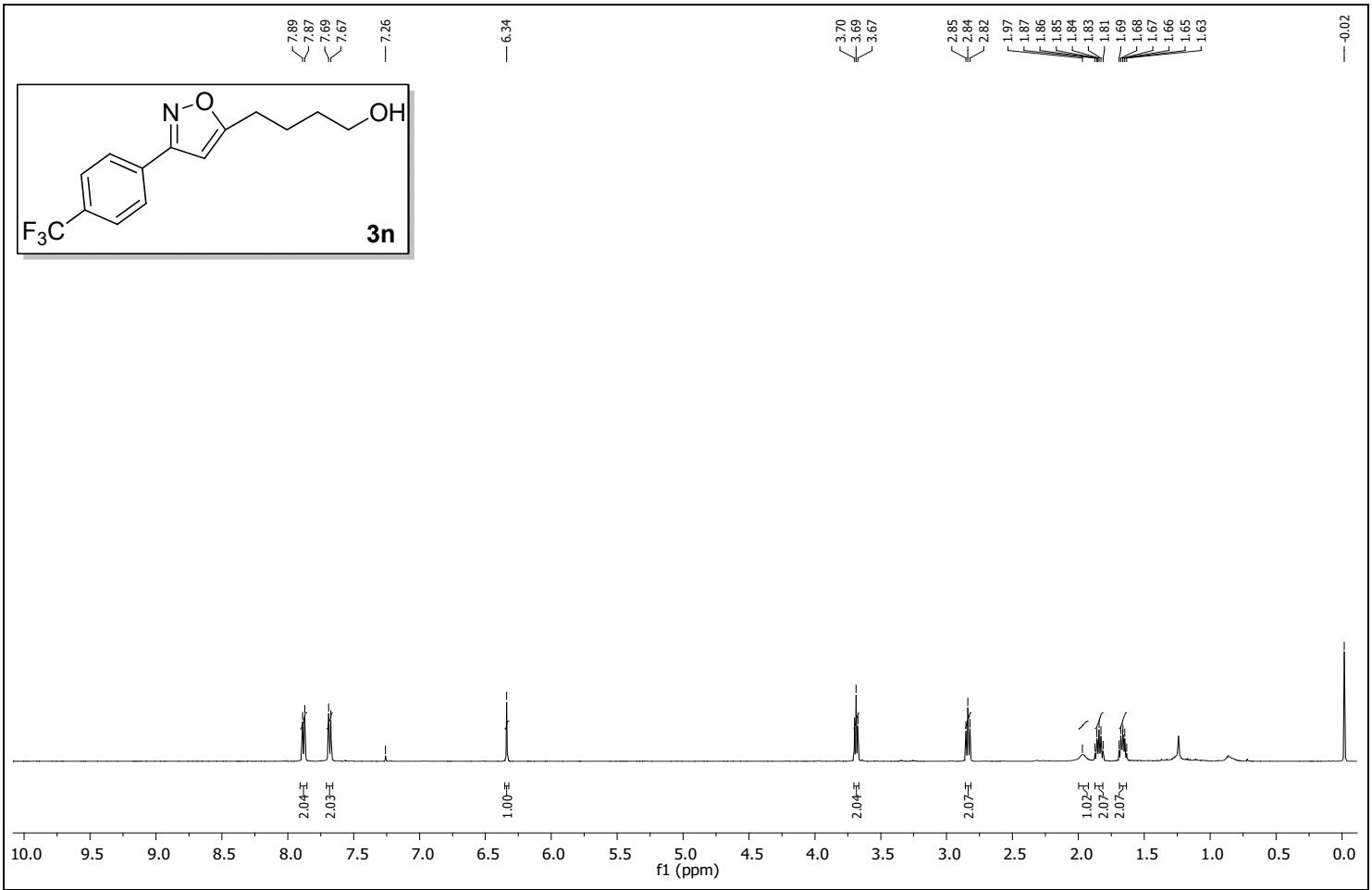
f1 (ppm)

N
O
OH
F3C
3n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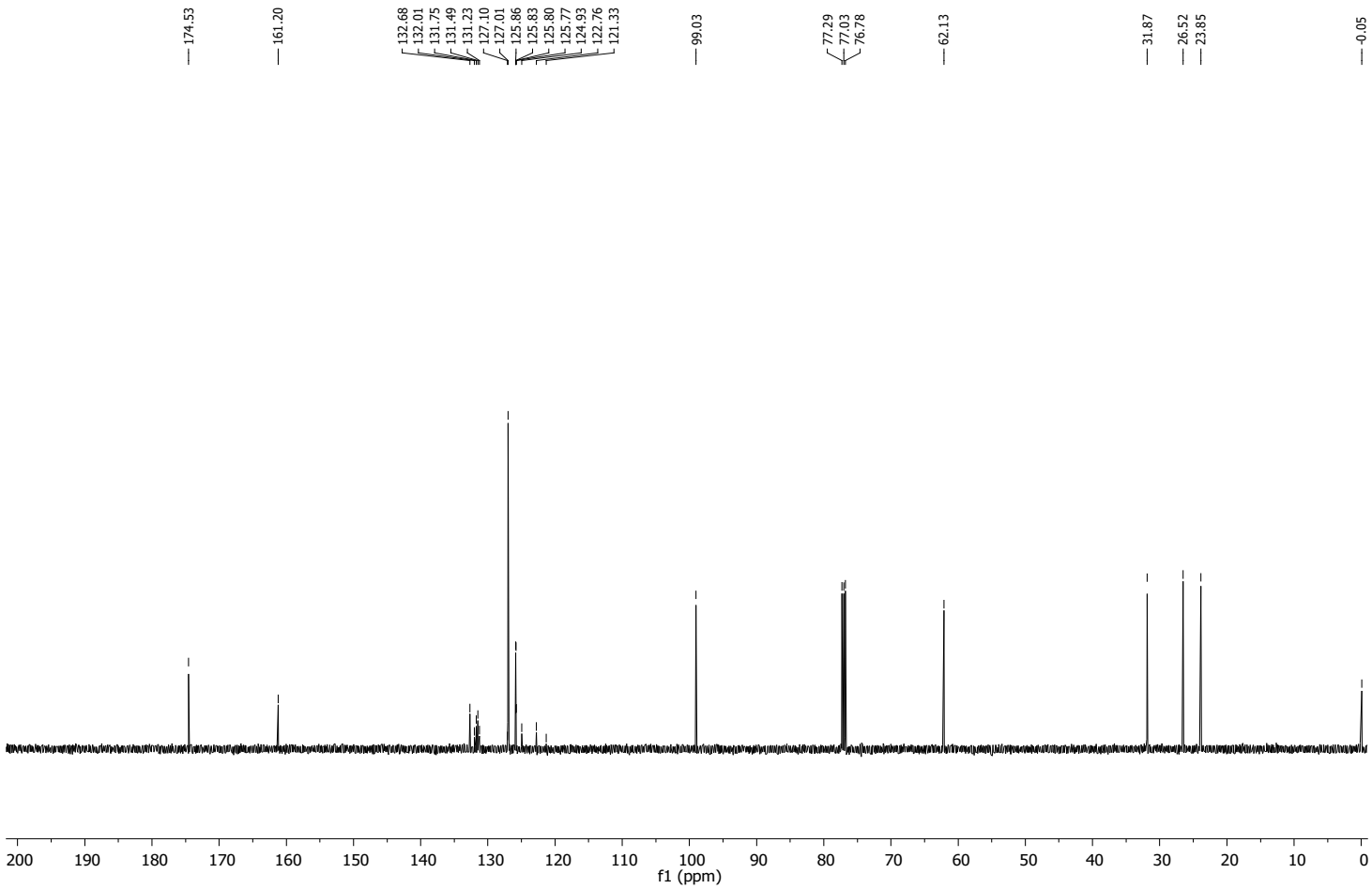
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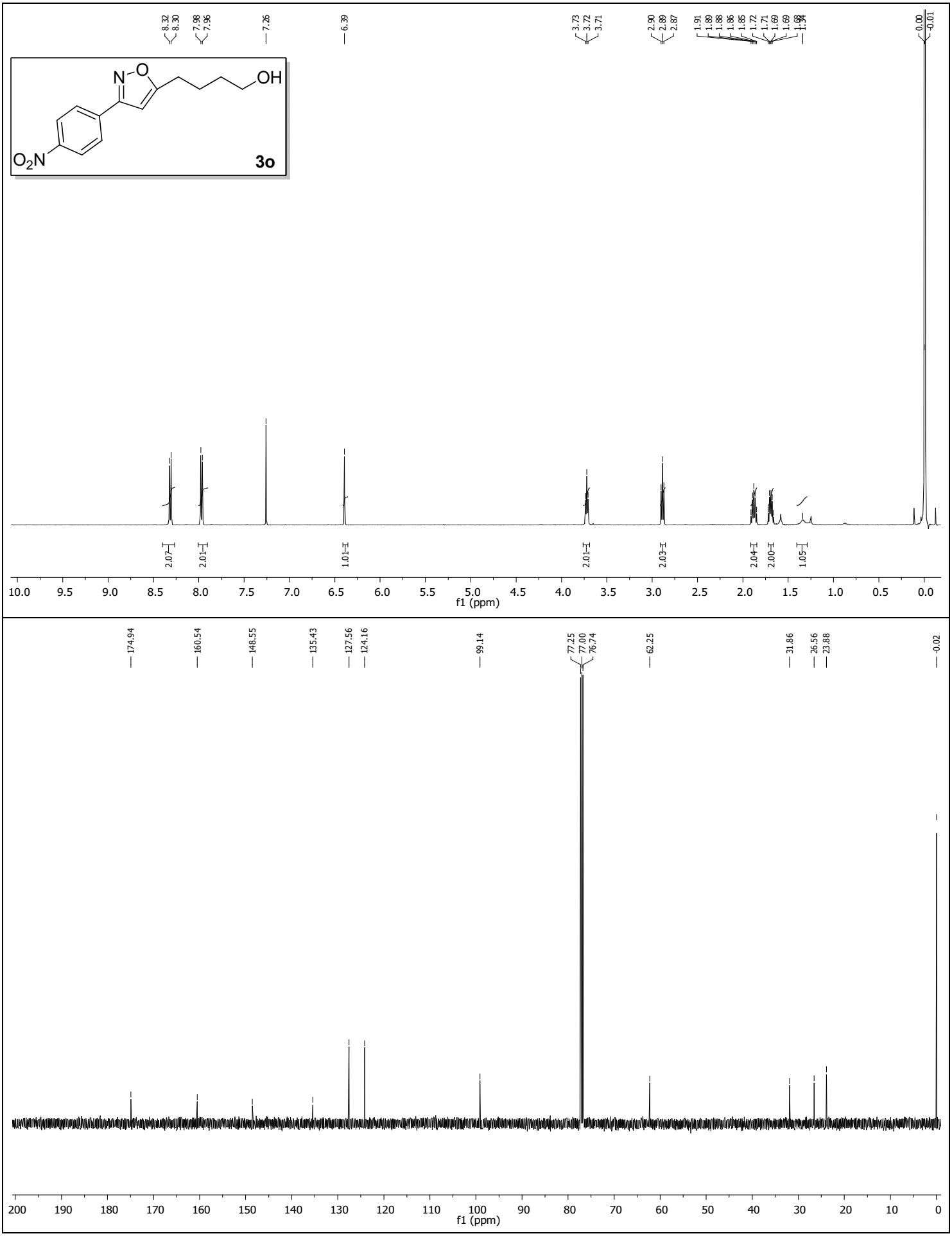
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2.01
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2.00
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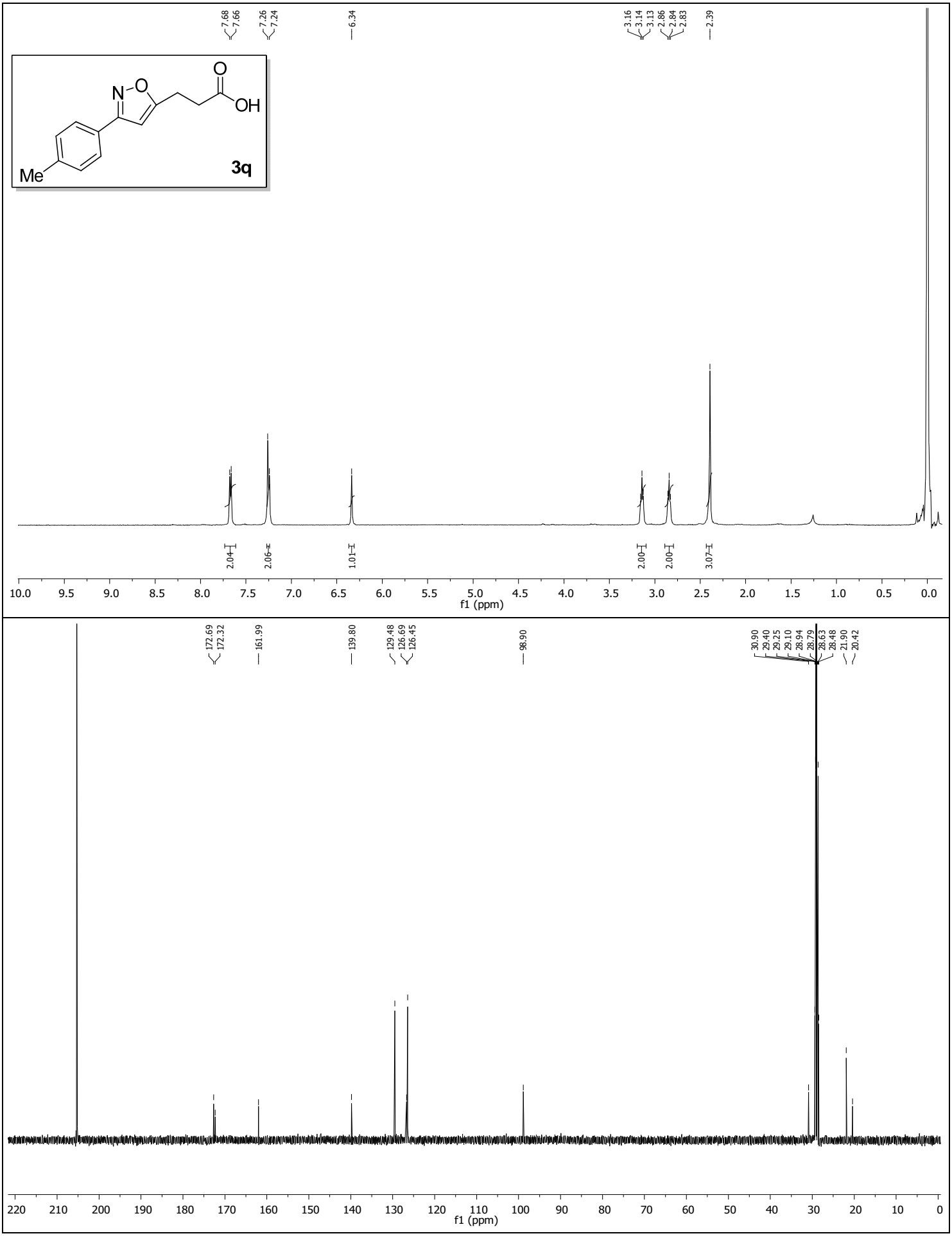
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OH
Me
3q
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2.00
3.07
f1 (ppm)
172.69
172.32
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126.45
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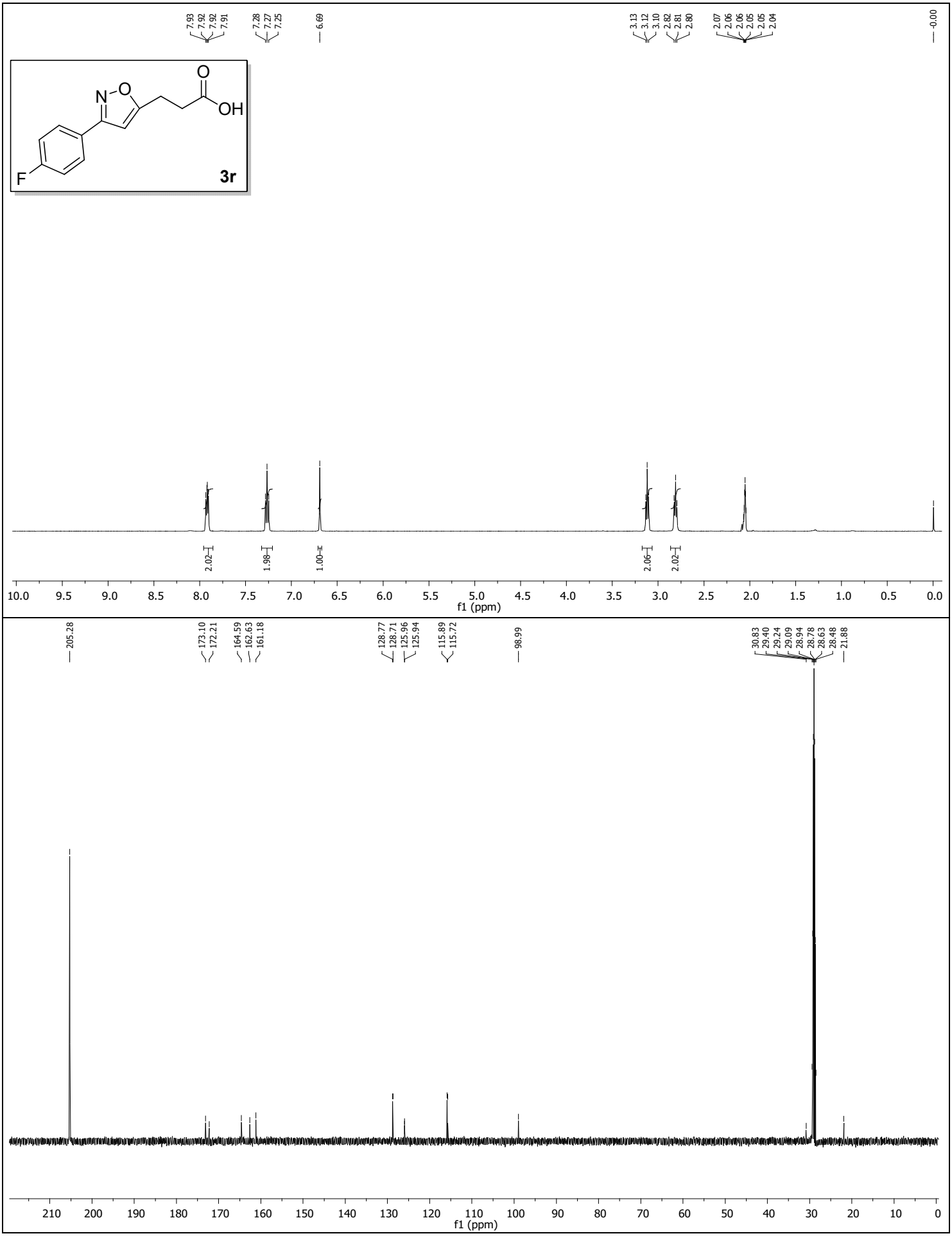
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OH
F
3r
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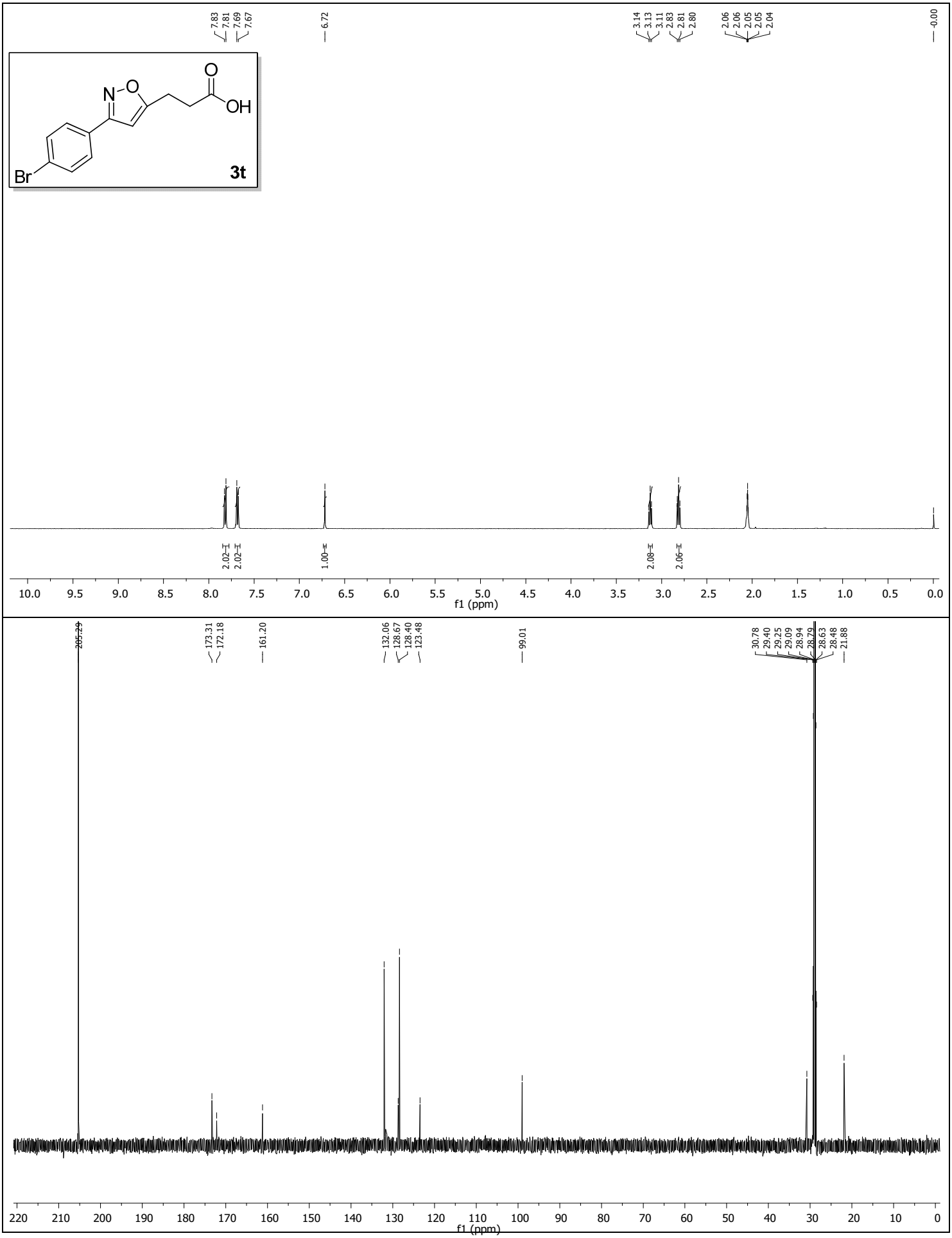
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Br
3t
2.02
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f1 (ppm)
205.29
173.31
172.18
161.20
132.06
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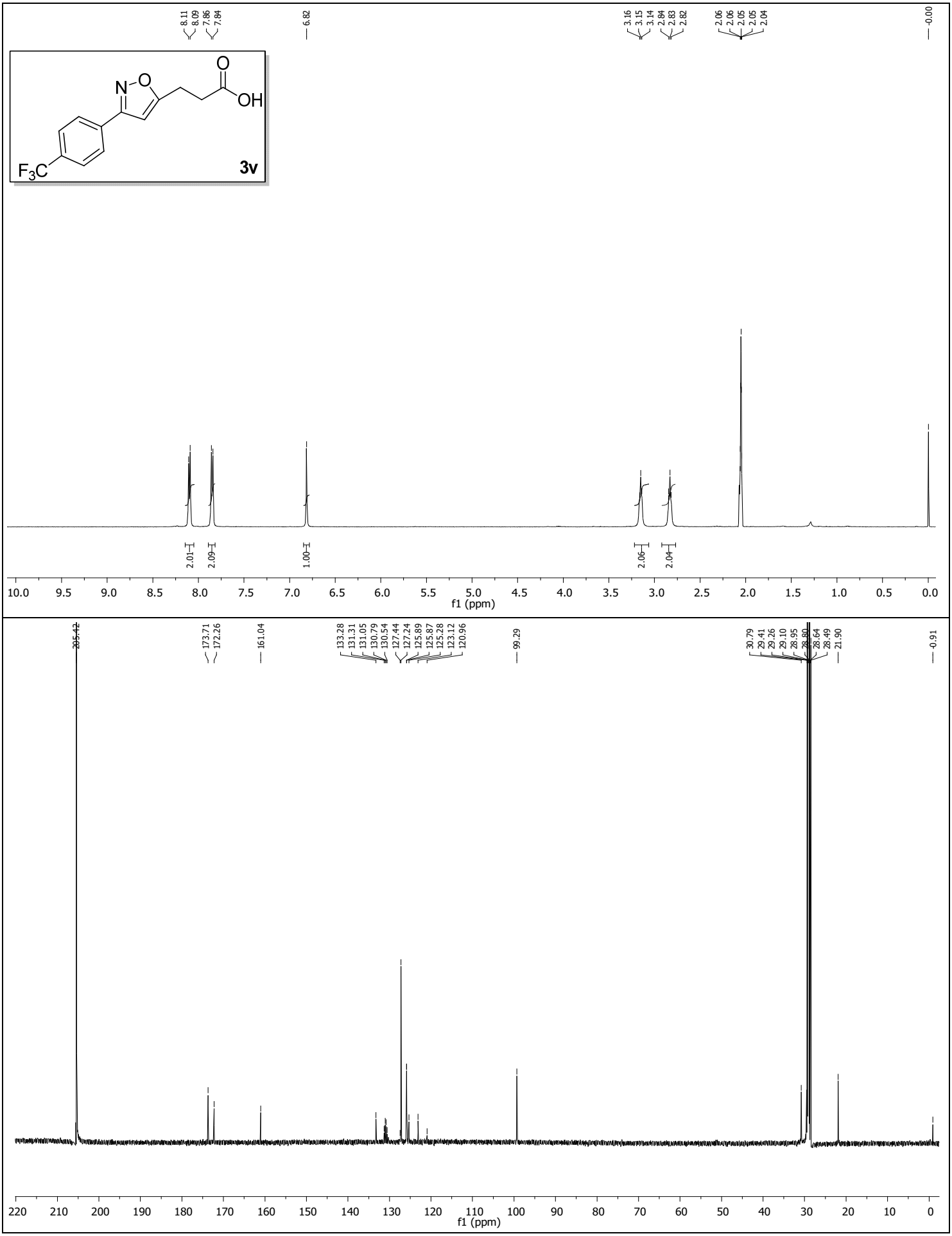
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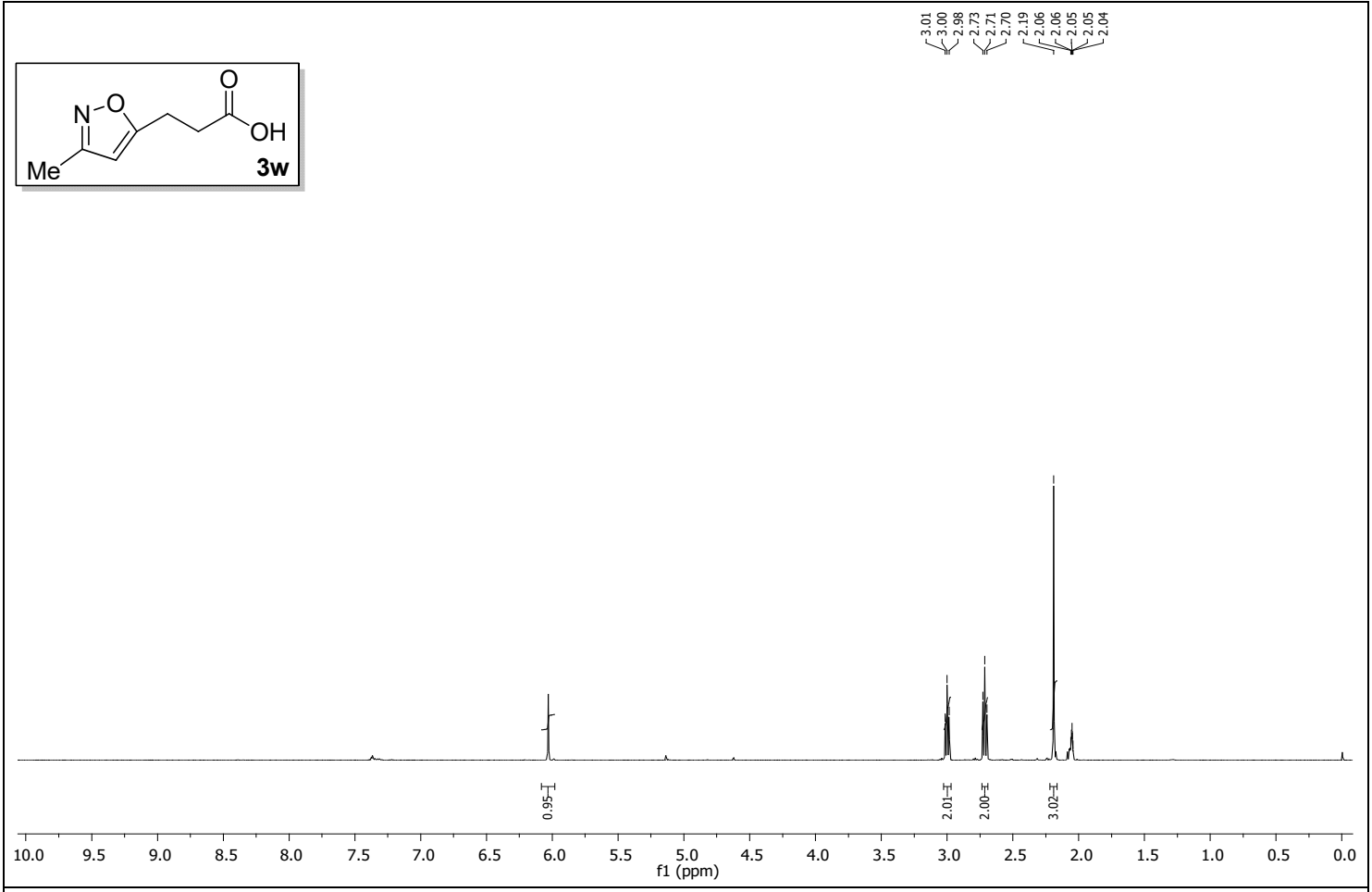
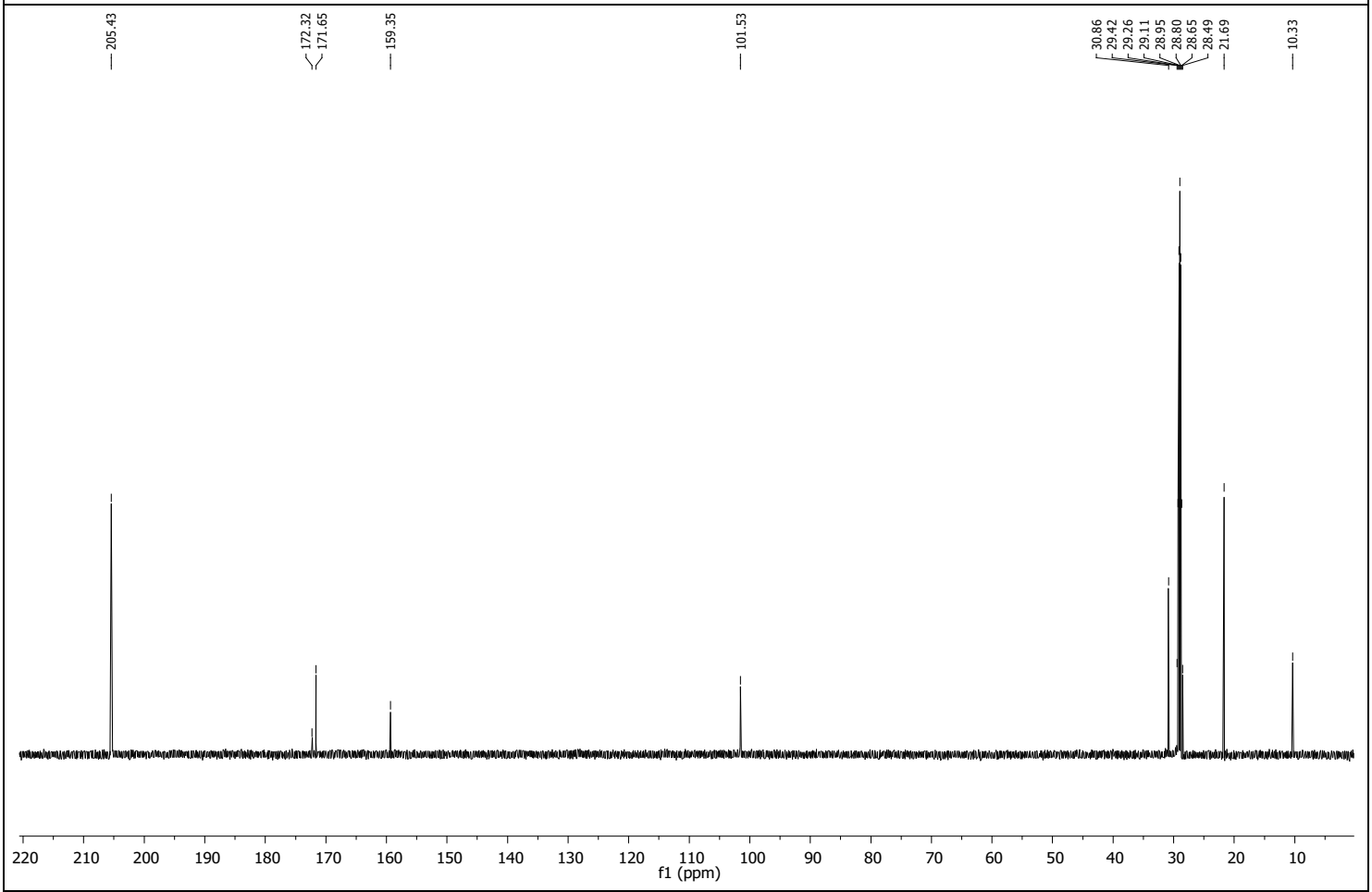
-0.91
f1 (ppm)

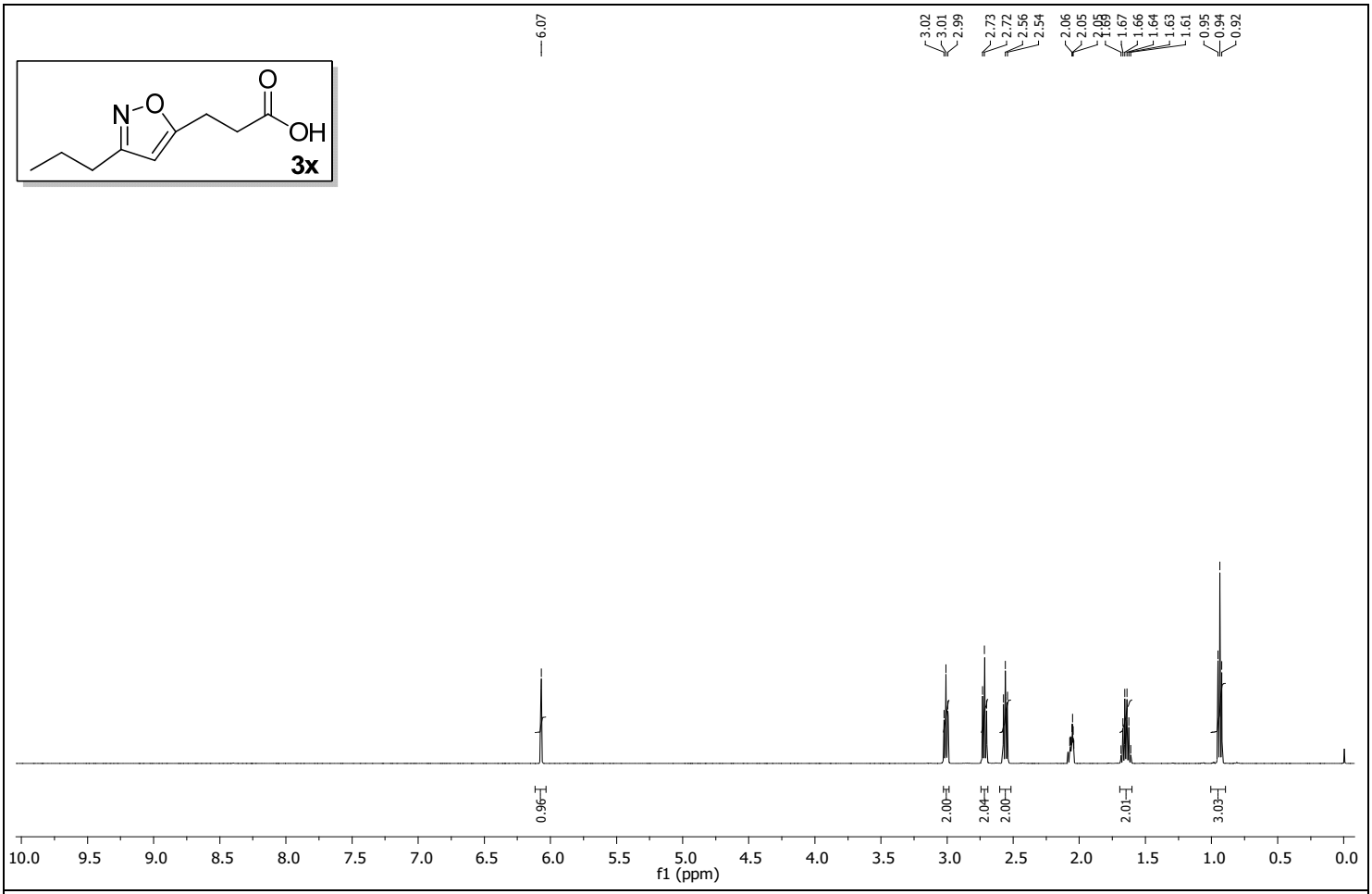
O
N
O
OH
Me
3w

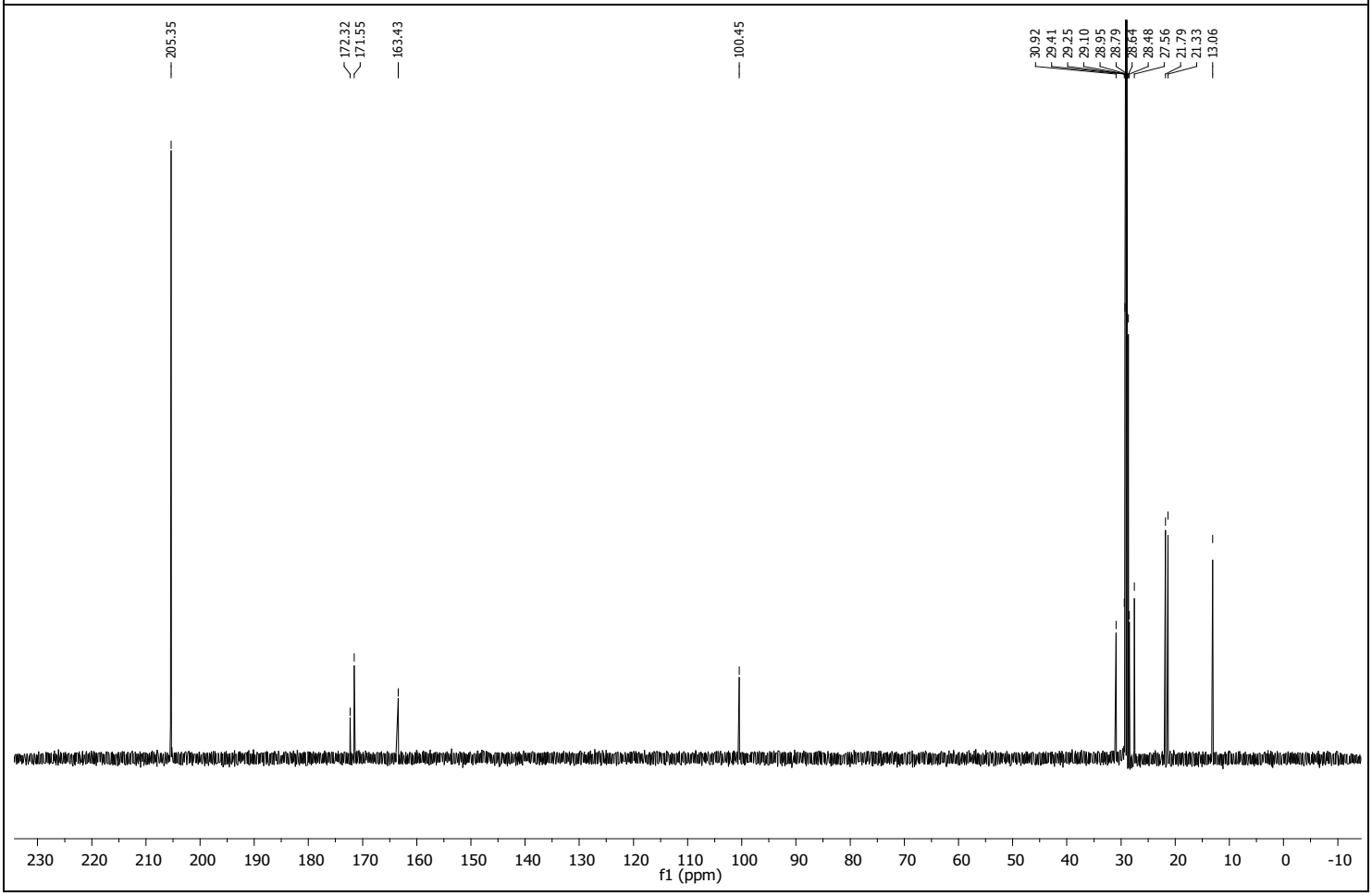

3.01
3.00
2.98
2.73
2.71
2.70
2.19
2.06
2.06
2.05
2.05
2.04
0.95
2.01
2.00
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

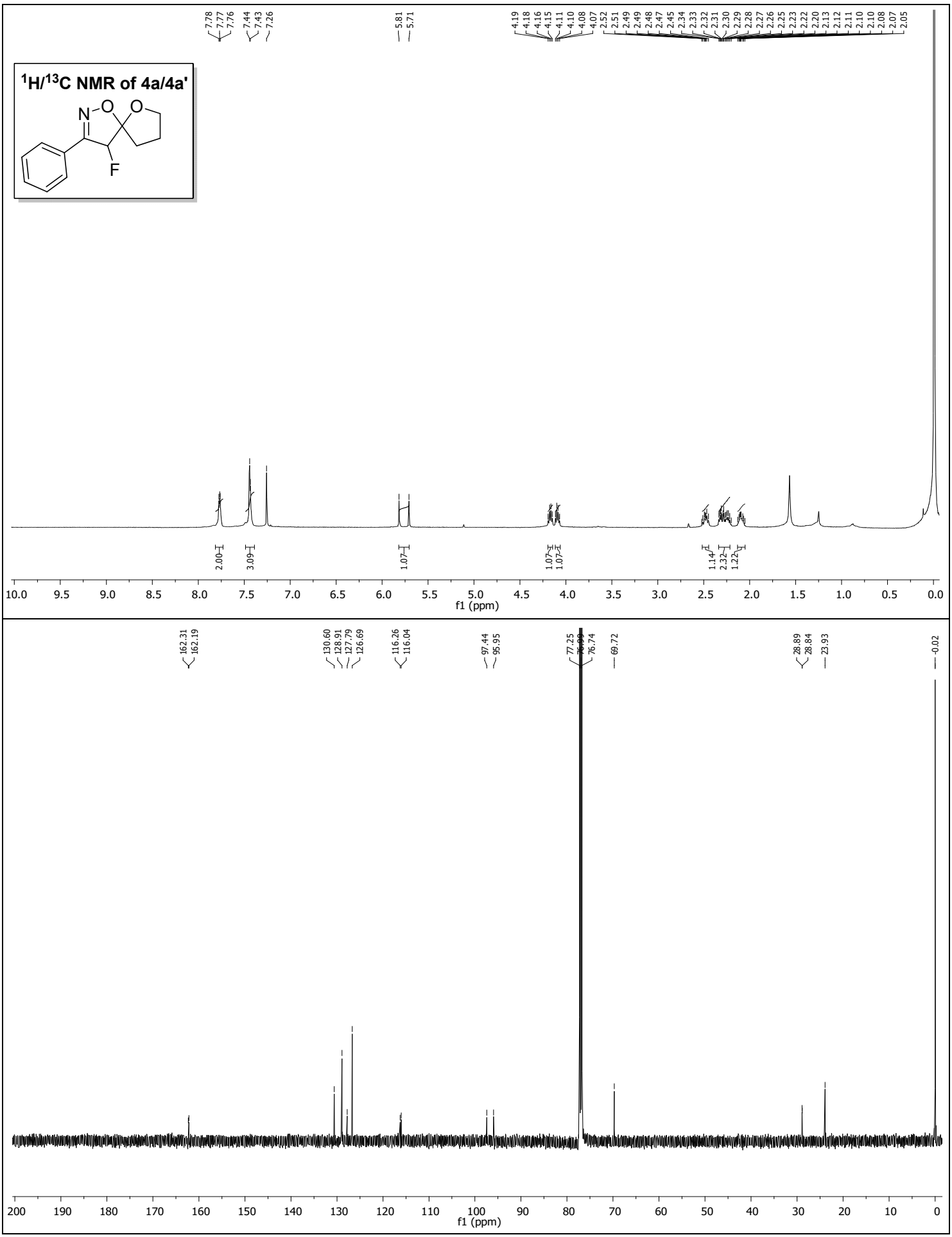

205.43
172.32
171.65
159.35
101.53
30.86
29.42
29.26
29.11
28.95
28.80
28.65
28.49
21.69
10.33
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

