Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Racemic and Enantioselective Metal-Catalyzed Synthesis of SF_5-Containing Diarylmethanols

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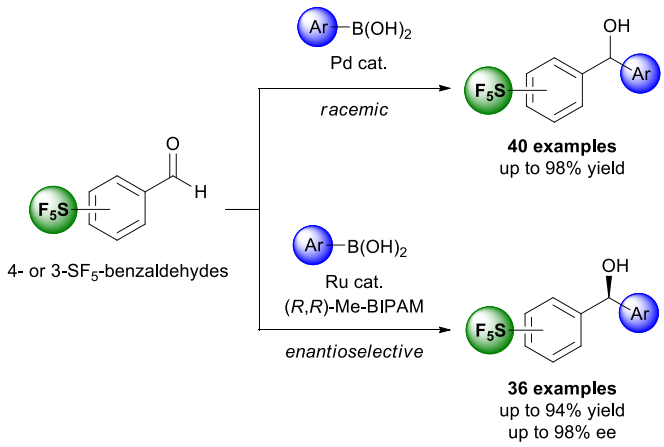

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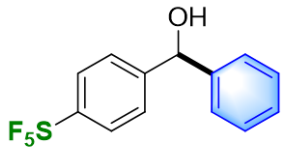
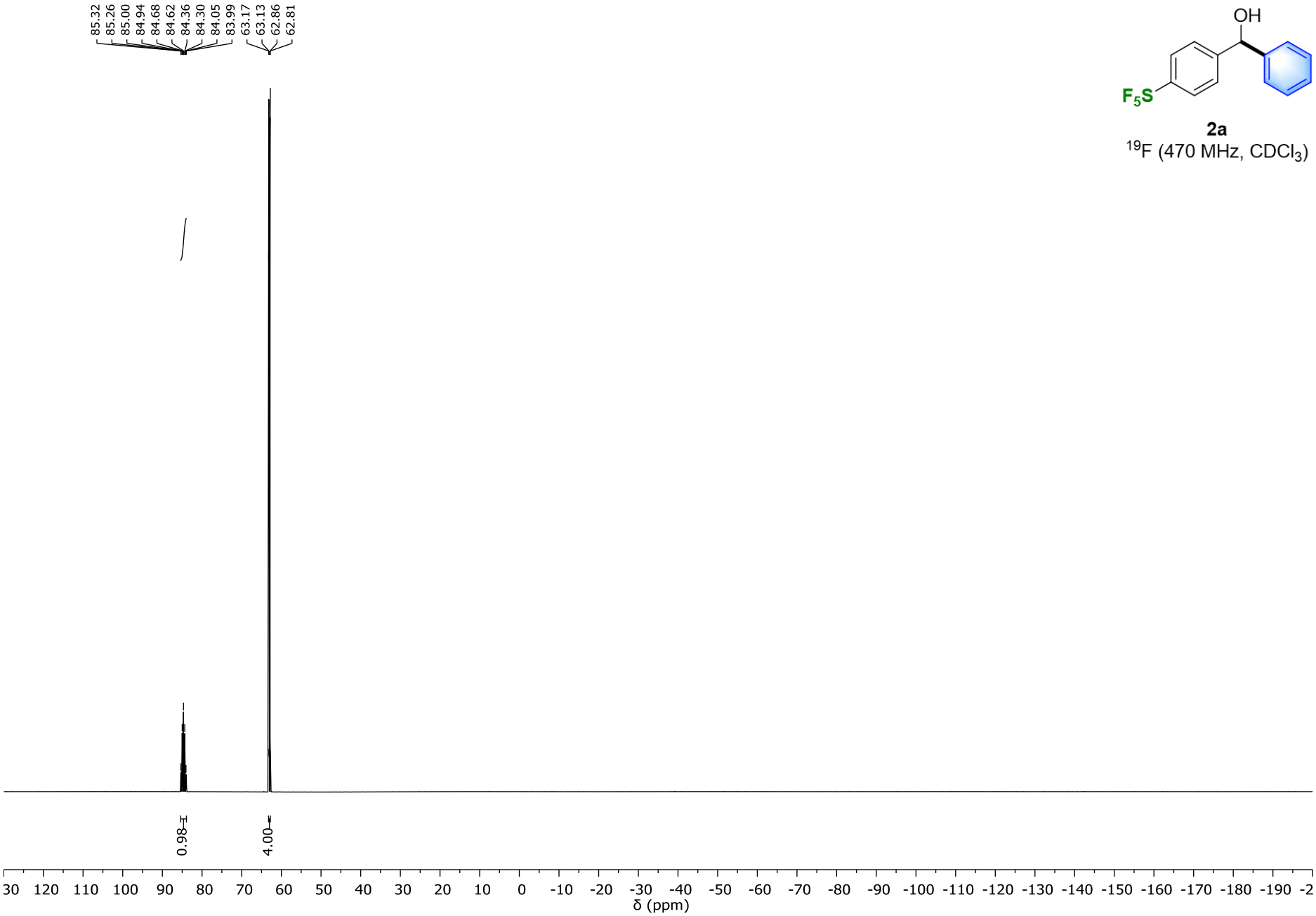
1. ^{1}H, ^{19}F and ^{13}C NMR Spectra

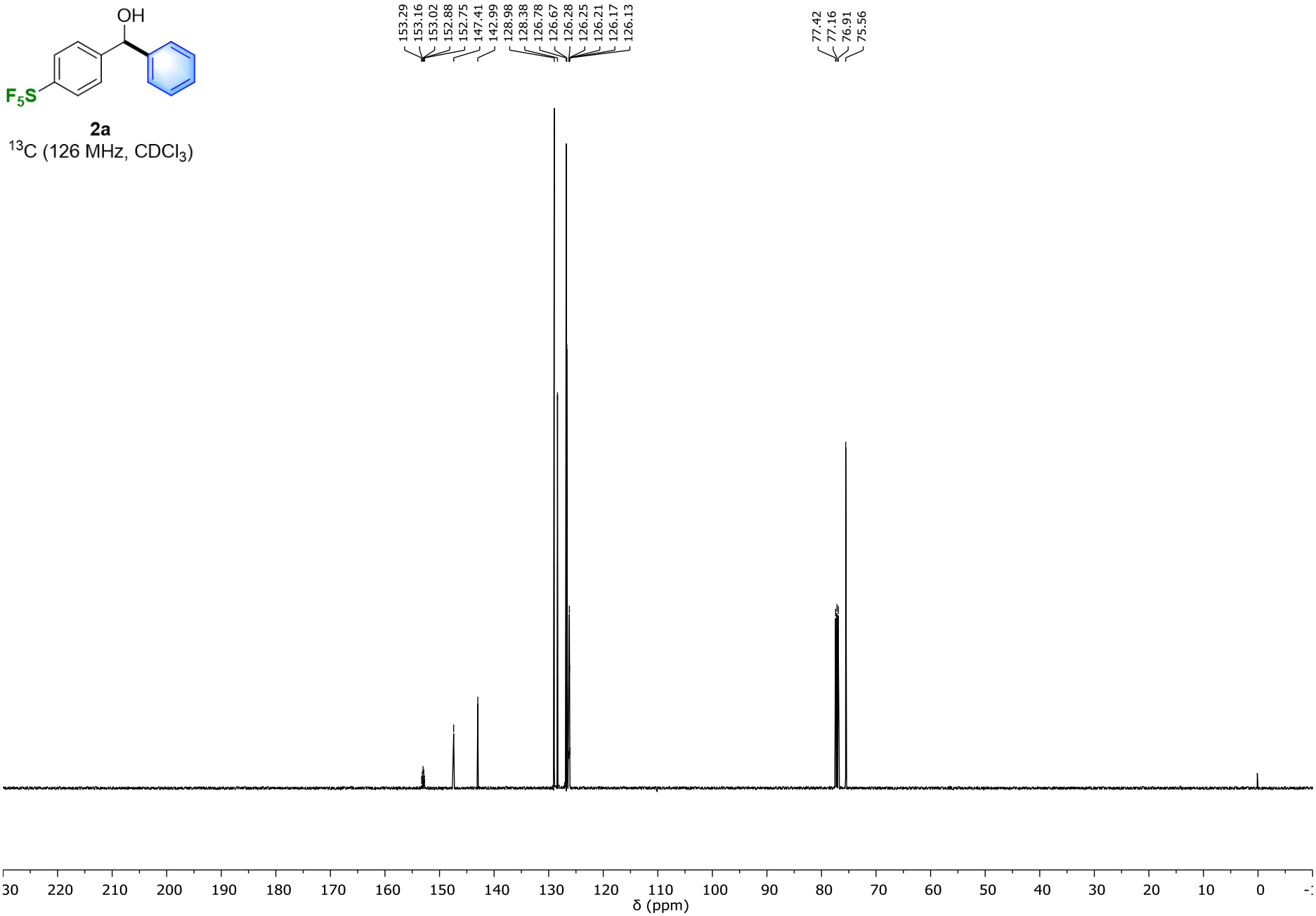
1.1. Compounds 2a-2t

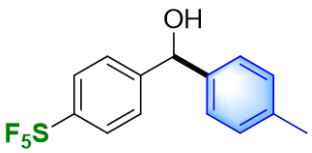


2a

^{1}H (500 MHz, $CDCl_3$)

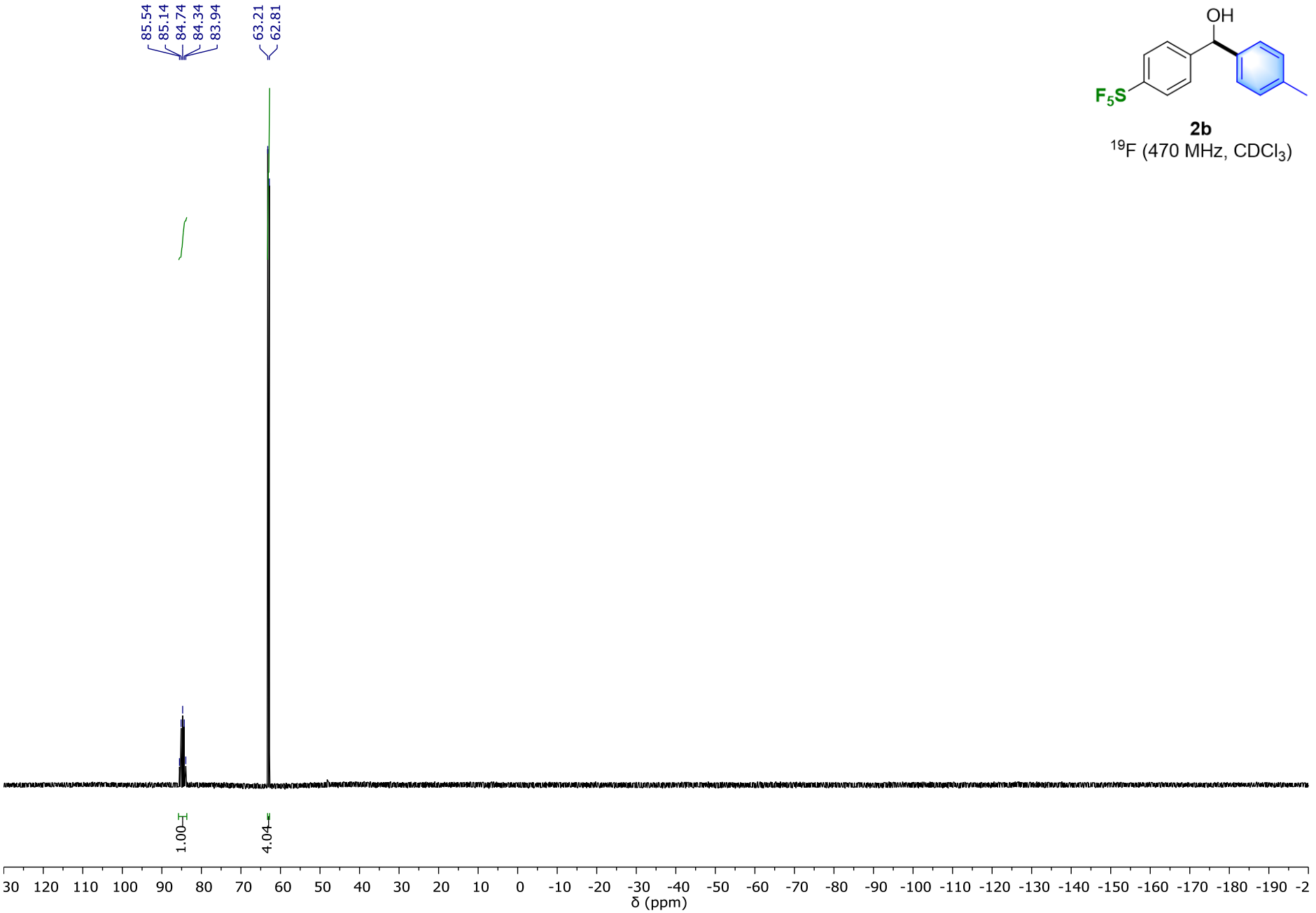

85.32
85.26
85.00
84.94
84.68
84.62
84.36
84.30
84.05
83.99
63.17
63.13
62.86
62.81
OH
F5S
2a
19F (470 MHz, CDCl3)
0.98
4.00
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

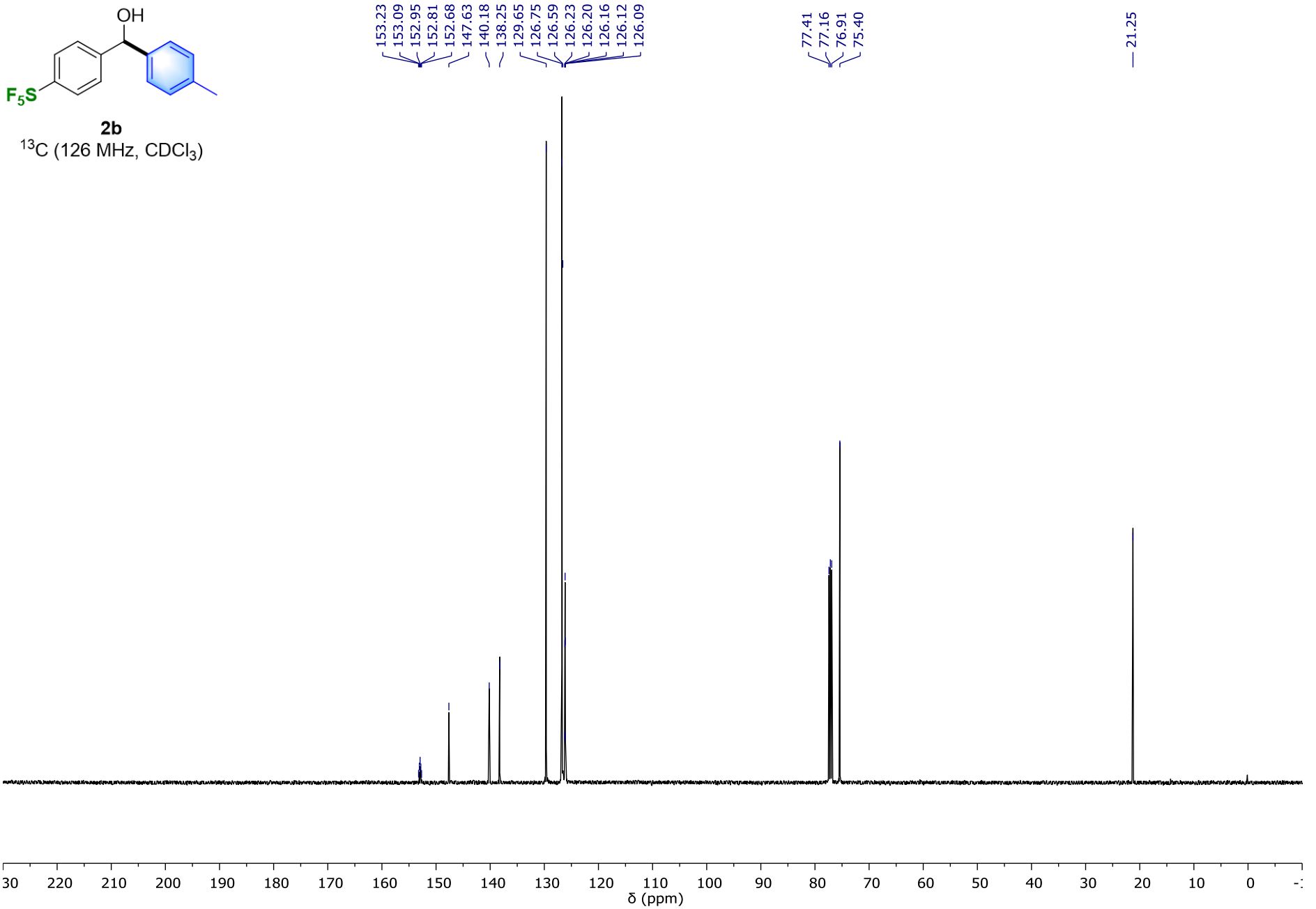

OH
F5S
2a
13C (126 MHz, CDCl3)
153.29
153.16
153.02
152.88
152.75
147.41
142.99
128.98
128.38
126.78
126.67
126.28
126.25
126.21
126.17
126.13
77.42
77.16
76.91
75.56
δ (ppm)

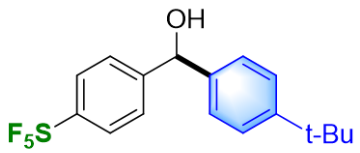


2b

^{1}H (500 MHz, $CDCl_3$)

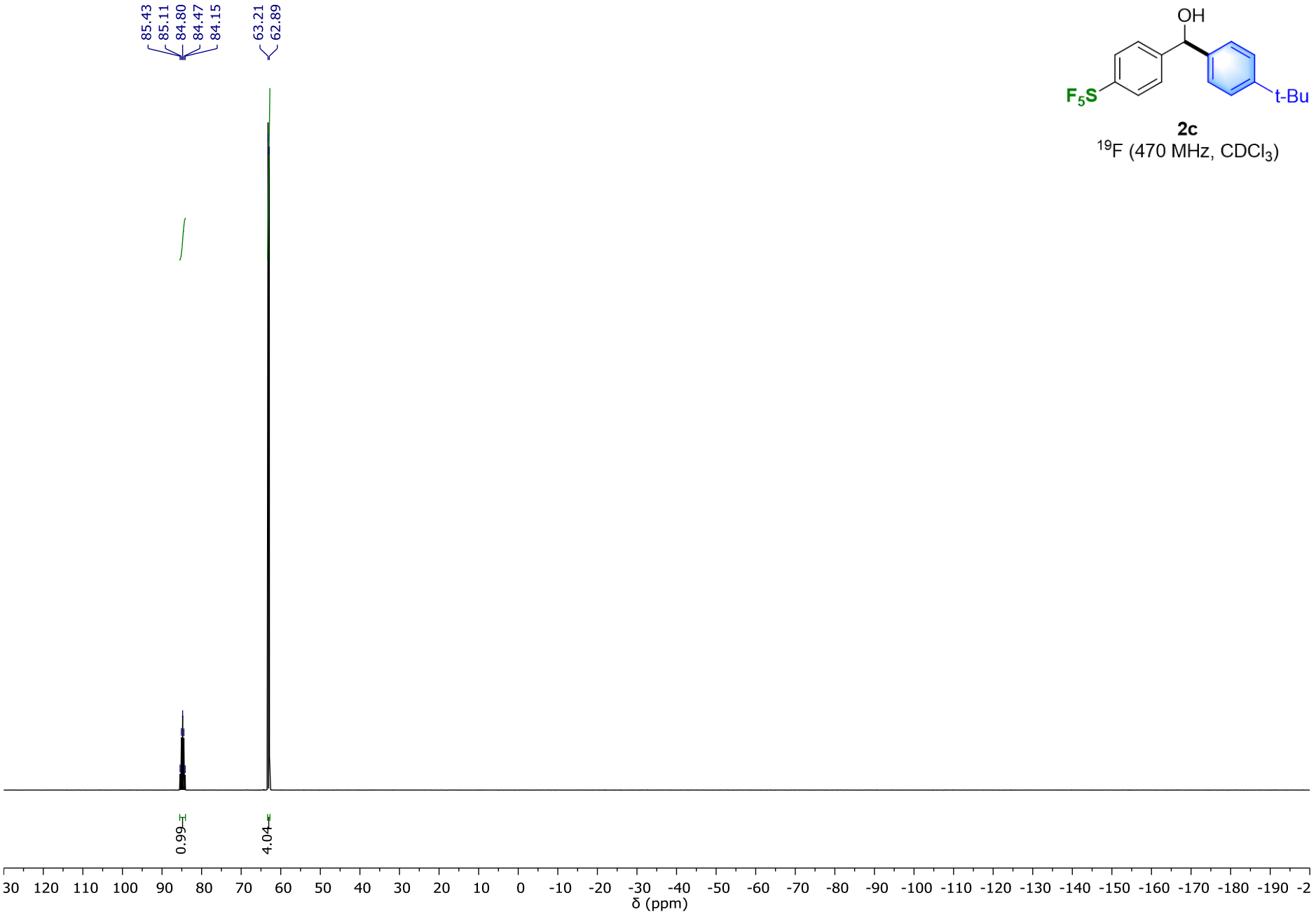

85.54
85.14
84.74
84.34
83.94
63.21
62.81
OH
F5S
2b
19F (470 MHz, CDCl3)
1.00
4.04
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

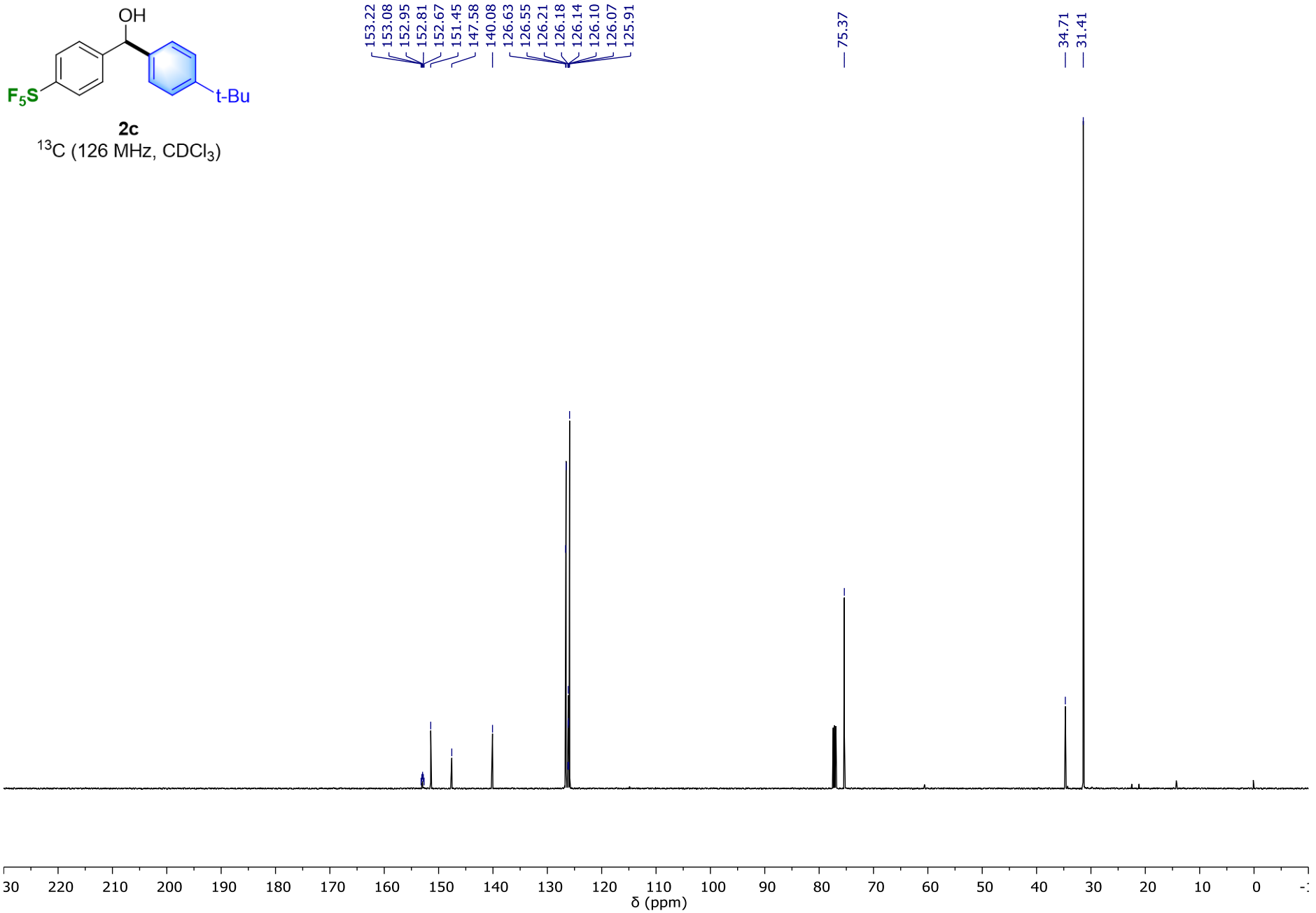

OH
F5S
2b
13C (126 MHz, CDCl3)
153.23
153.09
152.95
152.81
152.68
147.63
140.18
138.25
129.65
126.75
126.59
126.23
126.20
126.16
126.12
126.09
77.41
77.16
76.91
75.40
21.25
δ (ppm)

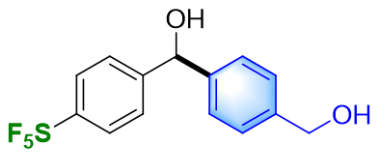


2c

^{1}H (500 MHz, $CDCl_3$)

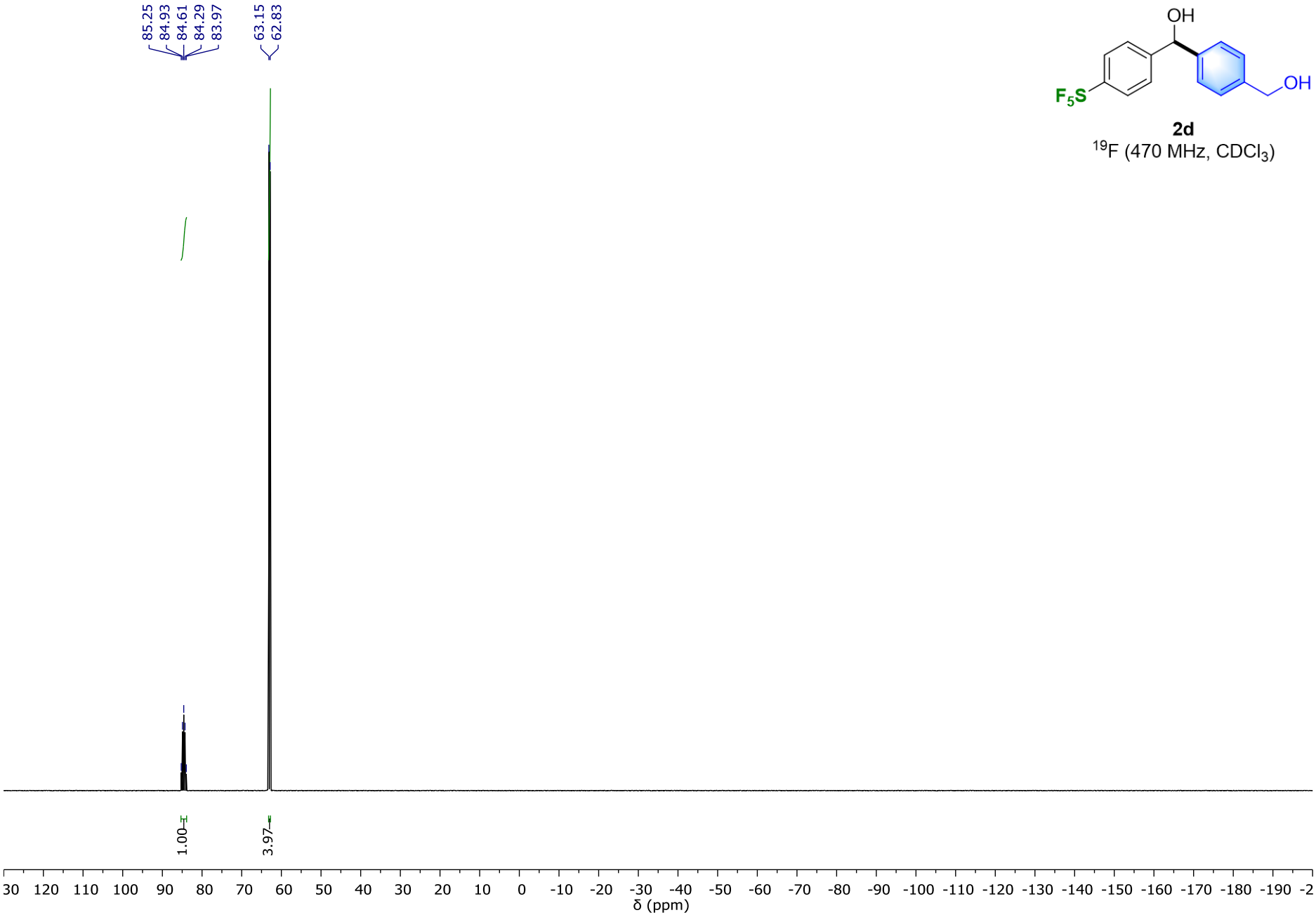

85.43
85.11
84.80
84.47
84.15
63.21
62.89
OH
F5S
t-Bu
2c
19F (470 MHz, CDCl3)
0.99
4.04
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

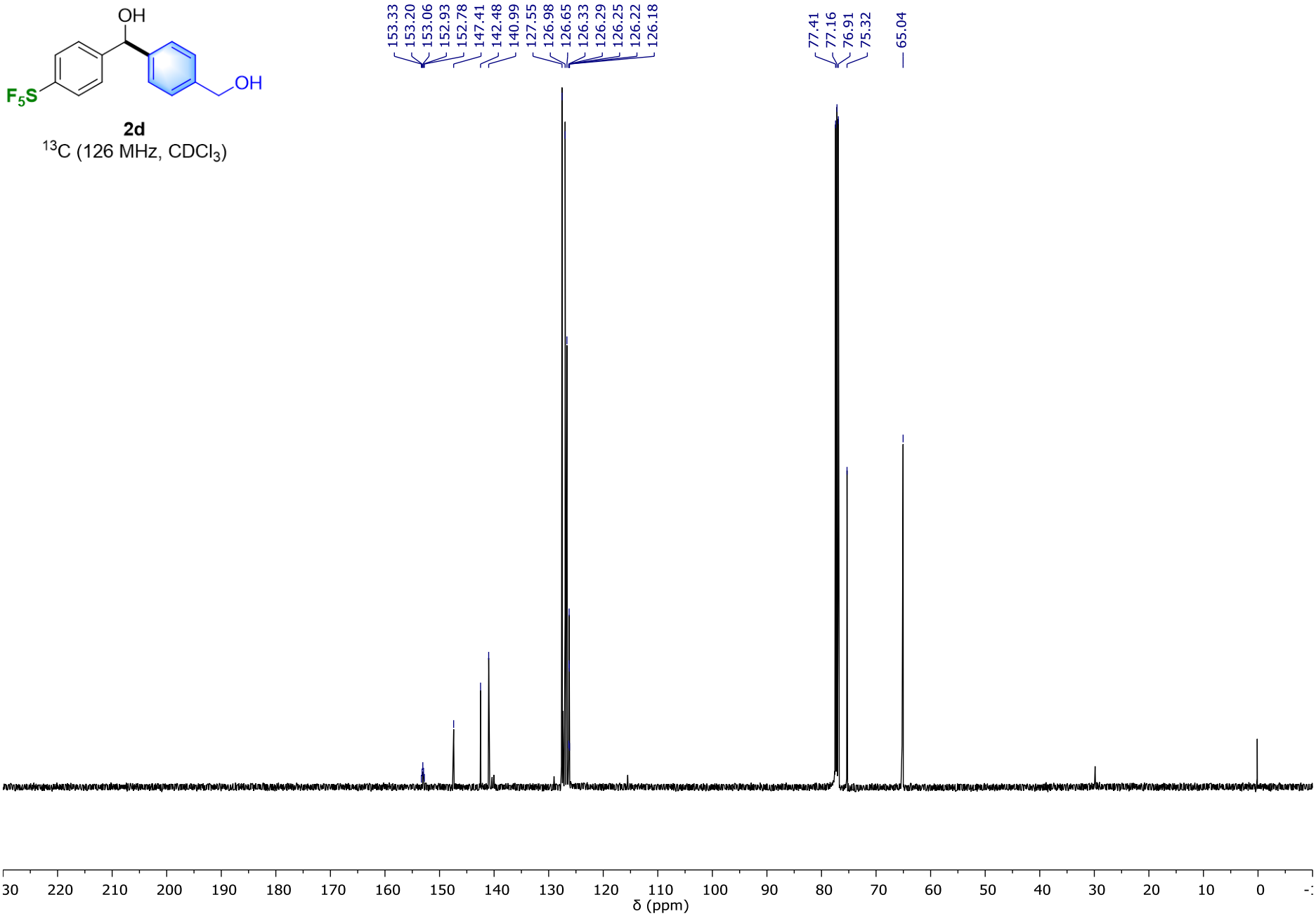

OH
F5S
t-Bu
2c
13C (126 MHz, CDCl3)
153.22
153.08
152.95
152.81
152.67
151.45
147.58
140.08
126.63
126.55
126.21
126.18
126.14
126.10
126.07
125.91
75.37
34.71
31.41
δ (ppm)

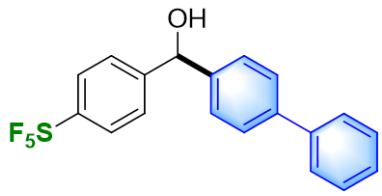


2d

^{1}H (500 MHz, $CDCl_3$)

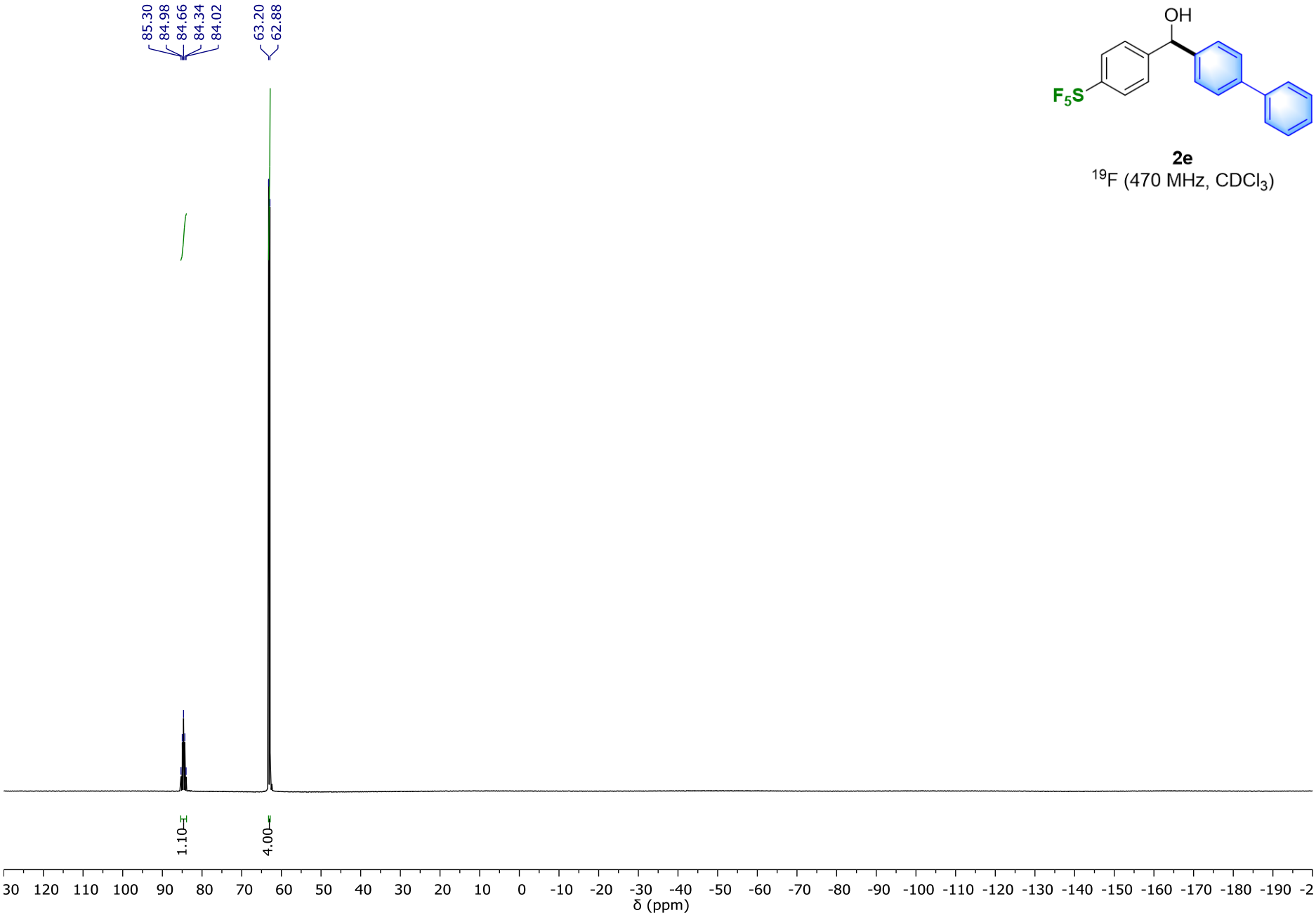

85.25
84.93
84.61
84.29
83.97
63.15
62.83
OH
OH
F5S
2d
19F (470 MHz, CDCl3)
1.00
3.97
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

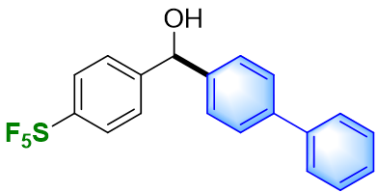

OH
F5S
OH
2d
13C (126 MHz, CDCl3)
153.33
153.20
153.06
152.93
152.78
147.41
142.48
140.99
127.55
126.98
126.65
126.33
126.29
126.25
126.22
126.18
77.41
77.16
76.91
75.32
65.04
30
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)



2e

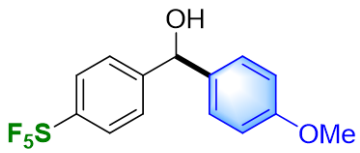
^{1}H (500 MHz, $CDCl_3$)


85.30
84.98
84.66
84.34
84.02
63.20
62.88
OH
F5S
2e
19F (470 MHz, CDCl3)
1.10
4.00
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



