

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

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[†] These authors contributed equally and are joint first authors.

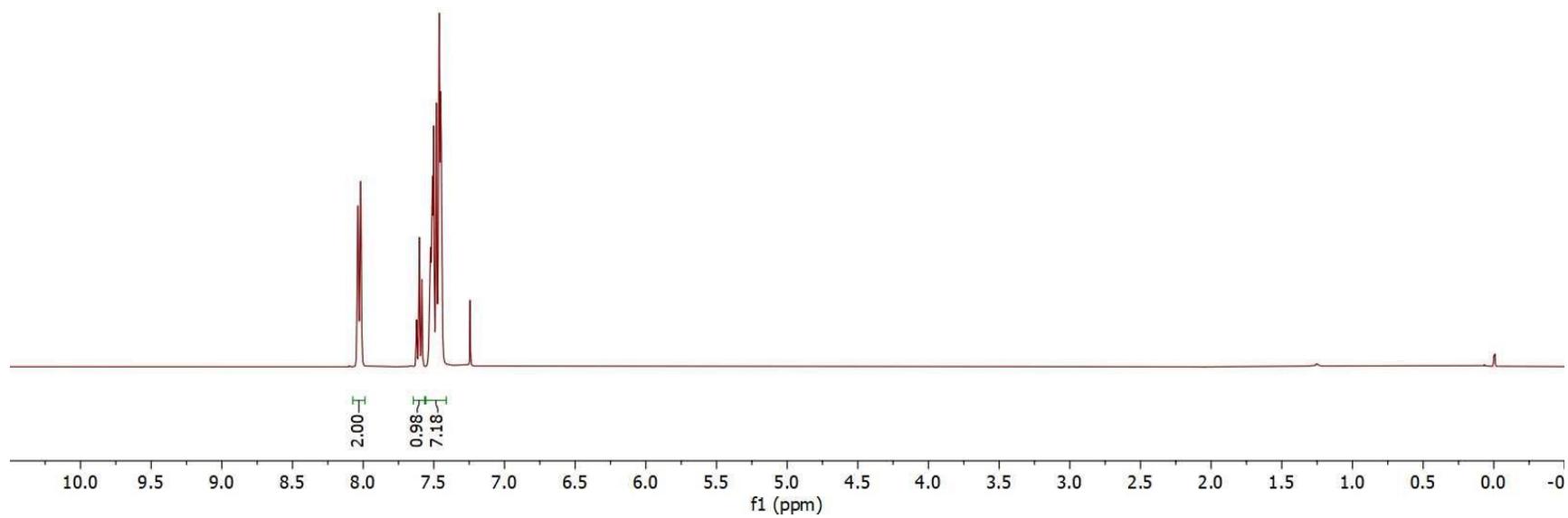
Copies of ¹H, ¹³C and ¹⁹F-NMR

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7.622
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7.588
7.585
7.581
7.533
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7.521
7.515
7.509
7.502
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7.444
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7.243

-0.000



(¹H NMR, 400 MHz, CDCl₃)



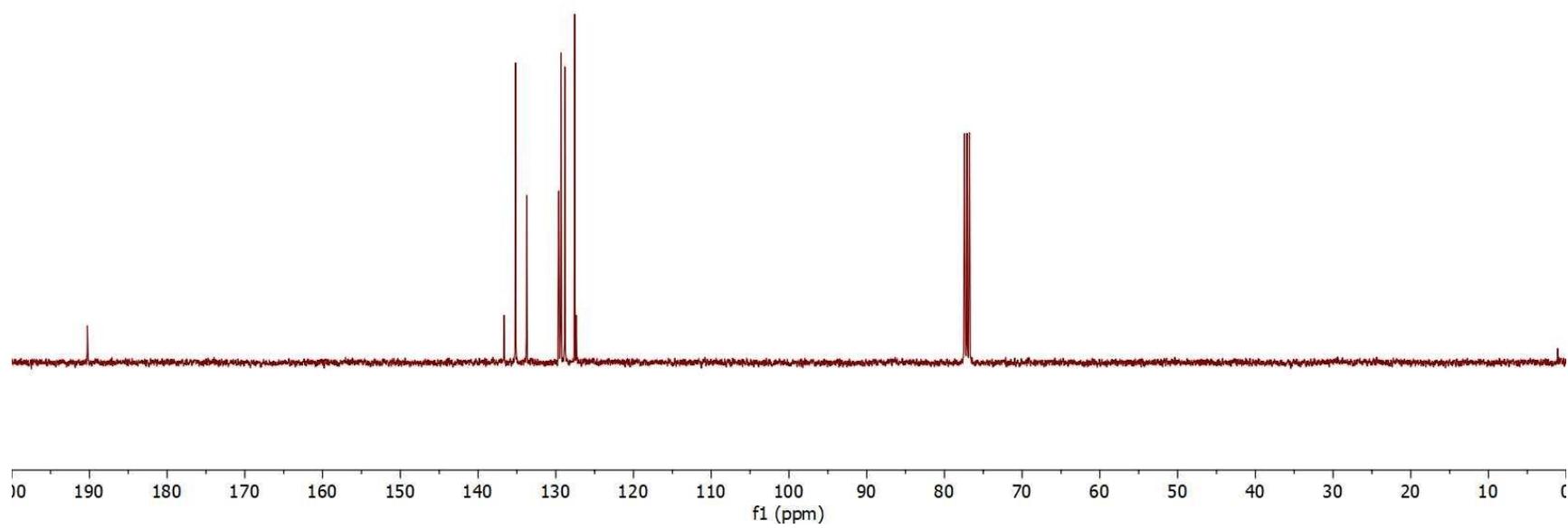
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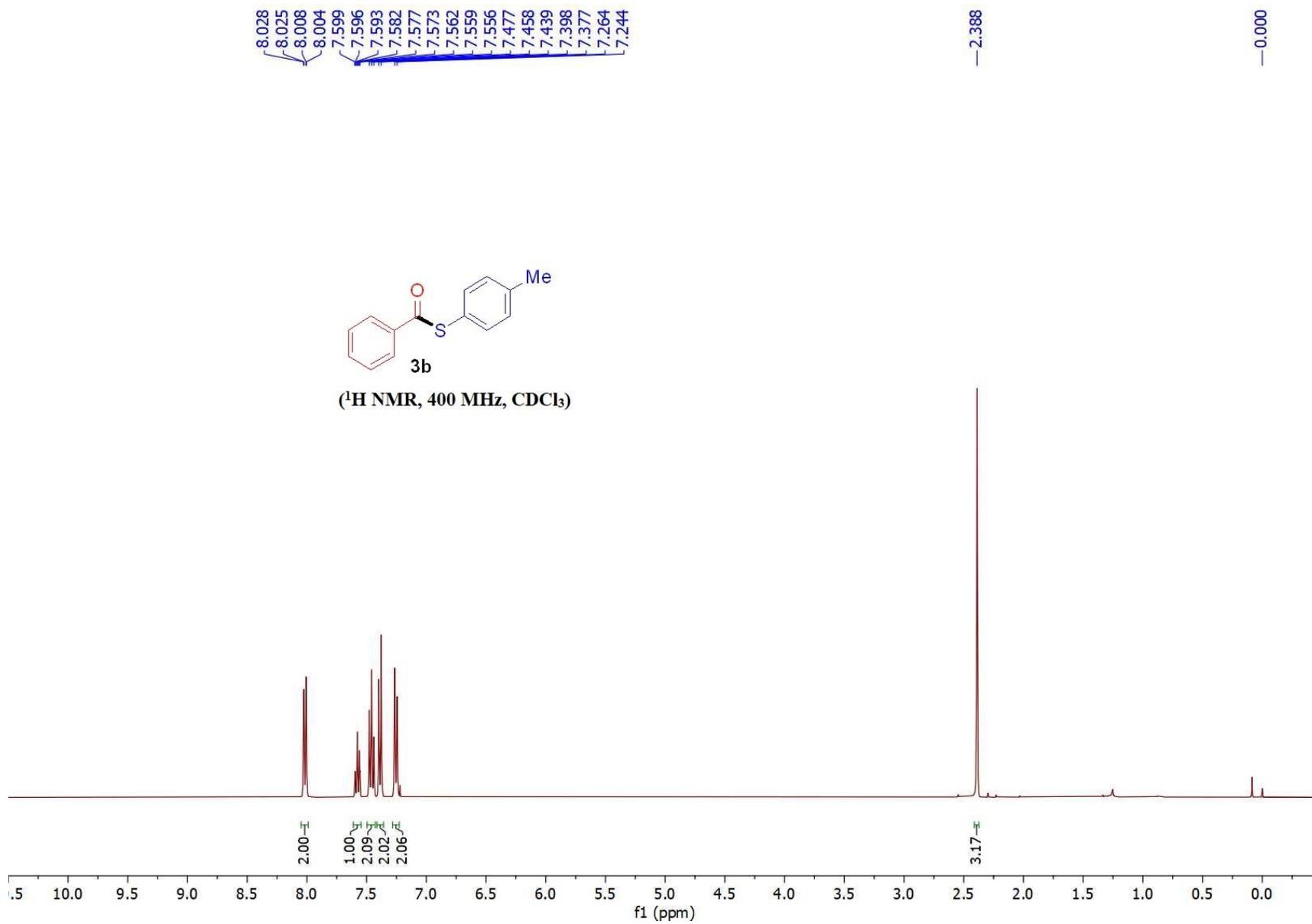
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77.42
77.10
76.78



(¹³C{¹H} NMR, 100 MHz, CDCl₃)



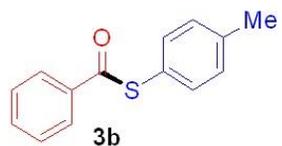


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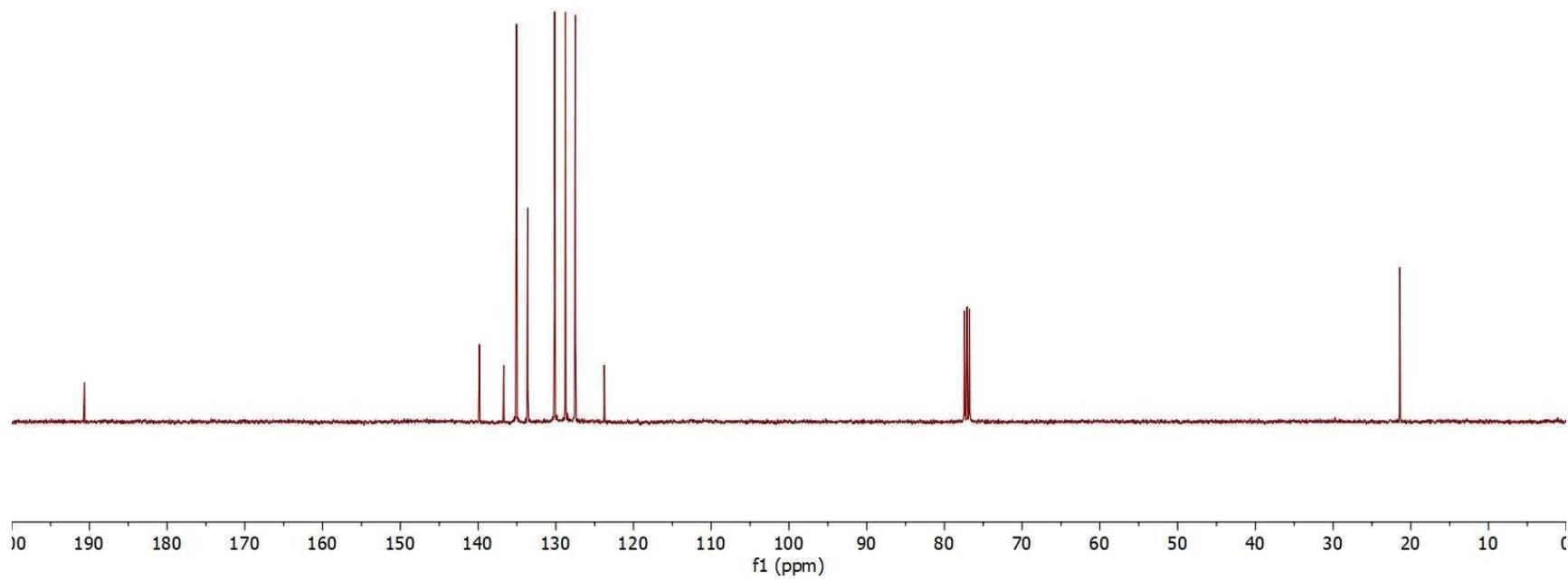
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76.78

—21.42



(¹³C{H} NMR, 100 MHz, CDCl₃)



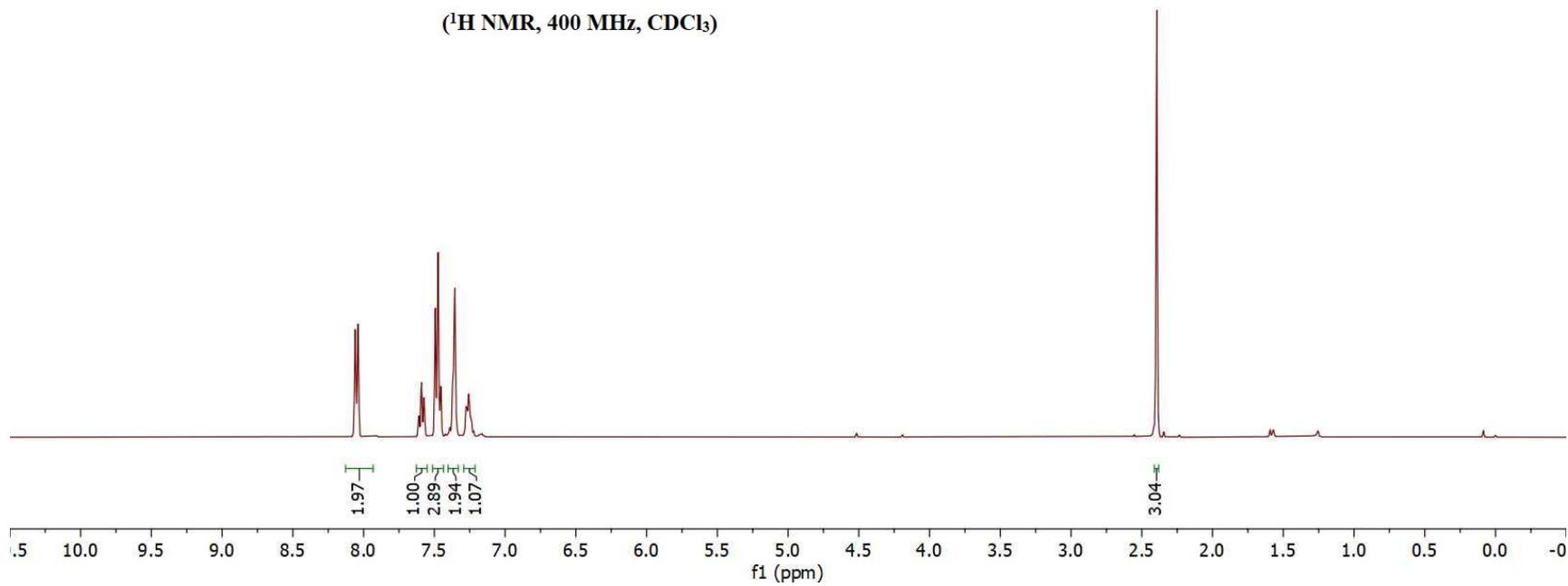
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7.354
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7.223
7.219

2.394

-0.000



(¹H NMR, 400 MHz, CDCl₃)



—189.69

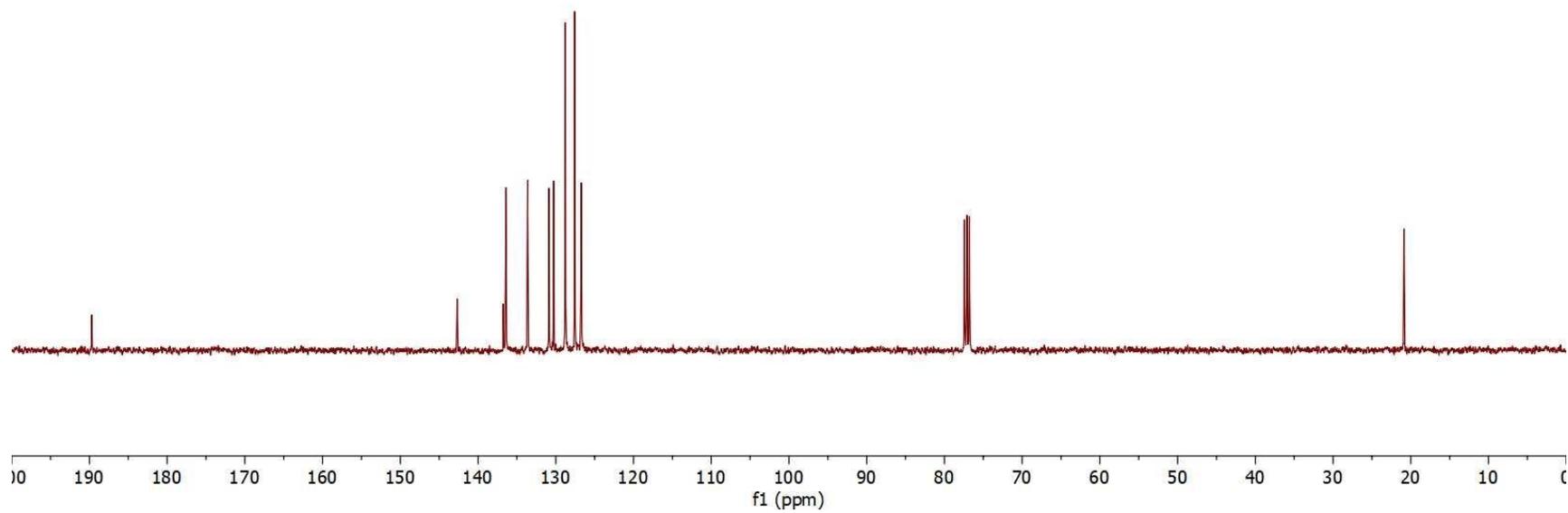
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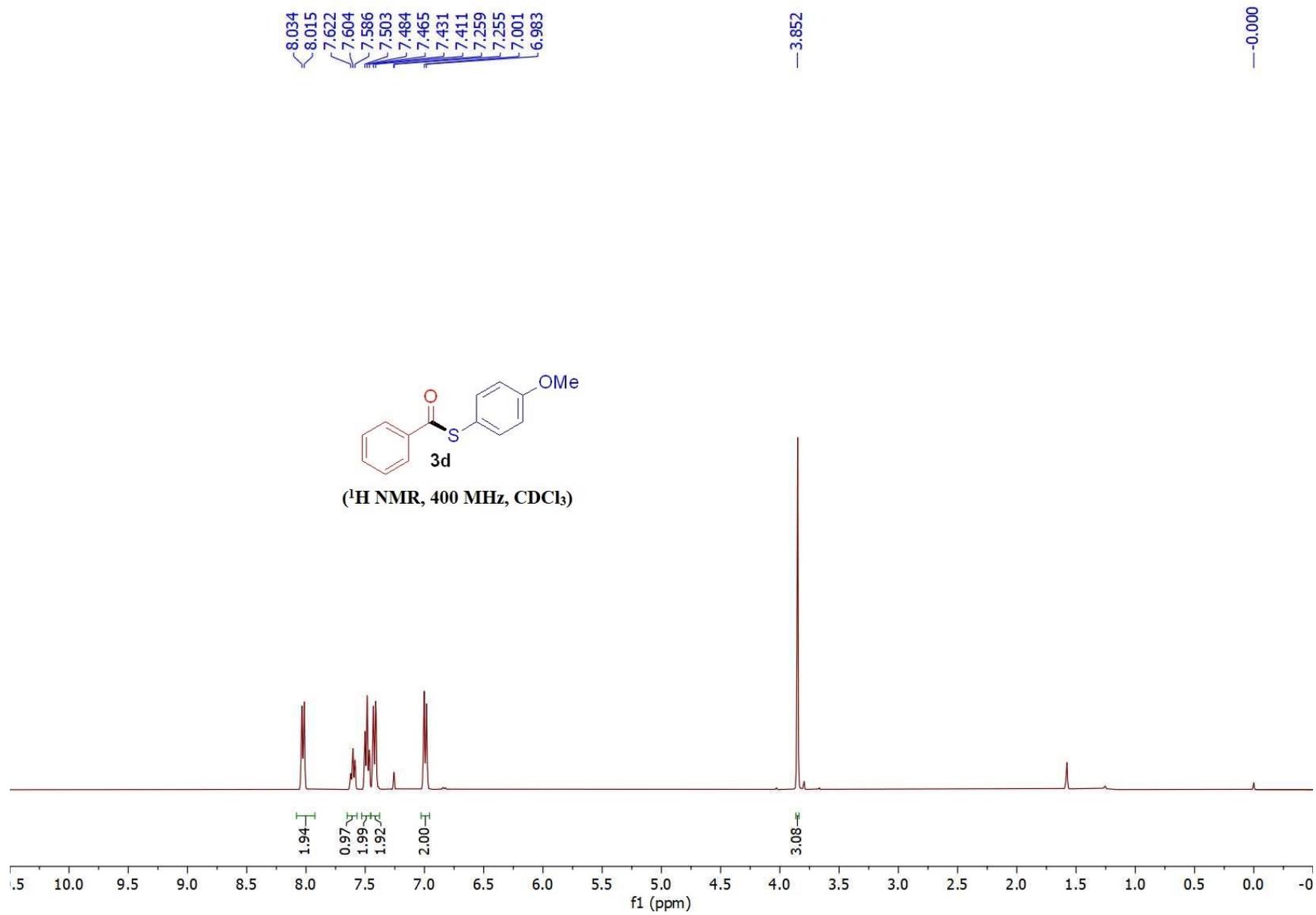
—77.42
—77.10
—76.78

—20.88



(¹³C{¹H} NMR, 100 MHz, CDCl₃)





