

Supporting information

Catalyst-Free Synthesis of Phenanthridines *via* Electrochemical Coupling of 2-Isocyanobiphenyls and Amines

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1. Experimental Setup



2. Cyclic Voltammetry studies of **3** and **5**

General Procedure for Cyclic Voltammetry (CV): Cyclic Voltammetry studies were carried out using IKA ElectraSyn 2.0 Pro with three electrode cell connected to a nitrogen balloon at room temperature. The working electrode was glassy carbon electrode, the counter electrode was a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous 3M KCl solution, and separated from reaction by a salt bridge. The scan rate is 0.1 V/s, ranging from -2.36 V to 1.6 V and the peak potential were measured vs. Ag/AgCl. The cyclic voltammetry (CV) experiments were carried out to study the redox potential of the substrate. All the experiment data taken 10 min after stirring. According to the CV data, we have confirmed the *in-situ* generation of diazonium salt see in details Fig S1 and S2. In Figure S1 and Figure S2 curve had cathodic reduction of **1a**, in fig S1 peak was observed at -0.26 V in nBu₄NBF₄ (0.05M) as an electrolyte in CH₃CN/H₂O (10:1), and in fig S2 two peaks was observed at -0.34 V and -1.92 V in nBu₄NBF₄ (0.05M) as a electrolyte in CH₃CN. In fig. S2 curve of **1a** gave two reduction peaks, corresponded to the reduction of aryl diazonium to aryl radicals and possibly further to aryl anion, respectively. In fig. S3, the anodic oxidation peak of nBu₄NBF₄ (0.05M) was observed at 0.77 V in CH₃CN (curve **a**). In fig. S4, the CV of the mixture of **1a** and **2a** substrate with nBu₄NBF₄, **1a** and **2a** had two oxidation peaks at 0.83 and 1.08 V (curve **b**). Interestingly, we found that the same voltage peaks but promoted oxidation was observed (curve **c**) when HFIP was used as co-solvent with CH₃CN.

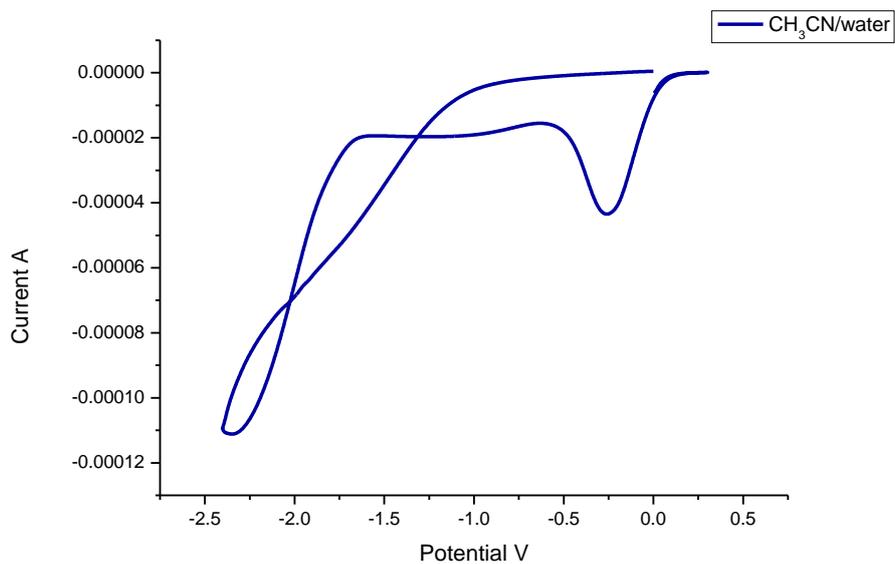


Figure S1. Cyclic voltammograms of CH₃CN/H₂O (10:1) as solution, using glassy carbon electrode as working electrode, a Pt wire as counter electrode, and Ag/AgCl as a reference electrode, scan rate of 0.1 V/s: (a) **1a**(0.01M) + *i*-AmONO (0.01M) + nBu₄NBF₄ (0.05M).

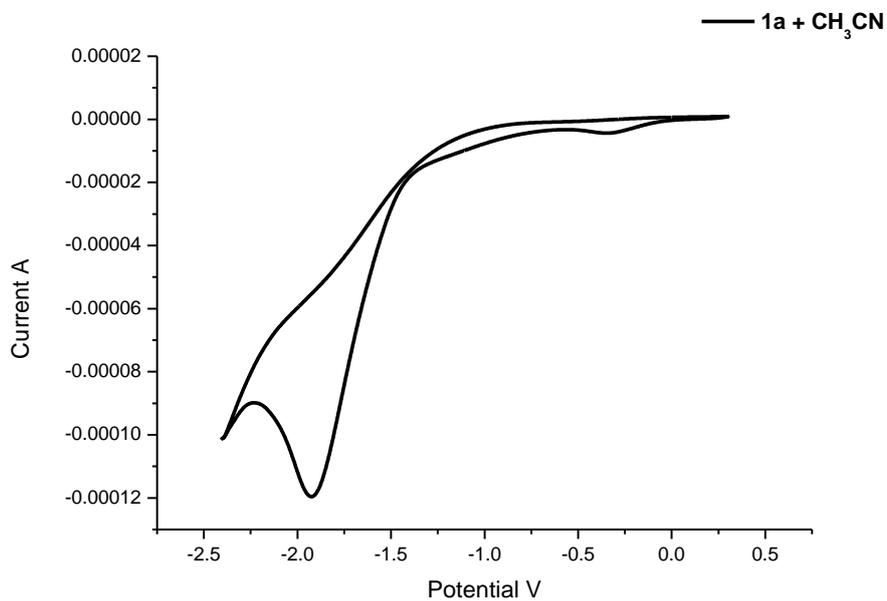


Figure S2. Cyclic voltammograms of CH₃CN as solution, using glassy carbon electrode as working electrode, a Pt wire as counter electrode, and Ag/AgCl as a reference electrode, scan rate of 0.1 V/s: (a) **1a**(0.01M) + *i*-AmONO(0.01M) + nBu₄NBF₄ (0.05M).

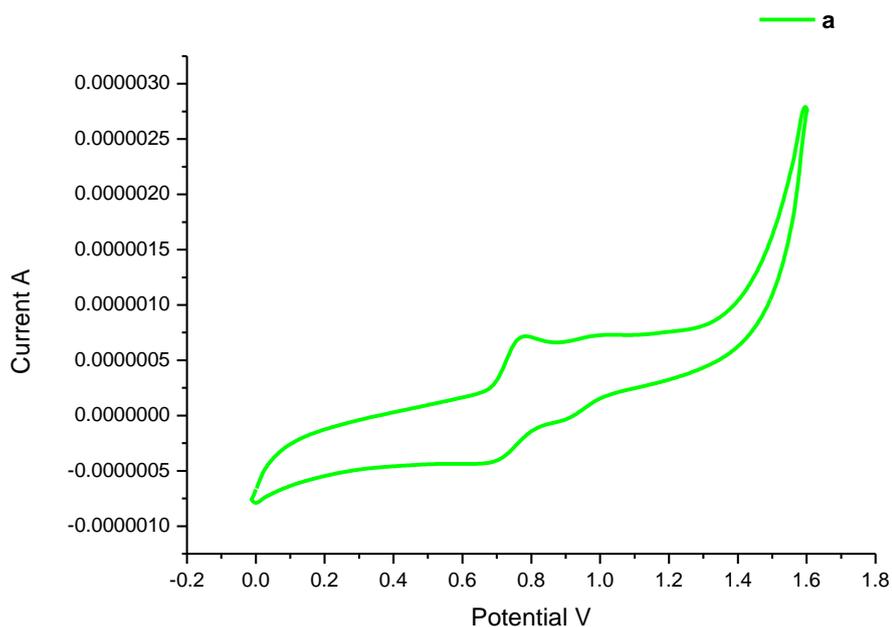


Figure S3. Cyclic voltammograms of CH_3CN as solution, using glassy carbon electrode as working electrode, a Pt wire as counter electrode, and Ag/AgCl as a reference electrode, scan rate of 0.1 V/s: (a) nBu_4NBF_4 (0.05M).

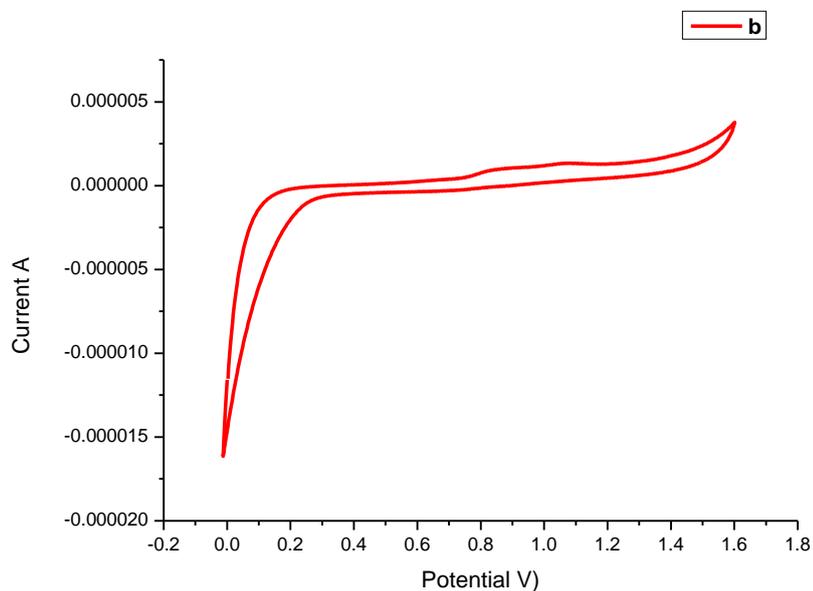


Figure S4. Cyclic voltammograms of CH_3CN as solution, using glassy carbon electrode as working electrode, a Pt wire as counter electrode, and Ag/AgCl as a reference electrode, scan rate of 0.1 V/s: (b) **1a** (0.01M) + *i*-AmONO(0.01M) + **2b**(0.01M) + nBu_4NBF_4 (0.05M).

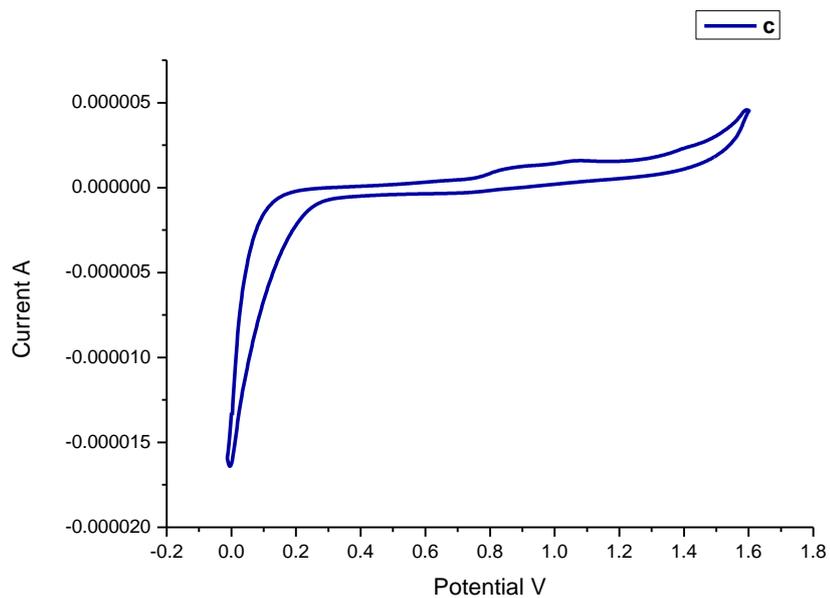
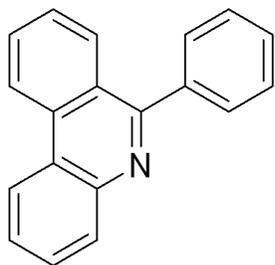


Figure S5. Cyclic voltammograms of CH_3CN as solution, using glassy carbon electrode as working electrode, a Pt wire as counter electrode, and Ag/AgCl as a reference electrode, scan rate of 0.1 V/s: (c) **1a** (0.01 M) + *i*-AmONO(0.01M) + **2a** (0.01 M) + nBu_4NBF_4 (0.05M) + HFIP (0.005 M)

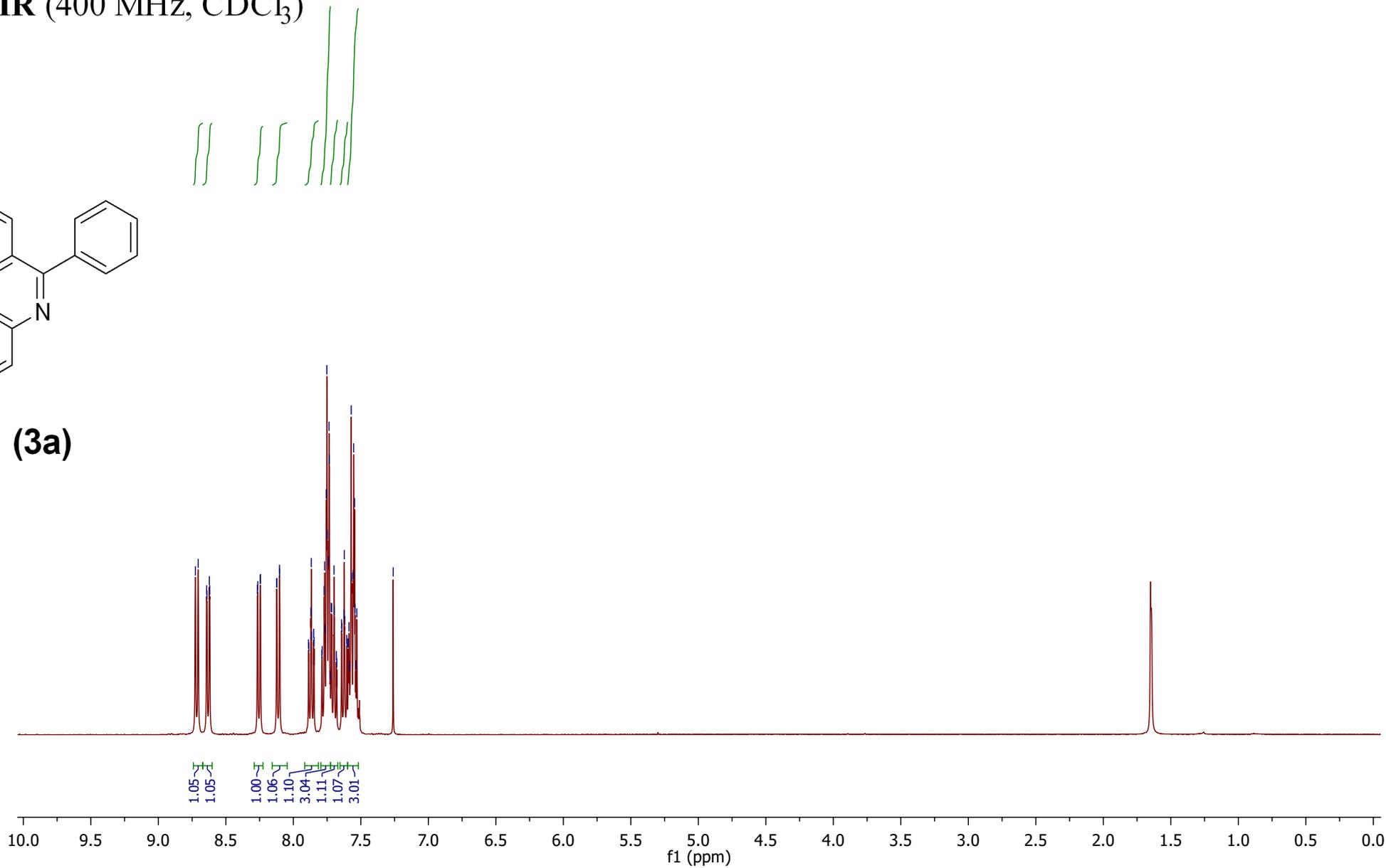
Feb11-2021
sb-101

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8.705
8.643
8.640
8.622
8.619
7.756
7.752
7.748
7.736
7.732
7.622
7.571
7.553
7.546

