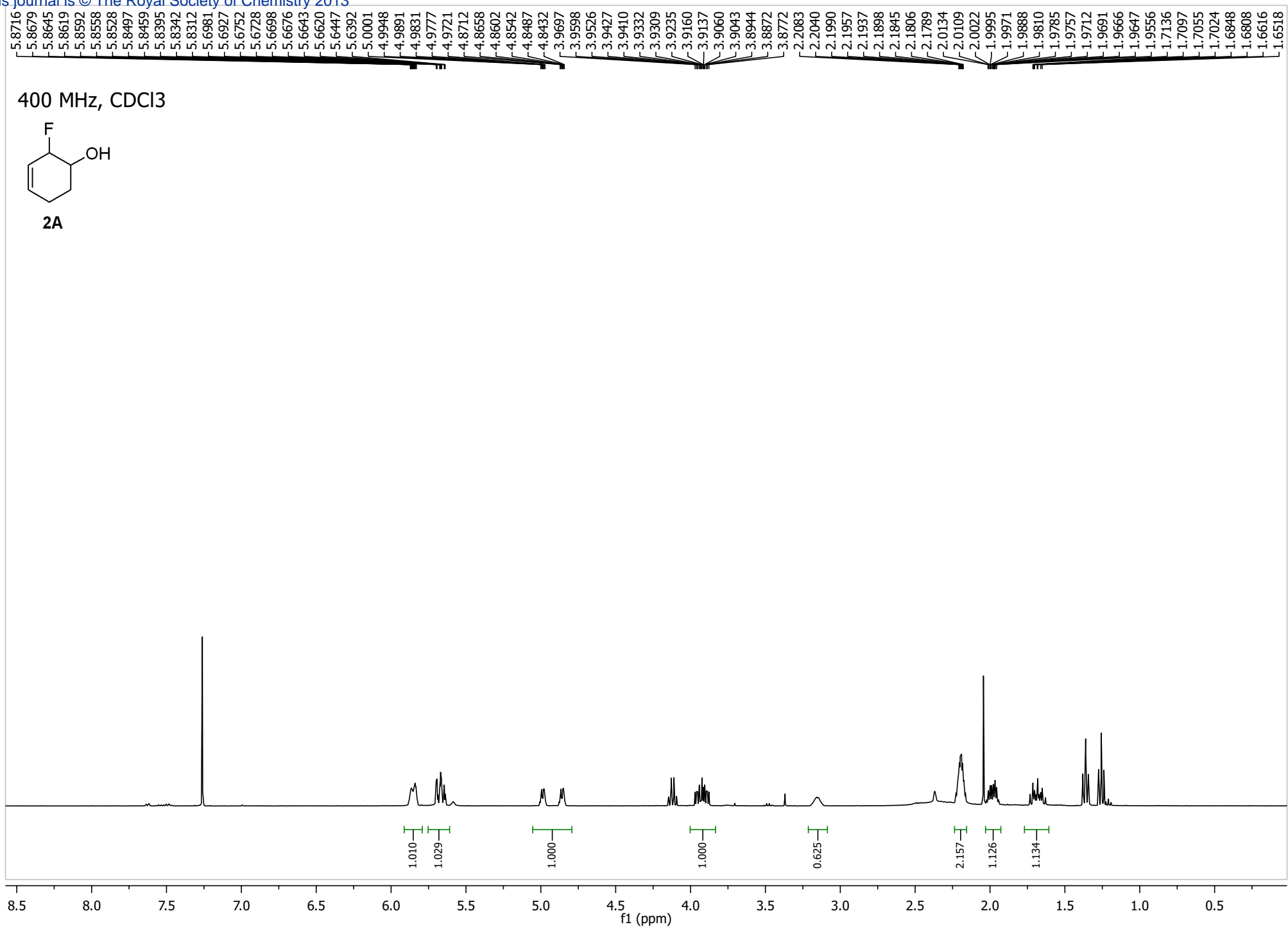


Rhodium-Catalyzed Regioselective Opening of Vinyl Epoxides with Et₃N·3HF Reagent - Formation of Allylic Fluorohydrins

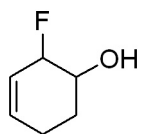
Qi Zhang, Hien M. Nguyen*

Department of Chemistry, University of Iowa, Iowa City, IA 52242

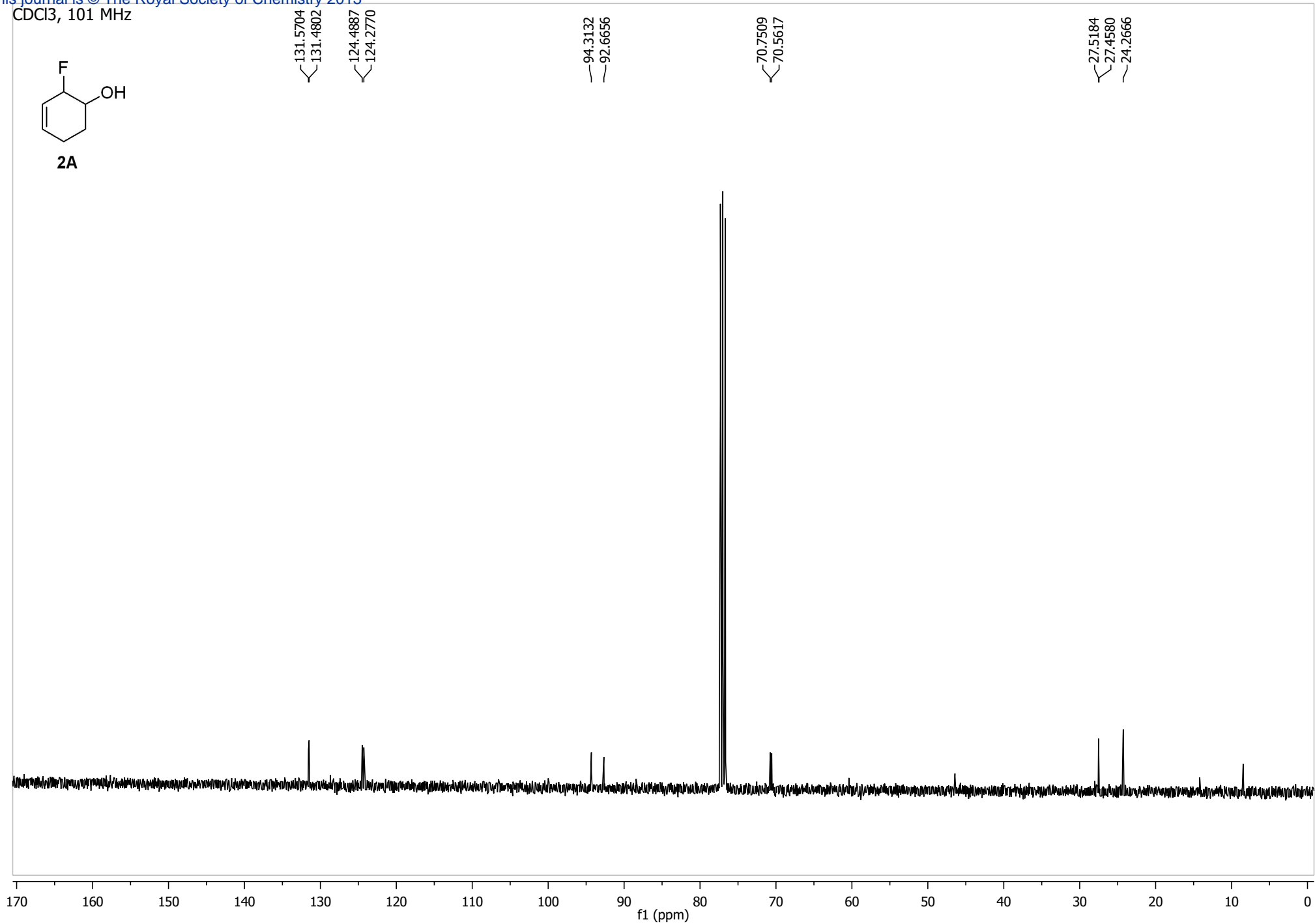
NMR SPECTRAL DATA FILE

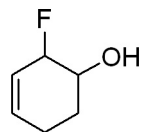


CDCl₃, 101 MHz

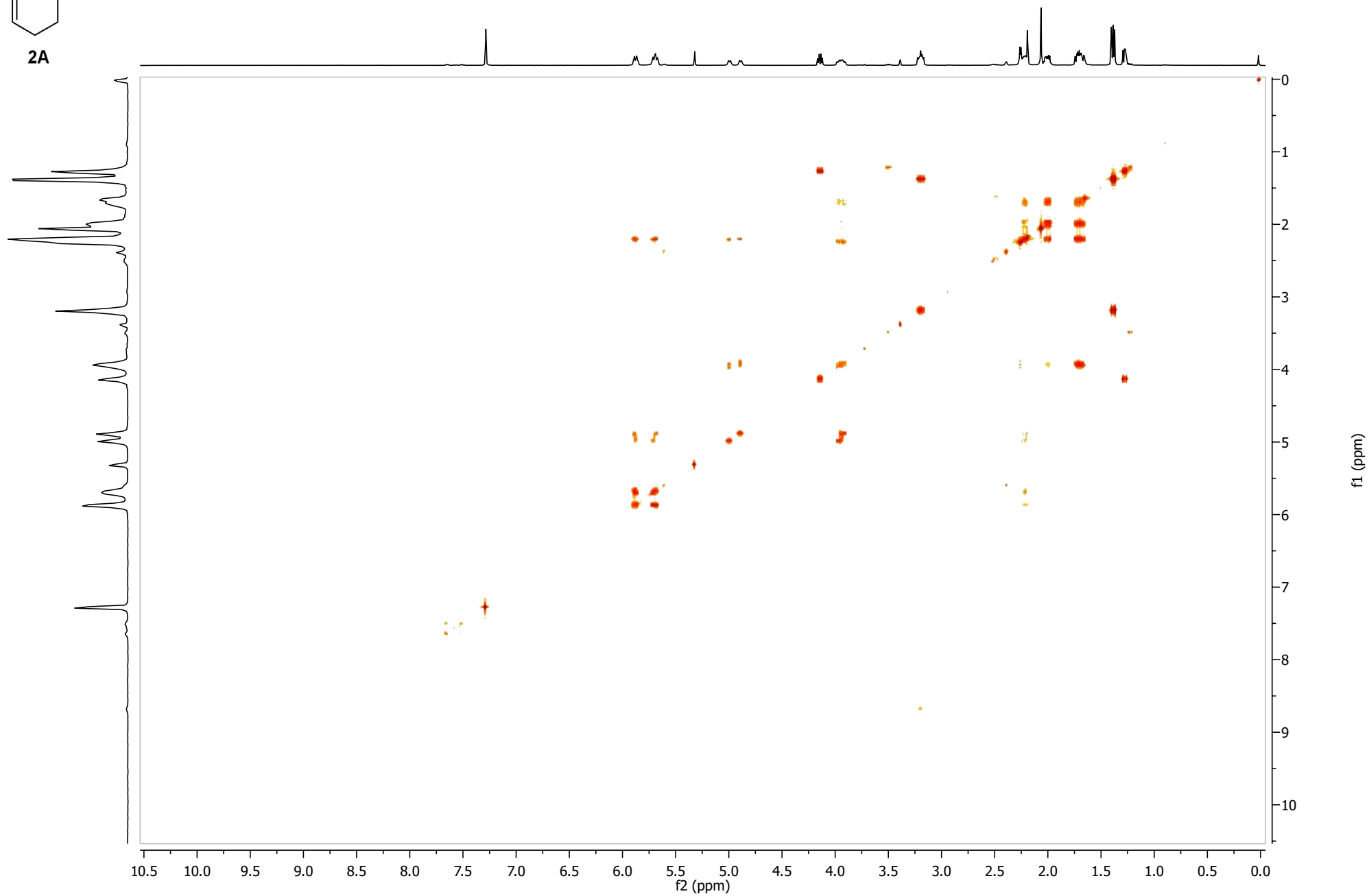


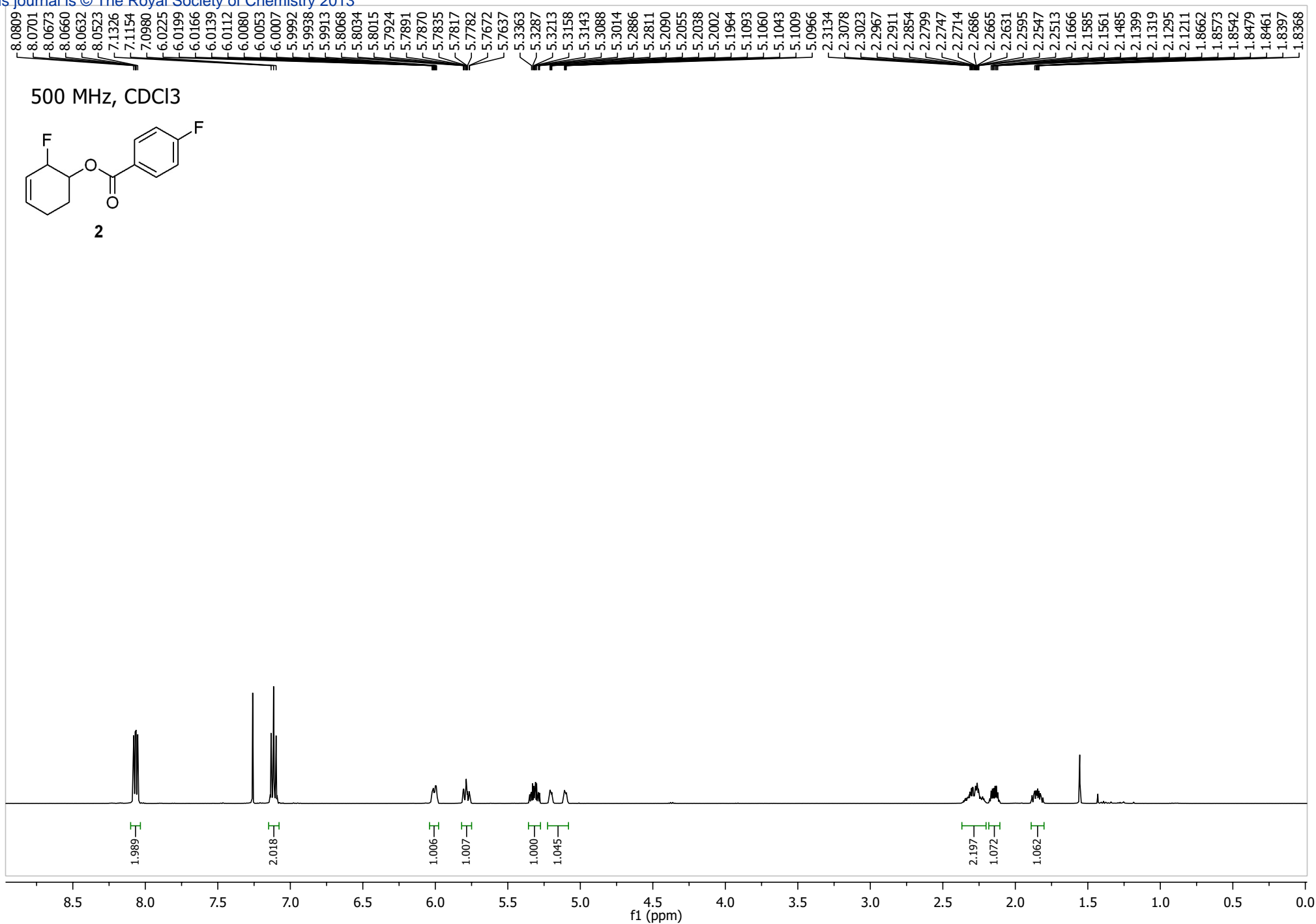
2A



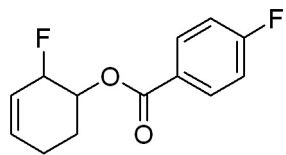


2A

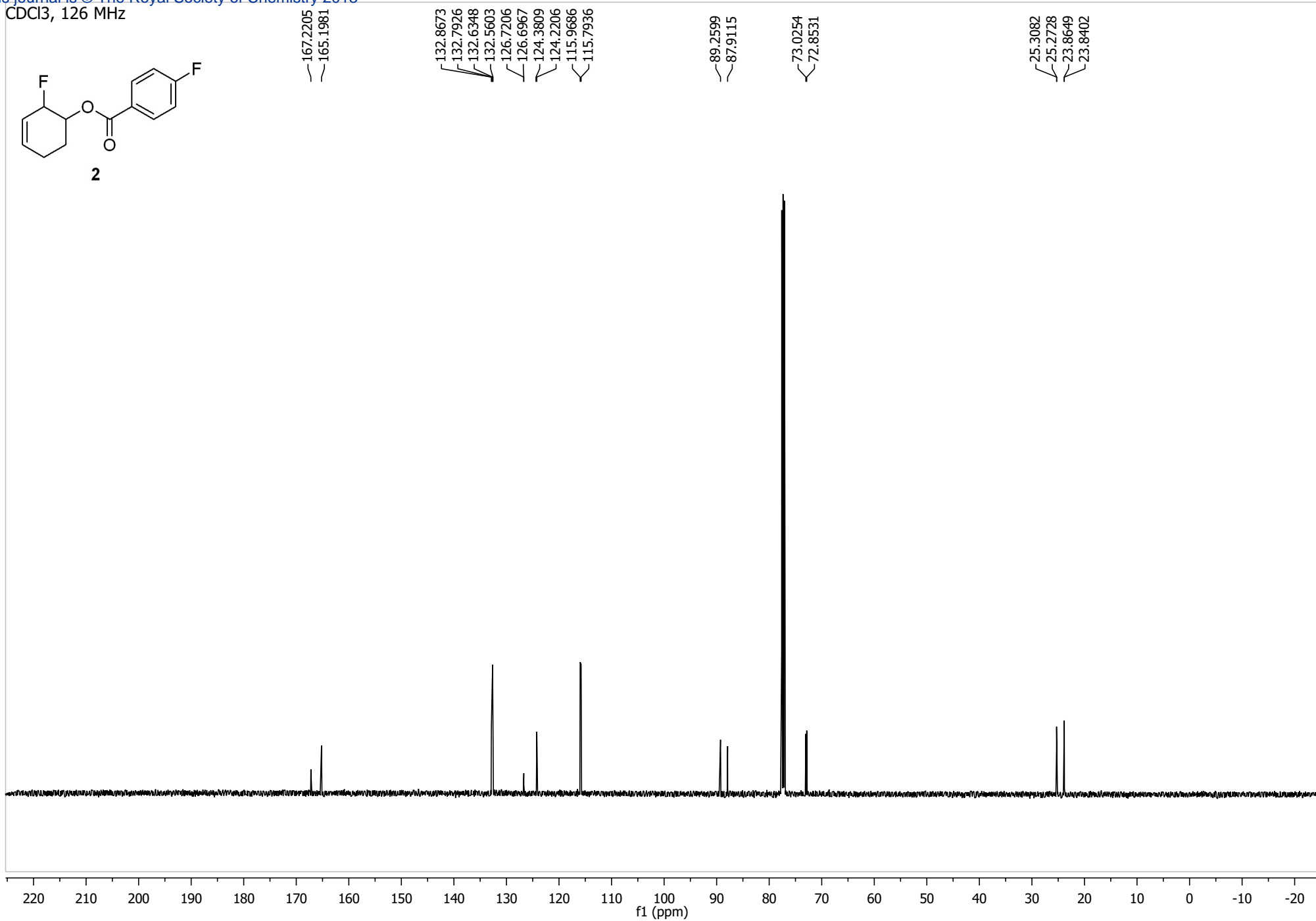




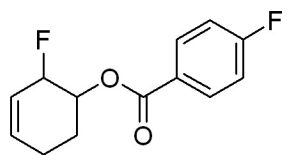
CDCl₃, 126 MHz



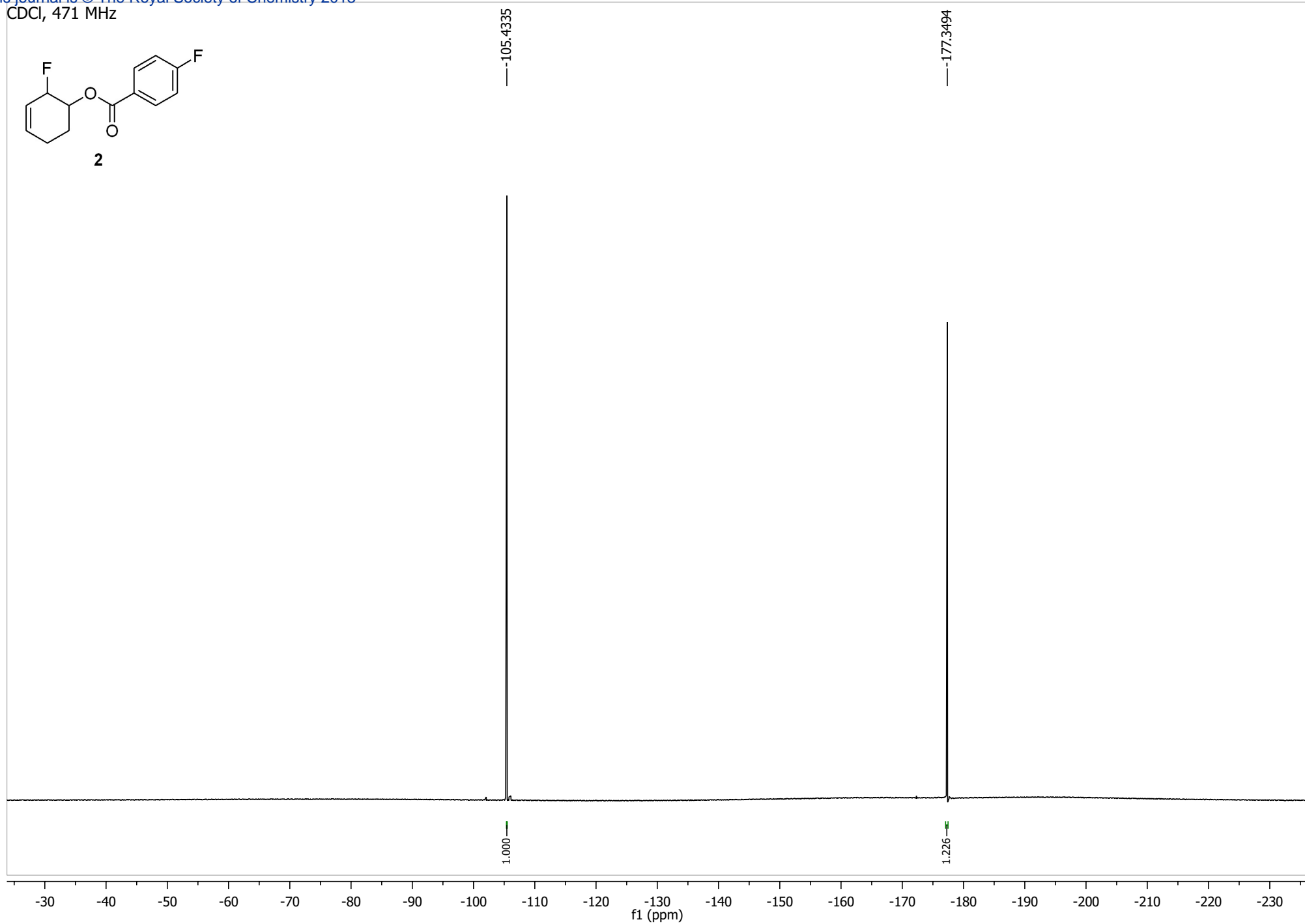
2

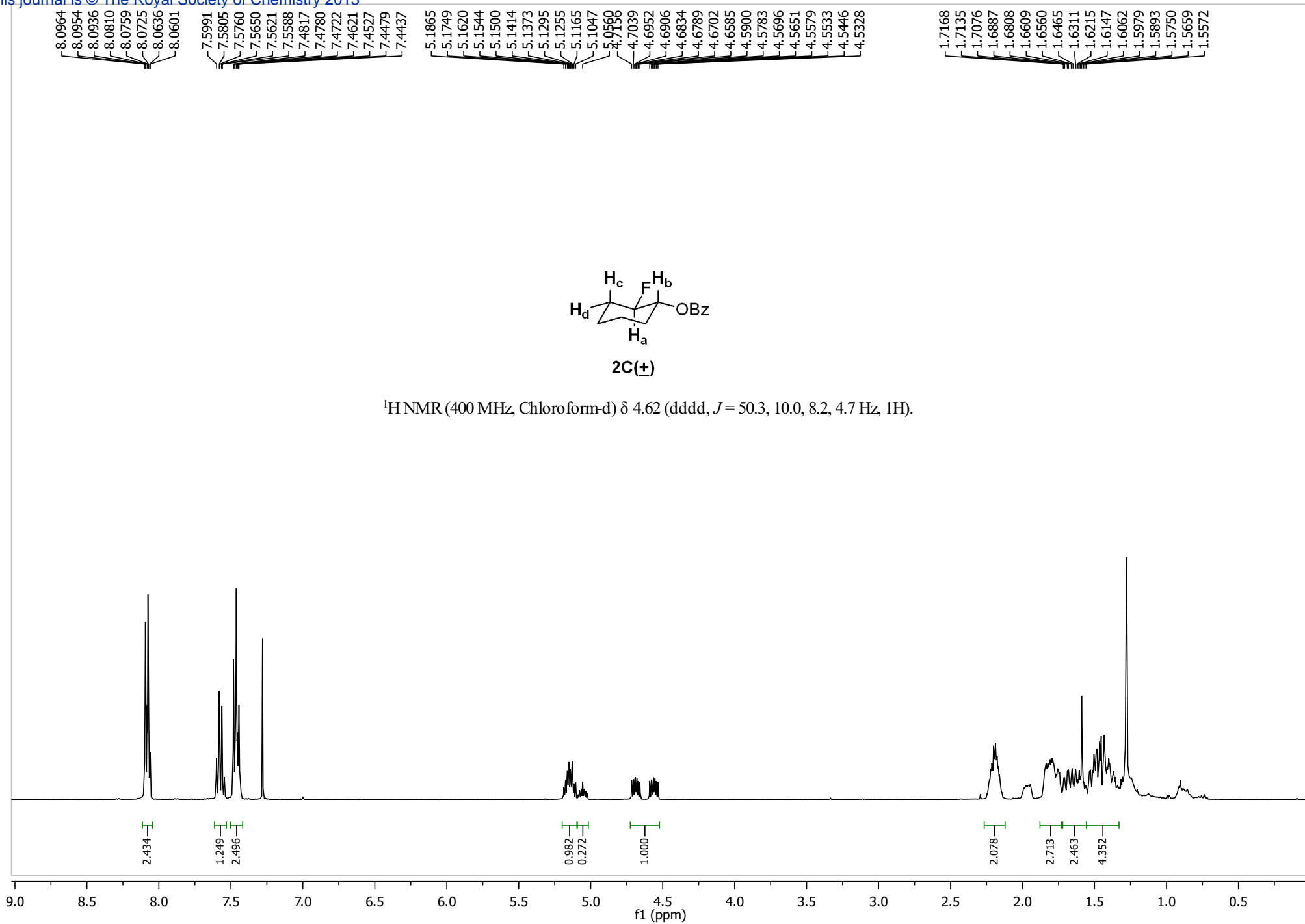


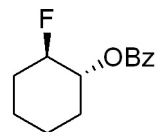
CDCl₃, 471 MHz



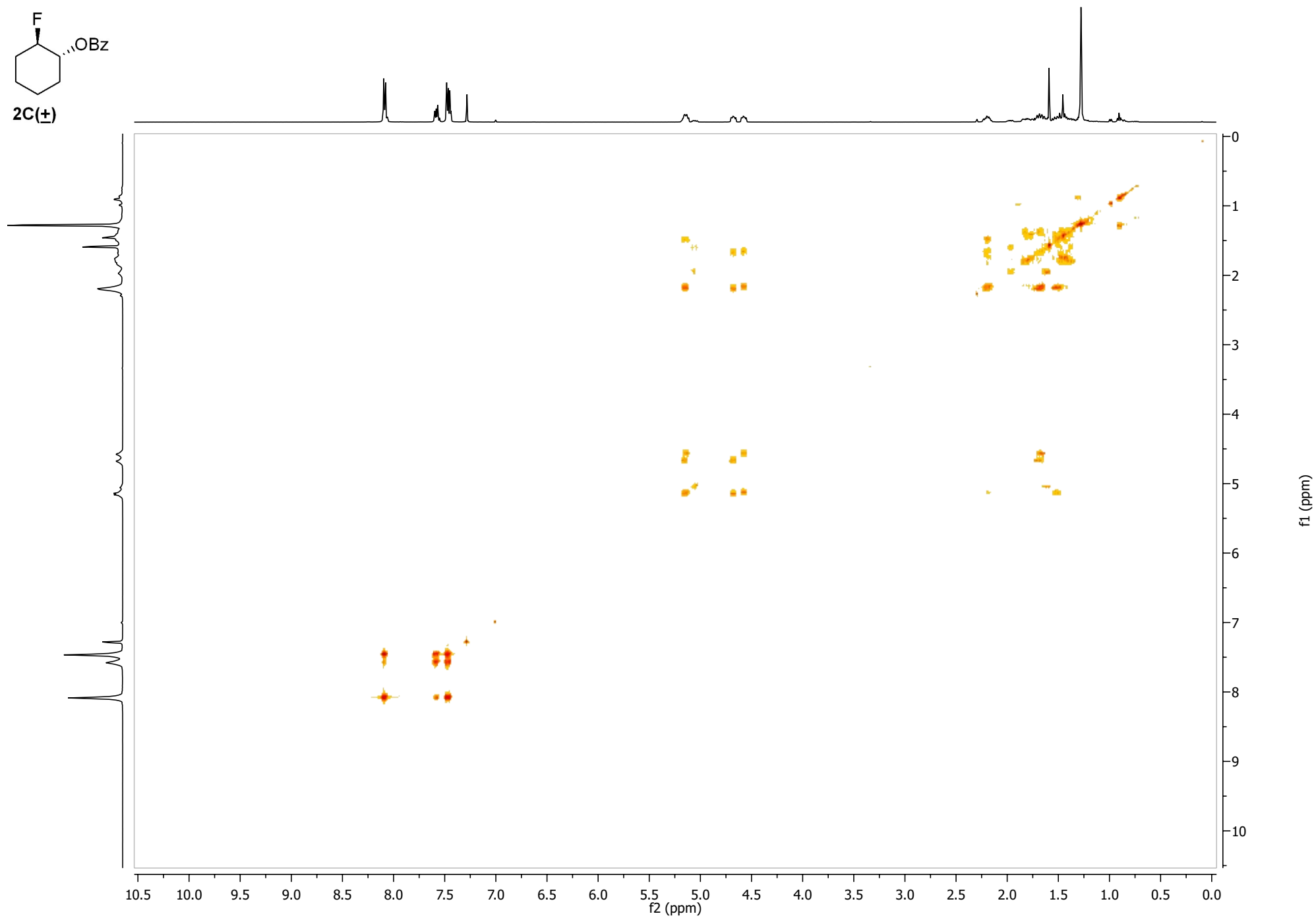
2

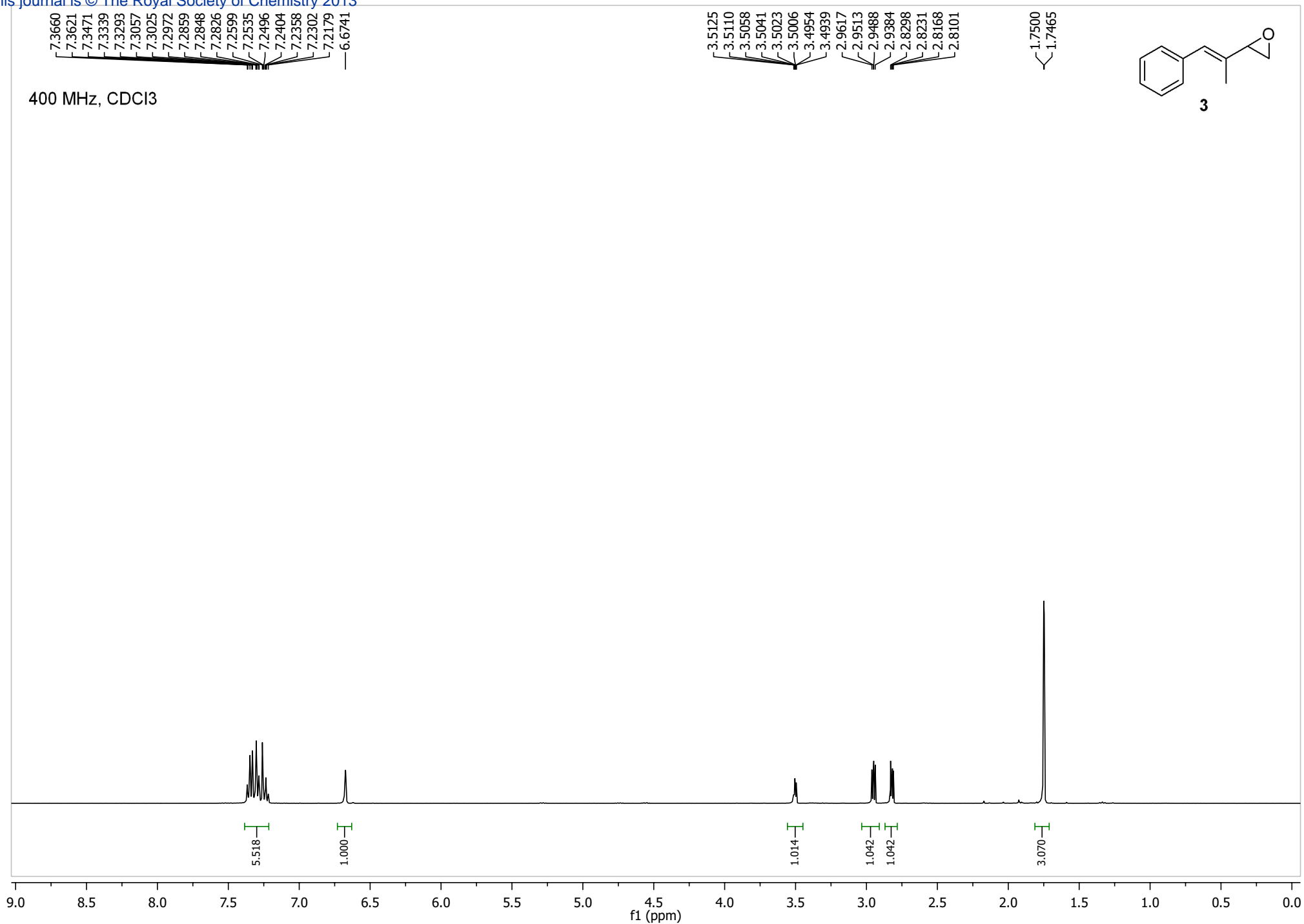






2C(±)