—191.14

—160.85

—136.70

—133.64

—128.78

—127.51

—117.91

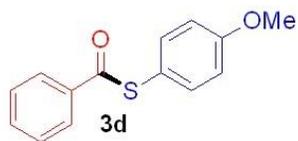
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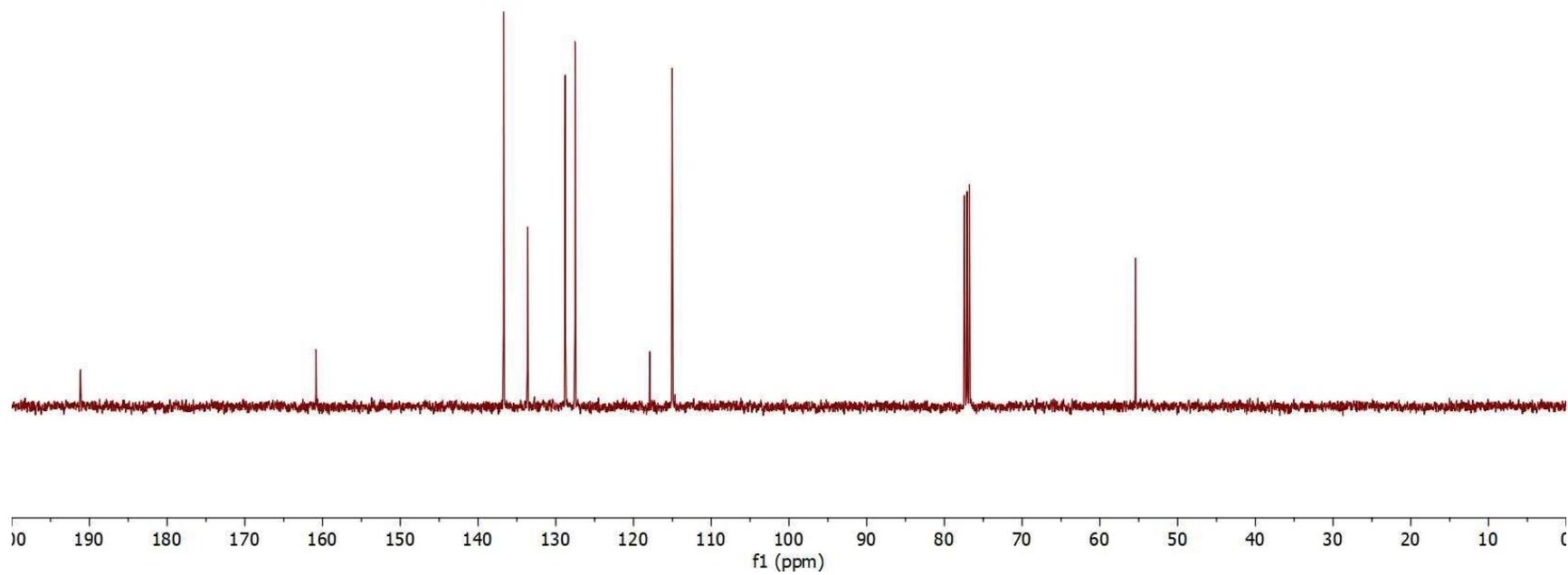
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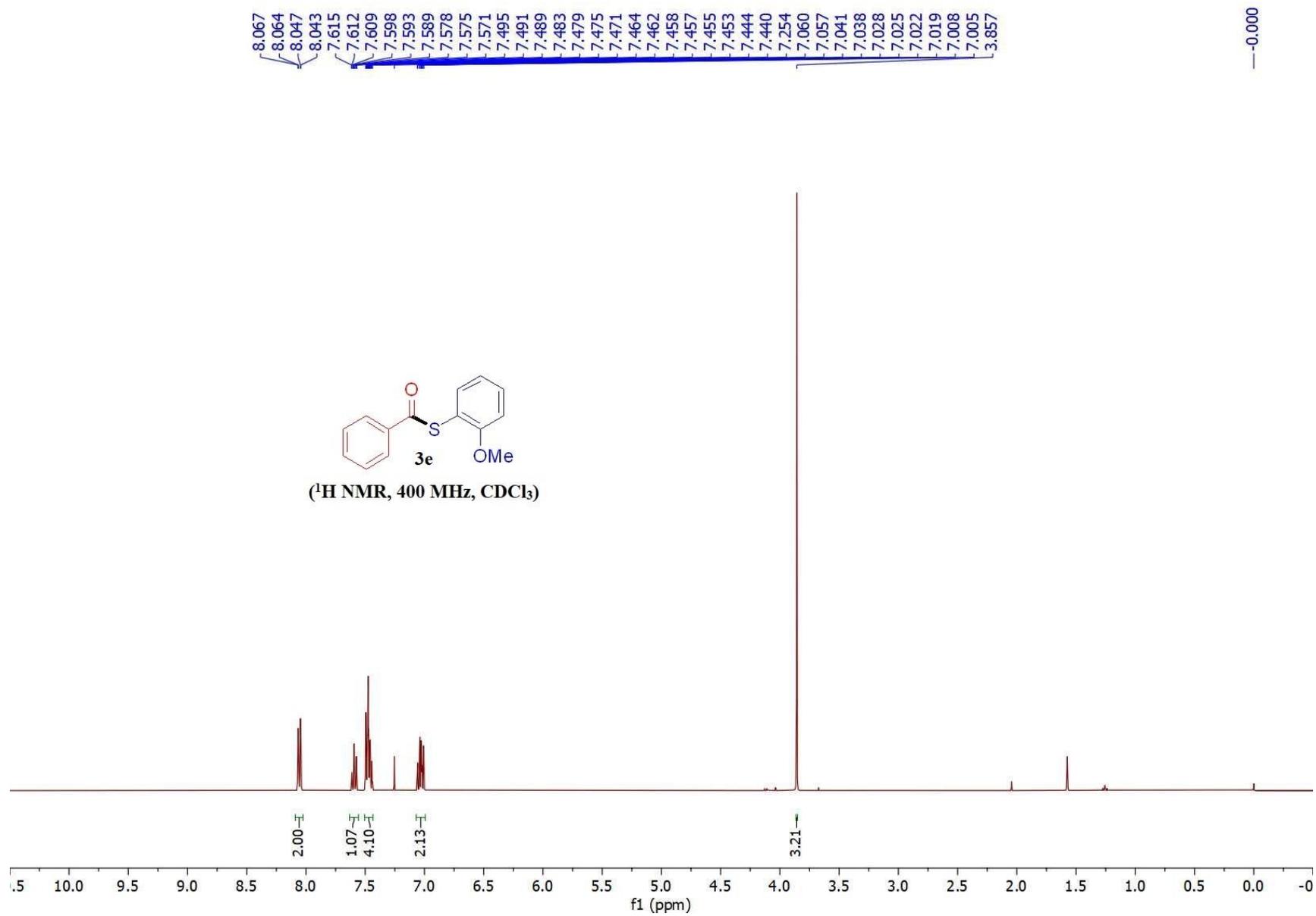
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—55.43



(¹³C{¹H} NMR, 100 MHz, CDCl₃)





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—159.78

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115.41

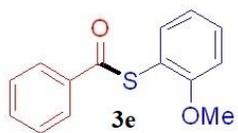
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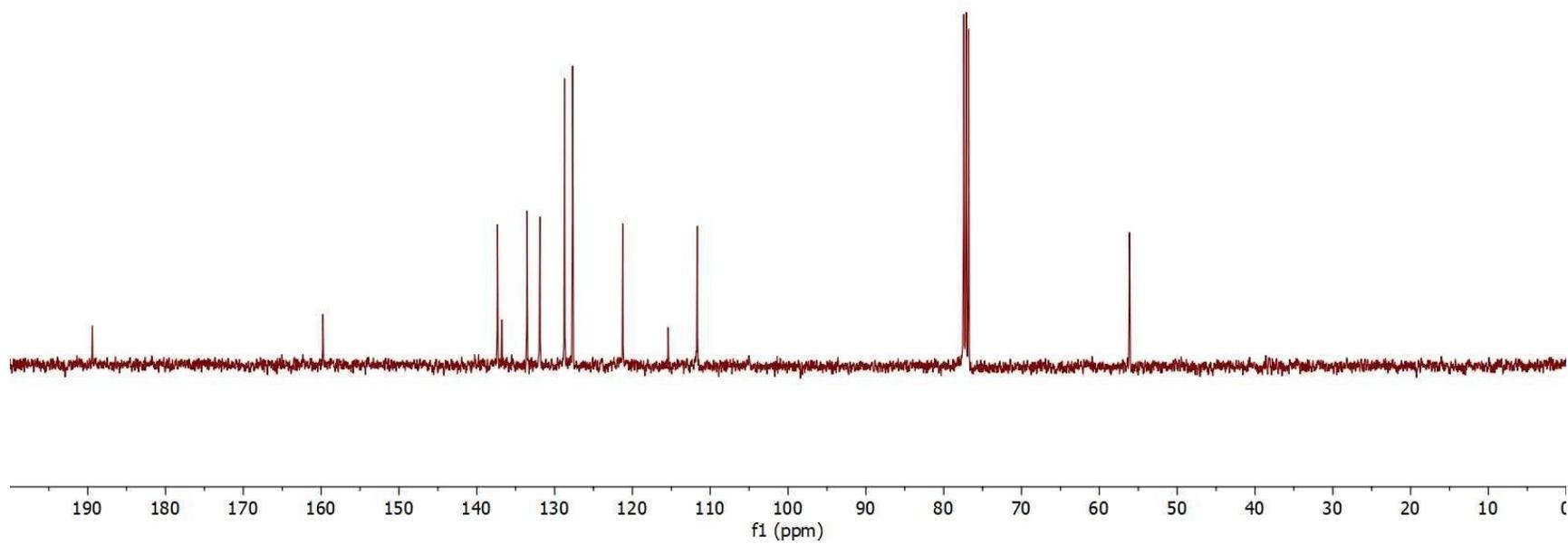
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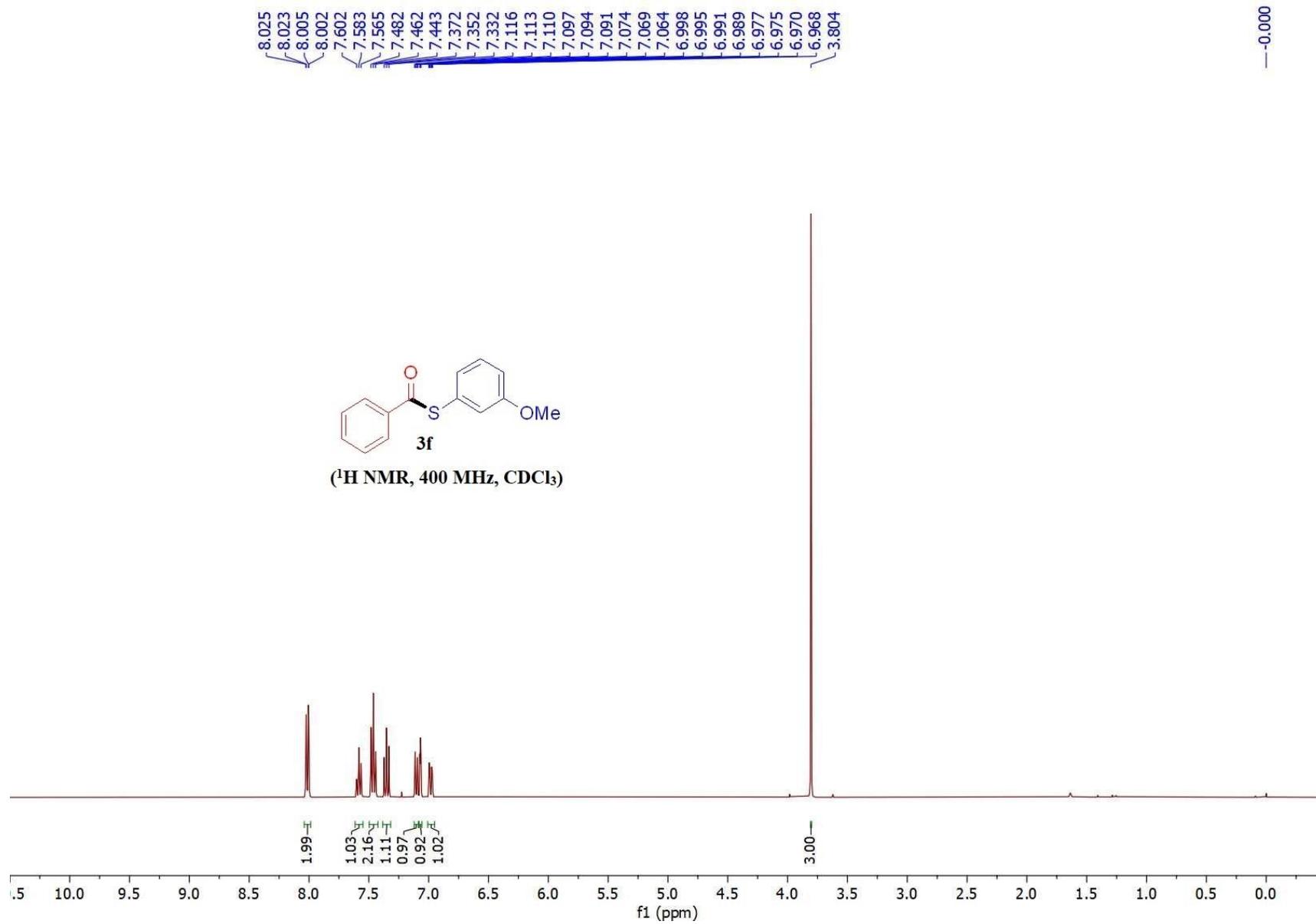
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—56.11



(¹³C{¹H} NMR, 100 MHz, CDCl₃)





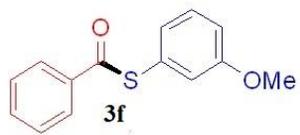
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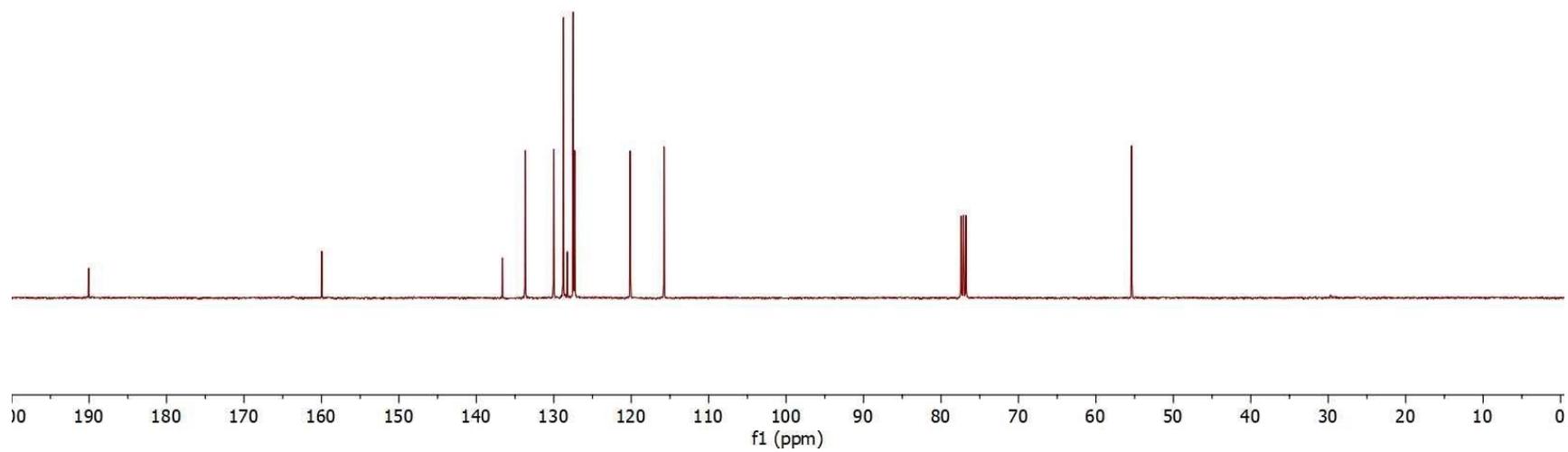
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76.78

—55.39

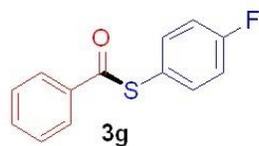


(¹³C{¹H} NMR, 100 MHz, CDCl₃)

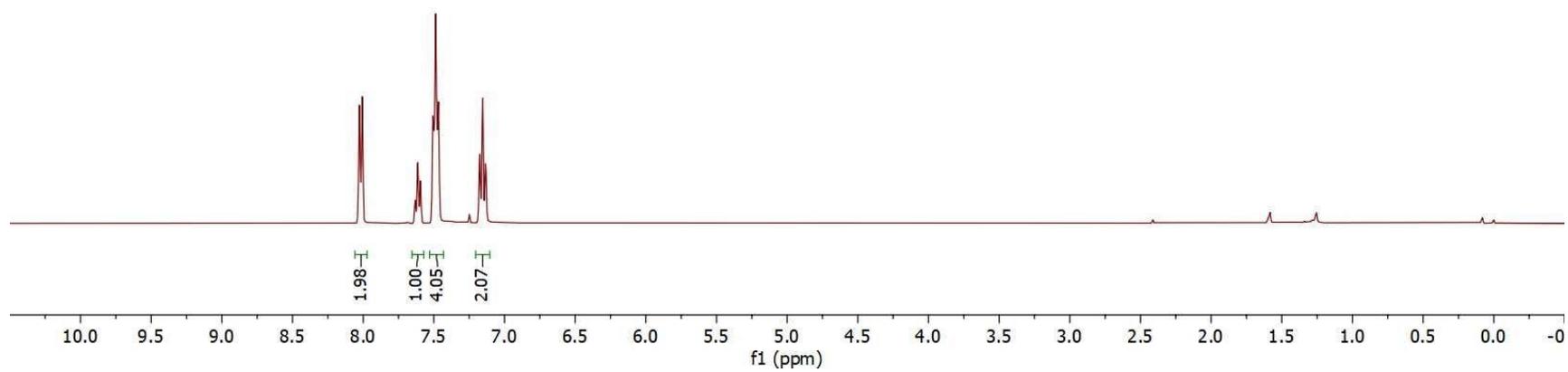


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7.632
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7.595
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7.154
7.134

-0.000



(¹H NMR, 400 MHz, CDCl₃)



—190.21

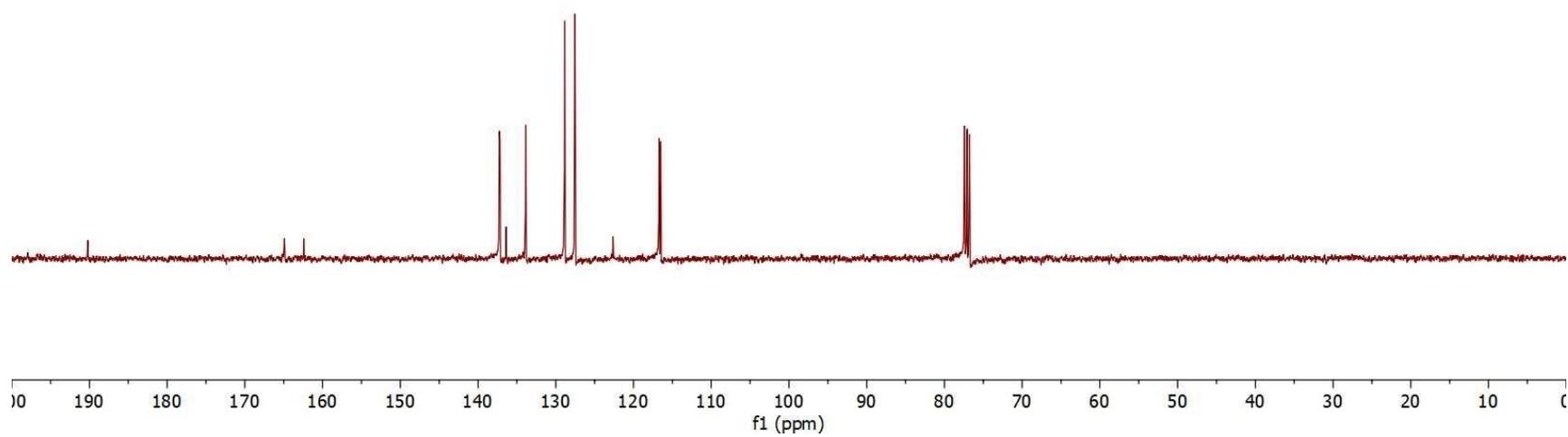
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—162.42

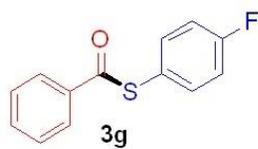
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76.78



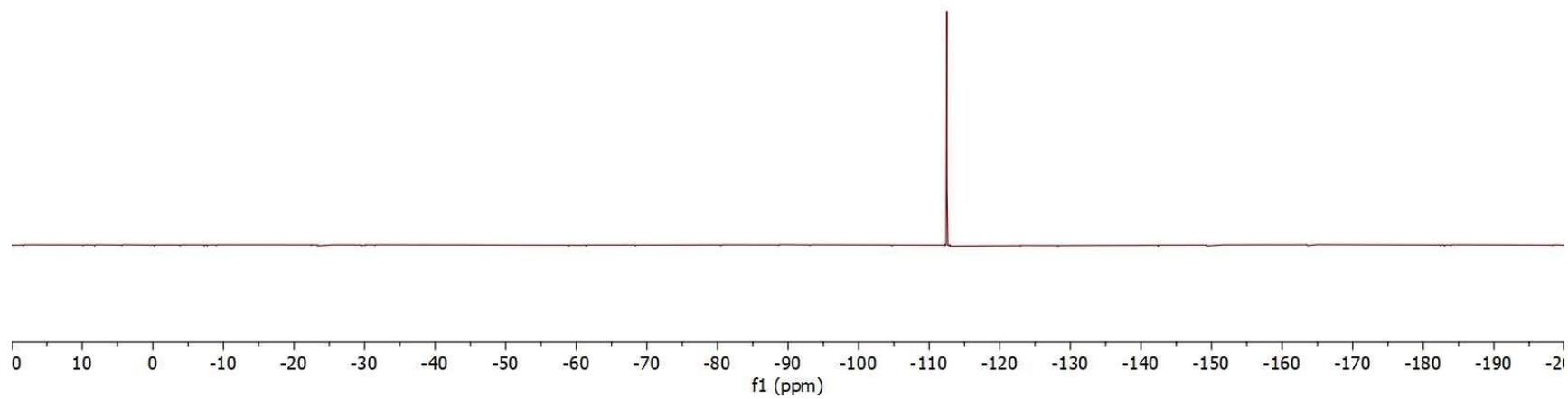
(¹³C{¹H} NMR, 100 MHz, CDCl₃)

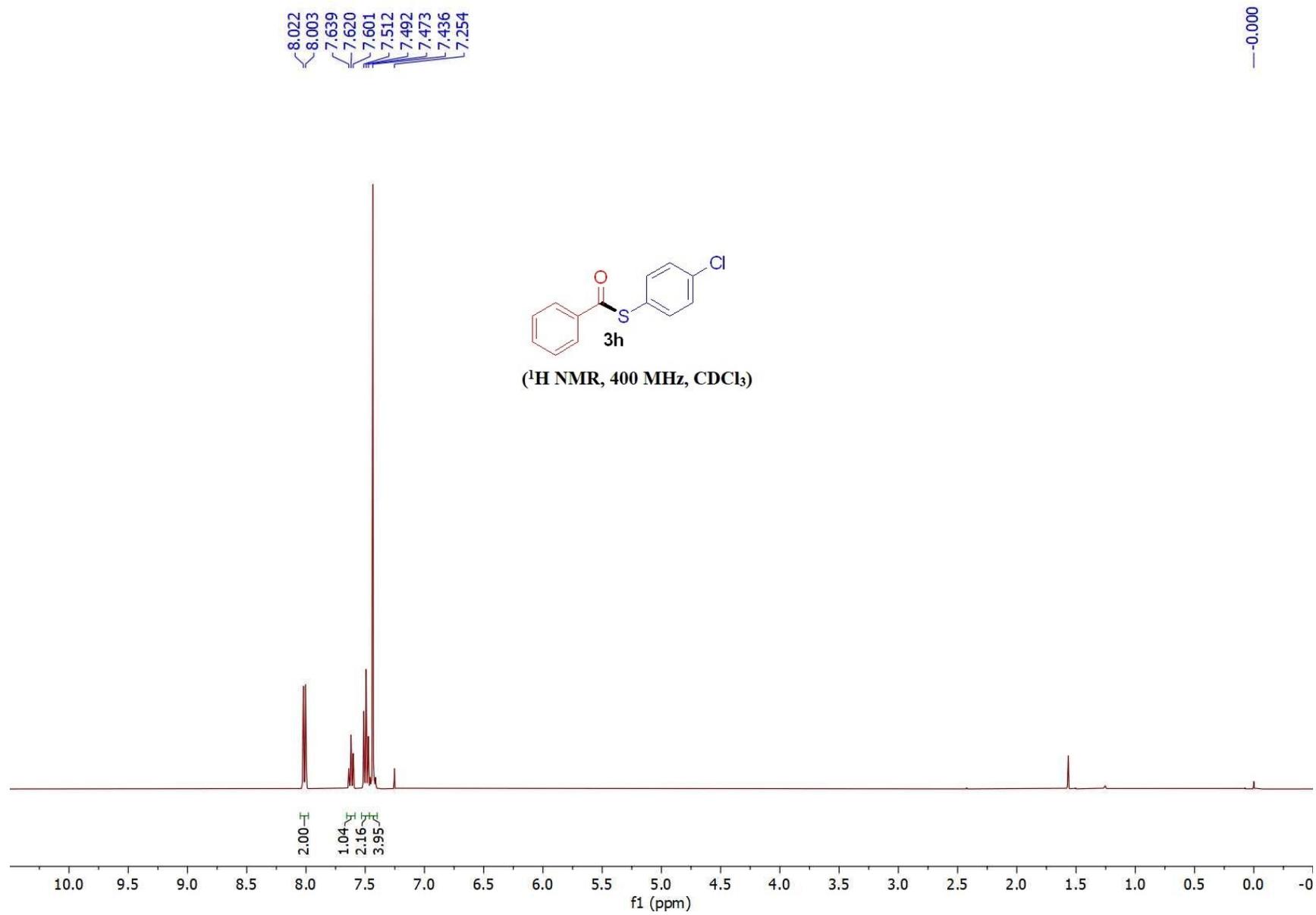




(¹⁹F NMR, 376 MHz, CDCl₃)

