

Supplementary Materials

2-Aryl-6-polyfluoroalkyl-4-pyrones as promising R^F-building-blocks: synthesis and application for construction of fluorinated azaheterocycles

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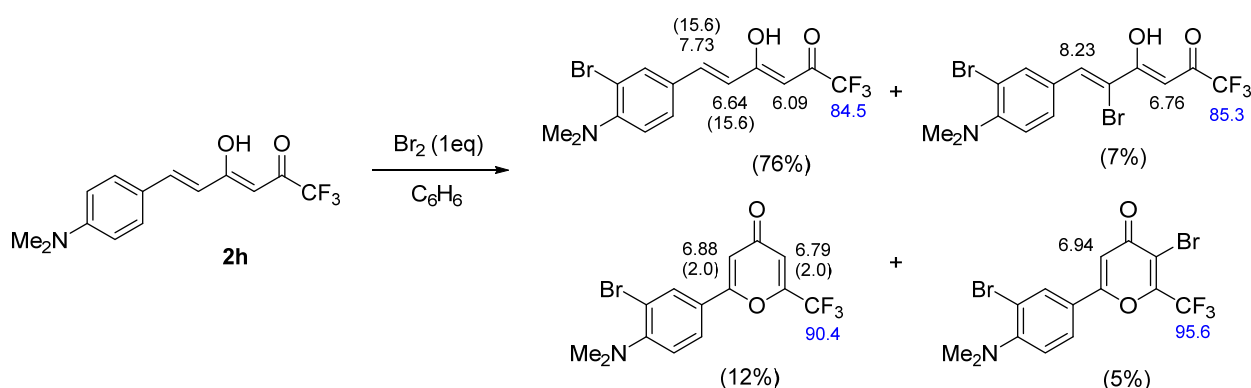
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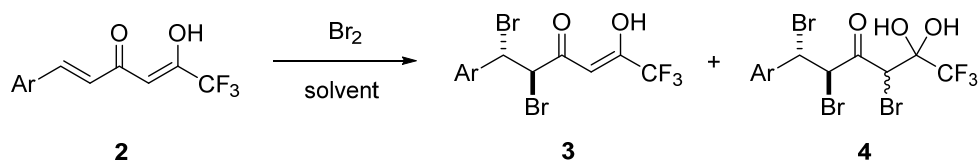
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Scheme S1. Reaction of (3*Z*,5*E*)-6-(4-(dimethylamino)phenyl)-1,1,1-trifluoro-4-hydroxyhexa-3,5-dien-2-one with Br₂ in benzene.



The presence of the strong donor and moderate basic substituent completely changed the composition of the reaction mixture in the case of dimethylaminophenyl derivative **2h**. Thus, when one equivalent of bromine was used in benzene, selective bromination of the aromatic fragment occurred with subsequent partial bromination at the double bond and methylene group followed by spontaneous dehydrobromination and ring closure to corresponding pyrones. The characteristic signals and coupling constants (in parentheses) in the ¹H (in black) and ¹⁹F (in blue) NMR spectra of the reaction mixture after benzene evaporation are shown in the scheme. Complete bromination of the dimethylaminophenyl group follows from the absence of signals for aromatic protons with $\delta < 7.5$ ppm. The treatment of enedione **2h** with a threefold excess of bromine led to a complex mixture of products. The absence of signals in the ¹⁹F NMR spectrum of the reaction mixture suggests that the reaction was accompanied by detrifluoroacetylation.

Table S1. Composition of reaction mixtures of bromination of enediones **2**.

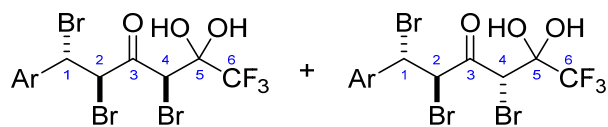
Ar	2,3,4	Br ₂ , equiv.	Solvent	2:3:4 ratio ^a
4-FC ₆ H ₄	b	1.0	dioxane	29:65:6
4-FC ₆ H ₄	b	1.3	dioxane	4:75:21
4-FC ₆ H ₄	b	1.0	<i>t</i> -BuOMe	17:(31+4 ^b):(39+9 ^b)
4-FC ₆ H ₄	b	1.0	CS ₂	25:(65+2 ^b):(7+1 ^b)
4-FC ₆ H ₄	b	1.0	AcOH	74:(7+2 ^b):(16+1 ^b)
4-FC ₆ H ₄	b	1.0	CH ₂ Cl ₂	42:(37+2 ^b):19
4-FC ₆ H ₄	b	1.5	CH ₂ Cl ₂	11:45:43
4-FC ₆ H ₄	b	2.5	CH ₂ Cl ₂	0:7 ^b :93
4-FC ₆ H ₄	b	1.0	benzene	12:77:11
4-FC ₆ H ₄	b	1.2	benzene	0:(75+4 ^b):(19+2 ^b)
4-FC ₆ H ₄	b	2.2	benzene	0:(48+9 ^b):(32+10 ^b)
Ph	a	1.0	CH ₂ Cl ₂	0:(86+2 ^b):12
Ph	a	1.0	benzene	55:28:17
Ph	a	2.2	benzene	0:(27+15 ^b):(42+16 ^b)
4-ClC ₆ H ₄	c	1.0	benzene	60:(9+2 ^b):(27+2 ^b)
4-ClC ₆ H ₄	c	2.2	benzene	0:(18+21 ^b):(47+13 ^b)
4-ClC ₆ H ₄	c	2.1	CHCl ₃	0:5 ^b :95
3-NO ₂ C ₆ H ₄	e	1.0	benzene	51:(14+3 ^b):(28+4 ^b)
3-NO ₂ C ₆ H ₄	e	2.0	CHCl ₃	0:(38+3 ^b):(55+4 ^b)
4-MeC ₆ H ₄	f	2.0	CHCl ₃	0:(25+9 ^b):(43+23 ^b)
4-MeOC ₆ H ₄	g	1.0	benzene	3:75:22
4-MeOC ₆ H ₄	g	2.0	CHCl ₃	0:(21+15 ^b):(43+22 ^b)
2-C ₄ H ₃ S	i	1.0	benzene	9:(80+8 ^c):3
2-C ₄ H ₃ S	i	1.0	CHCl ₃	16:(72+1 ^b +6 ^c):5
2-C ₄ H ₃ S	i	2.5	CH ₂ Cl ₂	0:0:(52+48 ^d)

^a Based on ¹H and ¹⁹F NMR spectra^b Cyclized to dihydropyrone **B** or **C**^c A product of dehydrobromination **A** was spontaneously formed^d A product of aromatic bromination was also formed

Table S2. Characteristic chemical shifts in the ^1H and ^{19}F NMR spectra of compounds **3** used for the analysis of reaction mixtures, δ , ppm (J , Hz)

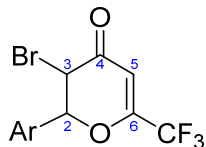
Ar	3	CF_3	6-CH	5-CH	3-CH
Ph	a	86.0	5.37 (11.6)	4.94 (11.6)	6.22
4-FC ₆ H ₄	b	86.0	5.36 (11.6)	4.88 (11.6)	6.21
4-ClC ₆ H ₄	c	86.0	5.34 (11.6)	4.88 (11.6)	6.20
4-BrC ₆ H ₄	d	86.0	5.26 (11.6)	4.81 (11.6)	6.13
3-O ₂ NC ₆ H ₄	e	86.0	5.45 (11.6)	4.94 (11.6)	6.23
4-MeC ₆ H ₄	f	86.0	5.35 (11.6)	4.93 (11.6)	6.21
4-MeOC ₆ H ₄	g	86.0	5.37 (11.6)	4.93 (11.6)	6.21
2-C ₄ H ₃ S	i	86.0	5.72 (11.4)	4.92 (11.4)	6.20

Table S3. Characteristic chemical shifts in the ^1H and ^{19}F NMR spectra of compounds **4** used for the analysis of reaction mixtures, δ , ppm (J , Hz)



Ar	4	CF ₃	1-CH	2-CH	4-CH	C(OH) ₂
Ph (<i>major</i>)	a	—	5.39 (11.3)	5.30 (11.3)	4.96	4.46; 4.79
Ph (<i>minor</i>)	a	—	5.30 (11.3)	5.24 (11.3)	5.00	4.04; 4.63
4-FC ₆ H ₄ (<i>major</i>)	b	79.7	5.38 (11.3)	5.24 (11.3)	4.95	4.48; 4.80
4-FC ₆ H ₄ (<i>minor</i>)	b	79.9	5.29 (11.3)	5.19 (11.3)	4.99	4.03; 4.61
4-ClC ₆ H ₄ (<i>major</i>)	c	79.7	5.35 (11.3)	5.24 (11.3)	4.95	4.45; 4.79
4-ClC ₆ H ₄ (<i>minor</i>)	c	—	5.27 (11.3)	5.19 (11.3)	4.98	3.94; 4.58
3-O ₂ NC ₆ H ₄ (<i>major</i>)	e	79.7	5.46 (11.3)	5.28 (11.3)	4.96	4.37; 4.75
3-O ₂ NC ₆ H ₄ (<i>minor</i>)	e	79.8	5.38 (11.2)	5.24 (11.2)	4.99	3.96; 4.58
4-MeC ₆ H ₄ (<i>major</i>)	f	79.7	5.37 (11.3)	5.29 (11.3)	4.96	4.43; 4.77
4-MeC ₆ H ₄ (<i>minor</i>)	f	79.8	5.28 (11.3)	5.23 (11.3)	5.00	4.01; 4.61
4-MeOC ₆ H ₄ (<i>major</i>)	g	79.7	5.40 (11.3)	5.29 (11.3)	4.96	4.48; 4.79
4-MeOC ₆ H ₄ (<i>minor</i>)	g	79.9	5.30 (11.3)	5.22 (11.3)	5.00	4.07; 4.50
2-C ₄ H ₃ S (<i>major</i>)	i	79.7	5.73 (11.1)	5.26 (11.1)	4.94	4.44; 4.78
2-(5-BrC ₄ H ₂ S) (<i>major</i>)	i-Br	—	5.61 (11.1)	5.16 (11.1)	4.96	4.44; 4.78

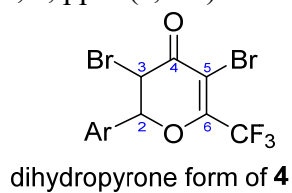
Table S4. Characteristic chemical shifts in the ^1H and ^{19}F NMR spectra of dihydropyrone form of **3** used for the analysis of reaction mixtures, δ , ppm (J , Hz)



dihydropyrone form of **3**

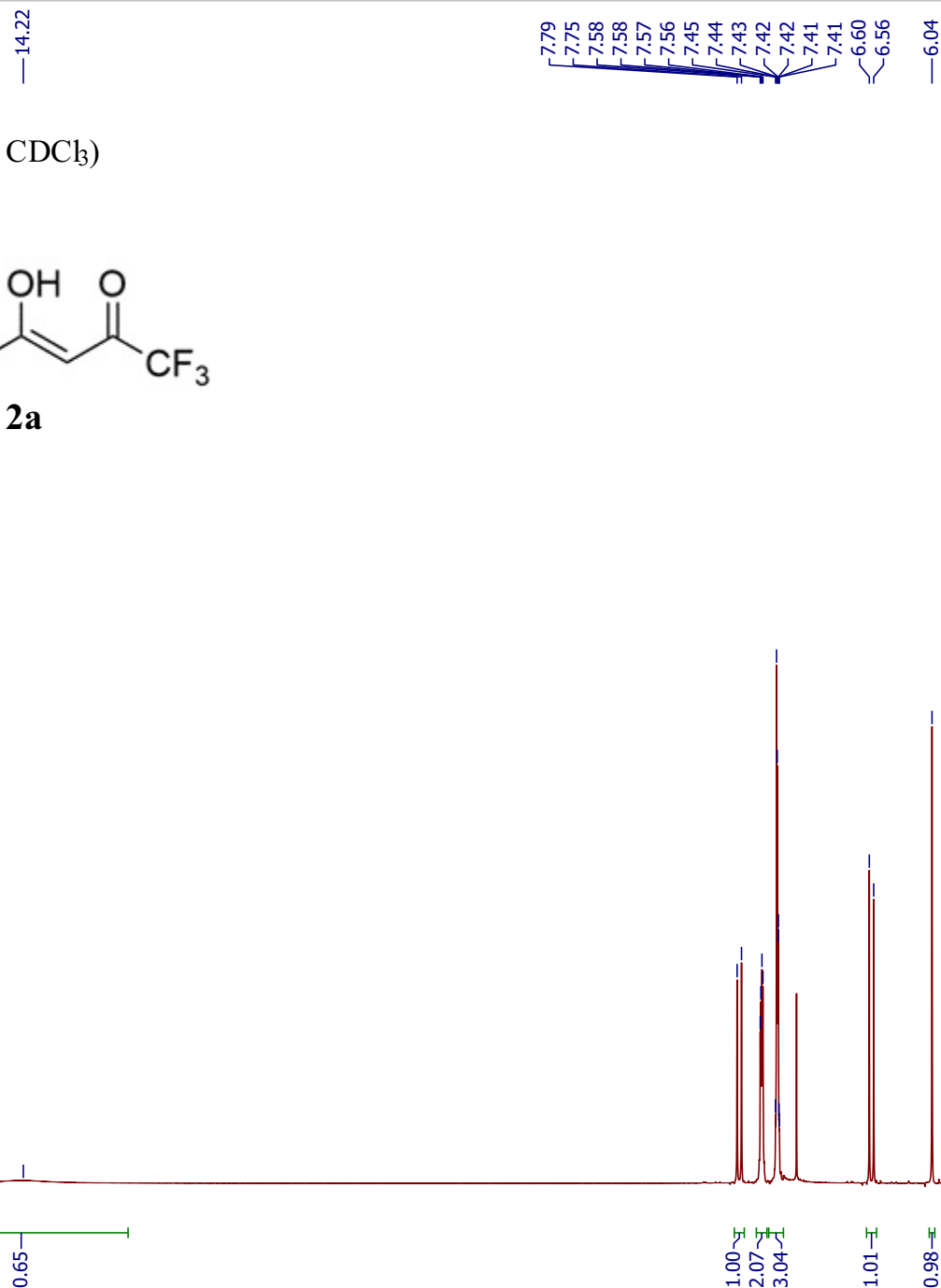
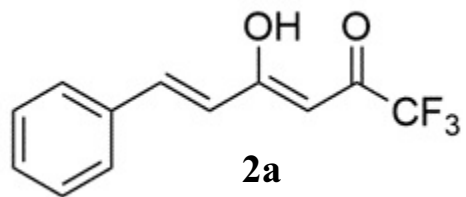
Ar	dihydropyrone form of 3	CF ₃	2-CH	3-CH	5-CH
Ph	a	—	5.56 (11.3)	5.37 (11.3)	5.85
4-FC ₆ H ₄	b	86.7	5.51 (11.3)	5.36 (11.3)	5.84
4-ClC ₆ H ₄	c	—	5.51 (11.3)	5.34 (11.3)	5.84
3-O ₂ NC ₆ H ₄	e	86.7	5.56 (11.6)	overlaped	5.85
4-MeC ₆ H ₄	f	86.6	5.56 (11.3)	5.36 (11.3)	5.84
4-MeOC ₆ H ₄	g	86.7	5.55 (11.3)	5.37 (11.3)	5.84

Table S5. Characteristic chemical shifts in the ^1H and ^{19}F NMR spectra of dihydropyrone form of **4** used for the analysis of reaction mixtures, δ , ppm (J , Hz)



Ar	dihydropyrone form of 4	CF ₃	2-CH	3-CH
Ph	a	—	5.80 (11.5)	5.44 (11.5)
4-FC ₆ H ₄	b	90.2	5.74 (11.5)	5.43 (11.5)
4-ClC ₆ H ₄	c	—	5.73 (11.5)	5.41 (11.5)
3-O ₂ NC ₆ H ₄	e	90.2	5.75 (11.3)	5.51 (11.3)
4-MeC ₆ H ₄	f	90.2	5.79 (11.5)	5.43 (11.6)
4-MeOC ₆ H ₄	g	90.2	5.79 (11.4)	5.45 (11.4)

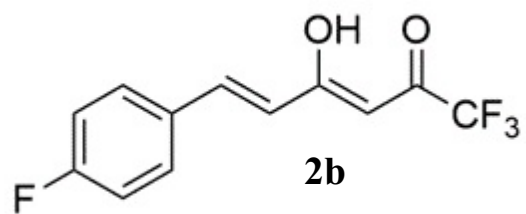
^1H NMR (500 MHz, CDCl_3)



^1H NMR (ppm)

S8

¹H NMR (500 MHz, CDCl₃)



14.24

7.75
7.72
7.58
7.57
7.56
7.55
7.14
7.12
7.10
6.52
6.48
6.02

1.03

1.04
2.07

2.16

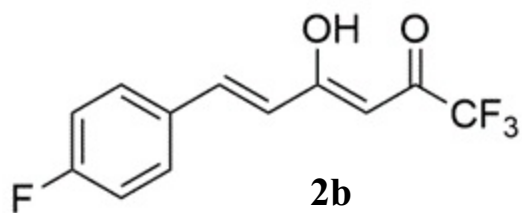
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1.00

¹H NMR (ppm)

S9

^{19}F NMR (471 MHz, CDCl_3)



84.65

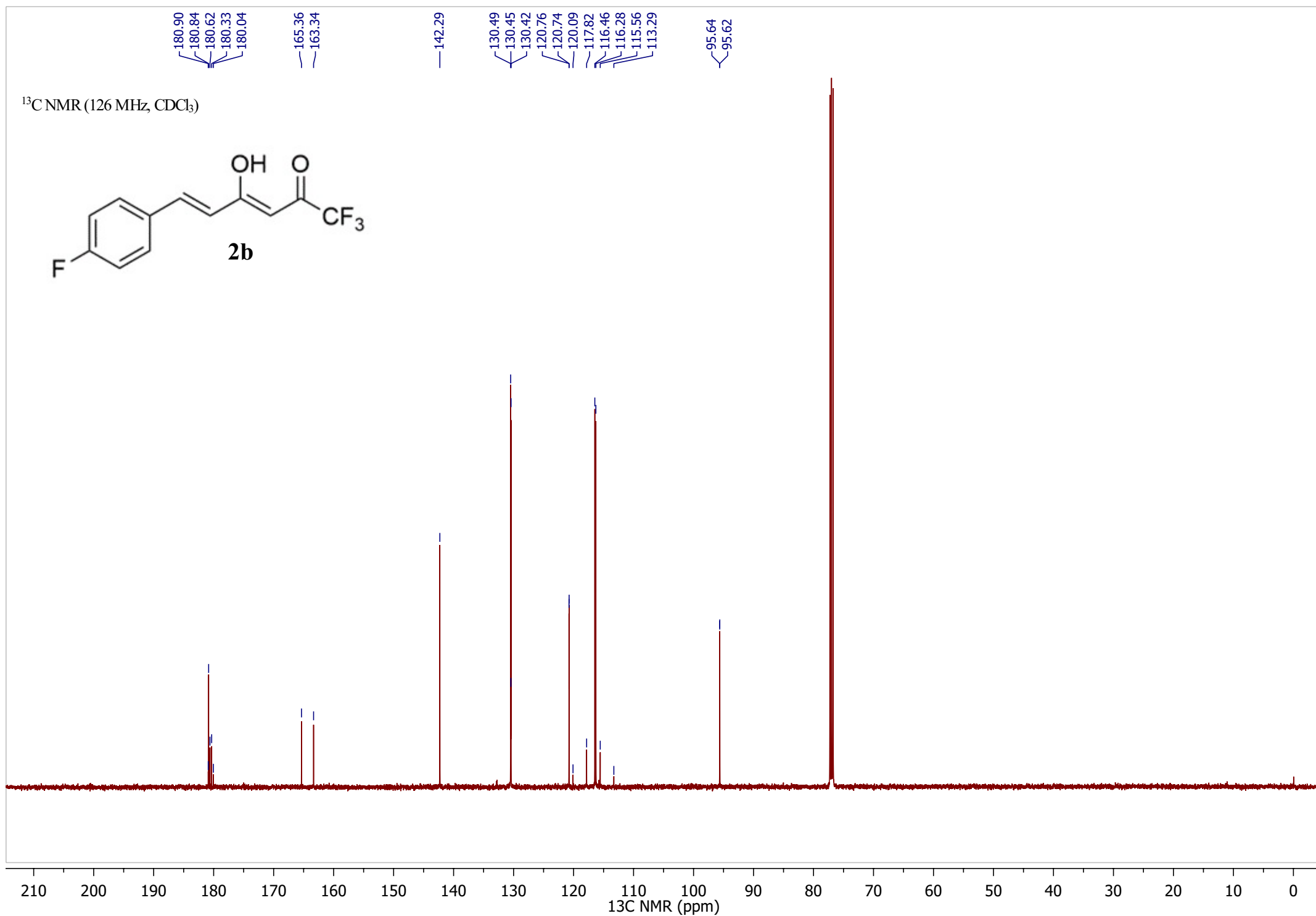
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53.94
53.94
53.93
53.93
53.92
53.92
53.91
53.90

3.02

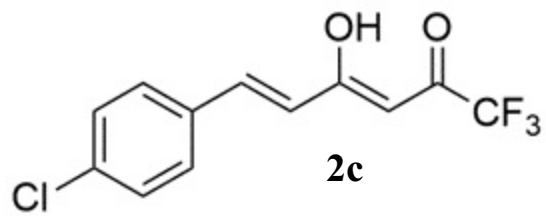
0.99

^{19}F NMR (ppm)

S10



^1H NMR (500 MHz, CDCl_3)



14.17

7.73

7.70

7.51

7.49

7.41

7.39

6.56

6.53

6.03

1.23

1.01

2.00

2.00

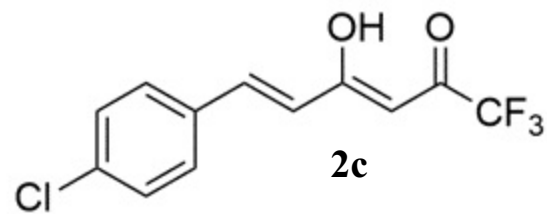
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0.97

^1H NMR (ppm)

S12

^{19}F NMR (471 MHz, CDCl_3)



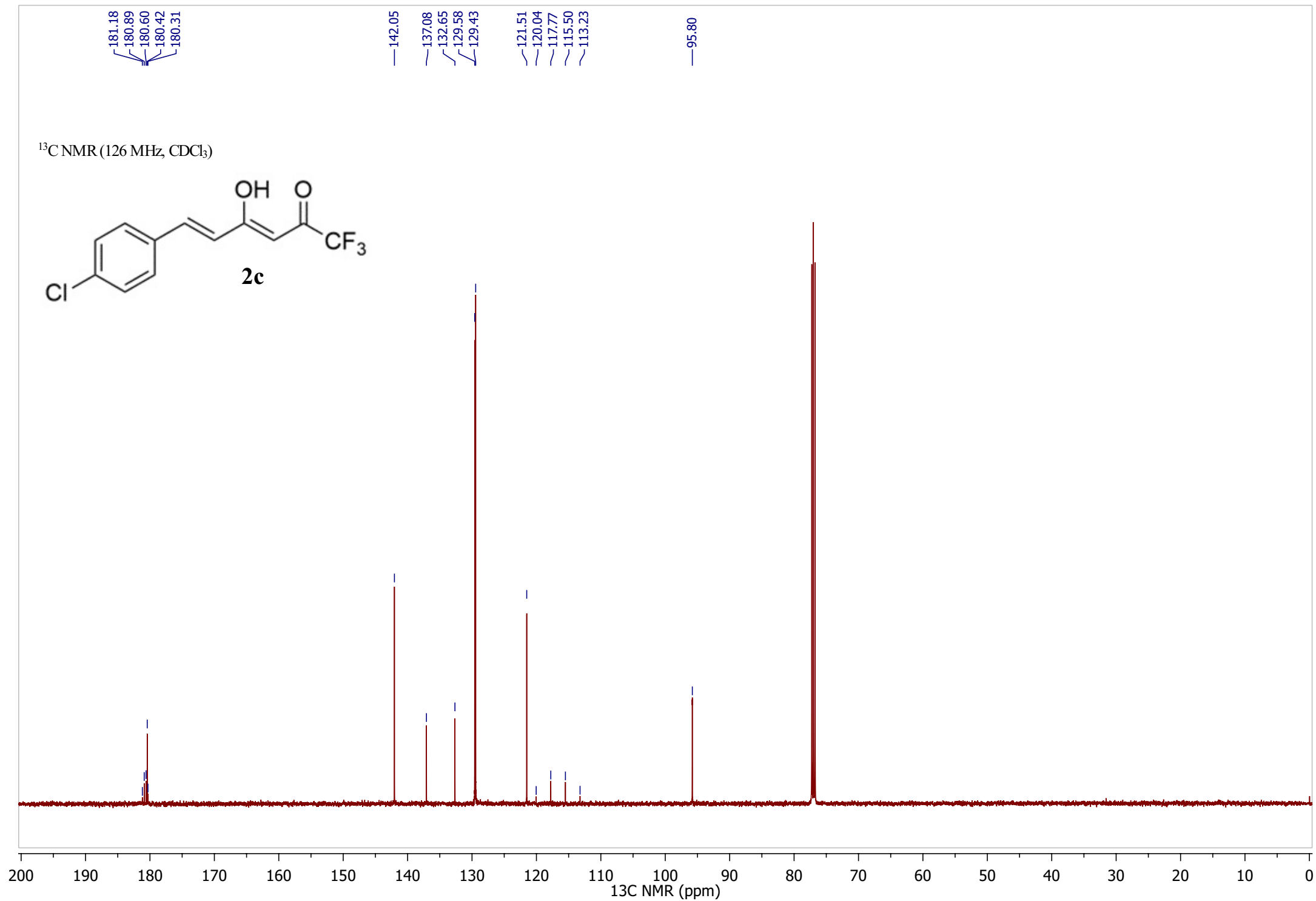
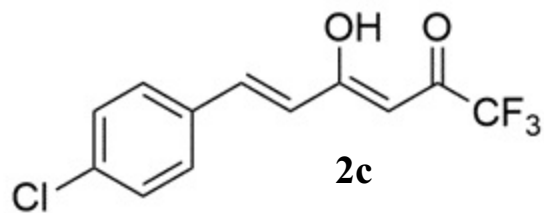
84.61

1.01

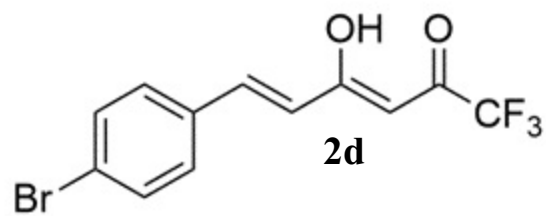
^{19}F NMR (ppm)

S13

^{13}C NMR (126 MHz, CDCl_3)

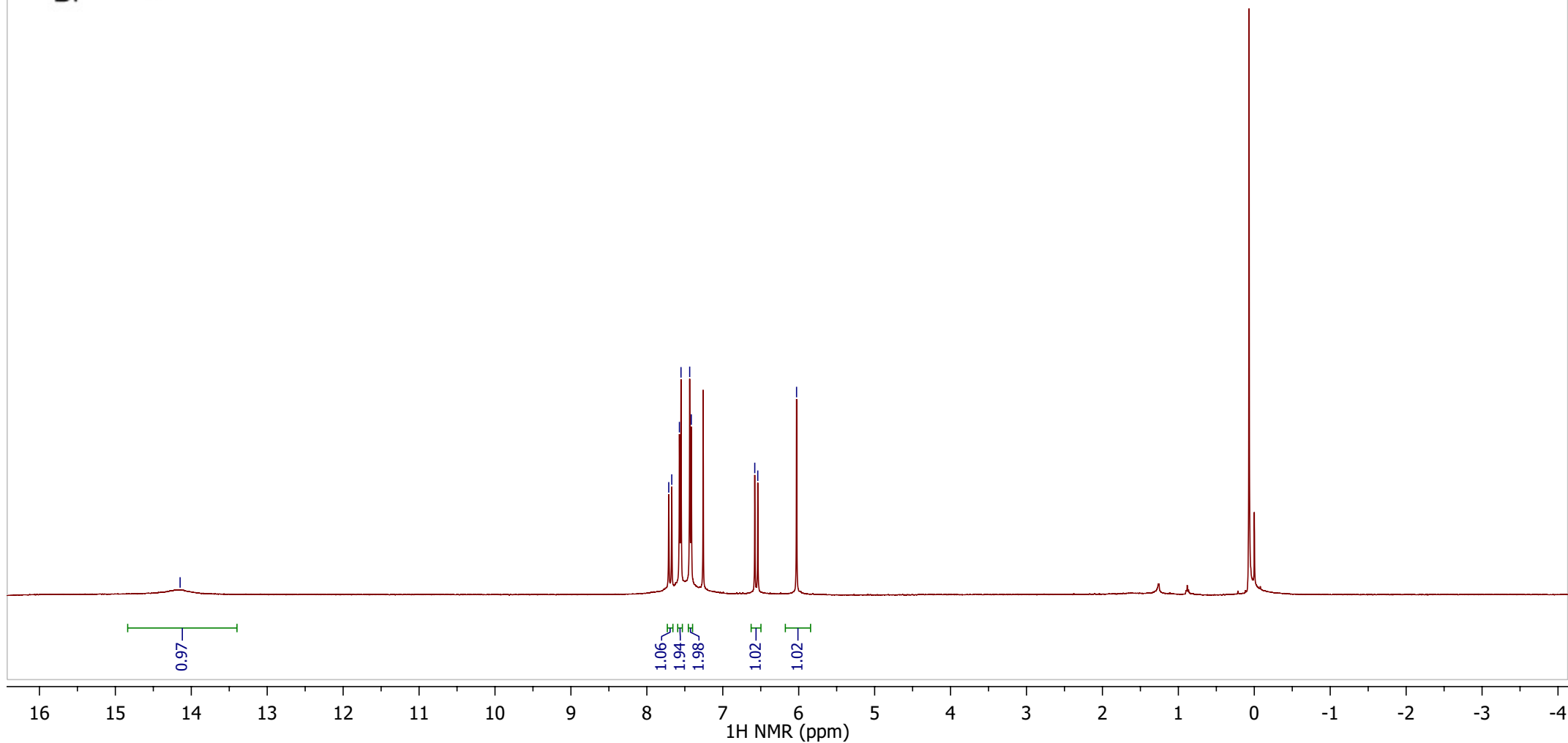


¹H NMR (400 MHz, CDCl₃)

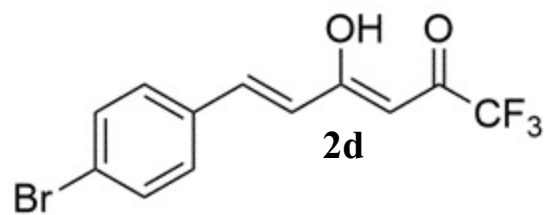


14.15

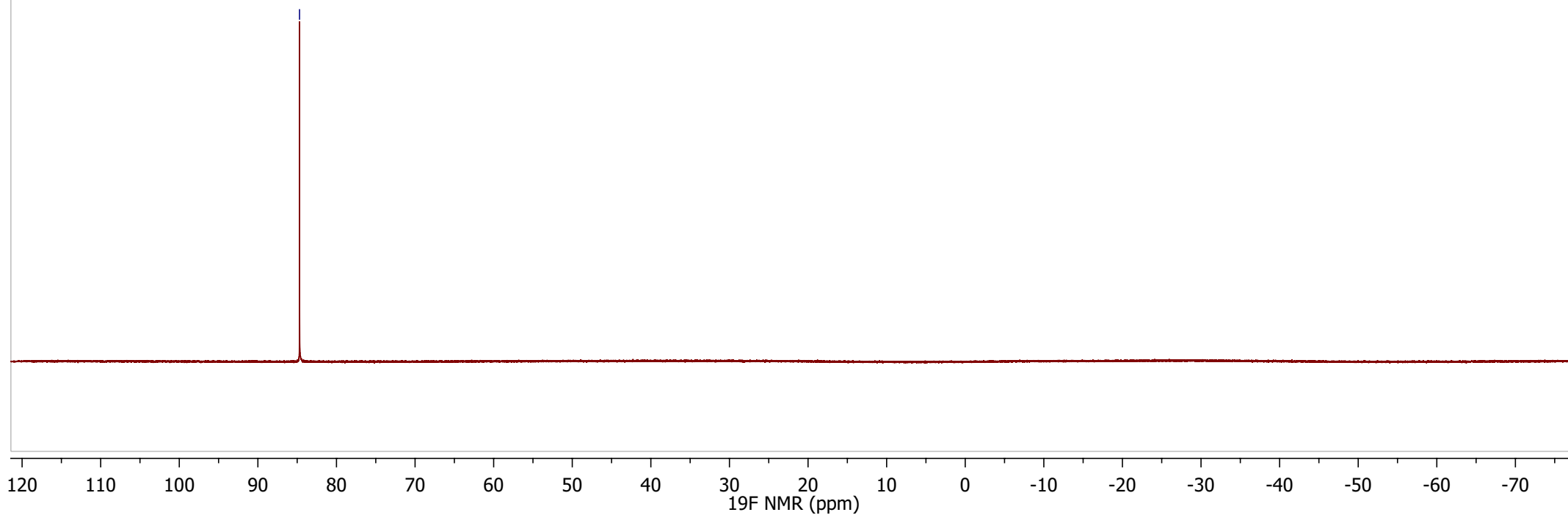
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6.58
6.54
6.03

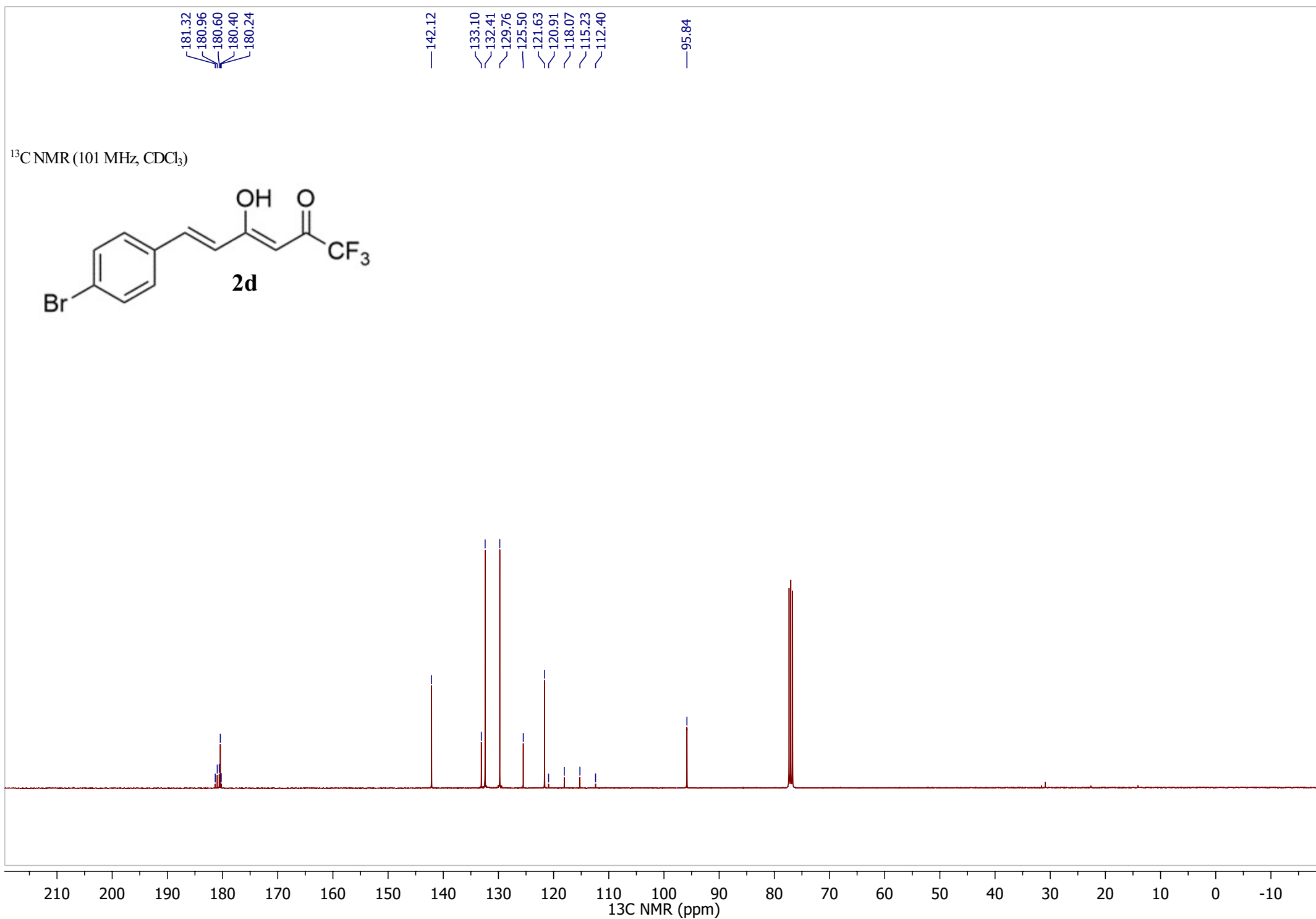


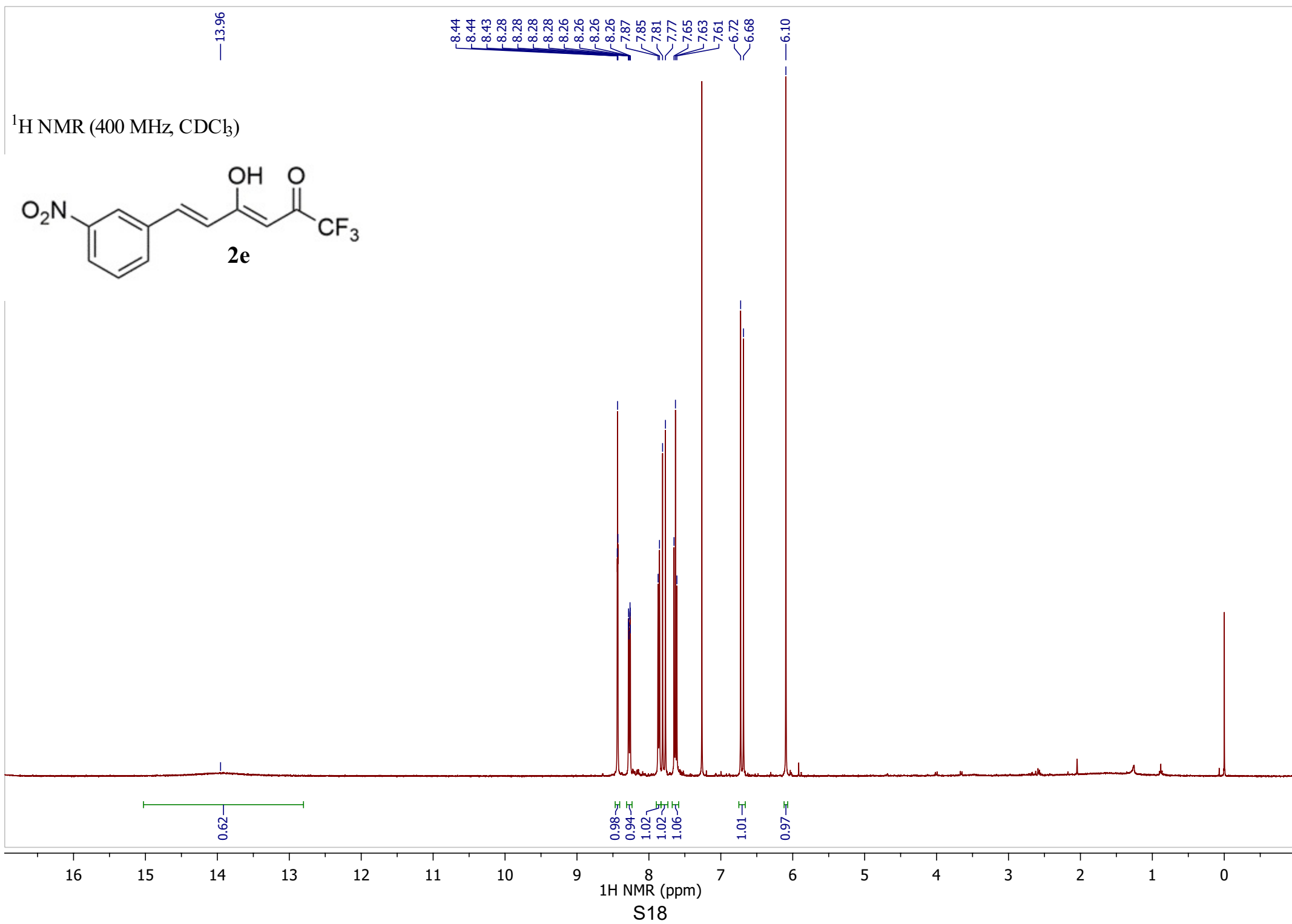
^{19}F NMR (376 MHz, CDCl_3)



