Palladium-catalyzed reductive cross-coupling reaction of carboxylic acids with thiols: An alternative strategy to access thioesters

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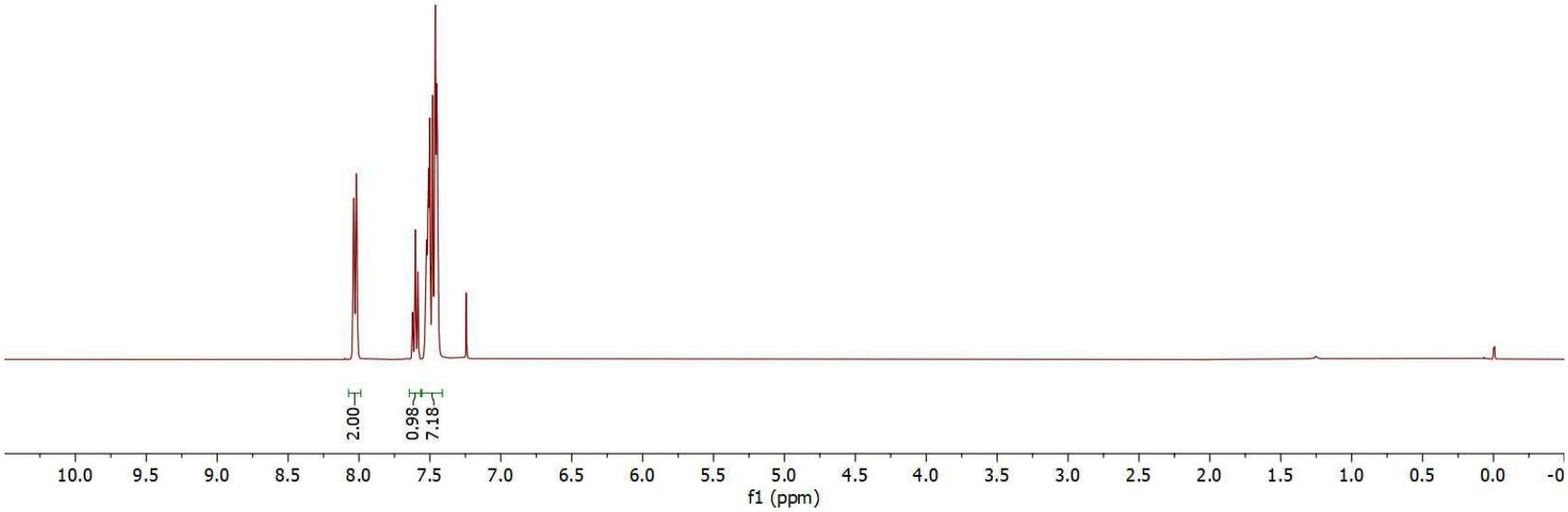
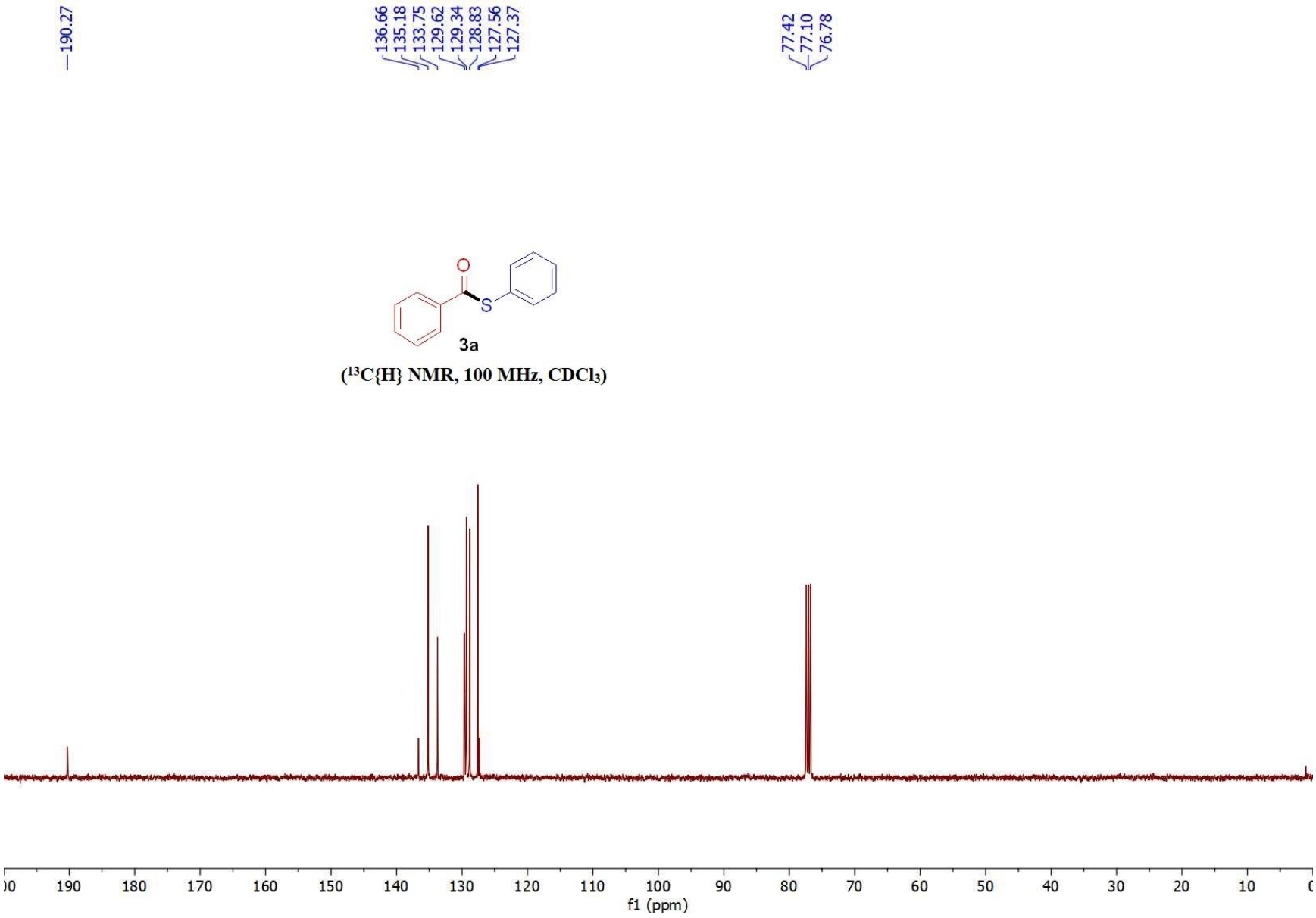
Copies of ^{1}H, ^{13}C and ^{19}F-NMR

3a

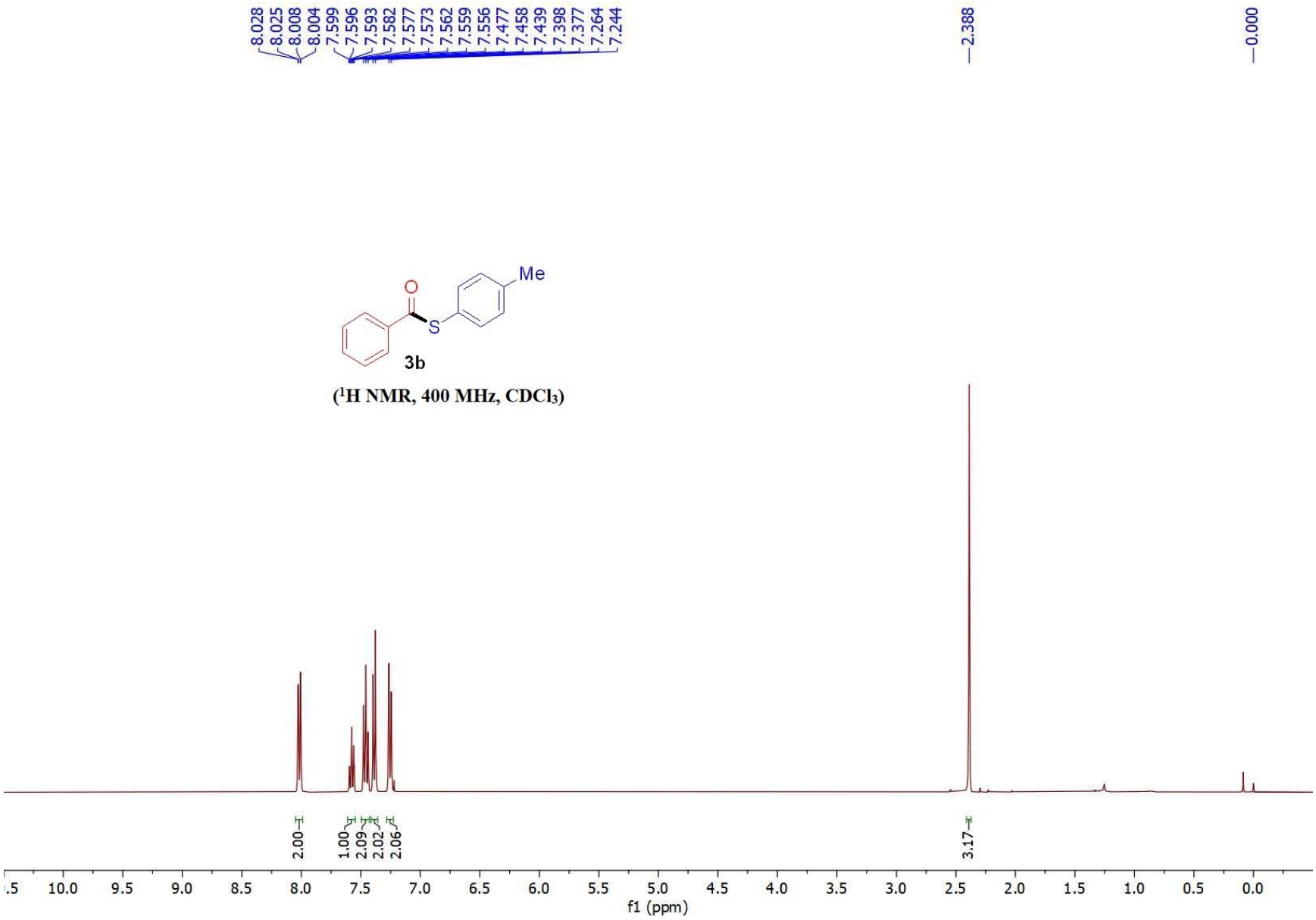
(^{1}H NMR, 400 MHz, $CDCl_3$)





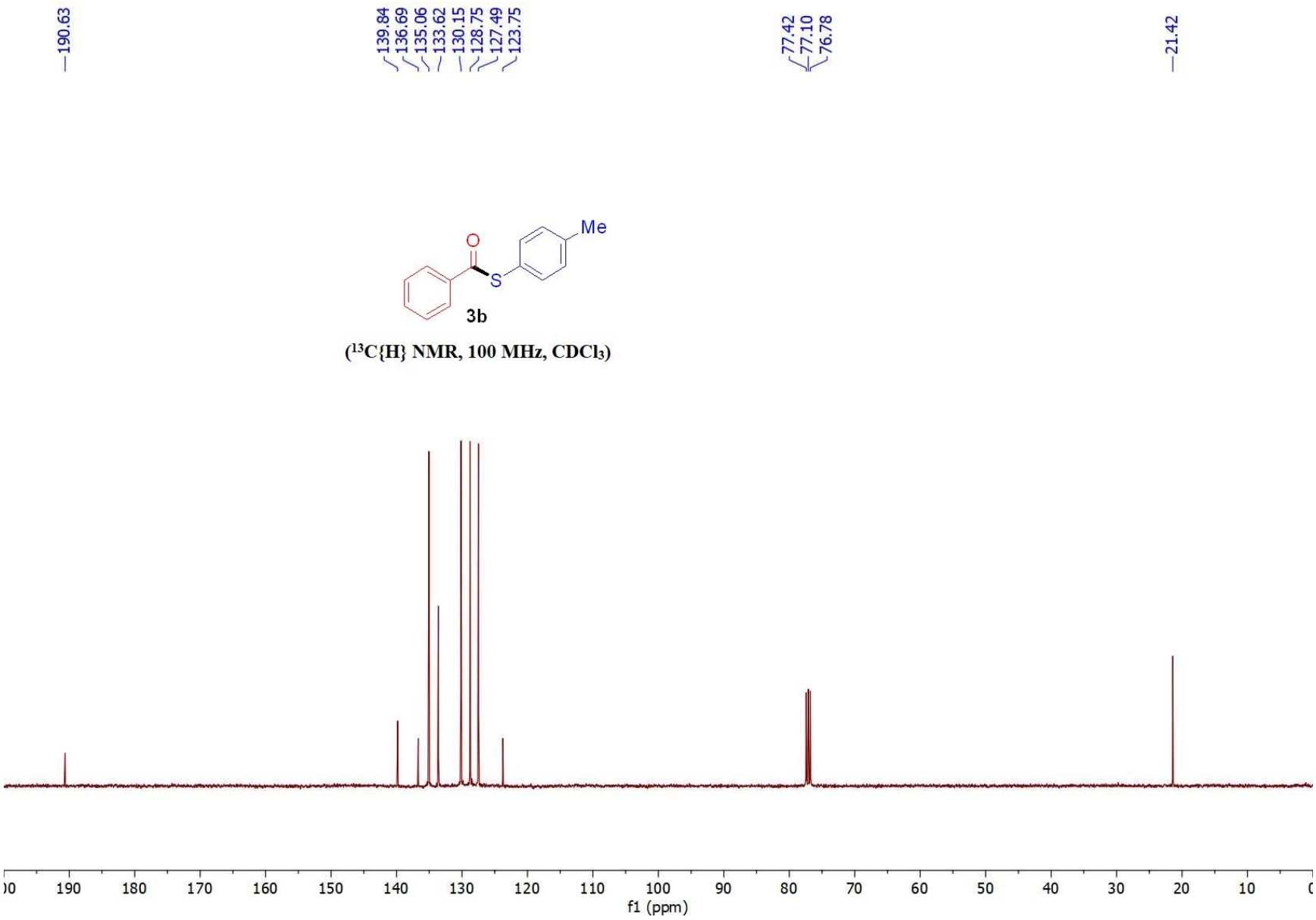
3a

($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



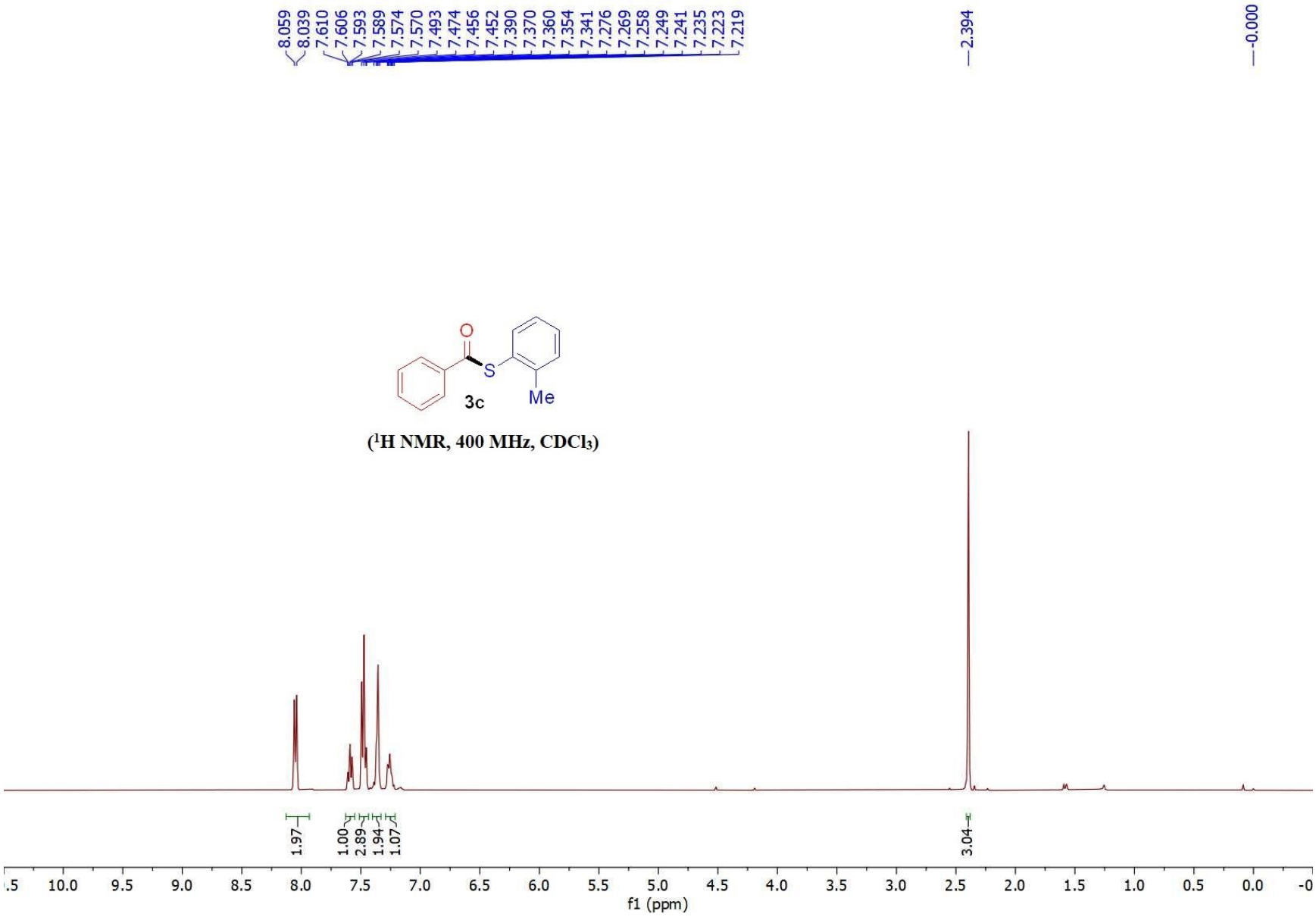
3b

(^{1}H NMR, 400 MHz, $CDCl_3$)

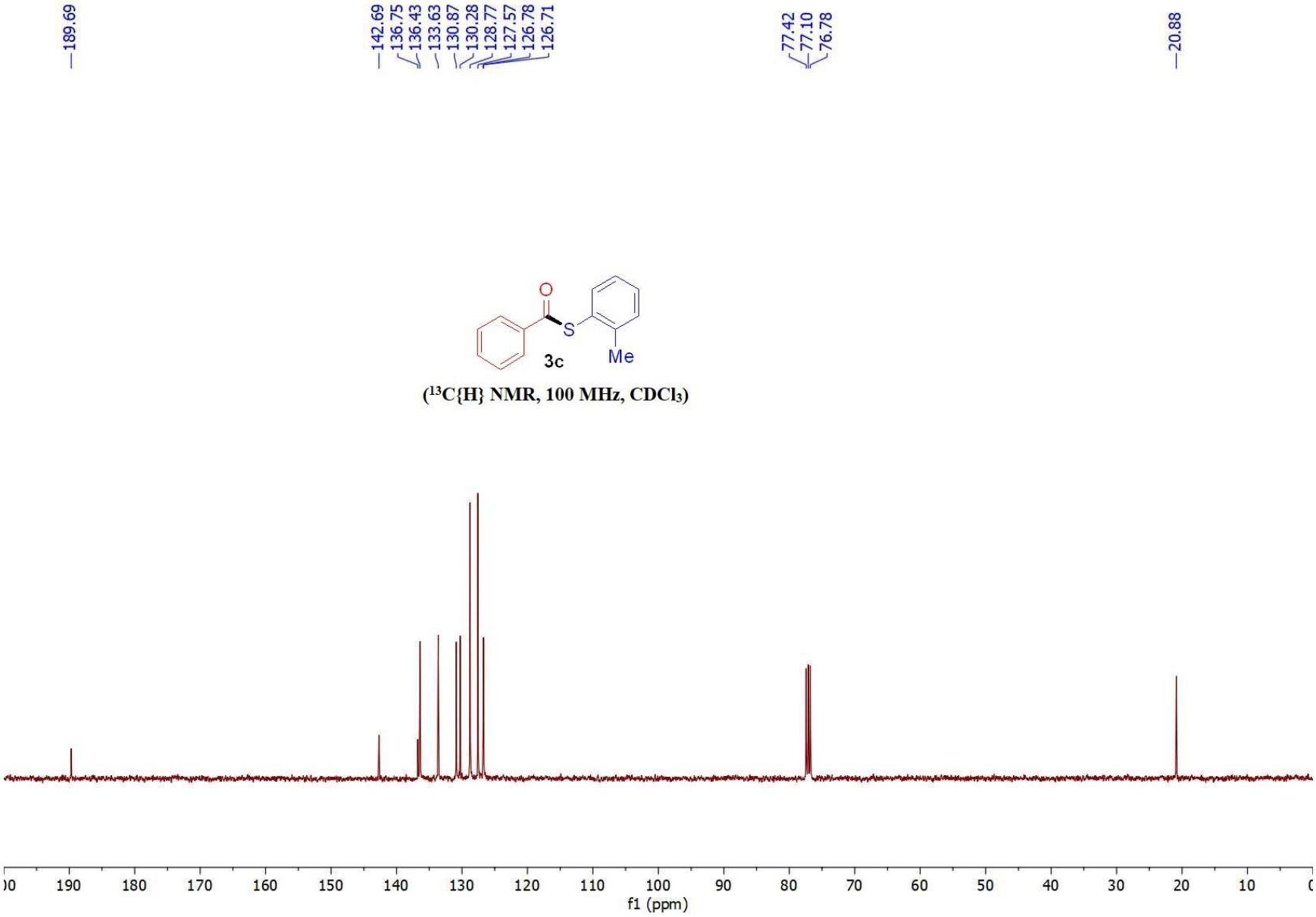


3b

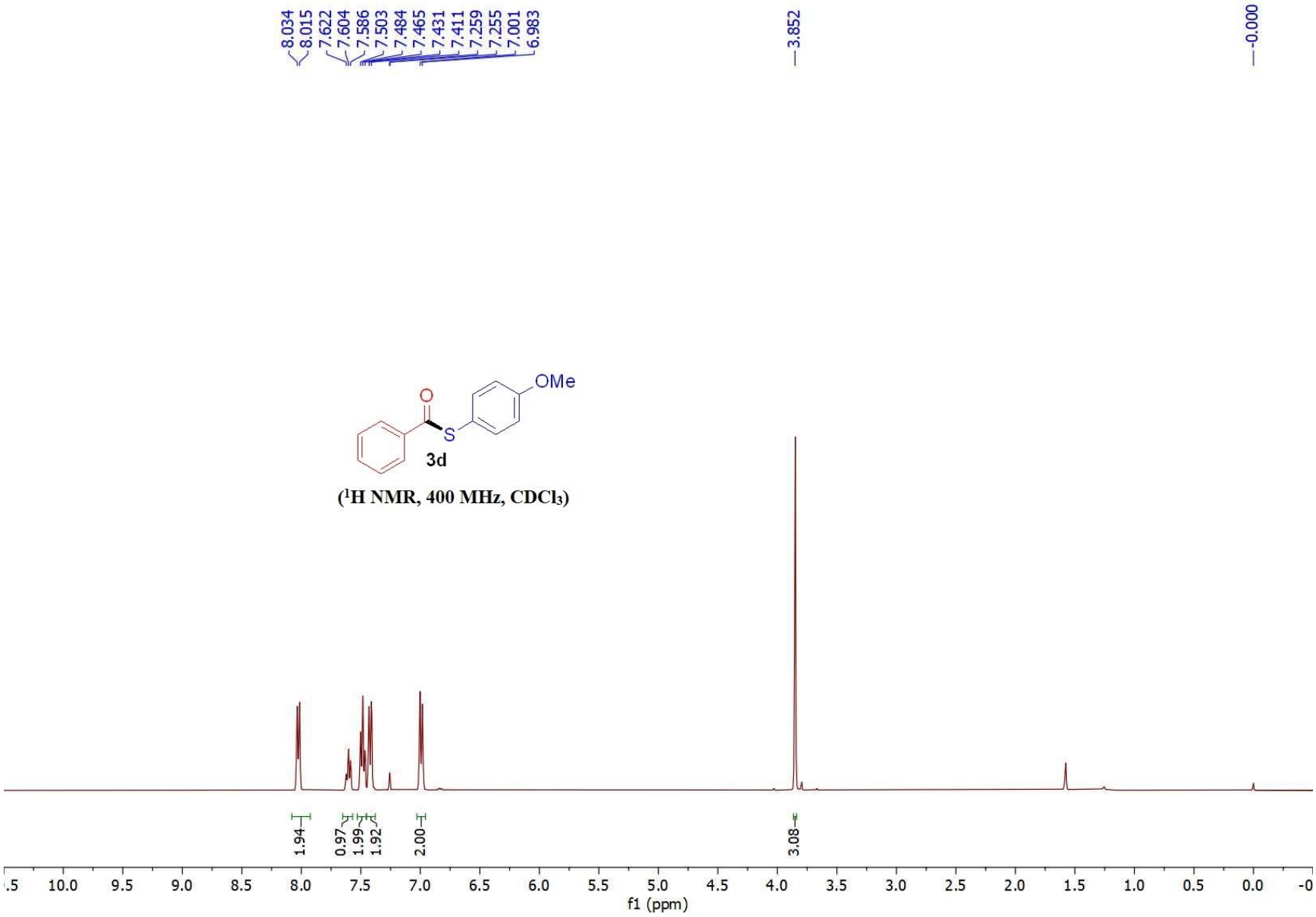
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



(^{1}H NMR, 400 MHz, $CDCl_3$)