---112.486





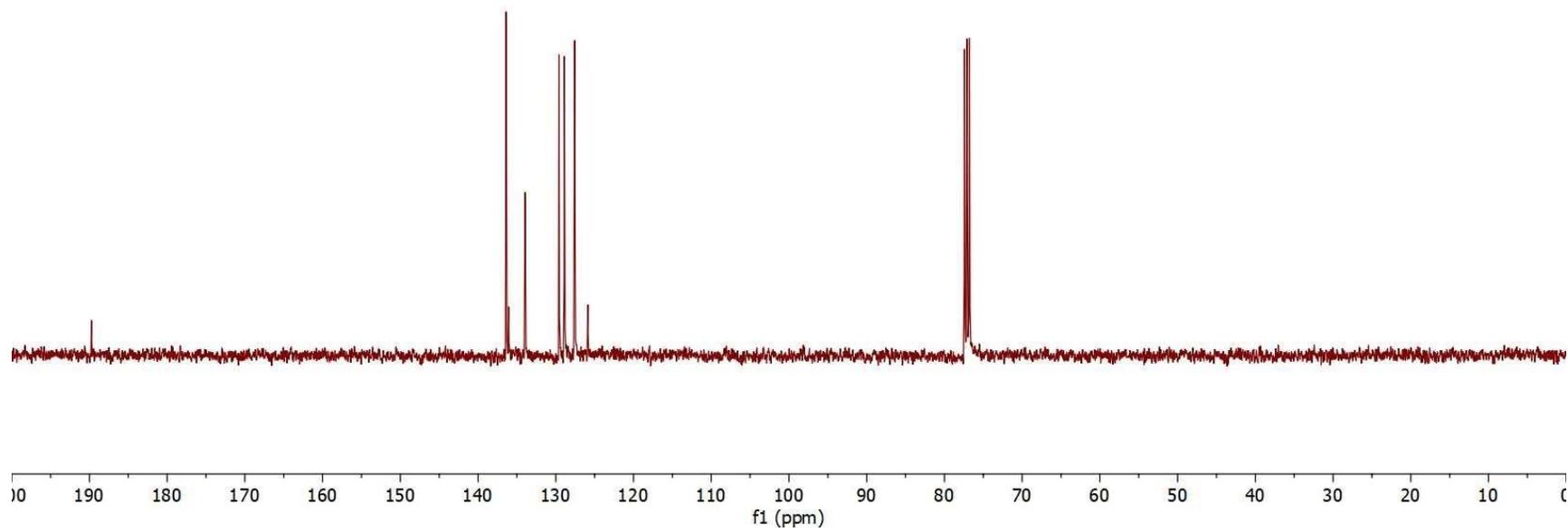
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136.40
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127.58
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77.42
77.10
76.78



(¹³C{H} NMR, 100 MHz, CDCl₃)

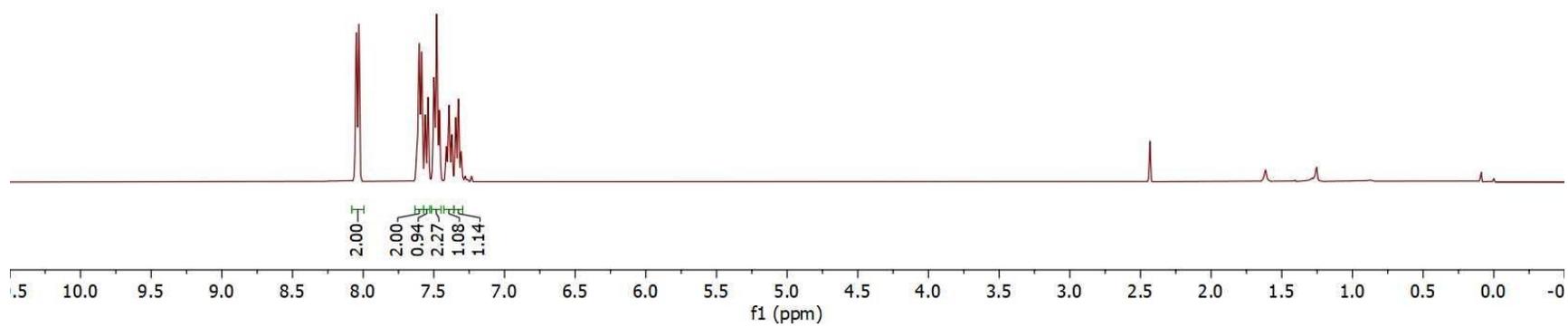


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7.604
7.599
7.590
7.585
7.580
7.561
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7.307

-0.000



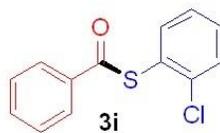
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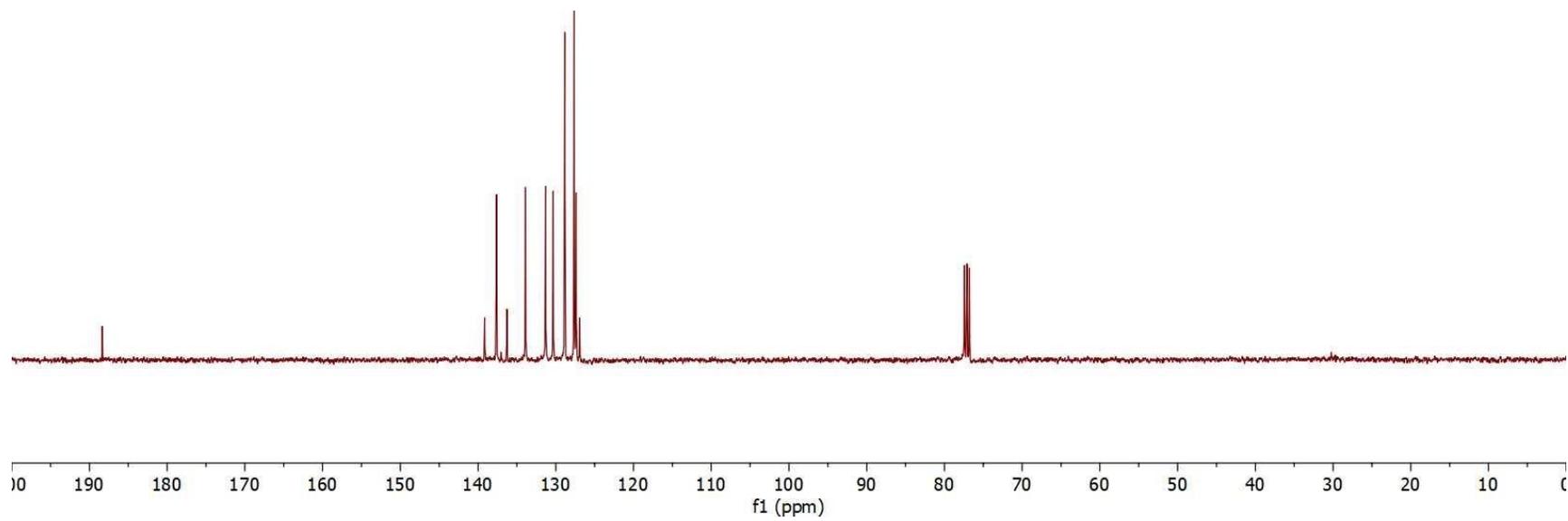
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139.15
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128.84
127.64
127.39
126.92

77.42
77.10
76.78

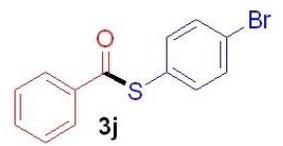


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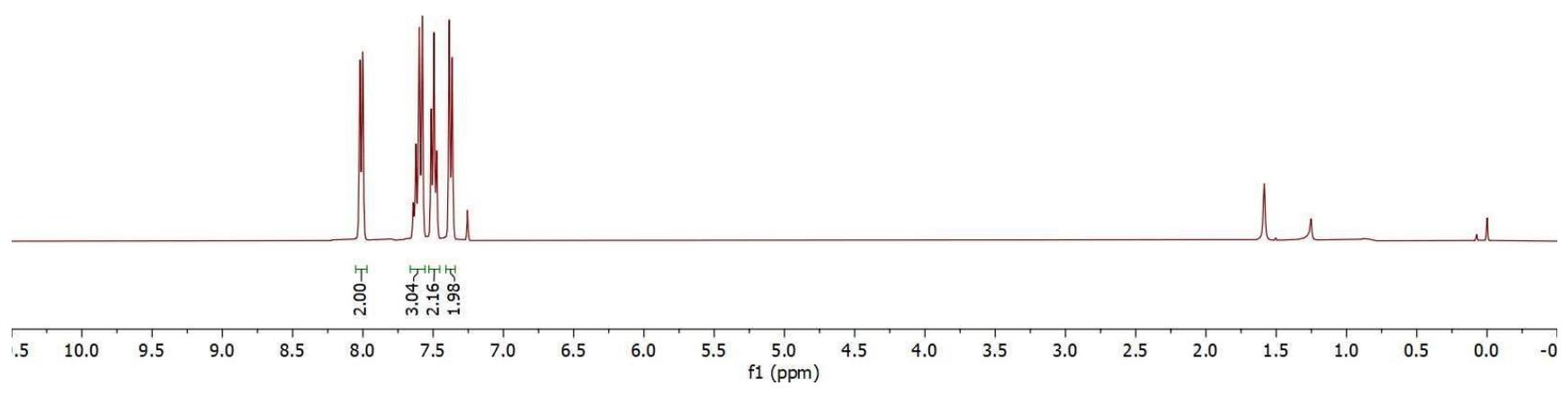


8.021
8.003
7.640
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-0.000



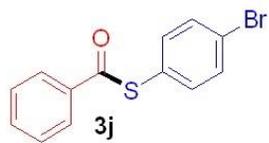
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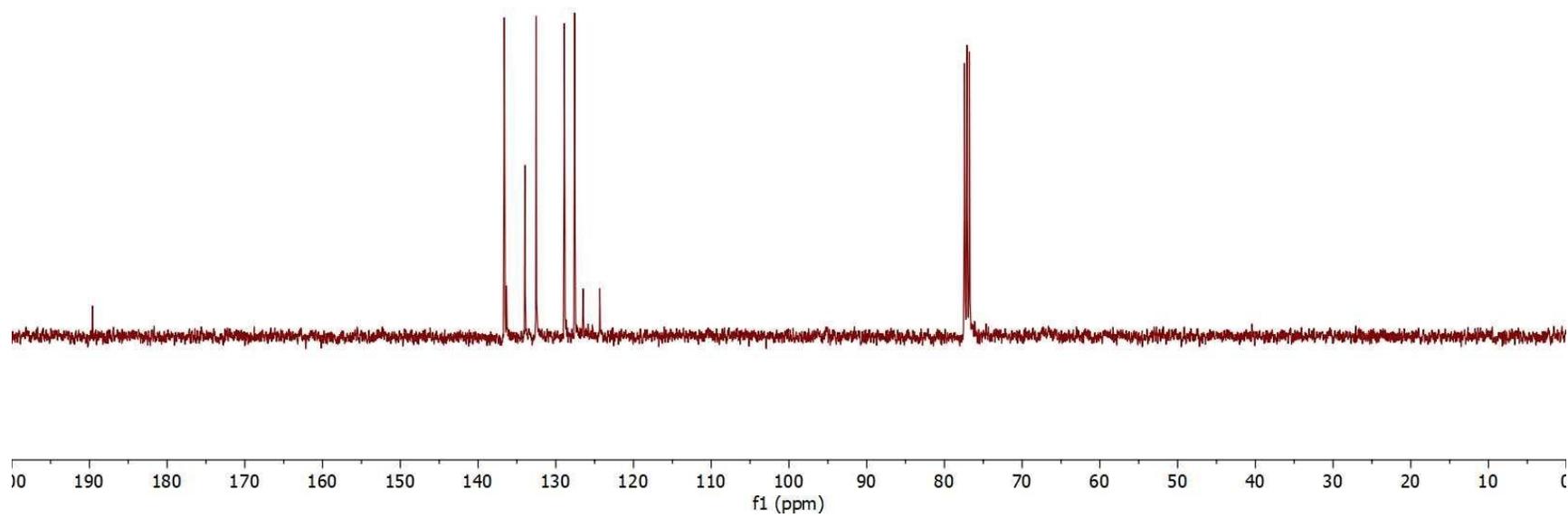
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77.42
77.10
76.78

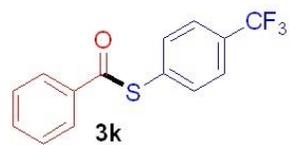


(¹³C{H} NMR, 100 MHz, CDCl₃)

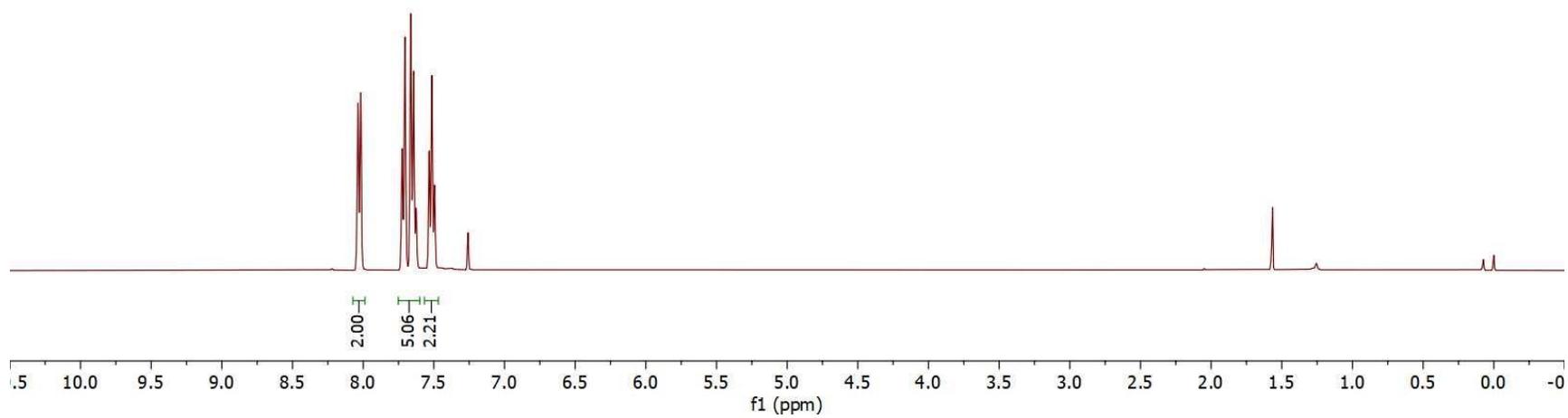


8.037
8.018
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7.704
7.663
7.643
7.625
7.533
7.514
7.495
7.258

-0.000



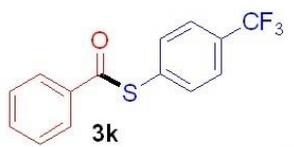
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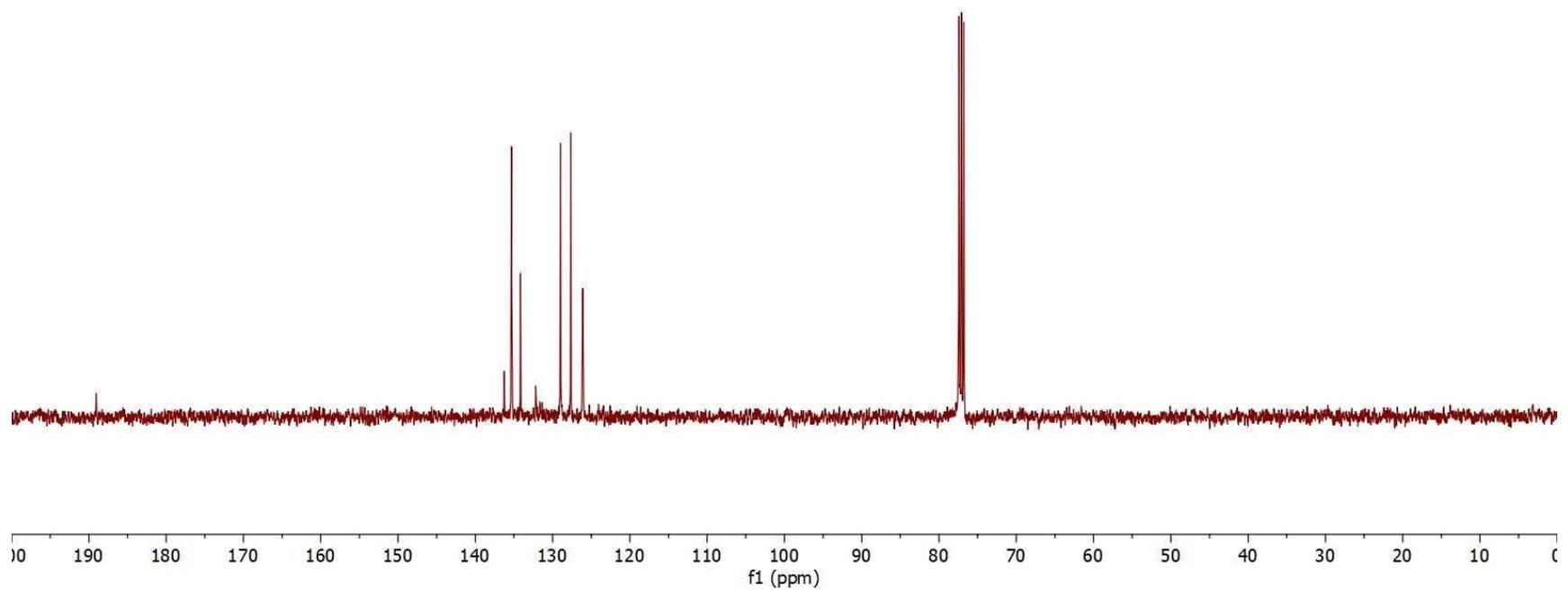
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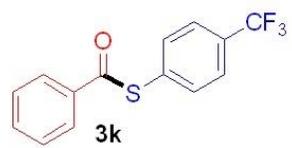
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77.10
76.78



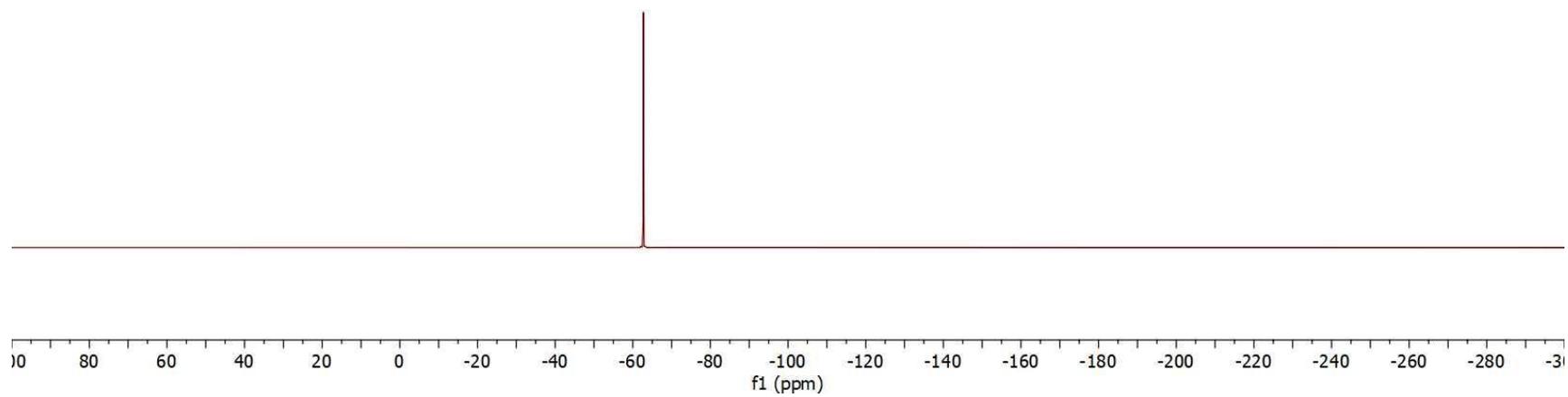
(¹³C{¹H} NMR, 100 MHz, CDCl₃)

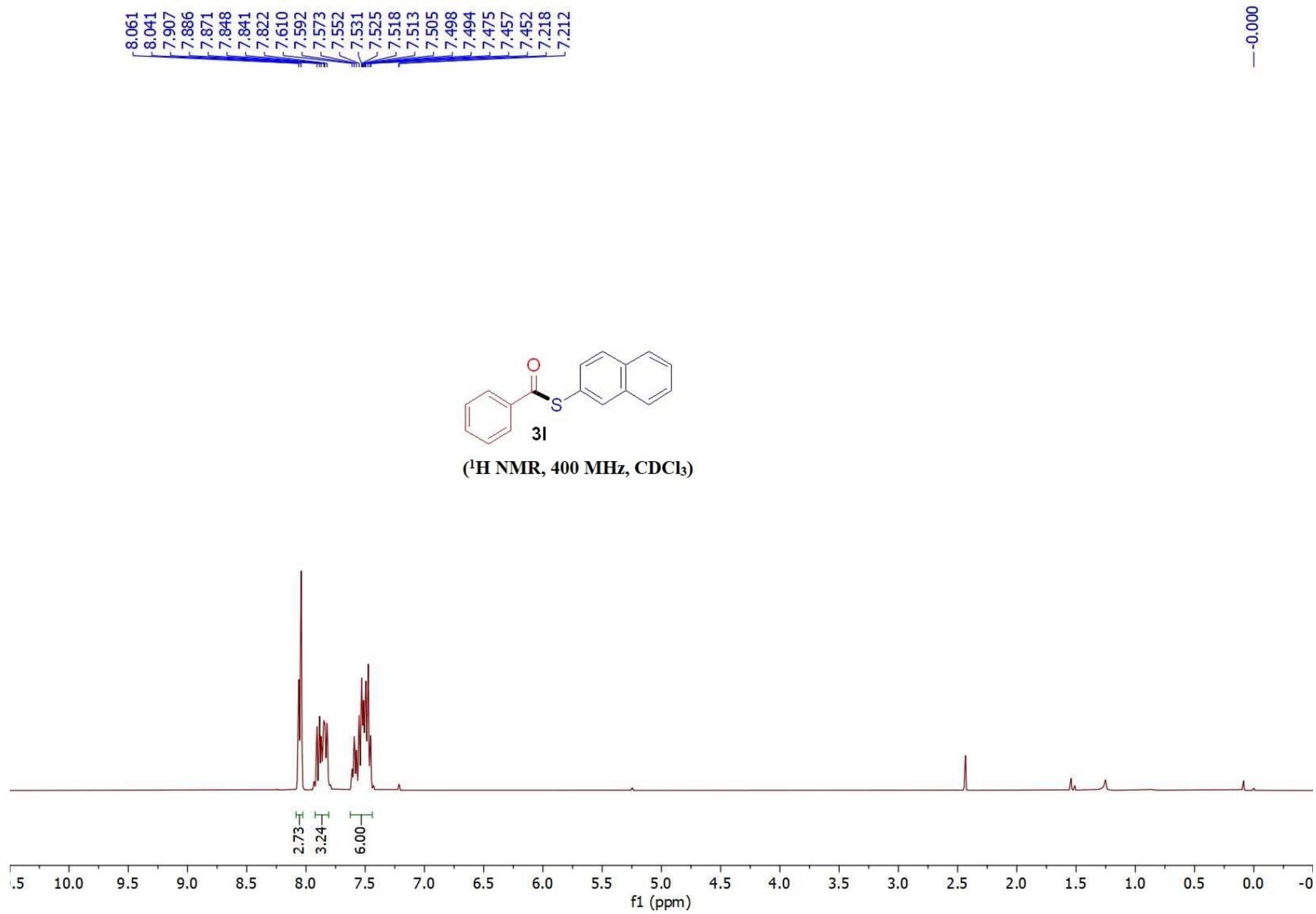


-62.712



(¹⁹F NMR, 376 MHz, CDCl₃)