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



(3a)



Feb11-2021 copy
sb-101

161.27

143.78

139.78

130.55

130.35

129.72

128.91

128.84

128.70

128.43

127.12

126.93

125.24

123.73

122.19

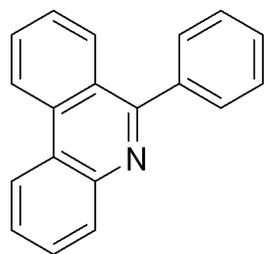
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77.35

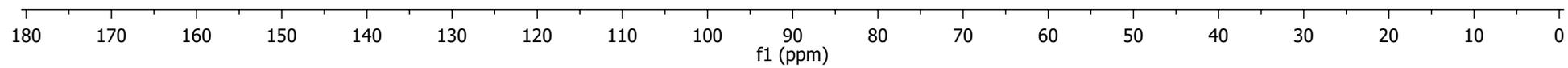
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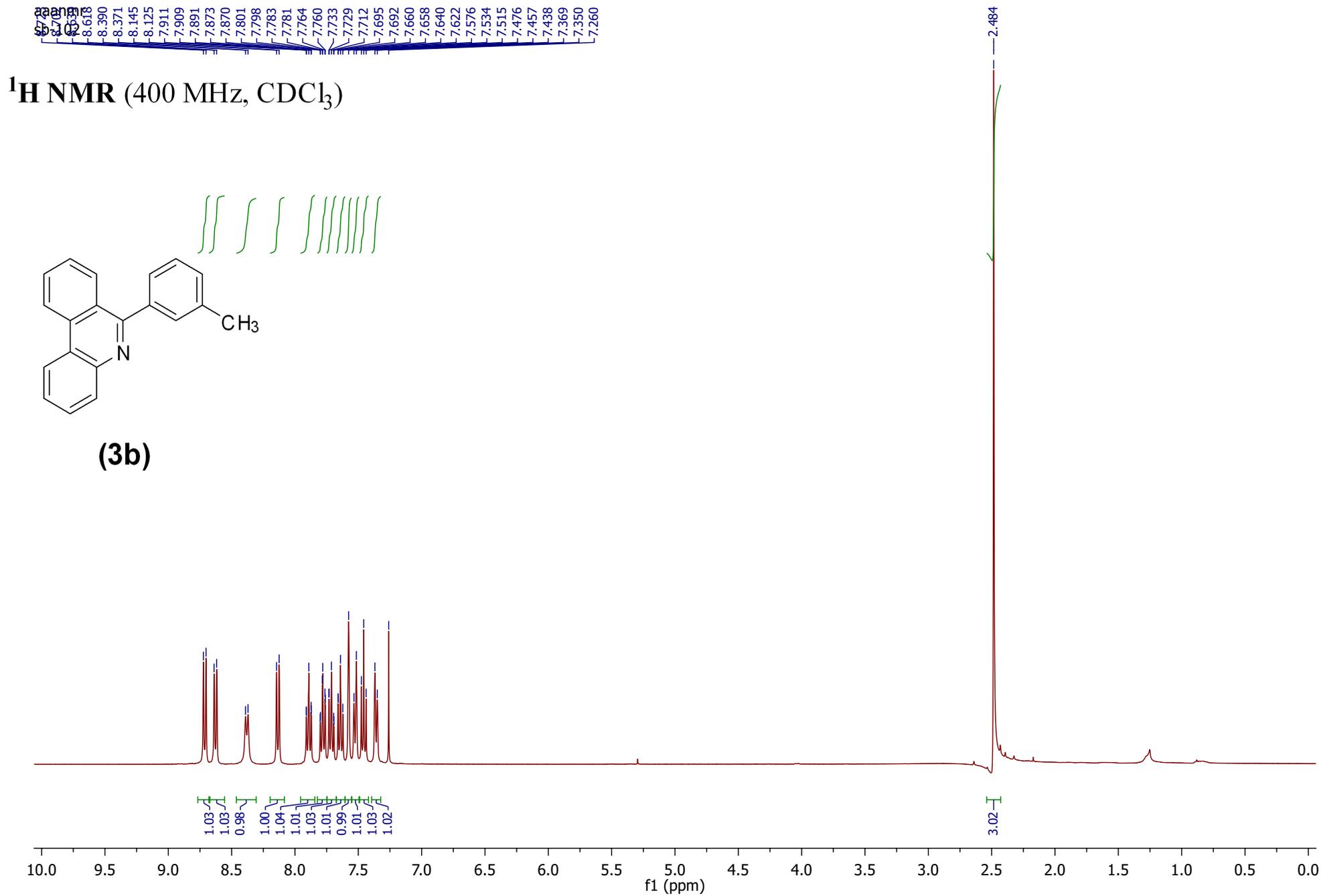
76.71

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



(3a)





aaanmr
sb-102

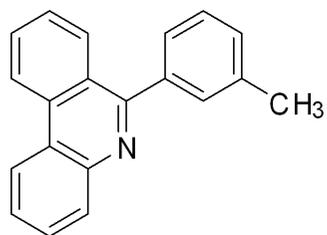
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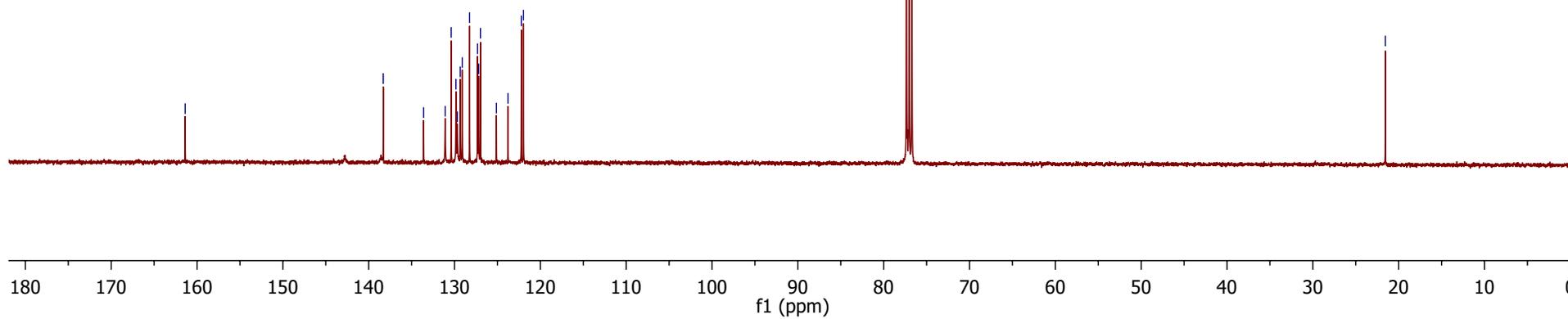
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77.03
76.71

21.55

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



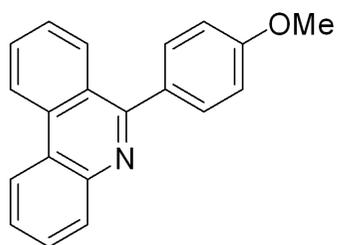
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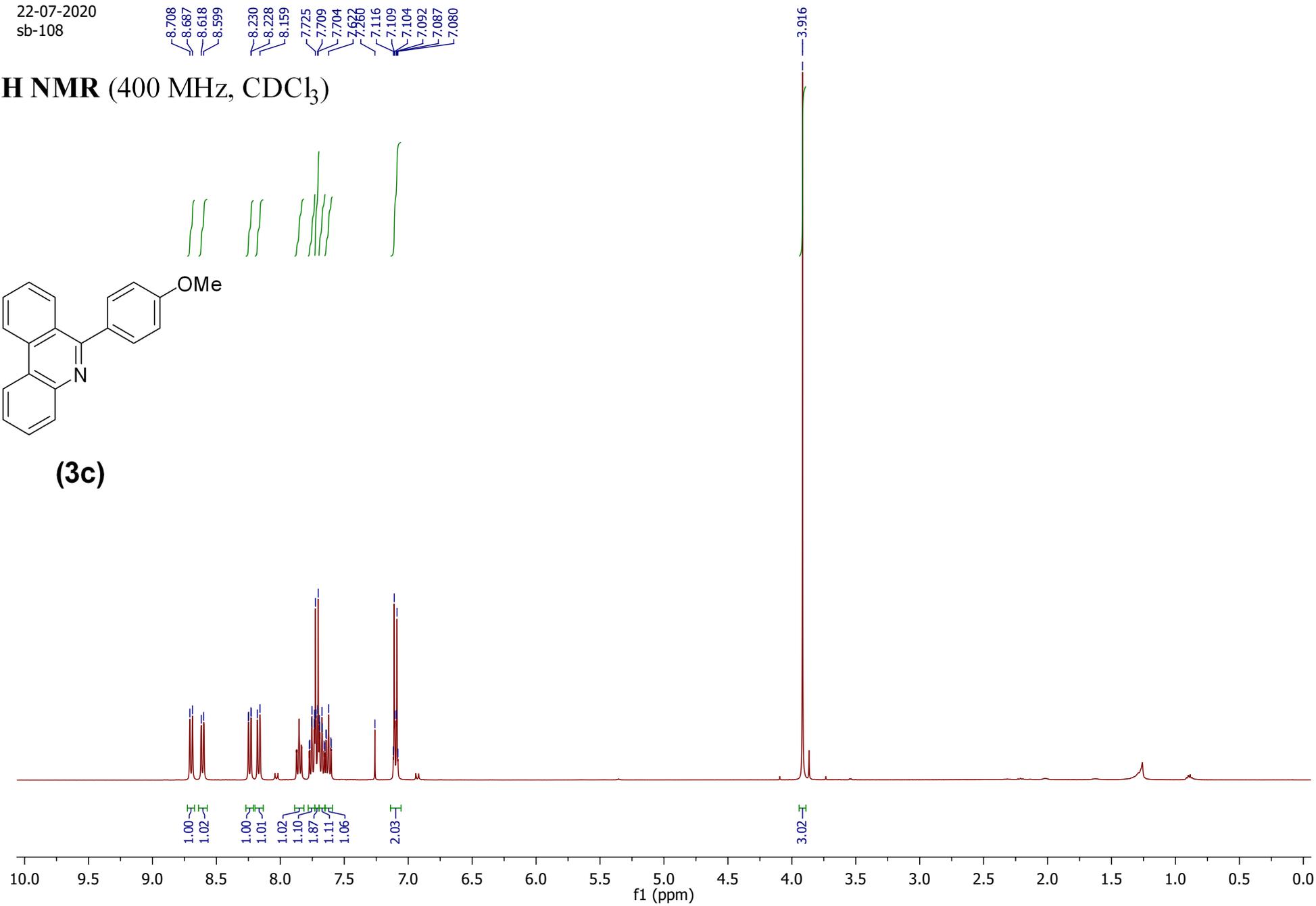
22-07-2020
sb-108

8.708
8.687
8.618
8.599
8.230
8.228
8.159
7.725
7.709
7.704
7.666
7.660
7.116
7.109
7.104
7.092
7.087
7.080

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



(3c)



22-07-2020
sb-108

160.89
160.14

143.86

132.28

131.19

130.47

130.24

128.96

128.80

127.07

126.74

123.63

122.21

113.96

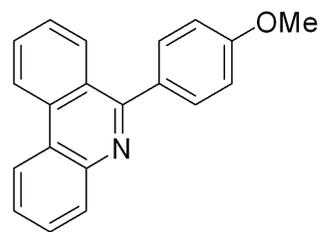
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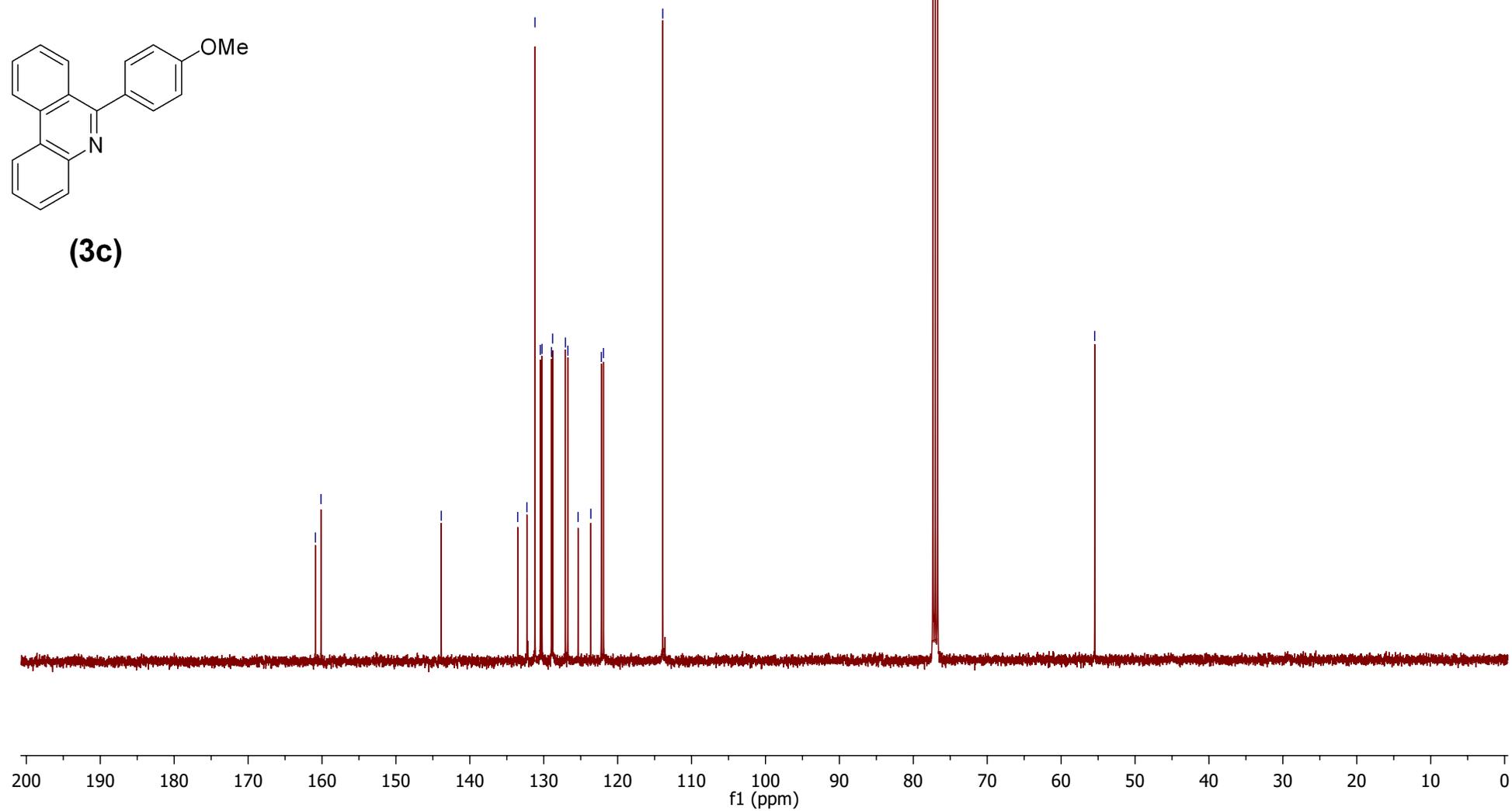
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55.46