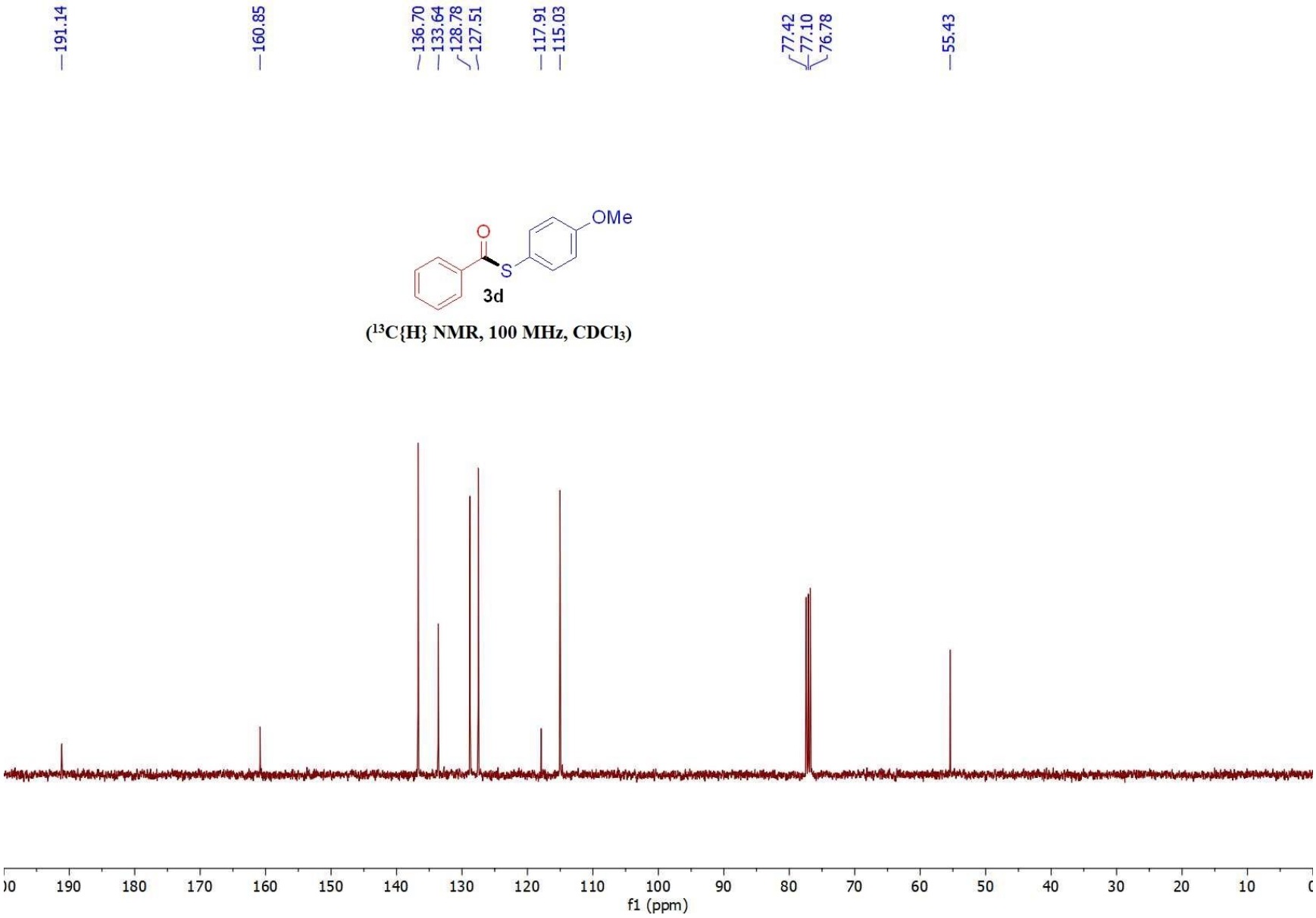


($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

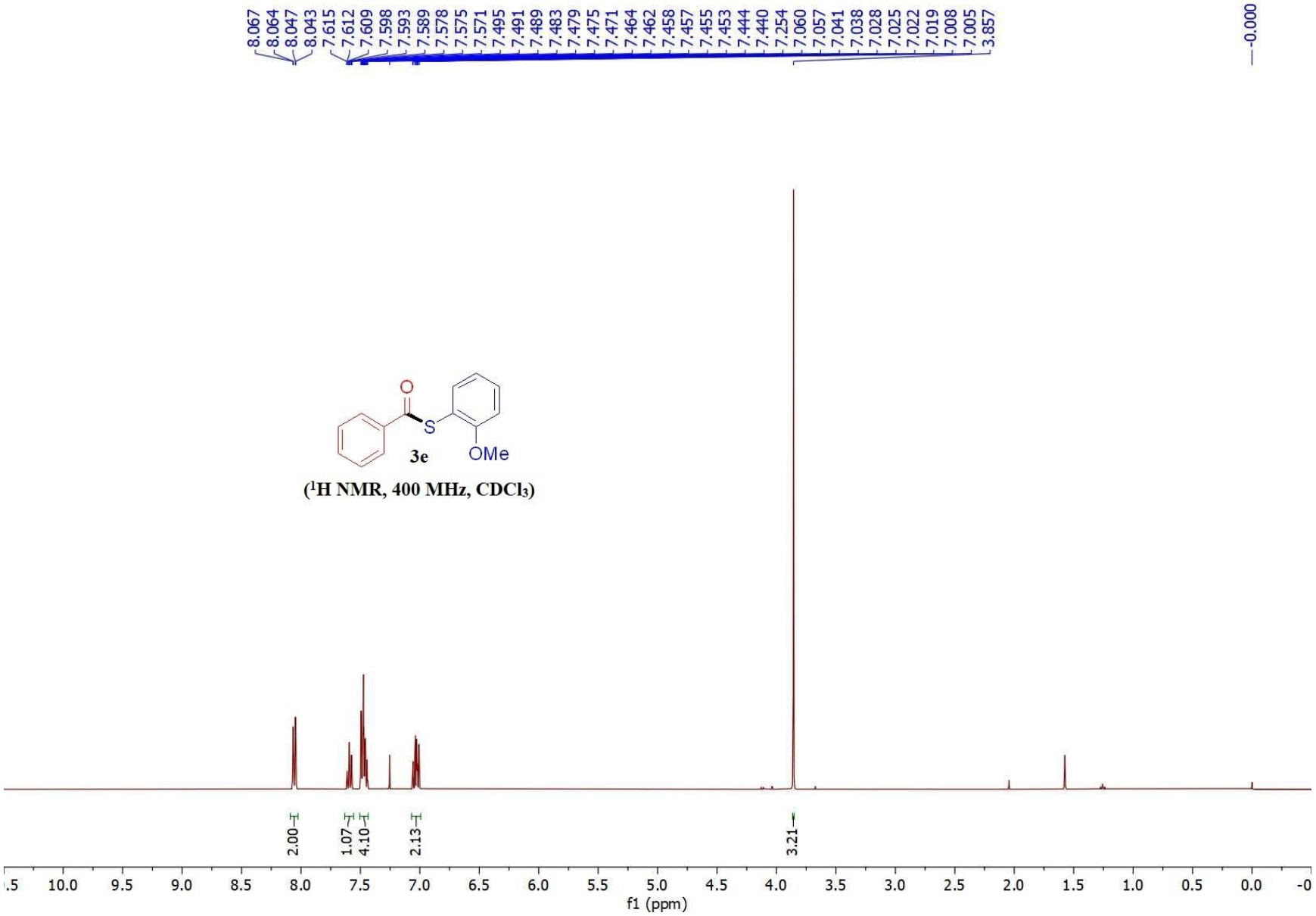


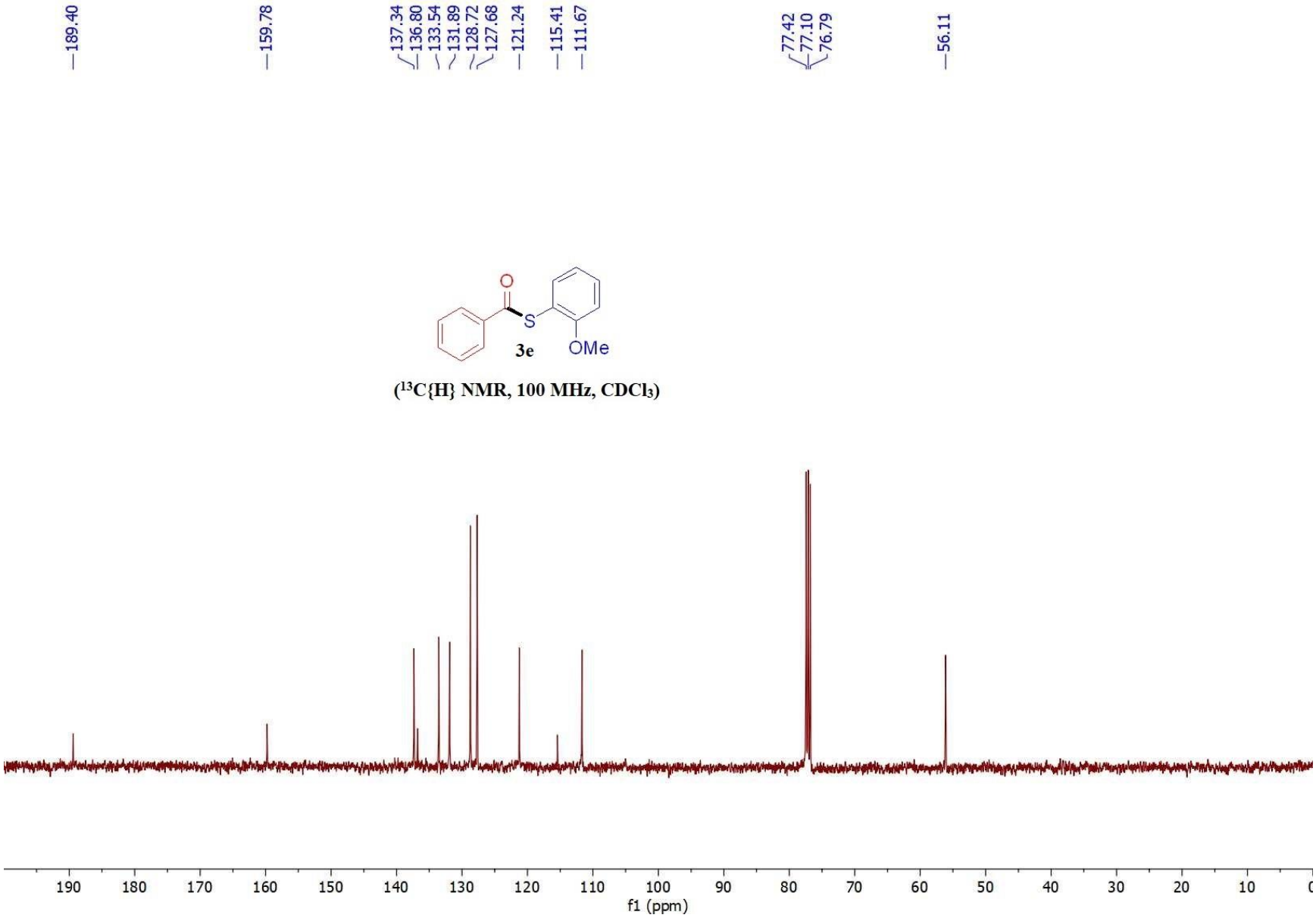
3d

(^{1}H NMR, 400 MHz, $CDCl_3$)

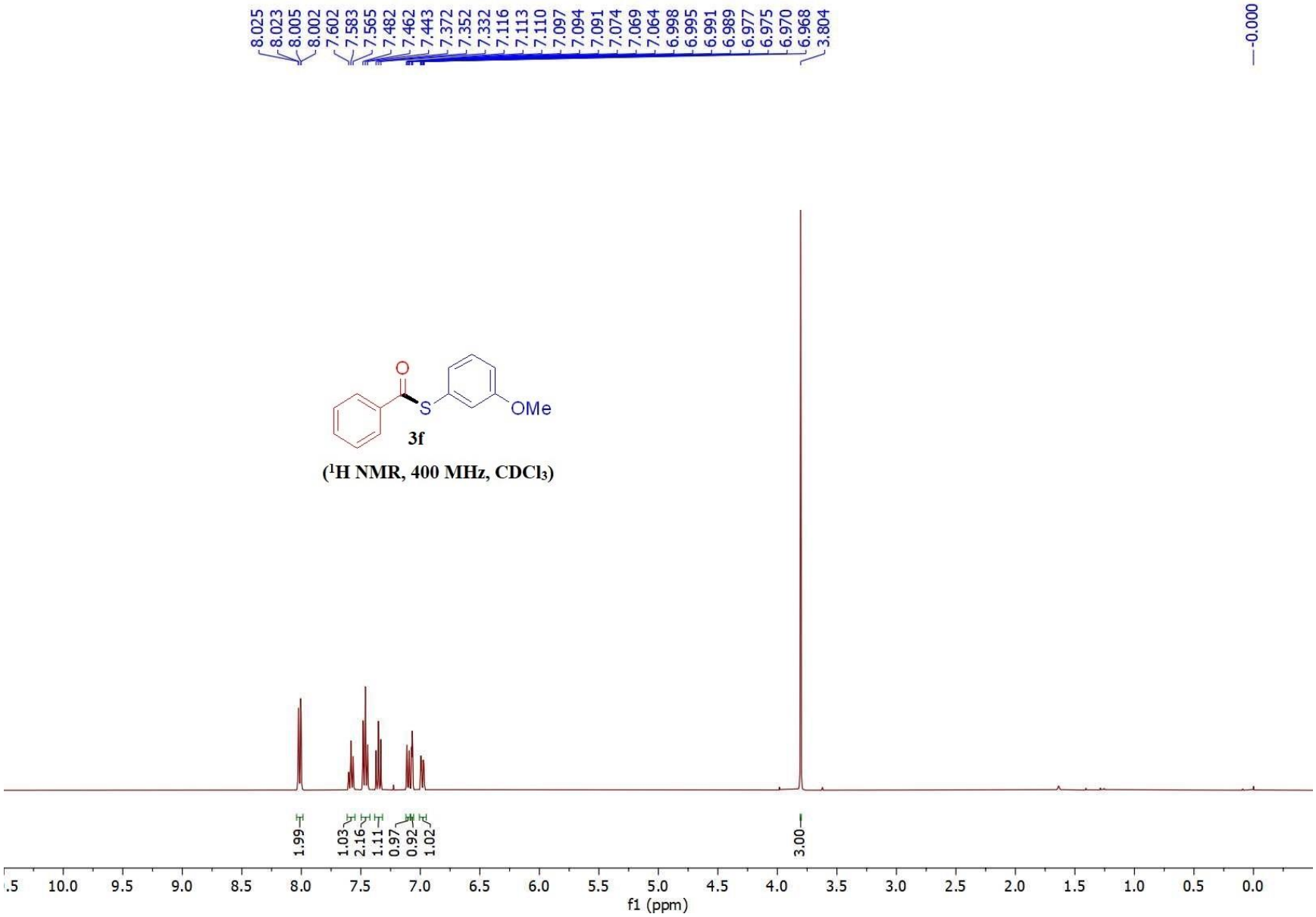


($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)


8.067
8.064
8.047
8.043
7.615
7.612
7.609
7.598
7.593
7.589
7.578
7.575
7.571
7.495
7.491
7.489
7.483
7.479
7.475
7.471
7.464
7.462
7.458
7.457
7.455
7.453
7.444
7.440
7.254
7.060
7.057
7.041
7.038
7.028
7.025
7.022
7.019
7.008
7.005
3.857
-0.000
O
S
OMe
3e
(1H NMR, 400 MHz, CDCl3)
2.00
1.07
4.10
2.13
3.21
f1 (ppm)

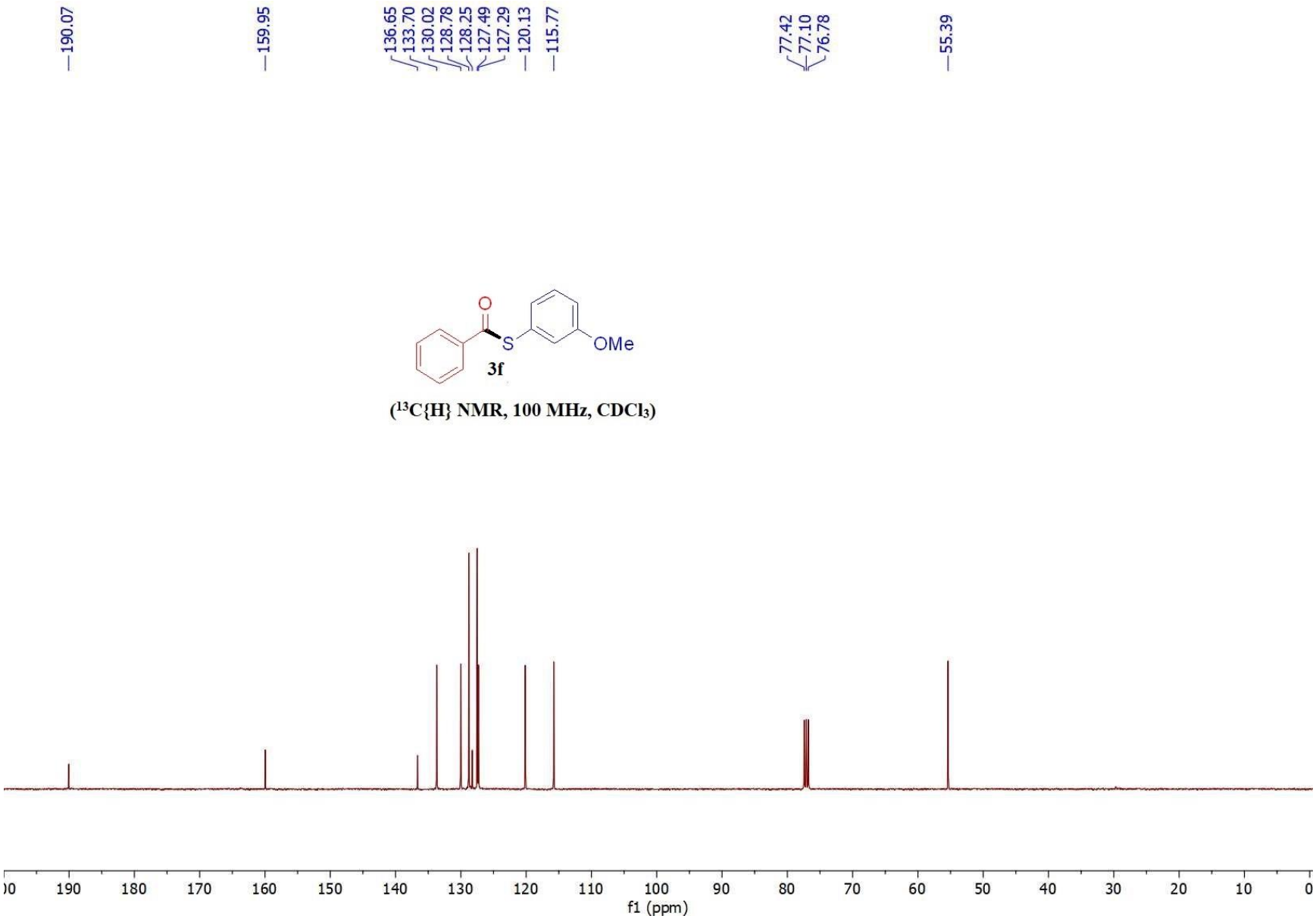


($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

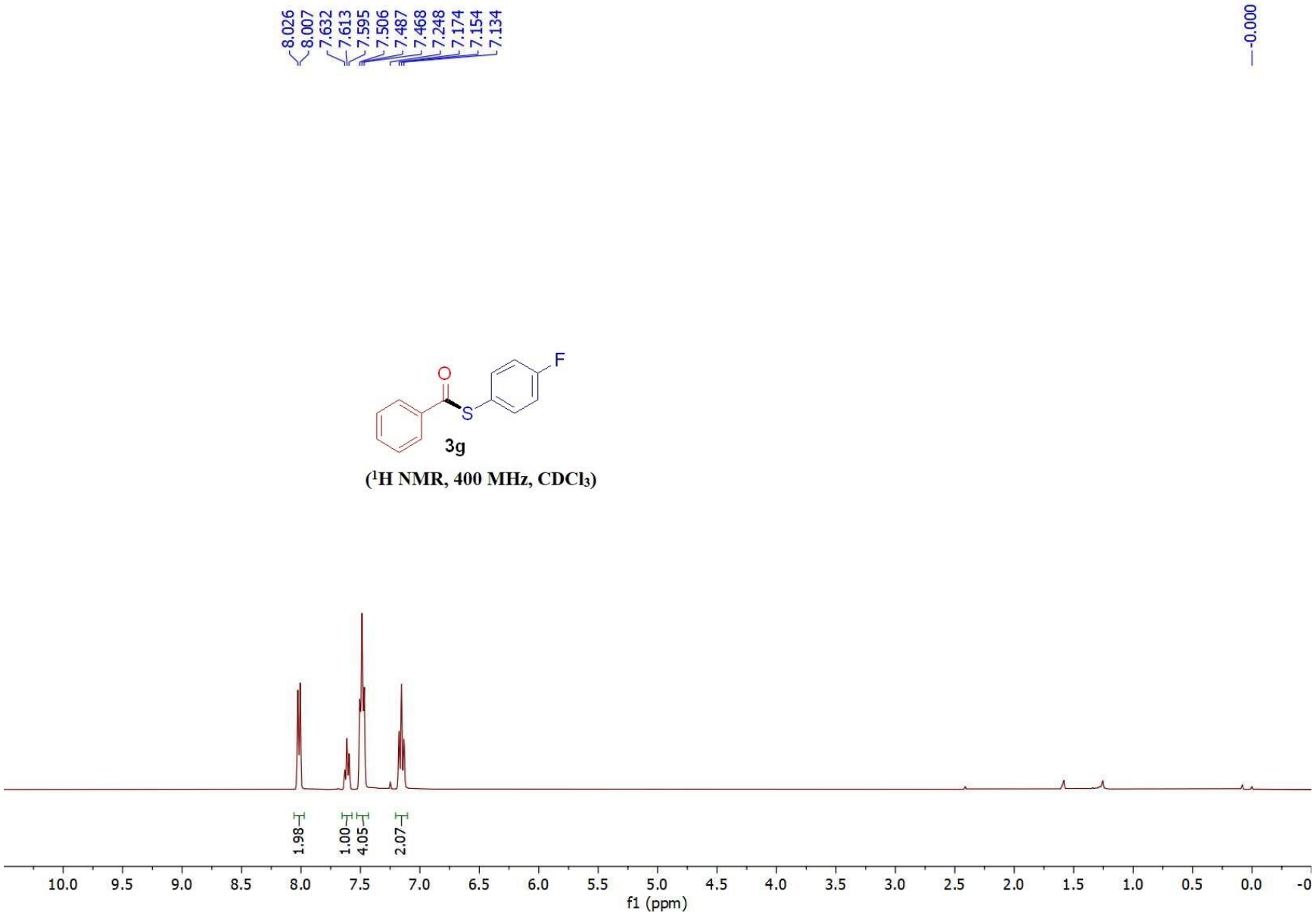


3f

(^{1}H NMR, 400 MHz, $CDCl_3$)

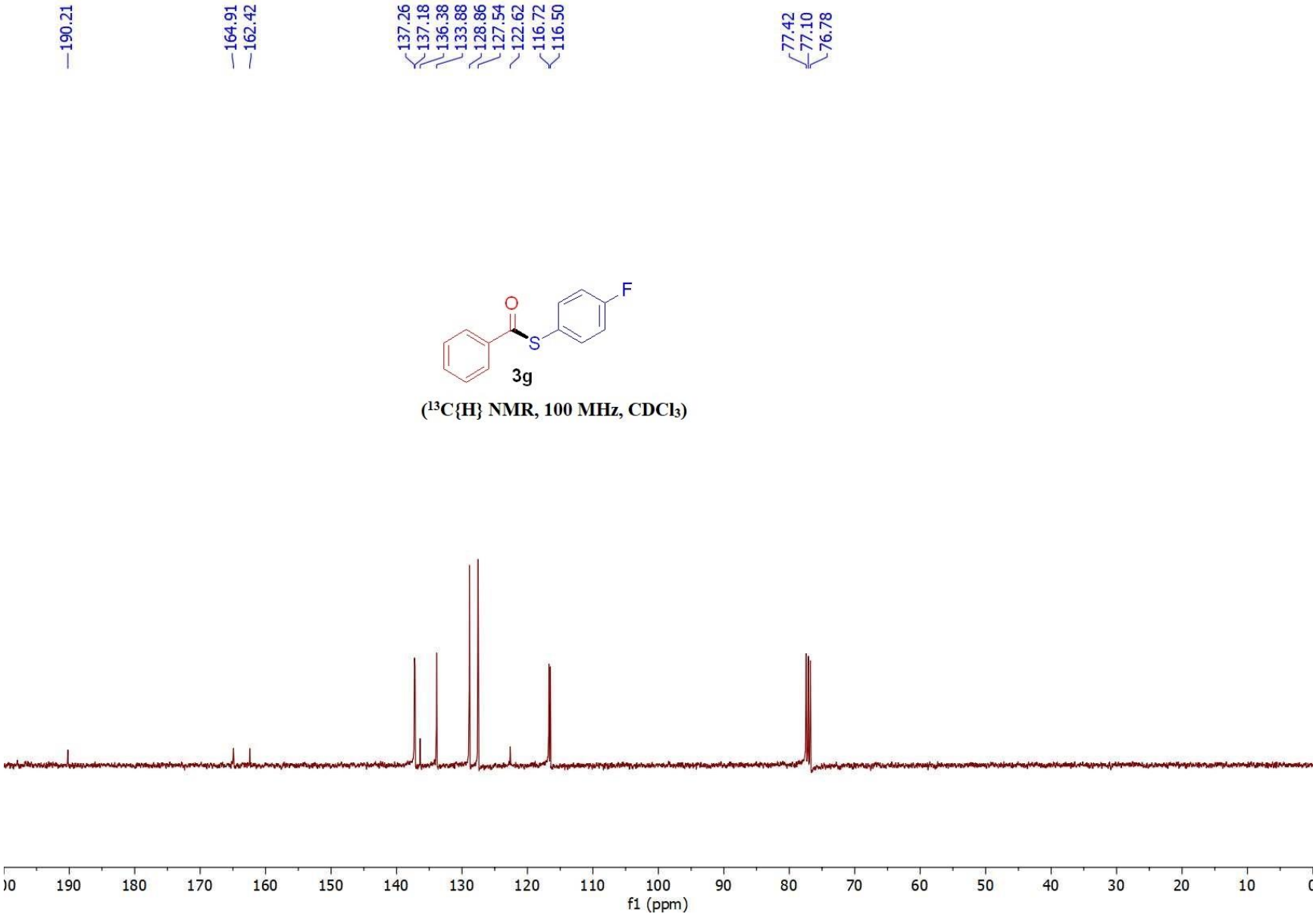


($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



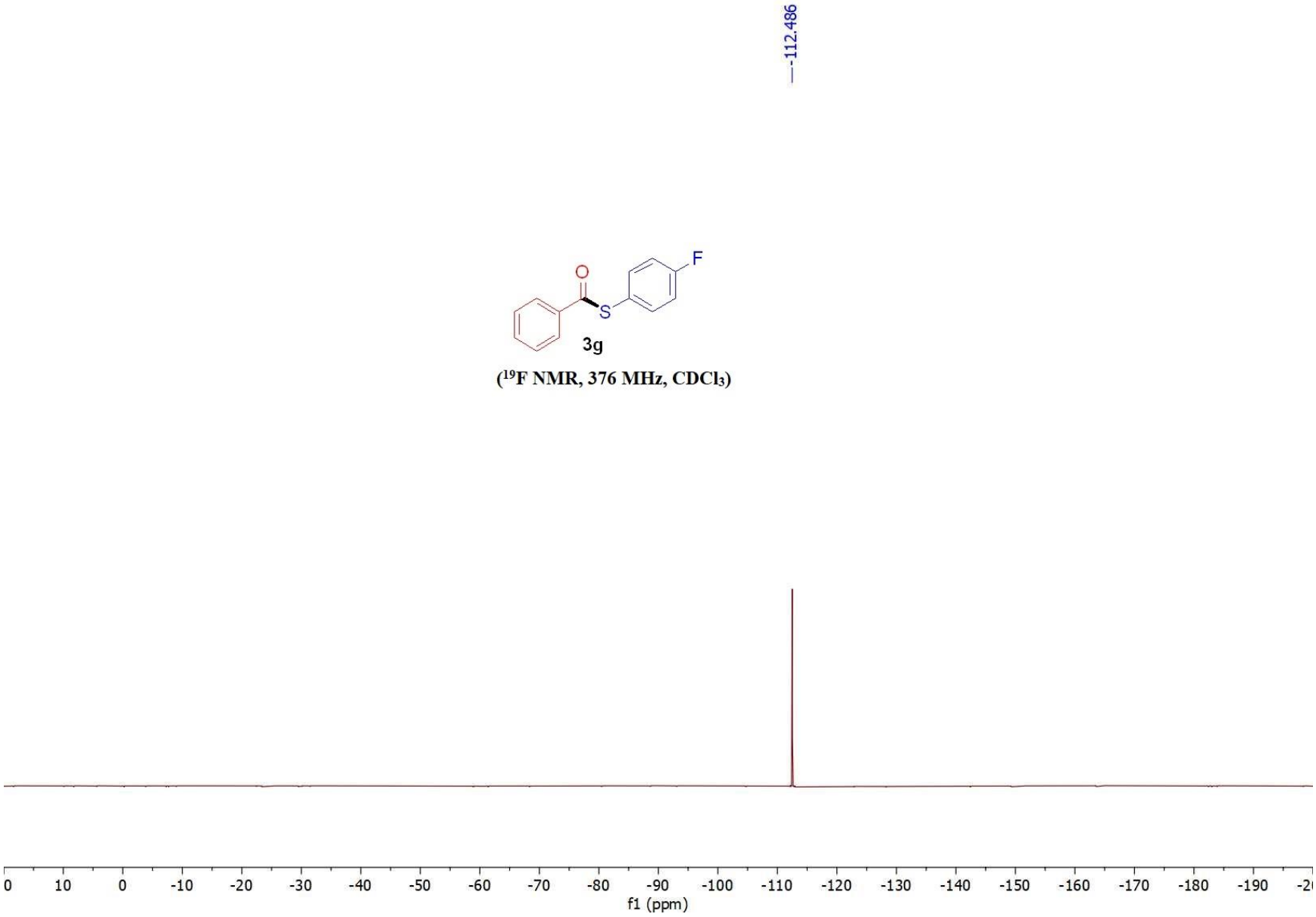
3g

(^{1}H NMR, 400 MHz, $CDCl_3$)