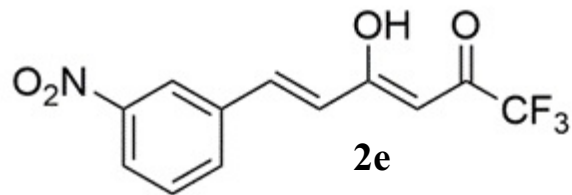
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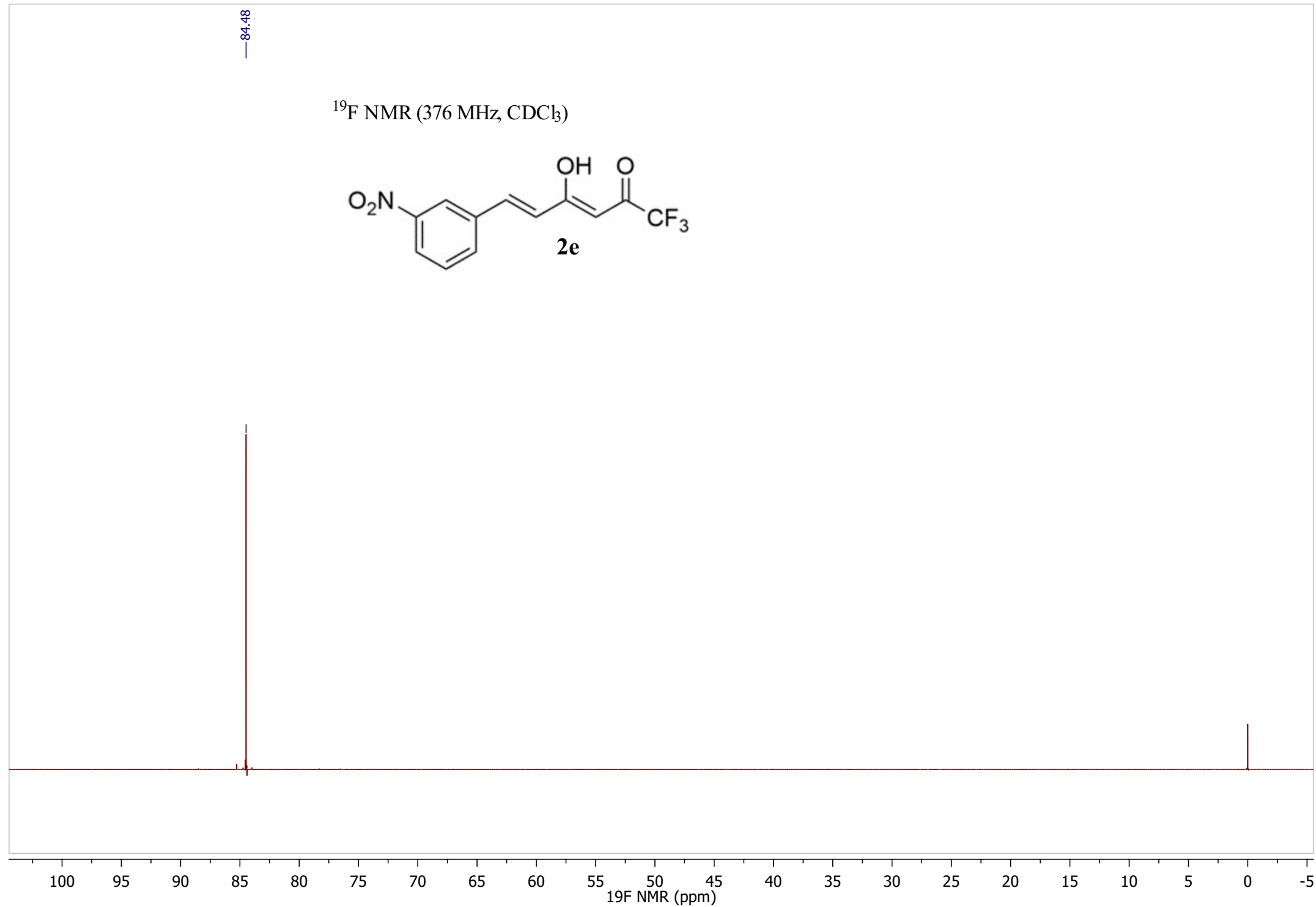




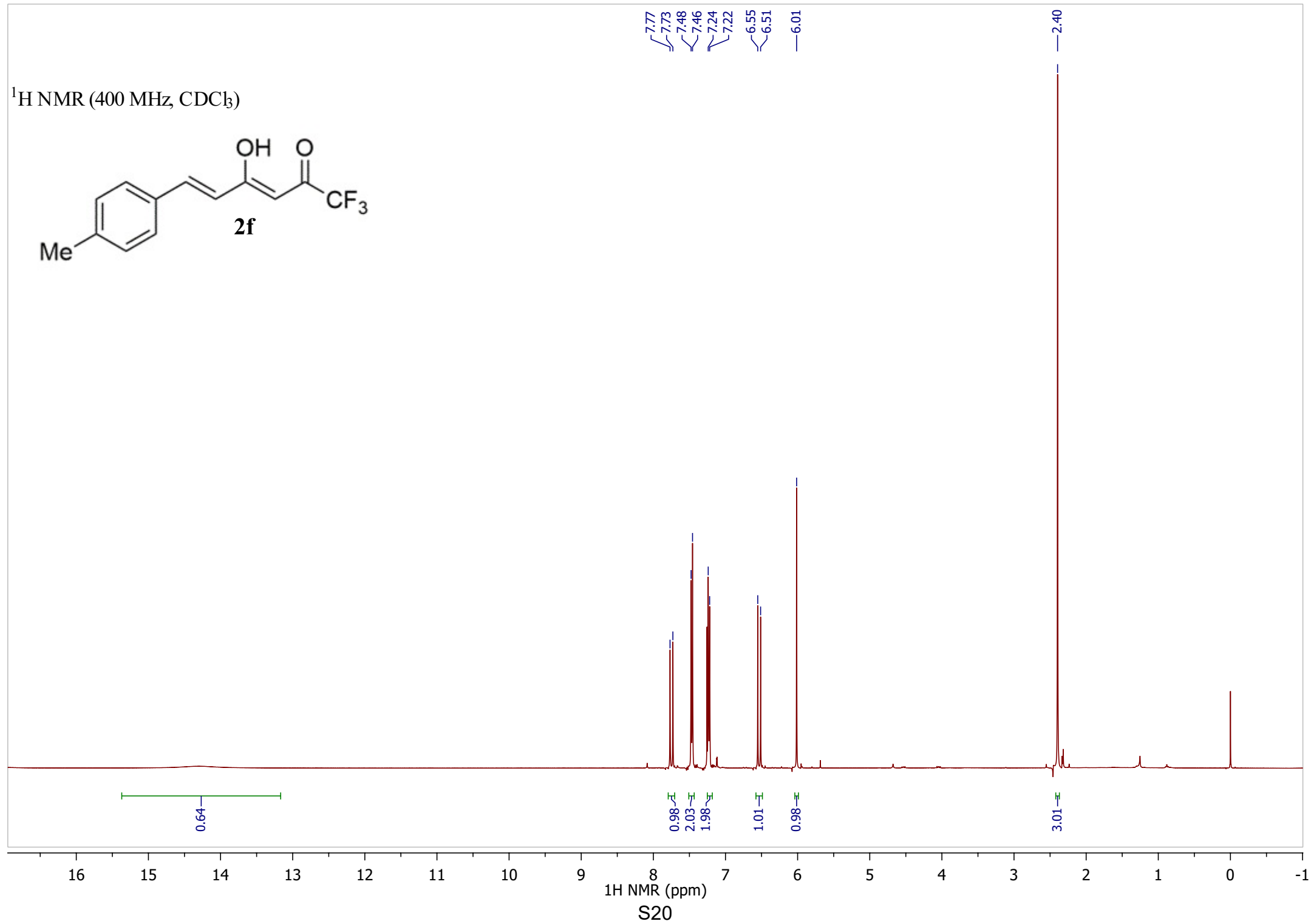
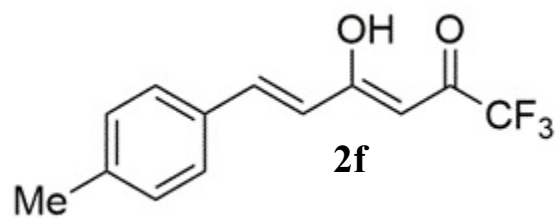
^{19}F NMR (376 MHz, CDCl_3)



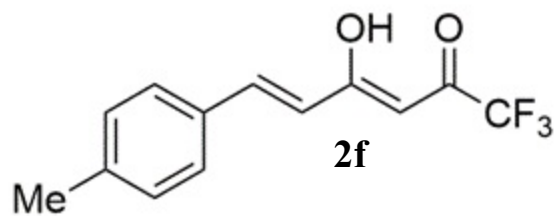
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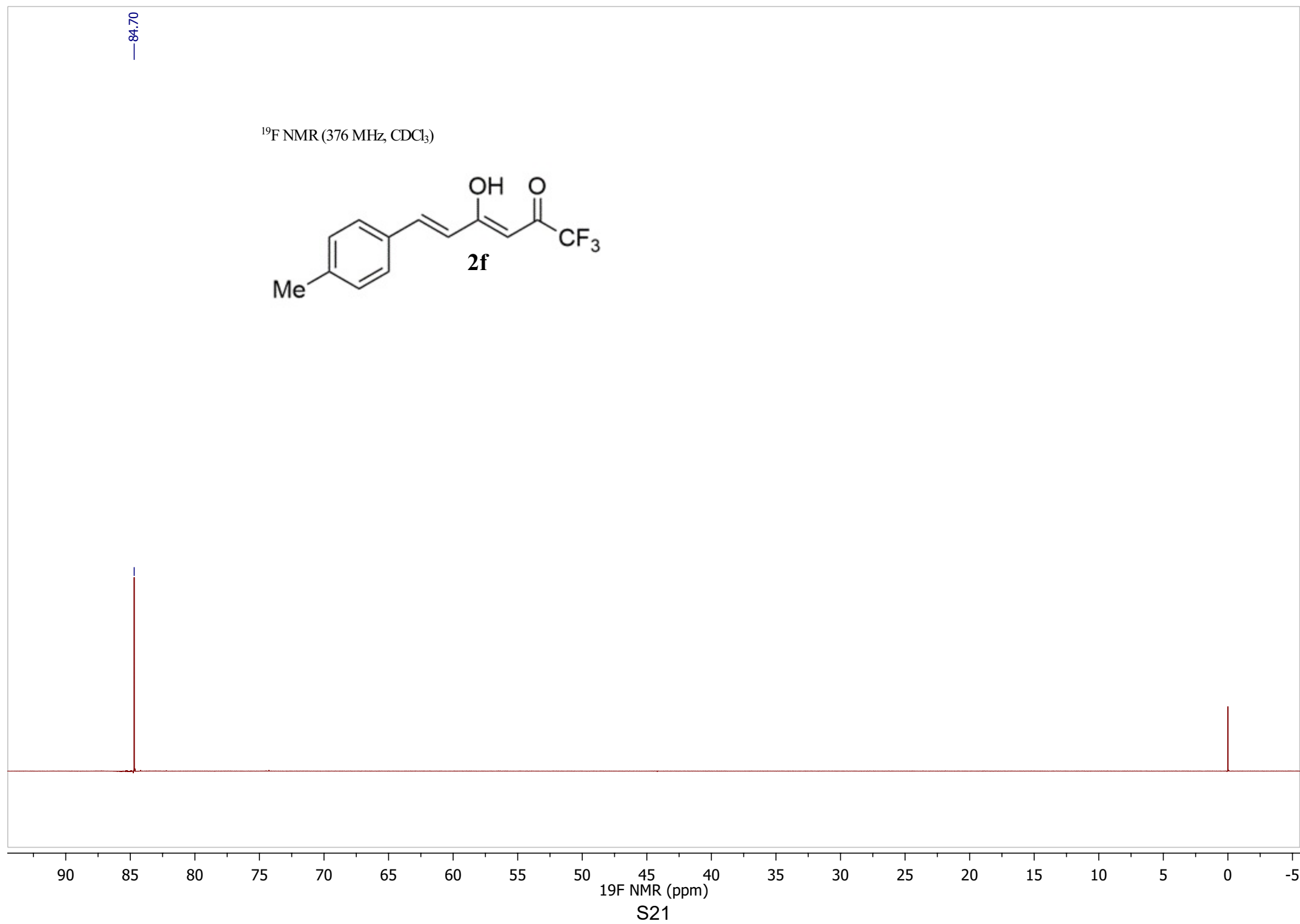
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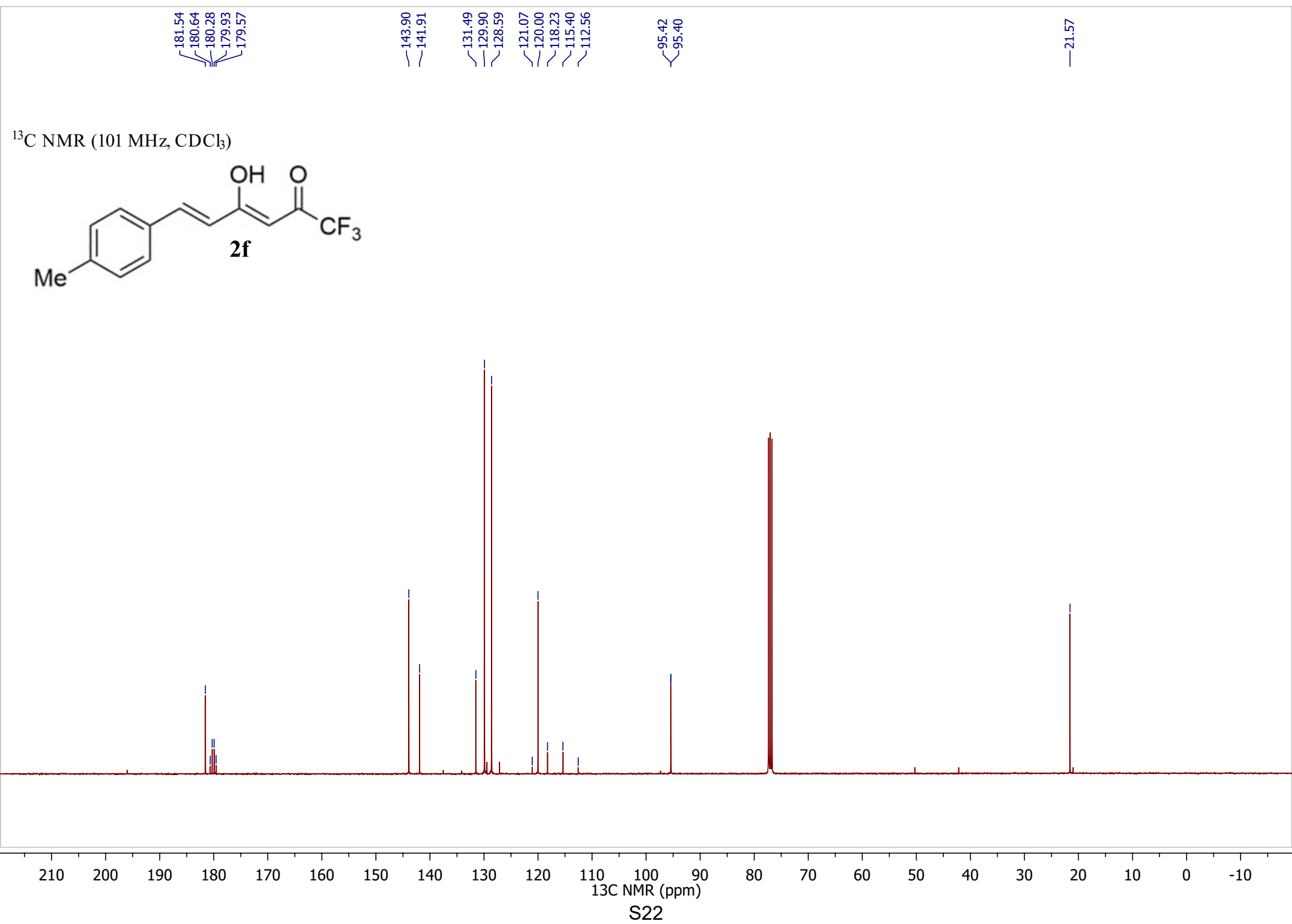


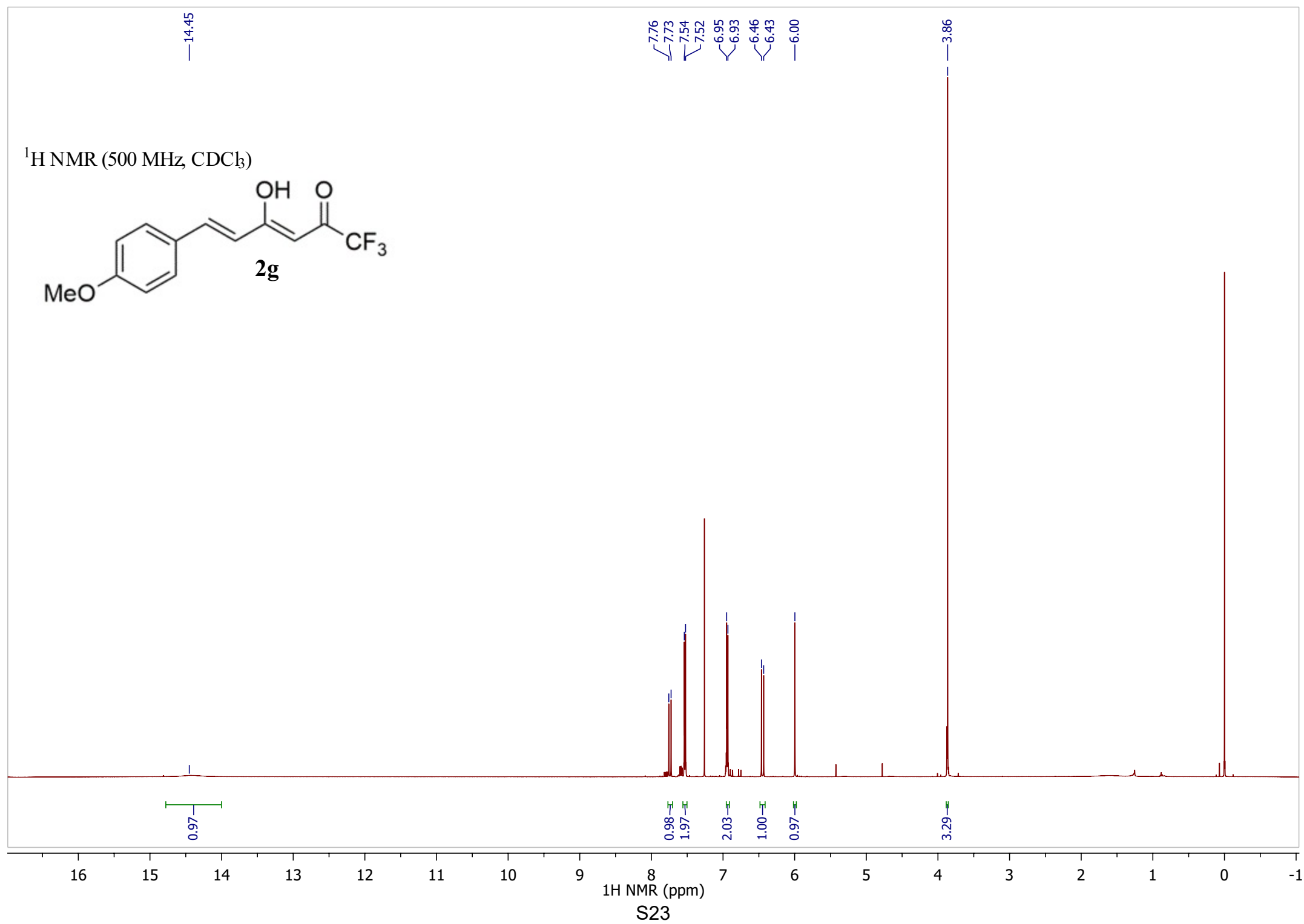
^{19}F NMR (376 MHz, CDCl_3)



—84.70

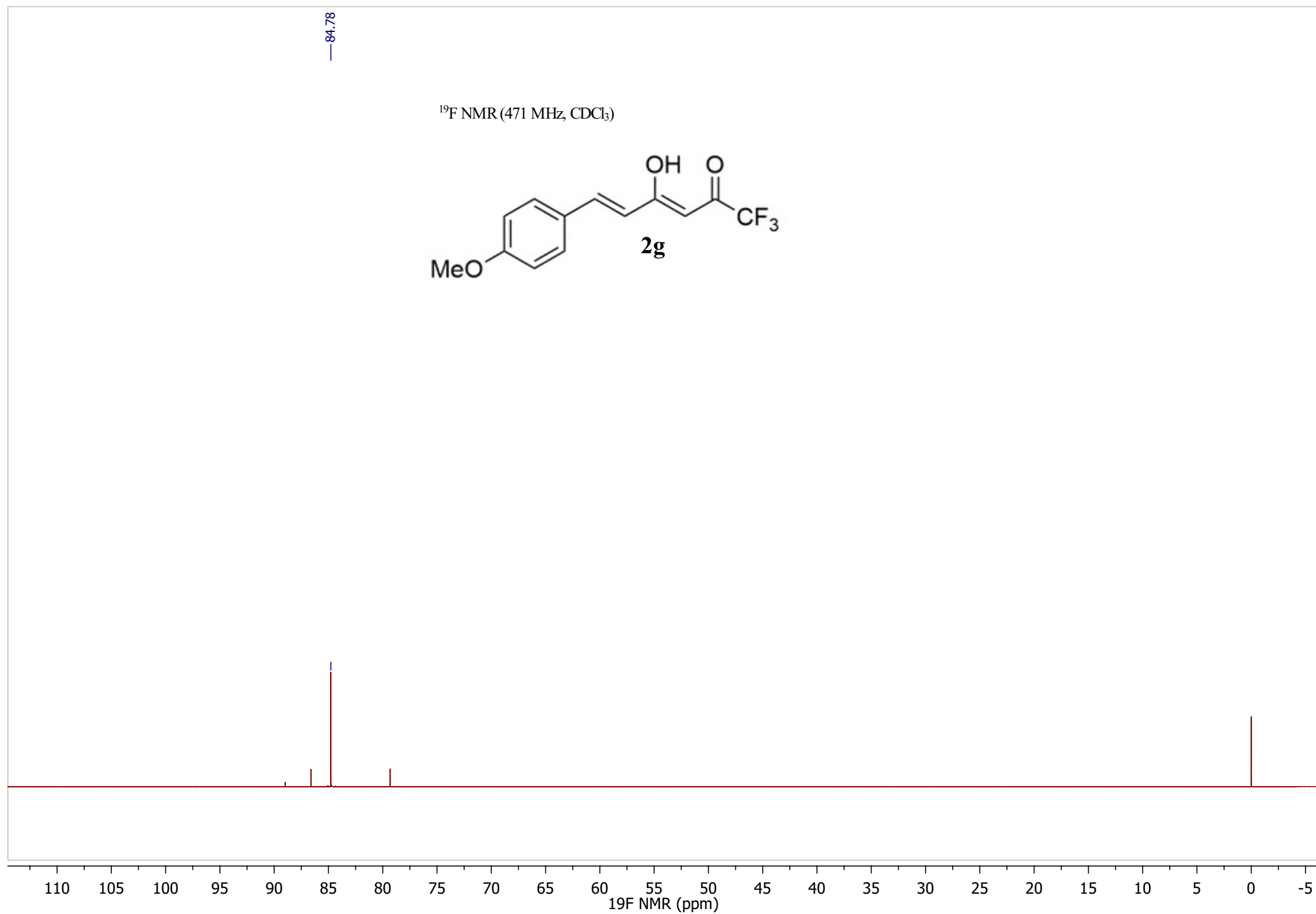
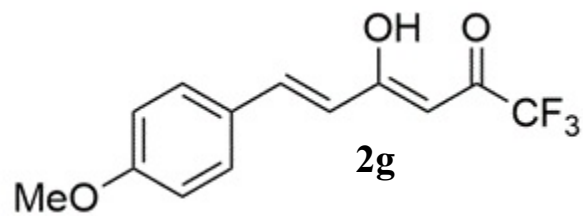






— 84.78

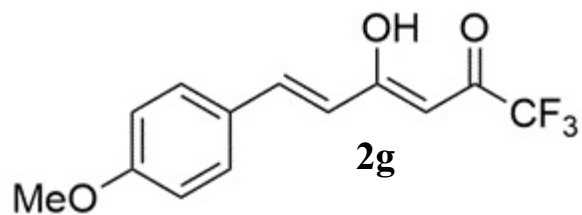
^{19}F NMR (471 MHz, CDCl_3)



^{19}F NMR (ppm)

S24

^{13}C NMR (101 MHz, CDCl_3)



181.90
180.21
179.86
179.50
179.14

162.25

143.71

130.45

126.95

121.14

118.55

118.30

115.47

114.65

112.64

95.19

95.18

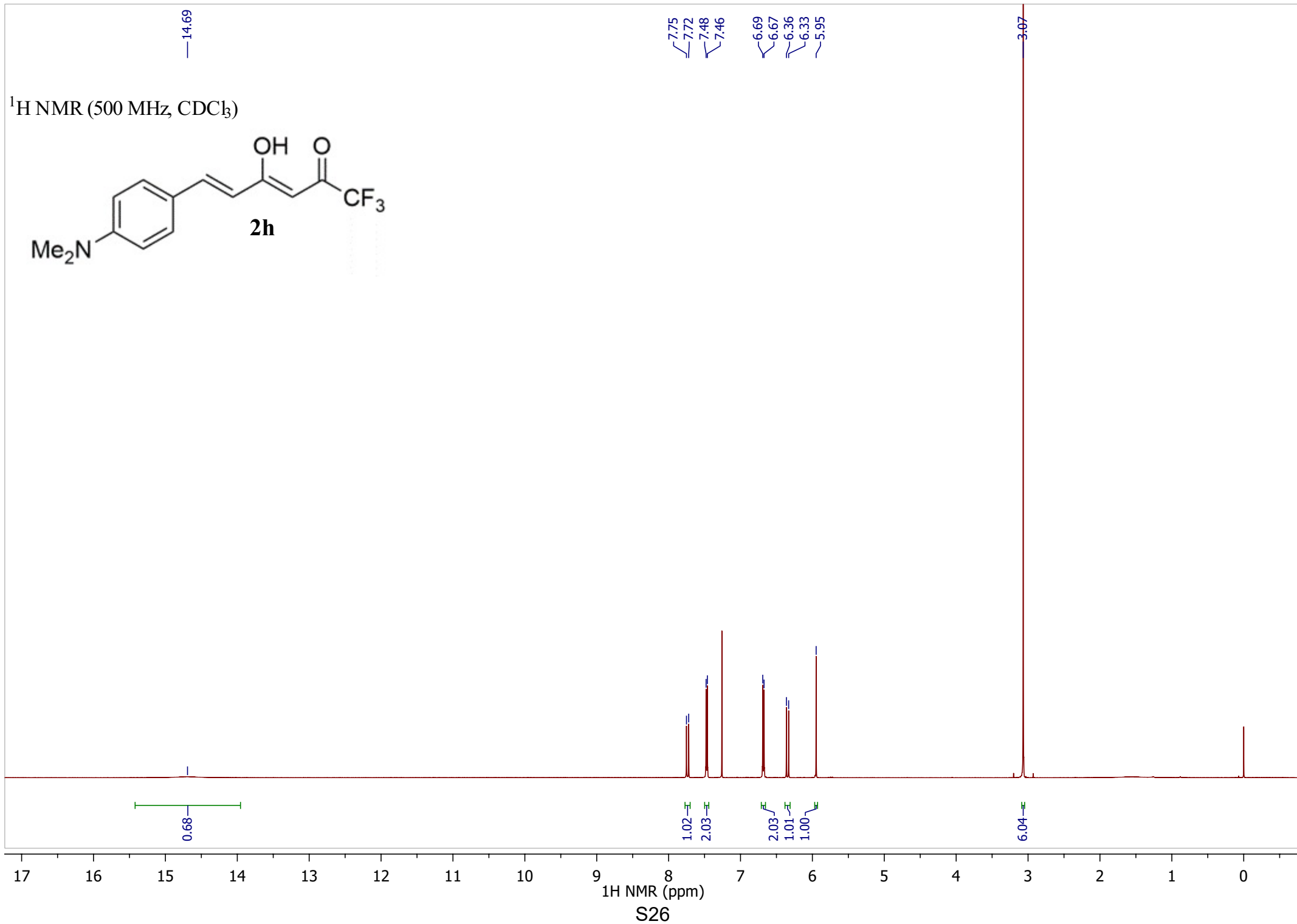
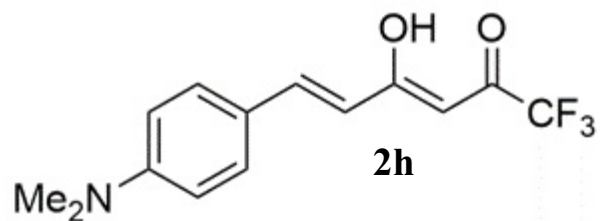
55.46

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

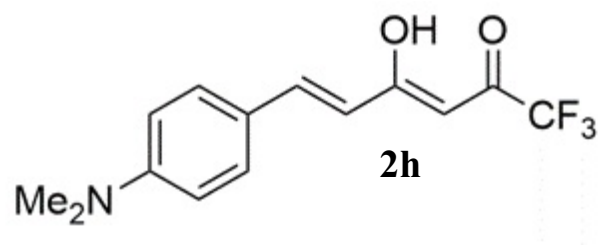
^{13}C NMR (ppm)

S25

^1H NMR (500 MHz, CDCl_3)



^{19}F NMR (471 MHz, CDCl_3)



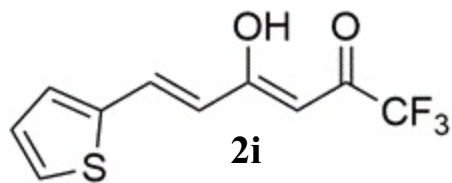
— 84.98



^{19}F NMR (ppm)

S27

¹H NMR (400 MHz, CDCl₃)



14.28

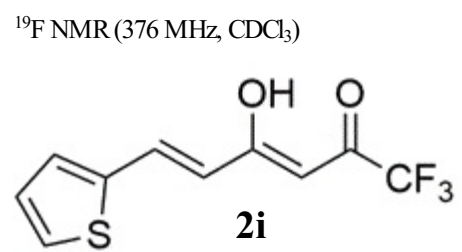
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7.34
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7.11
7.11
7.10
6.38
6.34
5.99

0.78

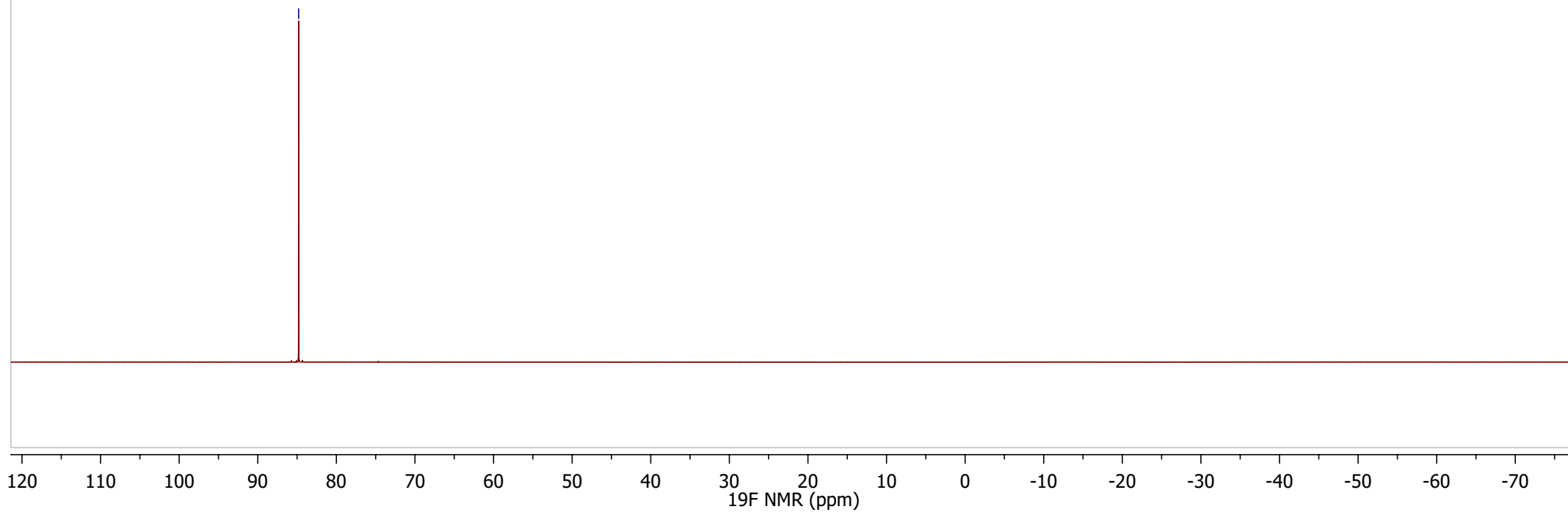
1.00
0.98
1.04
1.01
1.03
1.04

¹H NMR (ppm)

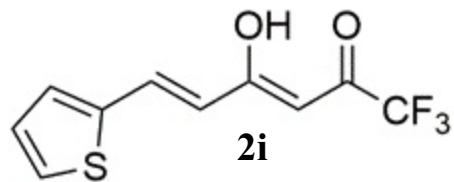
S28



84.80



¹³C NMR (101 MHz, CDCl₃)