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



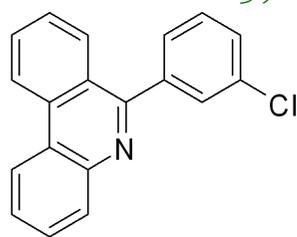
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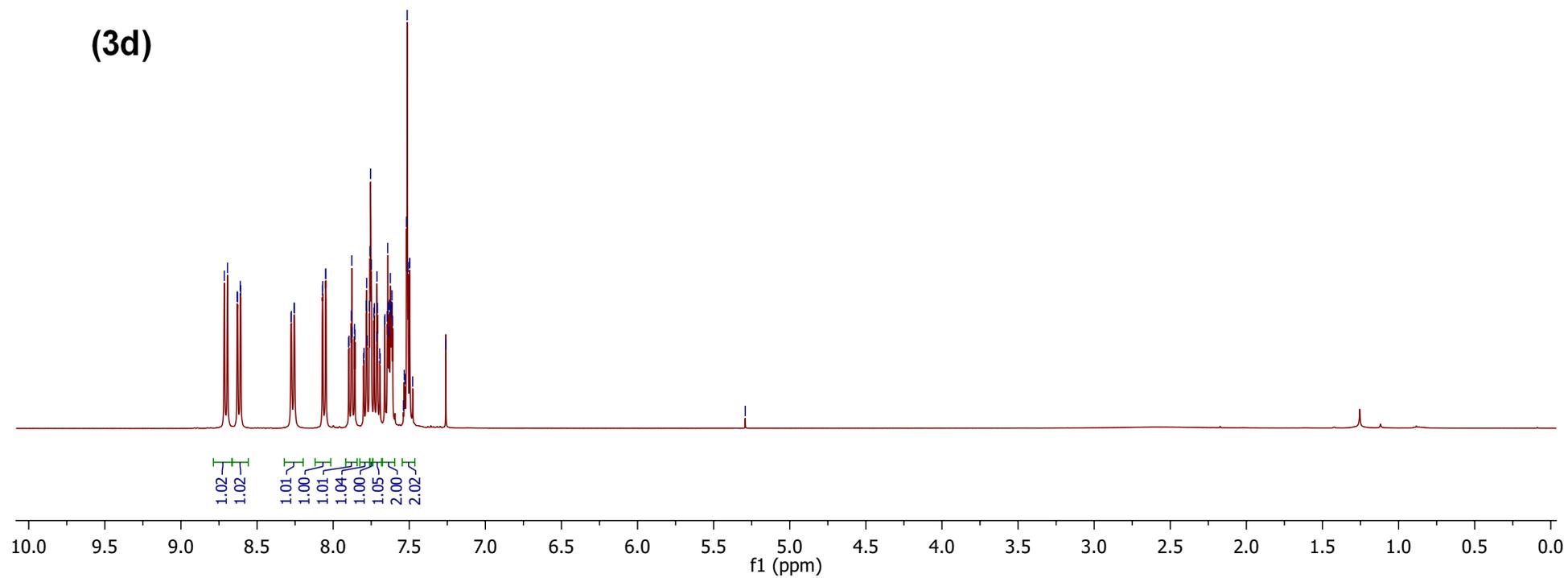
aa
sb-107

8.715
8.694
8.631
8.627
8.610
8.607
8.256
8.070
8.068
8.049
8.048
7.877
7.783
7.780
7.763
7.758
7.754
7.749
7.712
7.709
7.642
7.639
7.630
7.624
7.615
7.613
7.518
7.514
7.508
7.498
7.497

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



(3d)



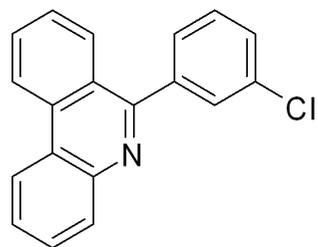
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sb-107

159.63

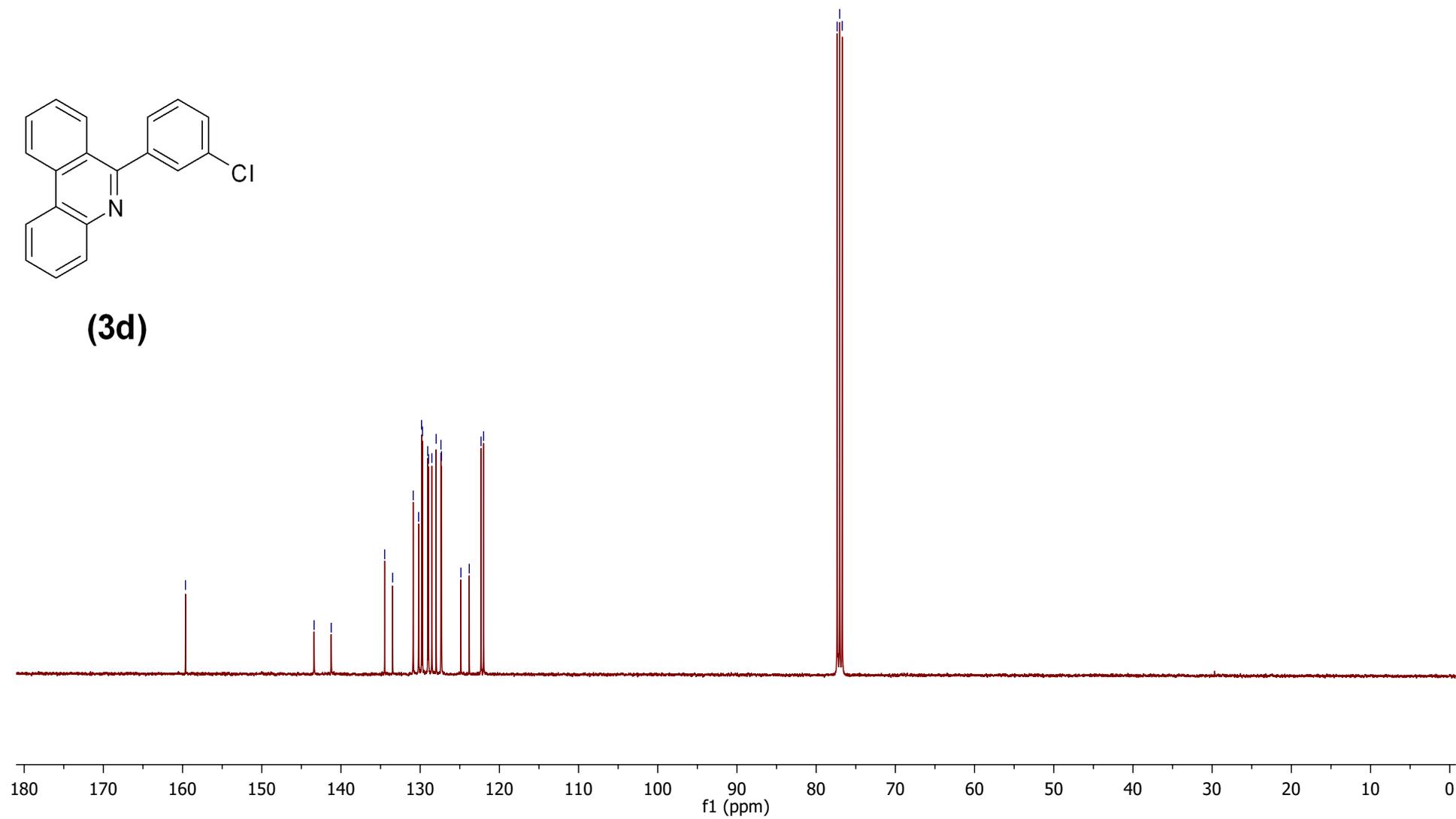
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129.04
128.94
128.52
127.98
127.38
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124.86
123.80
122.32
121.99

77.35
77.03
76.71

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



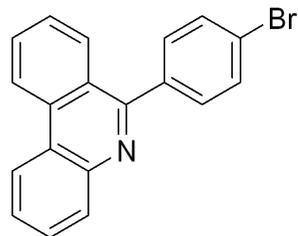
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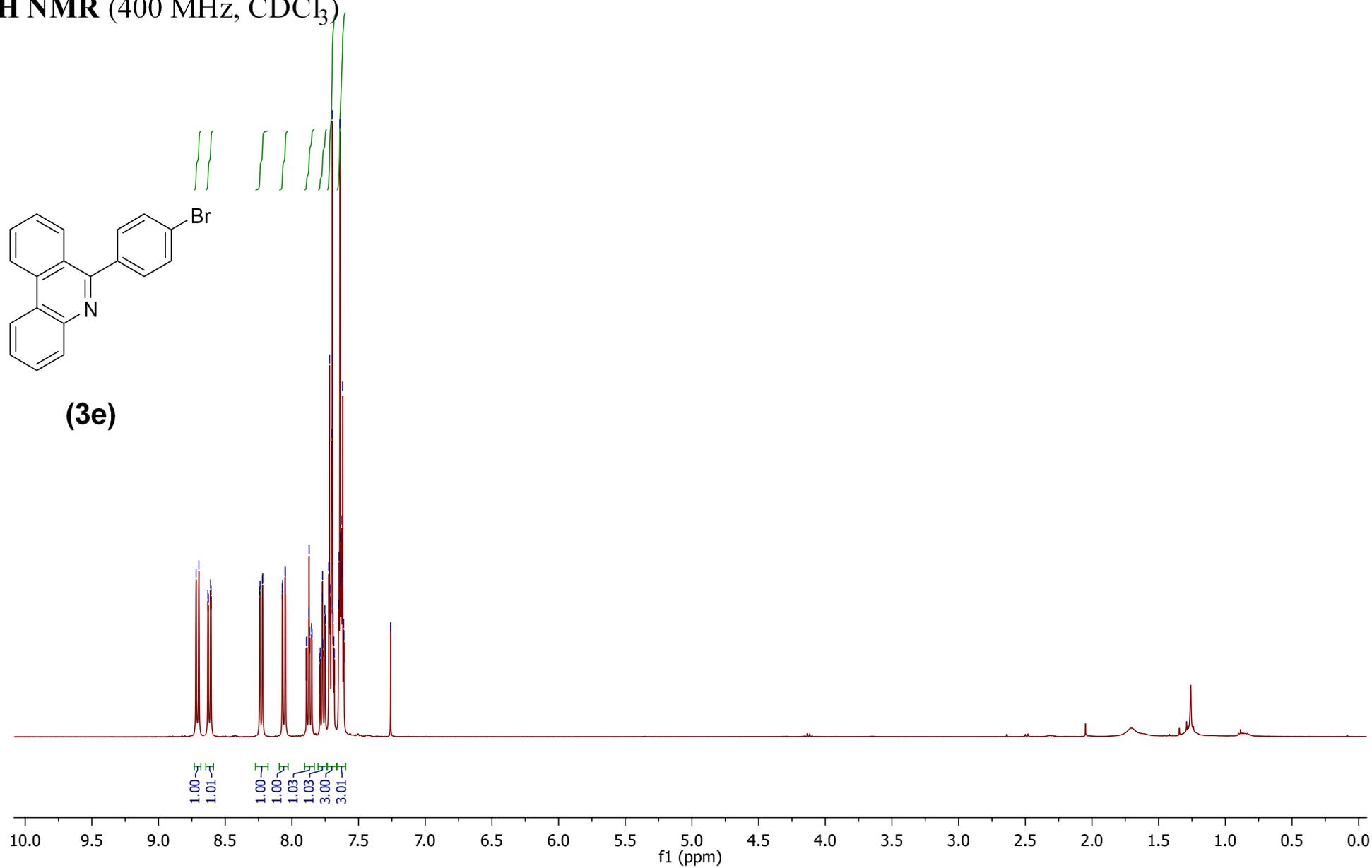
22-07-2020
sb-103

8.719
8.698
8.630
8.627
8.610
8.606
7.870
7.718
7.702
7.697
7.647
7.641
7.636
7.629
7.619

¹H NMR (400 MHz, CDCl₃)

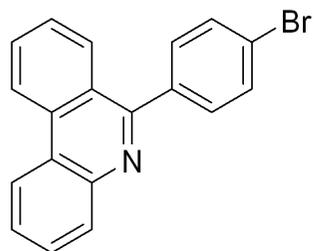


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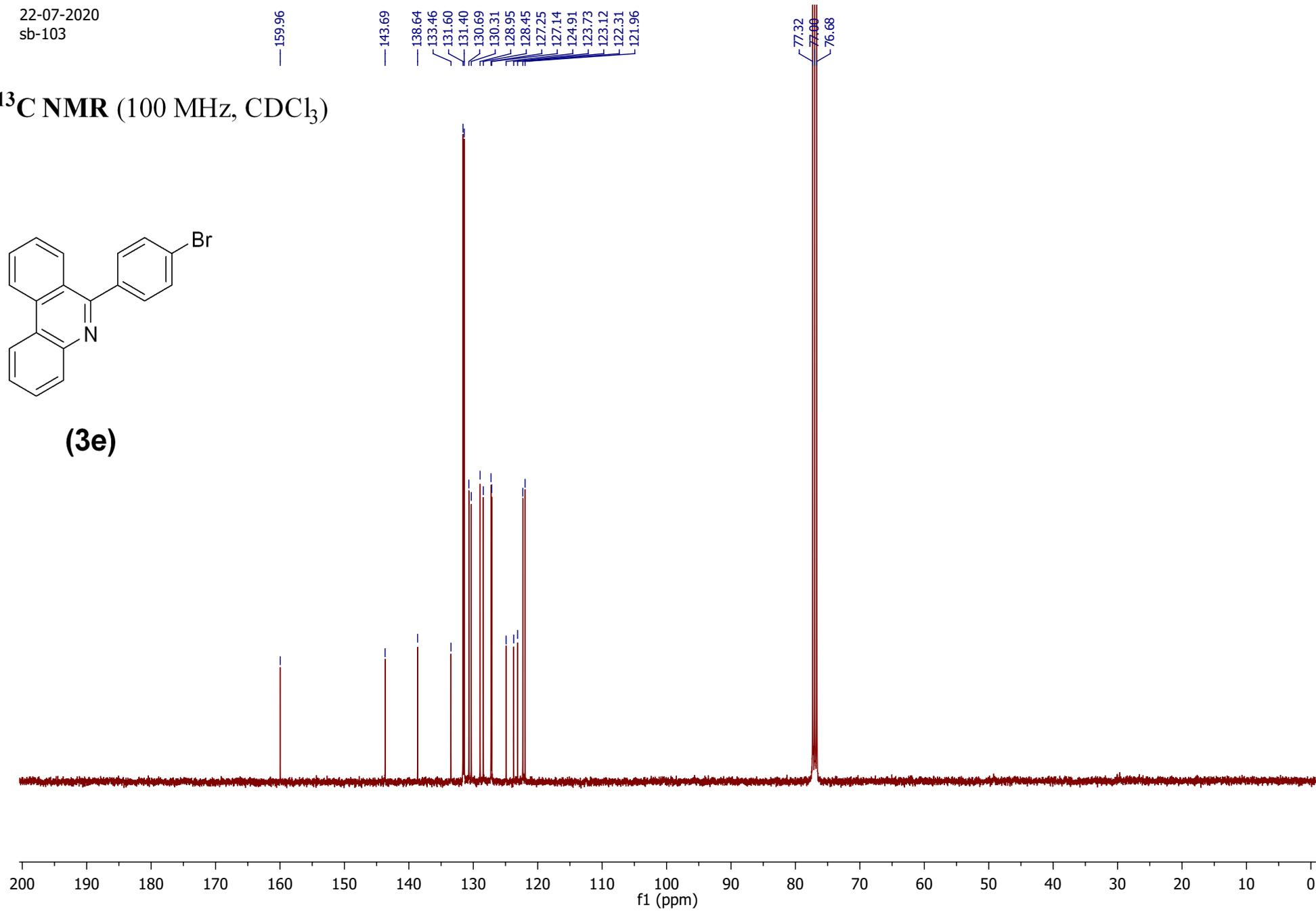