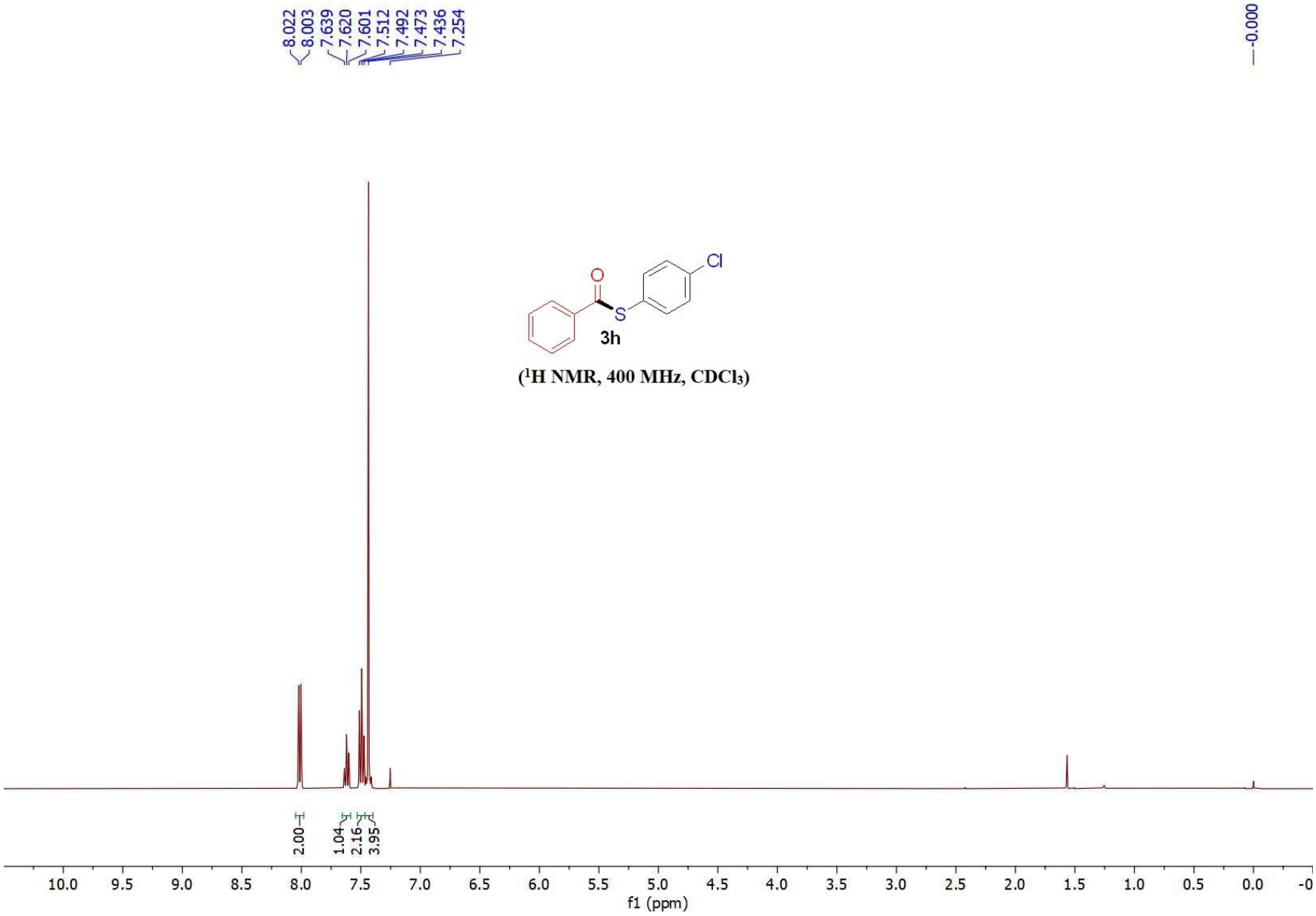
3g

($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

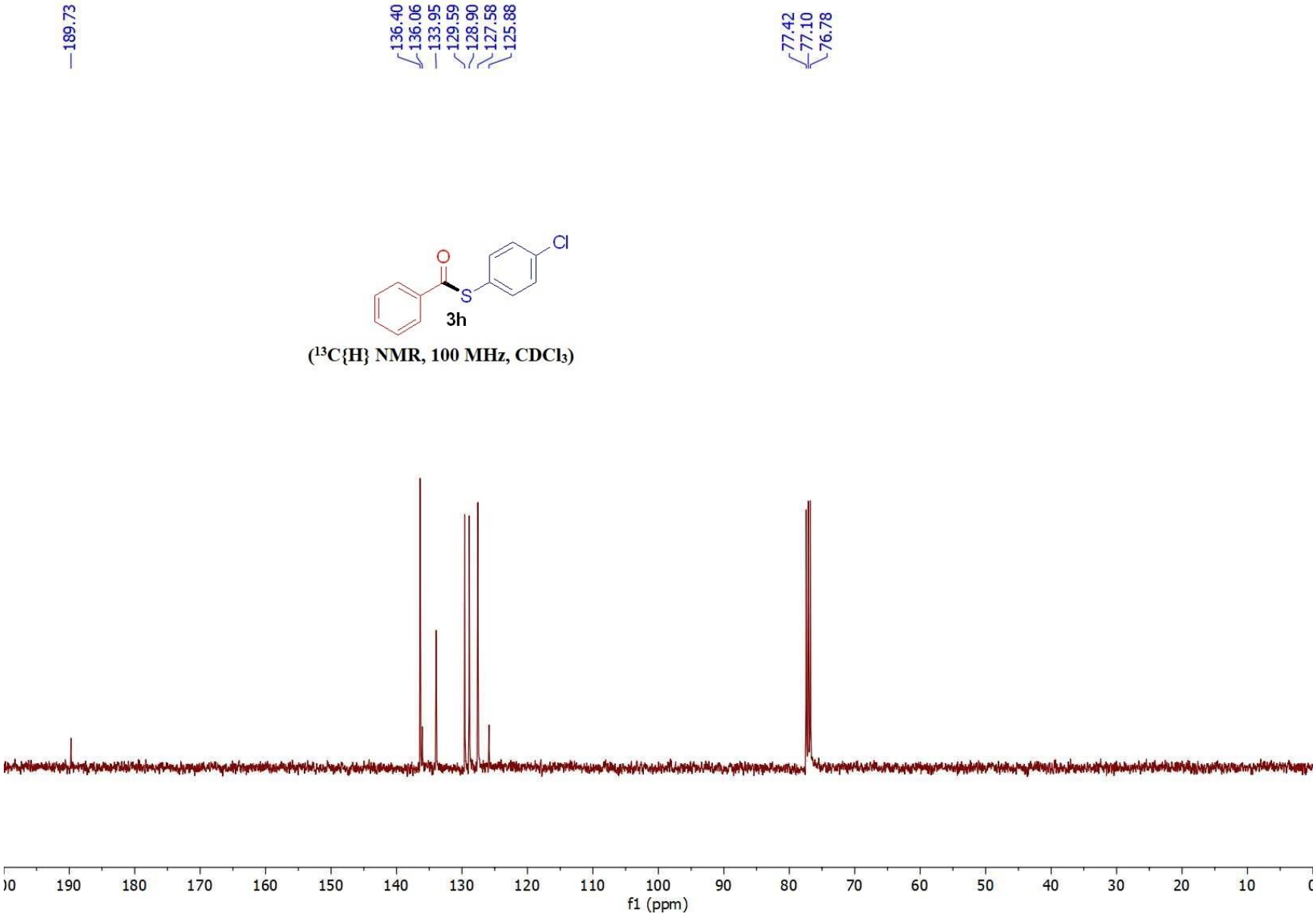


3g

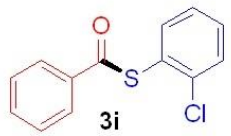
(^{19}F NMR, 376 MHz, $CDCl_3$)



(^{1}H NMR, 400 MHz, $CDCl_3$)

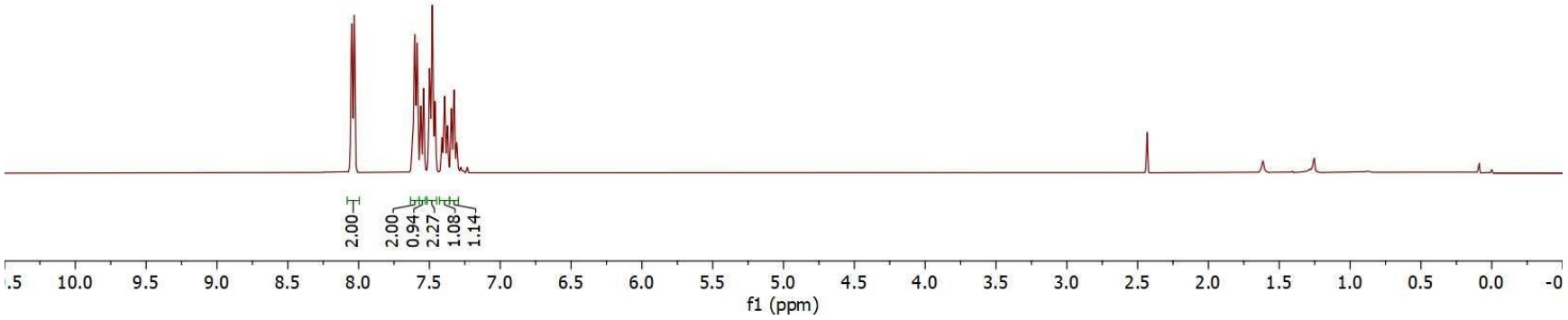


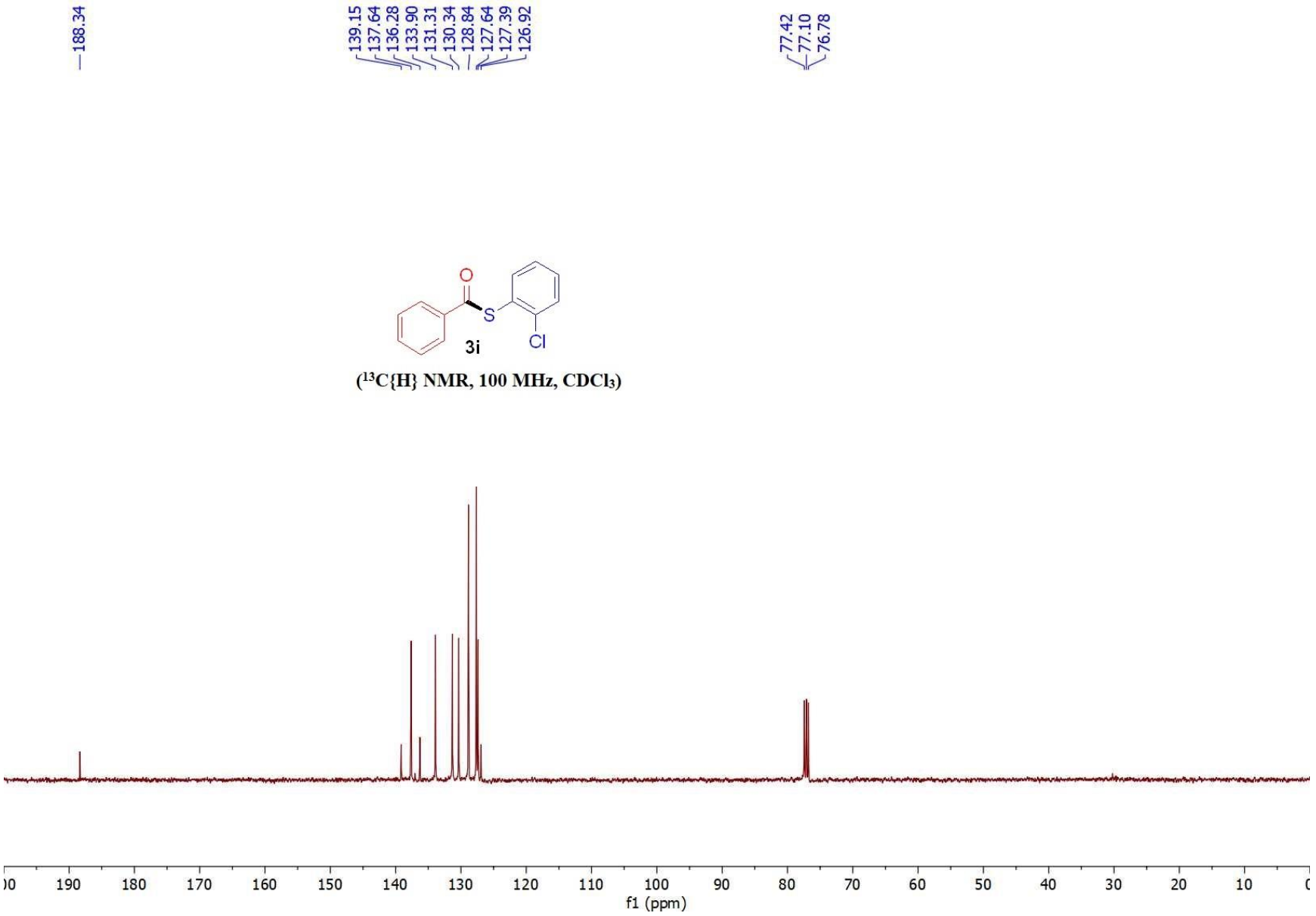
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



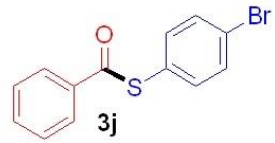
3i

(^{1}H NMR, 400 MHz, $CDCl_3$)



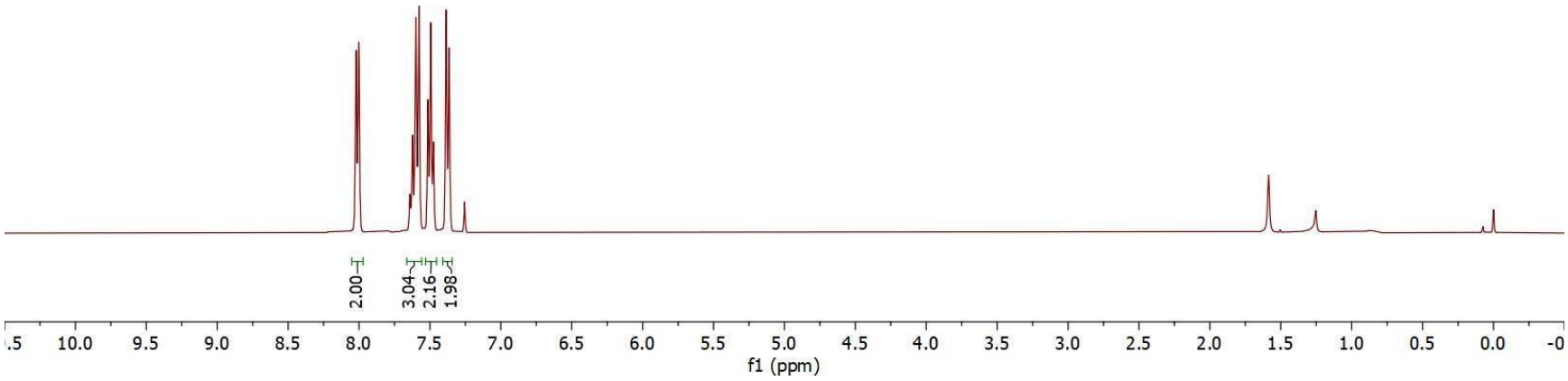


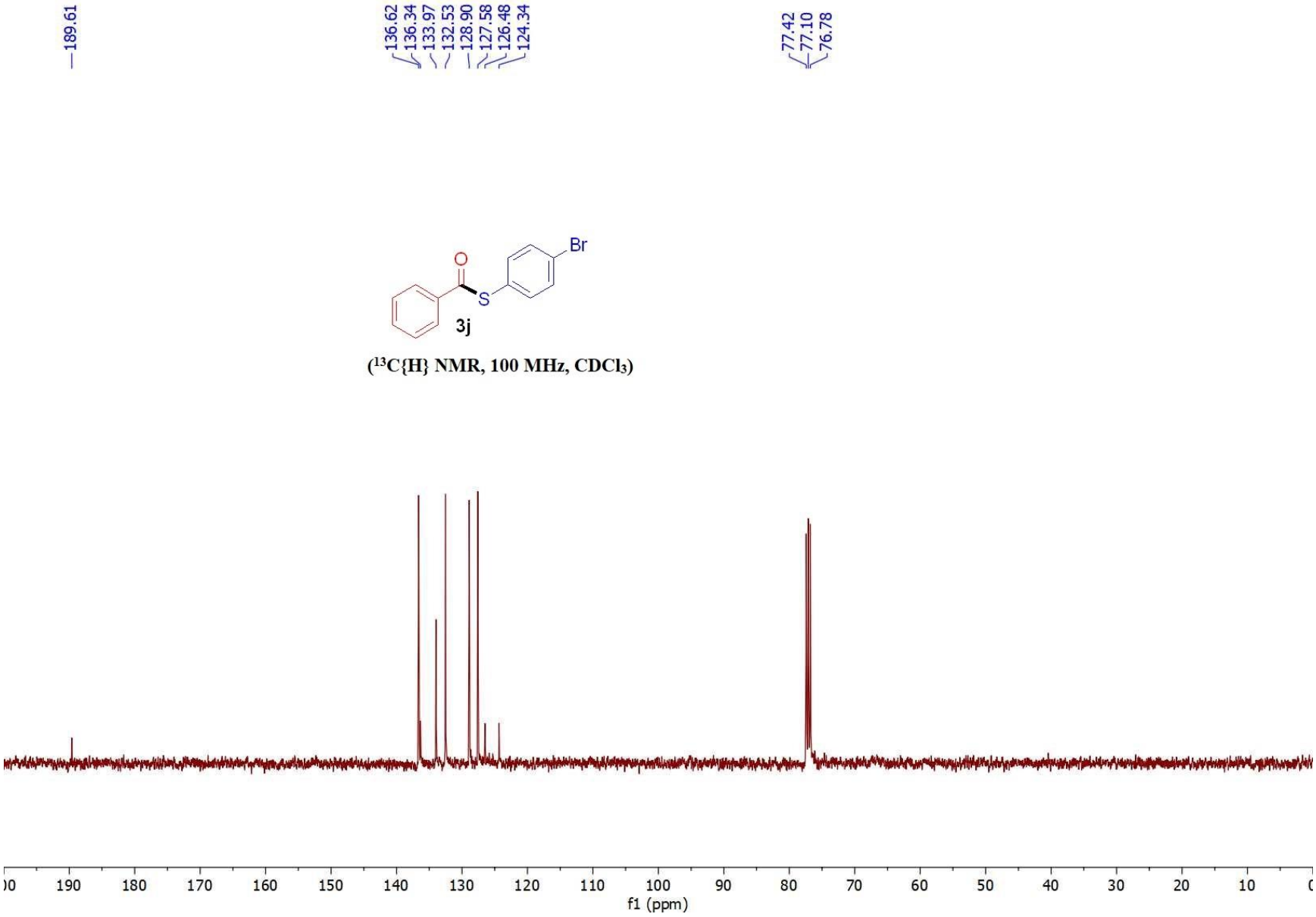
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



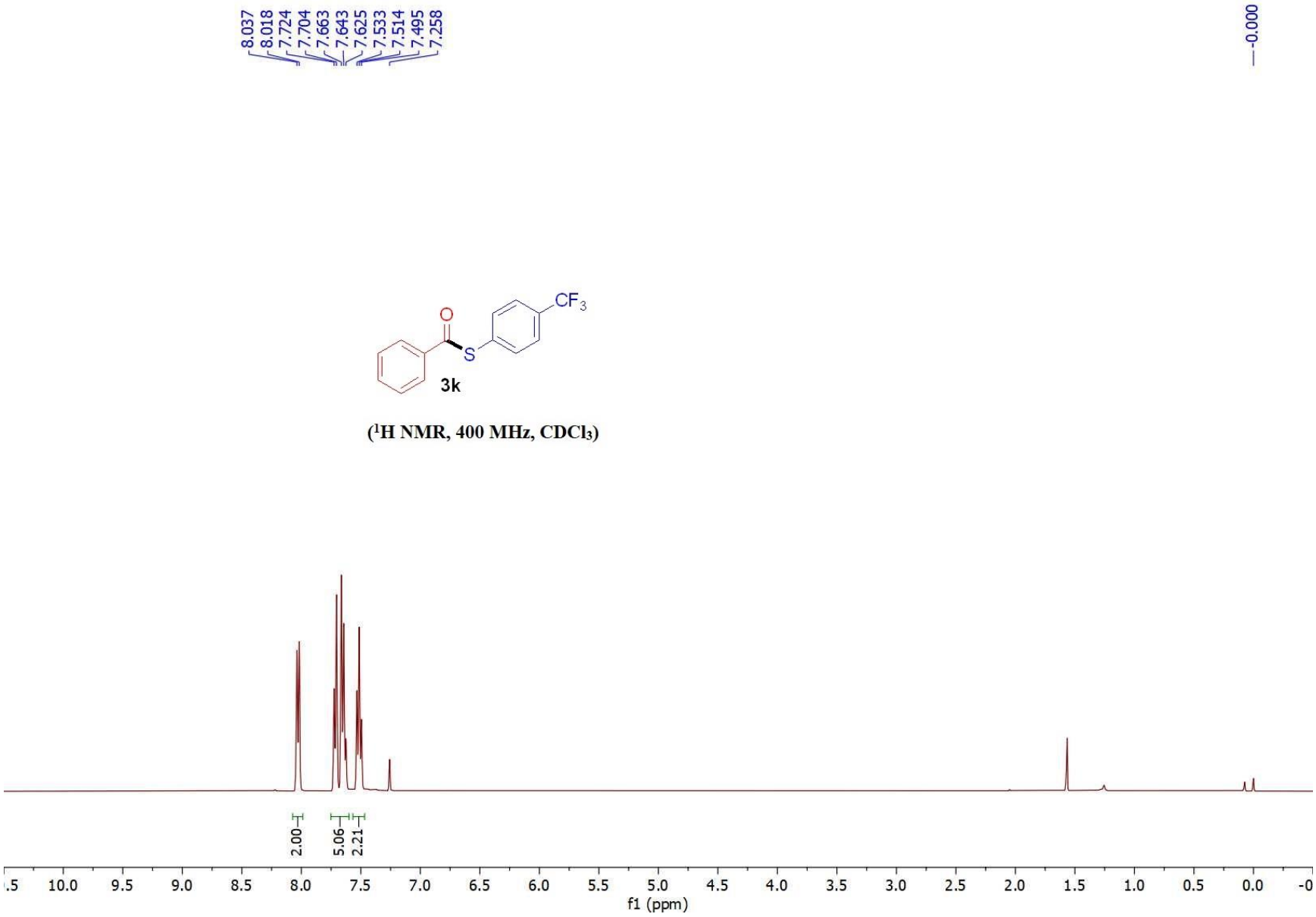
3j

(^{1}H NMR, 400 MHz, $CDCl_3$)



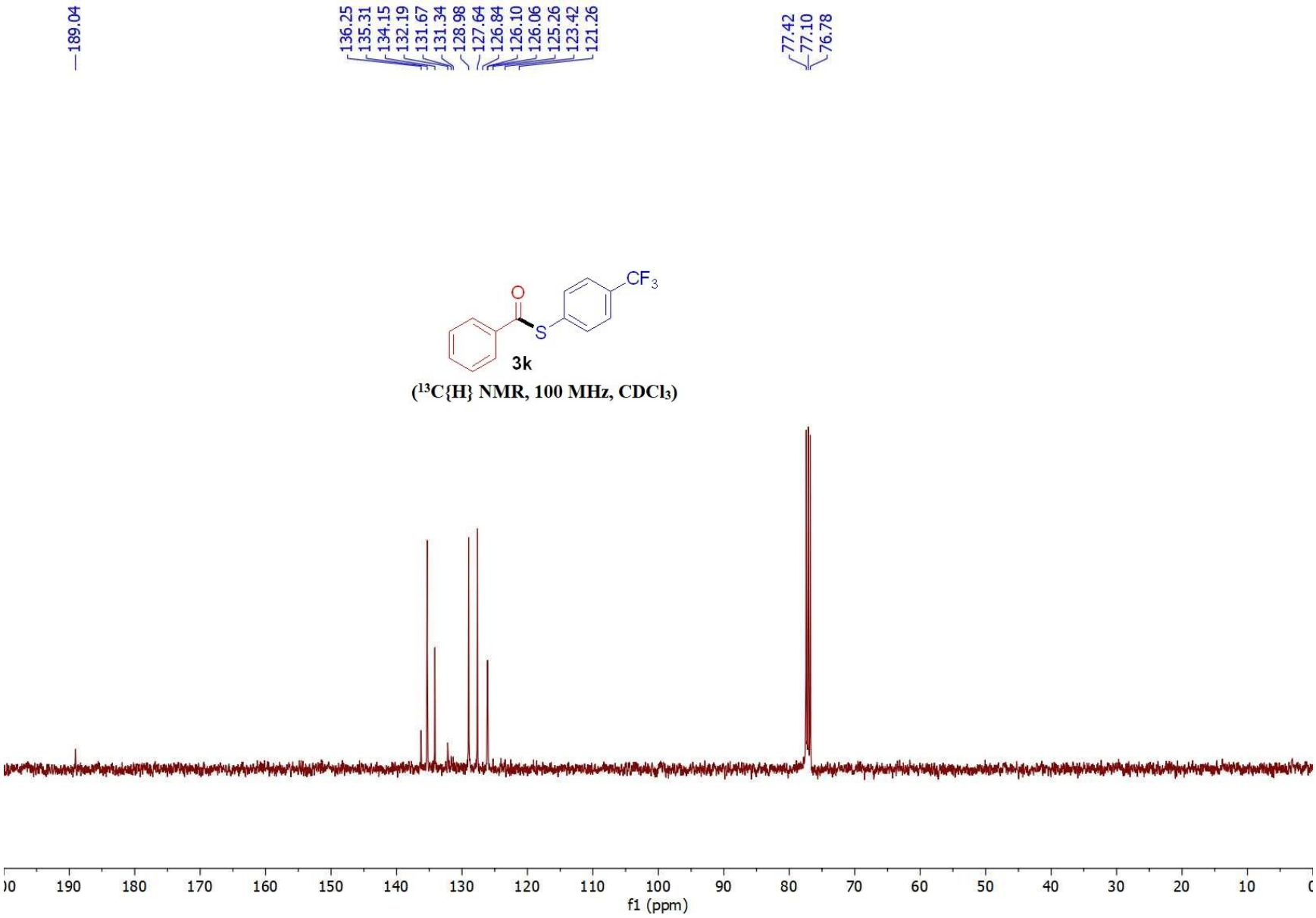


($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



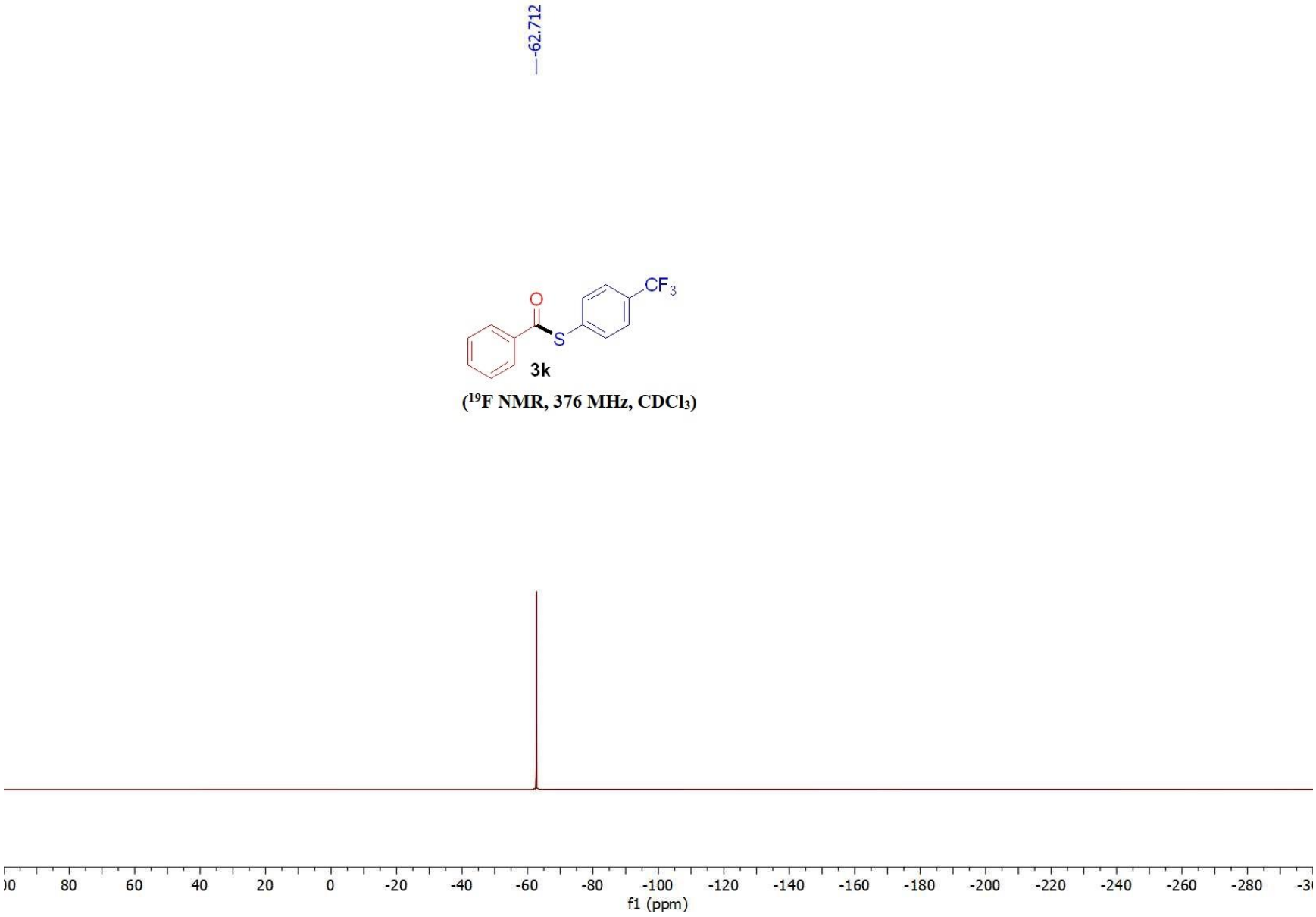
3k

(^{1}H NMR, 400 MHz, $CDCl_3$)