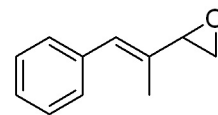
CDCl₃, 126 HMz

— 137.2287
— 134.2146
— 129.0486
— 128.9198
— 128.3339
— 126.8869

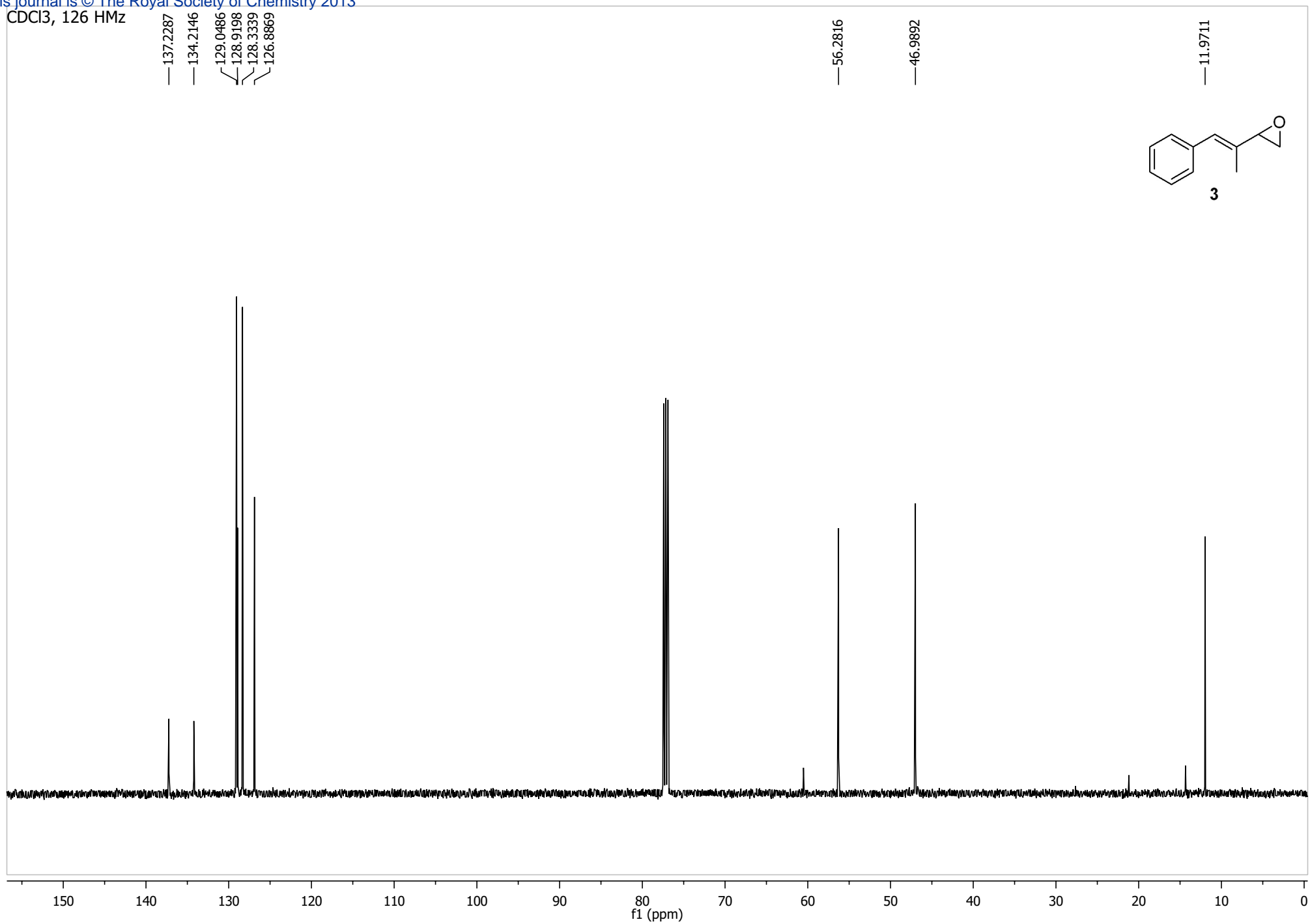
— 56.2816

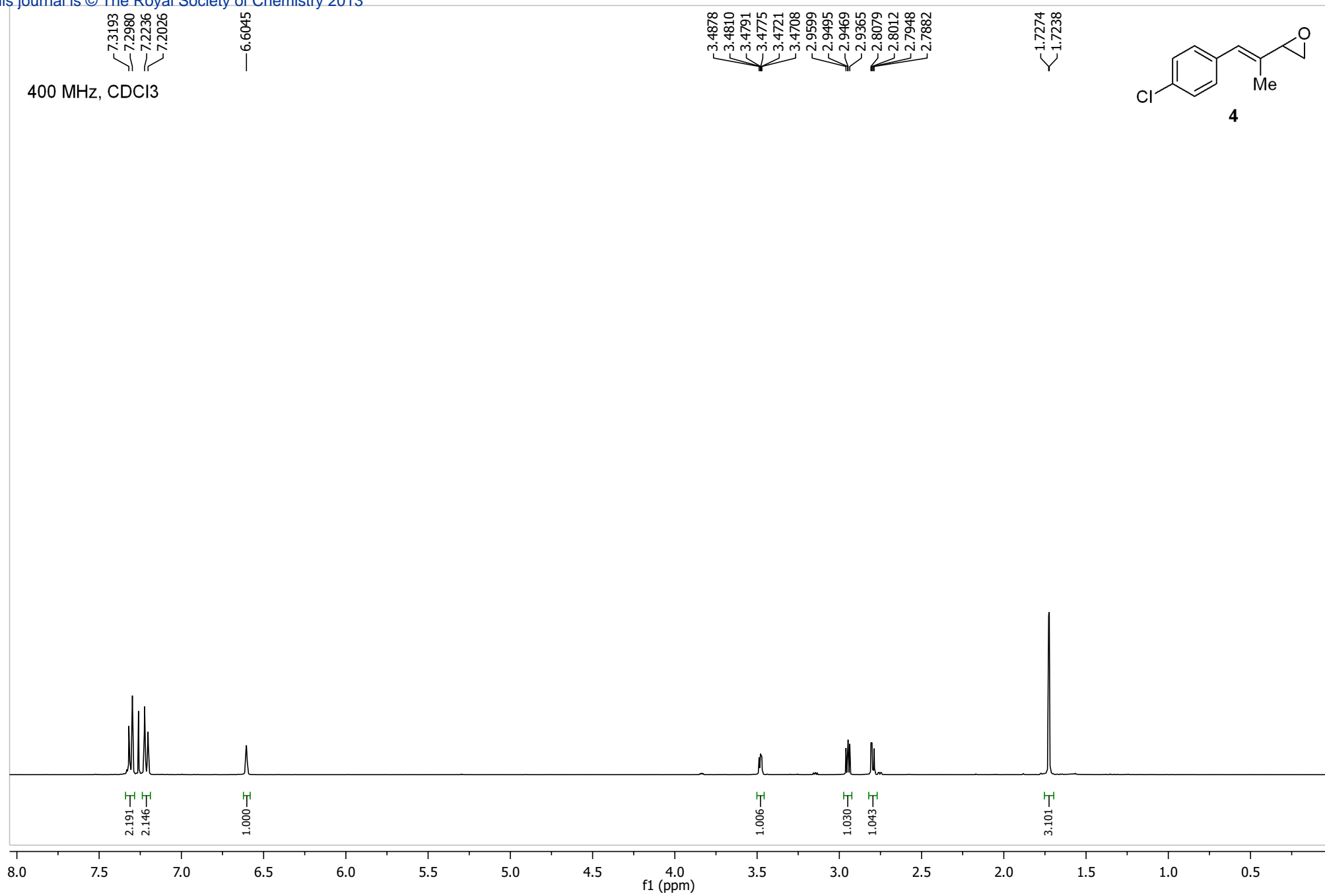
— 46.9892

— 11.9711



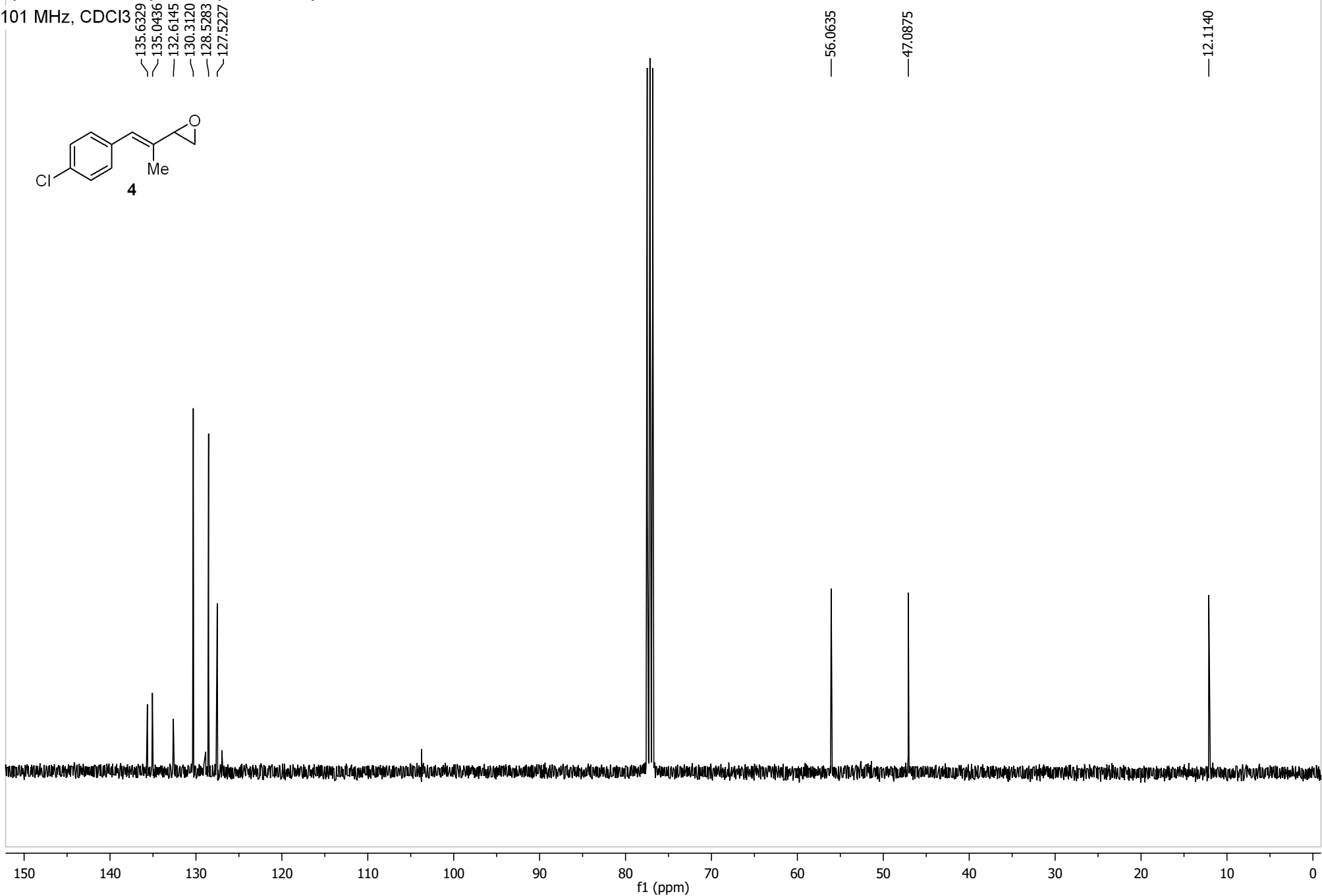
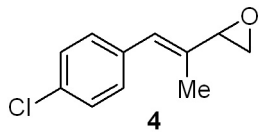
3



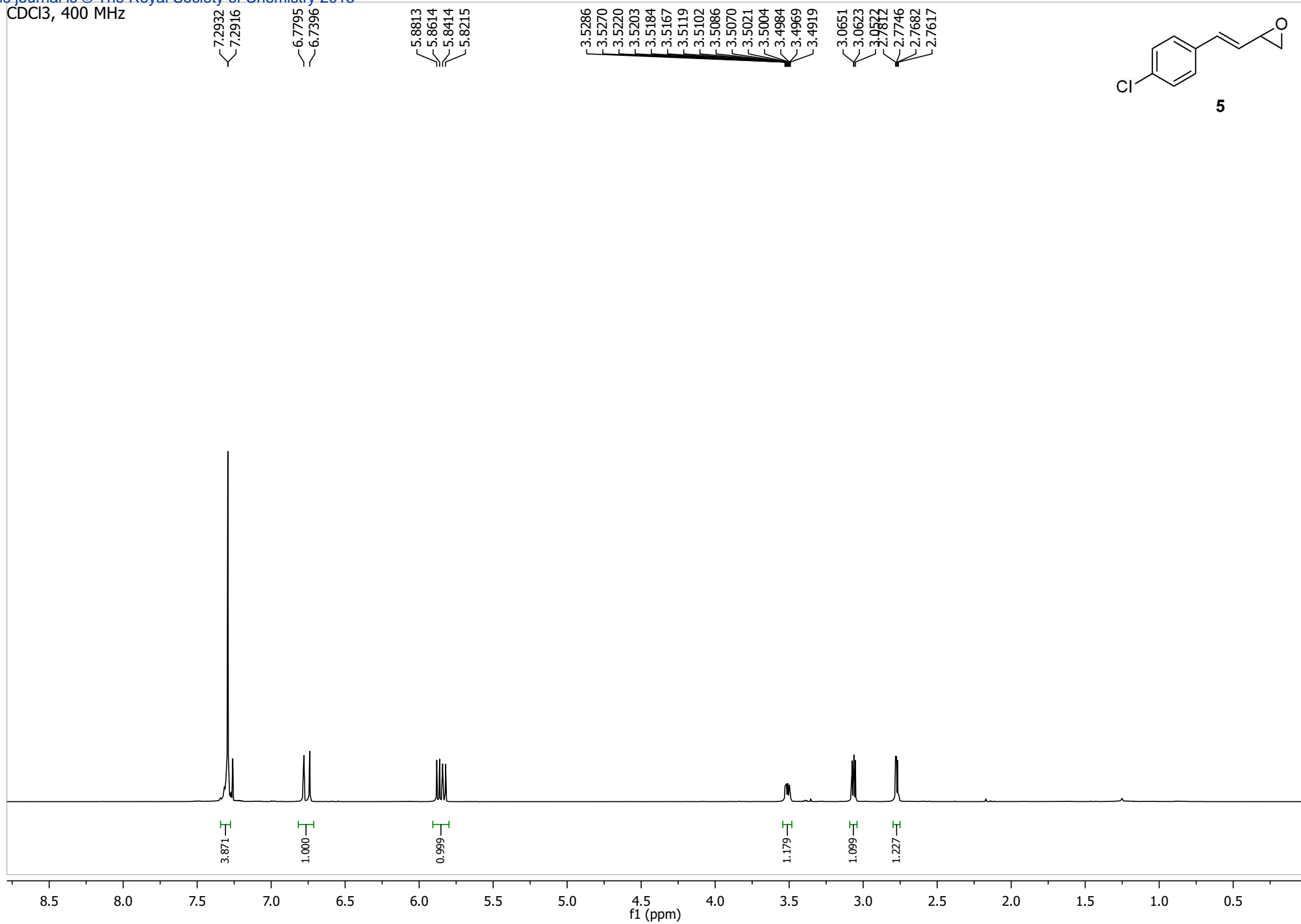


101 MHz, CDCl₃

135.6329
135.0436
132.6145
130.3120
128.5283
127.5227



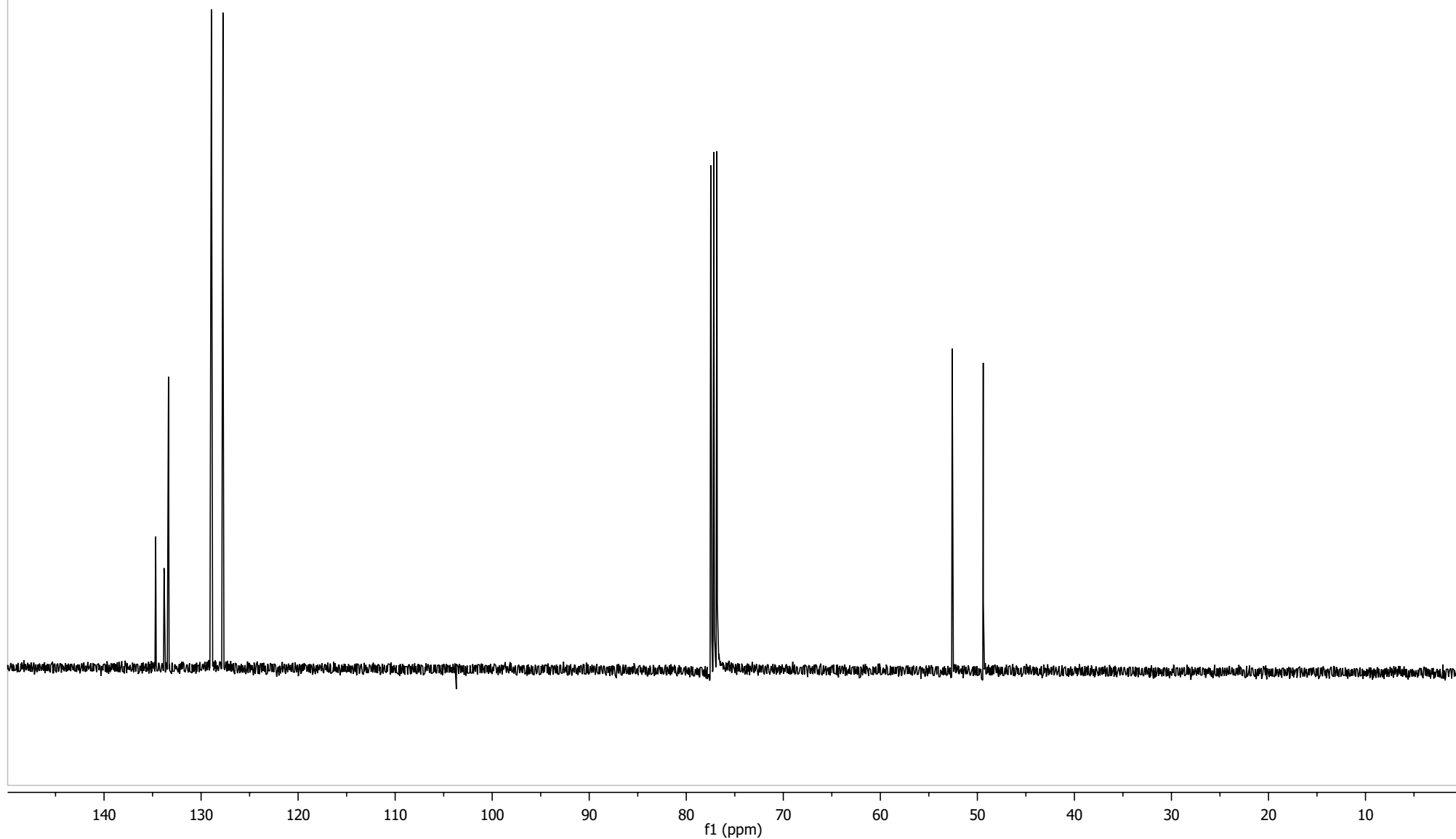
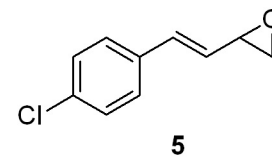
CDCl₃, 400 MHz



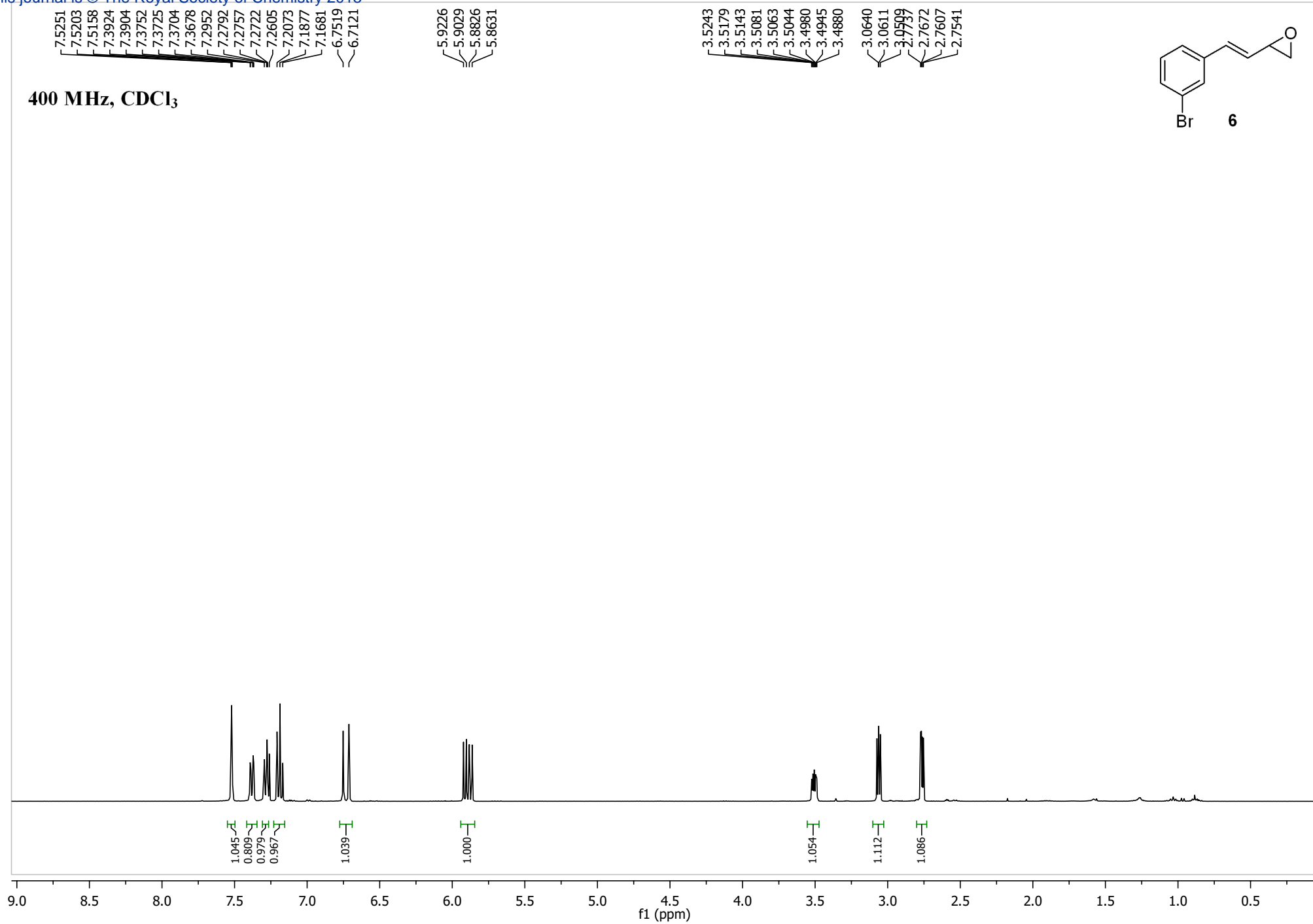
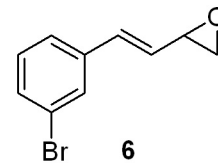
CDCl₃, 101 MHz

134.6818
133.8179
133.3595
128.9422
127.7768
127.7441

52.5938
49.3976



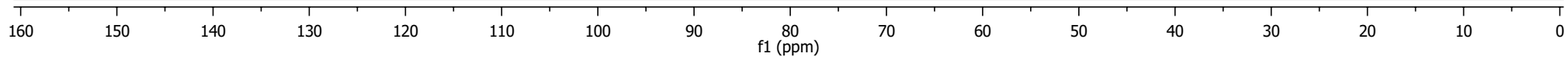
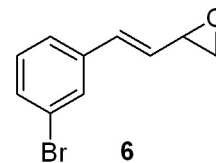
400 MHz, CDCl₃

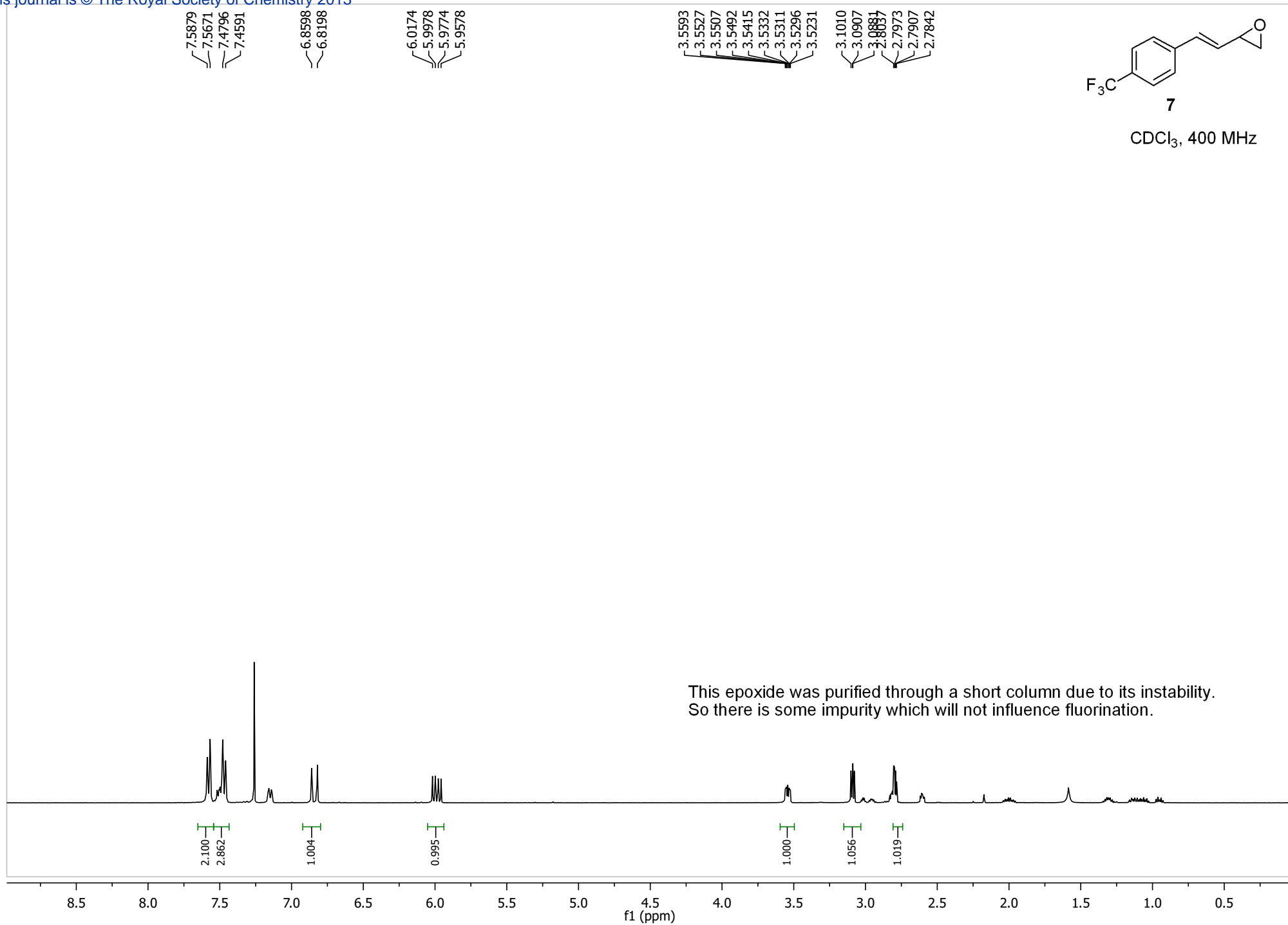


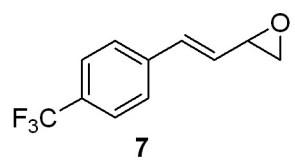
CDCl₃, 101 MHz

138.3804
132.9972
131.0352
130.2854
129.4550
128.8274
125.1892
122.9591

52.3945
49.3908



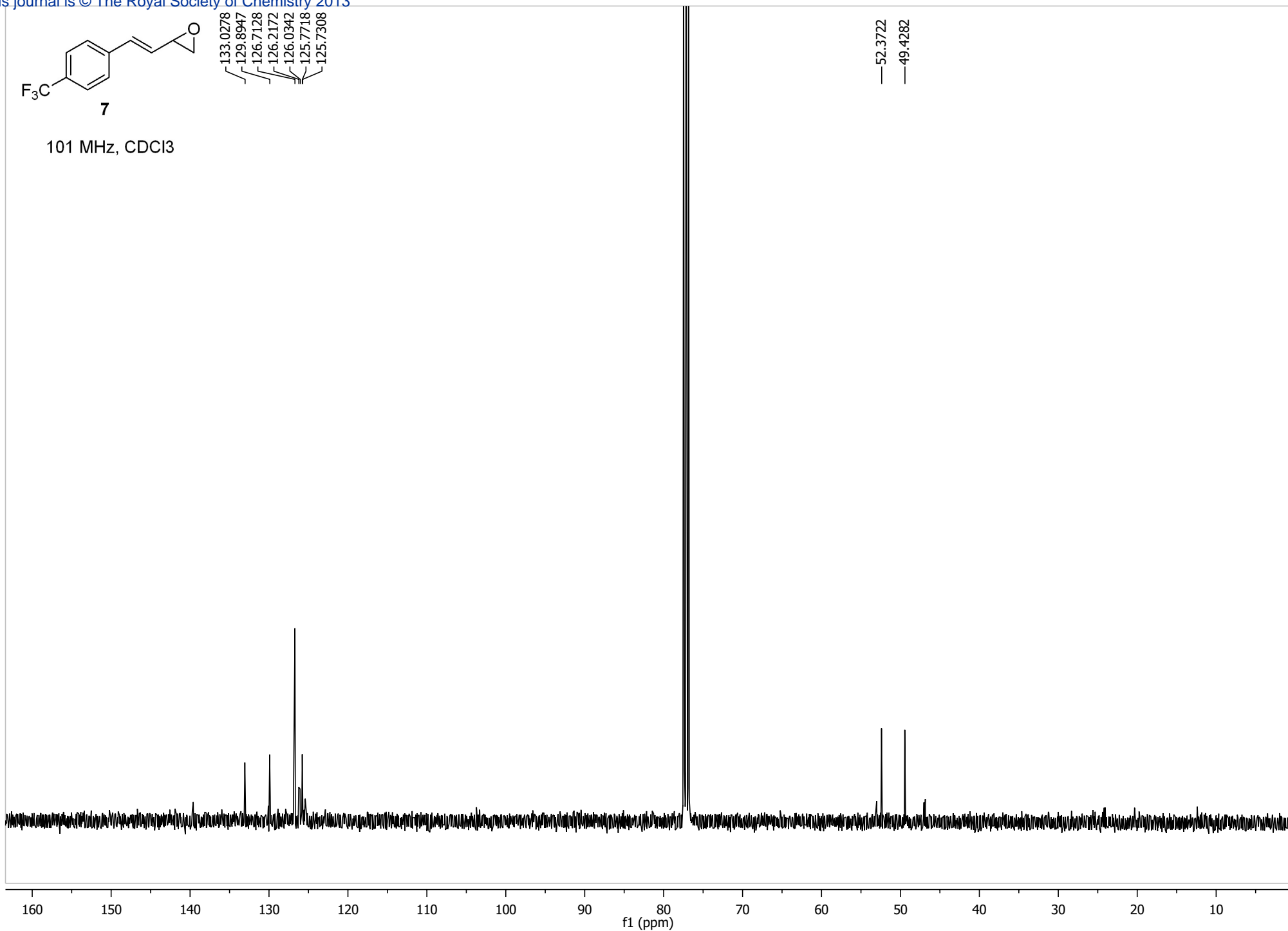




101 MHz, CDCl₃

133.0278
129.8947
126.7128
126.2172
126.0342
125.7718
125.7308

52.3722
49.4282



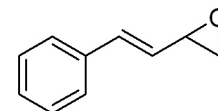
CDCl₃, 500 MHz

7.3896
7.3754
7.3418
7.3273
7.3118
7.2767
7.2604
6.8367
6.8048

5.9060
5.8901
5.8741
5.8582

3.5419
3.5411
3.5366
3.5357
3.5340
3.5331
3.5274
3.5264
3.5207
3.5197
3.5180
3.5126