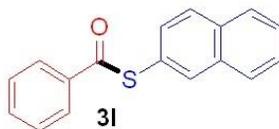




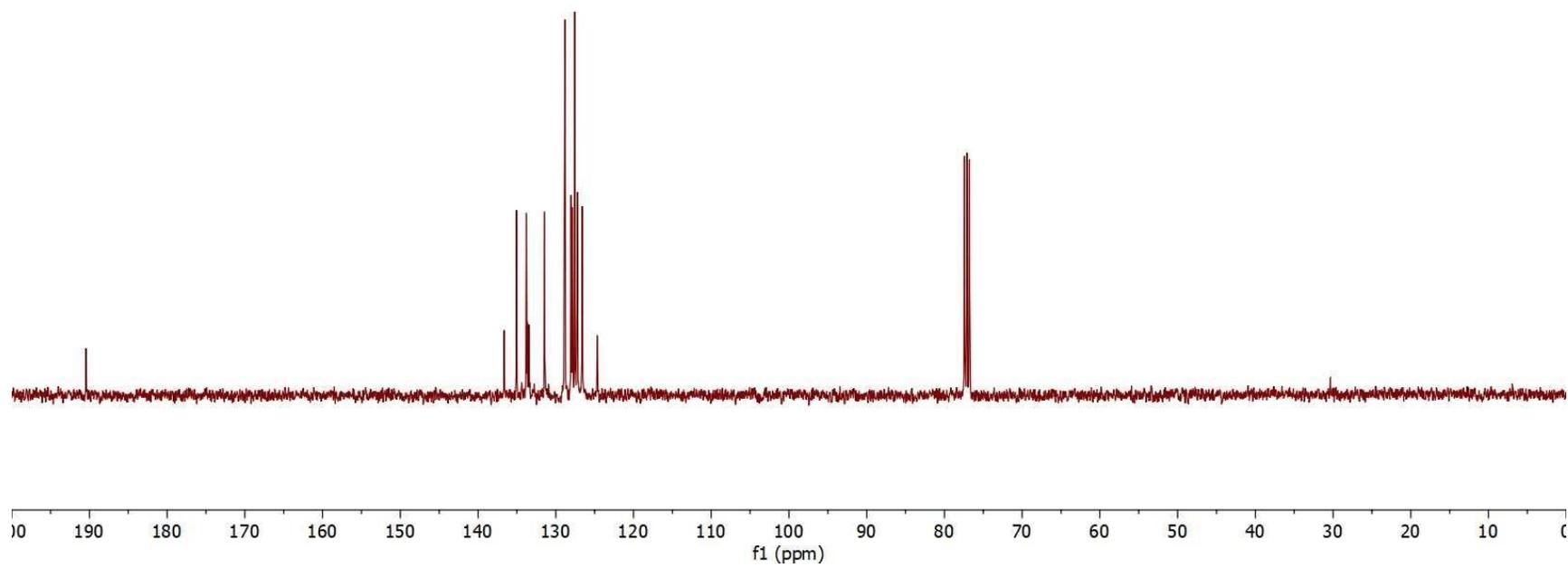
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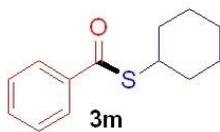
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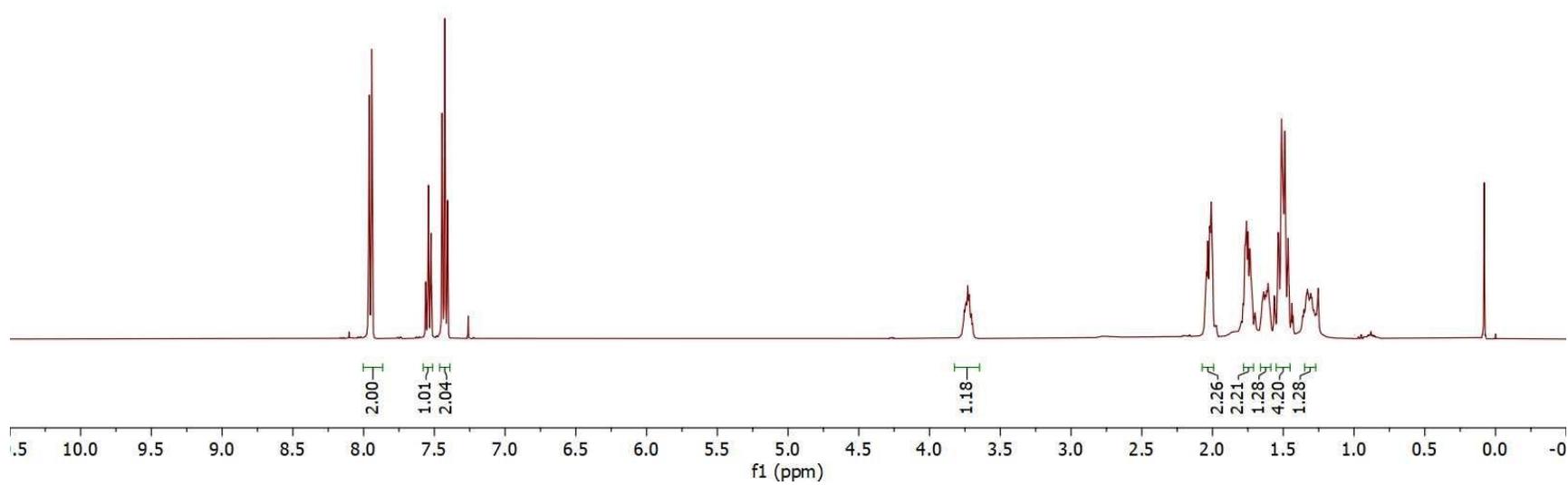
(¹³C{H} NMR, 100 MHz, CDCl₃)



7.961
7.940
7.560
7.542
7.523
7.445
7.425
7.406
7.261
3.765
3.755
3.745
3.739
3.730
3.720
3.714
3.705
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2.042
2.033
2.020
2.009
2.000
1.998
1.771
1.760
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1.507
1.500
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1.485
1.465
1.313
1.305
1.297
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0.000



(¹H NMR, 400 MHz, CDCl₃)



—191.90

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~133.16
~128.54
~127.17

~77.42
~77.10
~76.78

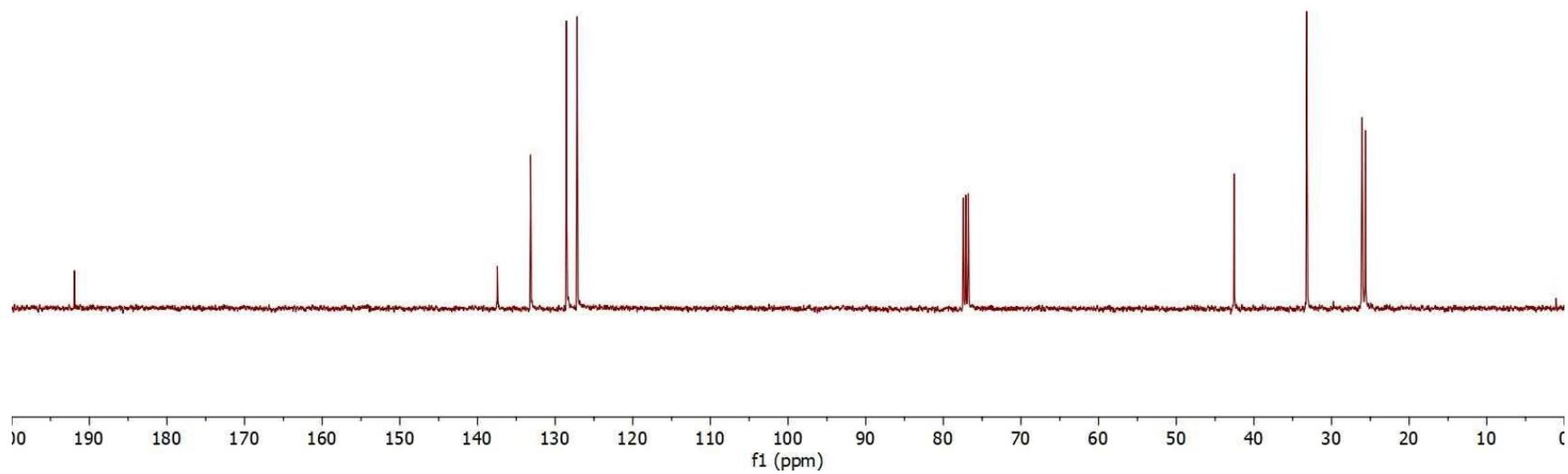
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—33.19

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~25.64



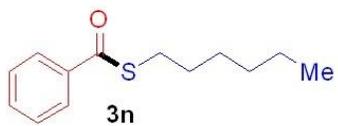
(¹³C{¹H} NMR, 100 MHz, CDCl₃)



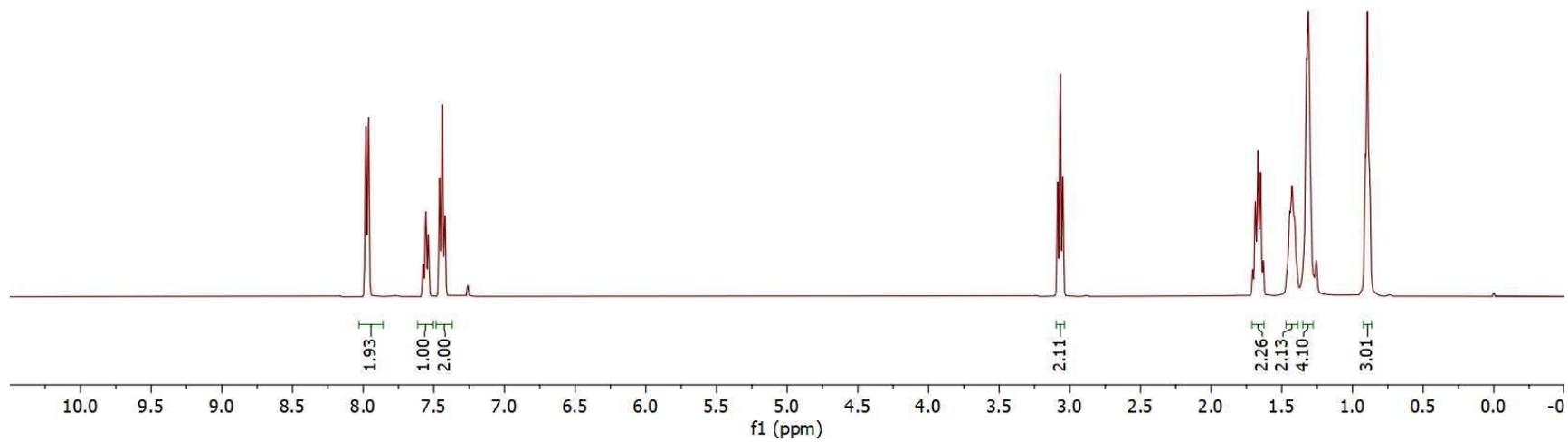
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(¹H NMR, 400 MHz, CDCl₃)



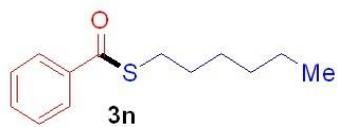
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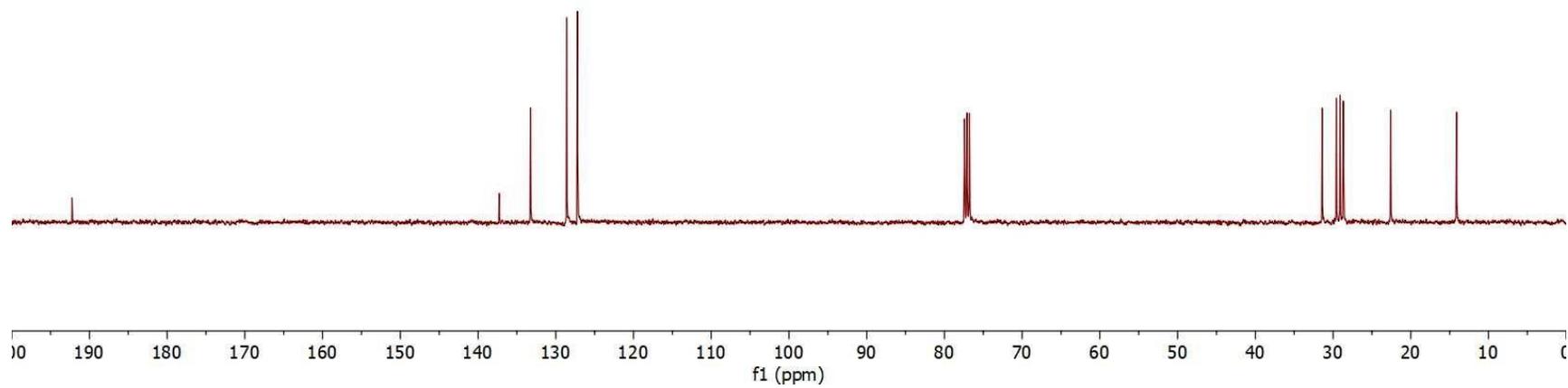
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~77.10
~76.78

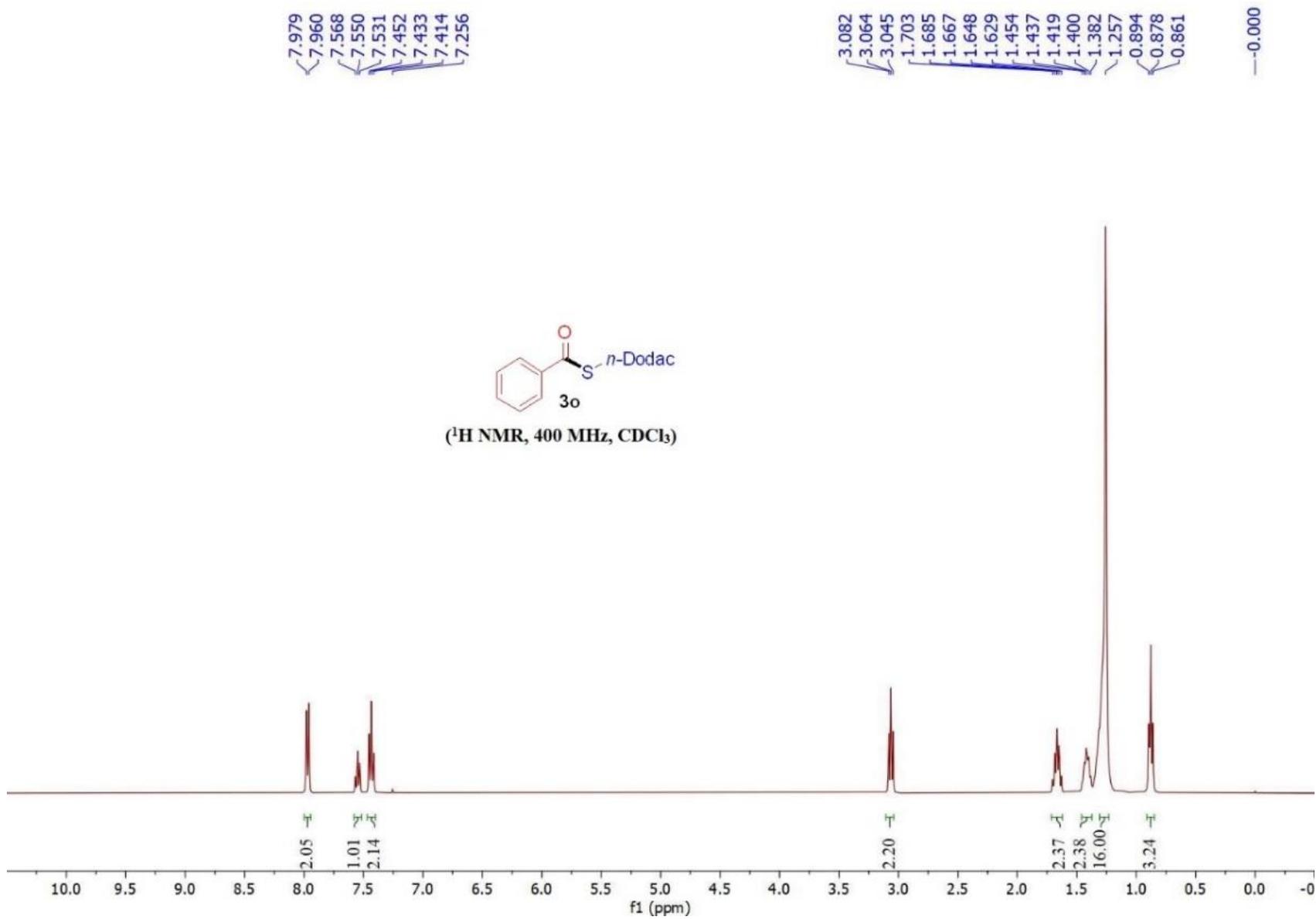
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—14.11



(¹³C{¹H} NMR, 100 MHz, CDCl₃)





—192.19

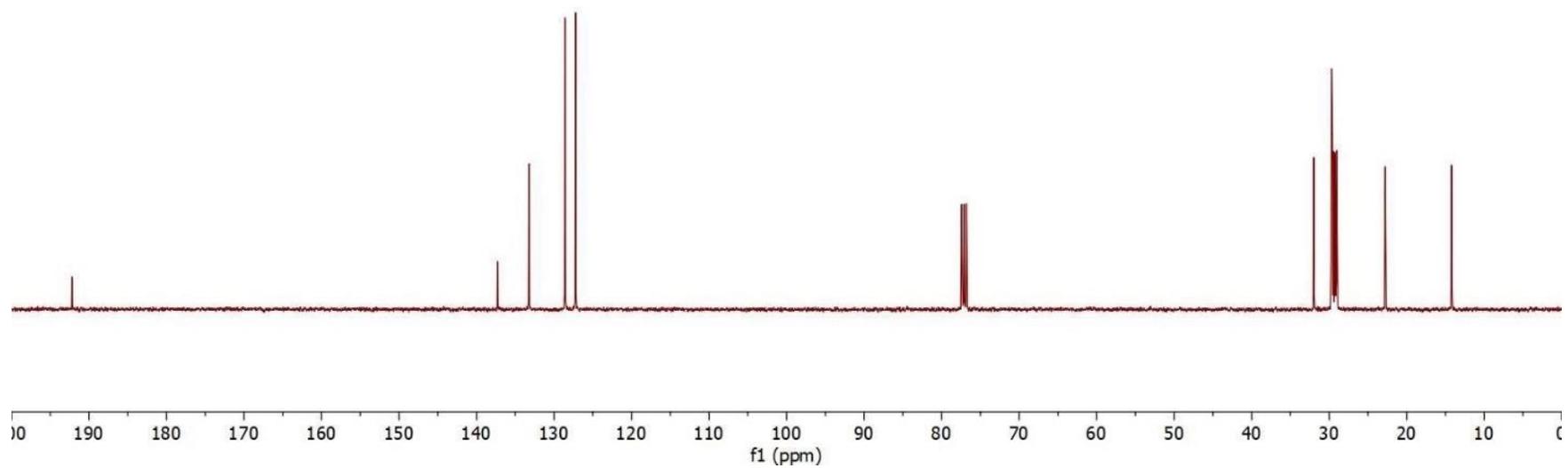
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76.78

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—14.20



(¹³C{¹H} NMR, 100 MHz, CDCl₃)



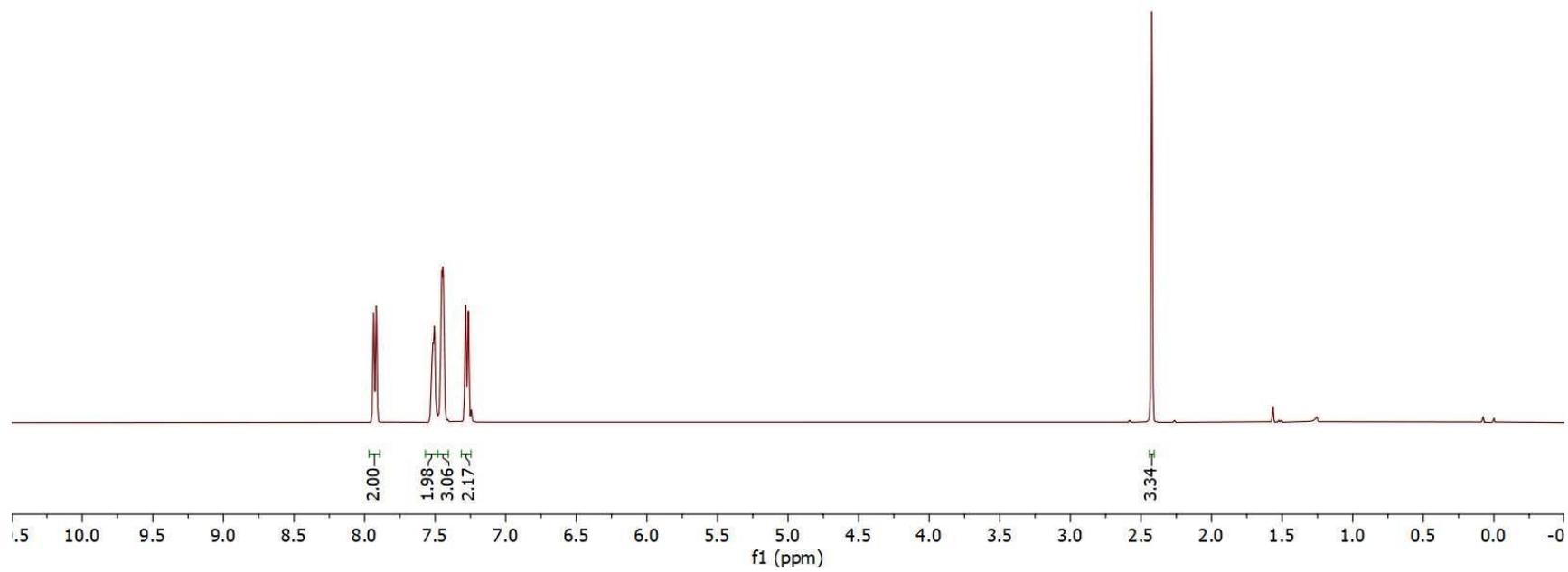
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7.285
7.265