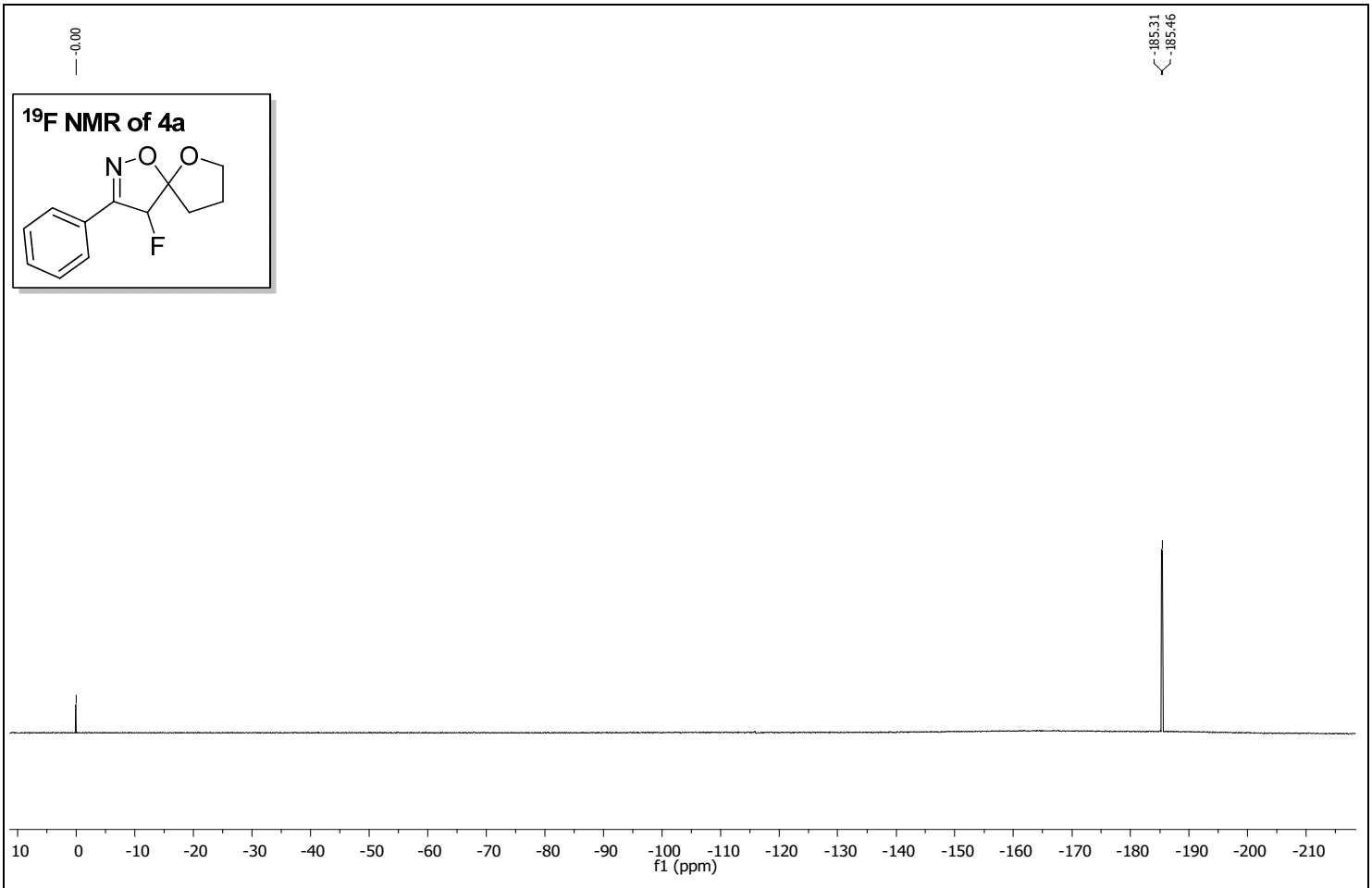
O
N
O
OH

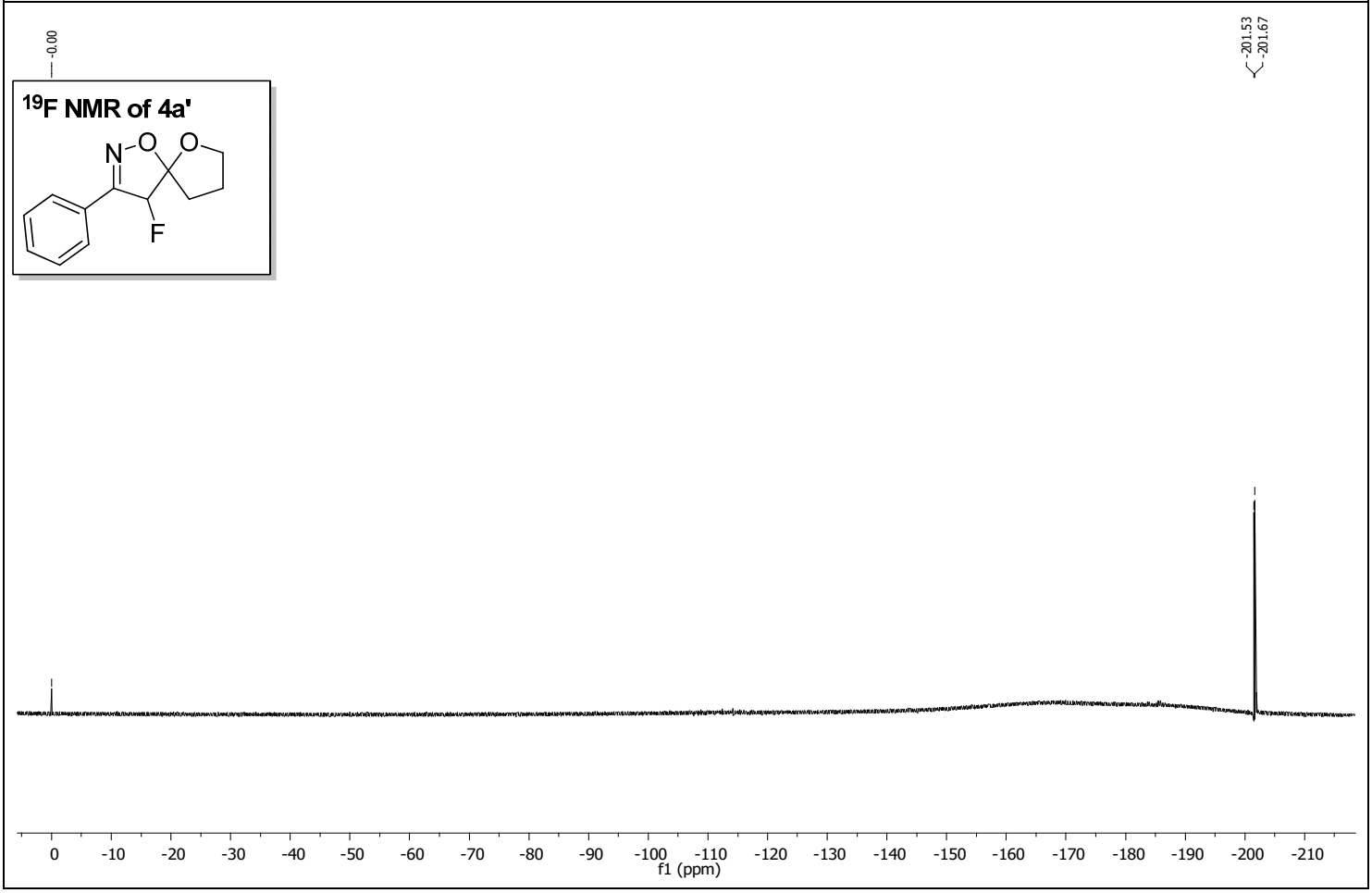
3x

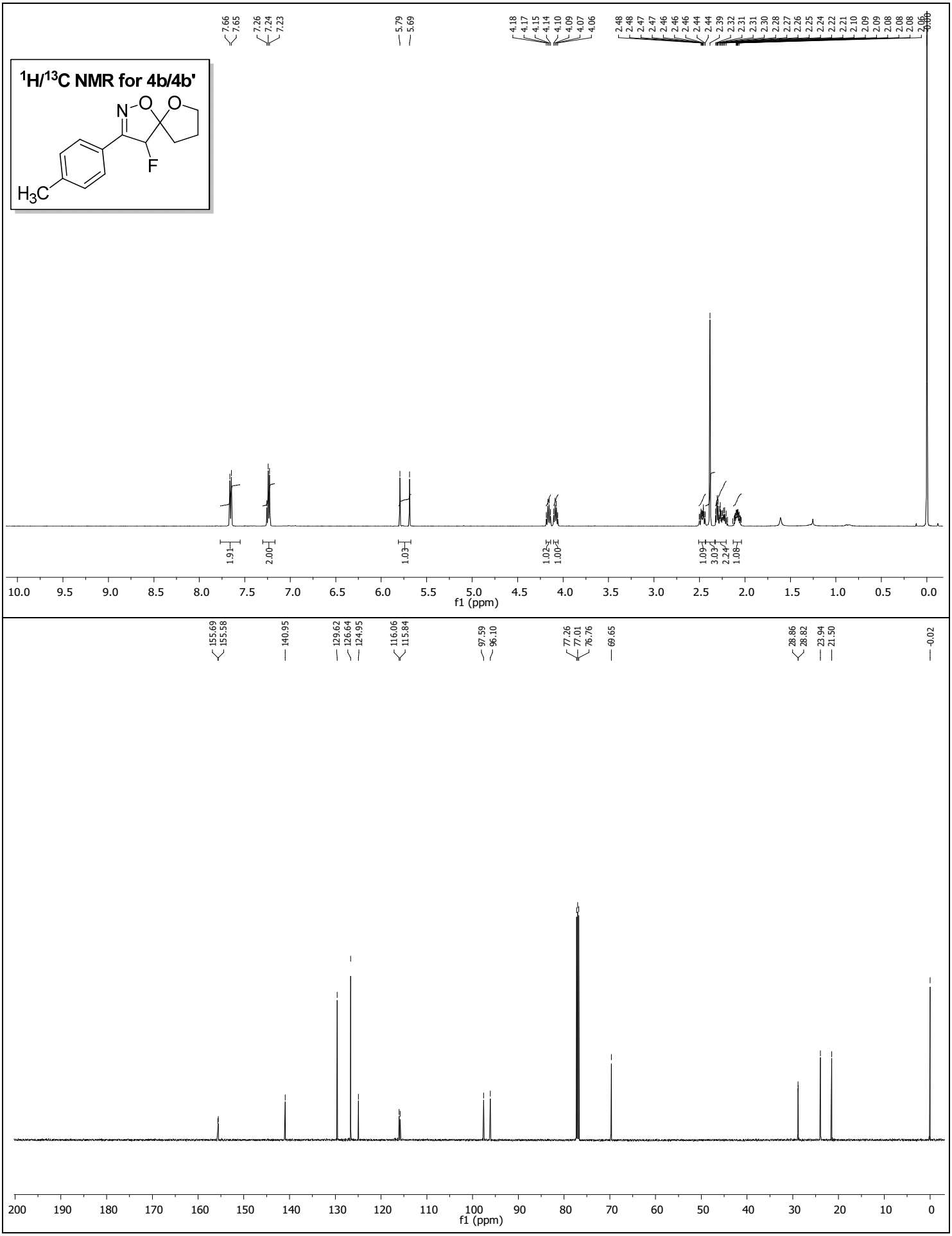

6.07
3.02
3.01
2.99
2.73
2.72
2.56
2.54
2.06
2.05
1.67
1.66
1.64
1.63
1.61
0.95
0.94
0.92
0.96
2.00
2.04
2.00
2.01
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


205.35
172.32
171.55
163.43
100.45
30.92
29.41
29.25
29.10
28.95
28.79
28.64
28.48
27.56
21.79
21.33
13.06
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

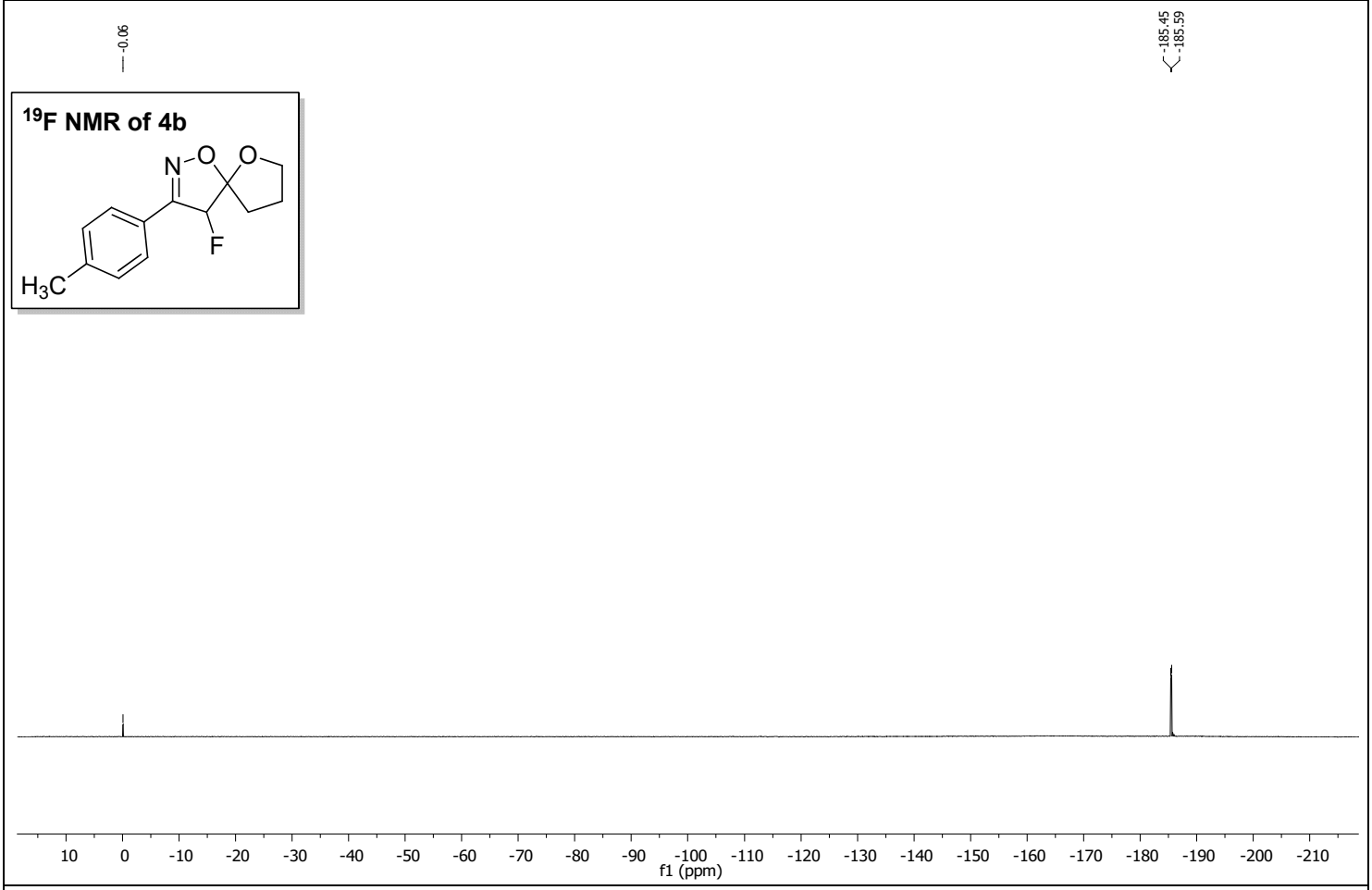

^{1}H/^{13}C NMR of 4a/4a'
N
O
O
F
7.78
7.77
7.76
7.44
7.43
7.26
5.81
5.71
4.19
4.18
4.16
4.15
4.11
4.10
4.08
4.07
2.52
2.51
2.49
2.49
2.48
2.47
2.45
2.34
2.33
2.32
2.31
2.30
2.29
2.28
2.27
2.26
2.25
2.23
2.22
2.20
2.13
2.12
2.11
2.10
2.10
2.08
2.07
2.05
2.00
3.09
1.07
1.07
1.07
1.14
2.32
1.22
f1 (ppm)
162.31
162.19
130.60
128.91
127.79
126.69
116.26
116.04
97.44
95.95
77.25
76.99
76.74
69.72
28.89
28.84
23.93
-0.02
f1 (ppm)


-0.00
-185.31
-185.46
19F NMR of 4a
N
O
O
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

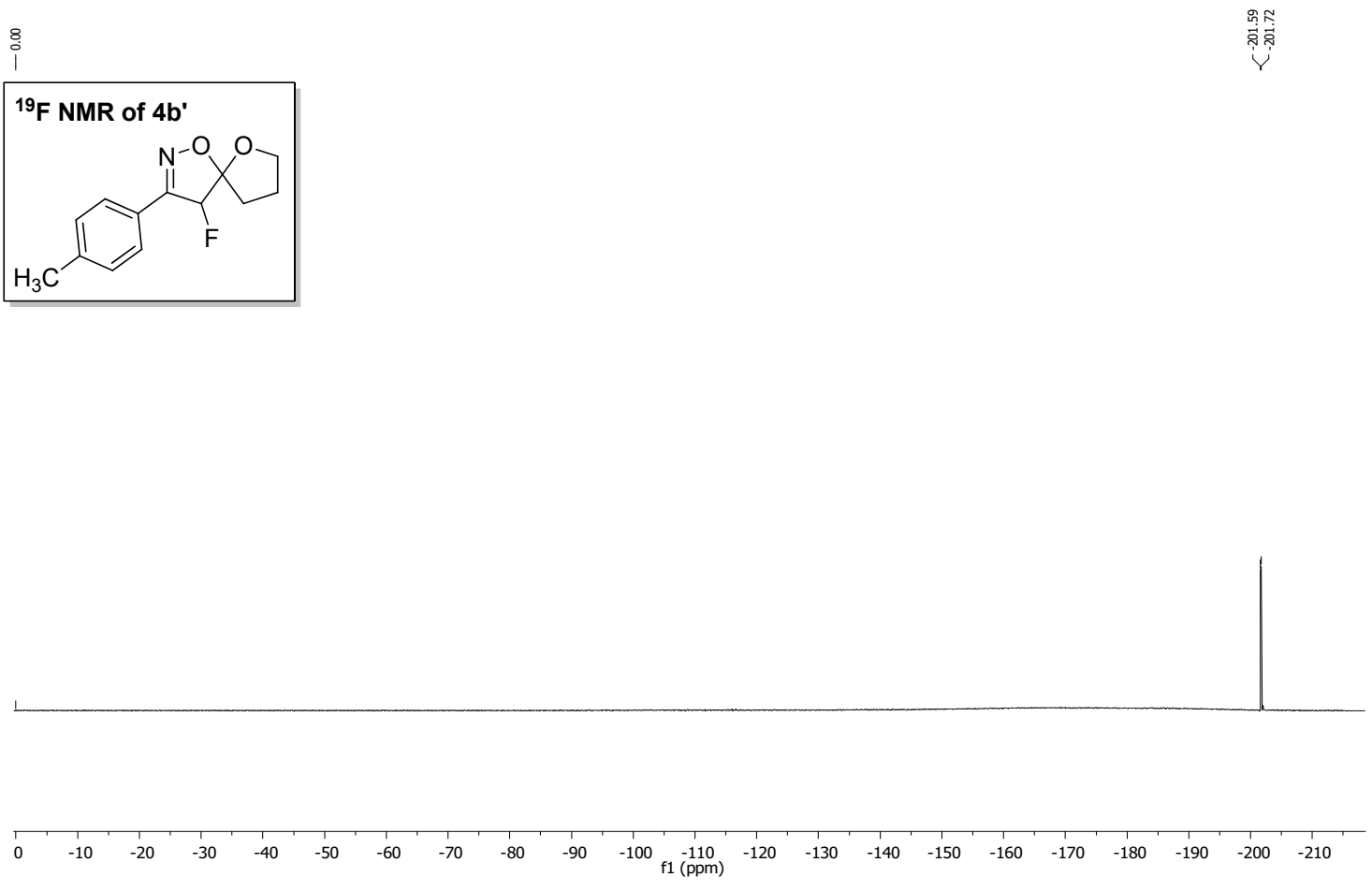

-0.00
-201.53
-201.67
19F NMR of 4a'
N
O
O
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

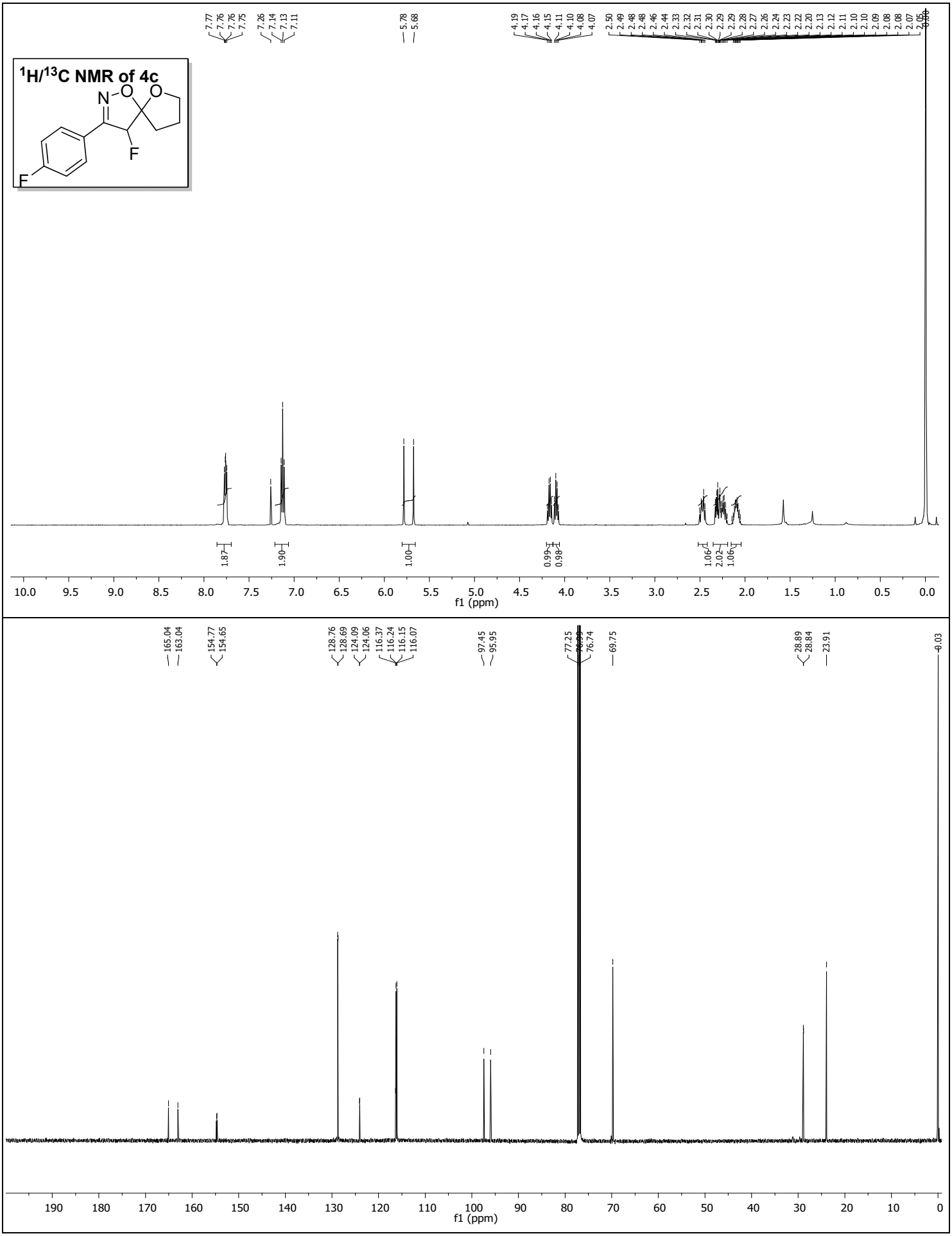

^{1}H/^{13}C NMR for 4b/4b'
N
O
O
F
H_3C
f1 (ppm)
f1 (ppm)

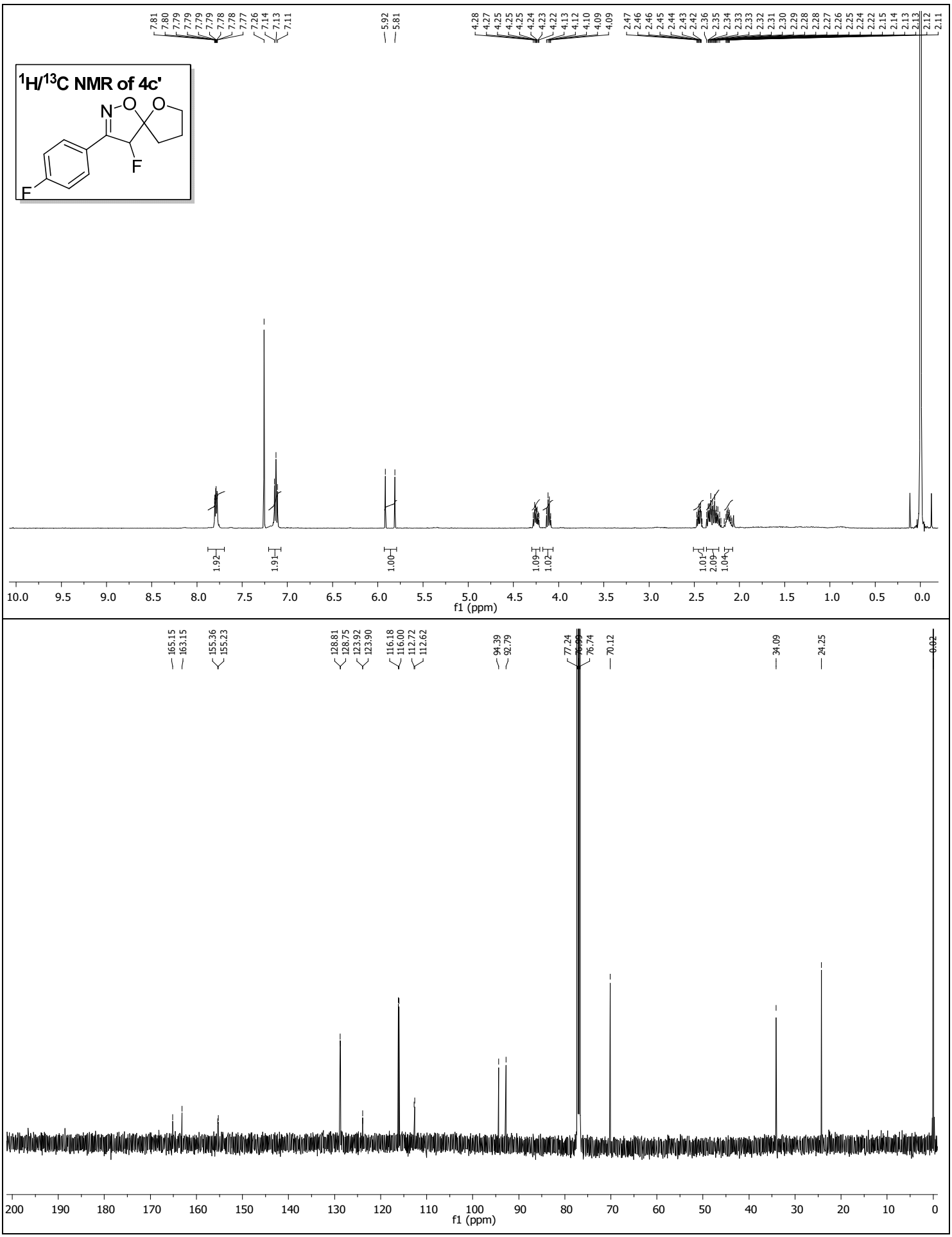
^{19}F NMR of 4b

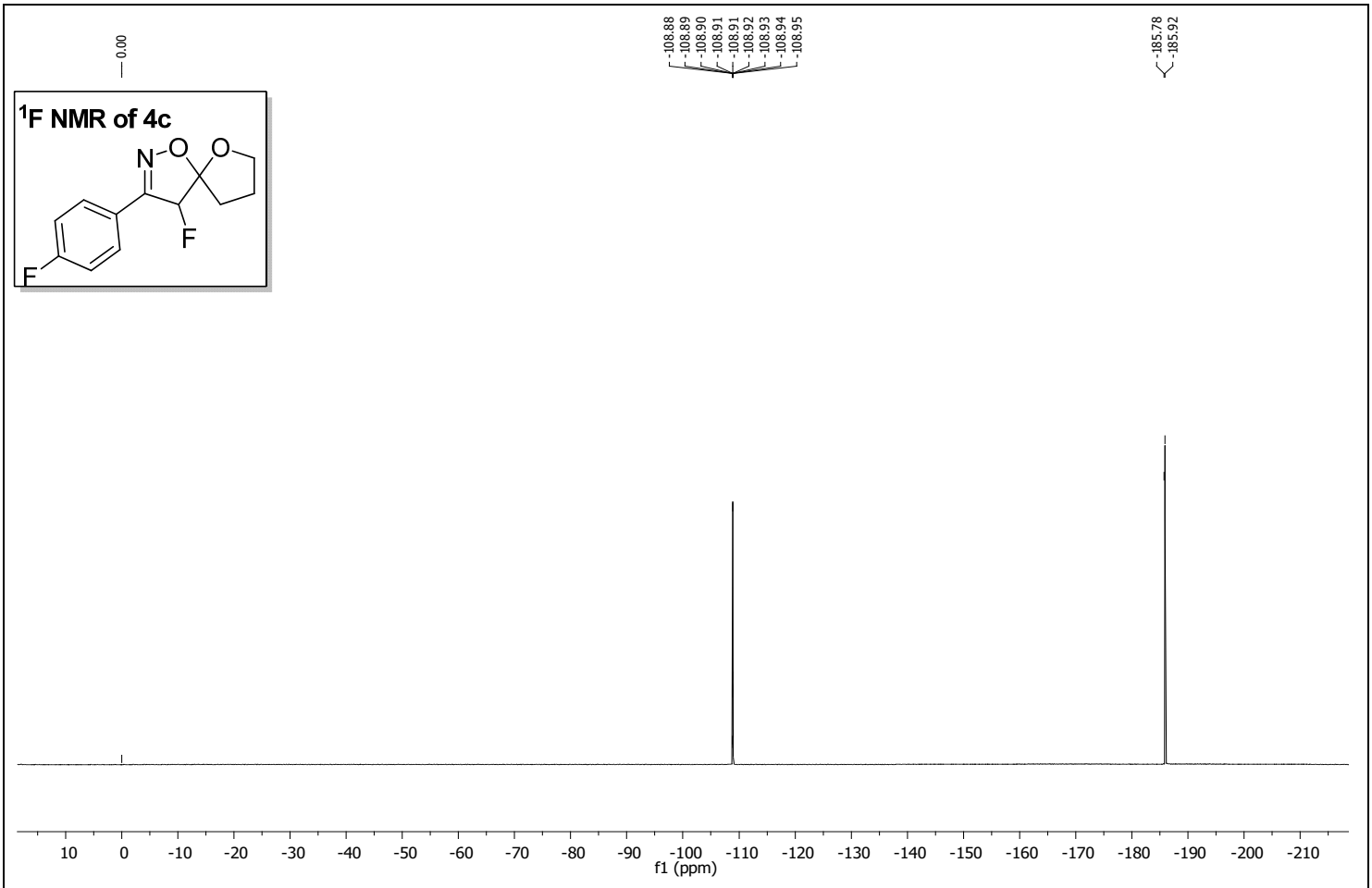


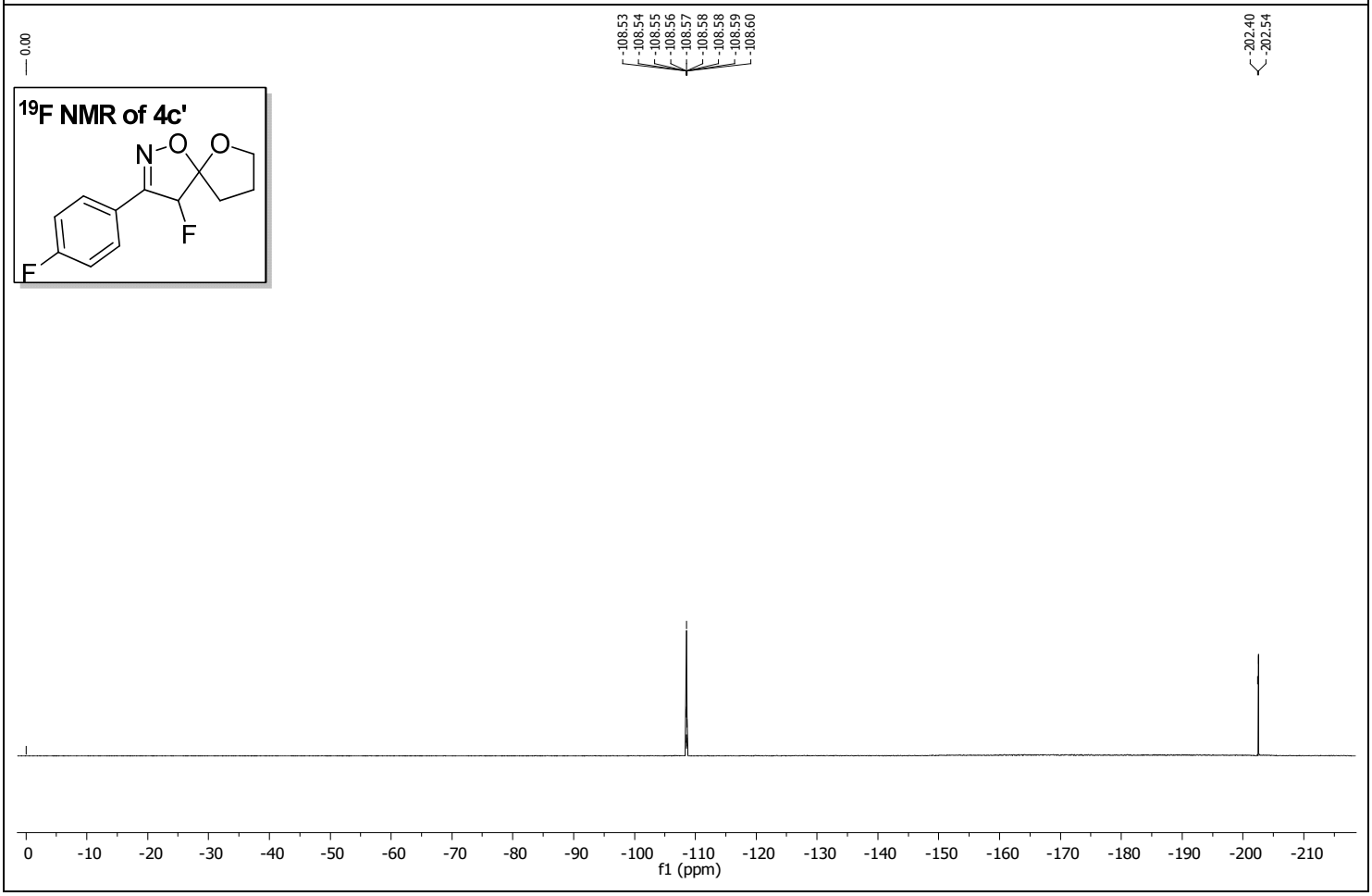
^{19}F NMR of 4b'

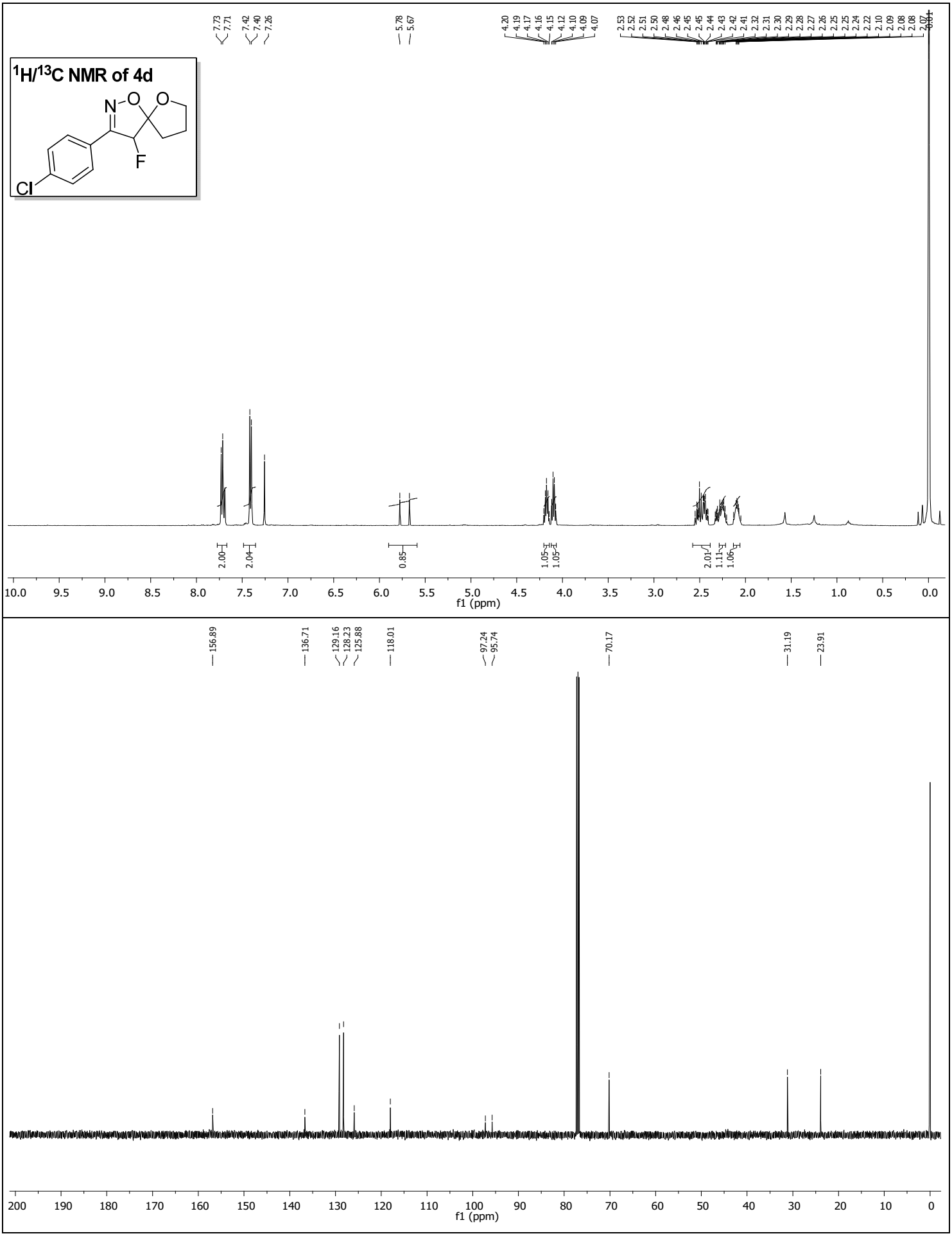


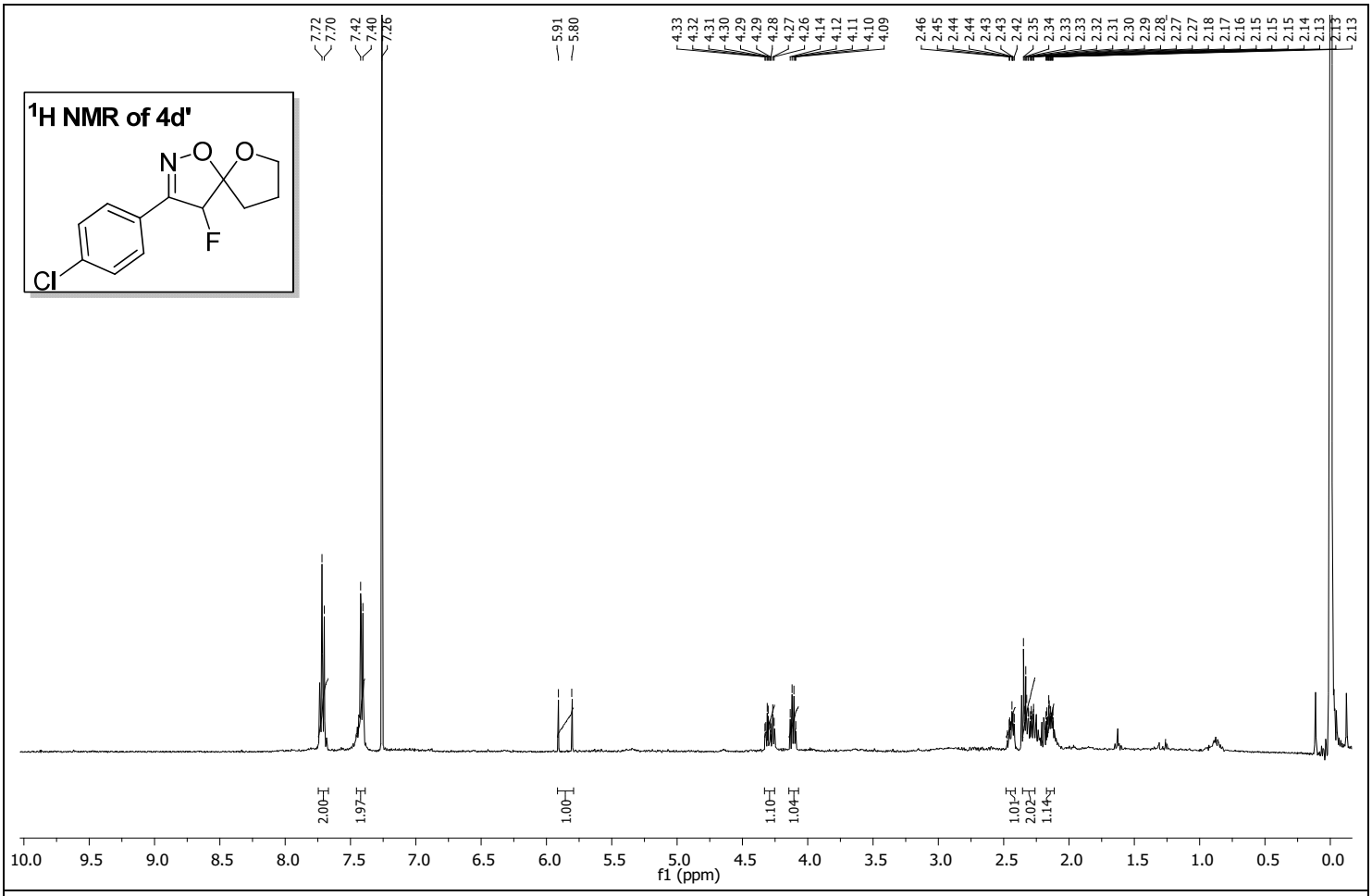

^{1}H/^{13}C NMR of 4c
f1 (ppm)
f1 (ppm)

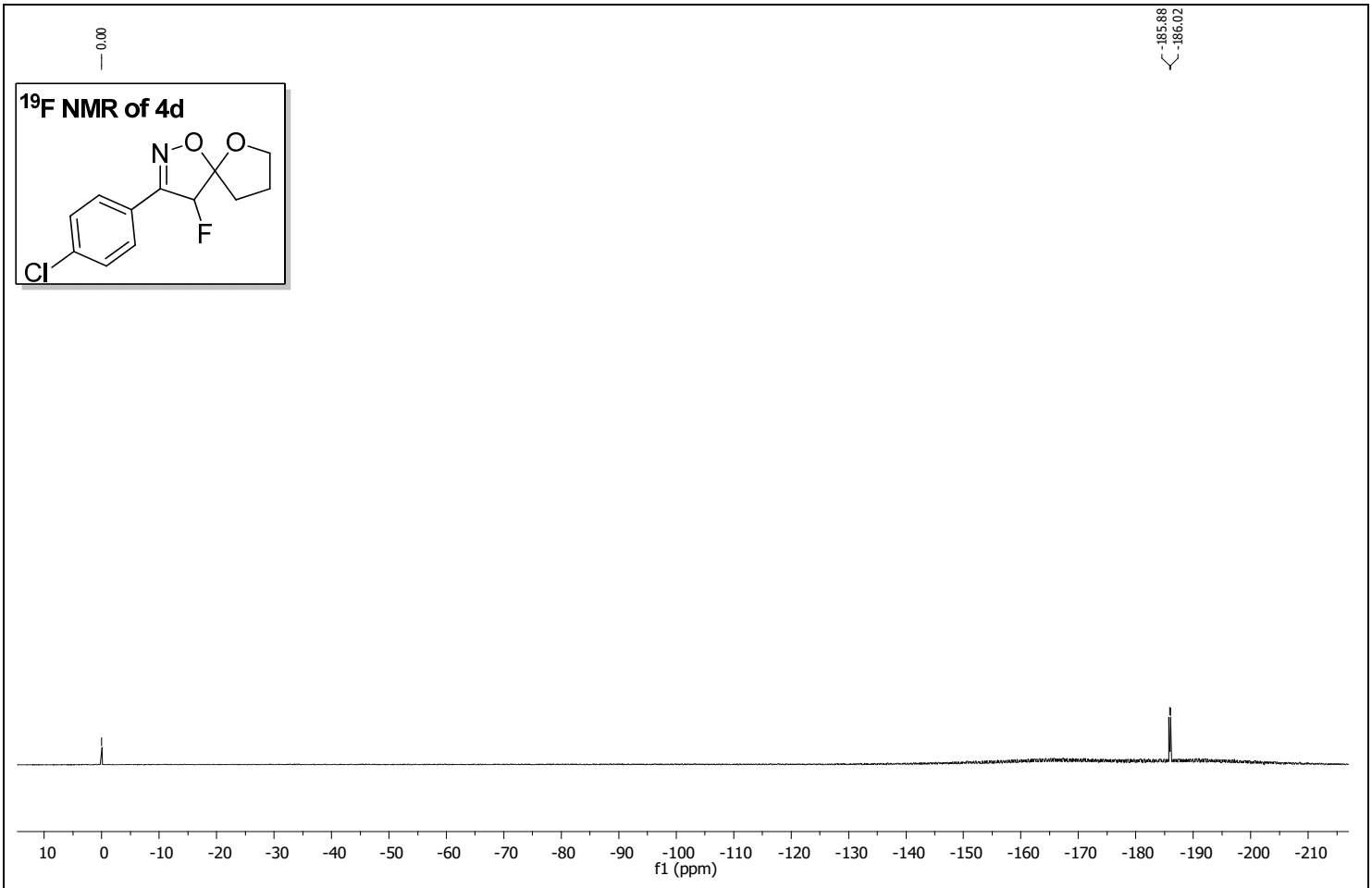

1H/13C NMR of 4c'
N
O
O
F
F
f1 (ppm)
f1 (ppm)

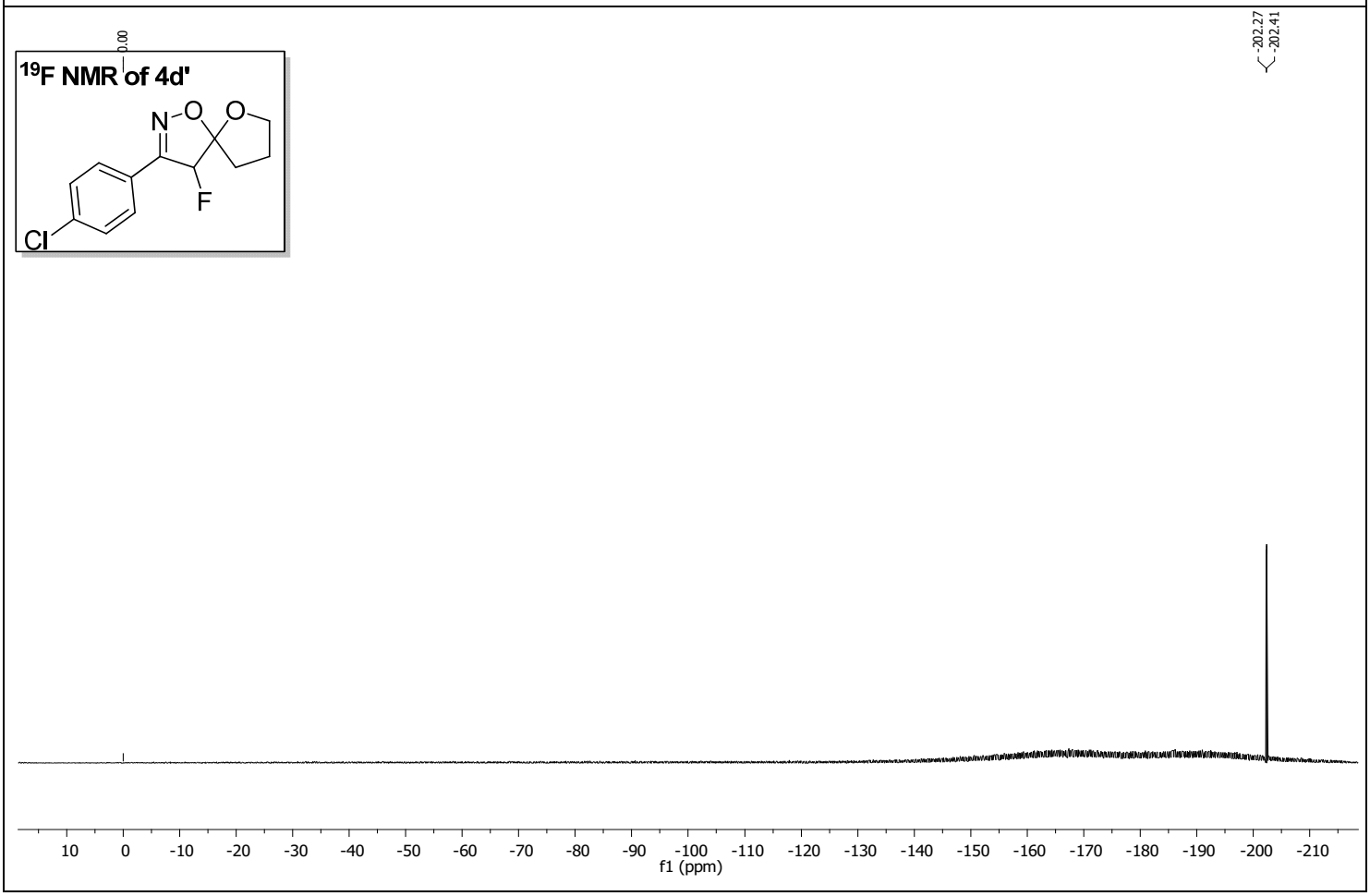

0.00
-108.88
-108.89
-108.90
-108.91
-108.91
-108.92
-108.93
-108.94
-108.95
-185.78
-185.92
19F NMR of 4c
N
O
O
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

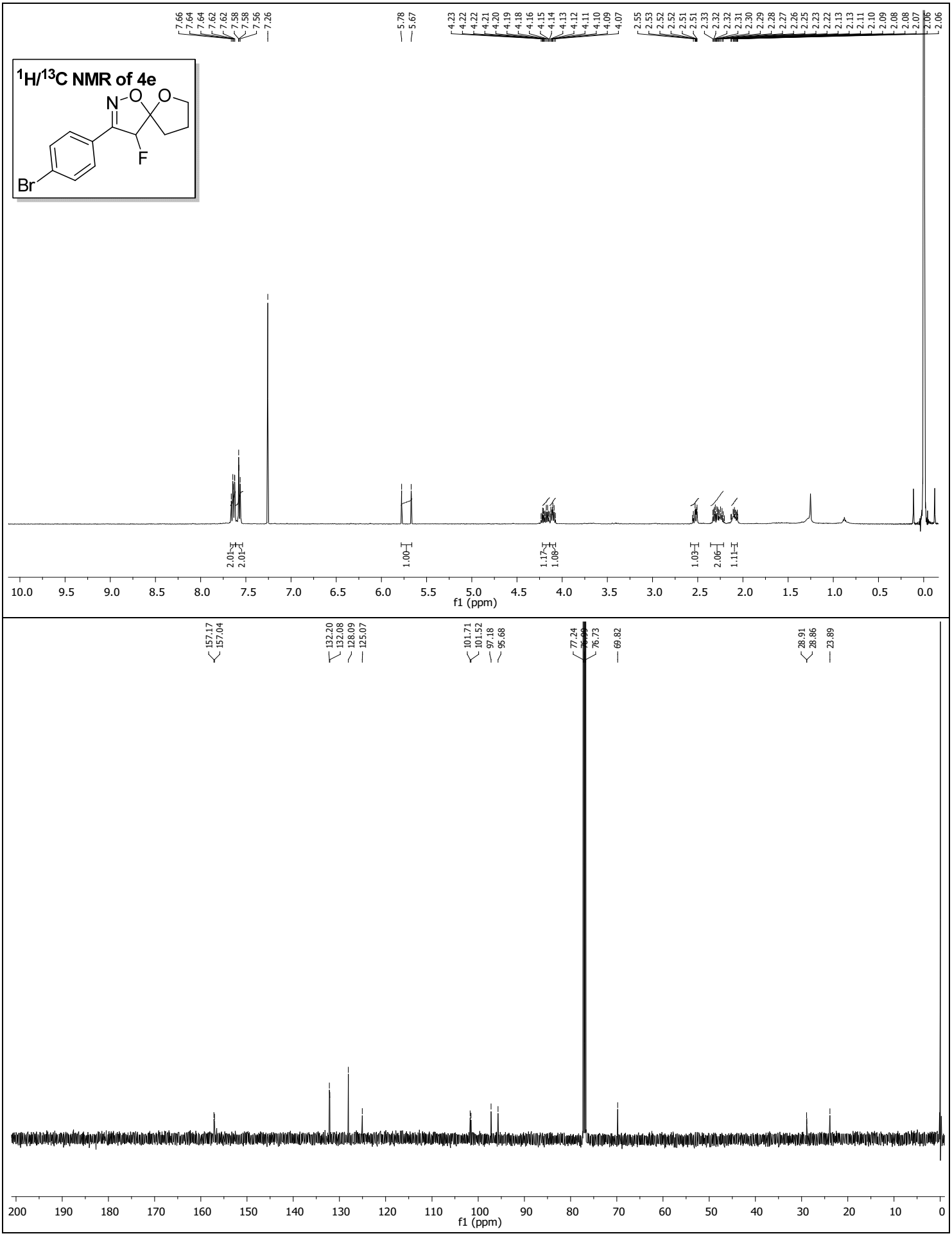

0.00
-108.53
-108.54
-108.55
-108.56
-108.57
-108.58
-108.58
-108.59
-108.60
-202.40
-202.54
19F NMR of 4c'
N
O
O
F
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