3.0658
3.0637
3.0555
2.7822
2.7771
2.7719



8

2.155
2.142
1.437

1.003

1.000

1.006

1.039

1.046

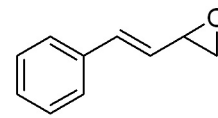
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

CDCl₃, 126 MHz

136.2656
134.7227
128.7901
128.2164
127.1165
126.5836

52.7746
49.3995

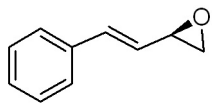


8

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

CDCl₃, 500 MHz



(R)-8

7.3896
7.3754
7.3418
7.3273
7.3118
7.2767
7.2604
6.8367
6.8048

5.9060
5.8901
5.8741
5.8582

3.5419
3.5411
3.5366
3.5357
3.5340
3.5331
3.5274
3.5264
3.5207
3.5197
3.5180
3.5126

3.0658
3.0637
3.0555
2.7822
2.7771
2.7719

2.155
2.142
1.437

1.003

1.000

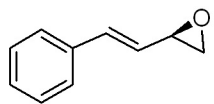
1.006

1.039

1.046

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

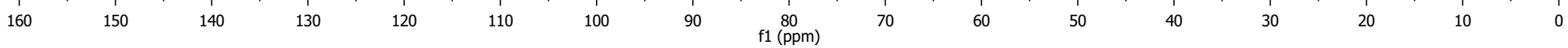
CDCl₃, 126 MHz

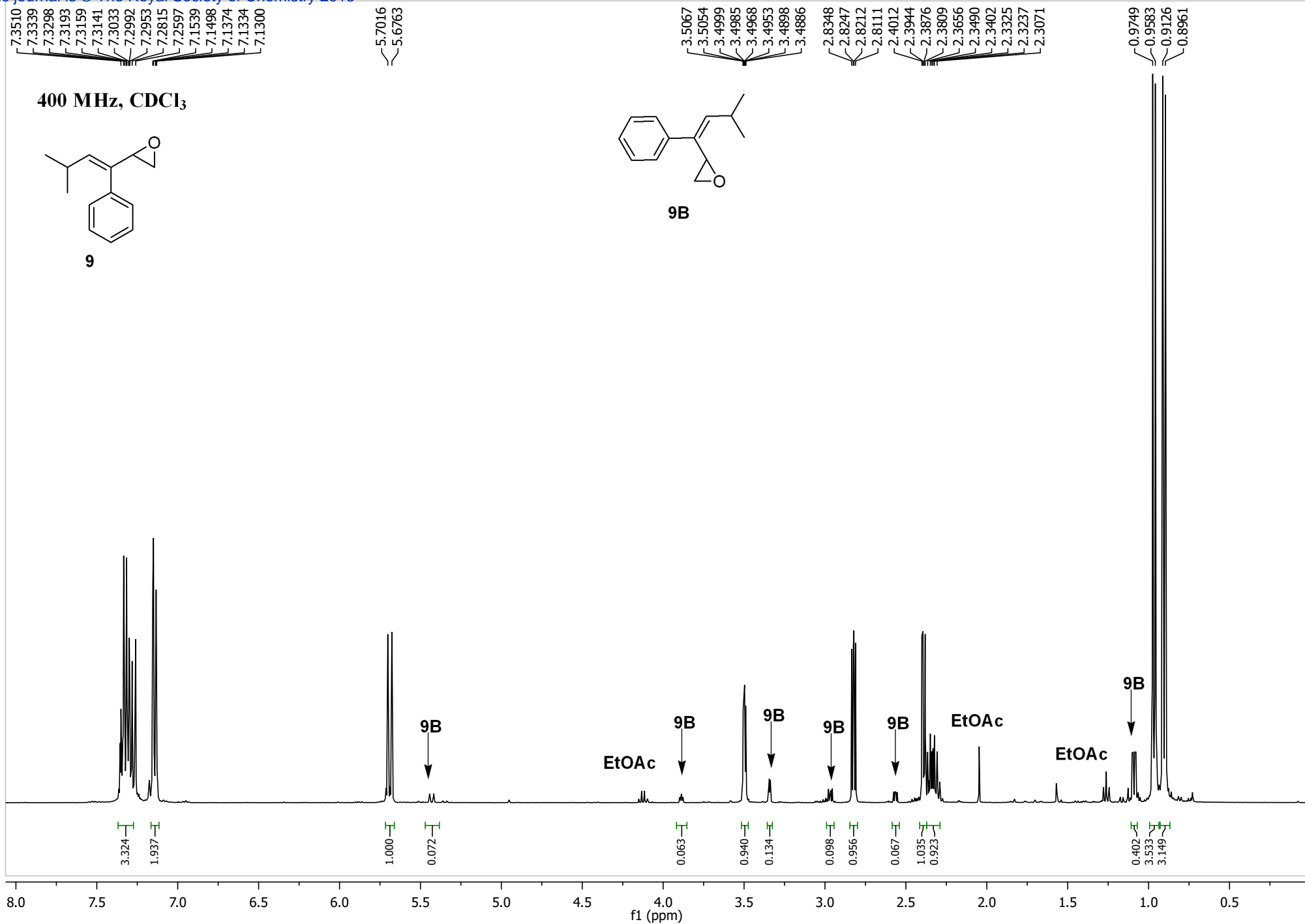


(*R*)-8

136.2656
134.7227
128.7901
128.2164
127.1165
126.5836

52.7746
49.3995