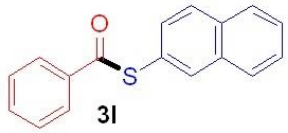
3k

($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



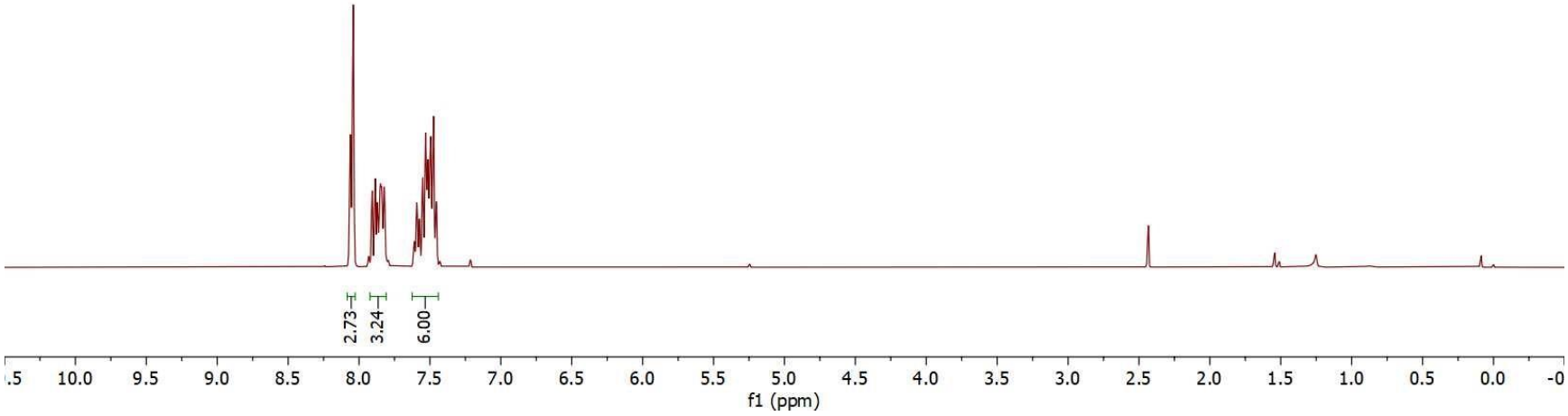
3k

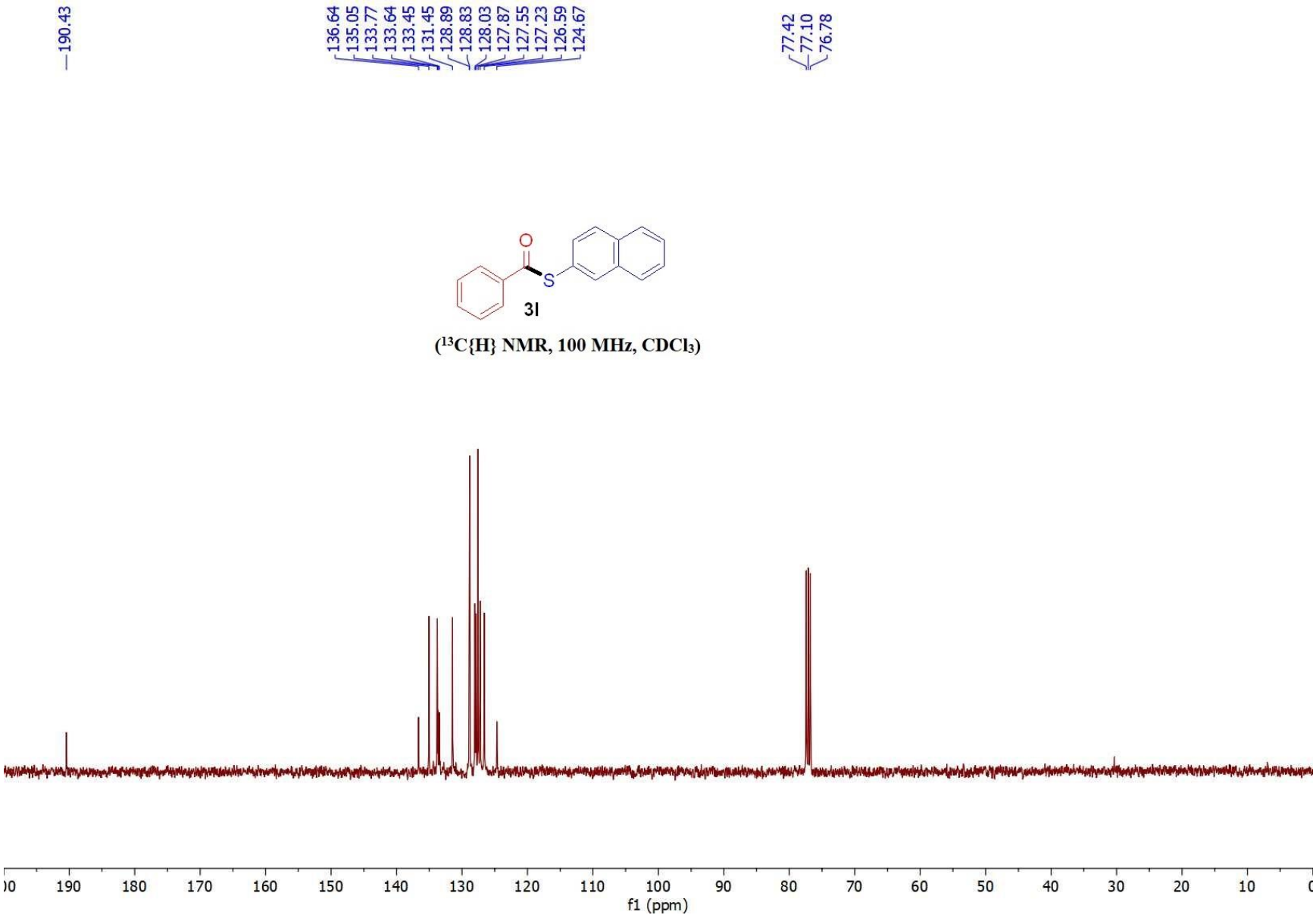
(^{19}F NMR, 376 MHz, $CDCl_3$)



3l

(^{1}H NMR, 400 MHz, $CDCl_3$)



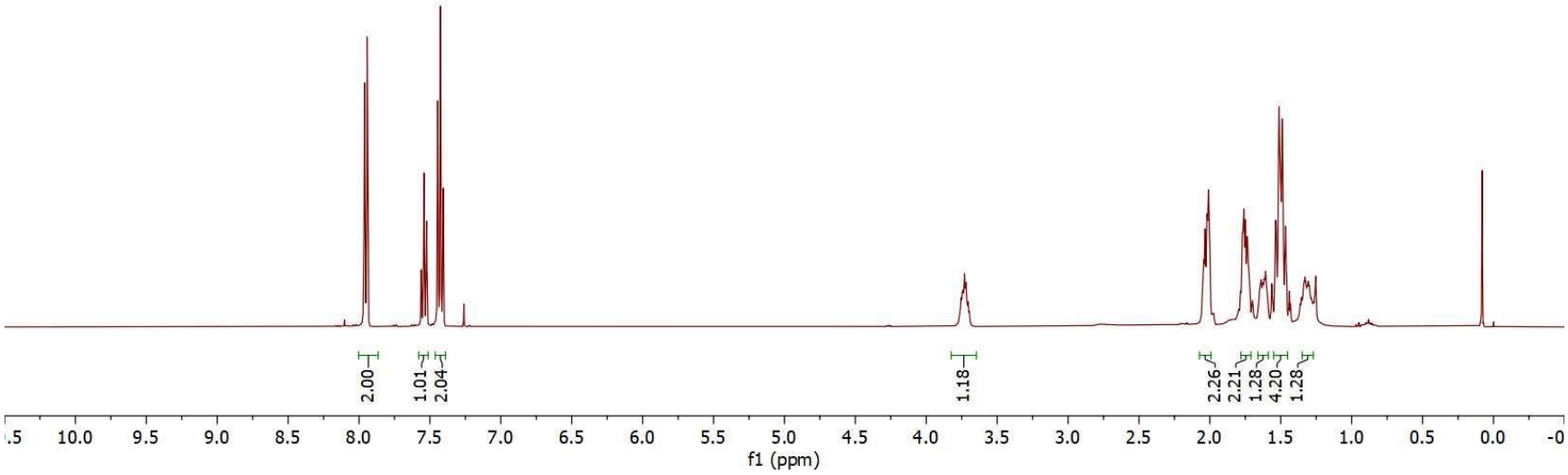


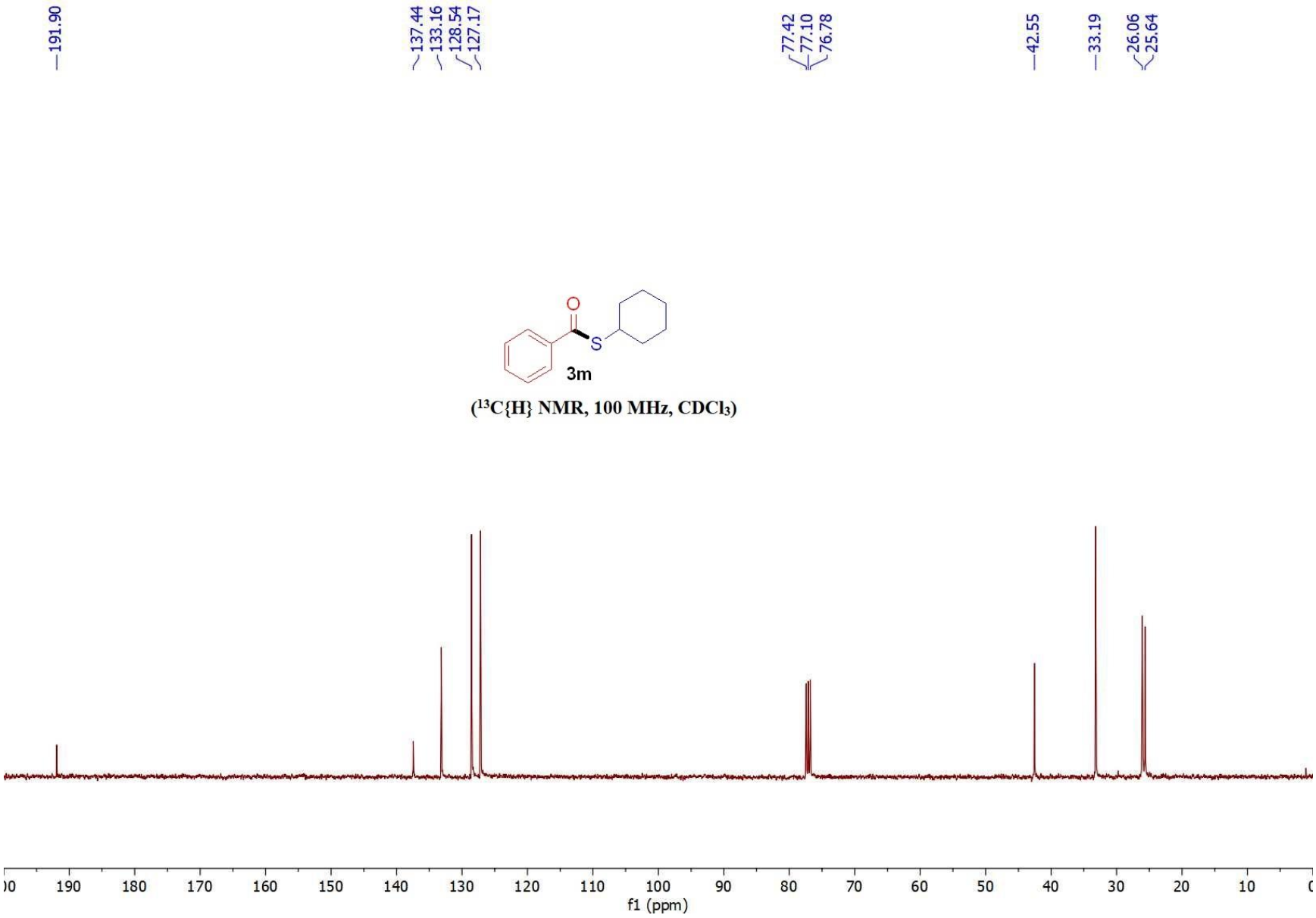
3l

($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

3m

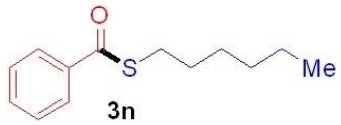
(^{1}H NMR, 400 MHz, $CDCl_3$)





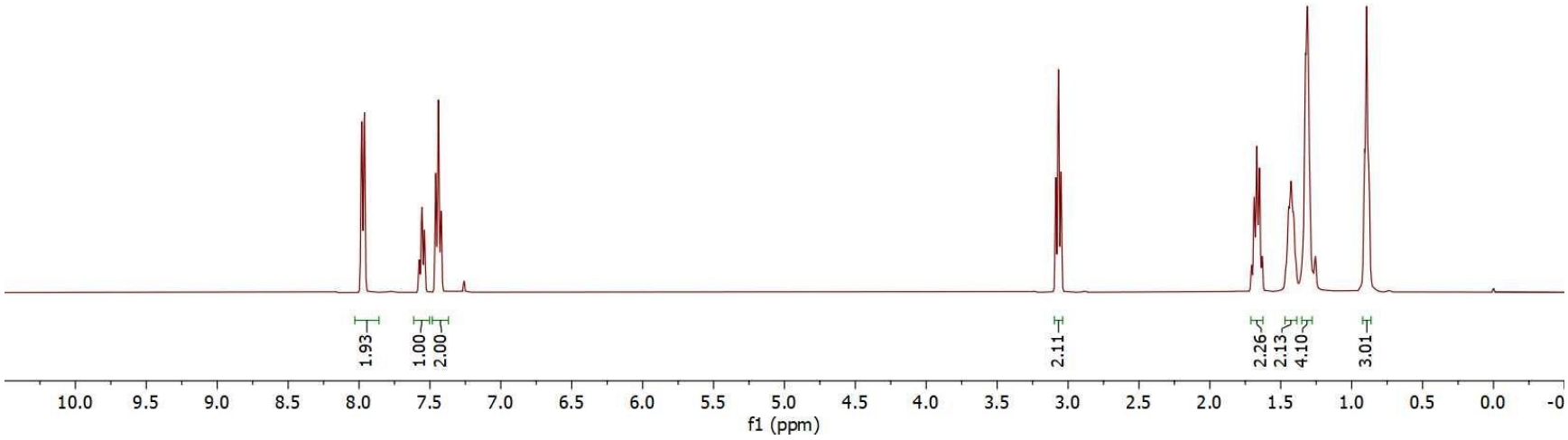
3m

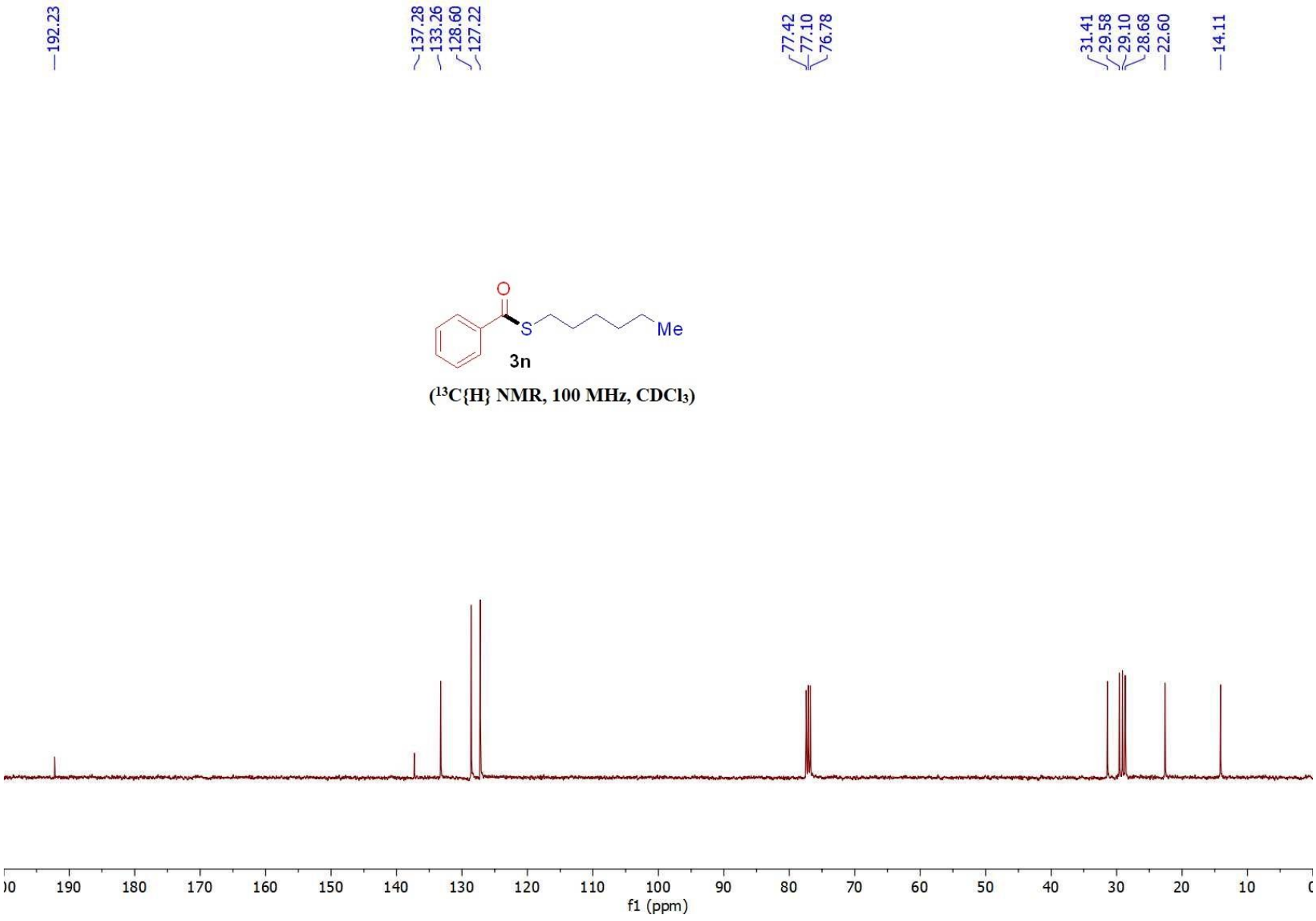
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



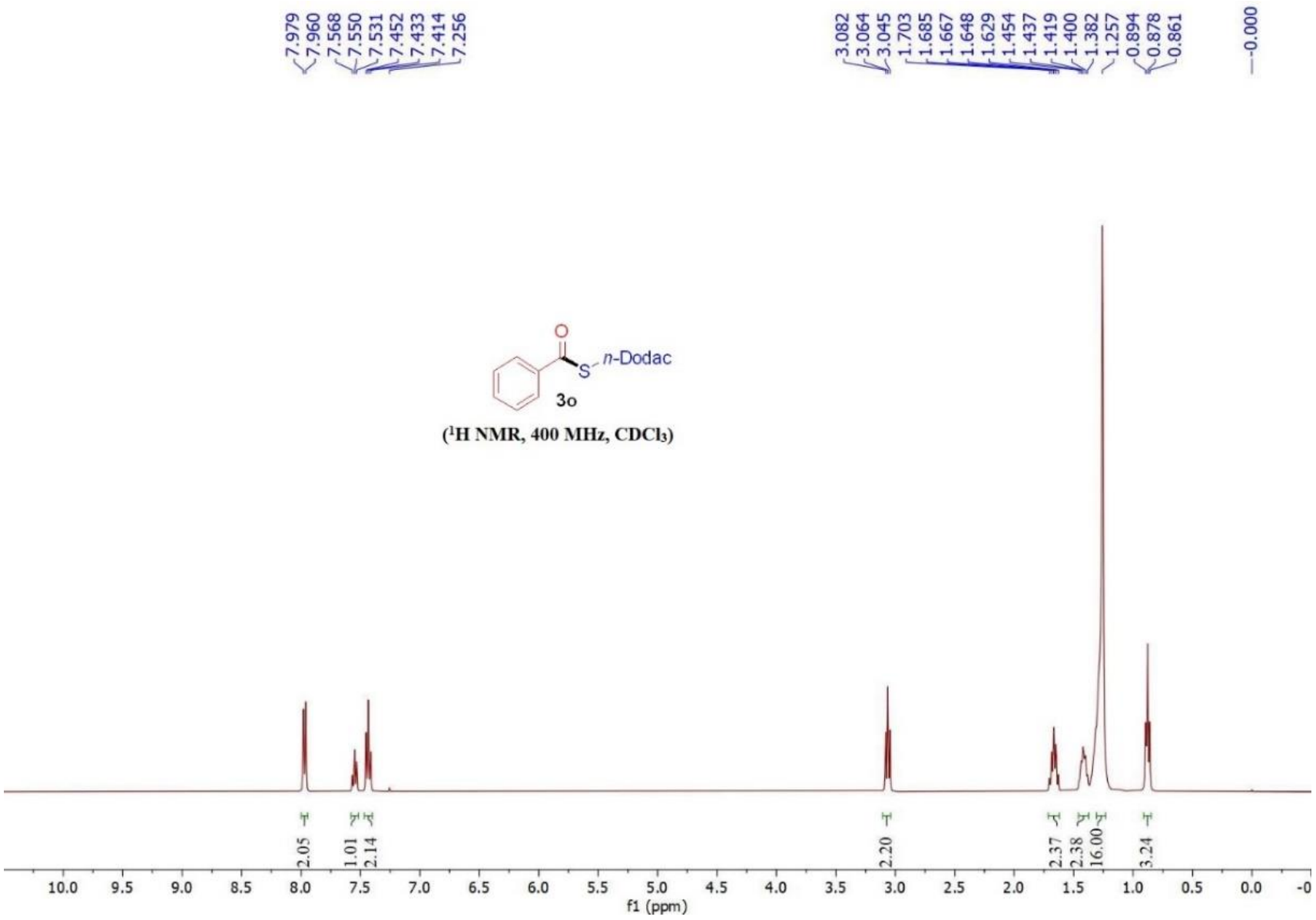
3n

(^{1}H NMR, 400 MHz, $CDCl_3$)





($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)