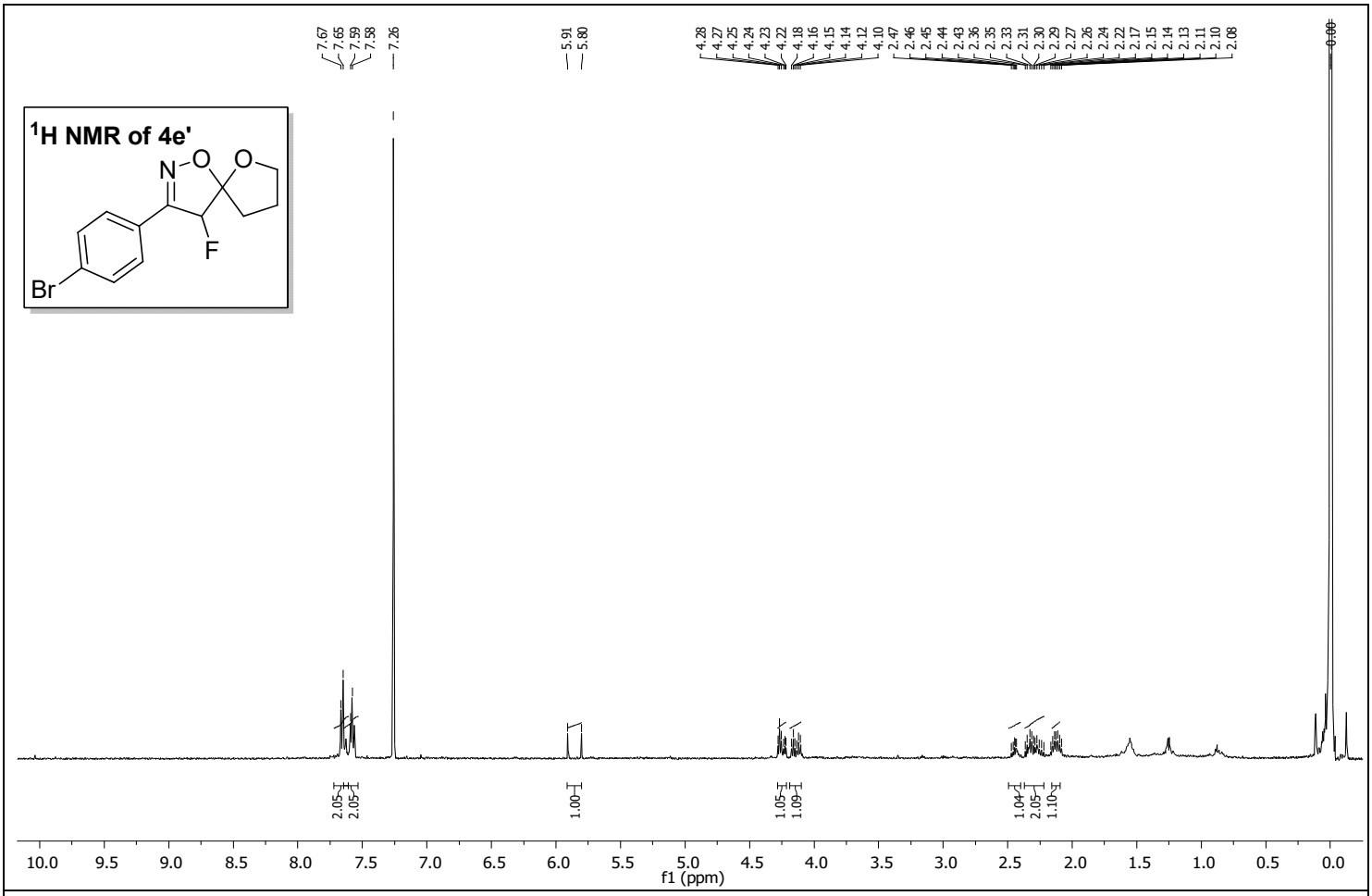

1H/13C NMR of 4d
N
O
O
F
Cl
7.73
7.71
7.42
7.40
7.26
5.78
5.67
4.20
4.19
4.17
4.16
4.15
4.12
4.10
4.09
4.07
2.53
2.52
2.51
2.50
2.48
2.46
2.45
2.45
2.44
2.43
2.42
2.41
2.32
2.31
2.30
2.29
2.28
2.27
2.26
2.25
2.25
2.24
2.22
2.10
2.09
2.08
2.08
2.07
0.01
2.00
2.04
0.85
1.05
1.05
2.01
1.11
1.06
10.0
9.5
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
0.0
f1 (ppm)
156.89
136.71
129.16
128.23
125.88
118.01
97.24
95.74
70.17
31.19
23.91
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

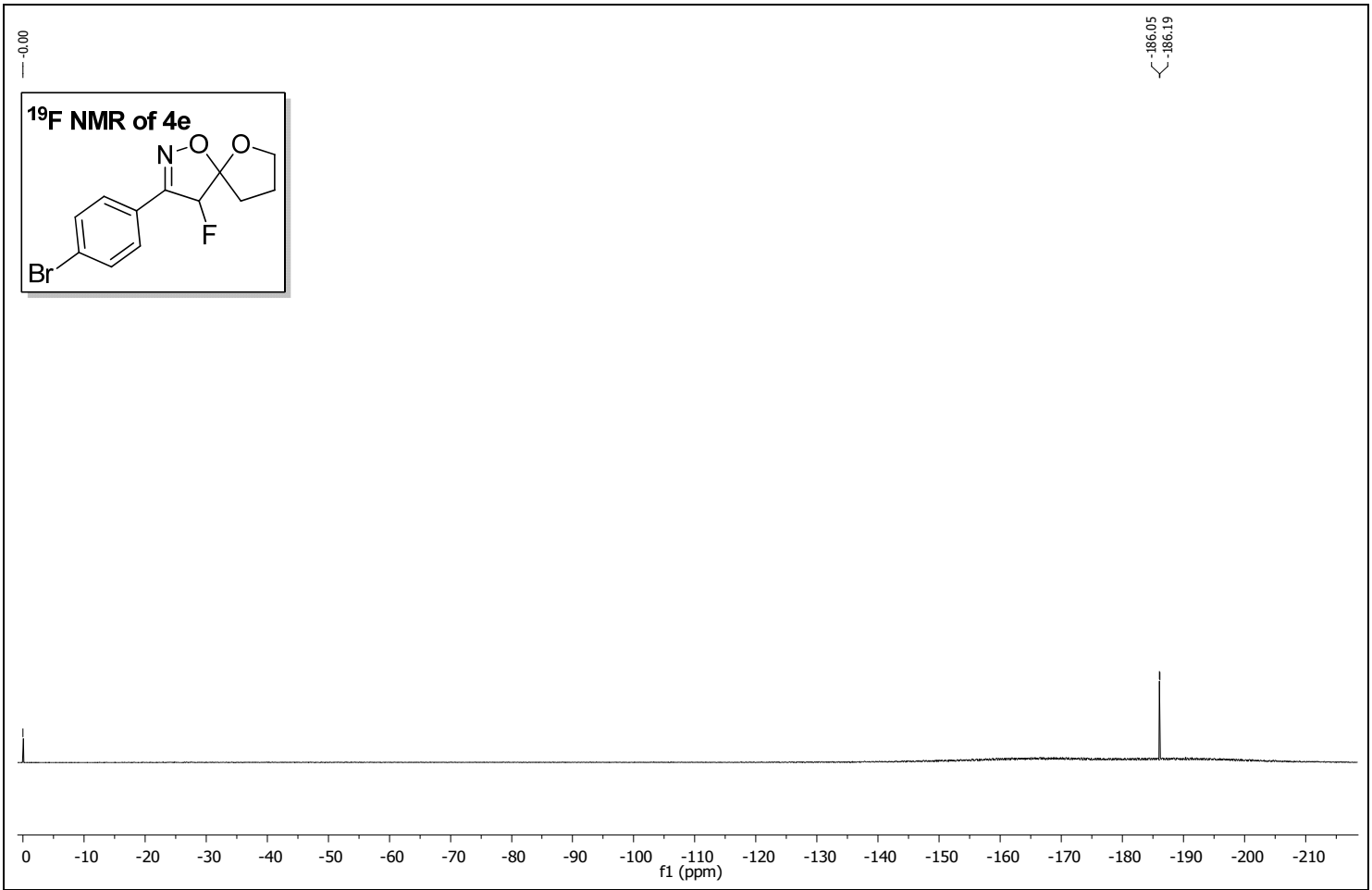

1H NMR of 4d'
N
O
O
F
Cl
7.72
7.70
7.42
7.40
7.26
5.91
5.80
4.33
4.32
4.31
4.30
4.29
4.29
4.28
4.27
4.26
4.14
4.12
4.11
4.10
4.09
2.46
2.45
2.44
2.44
2.43
2.43
2.42
2.35
2.34
2.33
2.33
2.32
2.31
2.30
2.29
2.28
2.27
2.27
2.18
2.17
2.16
2.15
2.15
2.15
2.14
2.13
2.13
2.13
2.00
1.97
1.00
1.10
1.04
1.01
2.02
1.14
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
0.0
f1 (ppm)

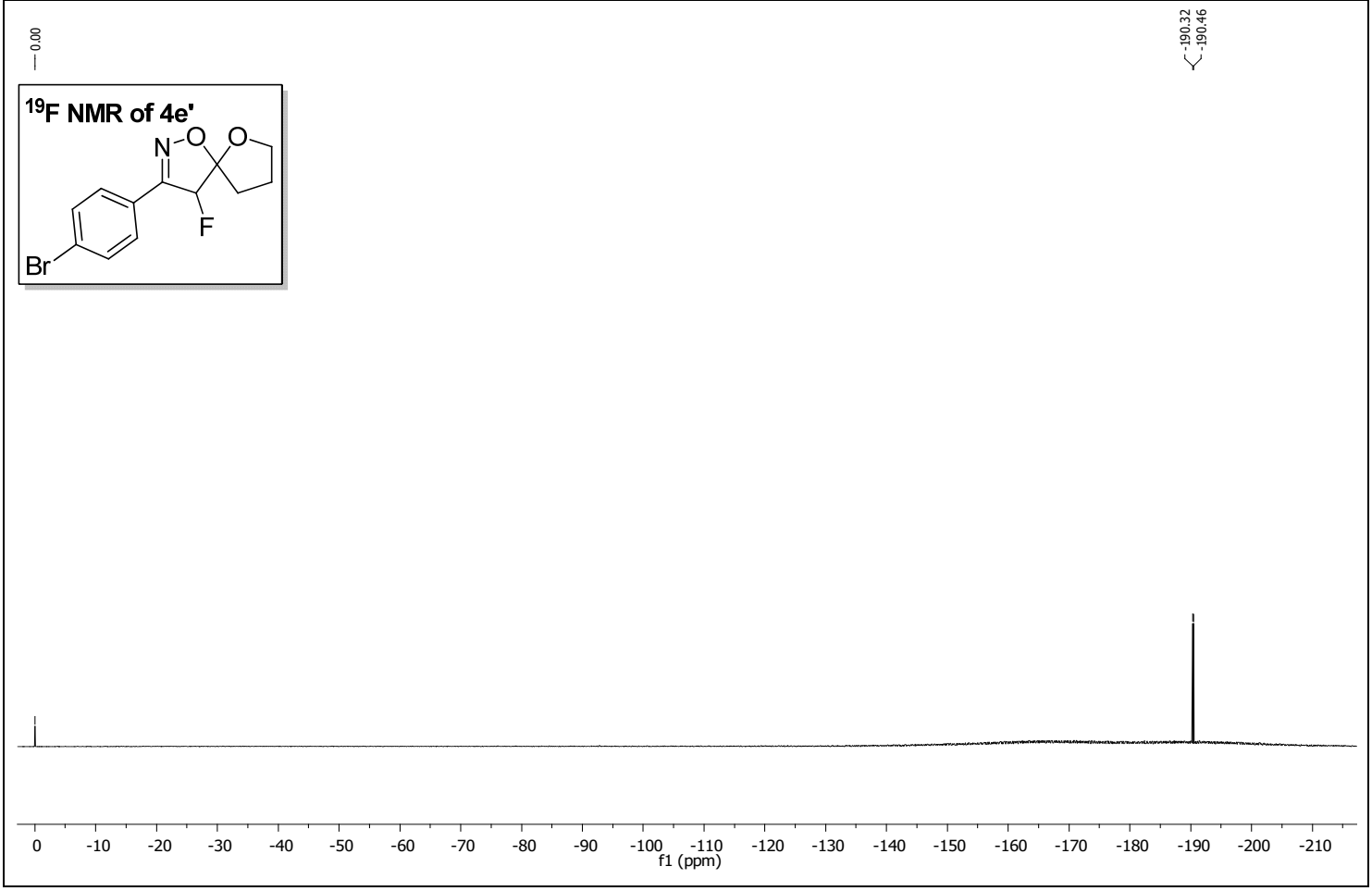

0.00
-185.88
-186.02
19F NMR of 4d
N
O
O
F
Cl
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

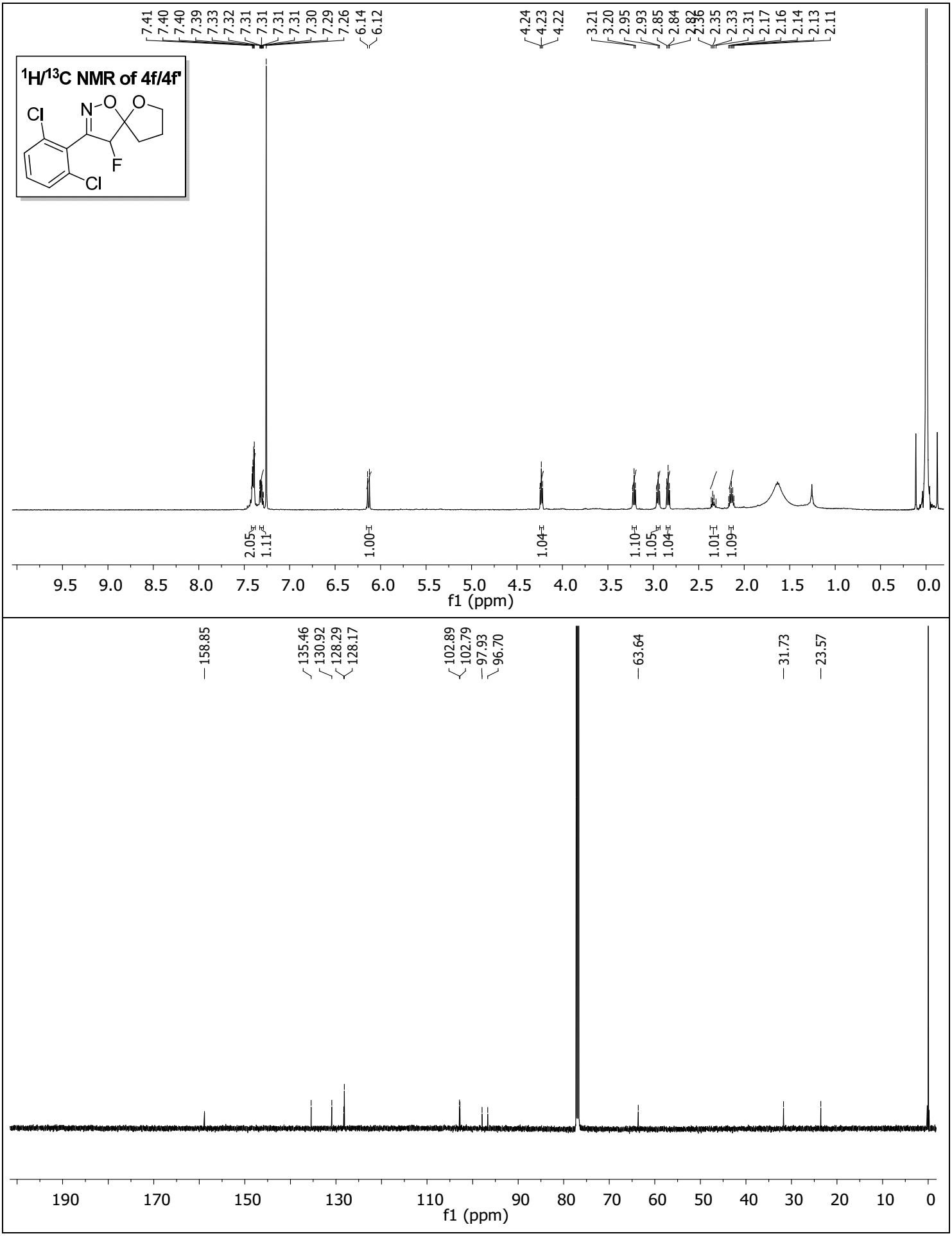

0.00
-202.27
-202.41
19F NMR of 4d'
N
O
O
F
Cl
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

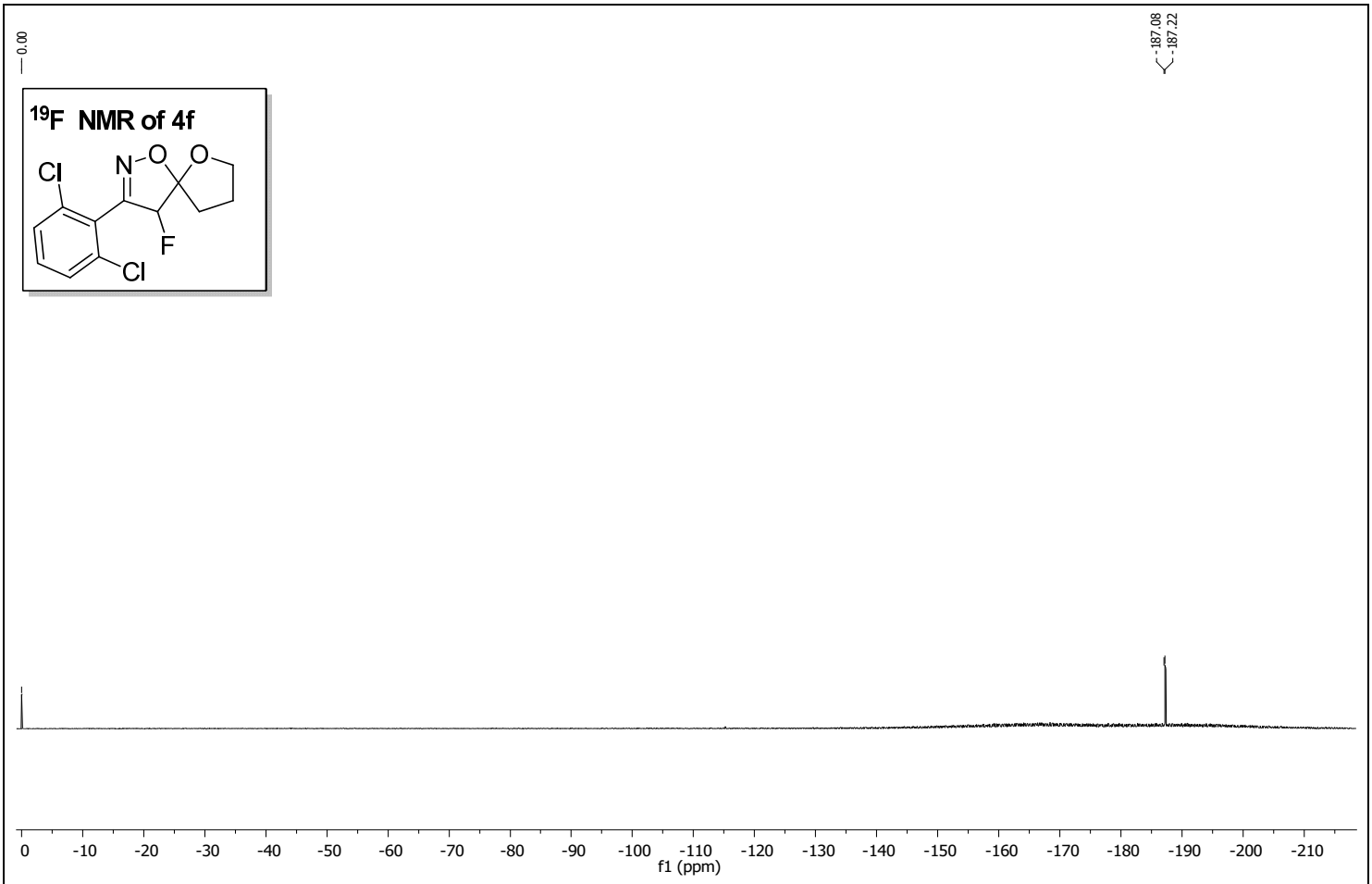

$^{1}H/^{13}C$ NMR of 4e
N
O
O
F
Br
f1 (ppm)
f1 (ppm)

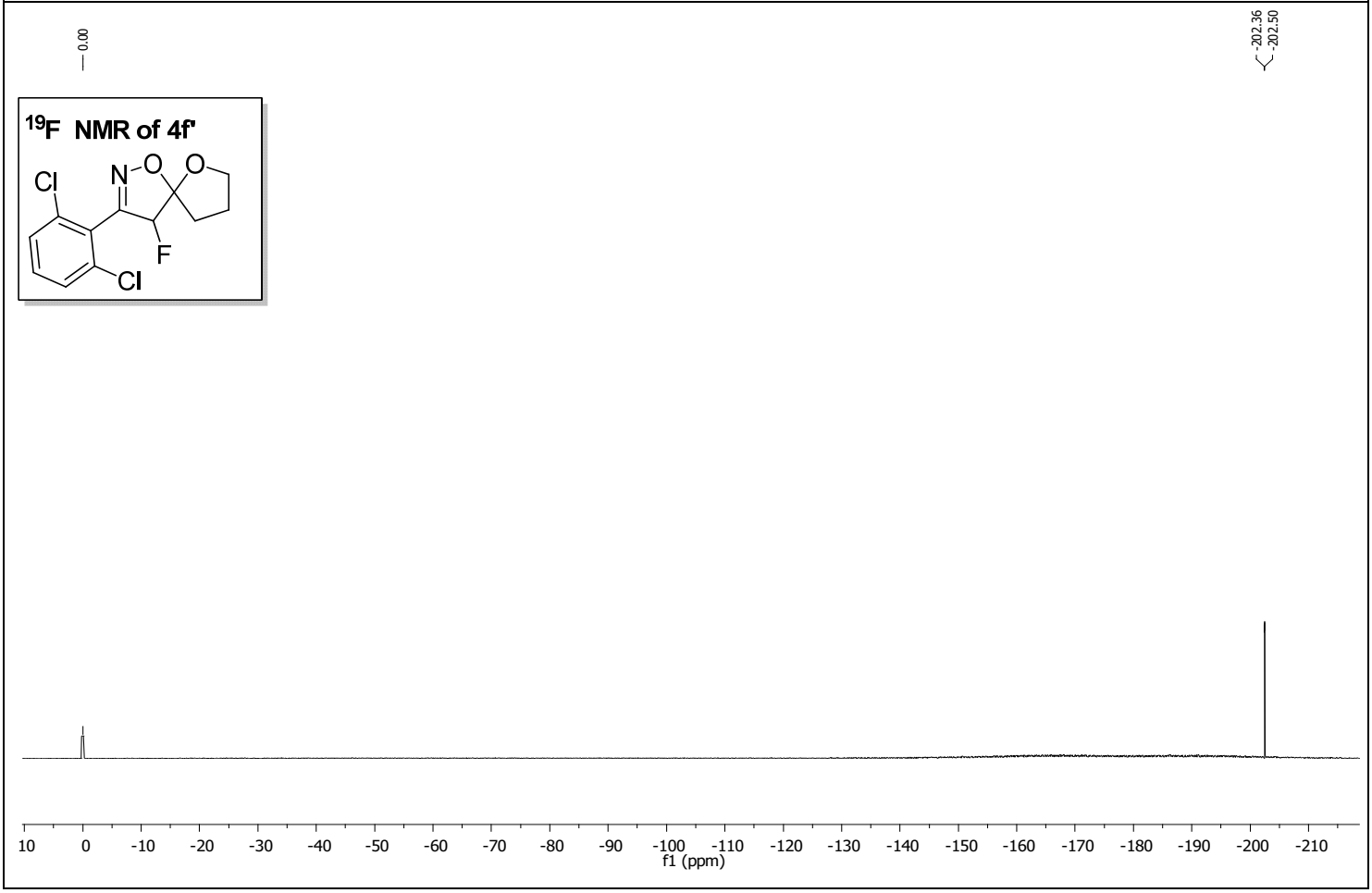

1H NMR of 4e'
N
O
O
F
Br
7.67
7.65
7.59
7.58
7.26
5.91
5.80
4.28
4.27
4.25
4.24
4.23
4.22
4.18
4.16
4.15
4.14
4.12
4.10
2.47
2.46
2.45
2.44
2.43
2.36
2.35
2.33
2.31
2.30
2.29
2.27
2.26
2.24
2.22
2.17
2.15
2.14
2.13
2.11
2.10
2.08
0.00
2.05
2.05
1.00
1.05
1.09
1.04
2.05
1.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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
0.0
f1 (ppm)

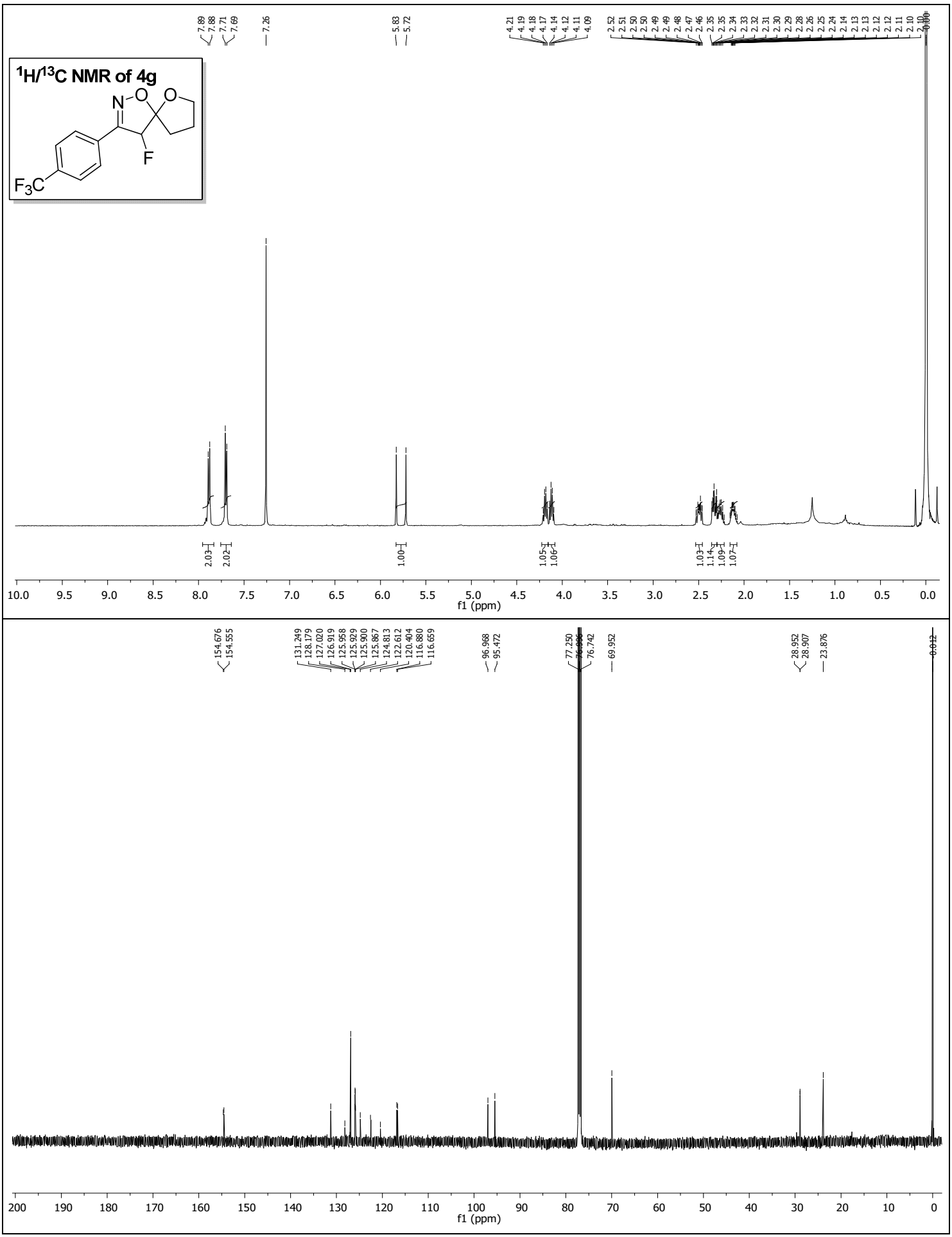

-0.00
-186.05
-186.19
19F NMR of 4e
N
O
O
F
Br
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

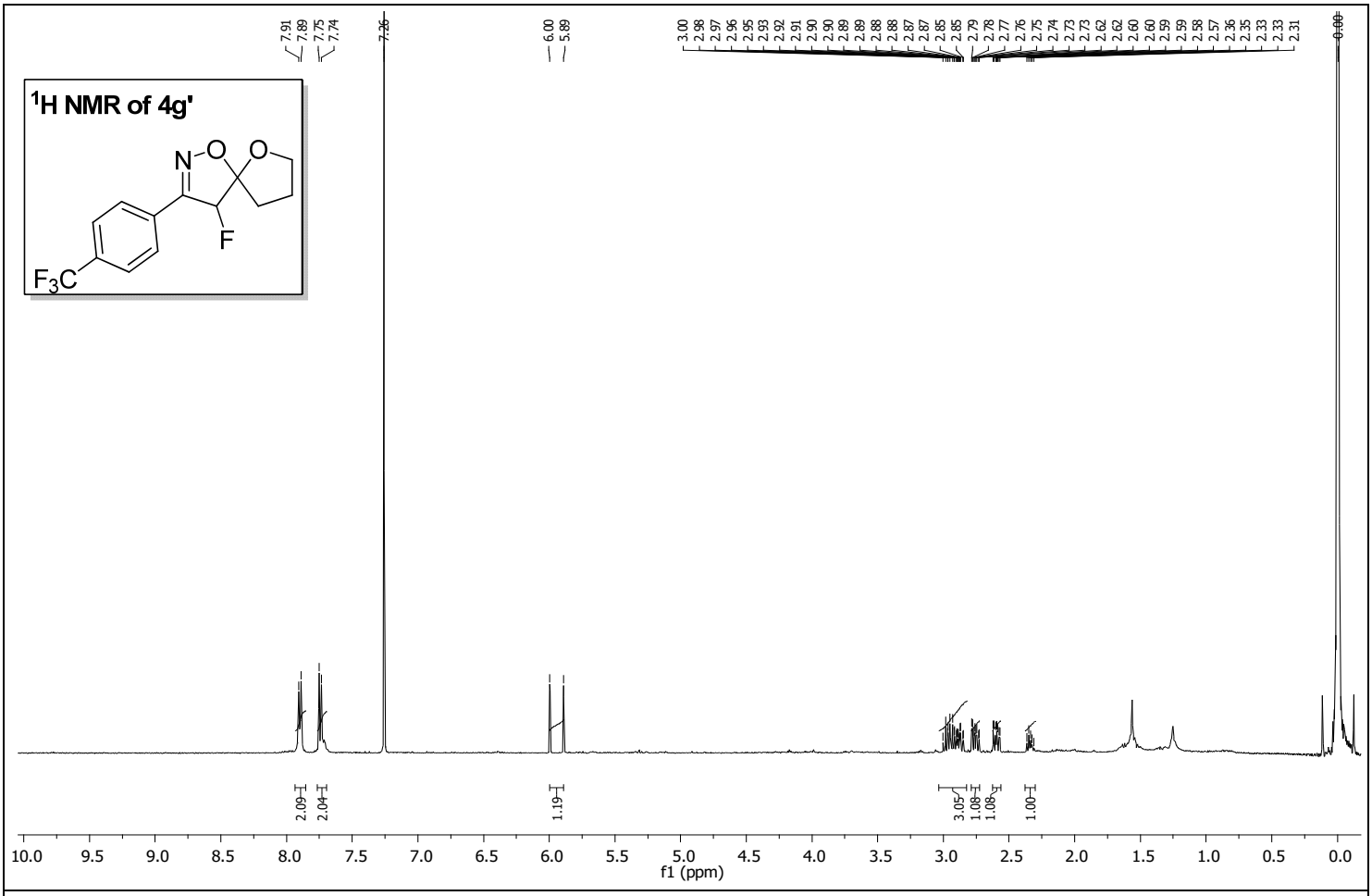

0.00
-190.32
-190.46
19F NMR of 4e'
N
O
O
F
Br
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

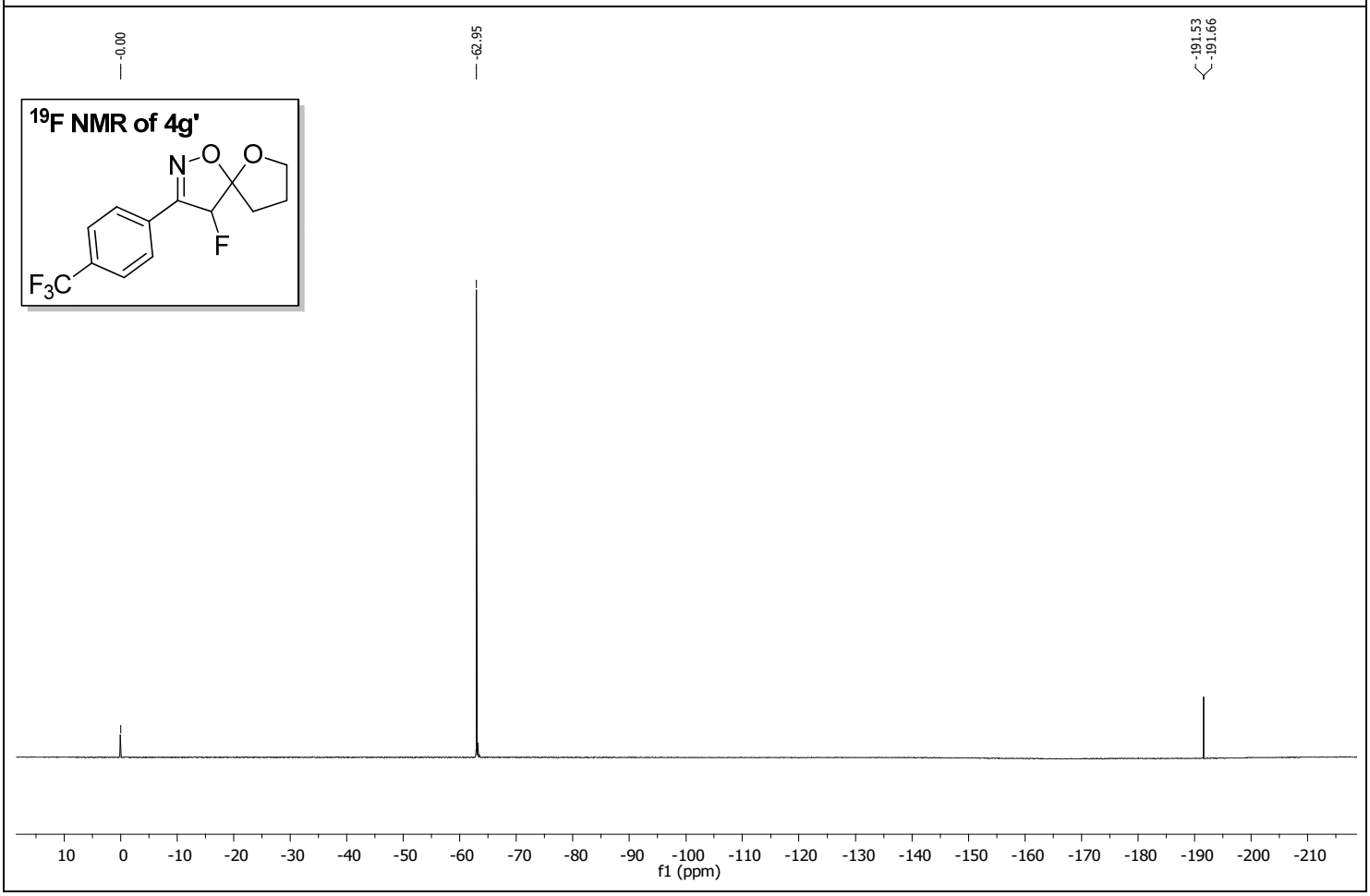

^{1}H/^{13}C NMR of 4f/4f'
Cl
N
O
O
F
Cl
7.41 7.40 7.40 7.39 7.33 7.32 7.31 7.31 7.31 7.31 7.30 7.29 7.26 6.14 6.12
4.24 4.23 4.22
3.21 3.20 2.95 2.93 2.85 2.84 2.82 2.36 2.35 2.33 2.31 2.17 2.16 2.14 2.13 2.11
2.05 1.11 1.00 1.04 1.10 1.05 1.04 1.01 1.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
158.85
135.46 130.92 128.29 128.17
102.89 102.79 97.93 96.70
63.64
31.73
23.57
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

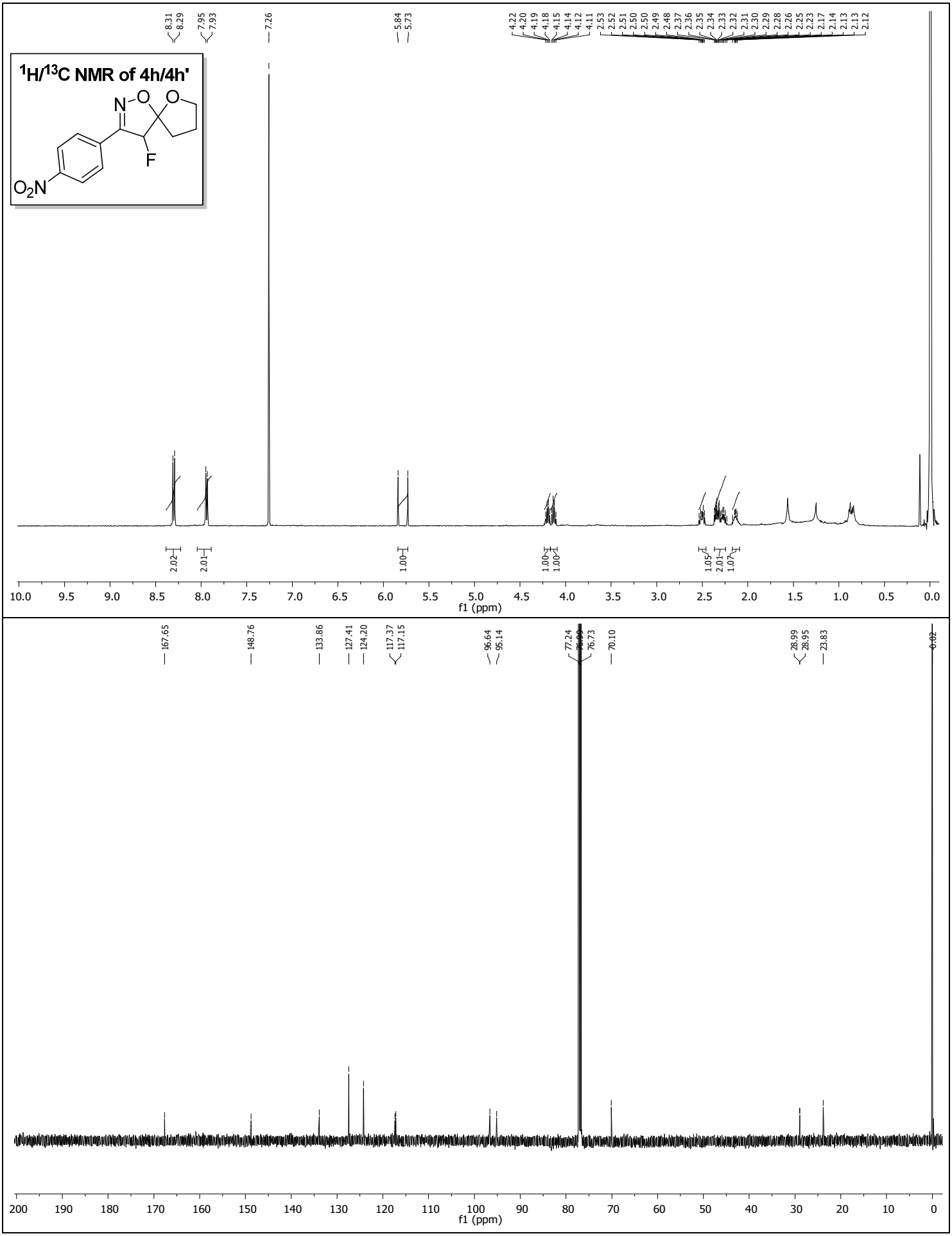

0.00
-187.08
-187.22
19F NMR of 4f
Cl
N
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

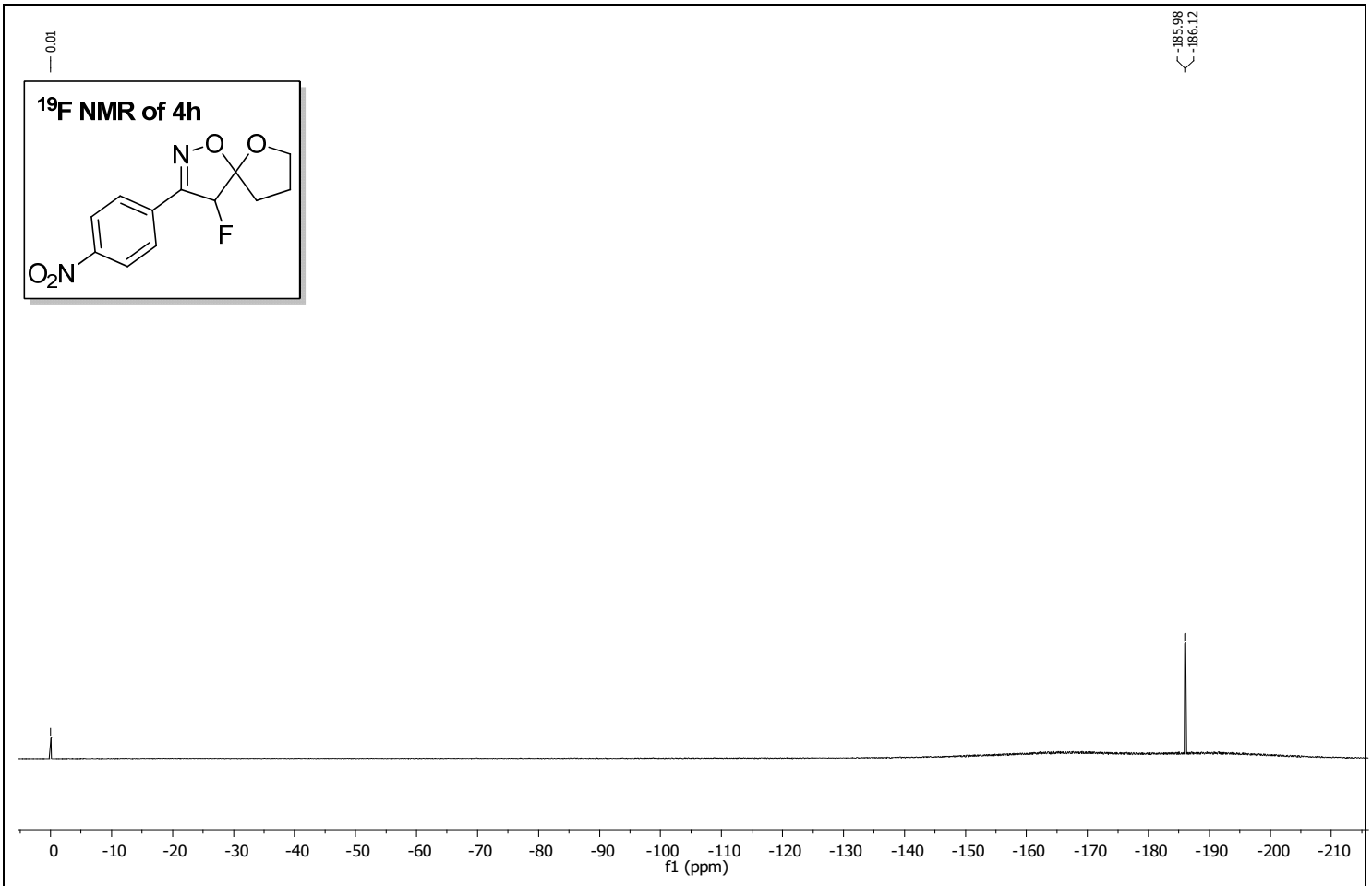

0.00
-202.36
-202.50
19F NMR of 4f'
Cl
N
O
O
F
Cl
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

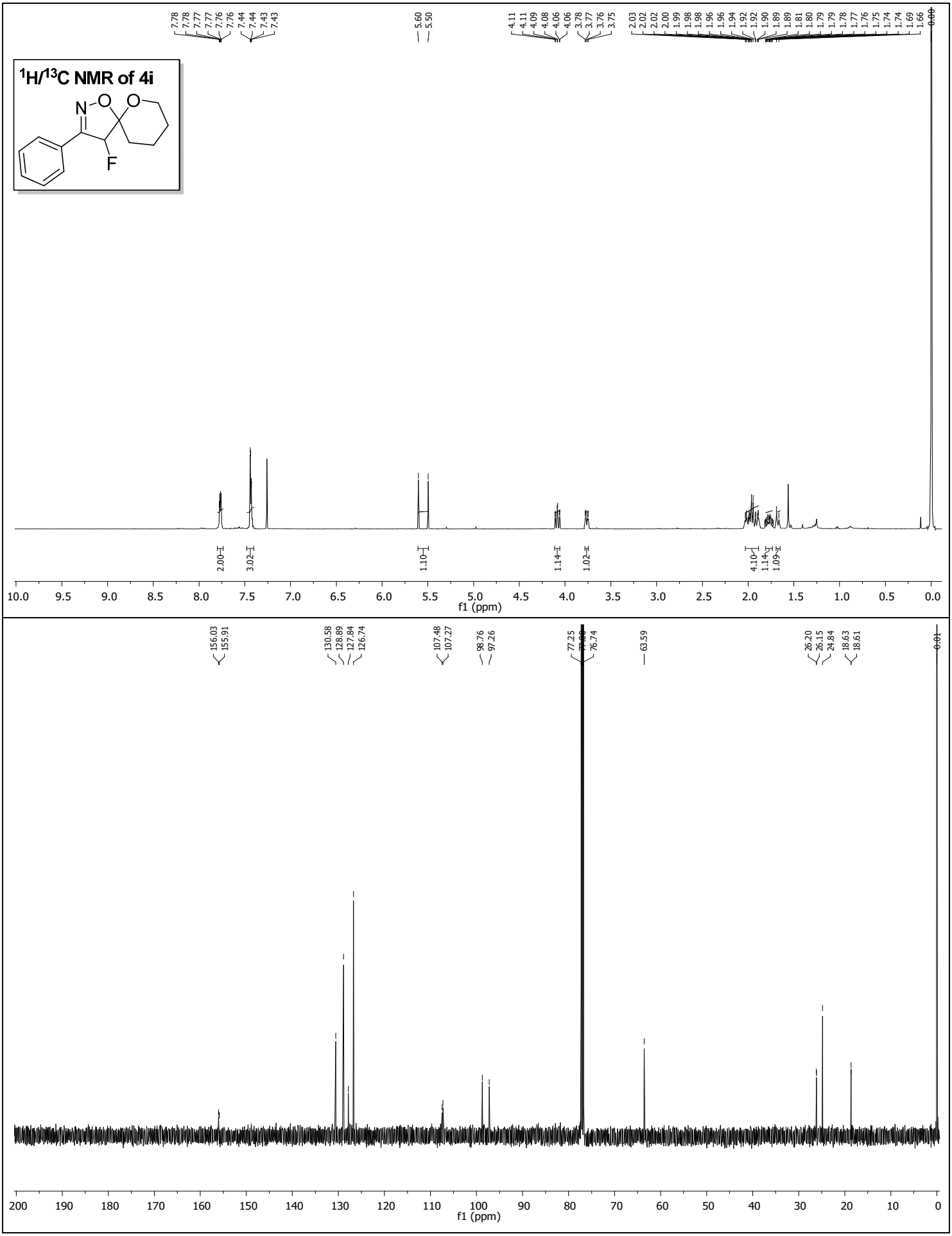

^{1}H/^{13}C NMR of 4g
N
O
O
F
F_3C
f1 (ppm)
f1 (ppm)