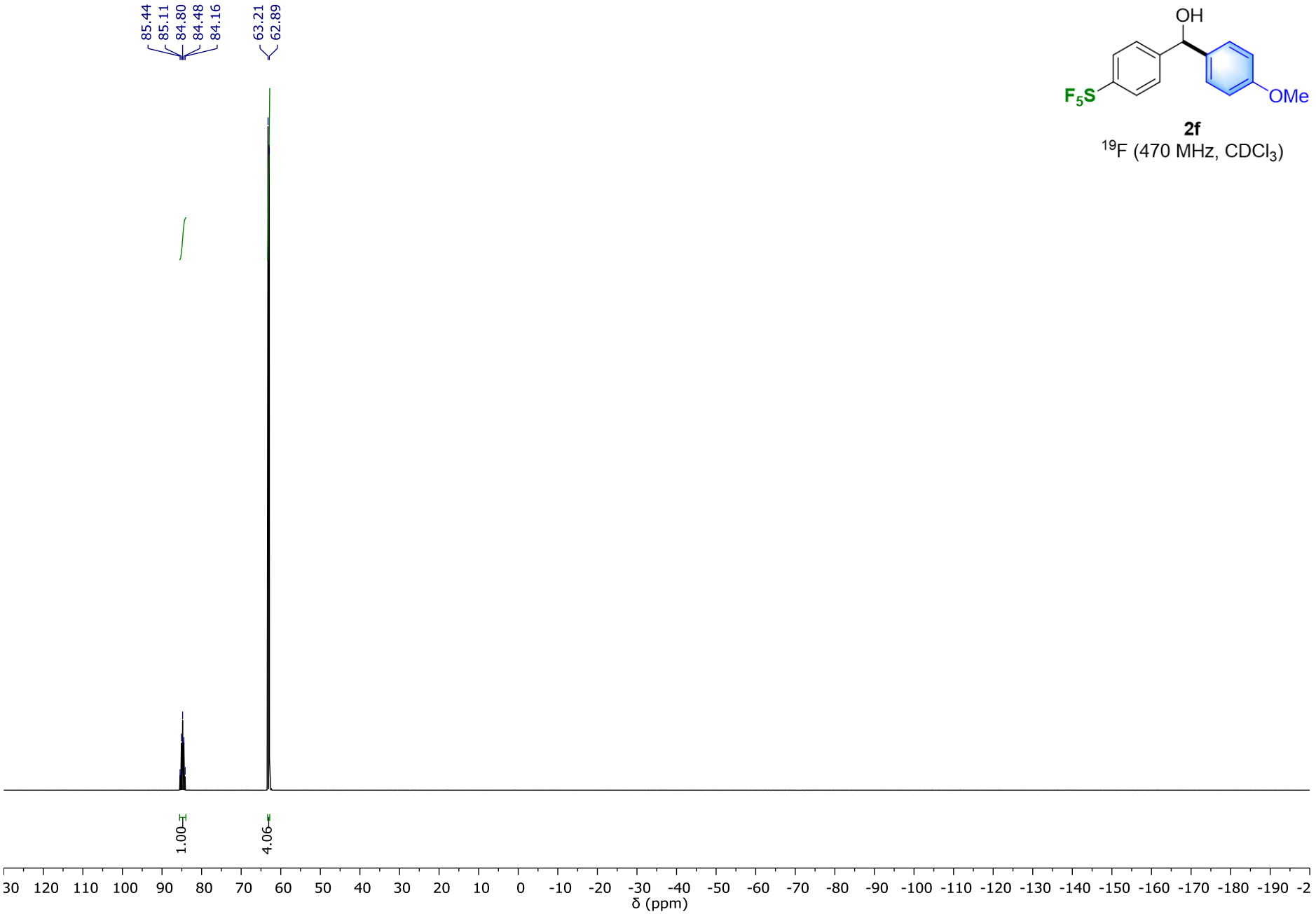
2e

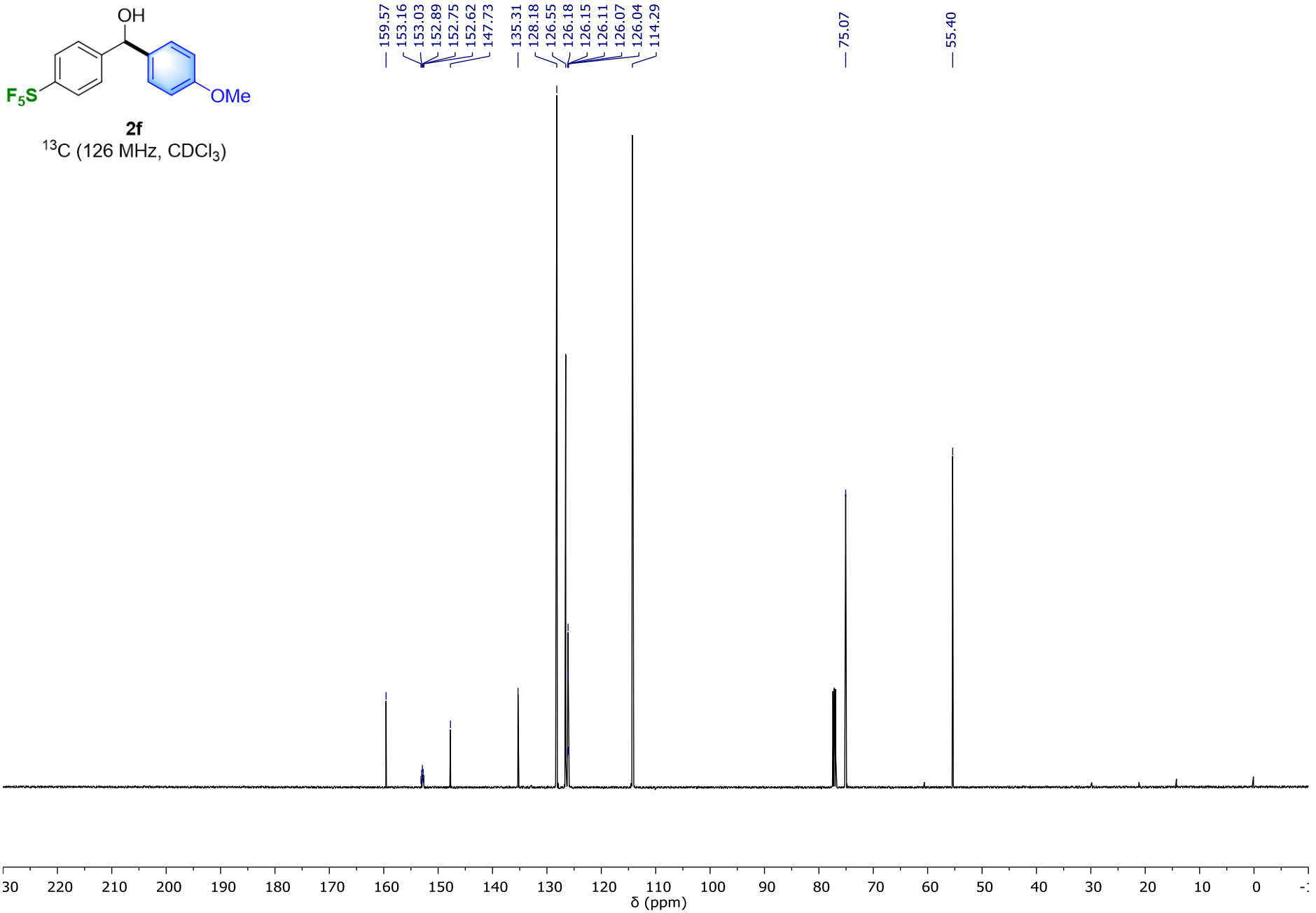
^{13}C (126 MHz, $CDCl_3$)

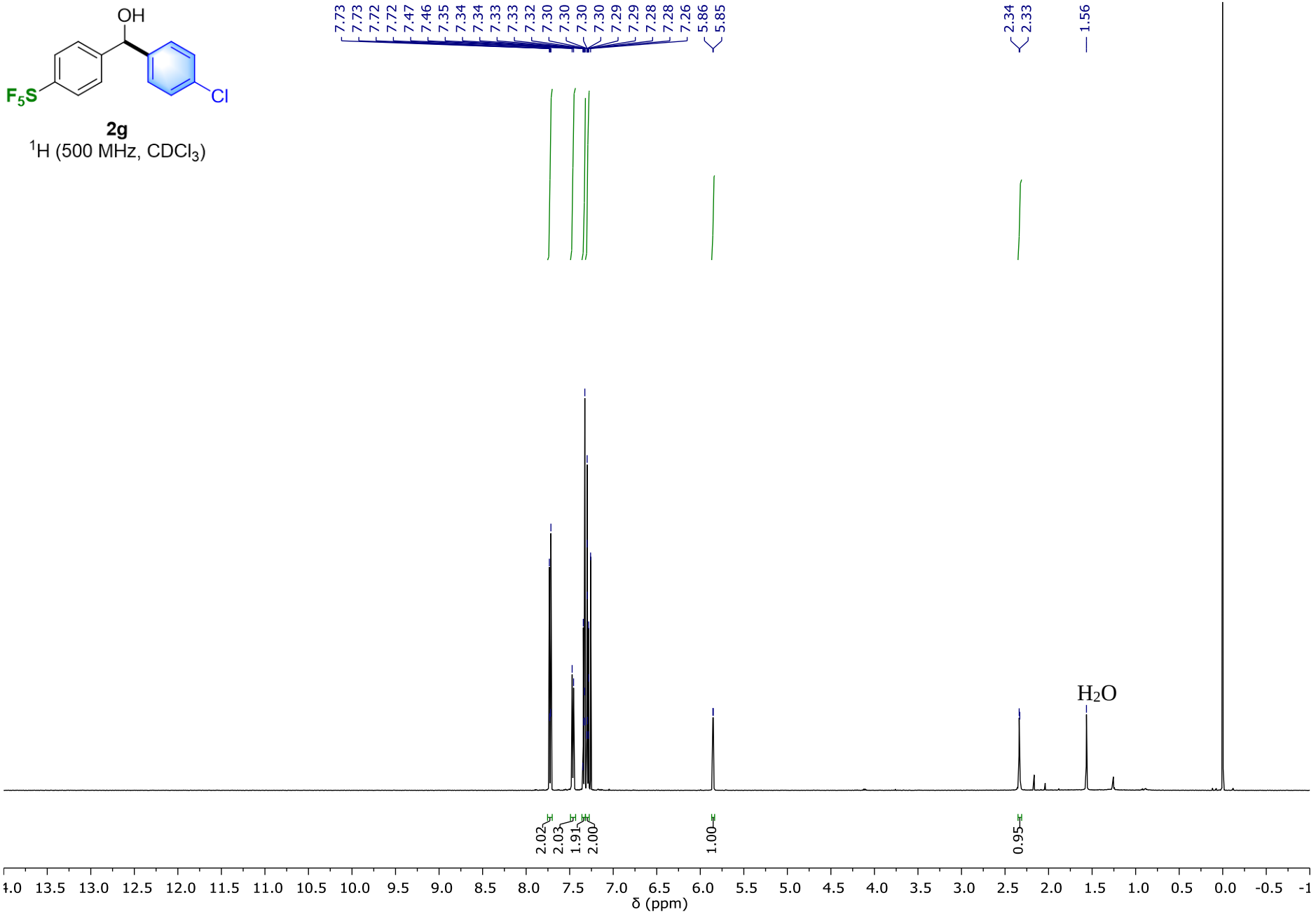


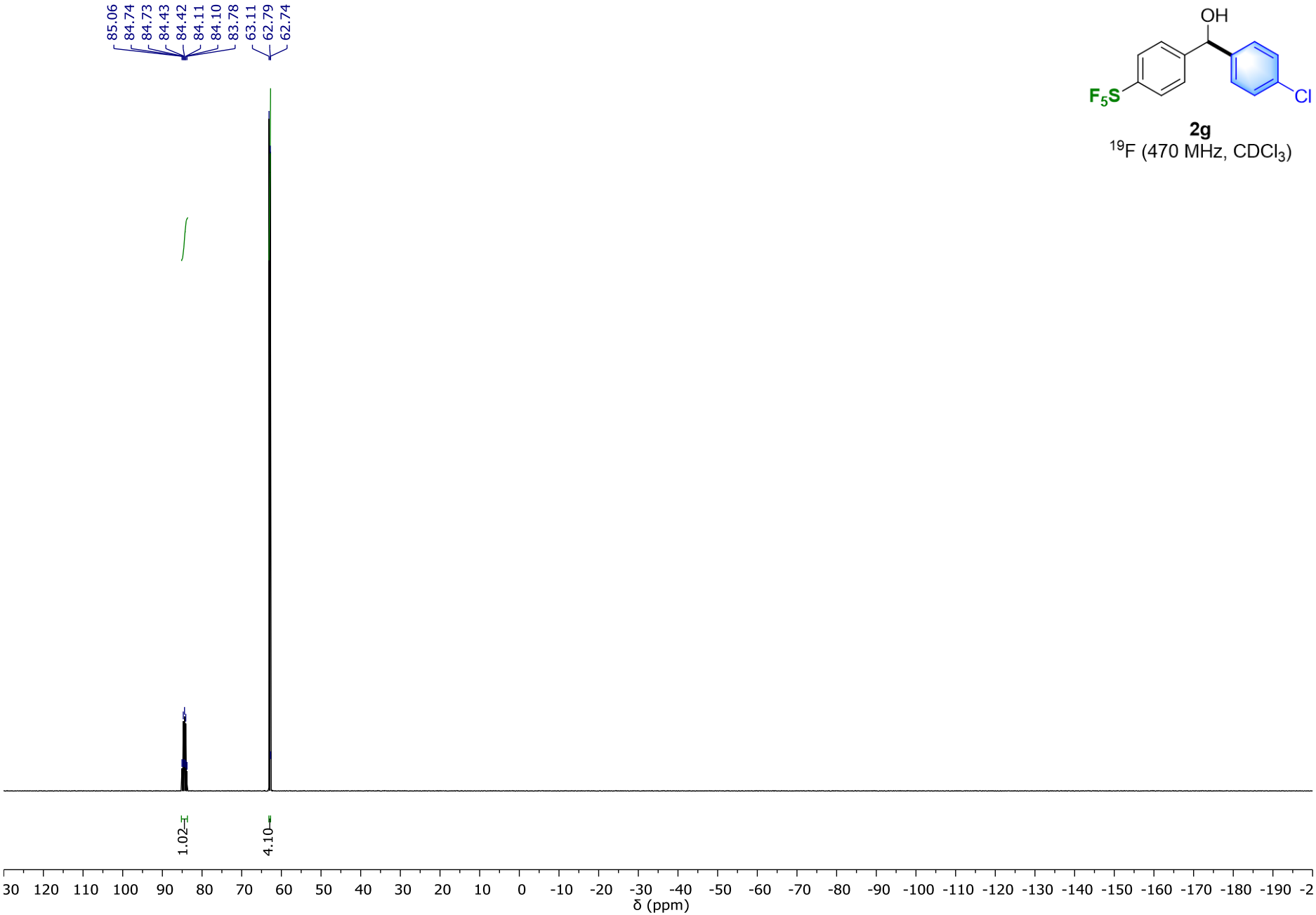
2f

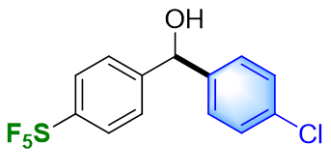
^{1}H (500 MHz, $CDCl_3$)


85.44
85.11
84.80
84.48
84.16
63.21
62.89
OH
F5S
OMe
2f
19F (470 MHz, CDCl3)
1.00
4.06
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)


OH
F5S
OMe
2f
13C (126 MHz, CDCl3)
159.57
153.16
153.03
152.89
152.75
152.62
147.73
135.31
128.18
126.55
126.18
126.15
126.11
126.07
126.04
114.29
75.07
55.40
δ (ppm)

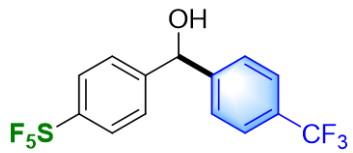

OH
F5S
Cl
2g
1H (500 MHz, CDCl3)
7.73
7.73
7.72
7.72
7.47
7.46
7.35
7.34
7.34
7.33
7.33
7.32
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.26
5.86
5.85
2.34
2.33
1.56
H2O
2.02
2.03
1.91
2.00
1.00
0.95
δ (ppm)


85.06
84.74
84.73
84.43
84.42
84.11
84.10
83.78
63.11
62.79
62.74
OH
F5S
Cl
2g
19F (470 MHz, CDCl3)
1.02
4.10
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



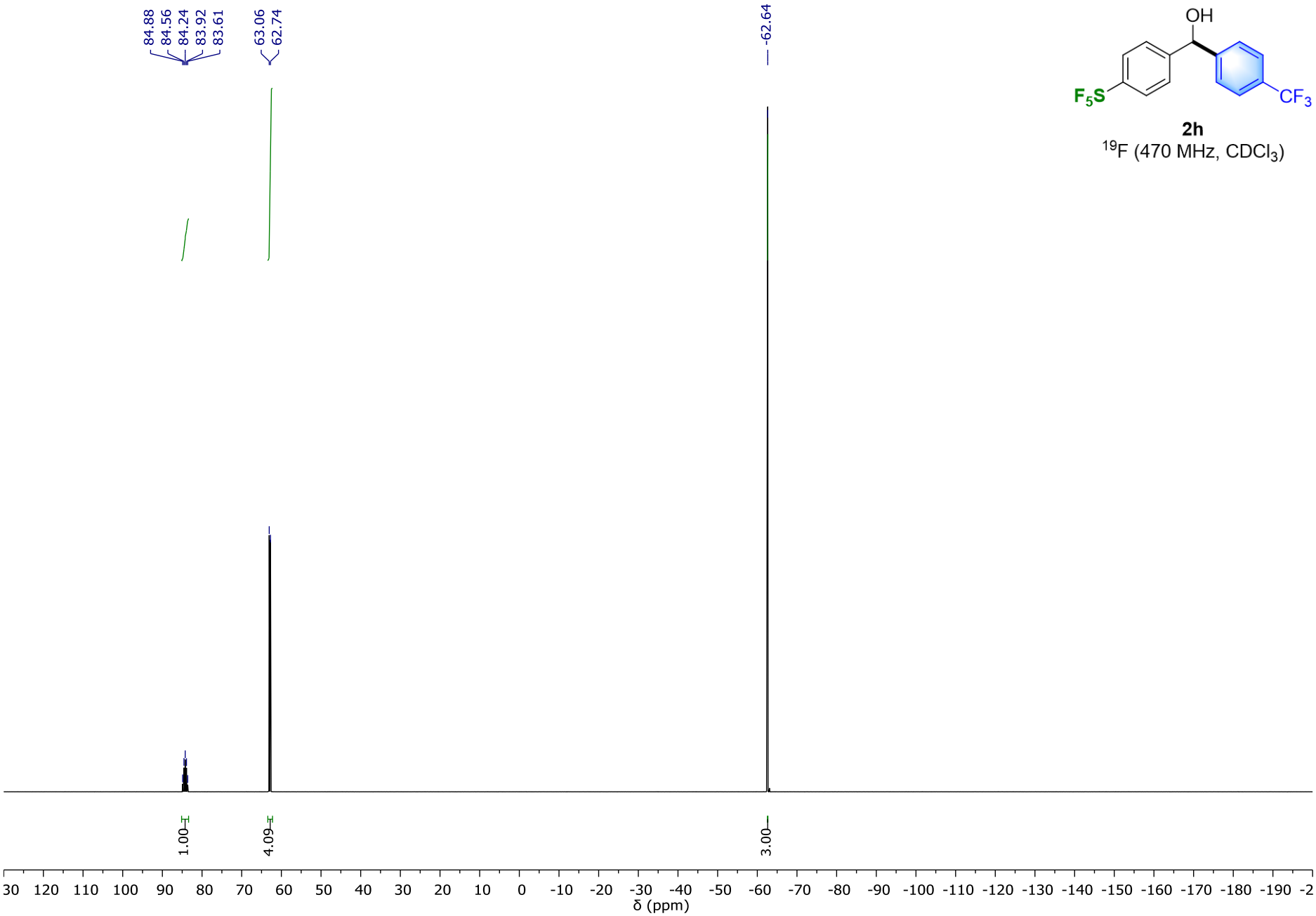
2g

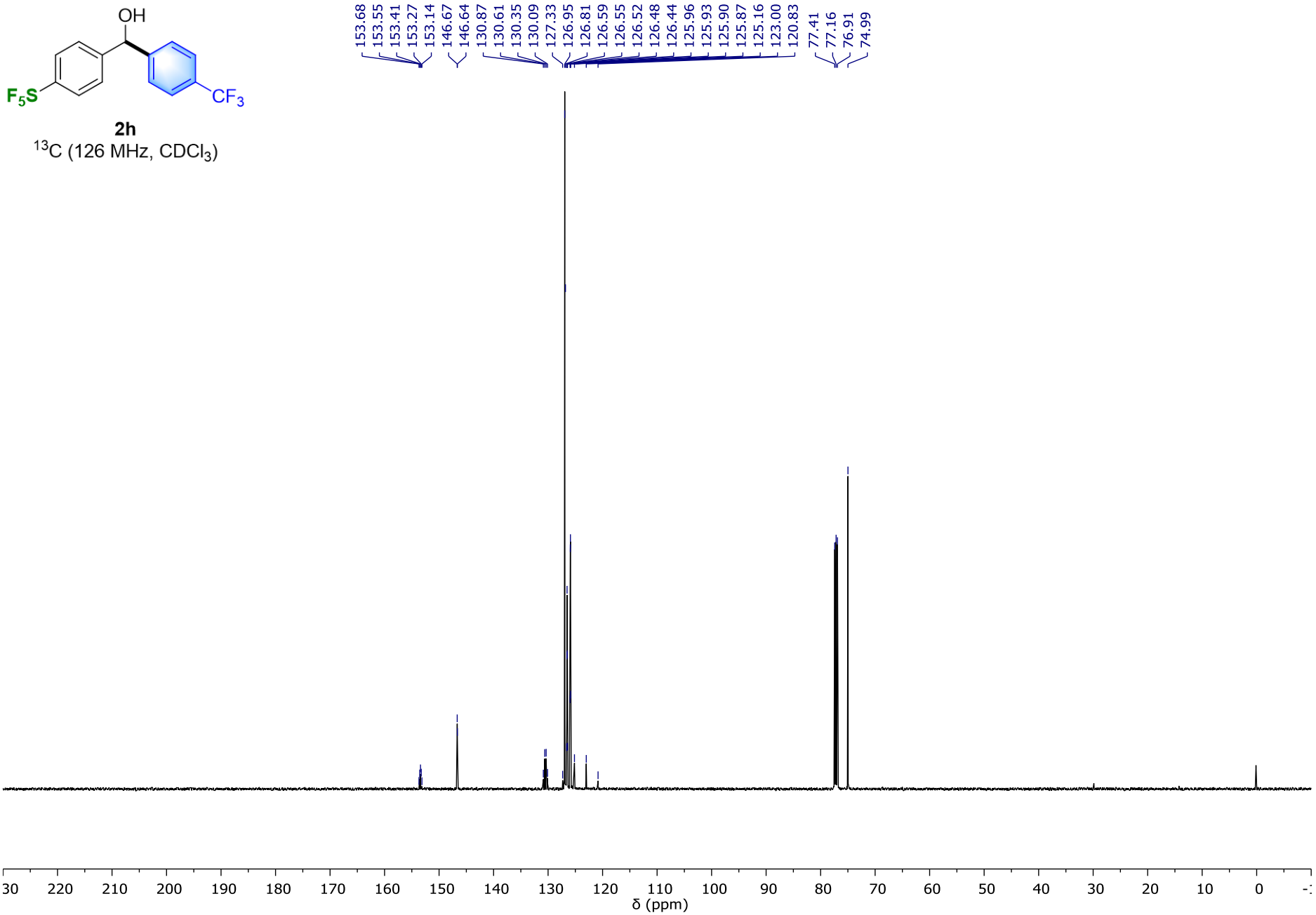
^{13}C (126 MHz, $CDCl_3$)

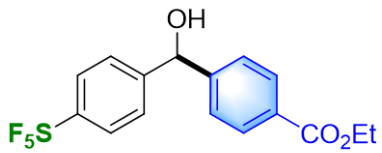


2h

^{1}H (500 MHz, $CDCl_3$)

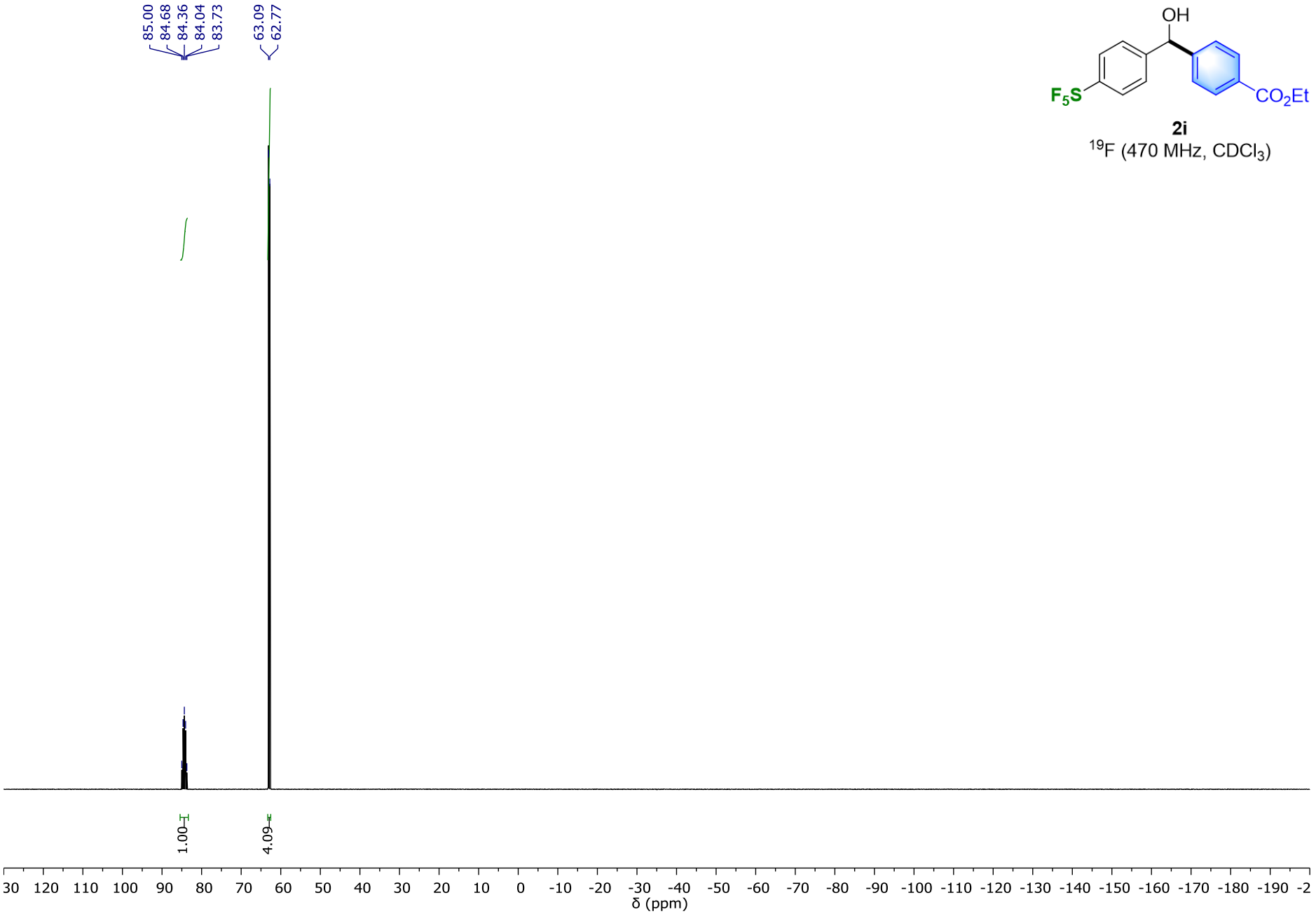

84.88
84.56
84.24
83.92
83.61
63.06
62.74
-62.64
OH
F5S
CF3
2h
19F (470 MHz, CDCl3)
1.00
4.09
3.00
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

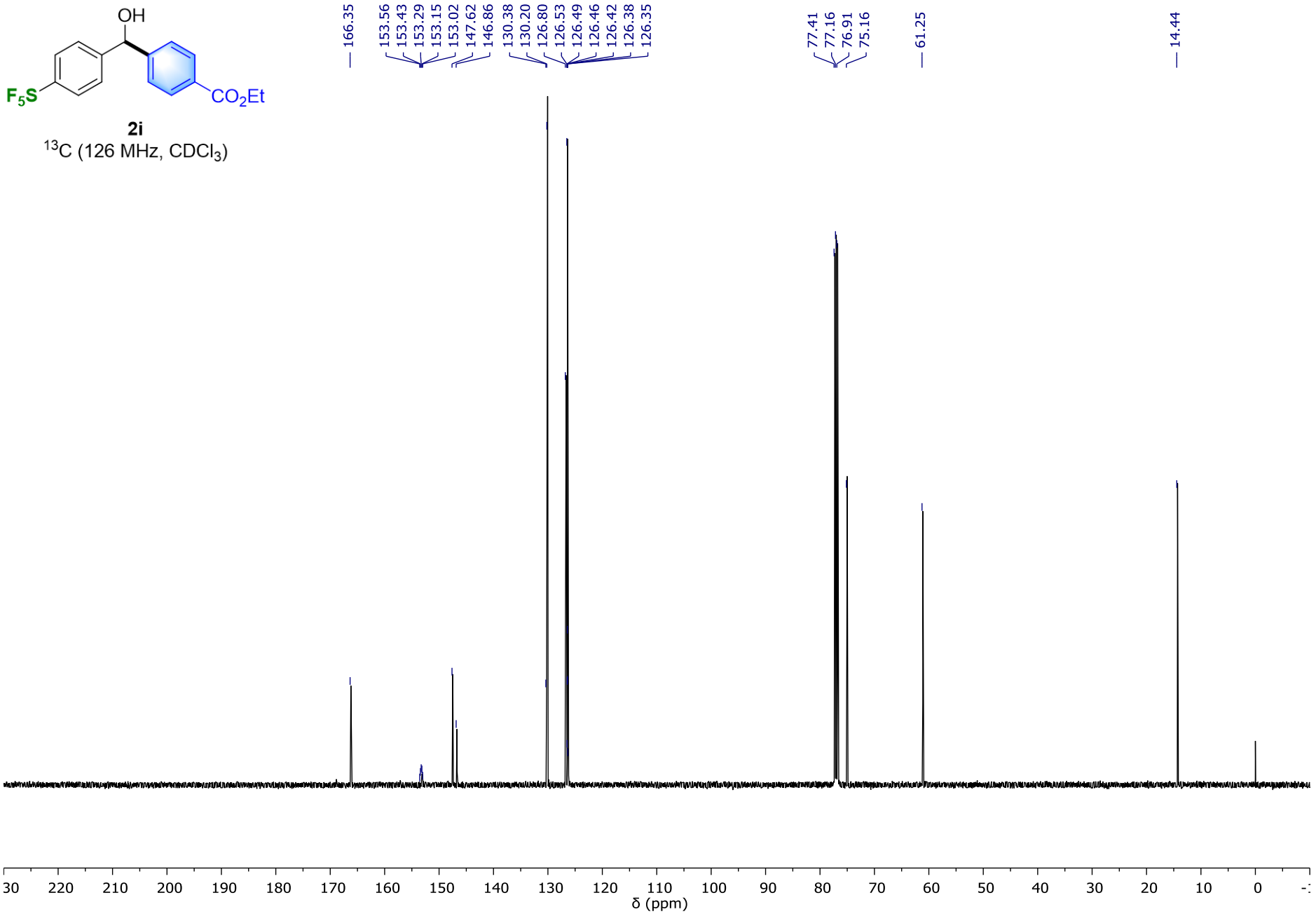

OH
F5S
CF3
2h
13C (126 MHz, CDCl3)
153.68
153.55
153.41
153.27
153.14
146.67
146.64
130.87
130.61
130.35
130.09
127.33
126.95
126.81
126.59
126.55
126.52
126.48
126.44
125.96
125.93
125.90
125.87
125.16
123.00
120.83
77.41
77.16
76.91
74.99
δ (ppm)

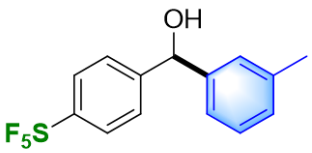


2i

^{1}H (500 MHz, $CDCl_3$)

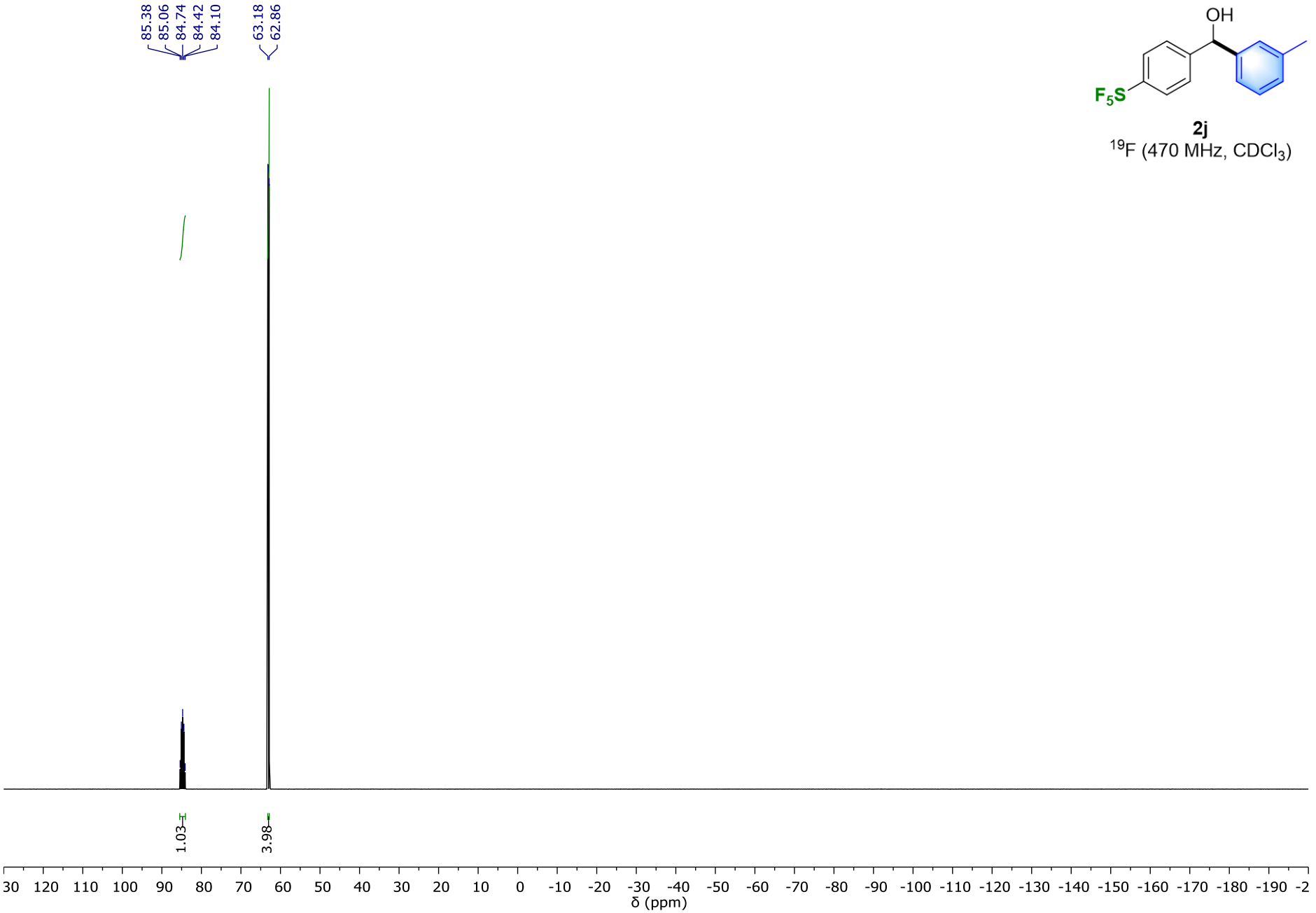

85.00
84.68
84.36
84.04
83.73
63.09
62.77
OH
F5S
CO2Et
2i
19F (470 MHz, CDCl3)
1.00
4.09
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

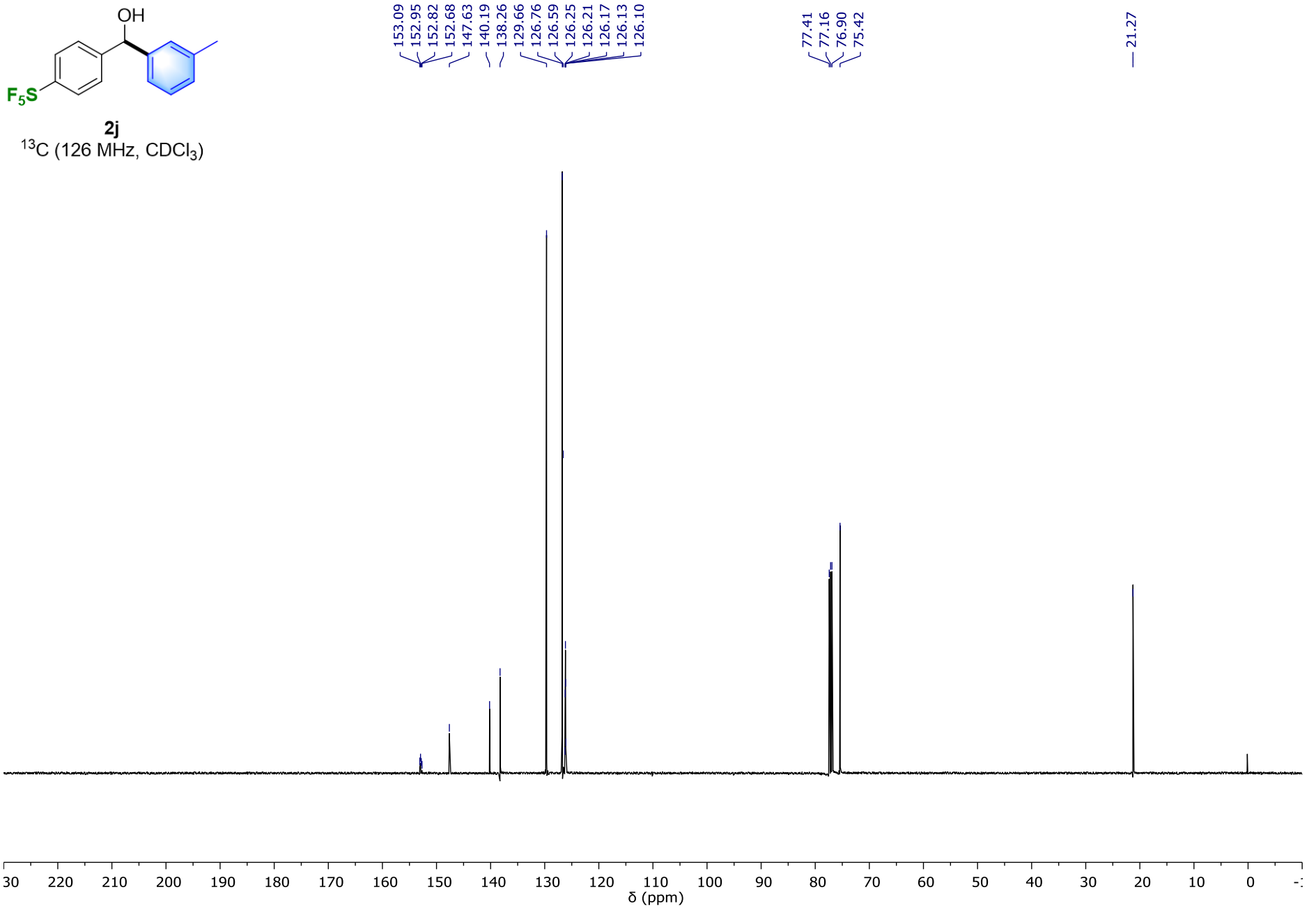

OH
F5S
CO2Et
2i
13C (126 MHz, CDCl3)
166.35
153.56
153.43
153.29
153.15
153.02
147.62
146.86
130.38
130.20
126.80
126.53
126.49
126.46
126.42
126.38
126.35
77.41
77.16
76.91
75.16
61.25
14.44
δ (ppm)



2j

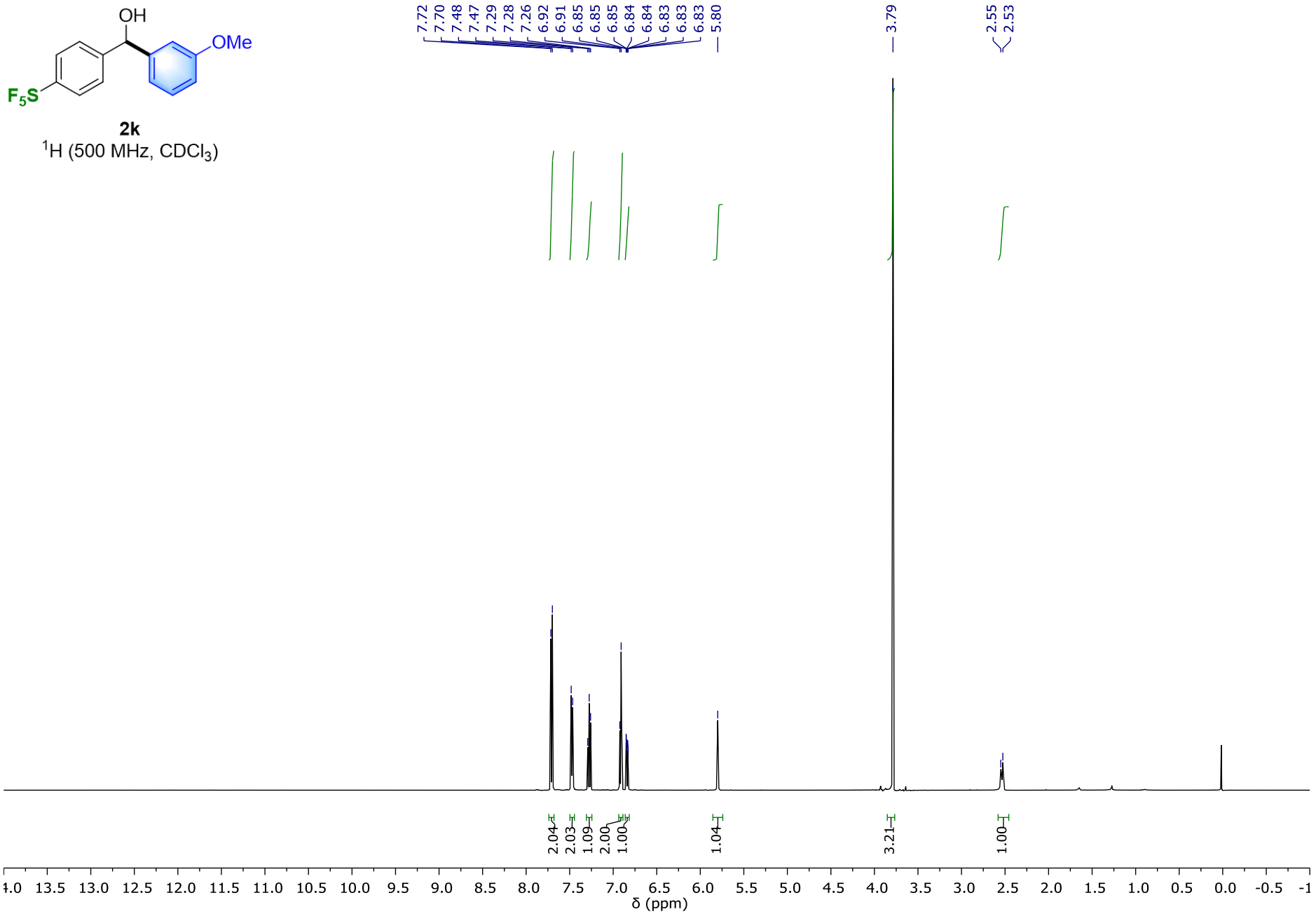
^{1}H (500 MHz, $CDCl_3$)