7.979
7.960
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7.452
7.433
7.414
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3.082
3.064
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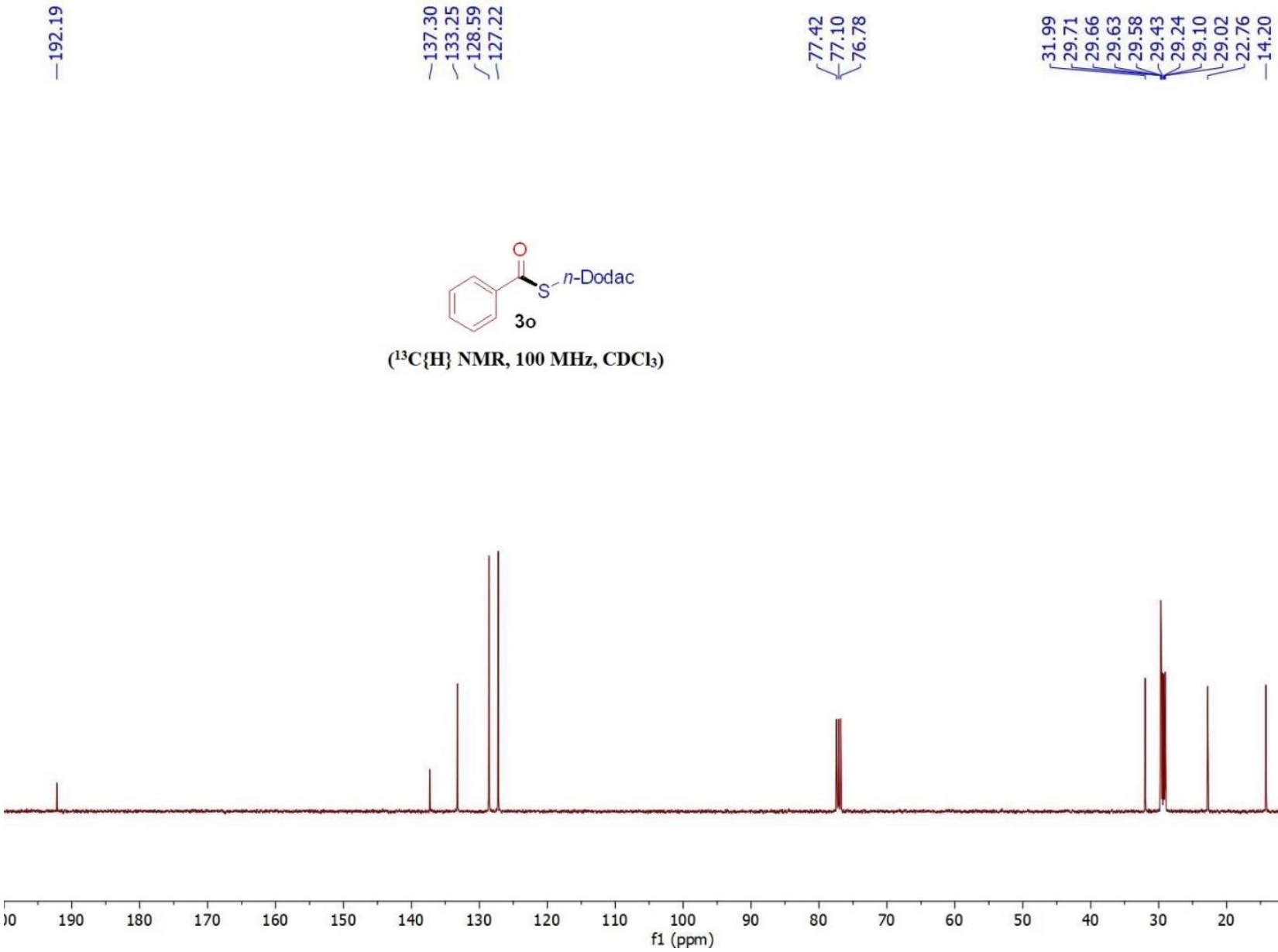
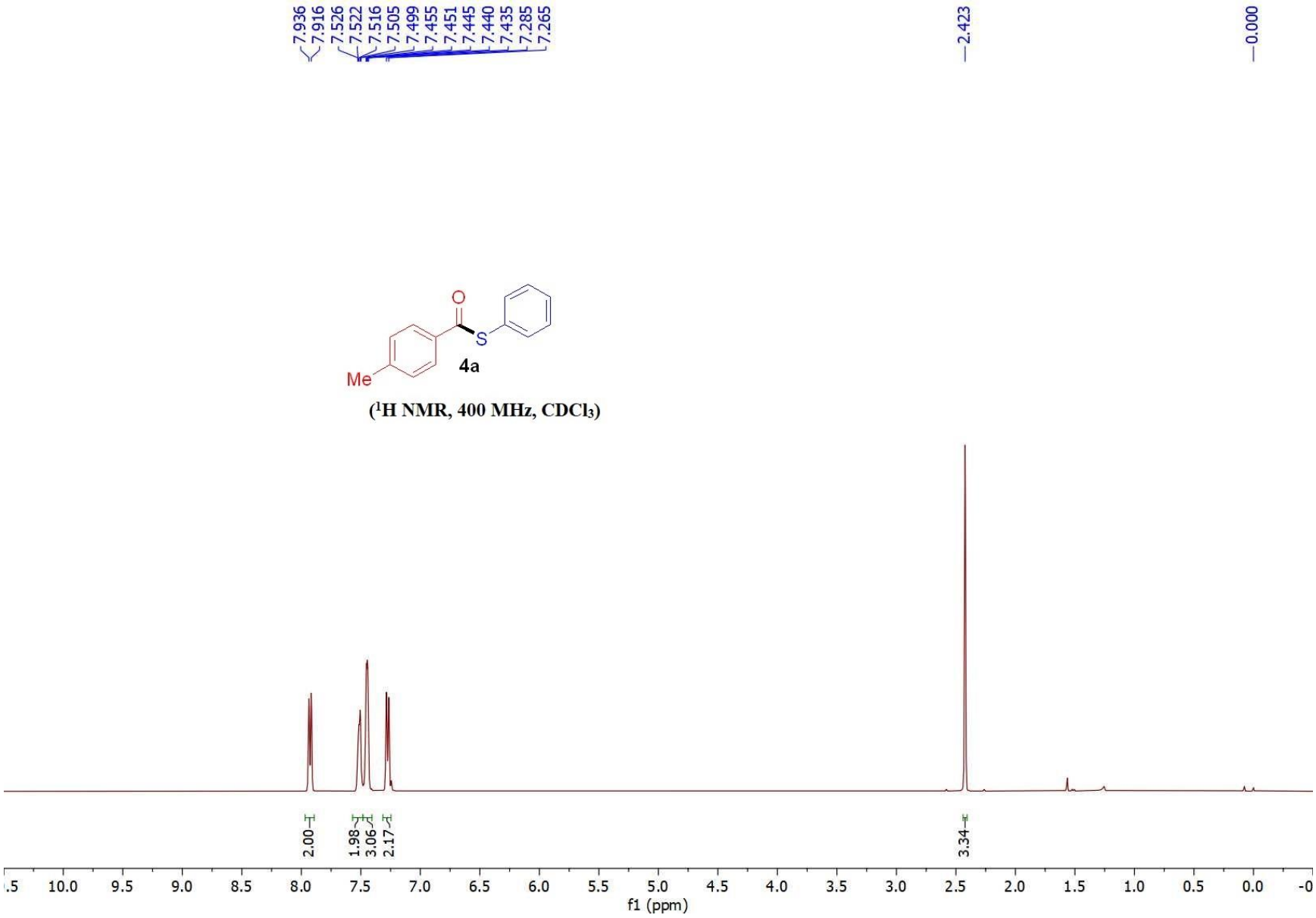
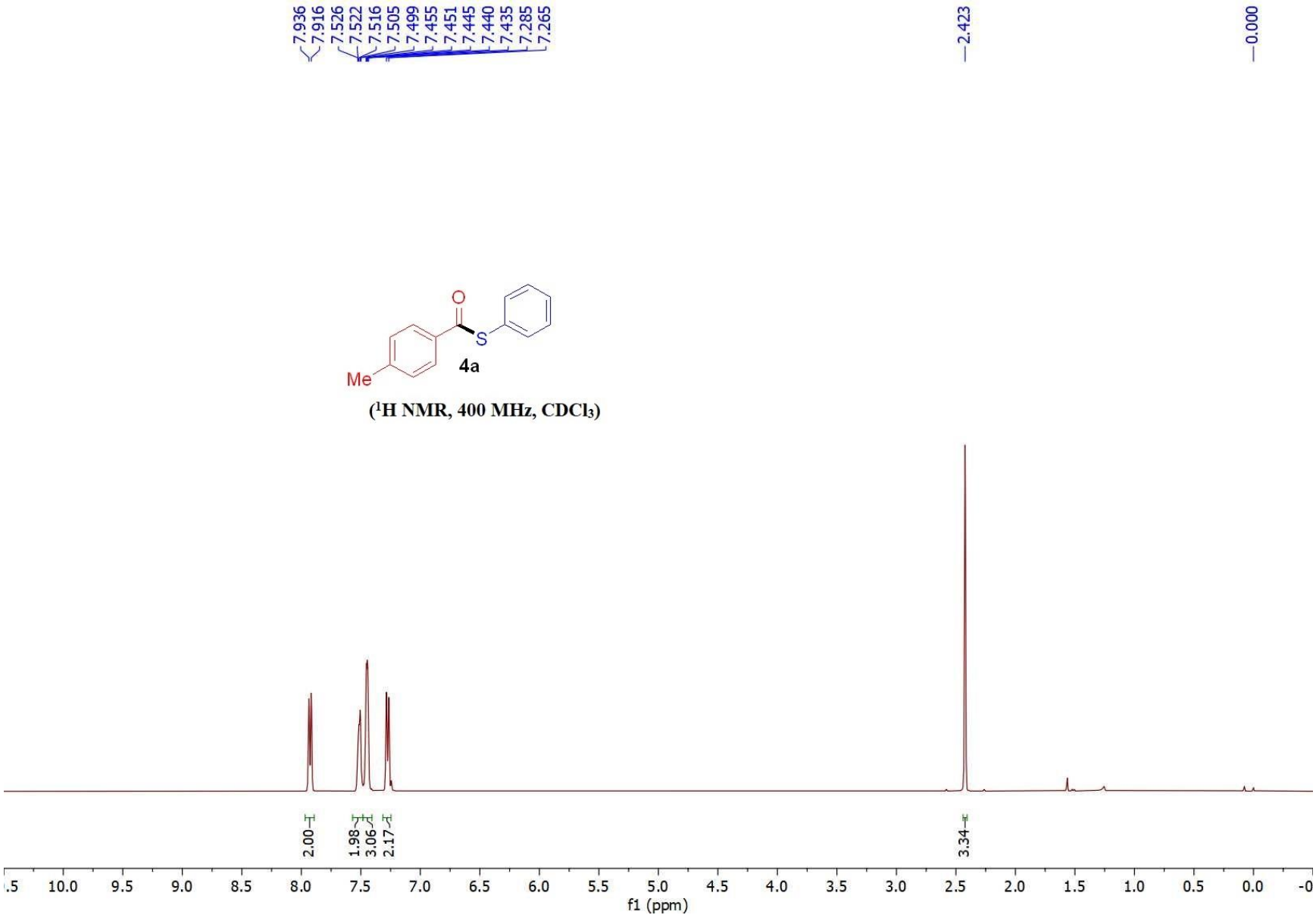
1.703
1.685
1.667
1.648
1.629
1.454
1.437
1.419
1.400
1.382
1.257
0.894
0.878
0.861
-0.000
O
S
n-Dodac
3o
(1H NMR, 400 MHz, CDCl3)
2.05
1.01
2.14
2.20
2.37
2.38
16.00
3.24
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)



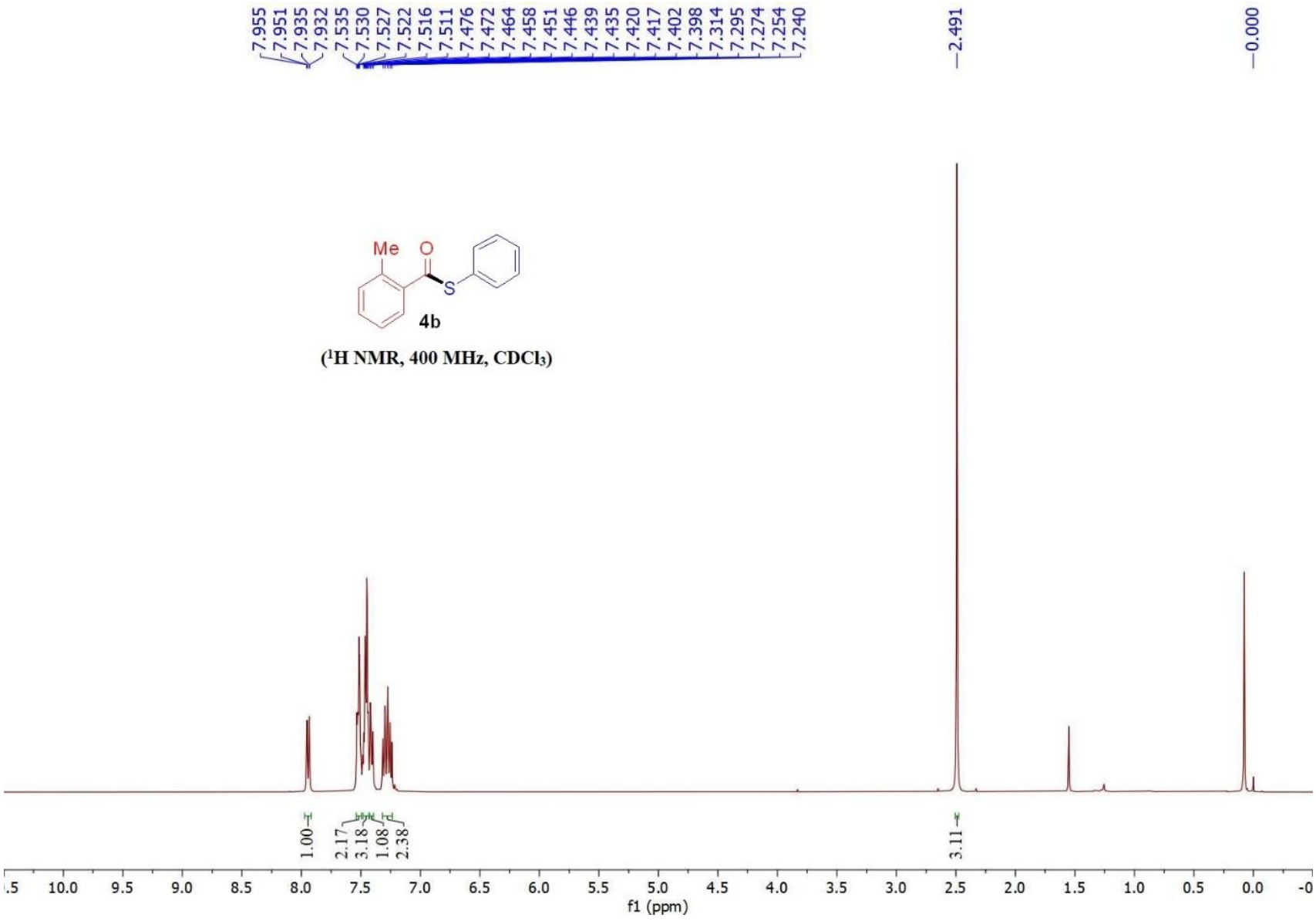
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

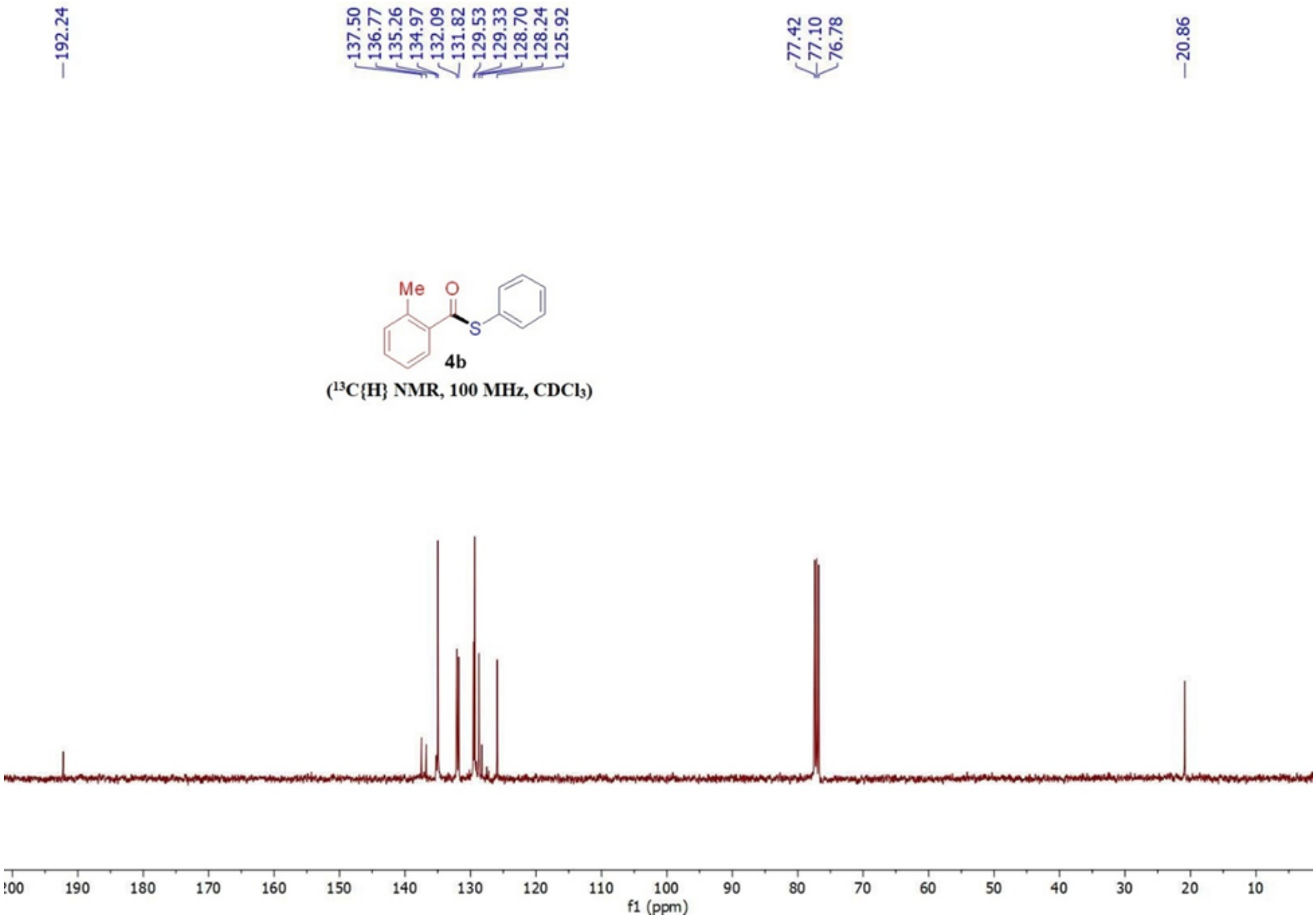


(^{1}H NMR, 400 MHz, $CDCl_3$)



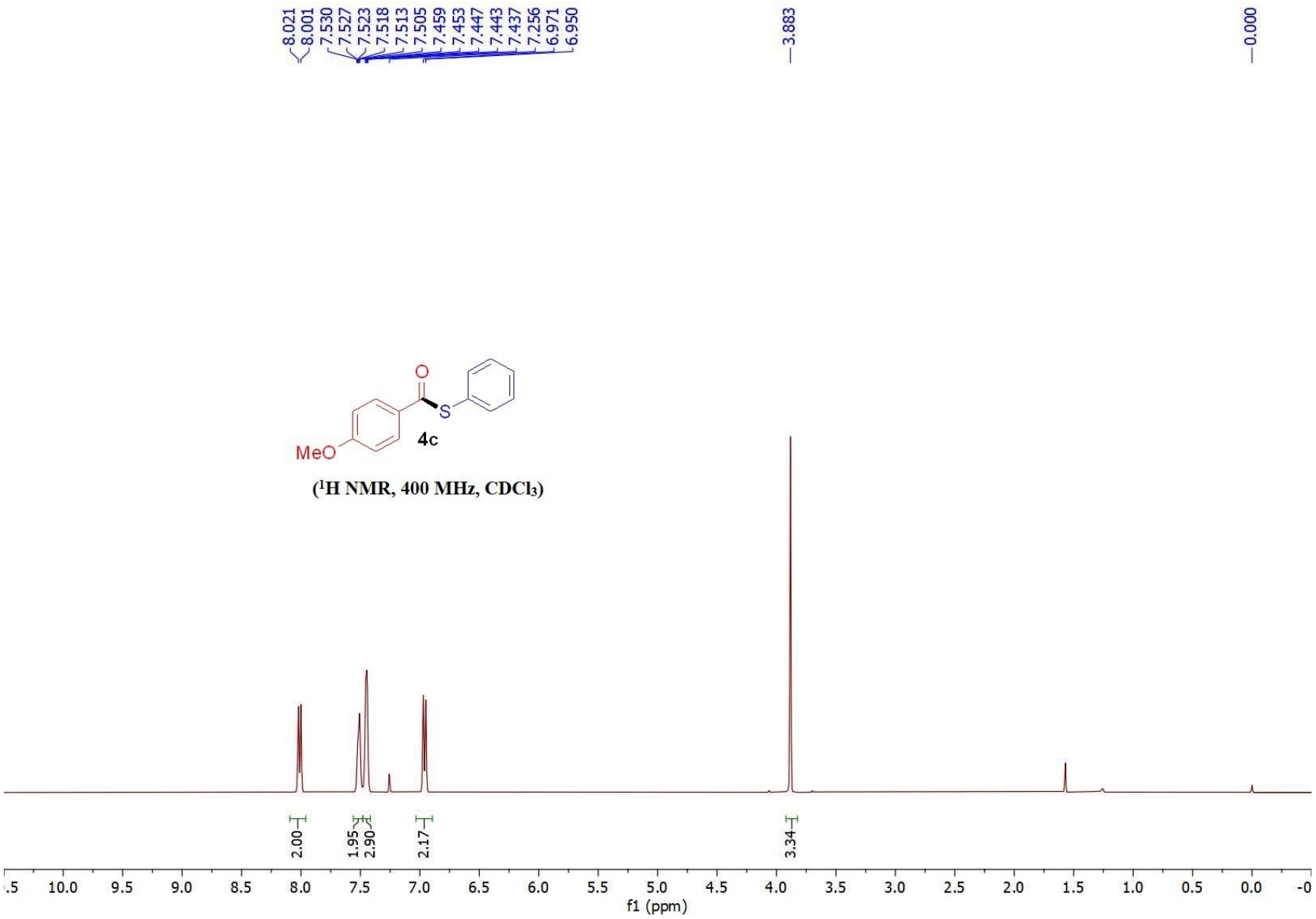
(¹H NMR, 400 MHz, $CDCl_3$)


7.955
7.951
7.935
7.932
7.535
7.530
7.527
7.522
7.516
7.511
7.476
7.472
7.464
7.458
7.451
7.446
7.439
7.435
7.420
7.417
7.402
7.398
7.314
7.295
7.274
7.254
7.240
2.491
0.000
Me
O
S
4b
(1H NMR, 400 MHz, CDCl3)
1.00
2.17
3.18
1.08
2.38
3.11
f1 (ppm)

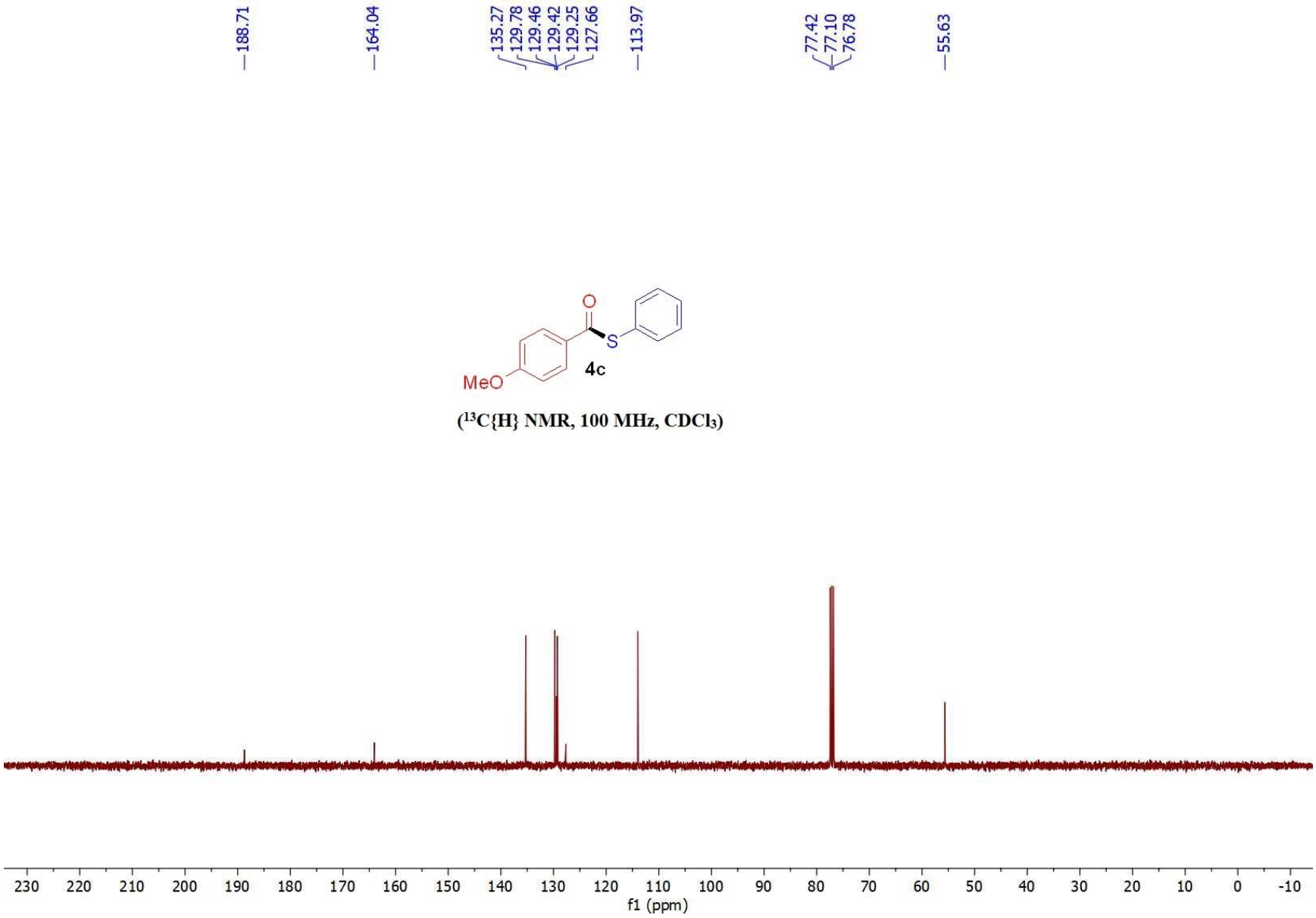


4b

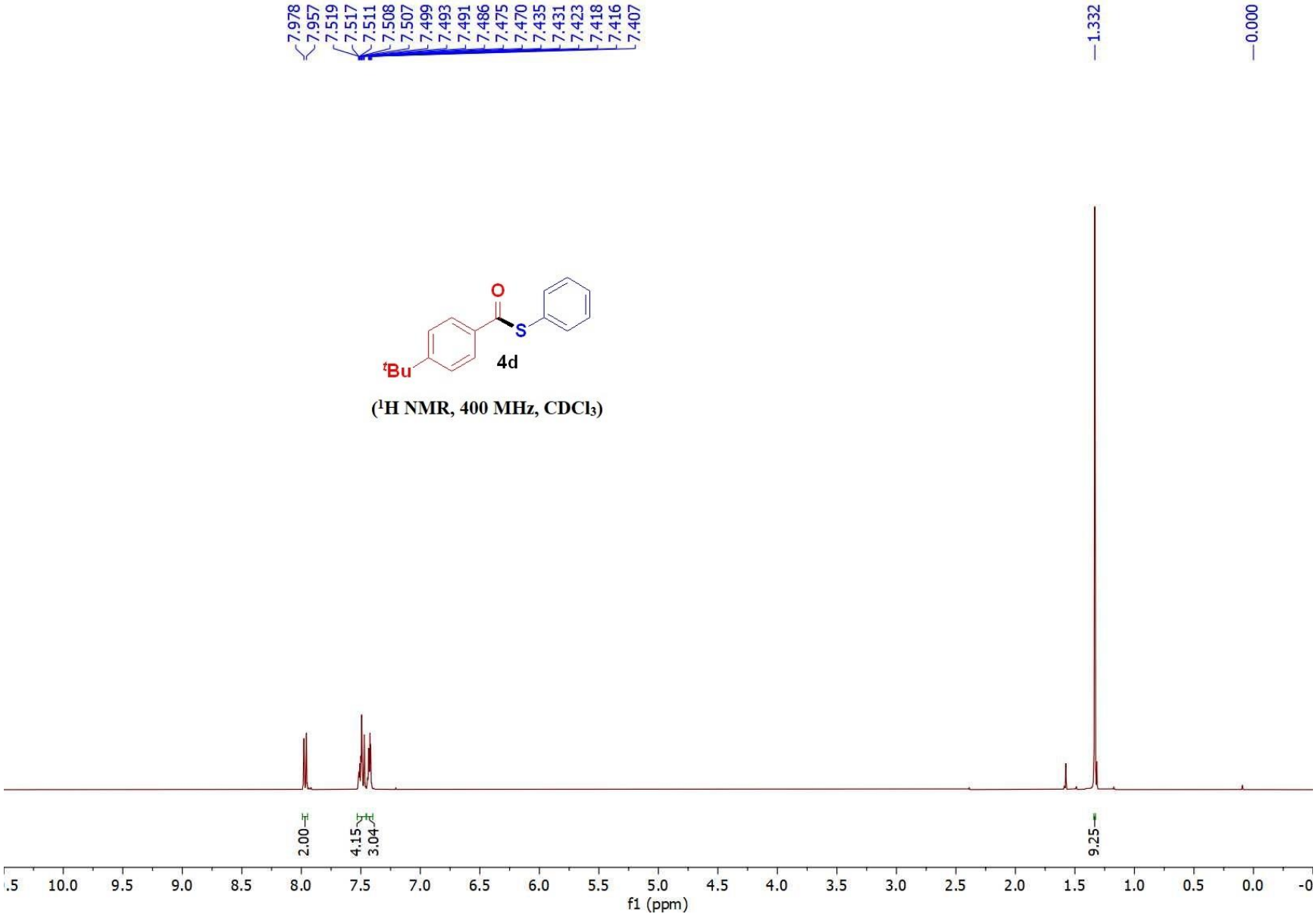
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)