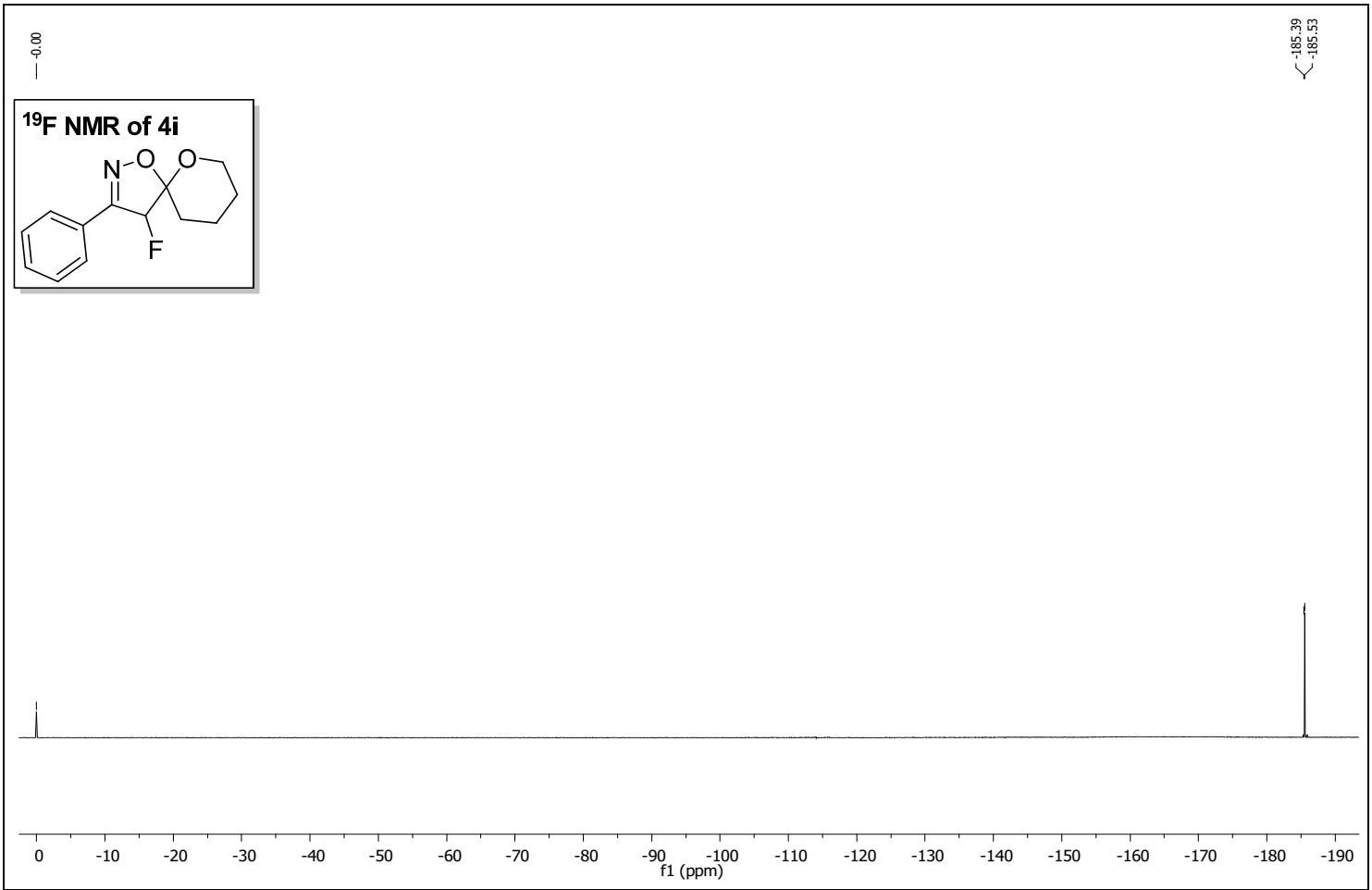

^{1}H NMR of 4g'
N
O
O
F
F_3C
7.91
7.89
7.75
7.74
7.26
6.00
5.89
3.00
2.98
2.97
2.96
2.95
2.93
2.92
2.91
2.90
2.90
2.89
2.89
2.88
2.88
2.87
2.87
2.85
2.85
2.79
2.78
2.77
2.76
2.75
2.74
2.73
2.73
2.62
2.62
2.60
2.60
2.59
2.59
2.58
2.57
2.36
2.35
2.33
2.31
0.00
2.09
2.04
1.19
3.05
1.08
1.08
1.00
10.0
9.5
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
0.0
f1 (ppm)

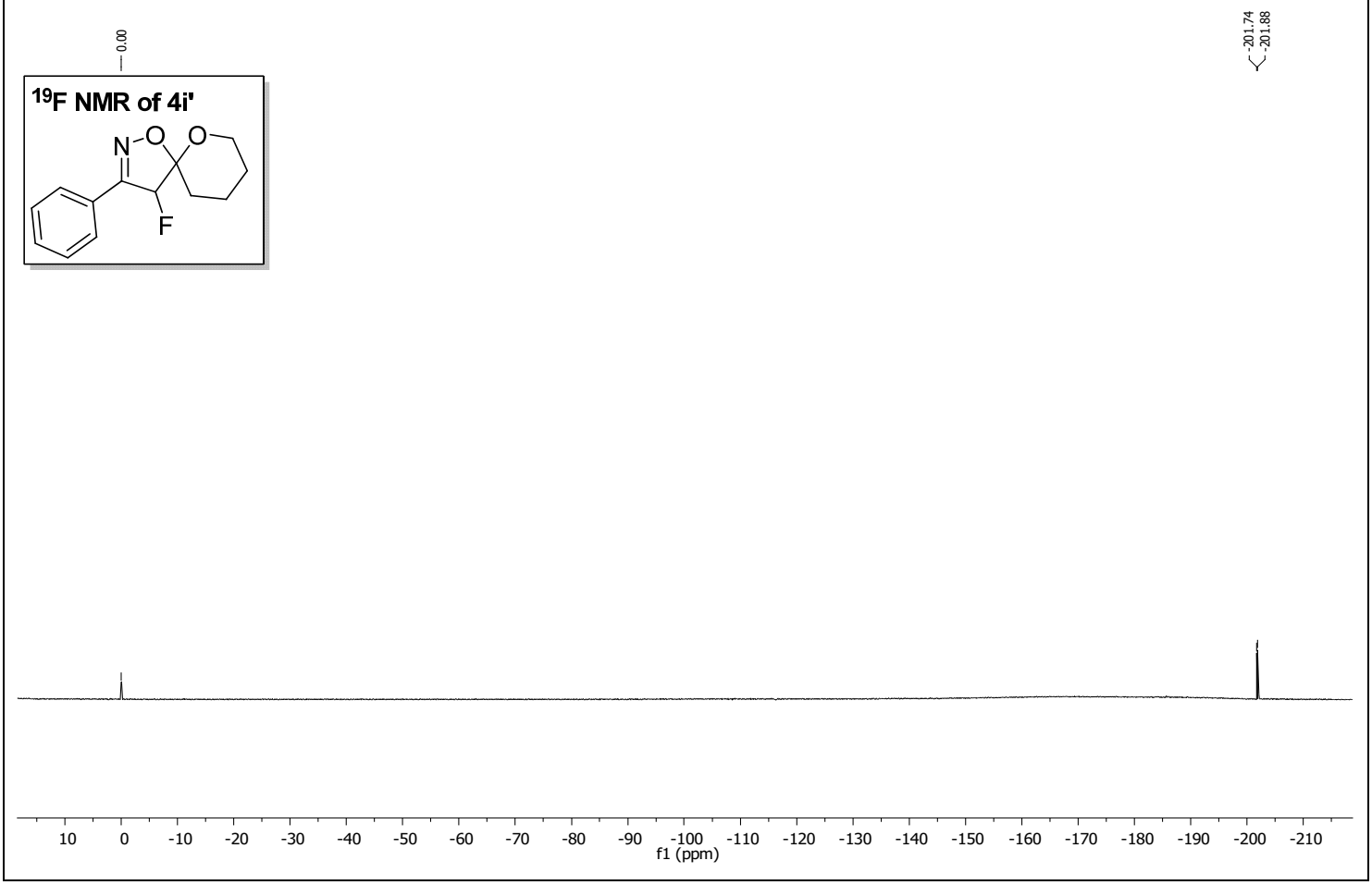

^{19}F NMR of 4g'
N
O
O
F
F_3C
-0.00
-62.95
-191.53
-191.66
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

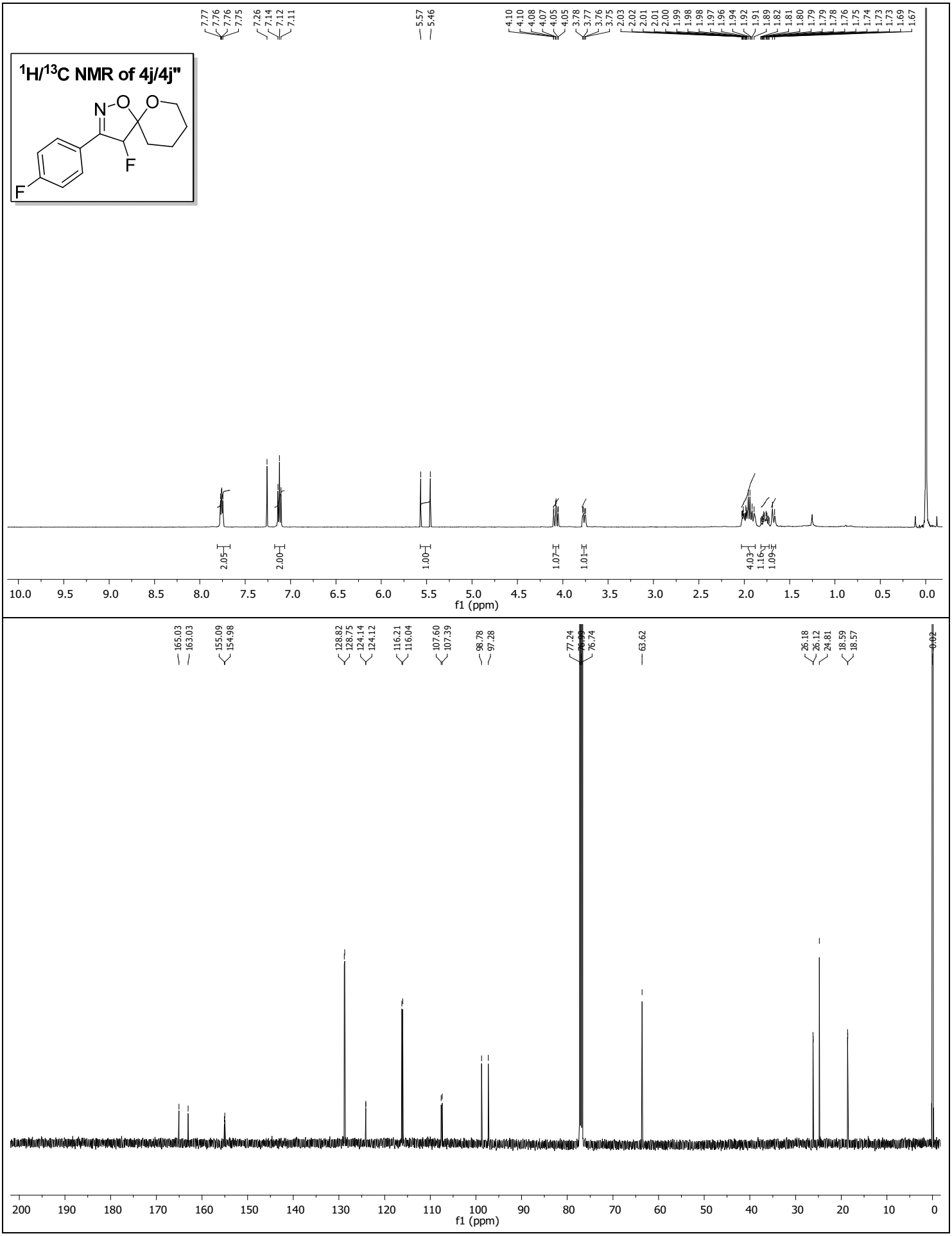

^{1}H/^{13}C NMR of 4h/4h'
f1 (ppm)
f1 (ppm)

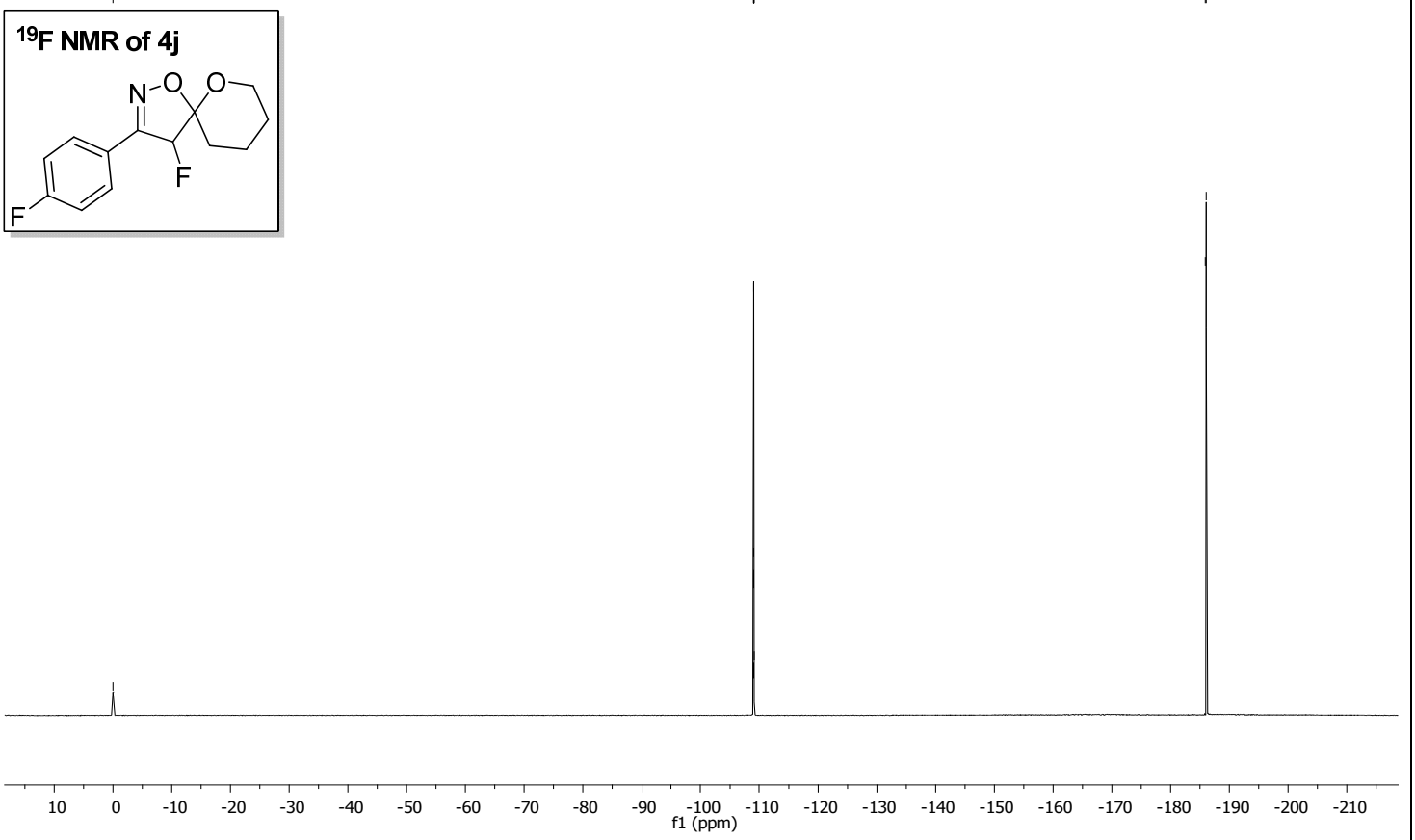

0.01
-185.98
-186.12
19F NMR of 4h
N
O
O
F
O2N
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

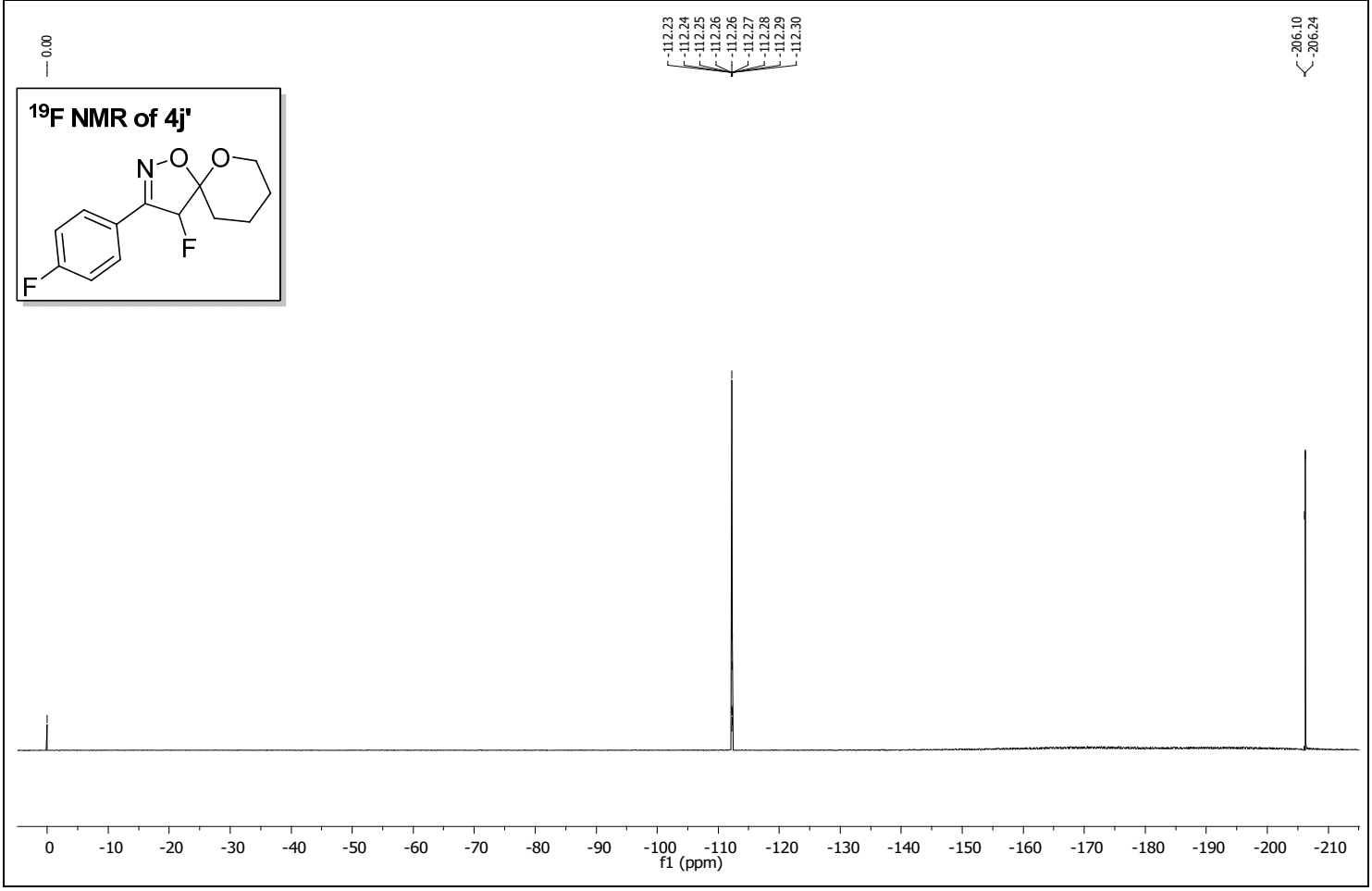

$^{1}H/^{13}C$ NMR of 4i
N
O
O
F
f1 (ppm)
f1 (ppm)

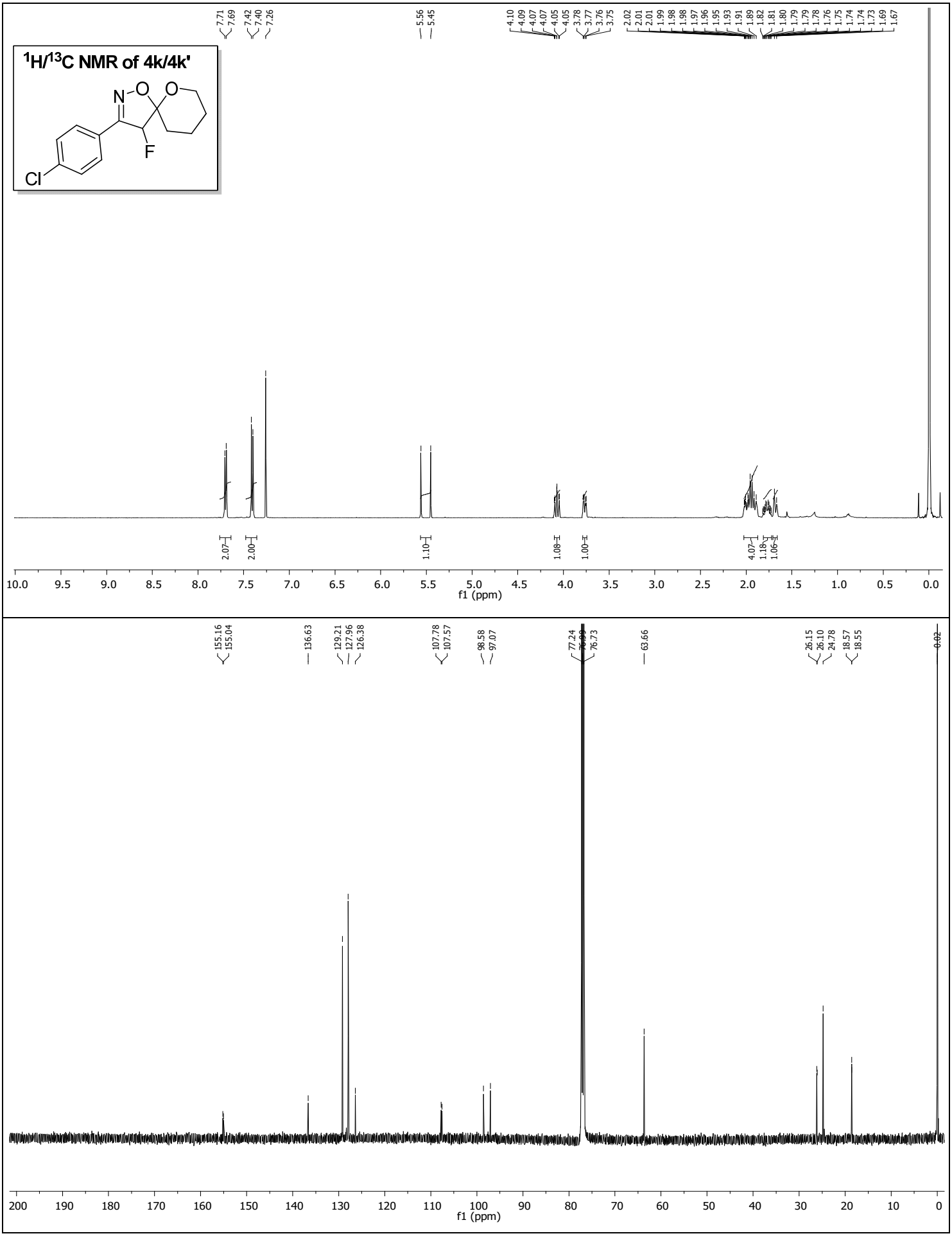

-0.00
-185.39
-185.53
19F NMR of 4i
N
O
O
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

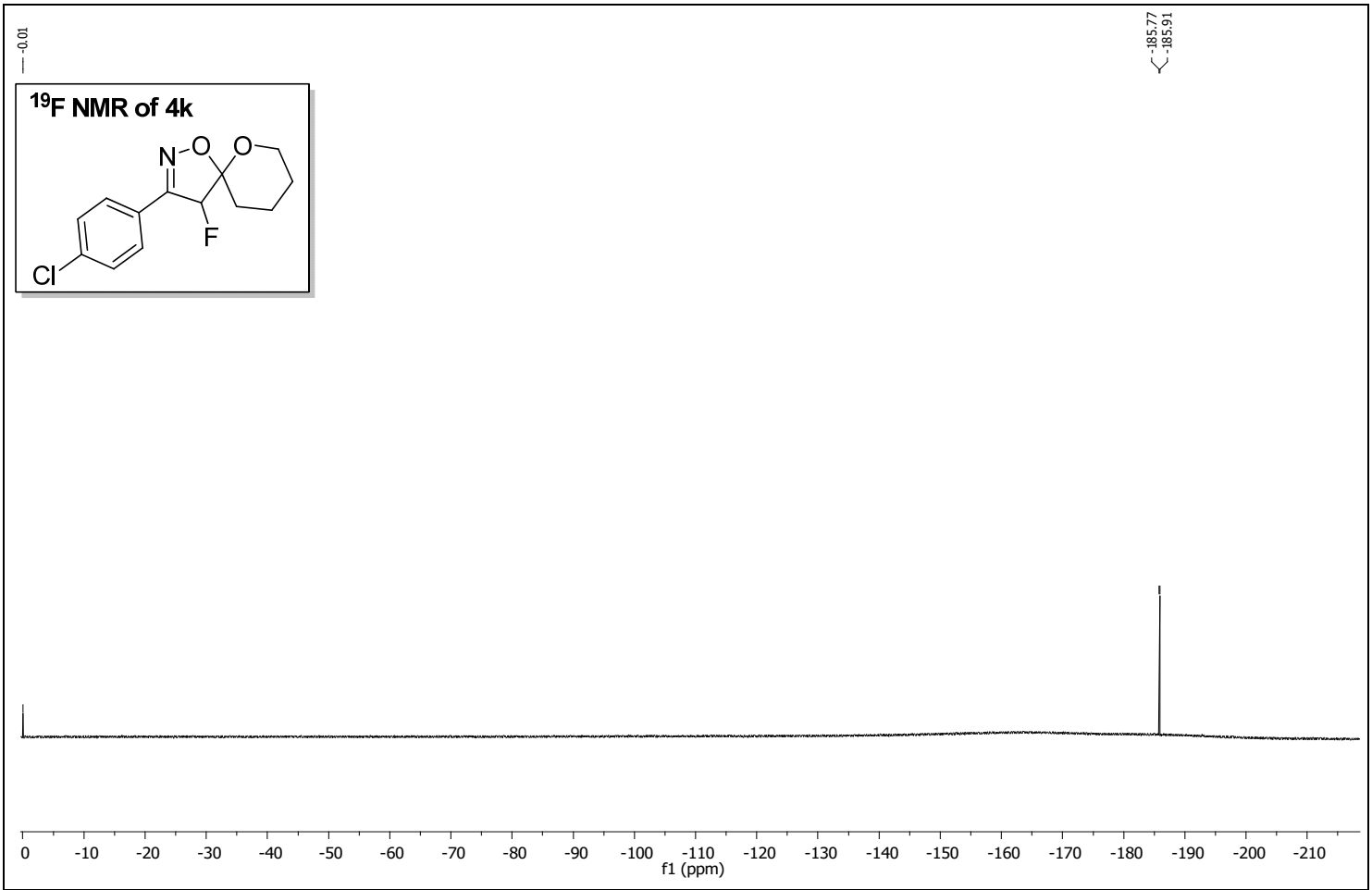

0.00
-201.74
-201.88
19F NMR of 4i'
N
O
O
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

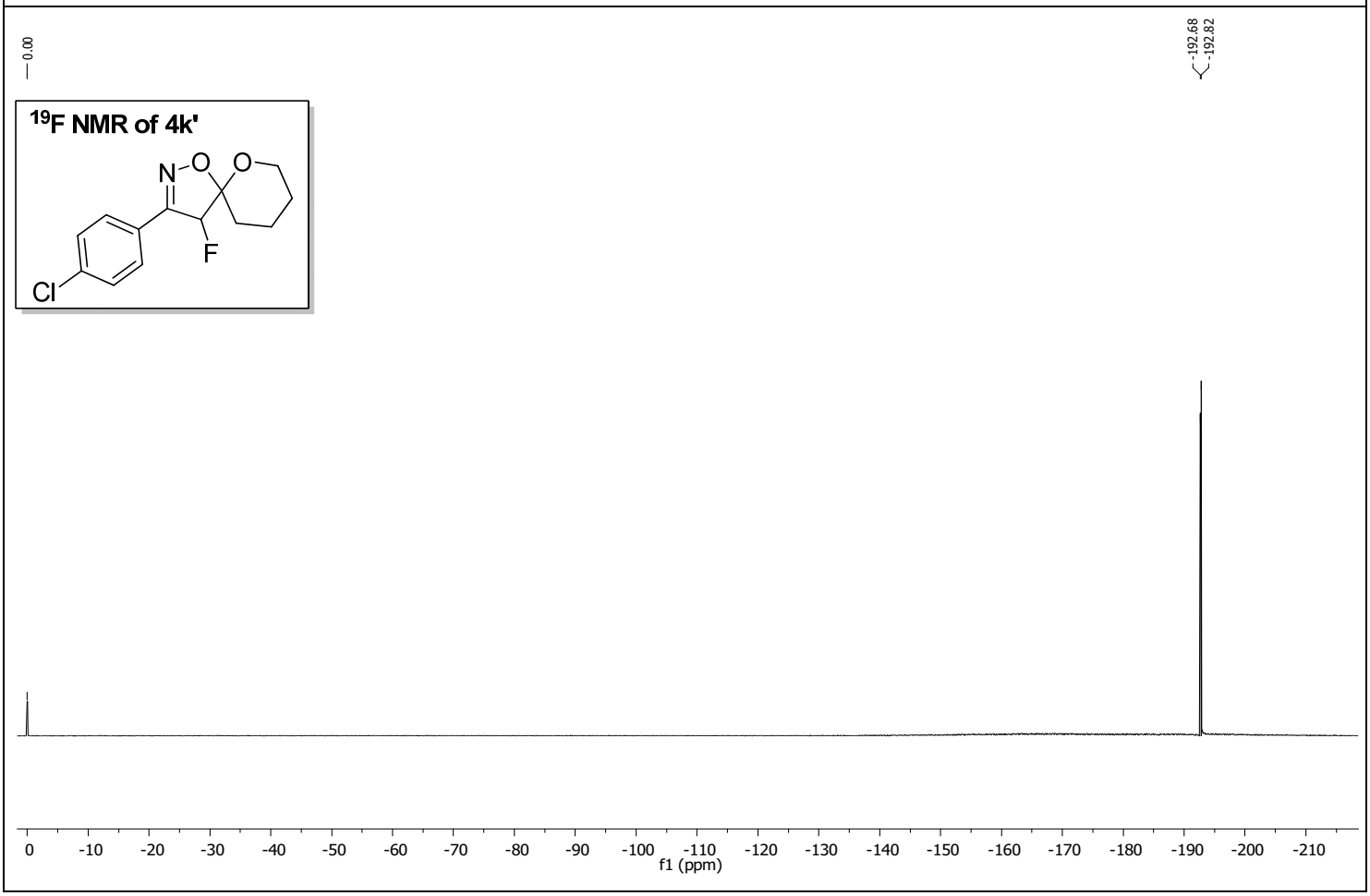

1H/13C NMR of 4j/4j"
N
O
O
F
F
f1 (ppm)
f1 (ppm)


0.00
-109.04
-109.05
-109.06
-109.06
-109.07
-109.08
-109.09
-109.09
-109.11
-185.94
-186.08
19F NMR of 4j
N
O
O
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

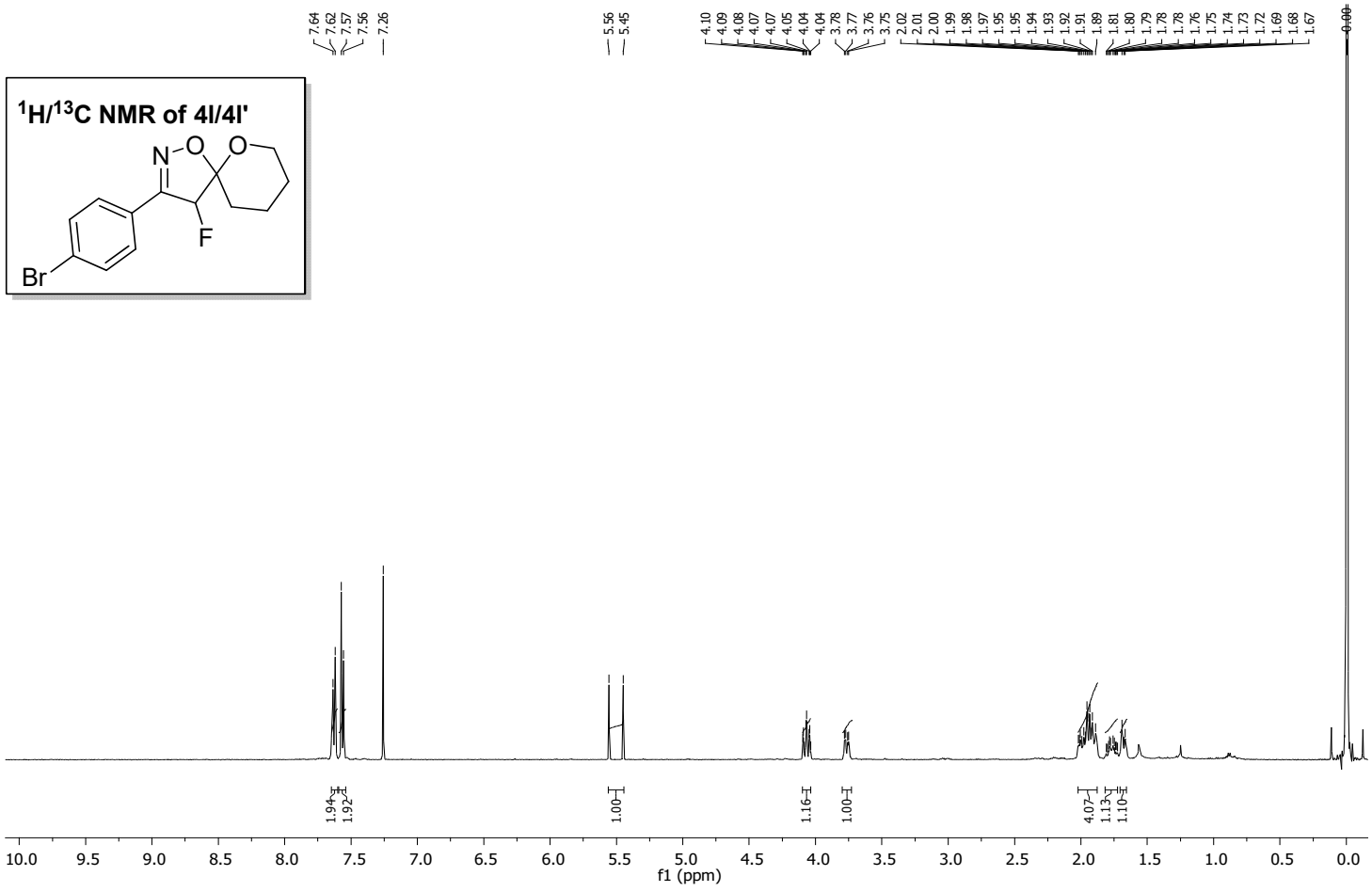

0.00
-112.23
-112.24
-112.25
-112.26
-112.26
-112.27
-112.28
-112.29
-112.30
-206.10
-206.24
19F NMR of 4j'
N
O
O
F
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

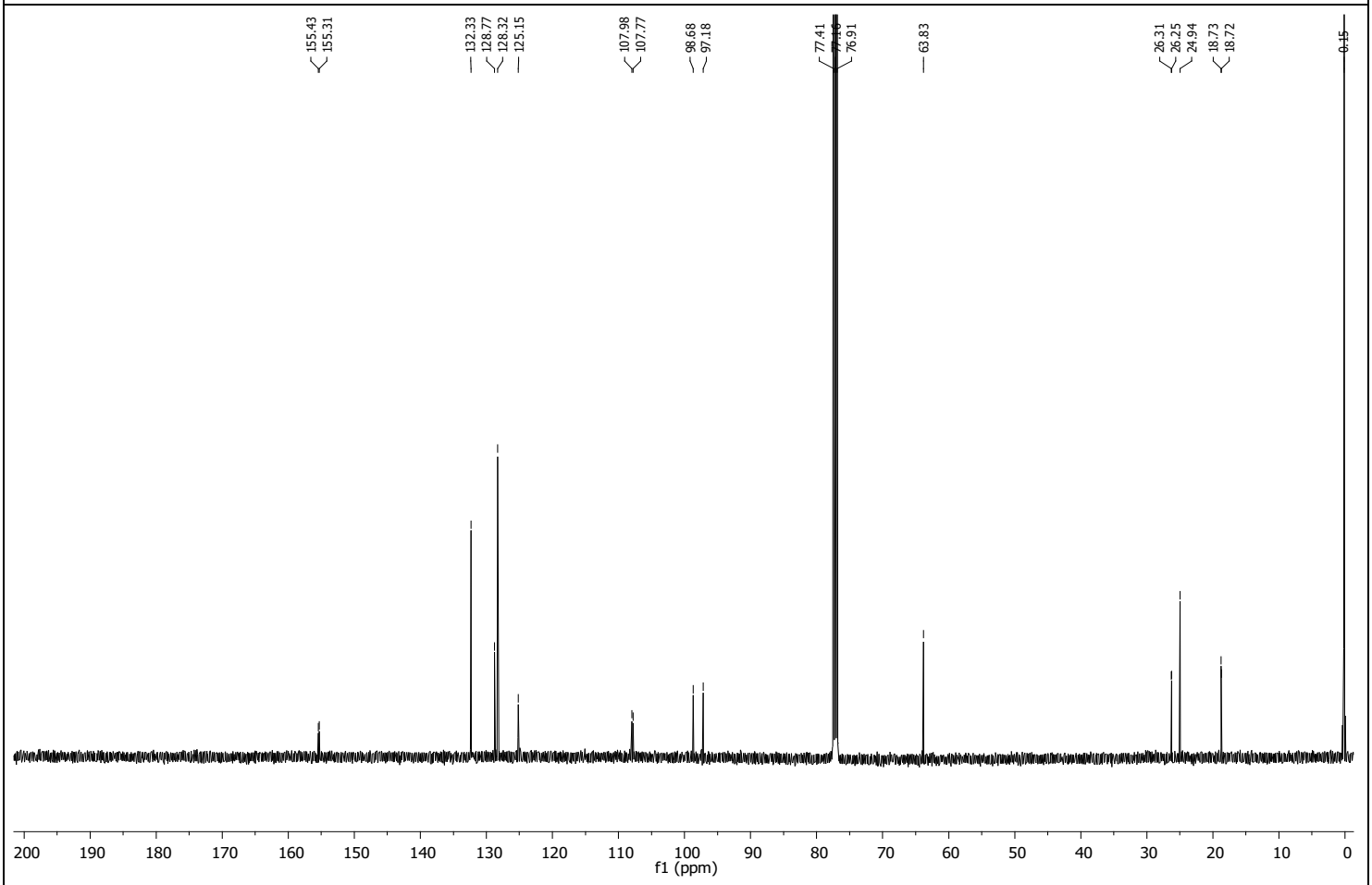

$^{1}H/^{13}C$ NMR of 4k/4k'
N
O
O
F
Cl
7.71
7.69
7.42
7.40
7.26
5.56
5.45
4.10
4.09
4.07
4.07
4.05
4.05
3.78
3.77
3.76
3.75
2.02
2.01
2.01
1.99
1.98
1.98
1.97
1.96
1.95
1.93
1.91
1.89
1.82
1.81
1.80
1.79
1.79
1.78
1.76
1.75
1.74
1.74
1.73
1.69
1.67
2.07
2.00
1.10
1.08
1.00
4.07
1.18
1.06
f1 (ppm)
155.16
155.04
136.63
129.21
127.96
126.38
107.78
107.57
98.58
97.07
77.24
76.73
63.66
26.15
26.10
24.78
18.57
18.55
0.02
f1 (ppm)

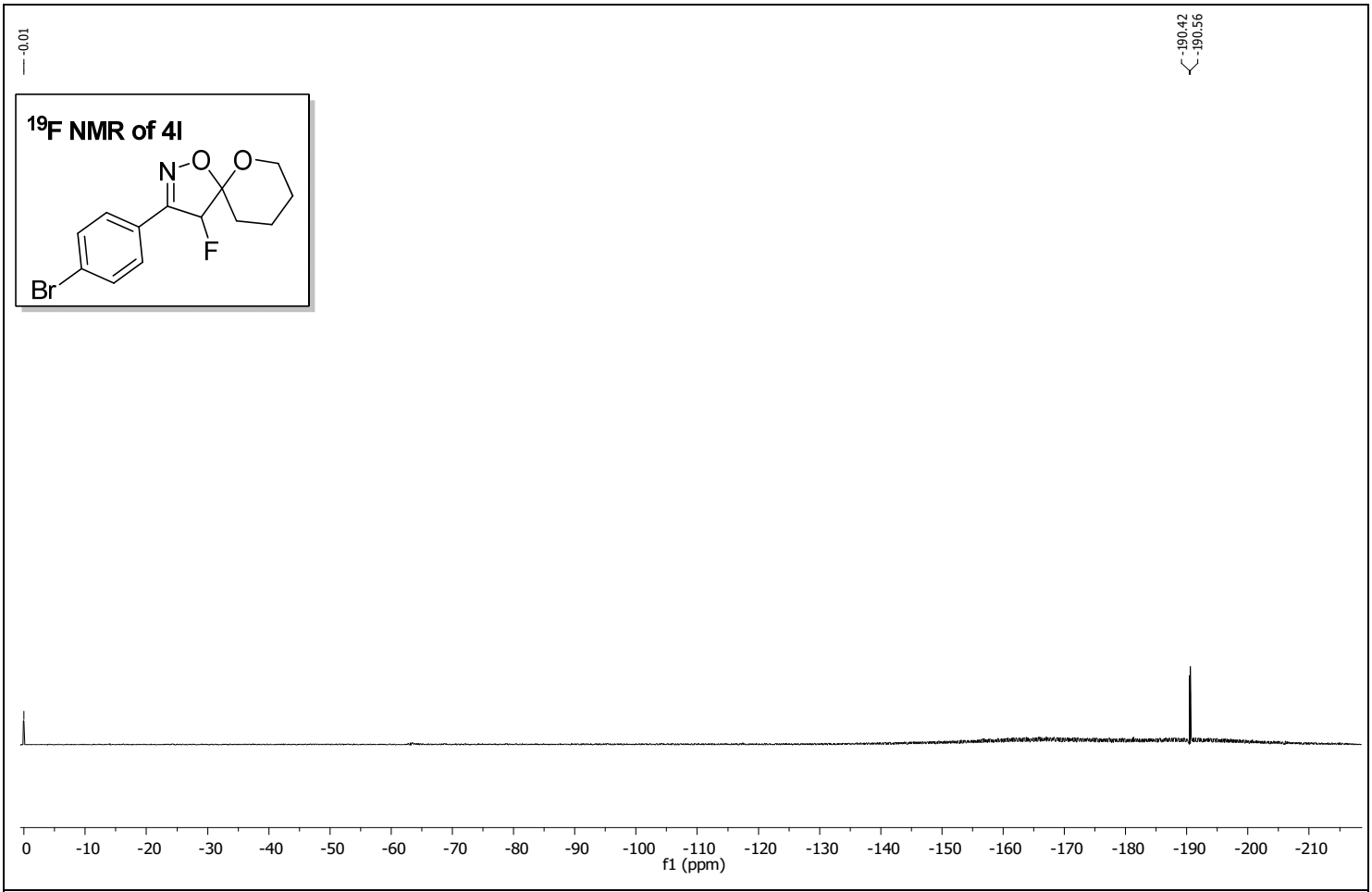

-0.01
-185.77
-185.91
19F NMR of 4k
N
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

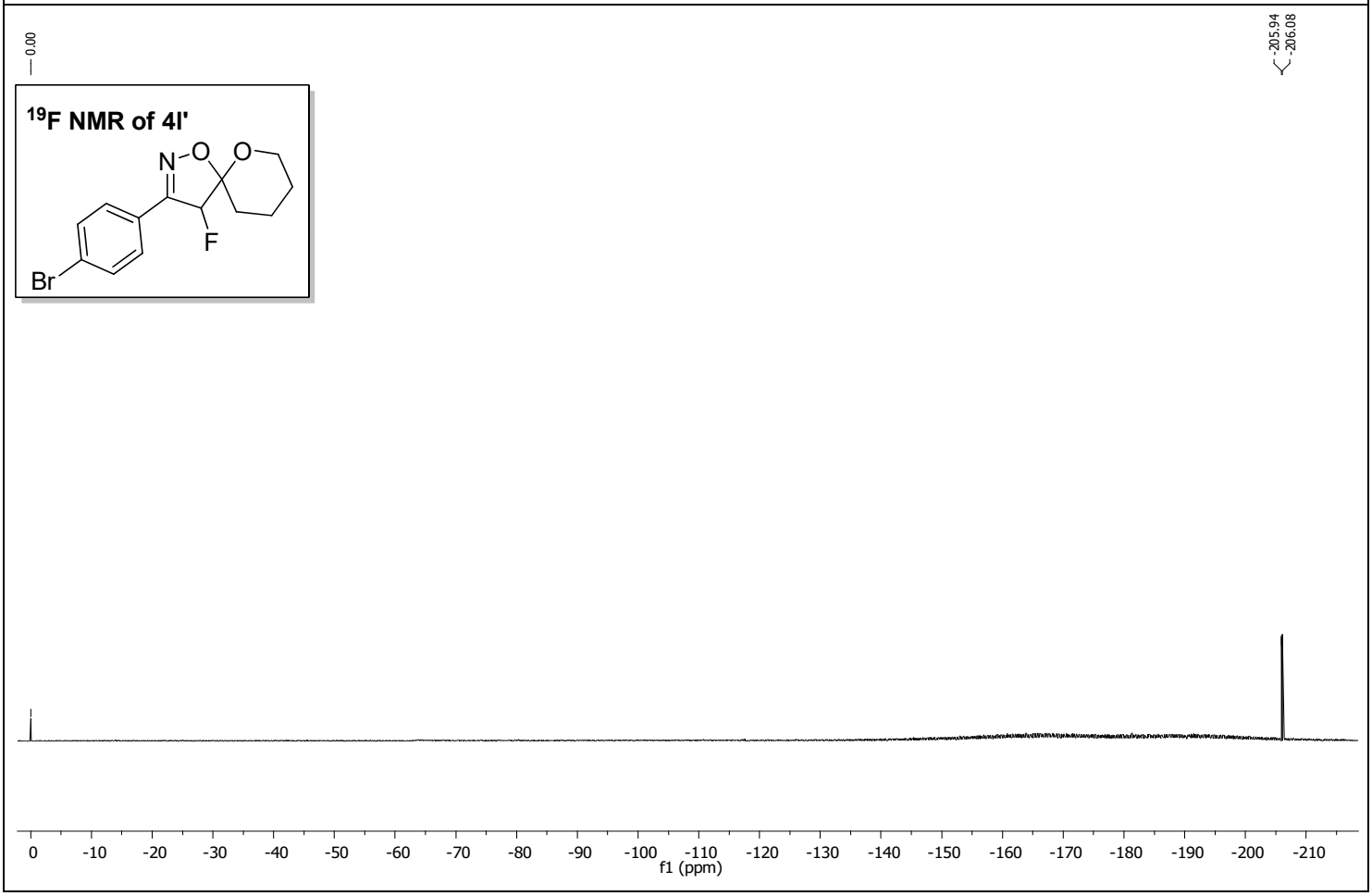

0.00
-192.68
-192.82
19F NMR of 4k'
N
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