22-07-2020
sb-103

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



(3e)

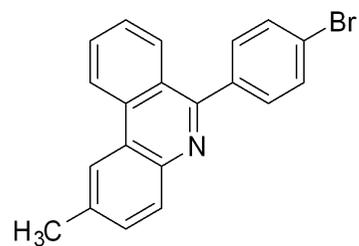


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sb-83

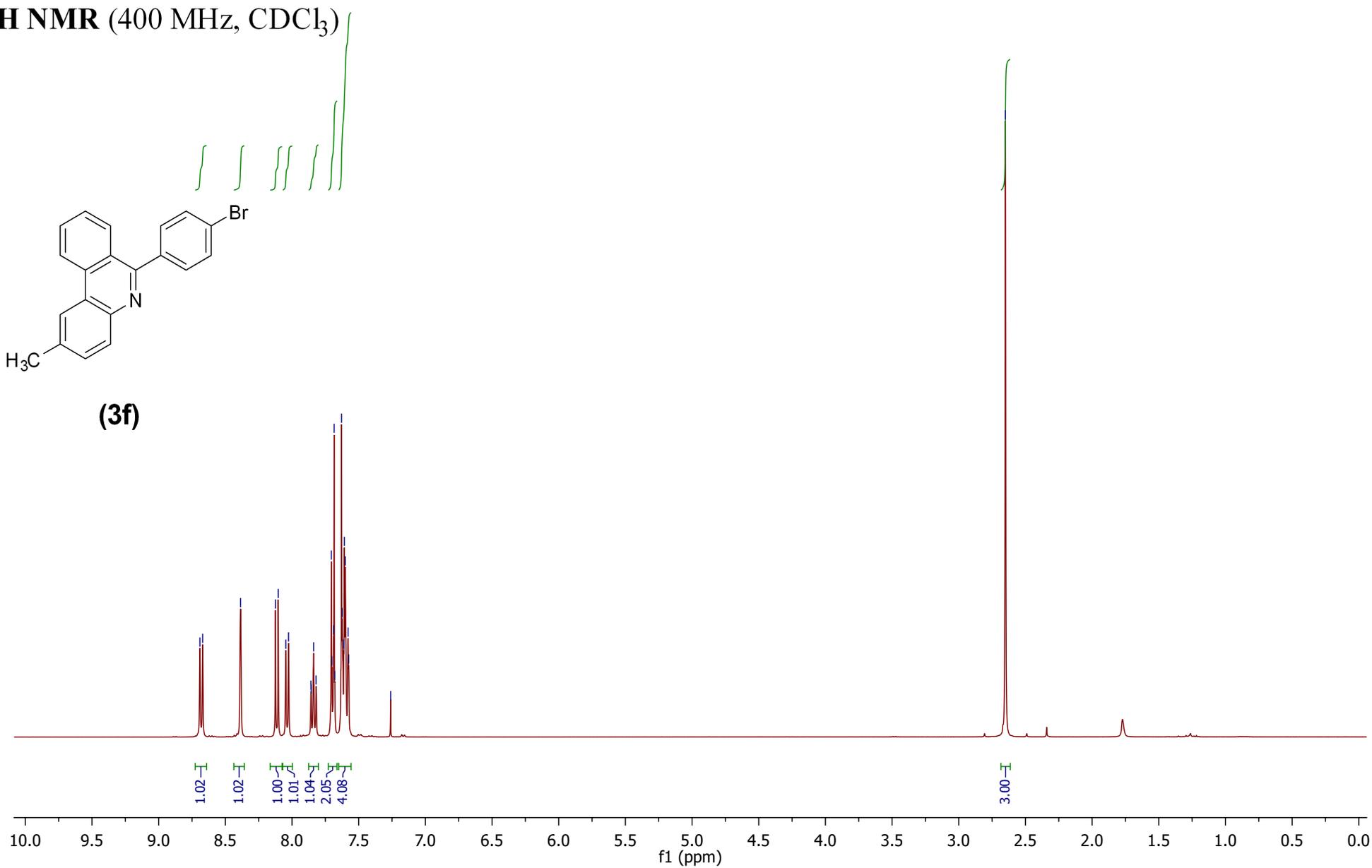
8.691
8.670
8.386
8.124
8.103
7.705
7.684
7.629
7.623
7.607
7.600

2.650

¹H NMR (400 MHz, CDCl₃)



(3f)



Oct26-2020 (1)
sb-83

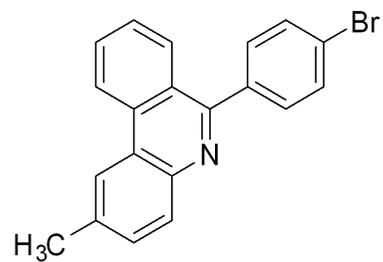
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142.03
138.77
137.08
133.19
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121.57

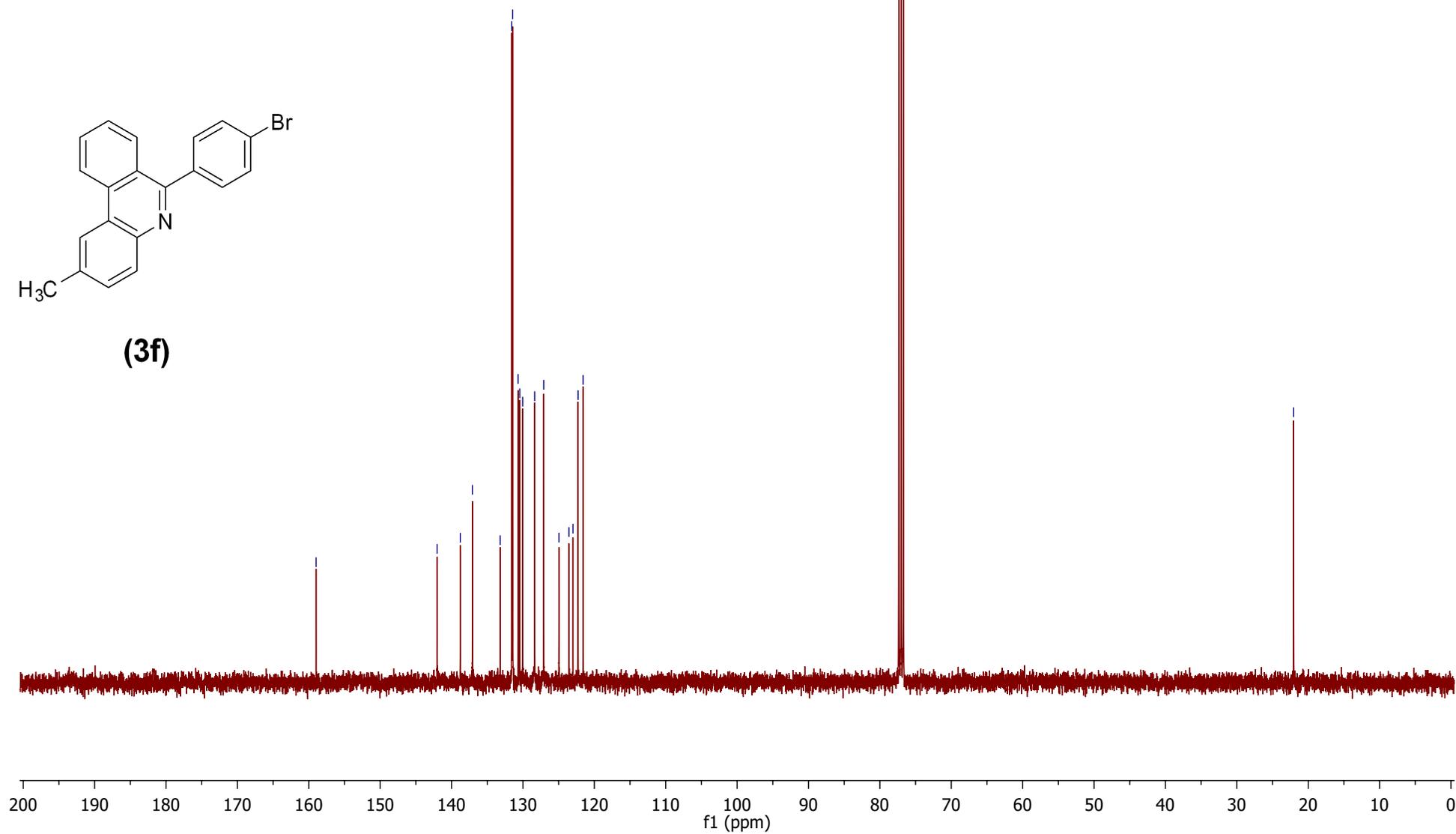
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77.03
76.71

22.04

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



(3f)



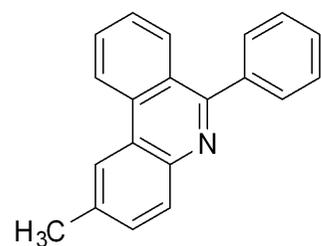
Phenenthridine NMR file
sb-77

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8.624
8.354
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7.765
7.726
7.711
7.549
7.522

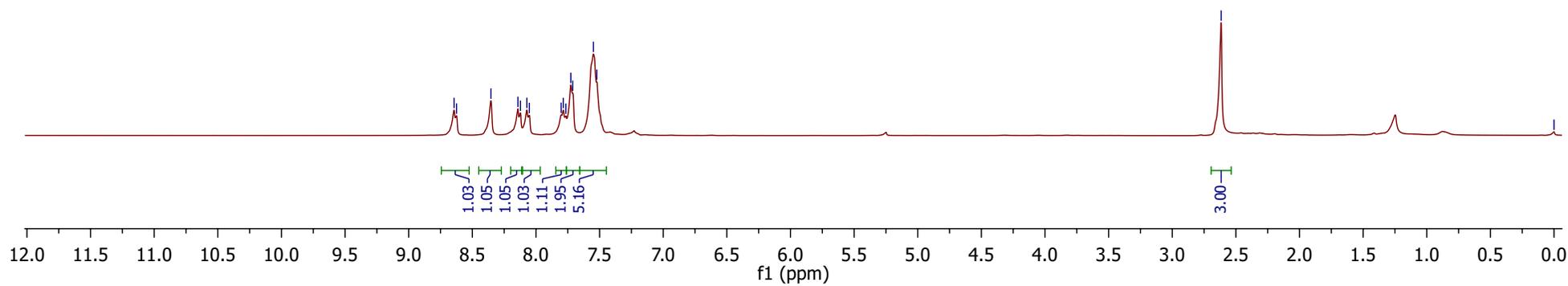
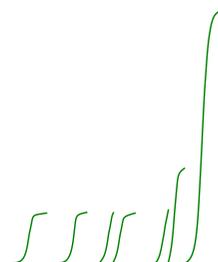
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0.000

^1H NMR (400 MHz, CDCl_3)



(3g)



Phenenthridine NMR file
sb-77

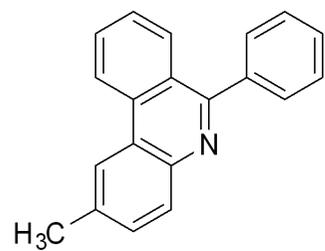
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141.99
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122.08
121.50

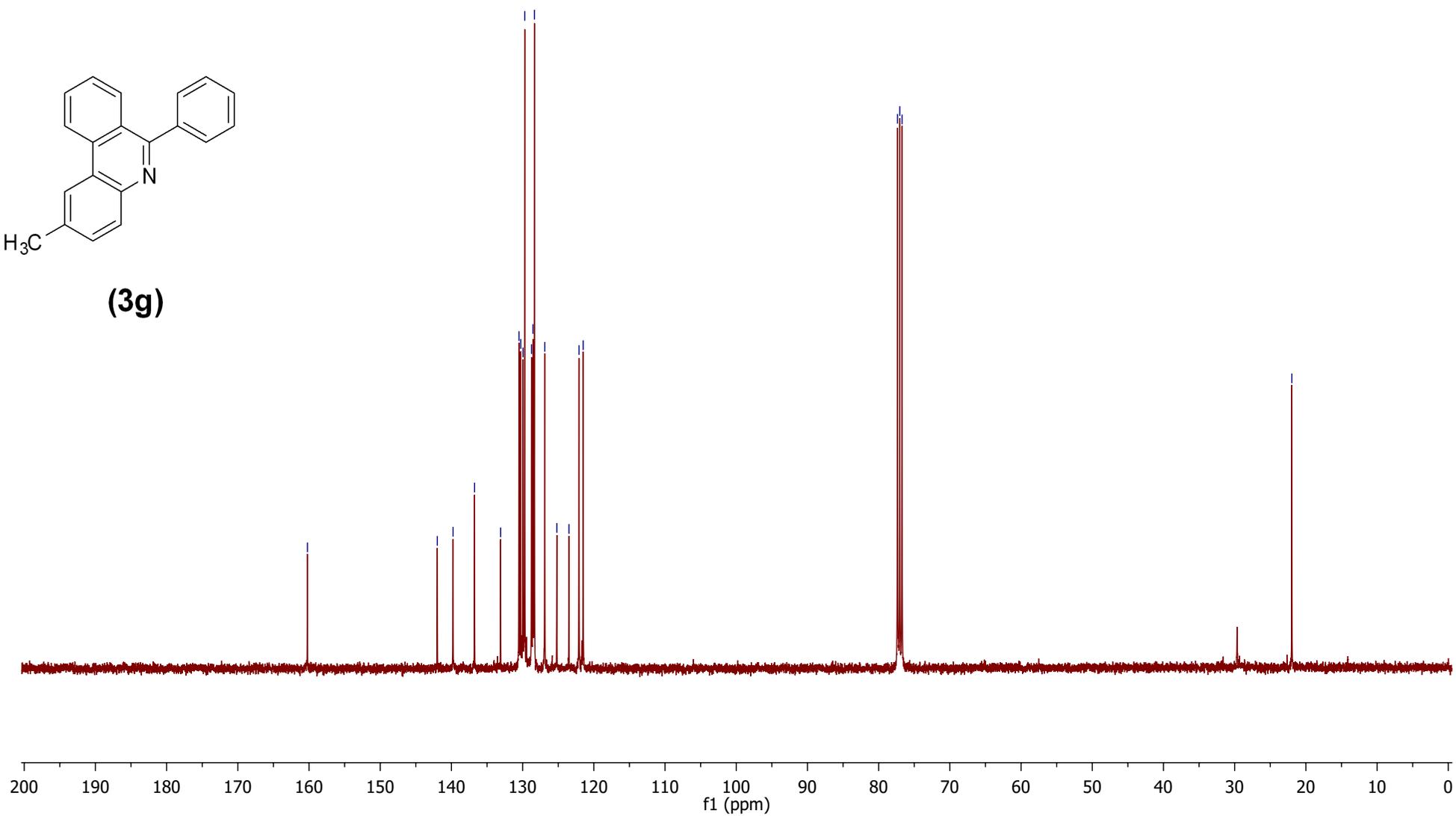
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77.03
76.71