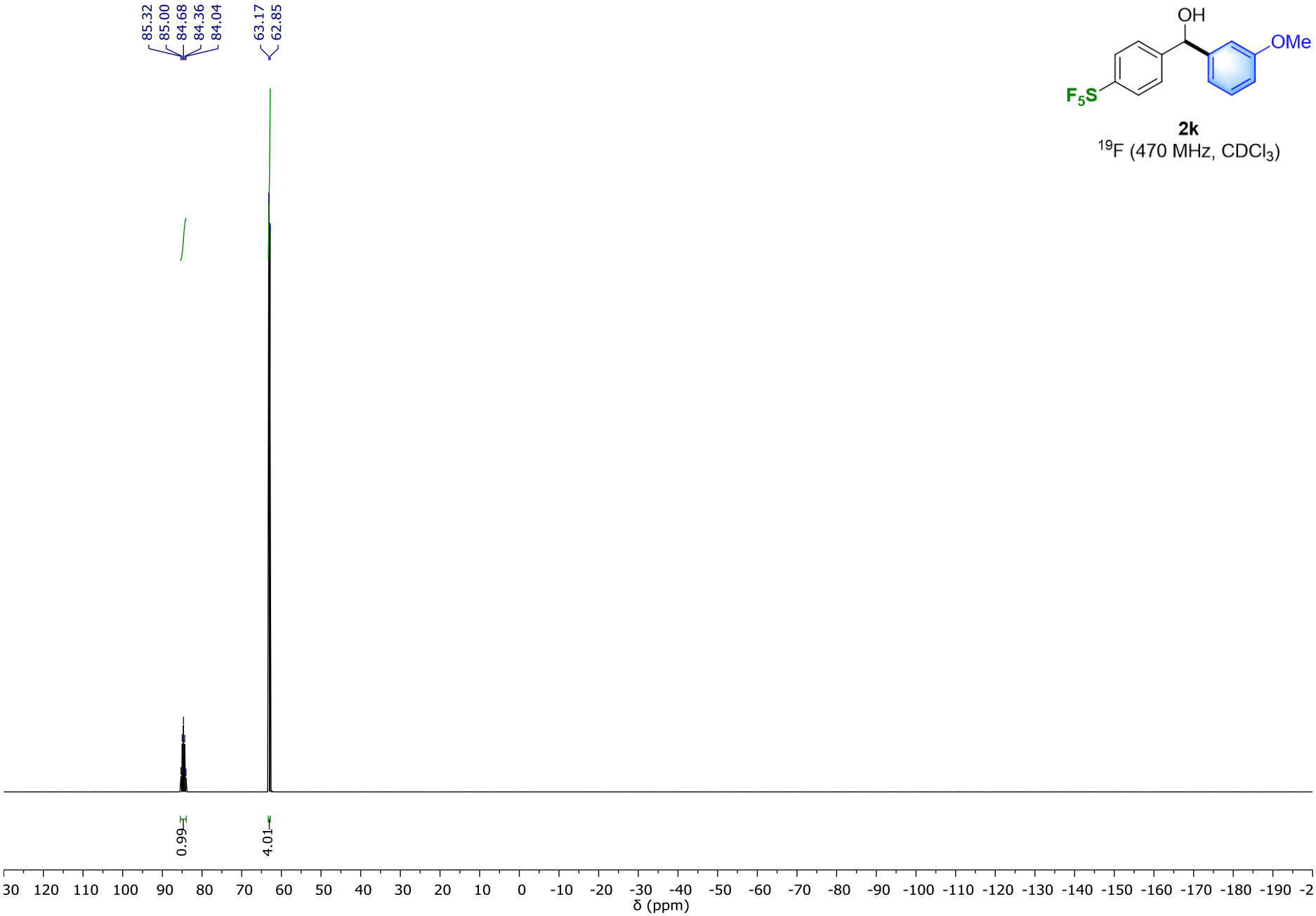

85.38
85.06
84.74
84.42
84.10
63.18
62.86
OH
F5S
2j
19F (470 MHz, CDCl3)
1.03
3.98
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

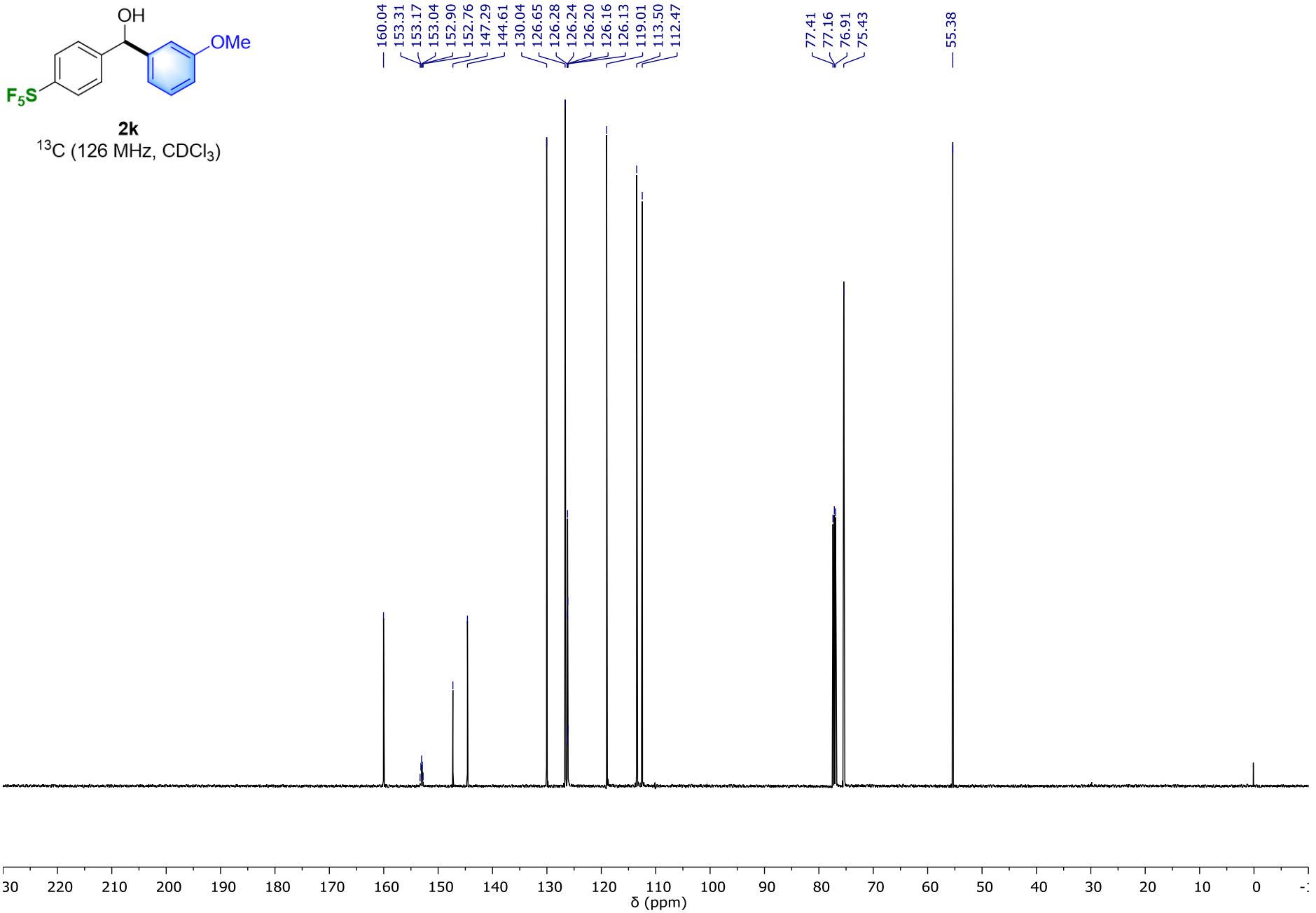


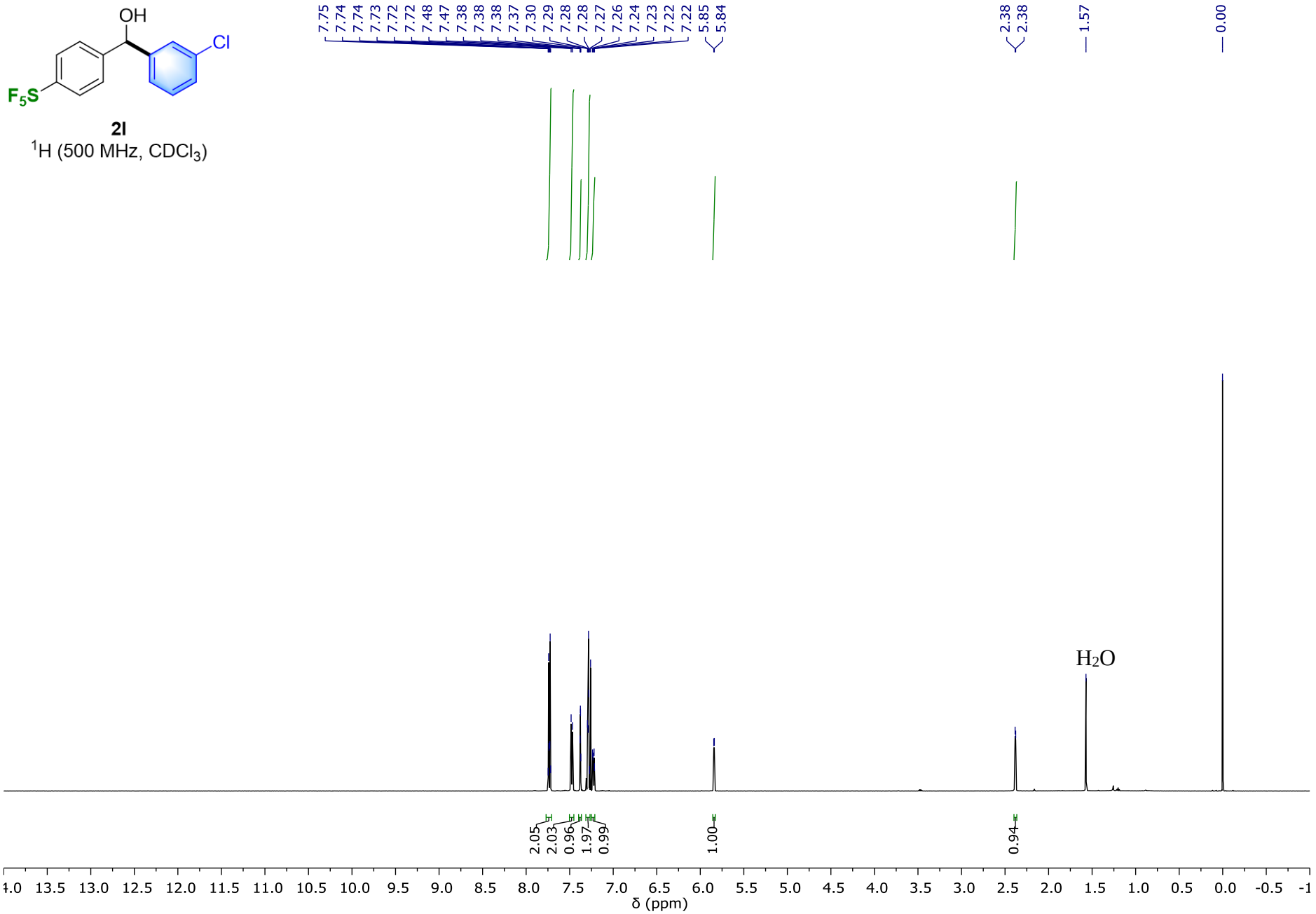
2j

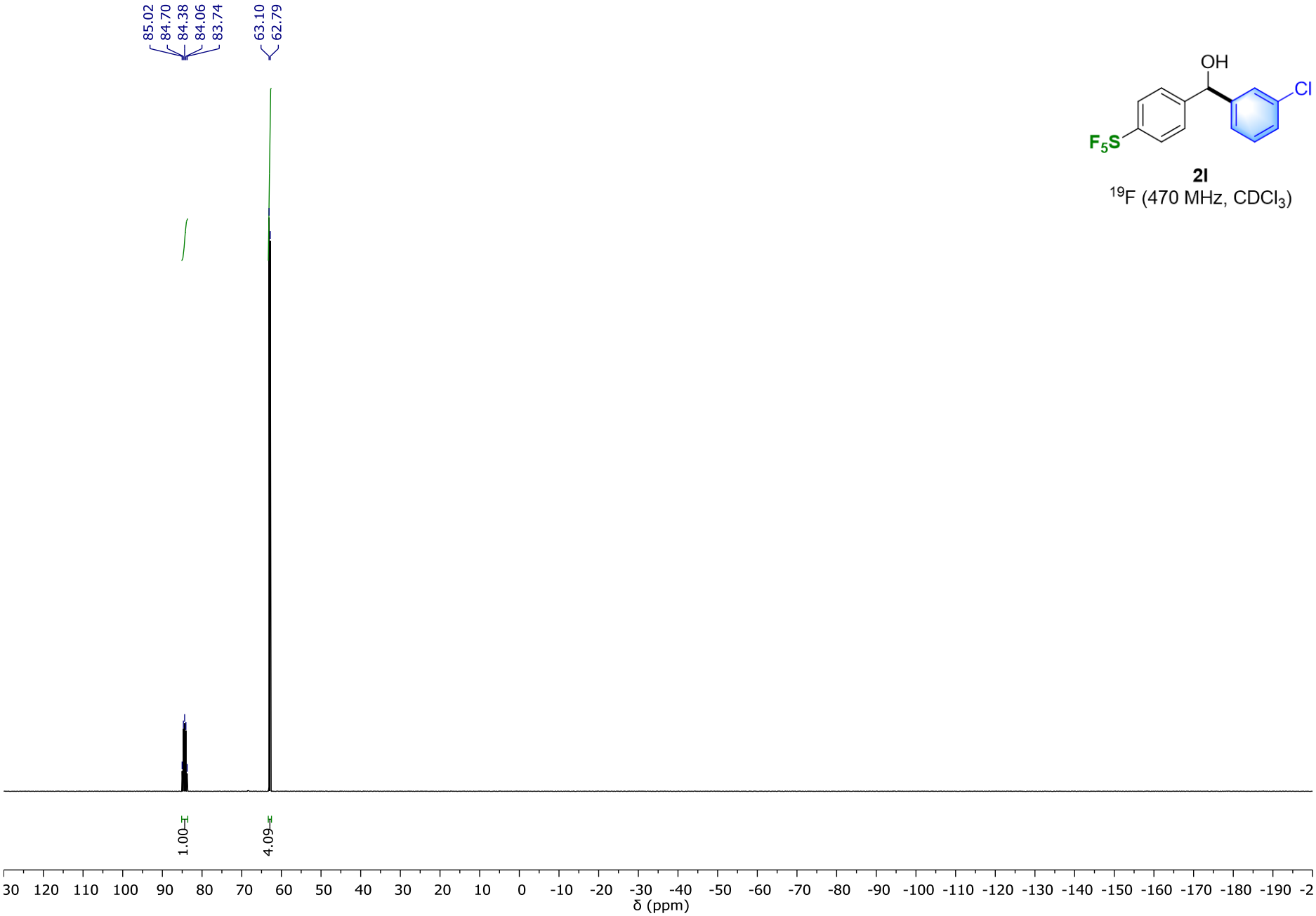
^{13}C (126 MHz, $CDCl_3$)

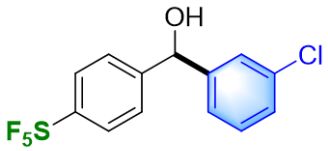

OH
OMe
F5S
2k
1H (500 MHz, CDCl3)
7.72
7.70
7.48
7.47
7.29
7.28
7.26
6.92
6.91
6.85
6.85
6.85
6.84
6.84
6.83
6.83
6.83
5.80
3.79
2.55
2.53
2.04
2.03
1.09
2.00
1.00
1.04
3.21
1.00
δ (ppm)


85.32
85.00
84.68
84.36
84.04
63.17
62.85
OH
OMe
F5S
2k
19F (470 MHz, CDCl3)
0.99
4.01
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)


OH
OMe
F5S
2k
13C (126 MHz, CDCl3)
160.04
153.31
153.17
153.04
152.90
152.76
147.29
144.61
130.04
126.65
126.28
126.24
126.20
126.16
126.13
119.01
113.50
112.47
77.41
77.16
76.91
75.43
55.38
δ (ppm)

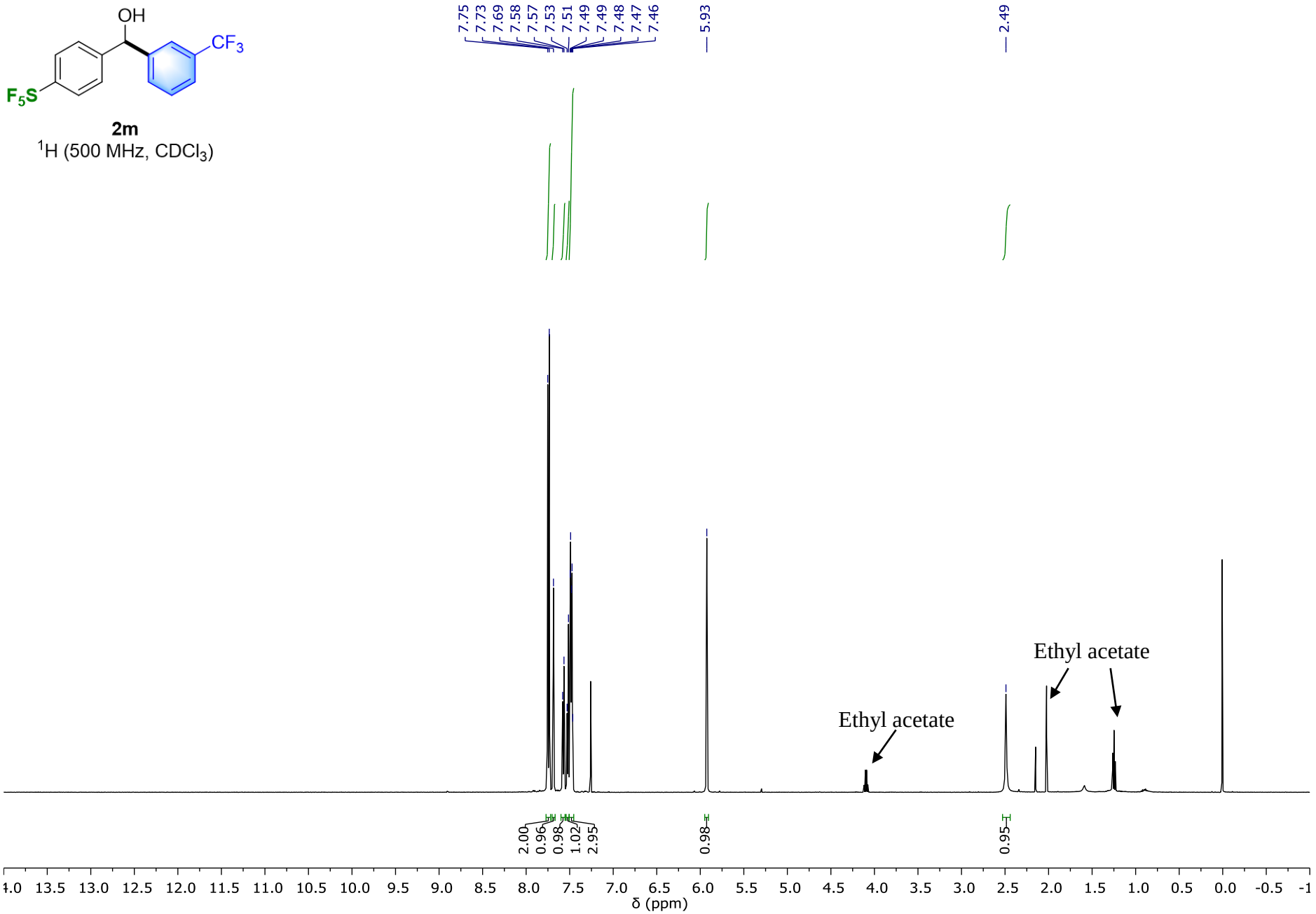

OH
Cl
F5S
2l
1H (500 MHz, CDCl3)
7.75 7.74 7.74 7.73 7.72 7.72 7.48 7.47 7.38 7.38 7.38 7.37 7.30 7.29 7.28 7.28 7.27 7.26 7.24 7.23 7.22 7.22 5.85 5.84
2.38 2.38
1.57
0.00
H2O
2.05 2.03 0.96 1.97 0.99
1.00
0.94
δ (ppm)

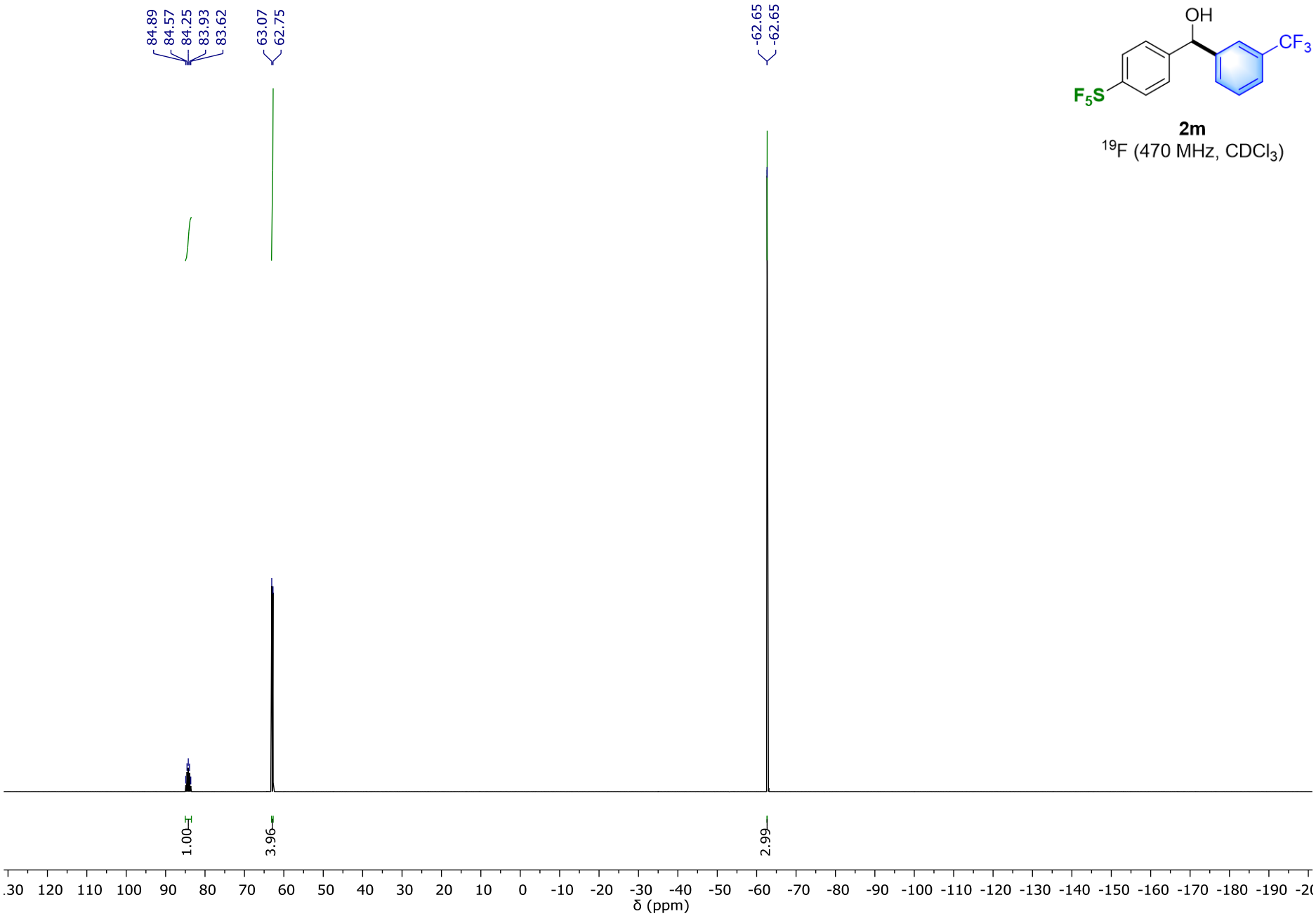

85.02
84.70
84.38
84.06
83.74
63.10
62.79
OH
Cl
F5S
2l
19F (470 MHz, CDCl3)
1.00
4.09
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

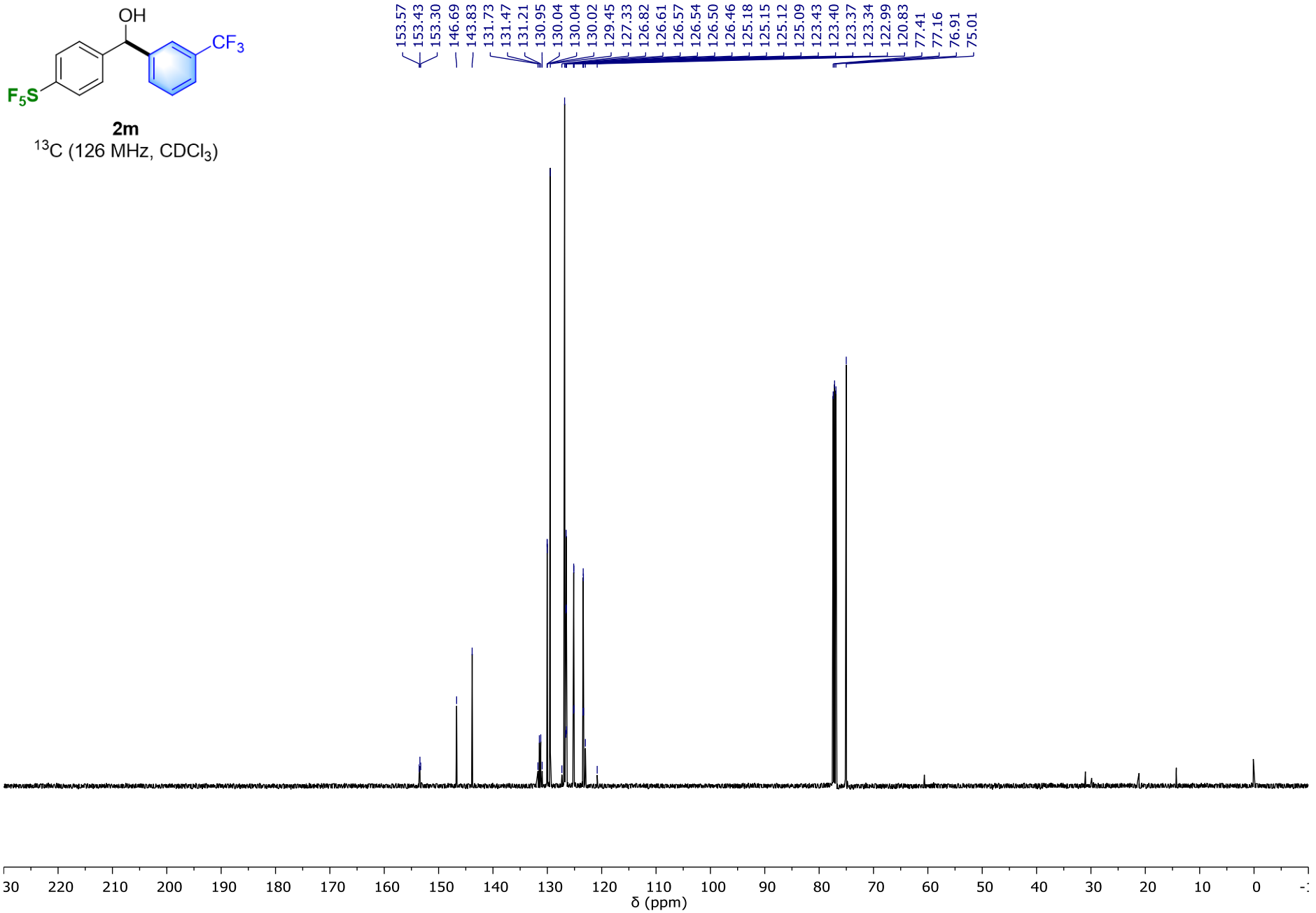


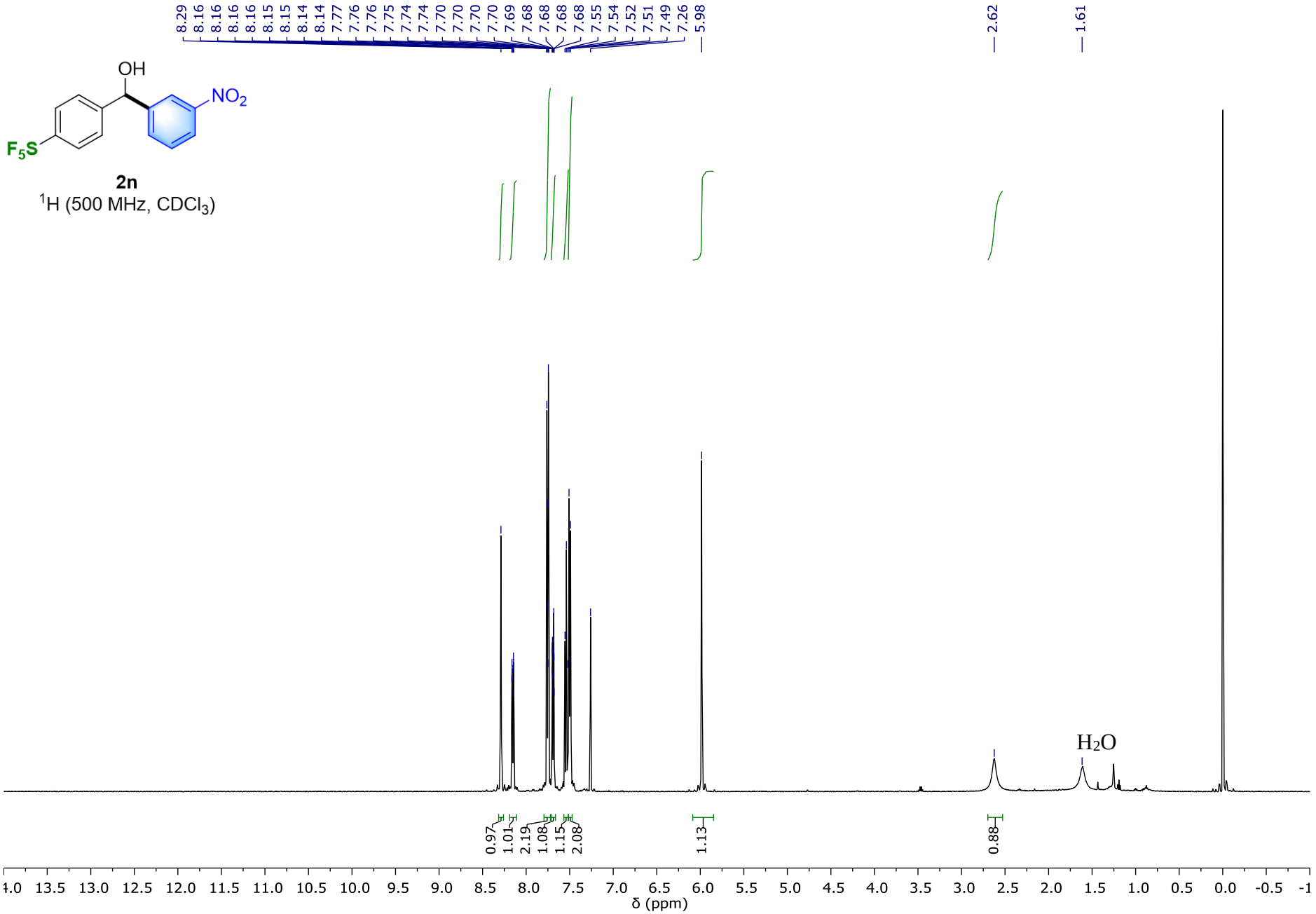
2l

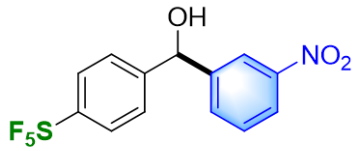
^{13}C (126 MHz, $CDCl_3$)


OH
CF3
F5S
2m
1H (500 MHz, CDCl3)
7.75
7.73
7.69
7.58
7.57
7.53
7.51
7.49
7.49
7.48
7.47
7.46
5.93
2.49
Ethyl acetate
Ethyl acetate
2.00
0.96
0.98
1.02
2.95
0.98
0.95
δ (ppm)


84.89
84.57
84.25
83.93
83.62
63.07
62.75
-62.65
-62.65
OH
CF3
F5S
2m
19F (470 MHz, CDCl3)
1.00
3.96
2.99
δ (ppm)

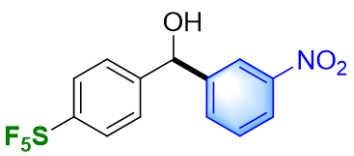

OH
CF3
F5S
2m
13C (126 MHz, CDCl3)
153.57
153.43
153.30
146.69
143.83
131.73
131.47
131.21
130.95
130.04
130.04
130.02
129.45
127.33
126.82
126.61
126.57
126.54
126.50
126.46
125.18
125.15
125.12
125.09
123.43
123.40
123.37
123.34
122.99
120.83
77.41
77.16
76.91
75.01
δ (ppm)


8.29
8.16
8.16
8.16
8.16
8.15
8.15
8.14
8.14
7.77
7.76
7.76
7.75
7.74
7.74
7.70
7.70
7.70
7.70
7.69
7.68
7.68
7.68
7.68
7.55
7.54
7.52
7.51
7.49
7.26
5.98
2.62
1.61
OH
NO2
F5S
2n
1H (500 MHz, CDCl3)
H2O
0.97
1.01
2.19
1.08
1.15
2.08
1.13
0.88
δ (ppm)



2n

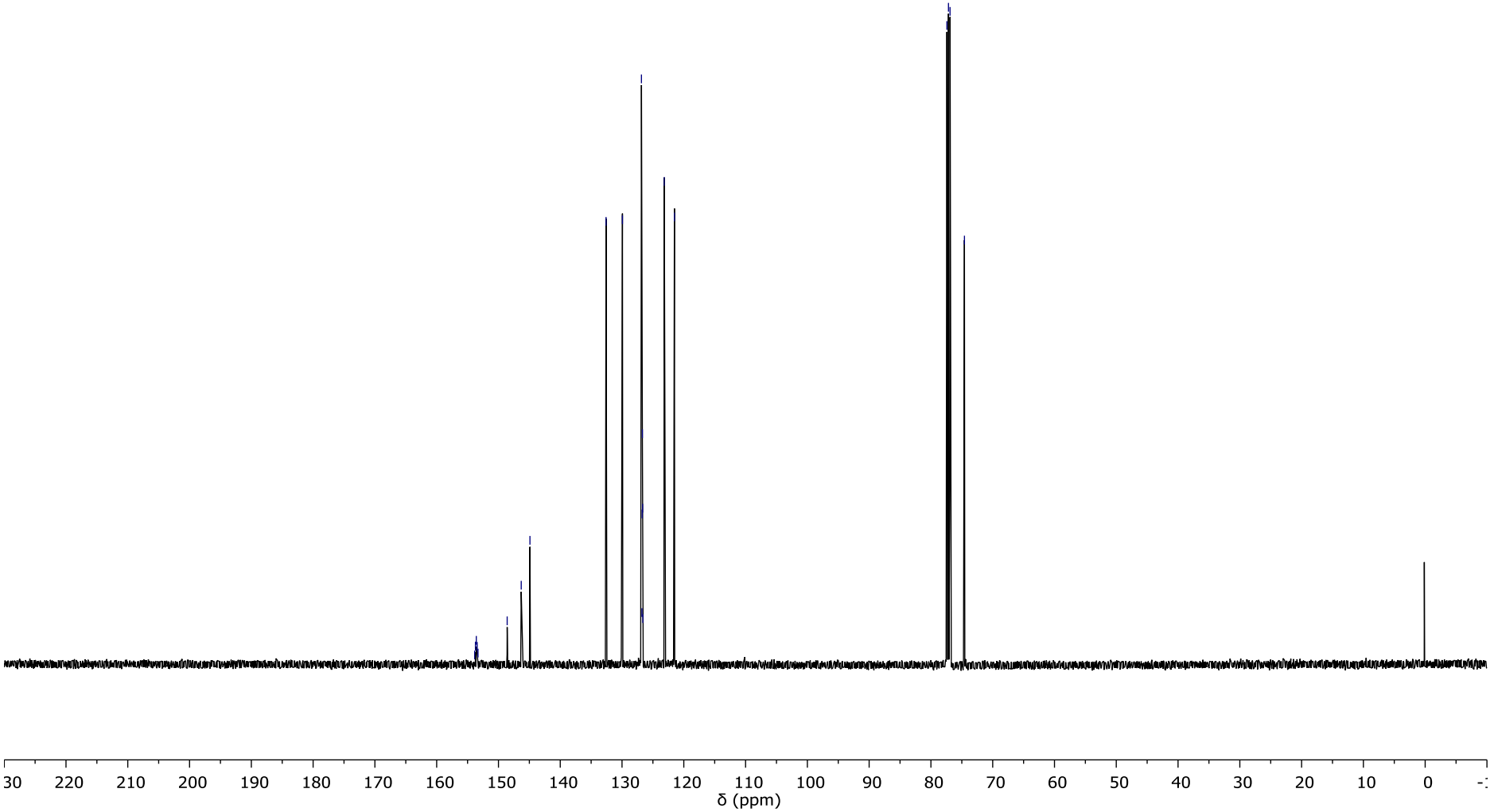
^{19}F (470 MHz, $CDCl_3$)

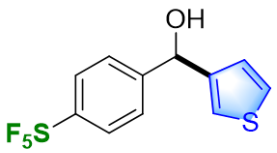


2n

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

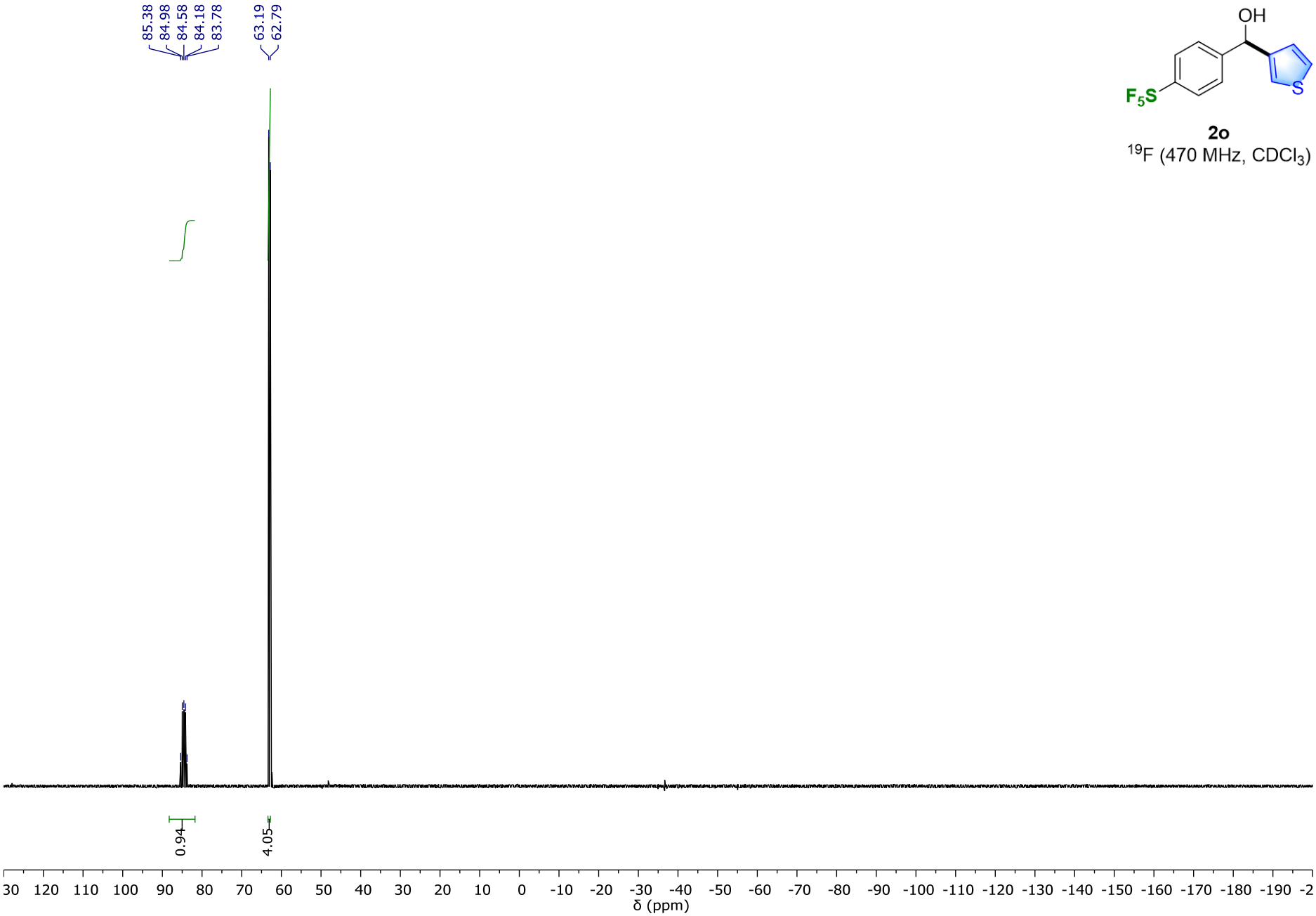
153.85
153.73
153.59
153.45
153.31
148.59
146.31
144.90
132.59
129.93
126.85
126.77
126.74
126.70
126.66
126.63
123.16
121.52
77.42
77.16
76.91
74.57