CDCl₃, 126 MHz

139.9737
136.3550
135.0573

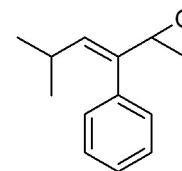
129.3068
128.1247
127.2828

55.1497

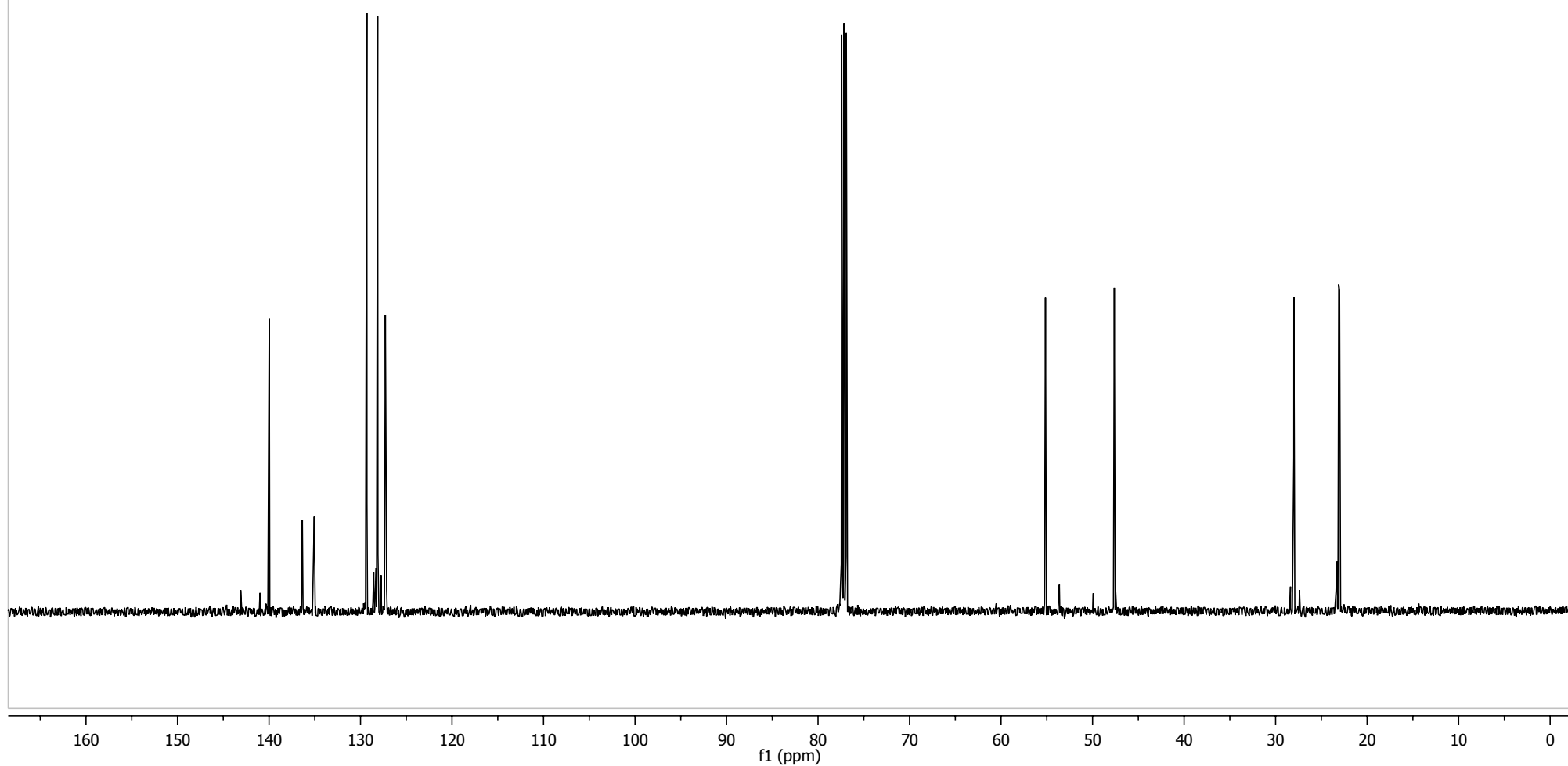
47.6236

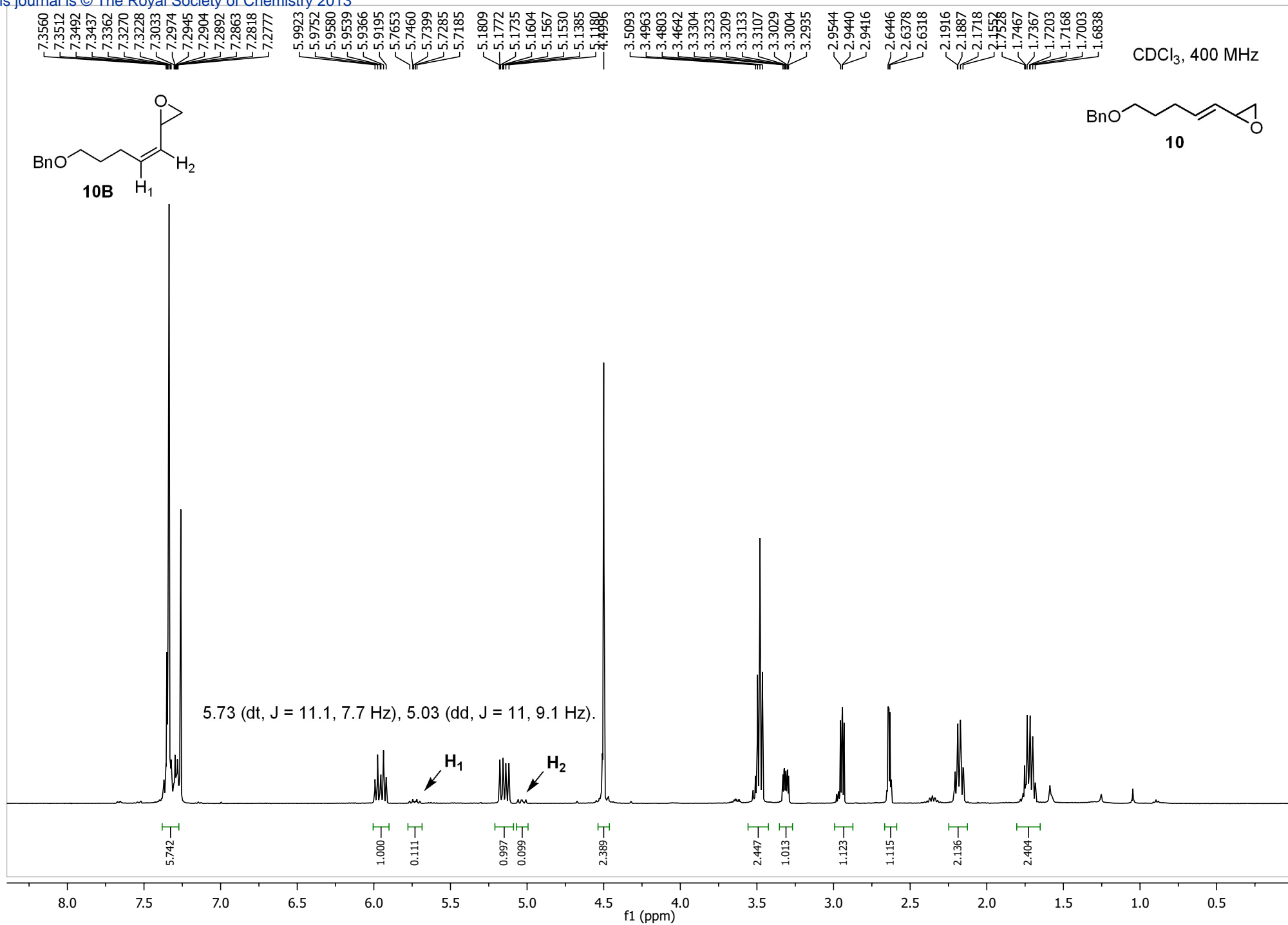
28.0070

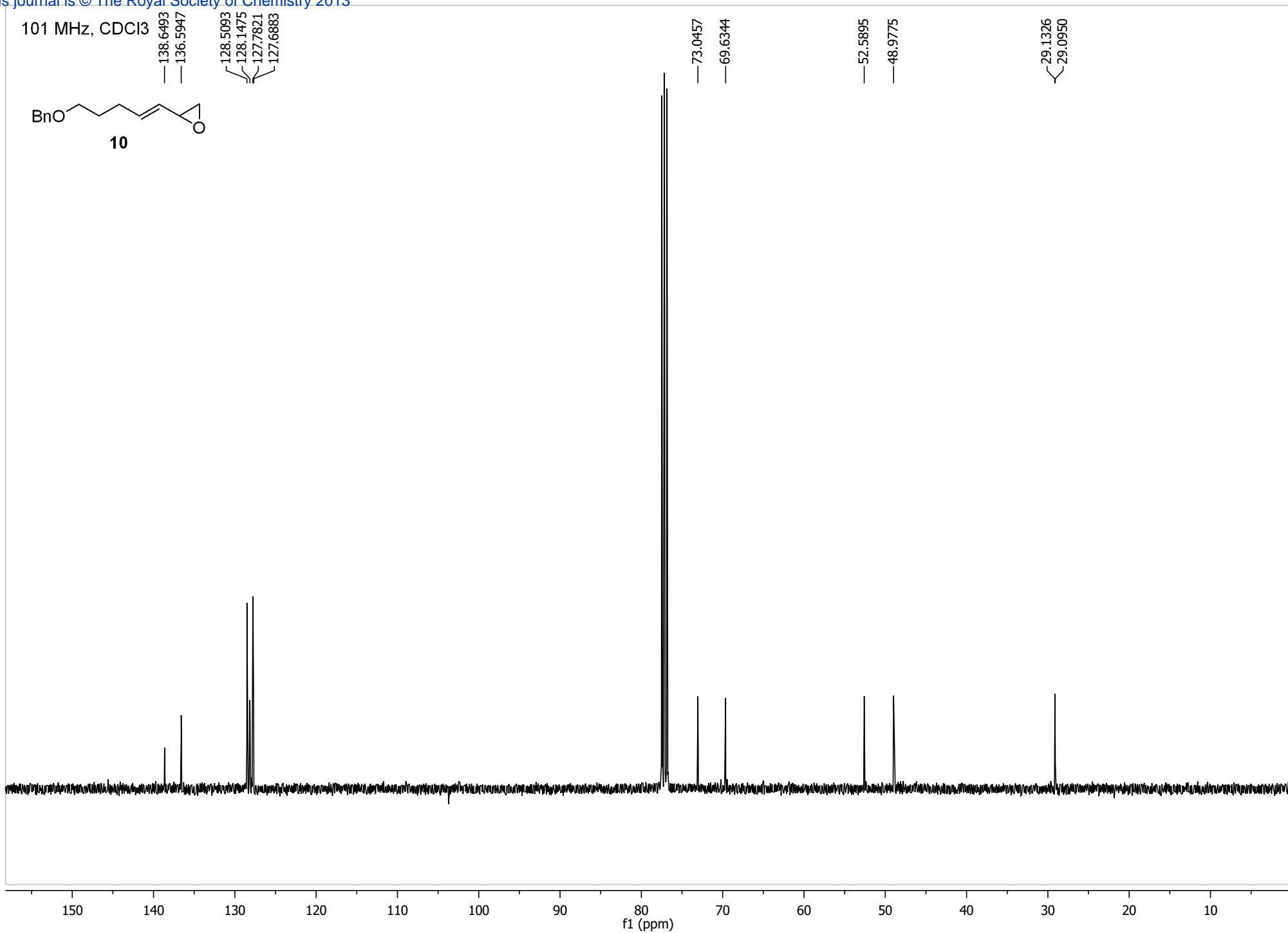
23.0964
23.0118



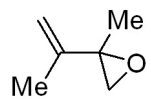
9



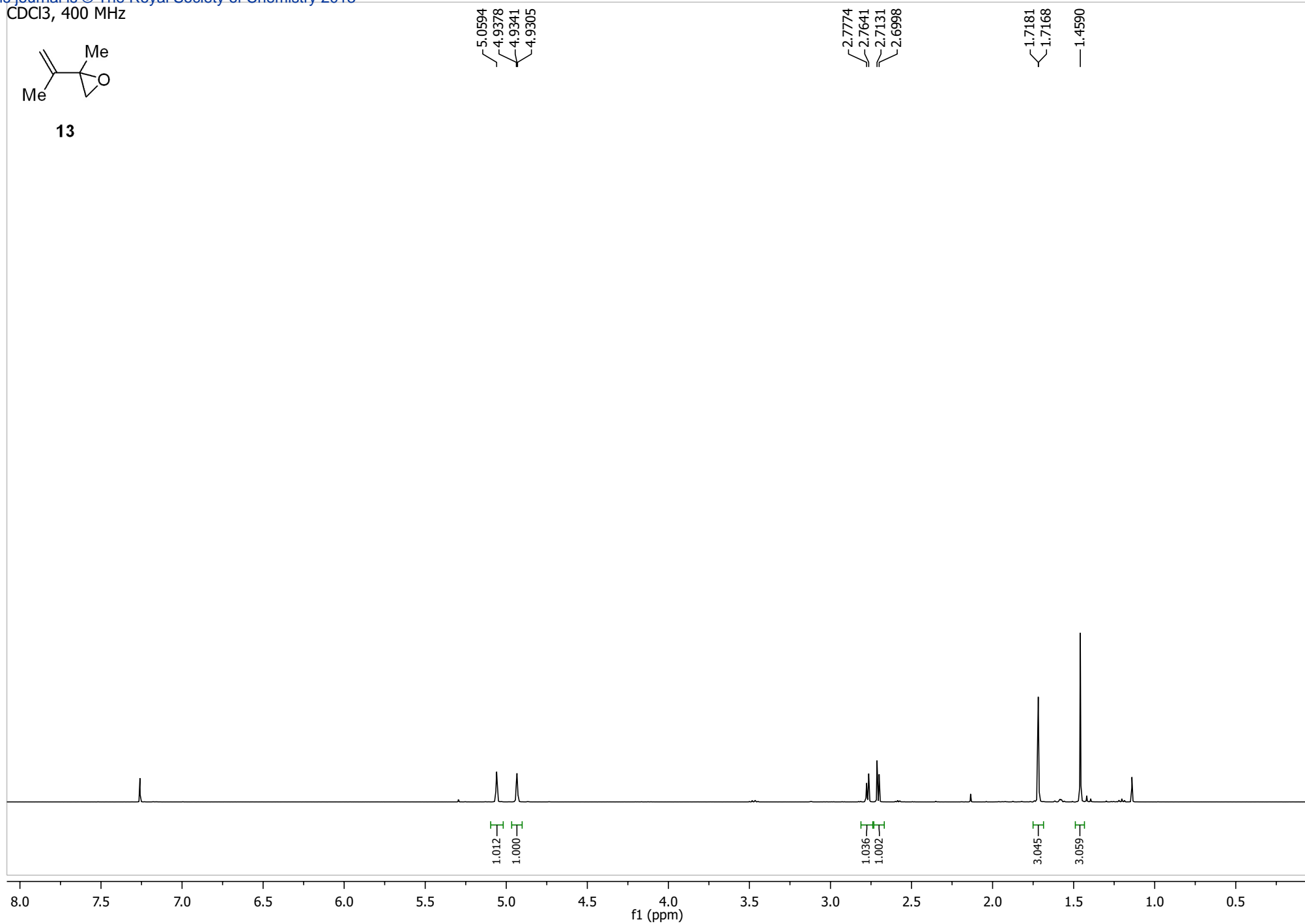




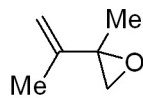
CDCl₃, 400 MHz



13



CDCl₃, 101 MHz



13

— 144.7985

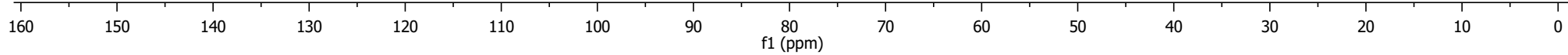
— 112.6811

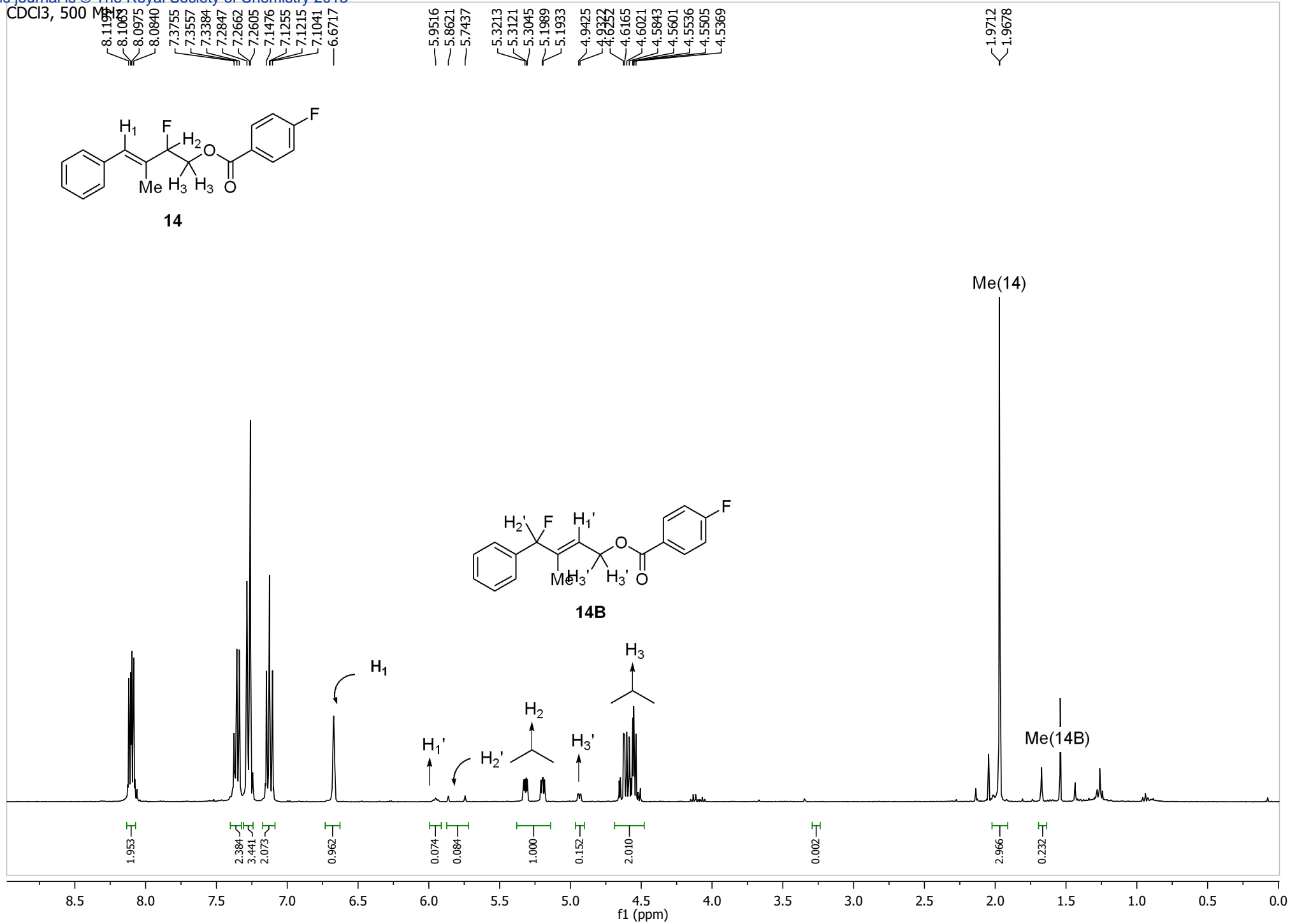
— 58.1058

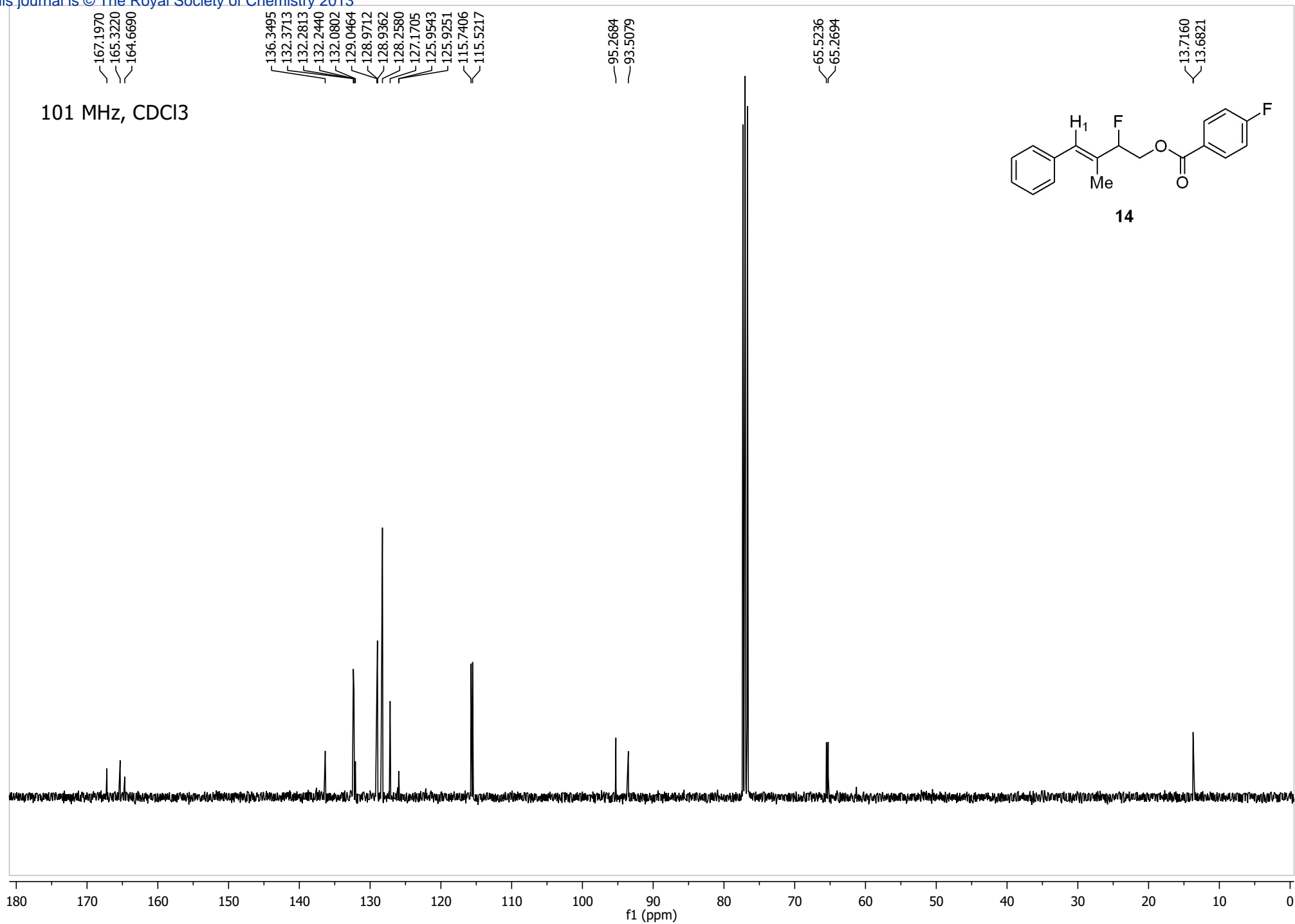
— 54.1785

— 20.7044

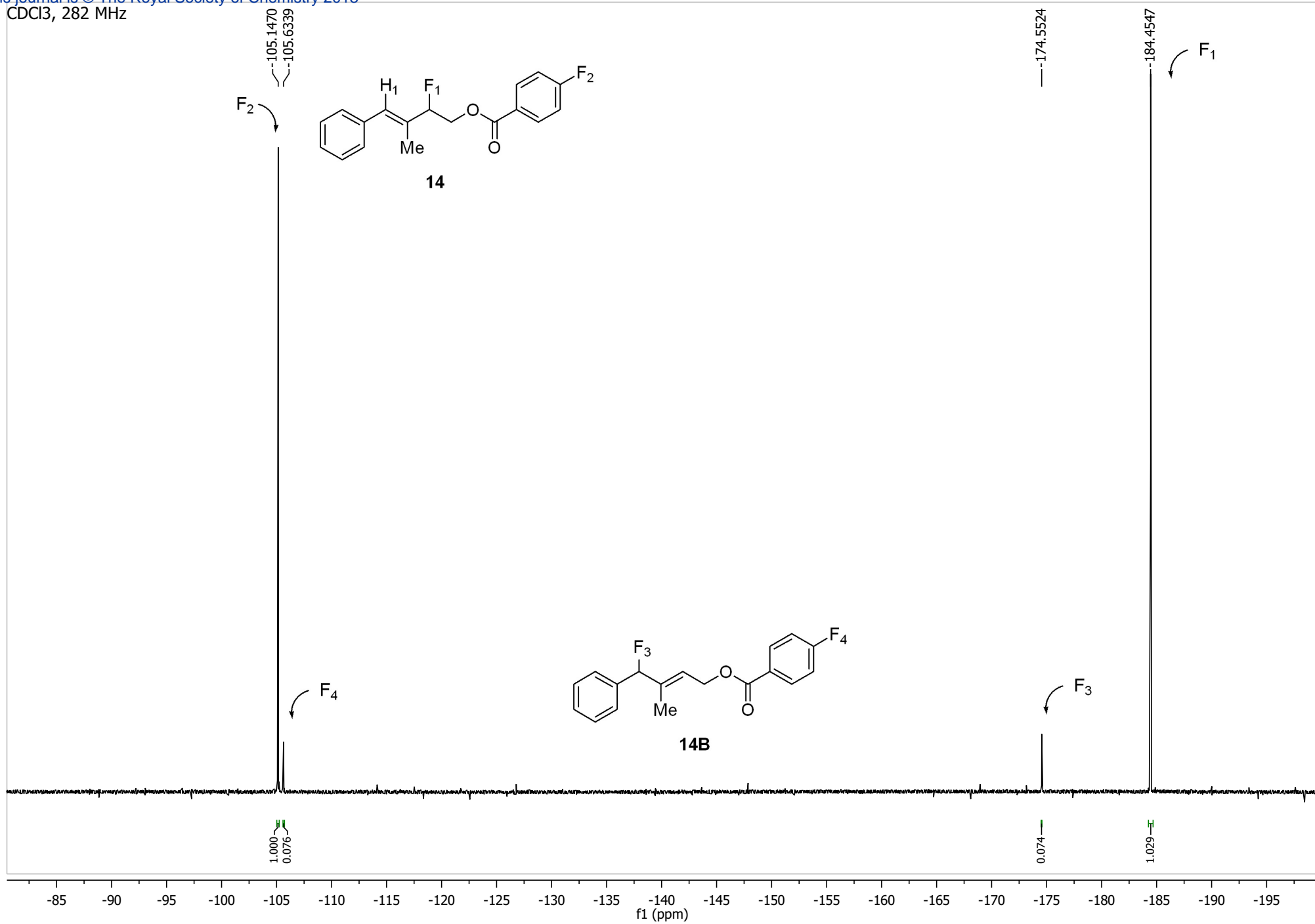
— 18.6010

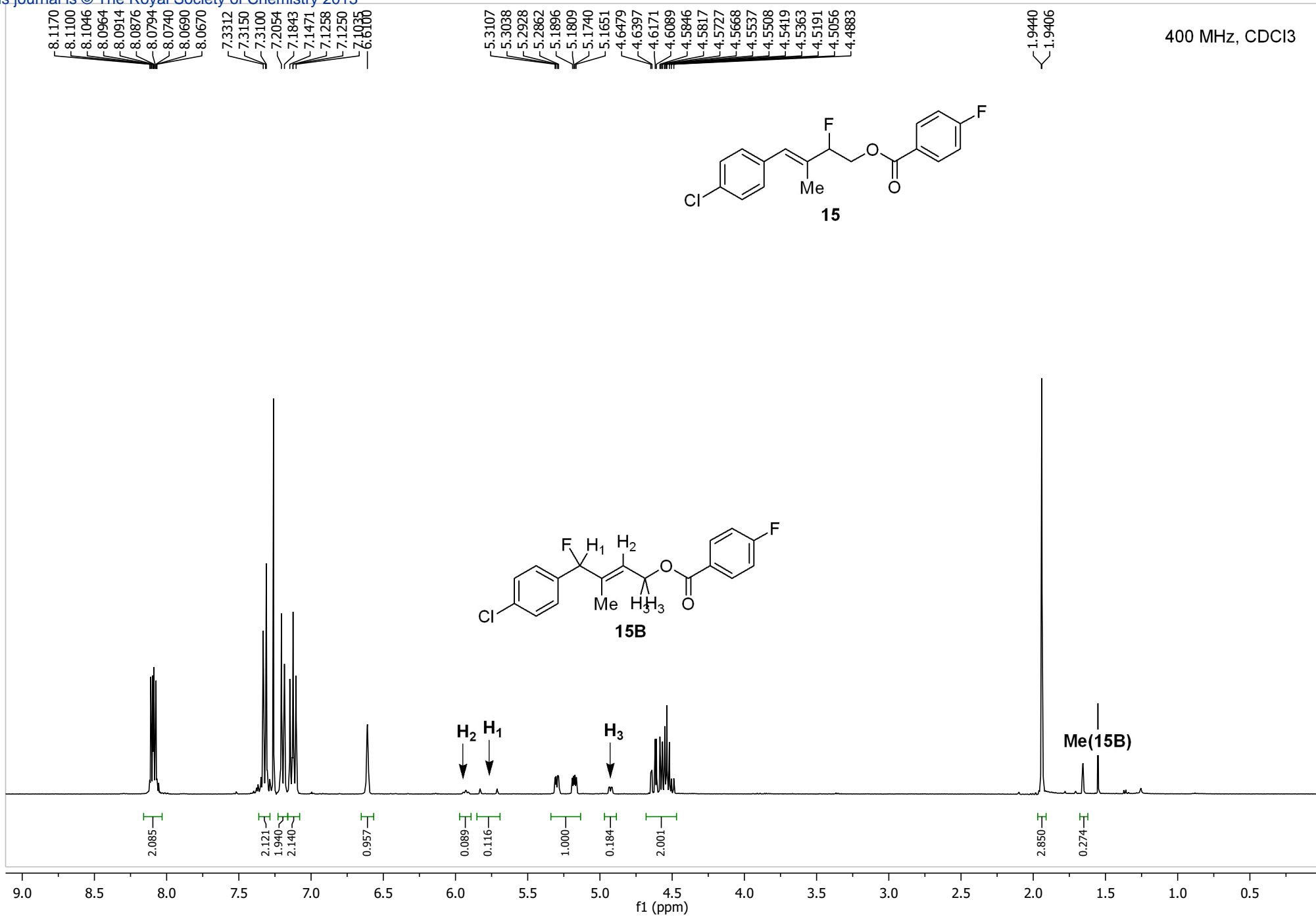


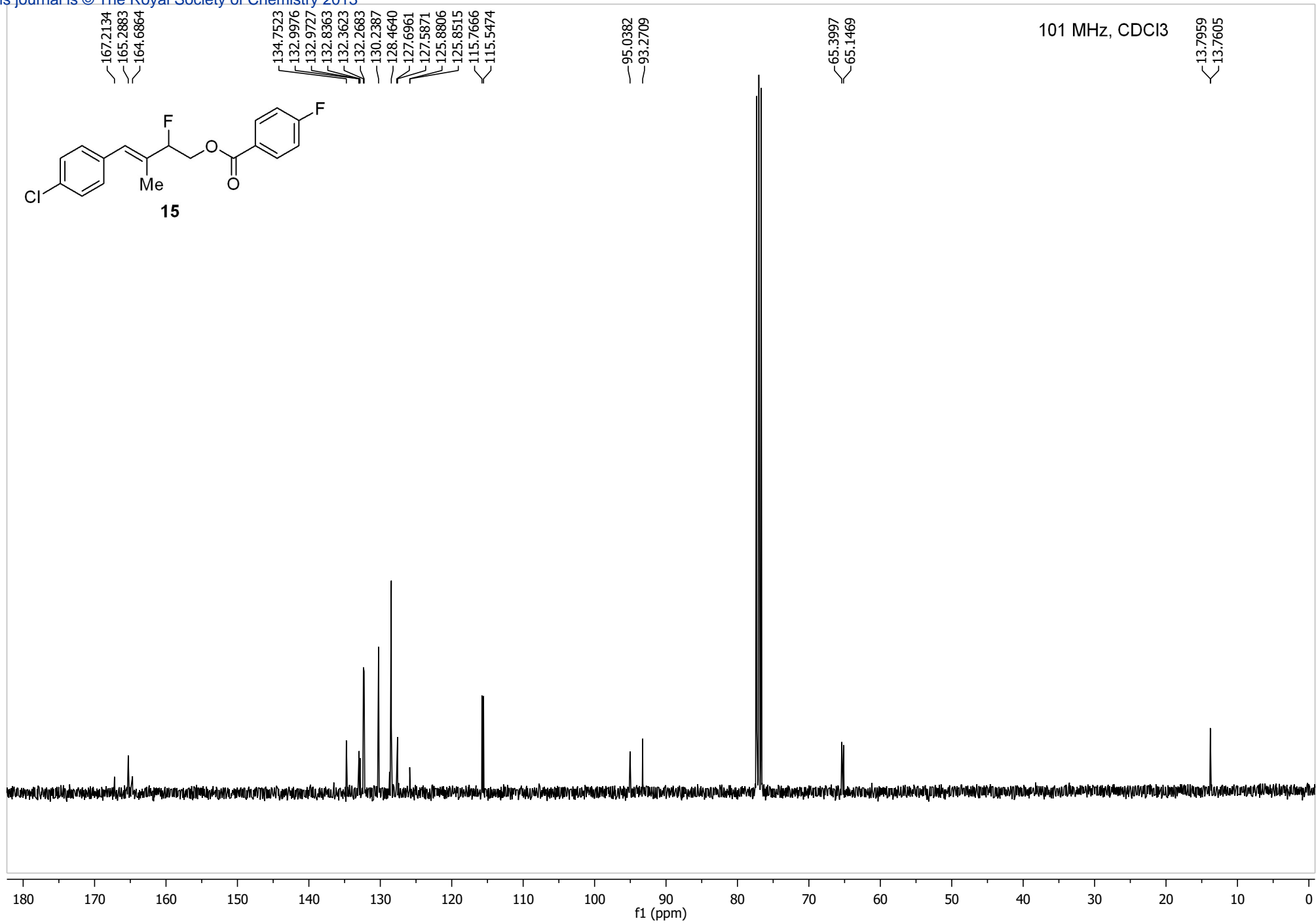




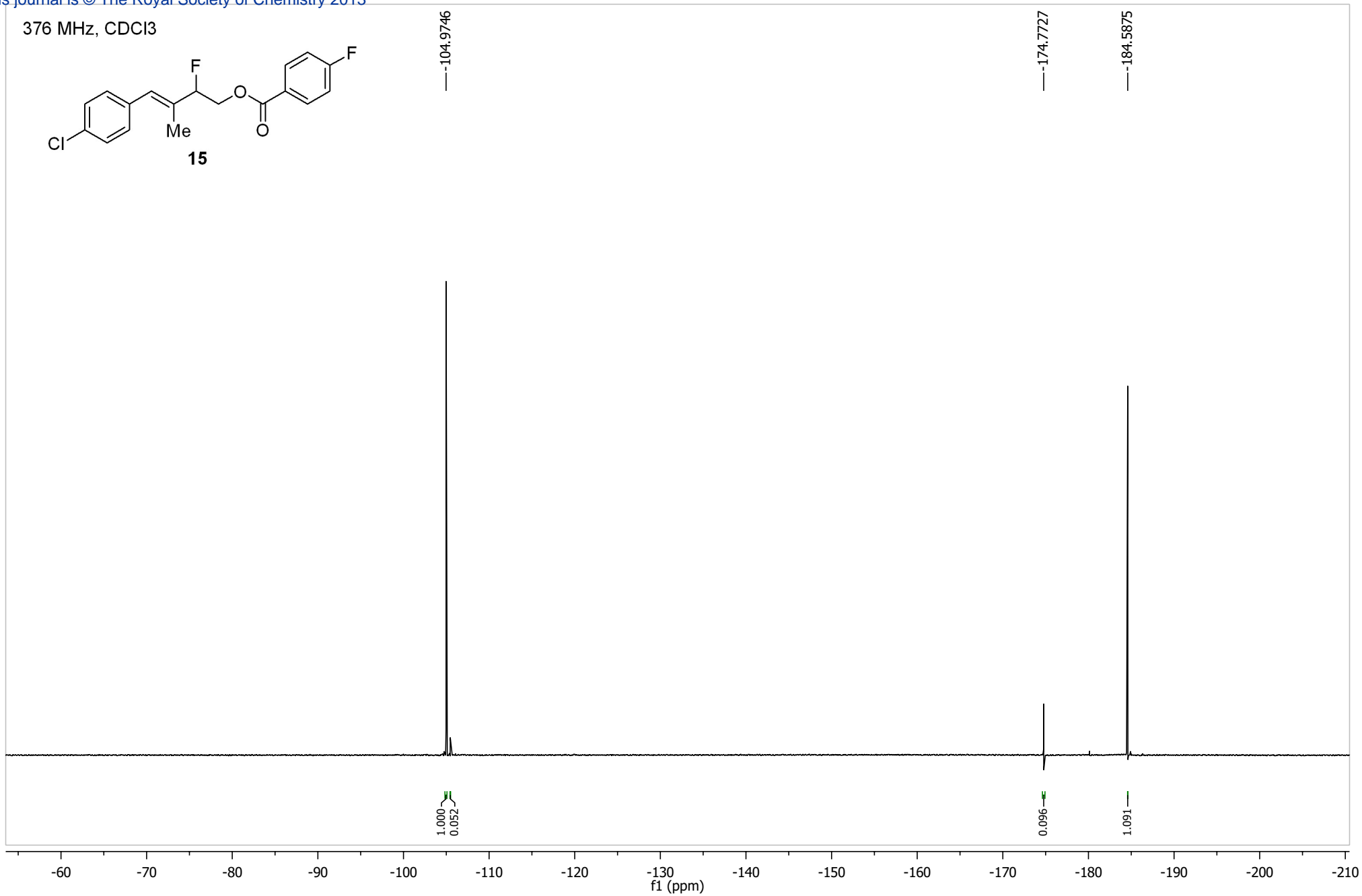
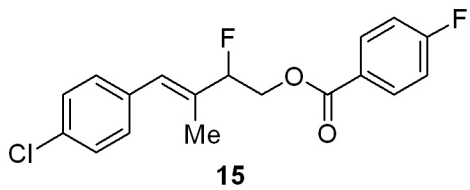
CDCl₃, 282 MHz



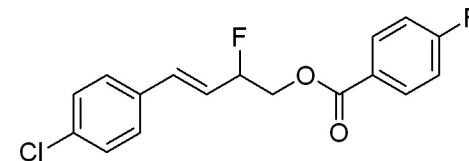
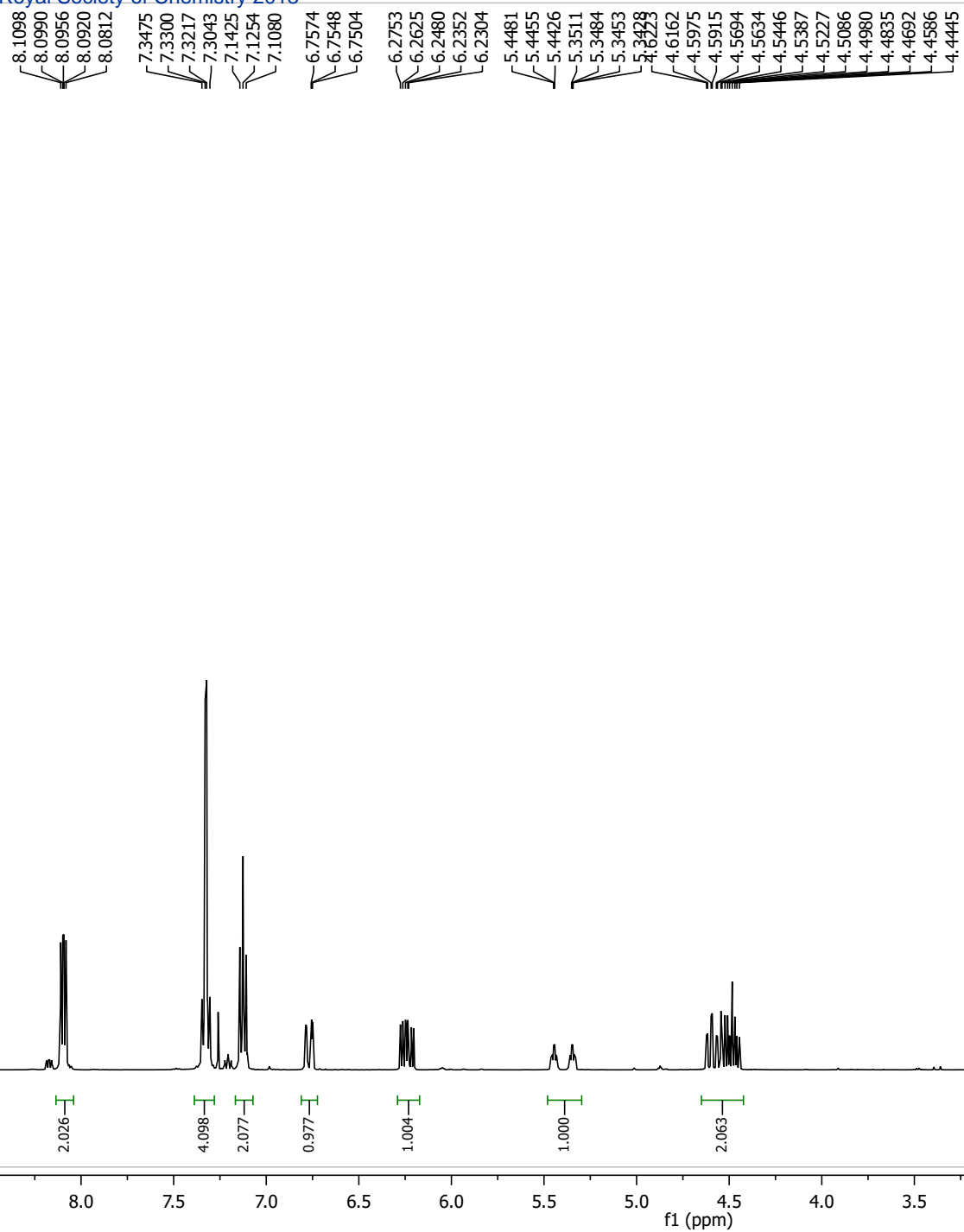