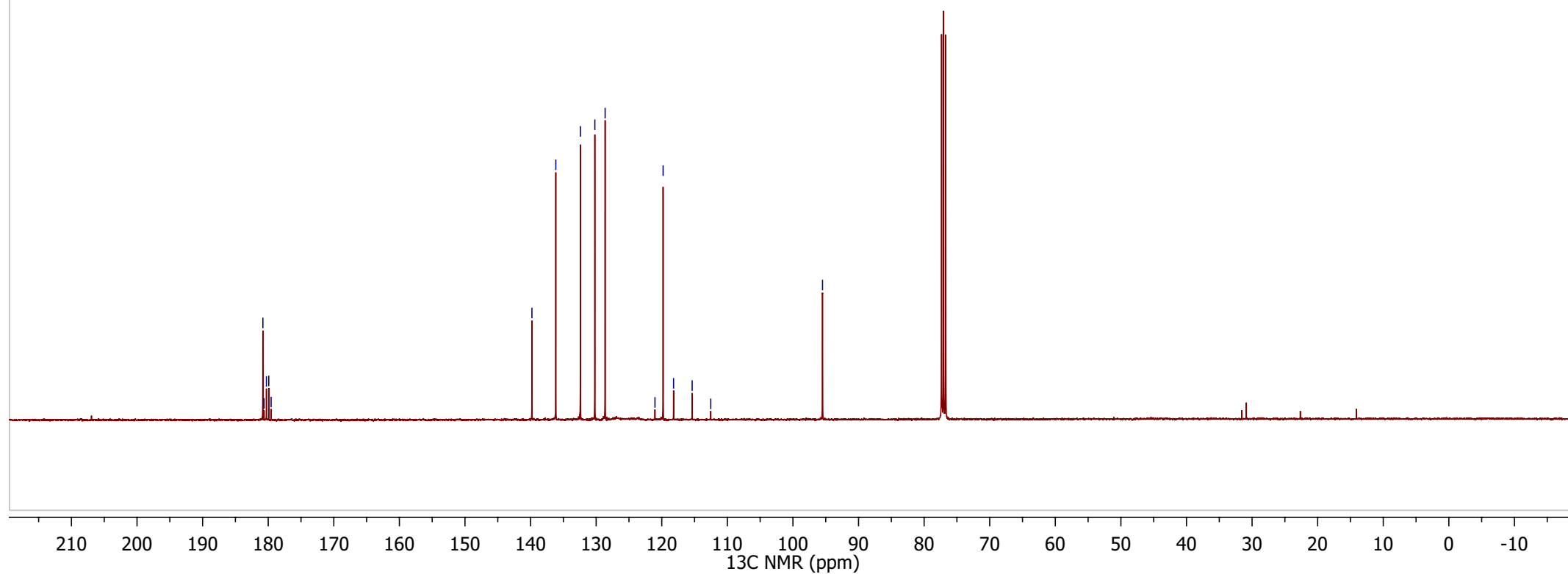


180.81
180.63
180.27
179.91
179.56

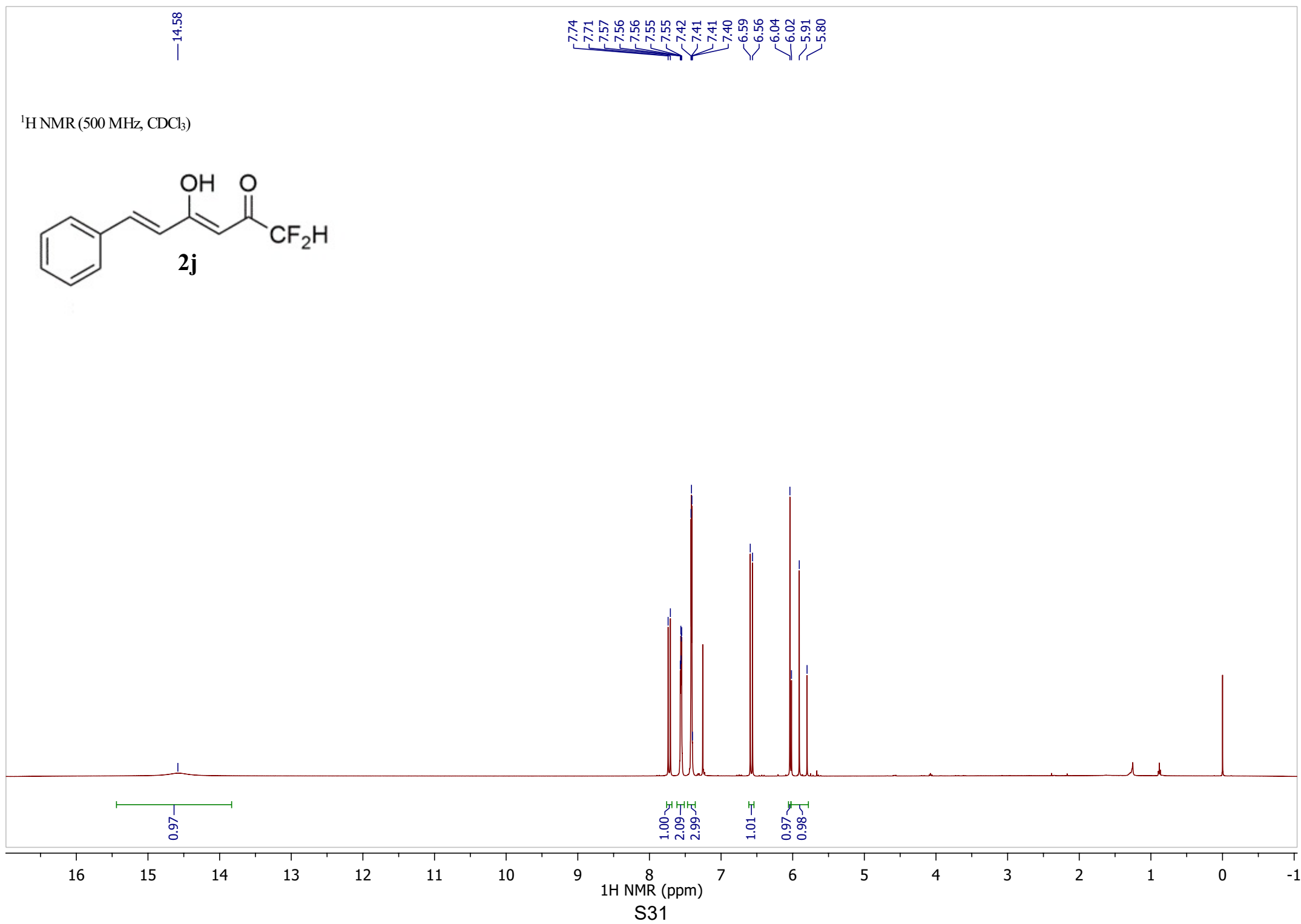
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128.63

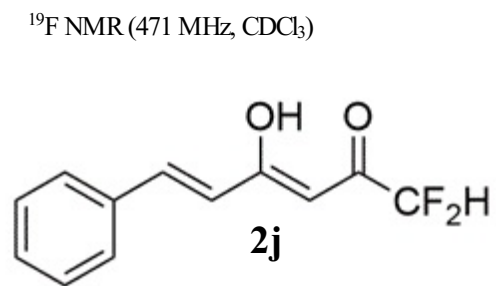
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95.49

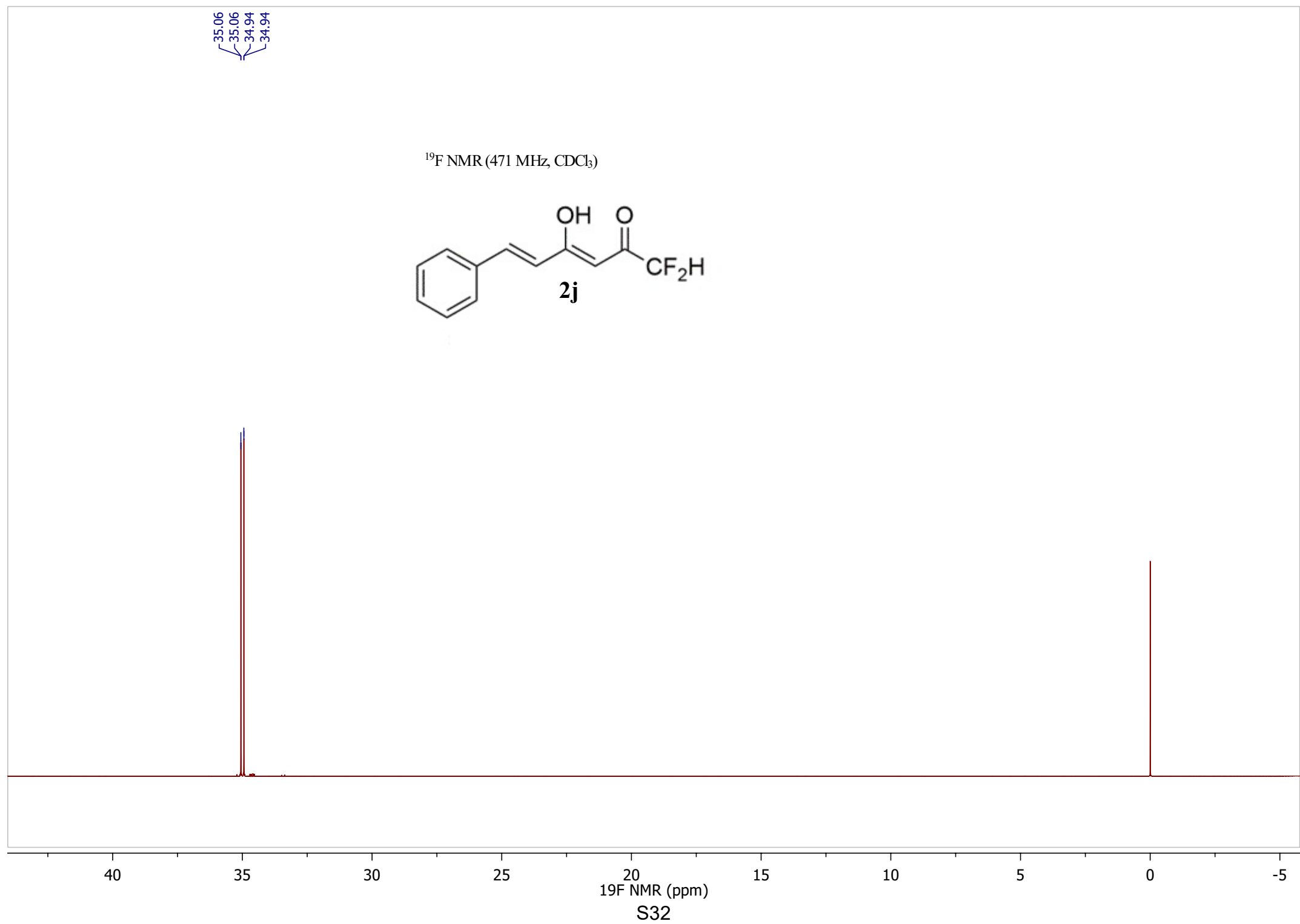


S30

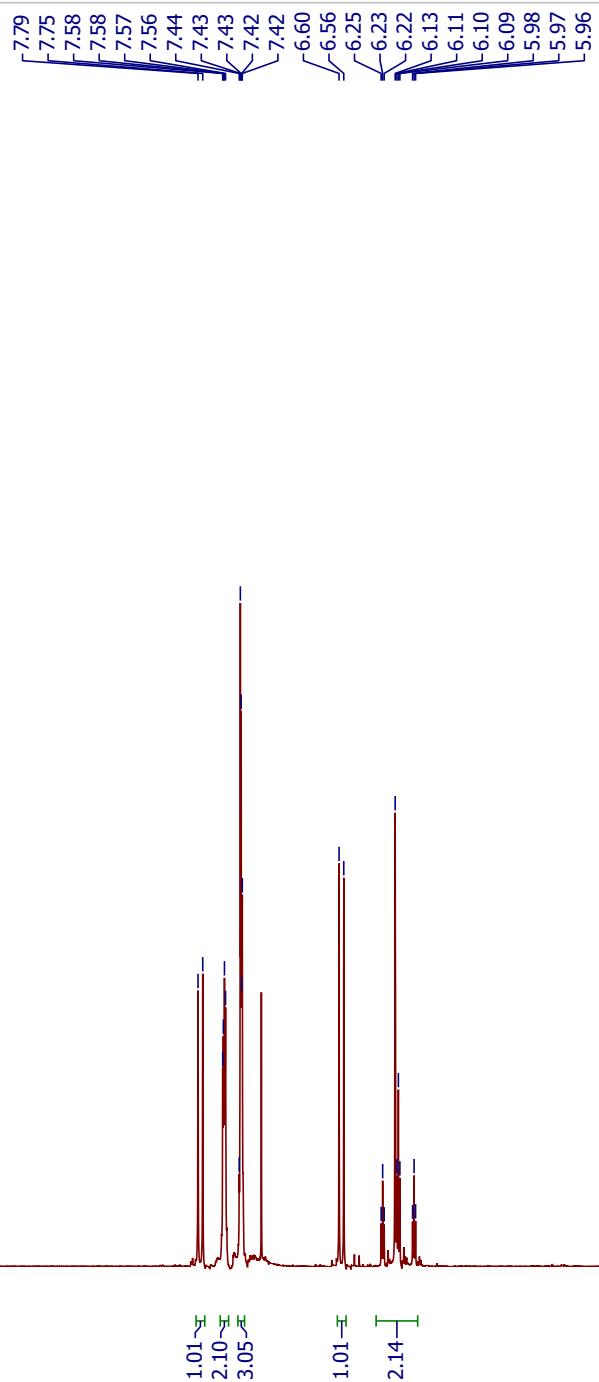
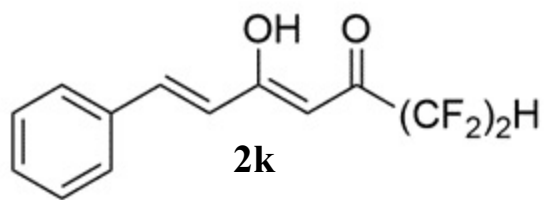




35.06
35.06
34.94
34.94



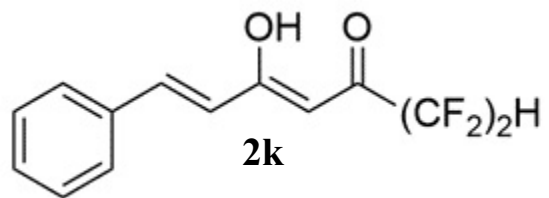
¹H NMR (400 MHz, CDCl₃)



1H NMR (ppm)

S33

^{19}F NMR (376 MHz, CDCl_3)



35.78
35.78
35.76
35.75
35.73
35.73

23.49
23.47
23.45
23.35
23.33
23.31

50

45

40

35

30

^{19}F NMR (ppm)

S34

25

20

15

10

5

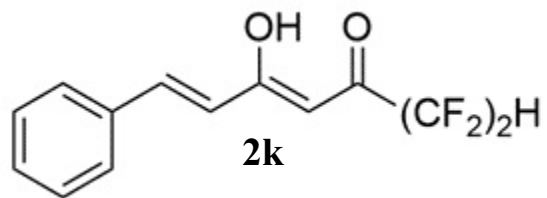
0

-5

2.00

2.04

¹³C NMR (126 MHz, CDCl₃)



184.78
184.57
184.36
180.88

143.63

134.27

131.03

129.11

128.49

121.31

111.34

111.08

109.51

109.35

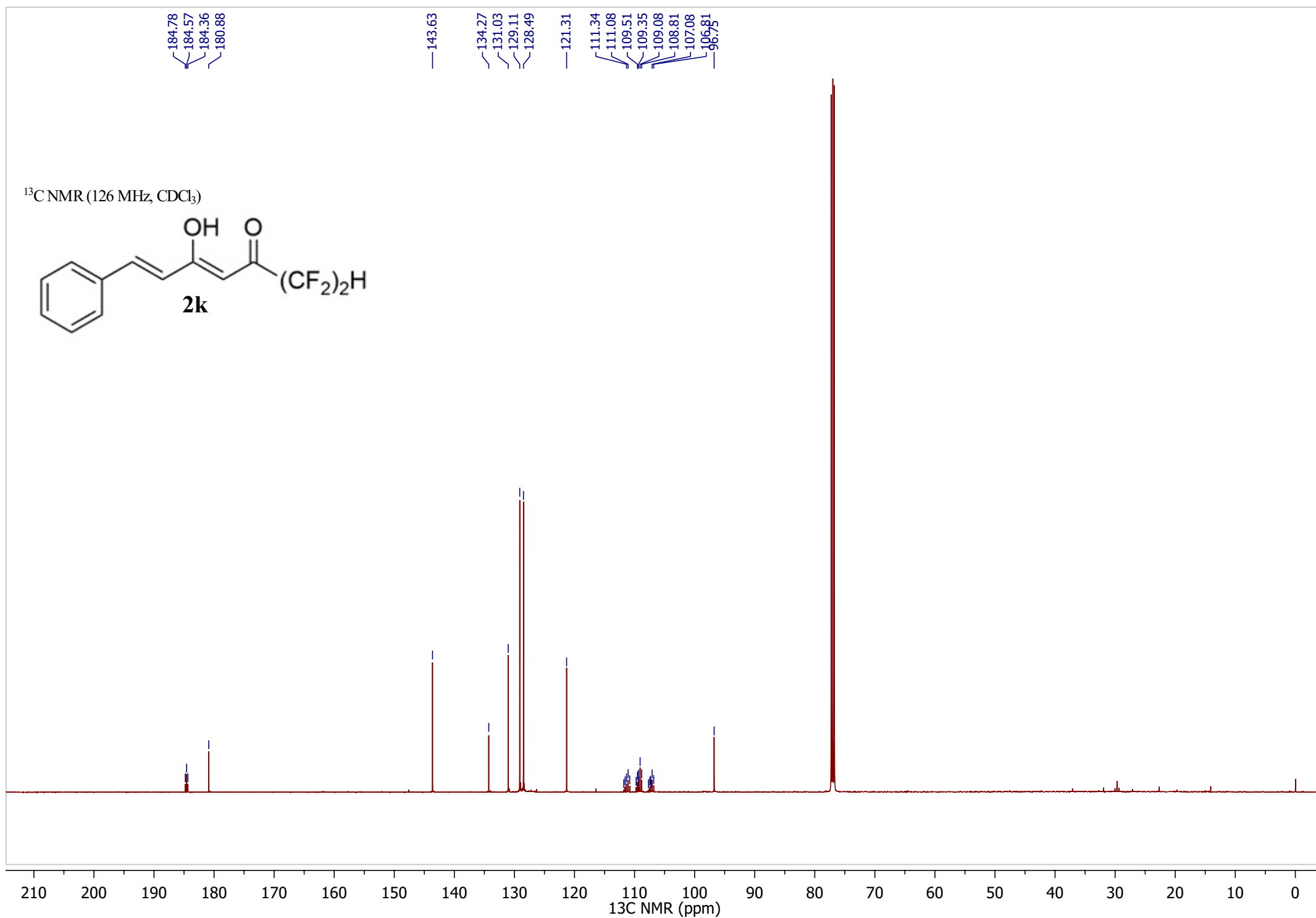
109.08

108.81

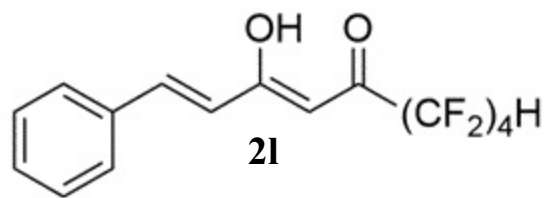
107.08

106.81

96.75



¹H NMR (500 MHz, CDCl₃)



14.33

7.83
7.81
7.80
7.77
7.59
7.58
7.57
7.56
7.55
7.44
7.44
7.43
7.42
7.42
7.41
7.26

6.60
6.56
6.47
6.44
6.23
6.22
6.21
6.19
6.18
6.17
6.13
6.12
6.11
6.08
6.02
6.01
6.00
5.99
5.97

1.03

1.02

2.10

3.09

1.00

2.13

16

15

14

13

12

11

10

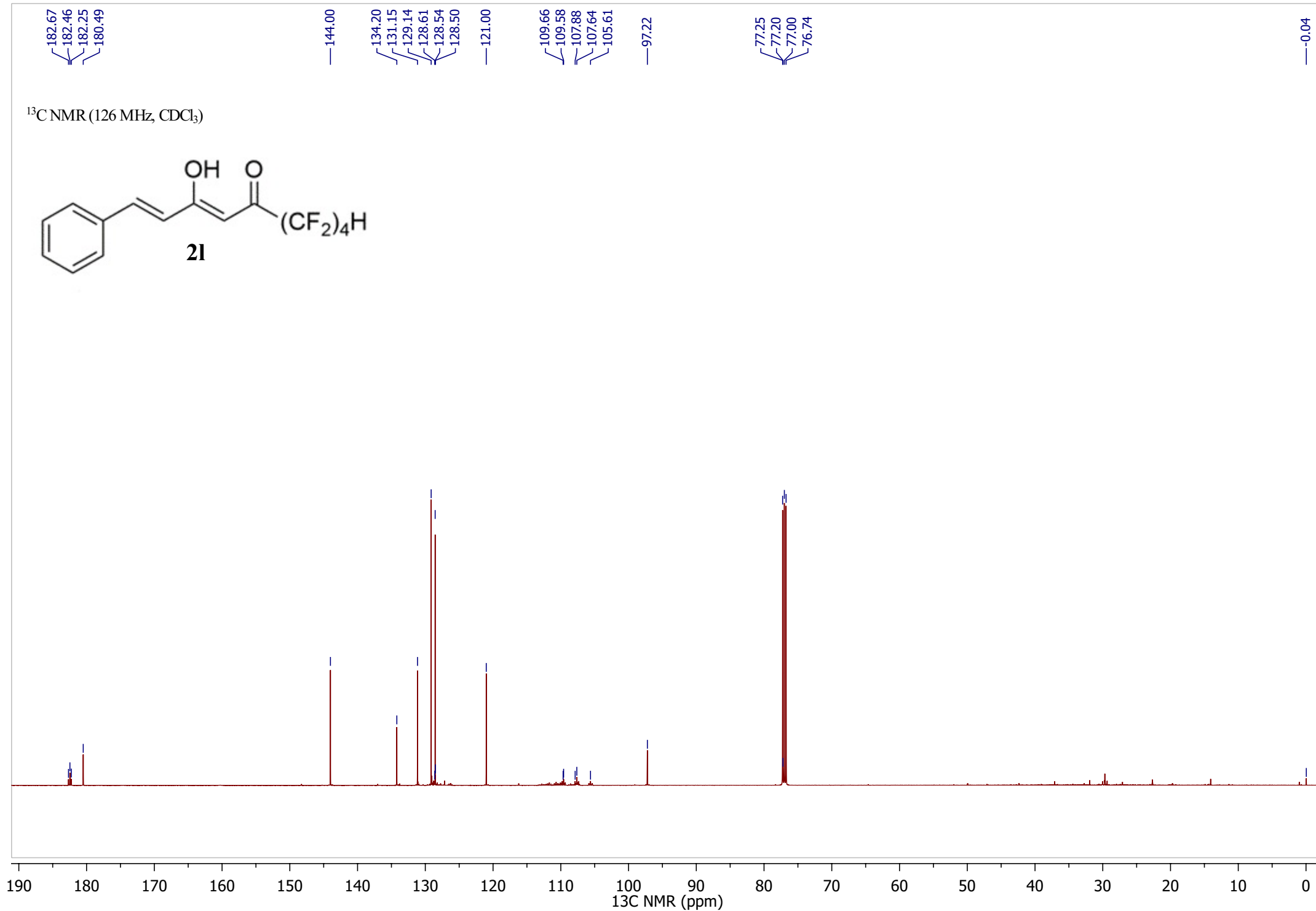
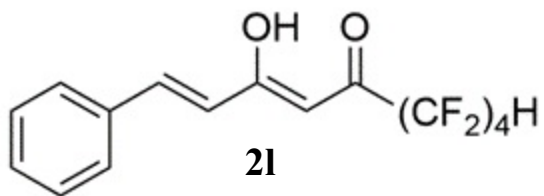
9

¹H NMR (ppm)

S36

0

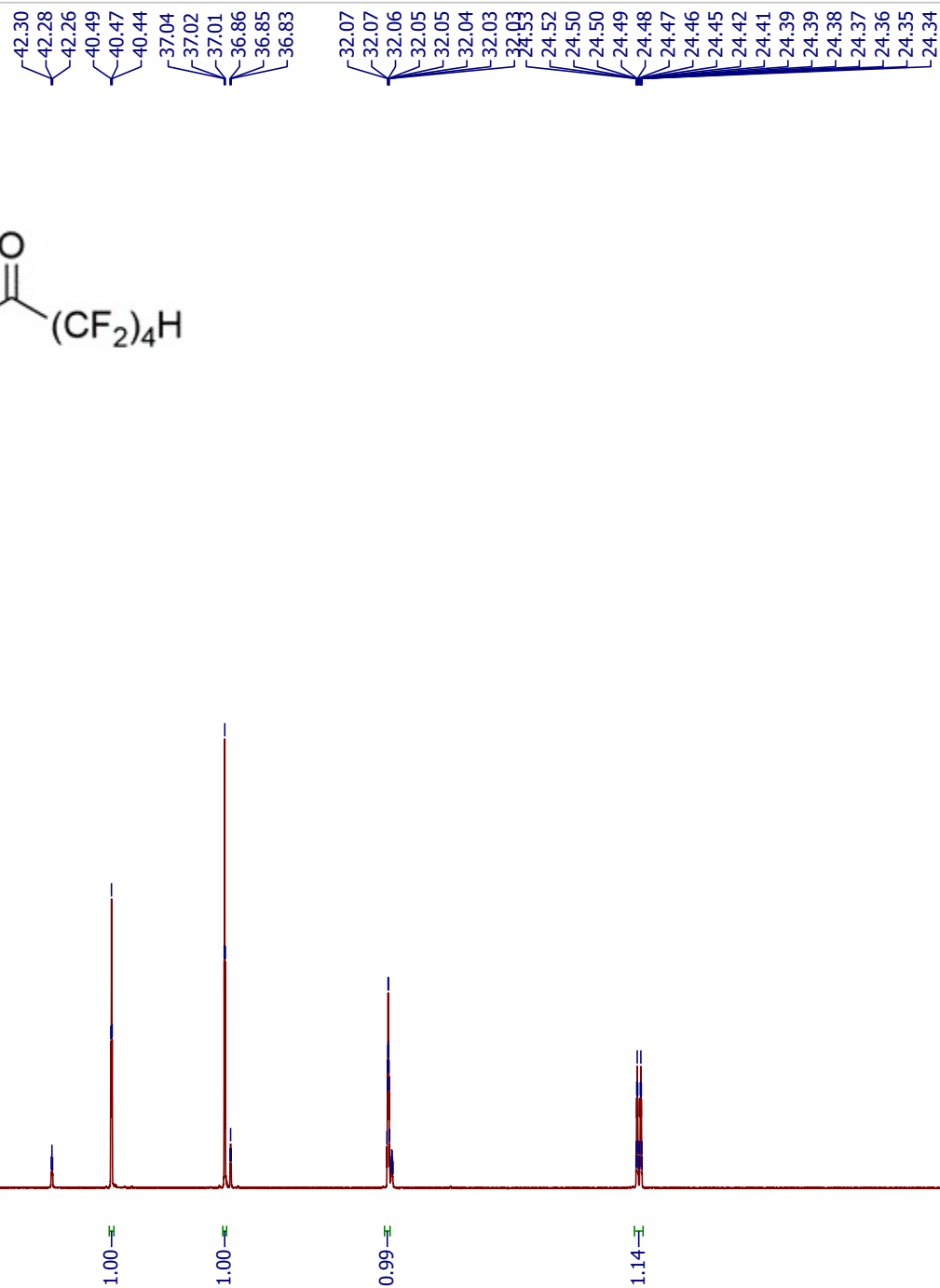
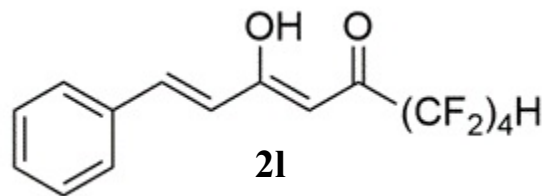
¹³C NMR (126 MHz, CDCl₃)



13C NMR (ppm)

S37

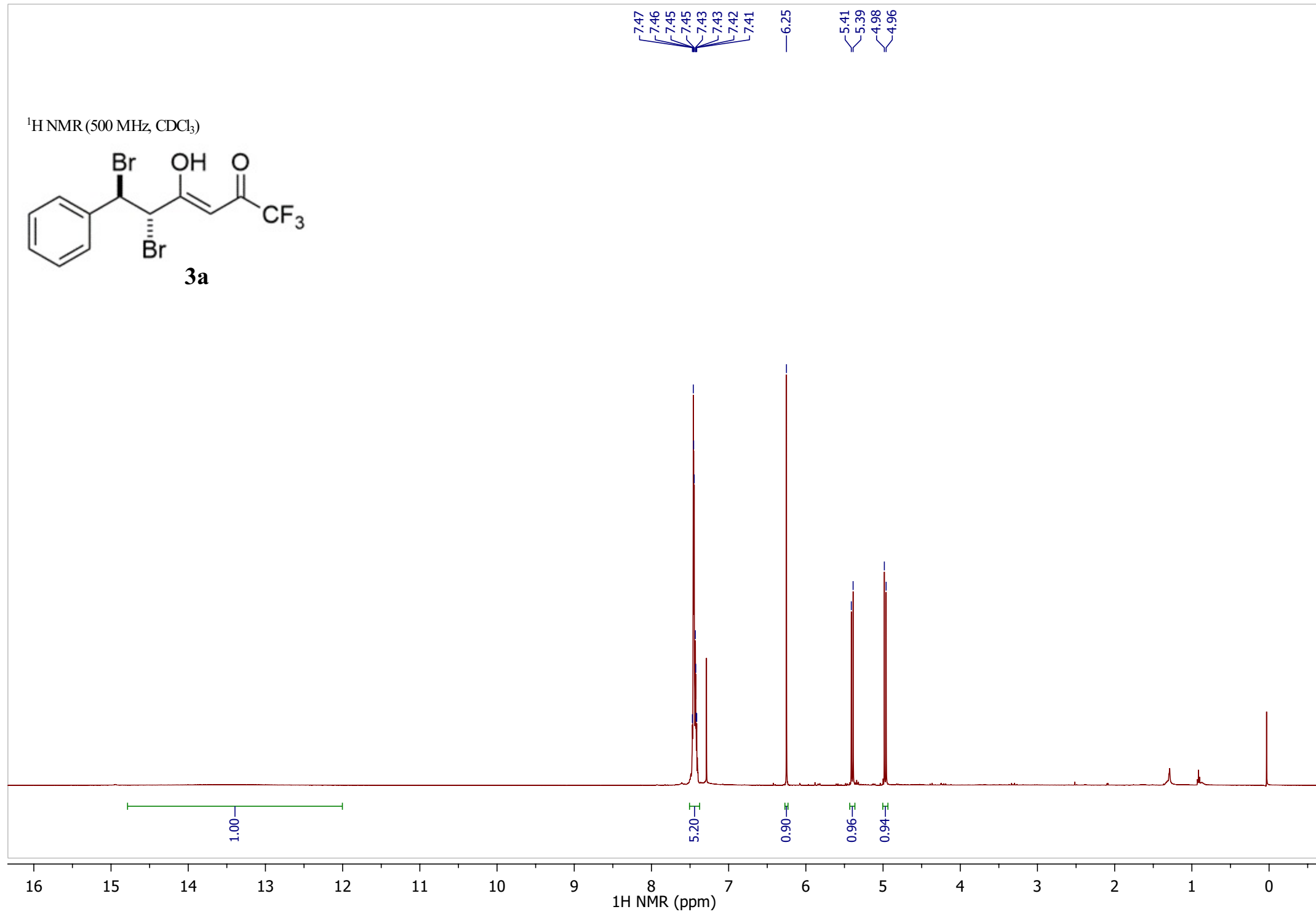
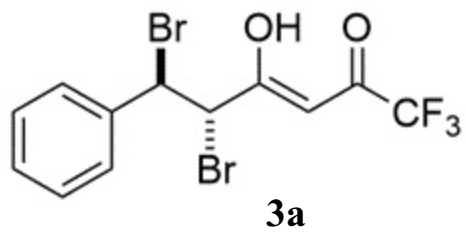
^{19}F NMR (471 MHz, CDCl_3)



^{19}F NMR (ppm)

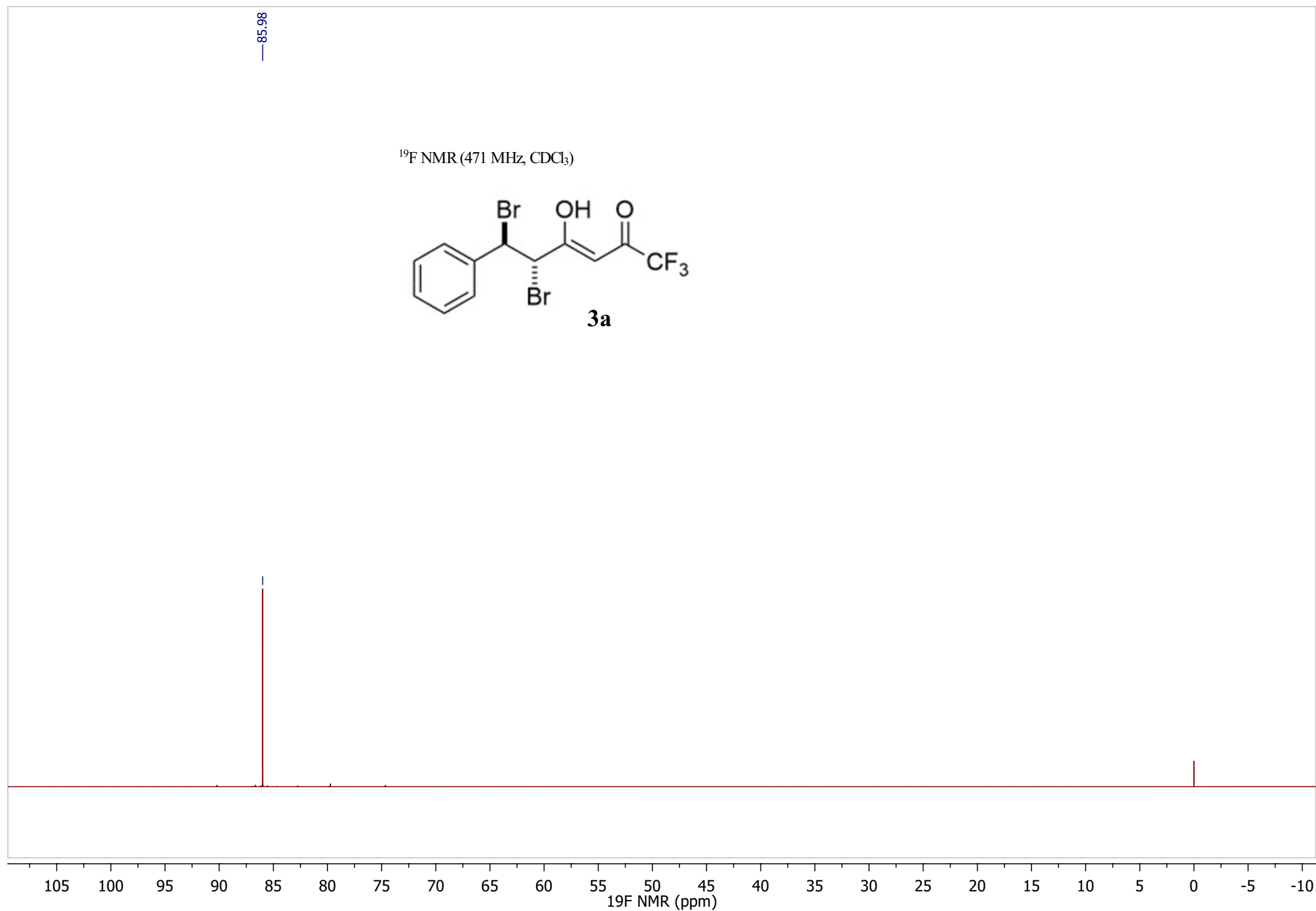
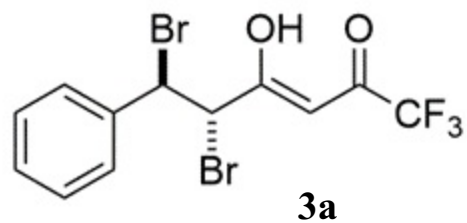
S38

^1H NMR (500 MHz, CDCl_3)



85.98

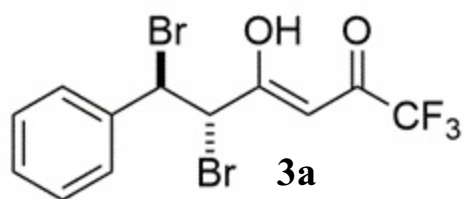
^{19}F NMR (471 MHz, CDCl_3)



^{19}F NMR (ppm)

S40

¹³C NMR (126 MHz, CDCl₃)