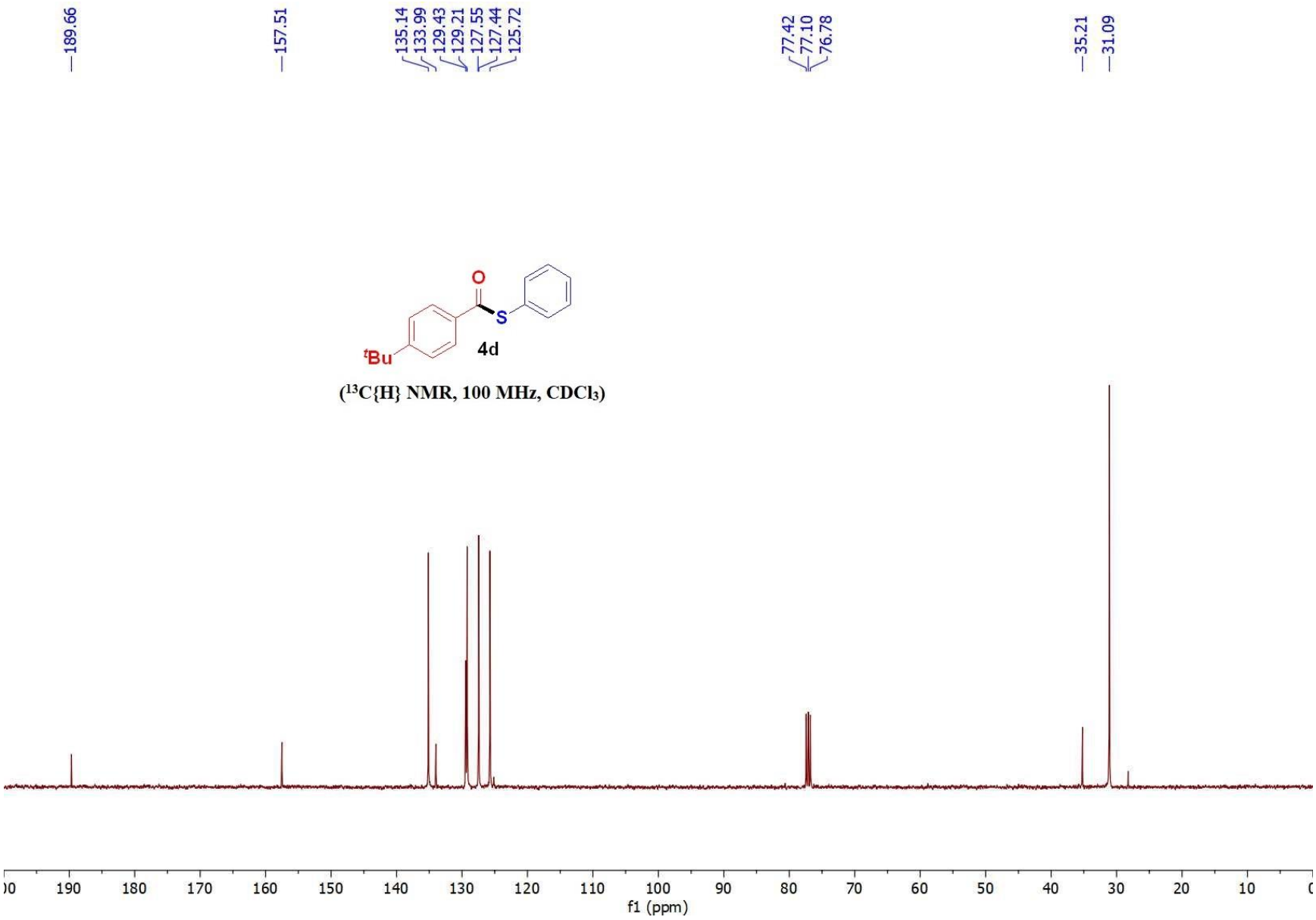
(^{1}H NMR, 400 MHz, $CDCl_3$)



($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

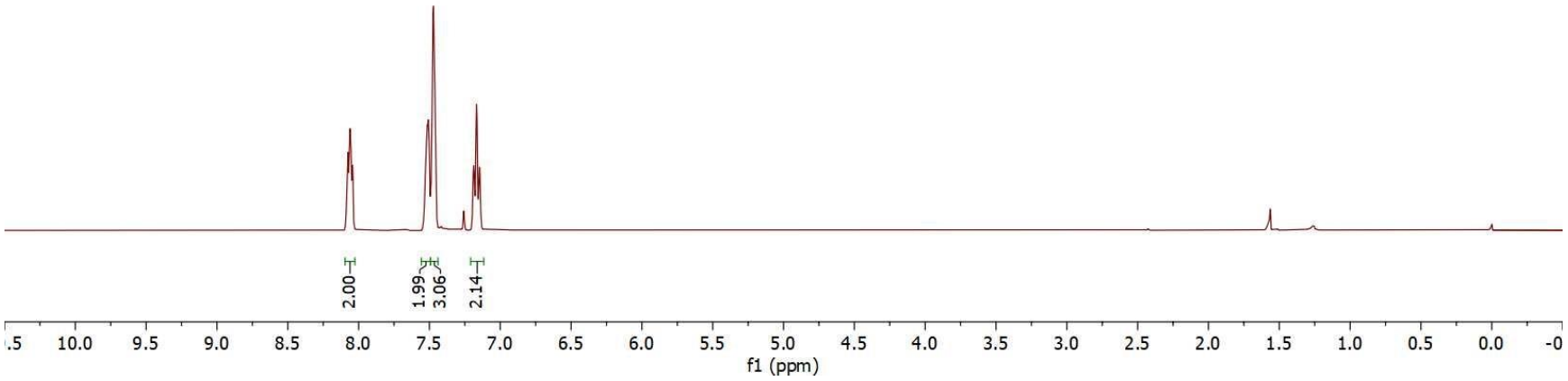


(¹H NMR, 400 MHz, $CDCl_3$)

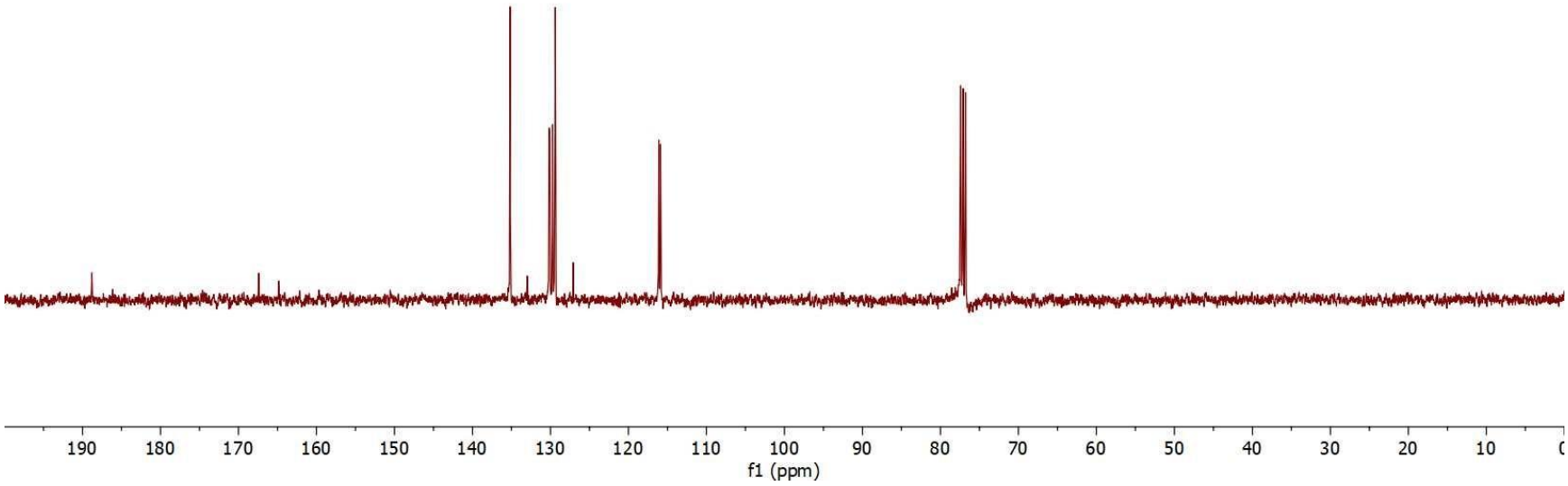

189.66
157.51
135.14
133.99
129.43
129.21
127.55
127.44
125.72
77.42
77.10
76.78
35.21
31.09
O
S
tBu
4d
(13C{H} NMR, 100 MHz, CDCl3)
f1 (ppm)

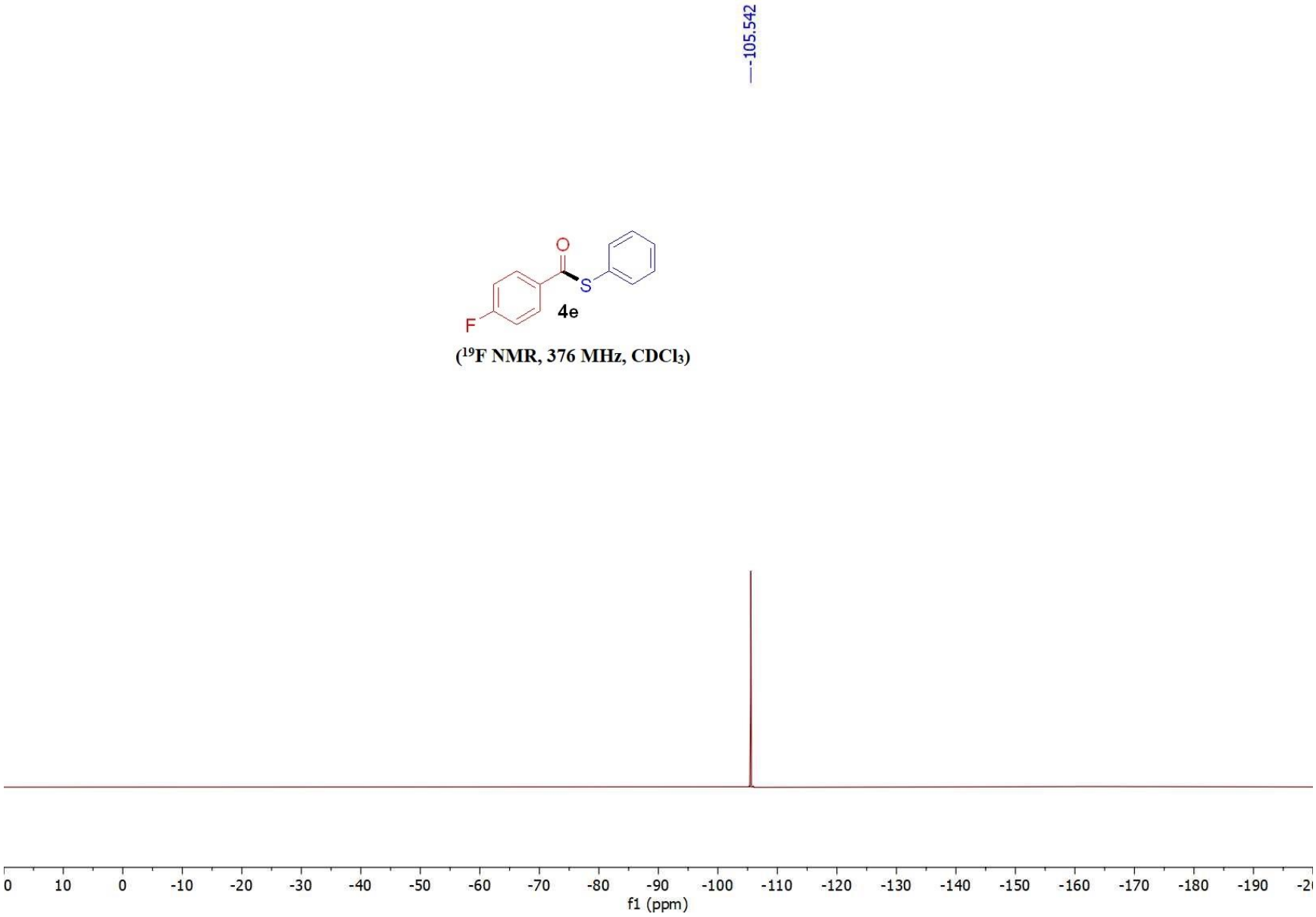
4e

(^{1}H NMR, 400 MHz, $CDCl_3$)



($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

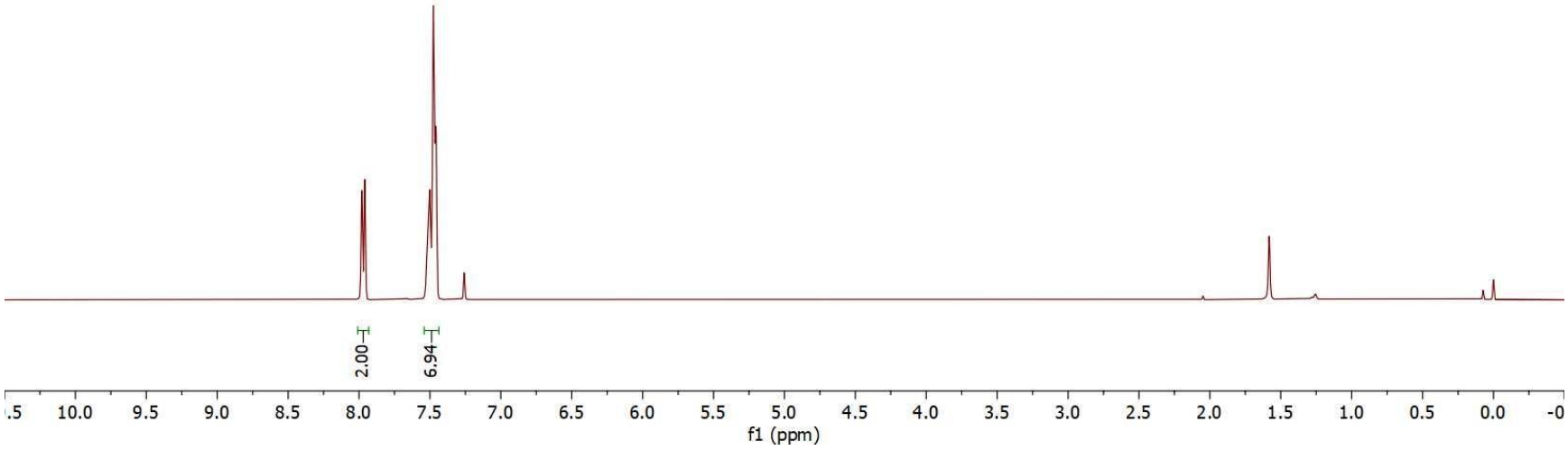


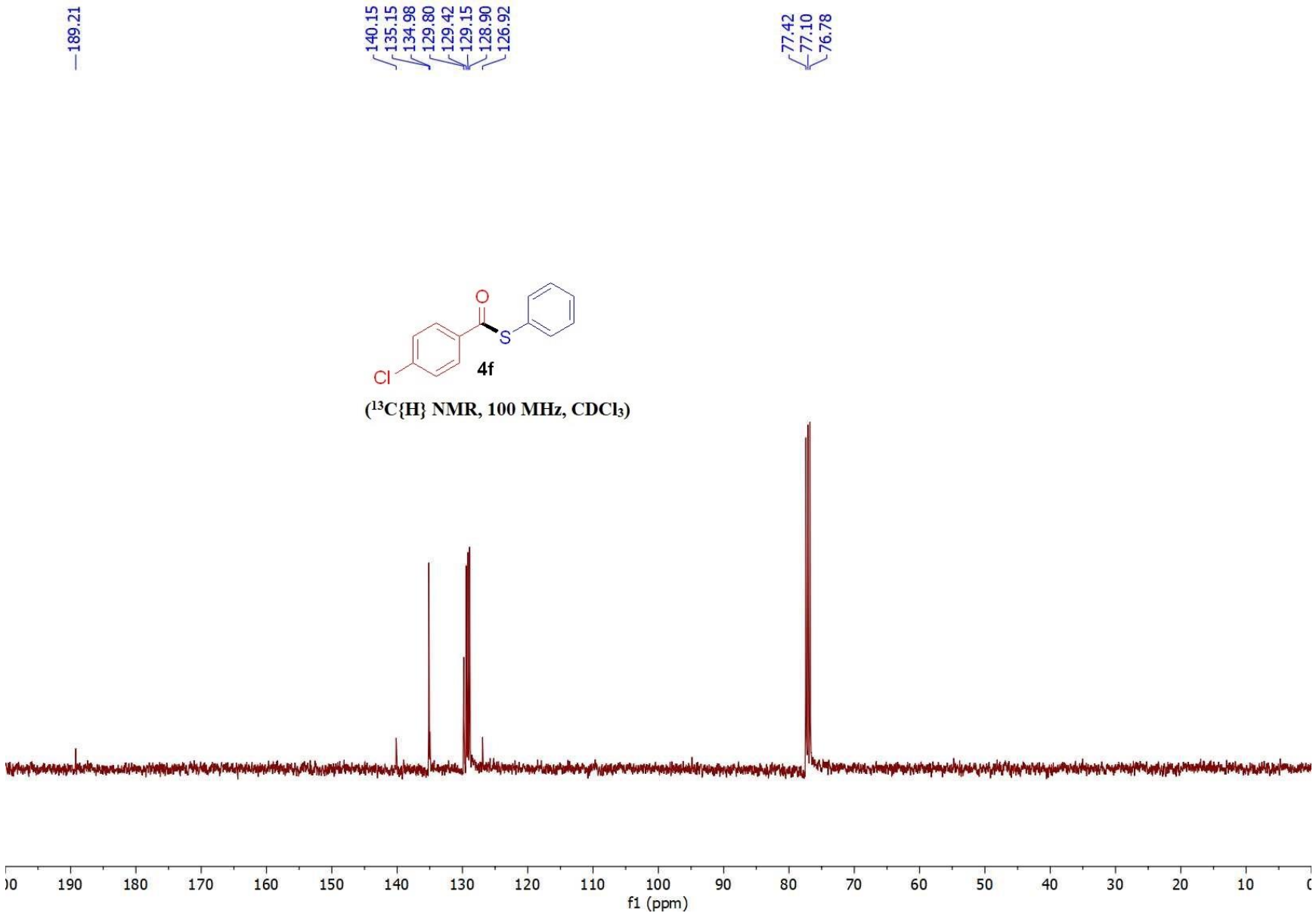


(^{19}F NMR, 376 MHz, $CDCl_3$)

4f

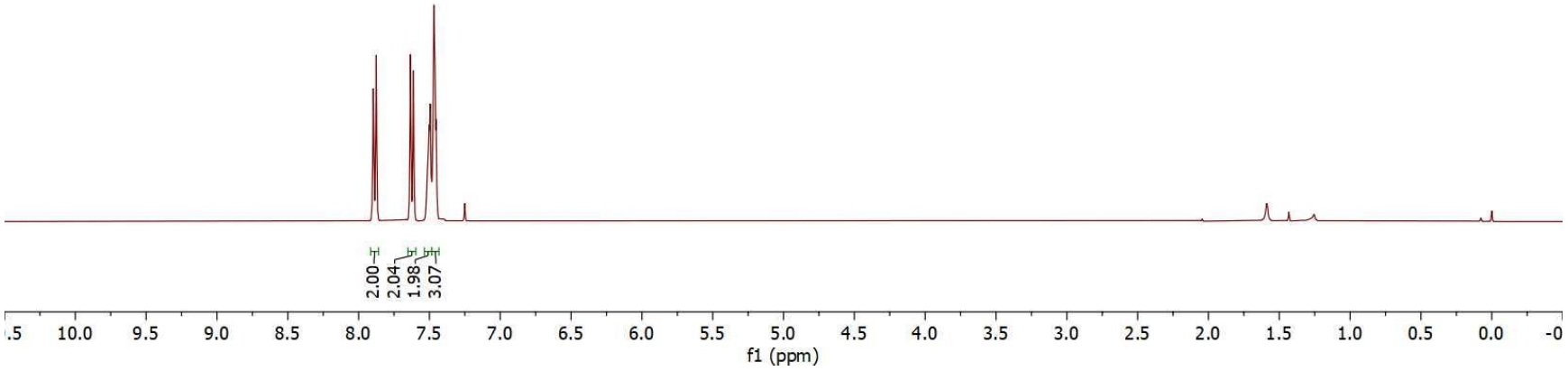
(^{1}H NMR, 400 MHz, $CDCl_3$)

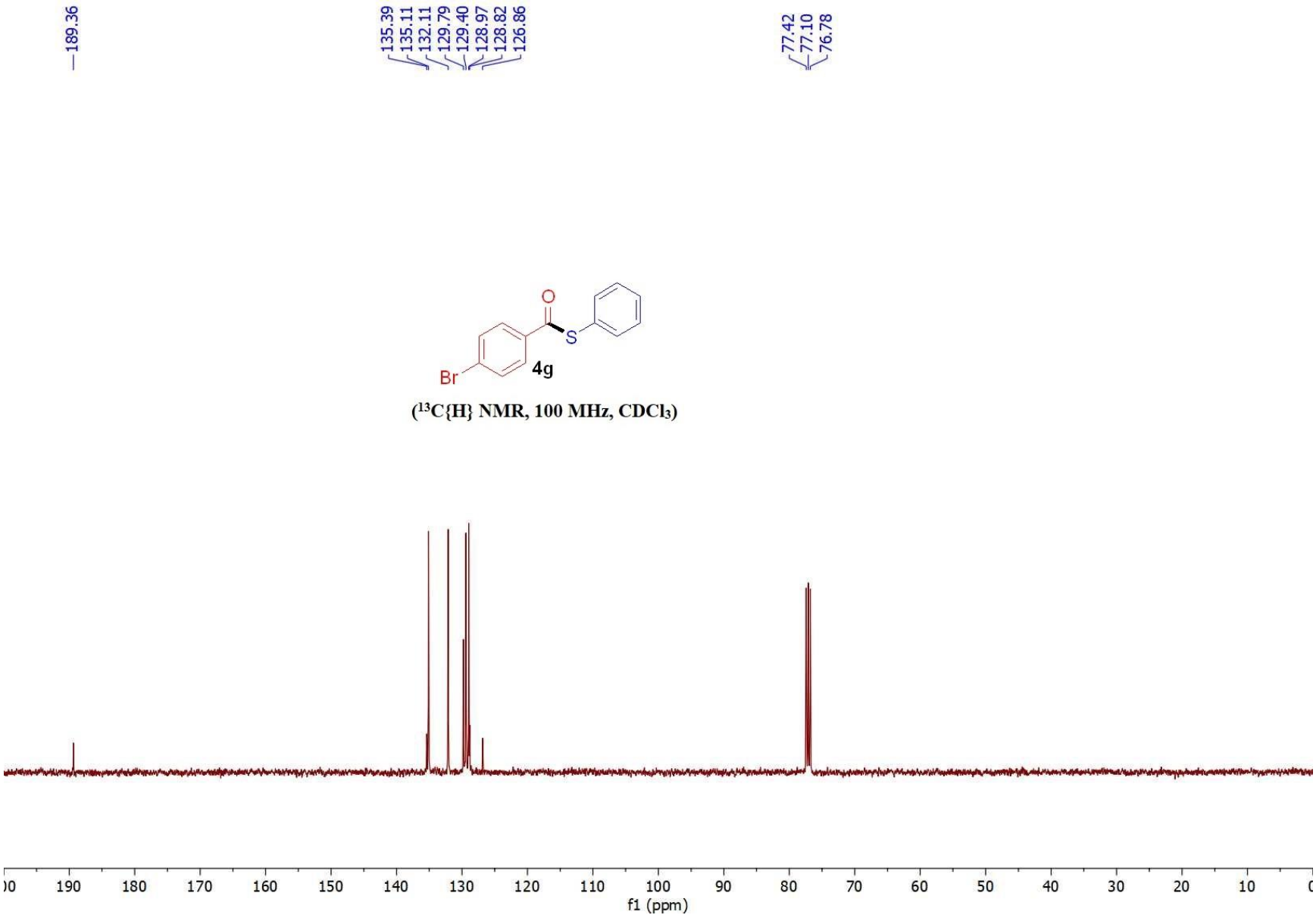



189.21
140.15
135.15
134.98
129.80
129.42
129.15
128.90
126.92
77.42
77.10
76.78
O
S
Cl
4f
(13C{H} NMR, 100 MHz, CDCl3)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

4g

(^{1}H NMR, 400 MHz, $CDCl_3$)