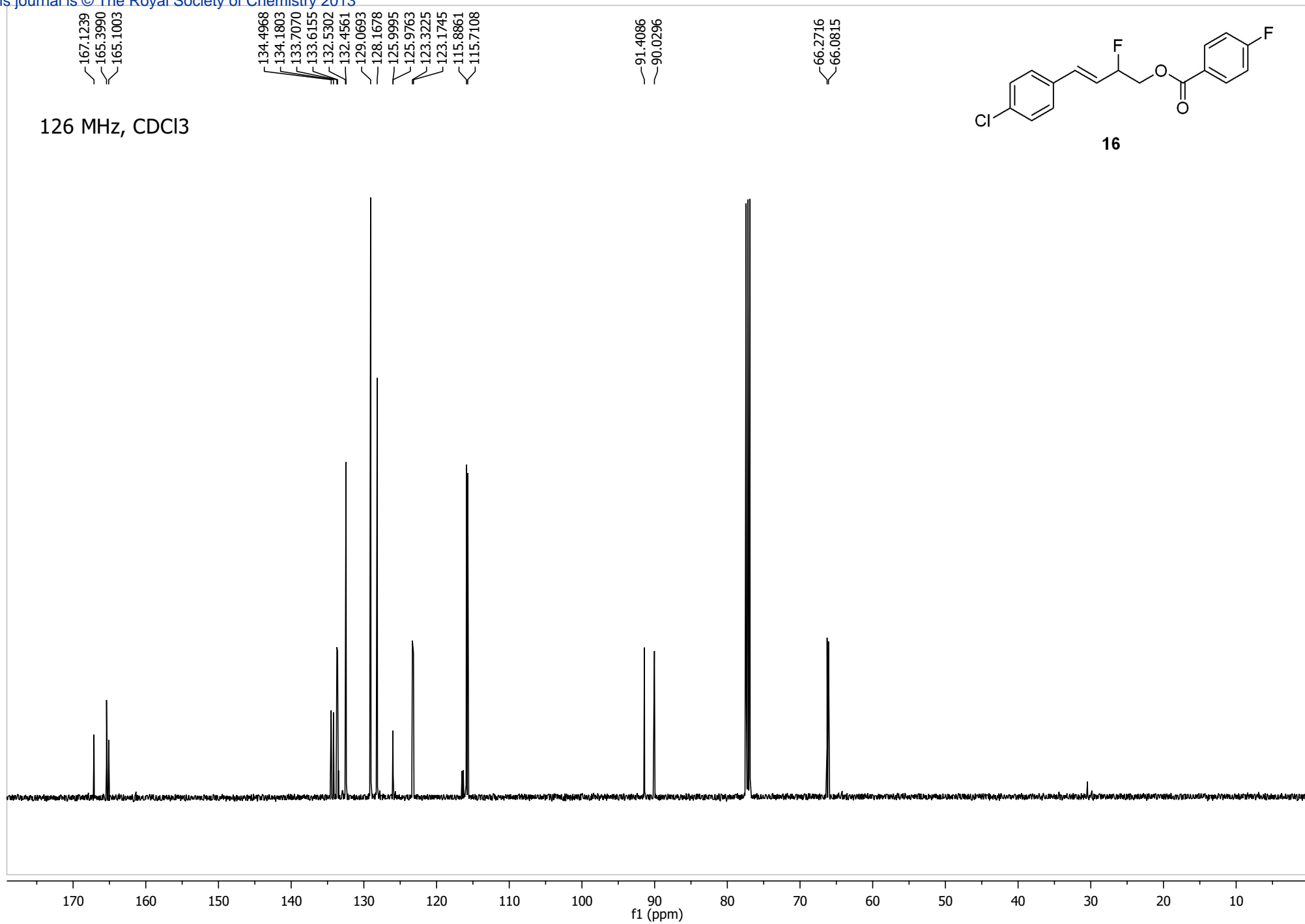
376 MHz, CDCl₃



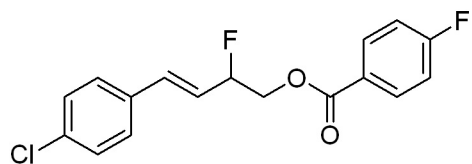
CDCl₃, 500 MHz



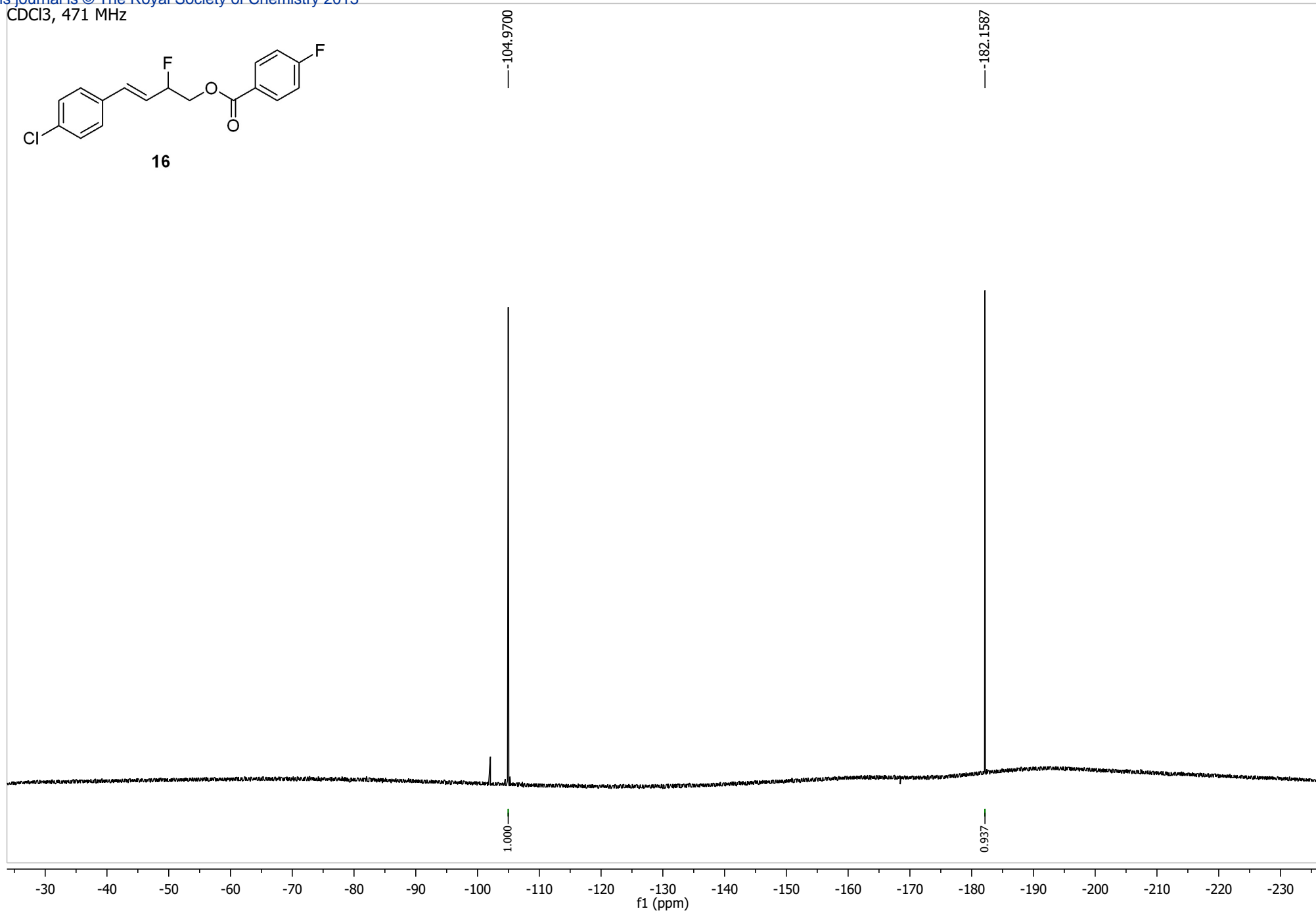
16

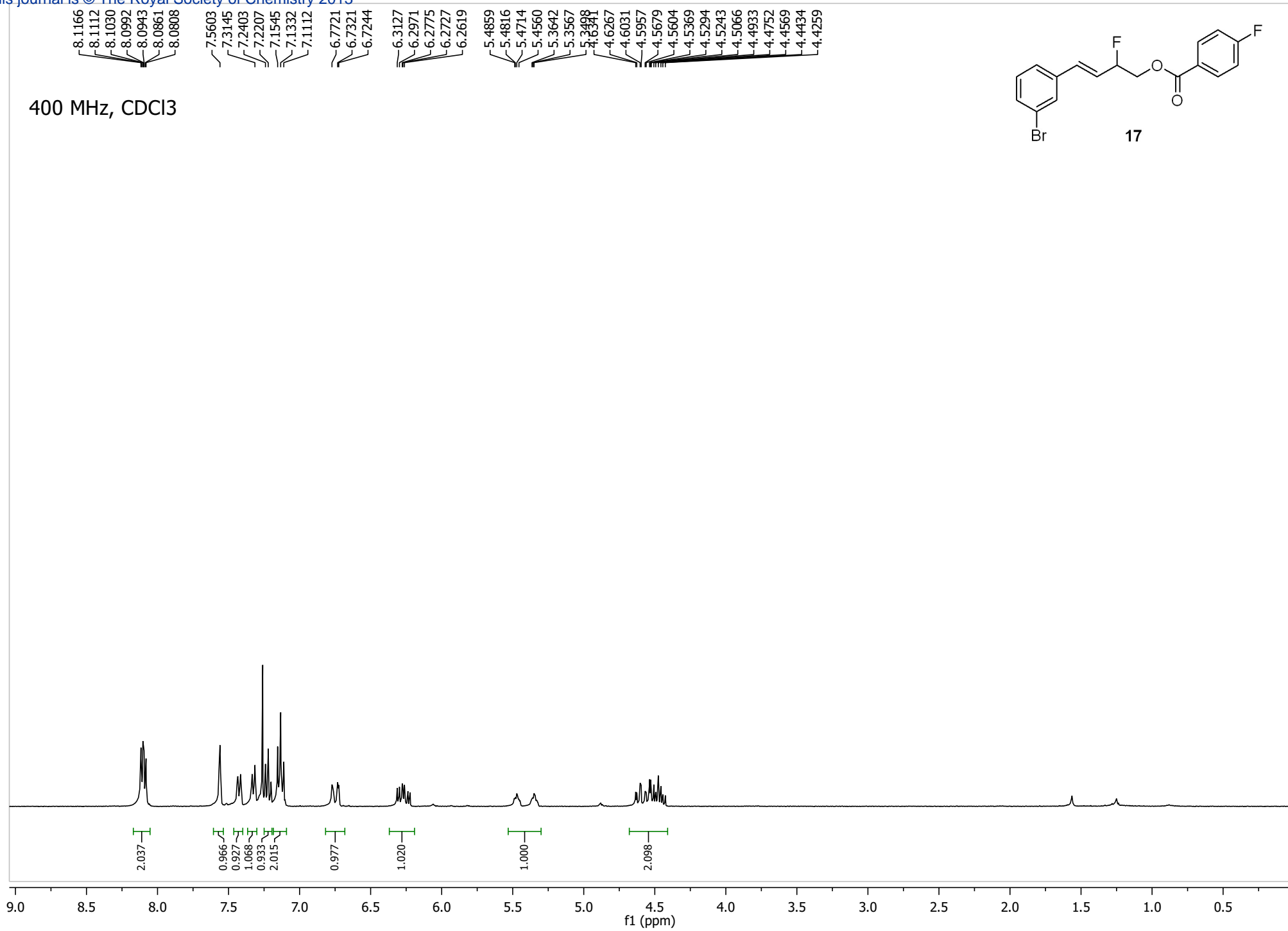


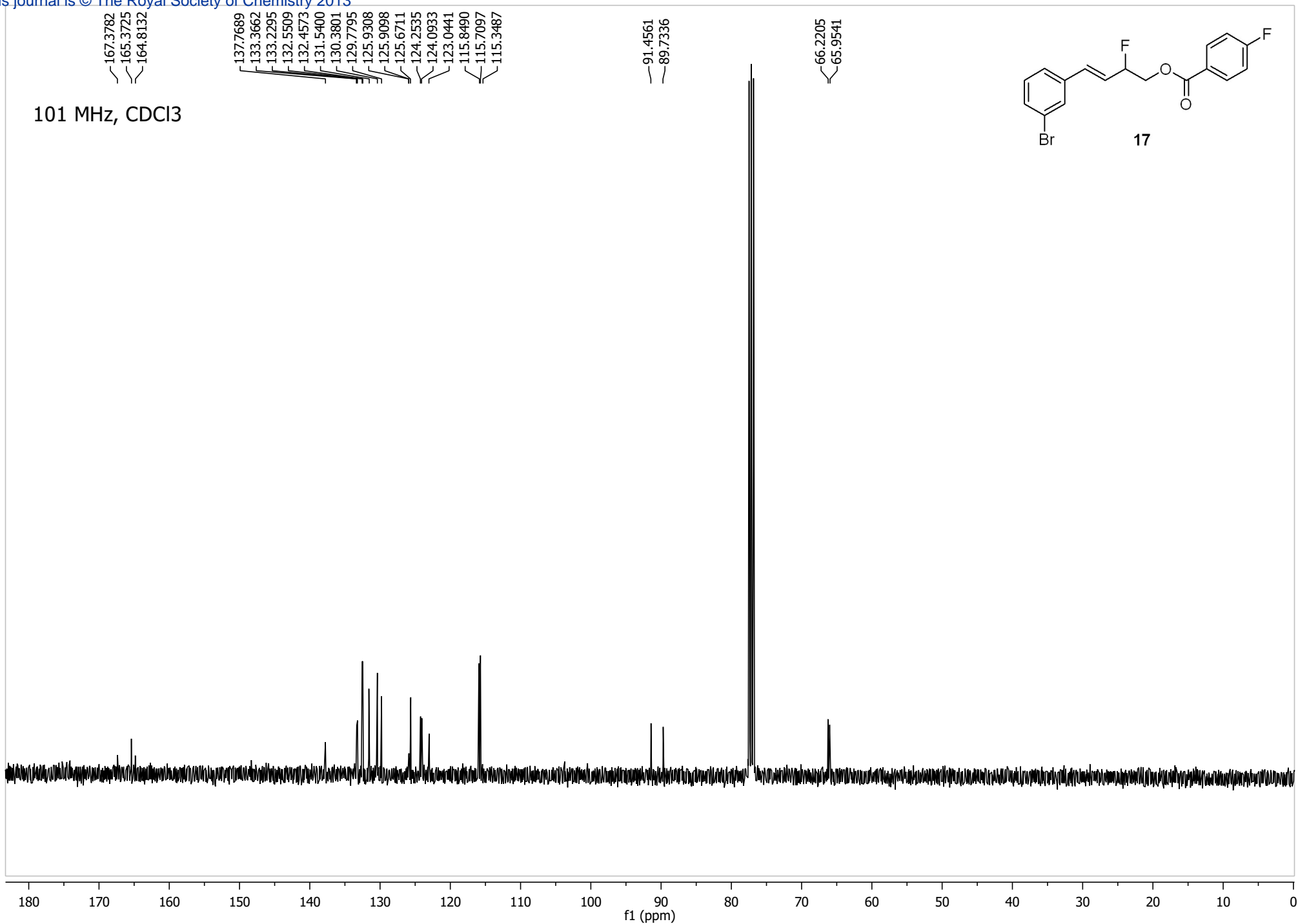
CDCl₃, 471 MHz



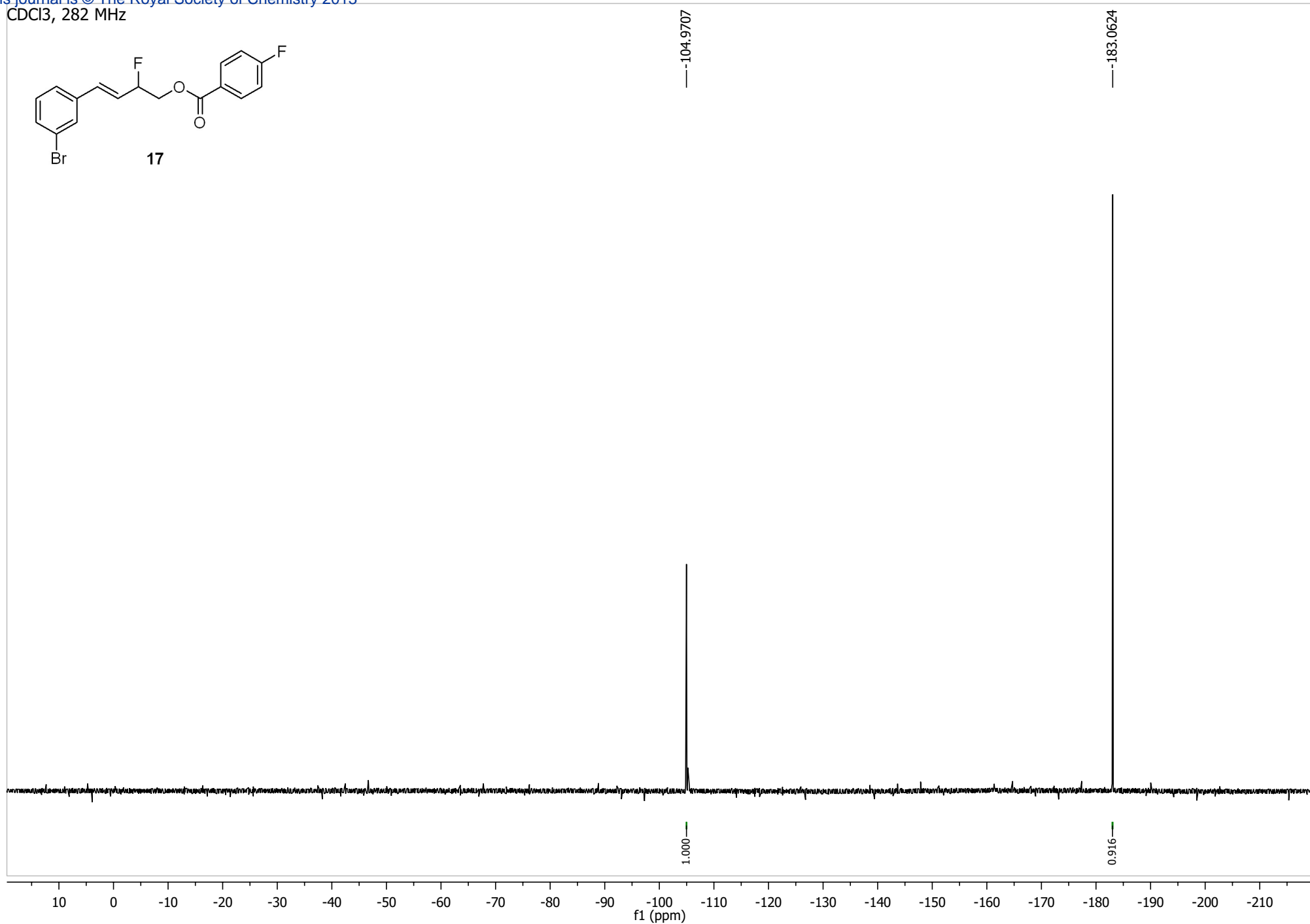
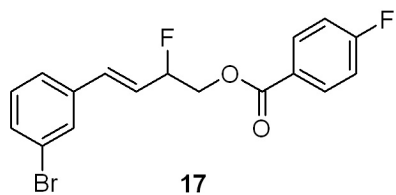
16