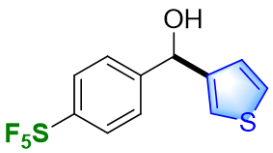




2o

^{1}H (500 MHz, $CDCl_3$)


85.38
84.98
84.58
84.18
83.78
63.19
62.79
OH
F5S
S
2o
19F (470 MHz, CDCl3)
0.94
4.05
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

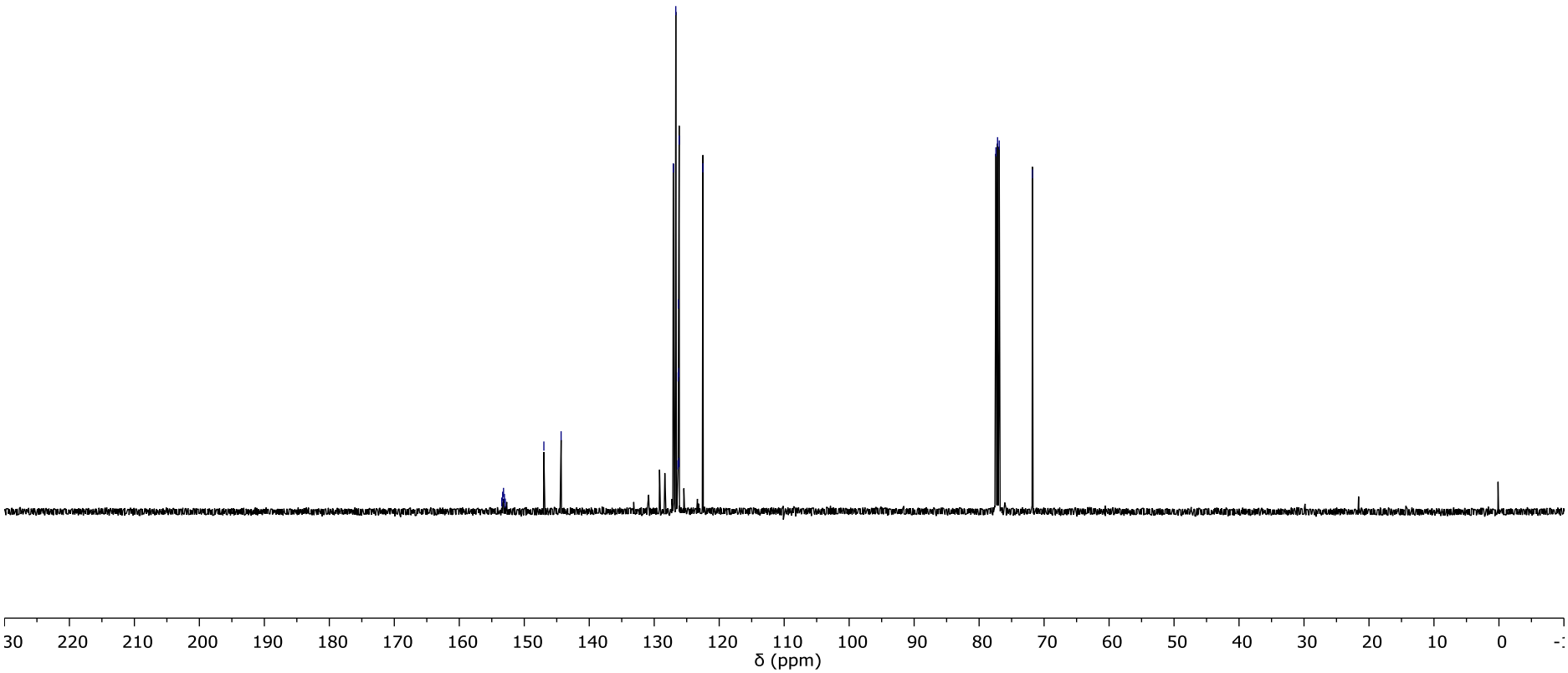


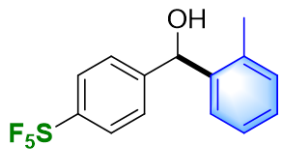
2o

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

153.46
153.33
153.19
153.05
152.92
146.98
144.33
127.07
126.68
126.35
126.31
126.28
126.24
126.20
126.16
122.52

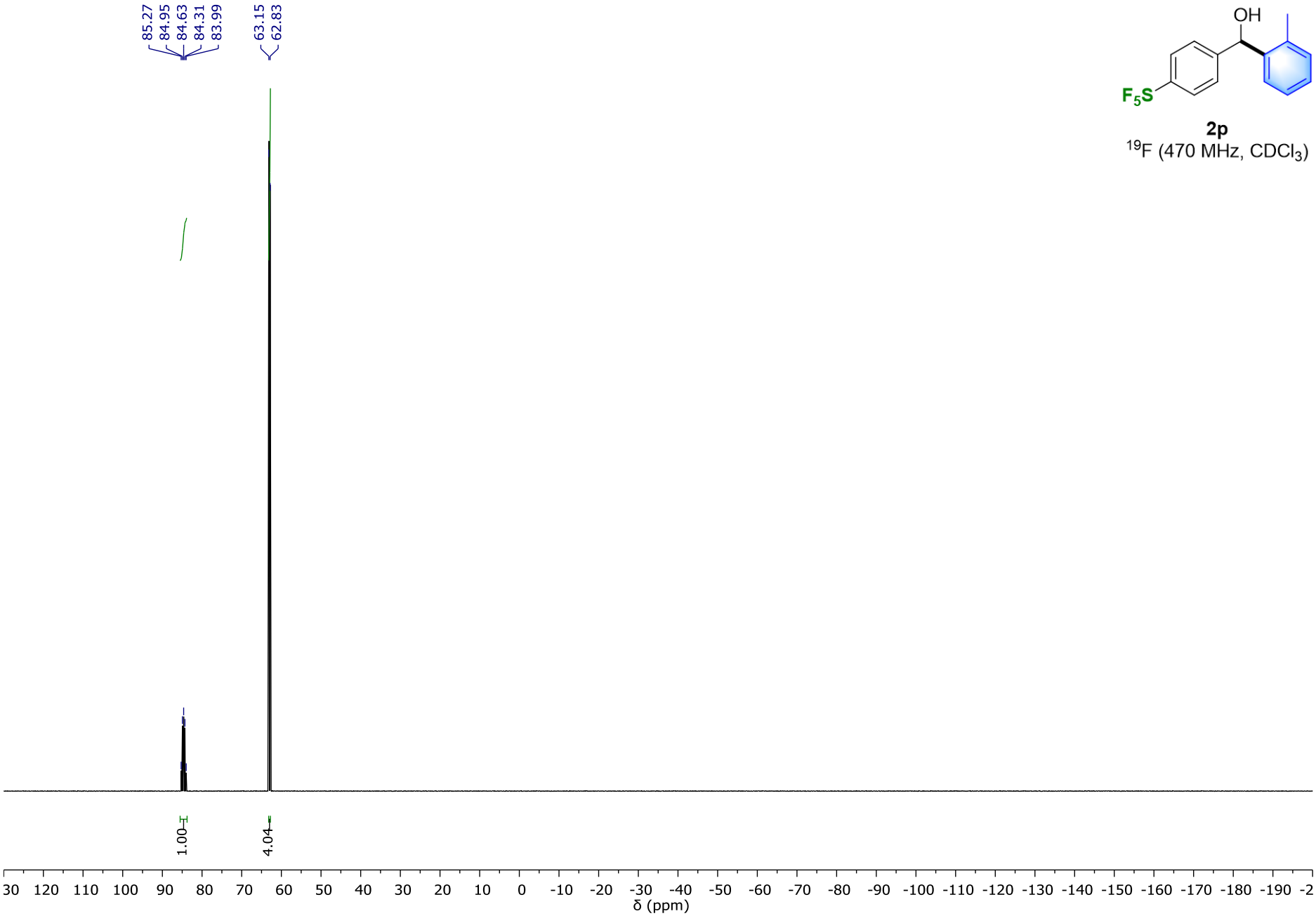
77.41
77.16
76.91
71.79

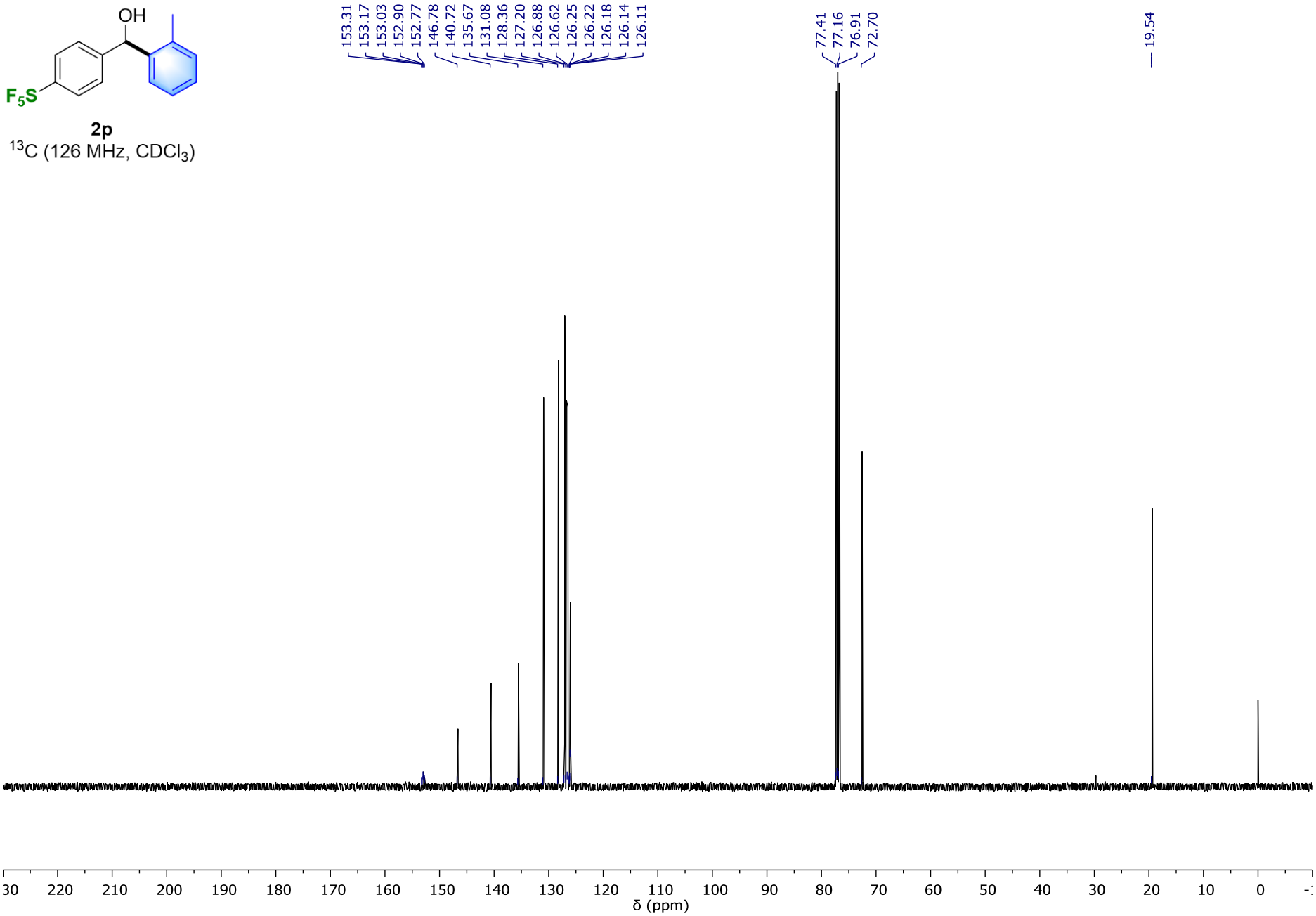


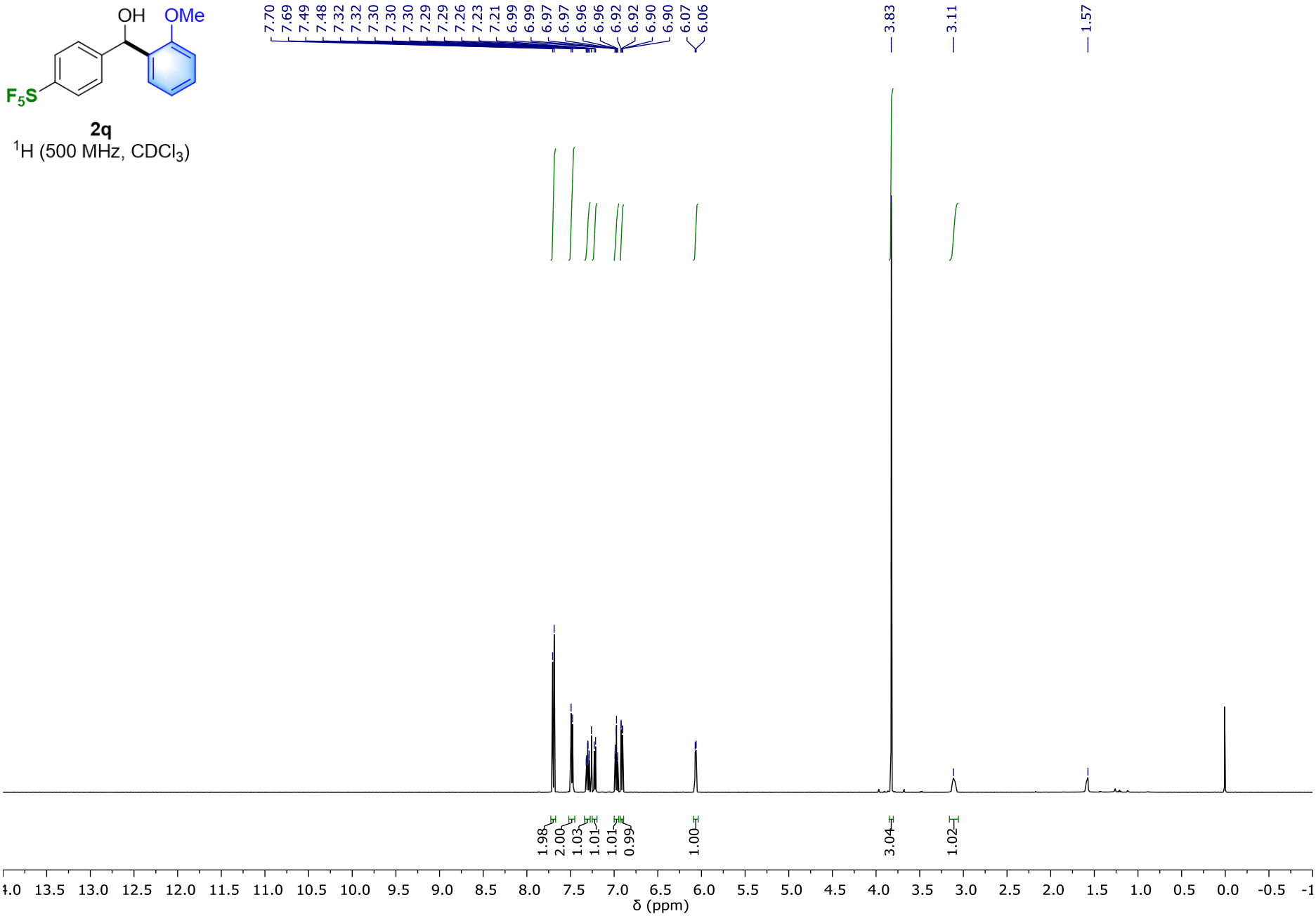


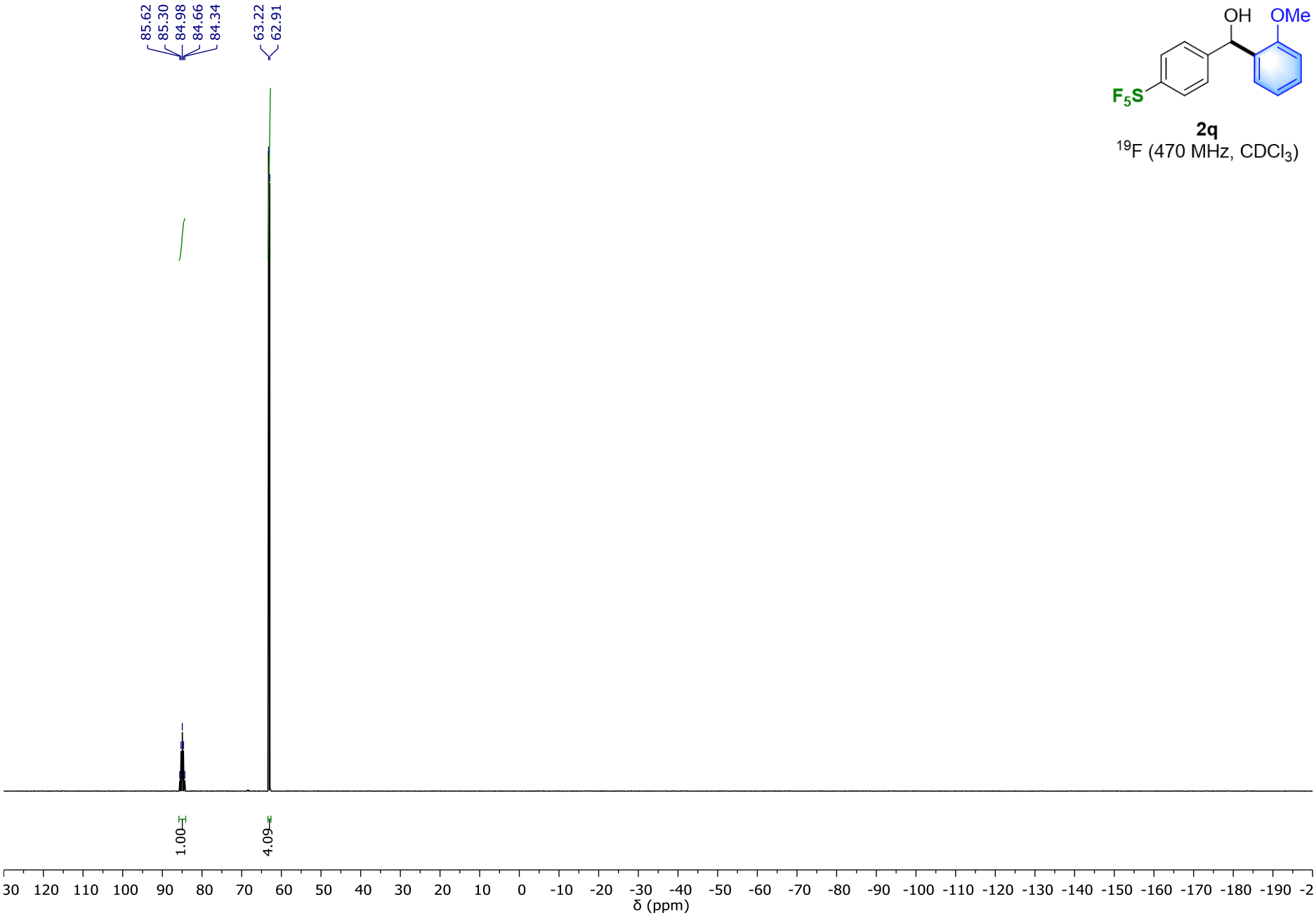
2p

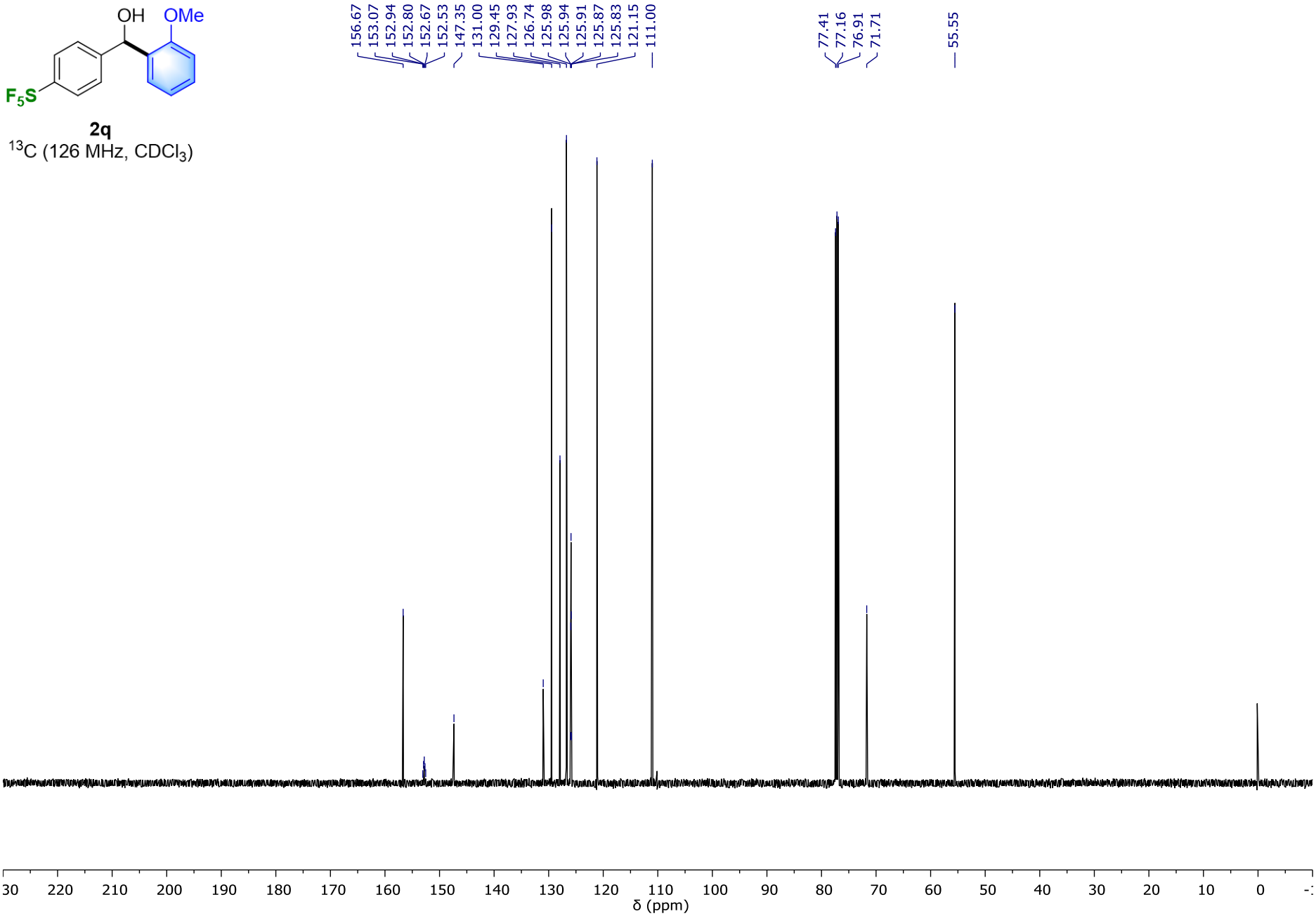
^{1}H (500 MHz, $CDCl_3$)

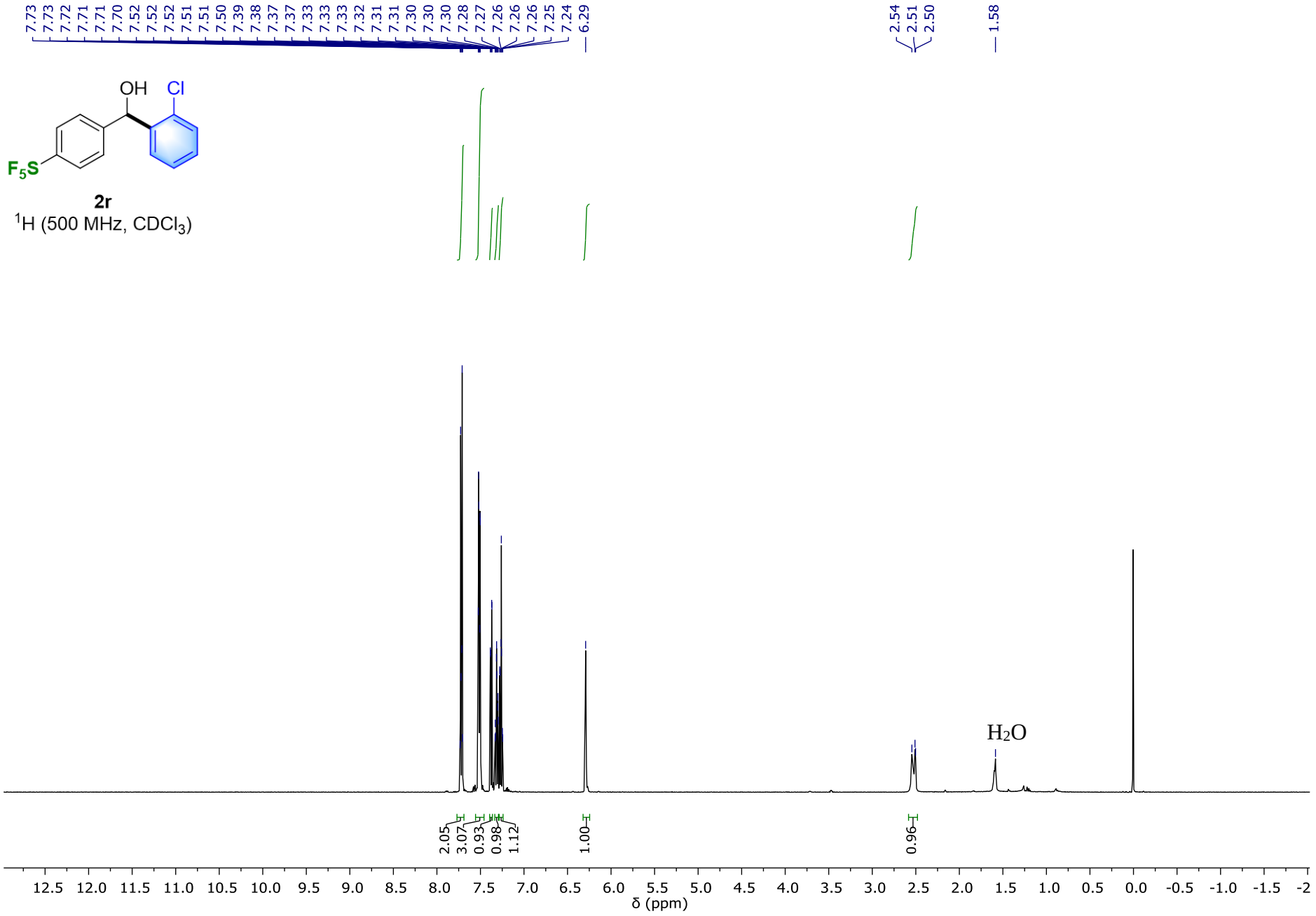

85.27
84.95
84.63
84.31
83.99
63.15
62.83
OH
F5S
2p
19F (470 MHz, CDCl3)
1.00
4.04
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

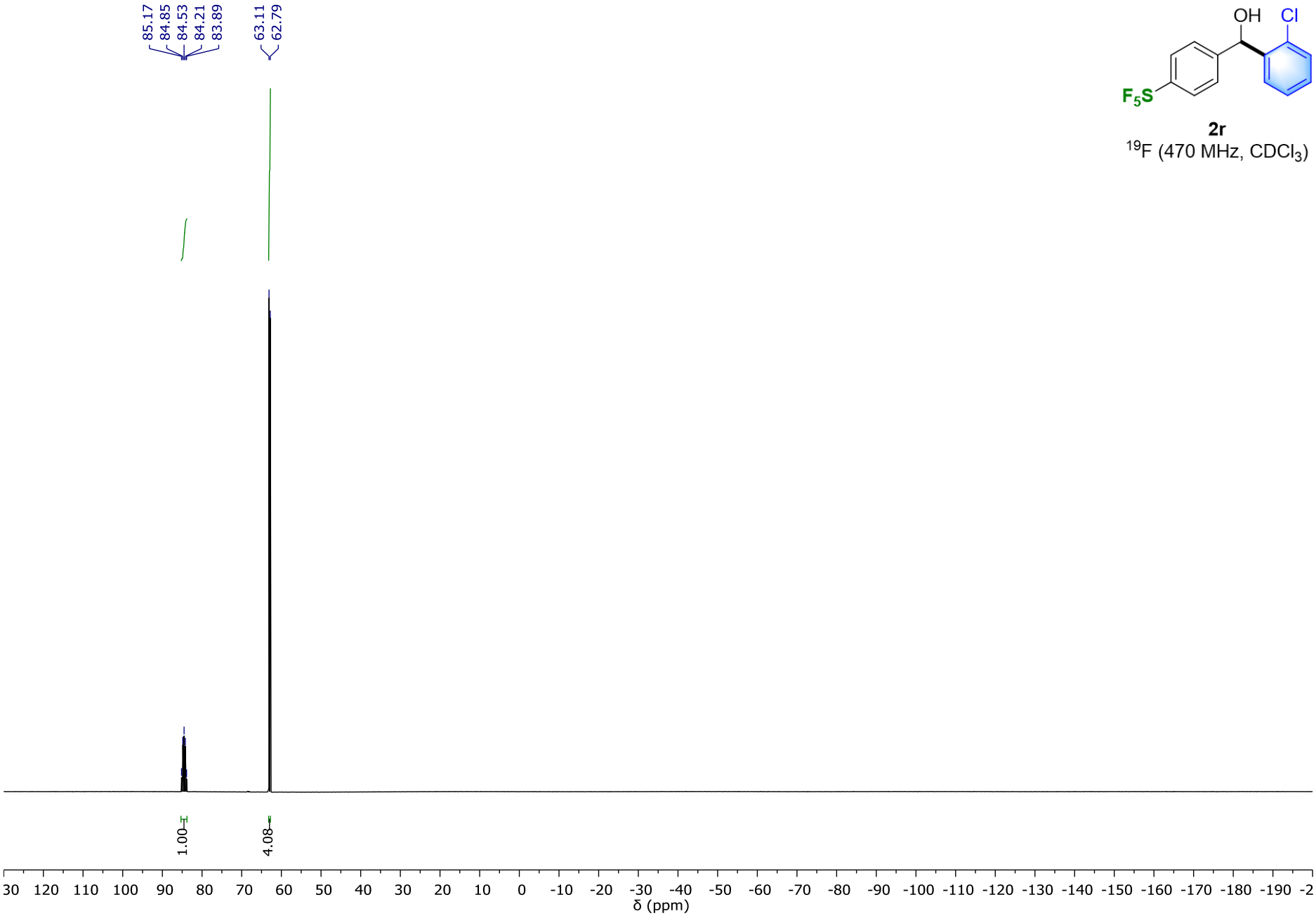

OH
F5S
2p
13C (126 MHz, CDCl3)
153.31
153.17
153.03
152.90
152.77
146.78
140.72
135.67
131.08
128.36
127.20
126.88
126.62
126.25
126.22
126.18
126.14
126.11
77.41
77.16
76.91
72.70
19.54
δ (ppm)

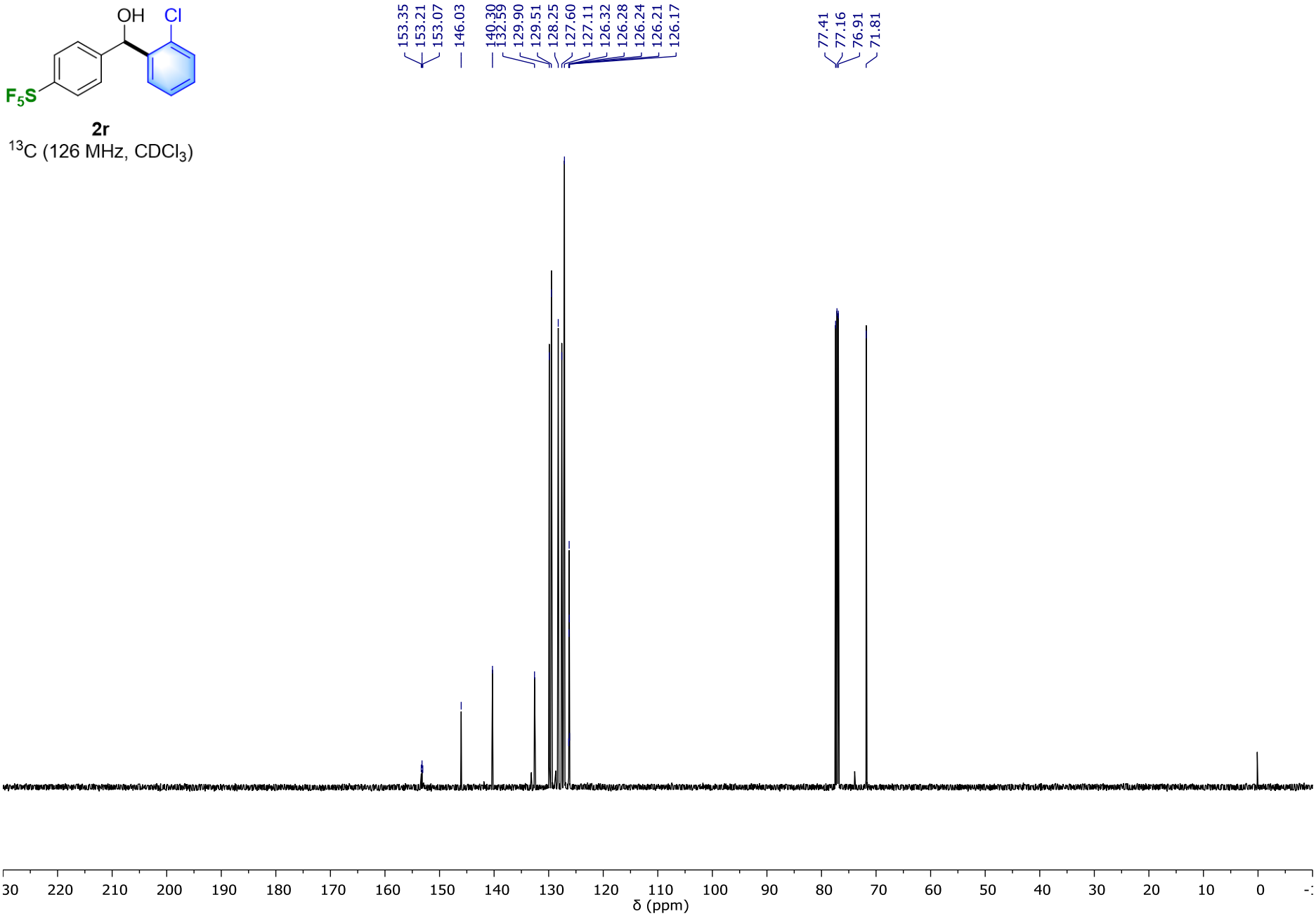

OH
OMe
F5S
2q
1H (500 MHz, CDCl3)
7.70
7.69
7.49
7.48
7.32
7.32
7.30
7.30
7.30
7.29
7.29
7.26
7.23
7.21
6.99
6.99
6.97
6.97
6.96
6.96
6.92
6.92
6.90
6.90
6.07
6.06
3.83
3.11
1.57
1.98
2.00
1.03
1.01
1.01
0.99
1.00
3.04
1.02
δ (ppm)


85.62
85.30
84.98
84.66
84.34
63.22
62.91
OH
OMe
F5S
2q
19F (470 MHz, CDCl3)
1.00
4.09
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)


OH
OMe
F5S
2q
13C (126 MHz, CDCl3)
156.67
153.07
152.94
152.80
152.67
152.53
147.35
131.00
129.45
127.93
126.74
125.98
125.94
125.91
125.87
125.83
121.15
111.00
77.41
77.16
76.91
71.71
55.55
δ (ppm)

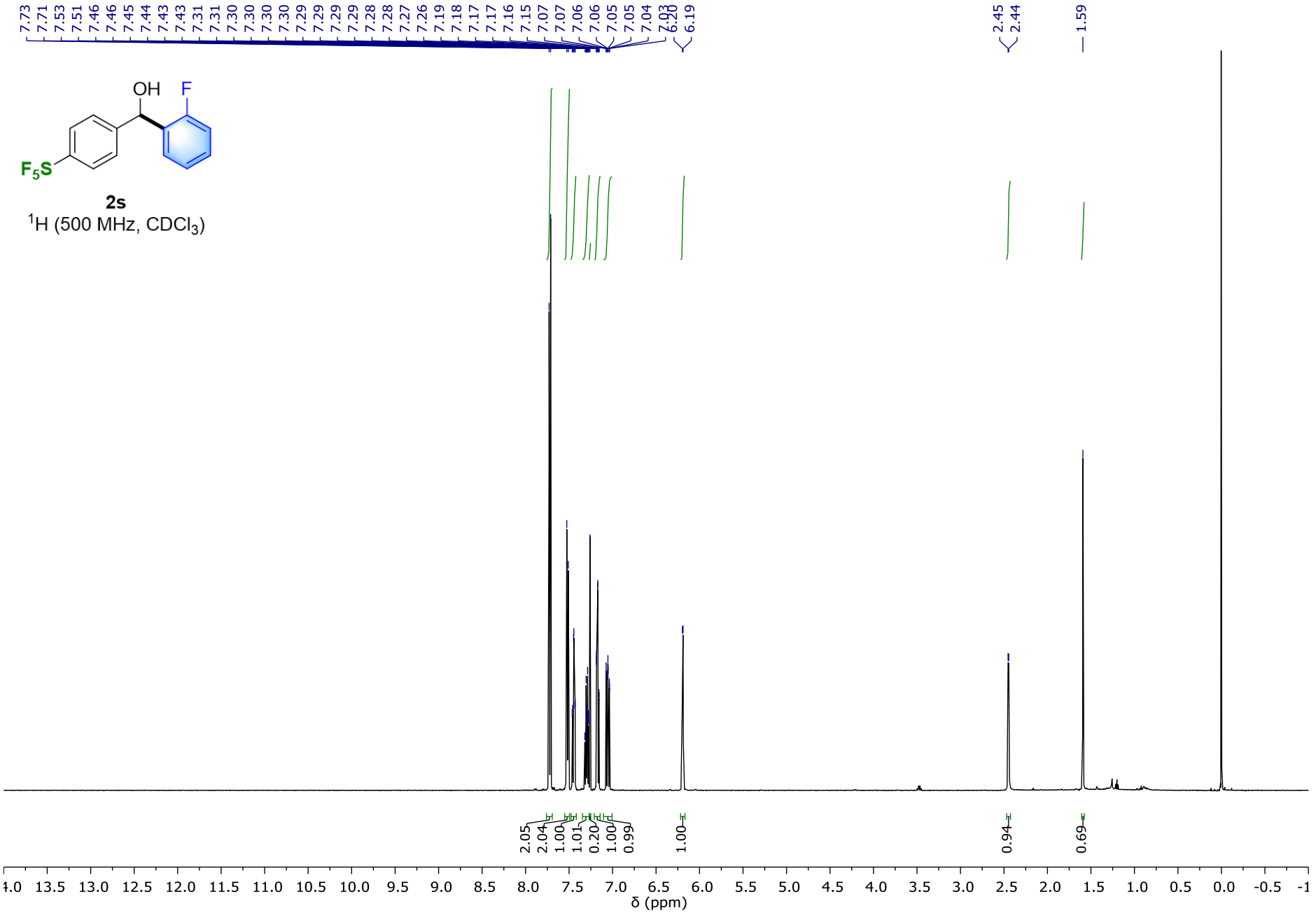

7.73 7.73 7.72 7.71 7.71 7.70 7.52 7.52 7.52 7.51 7.51 7.50 7.39 7.38 7.37 7.37 7.33 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.28 7.27 7.26 7.26 7.26 7.25 7.24 6.29
2.54 2.51 2.50
1.58
OH
Cl
F5S
2r
1H (500 MHz, CDCl3)
H2O
2.05 3.07 0.93 0.98 1.12 1.00 0.96
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 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 -0.5 -1.0 -1.5 -2
δ (ppm)