190.63
172.35
172.05
171.76
171.46

137.42
129.58
129.01
128.03
120.52
118.29
116.06
113.83

96.55
96.53
96.51
96.49

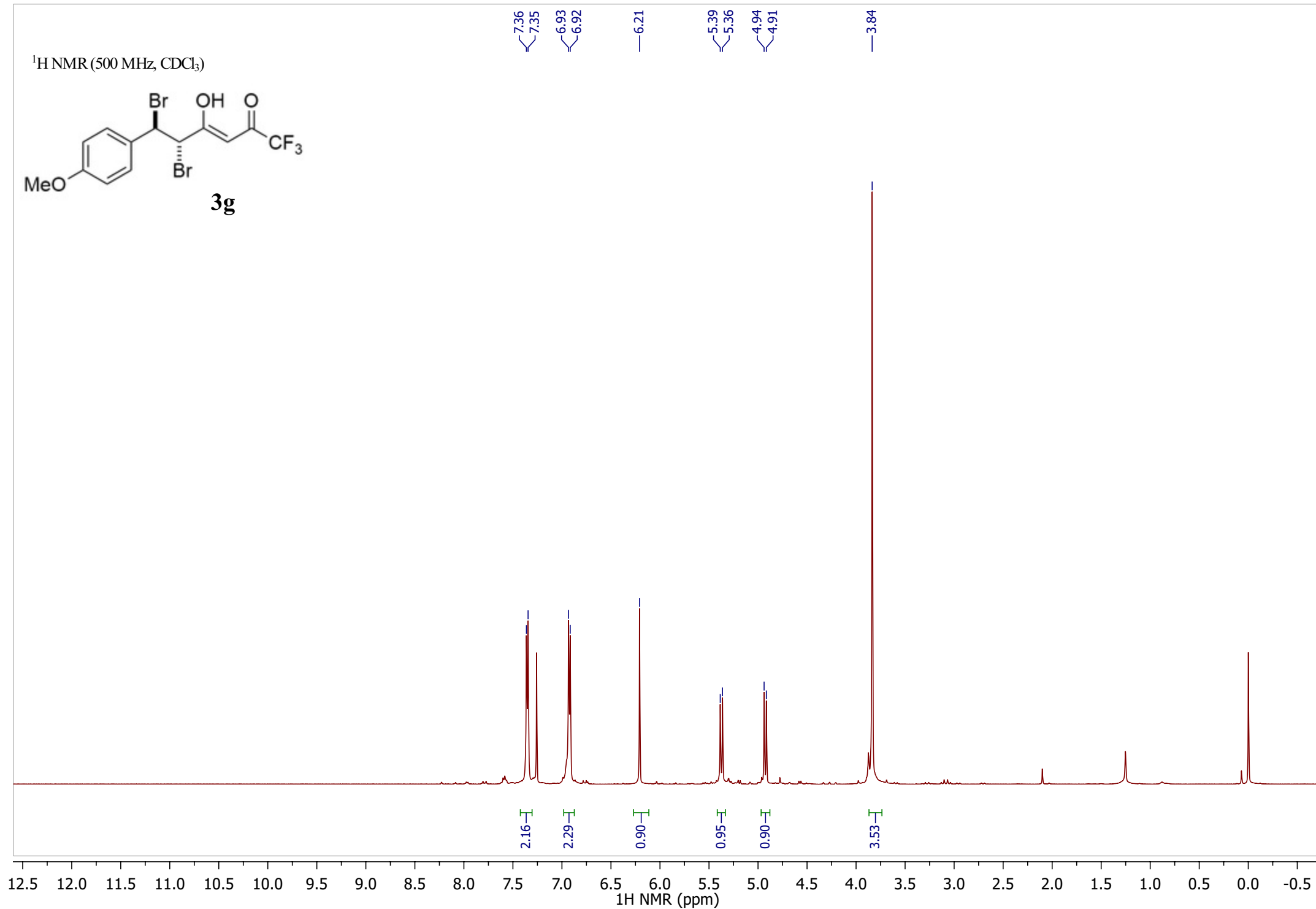
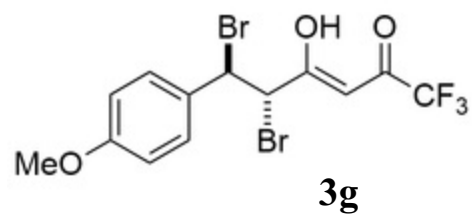
51.18
48.75

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

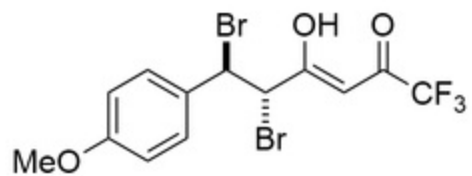
¹³C NMR (ppm)

S41

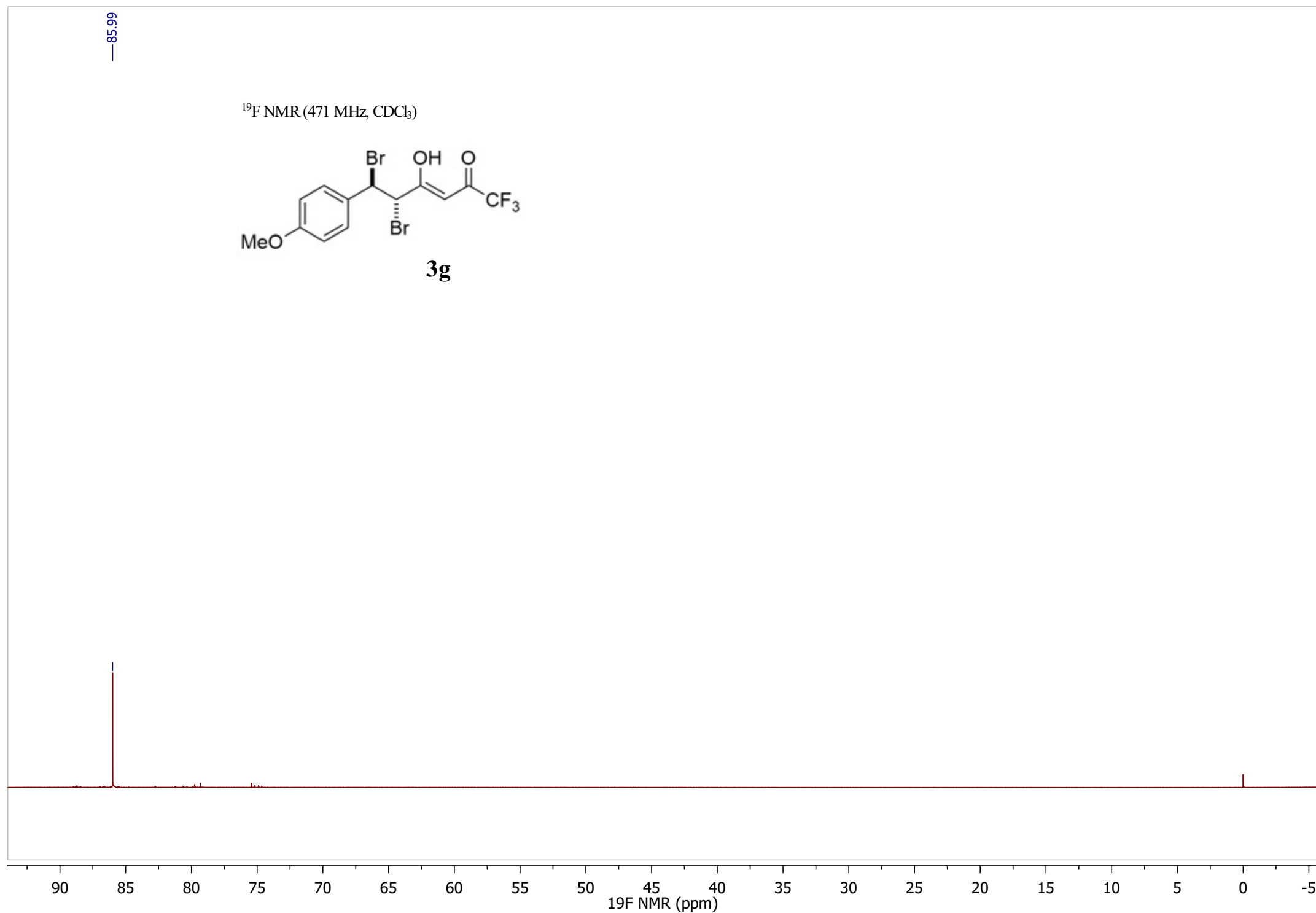
¹H NMR (500 MHz, CDCl₃)



^{19}F NMR (471 MHz, CDCl_3)



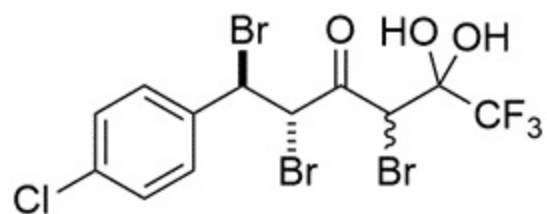
3g



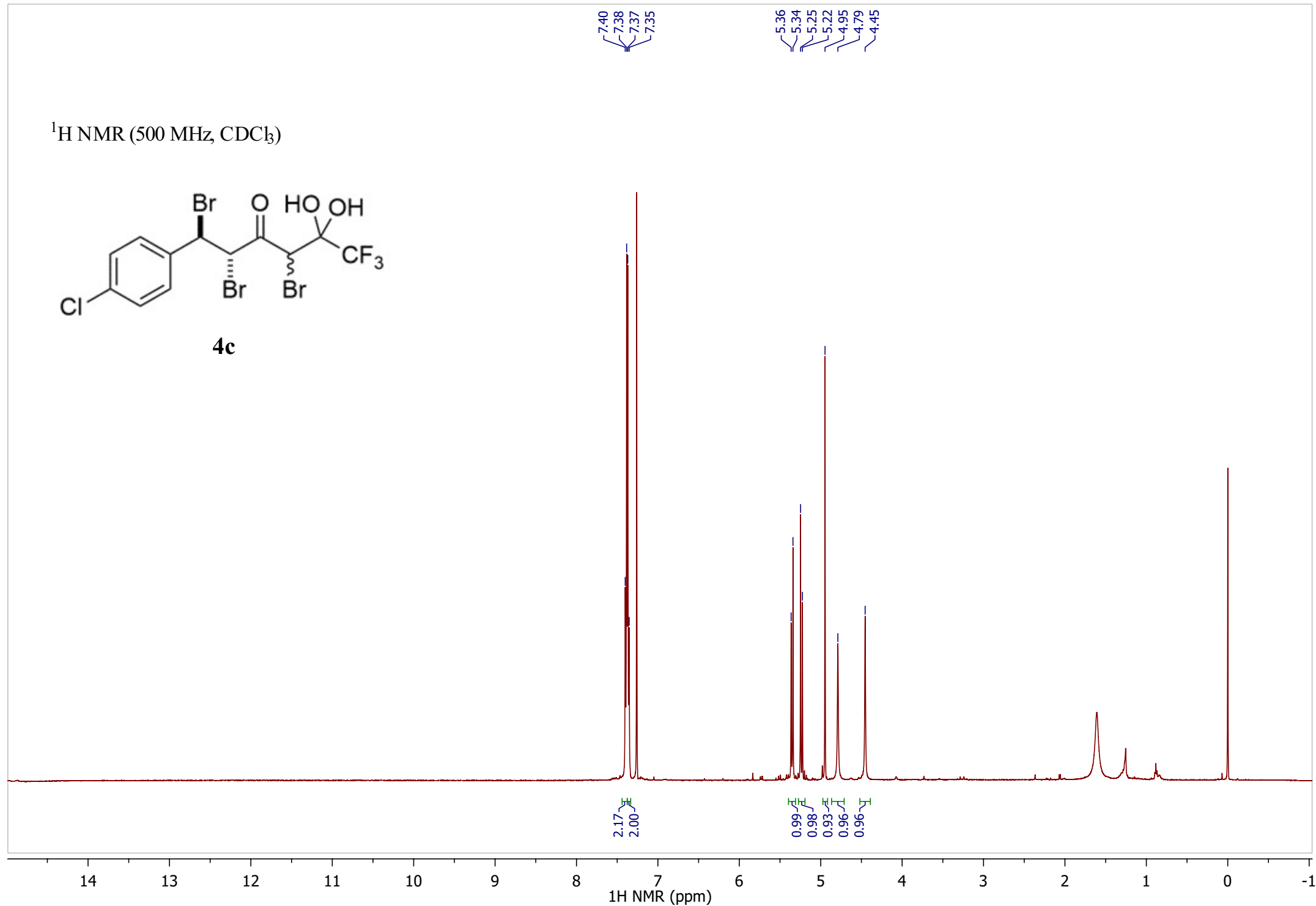
^{19}F NMR (ppm)

S43

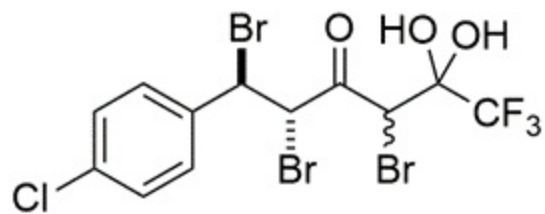
¹H NMR (500 MHz, CDCl₃)



4c

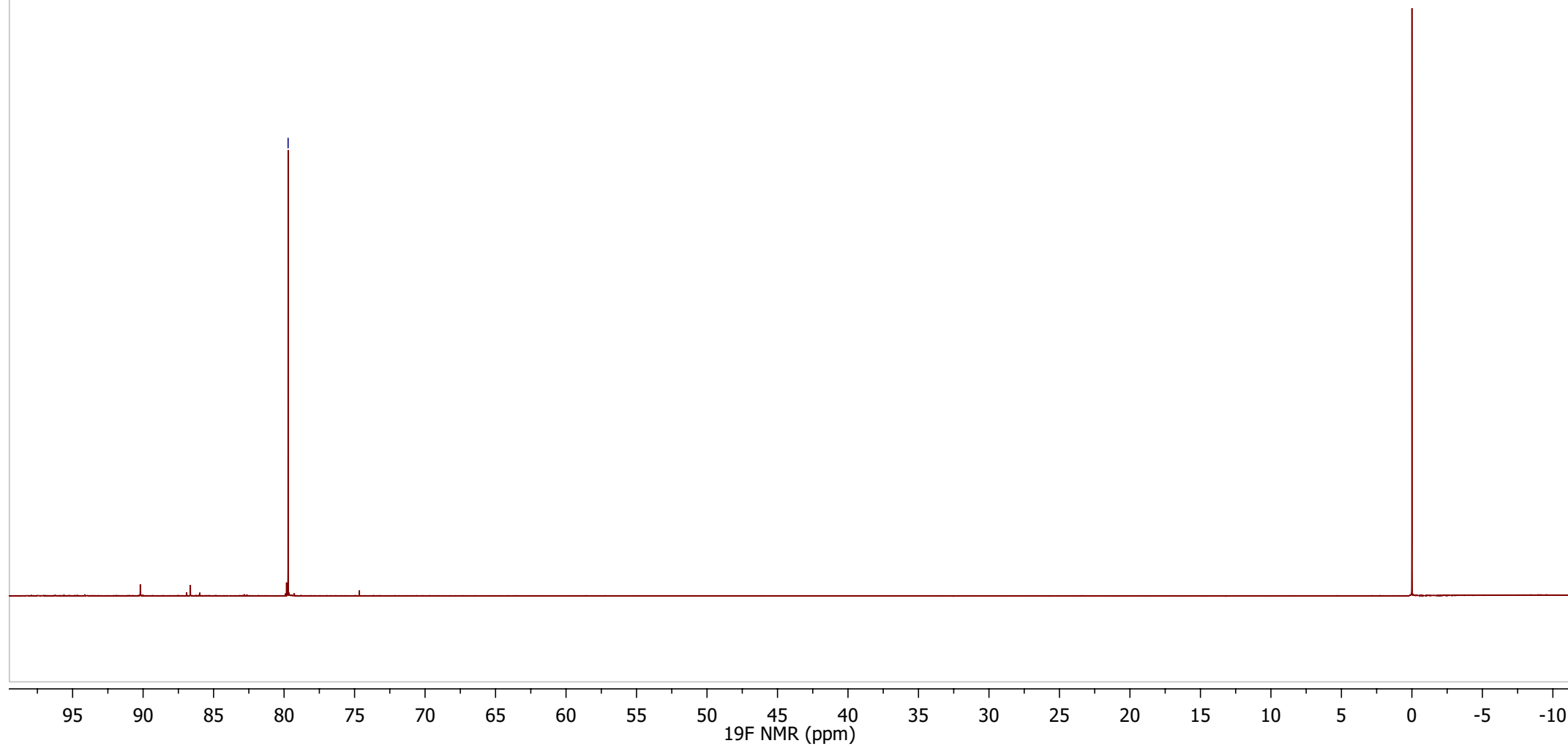


^{19}F NMR (471 MHz, CDCl_3)

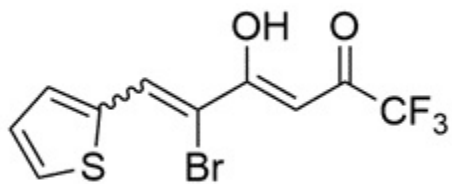


4c

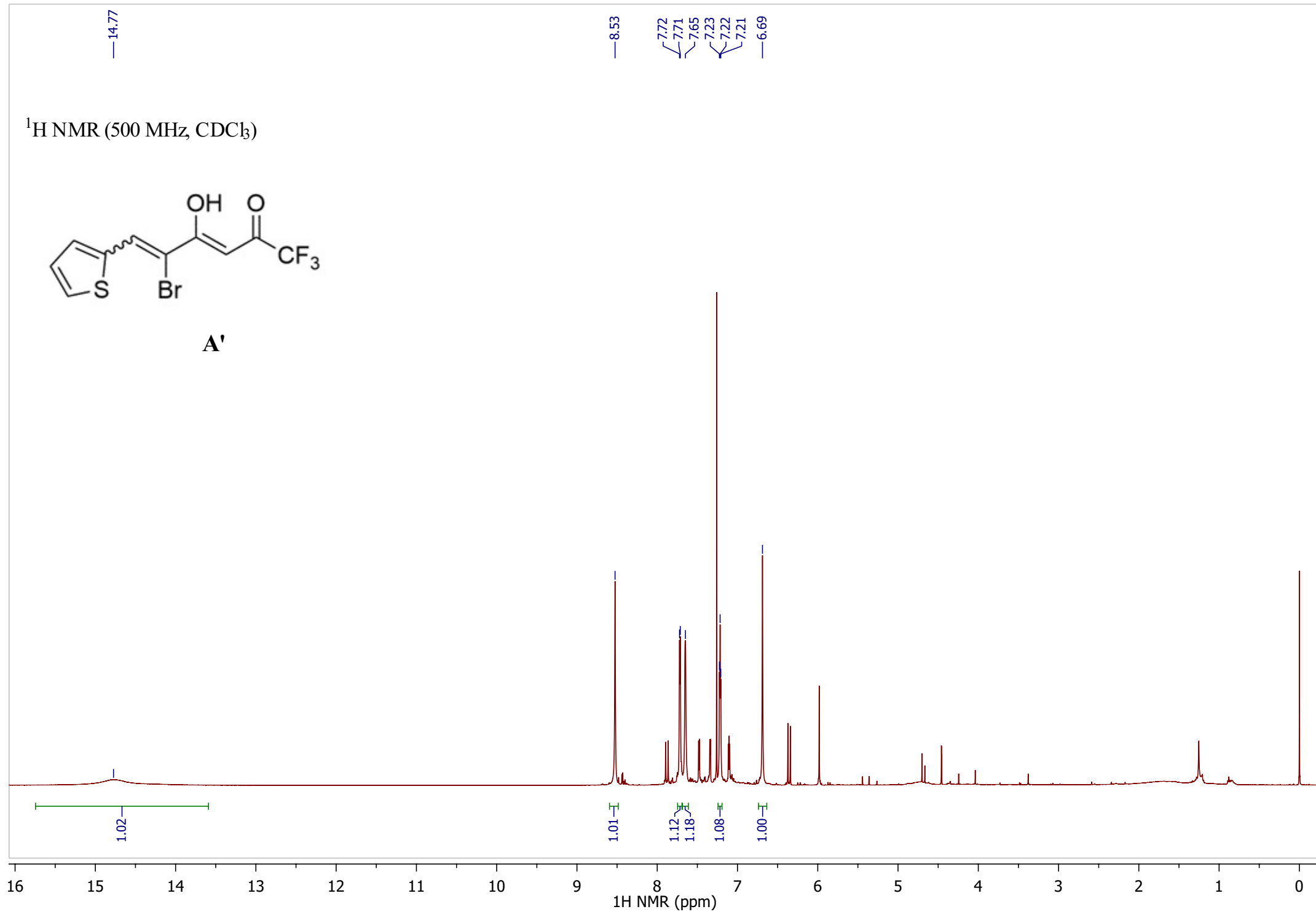
— 79.71



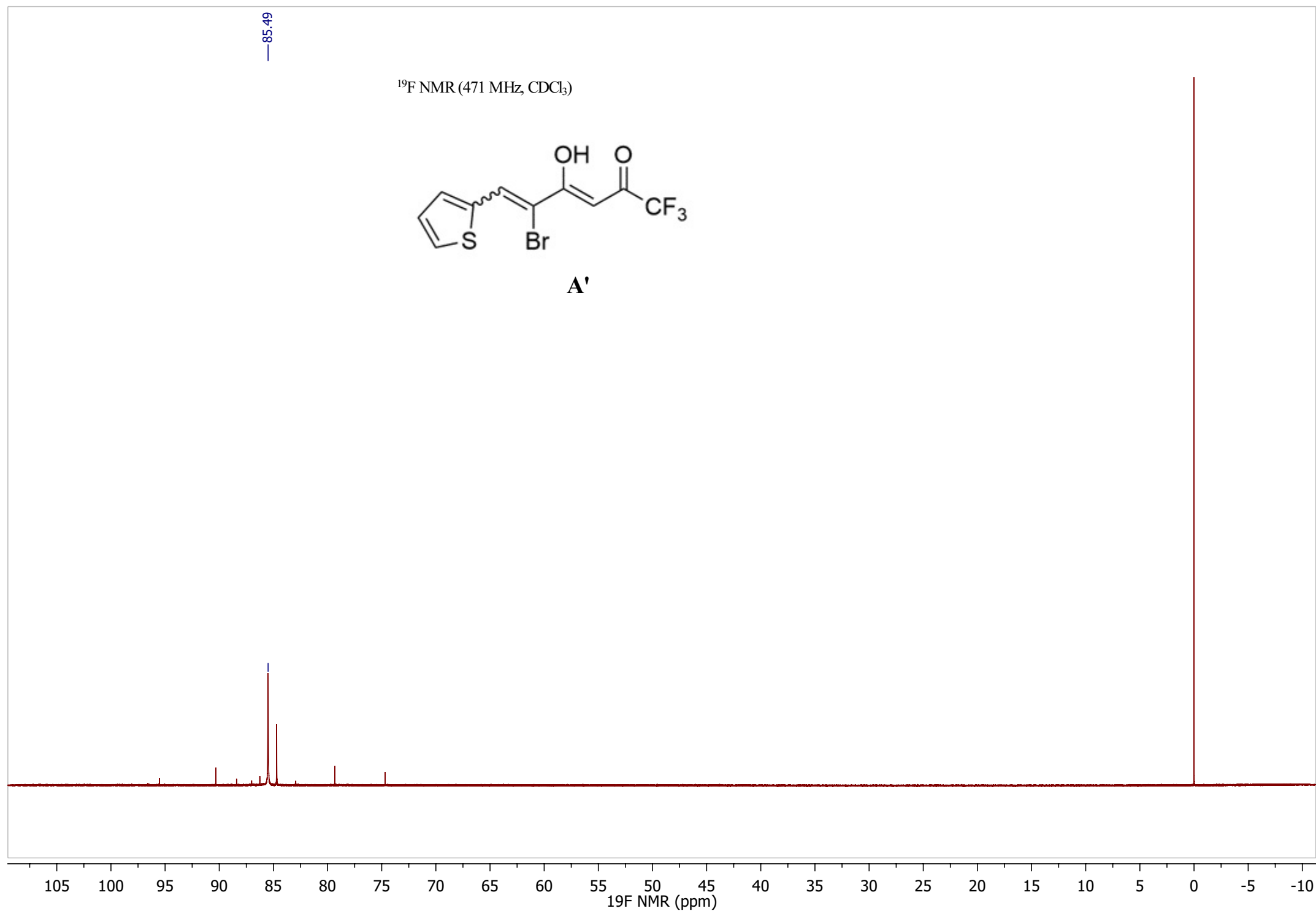
^1H NMR (500 MHz, CDCl_3)

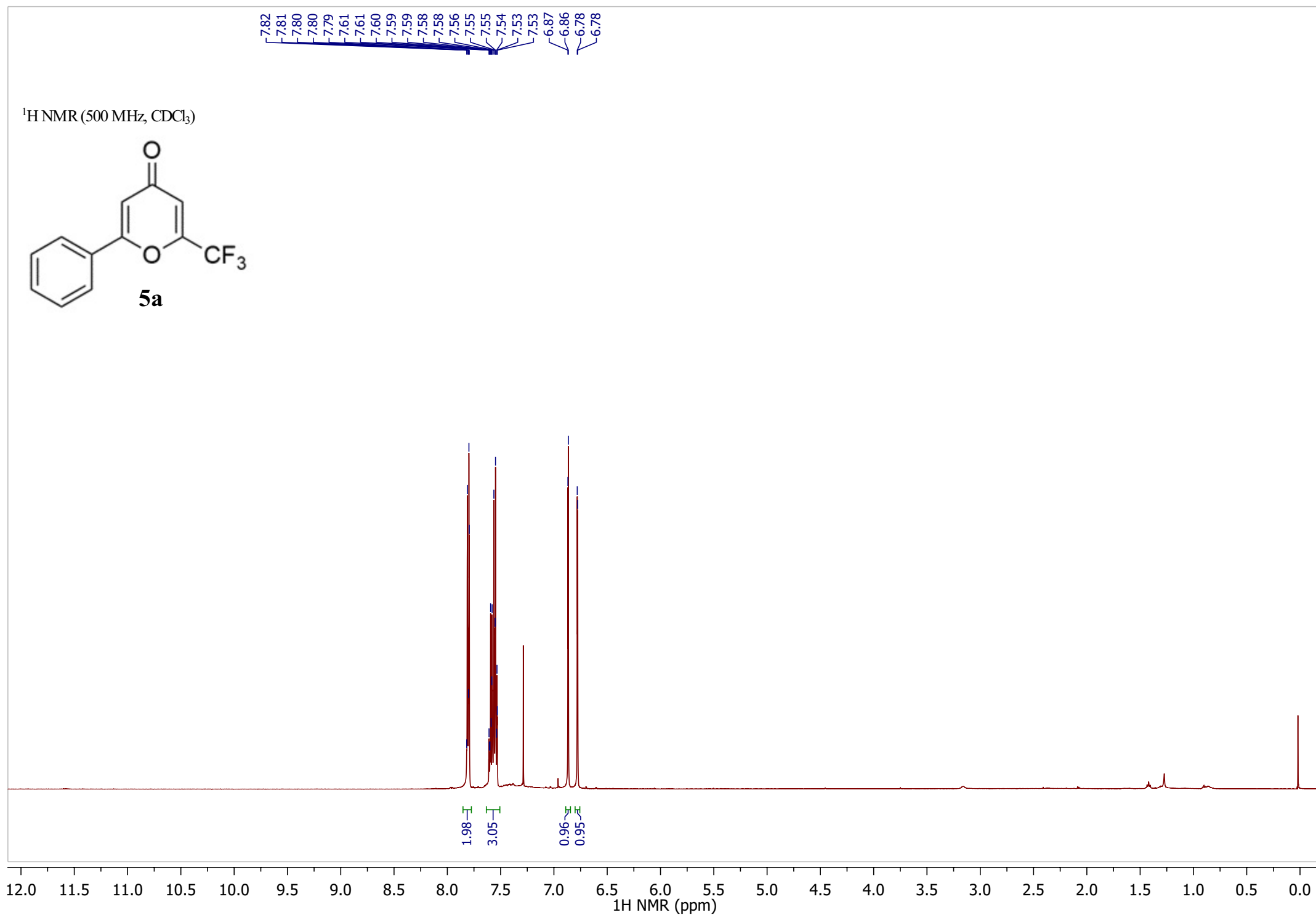


A'

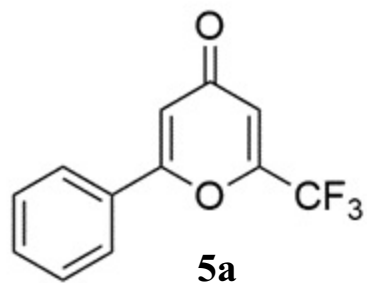


S46

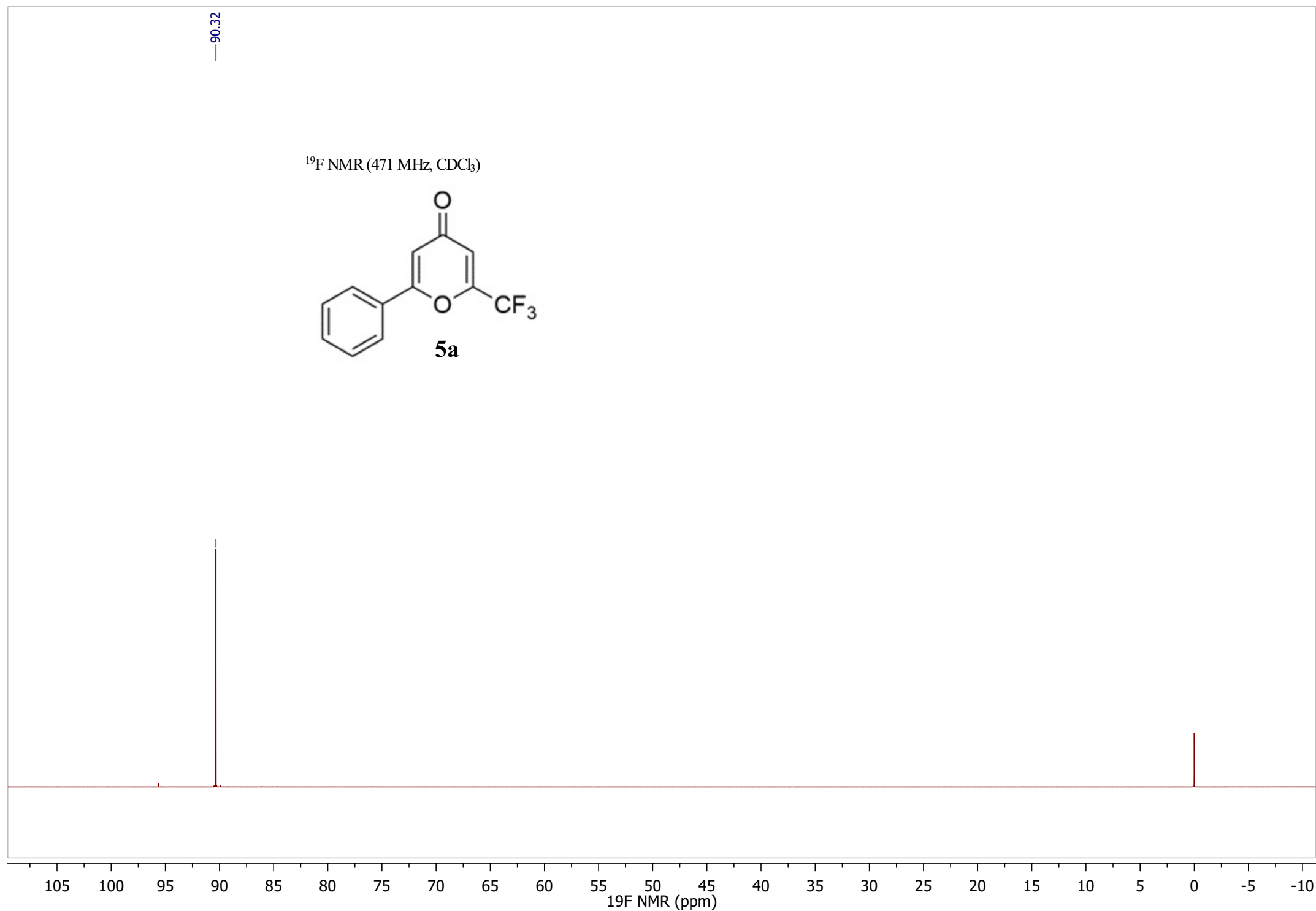




¹⁹F NMR (471 MHz, CDCl₃)

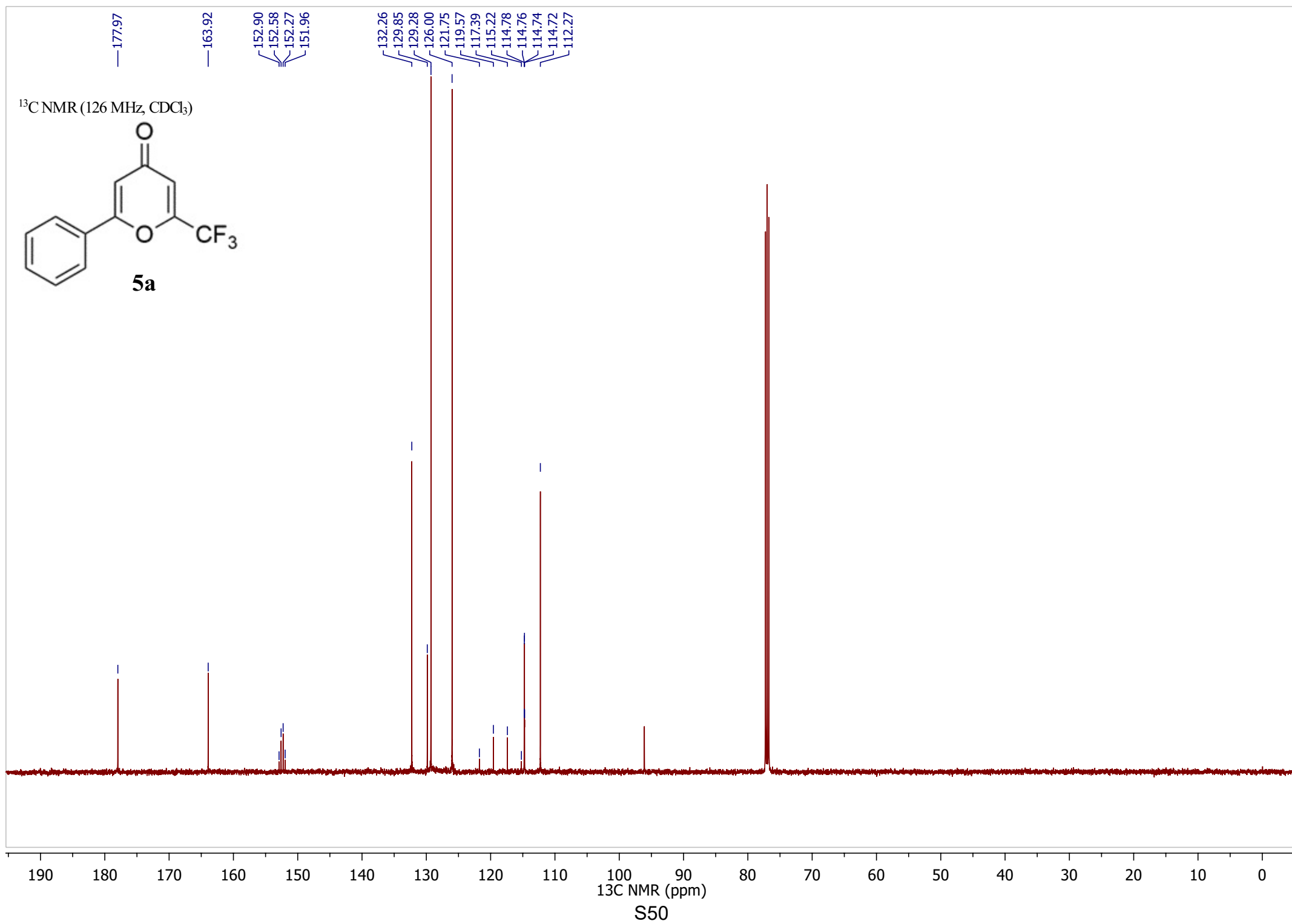


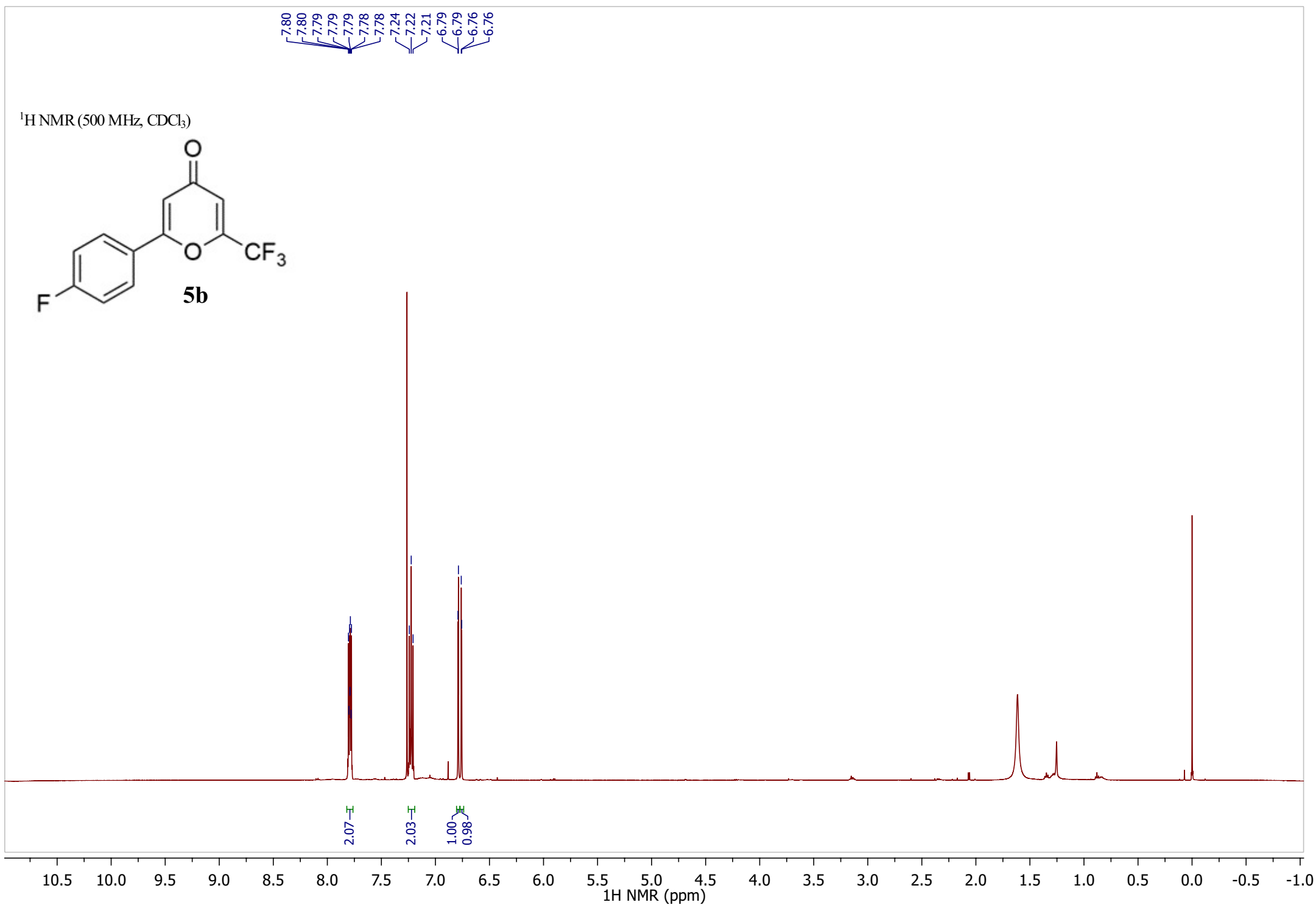
—90.32

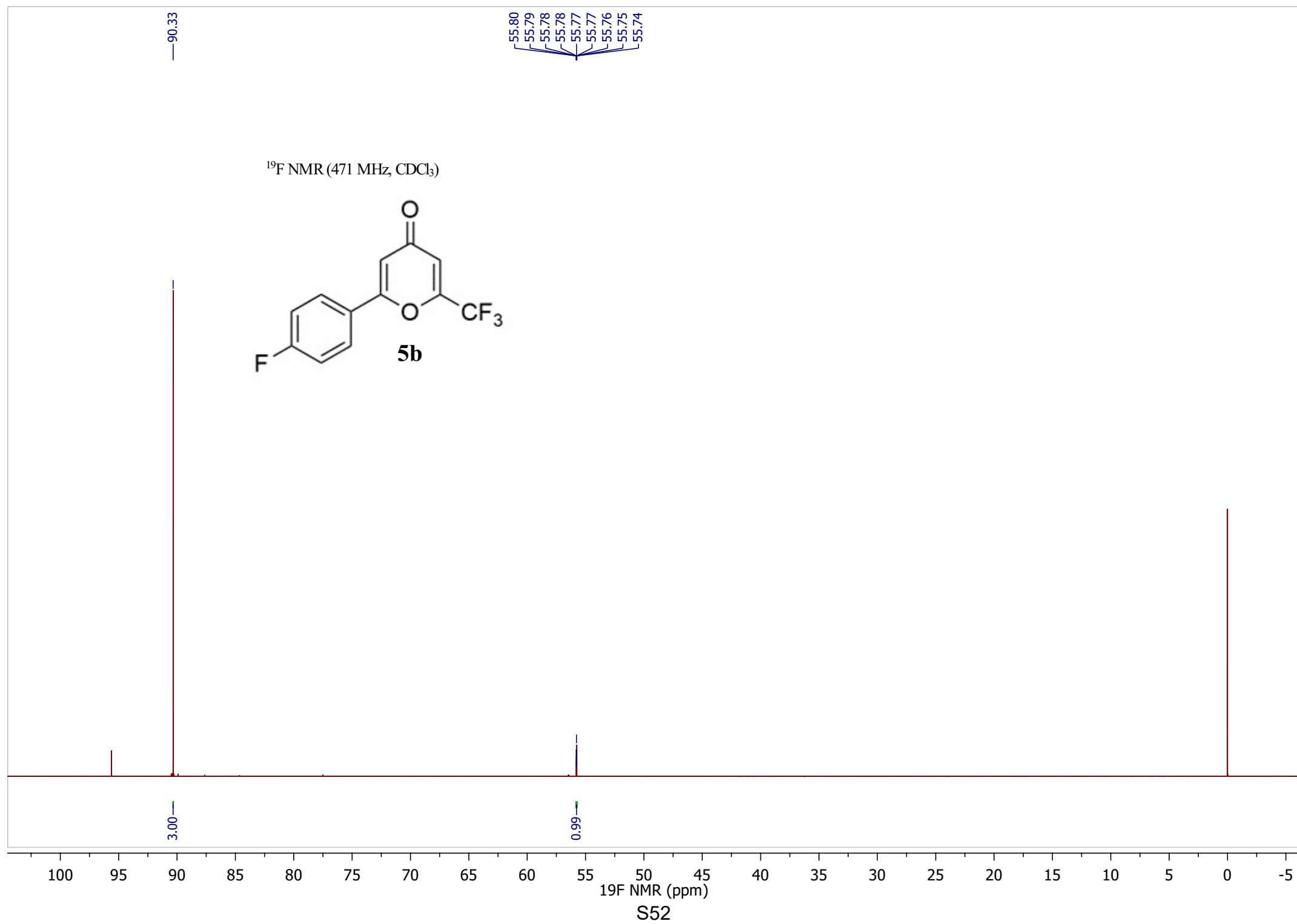


¹⁹F NMR (ppm)