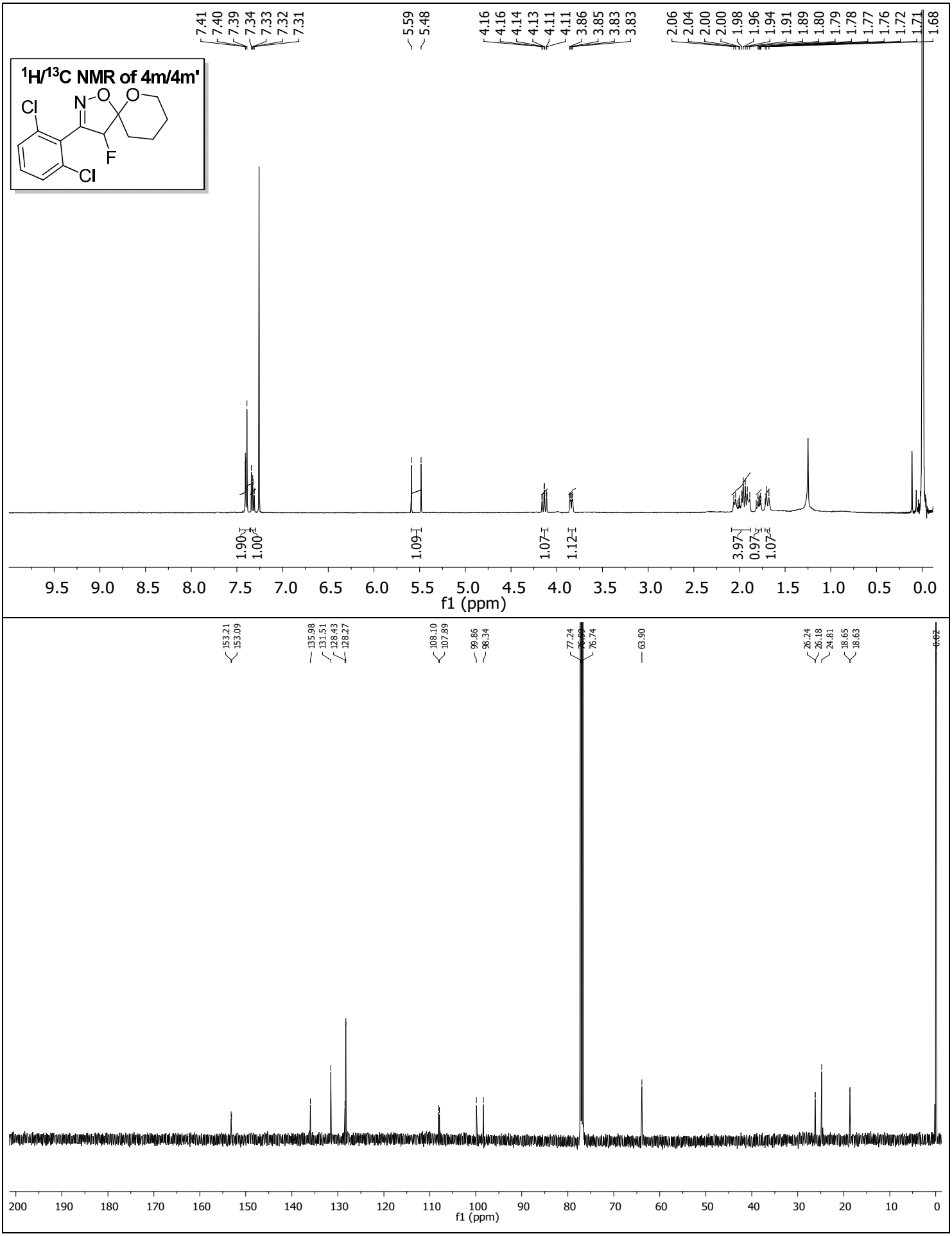
$^{1}H/^{13}C$ NMR of 4l/4l'

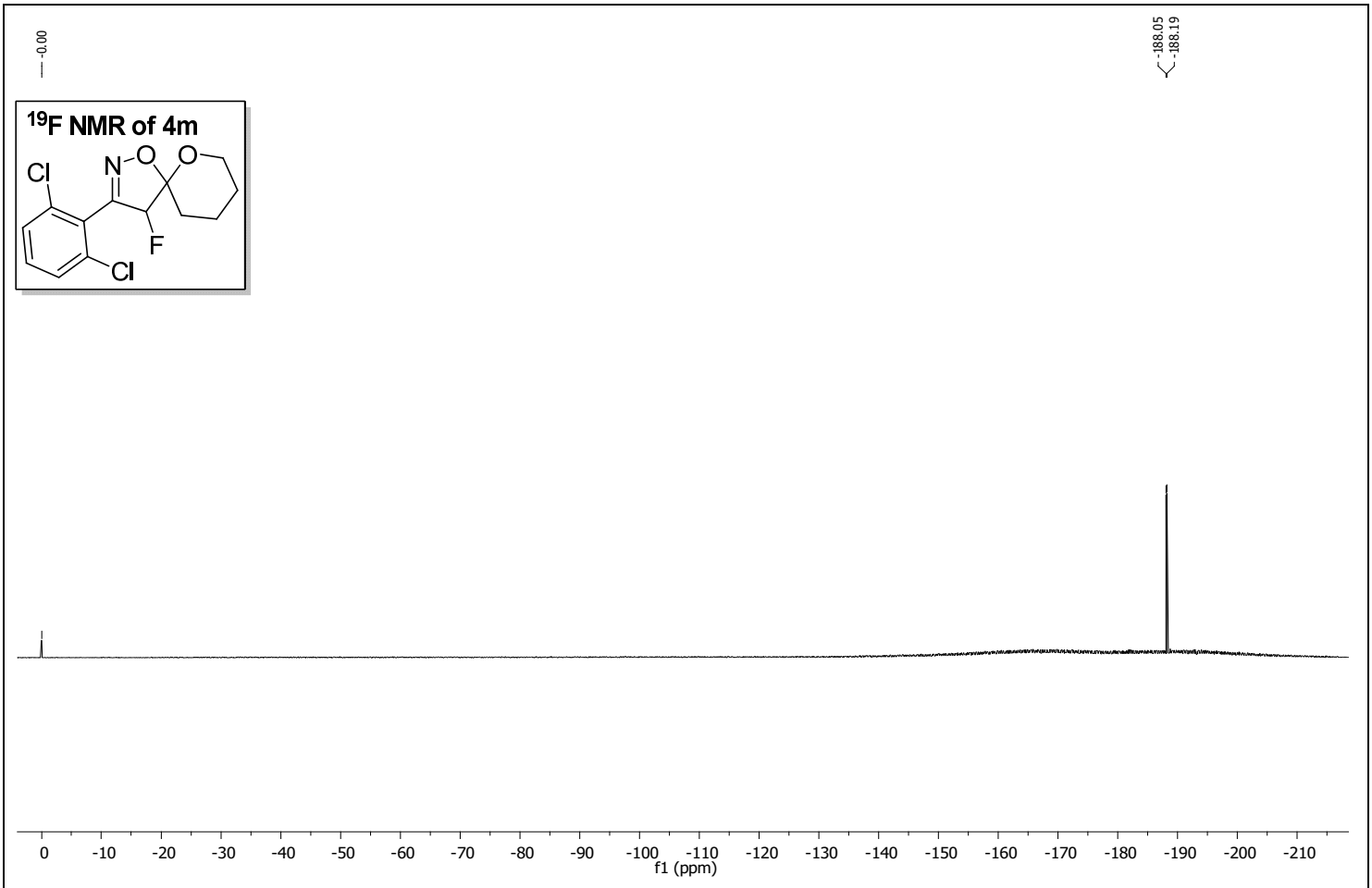


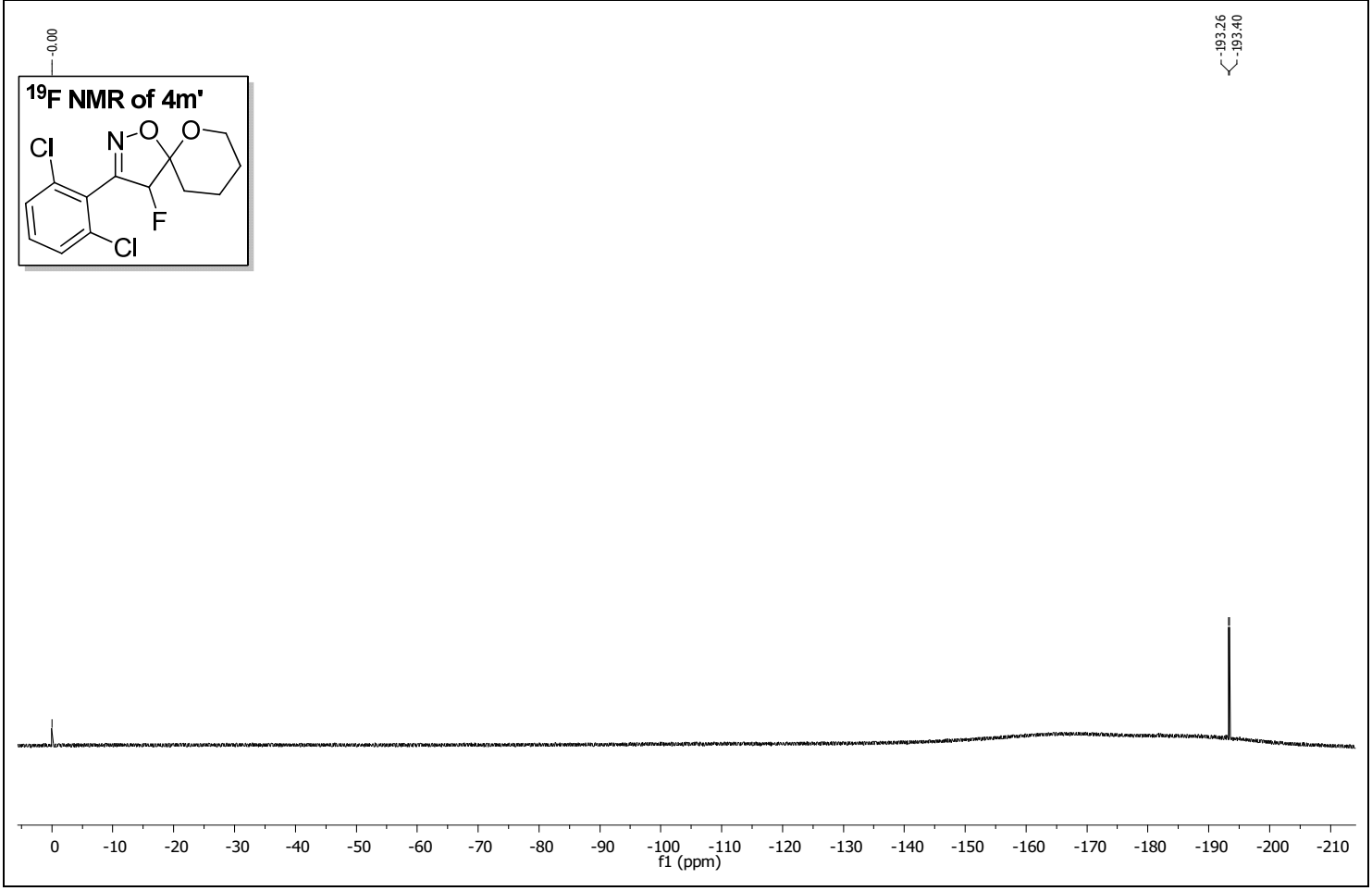


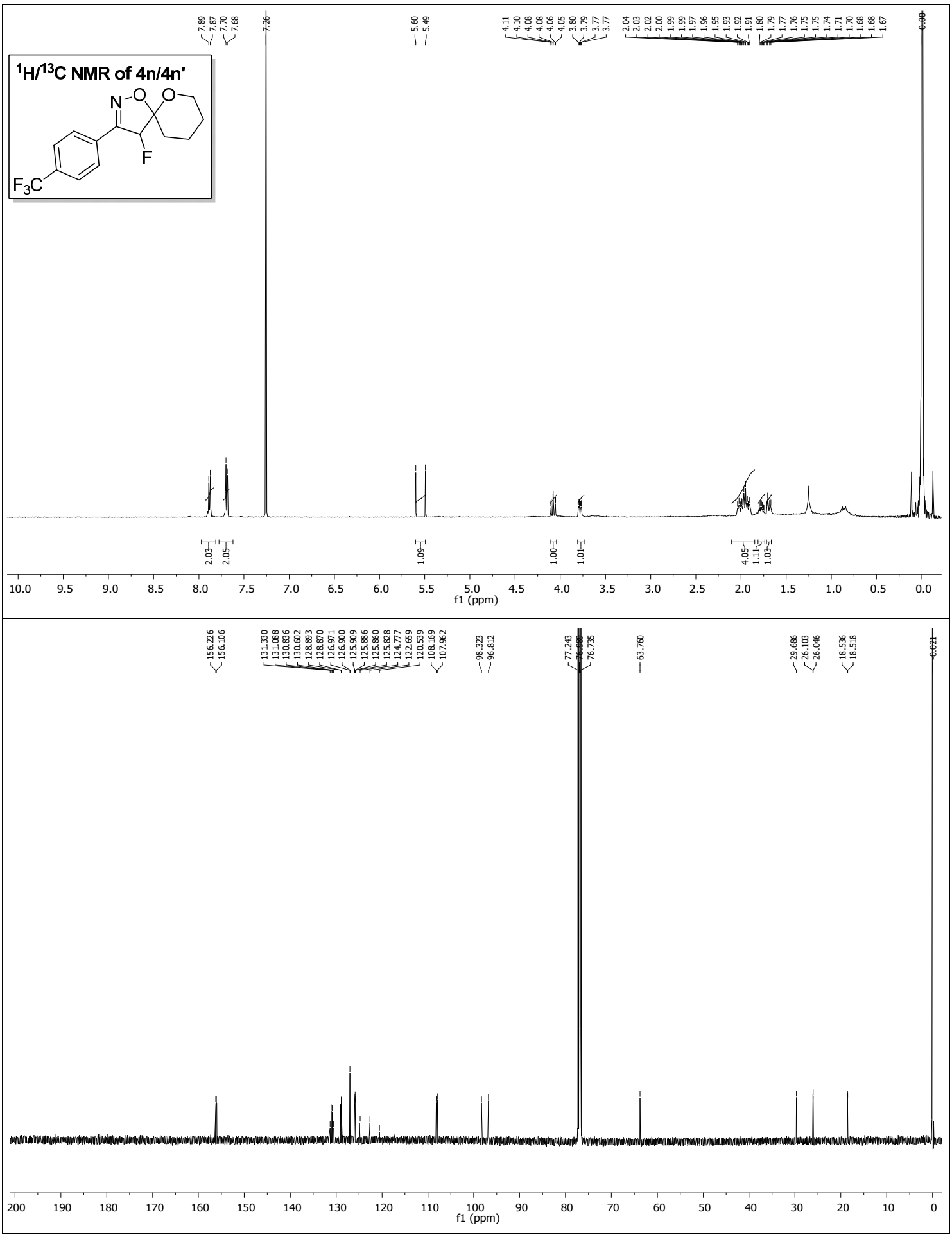

-0.01
-190.42
-190.56
19F NMR of 4l
N
O
O
F
Br
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

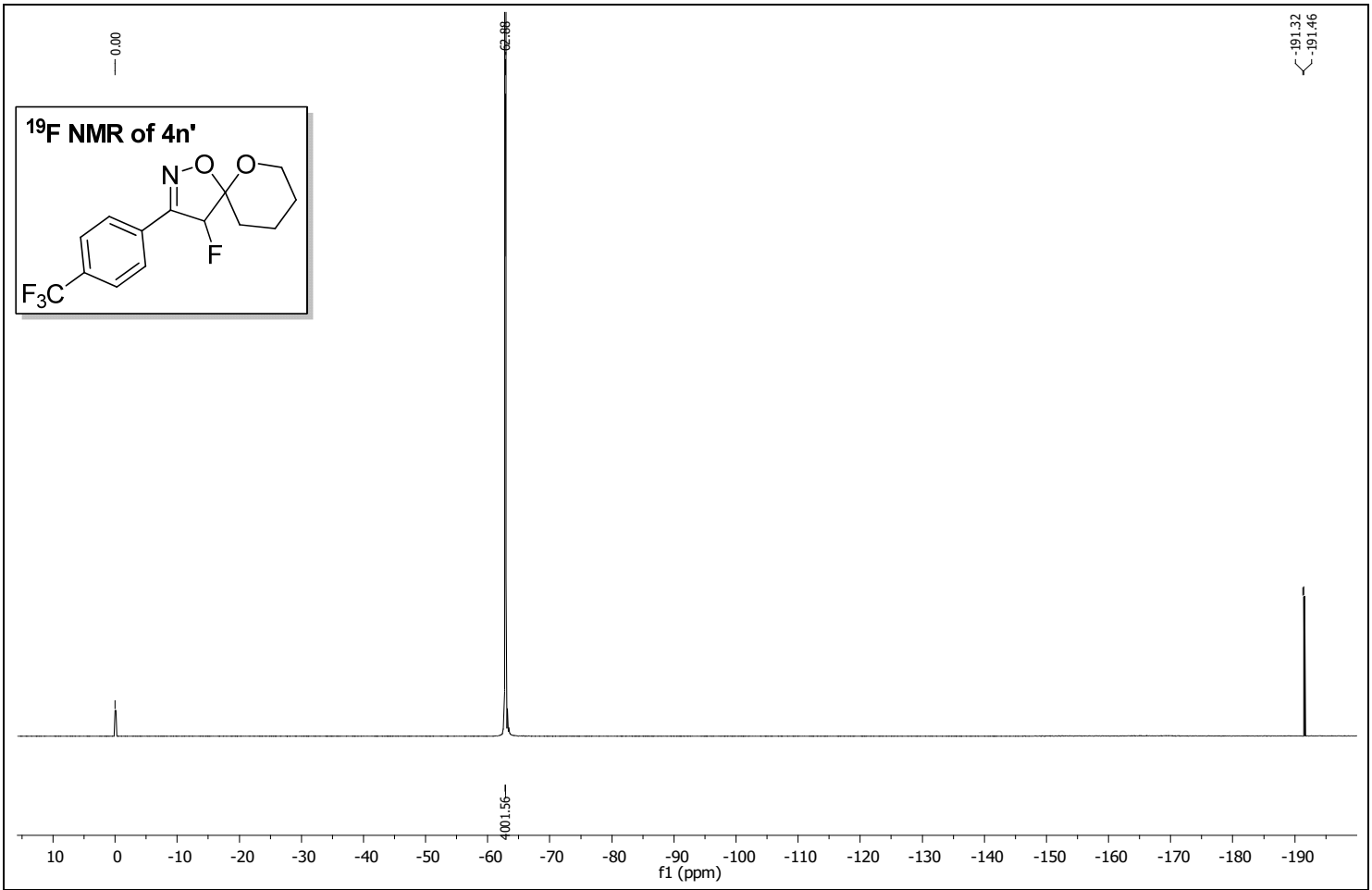

0.00
-205.94
-206.08
19F NMR of 4l'
N
O
O
F
Br
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

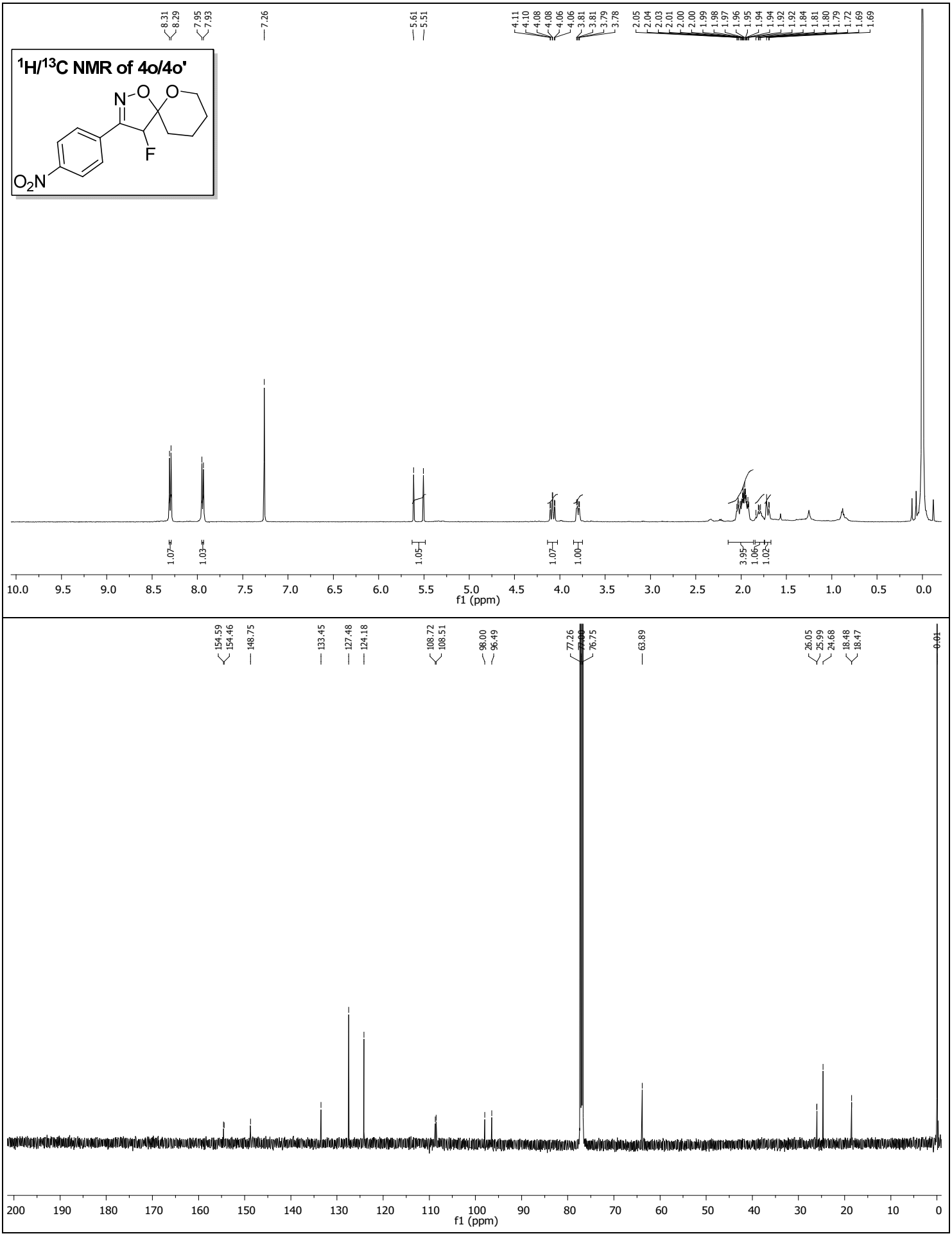

$^{1}H/^{13}C$ NMR of 4m/4m'
Cl
N
O
O
F
Cl
7.41 7.40 7.39 7.34 7.33 7.32 7.31
5.59 5.48
4.16 4.16 4.14 4.13 4.11 4.11
3.86 3.85 3.83 3.83
2.06 2.04 2.00 2.00 1.98 1.96 1.94 1.91 1.89 1.80 1.79 1.78 1.77 1.76 1.72 1.71 1.68
1.90 1.00 1.09 1.07 1.12 3.97 0.97 1.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
153.21 153.09
135.98 131.51 128.43 128.27
108.10 107.89
99.86 98.34
77.24 76.74
63.90
26.24 26.18 24.81
18.65 18.63
0.02
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

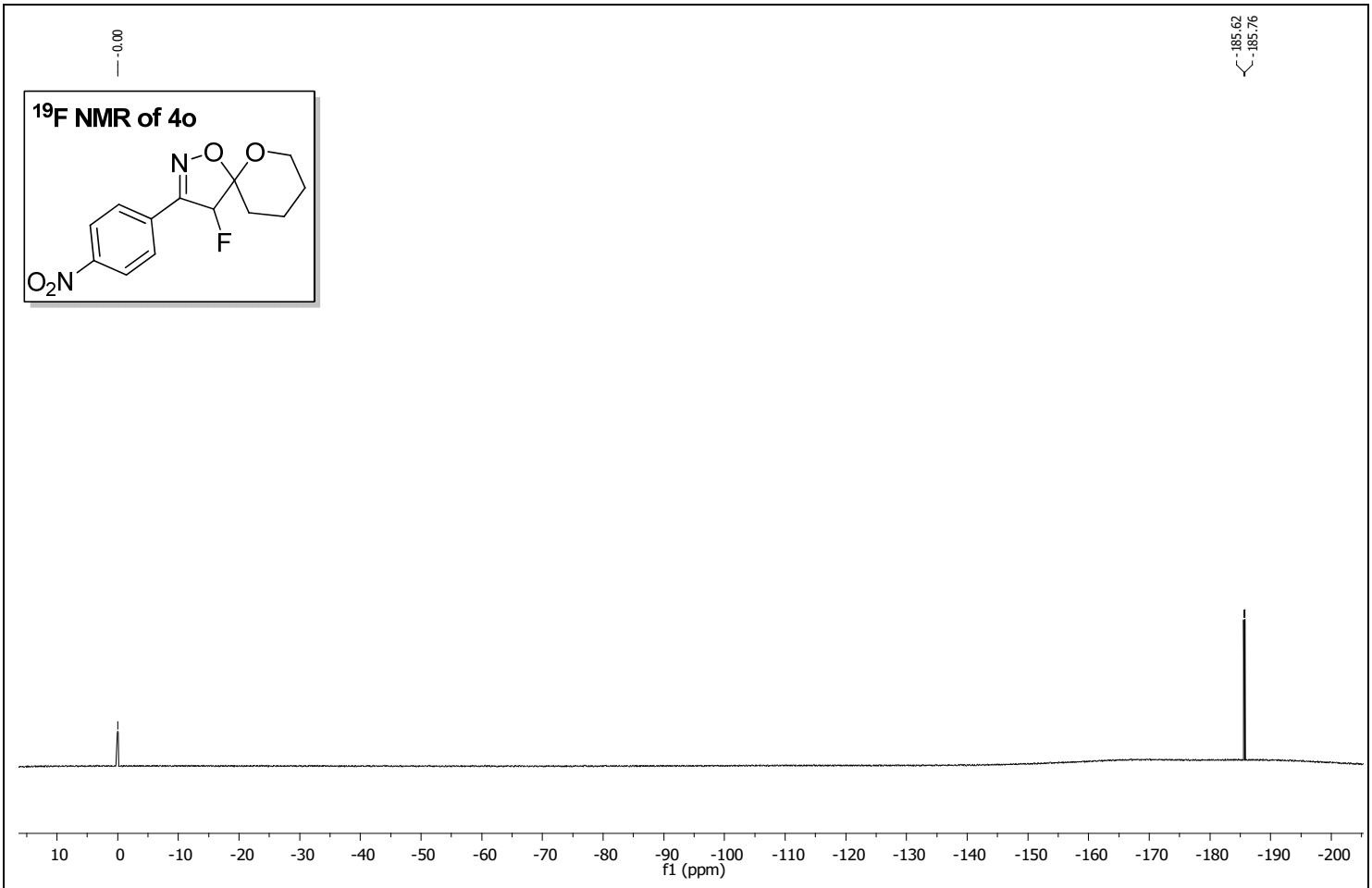

-0.00
-188.05
-188.19
19F NMR of 4m
Cl
N
O
O
F
Cl
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

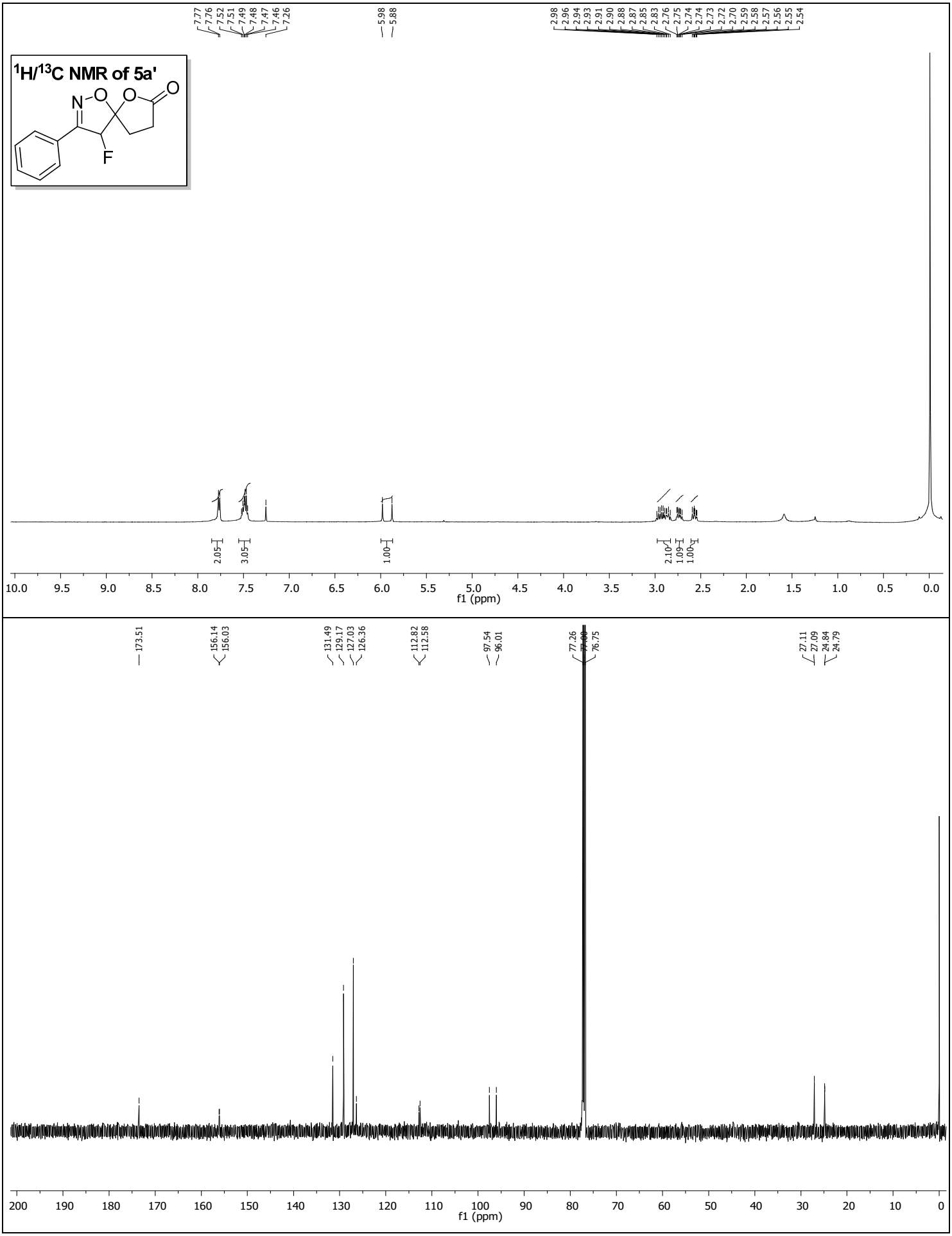

-0.00
-193.26
-193.40
19F NMR of 4m'
Cl
N
O
O
F
Cl
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


^{1}H/^{13}C NMR of 4n/4n'
N
O
O
F
F_3C
f1 (ppm)
f1 (ppm)

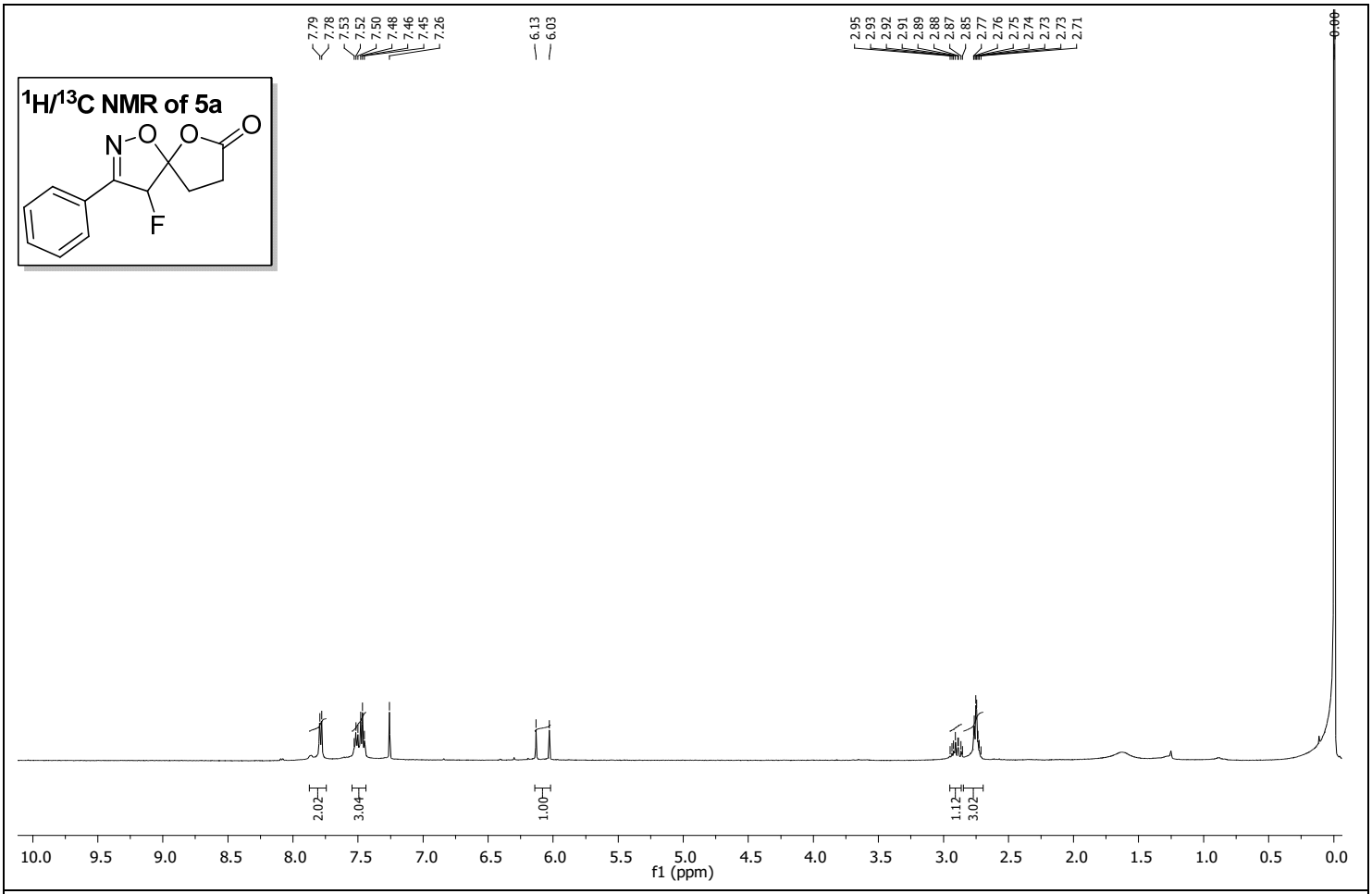

0.00
-62.88
-191.32
-191.46
19F NMR of 4n'
N
O
O
F
F3C
4001.56
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

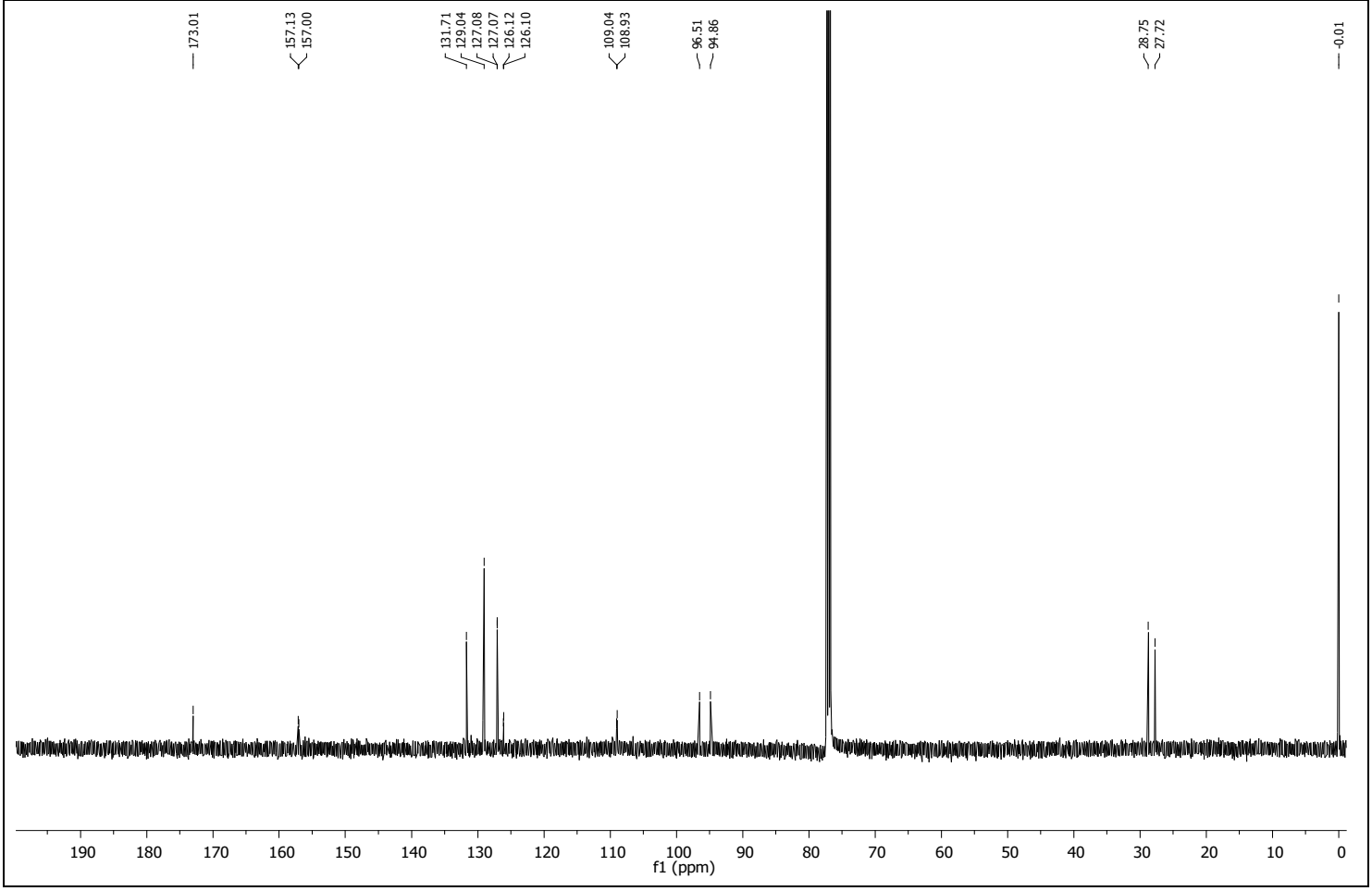

1H/13C NMR of 4o/4o'
f1 (ppm)
f1 (ppm)

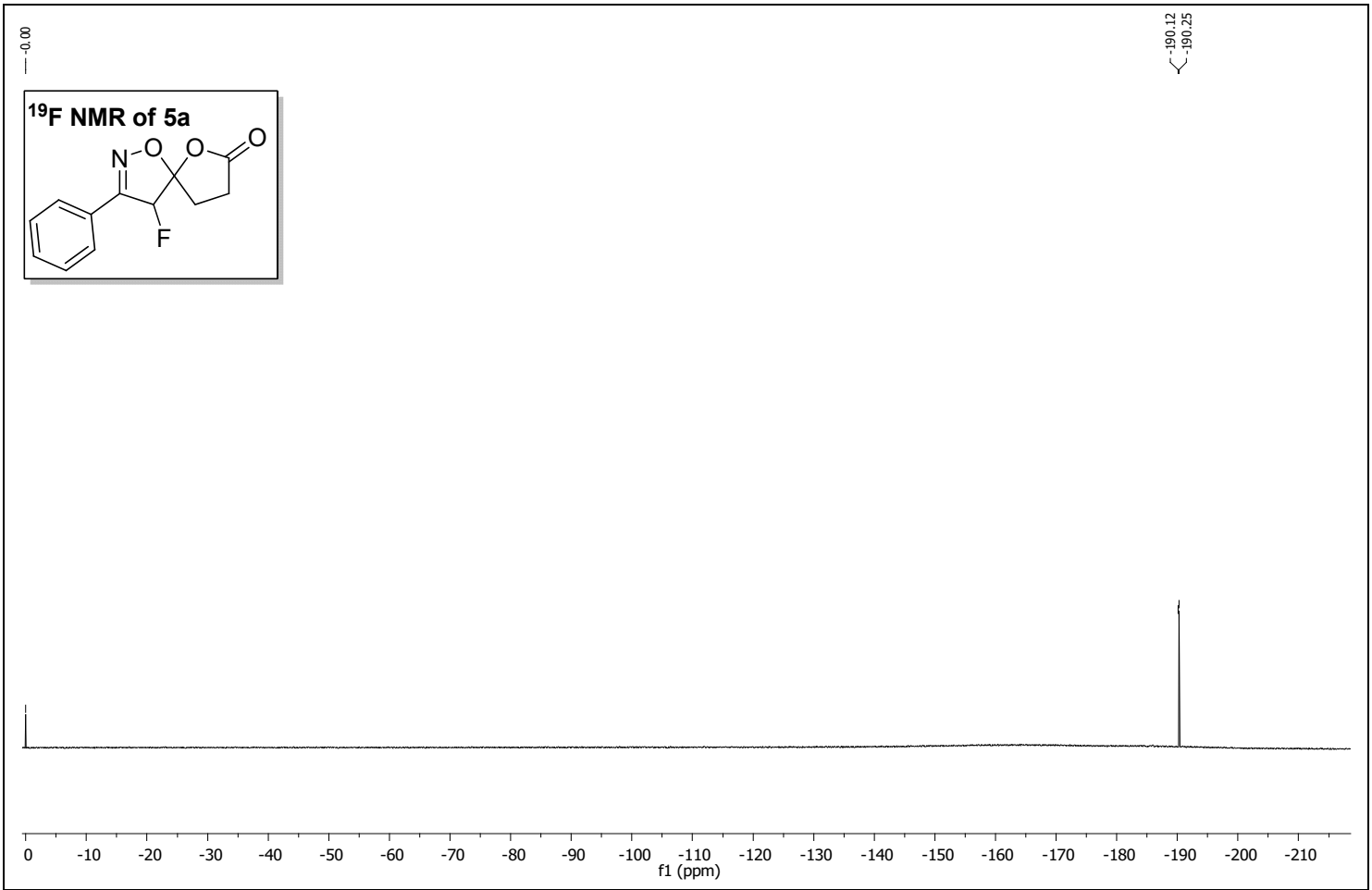

-0.00
-185.62
-185.76
19F NMR of 4o
N
O
O
F
O2N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

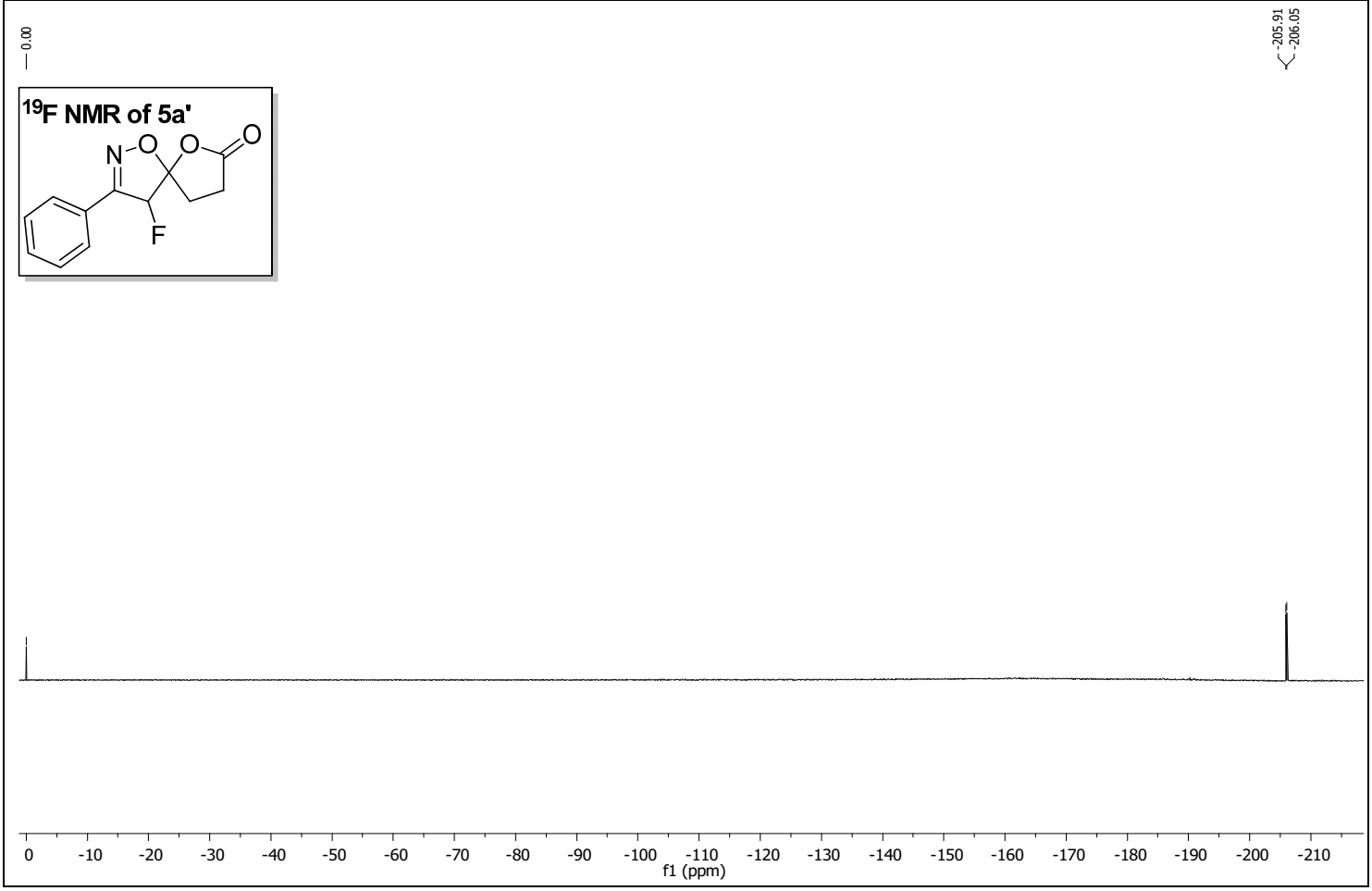

1H/13C NMR of 5a'
N
O
O
O
F
7.77
7.76
7.52
7.51
7.49
7.48
7.47
7.46
7.26
5.98
5.88
2.98
2.96
2.94
2.93
2.91
2.90
2.88
2.87
2.85
2.83
2.76
2.75
2.74
2.74
2.73
2.72
2.70
2.59
2.58
2.57
2.56
2.55
2.54
2.05
3.05
1.00
2.10
1.09
1.00
f1 (ppm)
173.51
156.14
156.03
131.49
129.17
127.03
126.36
112.82
112.58
97.54
96.01
77.26
77.00
76.75
27.11
27.09
24.84
24.79
f1 (ppm)