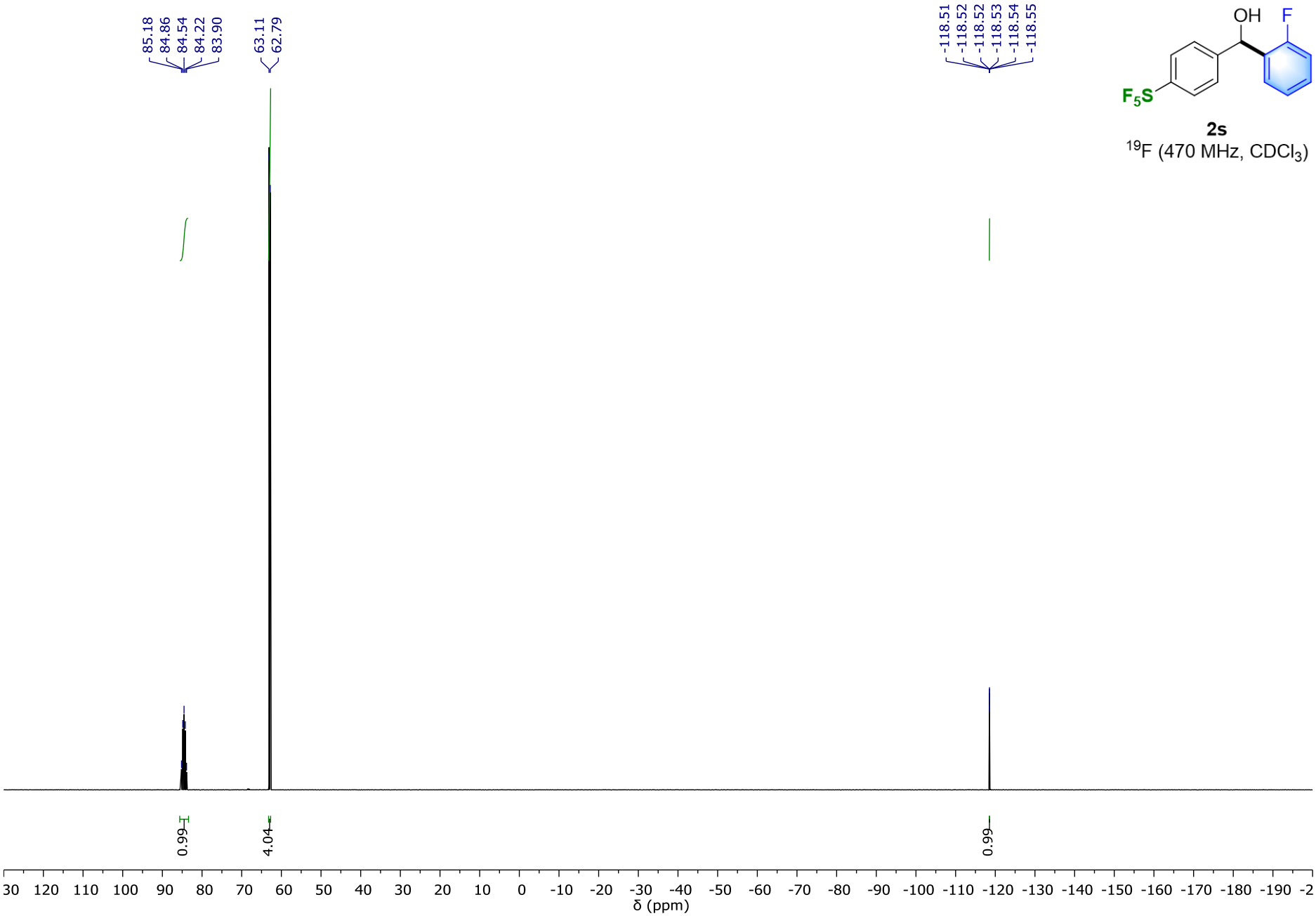

85.17
84.85
84.53
84.21
83.89
63.11
62.79
OH
Cl
F5S
2r
19F (470 MHz, CDCl3)
1.00
4.08
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



2r

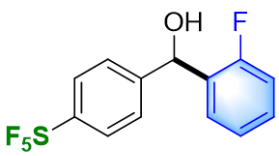
^{13}C (126 MHz, $CDCl_3$)


7.73
7.71
7.53
7.51
7.46
7.46
7.45
7.44
7.43
7.43
7.31
7.31
7.30
7.30
7.30
7.30
7.29
7.29
7.29
7.29
7.28
7.28
7.27
7.26
7.19
7.18
7.17
7.17
7.16
7.15
7.07
7.07
7.06
7.06
7.05
7.05
7.04
7.03
6.20
6.19
2.45
2.44
1.59
OH
F
F5S
2s
1H (500 MHz, CDCl3)
2.05
2.04
1.00
1.01
0.20
1.00
0.99
1.00
0.94
0.69
δ (ppm)



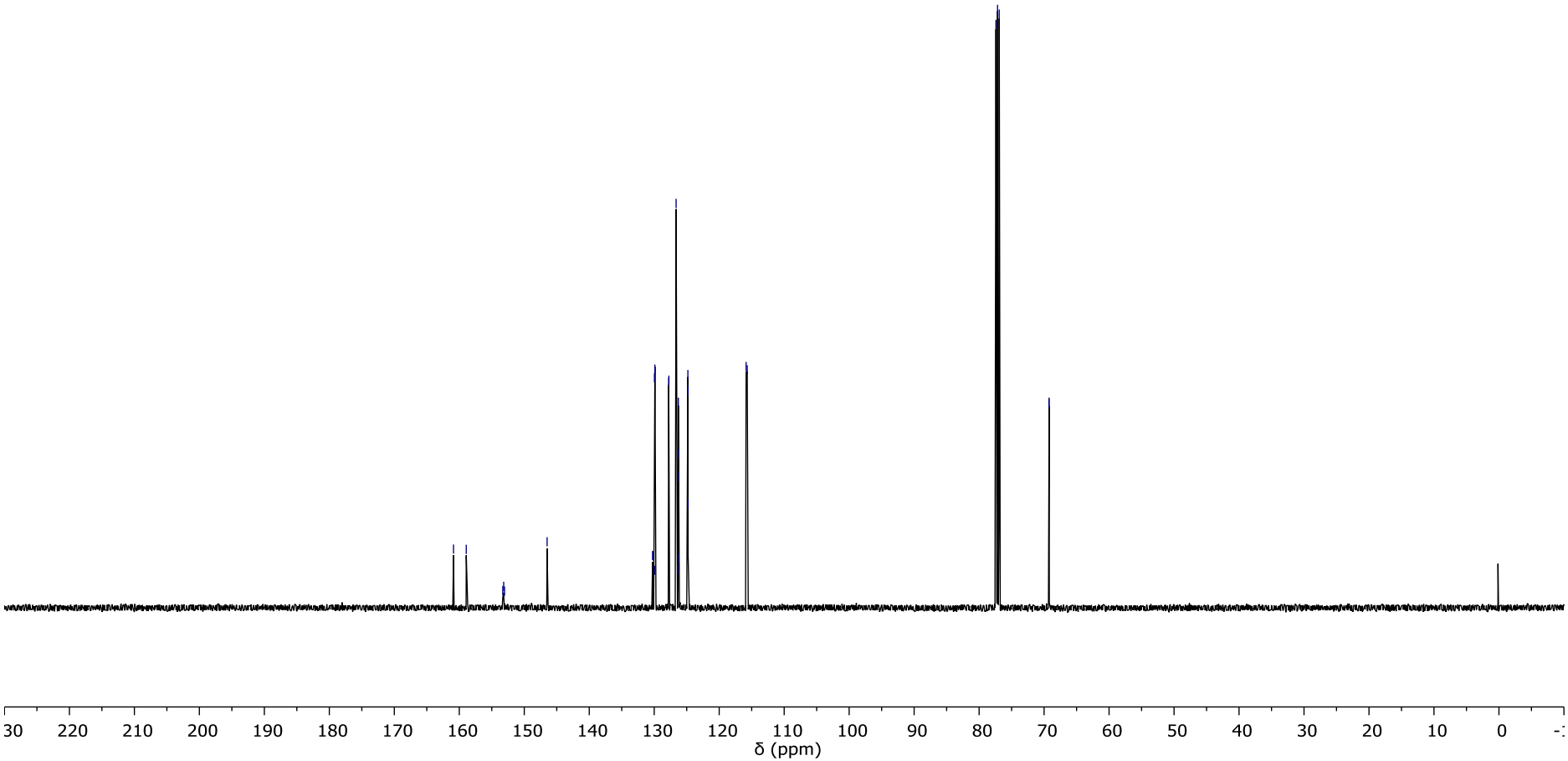
2s

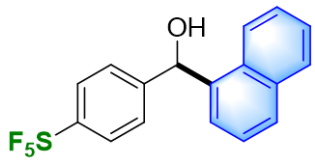
^{19}F (470 MHz, $CDCl_3$)



2s

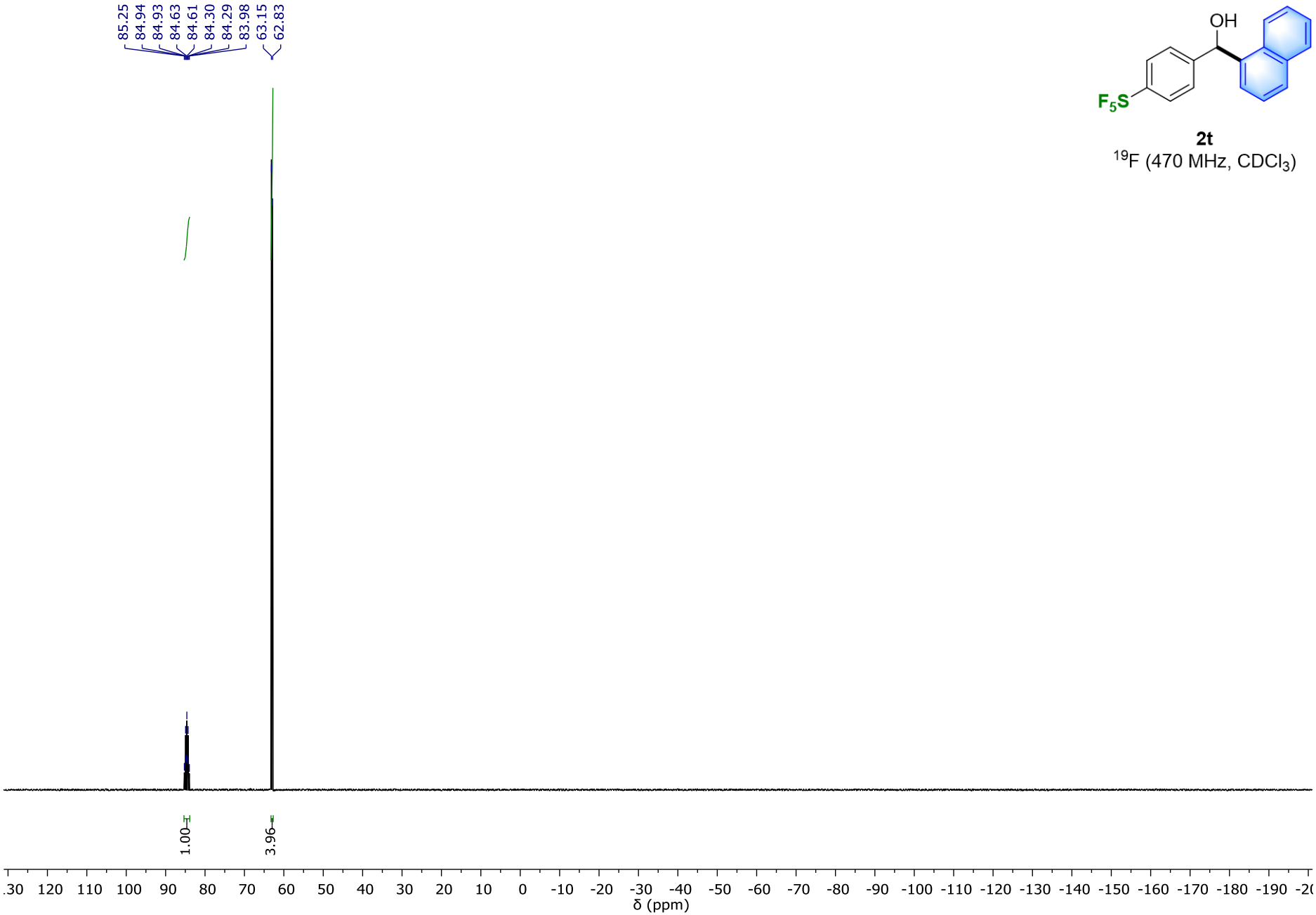
^{13}C (126 MHz, $CDCl_3$)





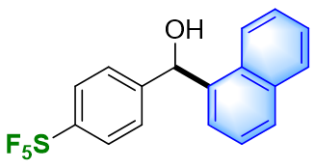
2t

^{1}H (500 MHz, $CDCl_3$)



2t

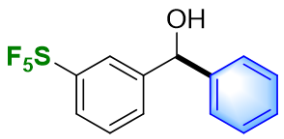
^{19}F (470 MHz, $CDCl_3$)



2t

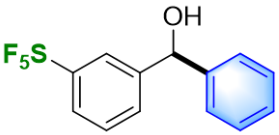
^{13}C (126 MHz, $CDCl_3$)

1.2. Compounds 4a-4t



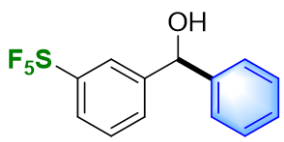
4a

^{1}H (500 MHz, $CDCl_3$)



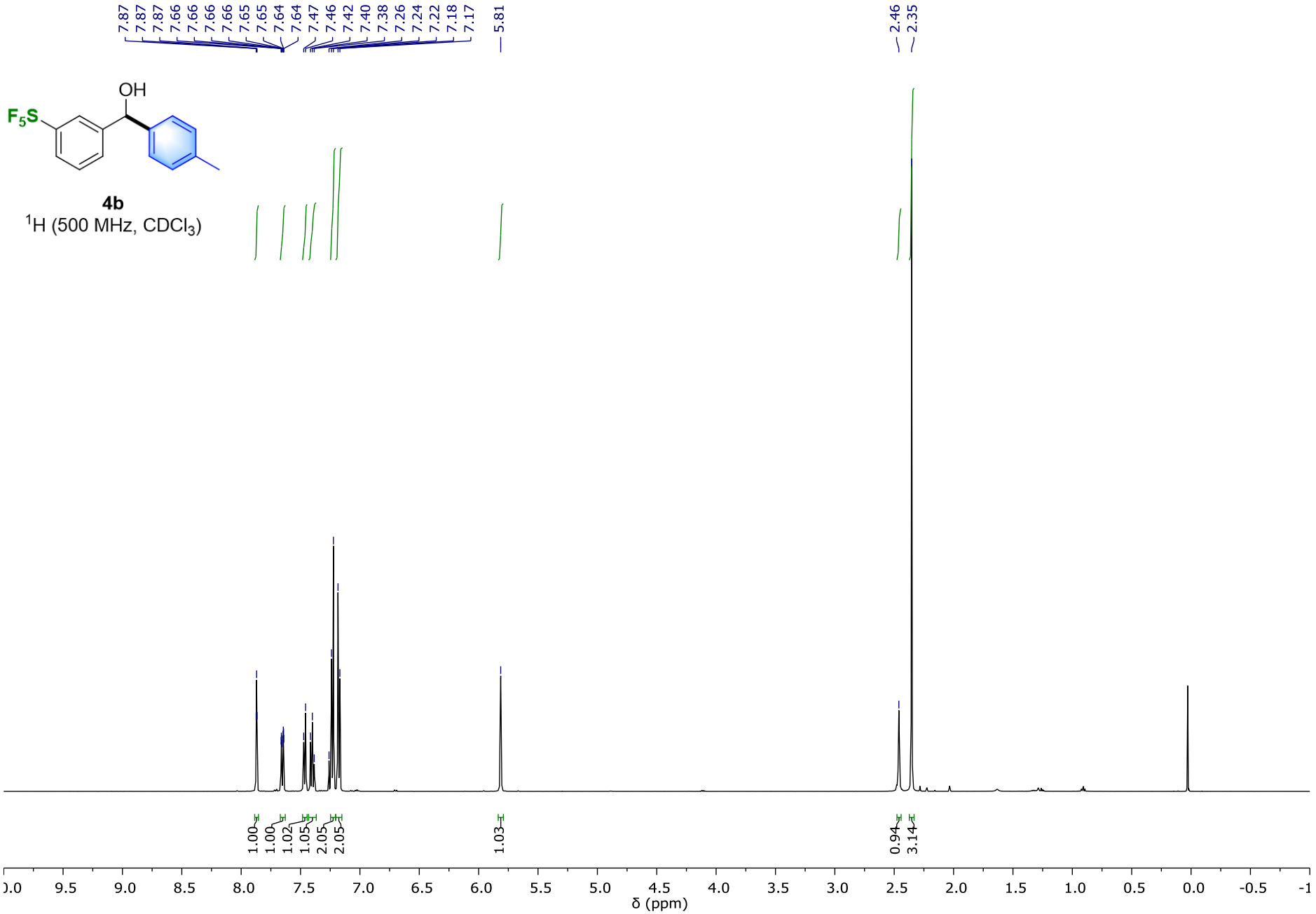
4a

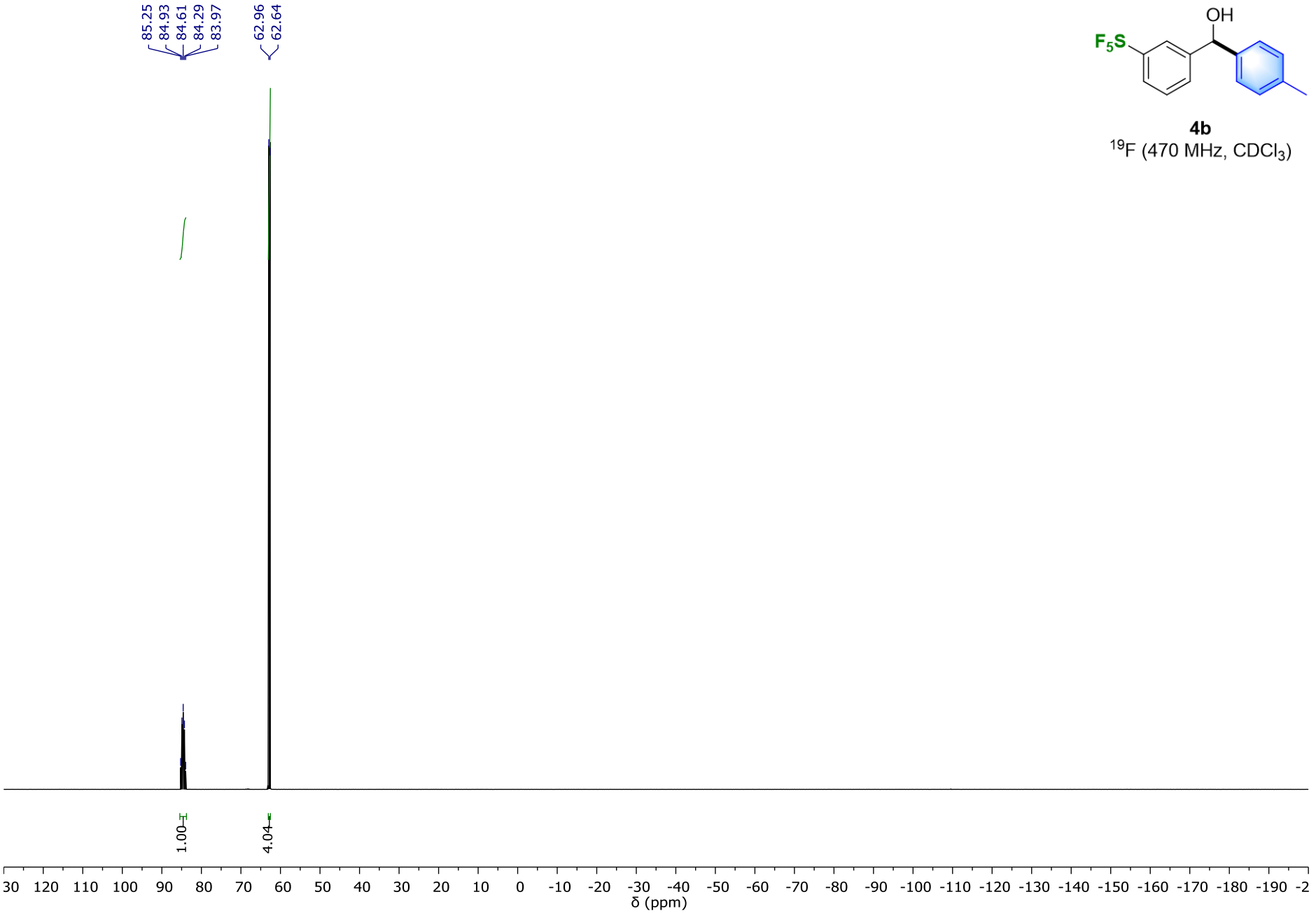
^{19}F (470 MHz, $CDCl_3$)

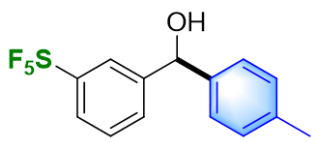


4a

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

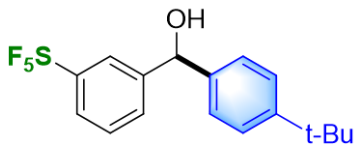

7.87
7.87
7.87
7.66
7.66
7.66
7.65
7.65
7.64
7.64
7.47
7.46
7.42
7.40
7.38
7.26
7.24
7.22
7.18
7.17
5.81
2.46
2.35
OH
F5S
4b
1H (500 MHz, CDCl3)
1.00
1.00
1.02
1.05
2.05
2.05
1.03
0.94
3.14
δ (ppm)


85.25
84.93
84.61
84.29
83.97
62.96
62.64
OH
F5S
4b
19F (470 MHz, CDCl3)
1.00
4.04
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



4b

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

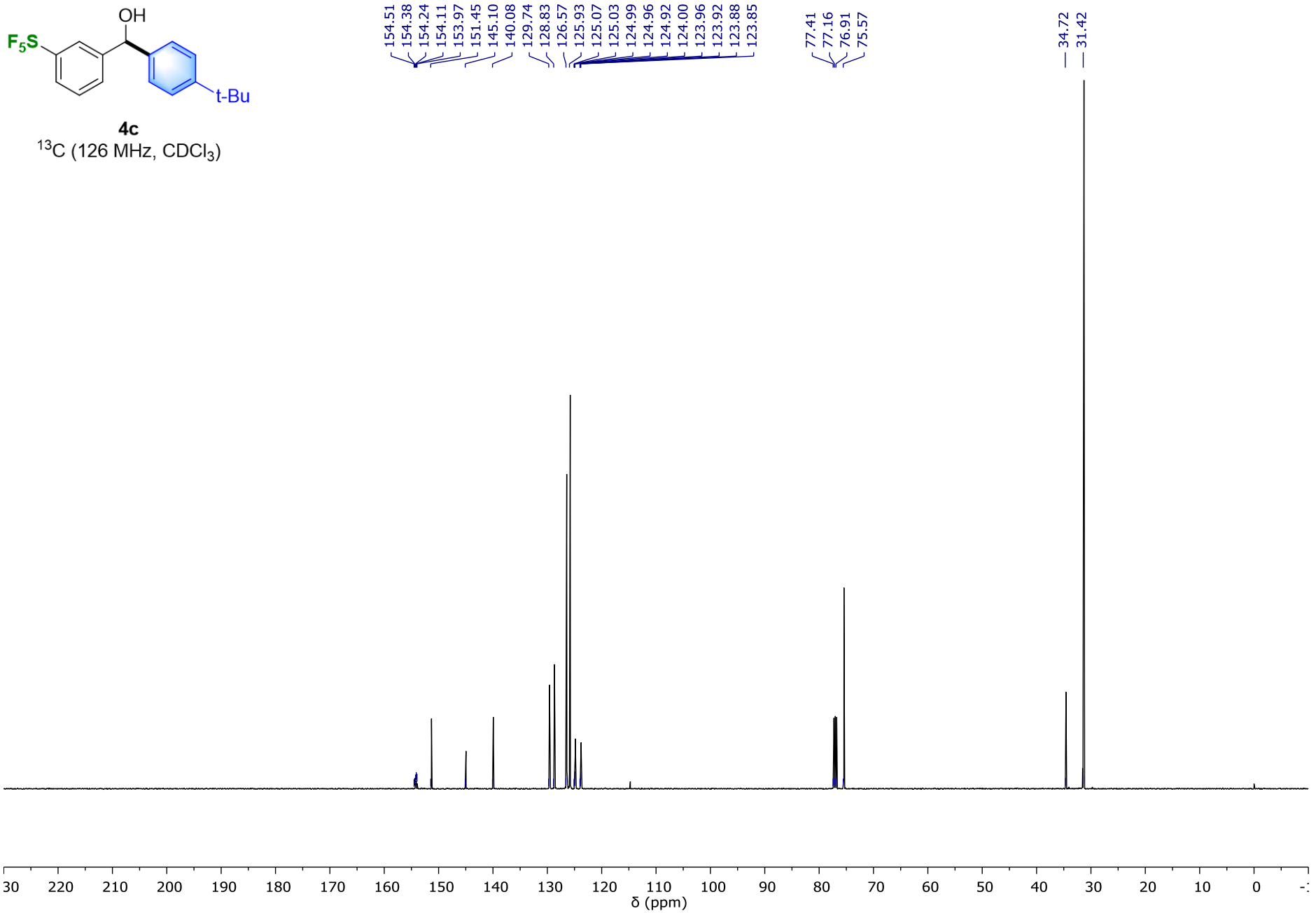


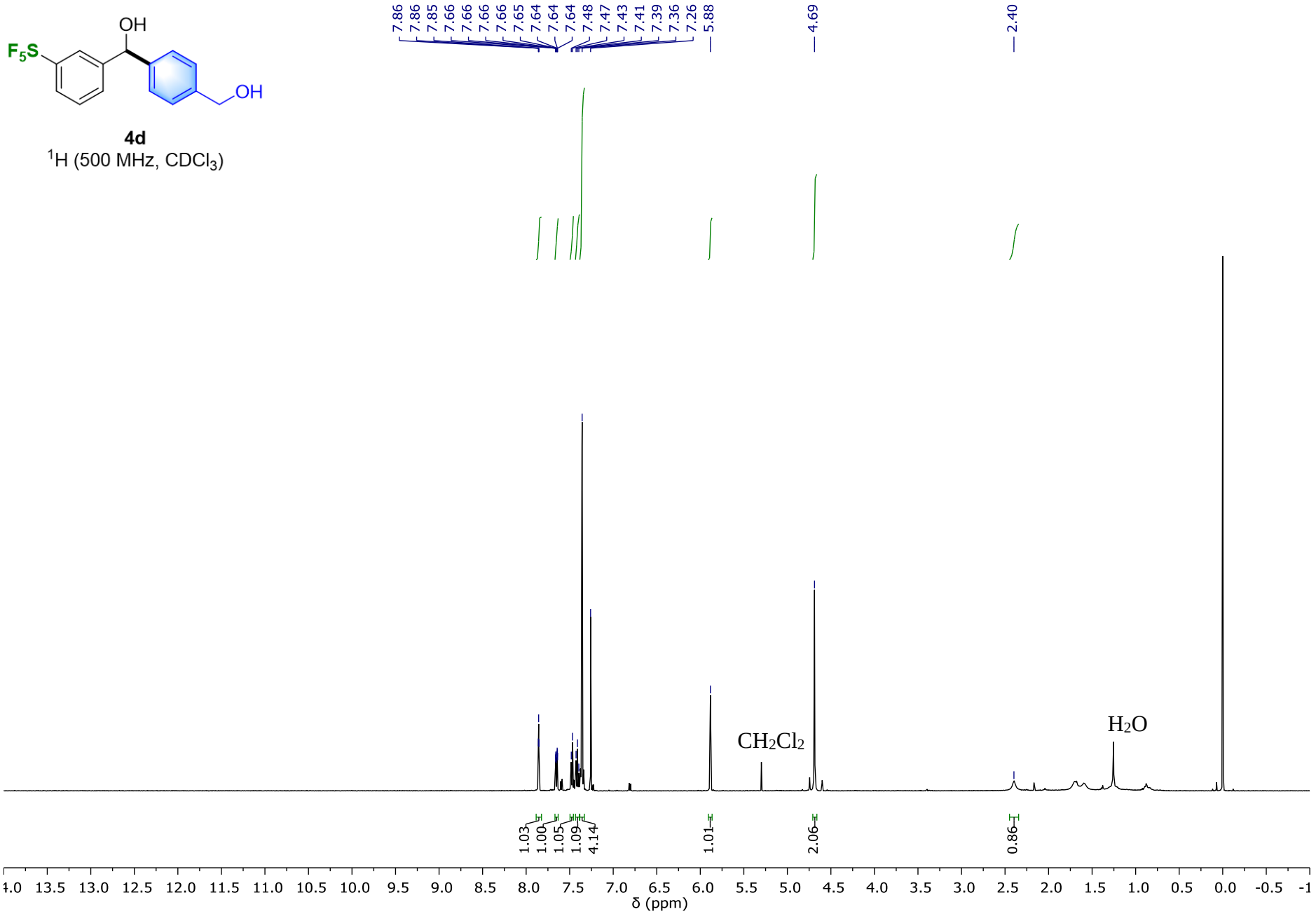
4c

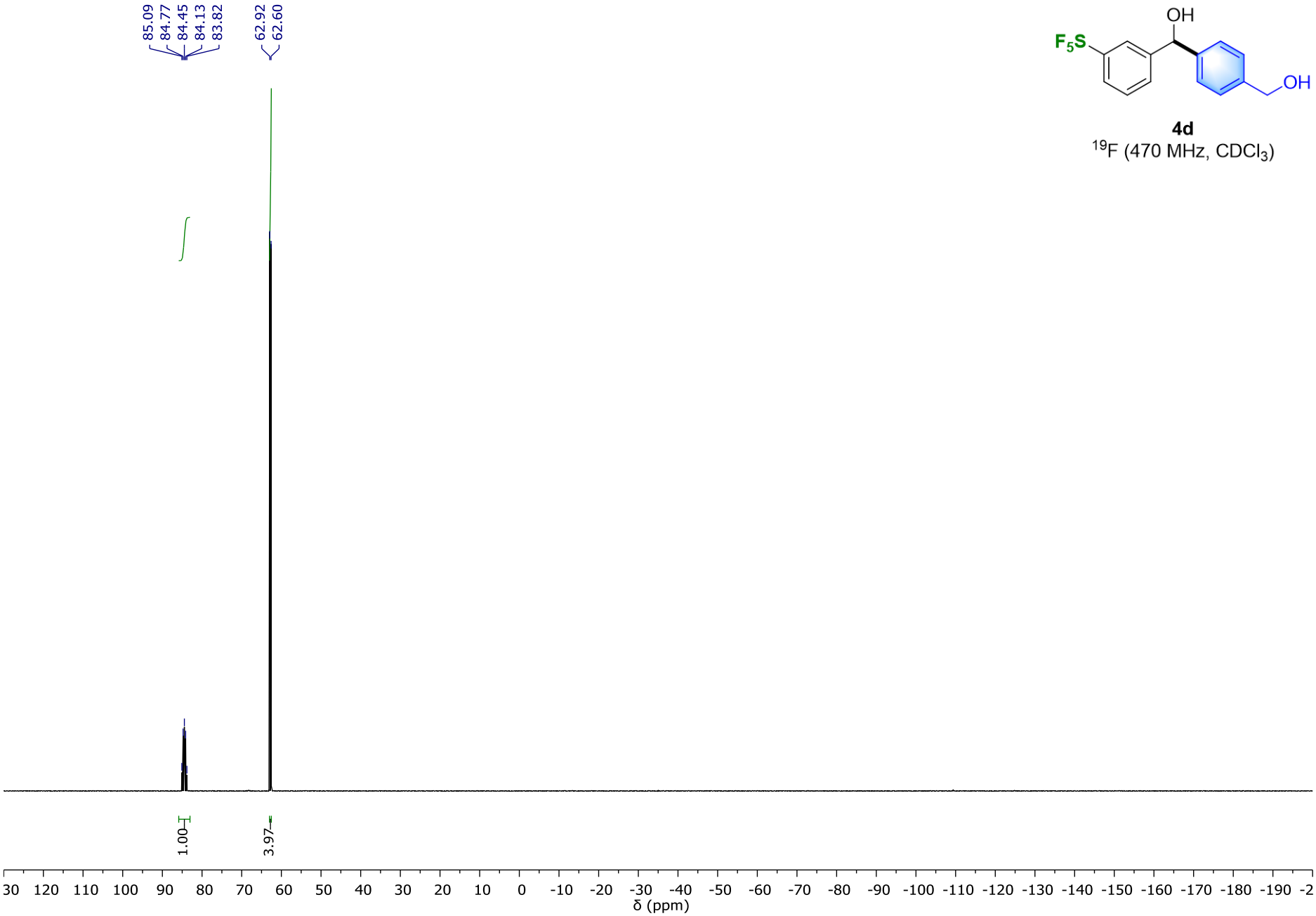
^{1}H (500 MHz, $CDCl_3$)

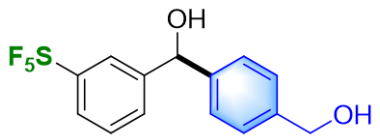
4c

^{19}F (470 MHz, $CDCl_3$)


OH
F5S
t-Bu
4c
13C (126 MHz, CDCl3)
154.51
154.38
154.24
154.11
153.97
151.45
145.10
140.08
129.74
128.83
126.57
125.93
125.07
125.03
124.99
124.96
124.92
124.00
123.96
123.92
123.88
123.85
77.41
77.16
76.91
75.57
34.72
31.42
δ (ppm)

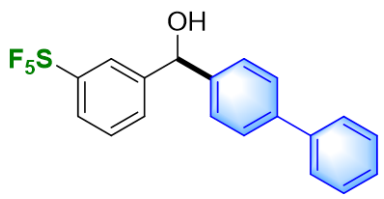

OH
F5S
OH
4d
1H (500 MHz, CDCl3)
7.86
7.86
7.85
7.66
7.66
7.66
7.66
7.65
7.64
7.64
7.64
7.48
7.47
7.43
7.41
7.39
7.36
7.26
5.88
4.69
2.40
CH2Cl2
H2O
1.03
1.00
1.05
1.09
4.14
1.01
2.06
0.86
δ (ppm)


85.09
84.77
84.45
84.13
83.82
62.92
62.60
OH
F5S
OH
4d
19F (470 MHz, CDCl3)
1.00
3.97
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



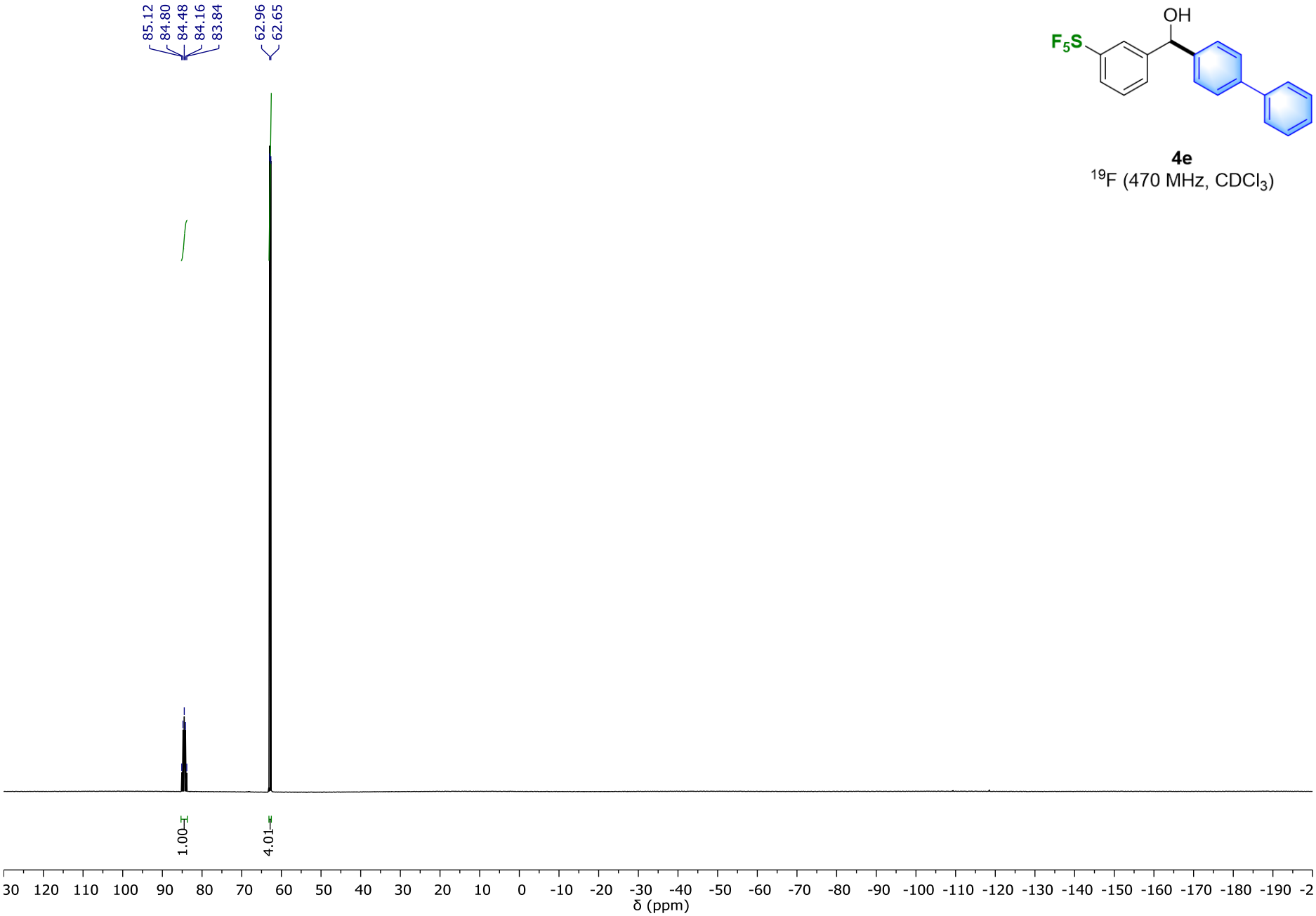
4d

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



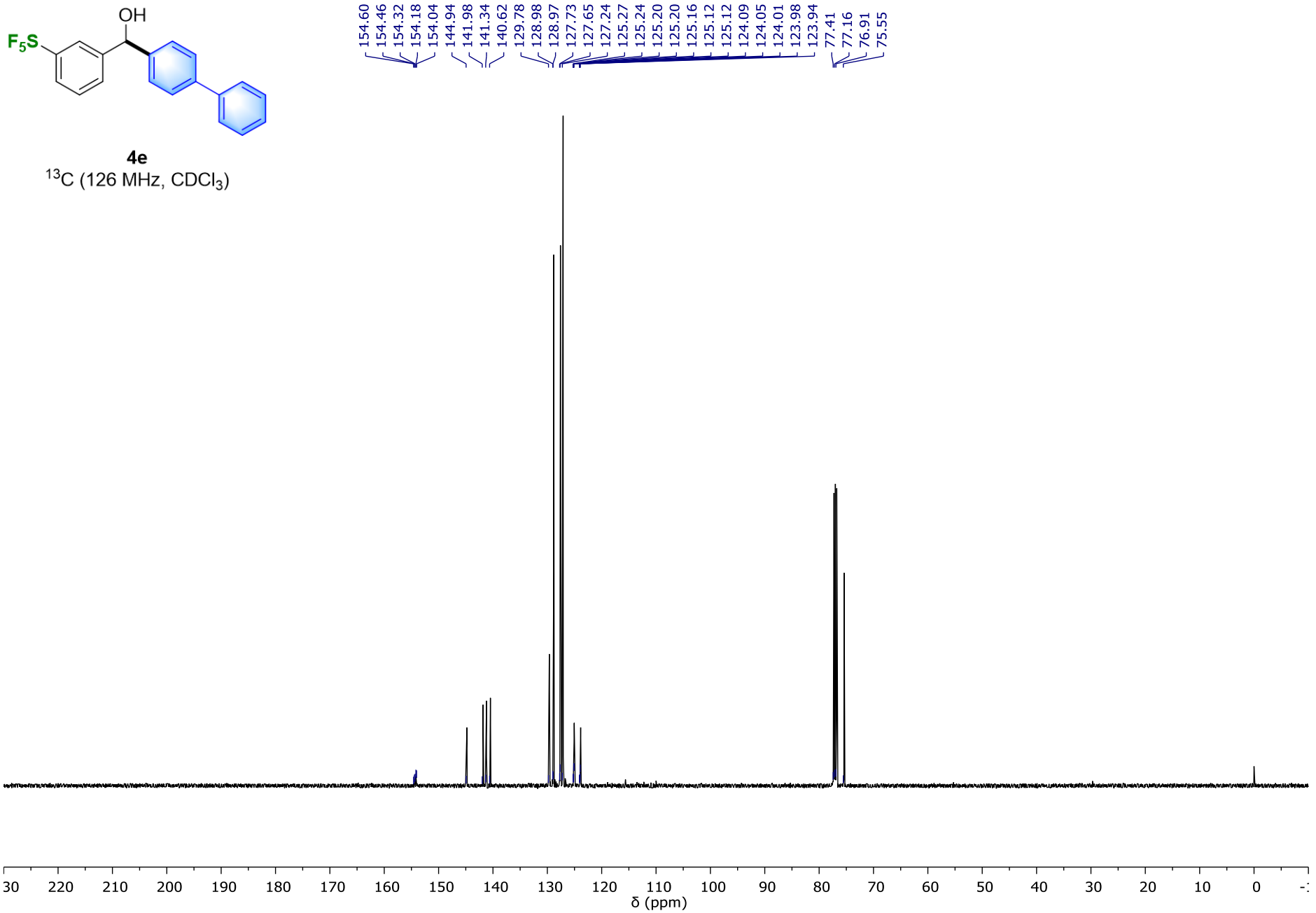
4e

^{1}H (500 MHz, $CDCl_3$)