21.97

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



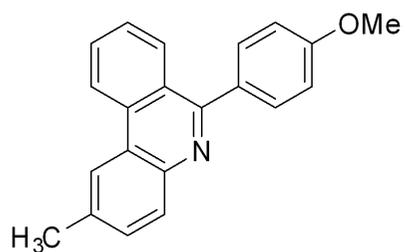
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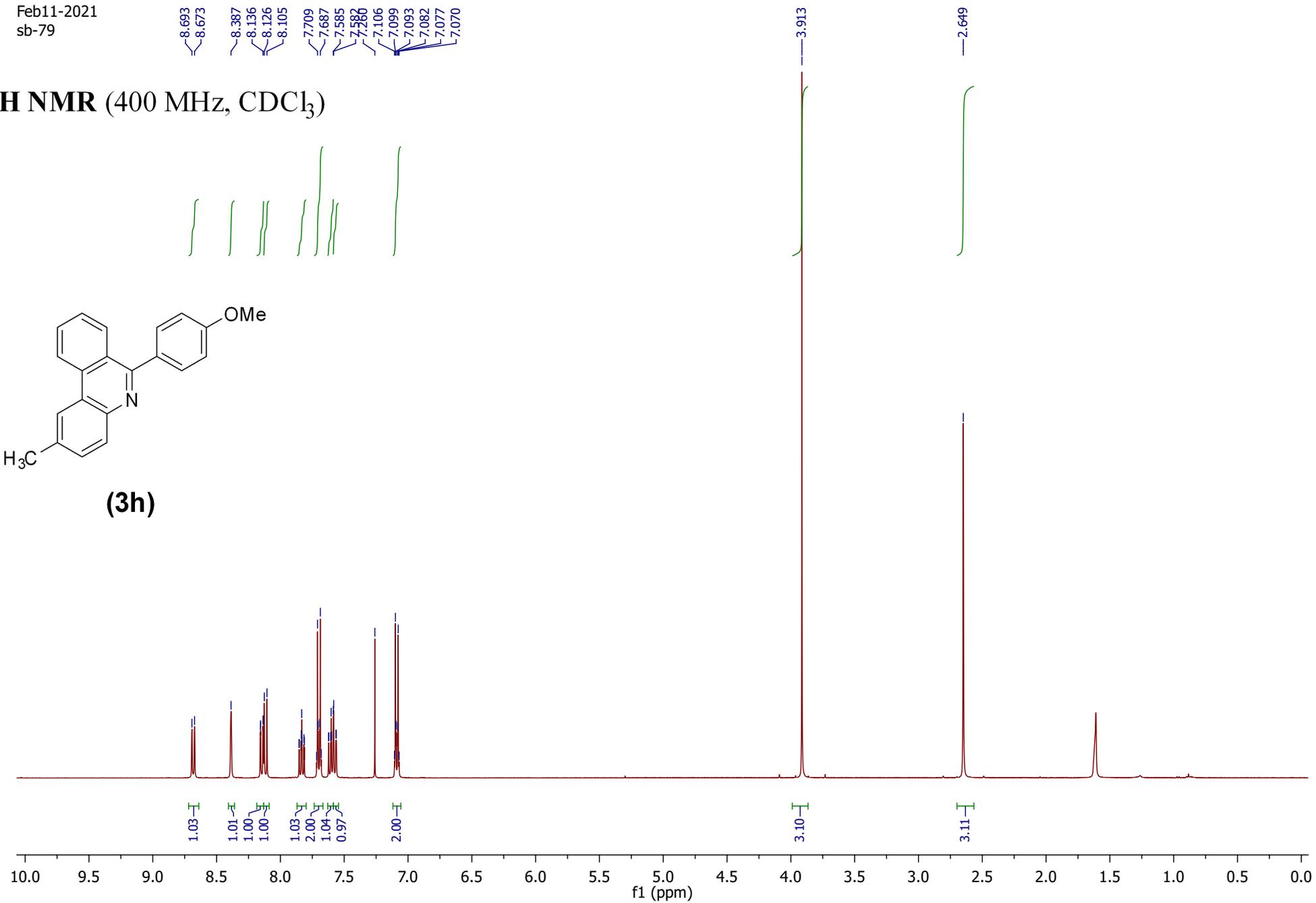
Feb11-2021
sb-79

8.693
8.673
8.387
8.136
8.126
8.105
7.709
7.687
7.585
7.582
7.280
7.106
7.099
7.093
7.082
7.077
7.070

^1H NMR (400 MHz, CDCl_3)



(3h)



Feb11-2021
sb-79

160.02
159.92

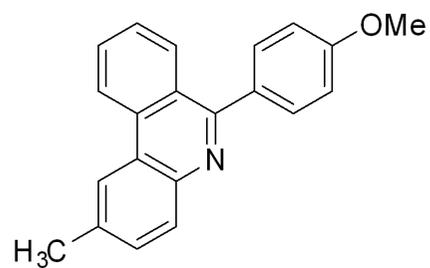
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123.43
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121.53
113.86

77.35
77.03
76.71

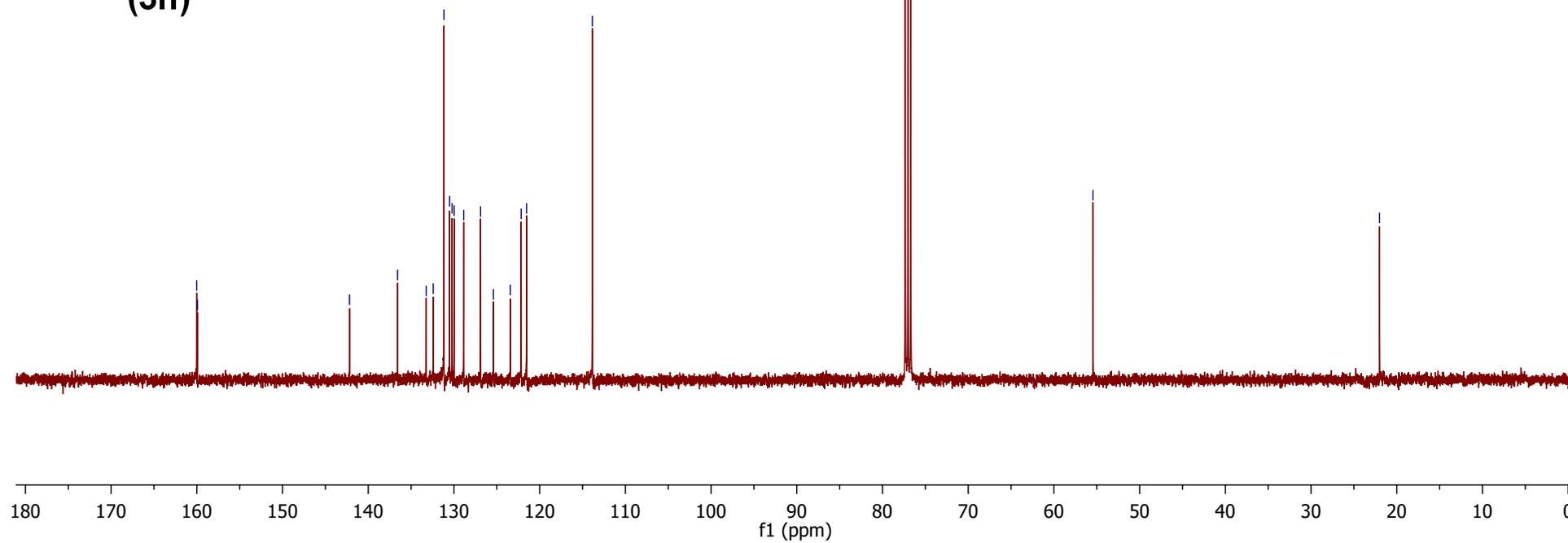
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22.02

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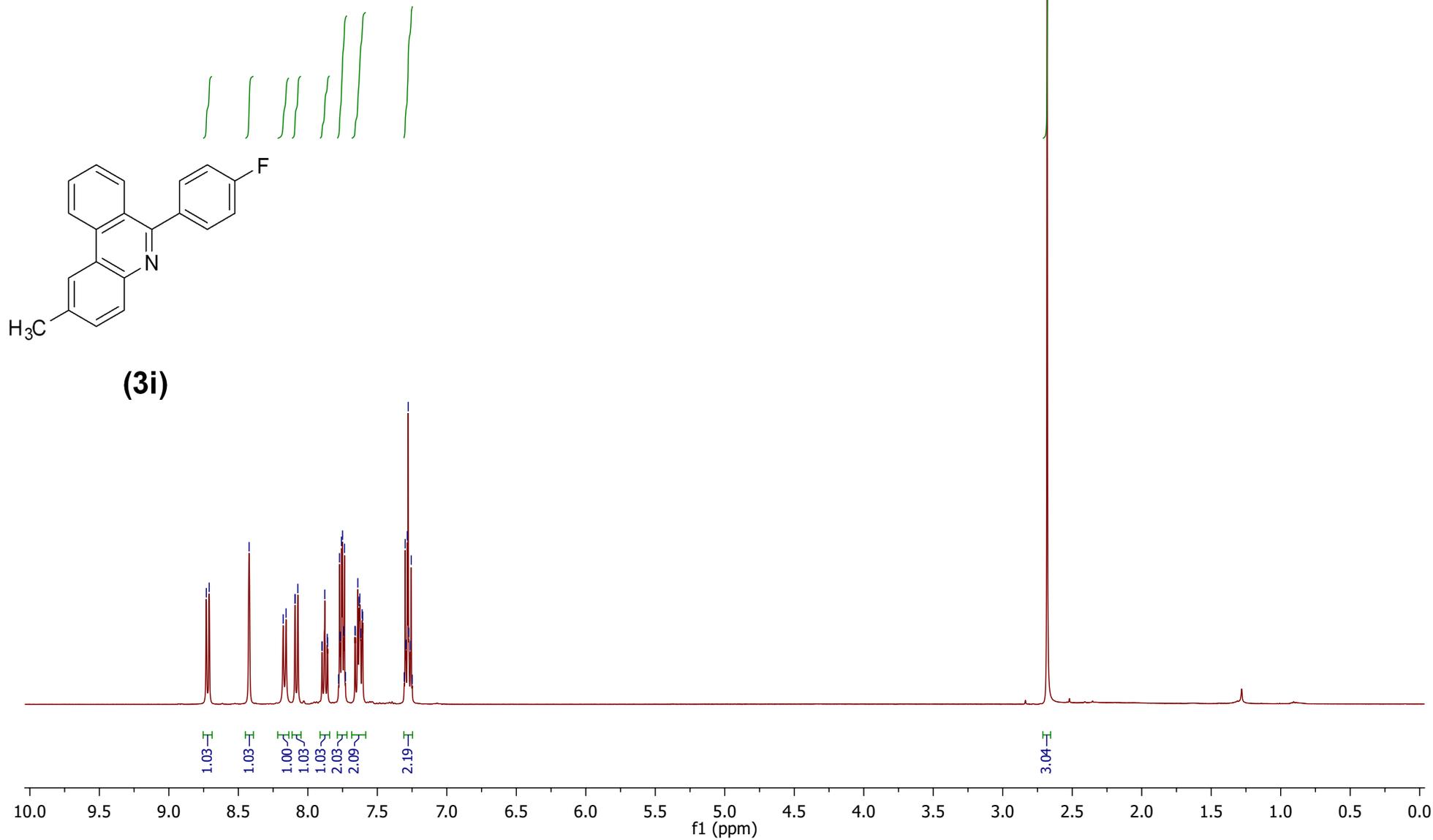
(3h)



22-07-2020
sb-85

8.731
8.710
8.423
8.072
7.878
7.772
7.758
7.750
7.737
7.649
7.299
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7.284
7.278
7.273
7.261
7.256
7.249

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



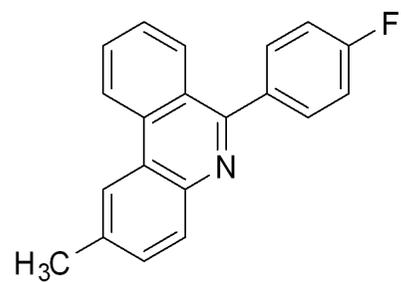
22-07-2020
sb-85

164.39
161.93
159.16
141.85
137.07
135.71
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128.61
127.12
125.18
123.59
122.29
121.58
115.55
115.33

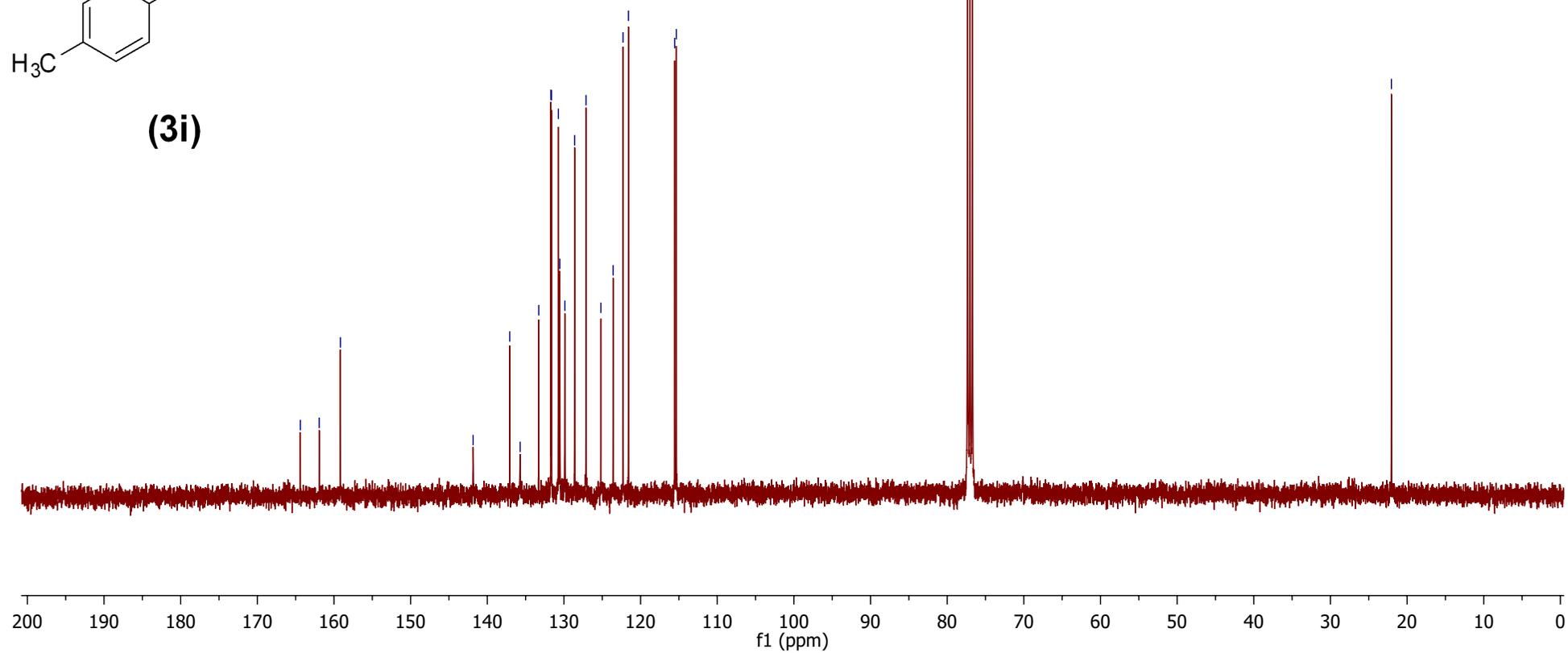
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77.03
76.71

22.05

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



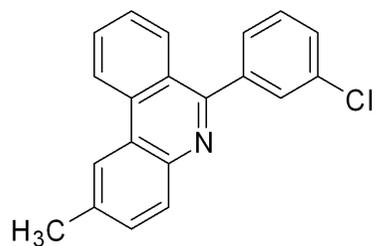
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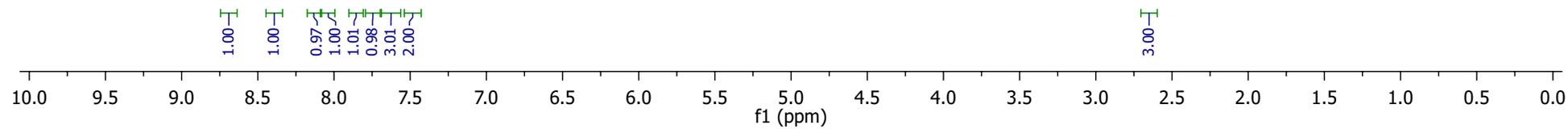
22-07-2020
sb-87