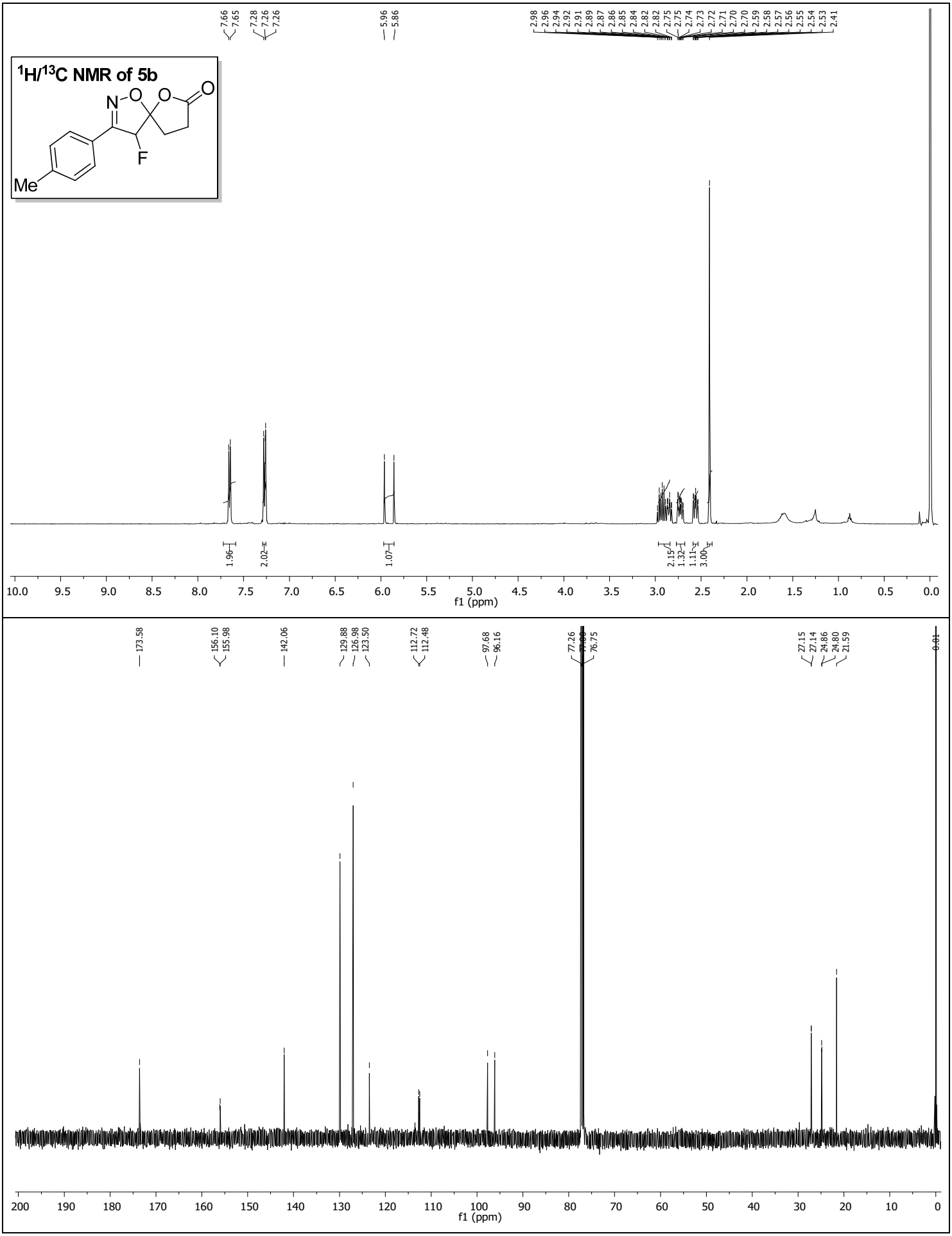
$^{1}H/^{13}C$ NMR of 5a

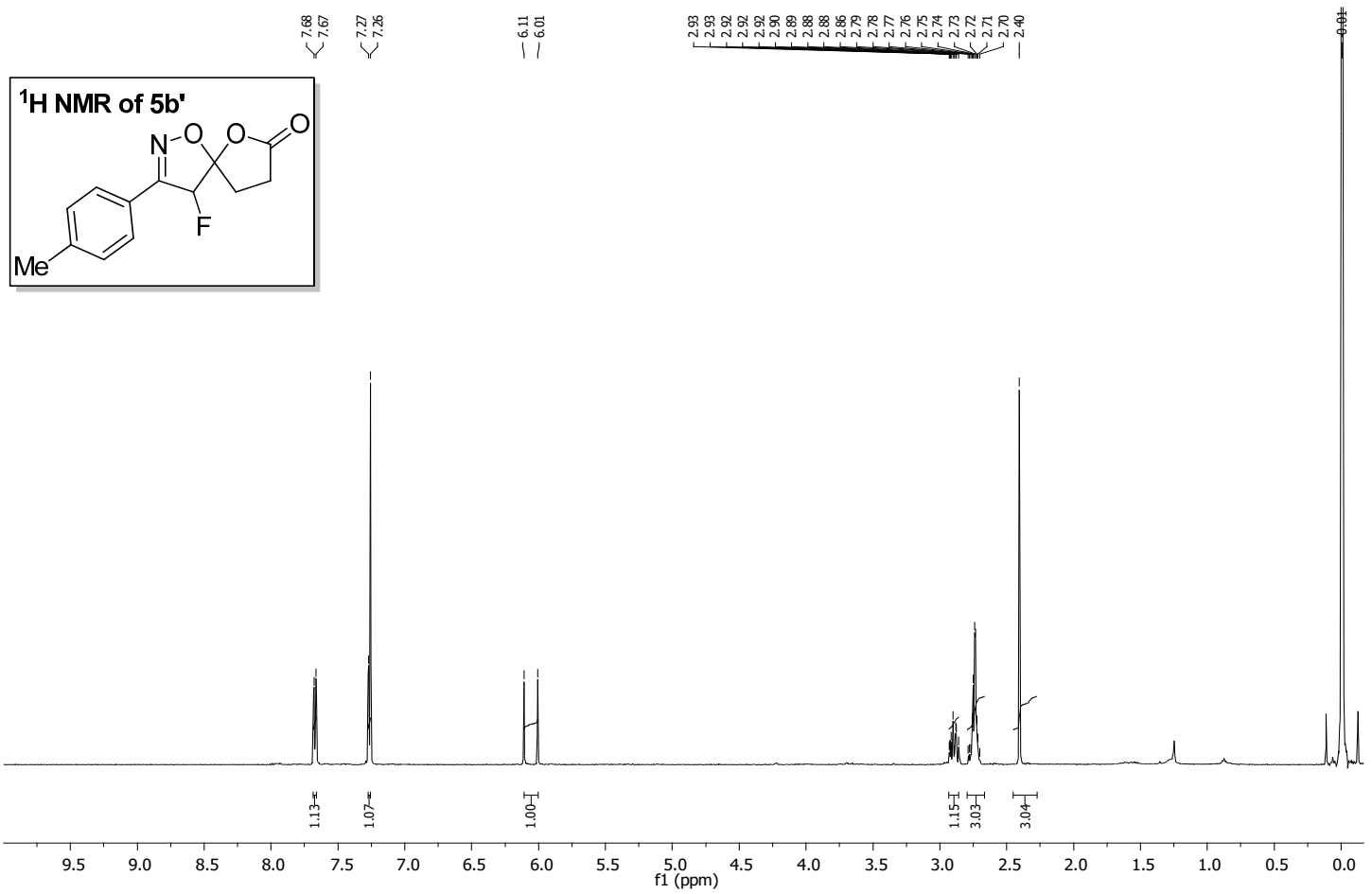


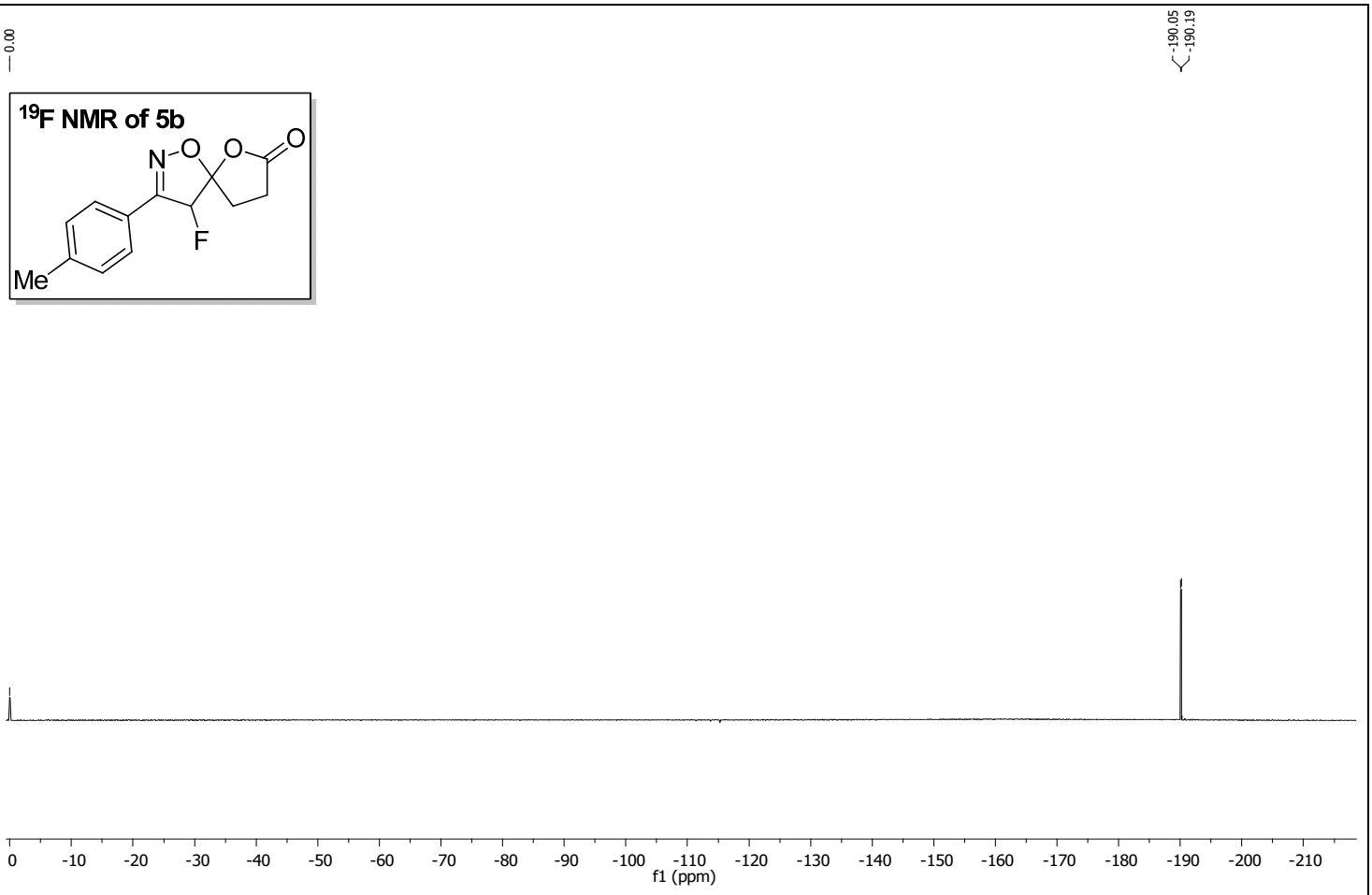


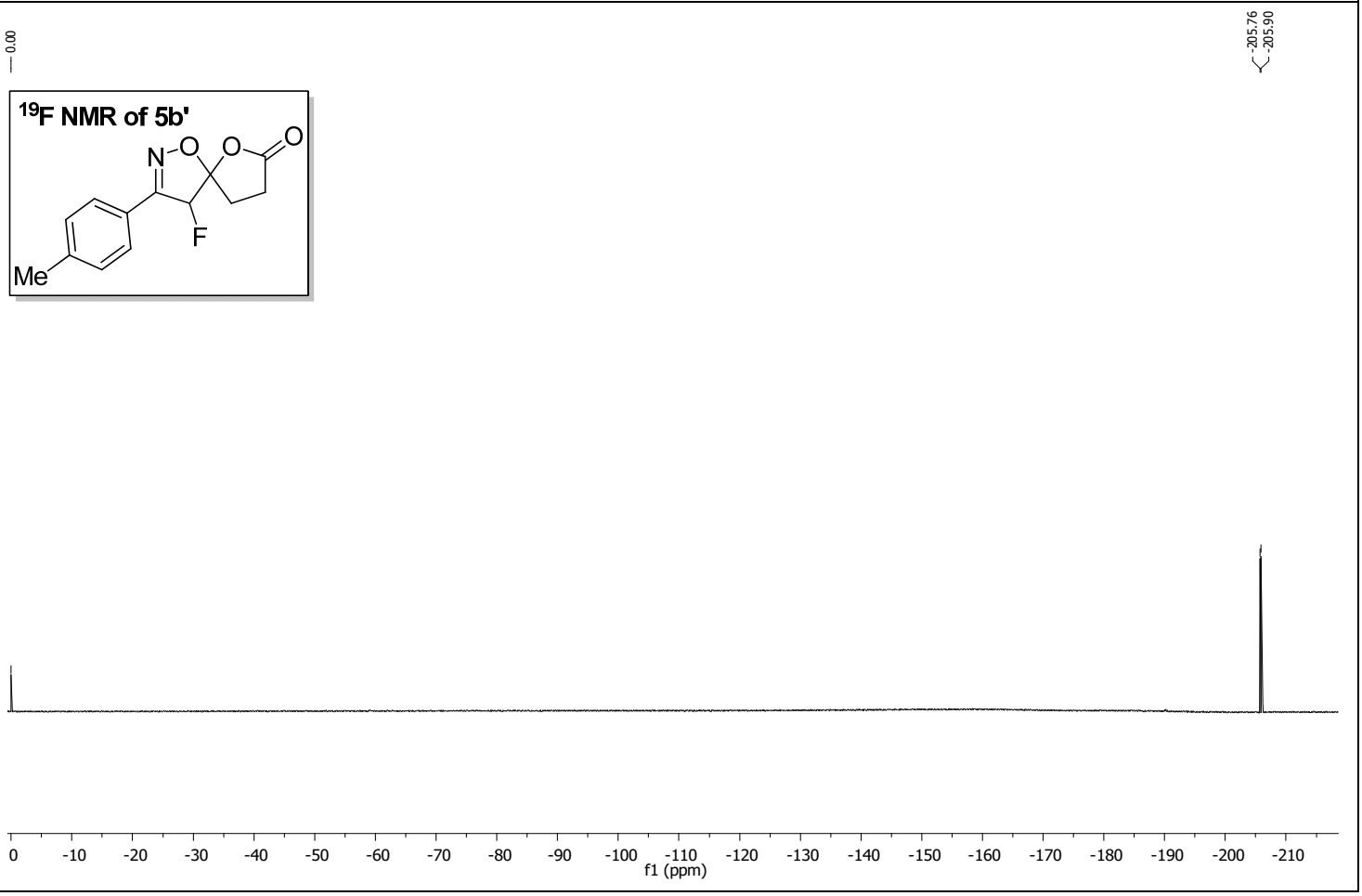

-0.00
-190.12
-190.25
19F NMR of 5a
N
O
O
O
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

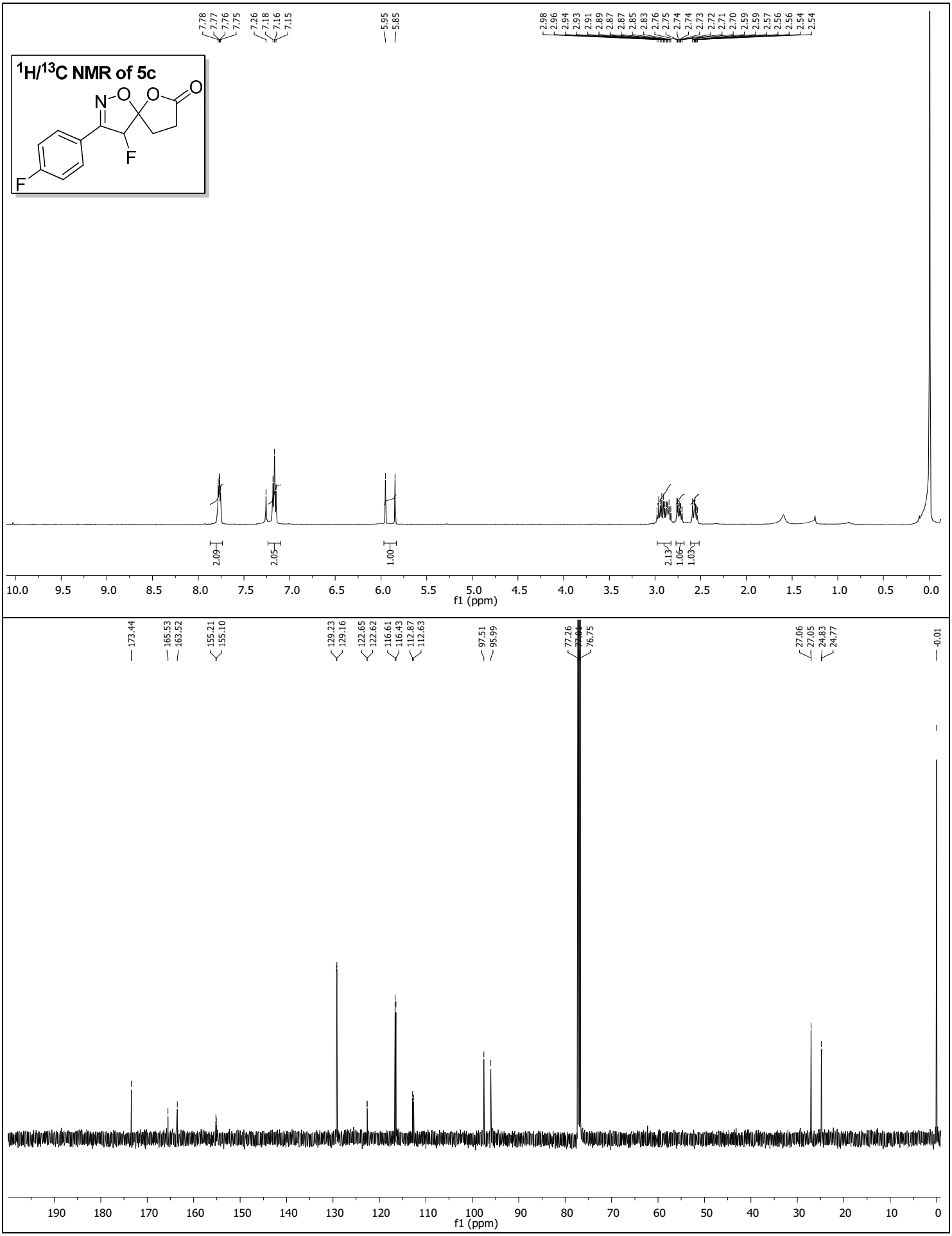

-0.00
-205.91
-206.05
19F NMR of 5a'
N
O
O
O
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

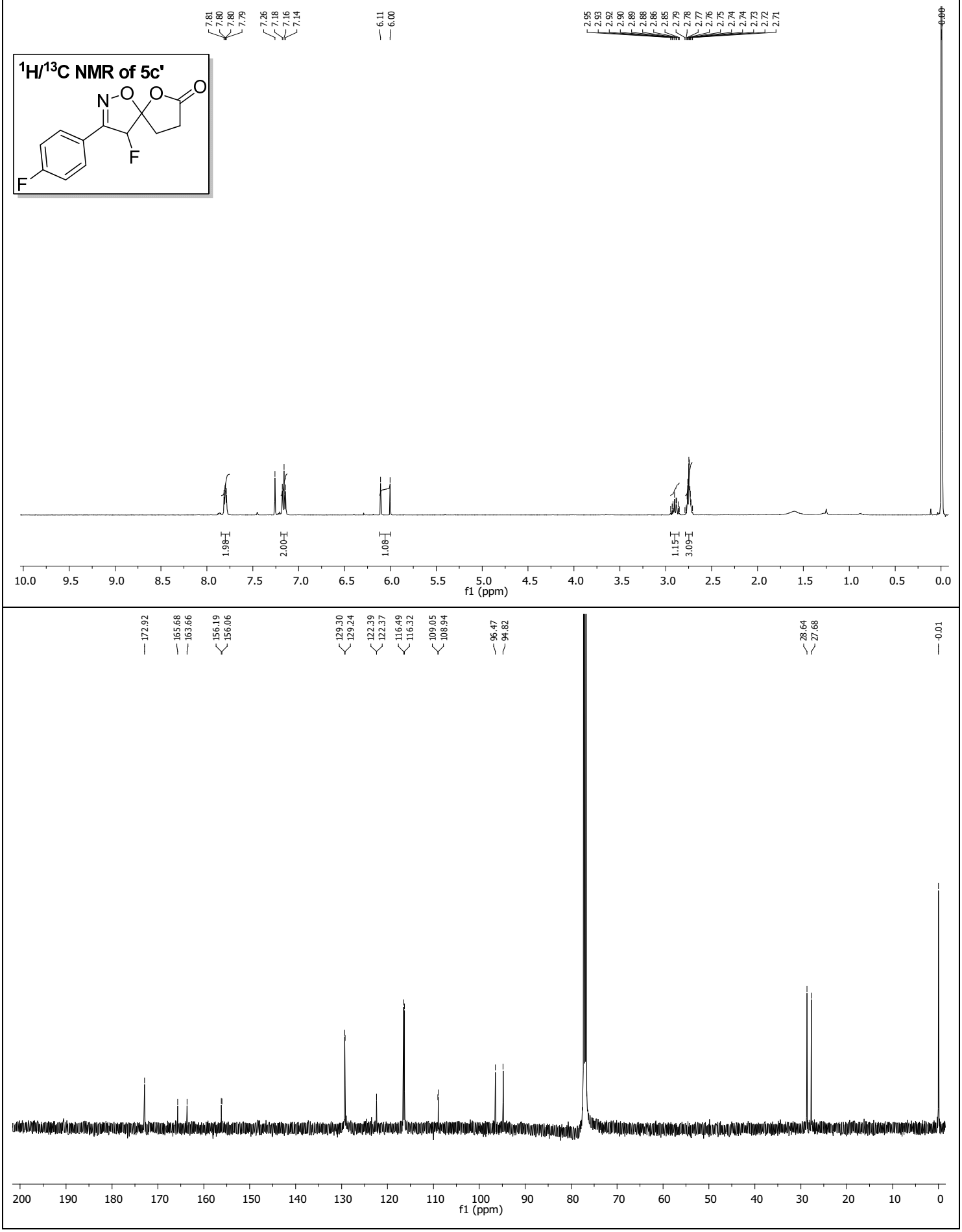

1H/13C NMR of 5b
Me
F
f1 (ppm)
f1 (ppm)

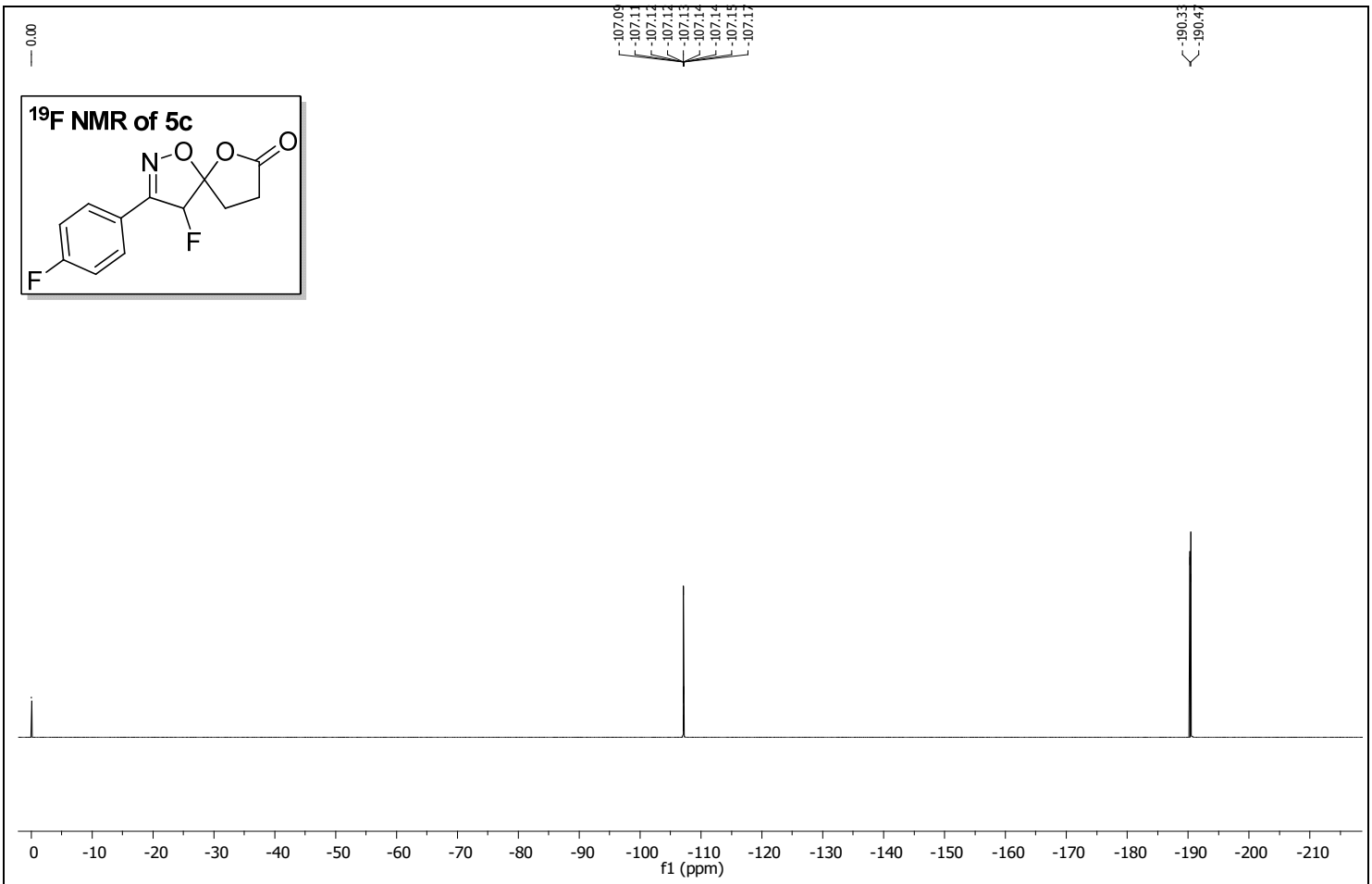

^{1}H NMR of 5b'
N
O
O
O
F
Me
7.68
7.67
7.27
7.26
6.11
6.01
2.93
2.93
2.92
2.92
2.92
2.90
2.89
2.88
2.88
2.86
2.79
2.78
2.77
2.76
2.75
2.74
2.73
2.72
2.71
2.70
2.40
0.01
1.13
1.07
1.00
1.15
3.03
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

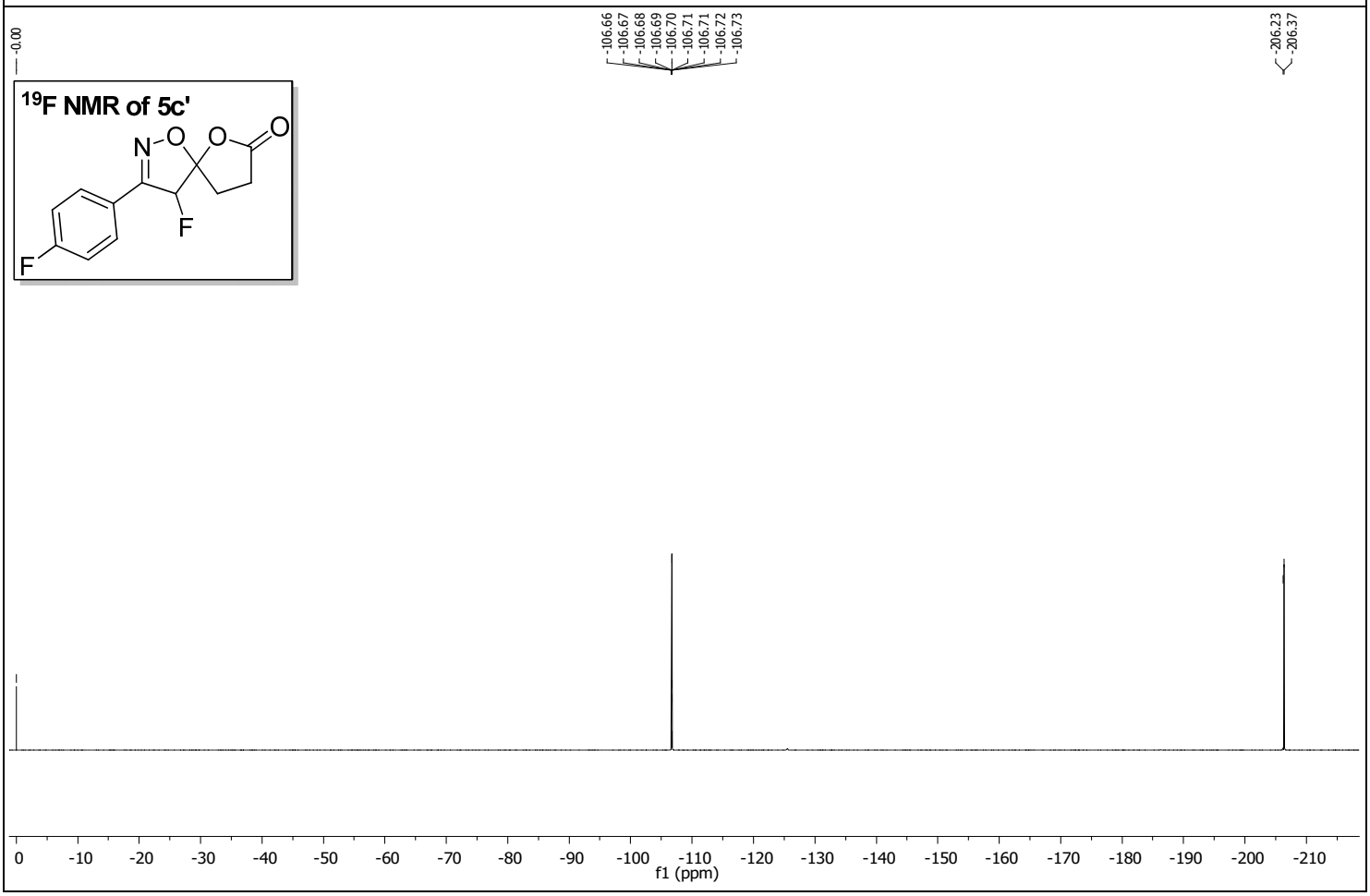

0.00
-190.05
-190.19
19F NMR of 5b
N
O
O
O
F
Me
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

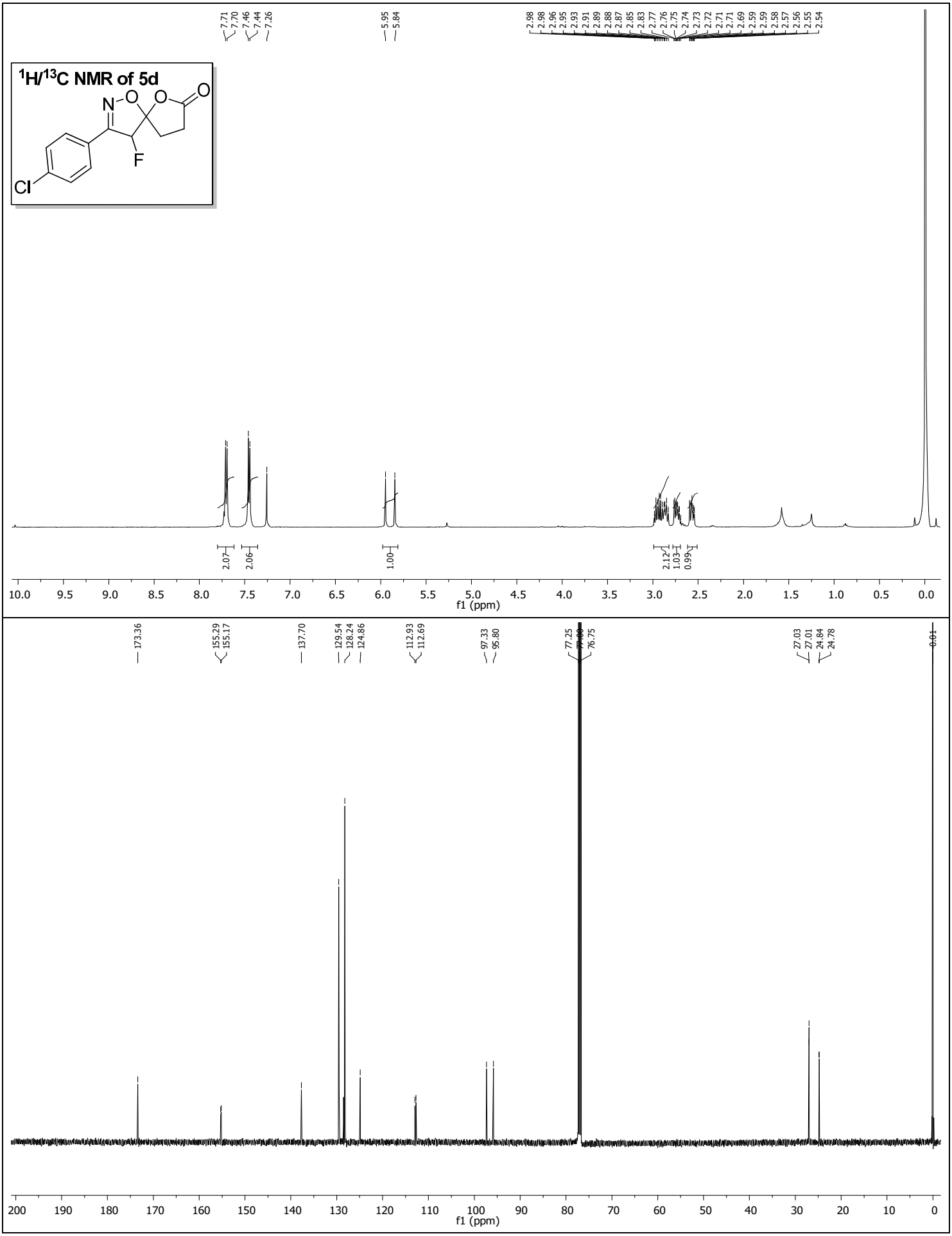

0.00
-205.76
-205.90
19F NMR of 5b'
N
O
O
O
F
Me
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

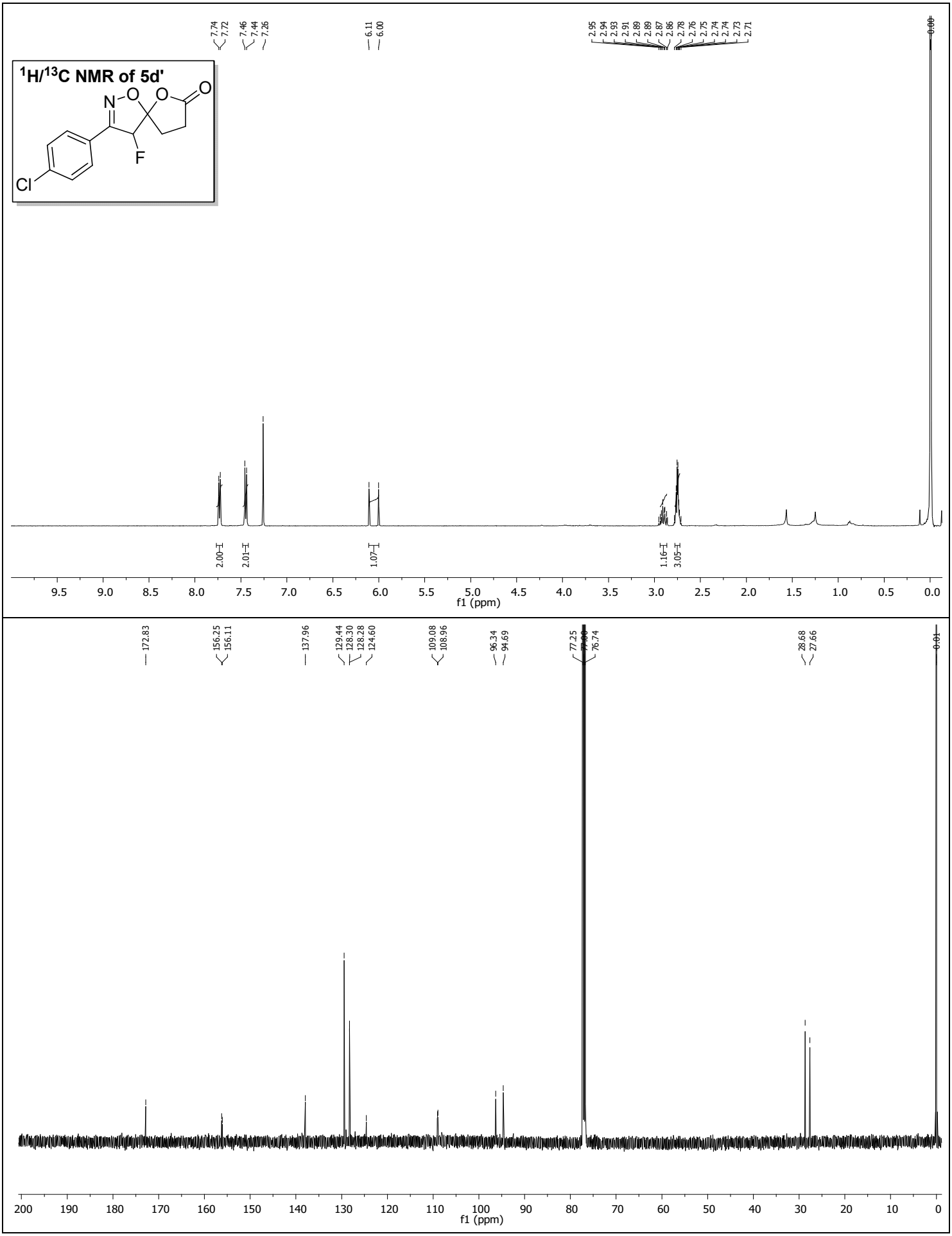

1H/13C NMR of 5c
f1 (ppm)
f1 (ppm)

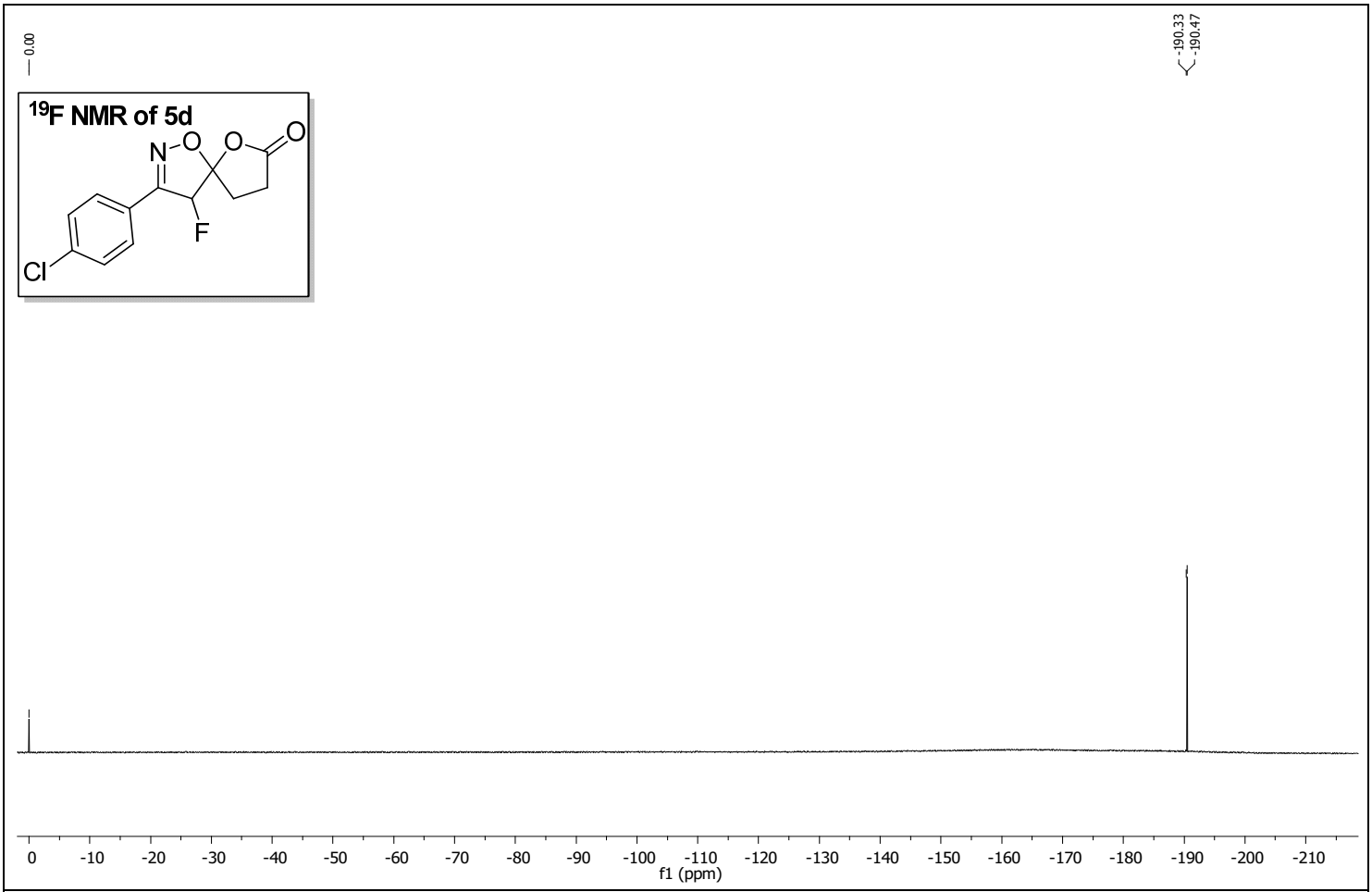

$^{1}H/^{13}C$ NMR of 5c'
f1 (ppm)
f1 (ppm)

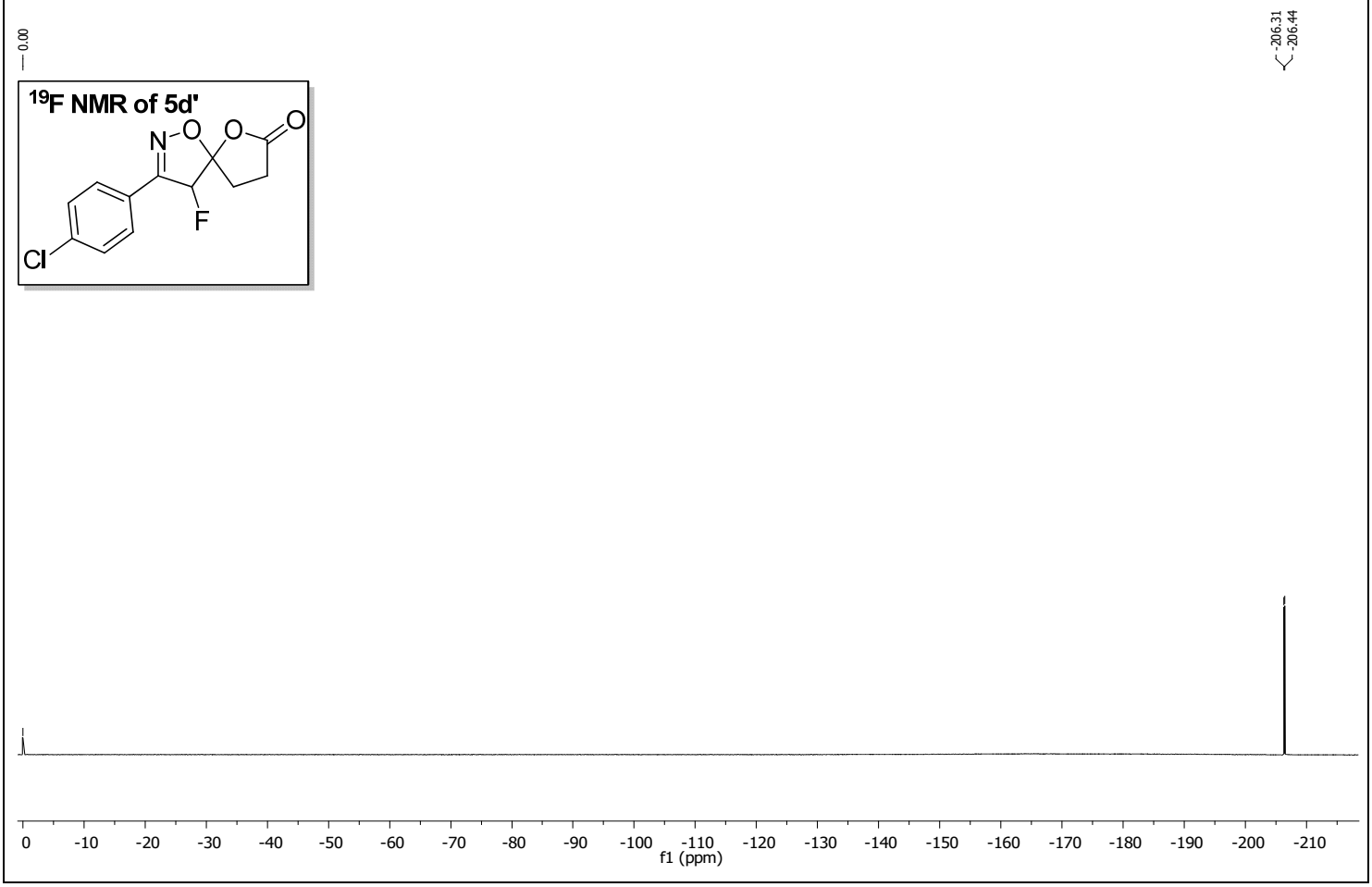

0.00
-107.09
-107.11
-107.12
-107.12
-107.13
-107.14
-107.14
-107.15
-107.17
-190.33
-190.47
19F NMR of 5c
N
O
O
O
F
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

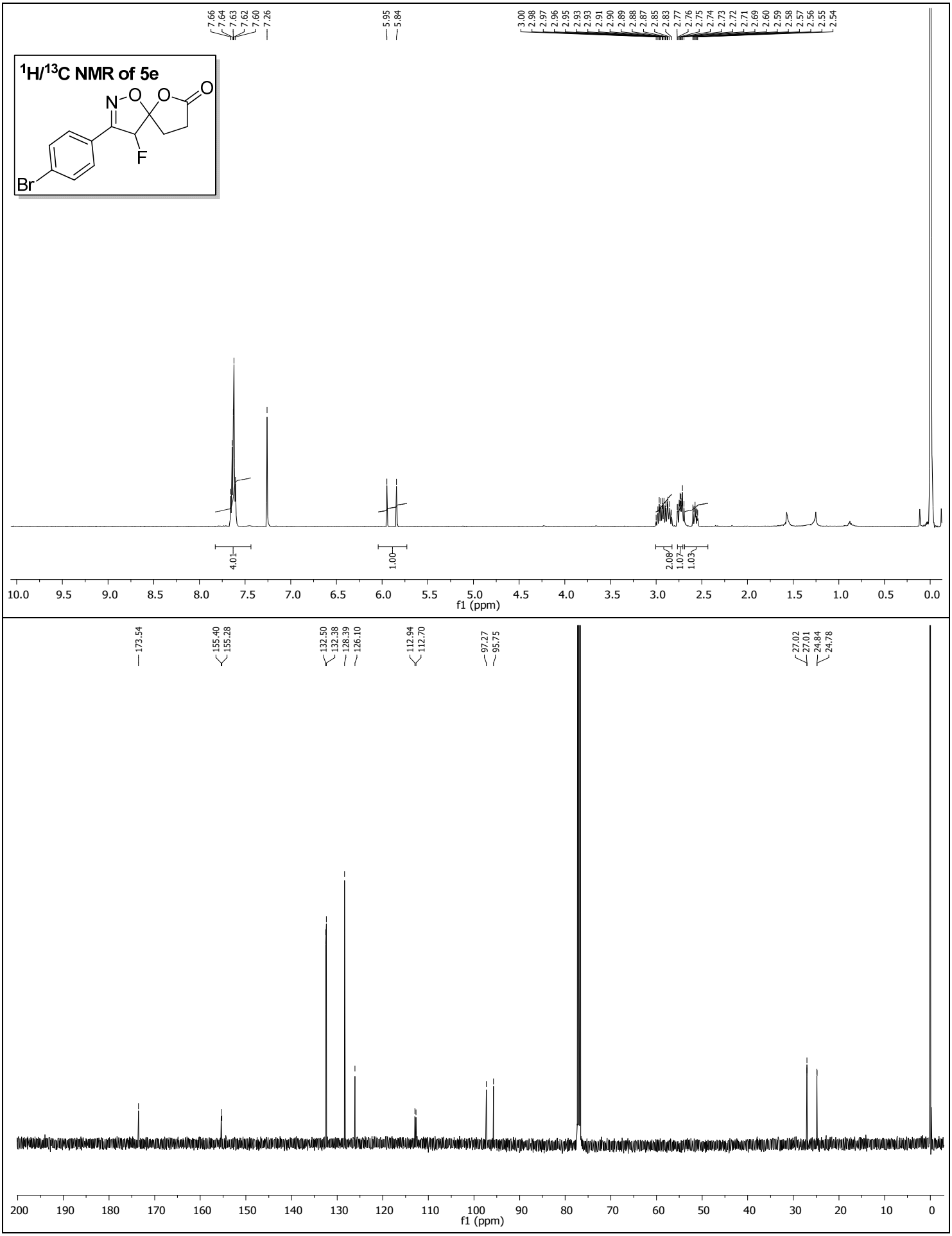

-0.00
-106.66
-106.67
-106.68
-106.69
-106.70
-106.71
-106.71
-106.72
-106.73
-206.23
-206.37
19F NMR of 5c'
N
O
O
O
F
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

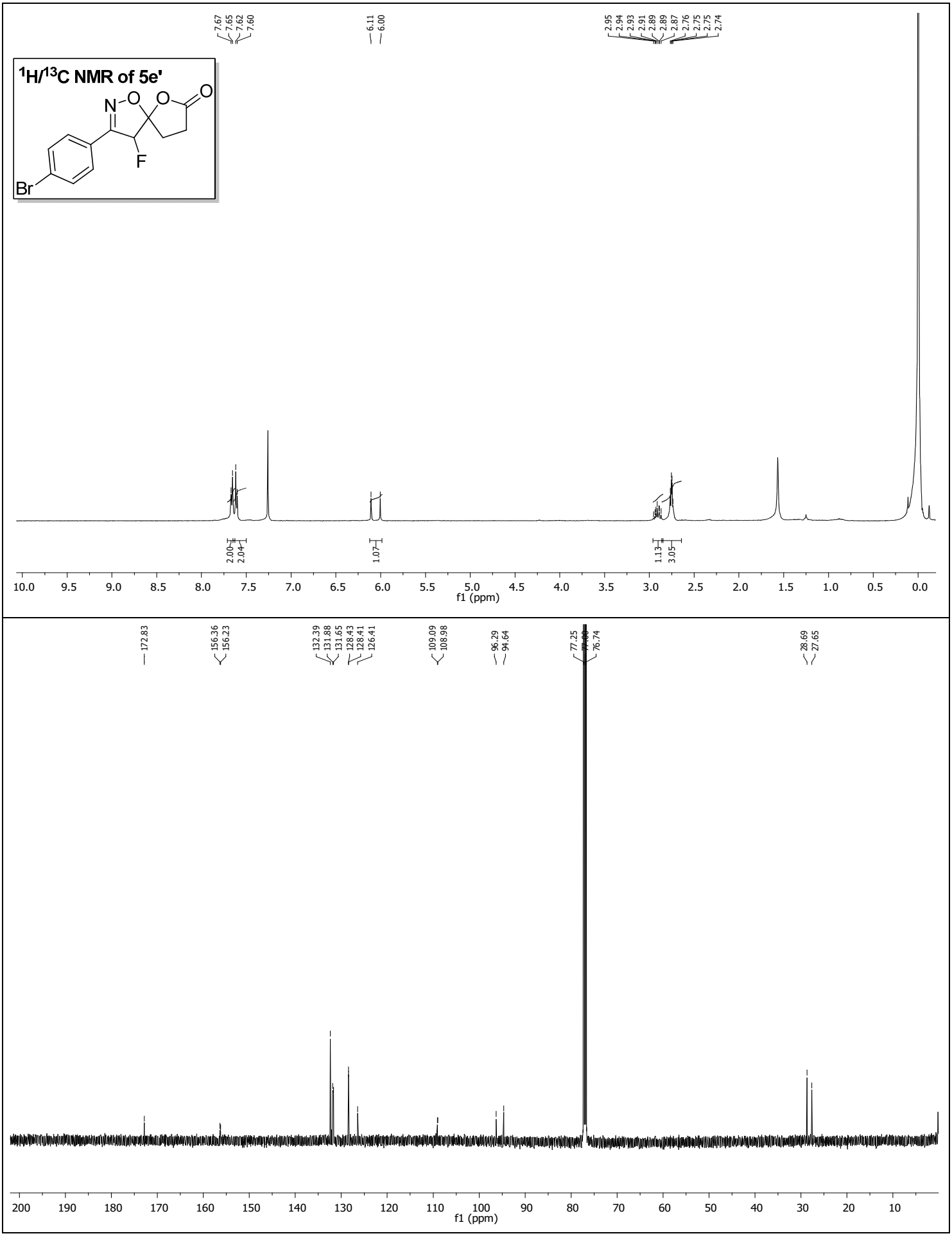

1H/13C NMR of 5d
N
O
O
O
F
Cl
7.71
7.70
7.46
7.44
7.26
5.95
5.84
2.98
2.96
2.95
2.93
2.91
2.89
2.88
2.87
2.85
2.83
2.77
2.76
2.75
2.74
2.73
2.72
2.71
2.71
2.69
2.59
2.59
2.58
2.57
2.56
2.55
2.54
2.07
2.06
1.00
2.12
1.03
0.99
f1 (ppm)
173.36
155.29
155.17
137.70
129.54
128.24
124.86
112.93
112.69
97.33
95.80
77.25
77.00
76.75
27.03
27.01
24.84
24.78
0.01
f1 (ppm)