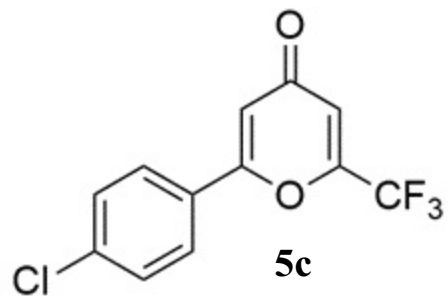
S49



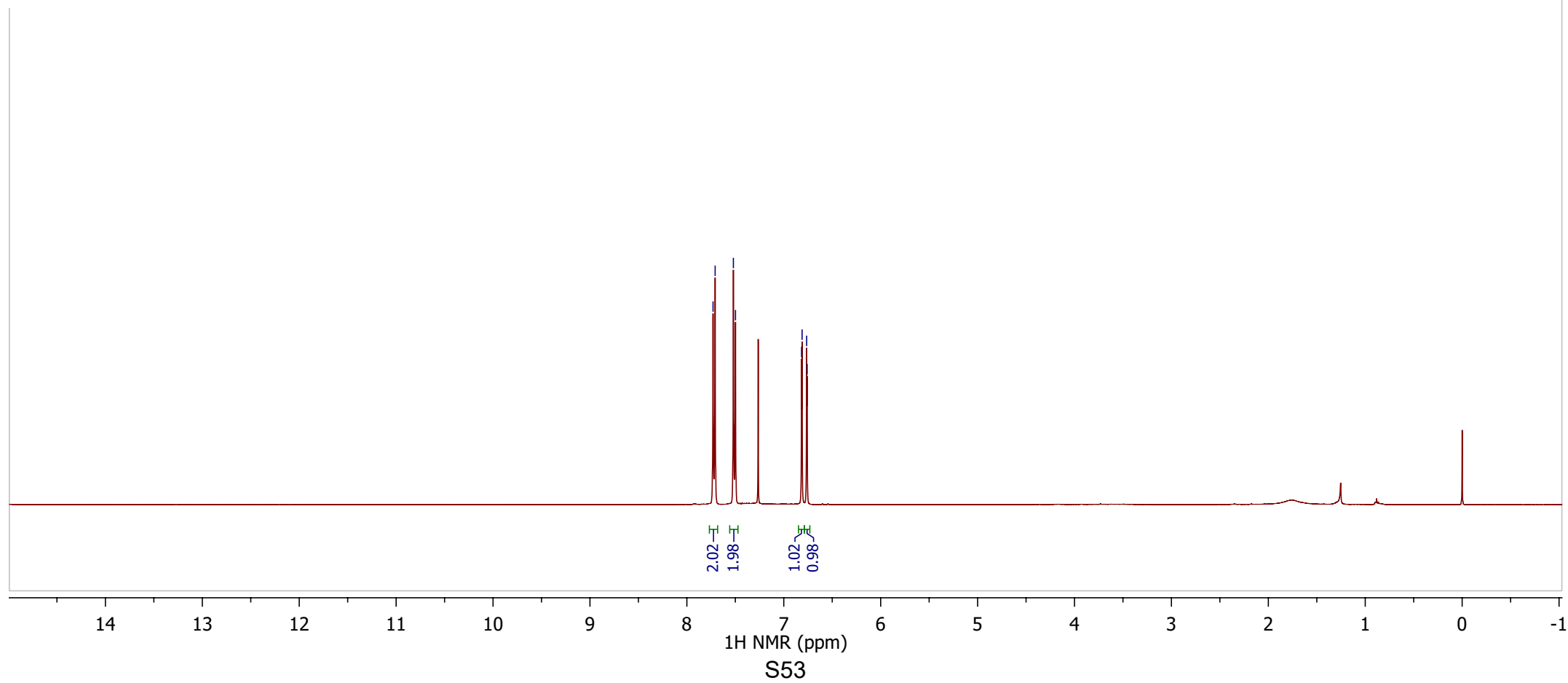




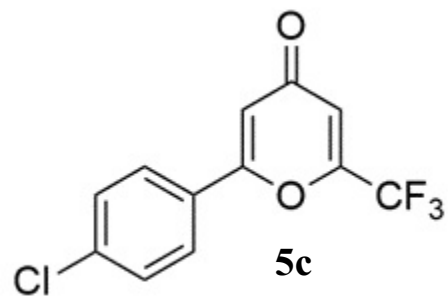
^1H NMR (400 MHz, CDCl_3)



7.73
7.71
7.52
7.50
6.82
6.81
6.76
6.76



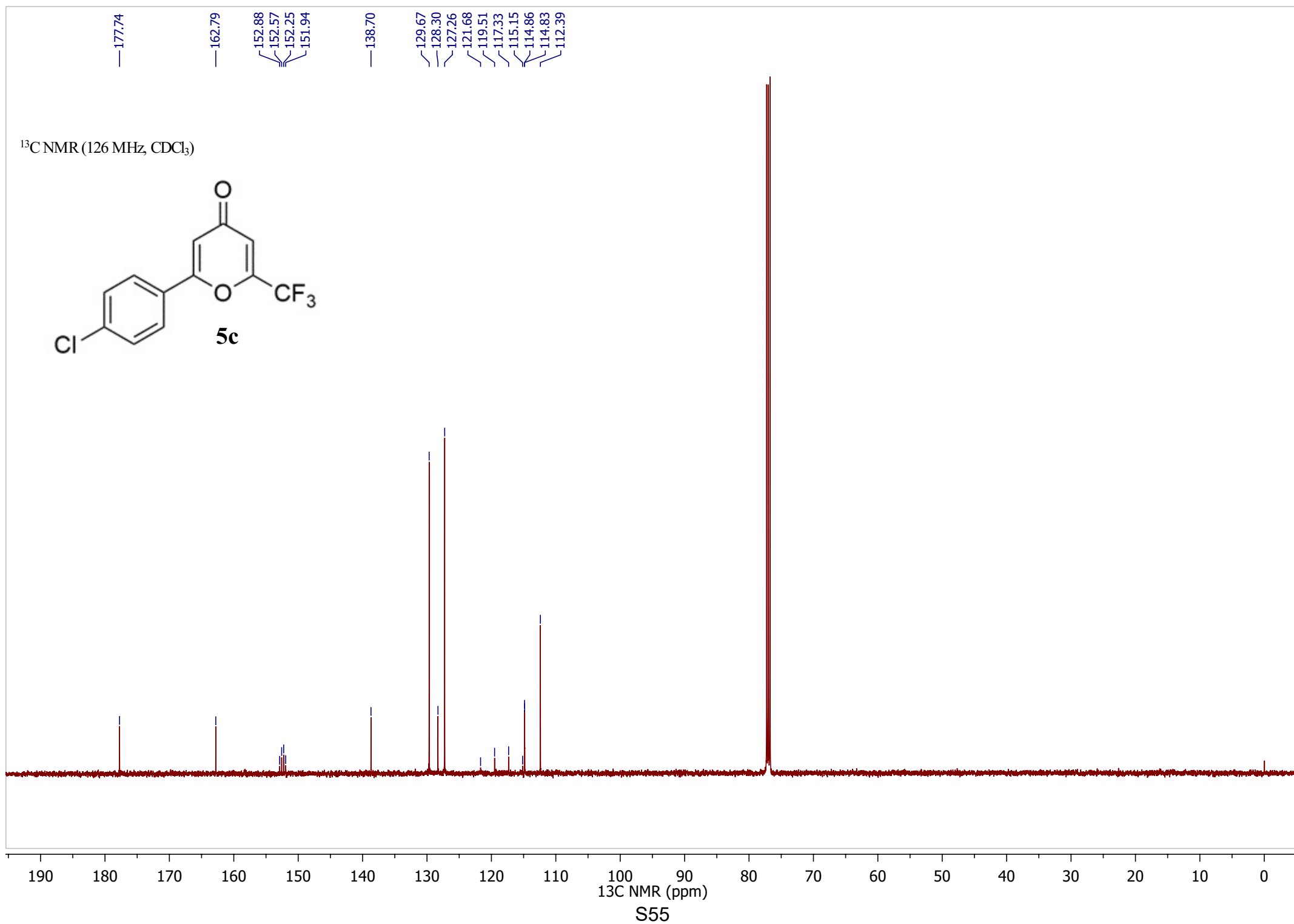
^{19}F NMR (376 MHz, CDCl_3)



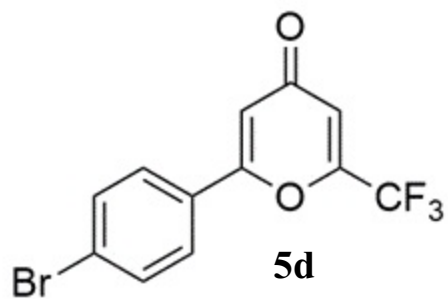
90.34

^{19}F NMR (ppm)

S54



^1H NMR (500 MHz, CDCl_3)



7.68
7.66
7.65
7.63

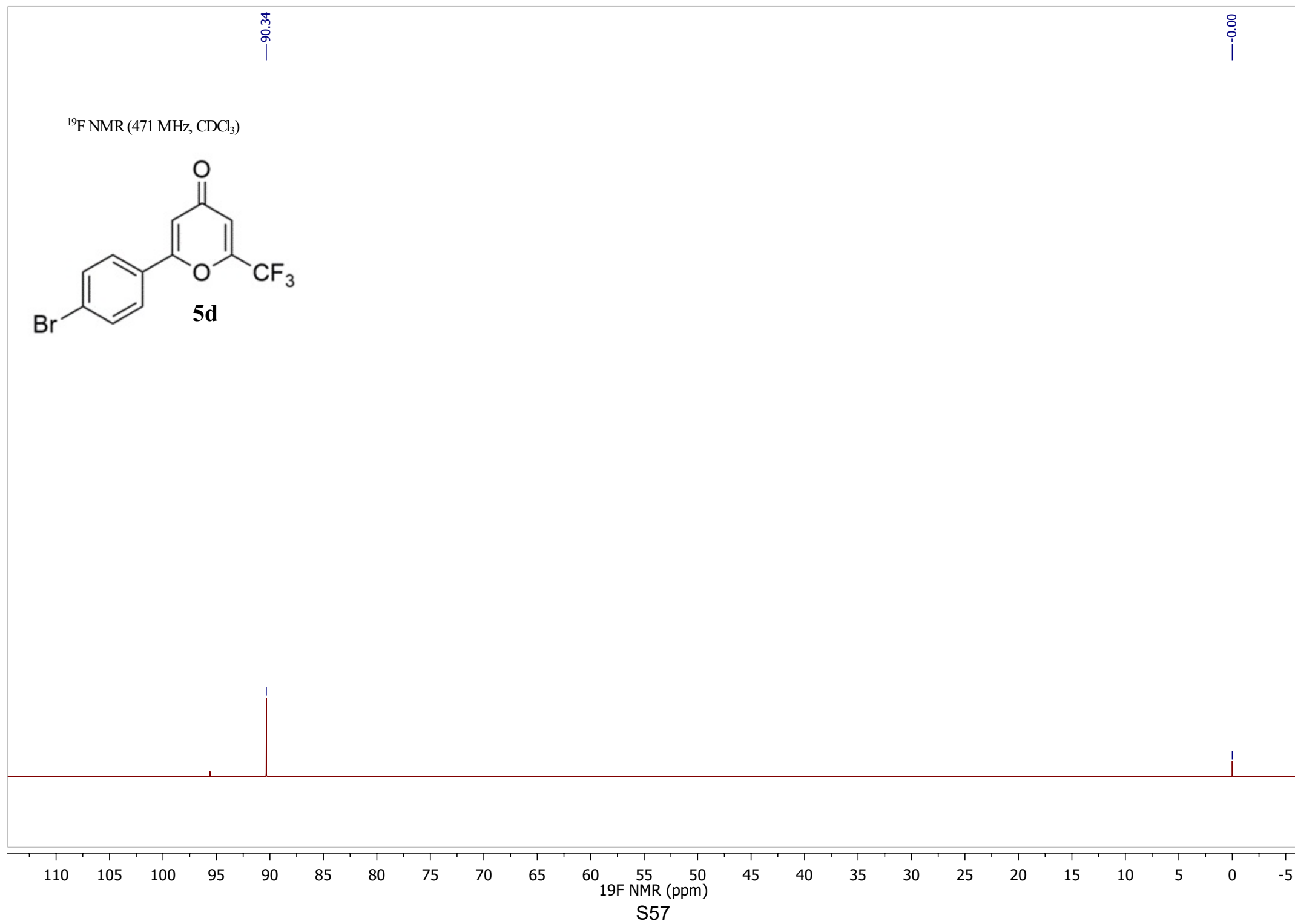
6.82
6.82
6.76
6.76

4.48

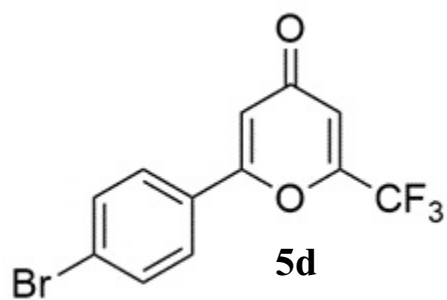
1.03
0.99

^1H NMR (ppm)

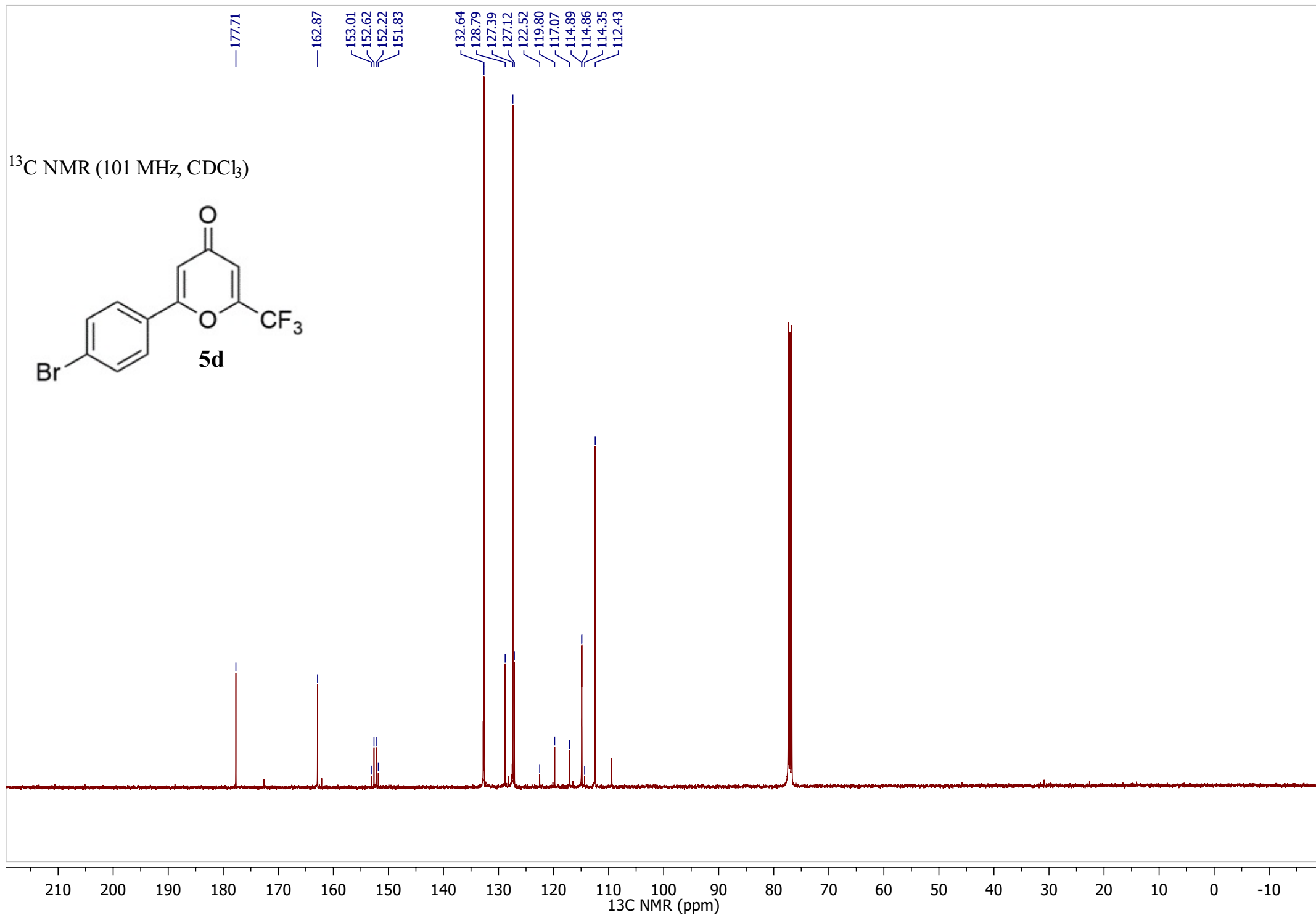
S56



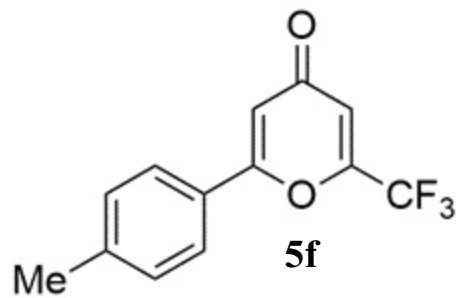
^{13}C NMR (101 MHz, CDCl_3)



177.71
162.87
153.01
152.62
152.22
151.83
132.64
128.79
127.39
127.12
122.52
119.80
117.07
114.89
114.86
114.35
112.43



¹H NMR (500 MHz, CDCl₃)



7.68
7.66
7.33
7.31
6.81
6.80
6.74
6.74

2.44

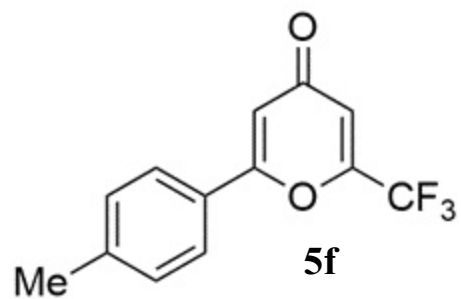
2.03
2.07
1.02
1.00

3.07

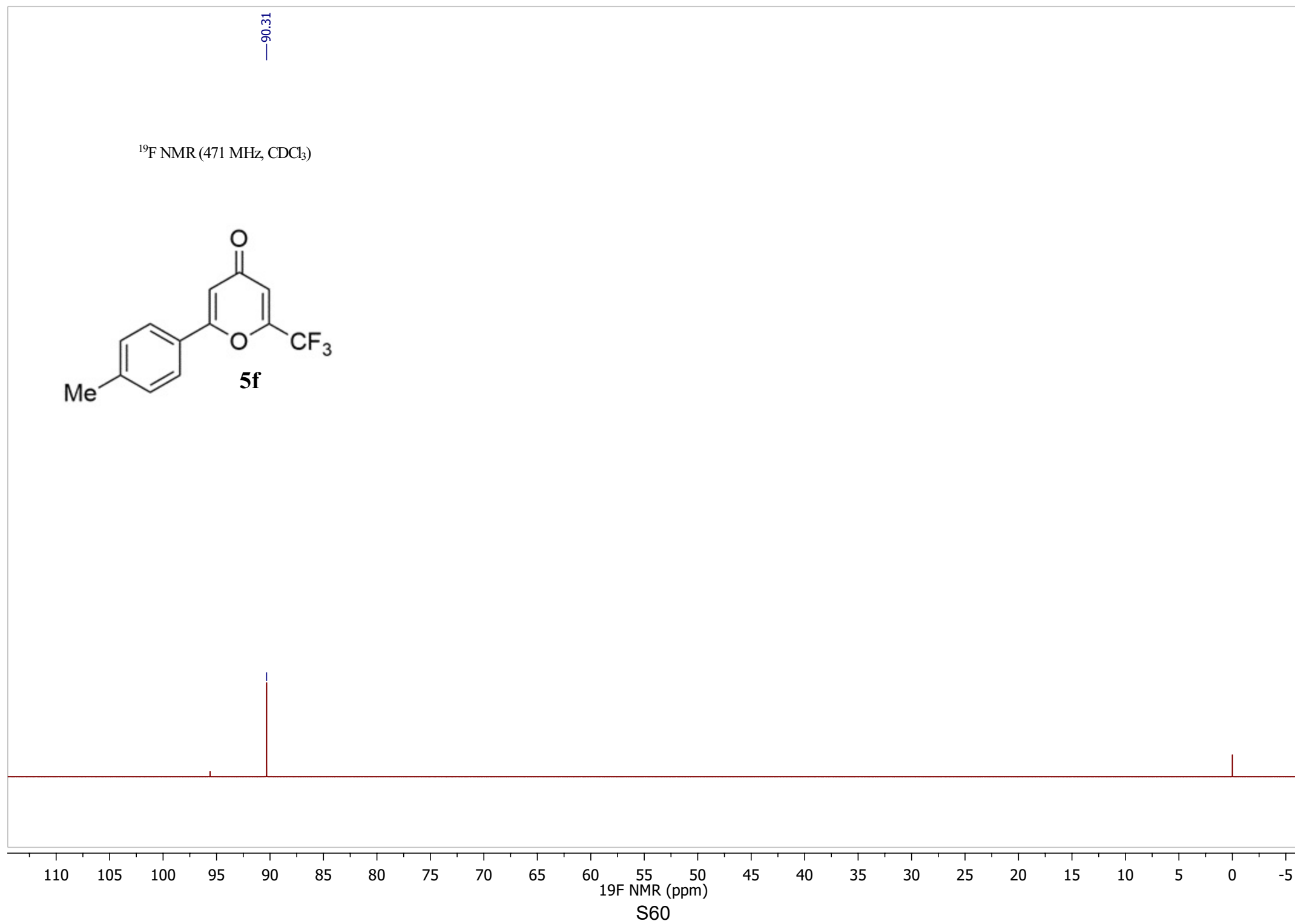
¹H NMR (ppm)

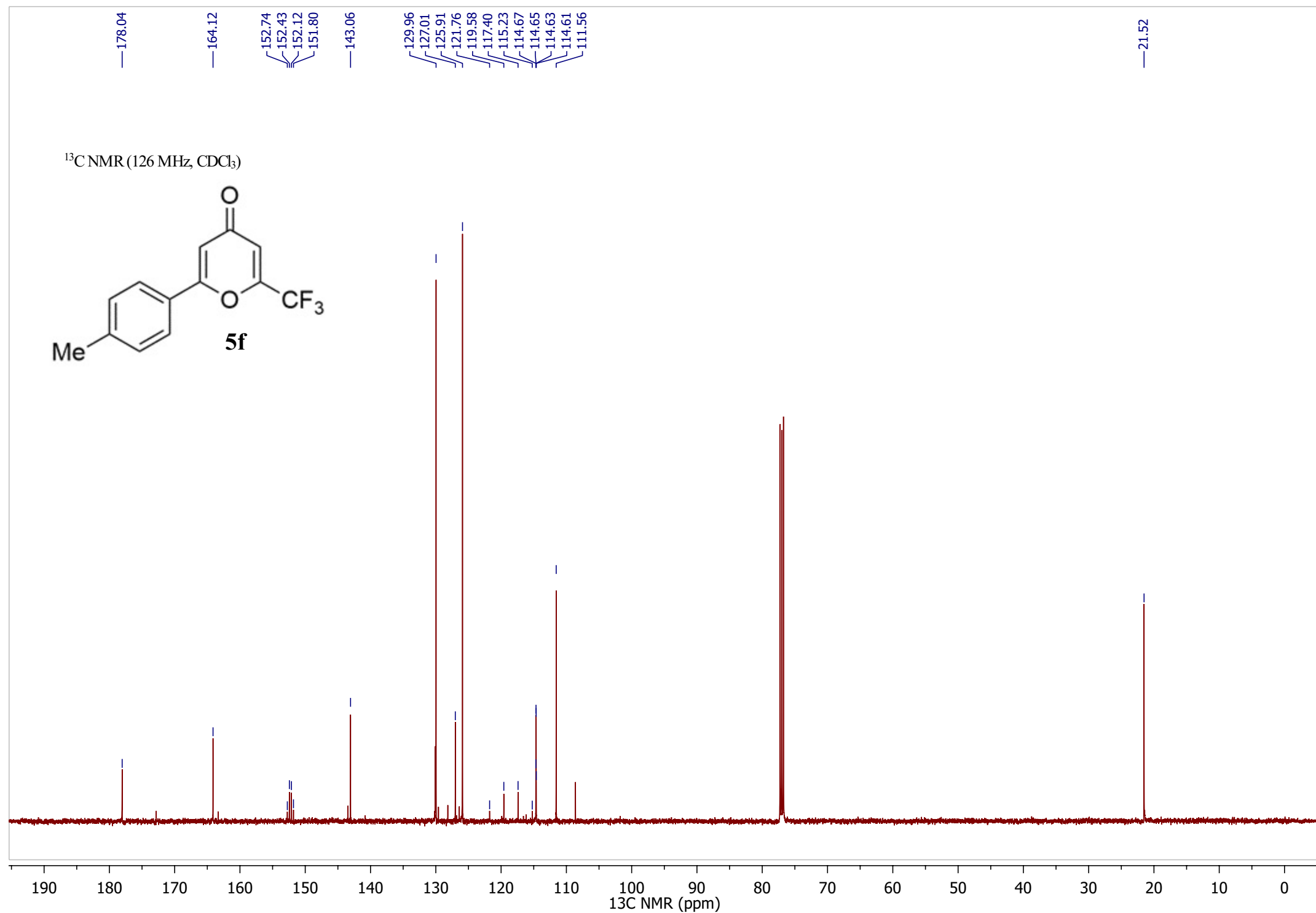
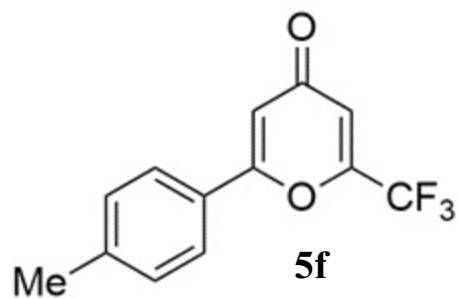
S59

^{19}F NMR (471 MHz, CDCl_3)

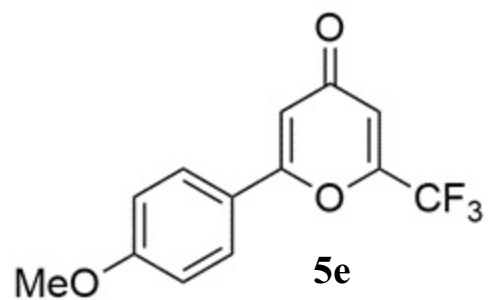


—90.31





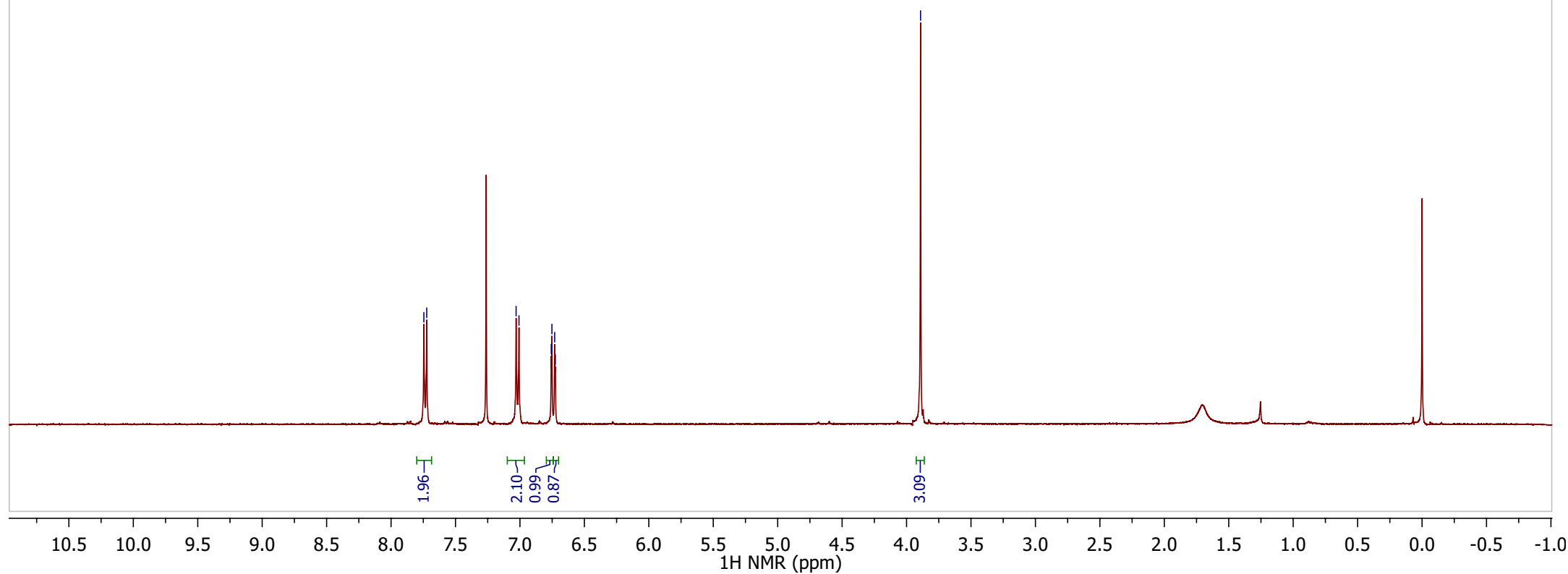
^1H NMR (400 MHz, CDCl_3)



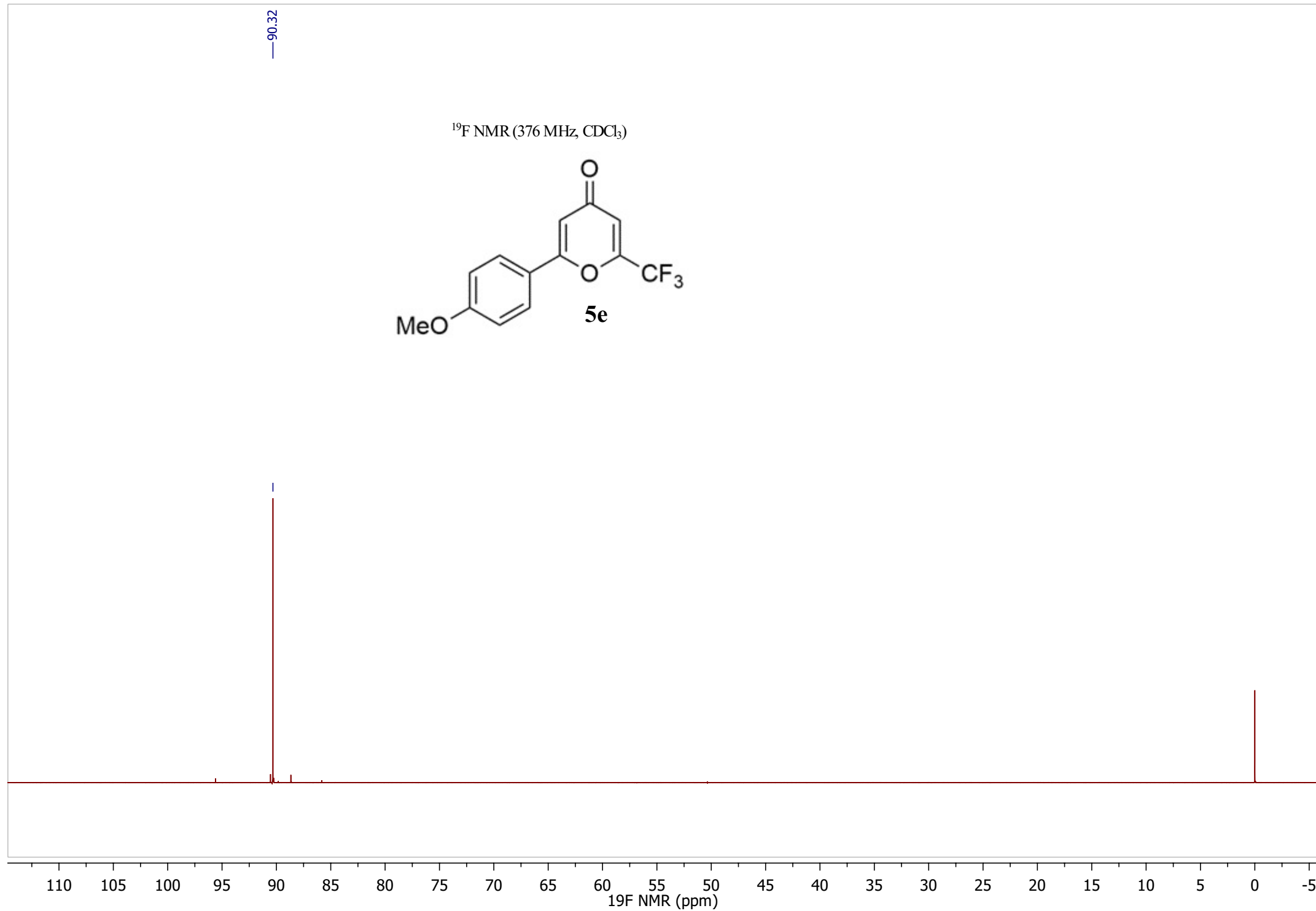
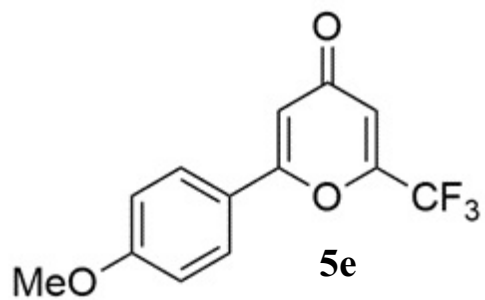
7.75
7.72