8.701
8.680
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7.636
7.619
7.613
7.607
7.605
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7.484
7.464
7.260

¹H NMR (400 MHz, CDCl₃)



(3j)



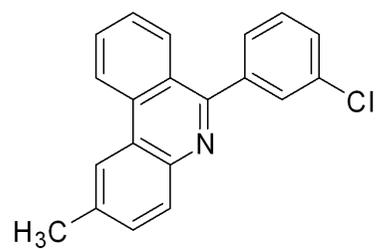
22-07-2020
sb-87

158.71
141.98
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137.20
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121.60

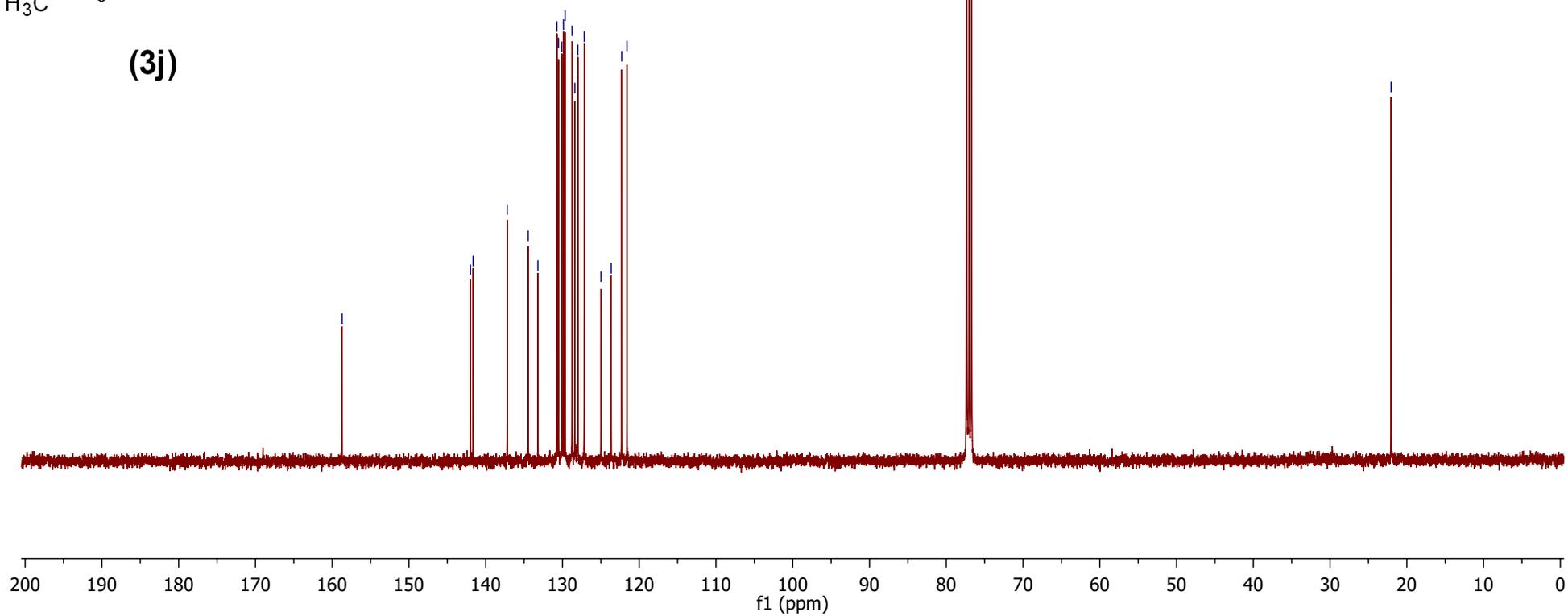
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(3j)



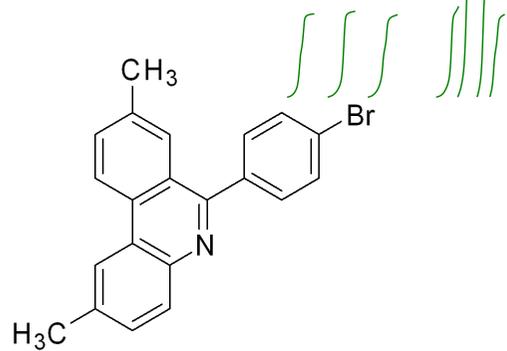
Phenenthridine NMR file
sb-84

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7.790
7.713
7.693
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7.604
7.568
7.547

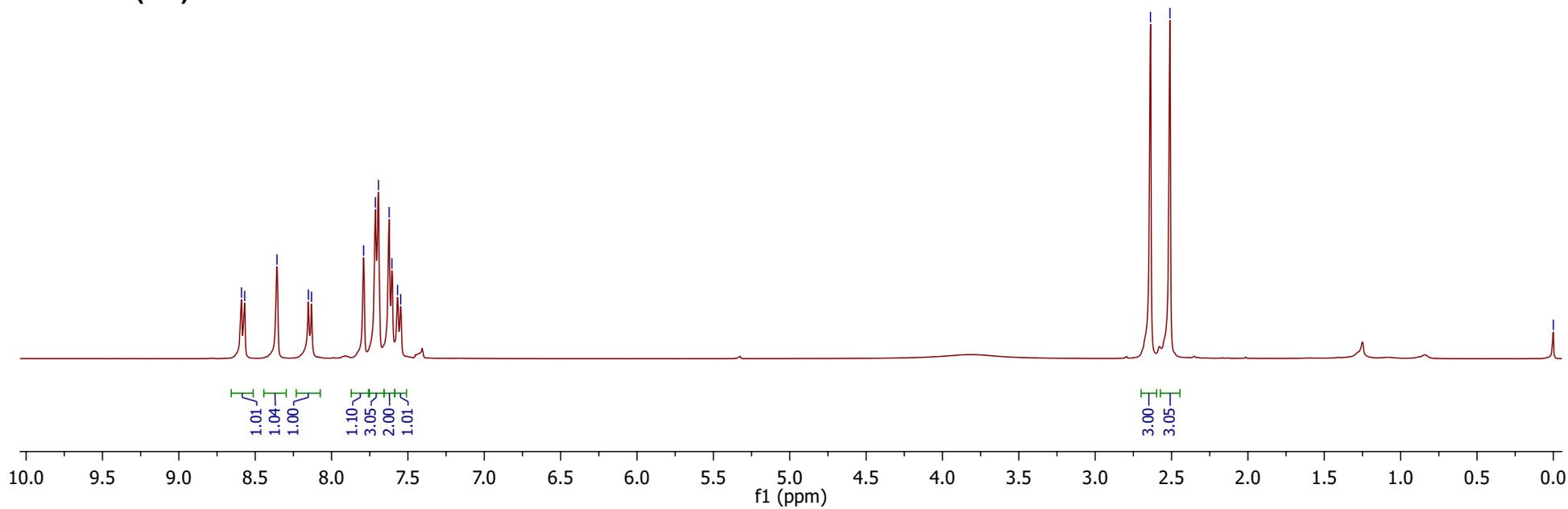
2.638
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0.000

¹H NMR (400 MHz, CDCl₃ + DMSO d₆)



(3k)



Phenenthridine NMR file
sb-84

158.19

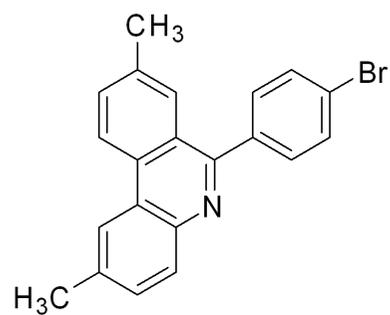
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77.35
77.03
76.71

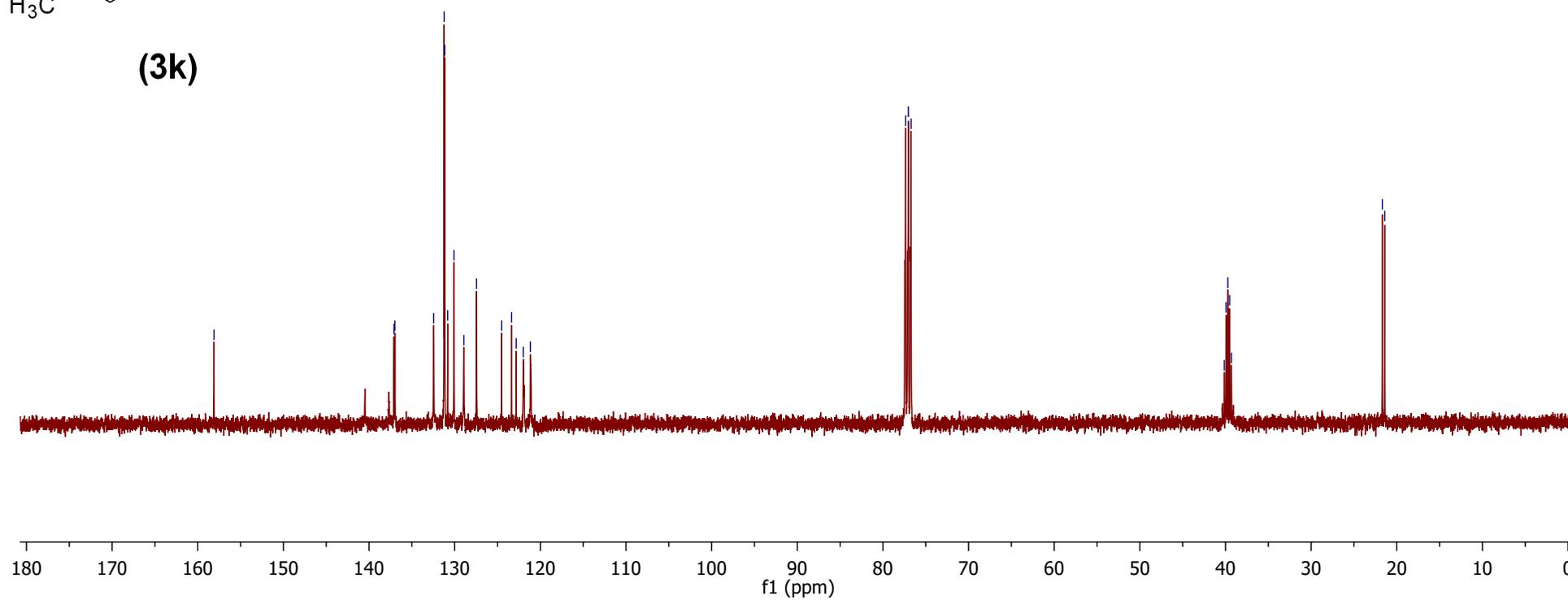
40.14
39.93
39.72
39.52
39.31

21.69
21.40

^{13}C NMR (100 MHz, $\text{CDCl}_3 + \text{DMSO } d_6$)



(3k)

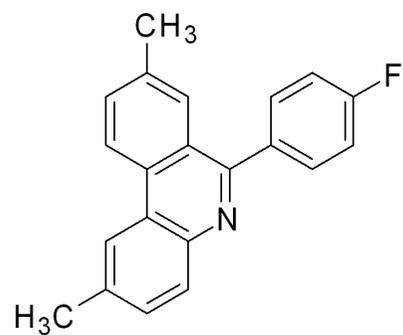
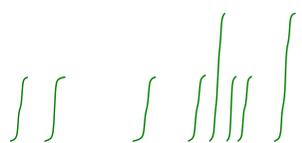


22-07-2020
sb-86

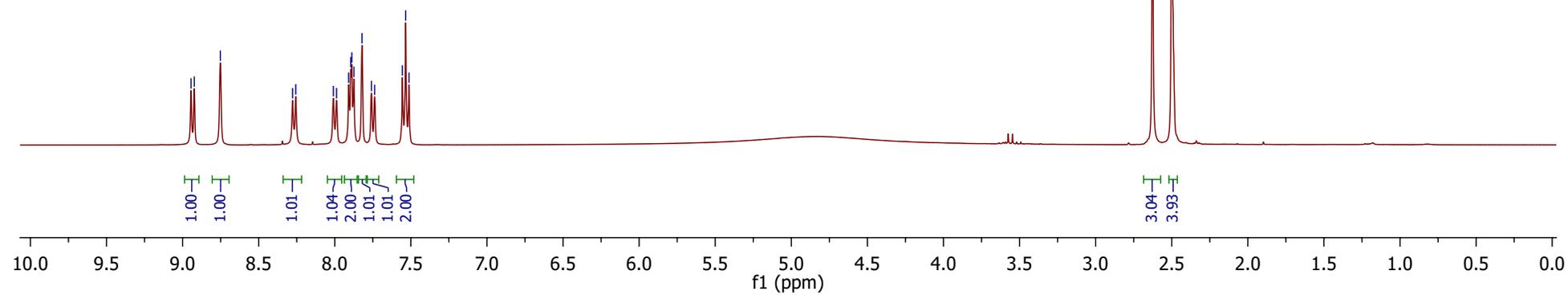
8.945
8.923
8.752
8.277
8.256
8.009
7.988
7.909
7.895
7.888
7.874
7.821
7.759
7.738
7.556
7.534
7.512

2.626
2.500

¹H NMR (400 MHz, CDCl₃)



(31)



22-07-2020
sb-86

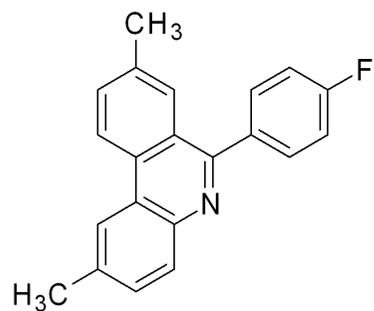
164.74
162.27
157.70

139.18
136.12
133.01
132.92
131.95
131.80
129.96
128.97
124.41
124.07
123.32
122.57
115.88
115.66

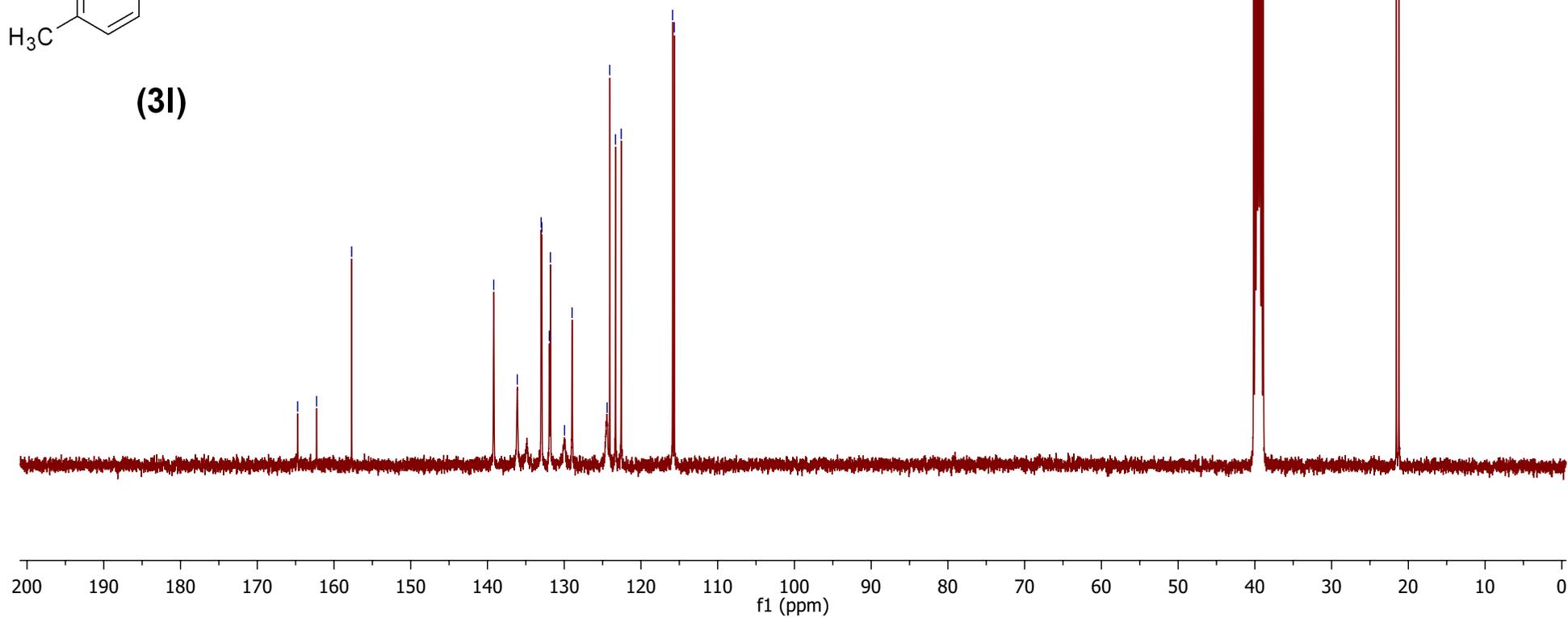
40.15
39.94
39.73
39.53
39.31
39.10
38.89