— 2.423

— 0.000



(¹H NMR, 400 MHz, CDCl₃)



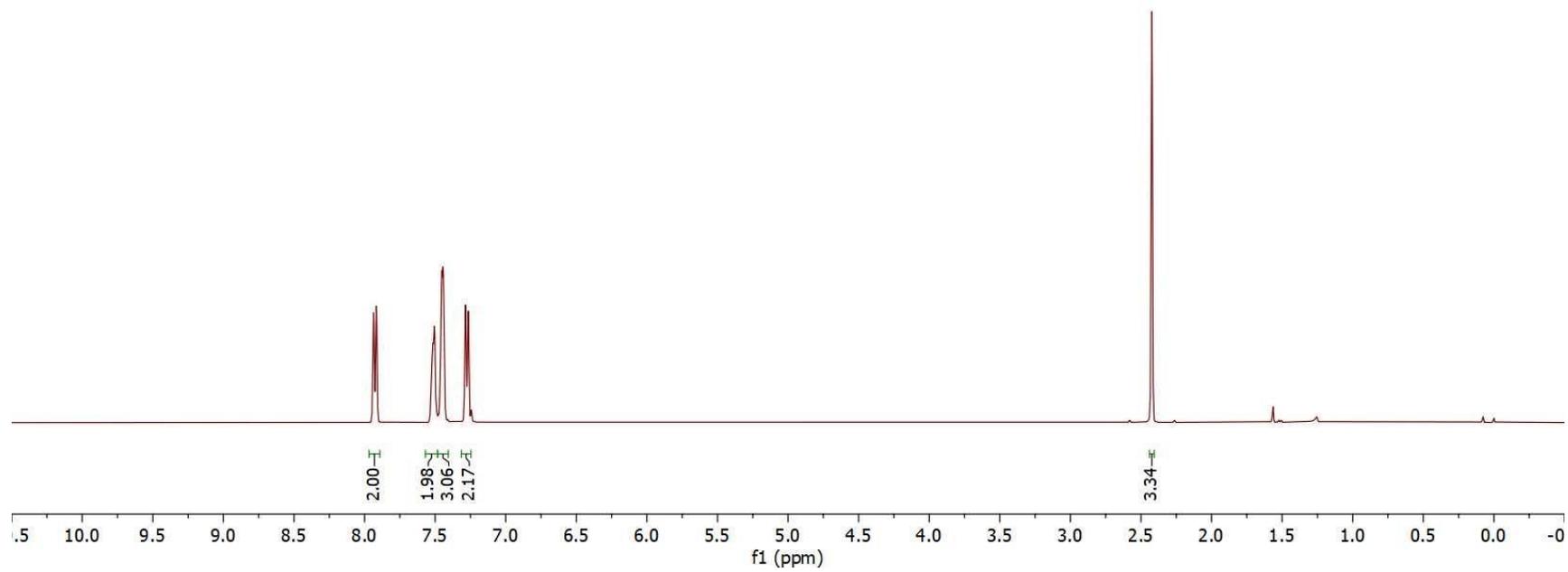
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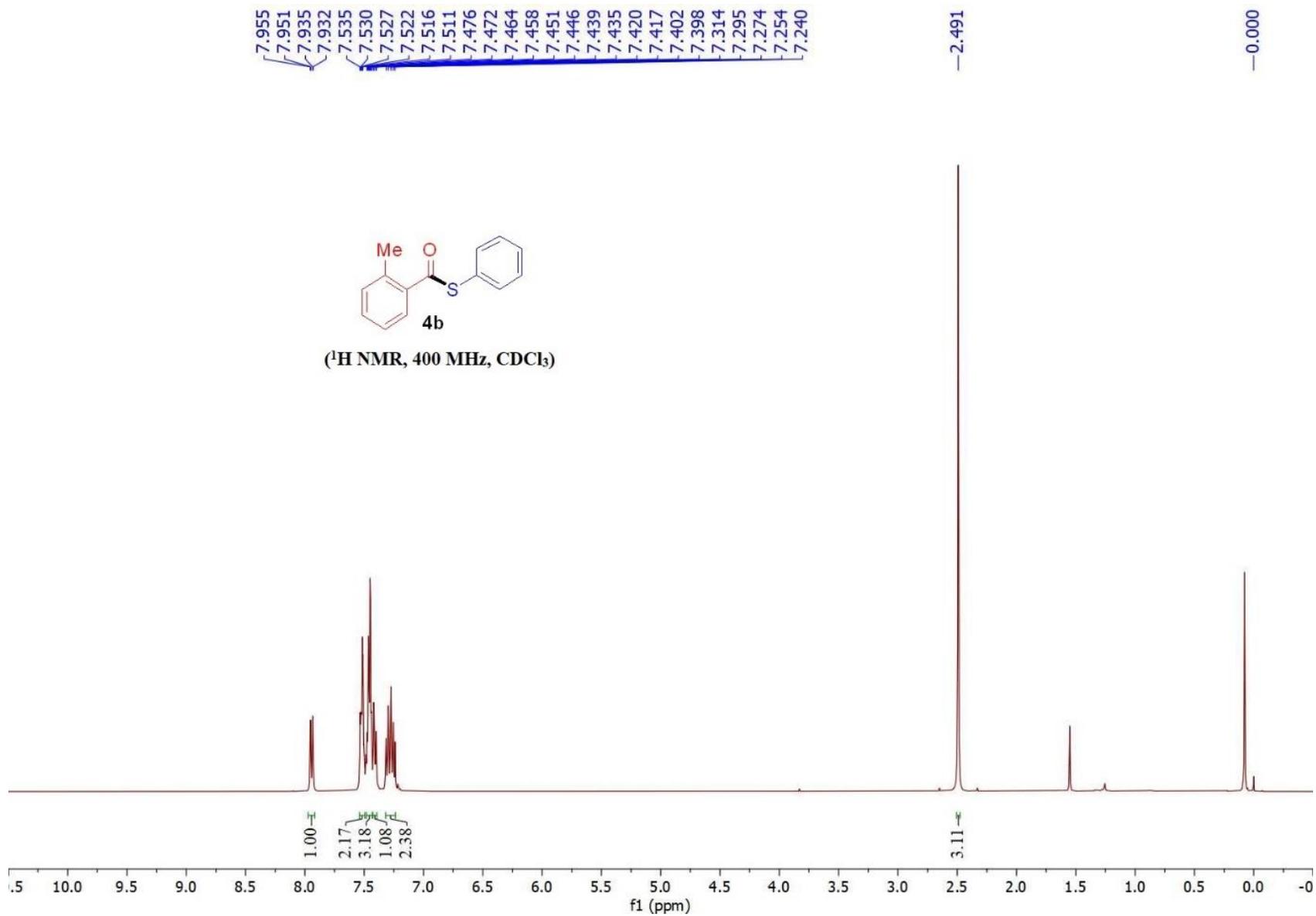
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(¹H NMR, 400 MHz, CDCl₃)





—192.24

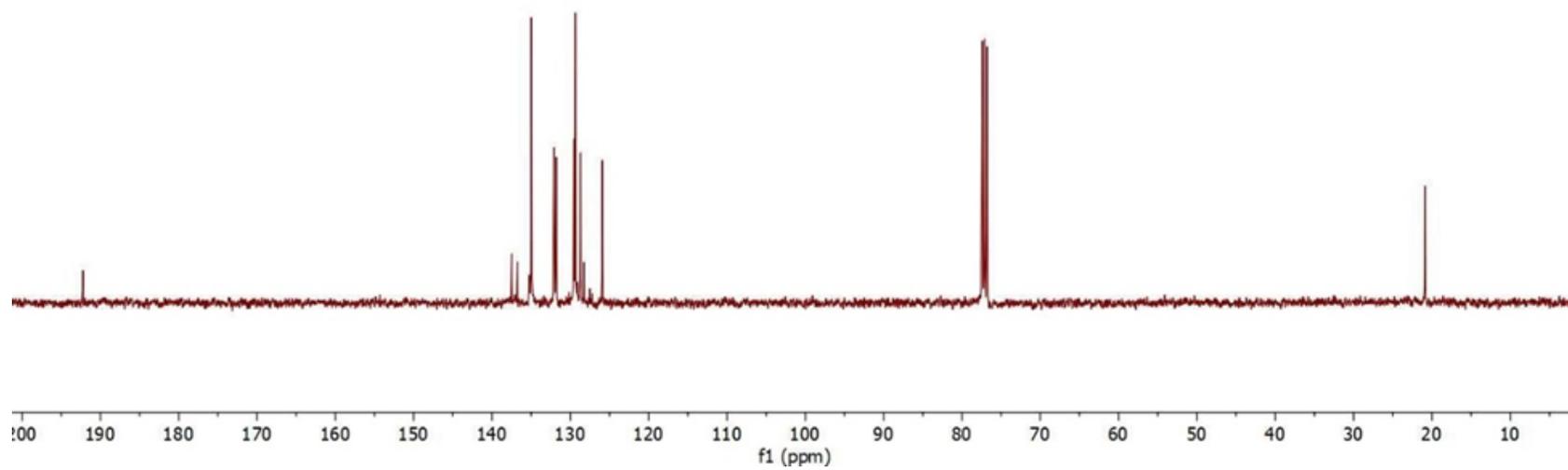
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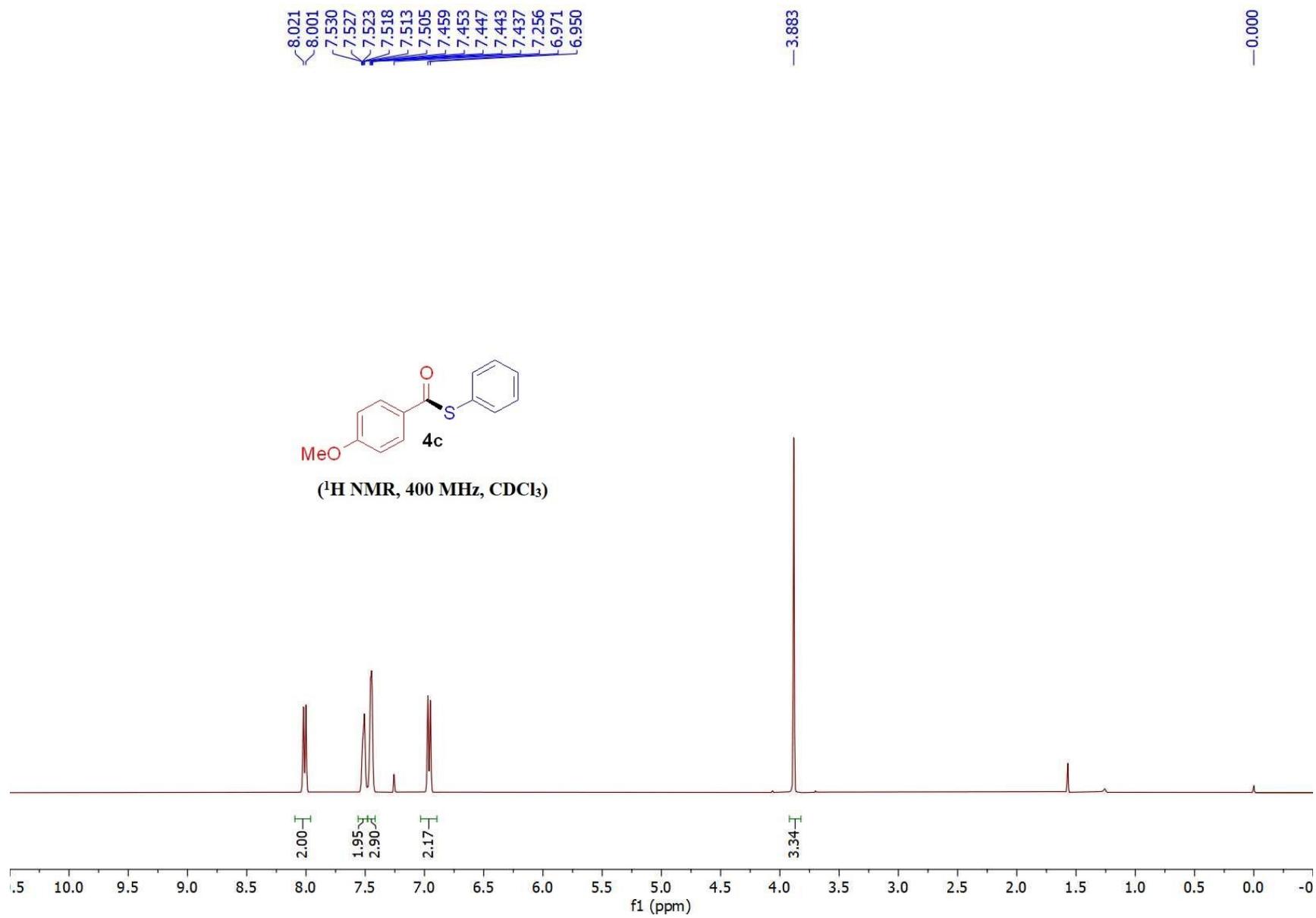
77.42
77.10
76.78

—20.86



(¹³C{H} NMR, 100 MHz, CDCl₃)





—188.71

—164.04

135.27

129.78

129.46

129.42

129.25

127.66

—113.97

77.42

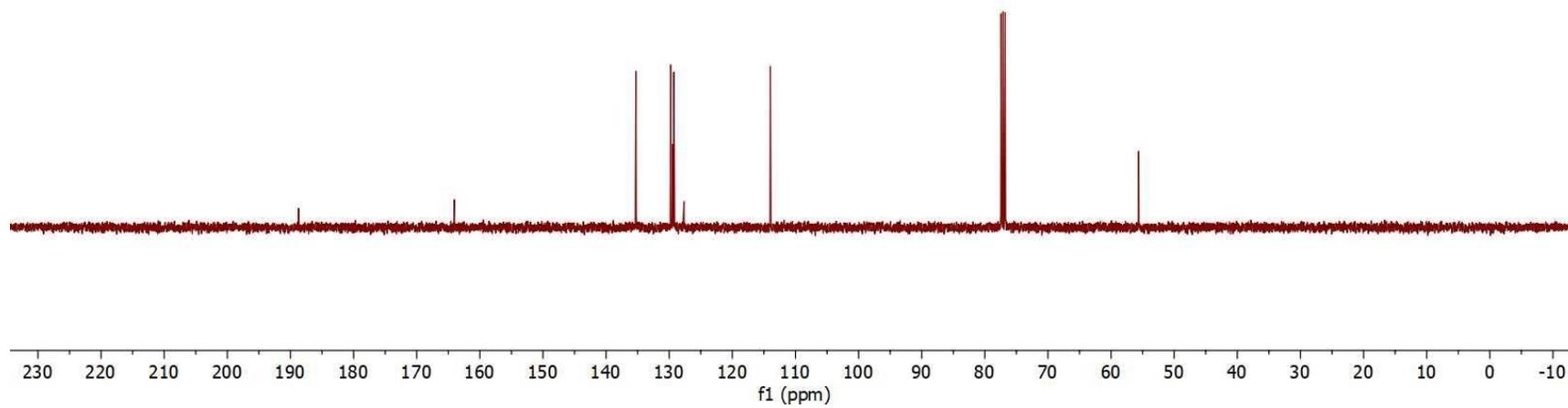
77.10

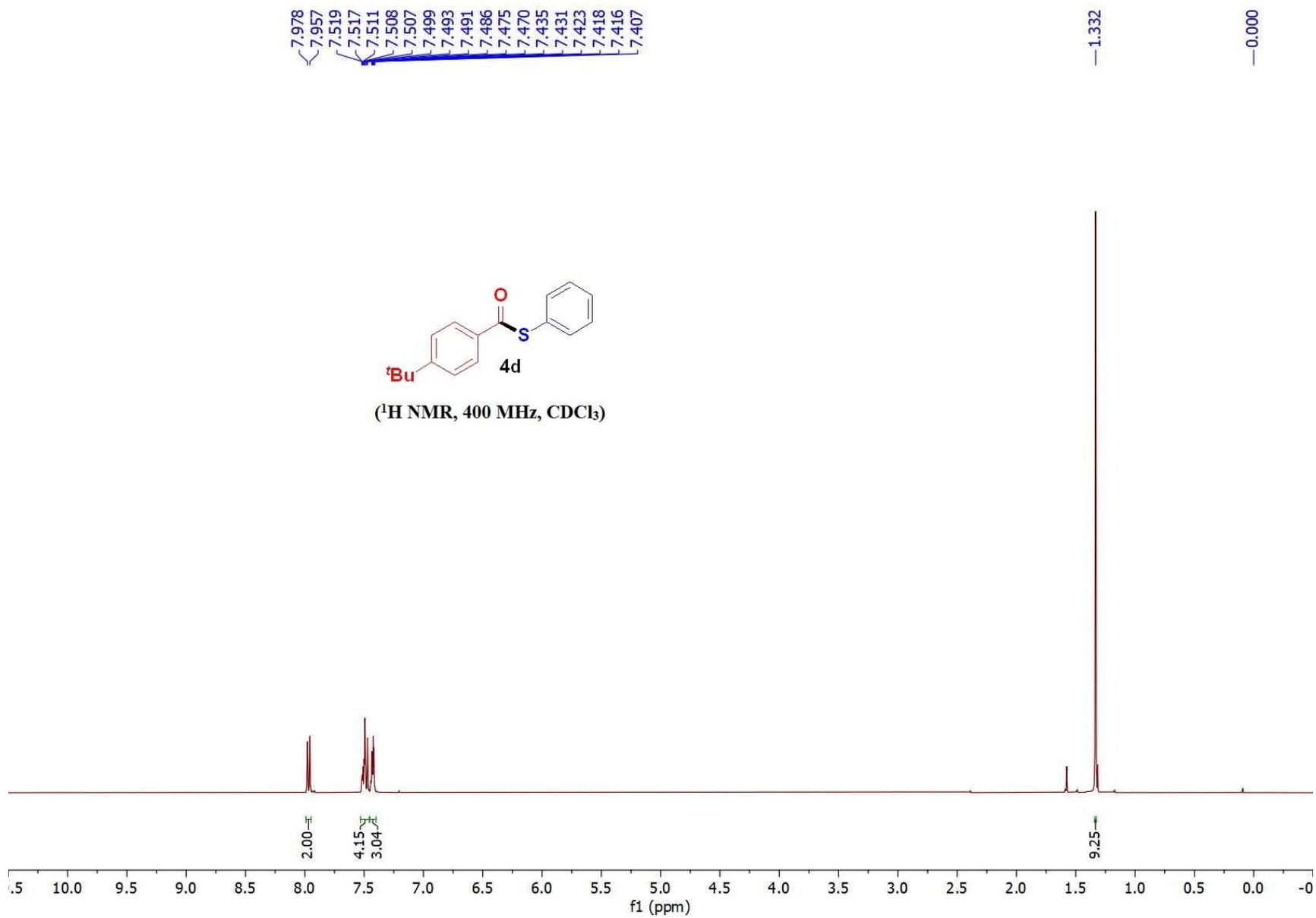
76.78

—55.63



(¹³C{H} NMR, 100 MHz, CDCl₃)





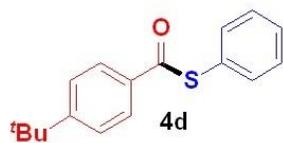
—189.66

—157.51

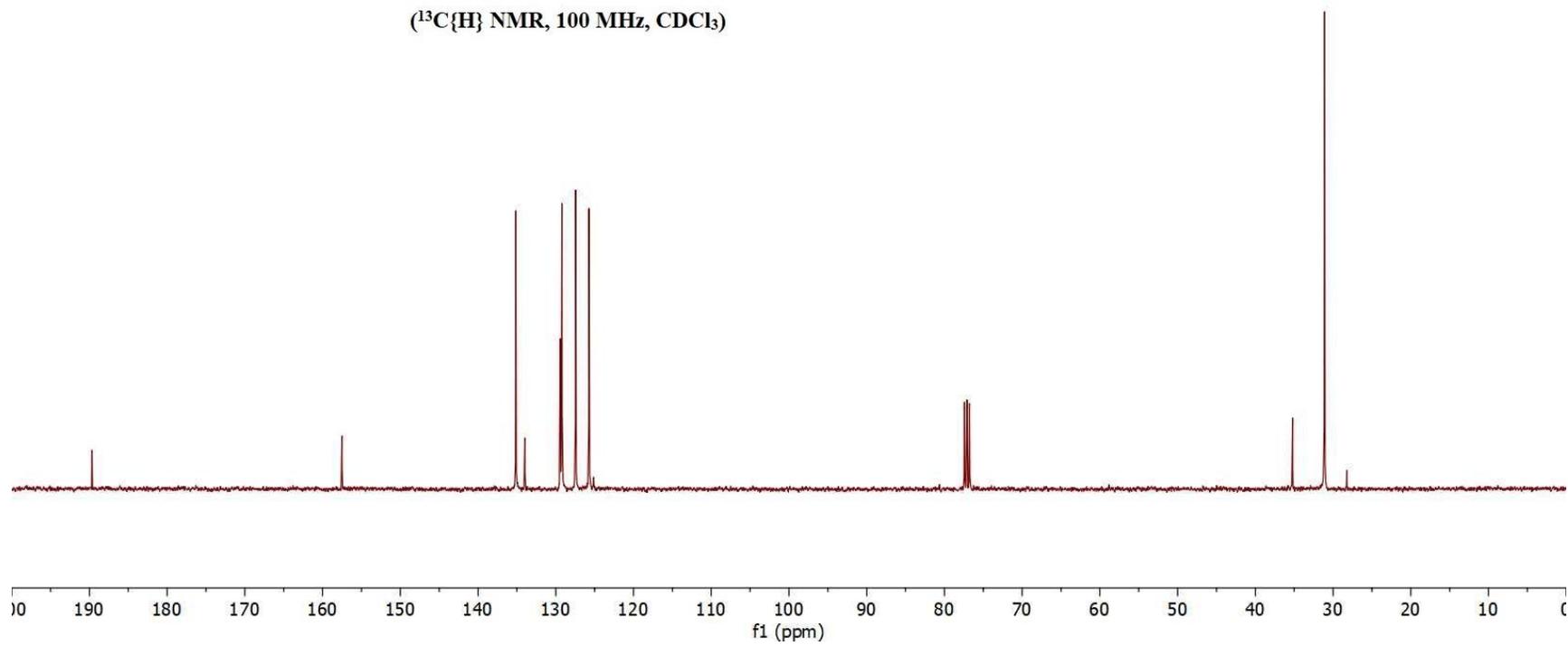
135.14
133.99
129.43
129.21
127.55
127.44
125.72