7.03
7.01
6.76
6.75
6.73
6.73

3.89



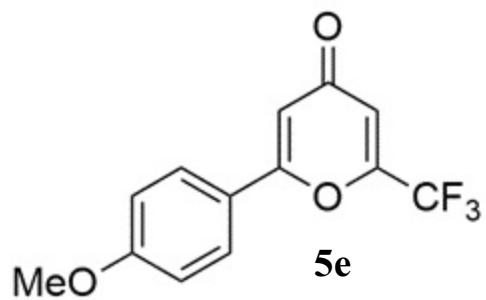
^{19}F NMR (376 MHz, CDCl_3)



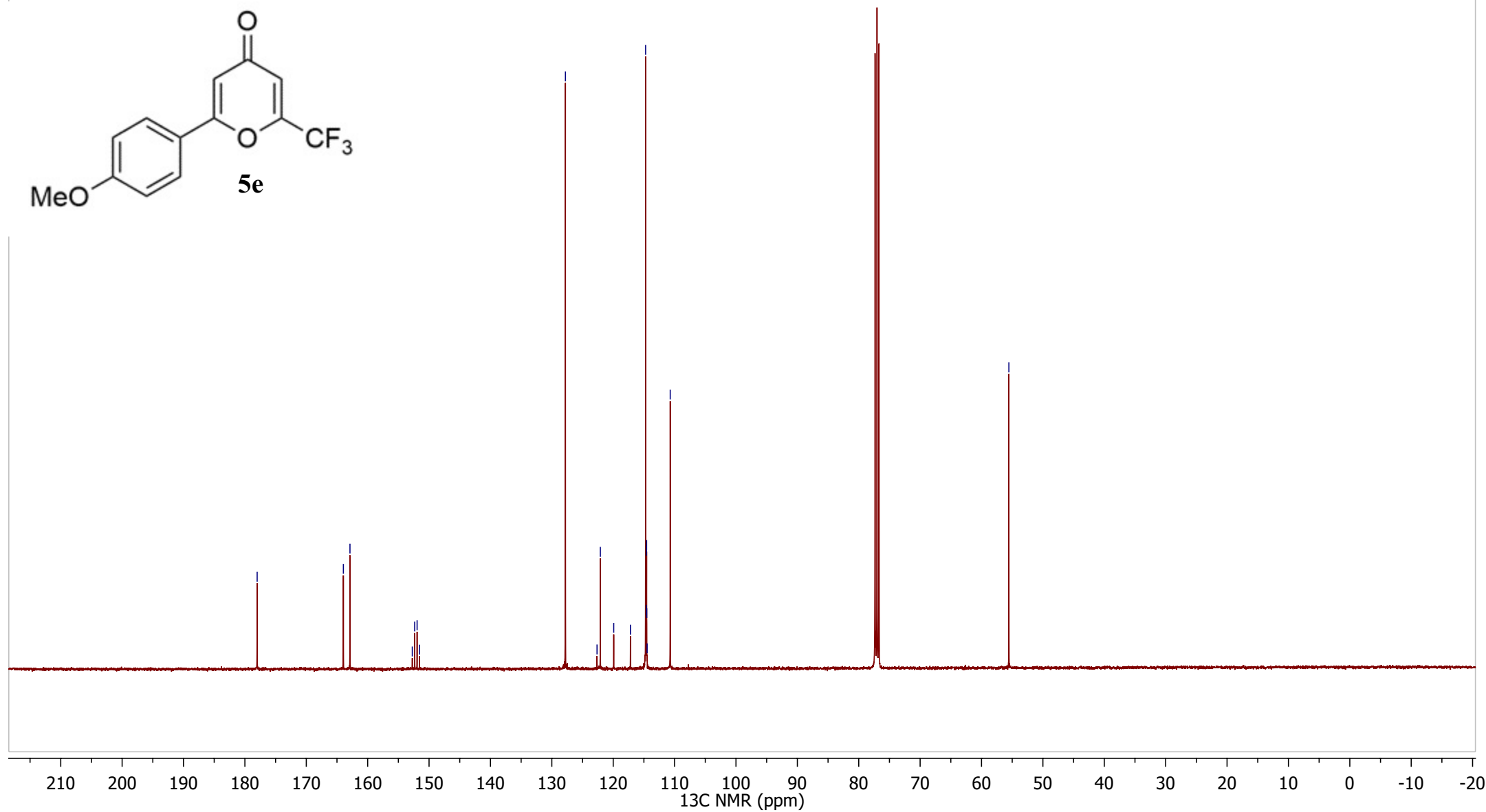
^{19}F NMR (ppm)

S63

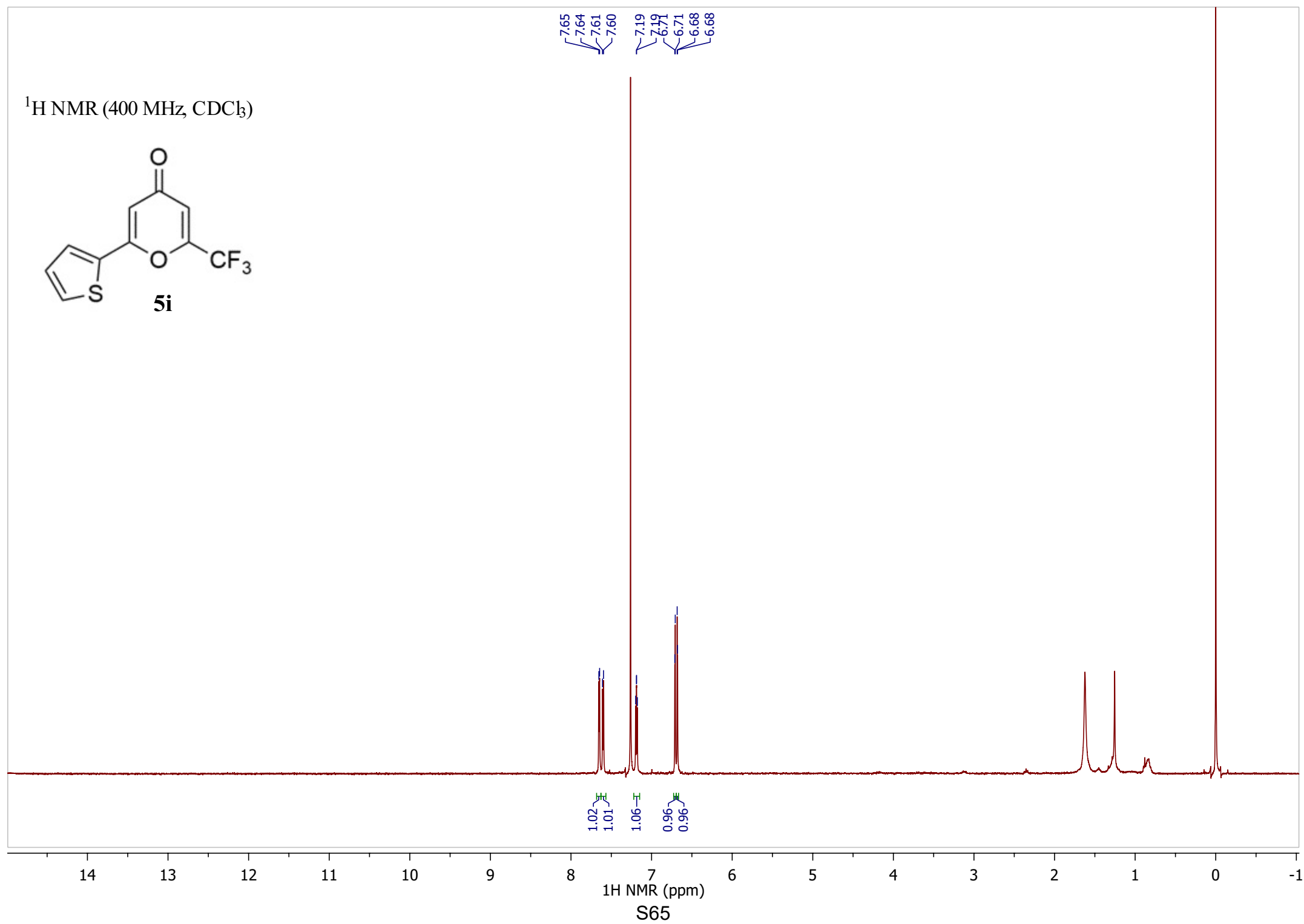
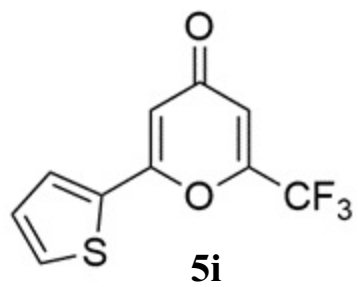
^{13}C NMR (101 MHz, CDCl_3)



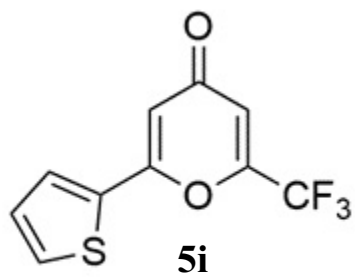
178.00
163.96 162.88
152.73 152.34 151.95 151.55
127.78 122.63 122.10 119.91 117.19 114.72 114.60 114.58 114.56 114.54 114.48 110.71
55.54



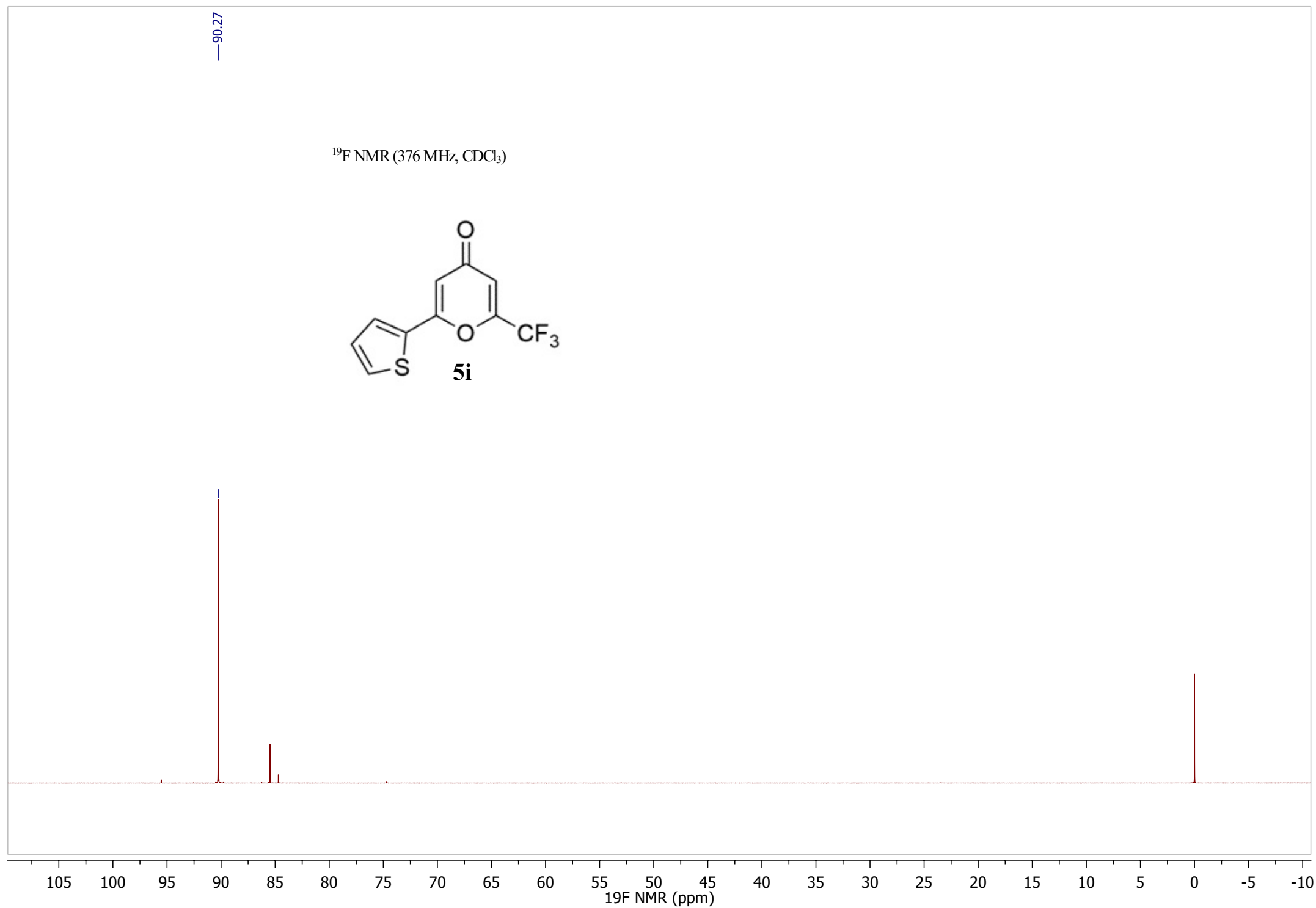
^1H NMR (400 MHz, CDCl_3)



¹⁹F NMR (376 MHz, CDCl₃)



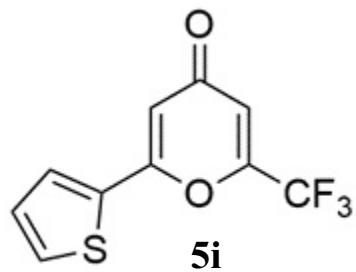
—90.27



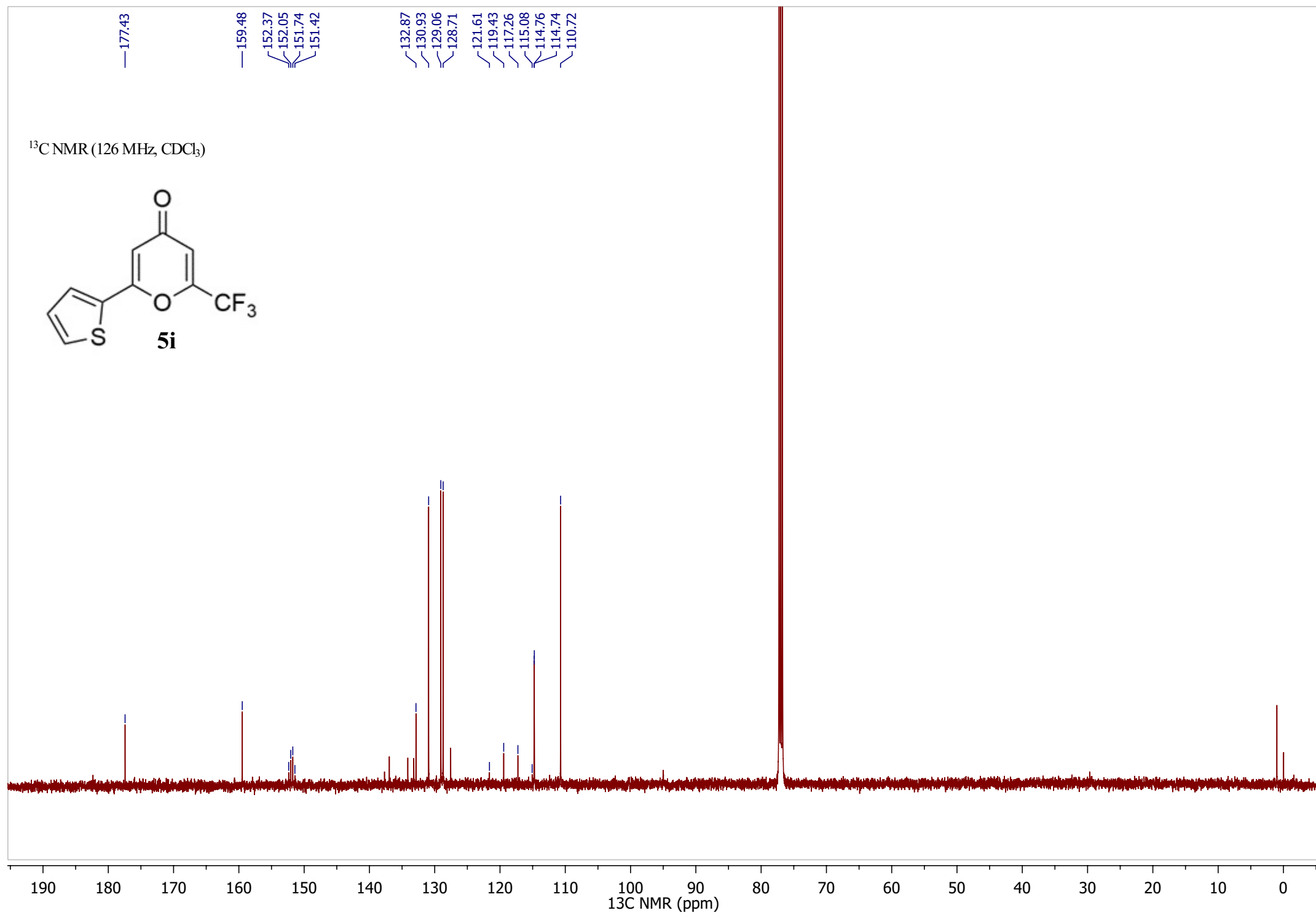
¹⁹F NMR (ppm)

S66

¹³C NMR (126 MHz, CDCl₃)

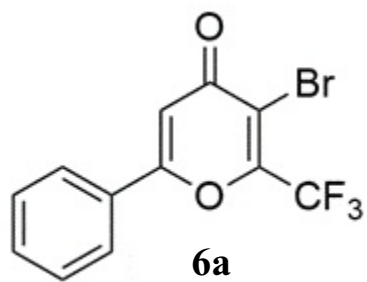


177.43
159.48
152.37
152.05
151.74
151.42
132.87
130.93
129.06
128.71
121.61
119.43
117.26
115.08
114.76
114.74
110.72



S67

^1H NMR (500 MHz, CDCl_3)

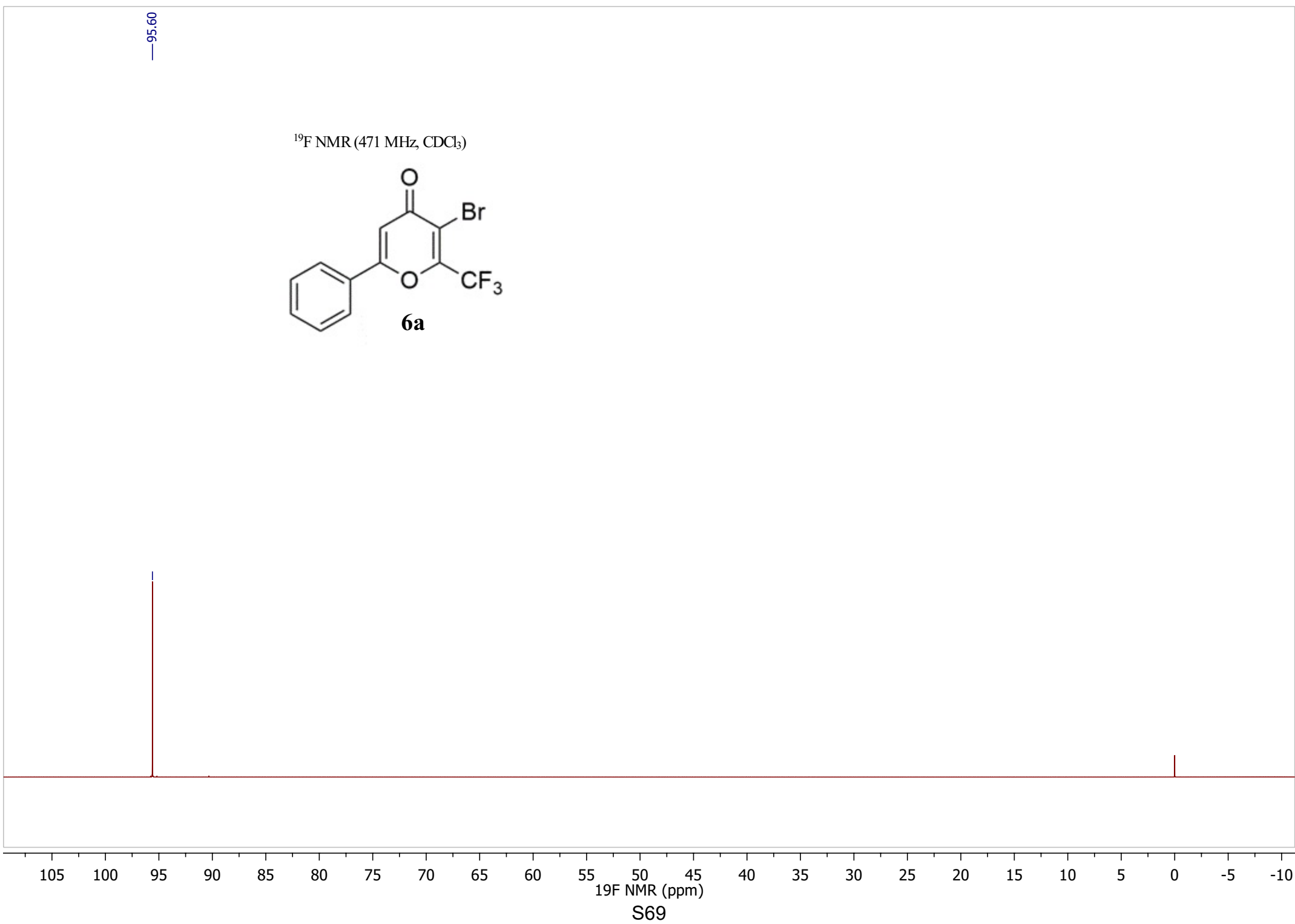


7.80
7.78
7.61
7.59
7.58
7.56
7.54
7.53
6.94

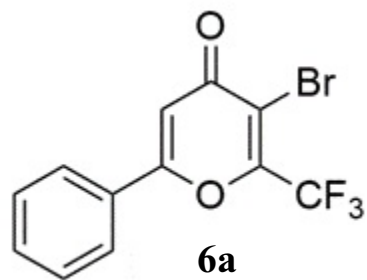
2.01
1.03
2.01
0.95

^1H NMR (ppm)

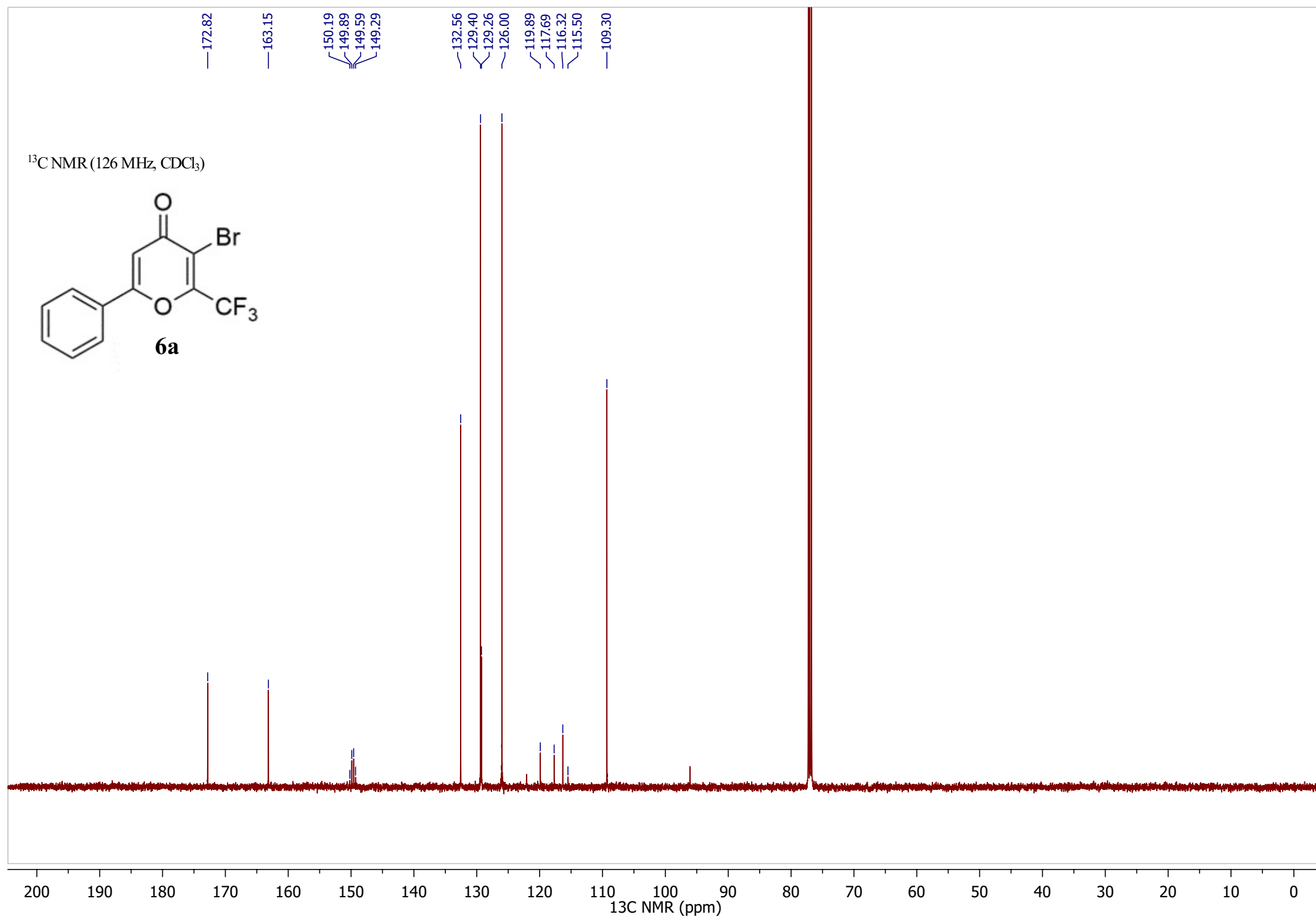
S68



^{13}C NMR (126 MHz, CDCl_3)

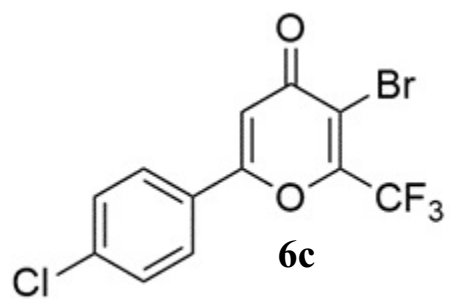


— 172.82
— 163.15
— 150.19
— 149.89
— 149.59
— 149.29
— 132.56
— 129.40
— 129.26
— 126.00
— 119.89
— 117.69
— 116.32
— 115.50
— 109.30

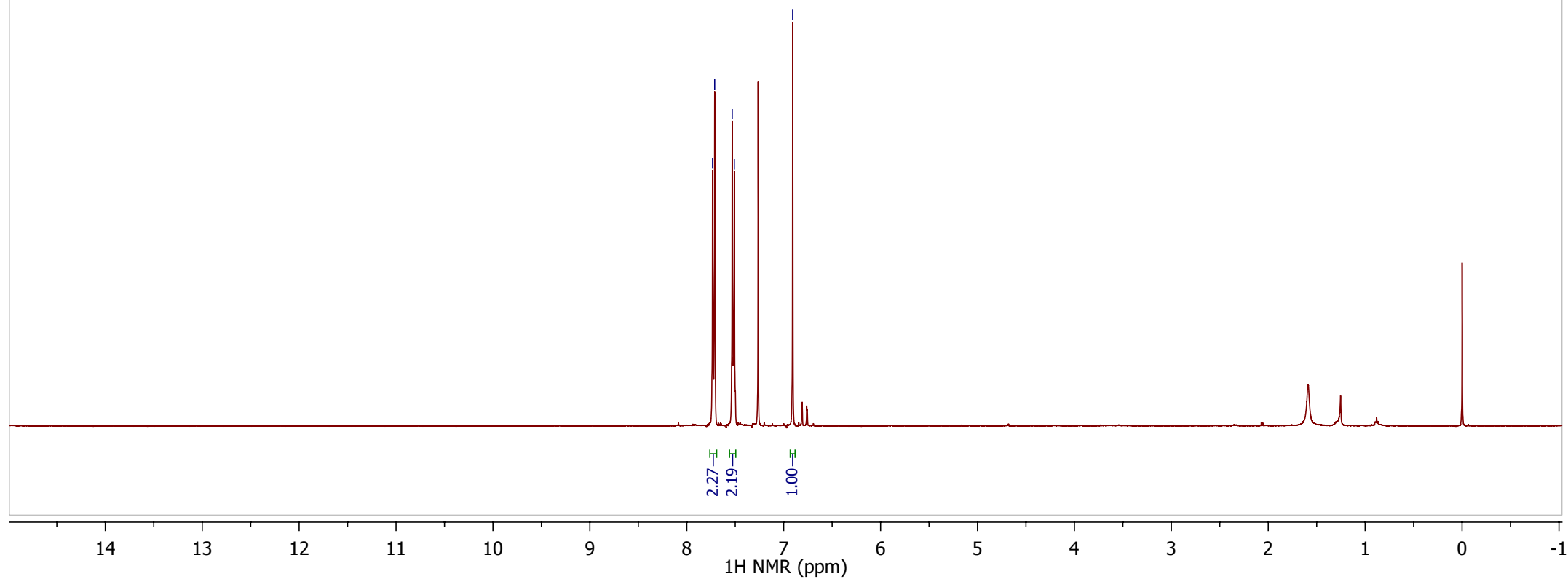


S70

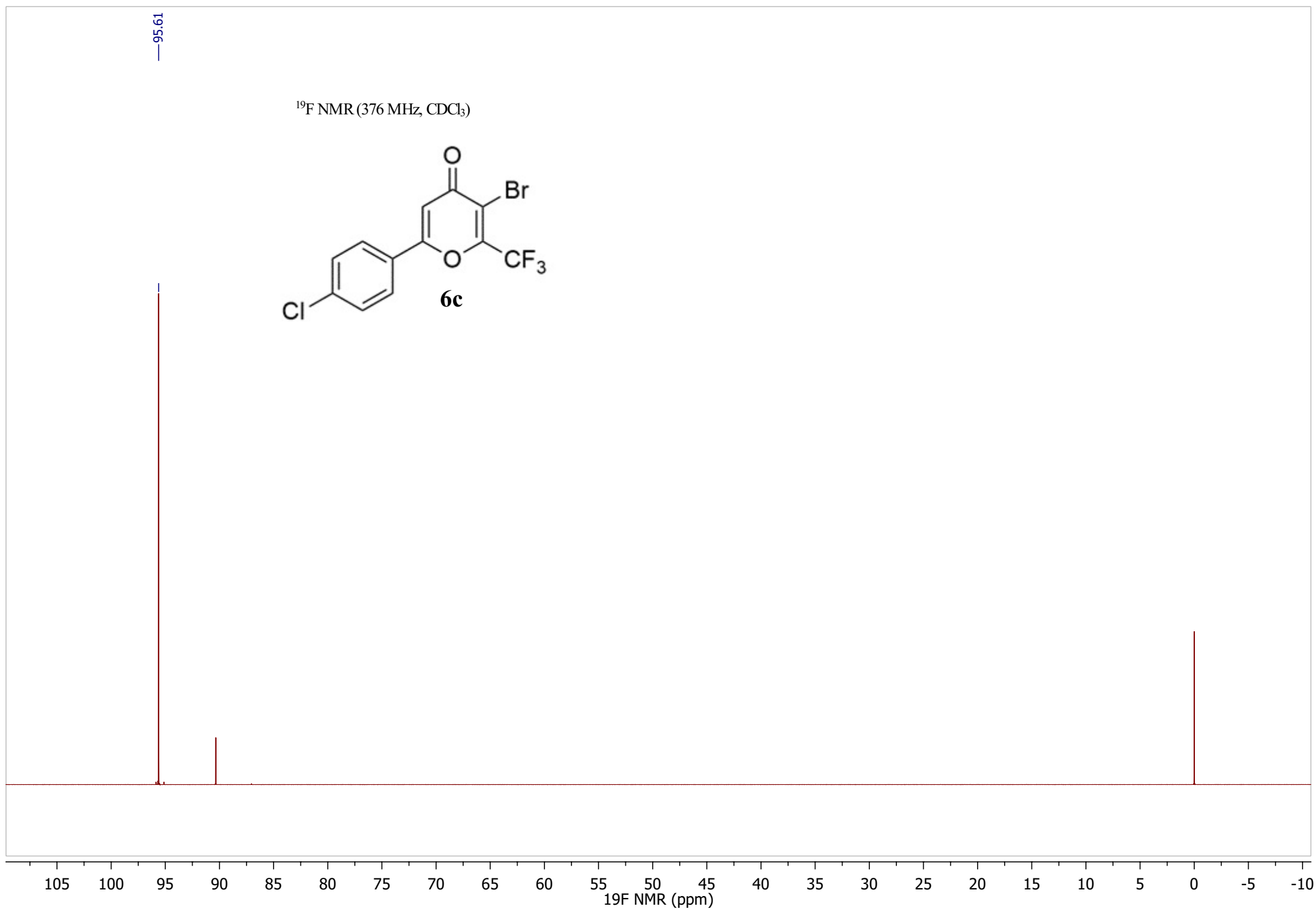
¹H NMR (400 MHz, CDCl₃)



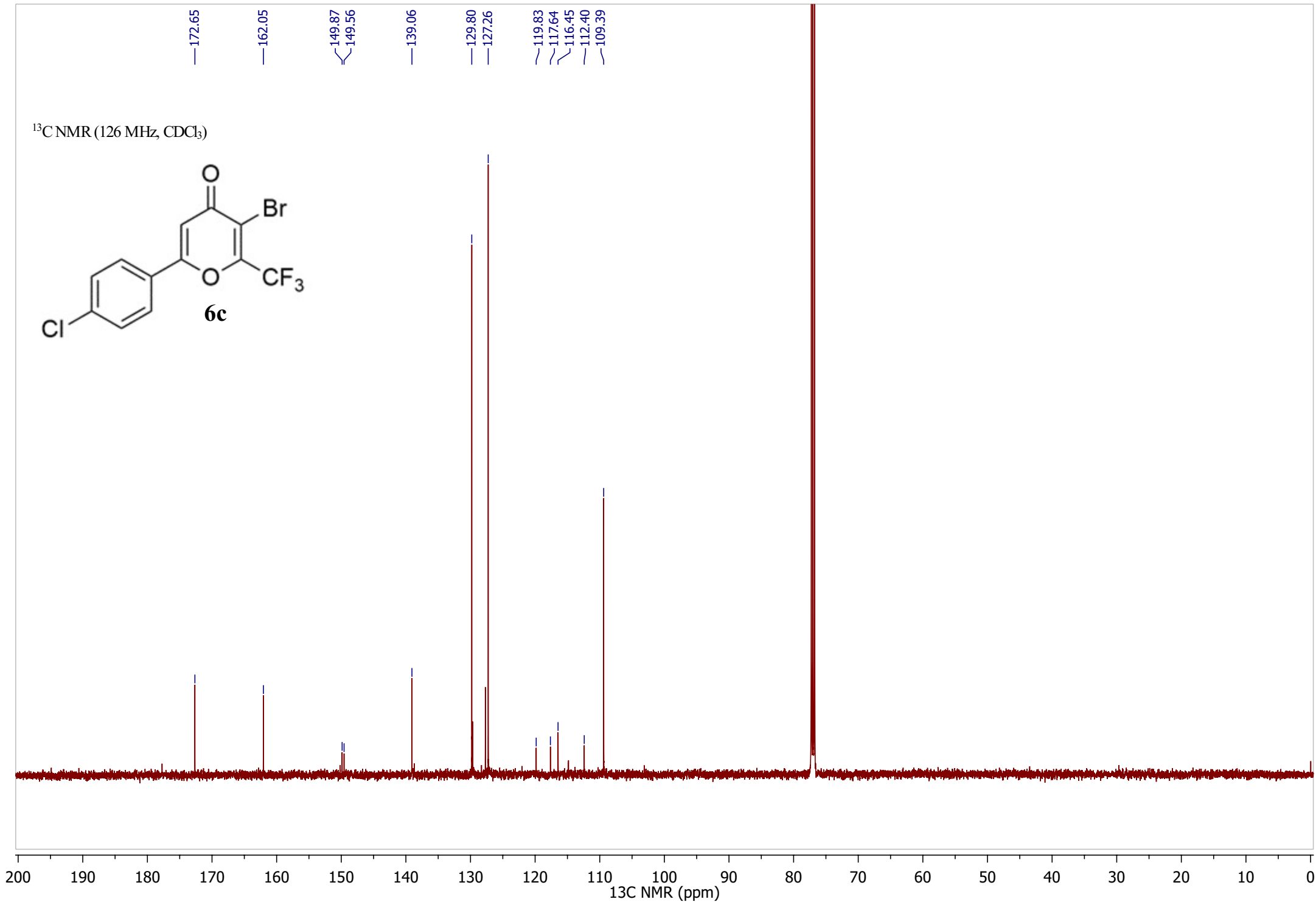
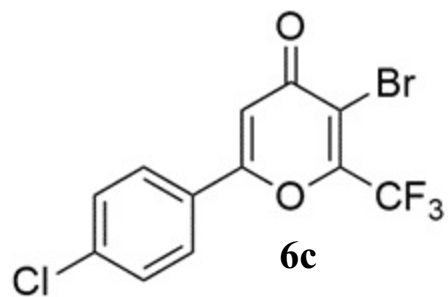
7.73
7.71
7.53
7.51
6.91