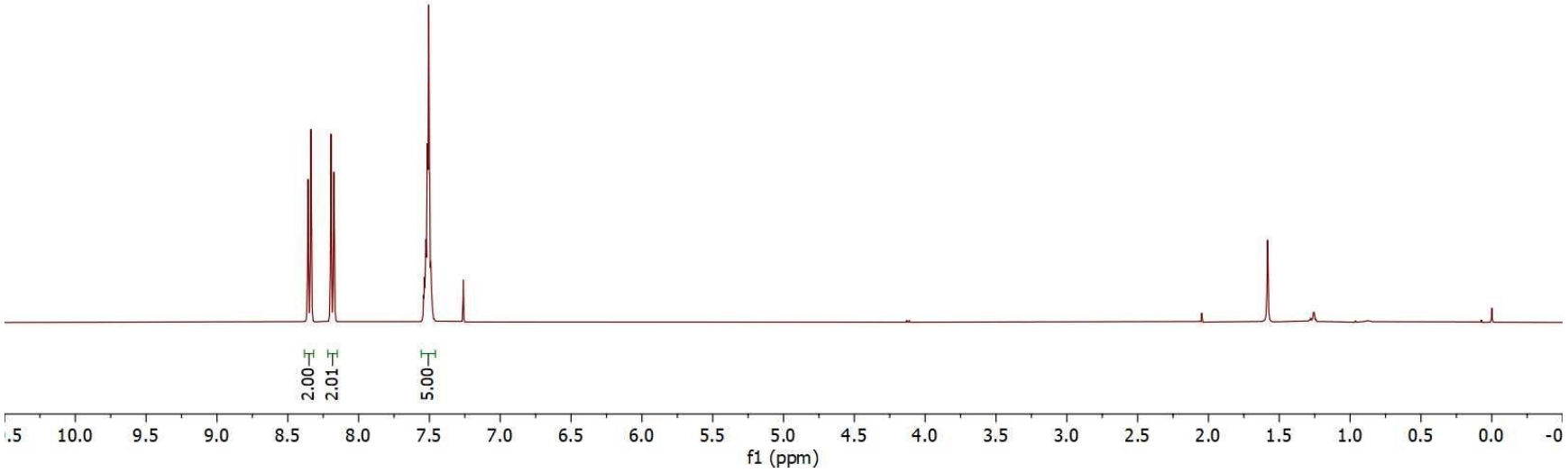


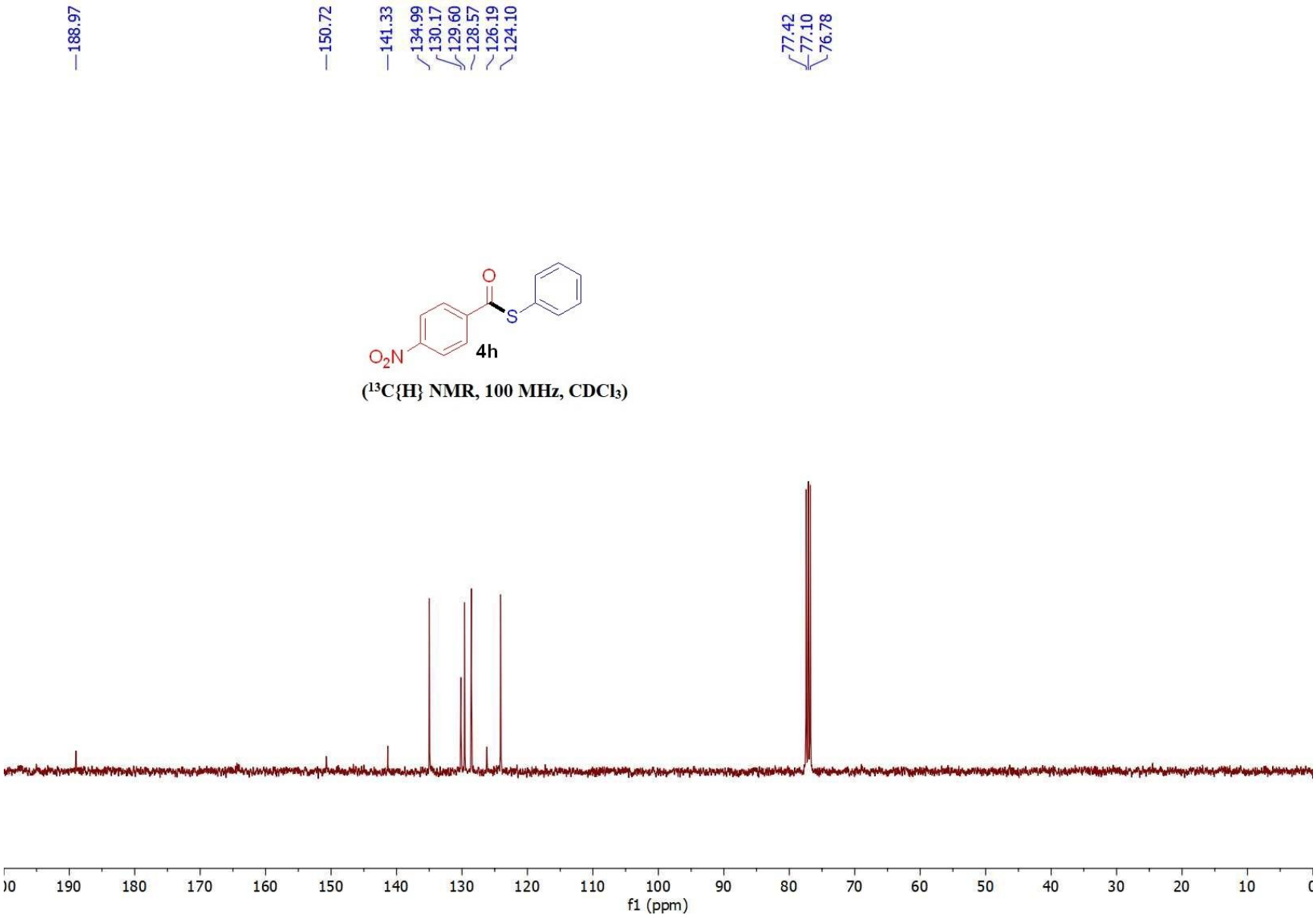


($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

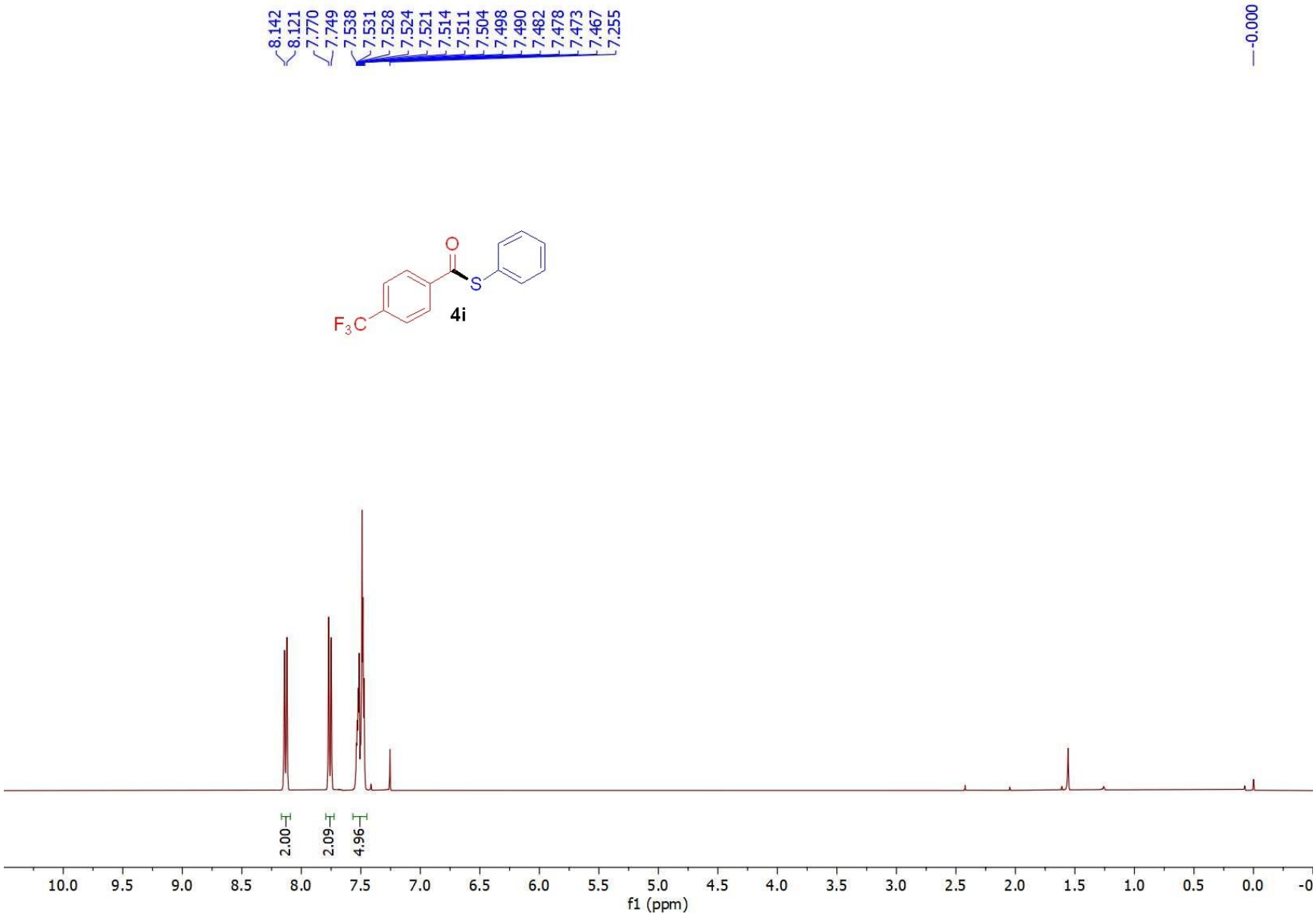
4h

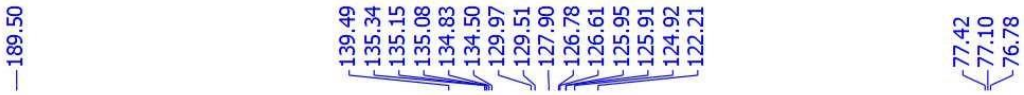
(^{1}H NMR, 400 MHz, $CDCl_3$)





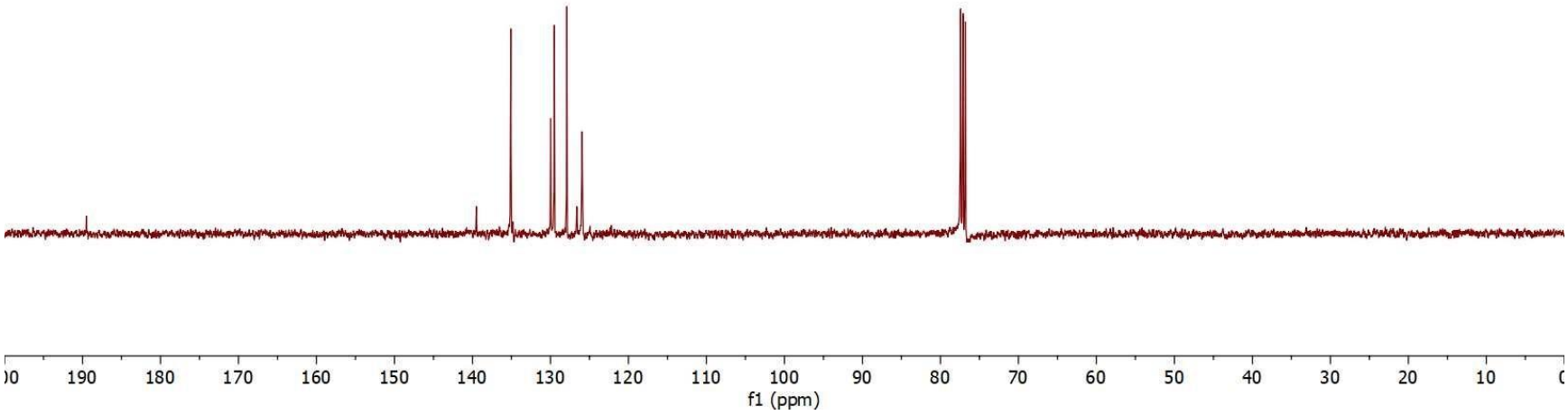
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

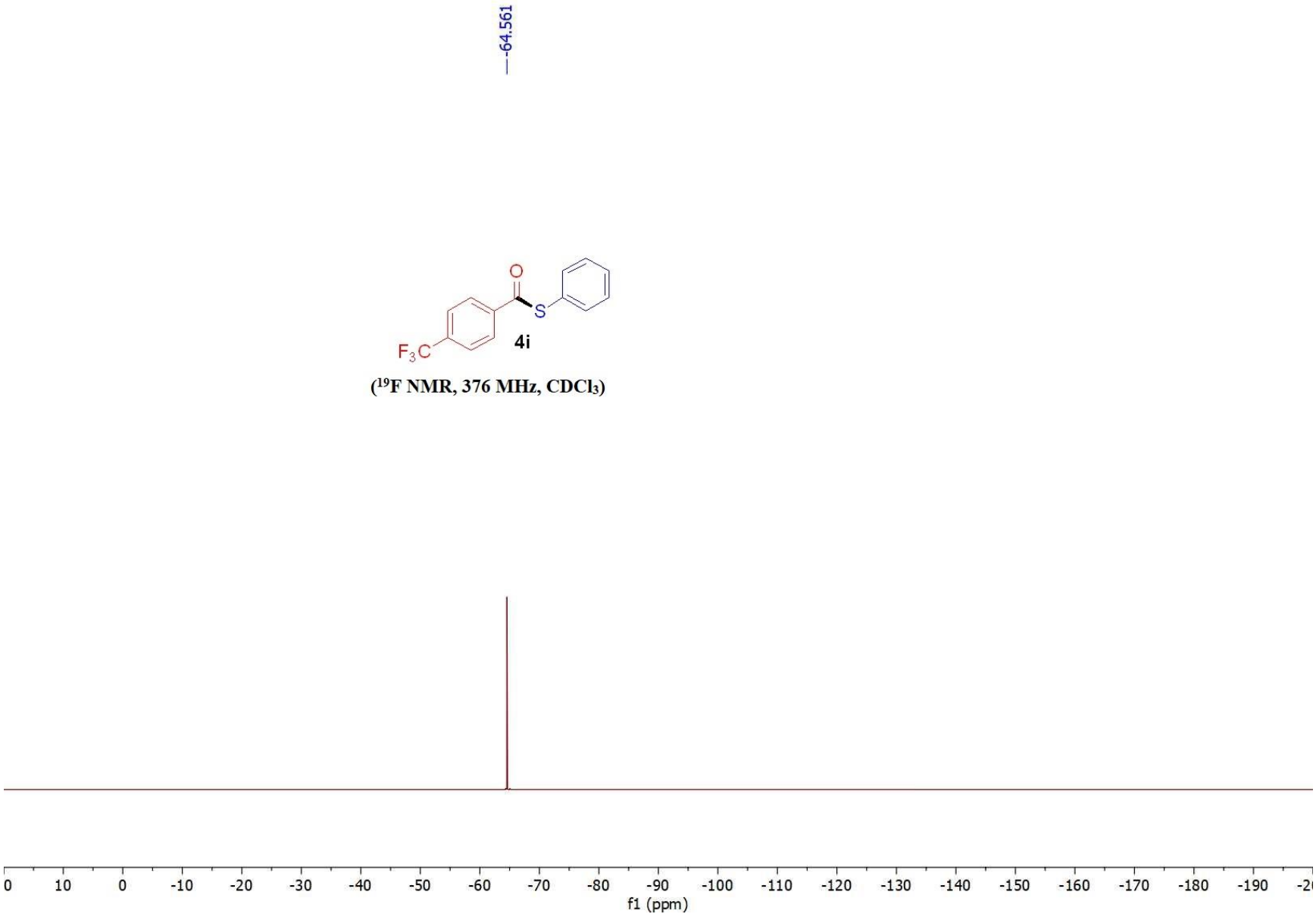

8.142
8.121
7.770
7.749
7.538
7.531
7.528
7.524
7.521
7.514
7.511
7.504
7.498
7.490
7.482
7.478
7.473
7.467
7.255
-0.000
O
S
F3C
4i
2.00
2.09
4.96
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)



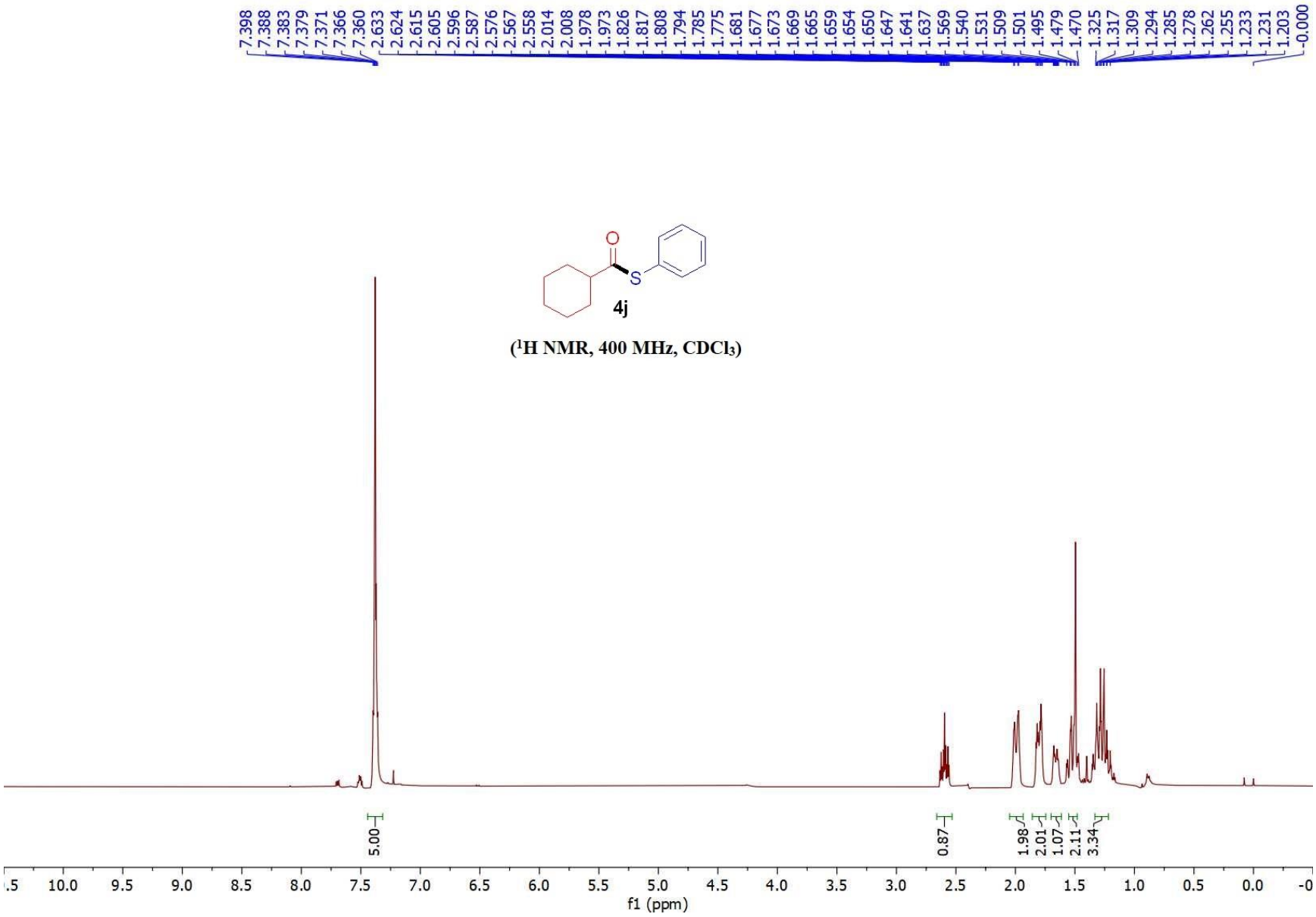
4i

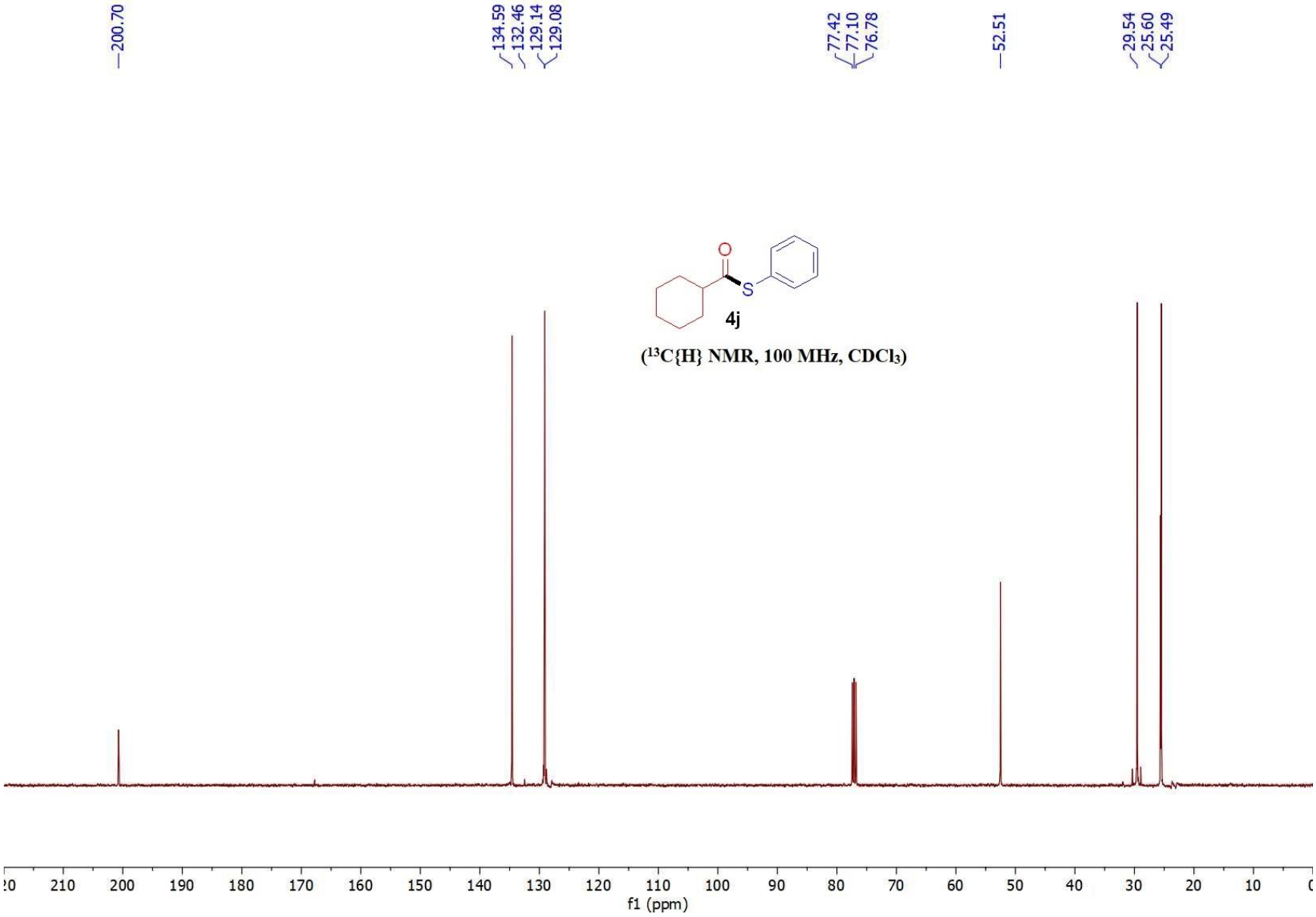
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

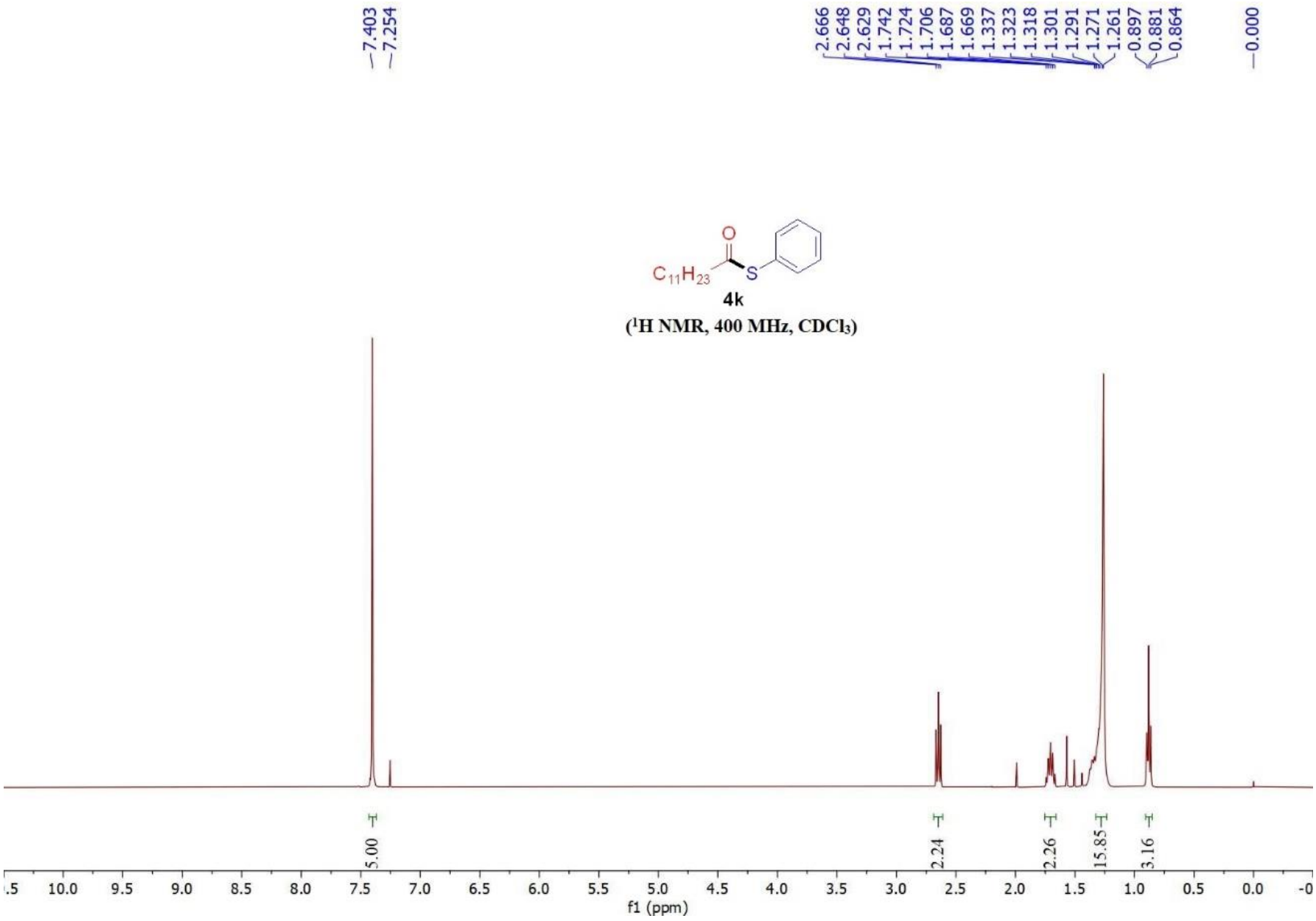




(^{19}F NMR, 376 MHz, $CDCl_3$)

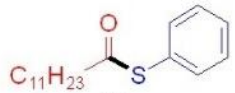

7.398
7.388
7.383
7.379
7.371
7.366
7.360
2.633
2.624
2.615
2.605
2.596
2.587
2.576
2.567
2.558
2.014
2.008
1.978
1.973
1.826
1.817
1.808
1.794
1.785
1.775
1.681
1.677
1.673
1.669
1.665
1.659
1.654
1.650
1.647
1.641
1.637
1.569
1.540
1.531
1.509
1.501
1.495
1.479
1.470
1.325
1.317
1.309
1.294
1.285
1.278
1.262
1.255
1.233
1.231
1.203
-0.000
O
S
4j
(1H NMR, 400 MHz, CDCl3)
5.00
0.87
1.98
2.01
1.07
2.11
3.34
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


200.70
134.59
132.46
129.14
129.08
77.42
77.10
76.78
52.51
29.54
25.60
25.49
O
S
4j
(13C{H} NMR, 100 MHz, CDCl3)
f1 (ppm)



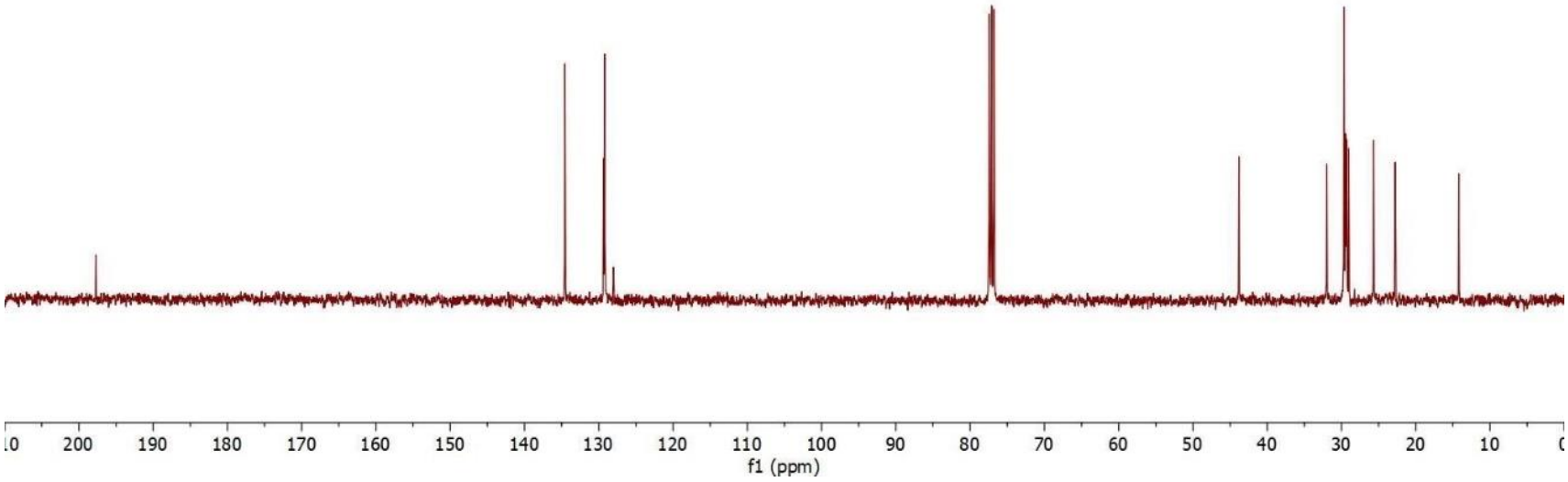
4k

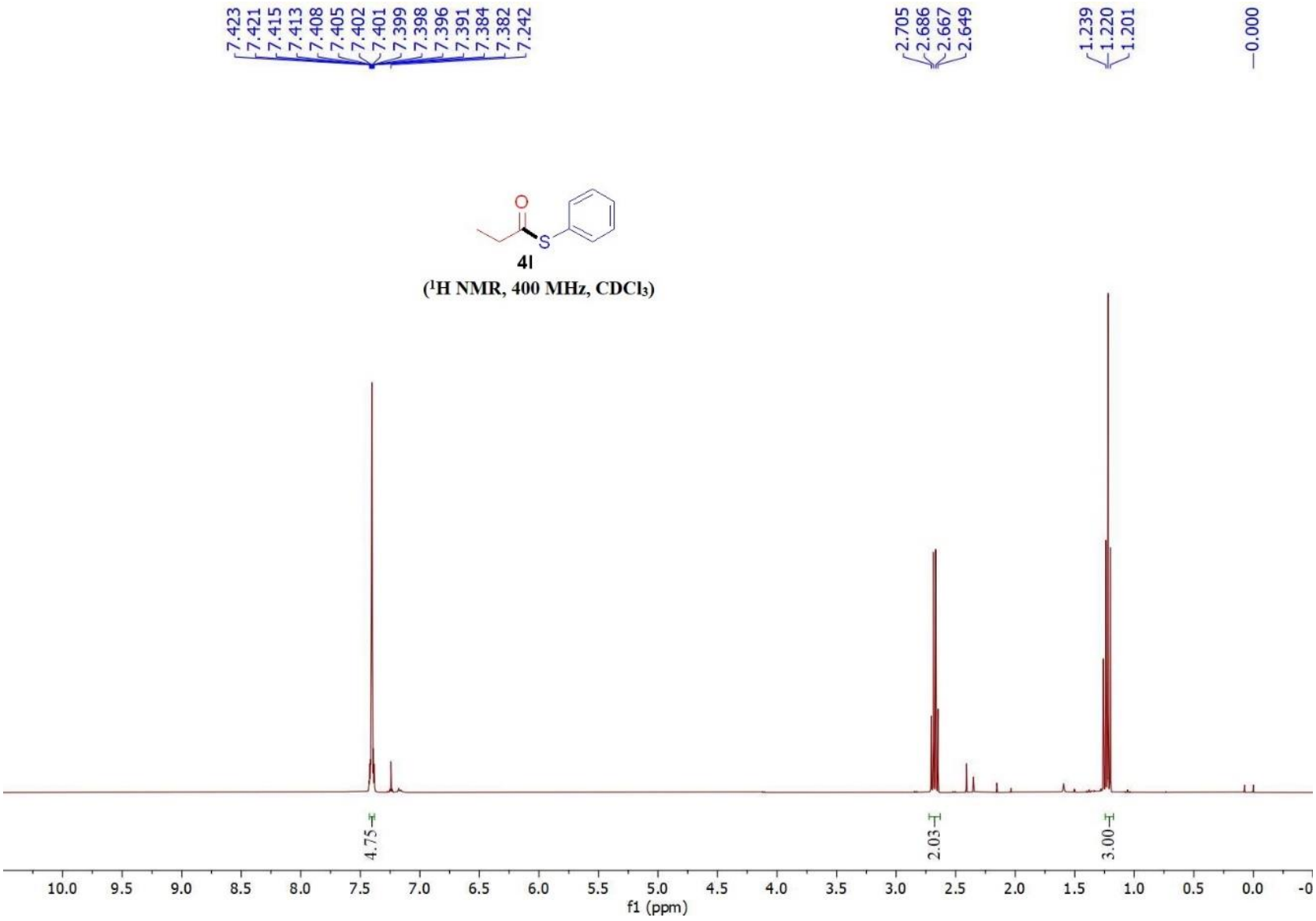
(^{1}H NMR, 400 MHz, $CDCl_3$)