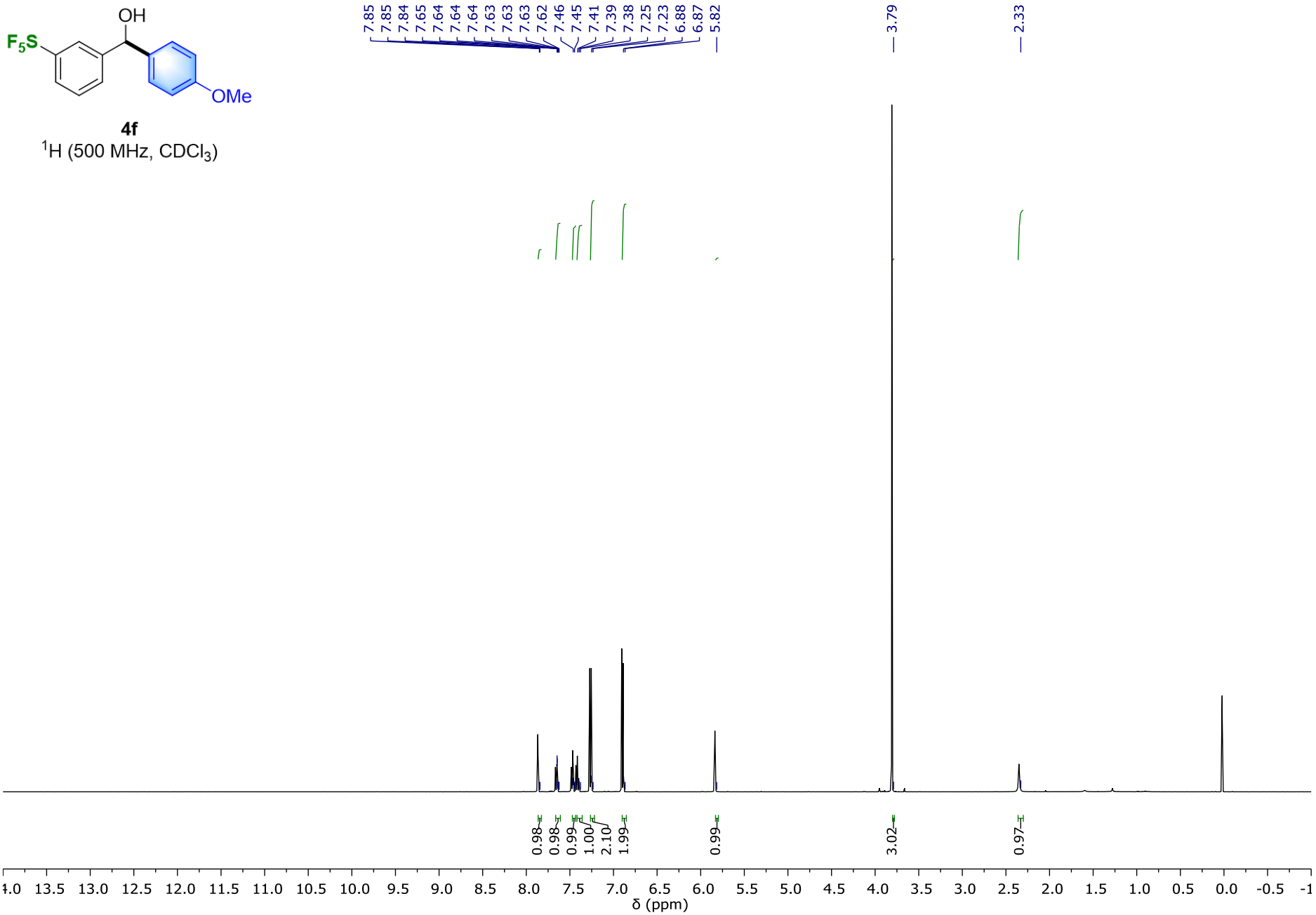
4e

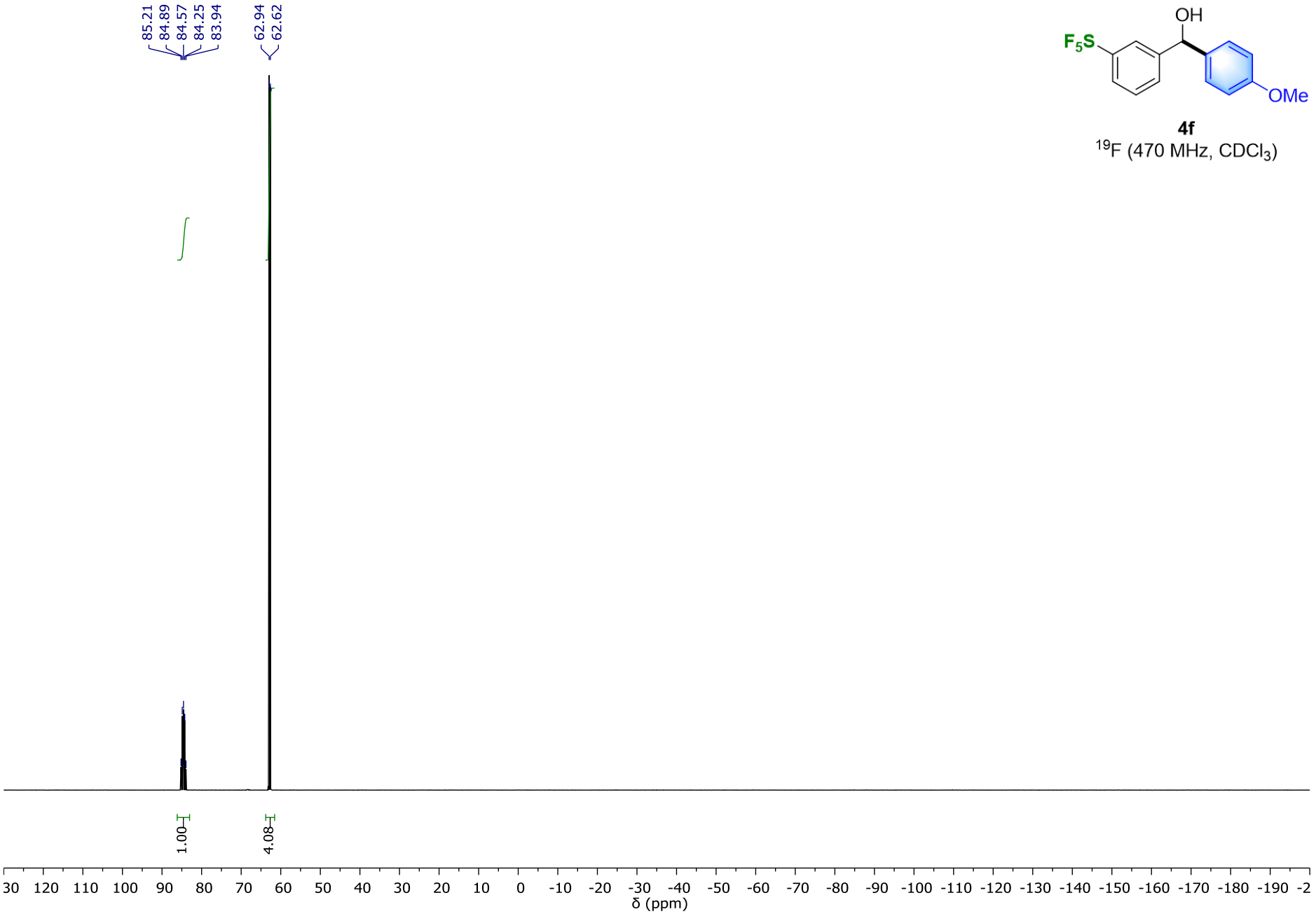
^{19}F (470 MHz, $CDCl_3$)

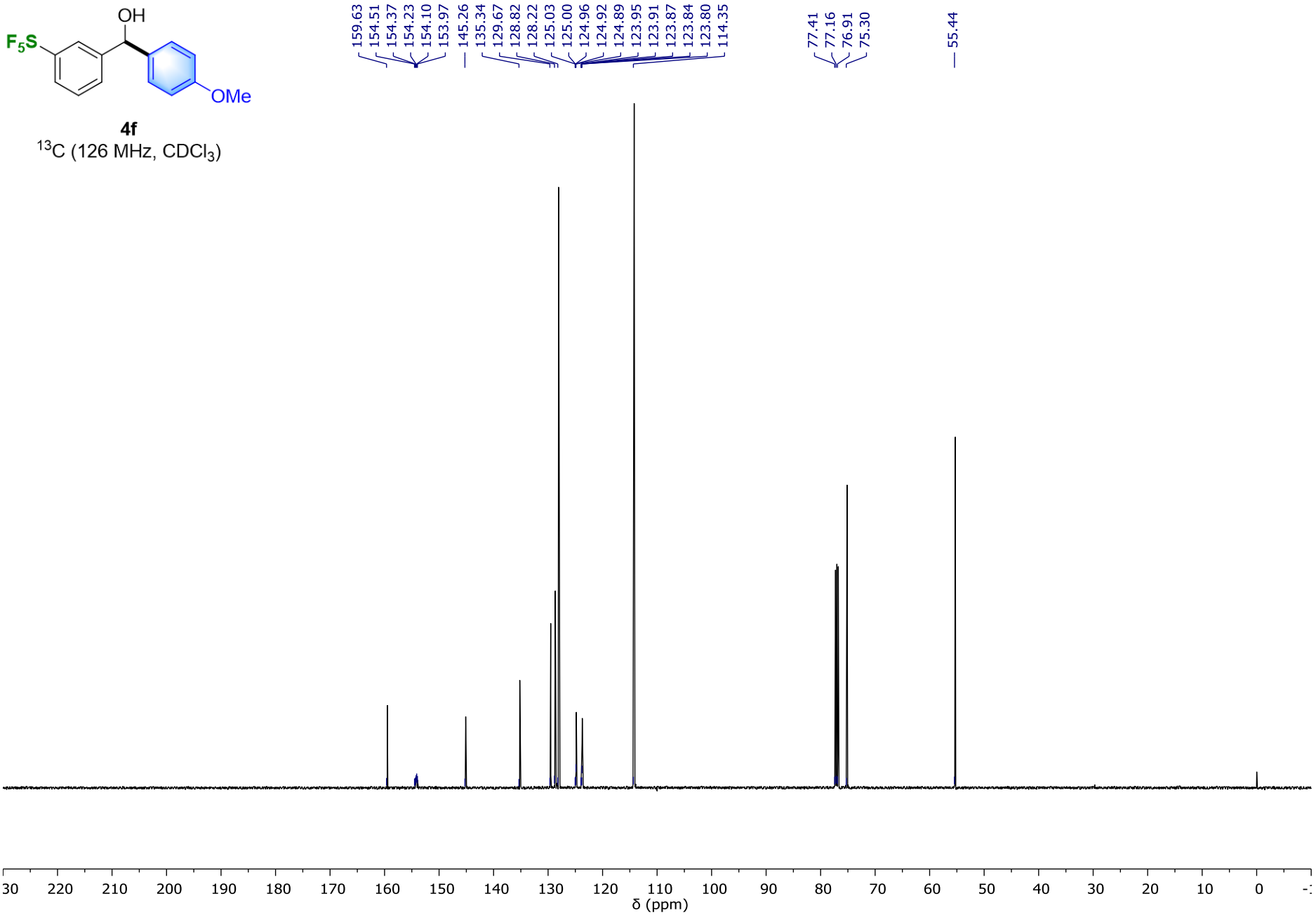


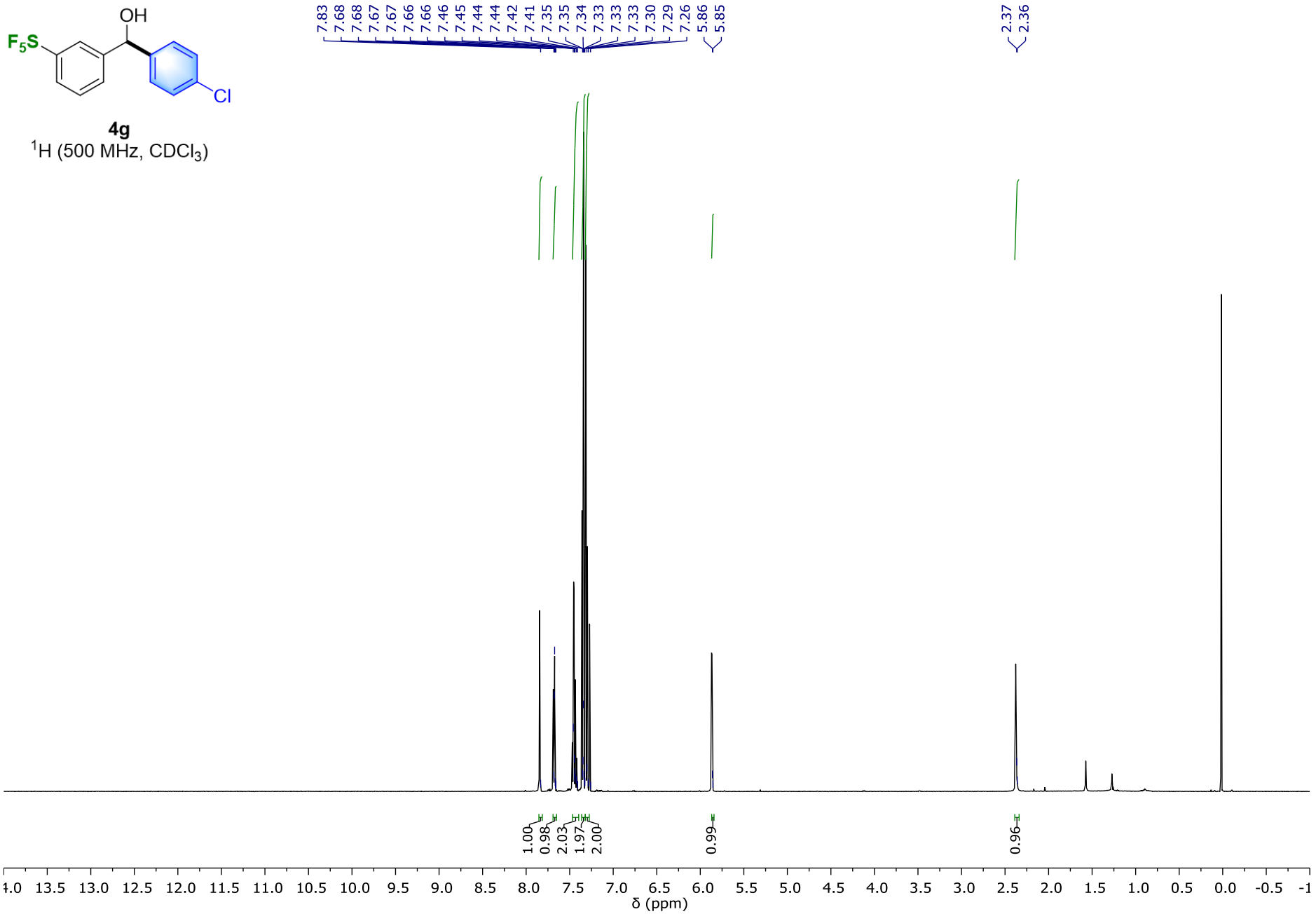
4e

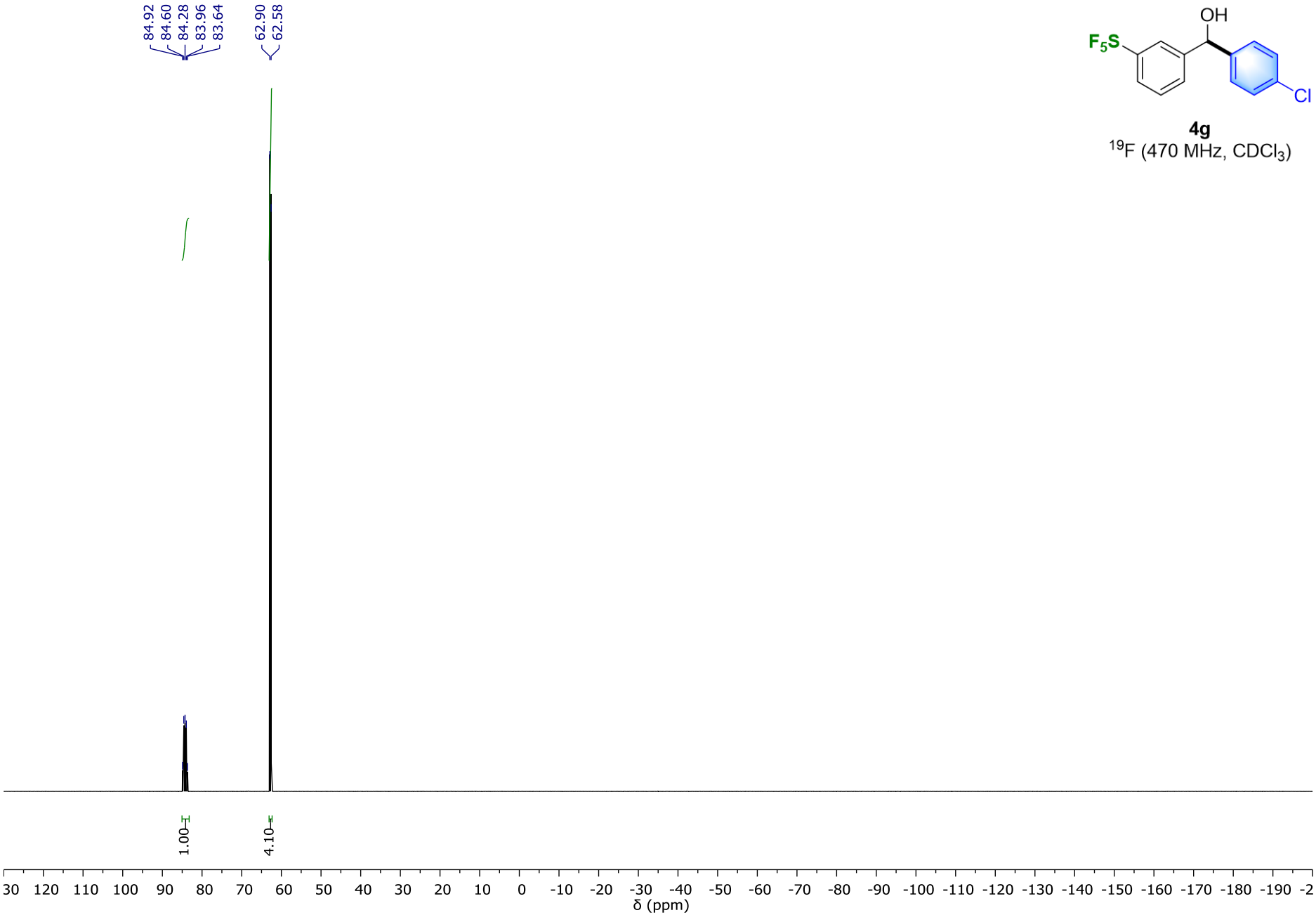
^{13}C (126 MHz, $CDCl_3$)

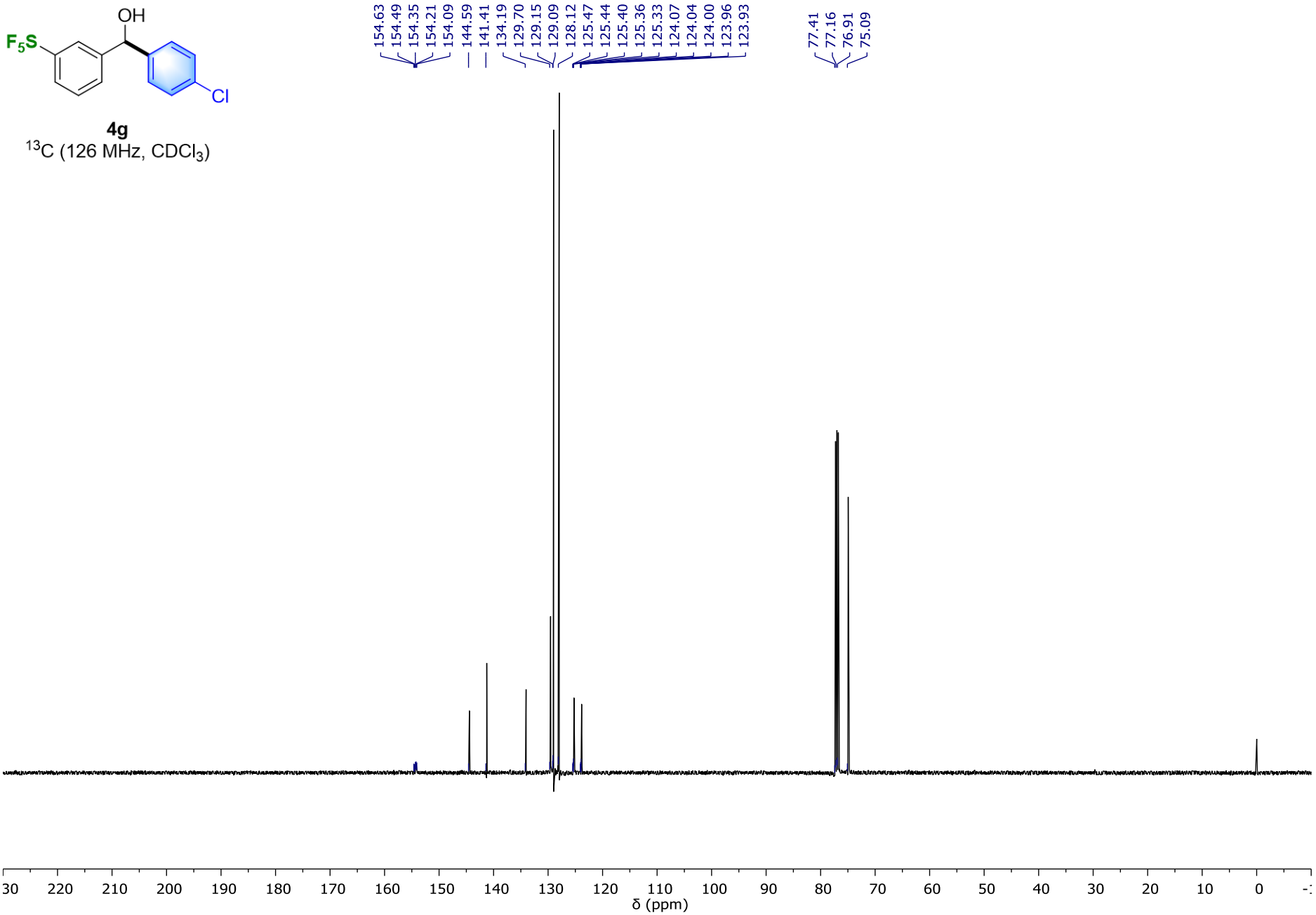

OH
F5S
OMe
4f
1H (500 MHz, CDCl3)
7.85
7.85
7.84
7.65
7.64
7.64
7.64
7.63
7.63
7.63
7.62
7.46
7.45
7.41
7.39
7.38
7.25
7.23
6.88
6.87
5.82
3.79
2.33
0.98
0.98
0.99
1.00
2.10
1.99
0.99
3.02
0.97
δ (ppm)

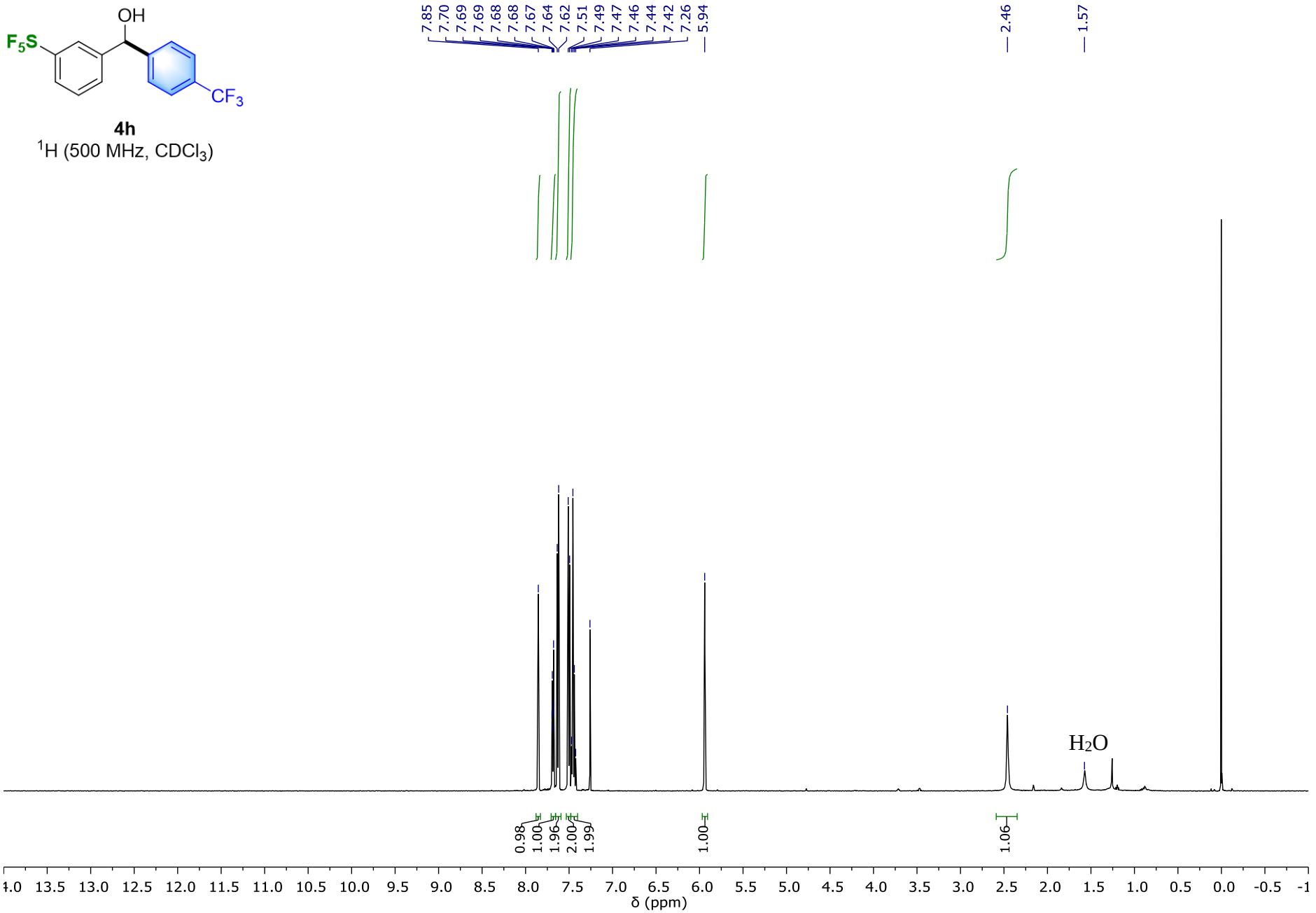

85.21
84.89
84.57
84.25
83.94
62.94
62.62
OH
F5S
OMe
4f
19F (470 MHz, CDCl3)
1.00
4.08
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

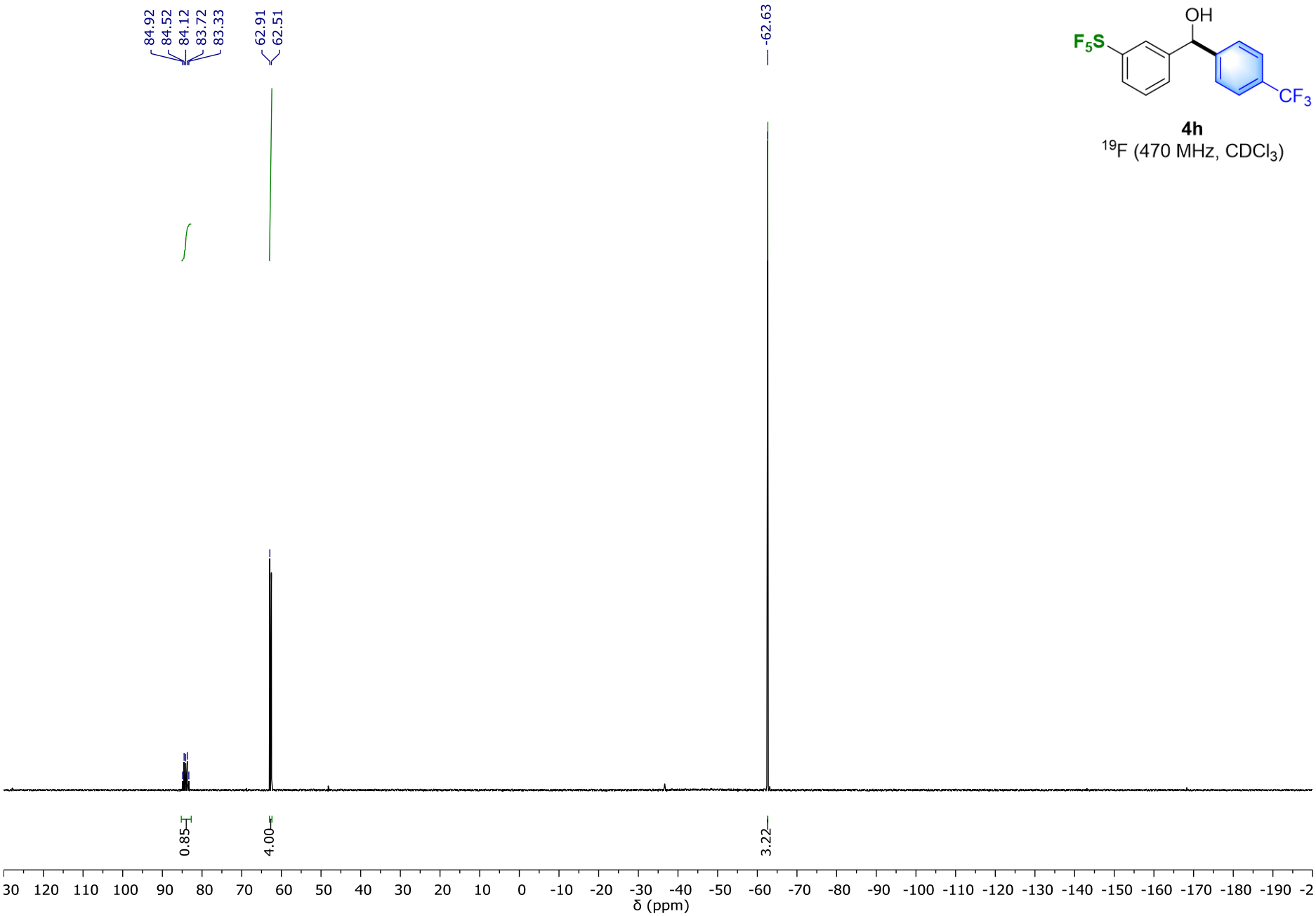

OH
F5S
OMe
4f
13C (126 MHz, CDCl3)
159.63
154.51
154.37
154.23
154.10
153.97
145.26
135.34
129.67
128.82
128.22
125.03
125.00
124.96
124.92
124.89
123.95
123.91
123.87
123.84
123.80
114.35
77.41
77.16
76.91
75.30
55.44
δ (ppm)

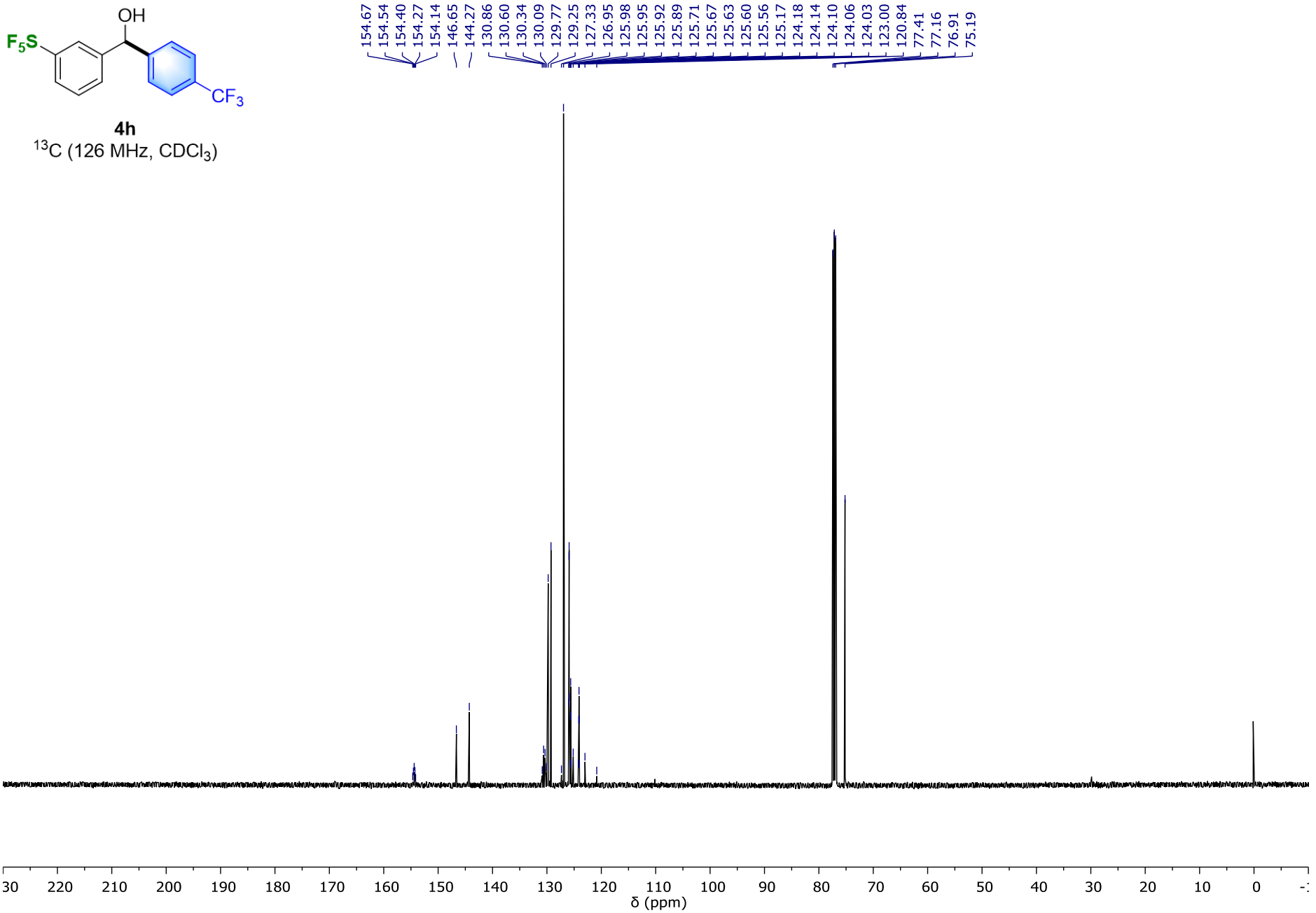

OH
F5S
Cl
4g
1H (500 MHz, CDCl3)
7.83
7.68
7.68
7.67
7.67
7.66
7.66
7.46
7.45
7.44
7.44
7.42
7.41
7.35
7.35
7.34
7.33
7.33
7.33
7.30
7.29
7.26
5.86
5.85
2.37
2.36
1.00
0.98
2.03
1.97
2.00
0.99
0.96
δ (ppm)

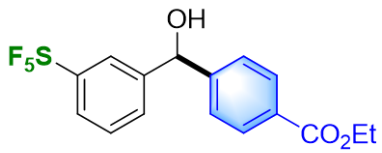

84.92
84.60
84.28
83.96
83.64
62.90
62.58
OH
F5S
Cl
4g
19F (470 MHz, CDCl3)
1.00
4.10
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)


OH
F5S
Cl
4g
13C (126 MHz, CDCl3)
154.63
154.49
154.35
154.21
154.09
144.59
141.41
134.19
129.70
129.15
129.09
128.12
125.47
125.44
125.40
125.36
125.33
124.07
124.04
124.00
123.96
123.93
77.41
77.16
76.91
75.09
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)


OH
F5S
CF3
4h
1H (500 MHz, CDCl3)
7.85
7.70
7.69
7.69
7.68
7.68
7.67
7.64
7.62
7.51
7.49
7.47
7.46
7.44
7.42
7.26
5.94
2.46
1.57
H2O
0.98
1.00
1.96
2.00
1.99
1.00
1.06
δ (ppm)

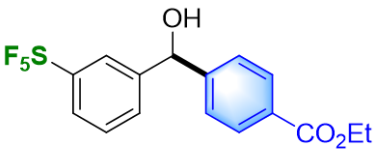

84.92
84.52
84.12
83.72
83.33
62.91
62.51
-62.63
OH
F5S
CF3
4h
19F (470 MHz, CDCl3)
0.85
4.00
3.22
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)


OH
F5S
CF3
4h
13C (126 MHz, CDCl3)
154.67
154.54
154.40
154.27
154.14
146.65
144.27
130.86
130.60
130.34
130.09
129.77
129.25
127.33
126.95
125.98
125.95
125.92
125.89
125.71
125.67
125.63
125.60
125.56
125.17
124.18
124.14
124.10
124.06
124.03
123.00
120.84
77.41
77.16
76.91
75.19
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)



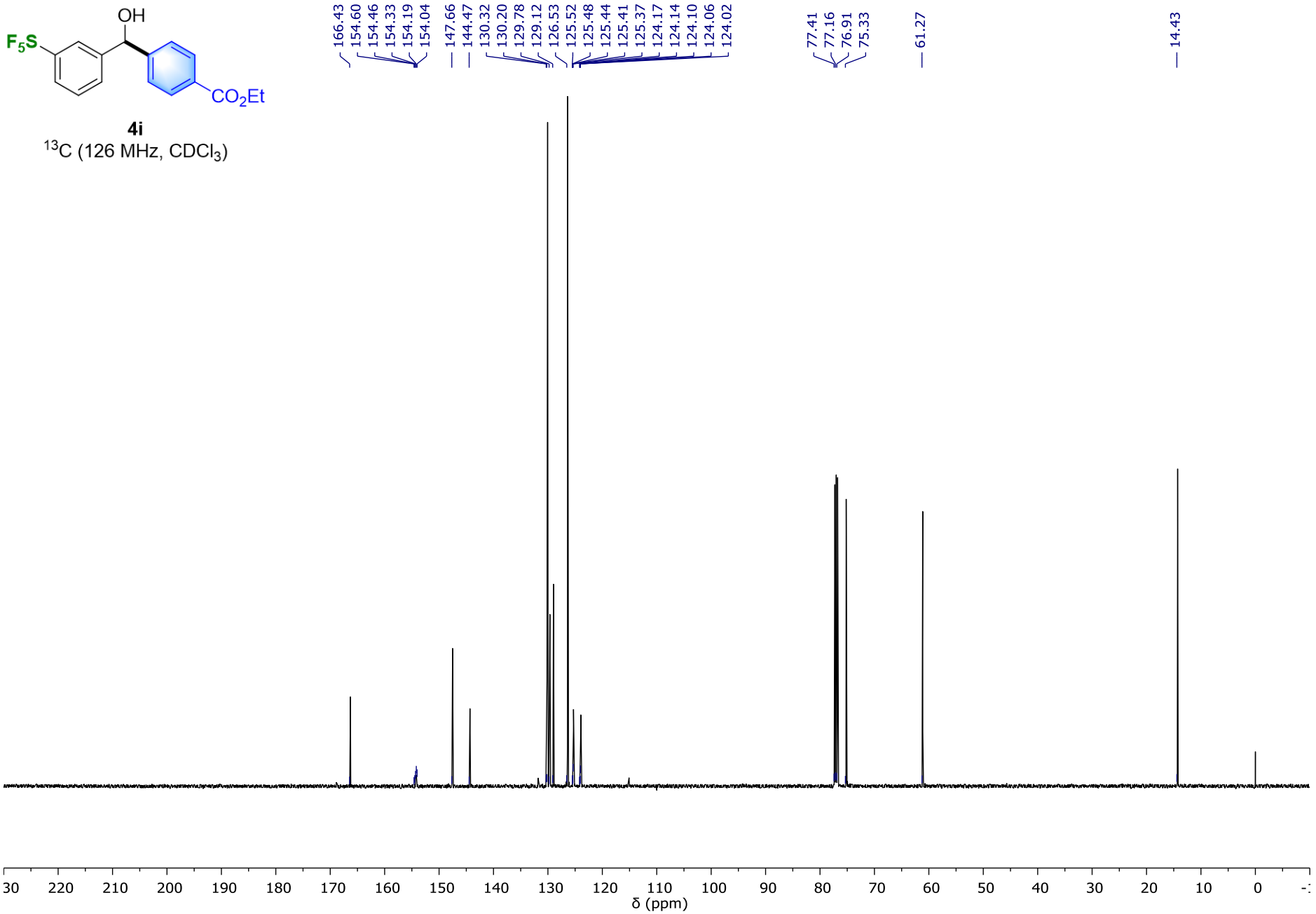
4i

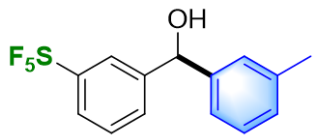
^{1}H (500 MHz, $CDCl_3$)