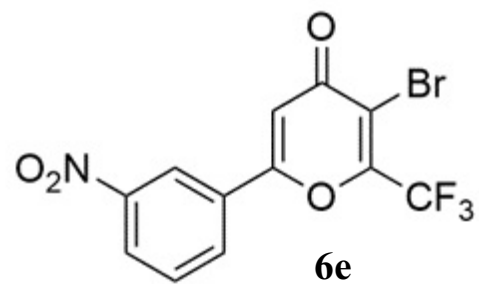
S71



¹³C NMR (126 MHz, CDCl₃)

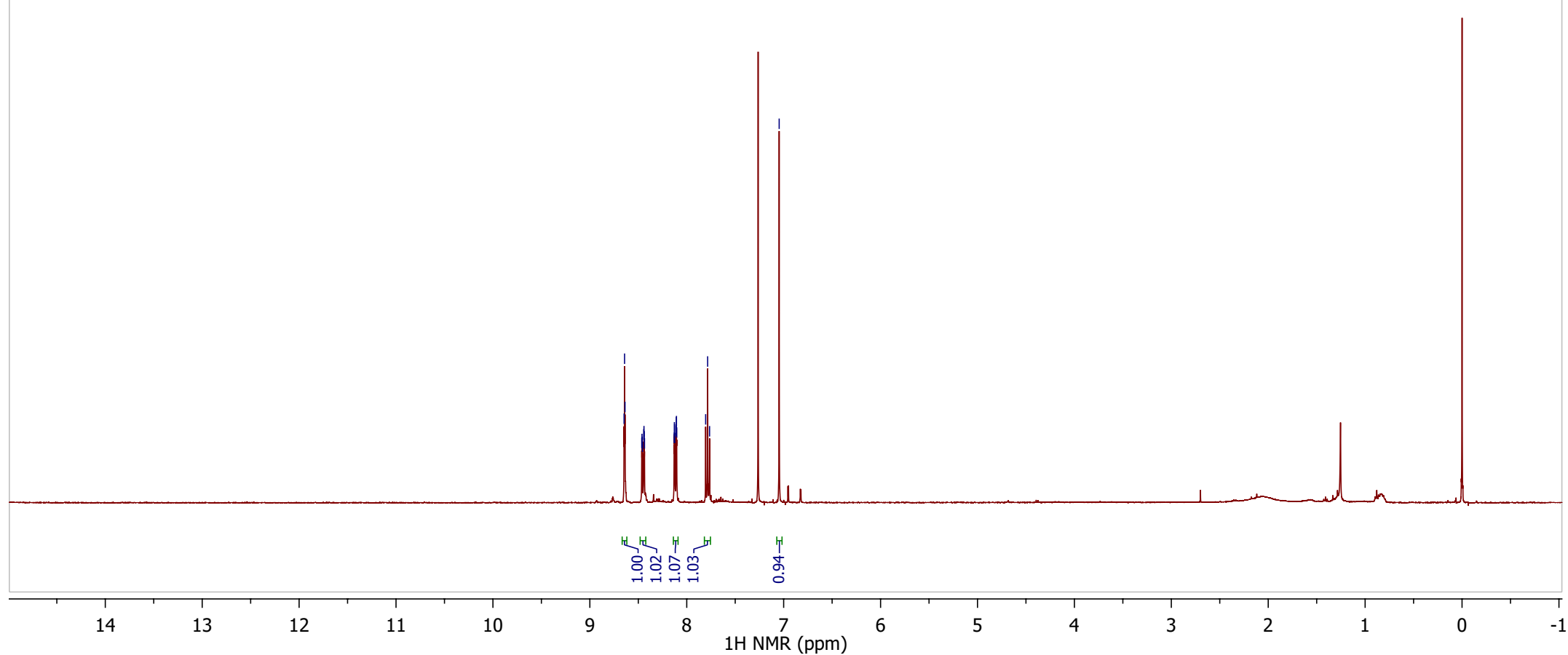


¹H NMR (400 MHz, CDCl₃)



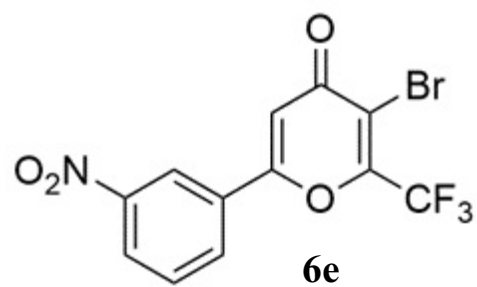
6e

8.65
8.64
8.64
8.46
8.46
8.46
8.46
8.44
8.44
8.44
8.13
8.13
8.13
8.12
8.11
8.11
8.11
8.10
7.80
7.78
7.76
7.05

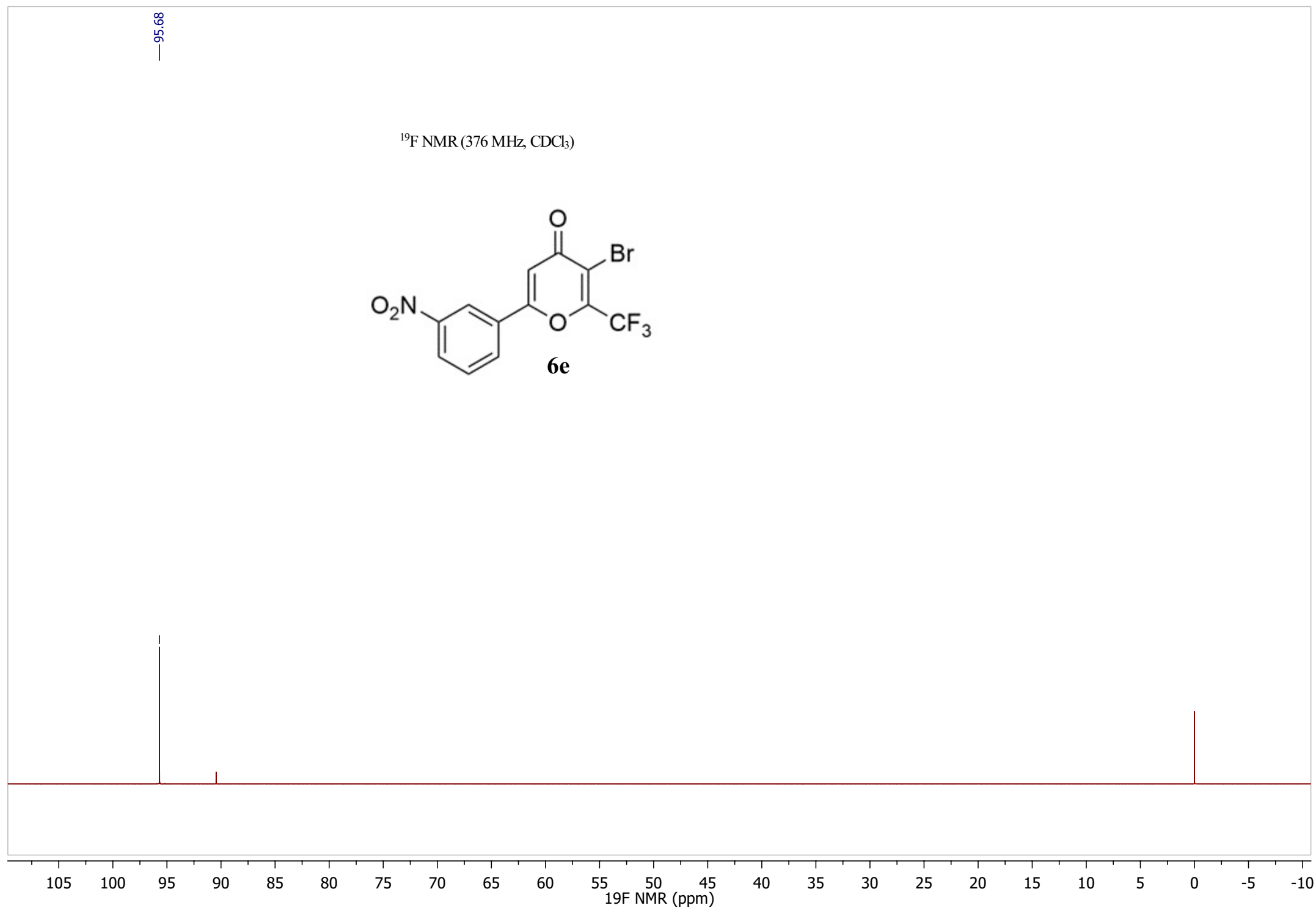


¹H NMR (ppm)

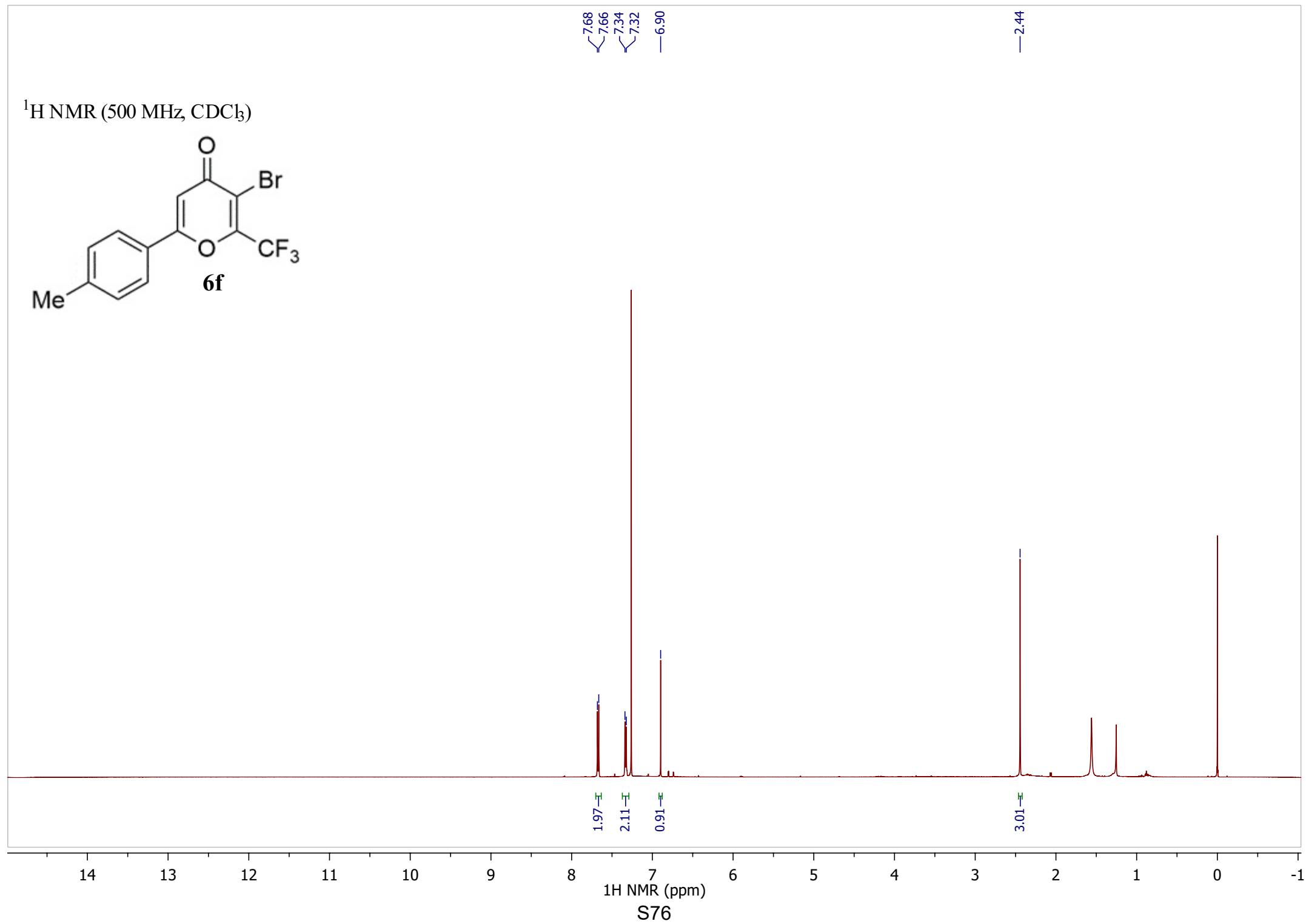
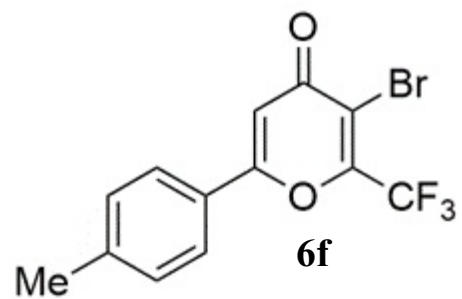
S74

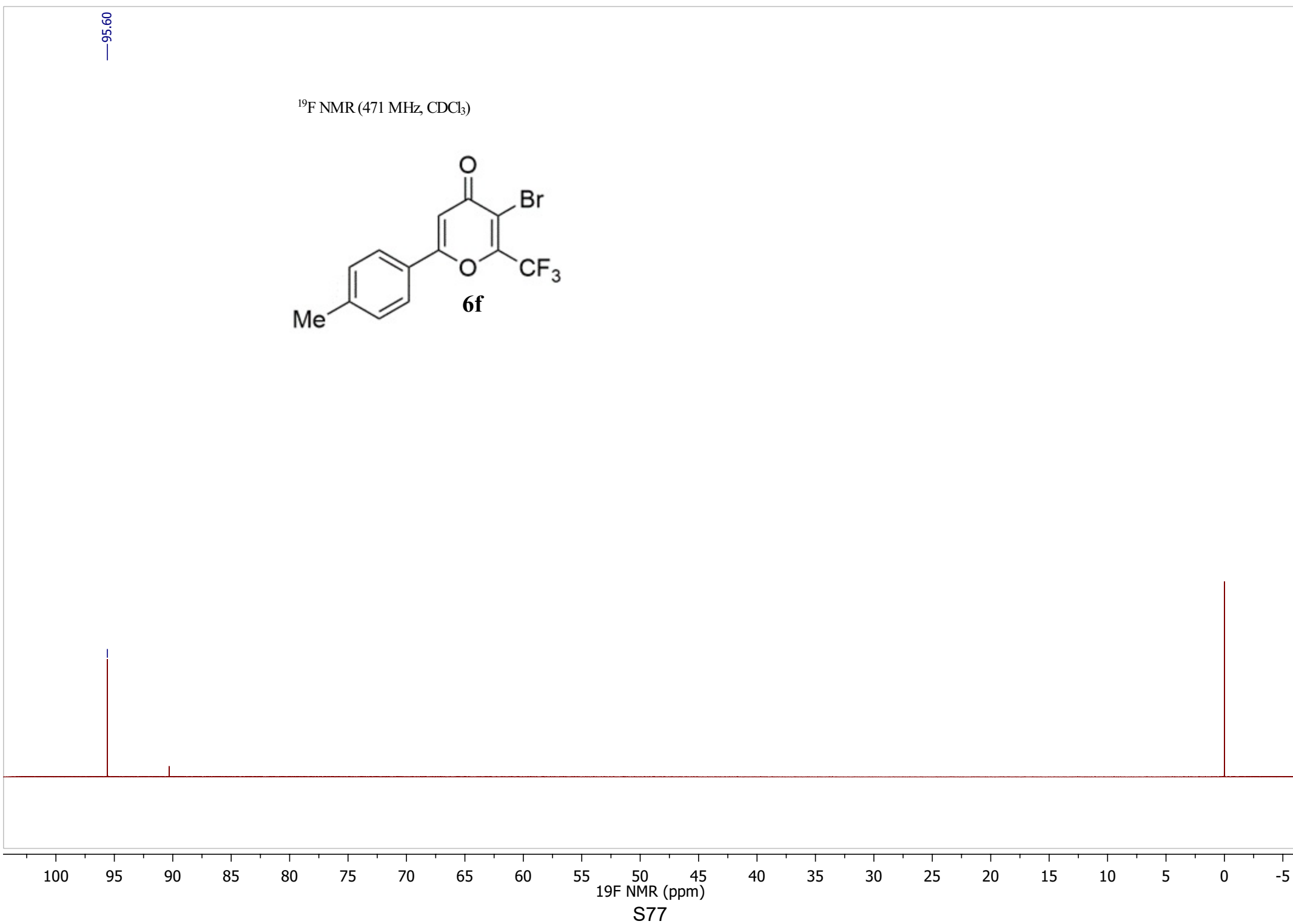


—95.68

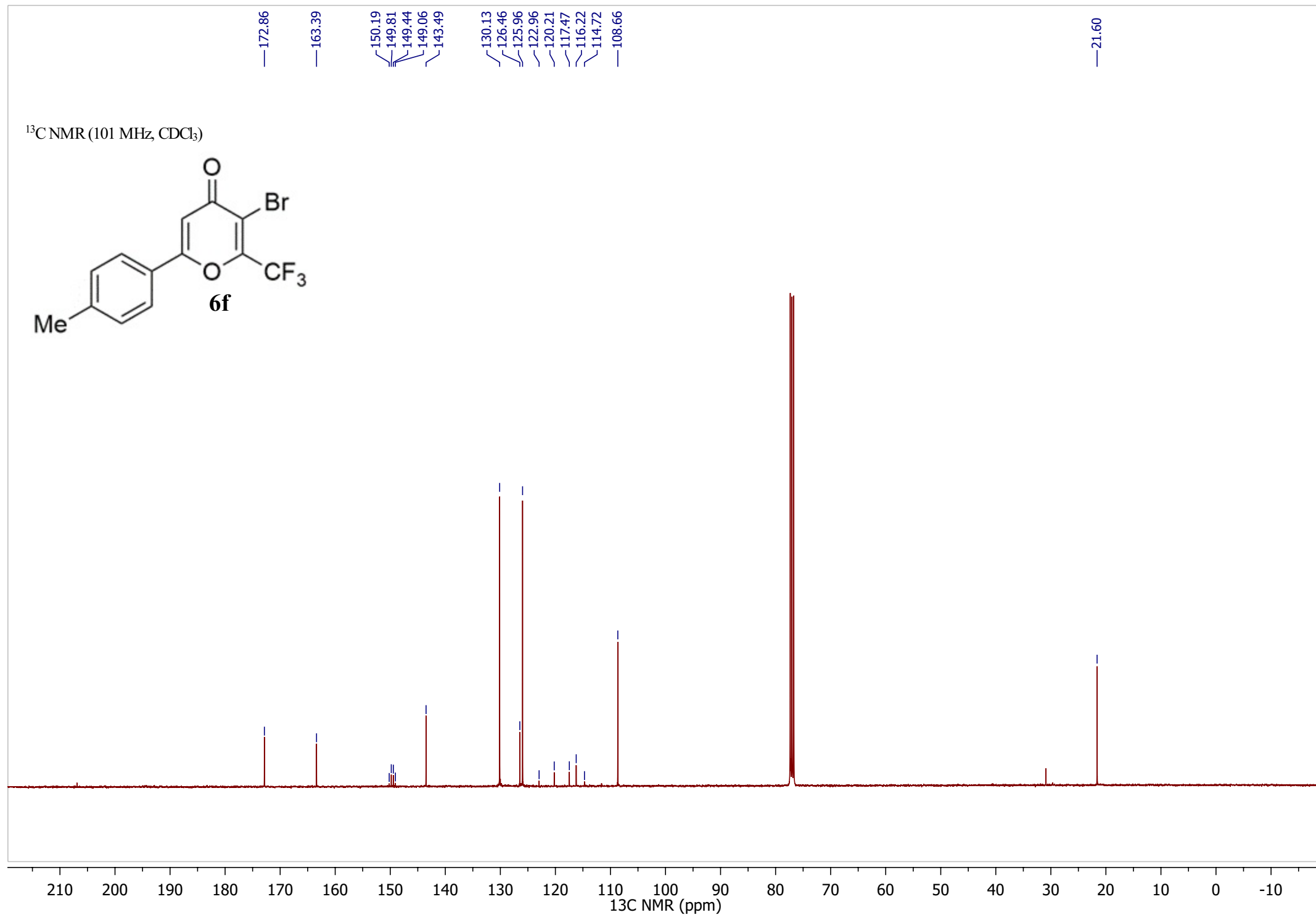
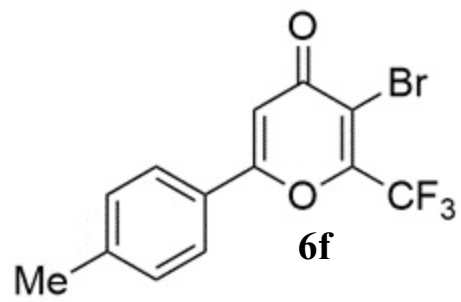


^1H NMR (500 MHz, CDCl_3)





^{13}C NMR (101 MHz, CDCl_3)

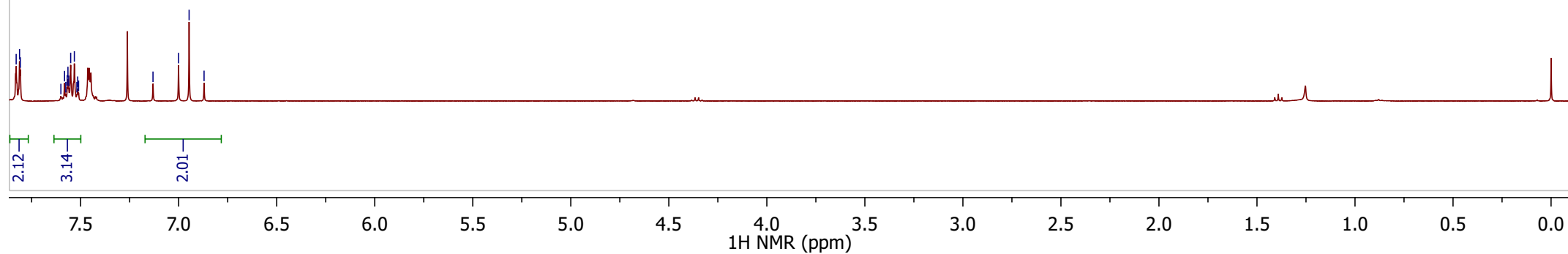
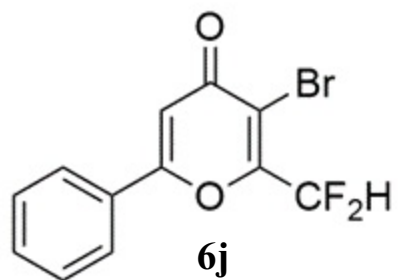


^{13}C NMR (ppm)

S78

7.81
7.58
7.57
7.56
7.55
7.53
7.00
6.95
6.87

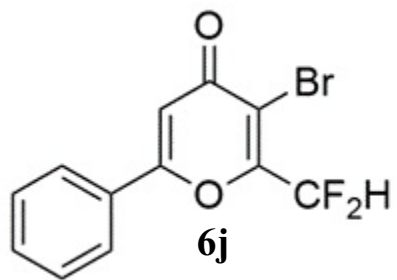
^1H NMR (400 MHz, CDCl_3)



^1H NMR (ppm)

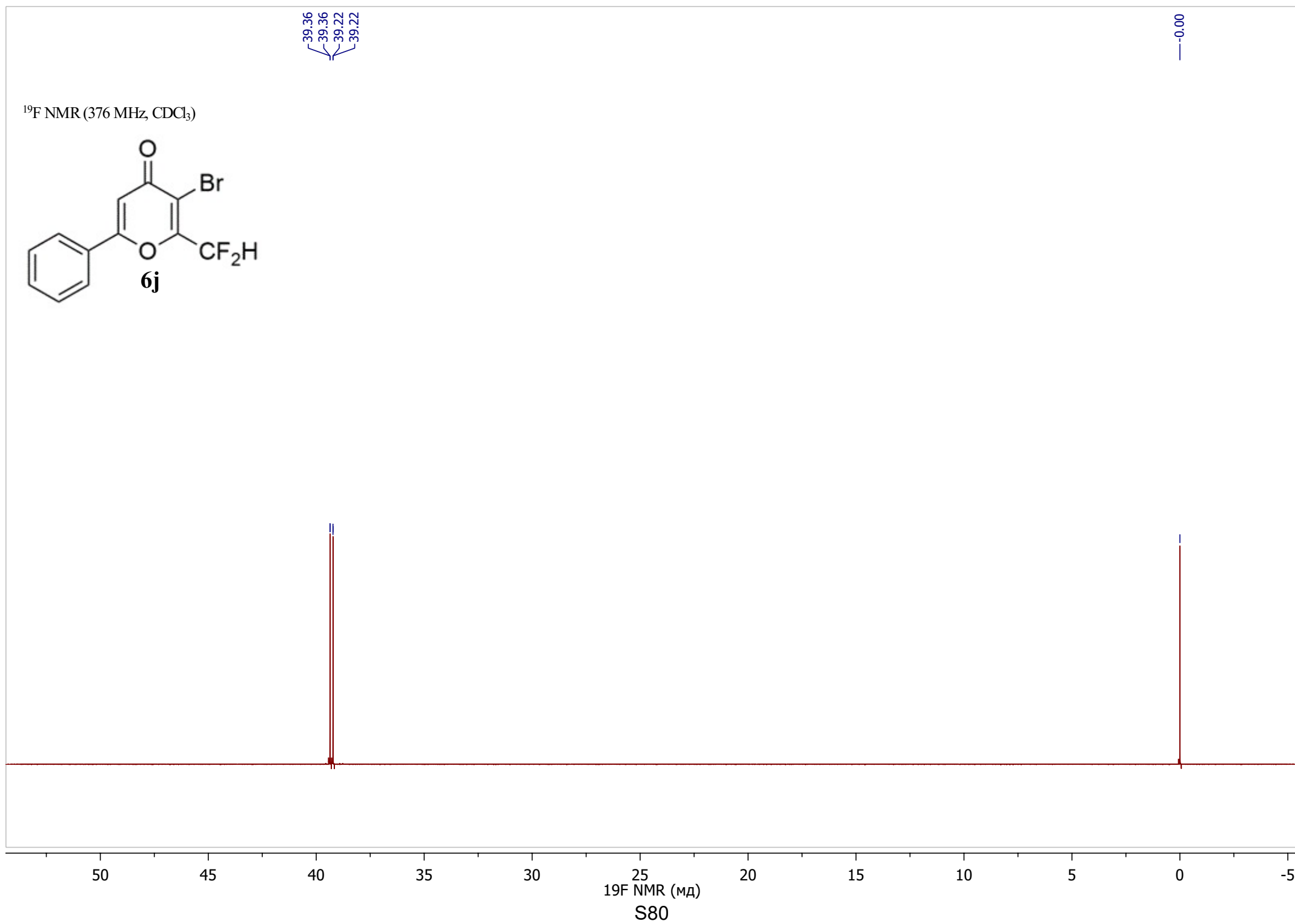
S79

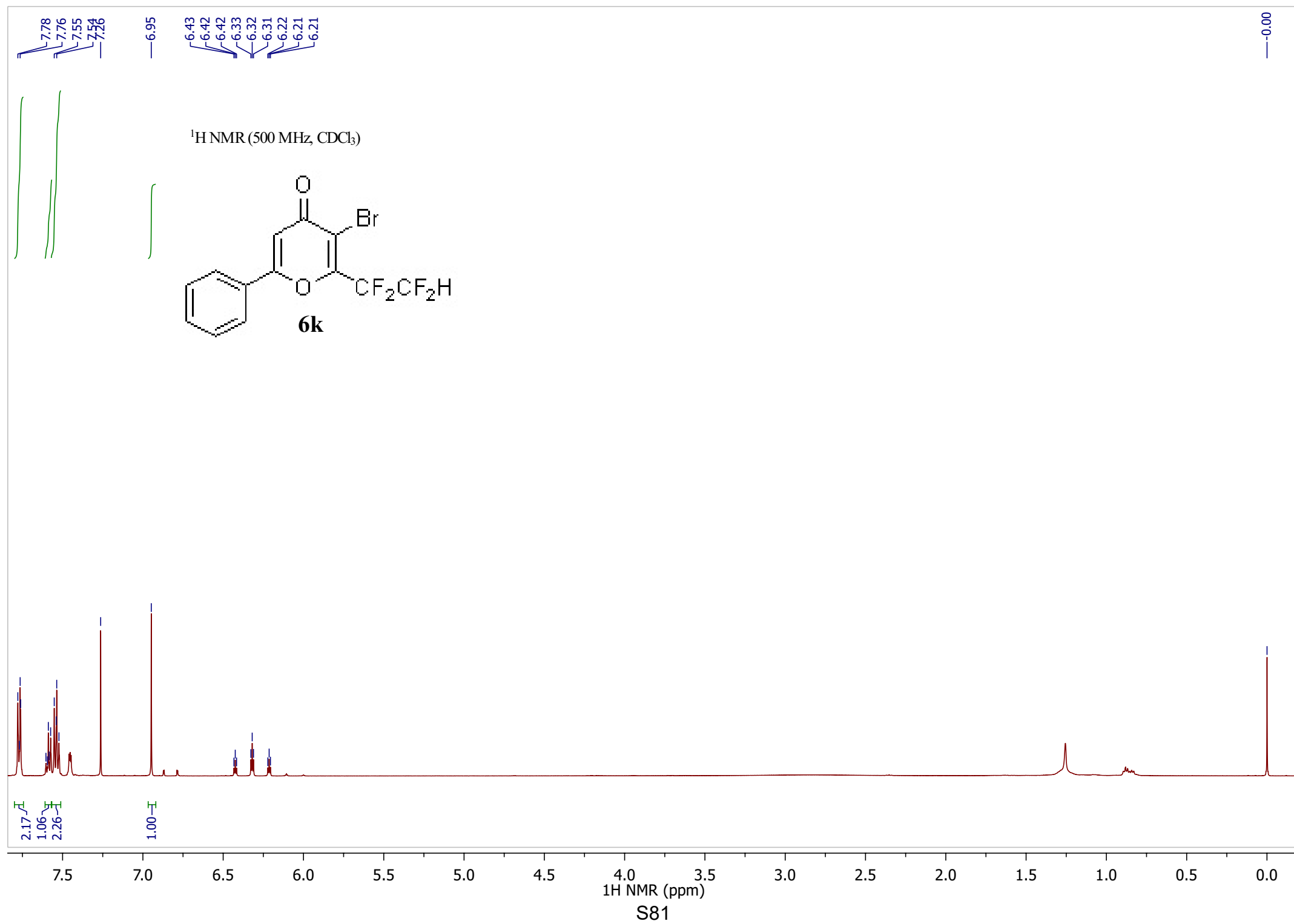
^{19}F NMR (376 MHz, CDCl_3)



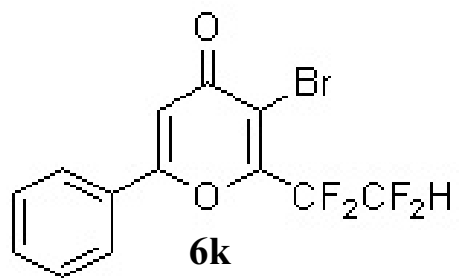
39.36
39.36
39.22
39.22

0.00





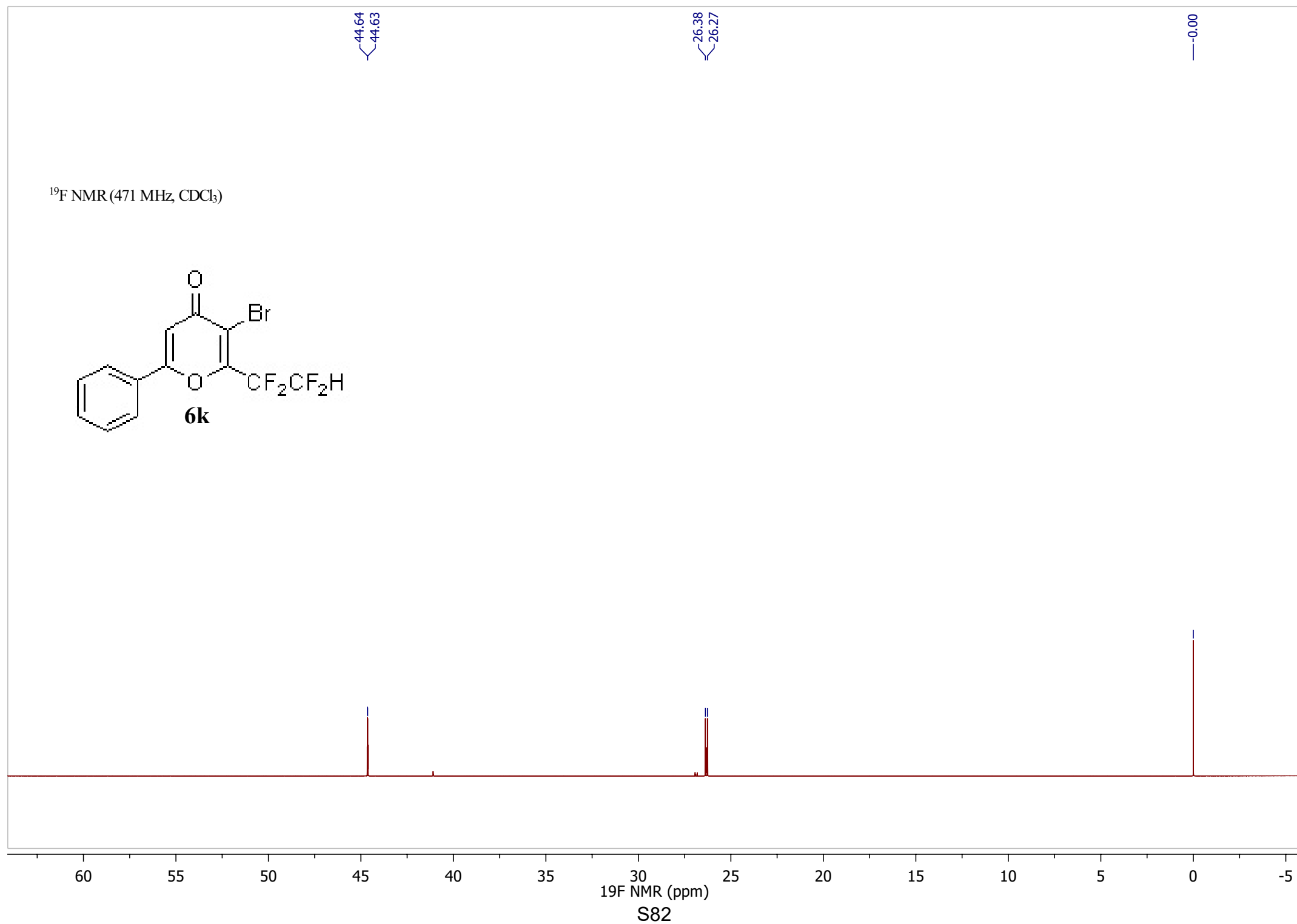
^{19}F NMR (471 MHz, CDCl_3)



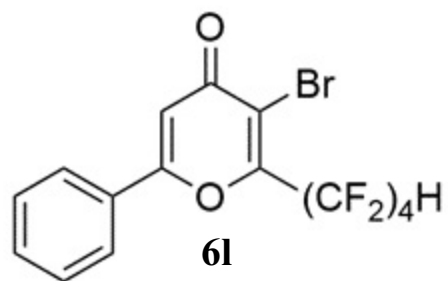
44.64
44.63

26.38
26.27

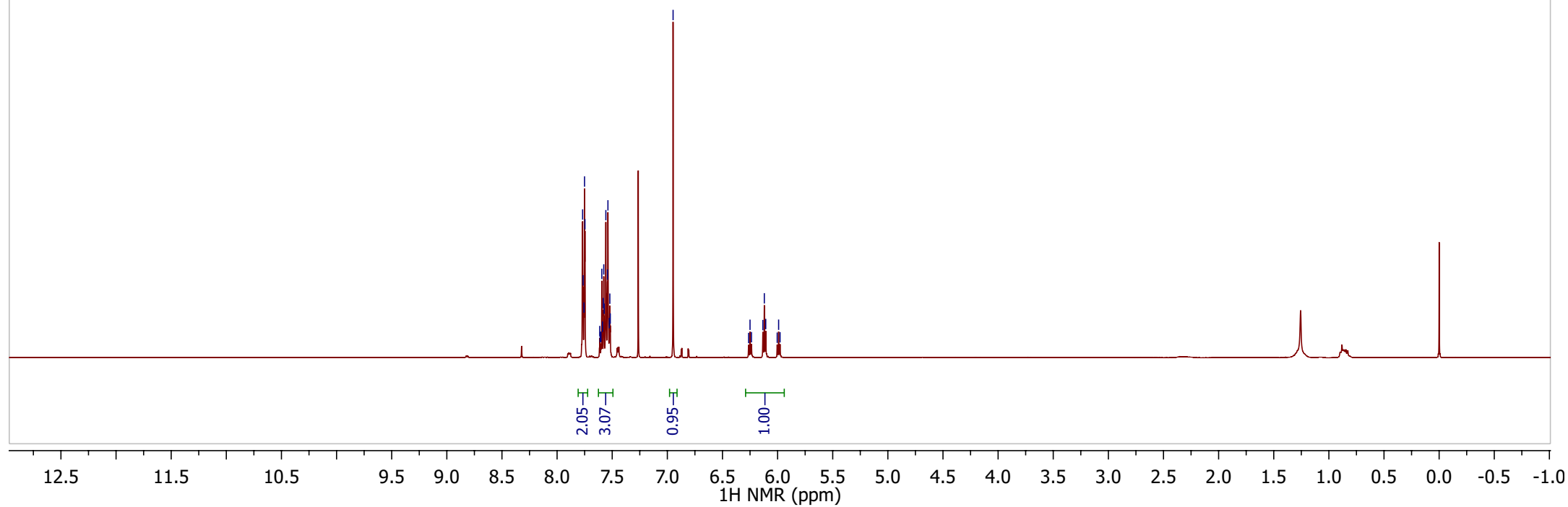
-0.00



¹H NMR (400 MHz, CDCl₃)