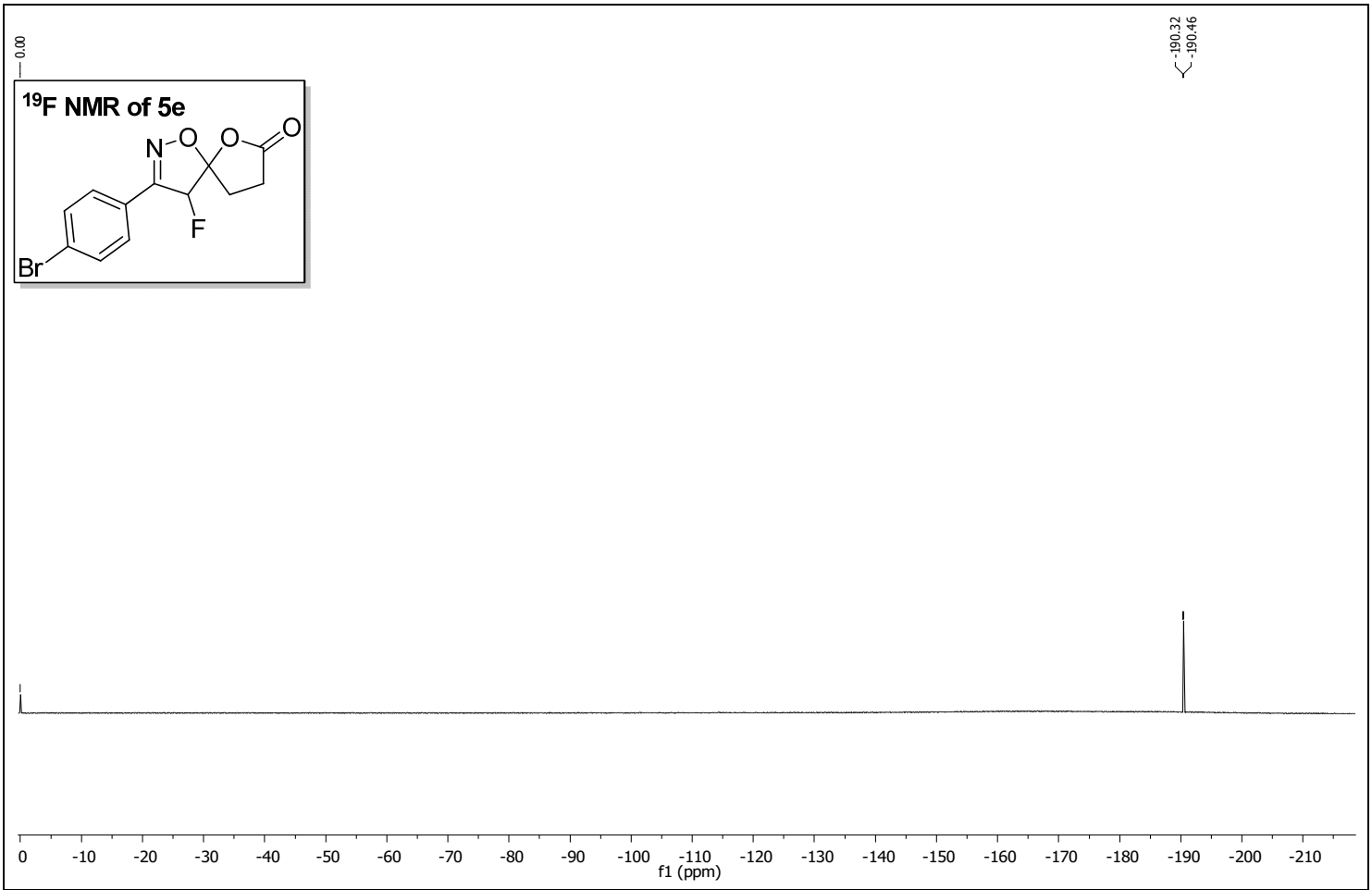

^{1}H/^{13}C NMR of 5d'
f1 (ppm)
f1 (ppm)

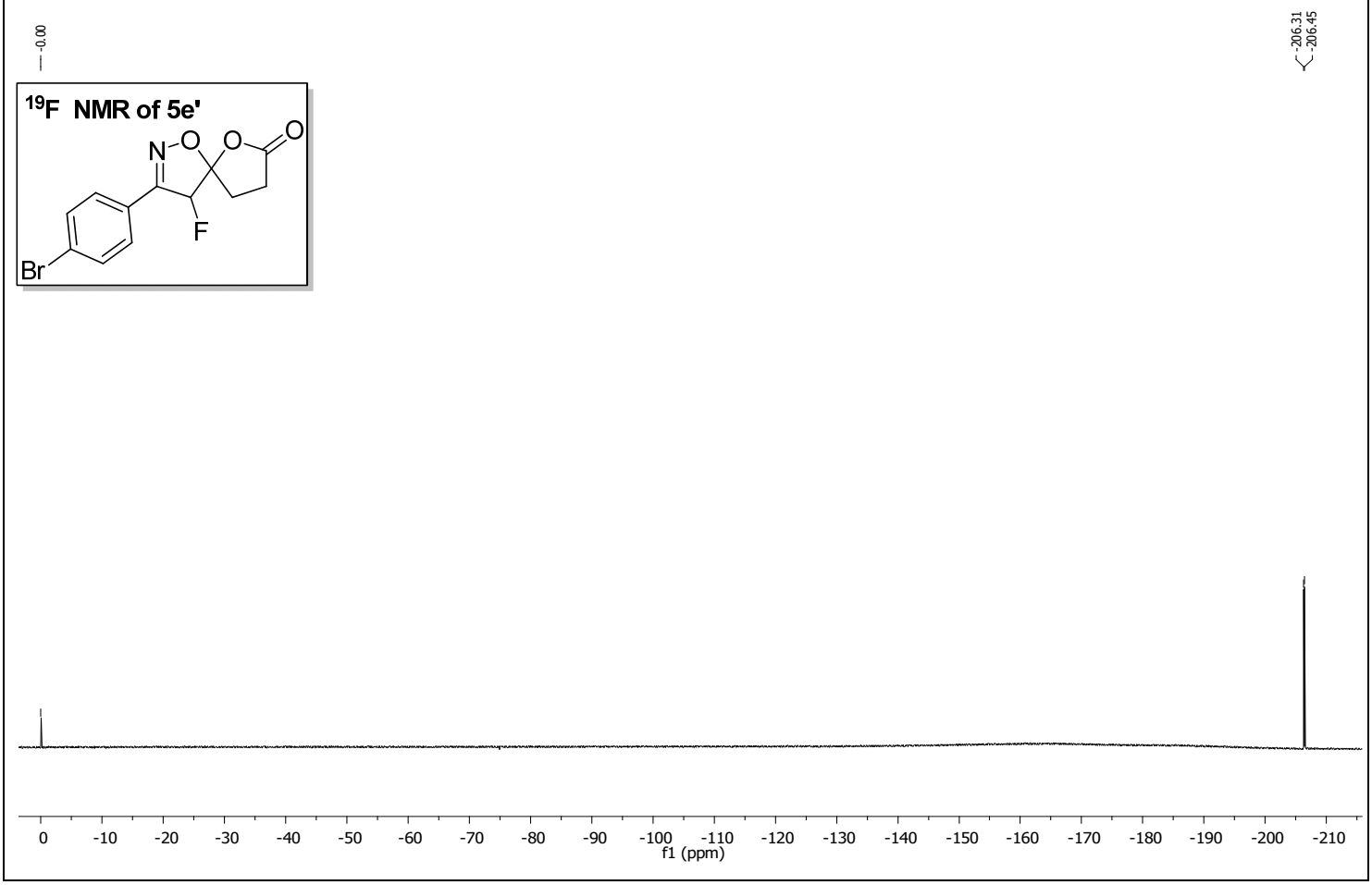

0.00
-190.33
-190.47
19F NMR of 5d
N
O
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

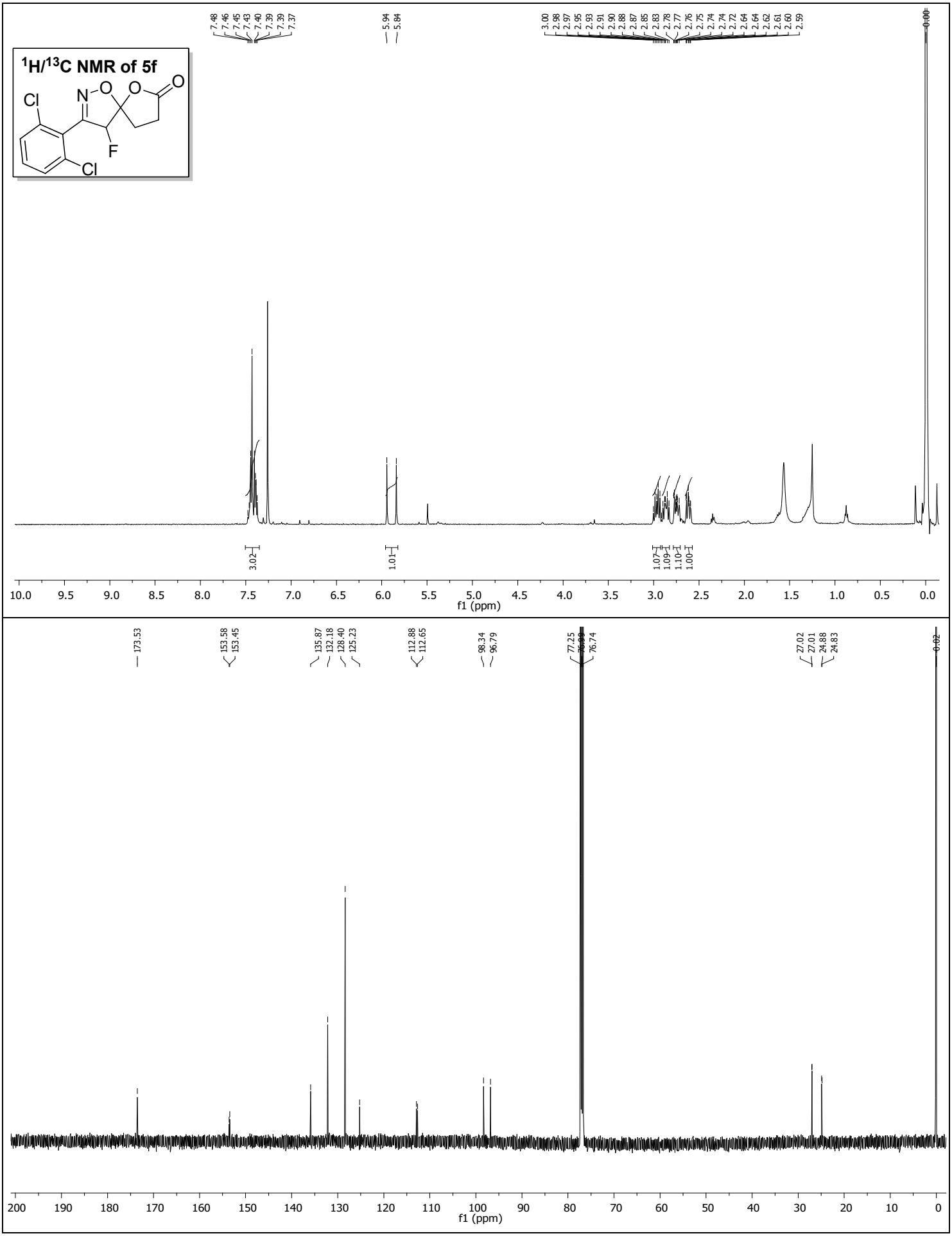

0.00
-206.31
-206.44
19F NMR of 5d'
N
O
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

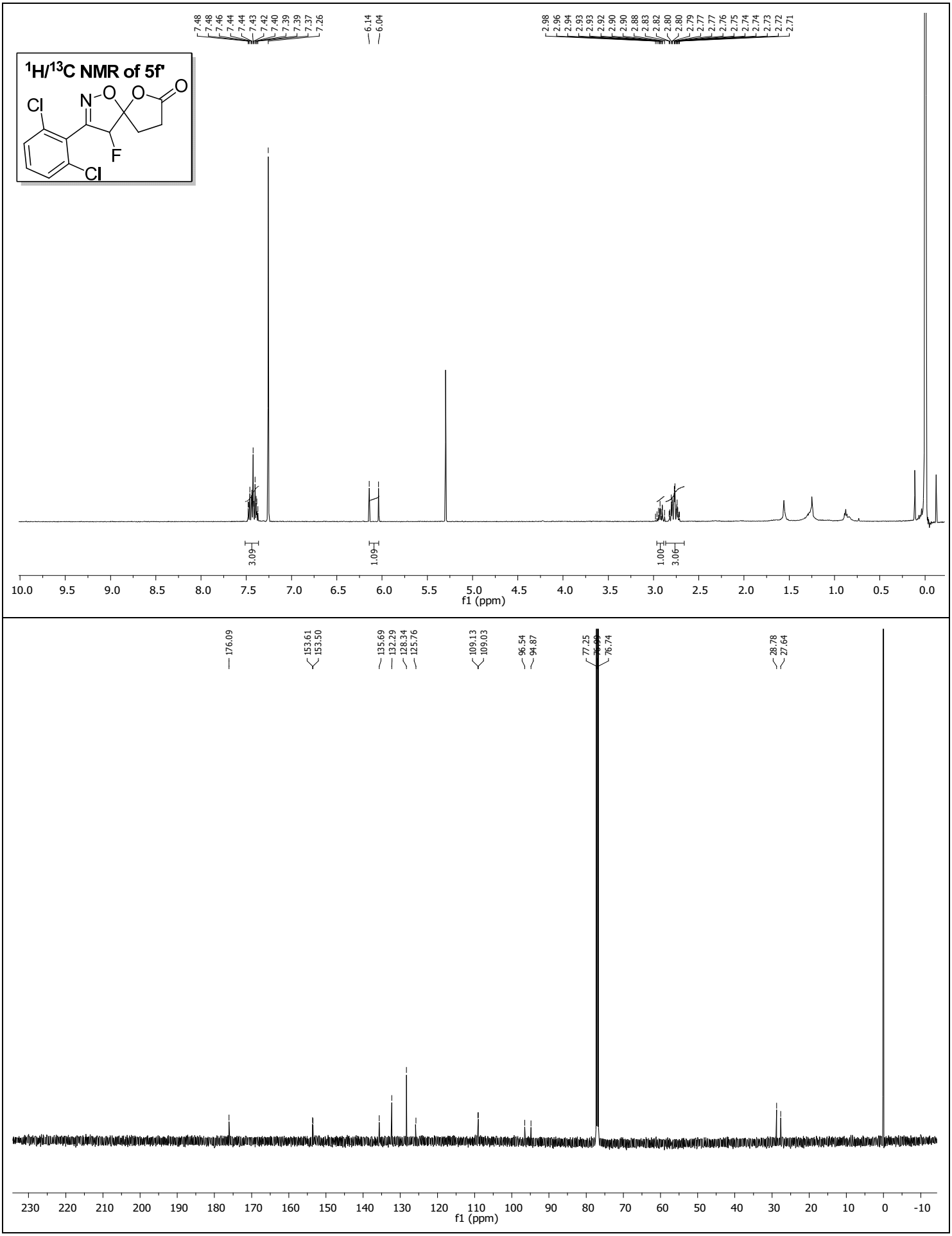

^{1}H/^{13}C NMR of 5e
Br
F
N
O
O
O
7.66
7.64
7.63
7.62
7.60
7.26
5.95
5.84
3.00
2.98
2.97
2.96
2.95
2.93
2.93
2.91
2.90
2.89
2.88
2.87
2.85
2.83
2.77
2.76
2.75
2.74
2.73
2.72
2.71
2.69
2.60
2.59
2.58
2.57
2.56
2.55
2.54
4.01
1.00
2.08
1.07
1.03
f1 (ppm)
173.54
155.40
155.28
132.50
132.38
128.39
126.10
112.94
112.70
97.27
95.75
27.02
27.01
24.84
24.78
f1 (ppm)

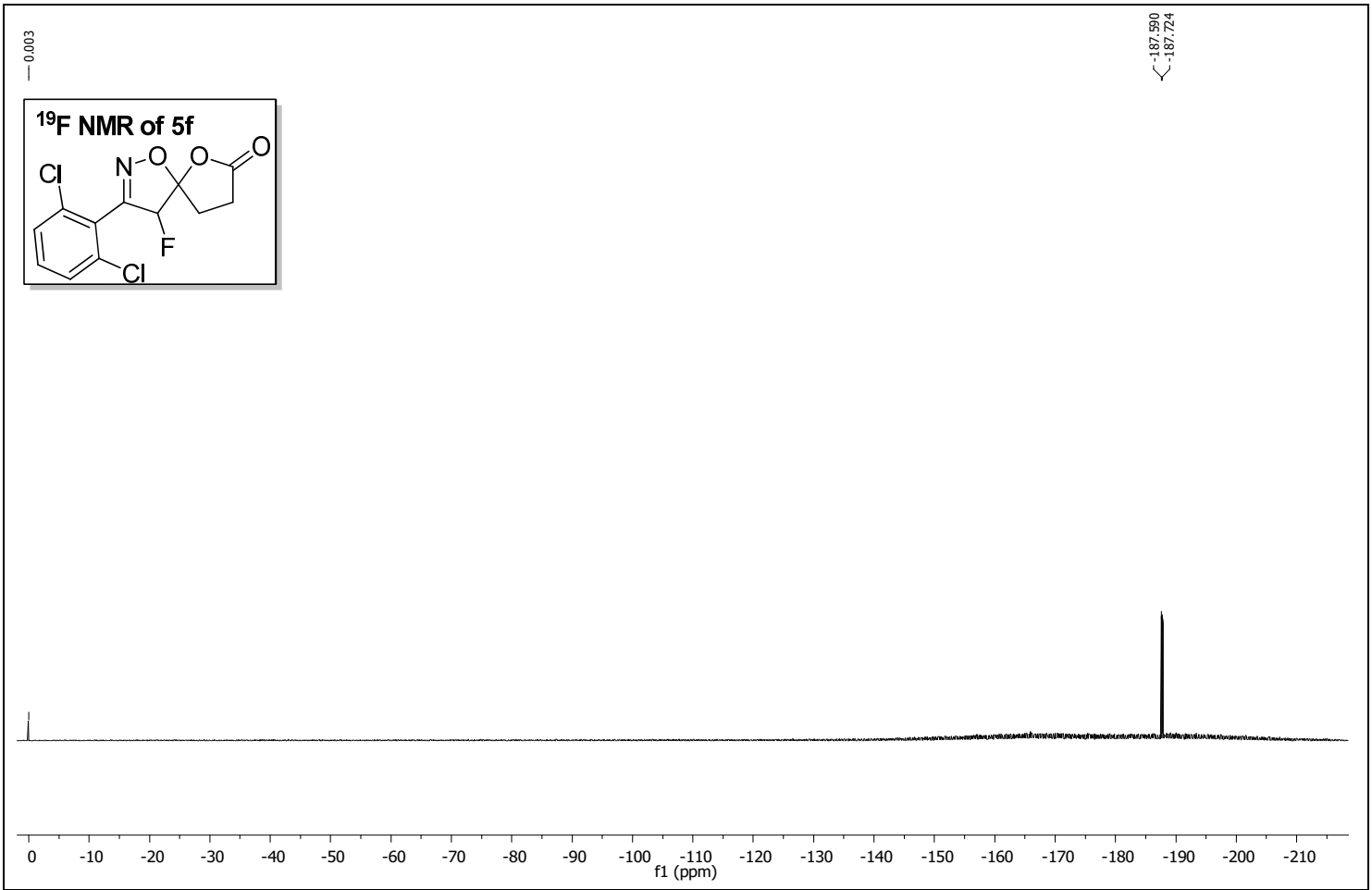

1H/13C NMR of 5e'
Br
F
f1 (ppm)
f1 (ppm)

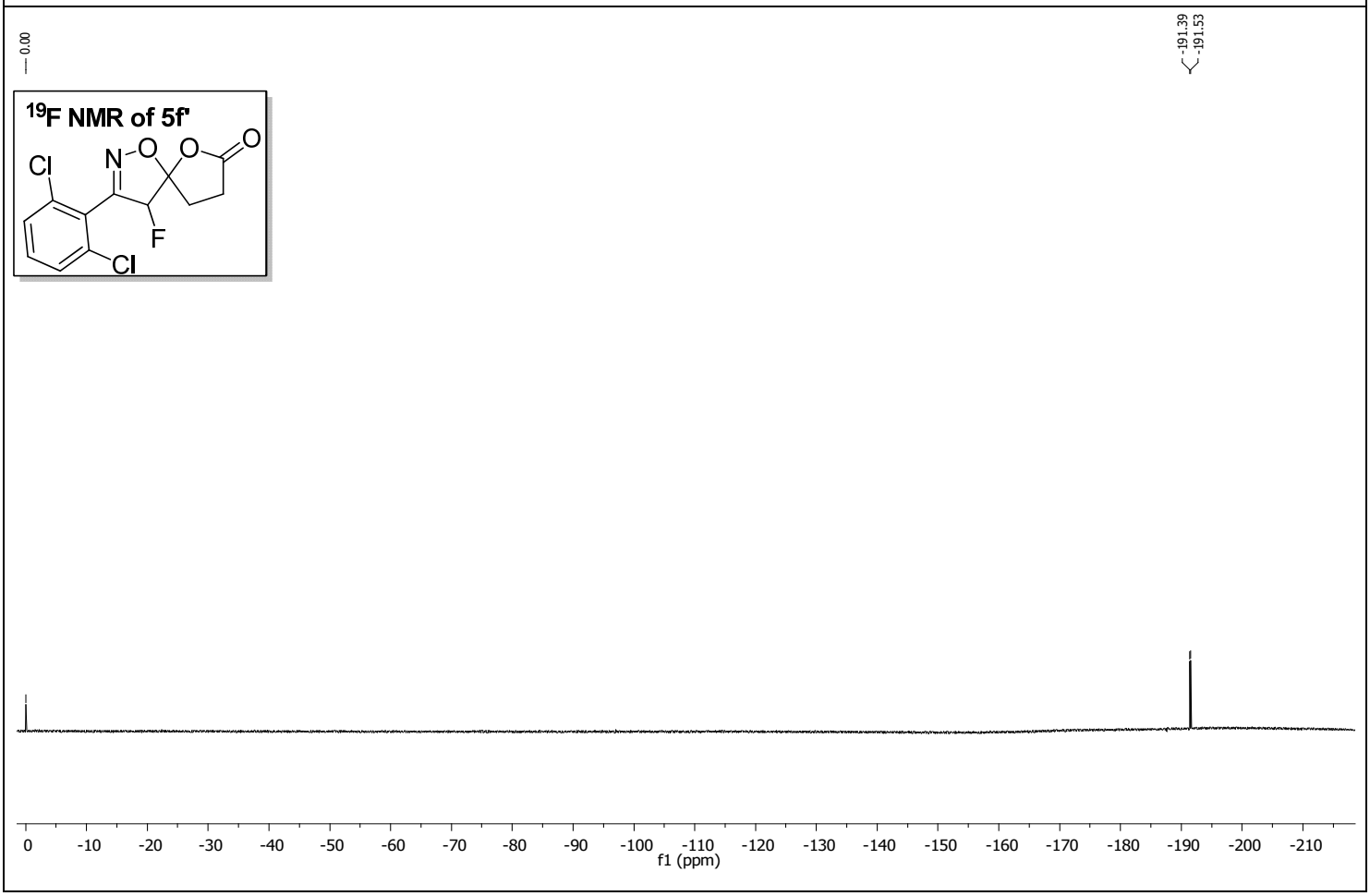

0.00
-190.32
-190.46
19F NMR of 5e
N
O
O
O
F
Br
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

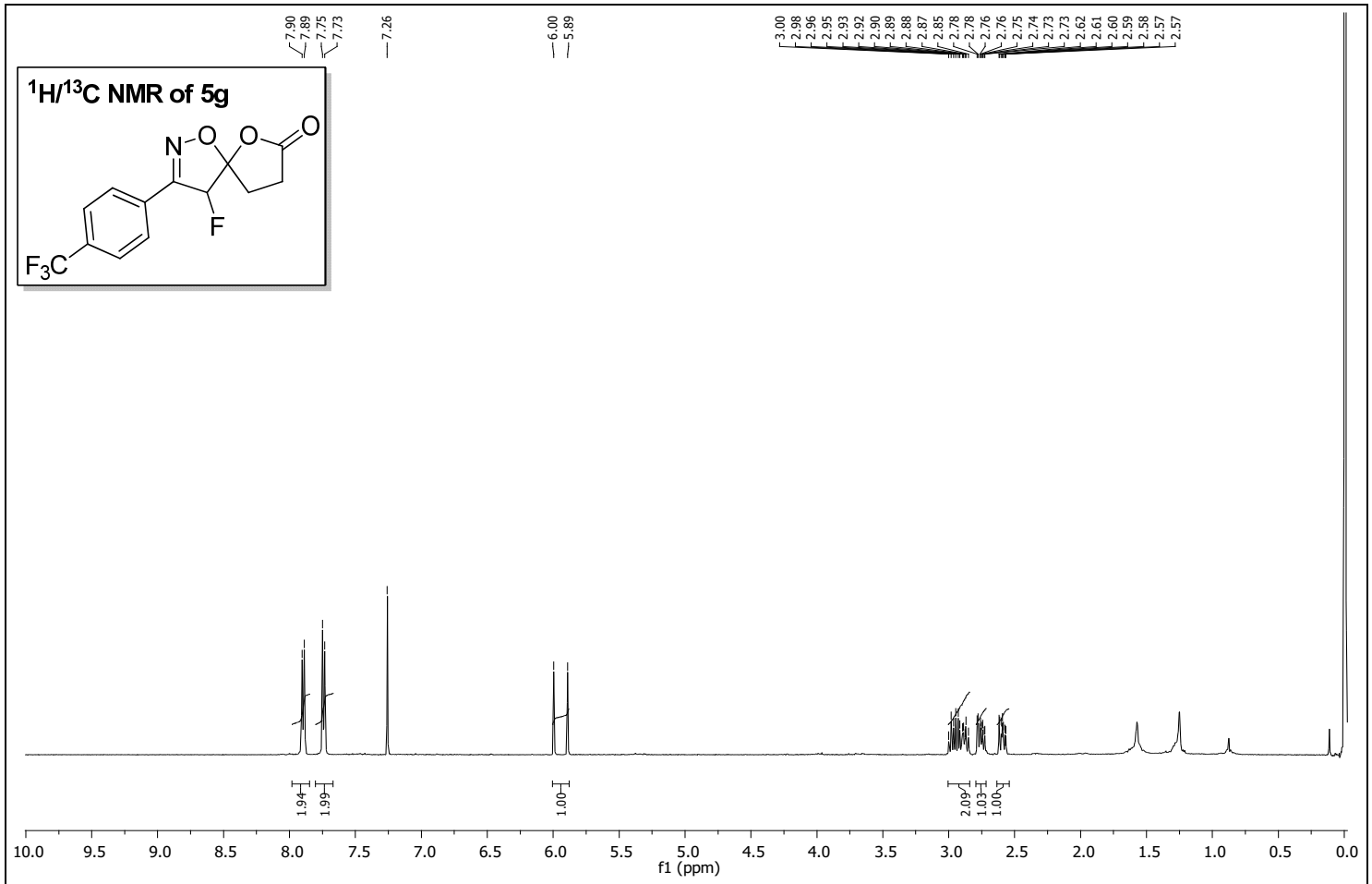

-0.00
-206.31
-206.45
19F NMR of 5e'
N
O
O
O
F
Br
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


$^{1}H/^{13}C$ NMR of 5f
Cl
N
O
O
O
F
Cl
7.48
7.46
7.45
7.43
7.40
7.39
7.39
7.37
5.94
5.84
3.00
2.98
2.97
2.95
2.93
2.91
2.90
2.88
2.87
2.85
2.83
2.78
2.77
2.76
2.75
2.74
2.74
2.72
2.64
2.64
2.62
2.61
2.60
2.59
0.00
3.02
1.01
1.07
1.09
1.10
1.00
f1 (ppm)
173.53
153.58
153.45
135.87
132.18
128.40
125.23
112.88
112.65
98.34
96.79
77.25
76.74
27.02
27.01
24.88
24.83
0.02
f1 (ppm)

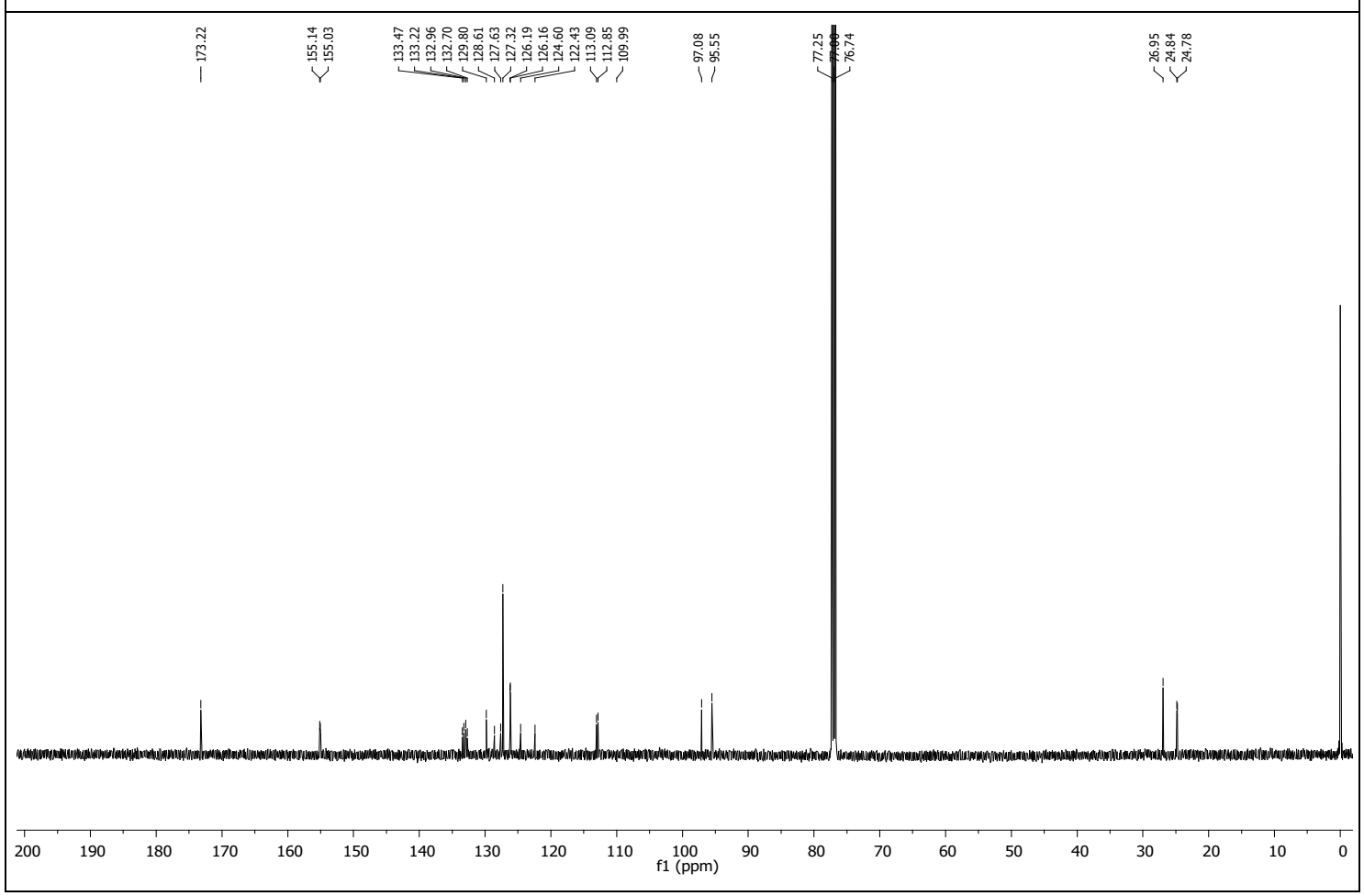

^{1}H/^{13}C NMR of 5f'
Cl
N
O
O
O
F
Cl
7.48
7.48
7.46
7.44
7.44
7.43
7.42
7.40
7.39
7.39
7.37
7.26
6.14
6.04
2.98
2.96
2.94
2.93
2.93
2.92
2.90
2.90
2.88
2.83
2.82
2.80
2.80
2.79
2.77
2.77
2.76
2.75
2.74
2.74
2.73
2.72
2.71
3.09
1.09
1.00
3.06
f1 (ppm)
176.09
153.61
153.50
135.69
132.29
128.34
125.76
109.13
109.03
96.54
94.87
77.25
76.74
28.78
27.64
f1 (ppm)


0.003
-187.590
-187.724
19F NMR of 5f
Cl
N
O
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

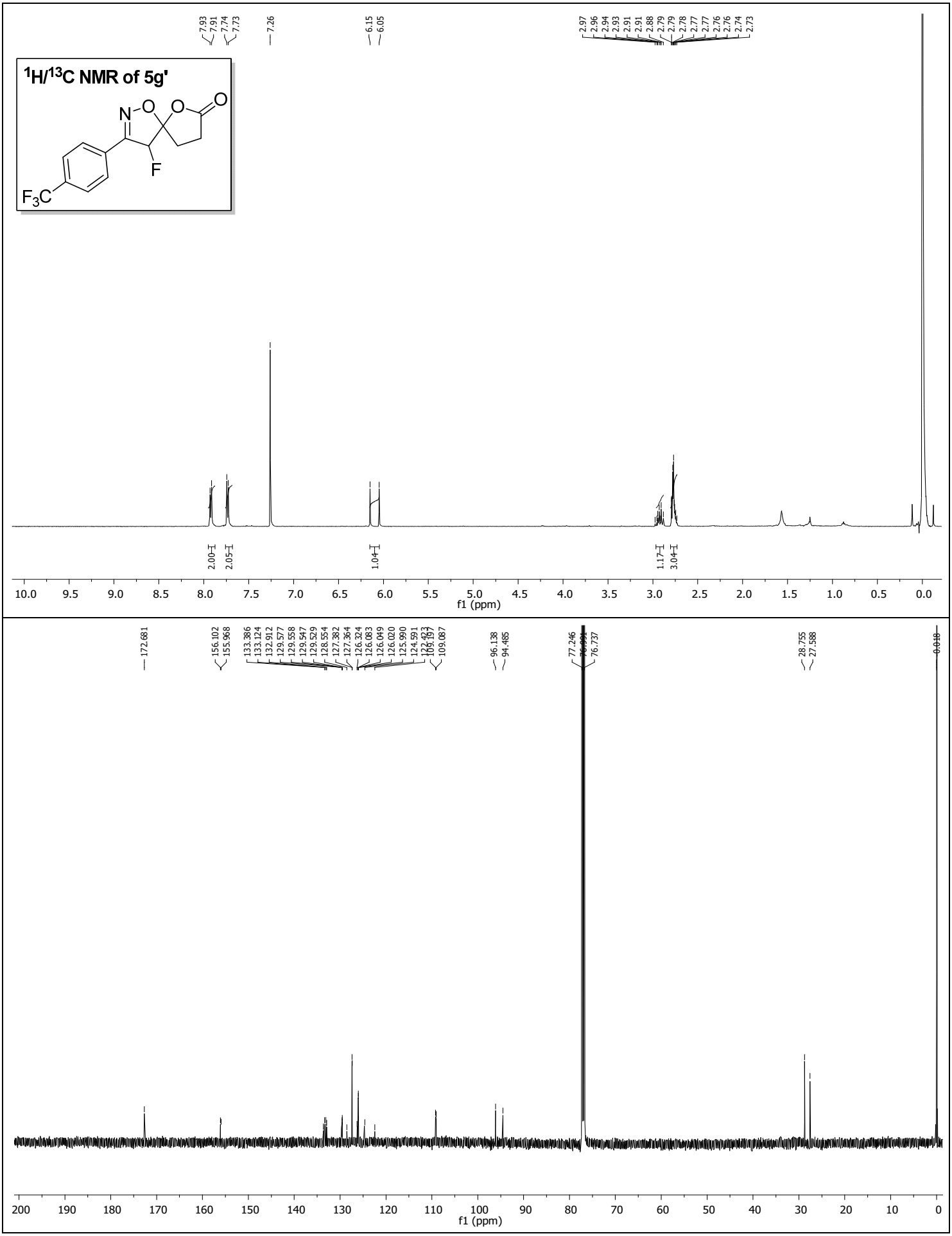

0.00
-191.39
-191.53
19F NMR of 5f'
Cl
N
O
O
O
F
Cl
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

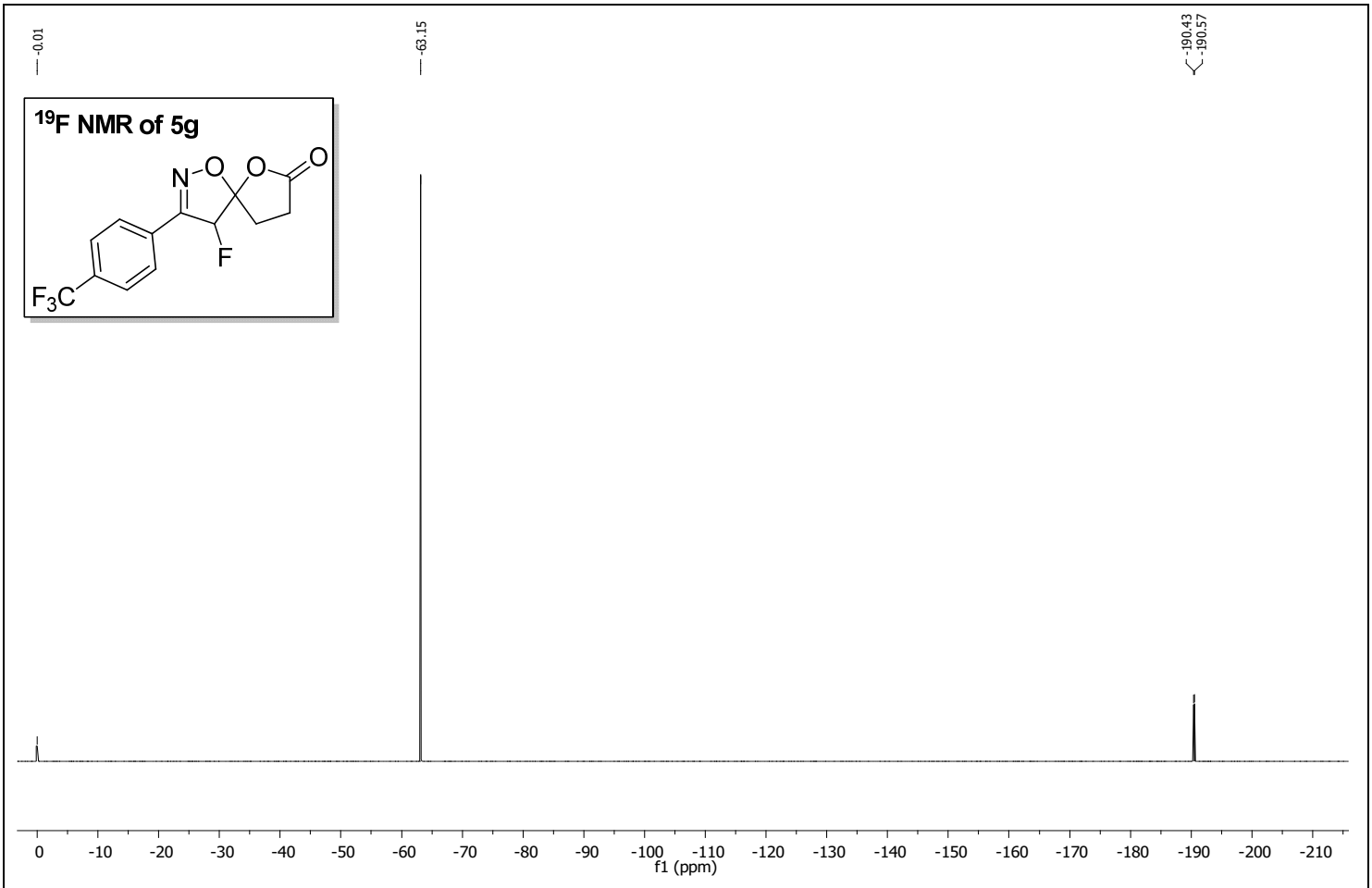


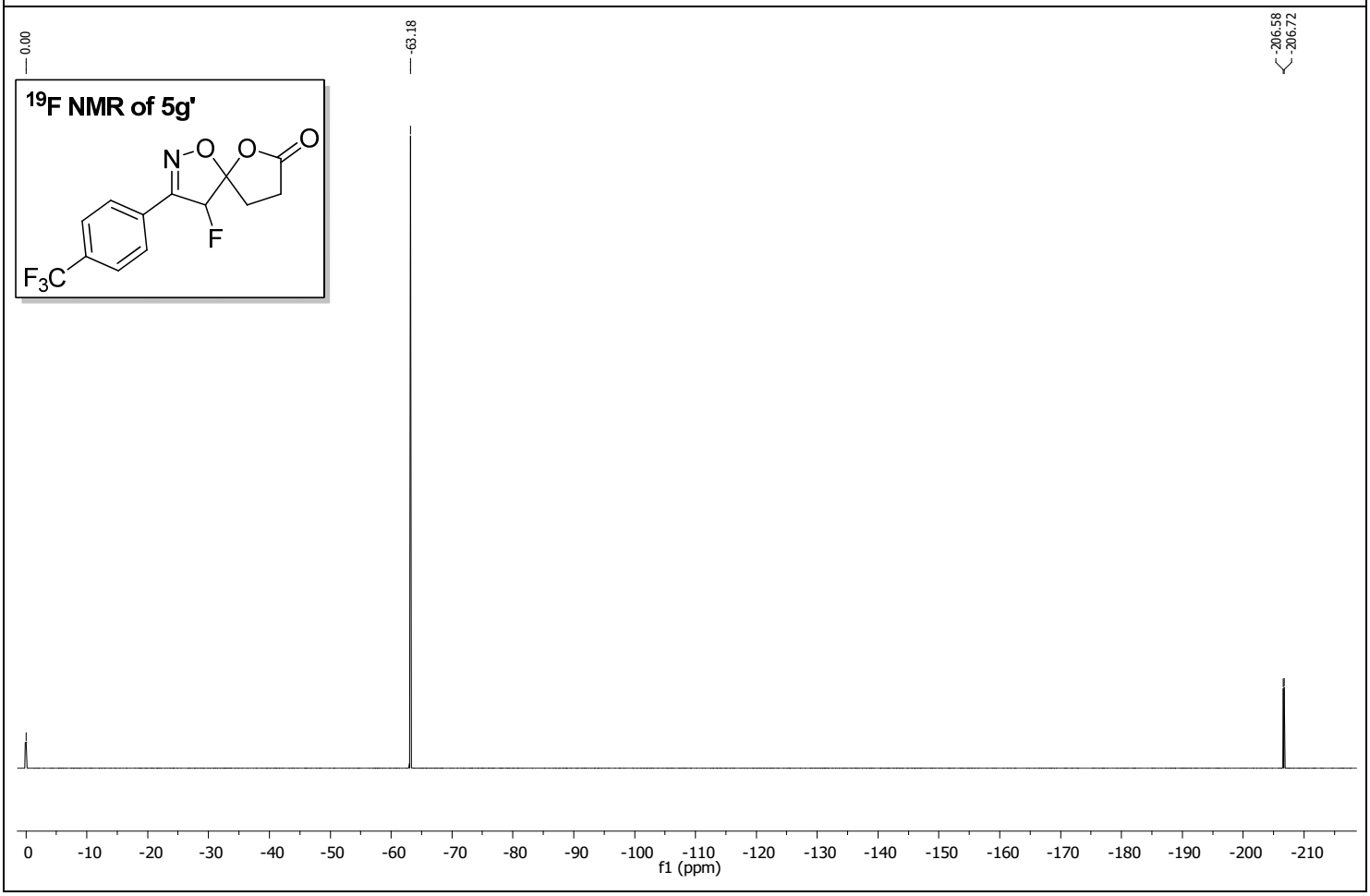
$^1H/^{13}C$ NMR of 5g
N
O
O
O
F
F_3C
7.90
7.89
7.75
7.73
7.26
6.00
5.89
3.00
2.98
2.96
2.95
2.93
2.92
2.90
2.89
2.88
2.87
2.85
2.78
2.78
2.76
2.76
2.75
2.74
2.73
2.73
2.62
2.61
2.60
2.59
2.58
2.57
2.57
1.94
1.99
1.00
2.09
1.03
1.00
f1 (ppm)