4k

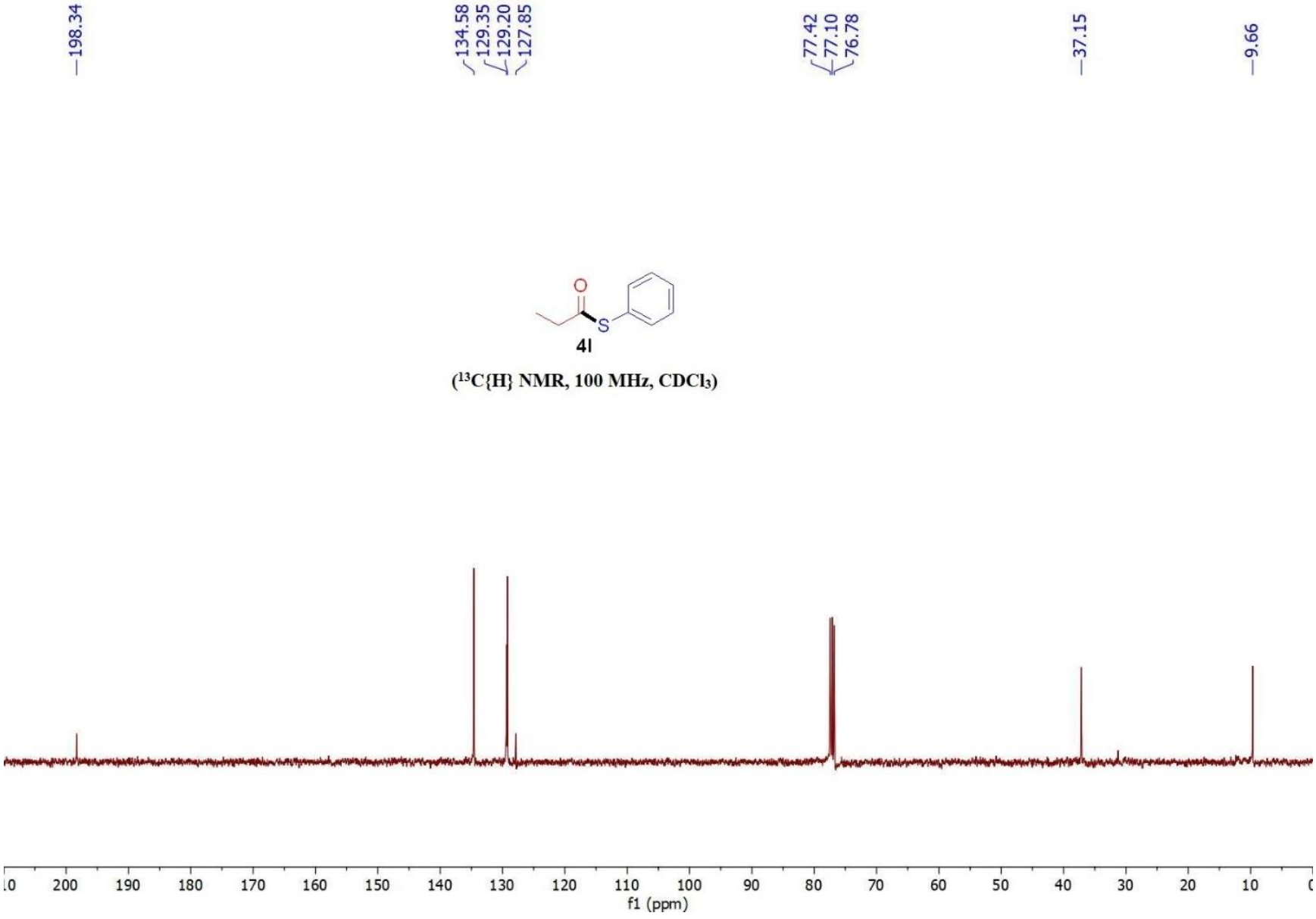
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)





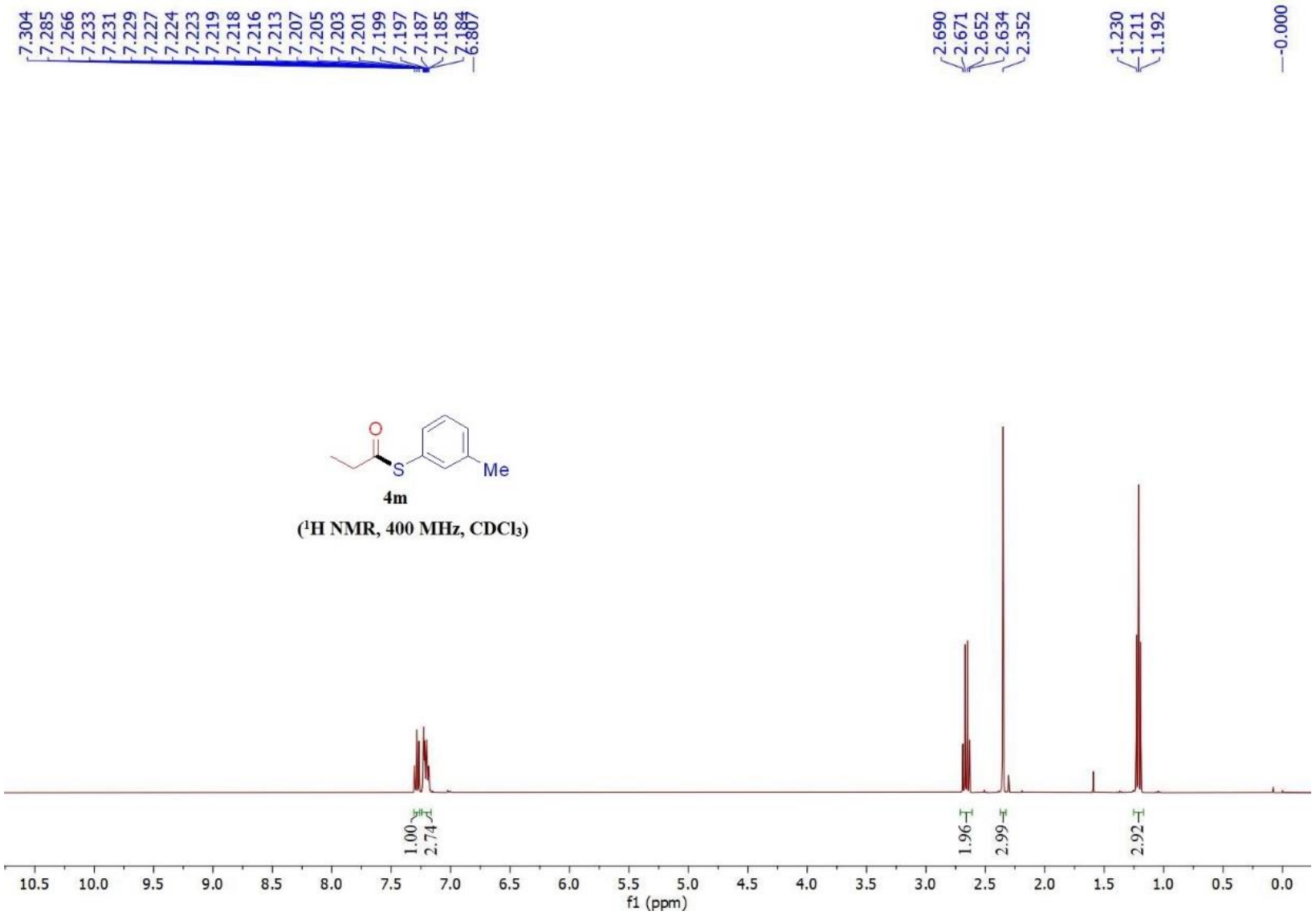
4l

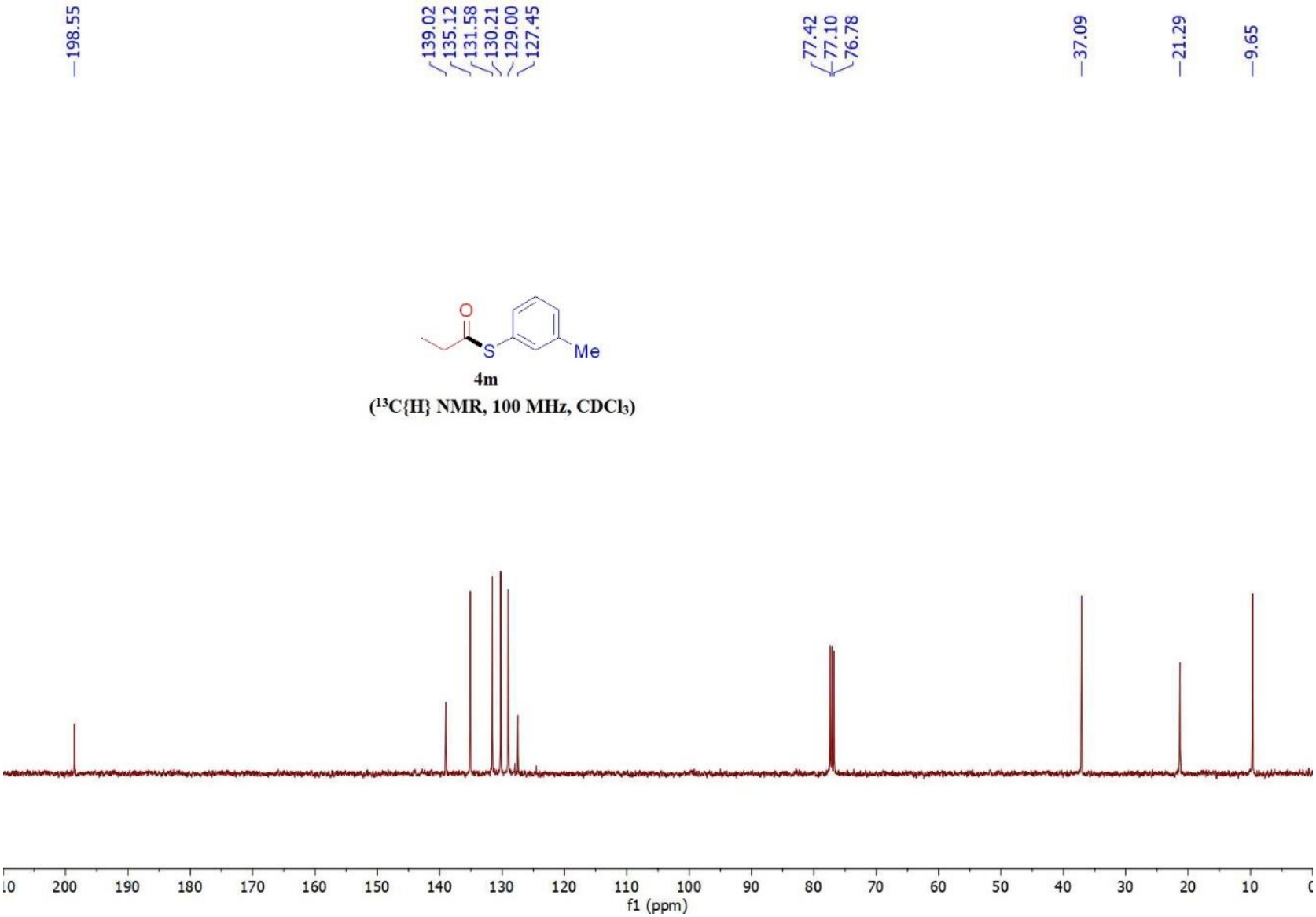
(^{1}H NMR, 400 MHz, $CDCl_3$)



4l

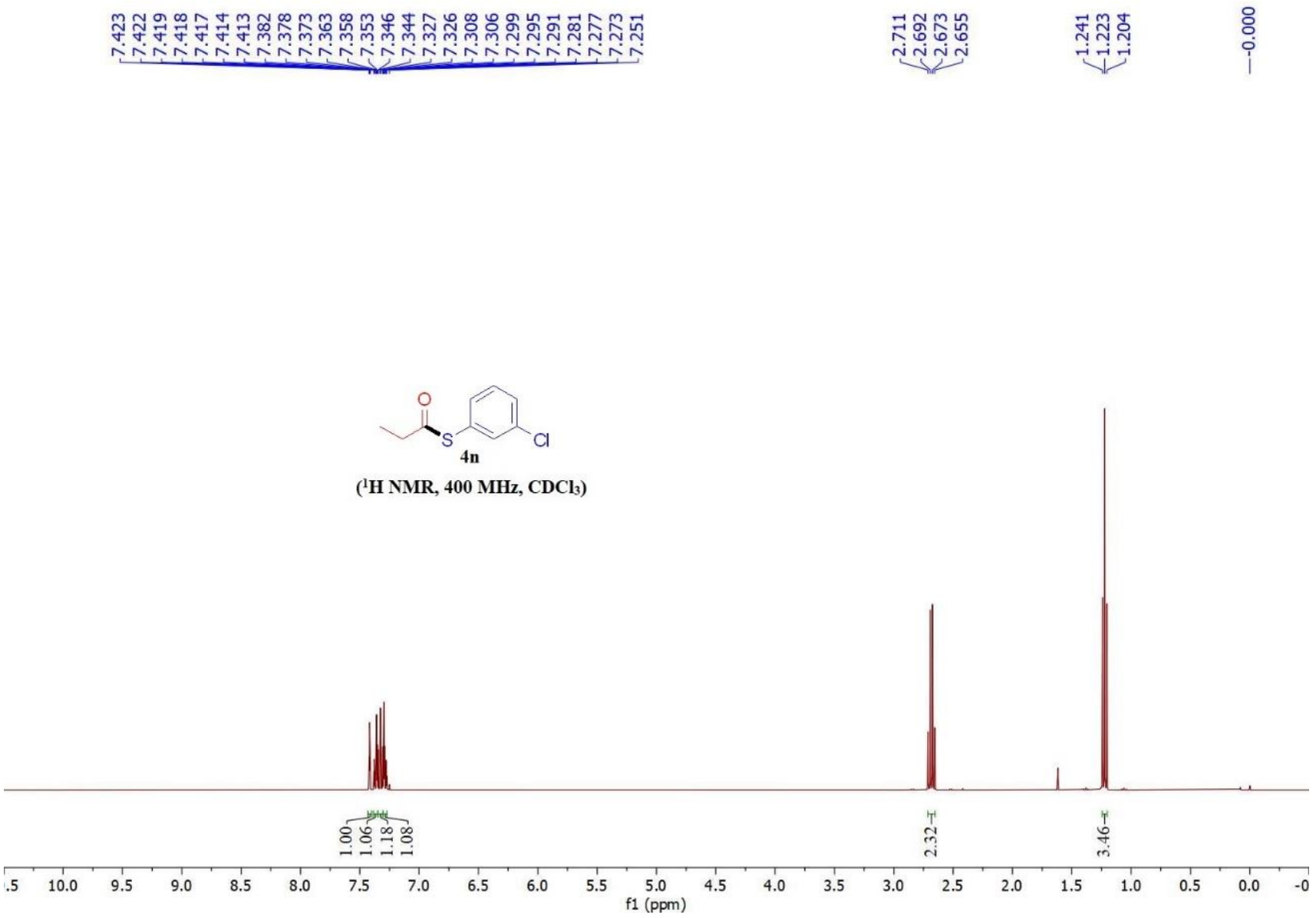
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

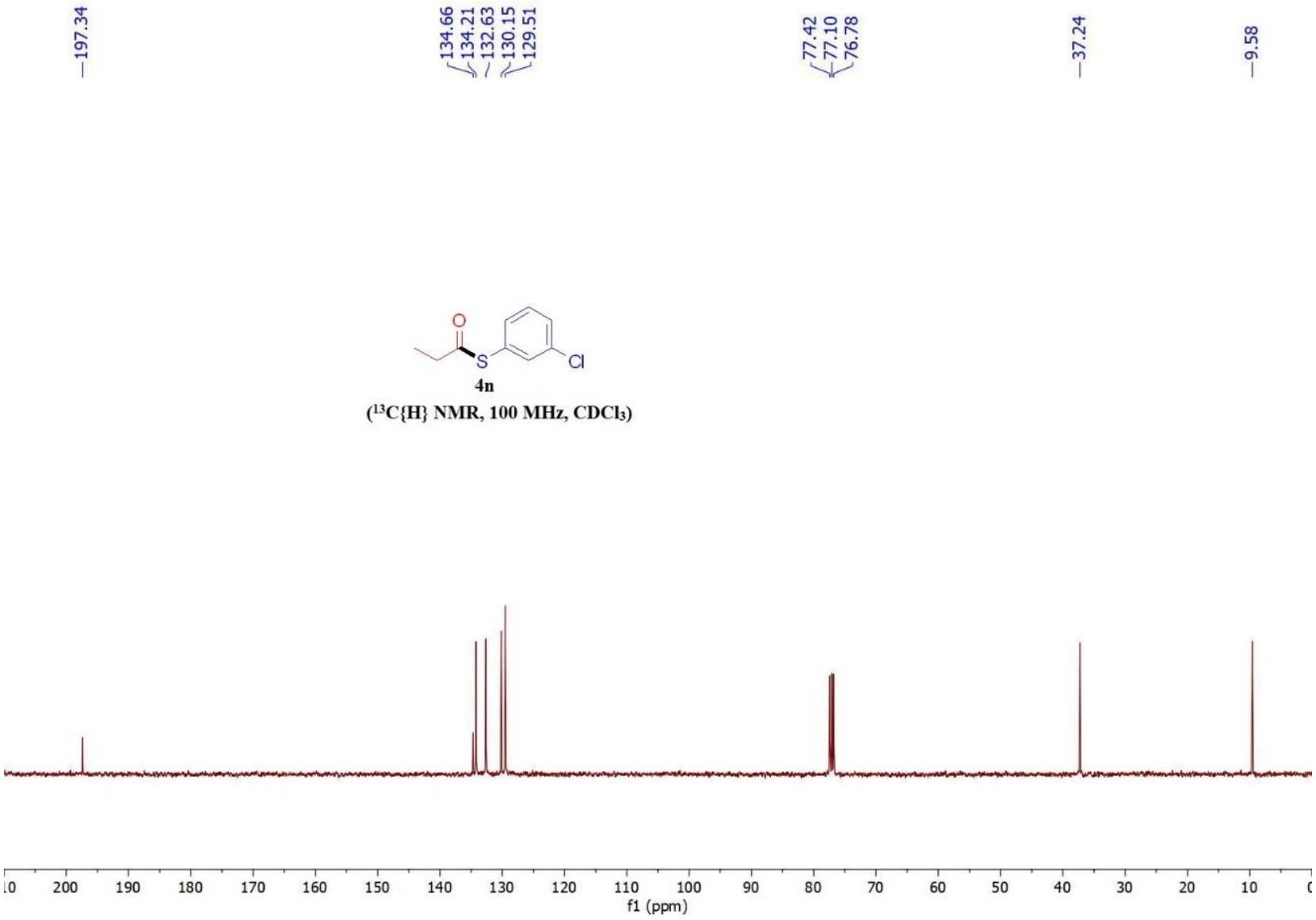

7.304
7.285
7.266
7.233
7.231
7.229
7.227
7.224
7.223
7.219
7.218
7.216
7.213
7.207
7.205
7.203
7.201
7.199
7.197
7.187
7.185
7.184
6.807
2.690
2.671
2.652
2.634
2.352
1.230
1.211
1.192
-0.000
O
S
Me
4m
(1H NMR, 400 MHz, CDCl3)
1.00
2.74
1.96
2.99
2.92
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



4m

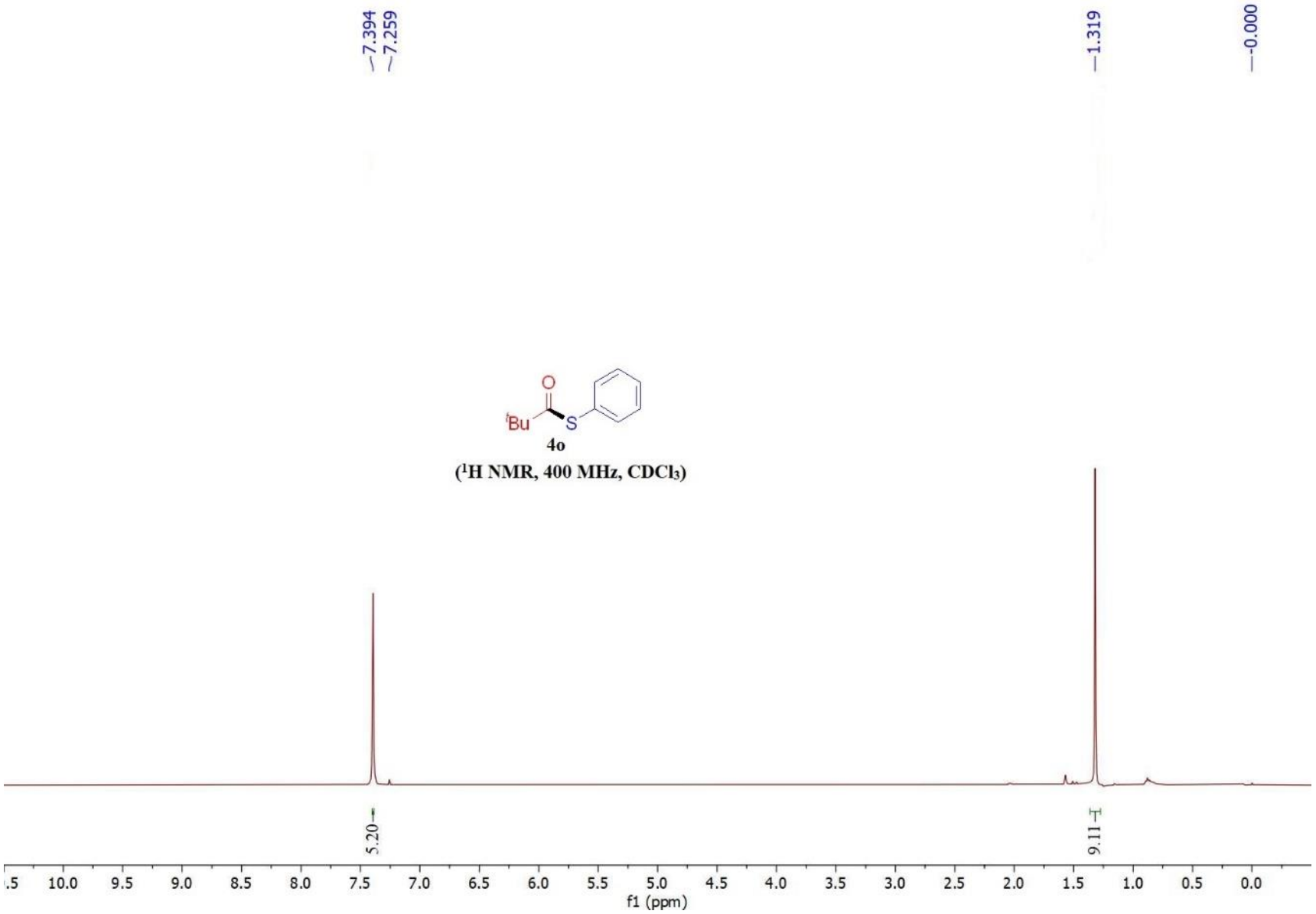
($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)

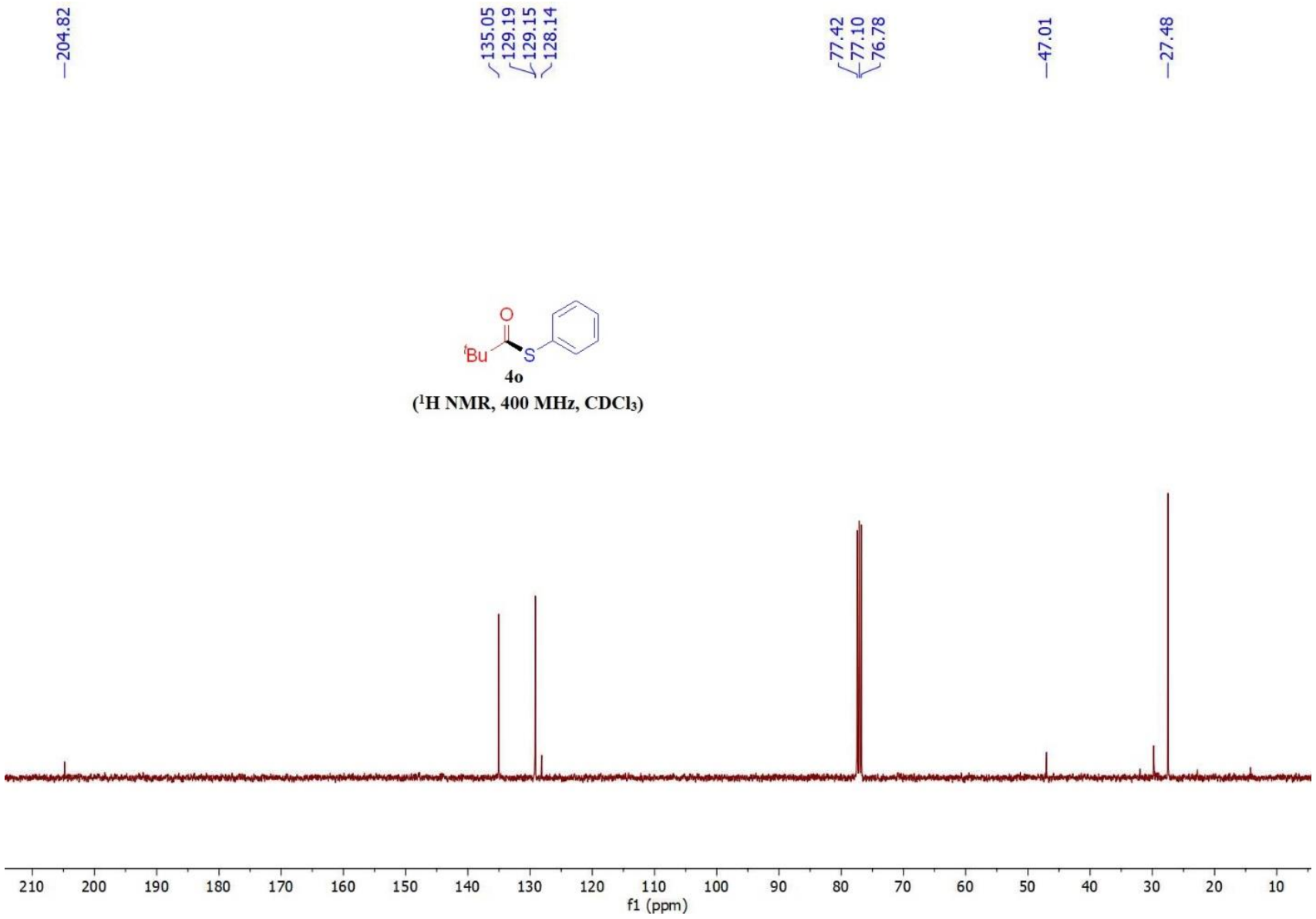

7.423
7.422
7.419
7.418
7.417
7.414
7.413
7.382
7.378
7.373
7.363
7.358
7.353
7.346
7.344
7.327
7.326
7.308
7.306
7.299
7.295
7.291
7.281
7.277
7.273
7.251
2.711
2.692
2.673
2.655
1.241
1.223
1.204
-0.000
O
S
Cl
4n
(1H NMR, 400 MHz, CDCl3)
1.00
1.06
1.18
1.08
2.32
3.46
f1 (ppm)



4n

($^{13}C\{H\}$ NMR, 100 MHz, $CDCl_3$)


7.394
7.259
1.319
0.000
O
tBu
S
4o
(1H NMR, 400 MHz, CDCl3)
5.20
9.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



4o

(^{1}H NMR, 400 MHz, $CDCl_3$)