4i

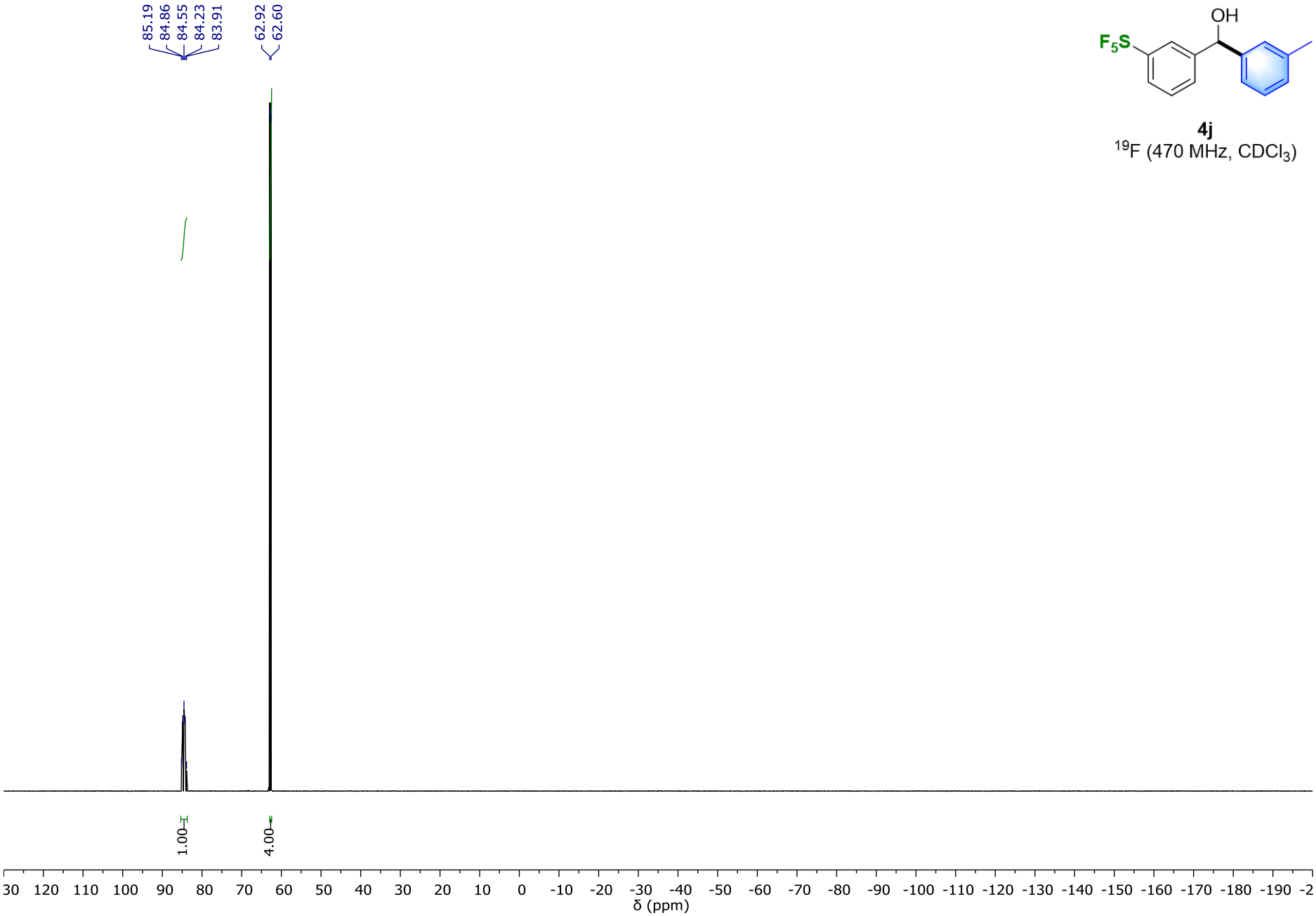
^{19}F (470 MHz, $CDCl_3$)

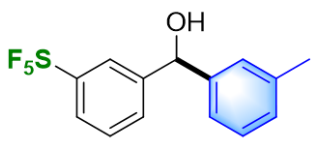

OH
F5S
CO2Et
4i
13C (126 MHz, CDCl3)
166.43
154.60
154.46
154.33
154.19
154.04
147.66
144.47
130.32
130.20
129.78
129.12
126.53
125.52
125.48
125.44
125.41
125.37
124.17
124.14
124.10
124.06
124.02
77.41
77.16
76.91
75.33
61.27
14.43
δ (ppm)



4j

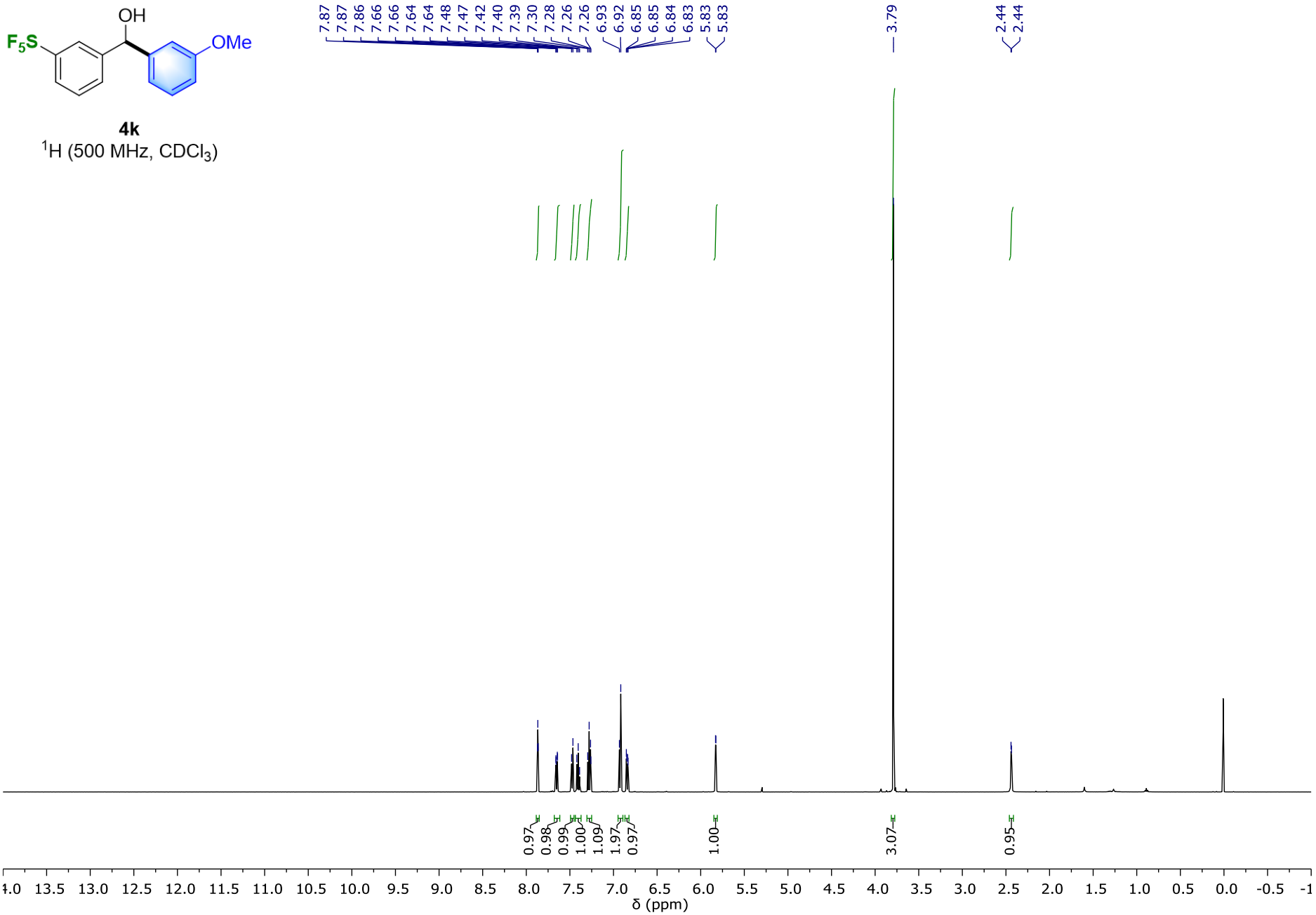
^{1}H (500 MHz, $CDCl_3$)

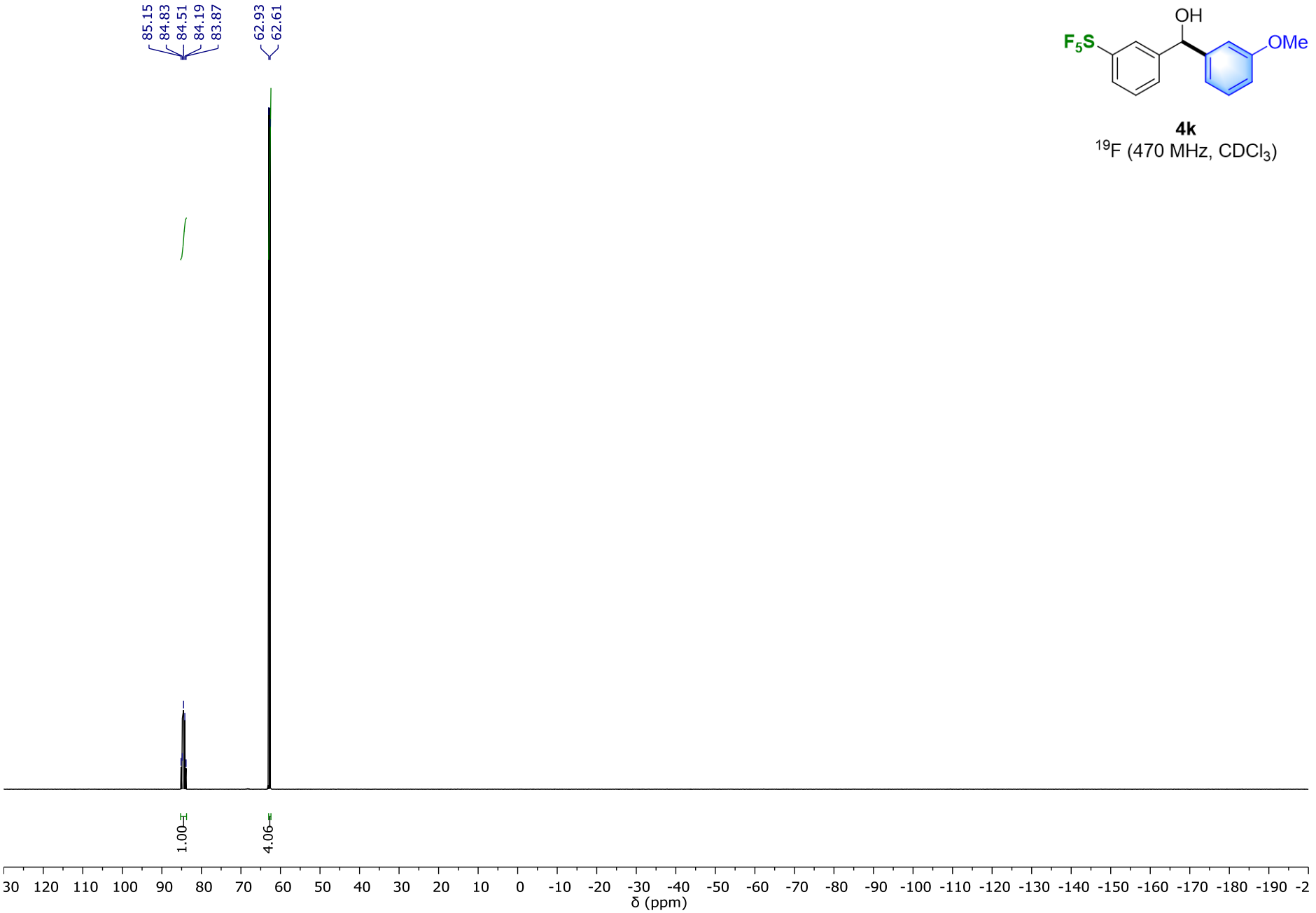

85.19
84.86
84.55
84.23
83.91
62.92
62.60
OH
F5S
4j
19F (470 MHz, CDCl3)
1.00
4.00
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

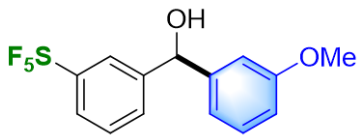


4j

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

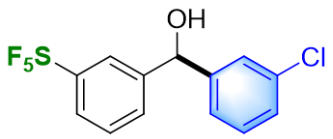

OH
F5S
OMe
4k
1H (500 MHz, CDCl3)
7.87
7.87
7.86
7.66
7.66
7.64
7.64
7.48
7.47
7.42
7.40
7.39
7.30
7.28
7.26
7.26
6.93
6.92
6.85
6.85
6.84
6.83
5.83
5.83
3.79
2.44
2.44
0.97
0.98
0.99
1.00
1.09
1.97
0.97
1.00
3.07
0.95
δ (ppm)


85.15
84.83
84.51
84.19
83.87
62.93
62.61
OH
F5S
OMe
4k
19F (470 MHz, CDCl3)
1.00
4.06
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



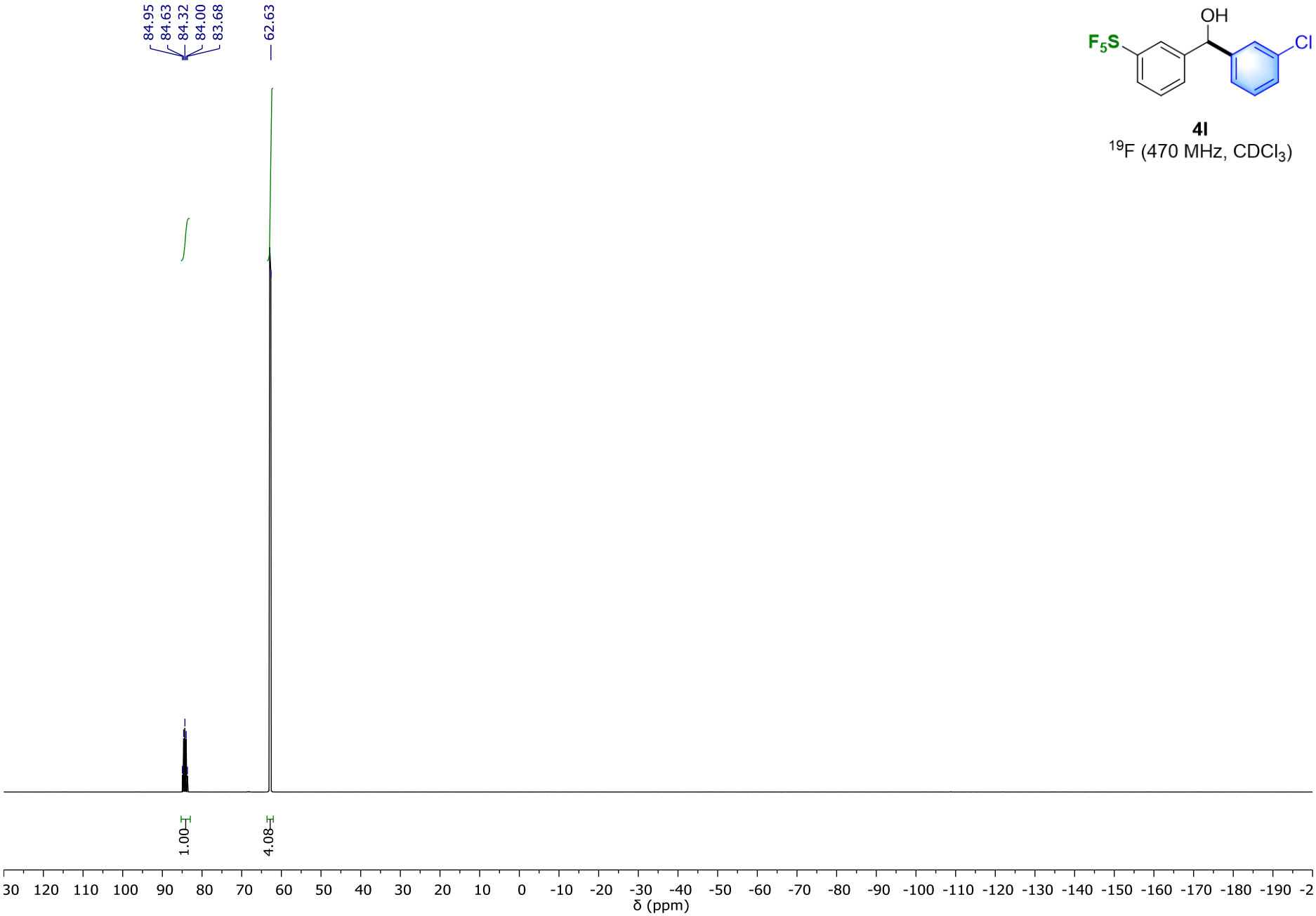
4k

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



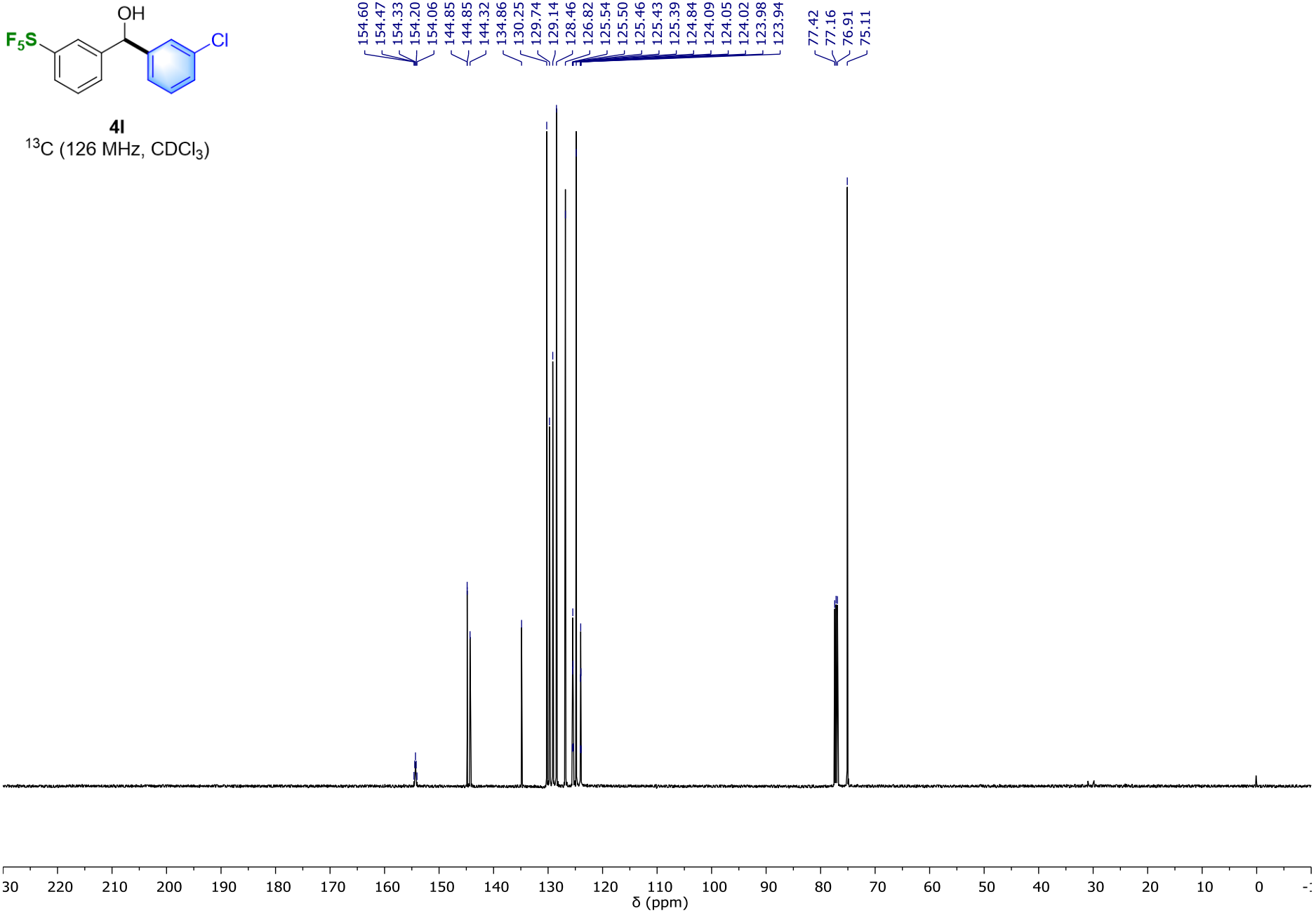
4l

^{1}H (500 MHz, $CDCl_3$)



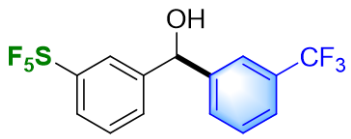
4l

^{19}F (470 MHz, $CDCl_3$)



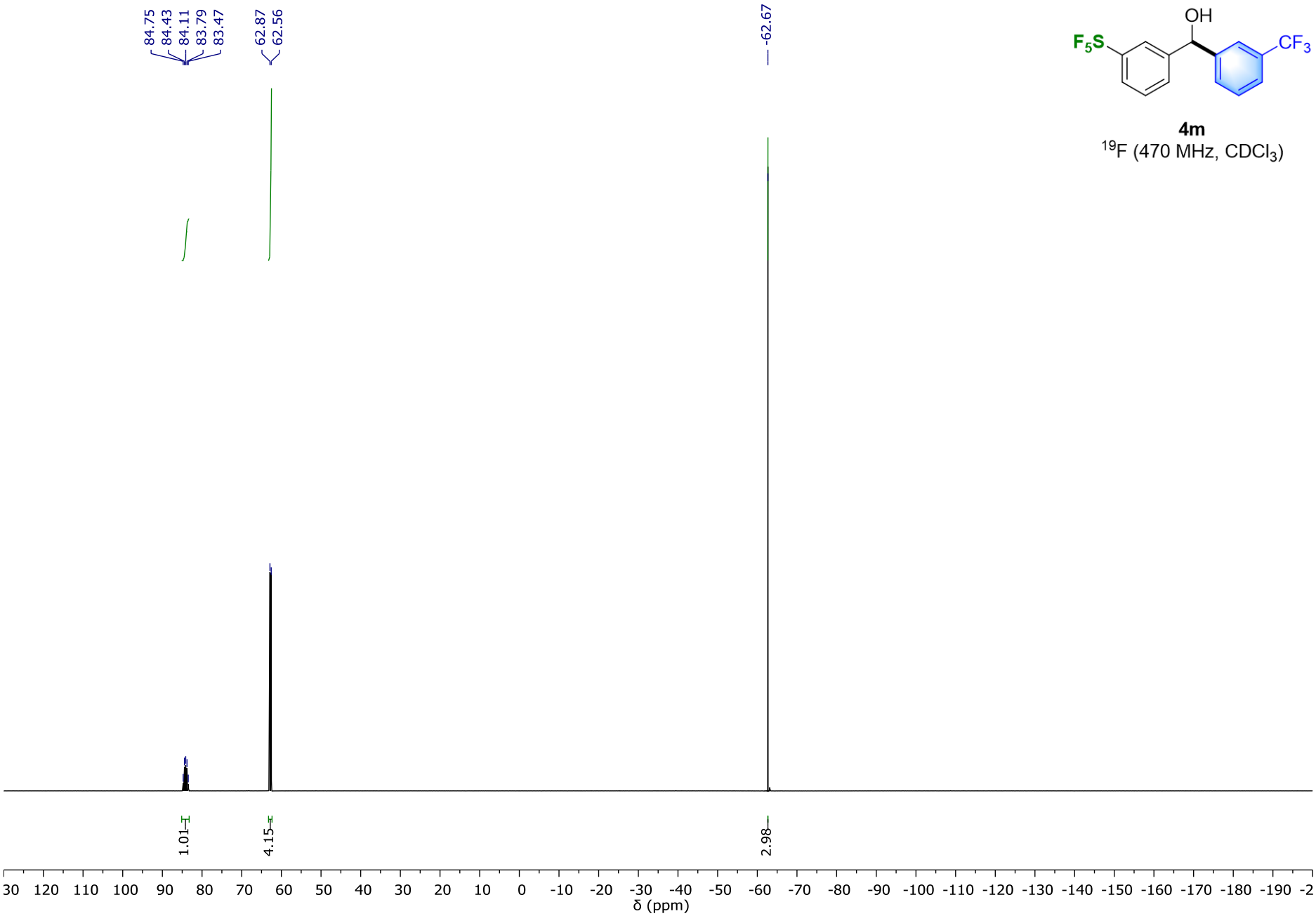
4l

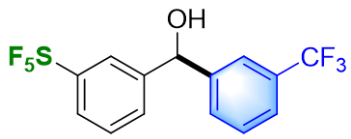
^{13}C (126 MHz, $CDCl_3$)



4m

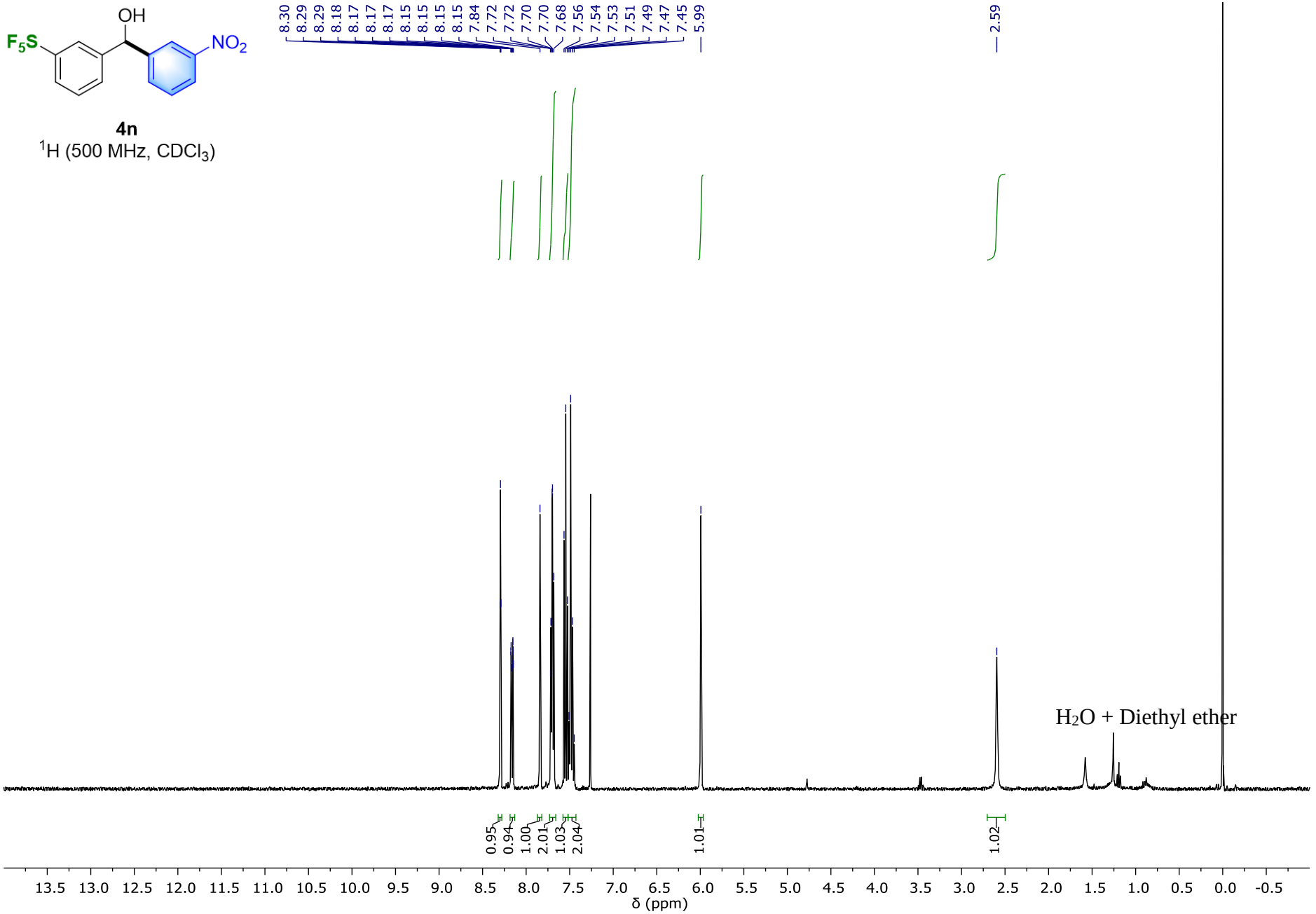
^{1}H (500 MHz, $CDCl_3$)

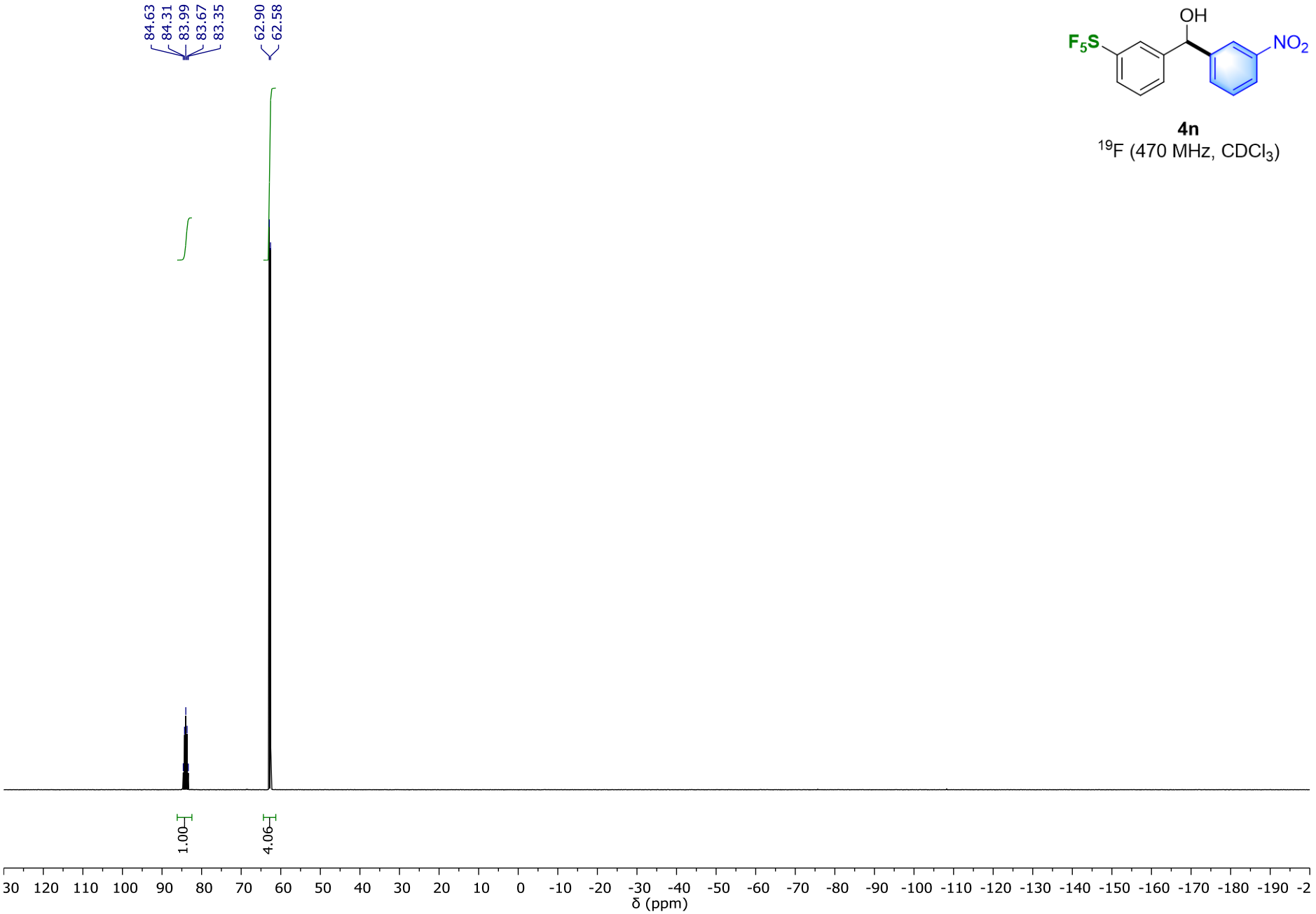

84.75
84.43
84.11
83.79
83.47
62.87
62.56
-62.67
OH
F5S
CF3
4m
19F (470 MHz, CDCl3)
1.01
4.15
2.98
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

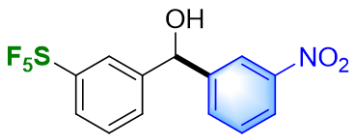


4m

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


OH
F5S
NO2
4n
1H (500 MHz, CDCl3)
8.30
8.29
8.29
8.18
8.17
8.17
8.17
8.15
8.15
8.15
8.15
7.84
7.72
7.72
7.70
7.70
7.68
7.56
7.54
7.53
7.51
7.49
7.47
7.45
5.99
2.59
H2O + Diethyl ether
0.95
0.94
1.00
2.01
1.03
2.04
1.01
1.02
δ (ppm)

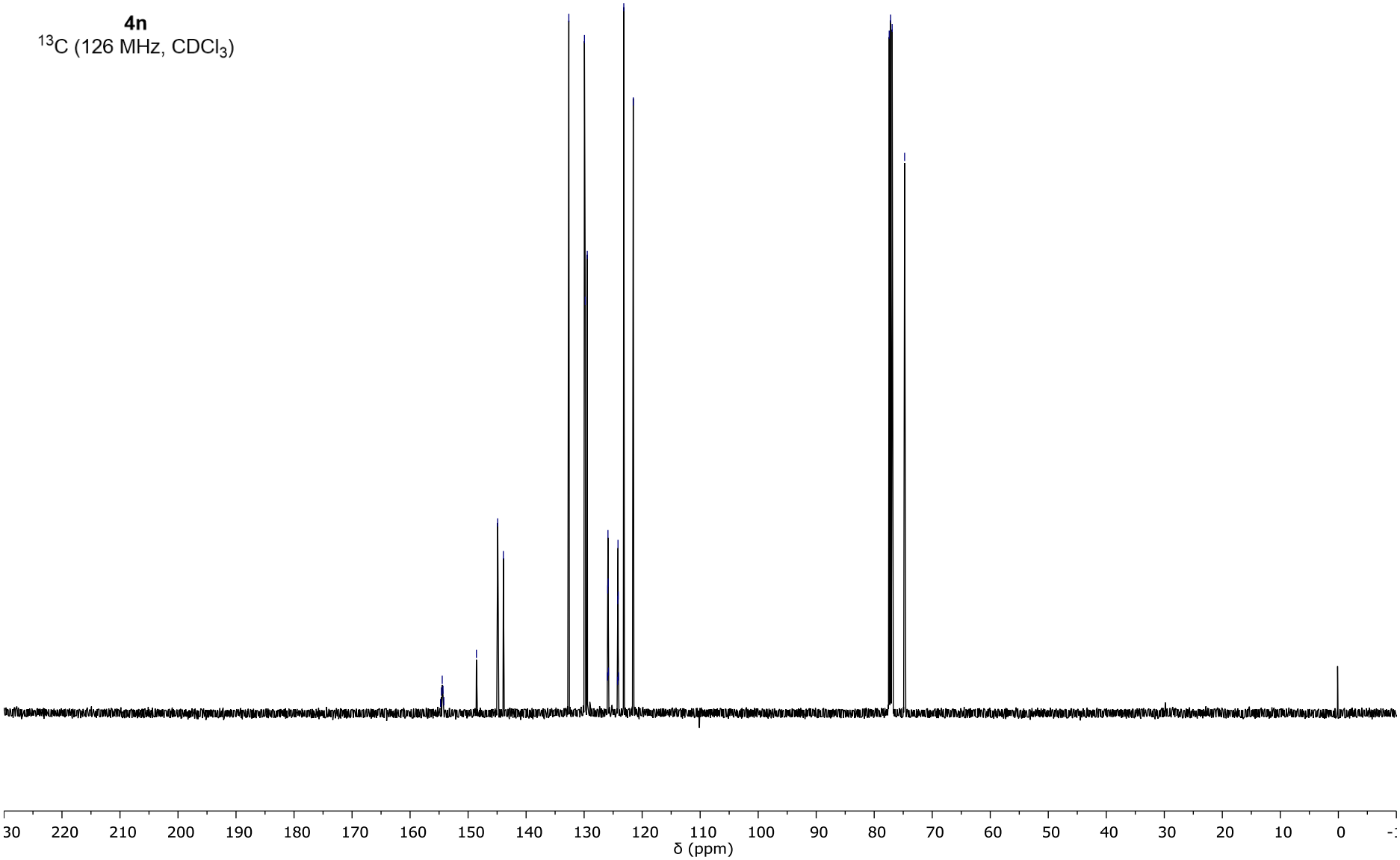

84.63
84.31
83.99
83.67
83.35
62.90
62.58
OH
F5S
NO2
4n
19F (470 MHz, CDCl3)
1.00
4.06
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

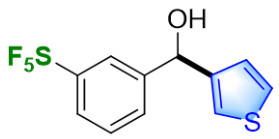


4n

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

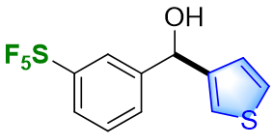
154.75
154.59
154.46
154.32
154.18
148.57
144.90
143.92
132.64
129.95
129.80
129.46
125.96
125.93
125.89
125.85
125.82
124.23
124.20
124.16
124.13
124.09
123.17
121.53
77.41
77.16
76.91
74.76





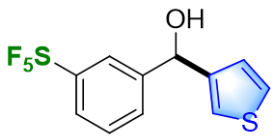
4o

^{1}H (500 MHz, $CDCl_3$)



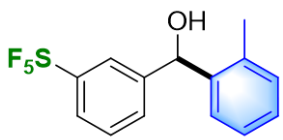
4o

^{19}F (470 MHz, $CDCl_3$)



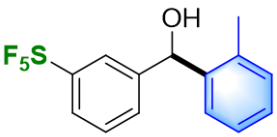
4o

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



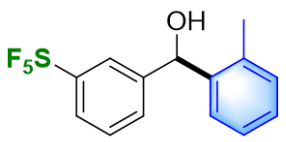
4p

^{1}H (500 MHz, $CDCl_3$)



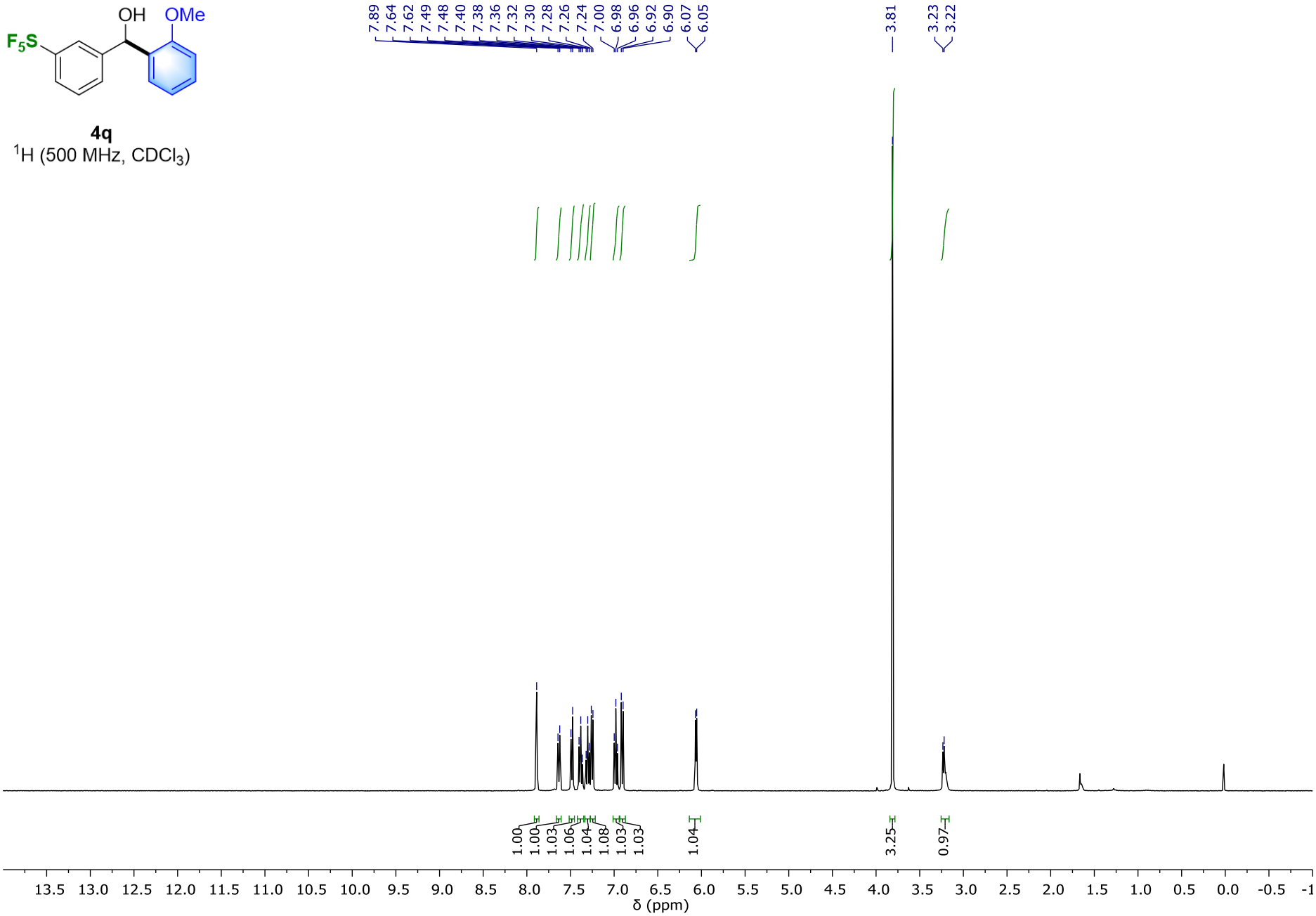
4p

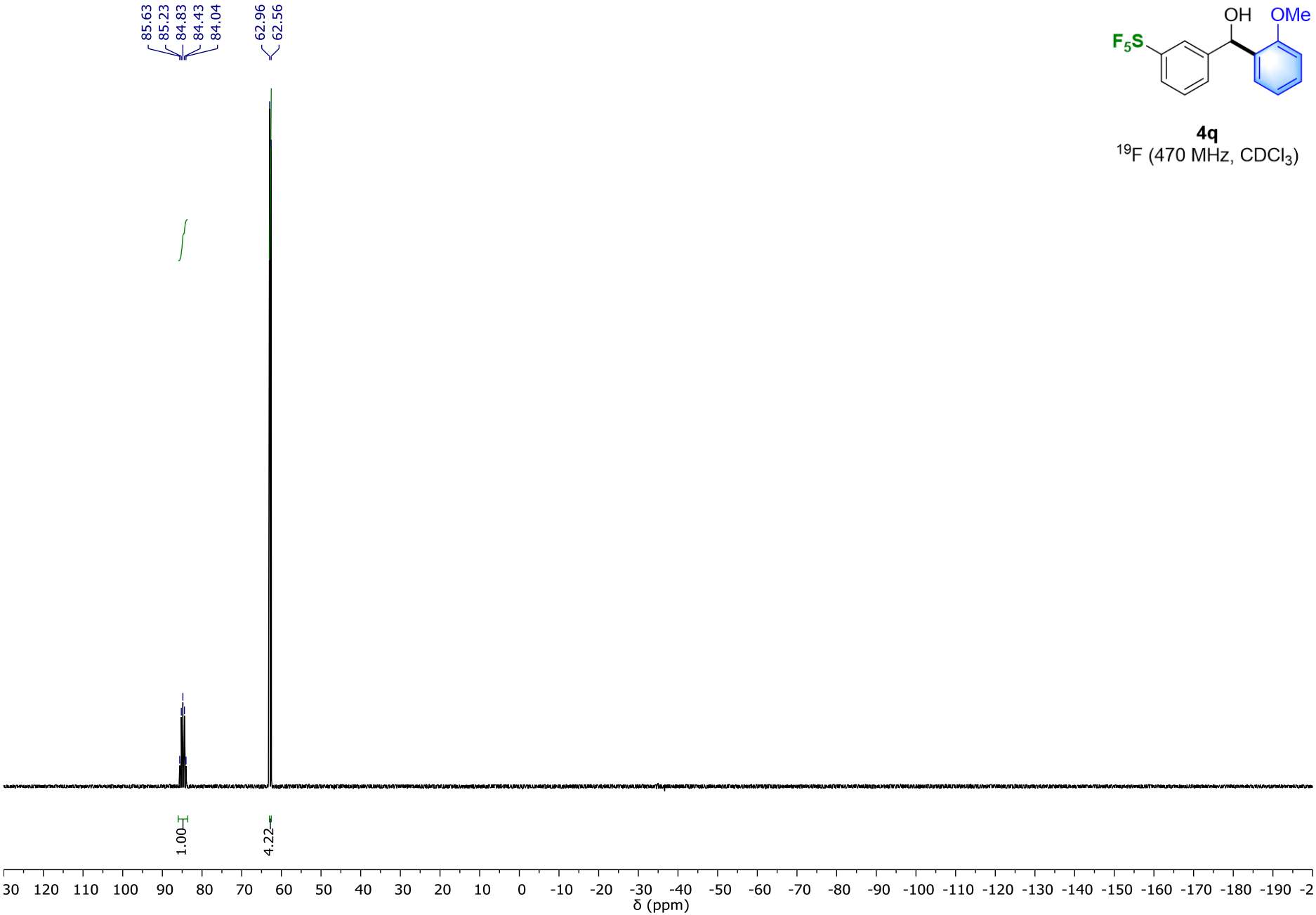
^{19}F (470 MHz, $CDCl_3$)