21.56
21.23

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



(31)



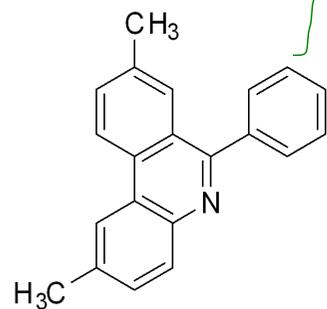
Phenenthridine NMR file
sb-78

8.553
8.532
8.330
8.161
8.140
7.834
7.727
7.709
7.557
7.539
7.520

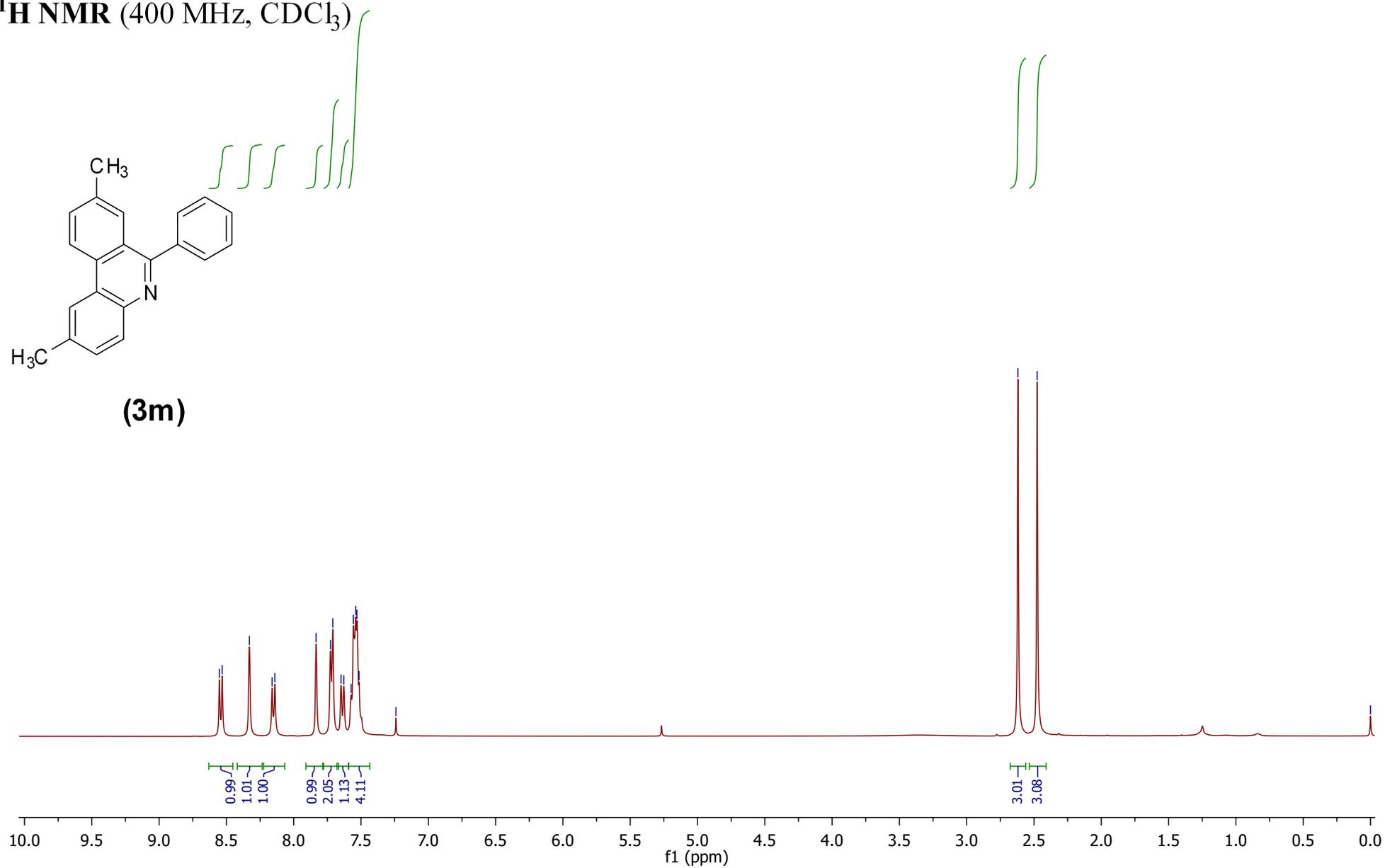
2.620
2.477

0.000

^1H NMR (400 MHz, CDCl_3)



(3m)



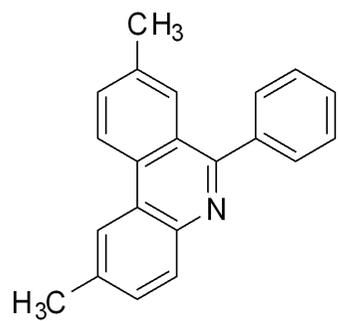
Phenenthridine NMR file
sb-78

159.41
141.38
139.62
136.99
136.81
132.26
131.08
130.17
129.74
129.69
128.60
128.39
128.17
125.32
123.65
122.07
121.35

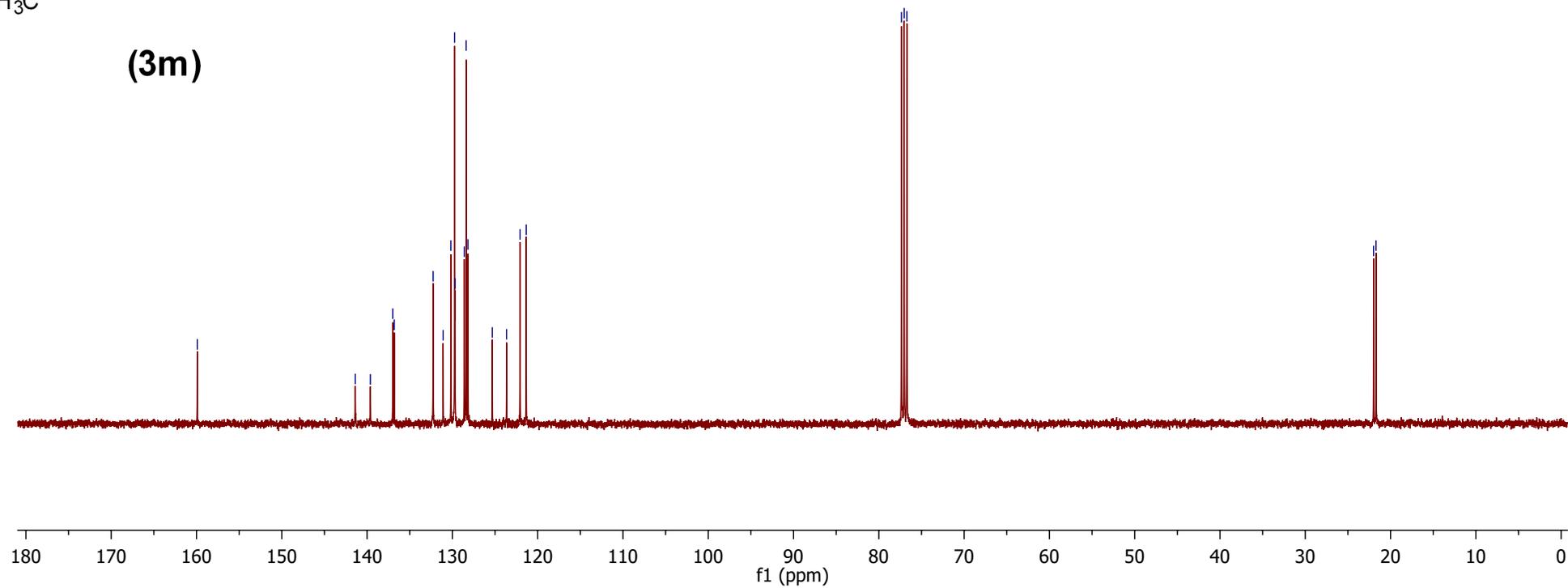
77.35
77.03
76.71

21.99
21.71

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



(3m)



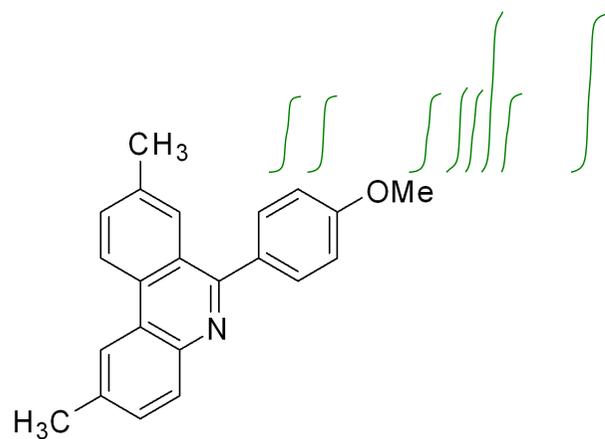
EXTRA SB-80
sb-80

8.748
8.727
8.544
8.004
7.983
7.824
7.765
7.744
7.667
7.646
7.585
7.564
7.152
7.131

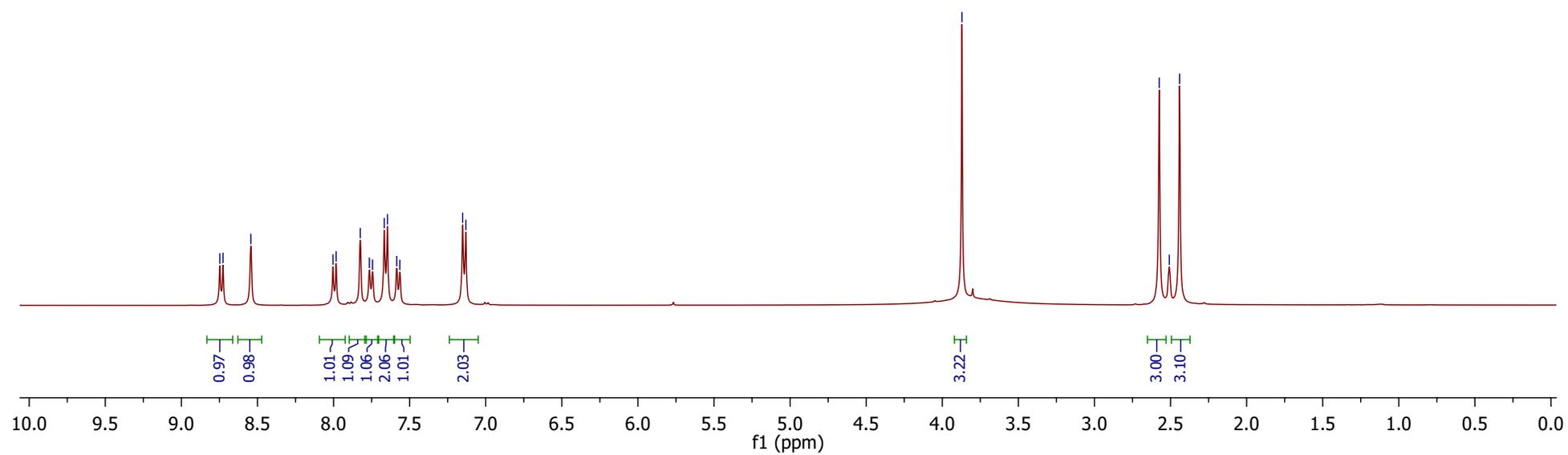
3.871

2.574
2.508
2.441

$^1\text{H NMR}$ (400 MHz, DMSO-d_6)



(3n)



EXTRA SB-80
sb-80

160.43
159.01

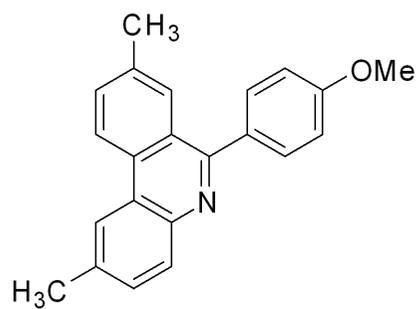
137.91
137.46
133.59
131.81
131.31
130.94
128.45
128.19
124.88
123.61
123.25
122.41
114.22

55.77

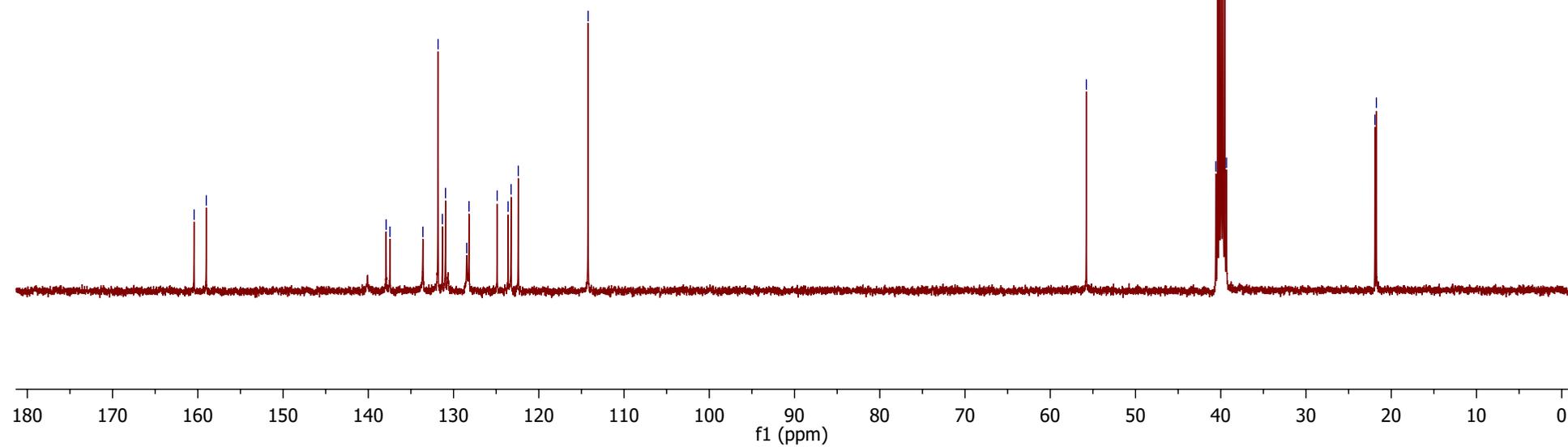
40.58
40.37
40.16
39.95
39.74
39.54
39.33

21.92
21.74

^{13}C NMR (100 MHz, DMSO d_6)



(3n)