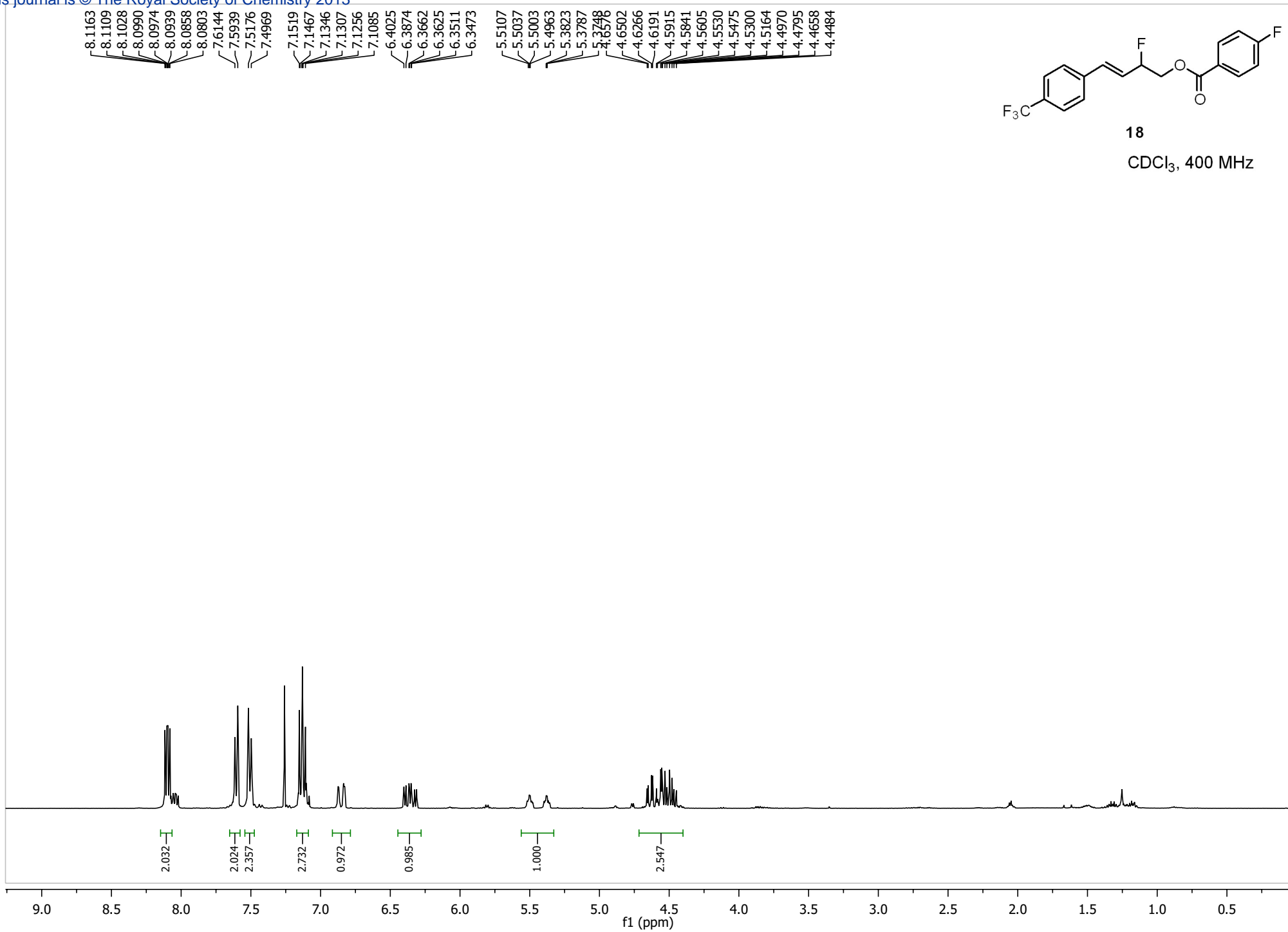


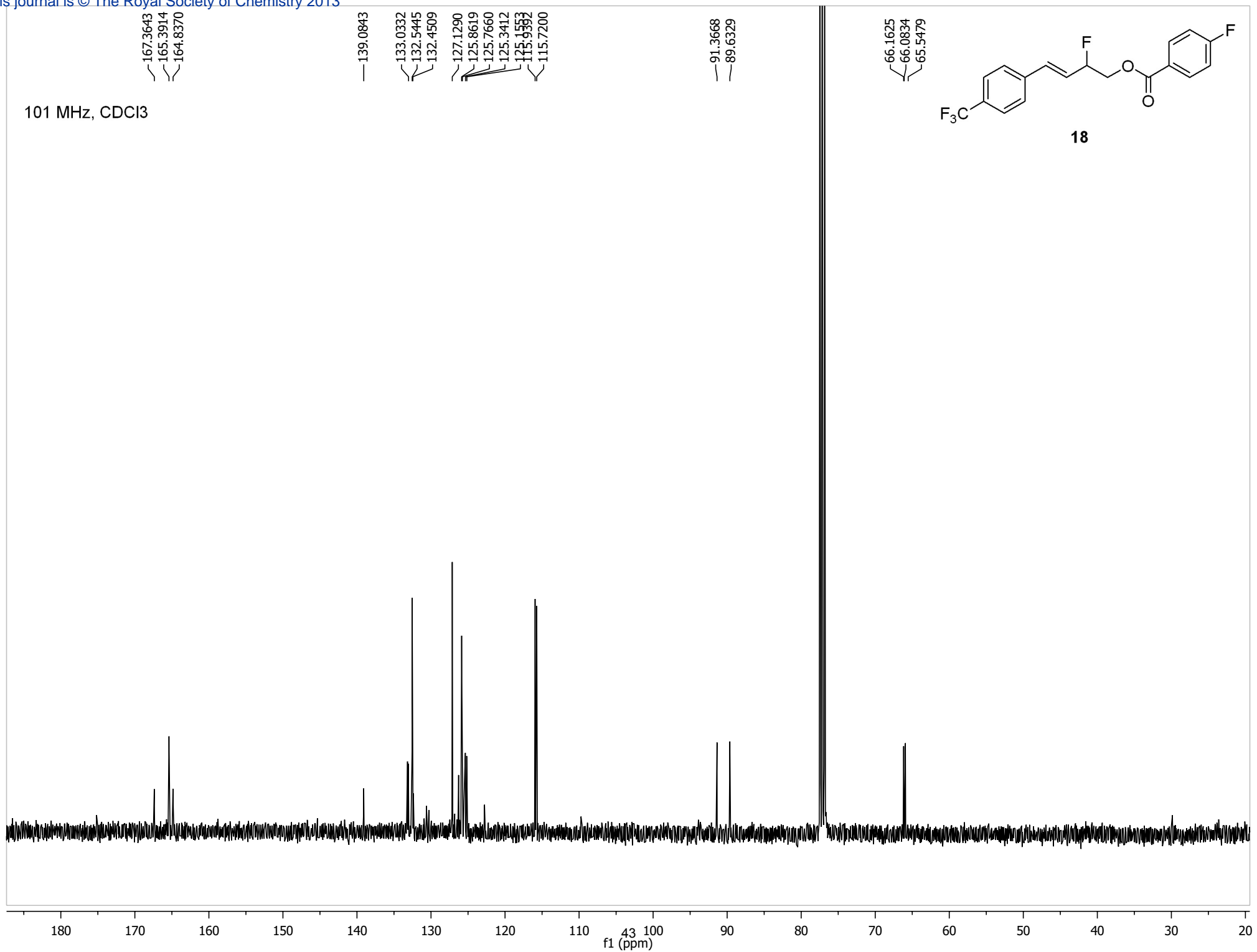


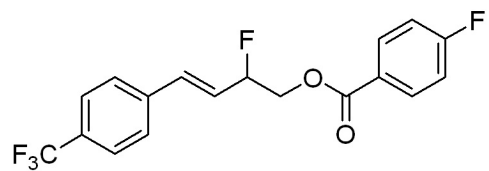


CDCl₃, 282 MHz



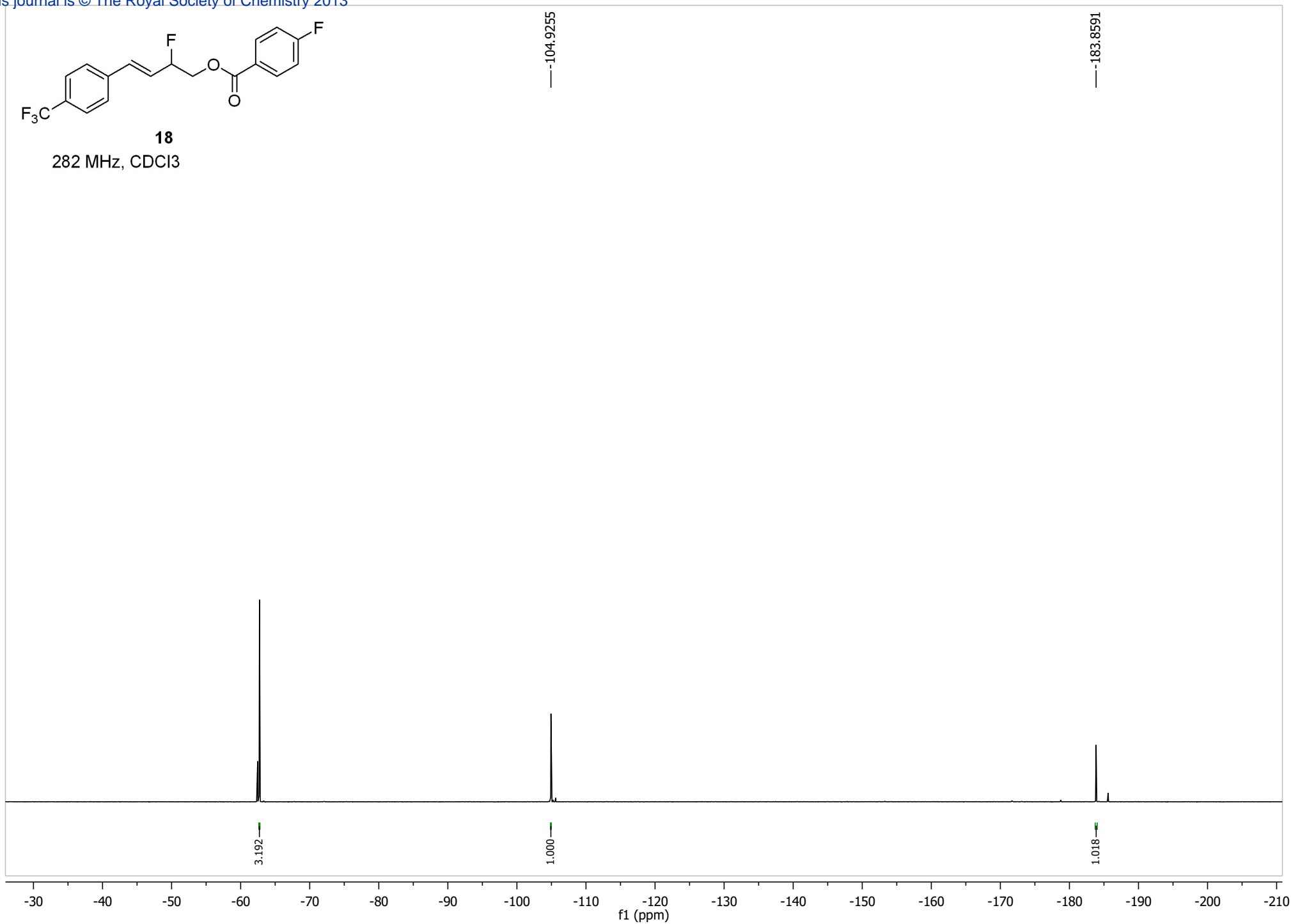




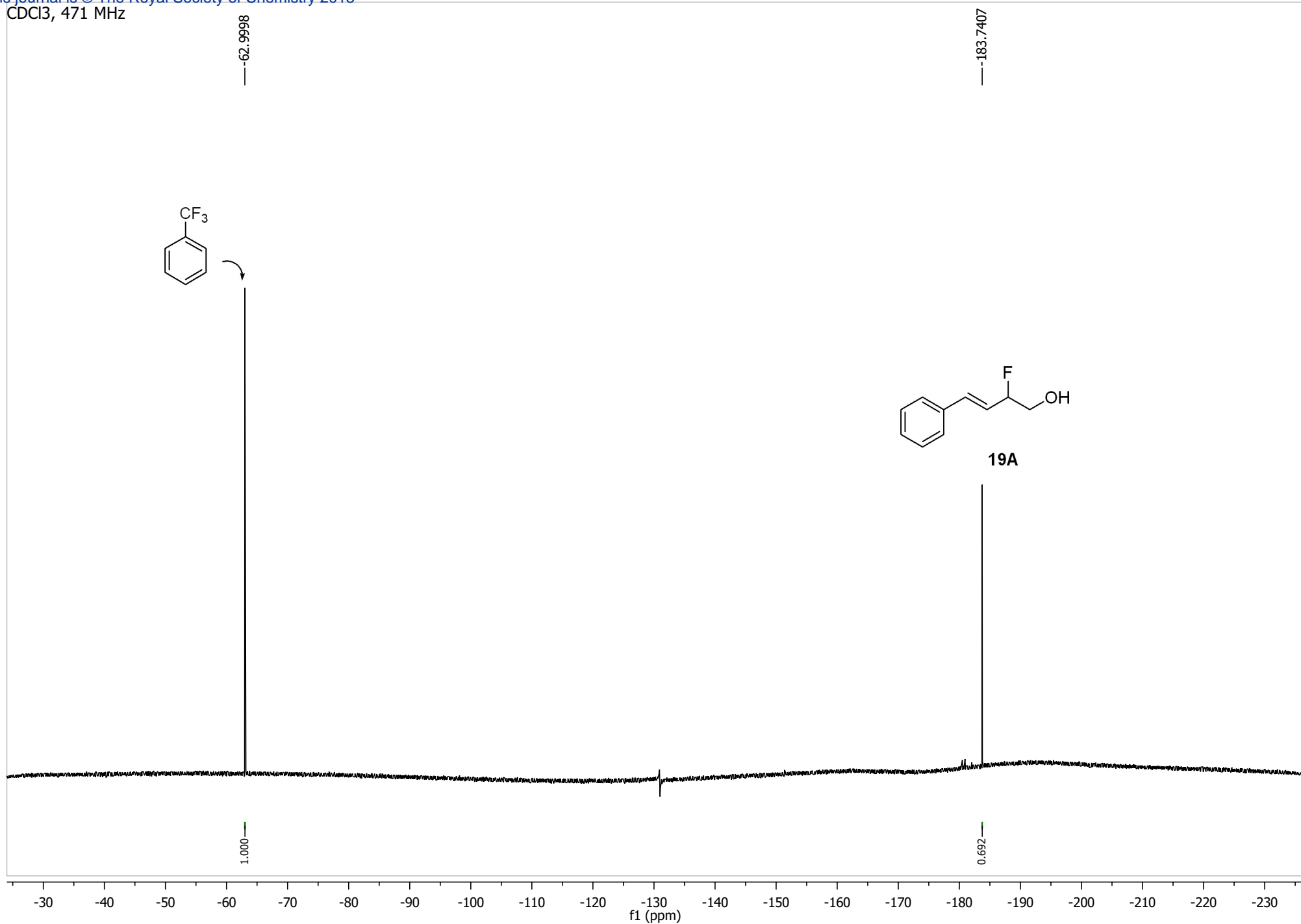


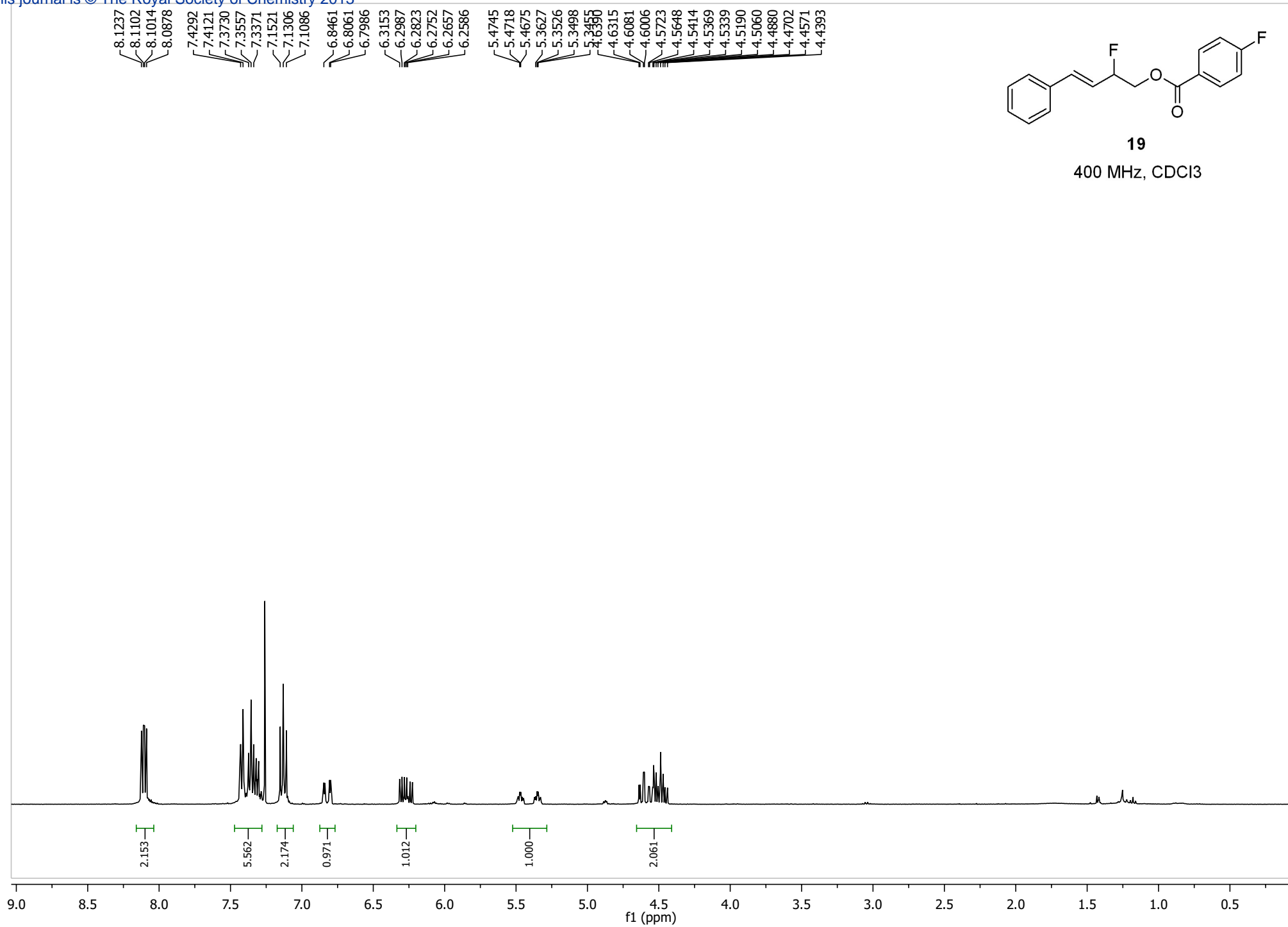
18

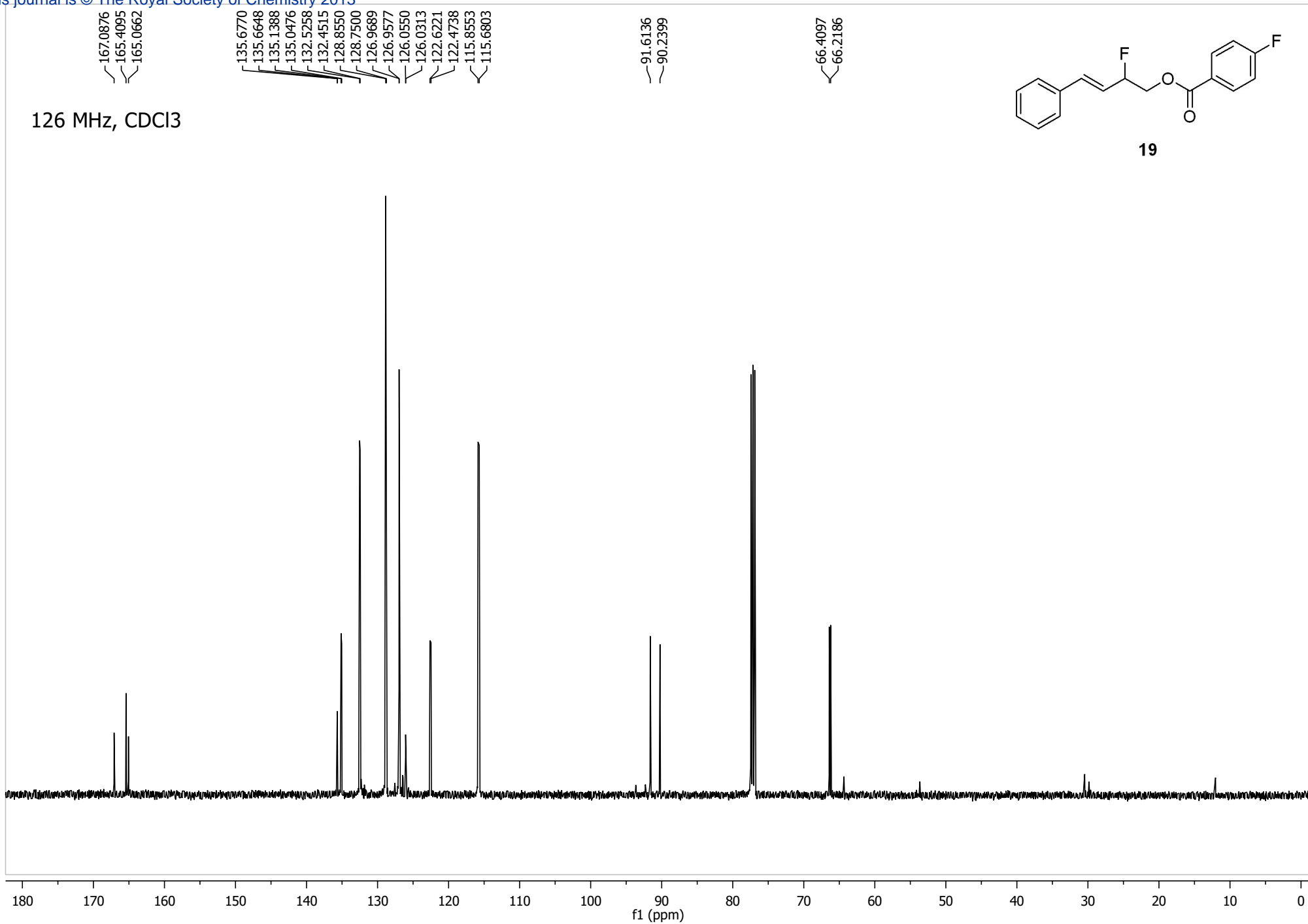
282 MHz, CDCl₃



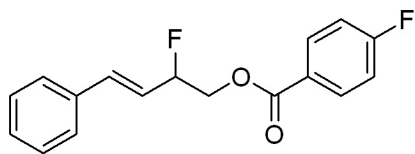
CDCl₃, 471 MHz



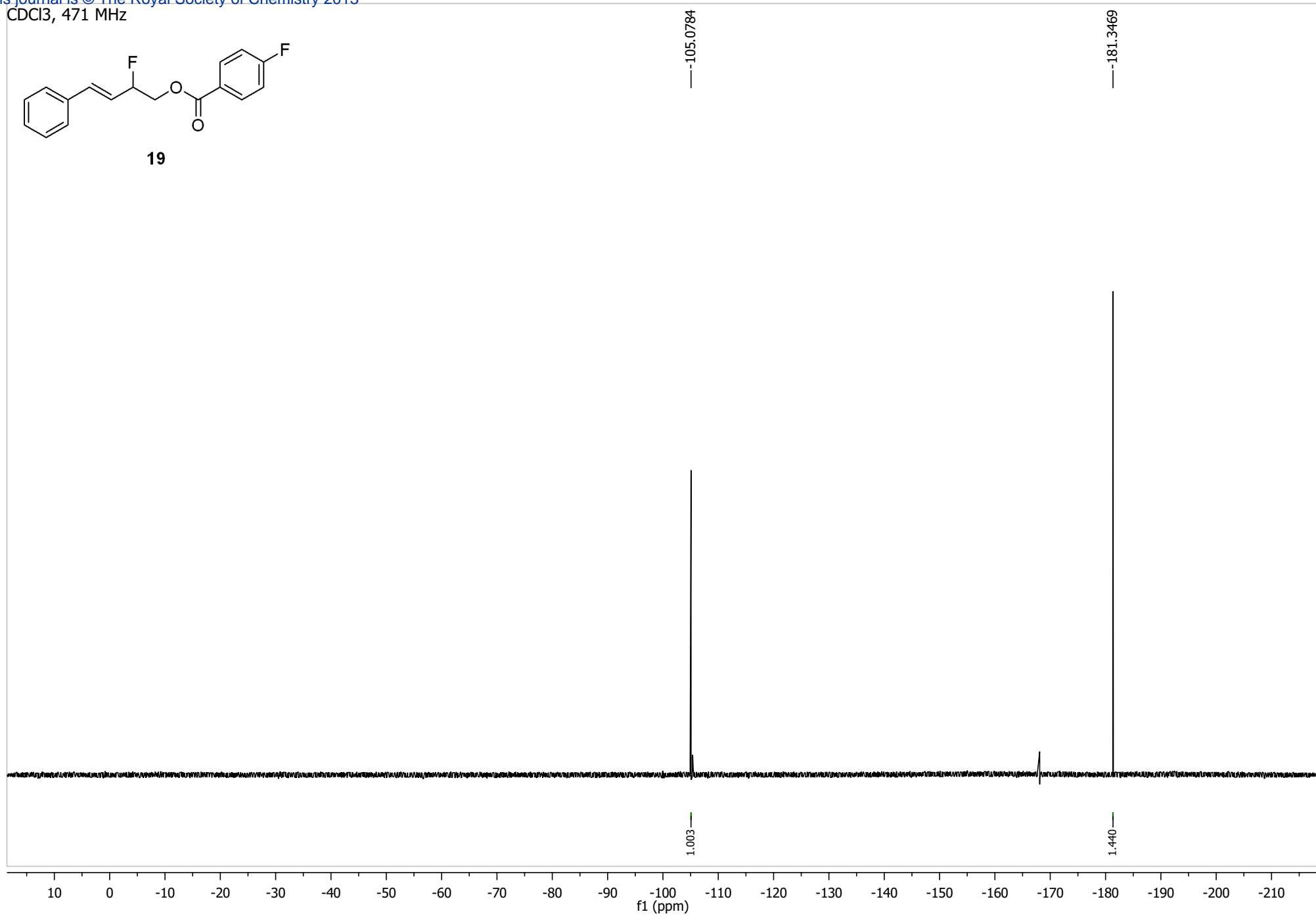


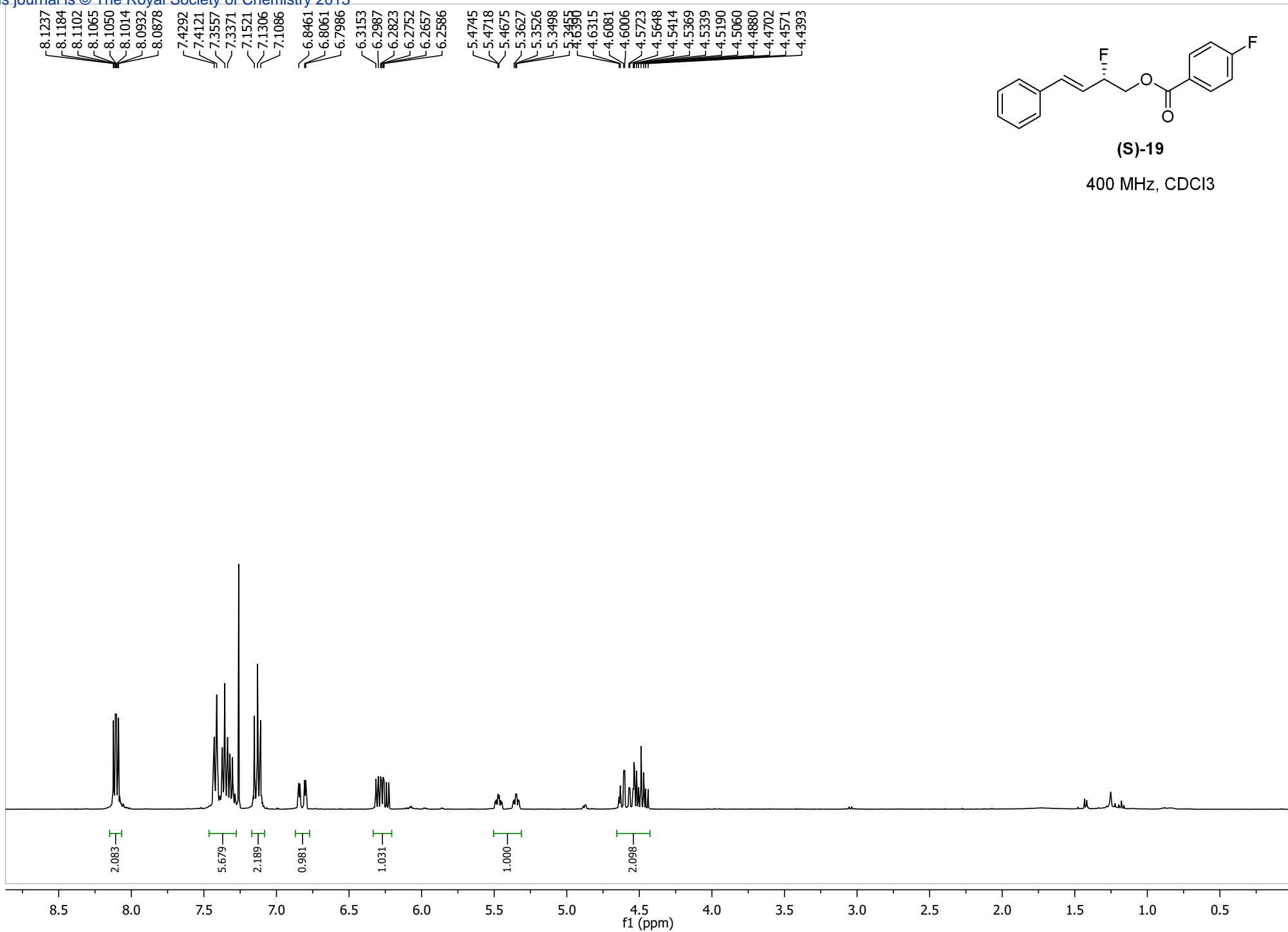


CDCl₃, 471 MHz

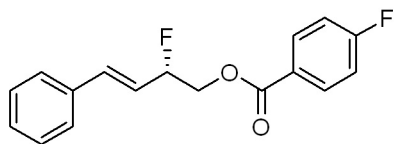


19

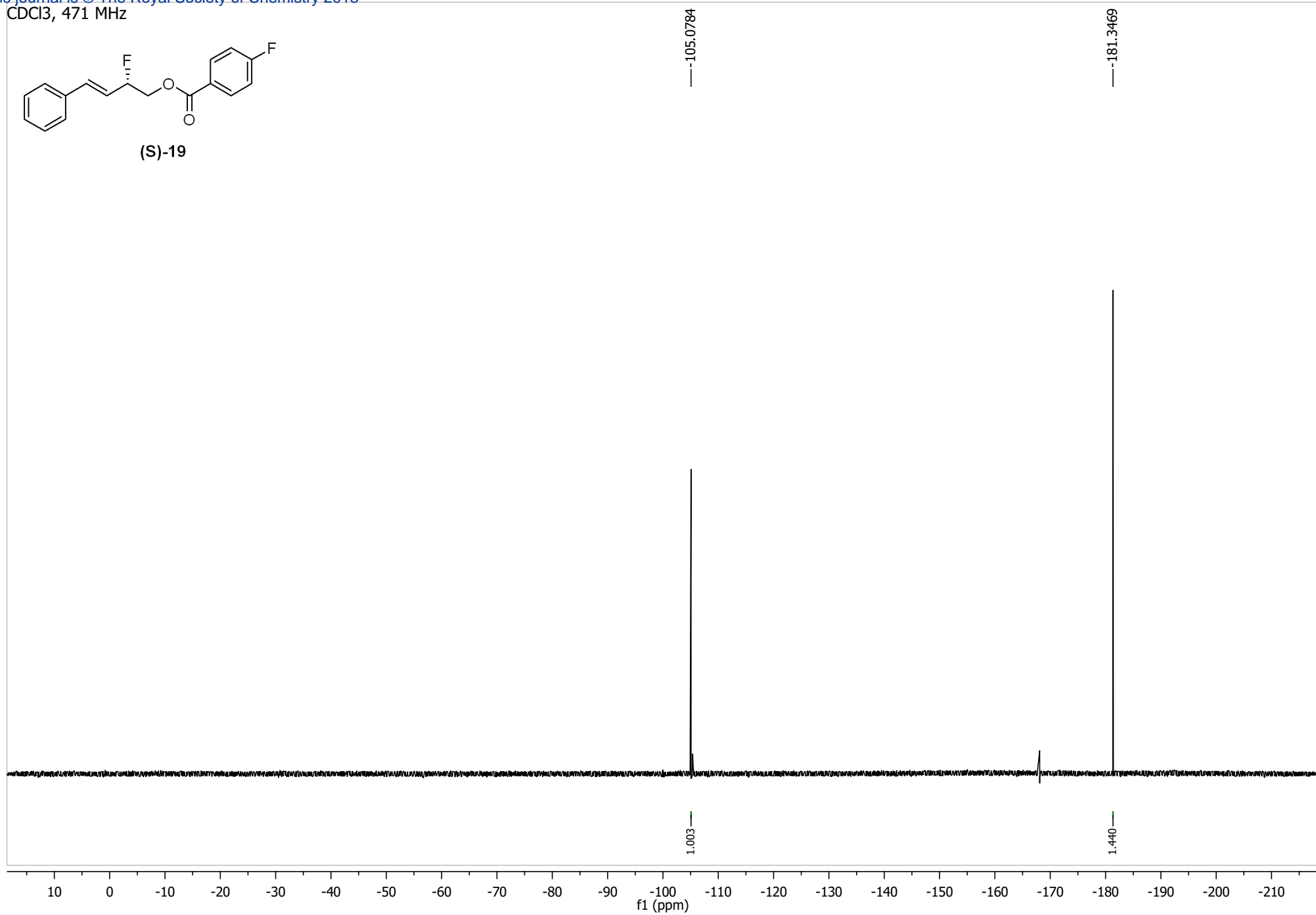




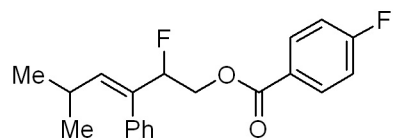
CDCl₃, 471 MHz



(S)-19



CDCl₃, 500 MHz



20

8.0335
7.3794
7.3654
7.3514
7.3280
7.3141
7.2307
7.2164
7.1989
7.1851
7.1176
7.1016
7.0857

5.7630
5.7432

5.3945
5.3800

5.2976
5.2837

4.4164
4.3913

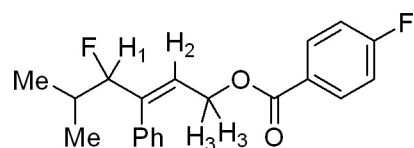
4.3613
4.3374

4.3291
4.3114

4.2877
4.2749

2.3345

0.9601
0.9430
0.9273



20B

H₂

H₁ & H₃

1.965

3.767

2.054

2.029

0.209

0.961

1.000

0.603

1.962

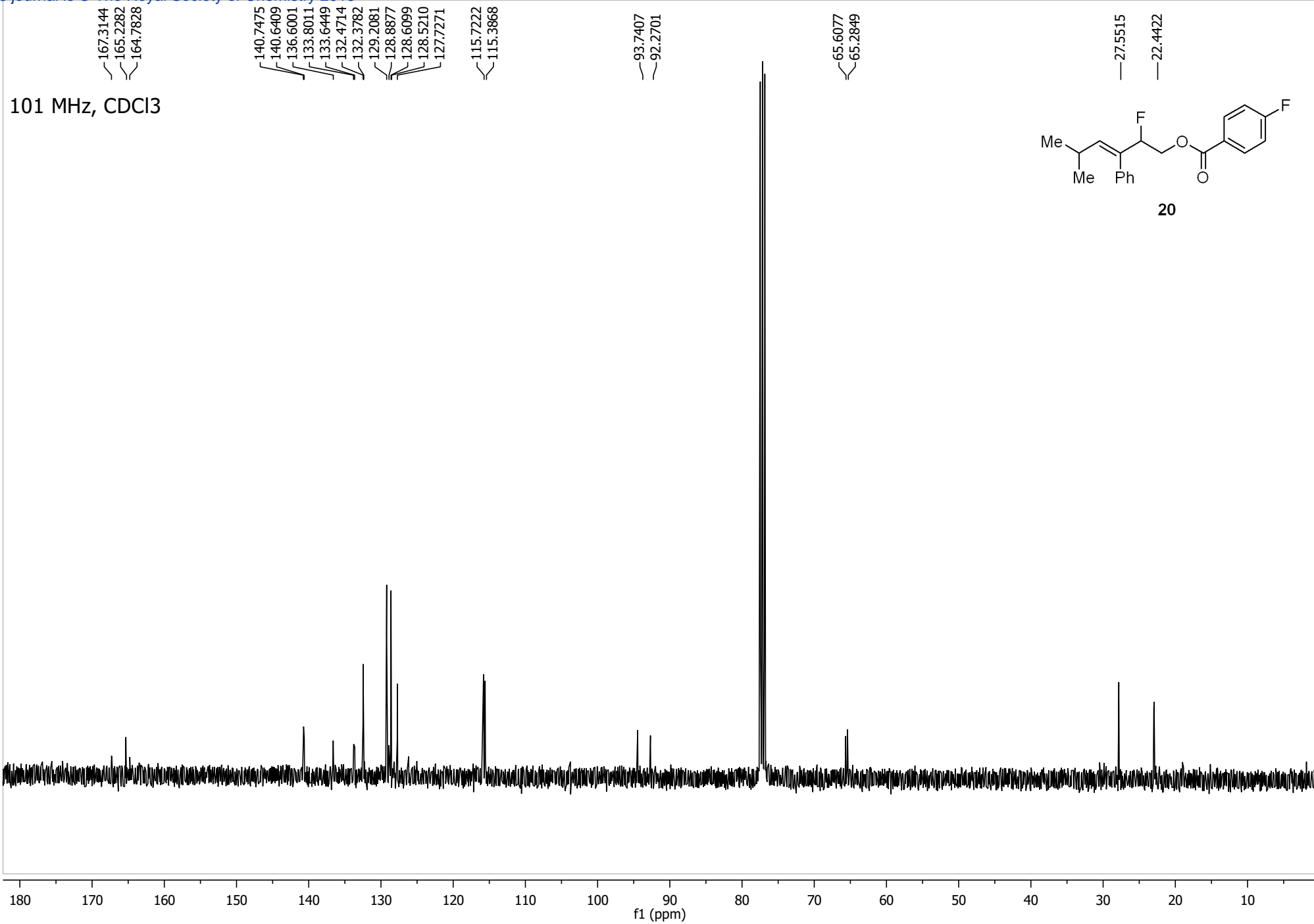
0.931

6.640

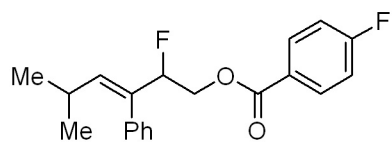
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