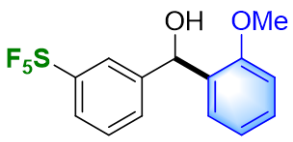


4p

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

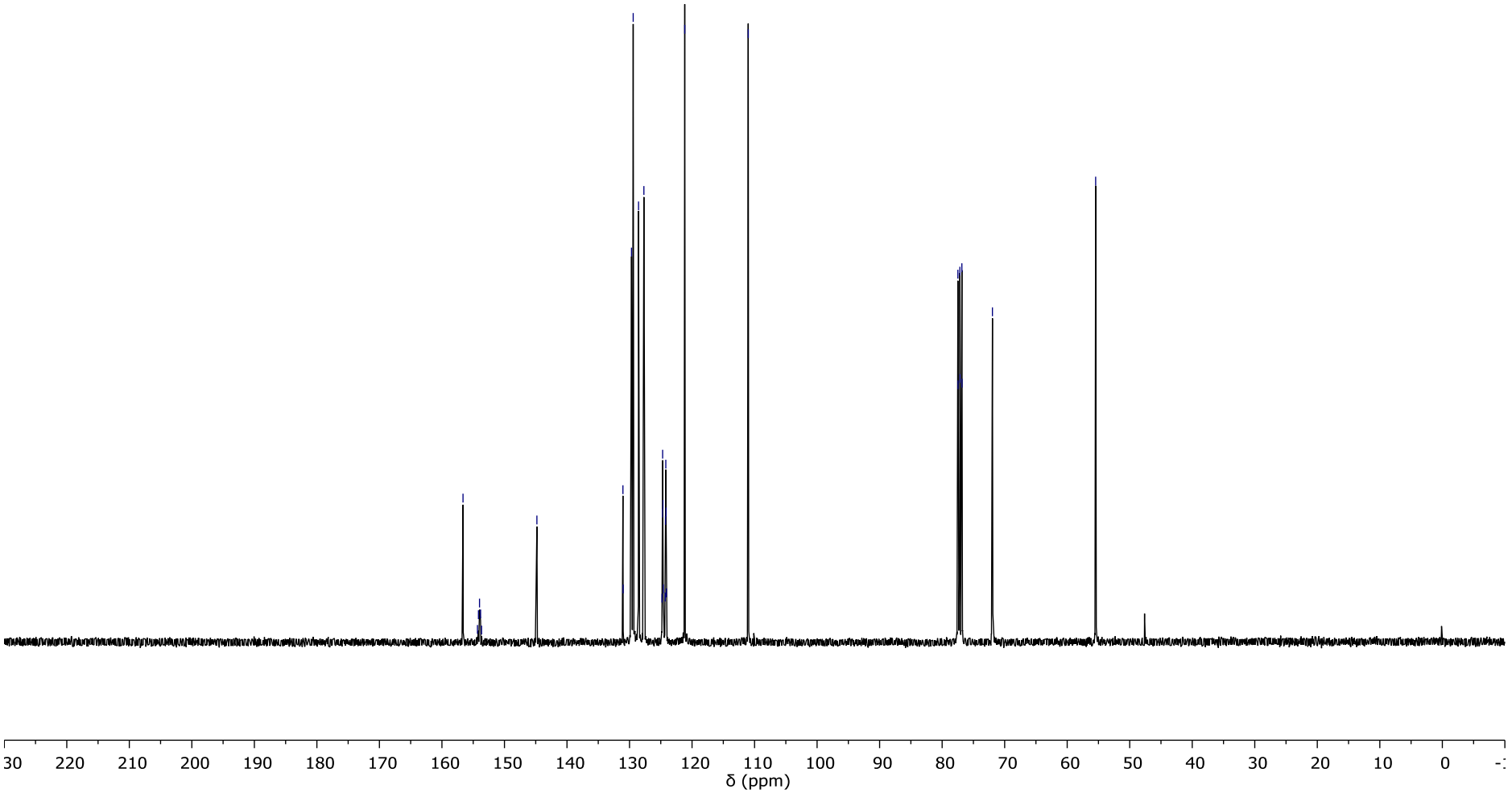

OH
OMe
F5S
4q
1H (500 MHz, CDCl3)
7.89
7.64
7.62
7.49
7.48
7.40
7.38
7.36
7.32
7.30
7.28
7.26
7.24
7.00
6.98
6.96
6.92
6.90
6.07
6.05
3.81
3.23
3.22
1.00
1.00
1.03
1.06
1.04
1.08
1.03
1.03
1.04
3.25
0.97
δ (ppm)

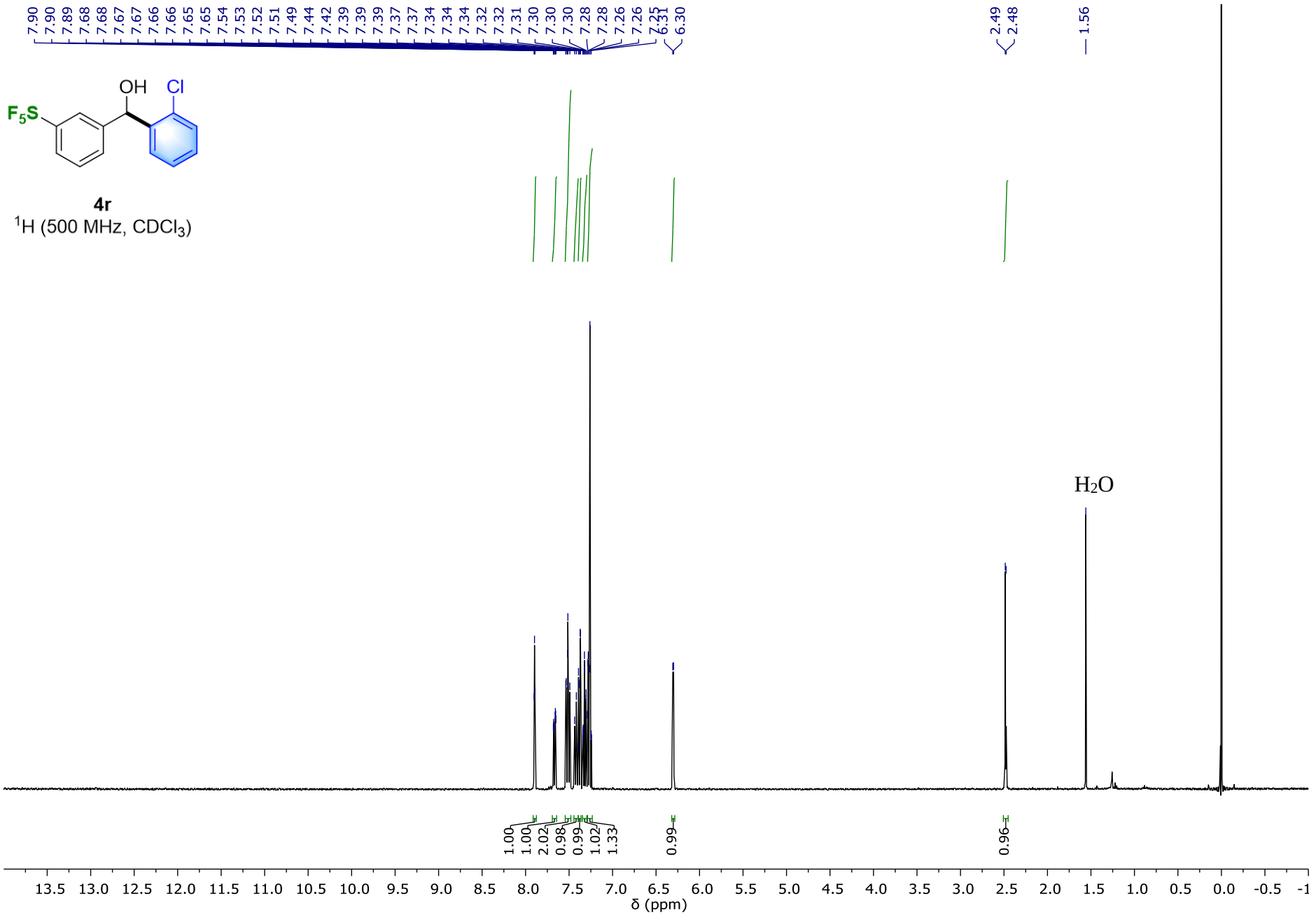

85.63
85.23
84.83
84.43
84.04
62.96
62.56
OH
OMe
F5S
4q
19F (470 MHz, CDCl3)
1.00
4.22
30 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)

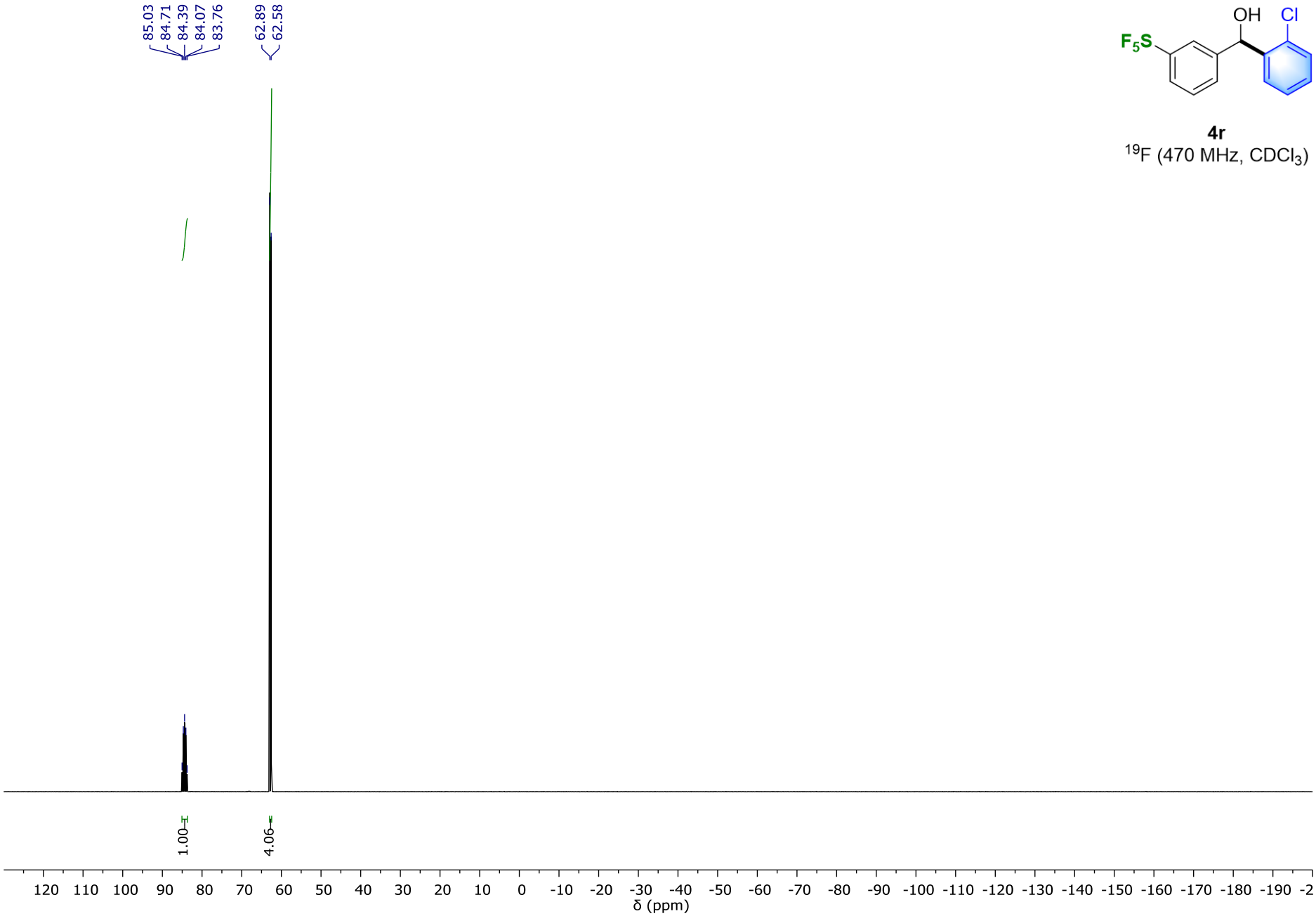


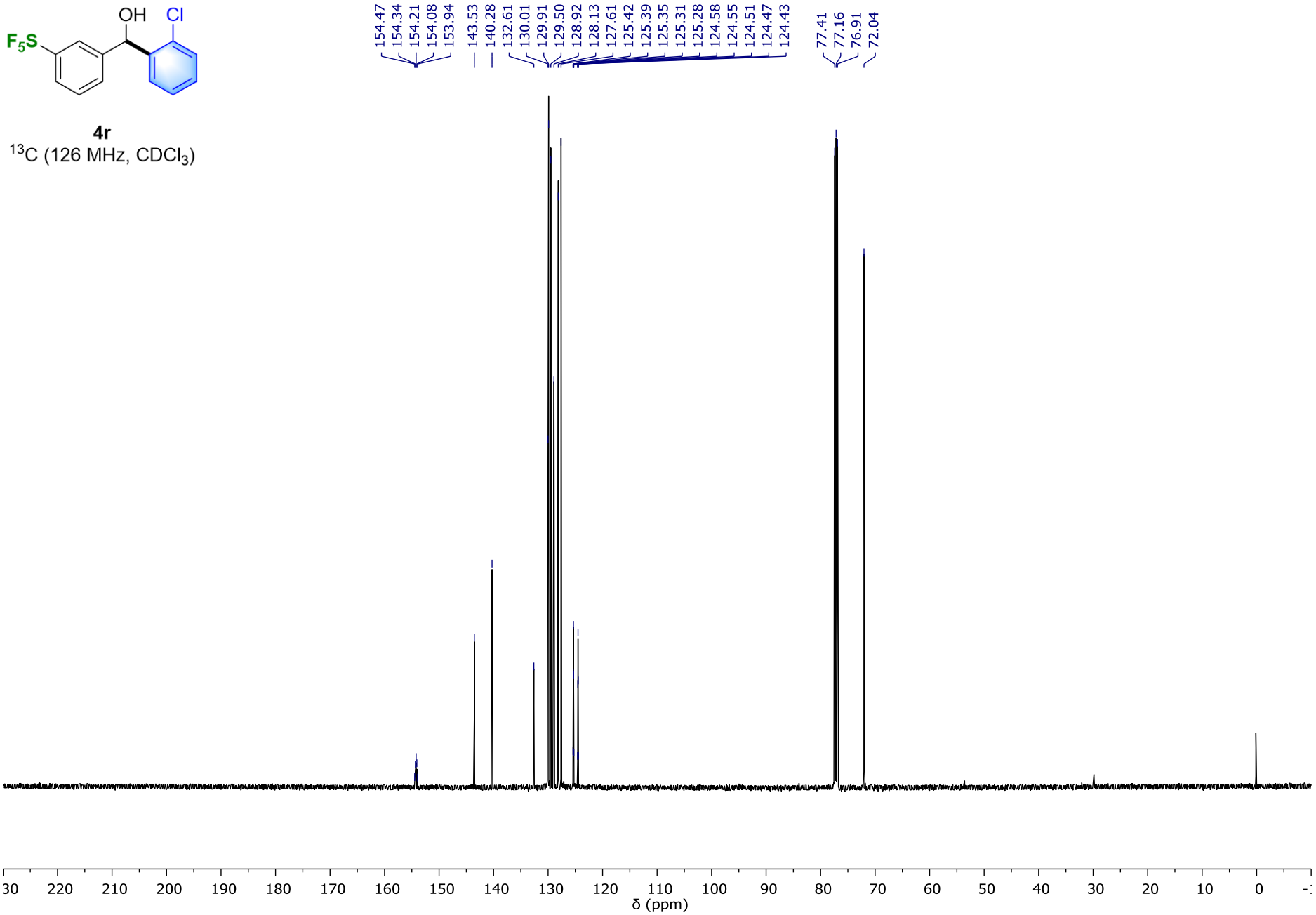
4q

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



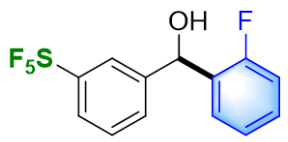

7.90
7.90
7.89
7.68
7.68
7.67
7.67
7.66
7.66
7.65
7.65
7.54
7.53
7.52
7.51
7.49
7.44
7.42
7.39
7.39
7.39
7.37
7.37
7.34
7.34
7.34
7.32
7.32
7.31
7.30
7.30
7.30
7.28
7.28
7.26
7.25
6.31
6.30
2.49
2.48
1.56
OH
Cl
F5S
4r
1H (500 MHz, CDCl3)
H2O
1.00
1.00
2.02
0.98
0.99
1.02
1.33
0.99
0.96
13.5 13.0 12.5 12.0 11.5 11.0 10.5 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 -0.5 -1
δ (ppm)


85.03
84.71
84.39
84.07
83.76
62.89
62.58
OH
Cl
F5S
4r
19F (470 MHz, CDCl3)
1.00
4.06
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
δ (ppm)



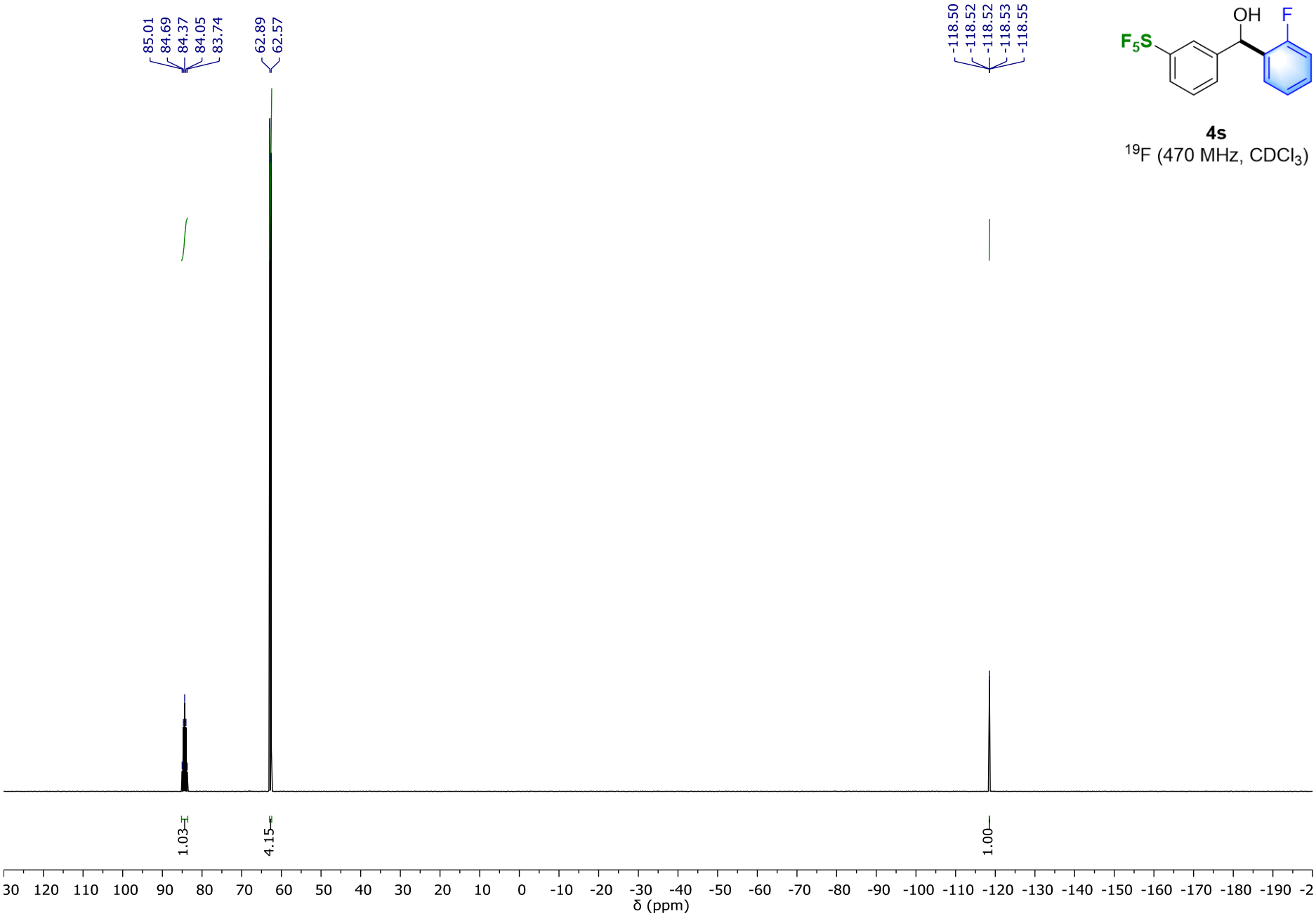
4r

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



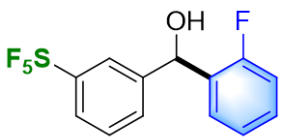
4s

^{1}H (500 MHz, $CDCl_3$)



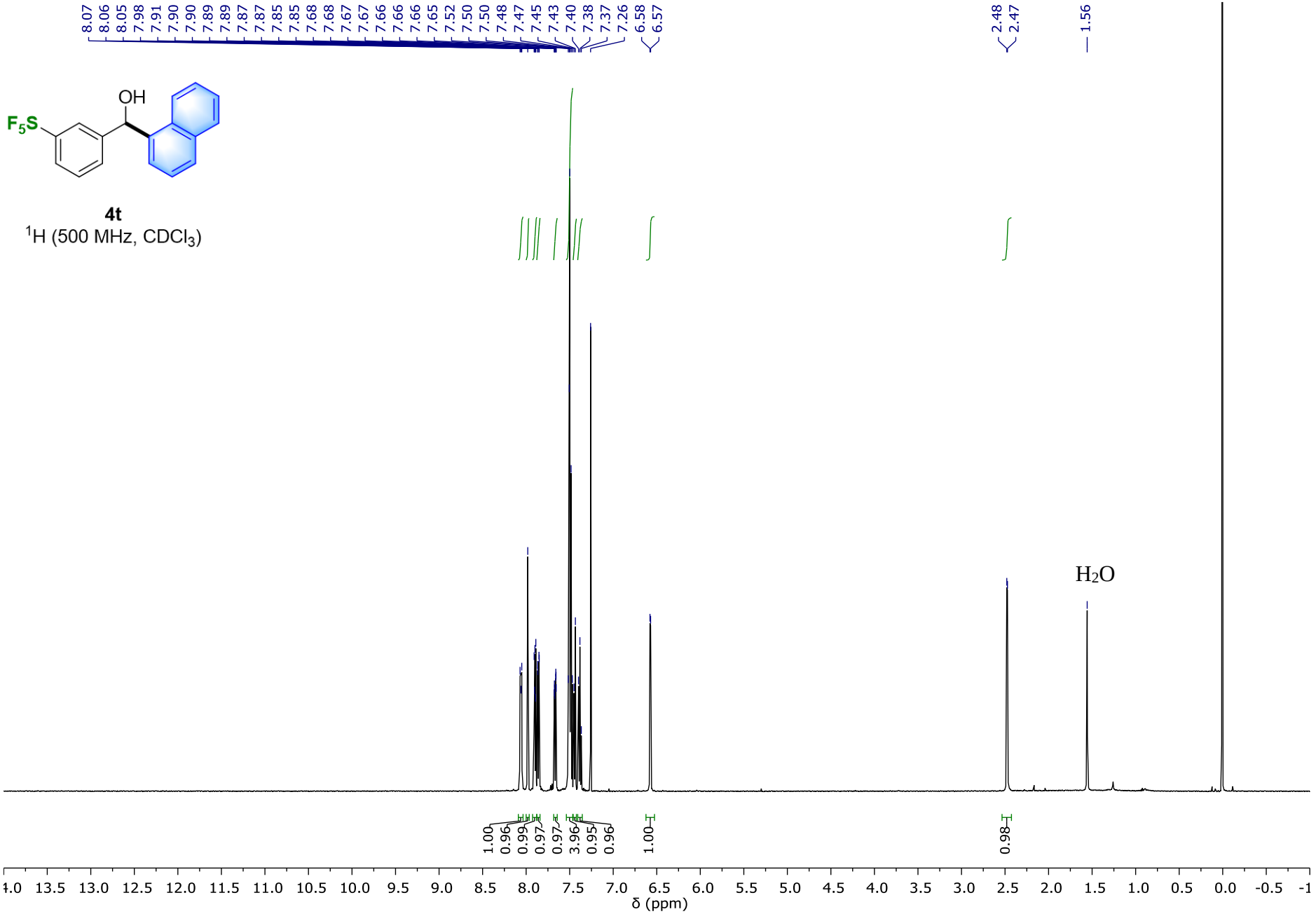
4s

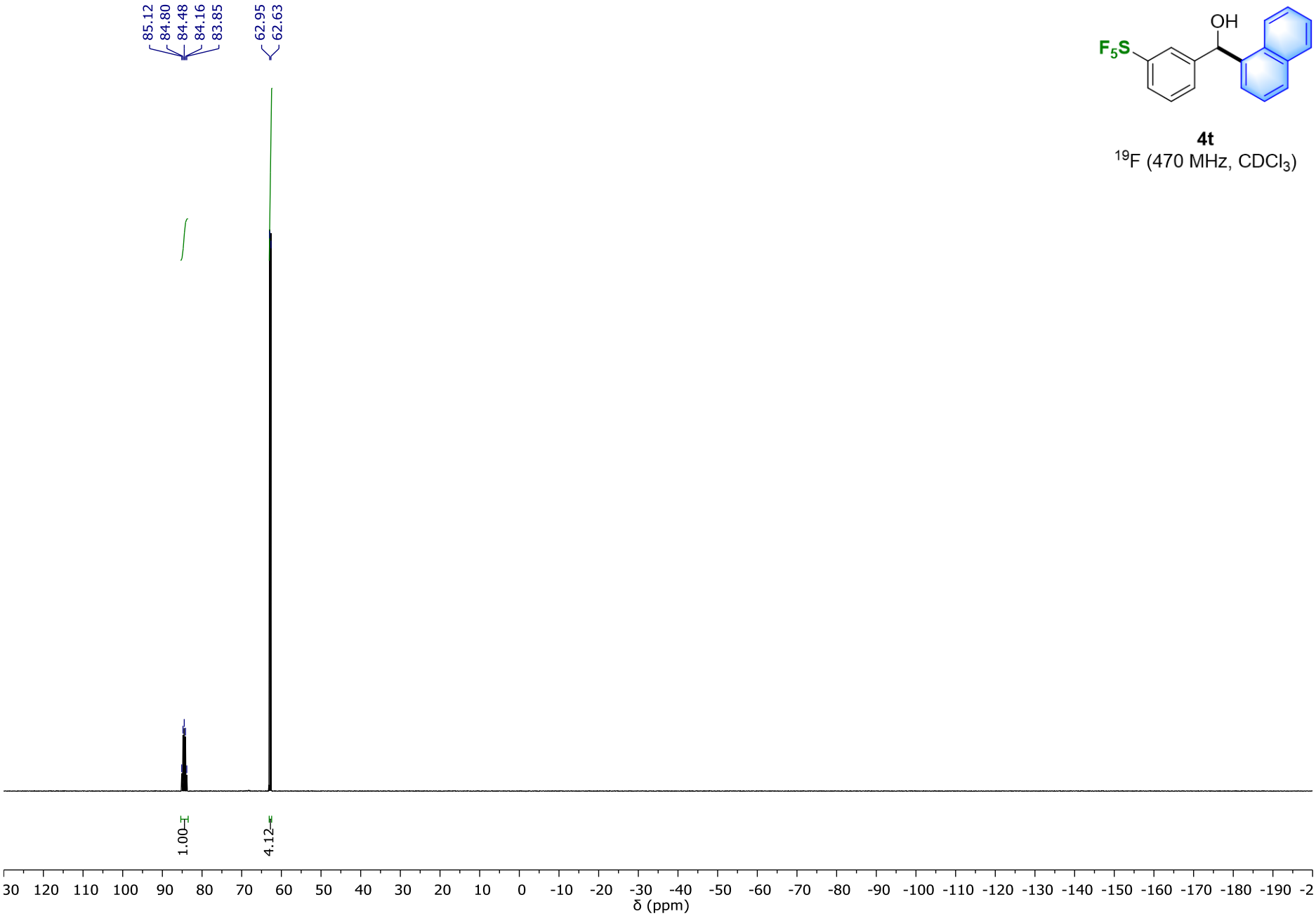
^{19}F (470 MHz, $CDCl_3$)



4s

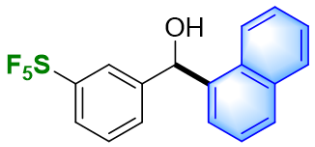
^{13}C (126 MHz, $CDCl_3$)


8.07
8.06
8.05
7.98
7.91
7.90
7.90
7.89
7.89
7.87
7.87
7.85
7.85
7.68
7.68
7.67
7.67
7.66
7.66
7.66
7.65
7.52
7.50
7.50
7.48
7.47
7.45
7.43
7.40
7.38
7.37
7.26
6.58
6.57
2.48
2.47
1.56
OH
F5S
4t
1H (500 MHz, CDCl3)
H2O
1.00
0.96
0.99
0.97
0.97
3.96
0.95
0.96
1.00
0.98
δ (ppm)



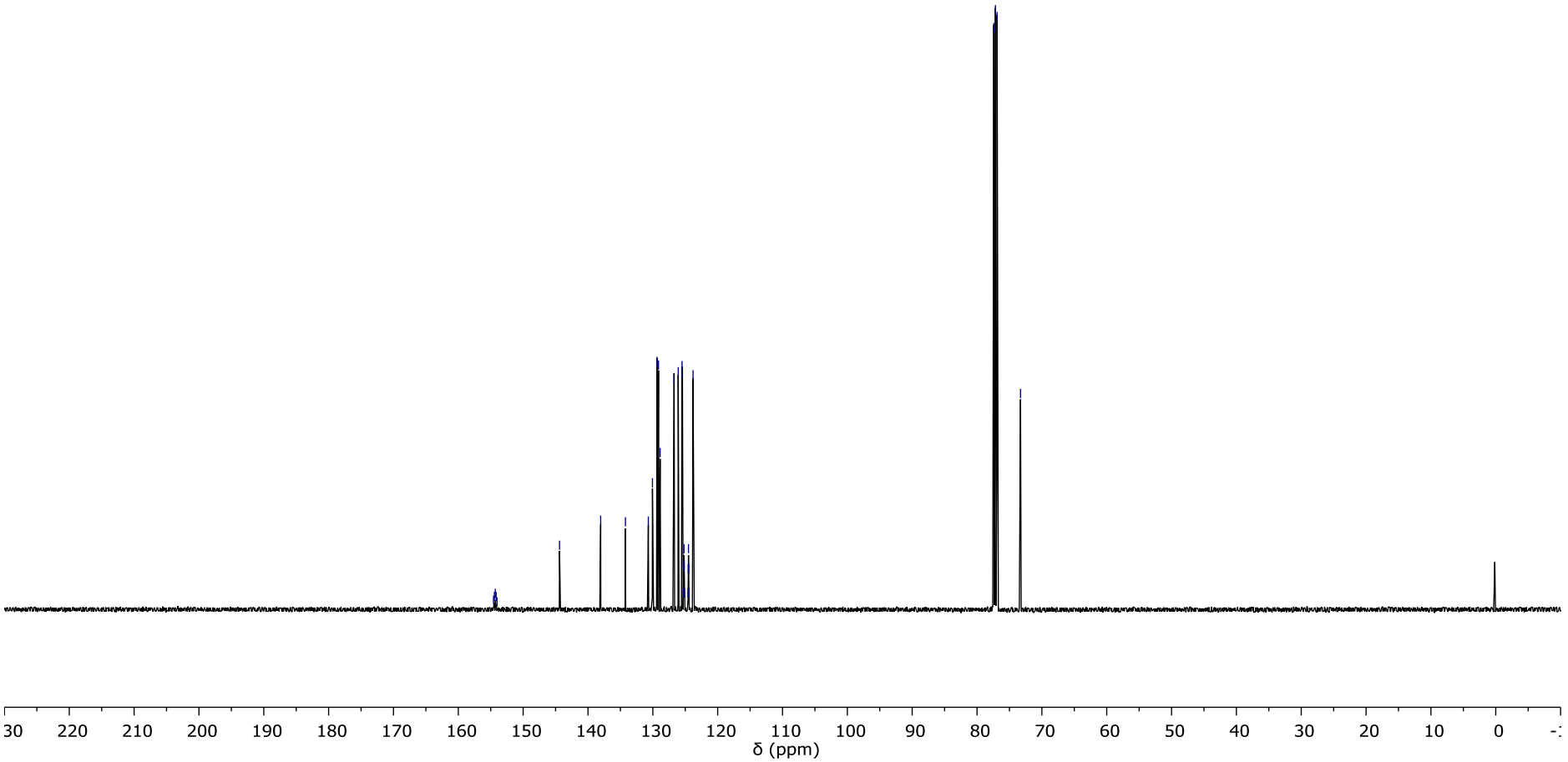
4t

^{19}F (470 MHz, $CDCl_3$)

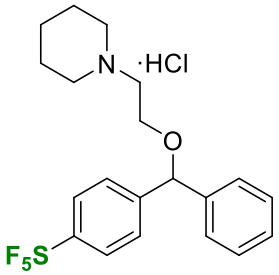


4t

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



1.3. Compound 5

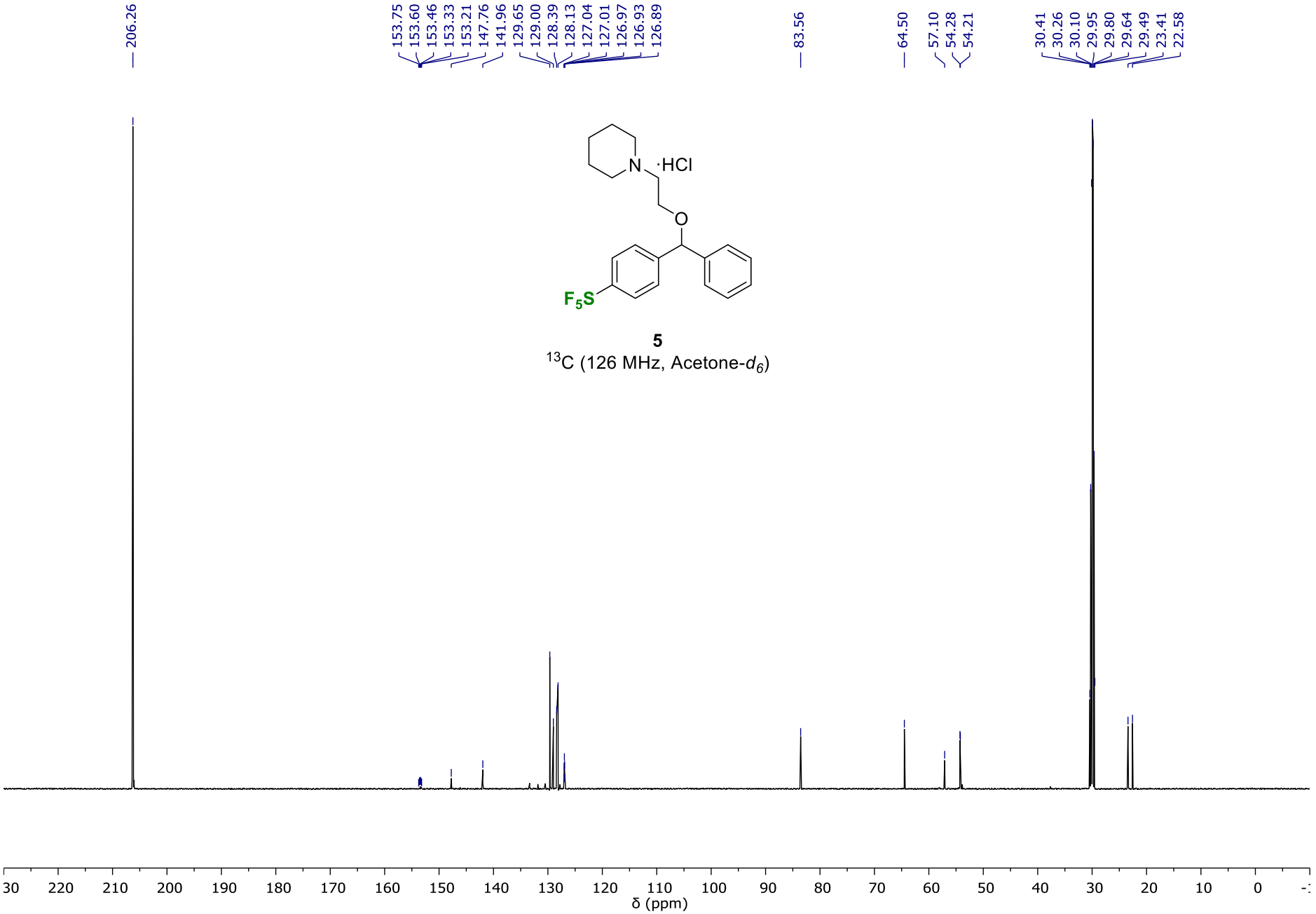


5

^{1}H (500 MHz, Acetone-d_6)

5

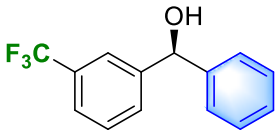
^{19}F (470 MHz, Acetone-d_6)



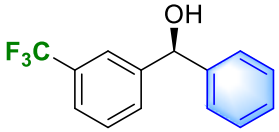
5

^{13}C (126 MHz, Acetone-d_6)

1.4. Compounds (*S*)-8 and (*S*)-10

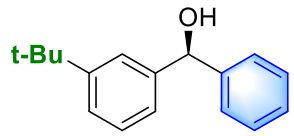


(*S*)-8
^{1}H (400 MHz, $CDCl_3$)



(*S*)-8

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



(*S*)-10
^{1}H (400 MHz, $CDCl_3$)