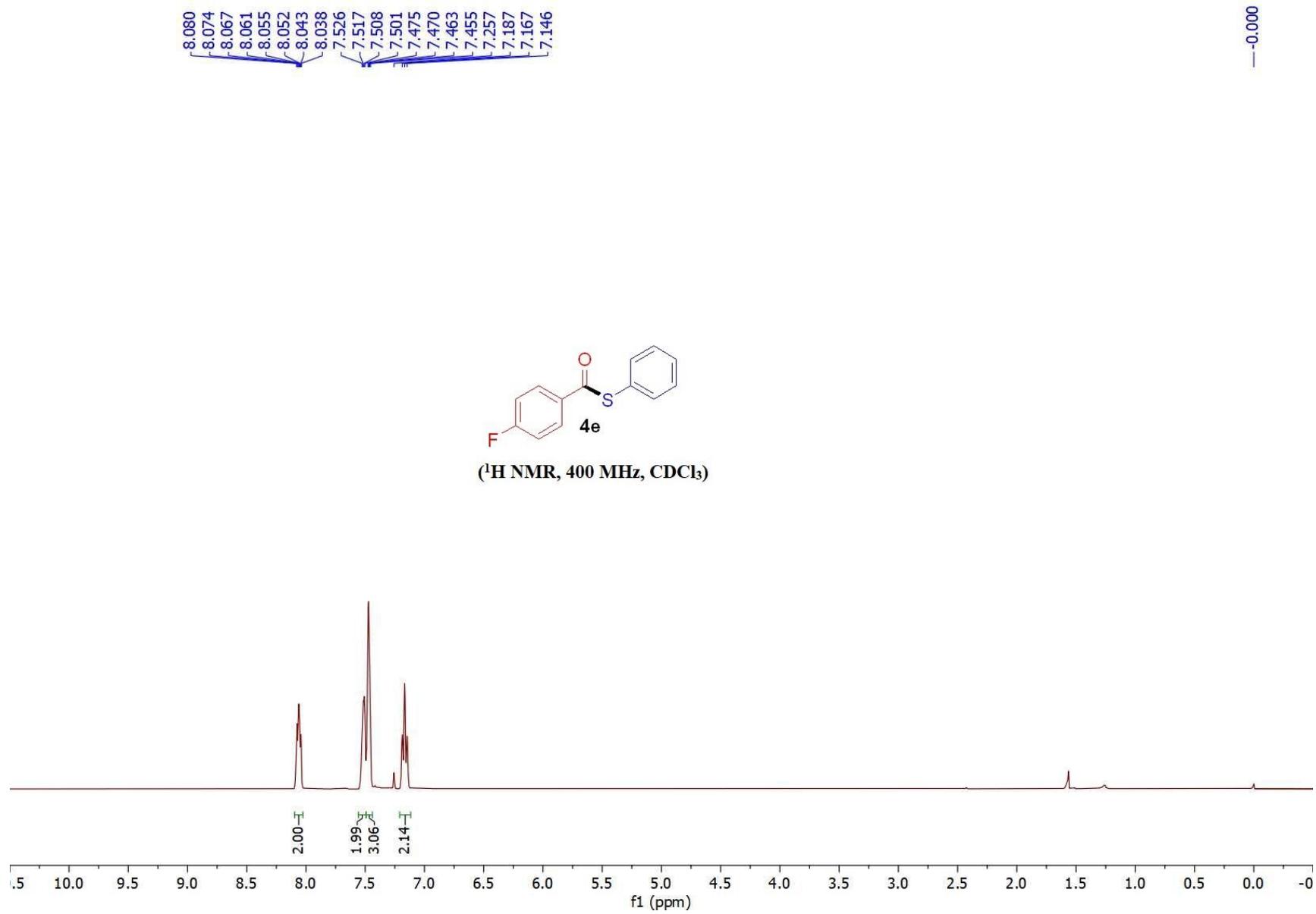
77.42
77.10
76.78

—35.21
—31.09



(¹³C{¹H} NMR, 100 MHz, CDCl₃)





—188.80

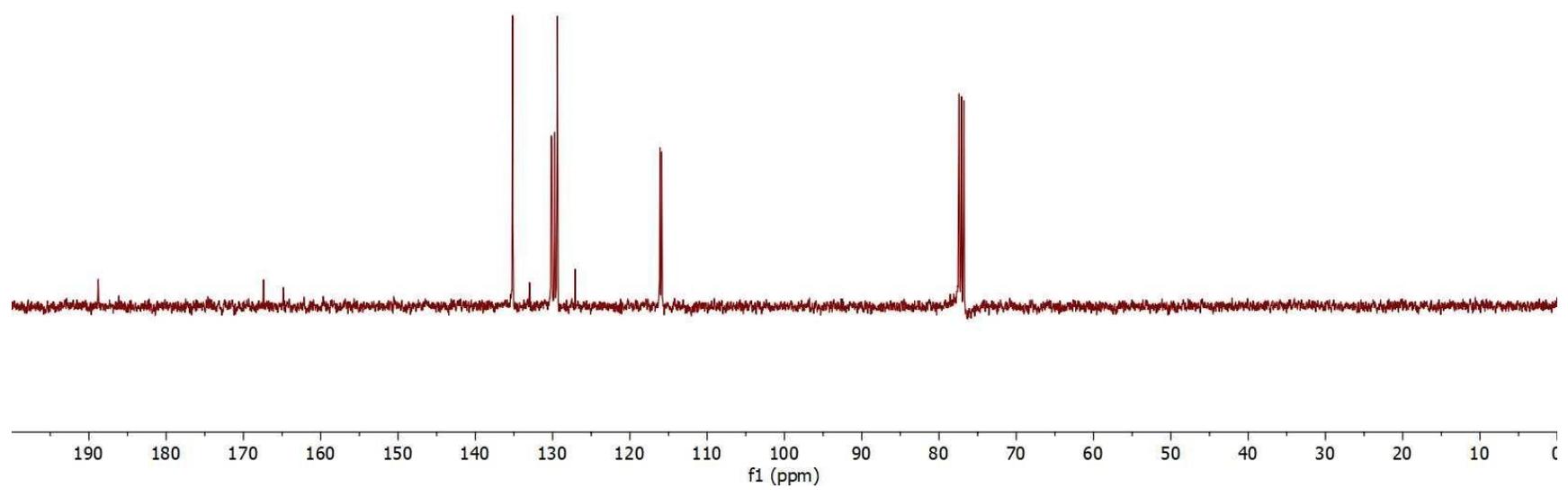
—167.39
—164.85

—135.18
—132.98
—132.95
—130.18
—130.08
—129.73
—129.38
—127.07
—116.11
—115.89

—77.42
—77.10
—76.78



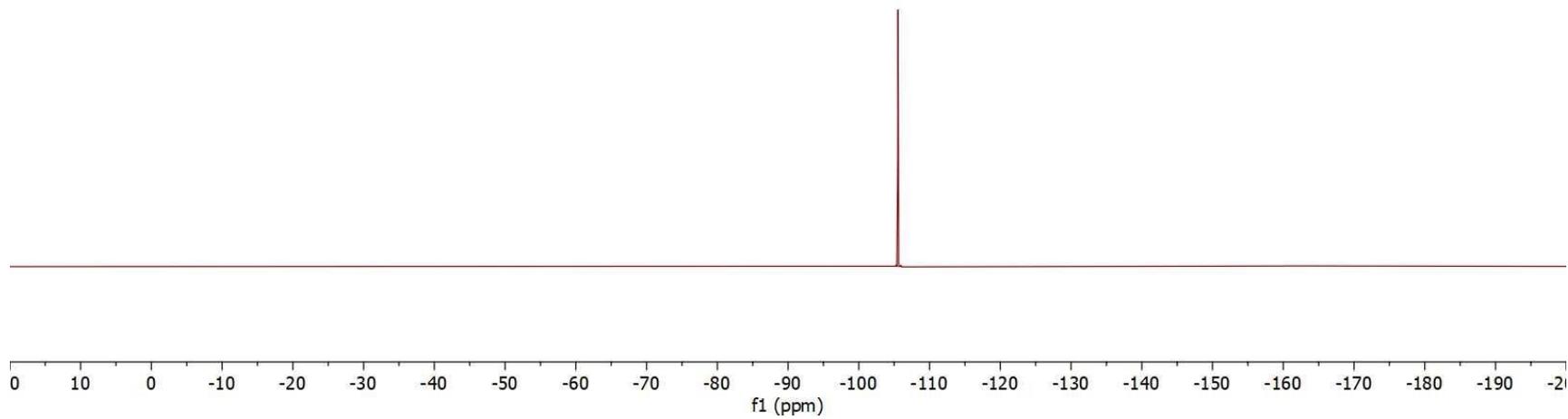
(¹³C{¹H} NMR, 100 MHz, CDCl₃)





(¹⁹F NMR, 376 MHz, CDCl₃)

-105.542

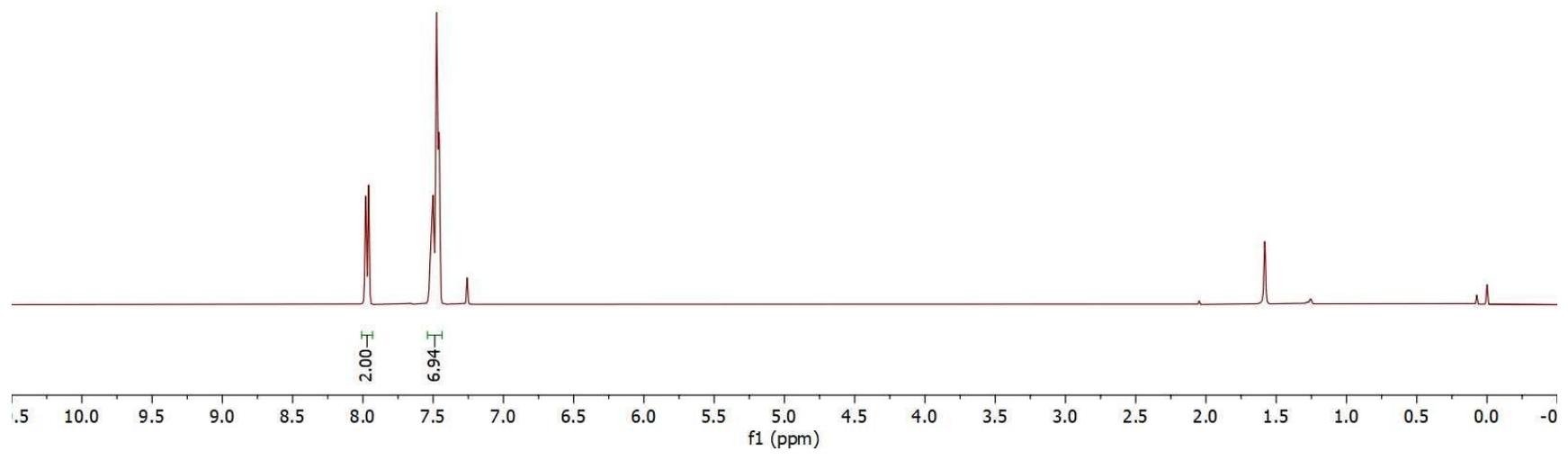


7.981
7.976
7.960
7.954
7.525
7.520
7.514
7.508
7.501
7.496
7.477
7.472
7.462
7.456
7.450
7.259

0.000



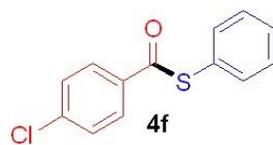
(¹H NMR, 400 MHz, CDCl₃)



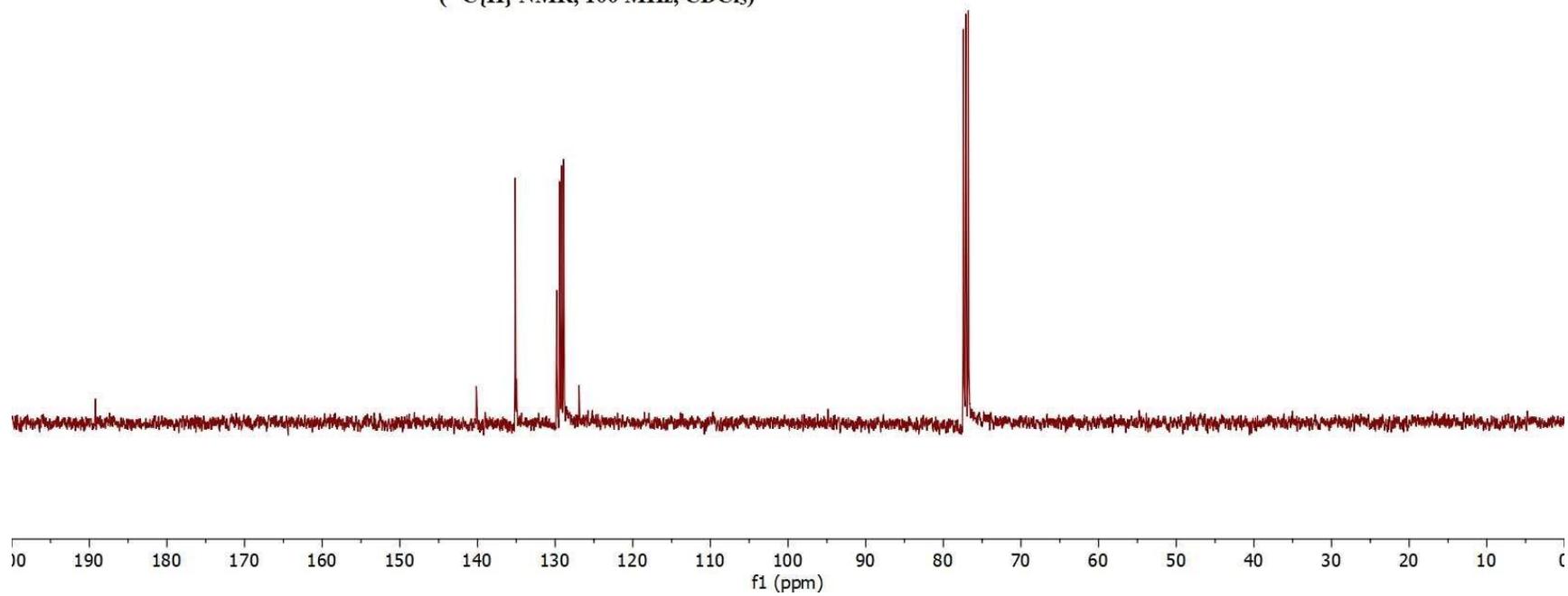
—189.21

140.15
135.15
134.98
129.80
129.42
129.15
128.90
126.92

77.42
77.10
76.78



(¹³C{H} NMR, 100 MHz, CDCl₃)

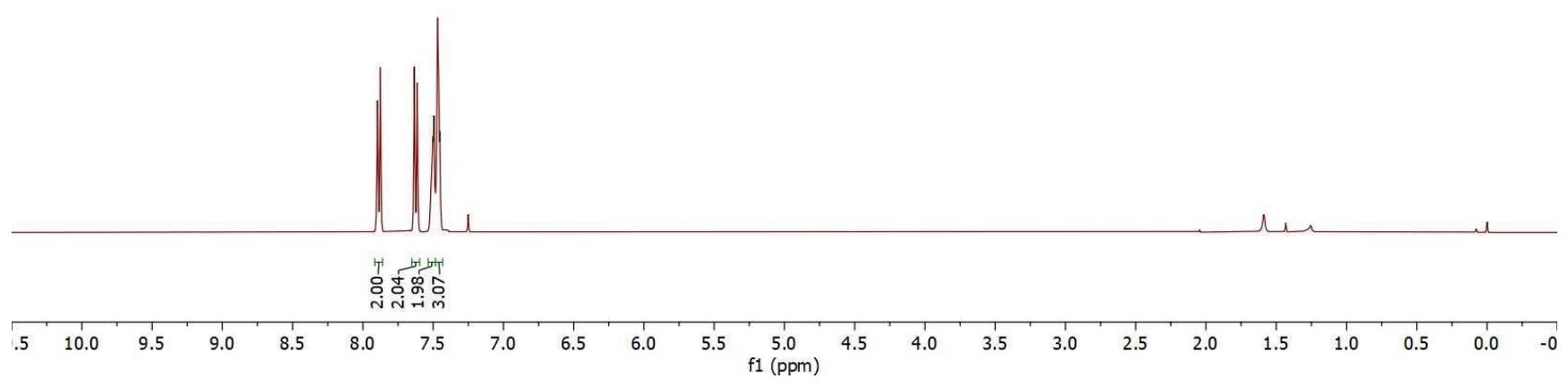


7.897
7.876
7.634
7.613
7.519
7.515
7.511
7.508
7.505
7.501
7.494
7.491
7.485
7.478
7.470
7.466
7.462
7.458
7.453
7.448
7.250

-0.000



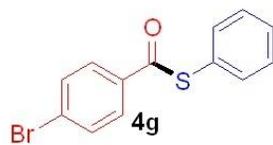
(¹H NMR, 400 MHz, CDCl₃)



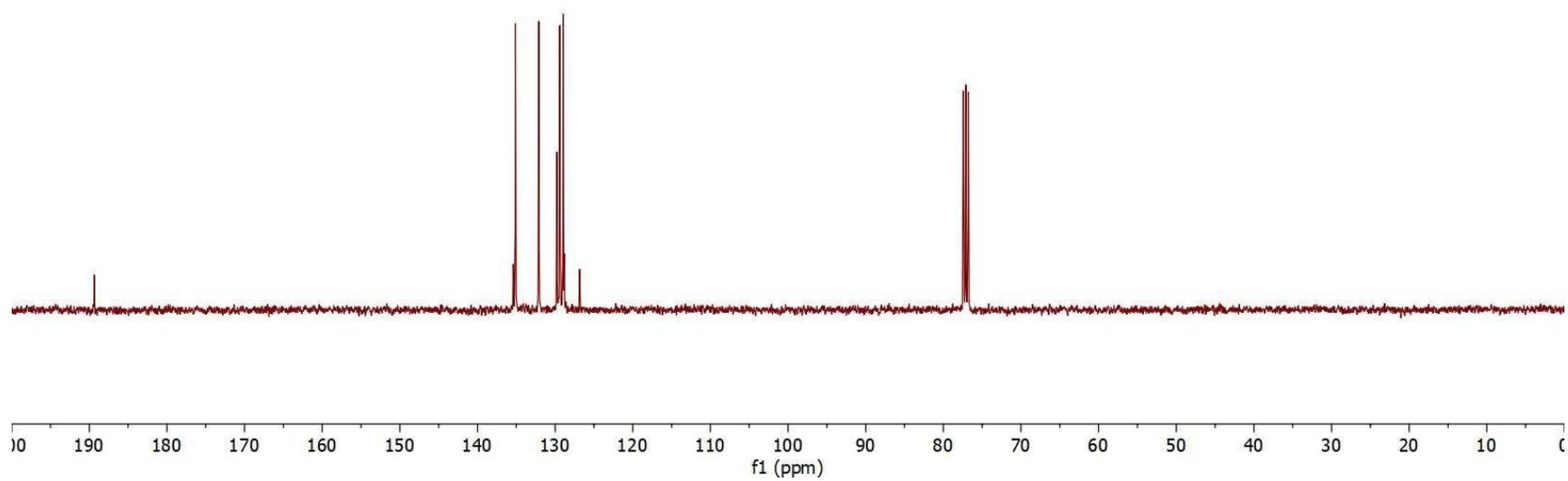
—189.36

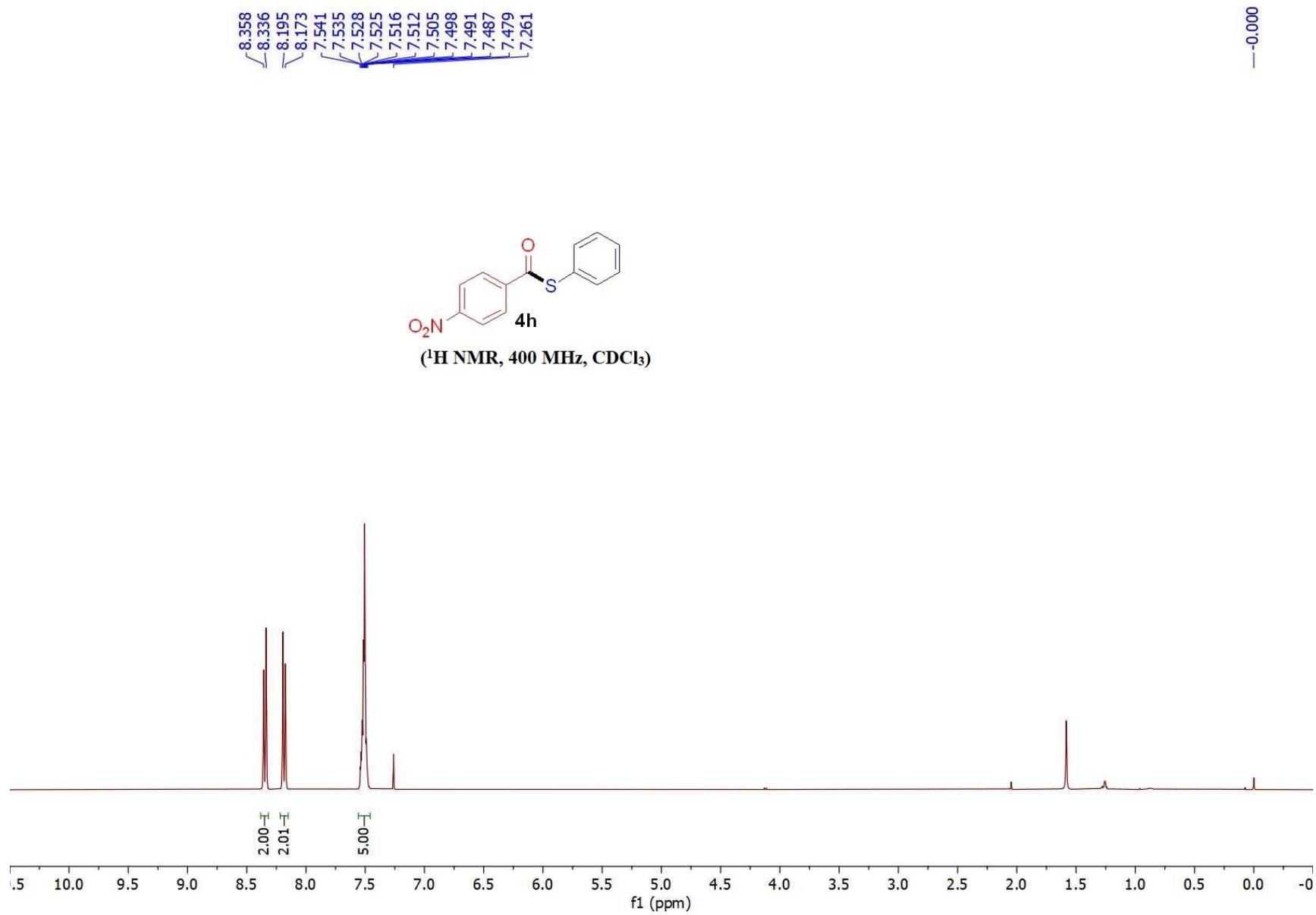
135.39
135.11
132.11
129.79
129.40
128.97
128.82
126.86

77.42
77.10
76.78



(¹³C{H} NMR, 100 MHz, CDCl₃)