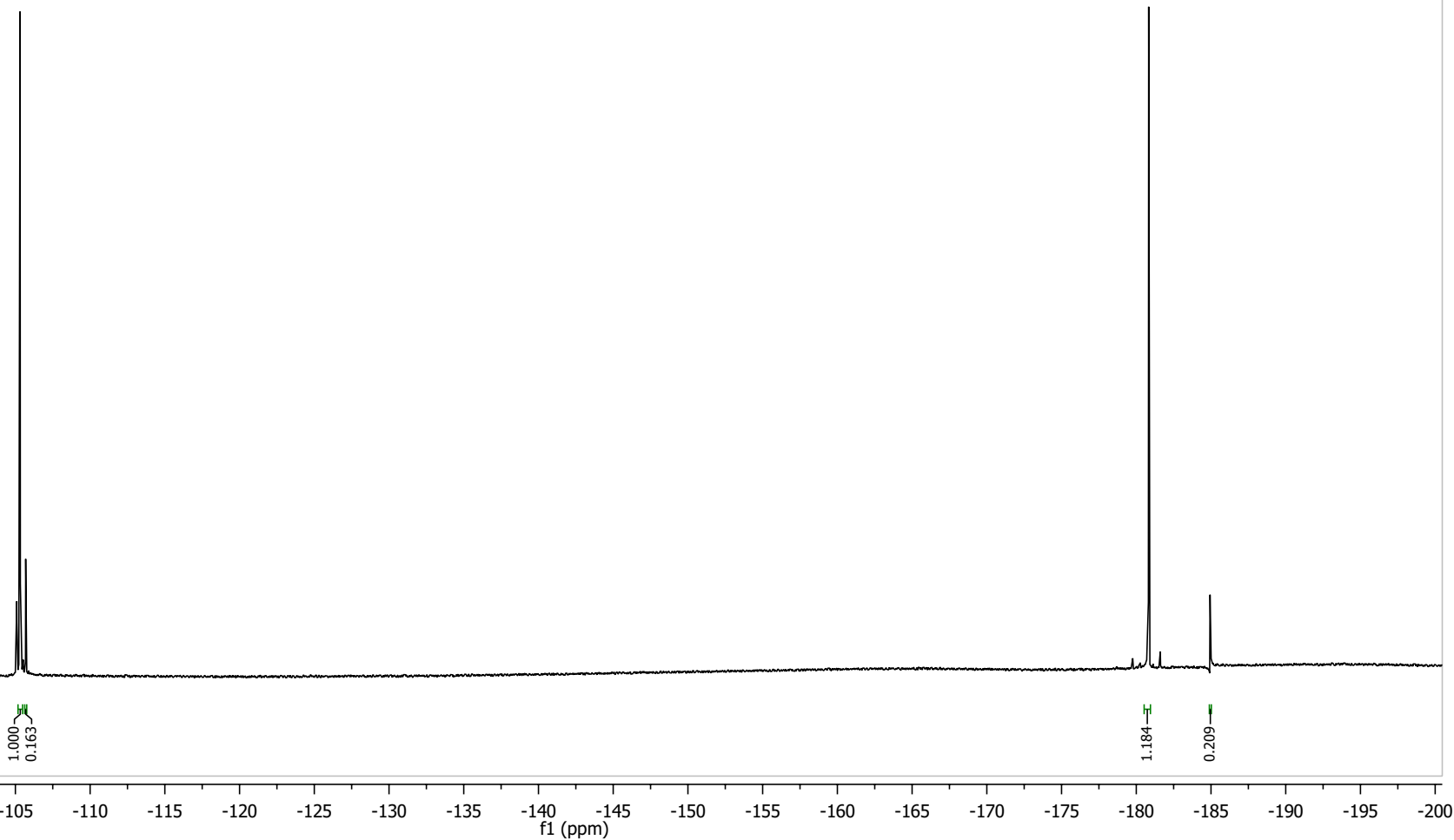
101 MHz, CDCl₃

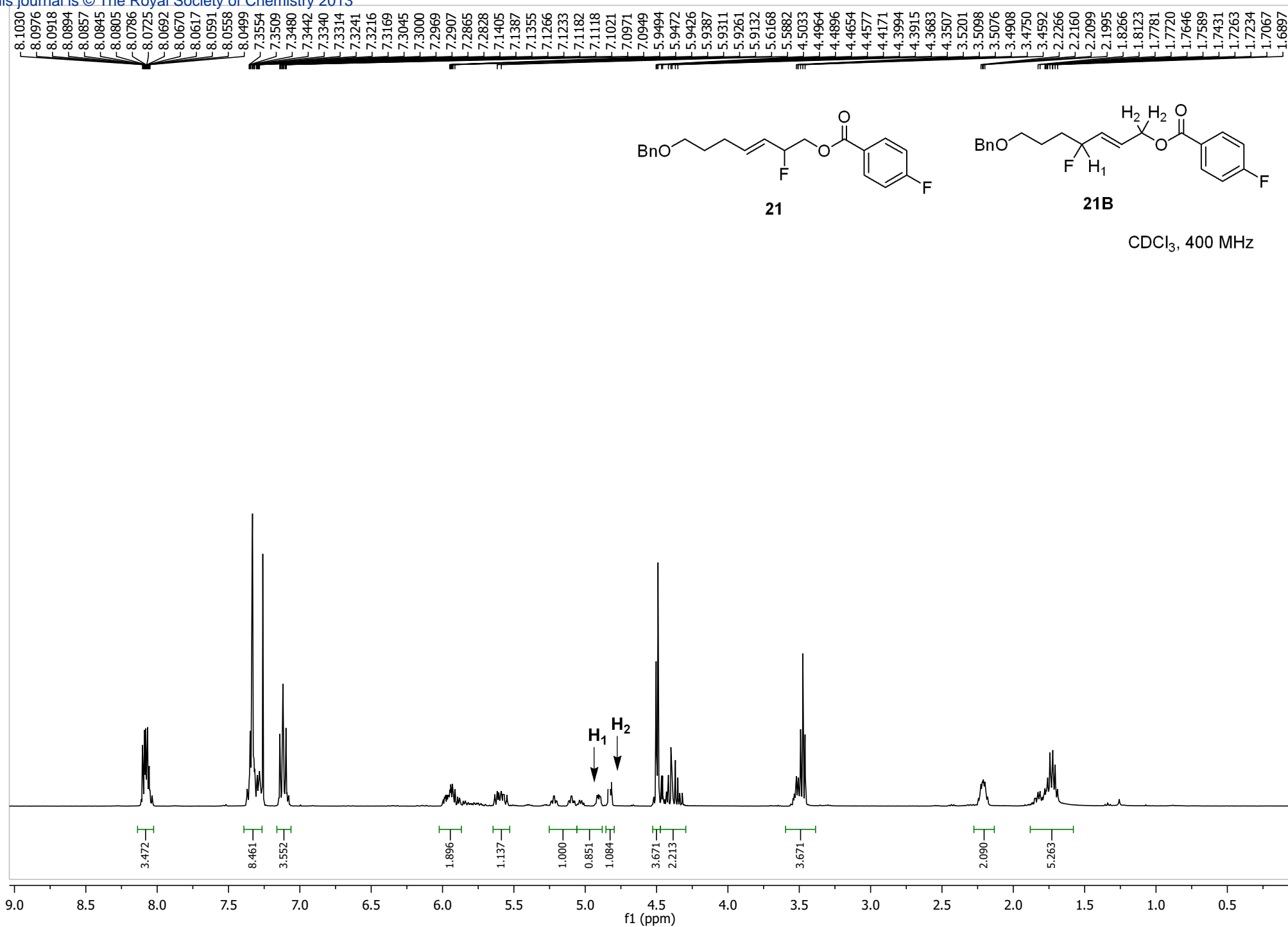


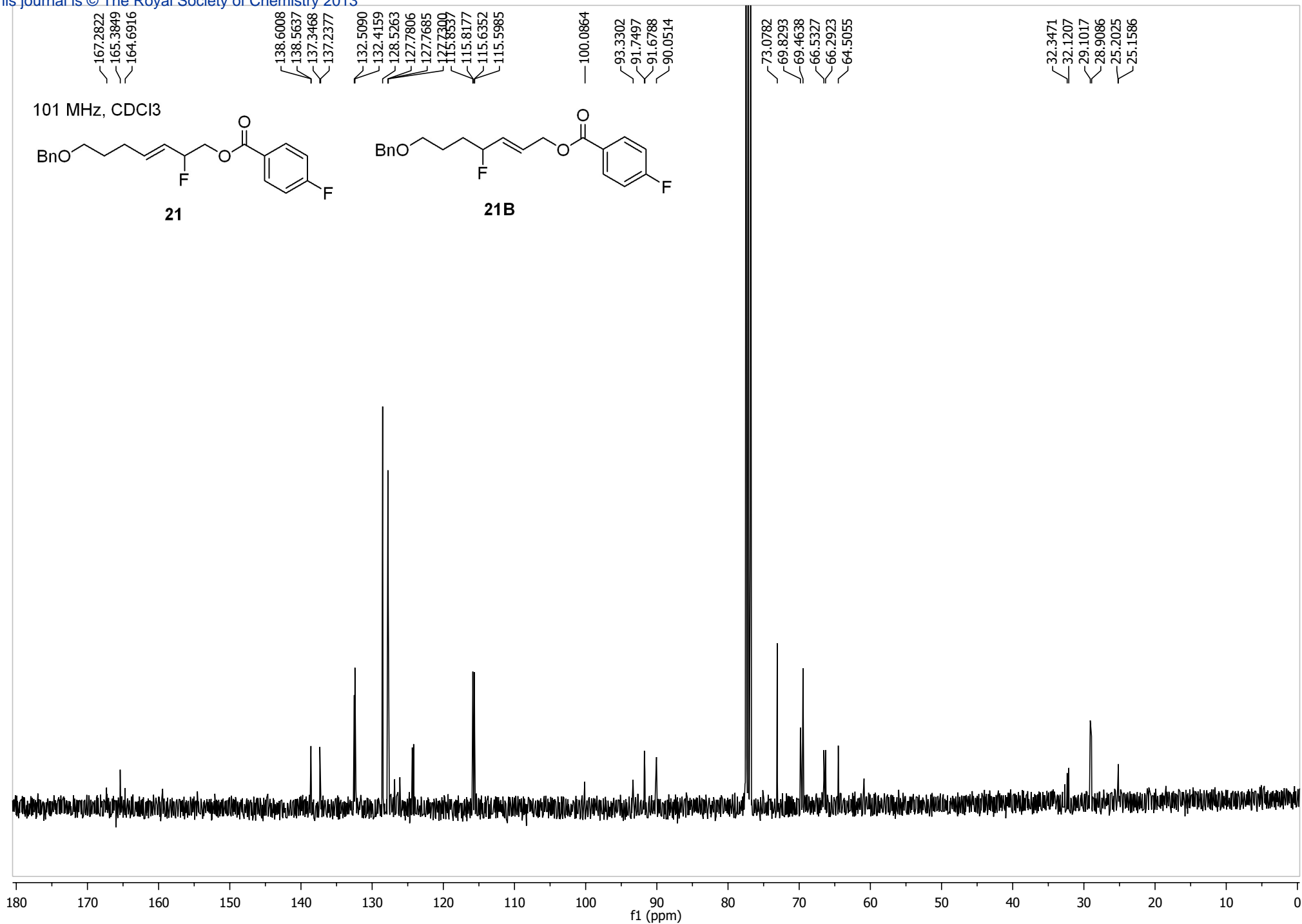
CDCl₃, 471 MHz

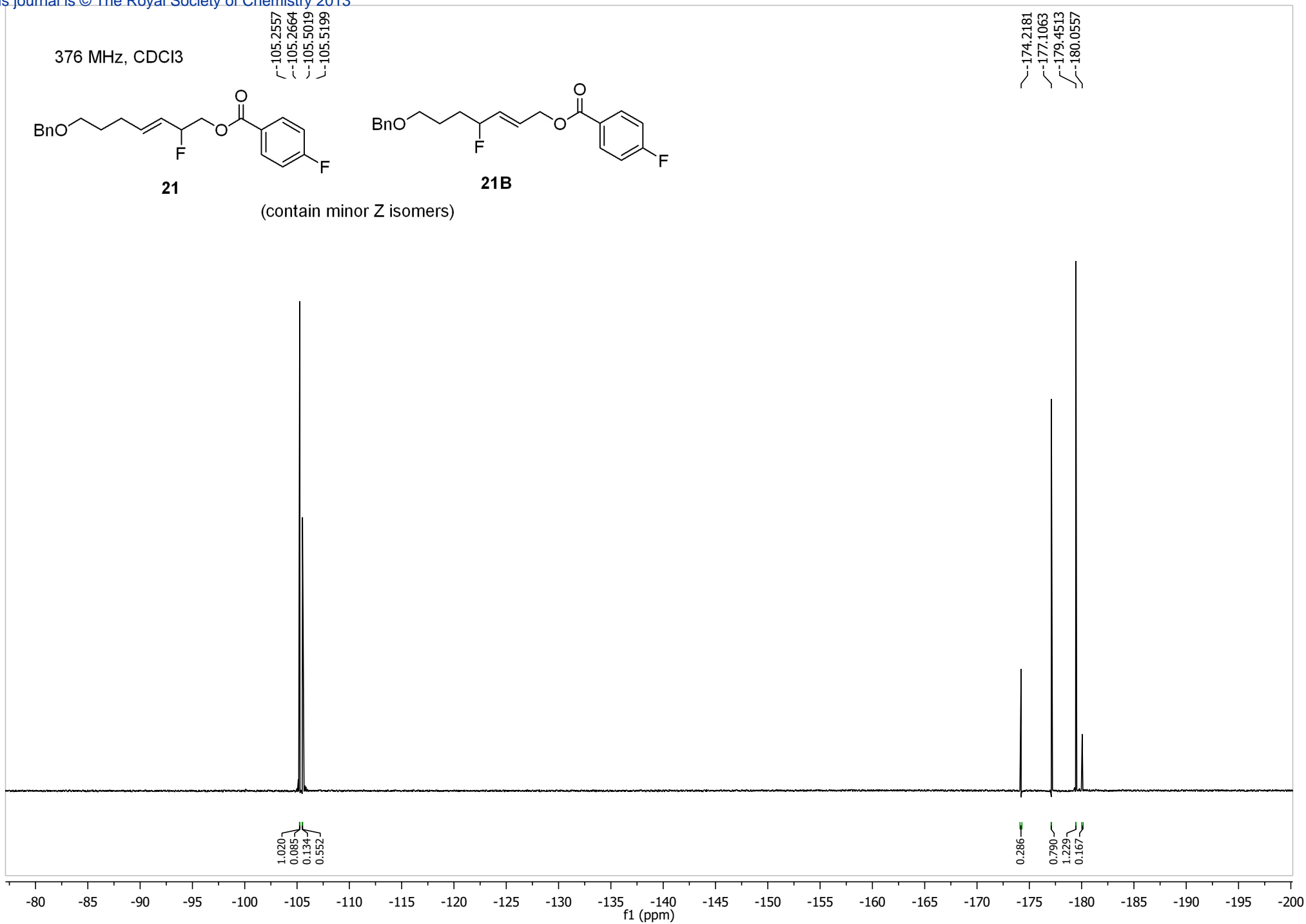


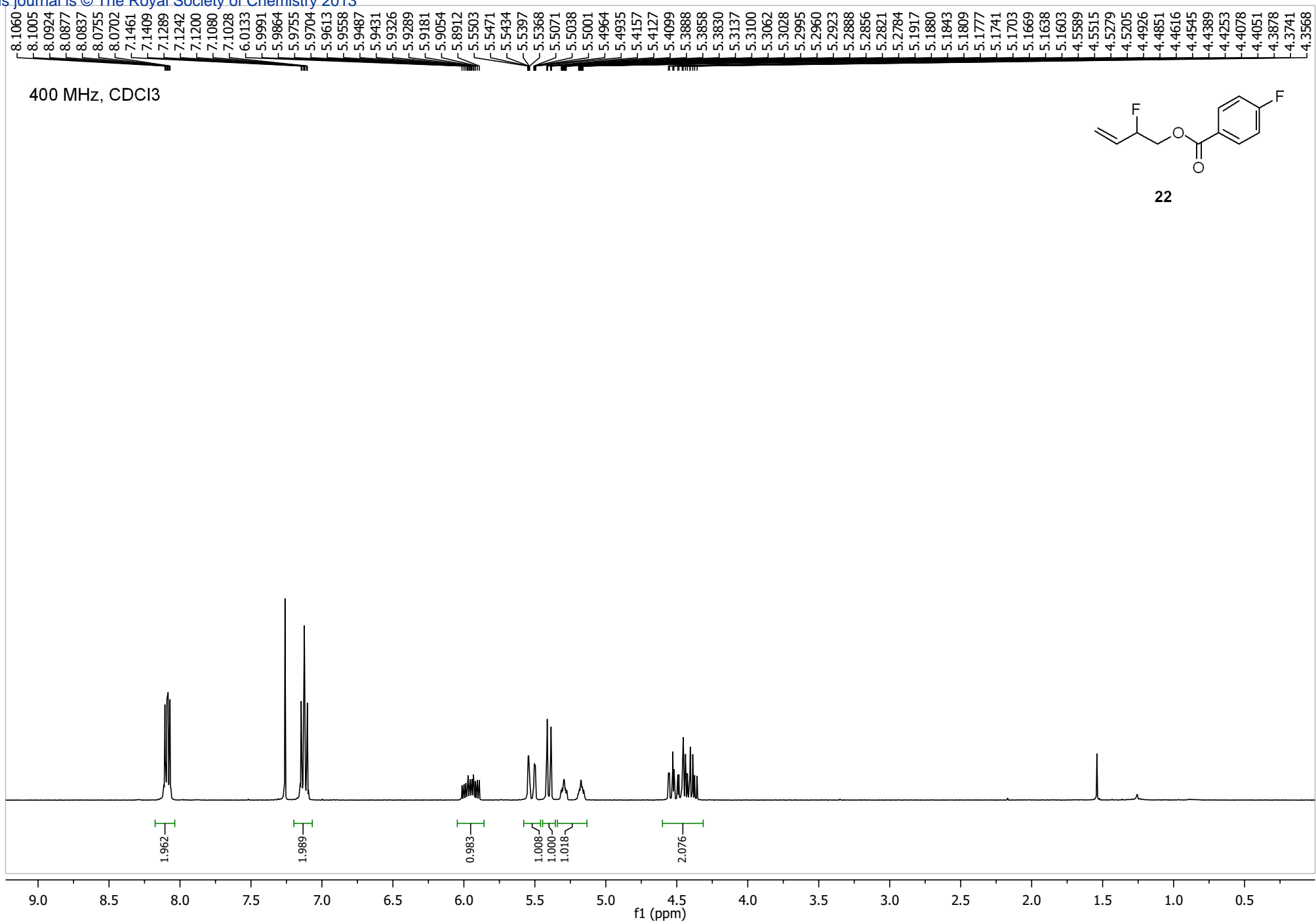
20

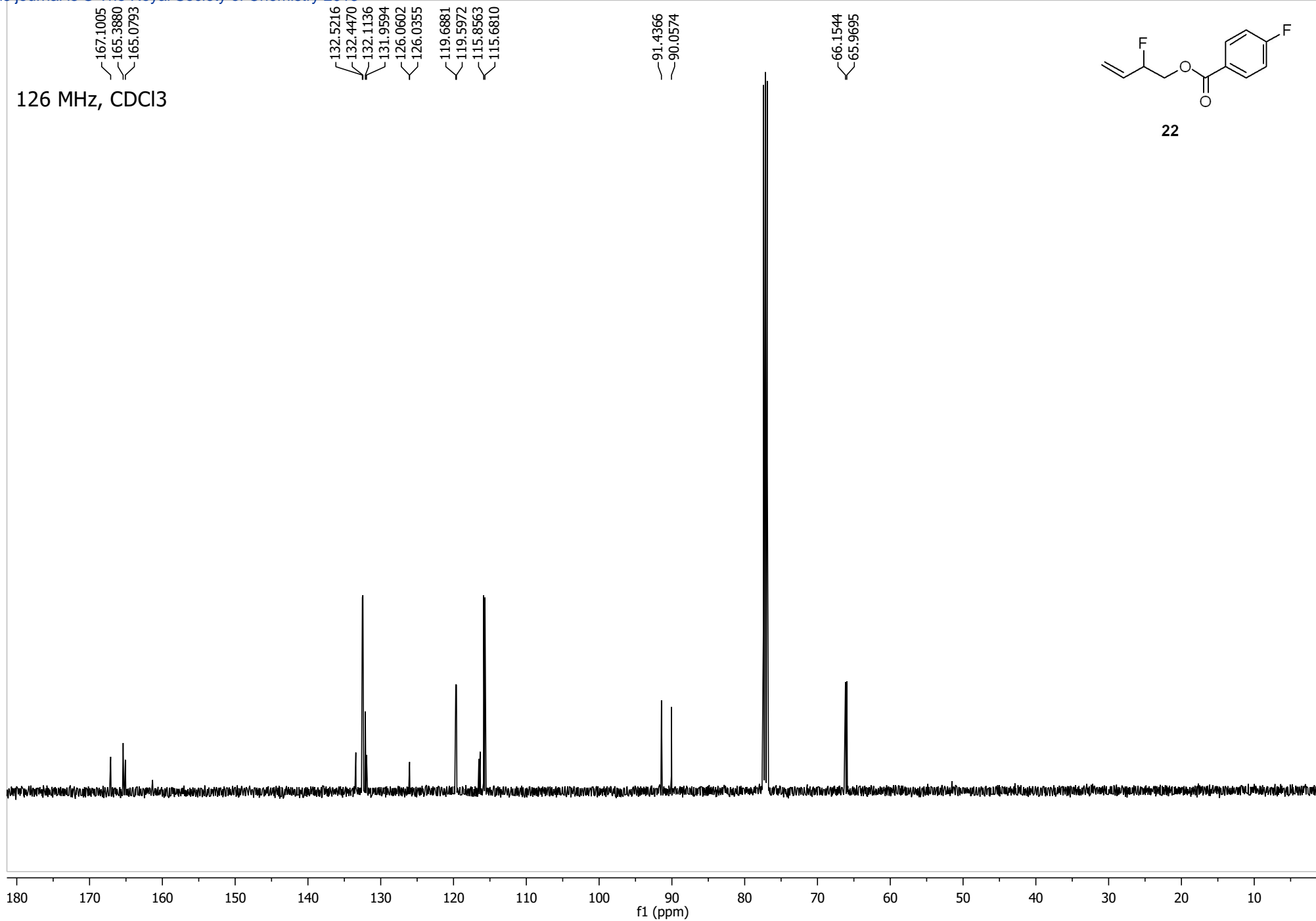




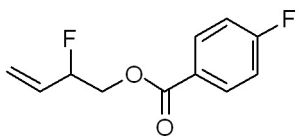




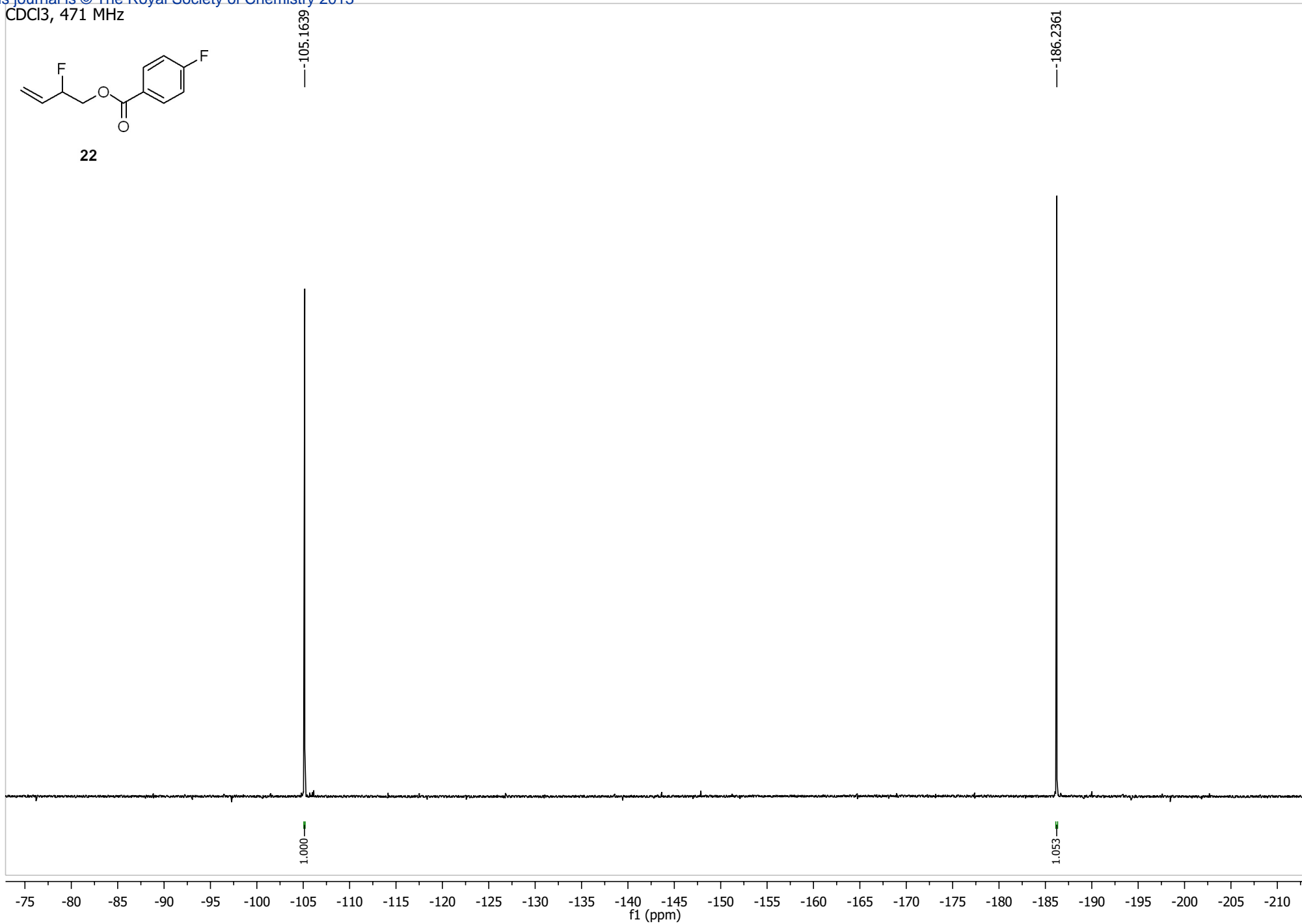


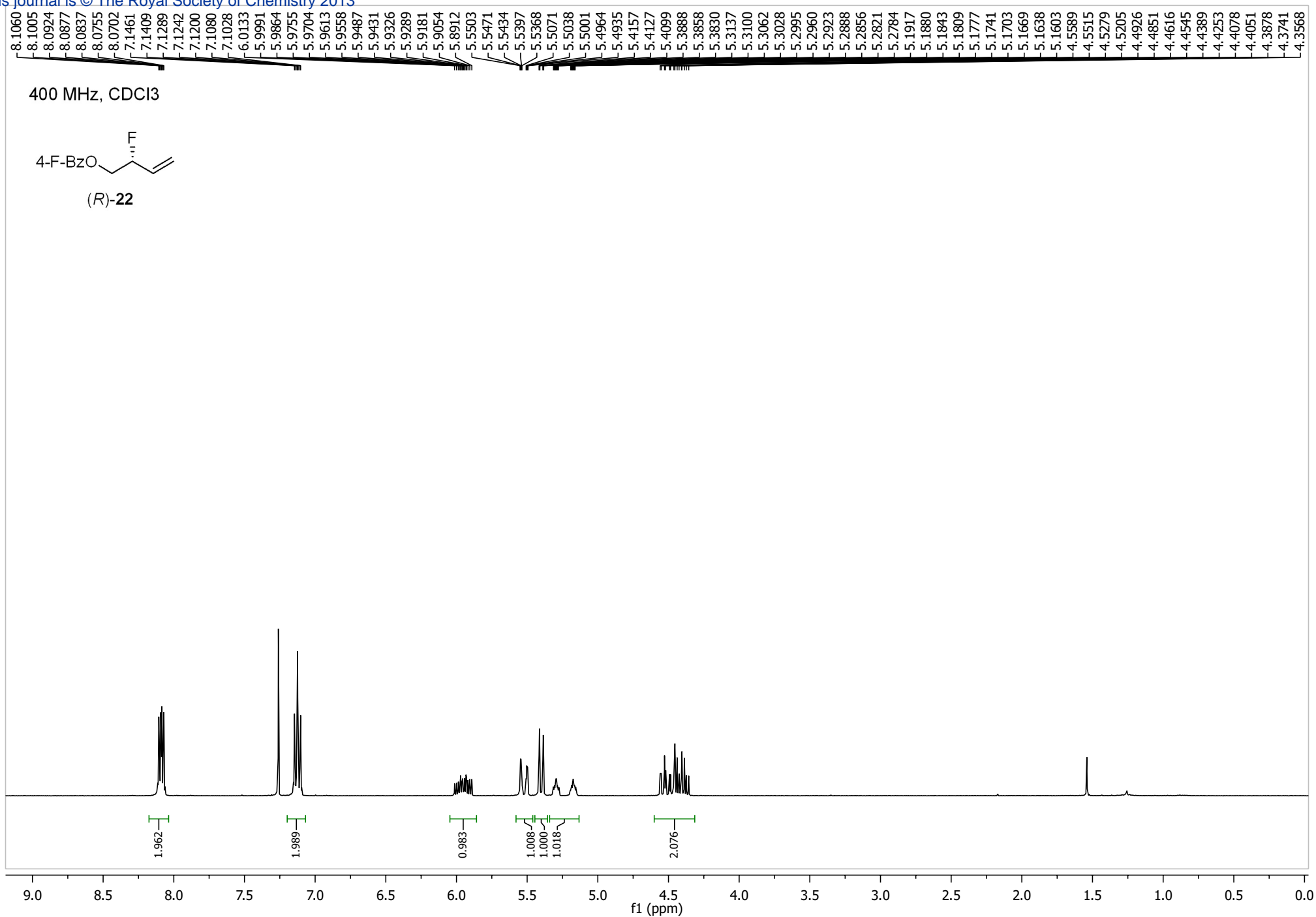


CDCl₃, 471 MHz

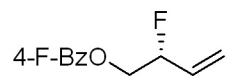


22





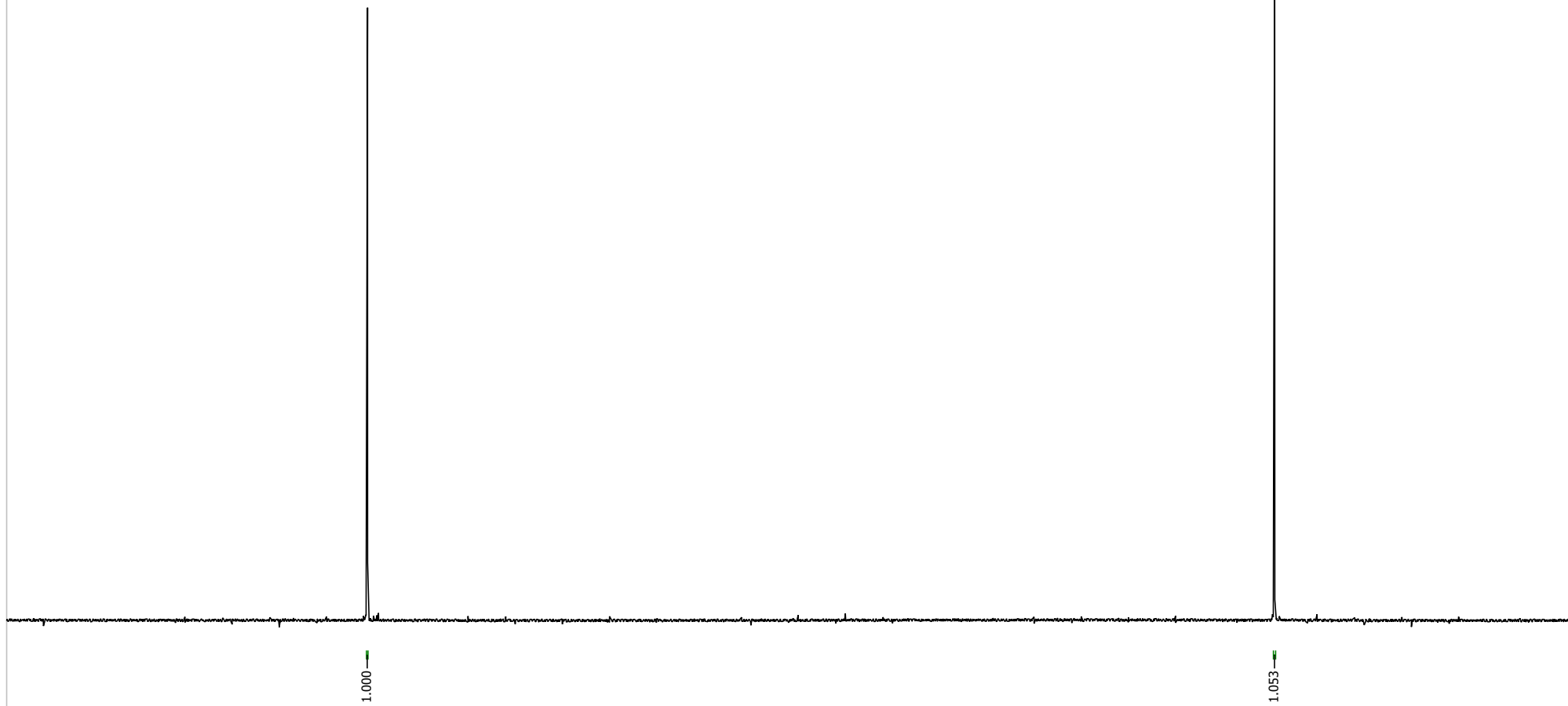
CDCl₃, 471 MHz



(*R*)-**22**

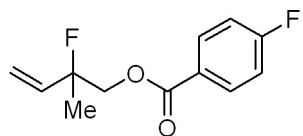
105.1639

186.2361

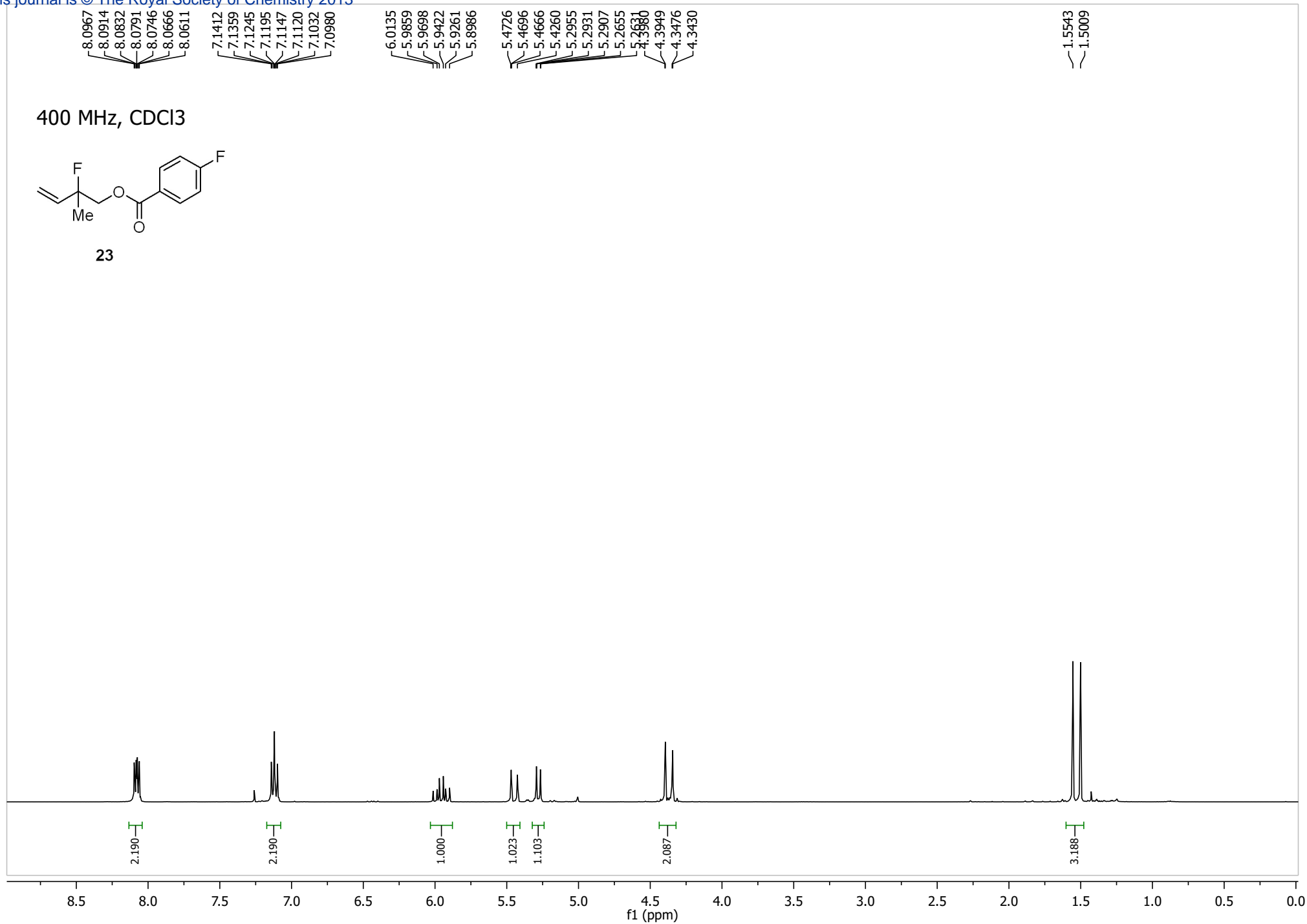


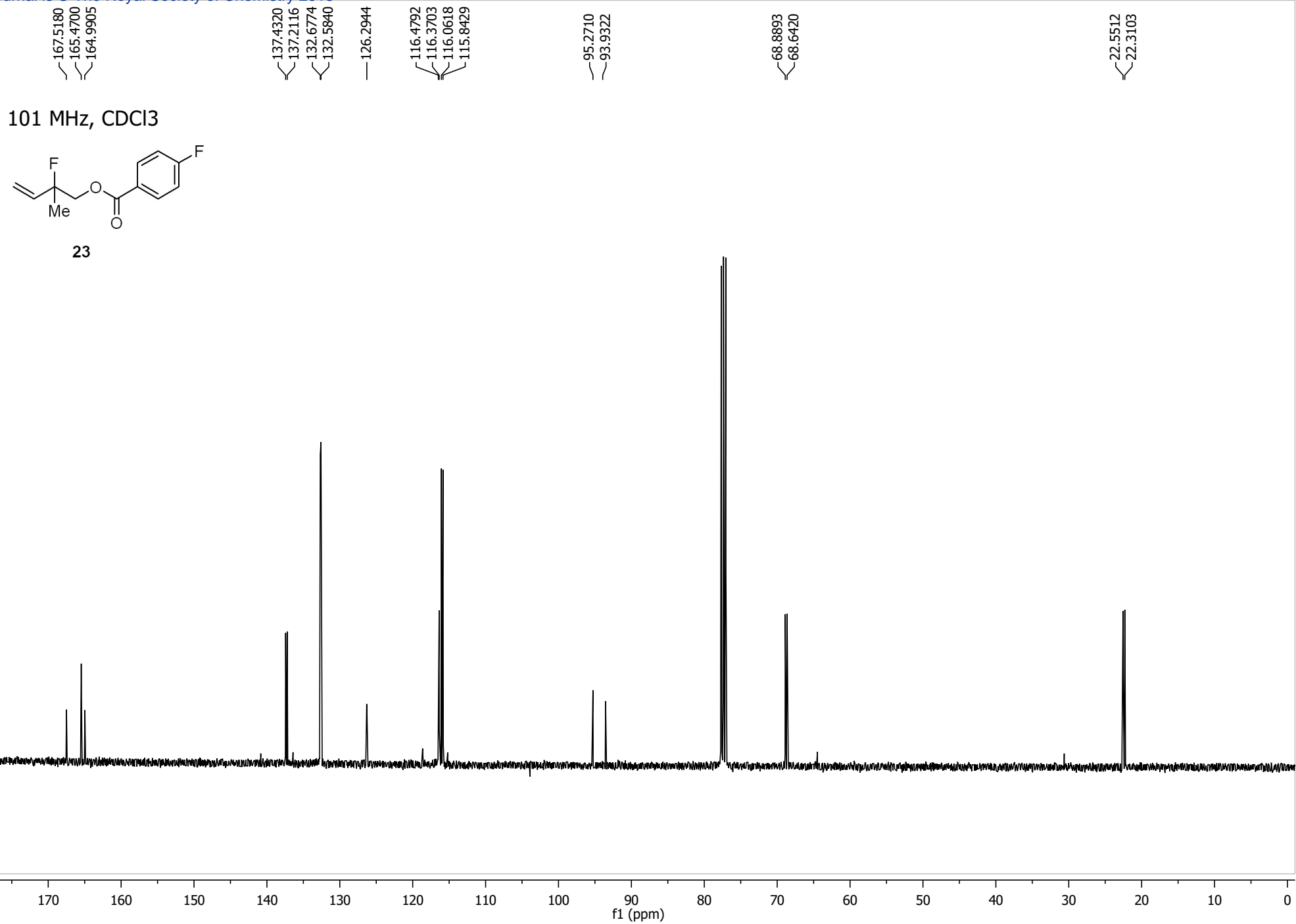
f1 (ppm)

400 MHz, CDCl₃

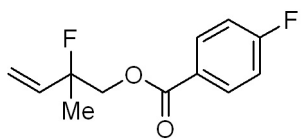


23

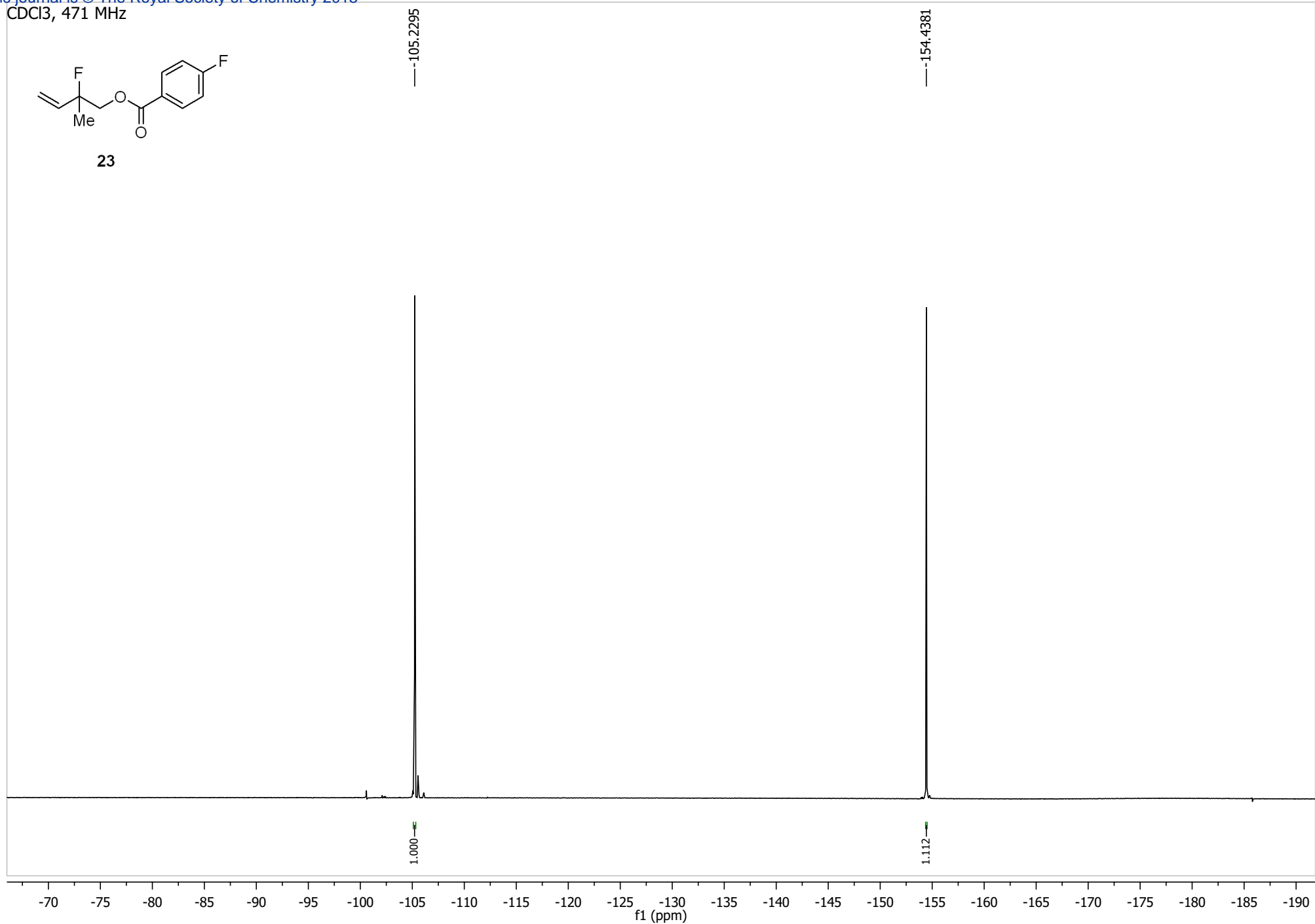




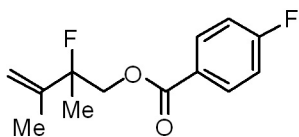
CDCl₃, 471 MHz



23



400 MHz, CDCl₃



24

8.0890
8.0835
8.0753
8.0719
8.0700
8.0666
8.0583
8.0530
7.1389
7.1335
7.1218
7.1179
7.1165
7.1124
7.1007
7.0955

5.1285
5.1259
5.1234
5.0199
5.0161
5.0124
5.0089
5.0064
5.0030
4.9994
4.9958
4.4586
4.4553
4.4058
4.4027