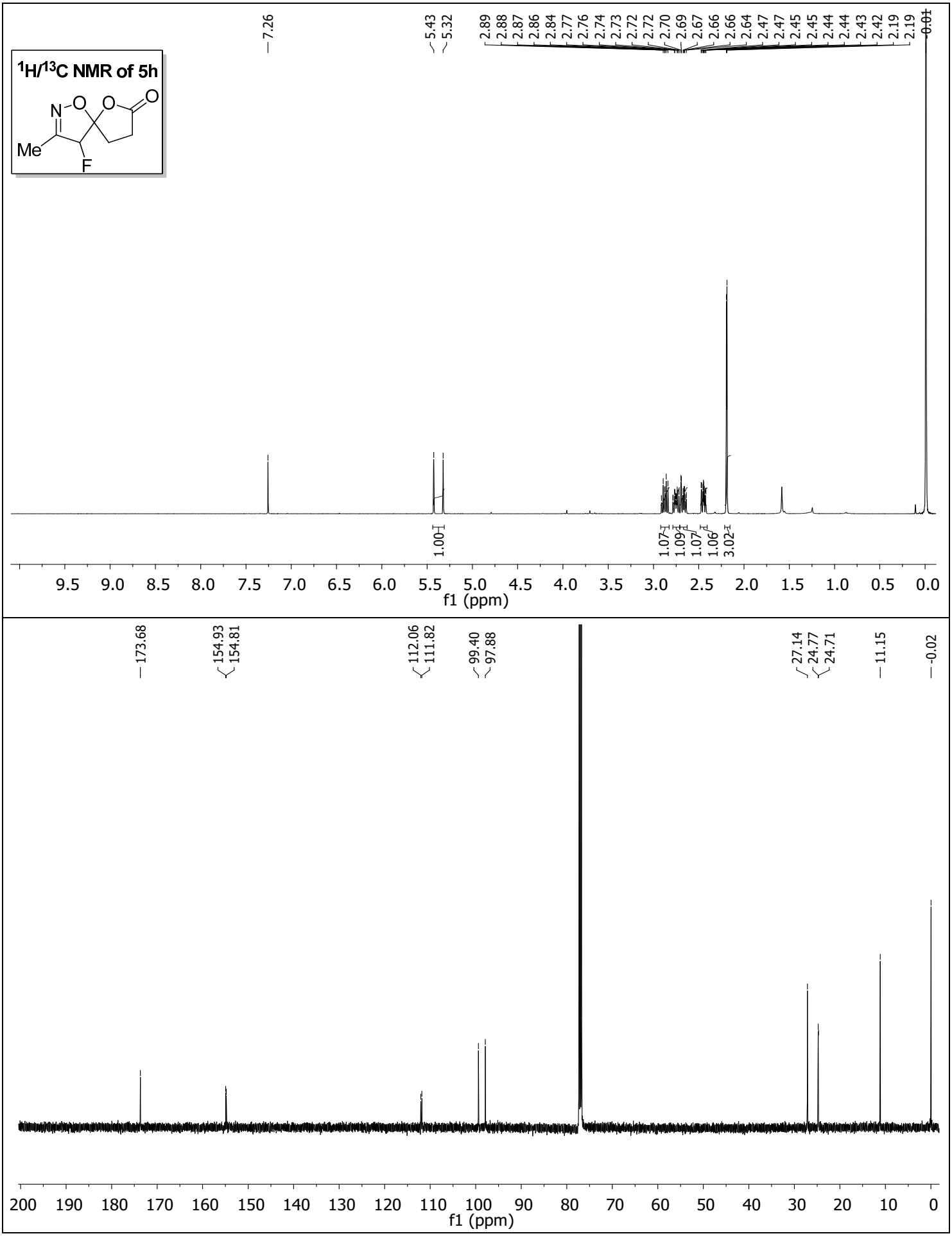


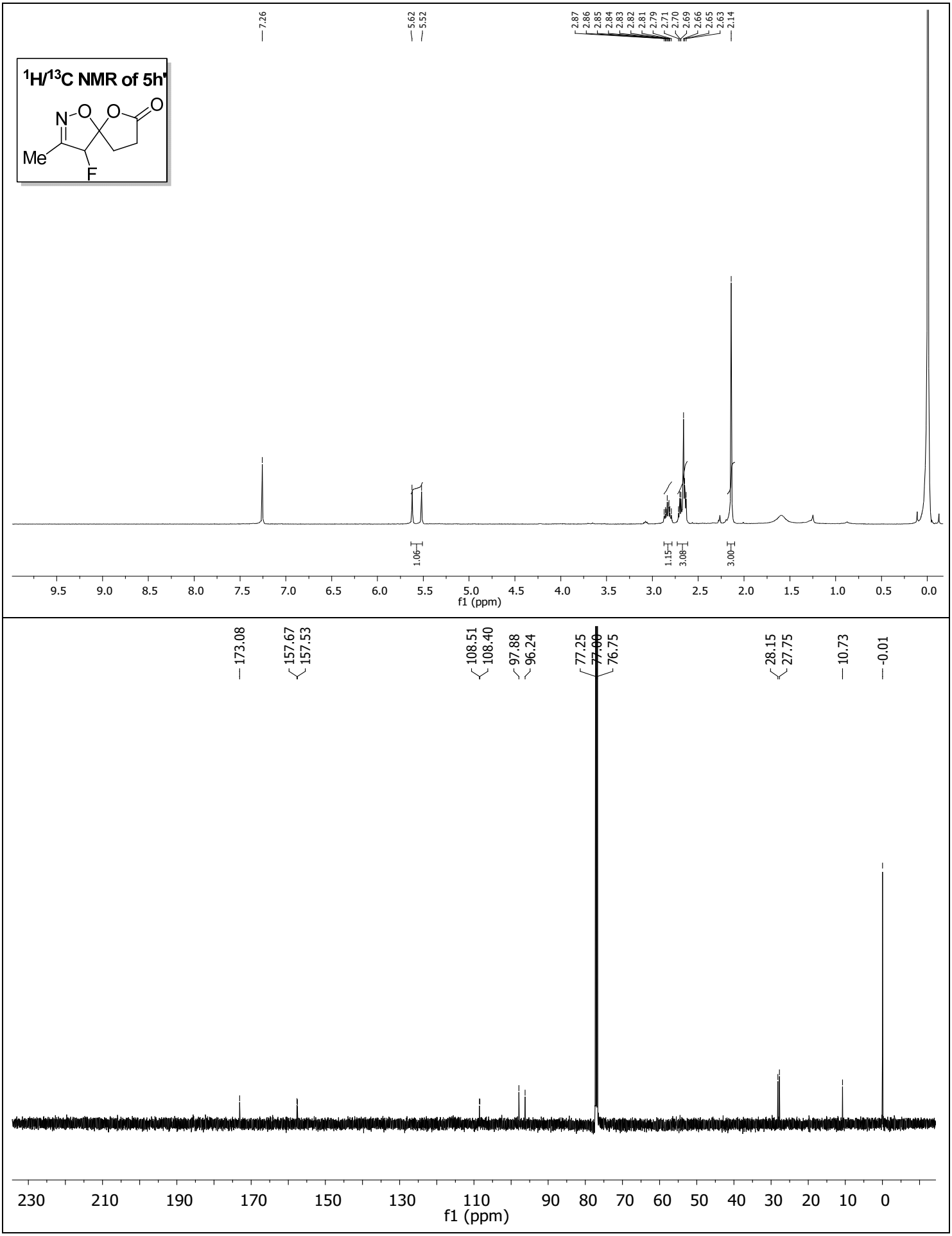
173.22
155.14
155.03
133.47
133.22
132.96
132.70
129.80
128.61
127.63
127.32
126.19
126.16
124.60
122.43
113.09
112.85
109.99
97.08
95.55
77.25
77.00
76.74
26.95
24.84
24.78
f1 (ppm)

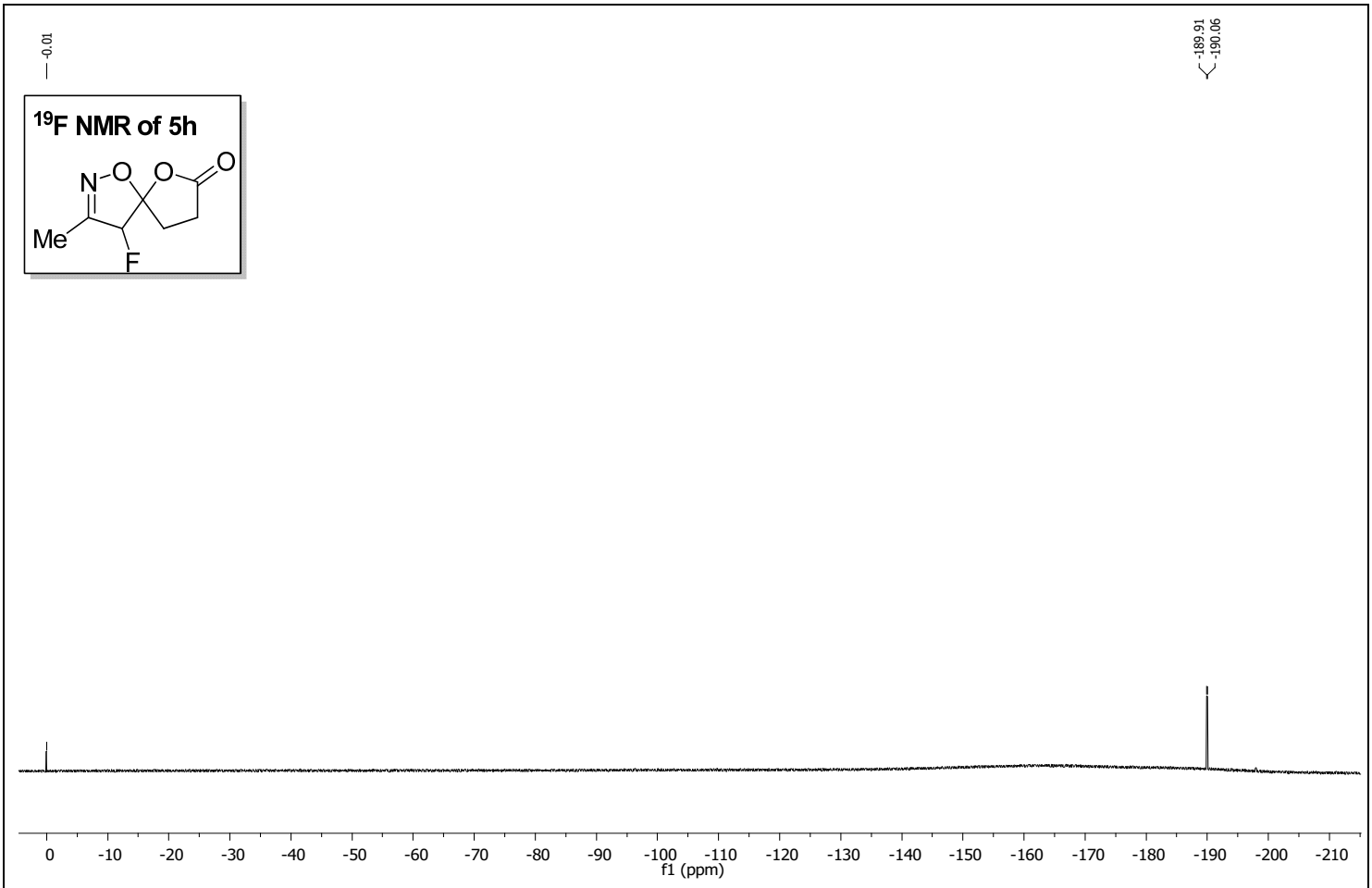

1H/13C NMR of 5g'
F3C
F
f1 (ppm)
f1 (ppm)

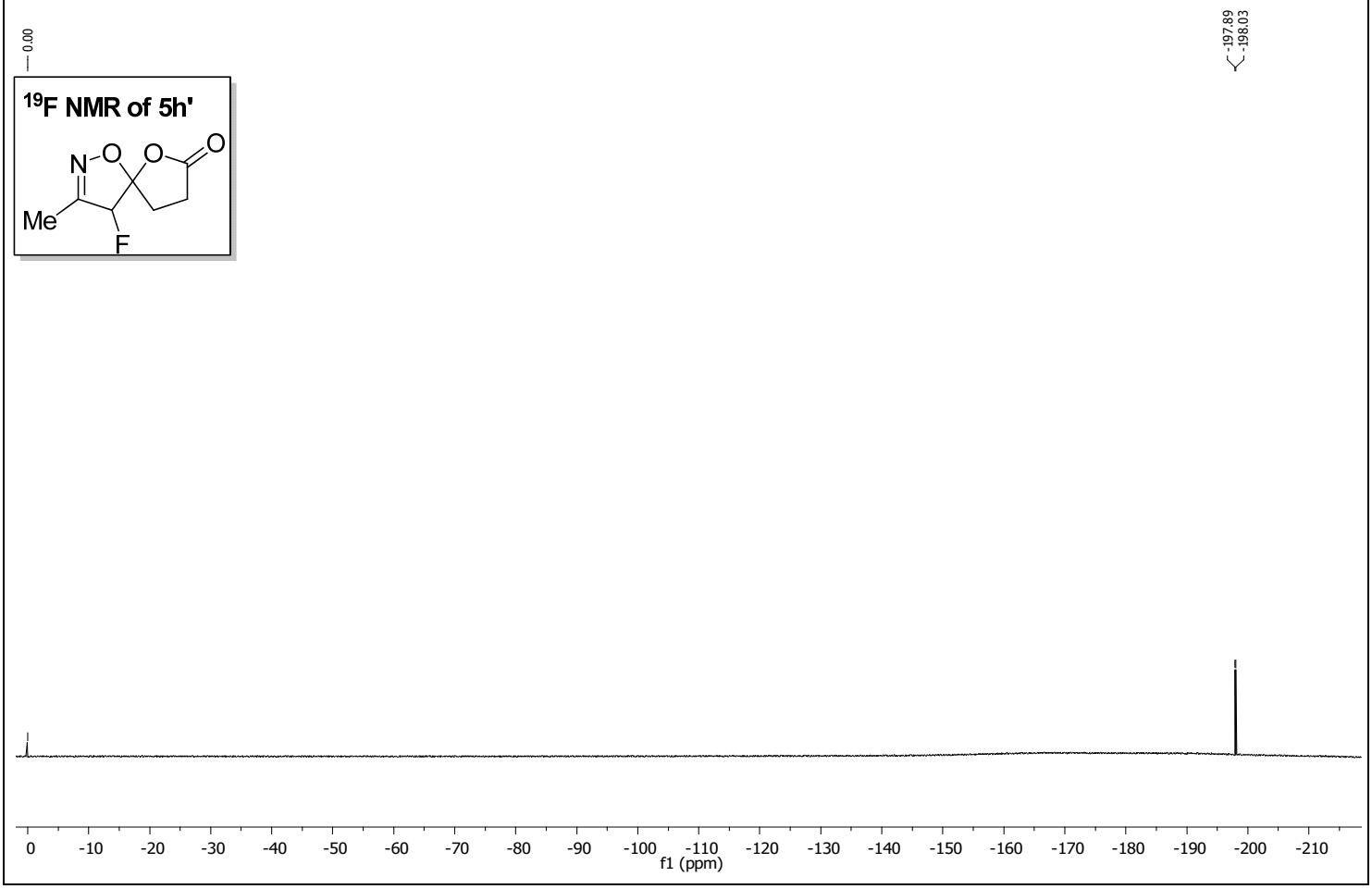

-0.01
-63.15
-190.43
-190.57
19F NMR of 5g
N
O
O
O
F
F3C
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

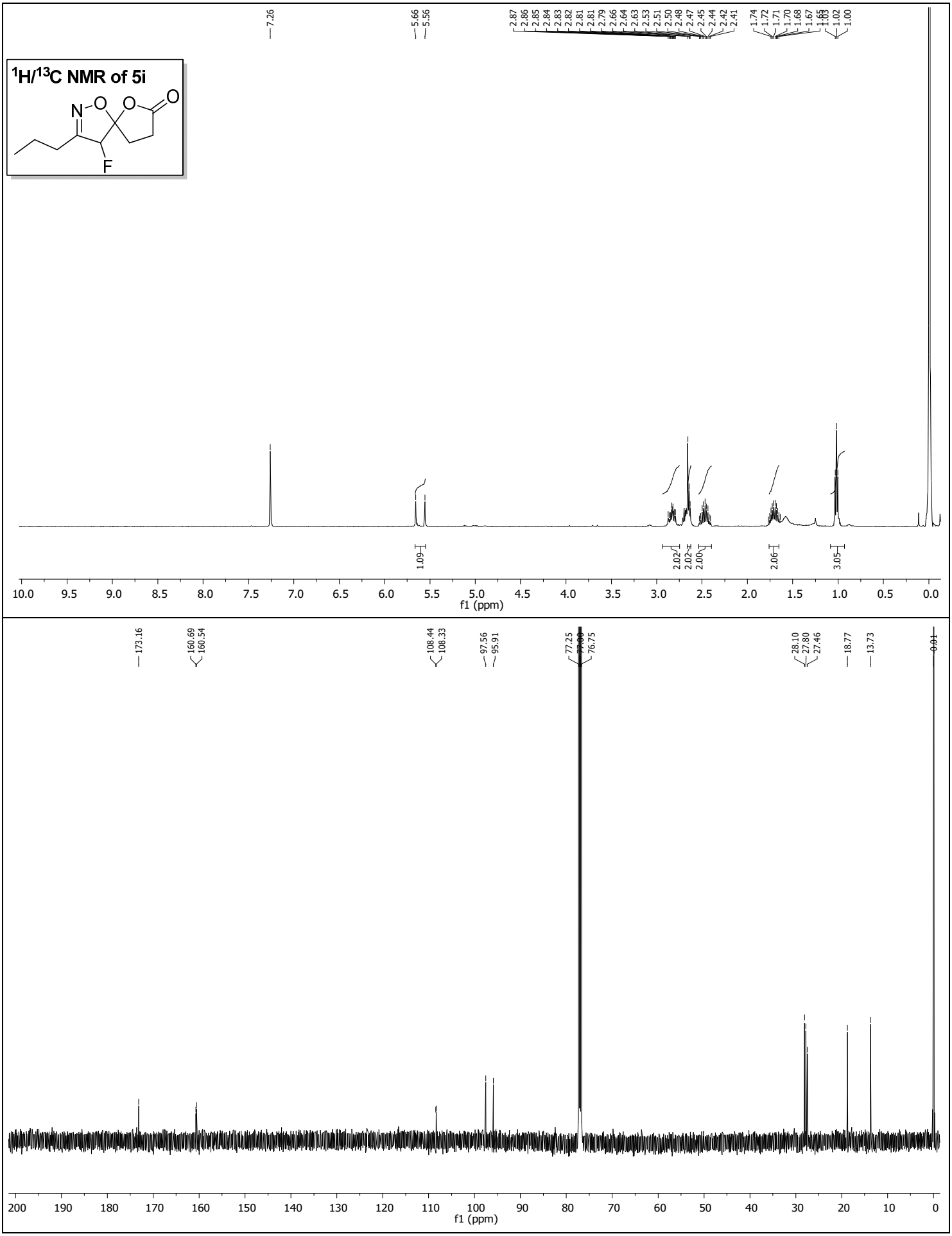

0.00
-63.18
-206.58
-206.72
19F NMR of 5g'
N
O
O
O
F
F3C
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

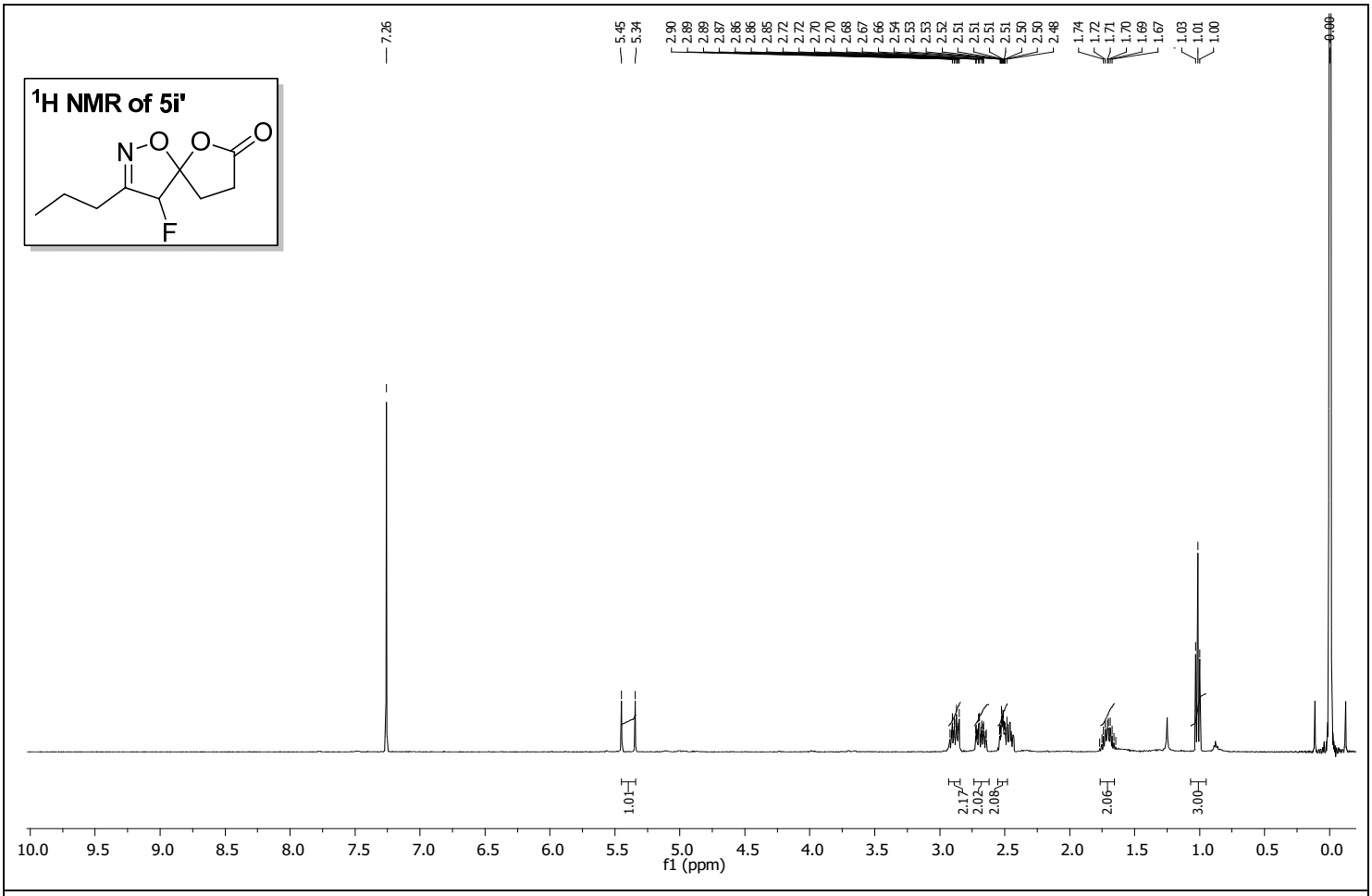

$^1H/^{13}C$ NMR of 5h
Me
F
7.26
5.43
5.32
2.89
2.88
2.87
2.86
2.84
2.77
2.76
2.74
2.73
2.72
2.72
2.70
2.69
2.67
2.66
2.66
2.64
2.47
2.47
2.45
2.45
2.44
2.44
2.43
2.42
2.19
2.19
0.01
1.00
1.07
1.09
1.07
1.06
3.02
f1 (ppm)
173.68
154.93
154.81
112.06
111.82
99.40
97.88
27.14
24.77
24.71
11.15
-0.02
f1 (ppm)

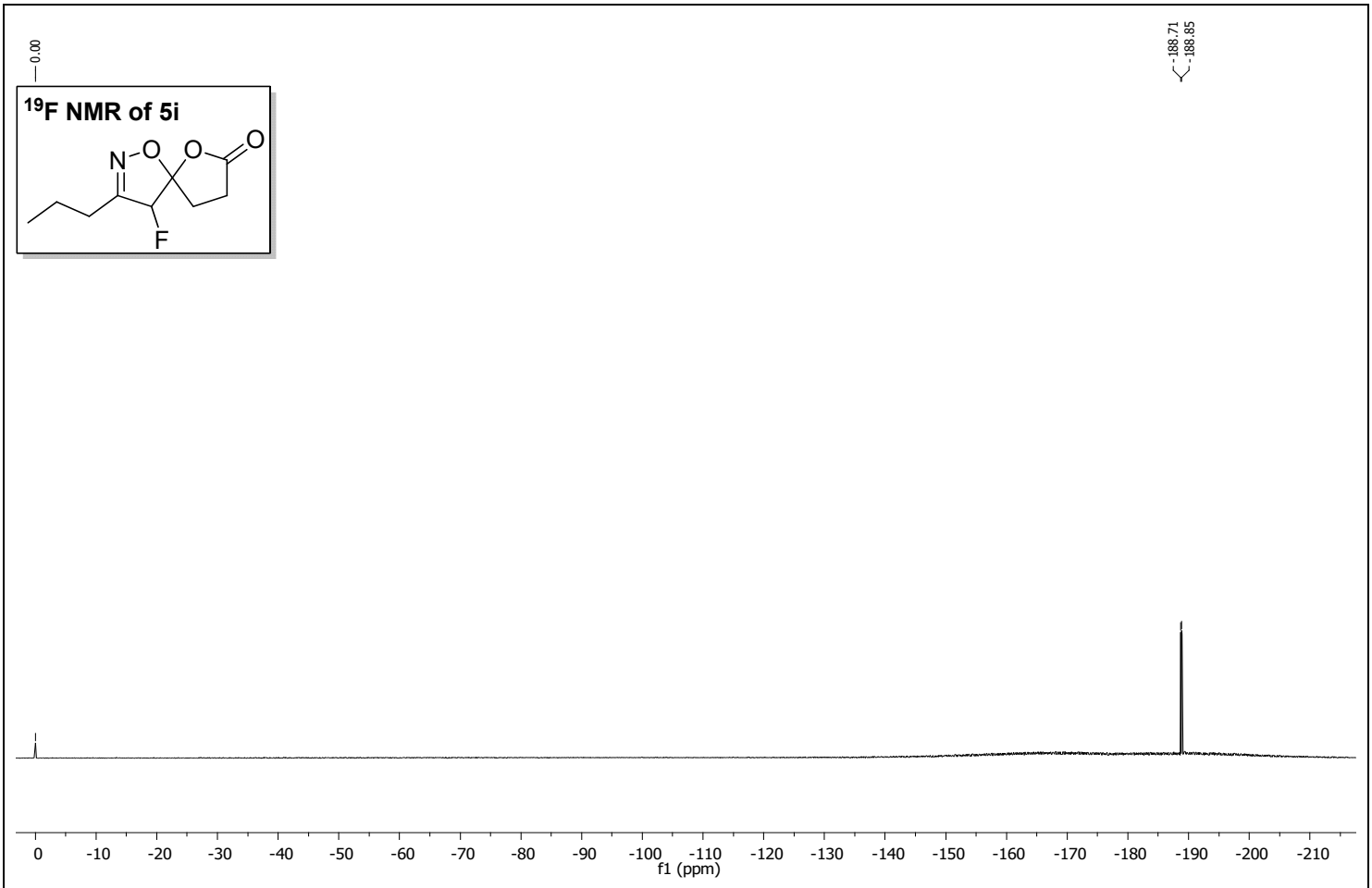

1H/13C NMR of 5h'
Me
F
7.26
5.62
5.52
2.87
2.86
2.85
2.84
2.83
2.82
2.81
2.79
2.71
2.70
2.69
2.66
2.65
2.63
2.14
1.06
1.15
3.08
3.00
f1 (ppm)
173.08
157.67
157.53
108.51
108.40
97.88
96.24
77.25
77.00
76.75
28.15
27.75
10.73
-0.01
f1 (ppm)

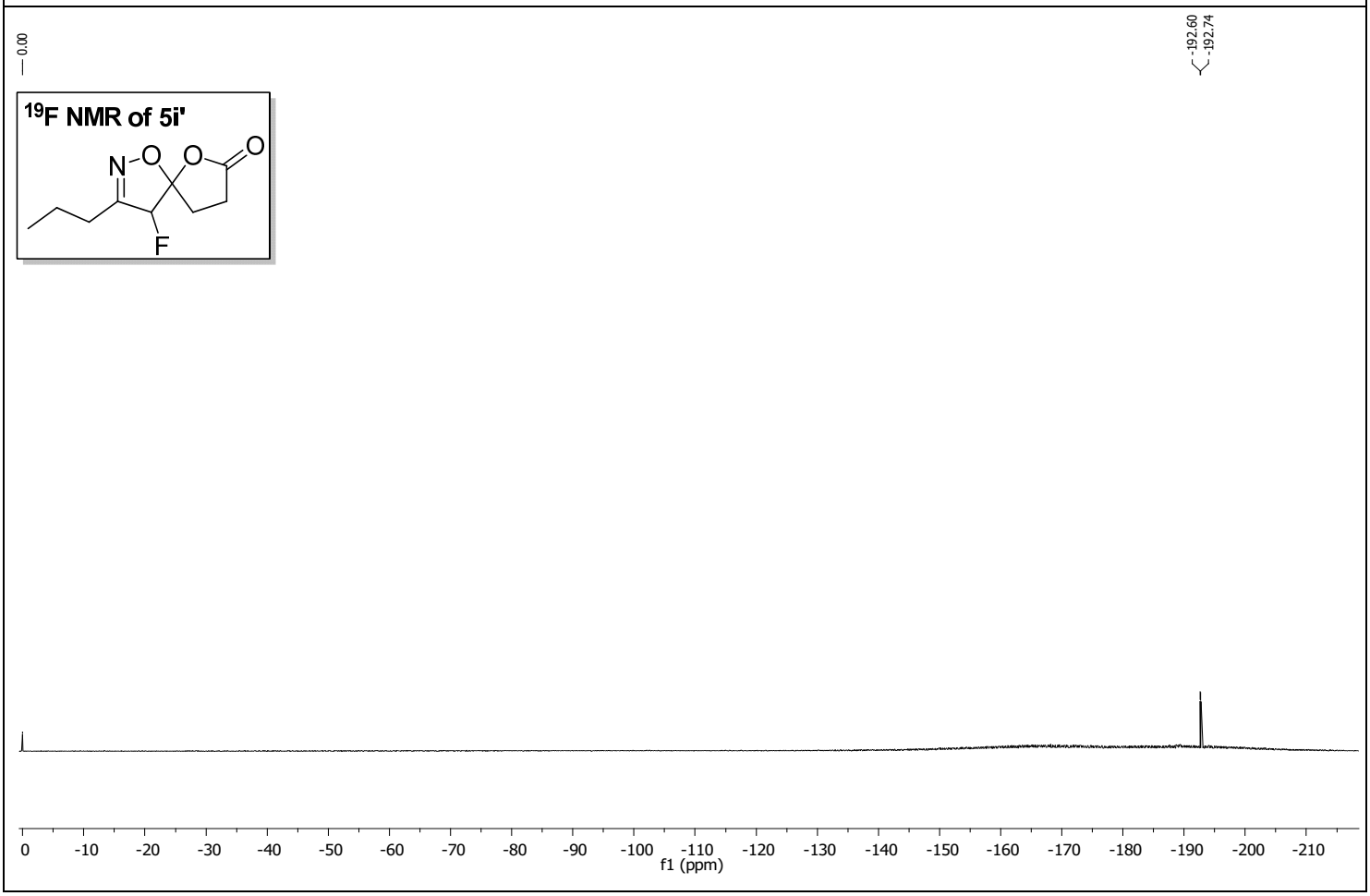

-0.01
-189.91
-190.06
19F NMR of 5h
N
O
O
O
Me
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


0.00
-197.89
-198.03
19F NMR of 5h'
N
O
O
O
Me
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

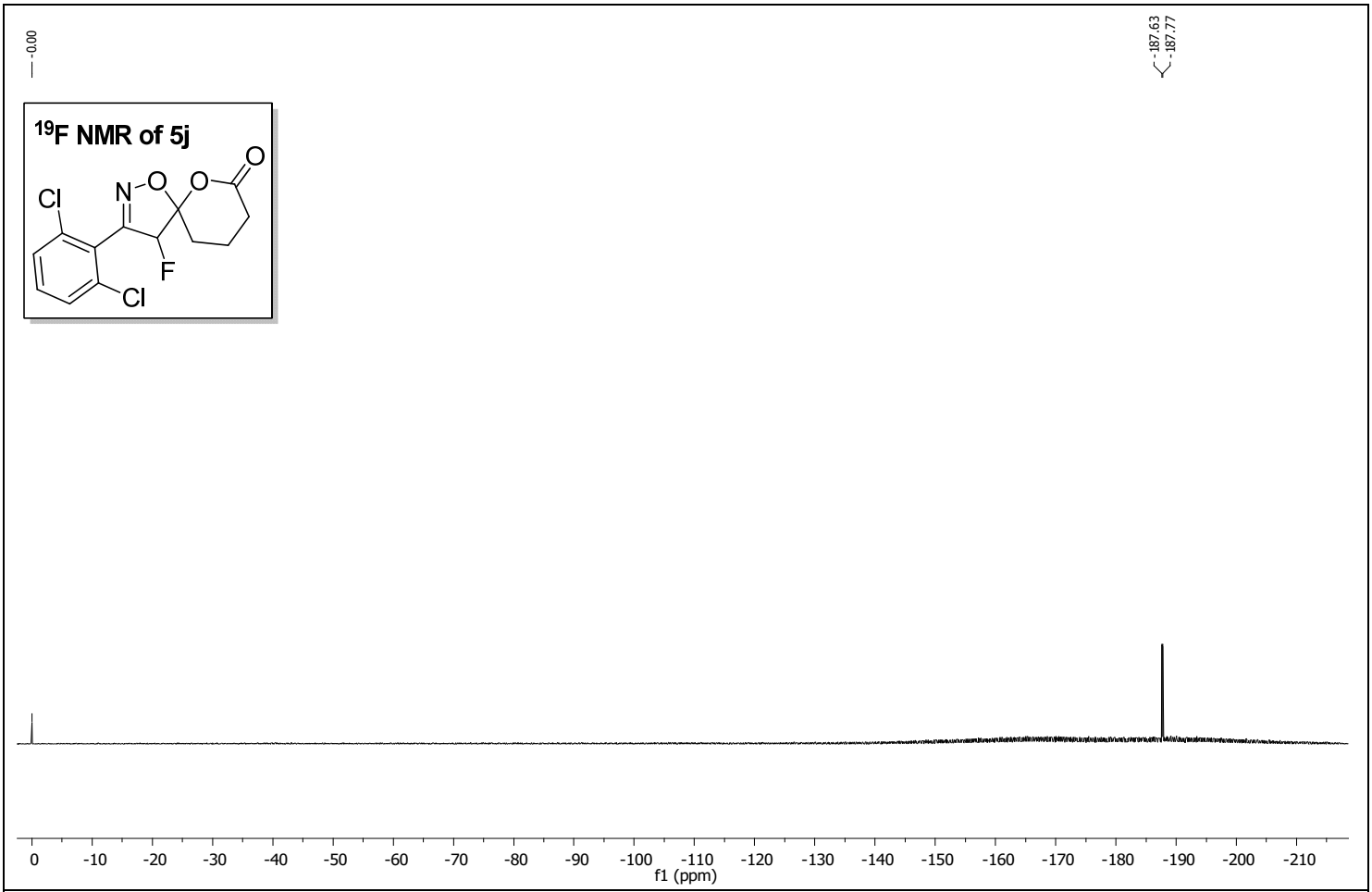

$^{1}H/^{13}C$ NMR of 5i
f1 (ppm)
f1 (ppm)

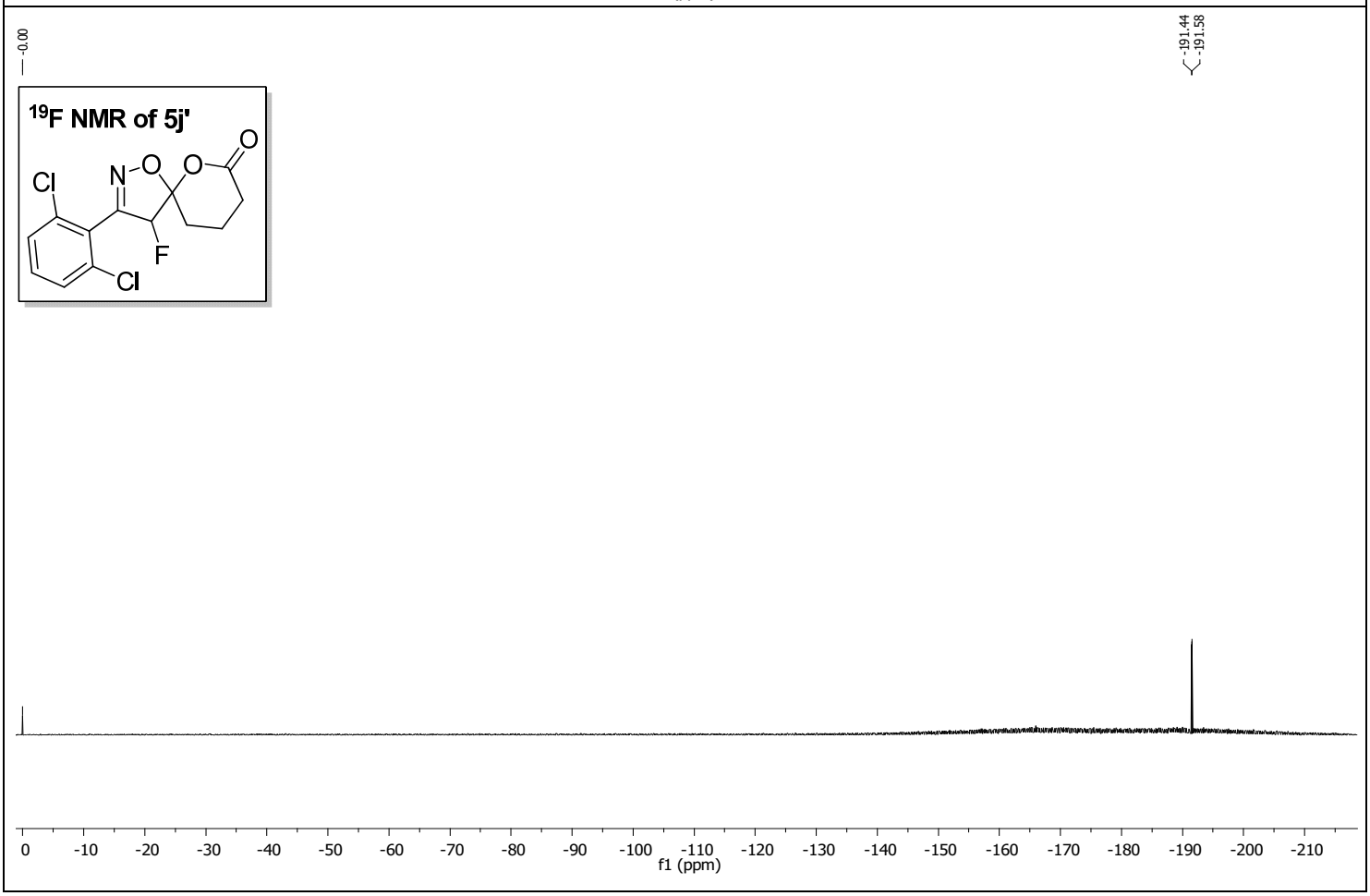

^{1}H NMR of 5i'
N
O
O
O
F
7.26
5.45
5.34
2.90
2.89
2.89
2.87
2.86
2.86
2.85
2.72
2.72
2.70
2.70
2.68
2.67
2.66
2.54
2.53
2.53
2.52
2.51
2.51
2.51
2.51
2.50
2.50
2.48
1.74
1.72
1.71
1.70
1.69
1.67
1.03
1.01
1.00
0.00
1.01
2.17
2.02
2.08
2.06
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

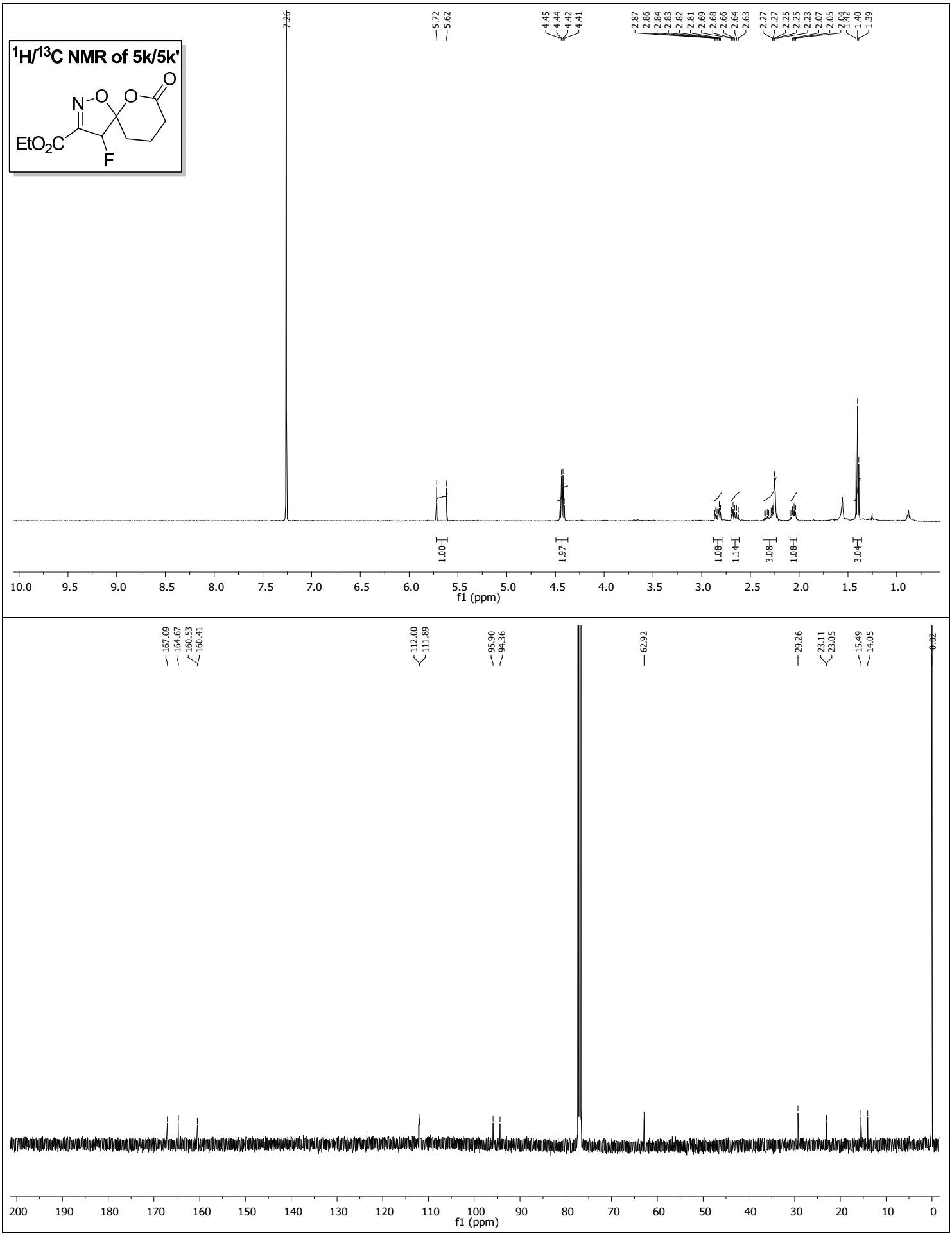

0.00
19F NMR of 5i
-188.71
-188.85
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

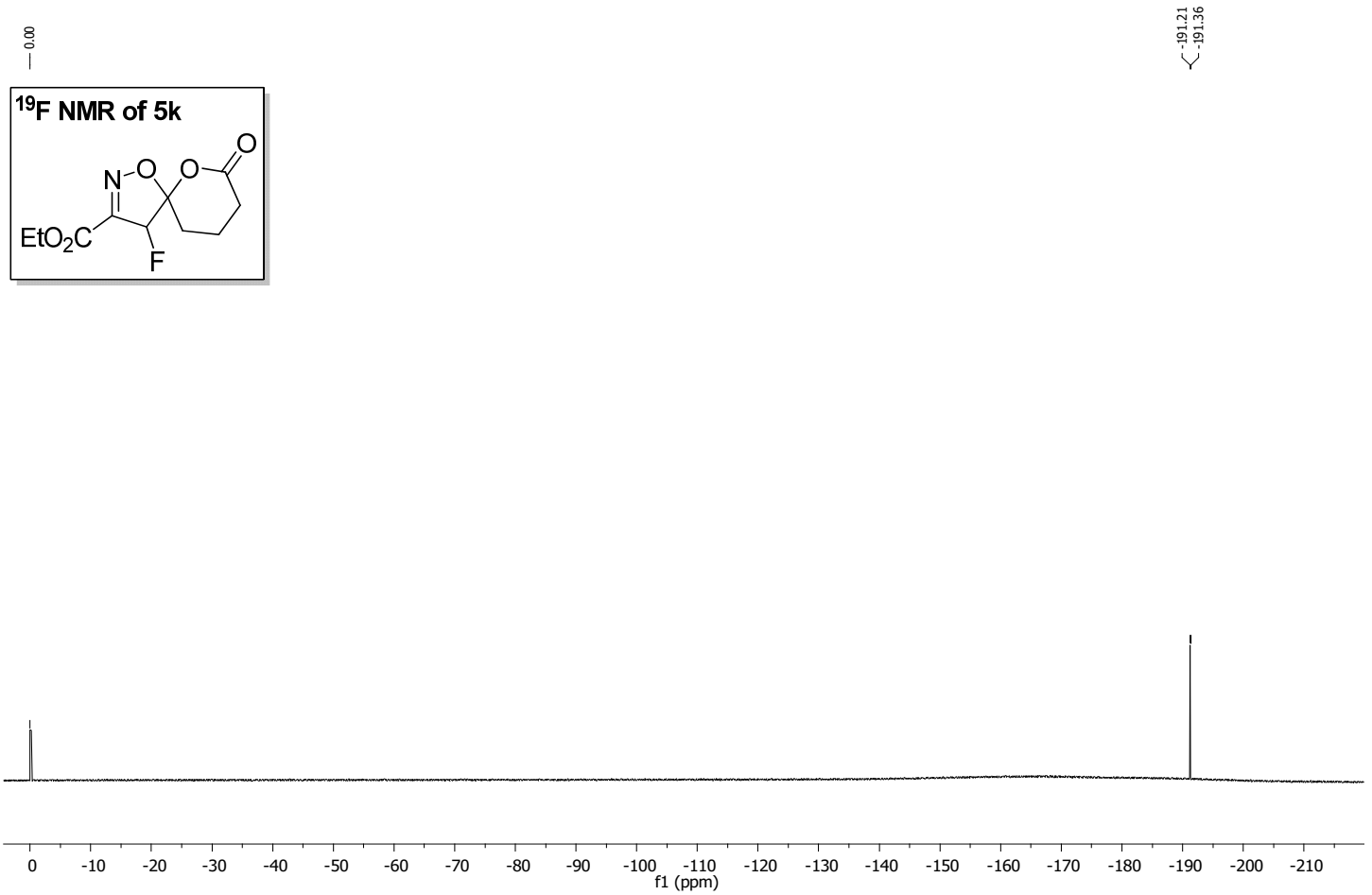

0.00
19F NMR of 5i'
-192.60
-192.74
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

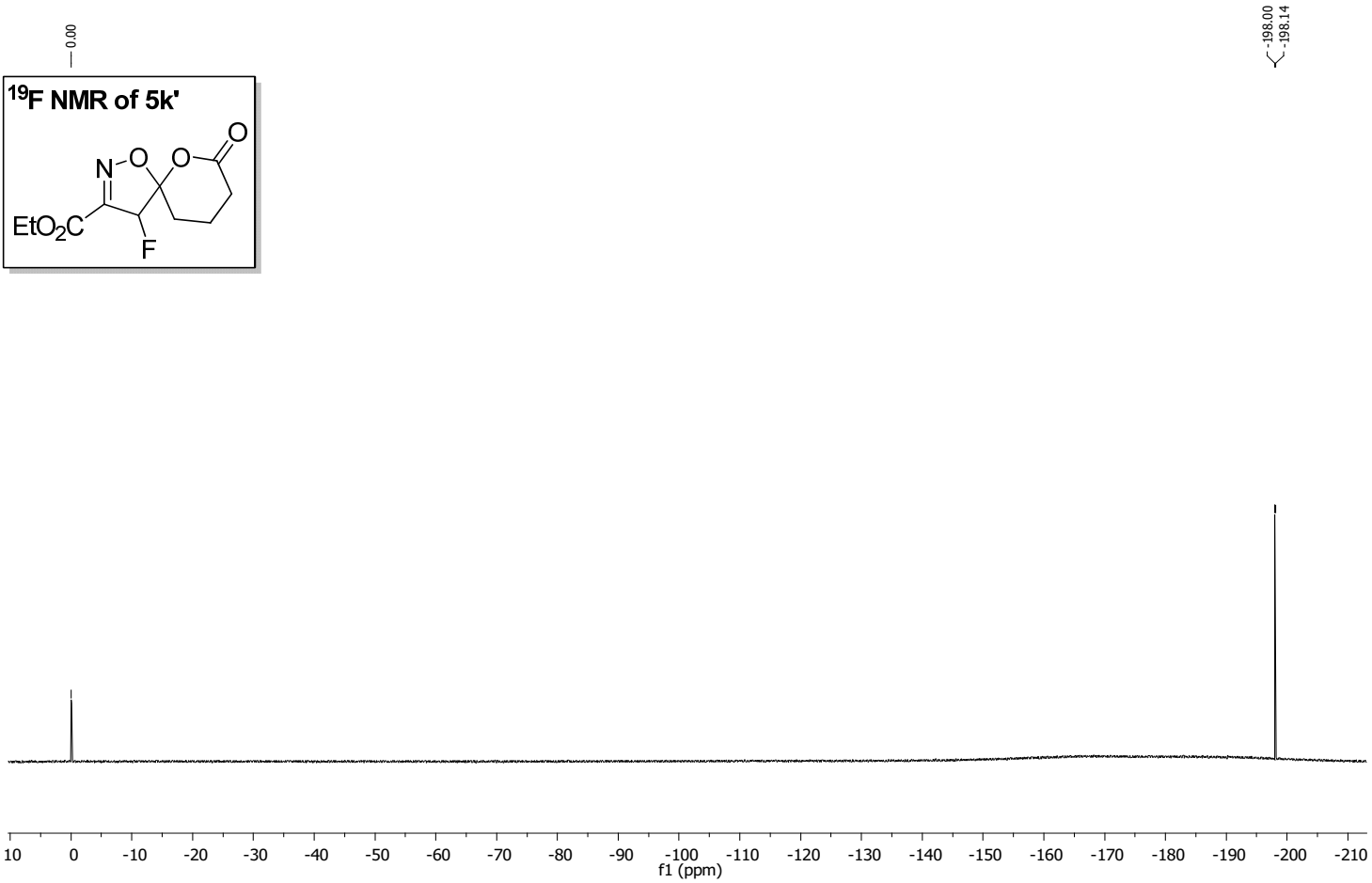
^{1}H/^{13}C NMR of 5j/5j'
Cl
N
O
O
O
F
Cl
7.46 7.44 7.44 7.43 7.42 7.39 7.38 7.37 7.36 7.26
5.90 5.79
2.91 2.90 2.89 2.88 2.86 2.85 2.75 2.74 2.73 2.71 2.70 2.68 2.67 2.66 2.64 2.62
2.35 2.34 2.34 2.32 2.31 2.31 2.30 2.30 2.29 2.27 2.25 2.25 2.24 2.09 2.07 2.07 2.07 2.06 2.06 2.05 2.04
3.02
1.07
1.00
2.06
2.01
1.06
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 0.0
f1 (ppm)
168.05
162.60
162.47
135.93
132.07
128.38
125.33
110.67
110.46
99.57
98.02
29.29
23.60
23.54
15.40
15.39
0.01
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-0.00
-187.63
-187.77
19F NMR of 5j
Cl
N
O
O
O
F
Cl
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


-0.00
-191.44
-191.58
19F NMR of 5j'
Cl
N
O
O
O
F
Cl
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


1H/13C NMR of 5k/5k'
EtO2C
F
f1 (ppm)
f1 (ppm)


0.00
-191.21
-191.36
19F NMR of 5k
O
N
O
O
EtO2C
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


0.00
-198.00
-198.14
19F NMR of 5k'
O
N
O
O
EtO2C
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)