—188.97

—150.72

—141.33

134.99

130.17

129.60

128.57

126.19

124.10

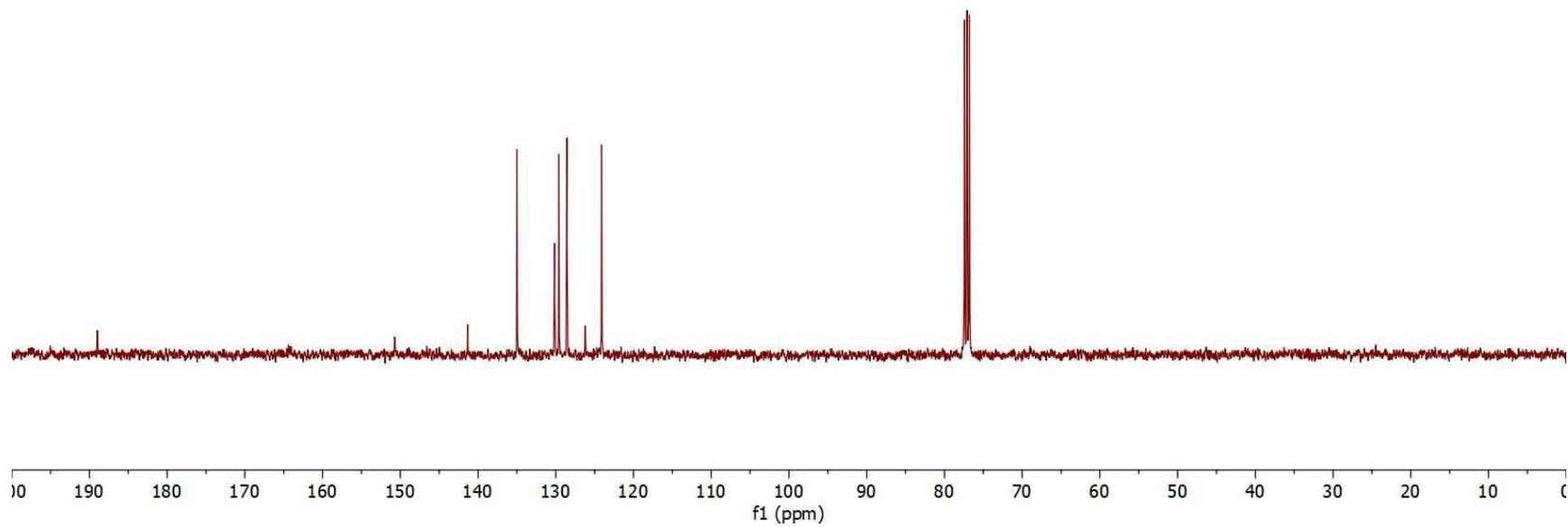
77.42

77.10

76.78

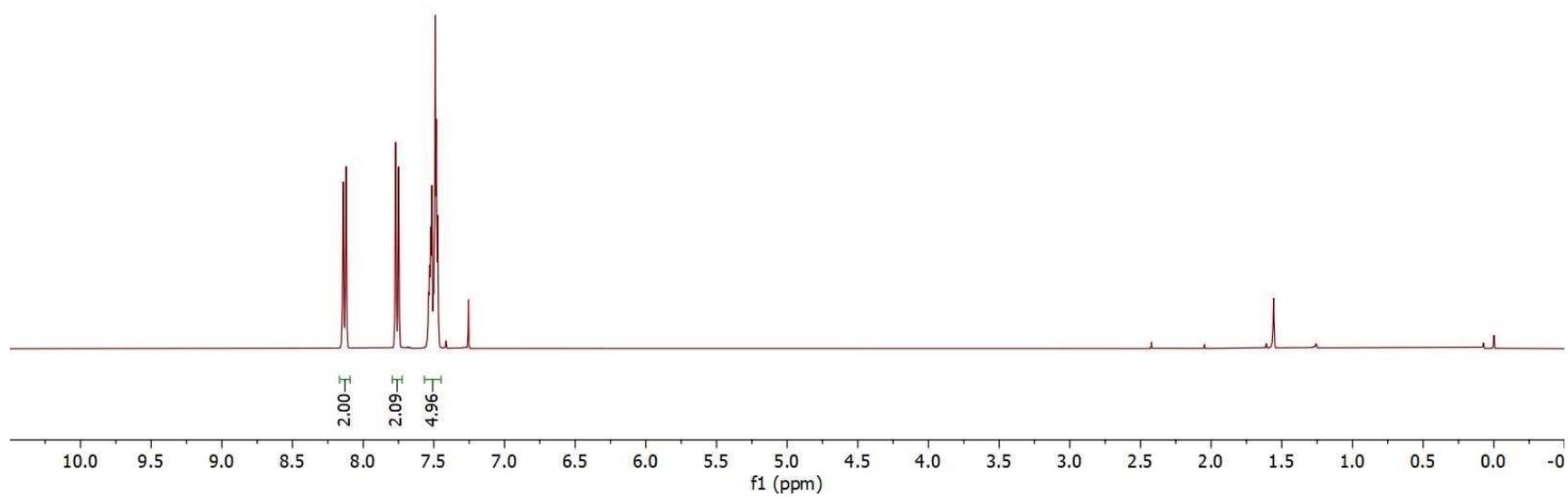


(¹³C{¹H} NMR, 100 MHz, CDCl₃)



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



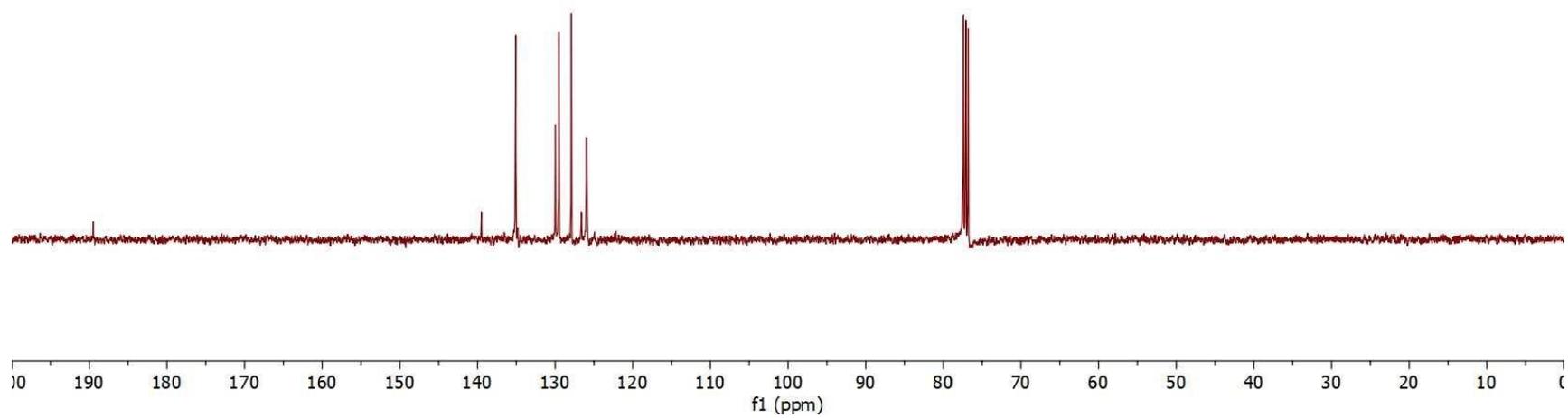
—189.50

139.49
135.34
135.15
135.08
134.83
134.50
129.97
129.51
127.90
126.78
126.61
125.95
125.91
124.92
122.21

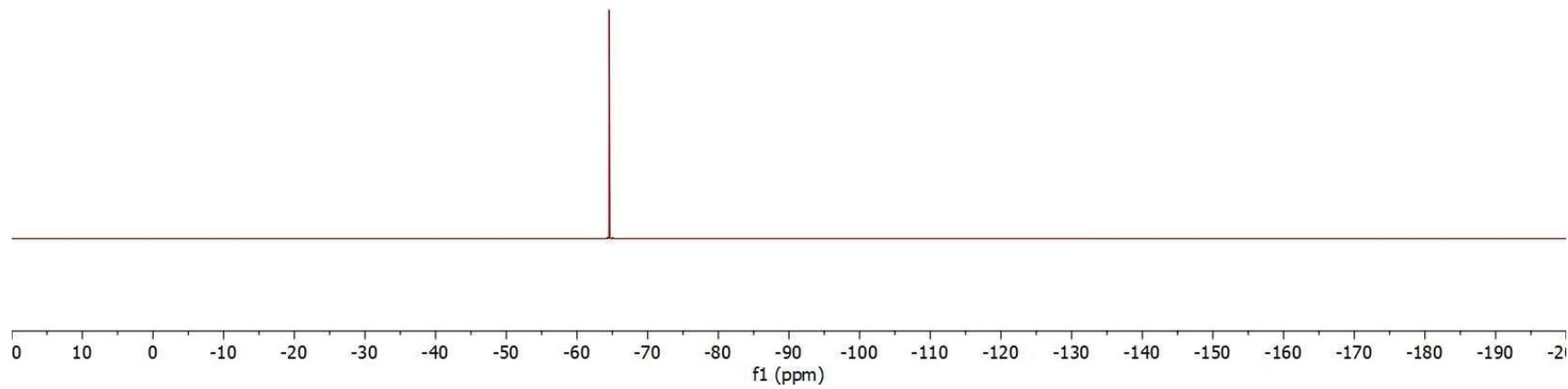
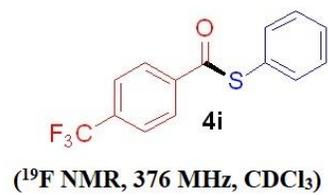
77.42
77.10
76.78

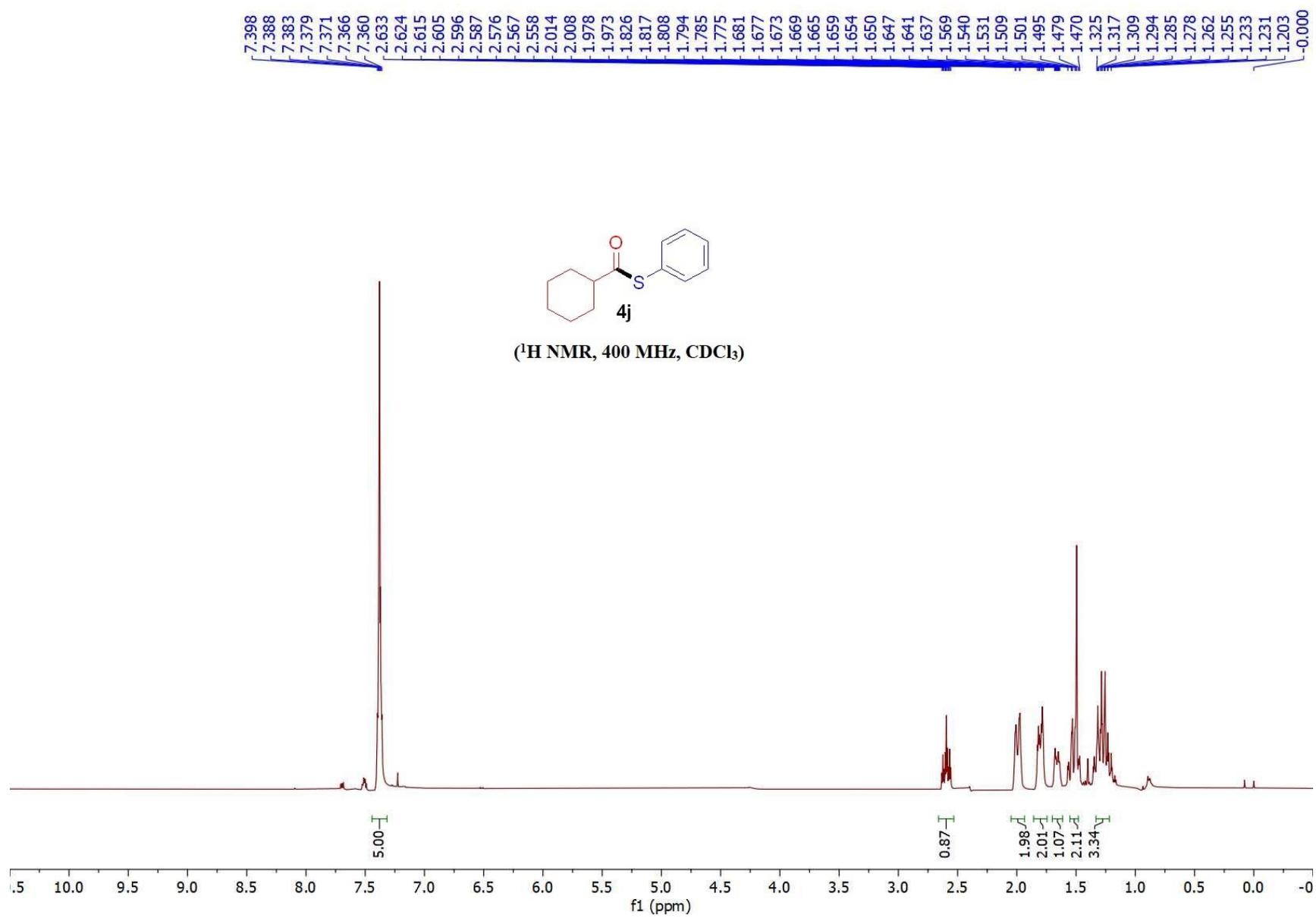


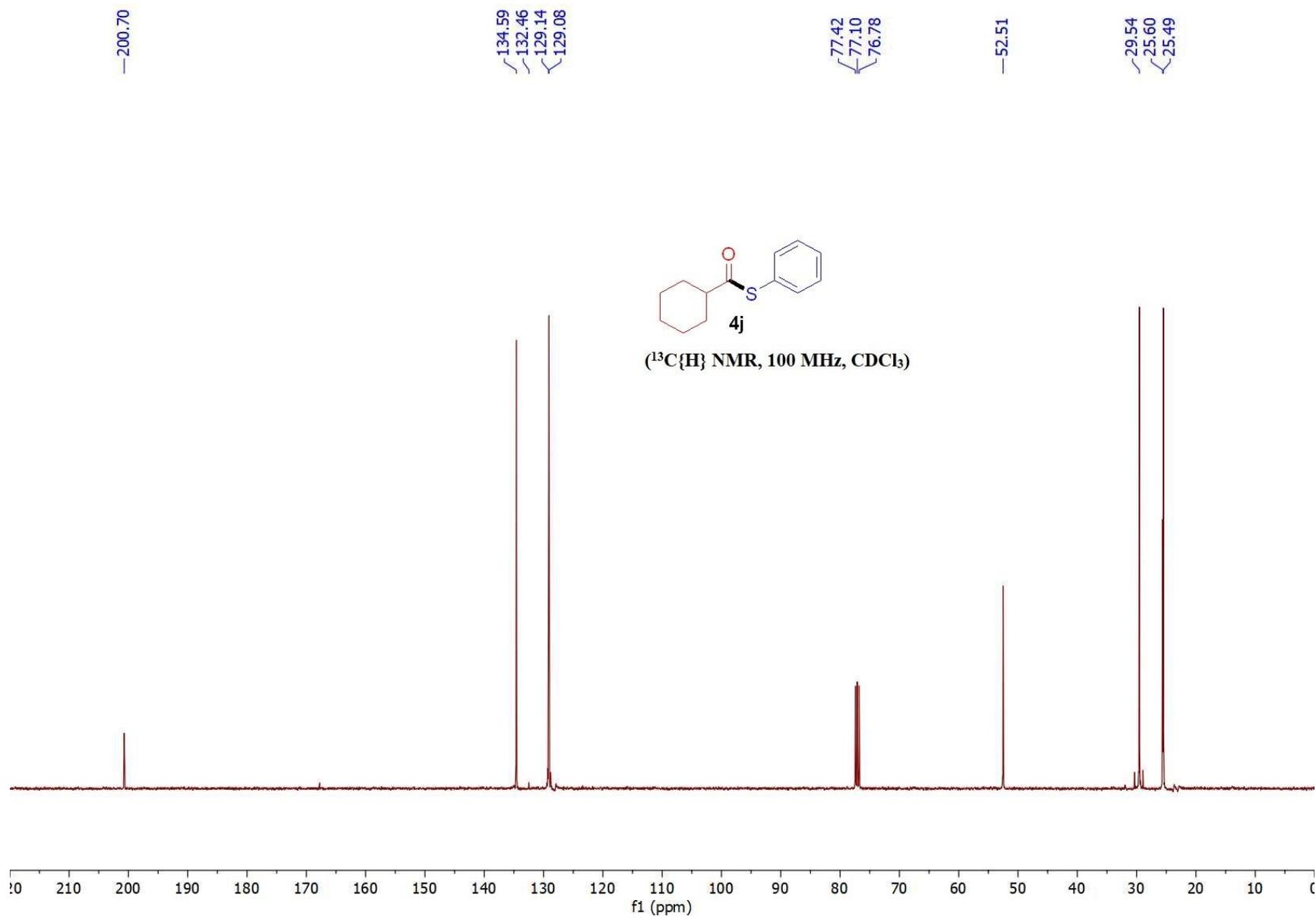
(¹³C{H} NMR, 100 MHz, CDCl₃)

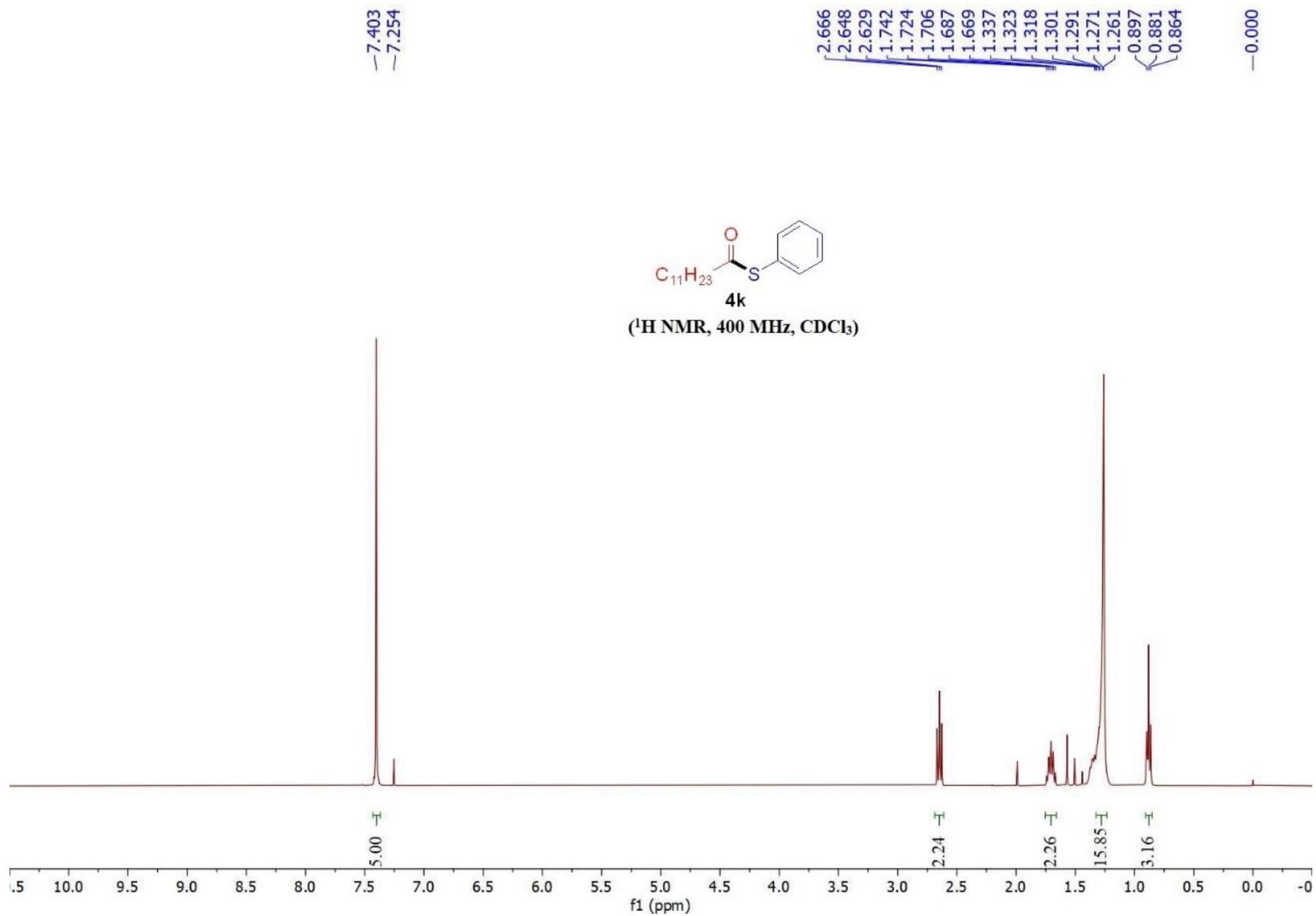


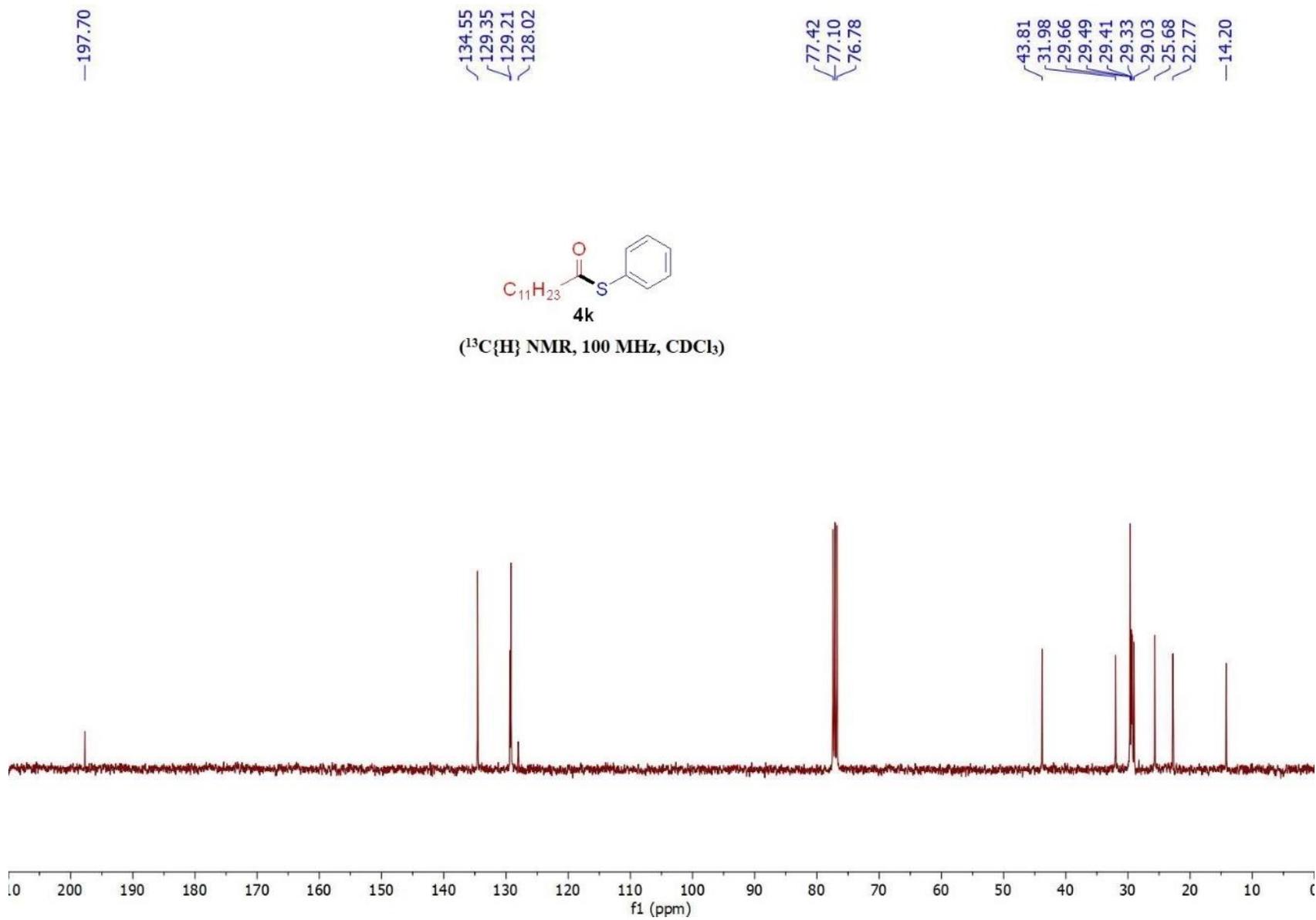
—64.561









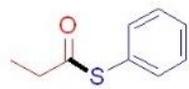


7.423
7.421
7.415
7.413
7.408
7.405
7.402
7.401
7.399
7.398
7.396
7.391
7.384
7.382
7.242