1.8424
1.8399
1.8380
1.8361
1.8337
1.5726
1.5179

2.072

2.070

1.000

1.004

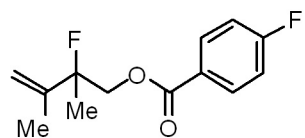
1.955

2.958

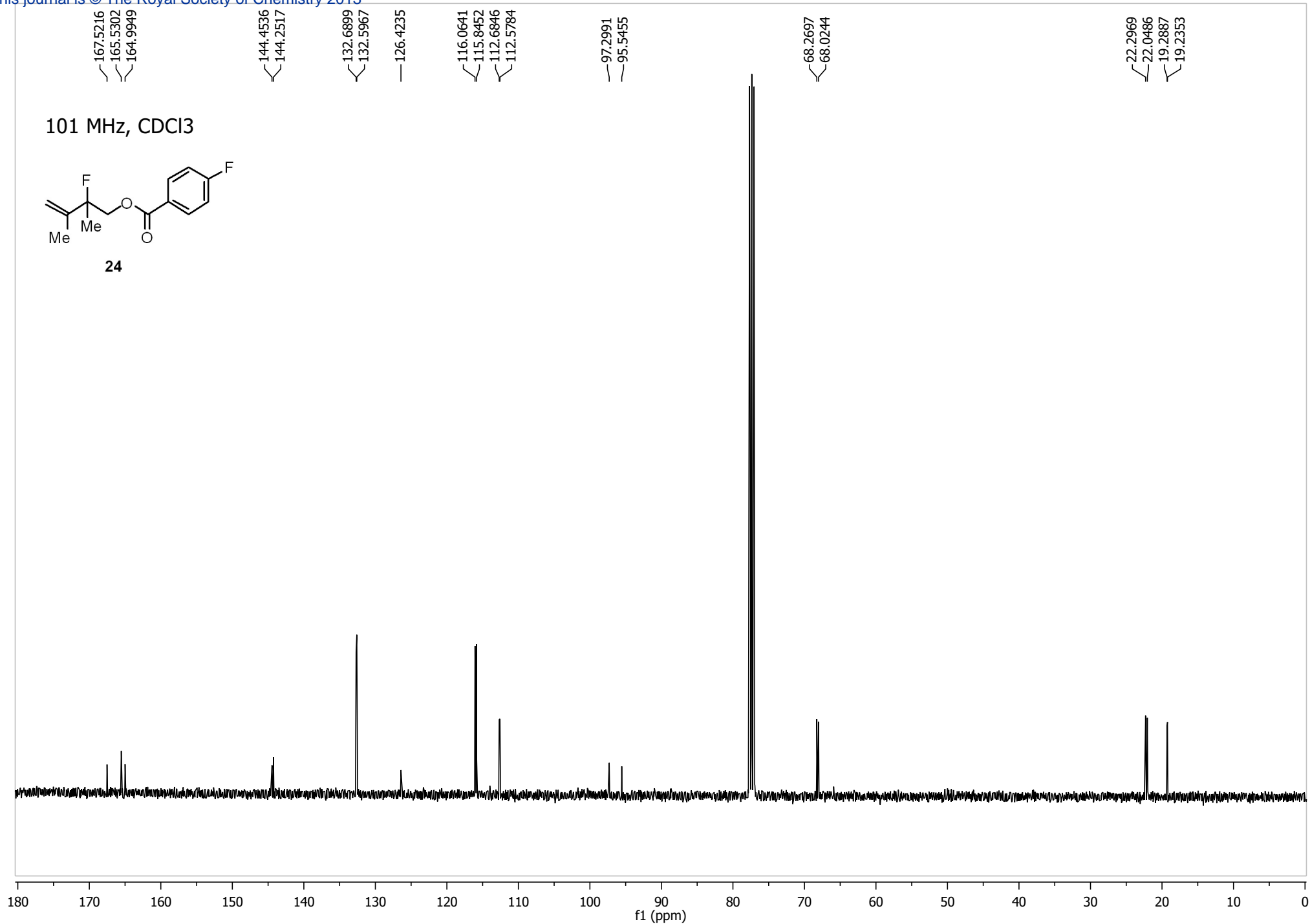
3.151

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

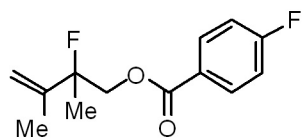
101 MHz, CDCl₃



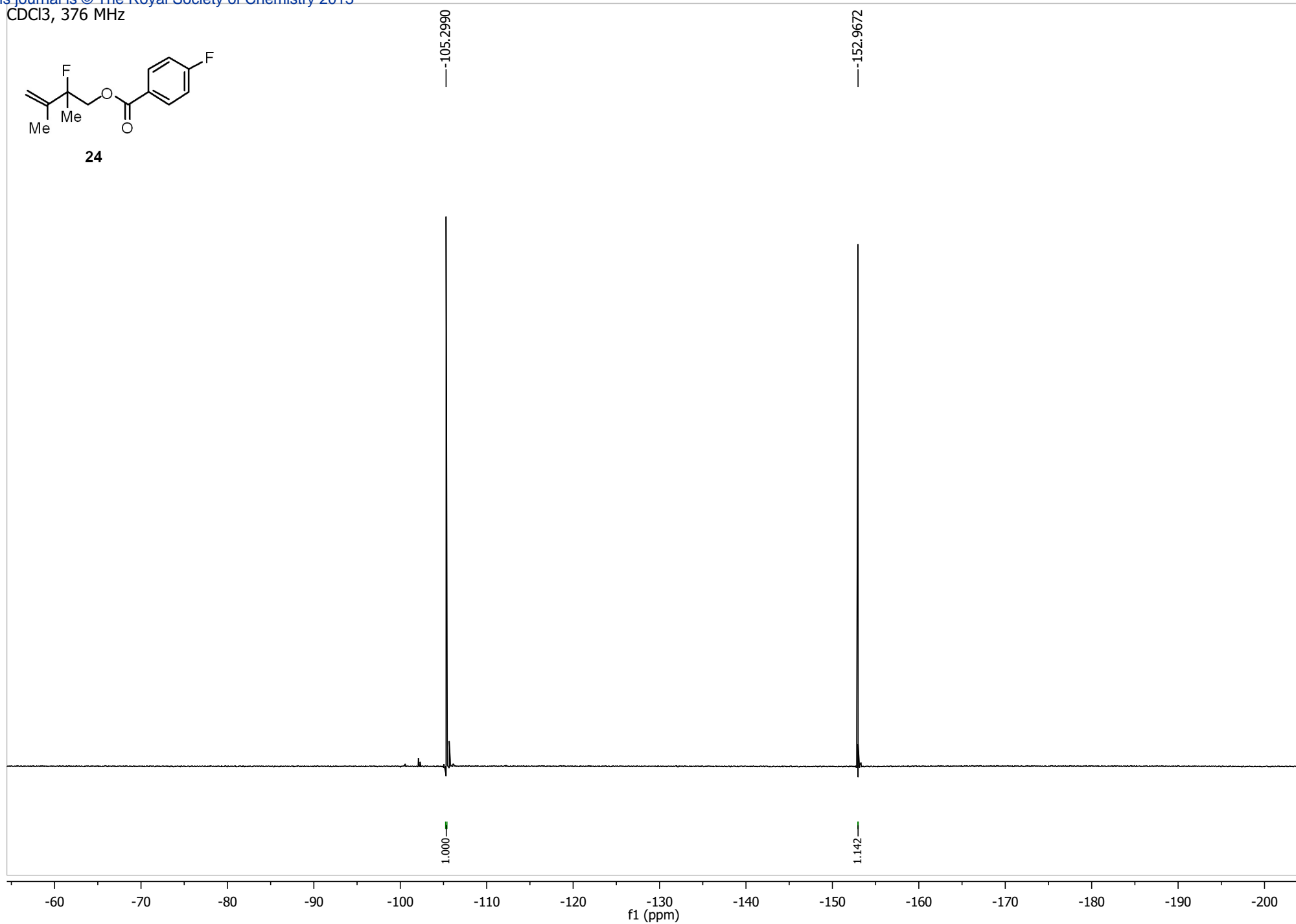
24

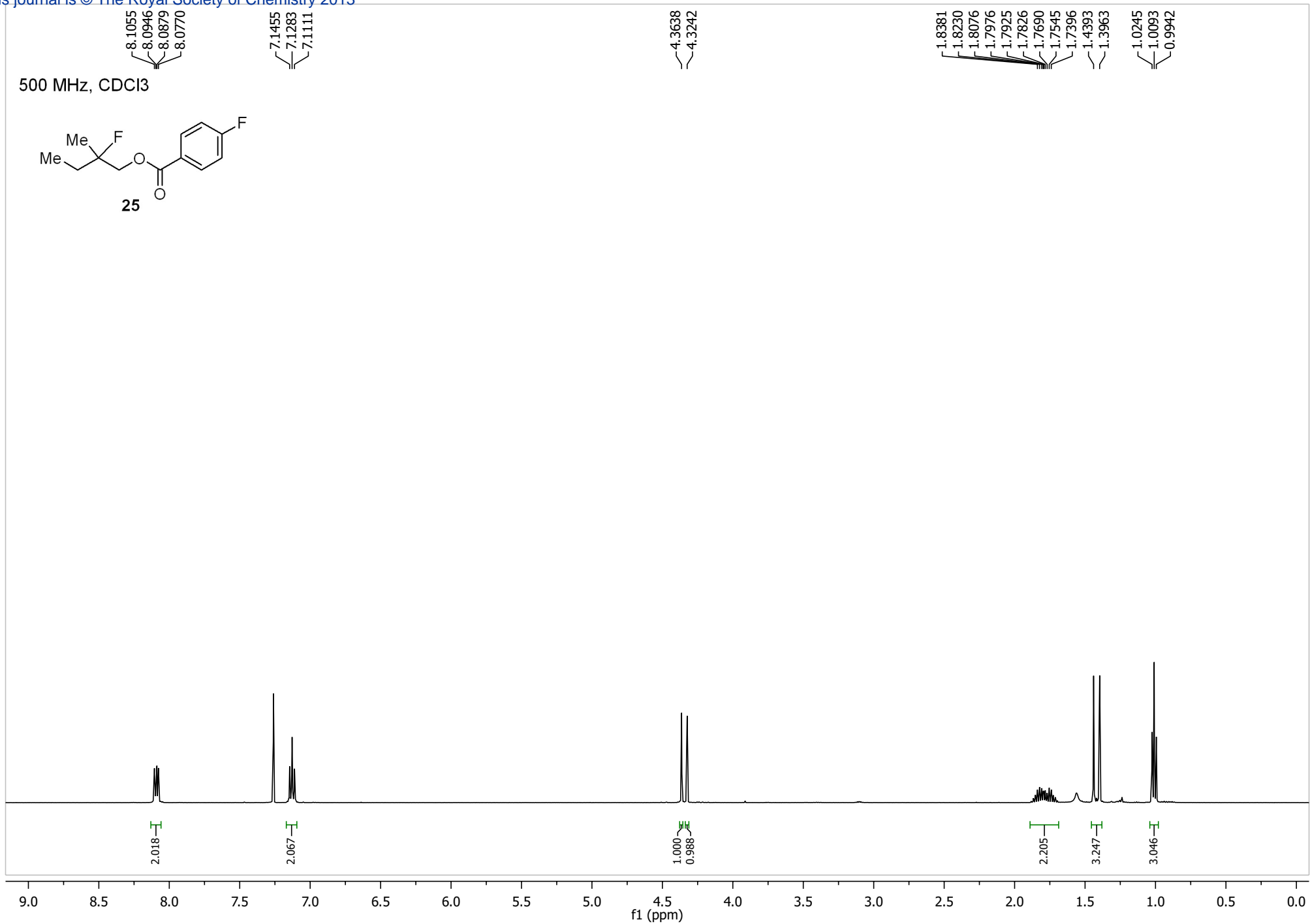


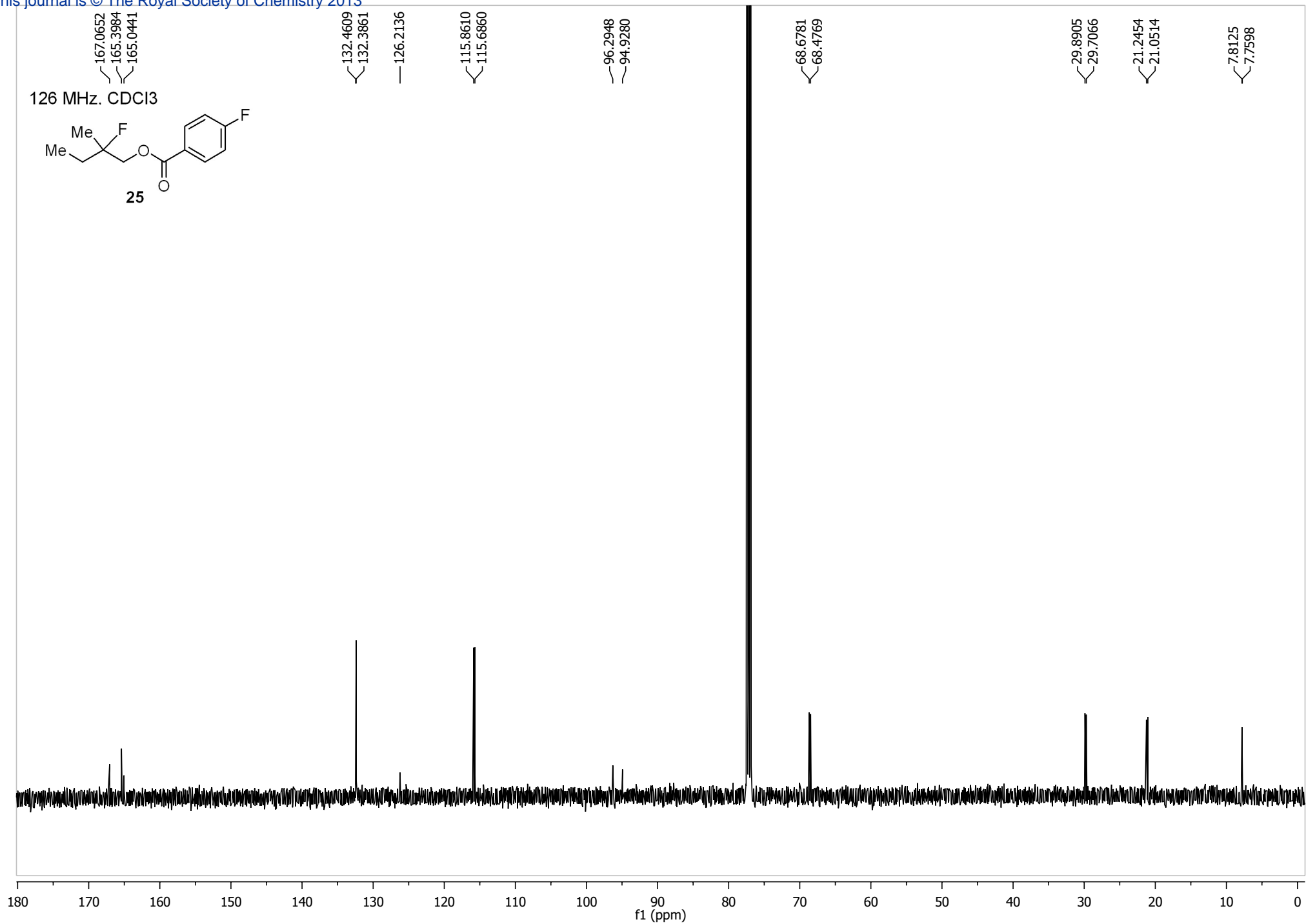
CDCl₃, 376 MHz



24

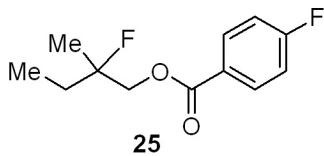






471 MHz, CDCl₃

-105.2476



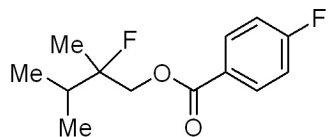
-153.6486

1.000

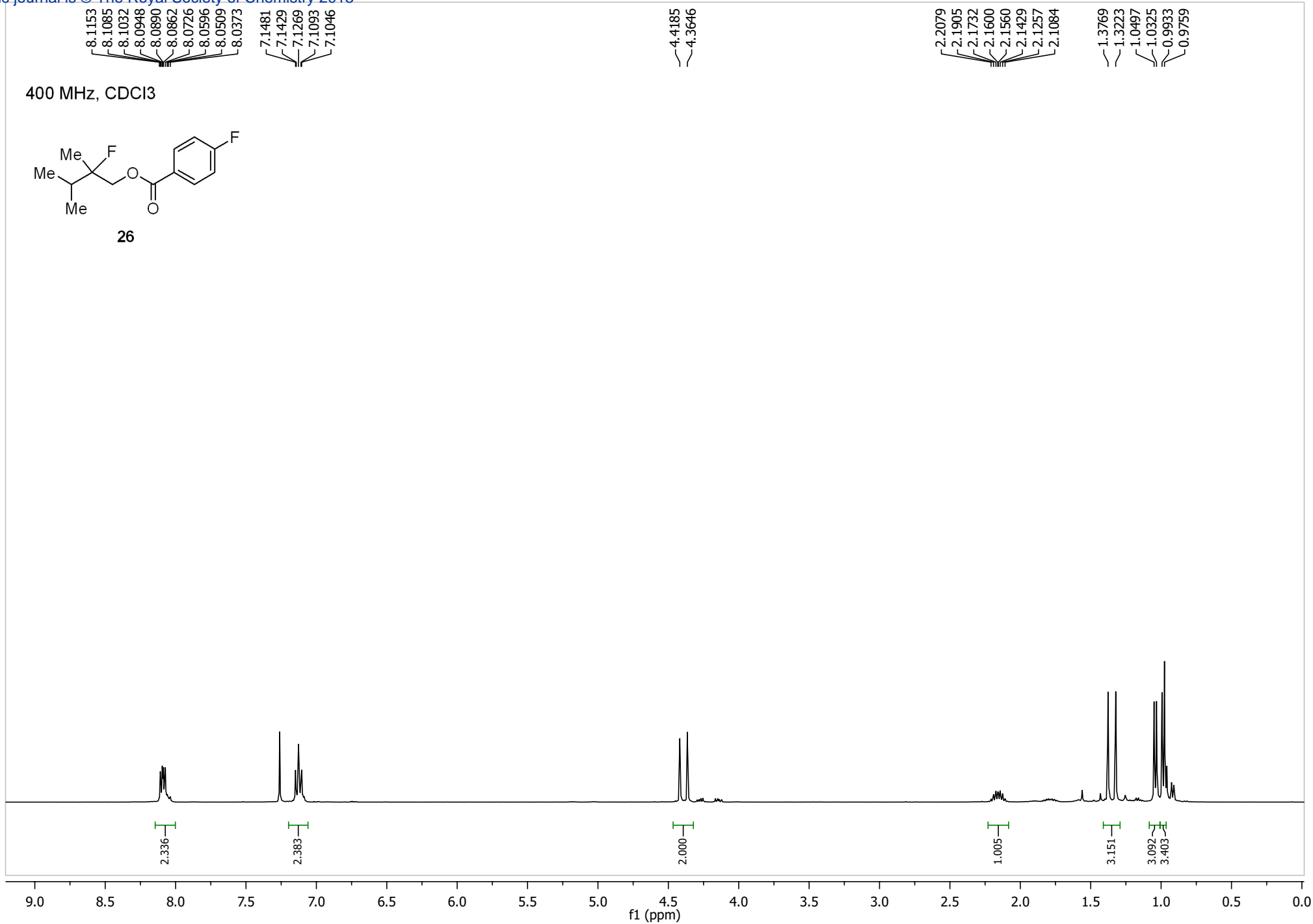
0.954

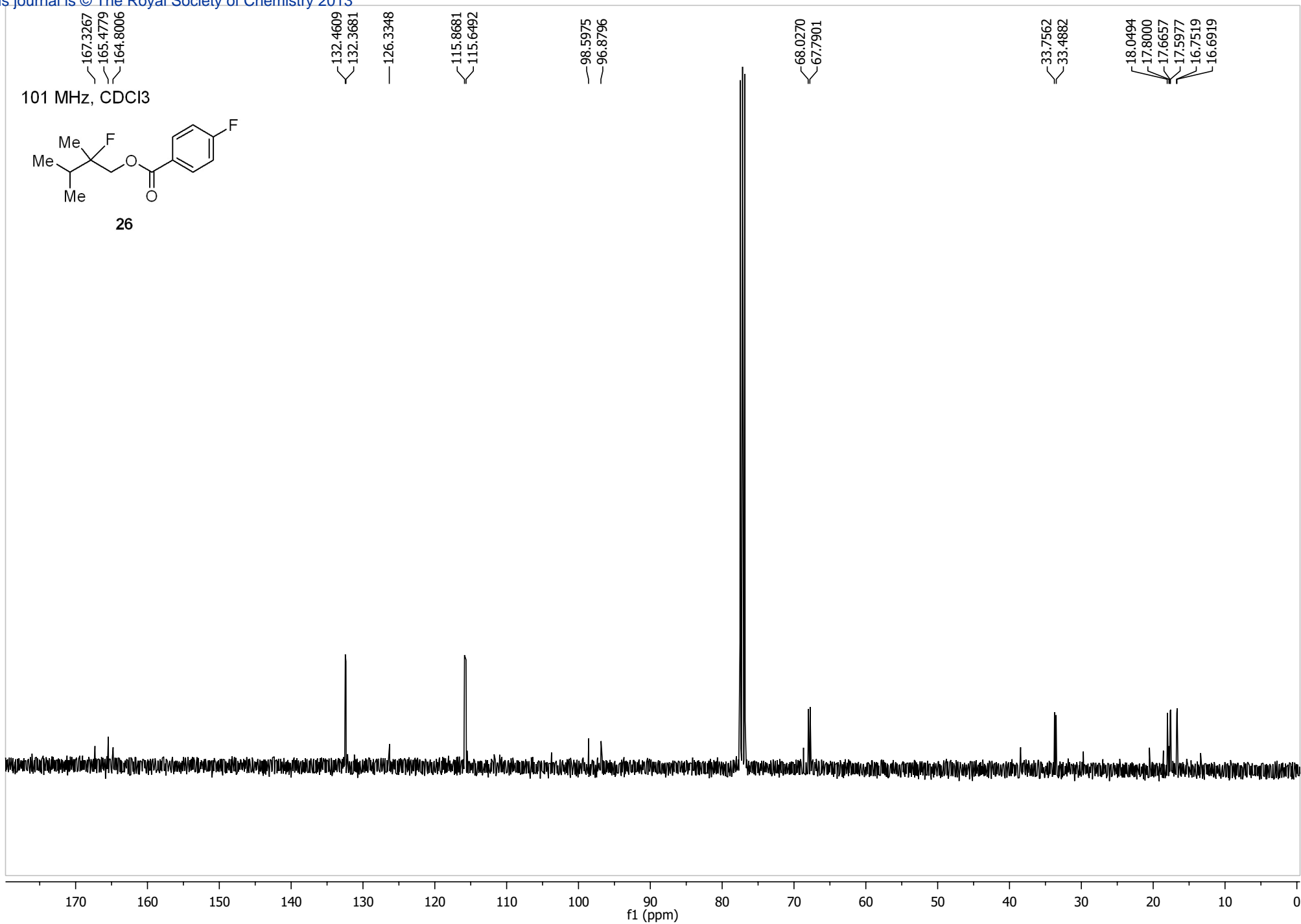
-95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165
f1 (ppm)

400 MHz, CDCl₃

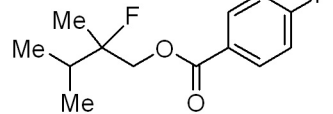


26





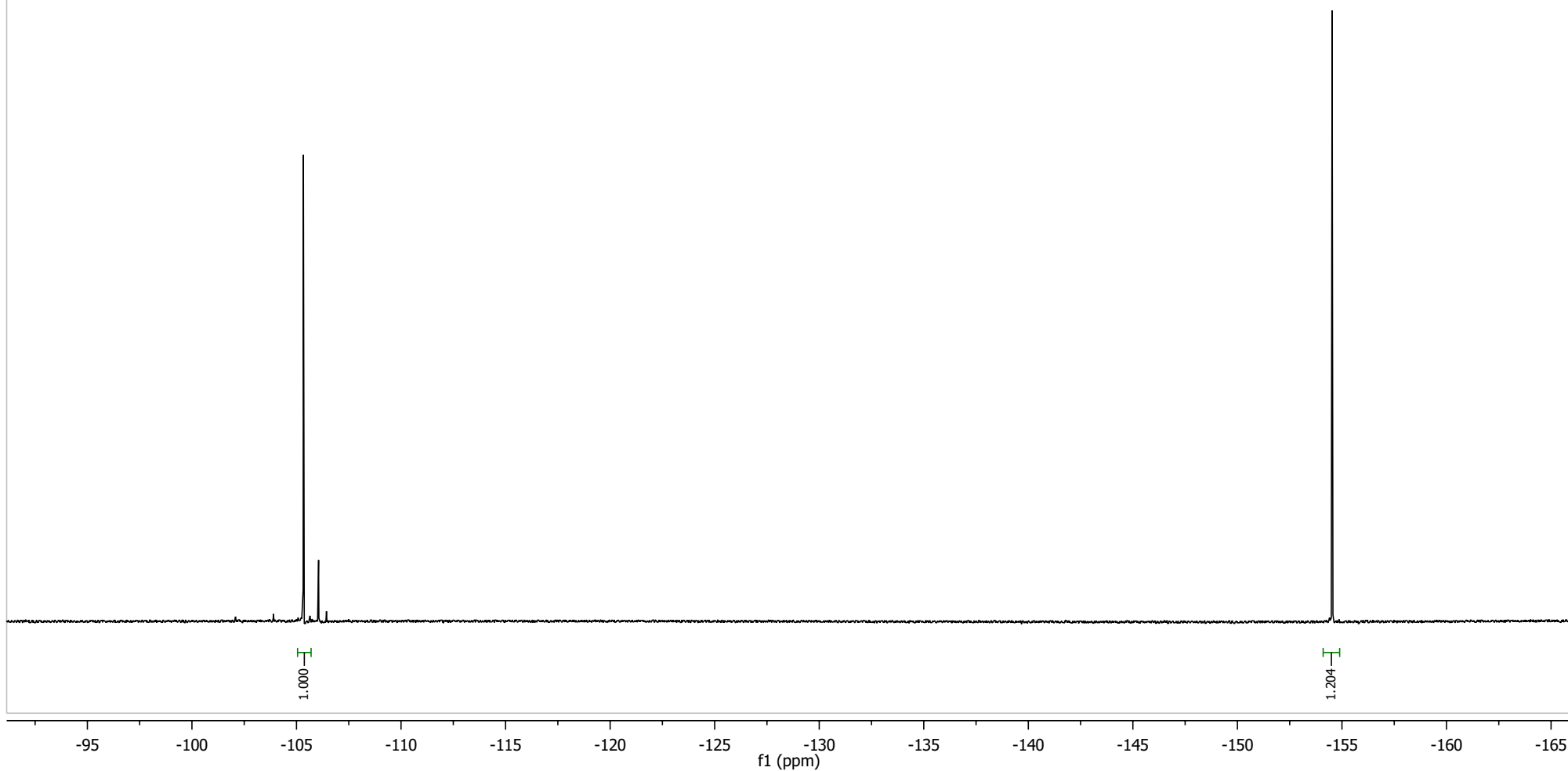
376 MHz, CDCl₃



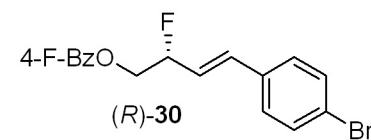
26

---105.3283

---154.5283



400 MHz, CDCl₃

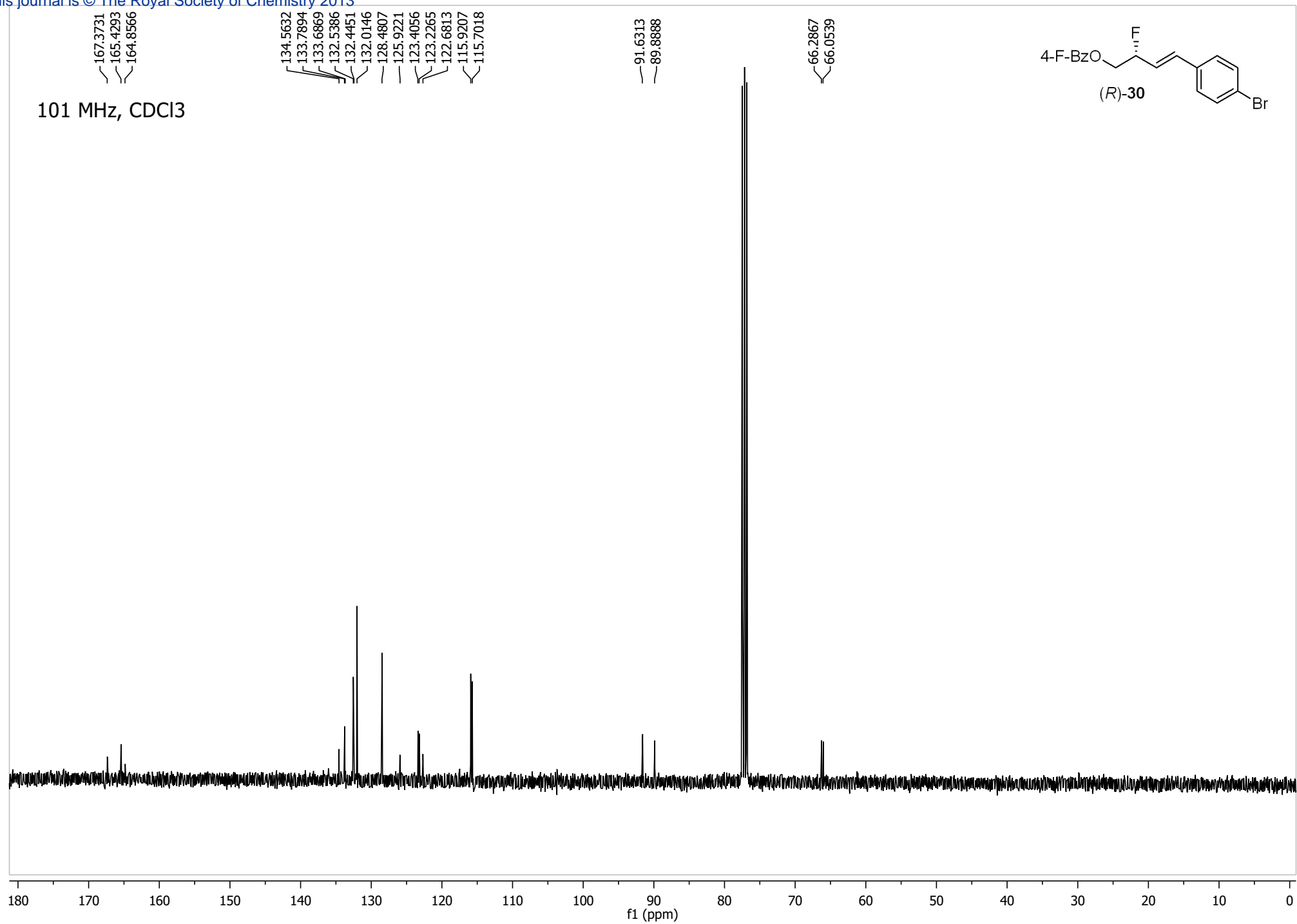


8.1088
8.0953
8.0866
8.0731
7.4799
7.4587
7.2813
7.2602
7.2551
7.1458
7.1240
6.7727
6.7328
6.7258
6.2951
6.2791
6.2608
6.2448
6.2390
5.4616
5.4535
5.4465
5.3428
5.3397
5.3319
5.3255
4.6289
4.6196
4.5959
4.5886
4.5604
4.5530
4.5294
4.5210
4.5027
4.4894
4.4711
4.4532
4.4399
4.4222

1.914
1.952
2.471
1.947
0.959
0.979
1.000
2.008

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

f1 (ppm)



CDCl₃, 282 MHz