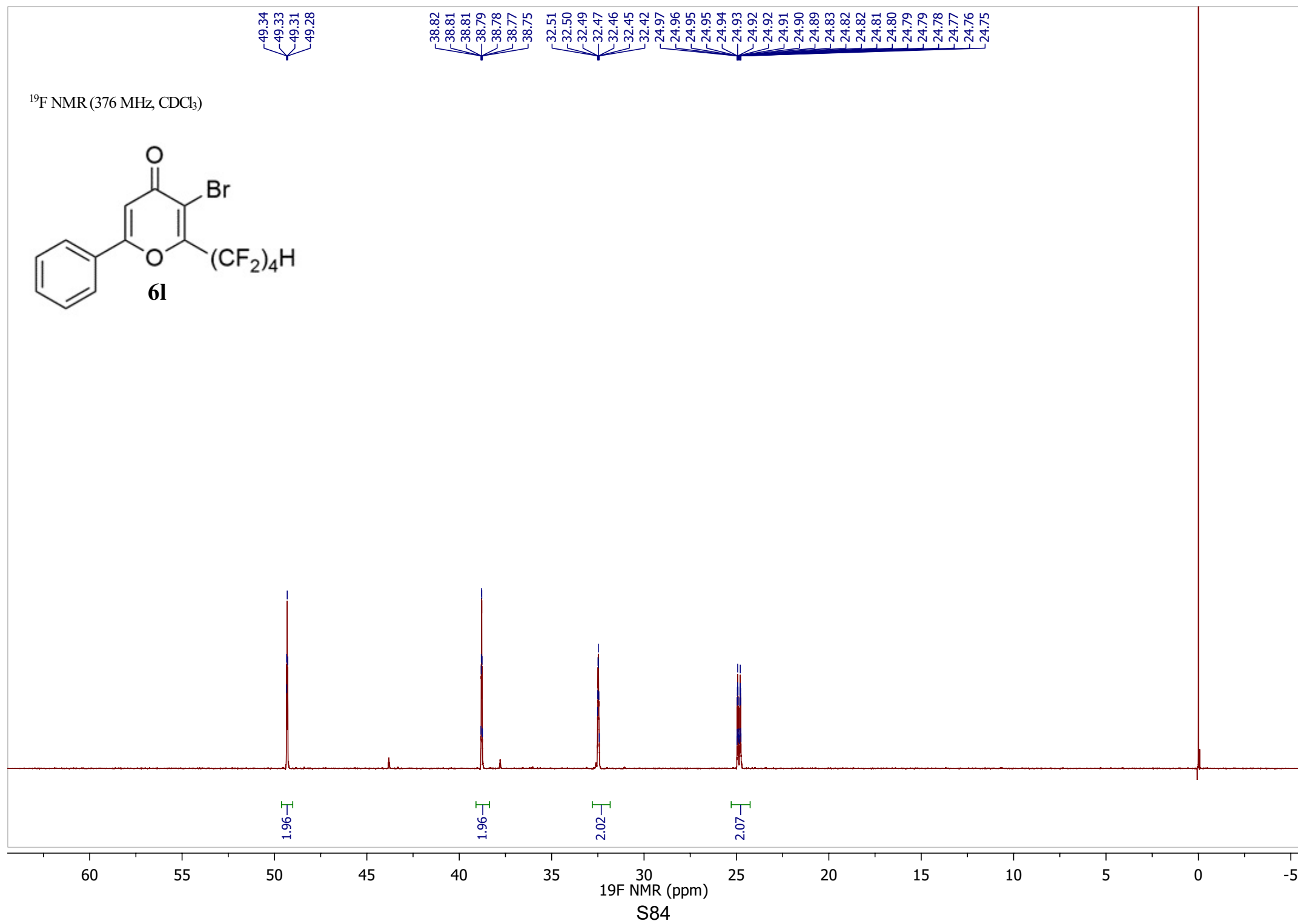
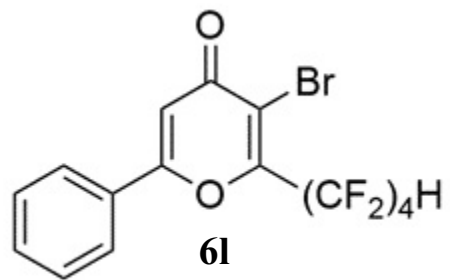


7.77
7.76
7.76
7.75
7.75
7.61
7.61
7.60
7.59
7.59
7.58
7.58
7.57
7.56
7.54
7.54
7.53
7.52
7.52
6.95
6.26
6.25
6.24
6.13
6.12
6.11
6.00
5.99
5.98



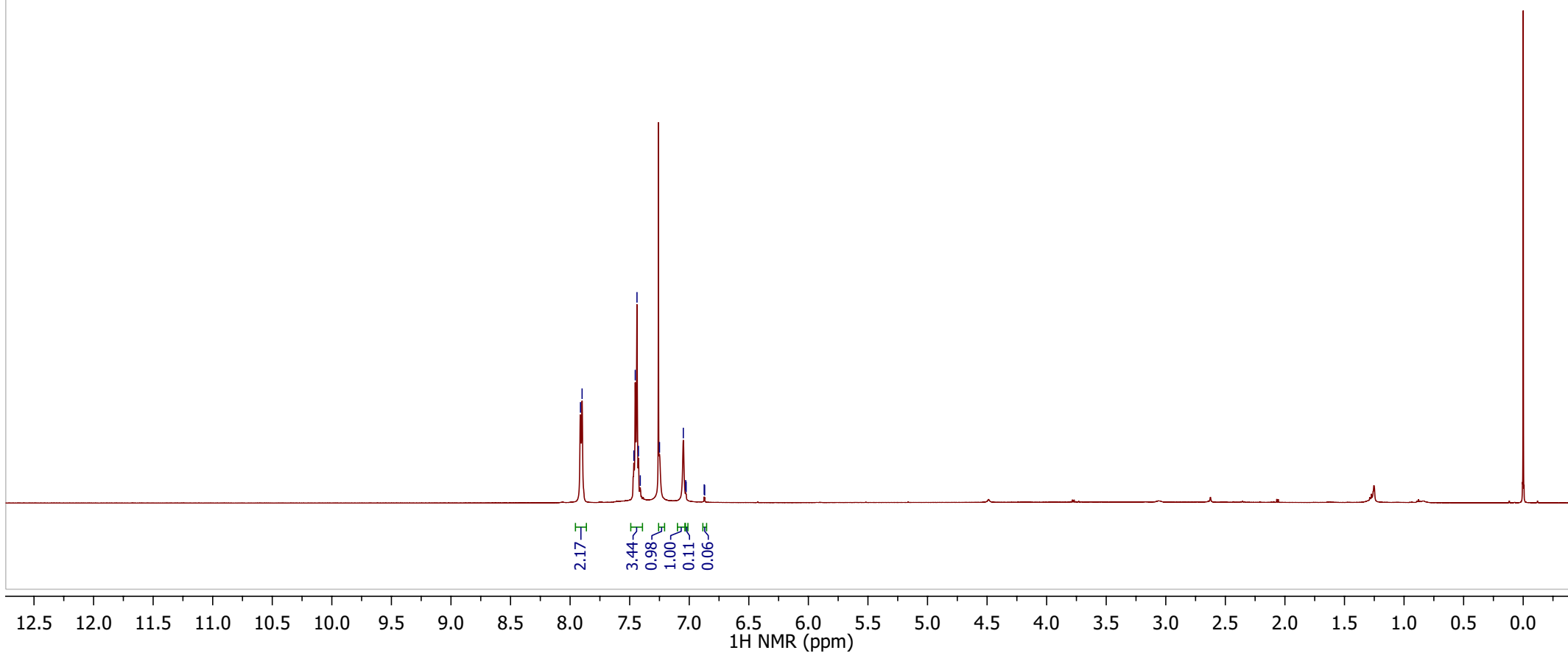
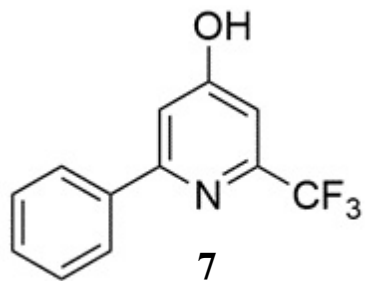
S83

¹⁹F NMR (376 MHz, CDCl₃)

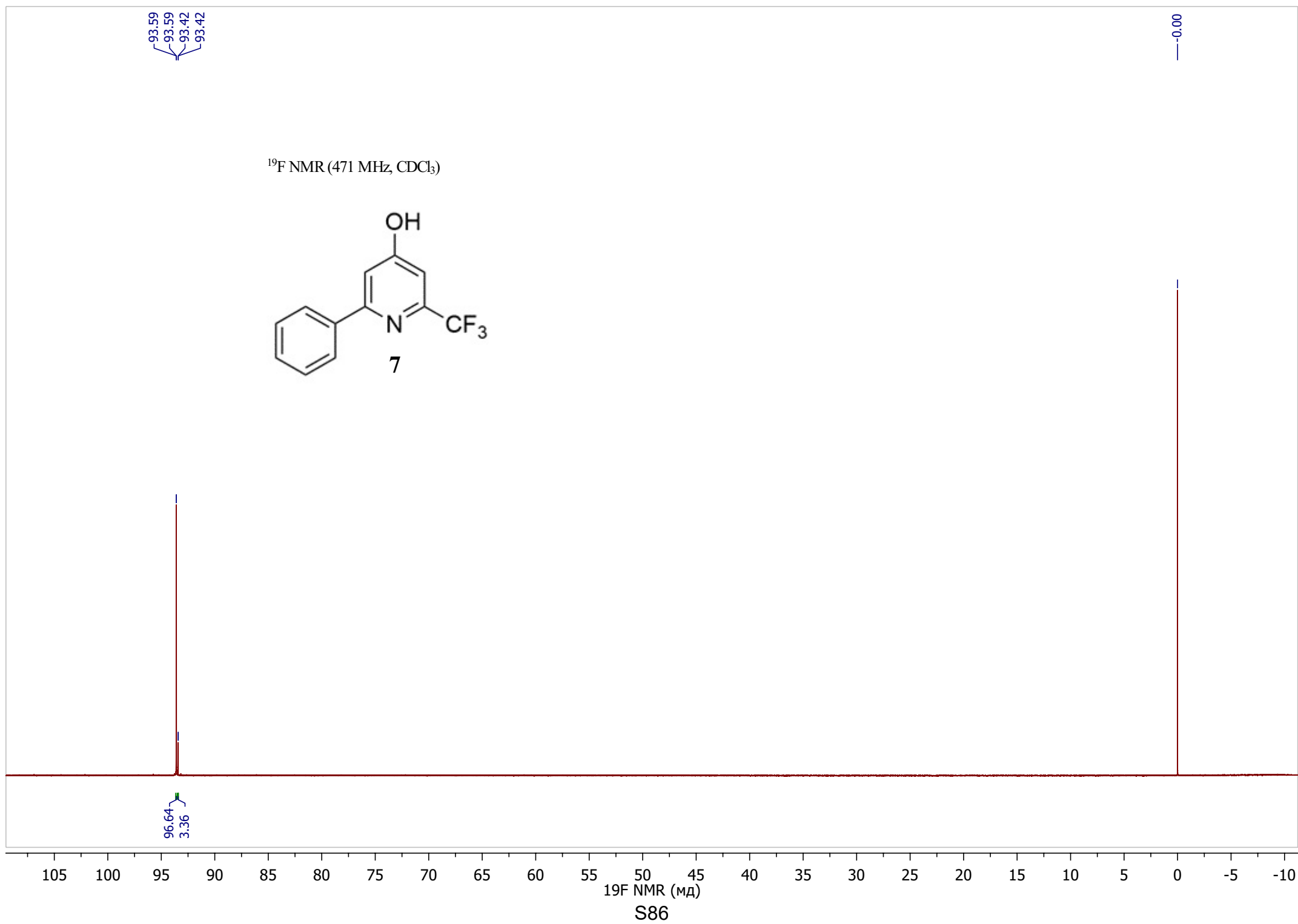


7.91
7.90
7.46
7.45
7.44
7.43
7.41
7.25
7.05
7.03
7.03
6.87
6.87

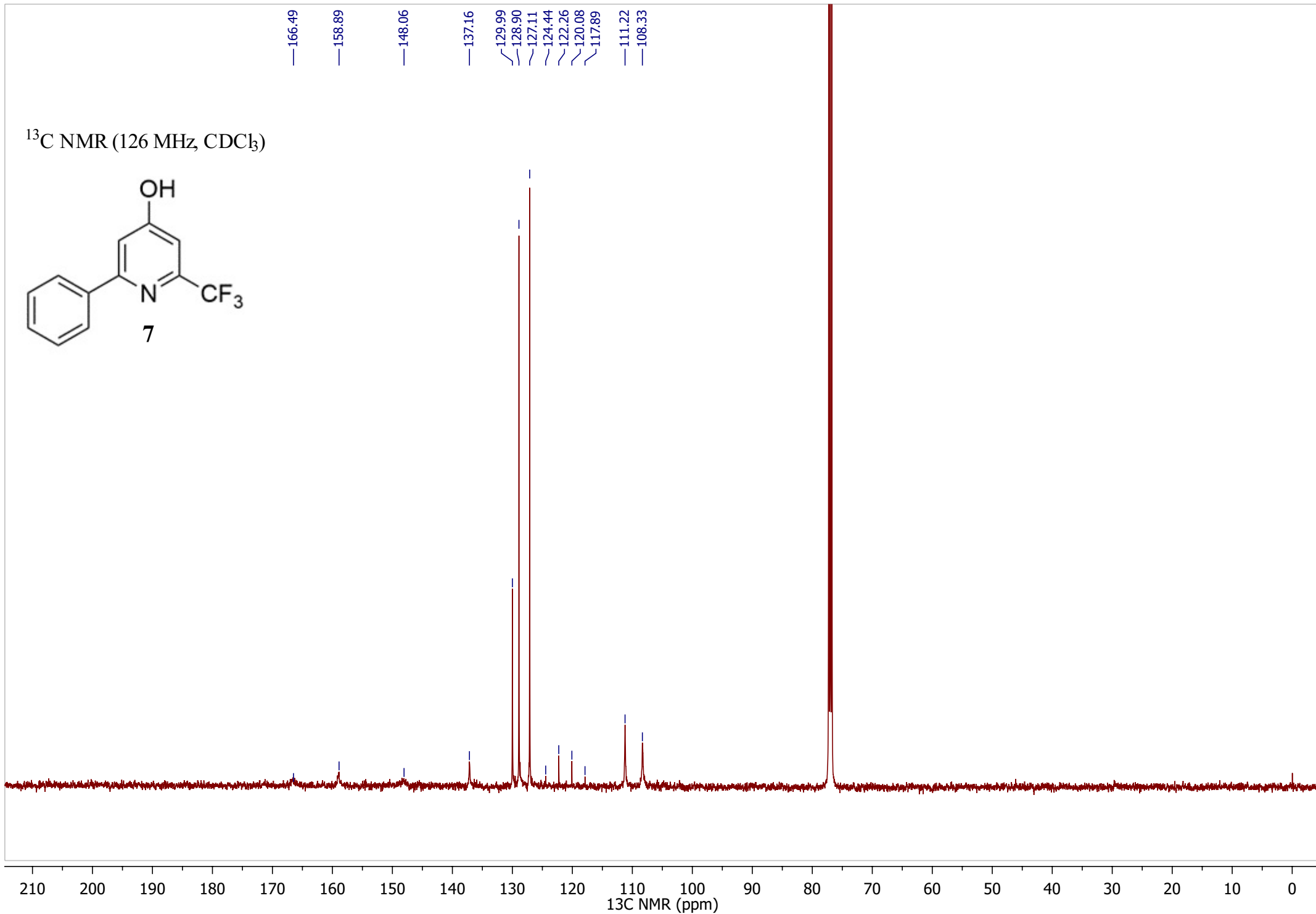
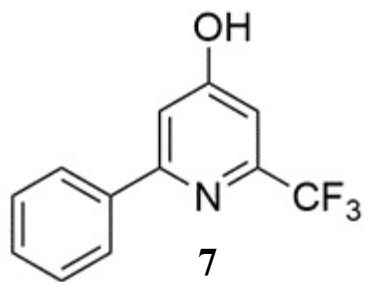
^1H NMR (500 MHz, CDCl_3)



S85

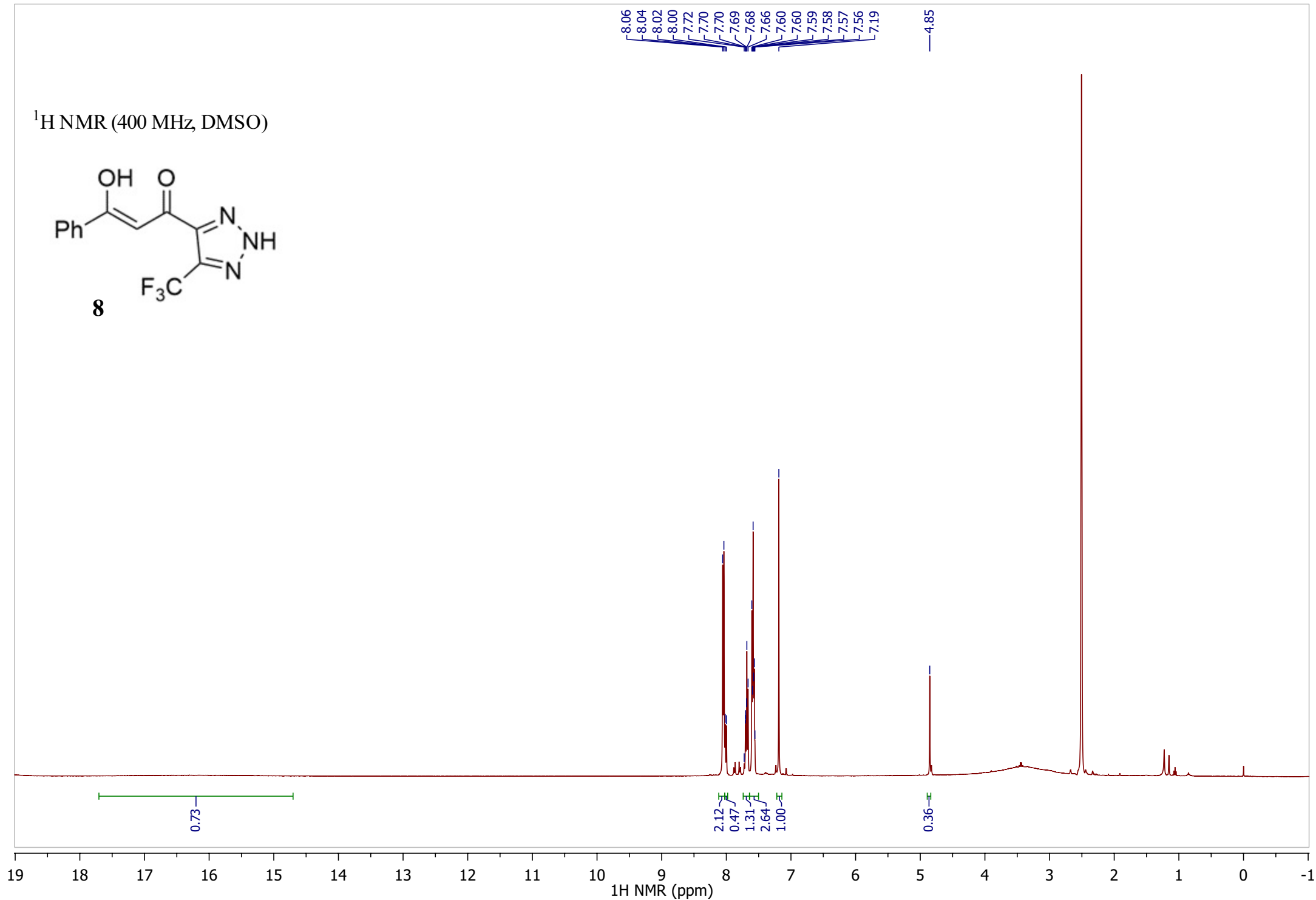
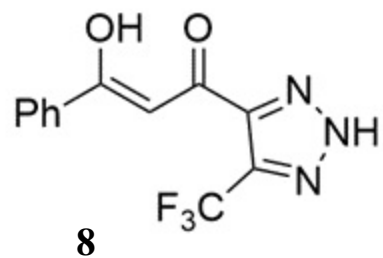


¹³C NMR (126 MHz, CDCl₃)

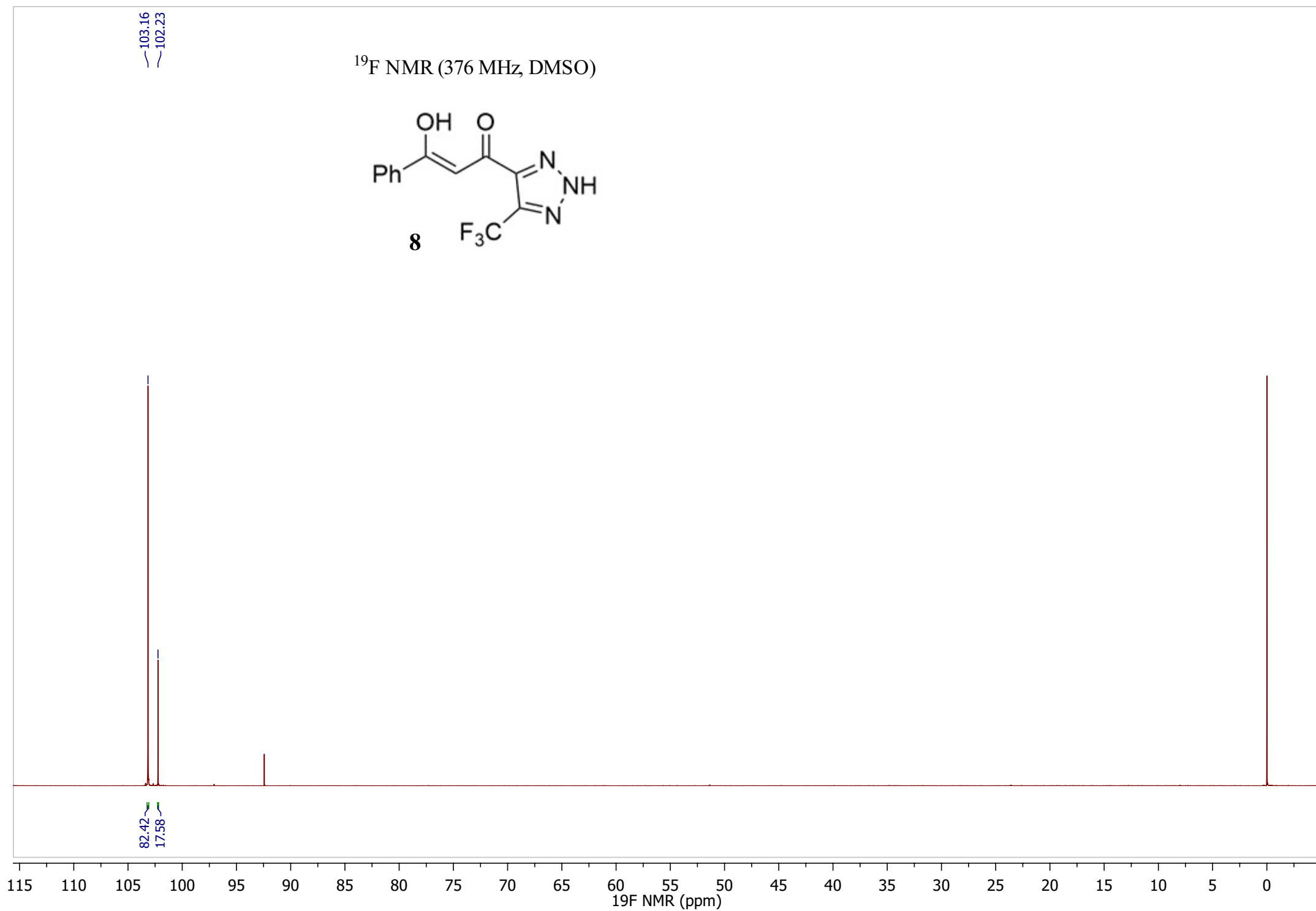
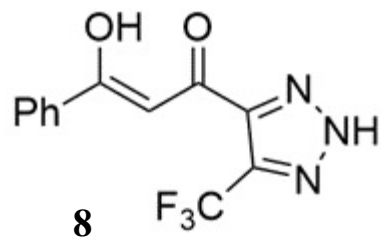


S87

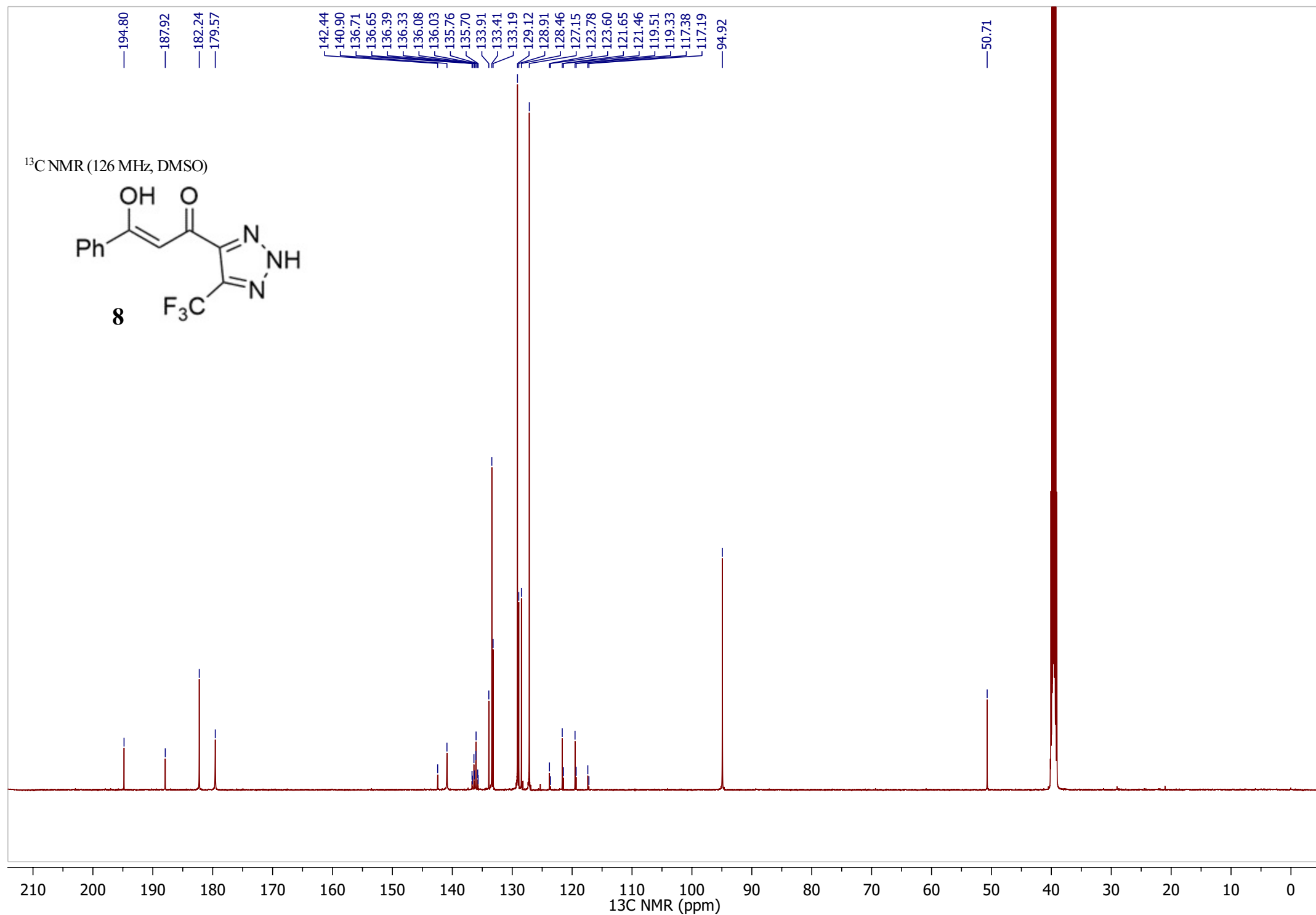
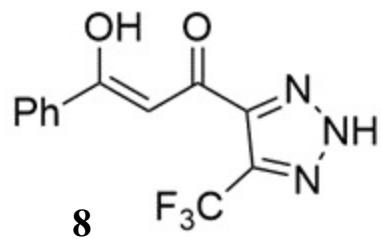
¹H NMR (400 MHz, DMSO)



¹⁹F NMR (376 MHz, DMSO)



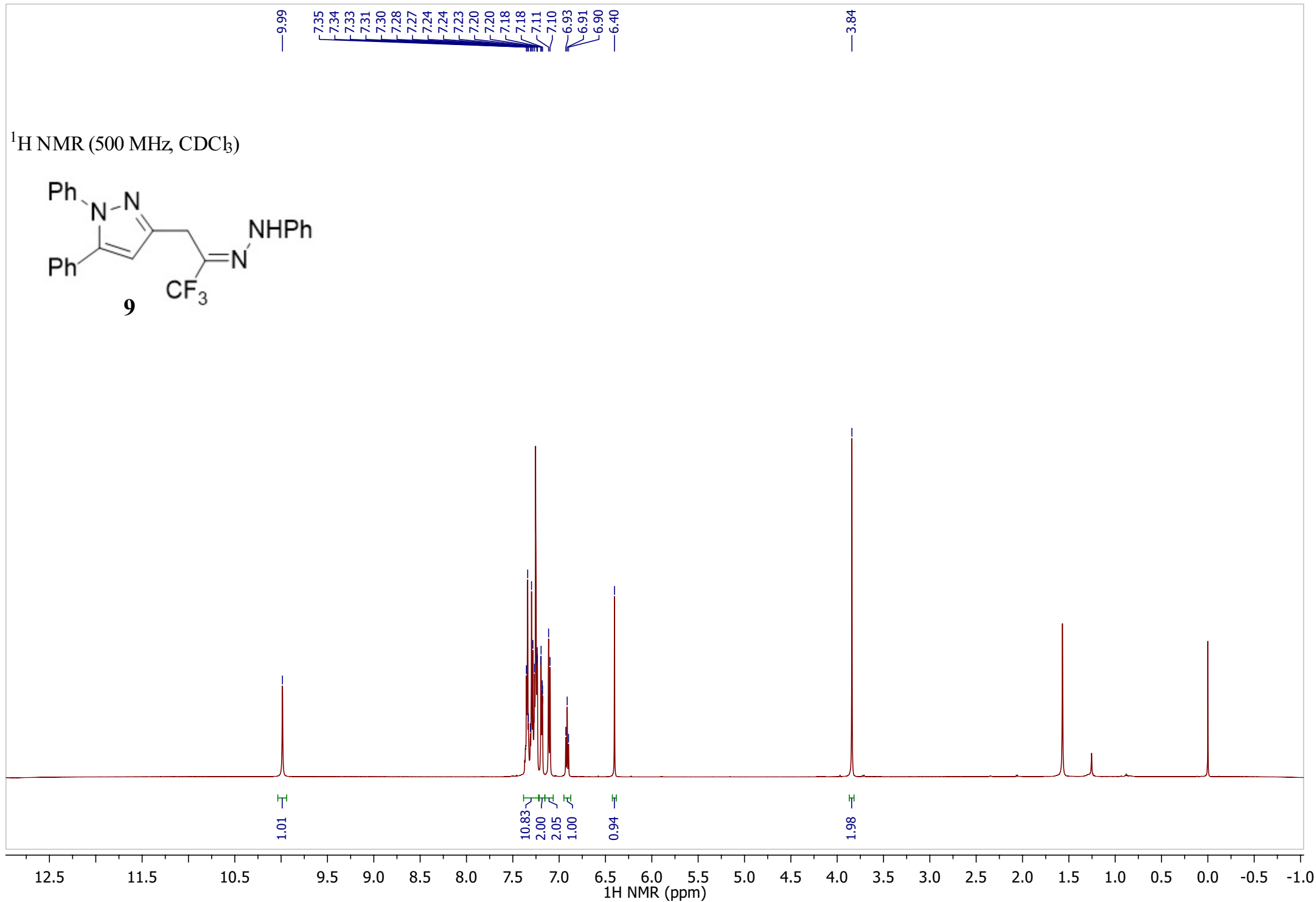
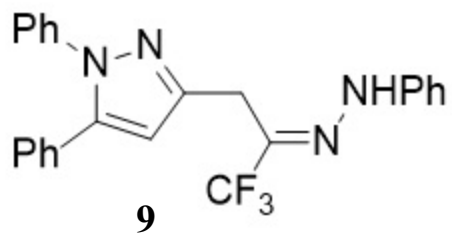
¹³C NMR (126 MHz, DMSO)



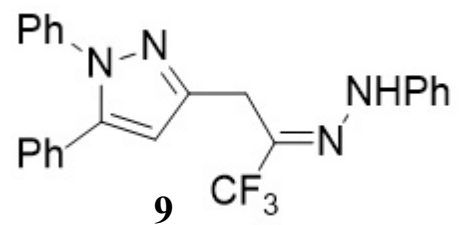
¹³C NMR (ppm)

S90

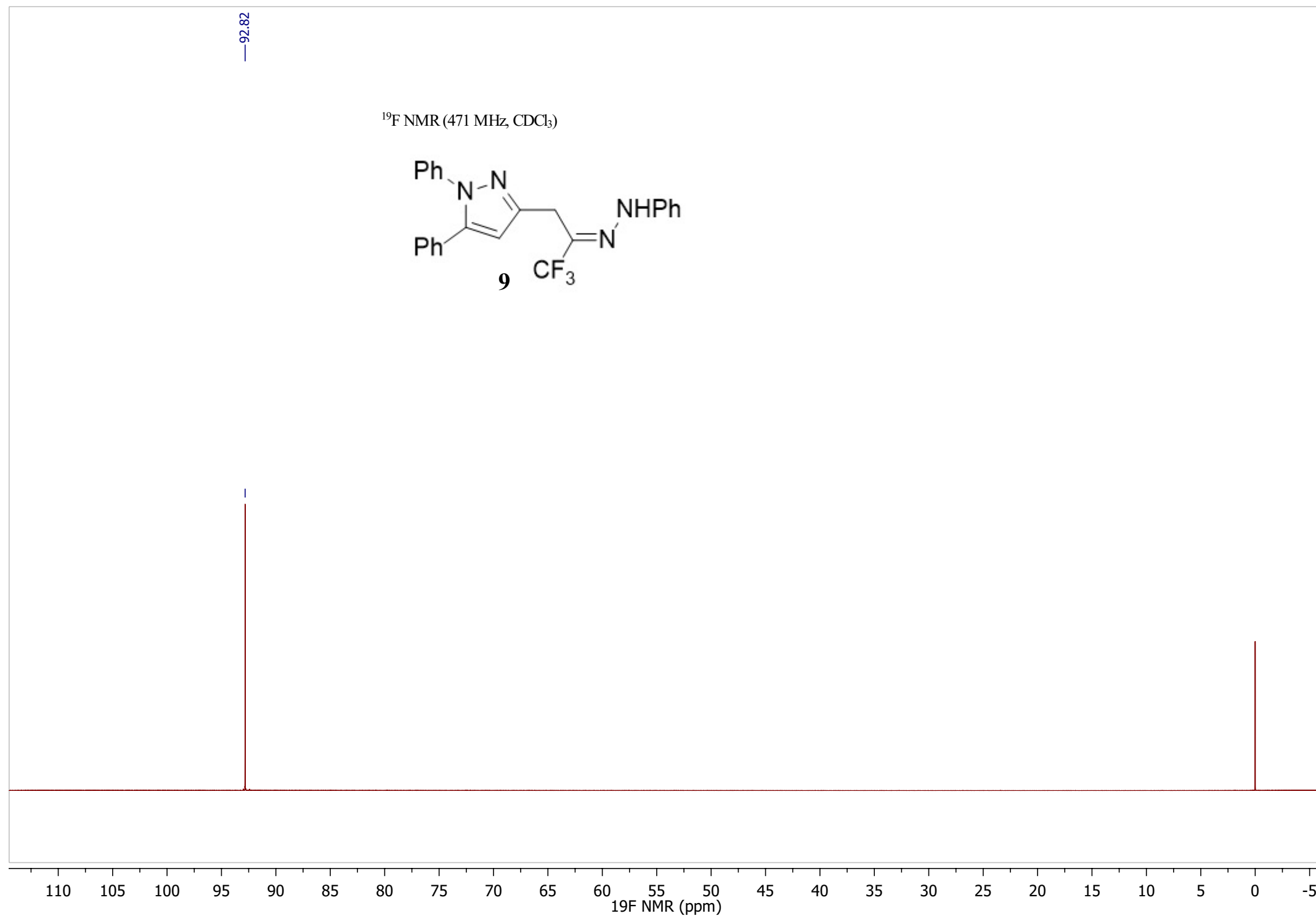
¹H NMR (500 MHz, CDCl₃)



¹⁹F NMR (471 MHz, CDCl₃)



—92.82



¹⁹F NMR (ppm)

S92