2.705
2.686
2.667
2.649

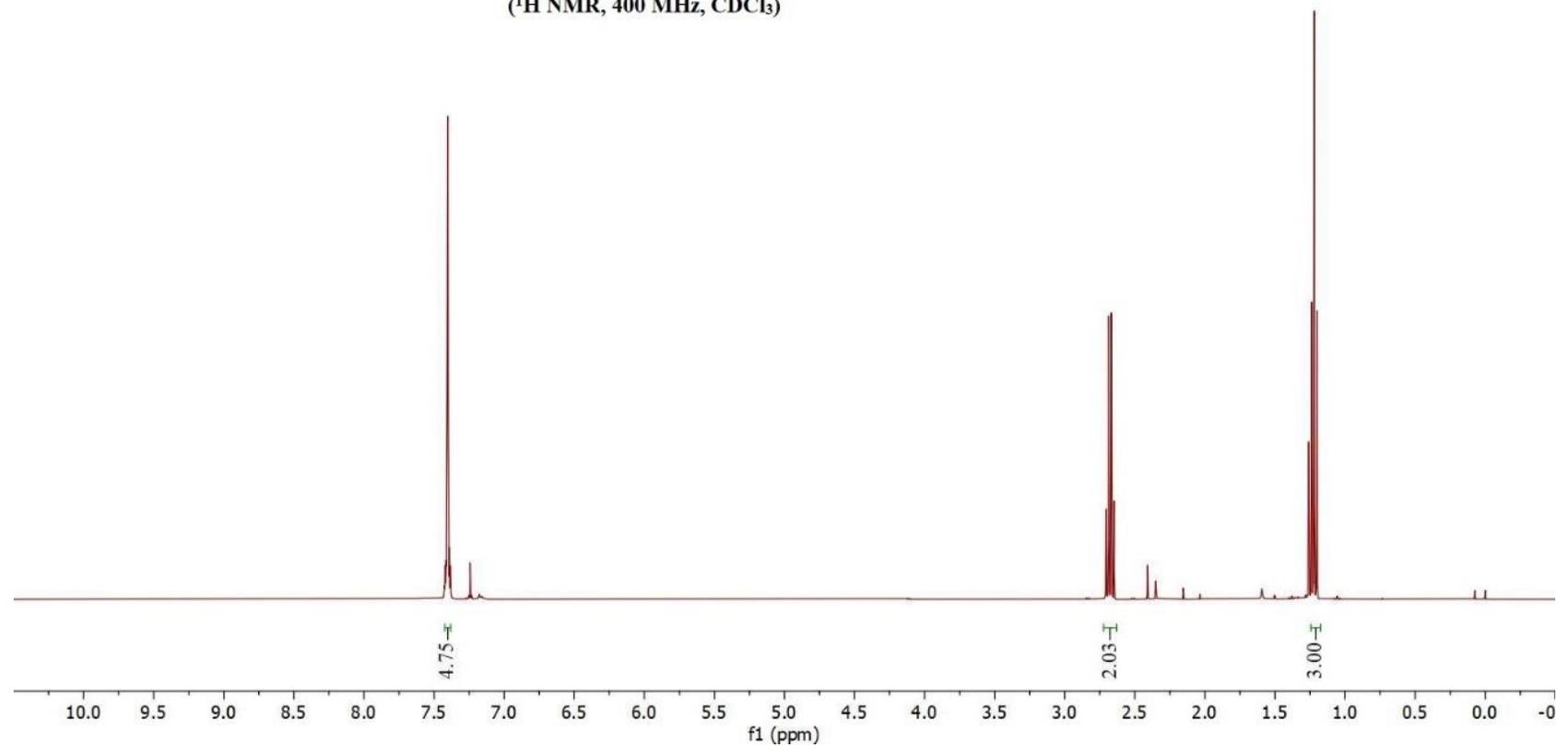
1.239
1.220
1.201

-0.000



4i

(¹H NMR, 400 MHz, CDCl₃)



—198.34

134.58
129.35
129.20
127.85

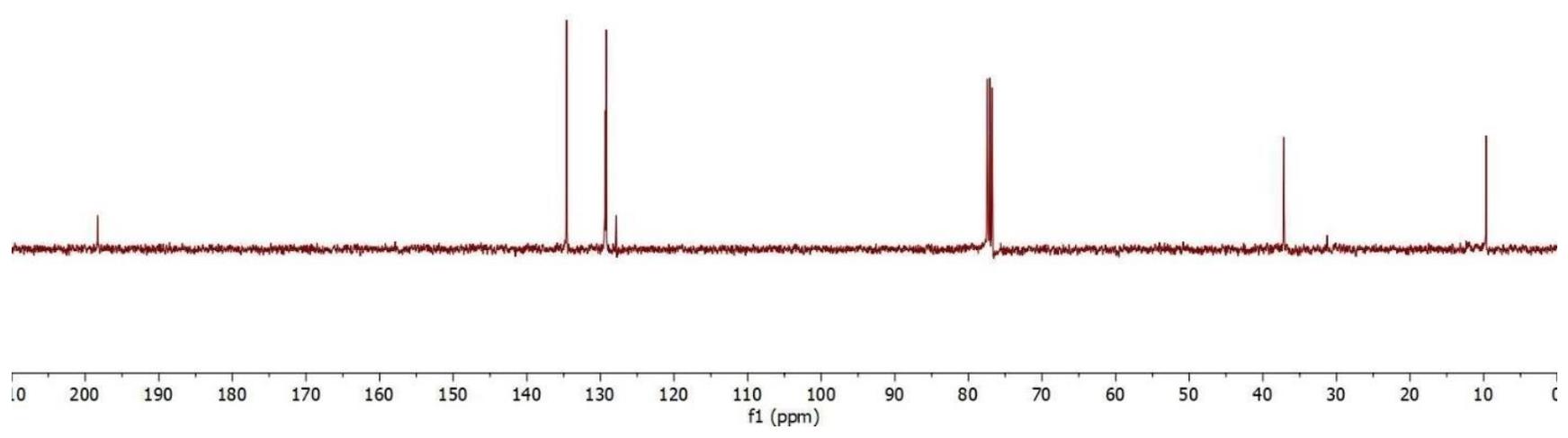
77.42
77.10
76.78

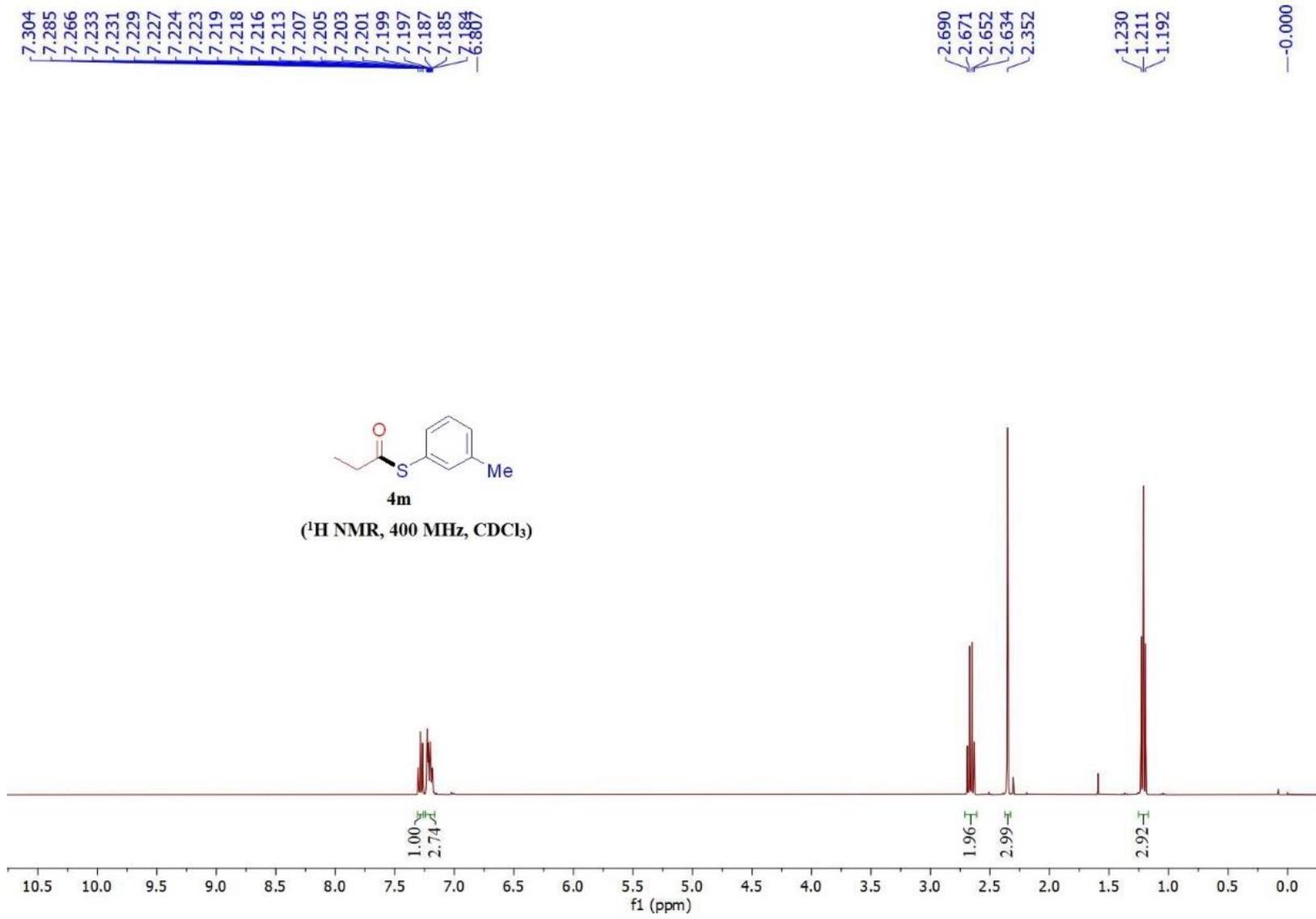
—37.15

—9.66



(¹³C{¹H} NMR, 100 MHz, CDCl₃)





—198.55

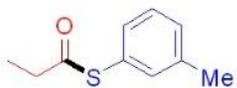
139.02
135.12
131.58
130.21
129.00
127.45

77.42
77.10
76.78

—37.09

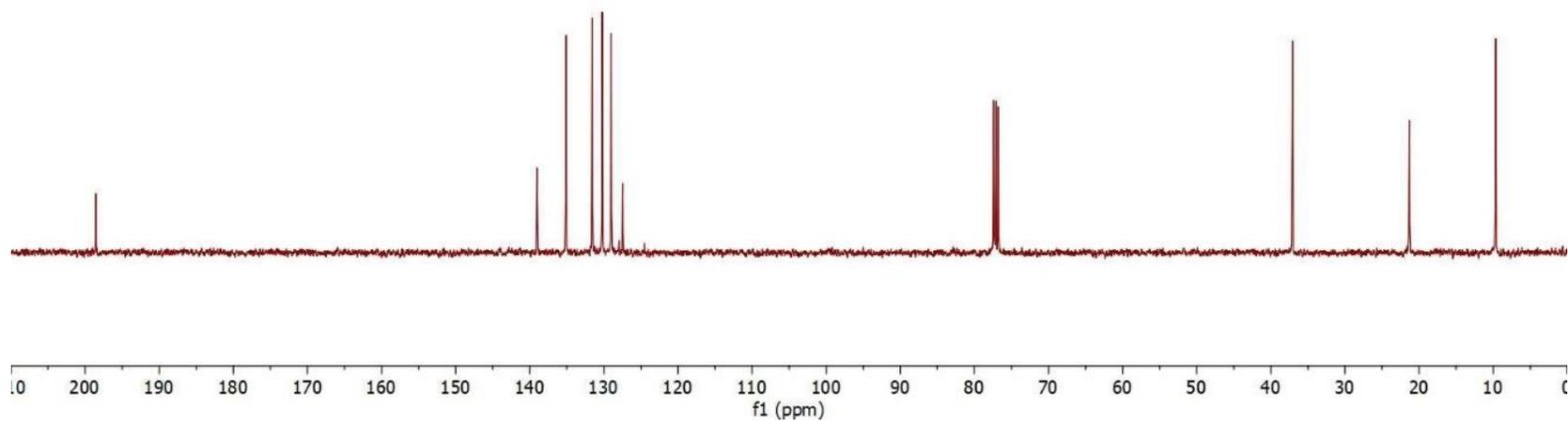
—21.29

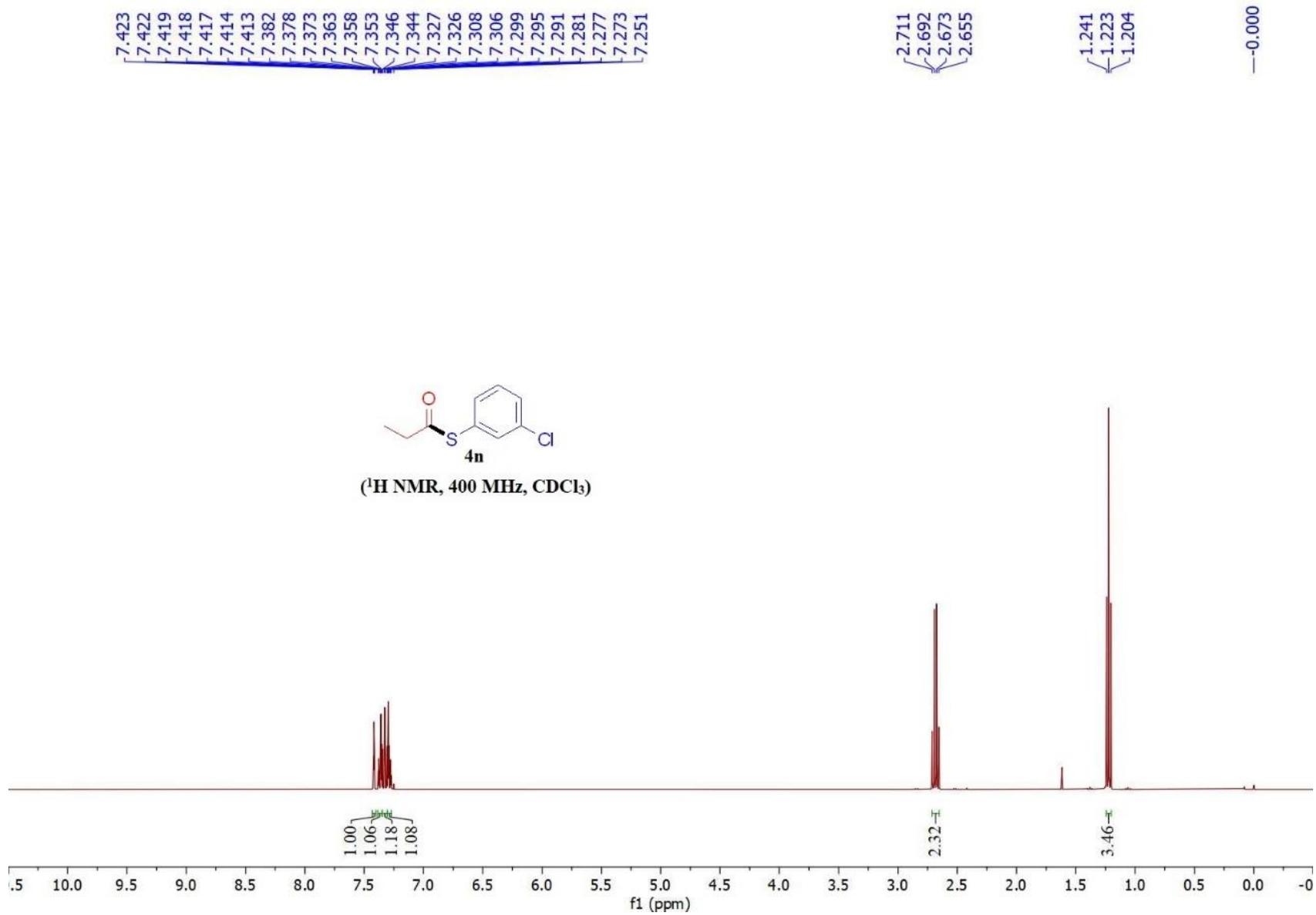
—9.65

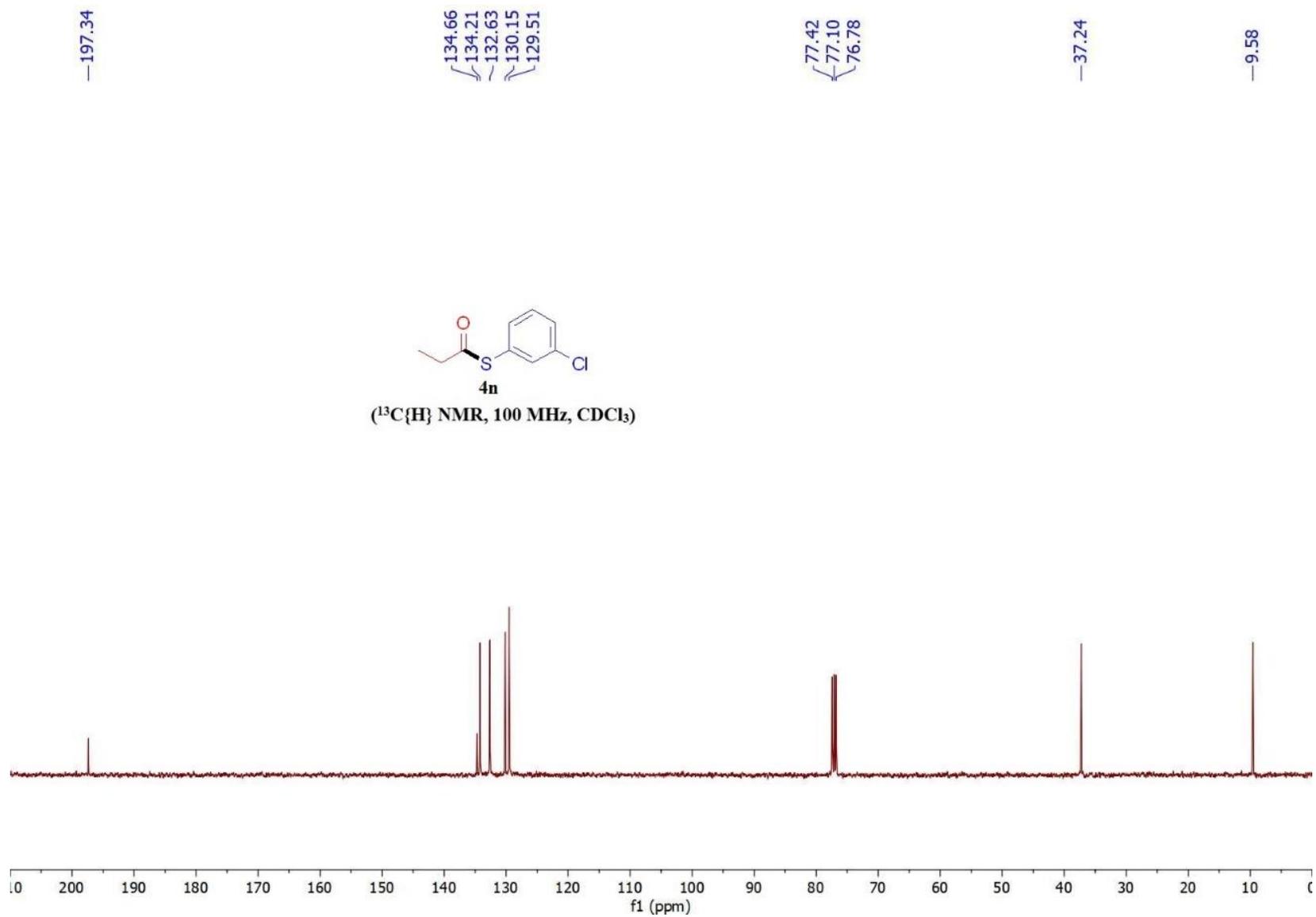


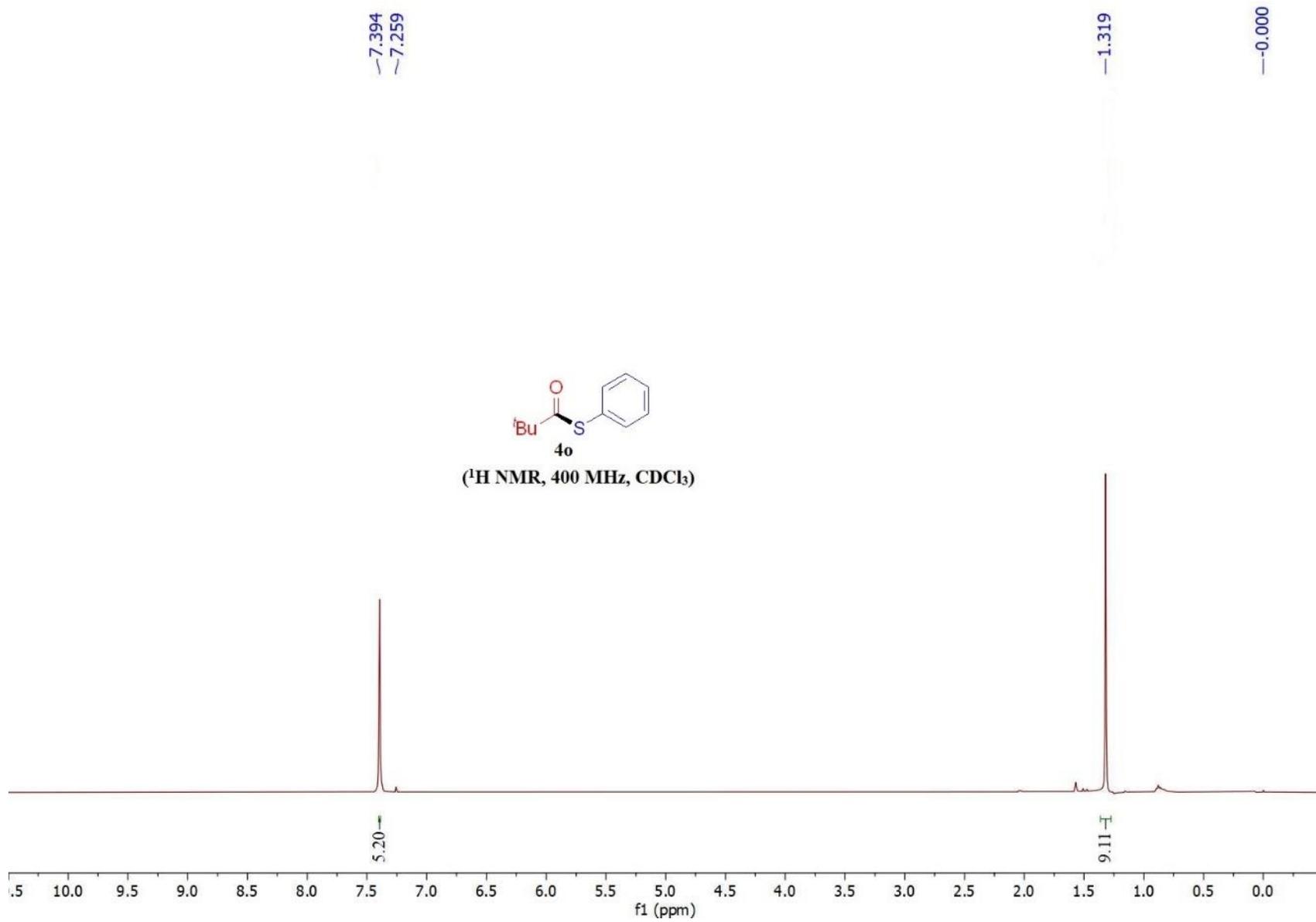
4m

(¹³C{H} NMR, 100 MHz, CDCl₃)









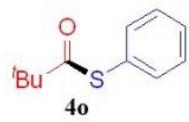
—204.82

135.05
129.19
129.15
128.14

77.42
77.10
76.78

—47.01

—27.48



(¹H NMR, 400 MHz, CDCl₃)