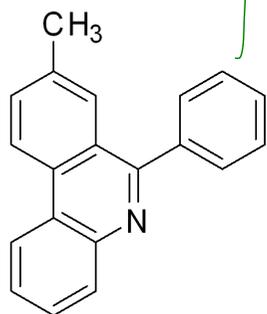
Phenenthridine NMR fit
sb-94

8.578
8.563
8.549
8.543
8.276
8.256
7.735
7.718
7.716
7.651
7.566
7.547
7.542

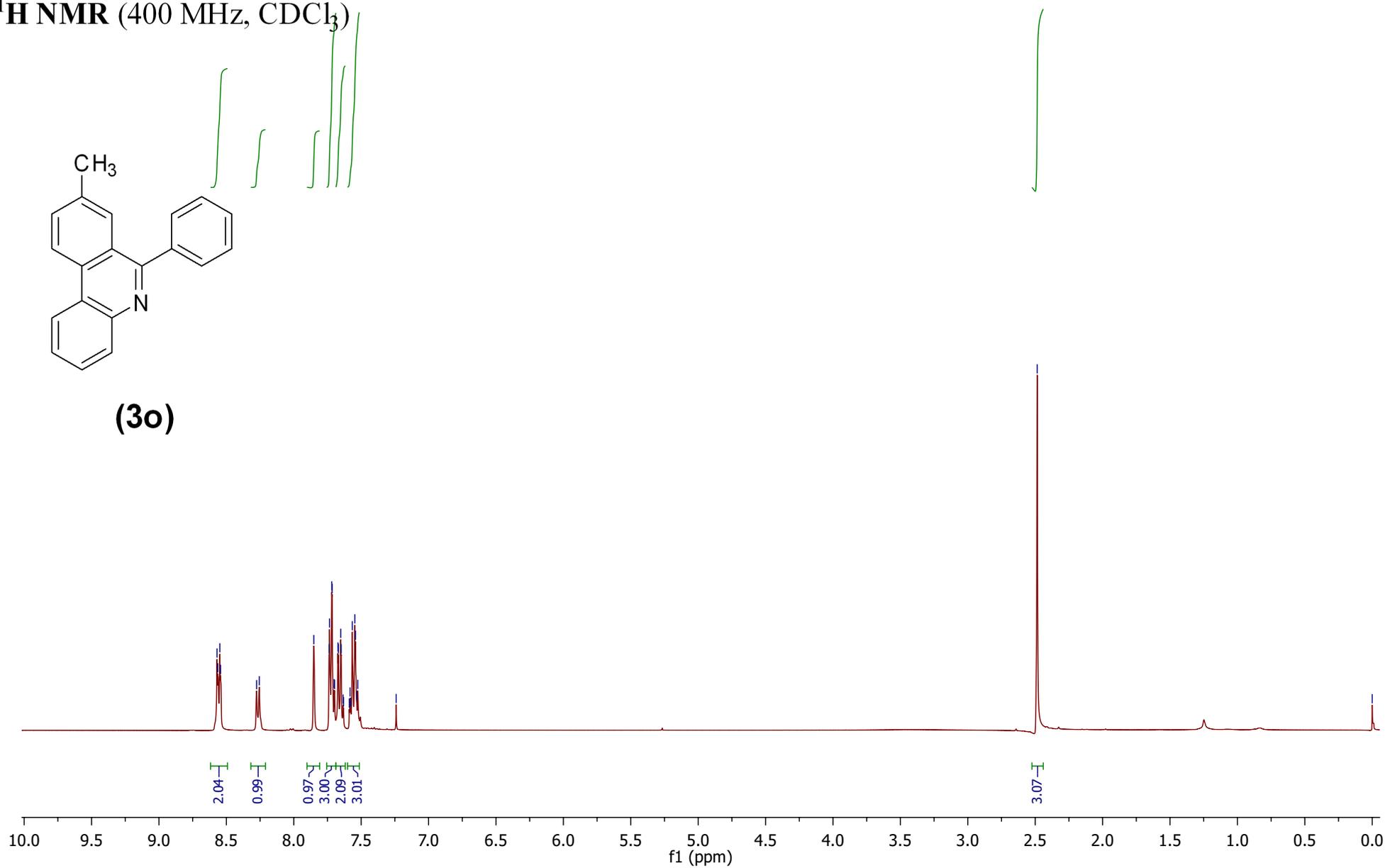
2.485

0.000

^1H NMR (400 MHz, CDCl_3)



(30)



Phenenthridine NMR file
sb-94

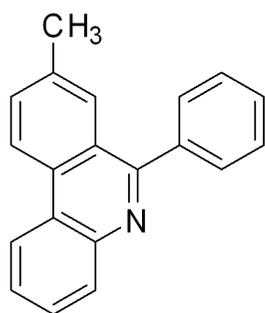
143.09
139.54
137.19
132.48
131.35
129.99
129.71
128.72
128.44
128.41
128.26
126.93
125.29
123.83
122.11
121.75

77.35
77.03
76.71

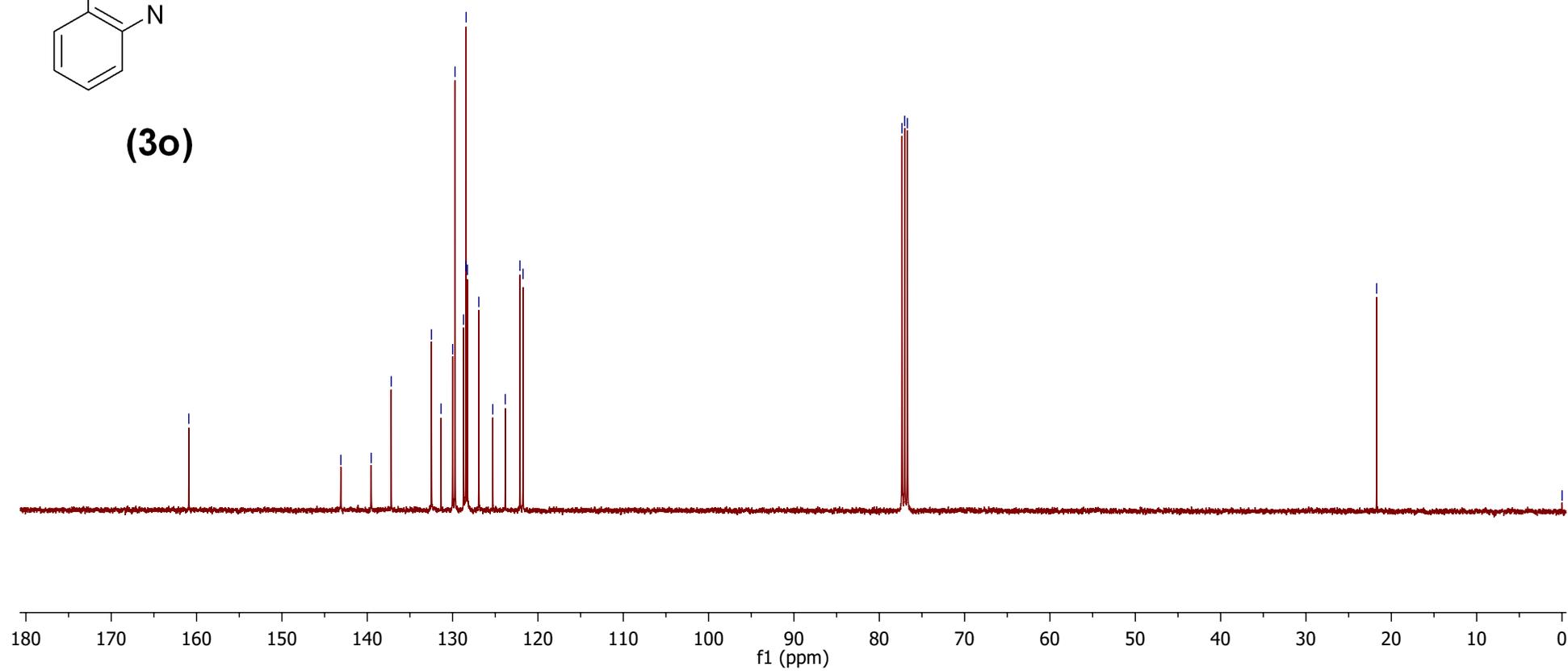
21.72

-0.01

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



(3o)



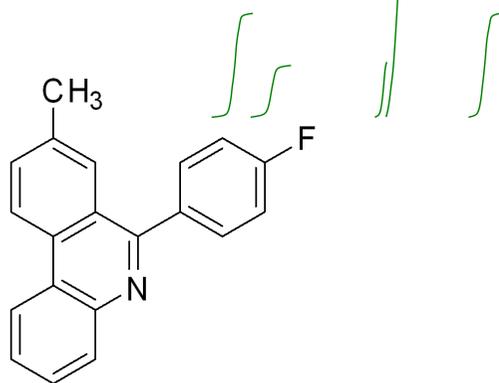
EXTRA SB-95
sb-95

8.684
8.674
8.663
8.653
8.639
8.634
8.466
7.814
7.803
7.790
7.785
7.774
7.748
7.327
7.309

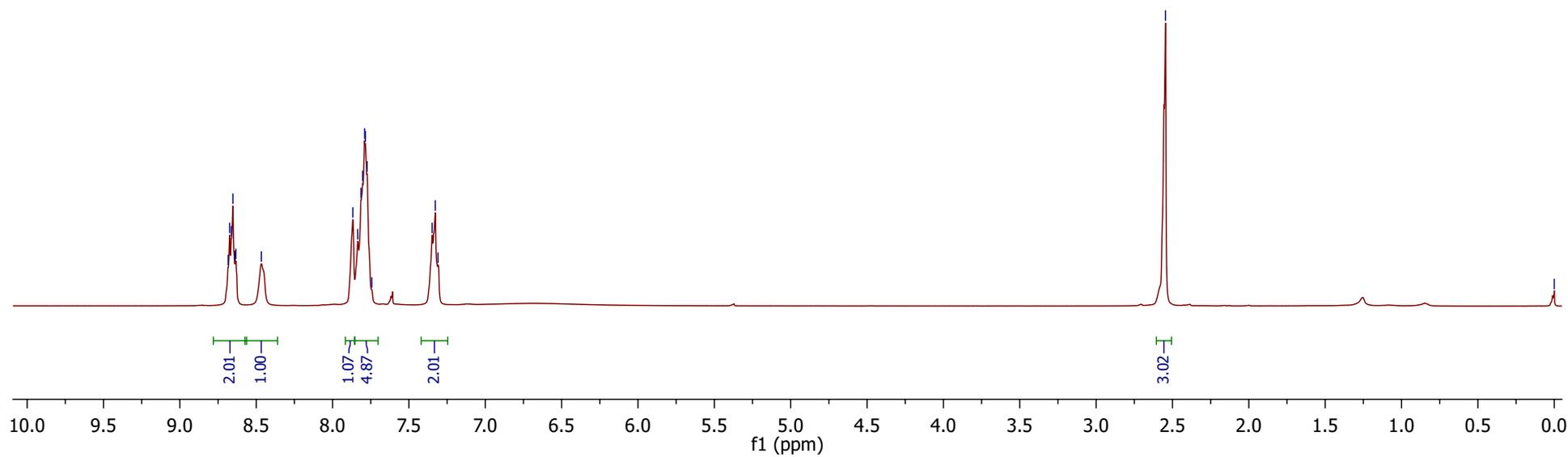
2.546

0.000

¹H NMR (400 MHz, CDCl₃ + DMSO d₆)



(3p)



EXTRA SB-95
sb-95

164.02
161.54
158.36

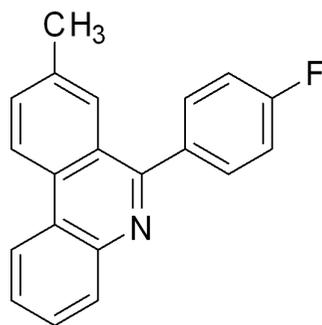
139.17
137.62
133.71
131.41
131.32
131.16
128.48
127.83
127.27
126.83
123.72
123.19
121.82
121.40
115.00
114.78

77.35
77.03
76.71

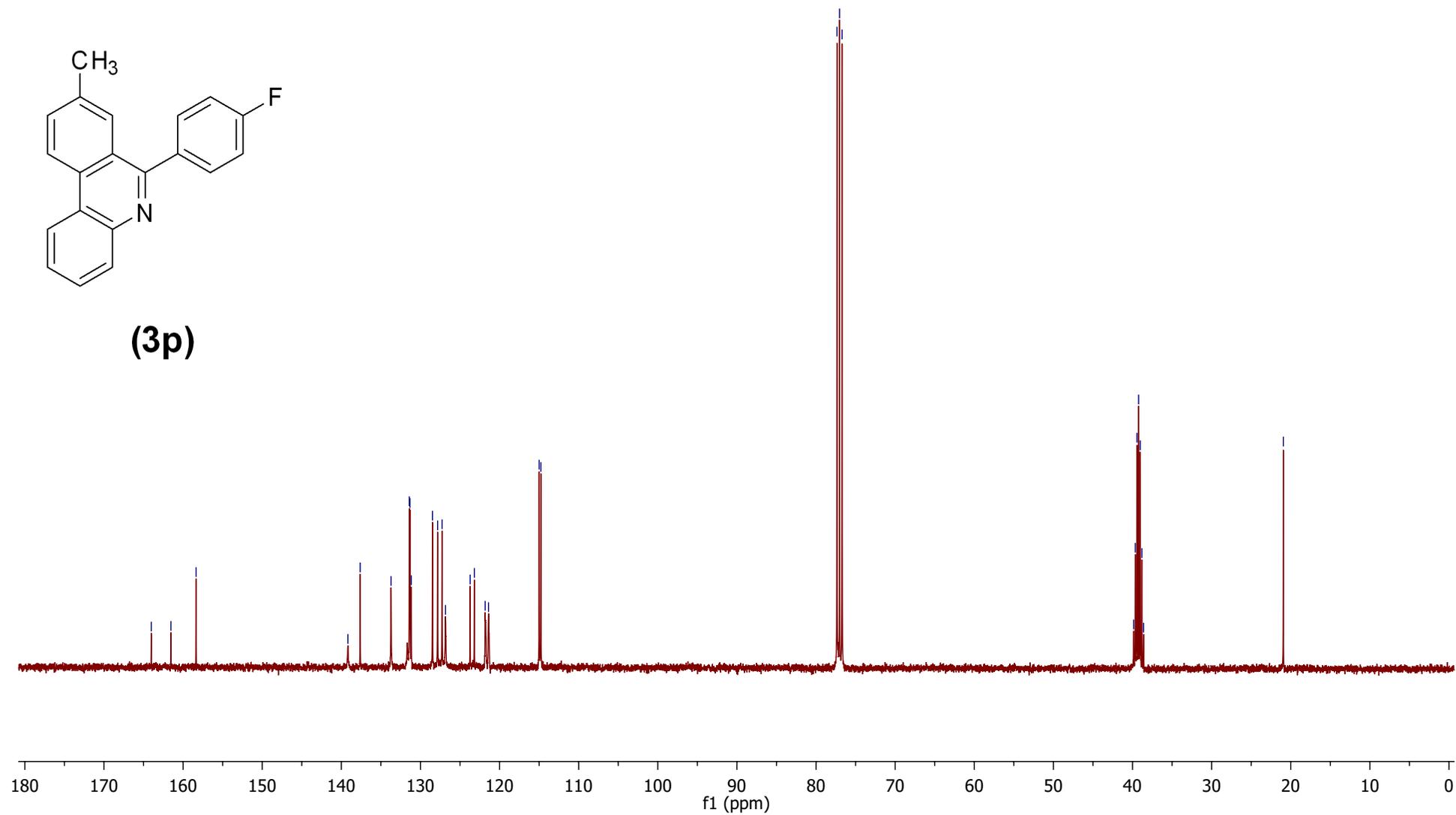
39.86
39.65
39.44
39.23
39.02
38.81
38.61

20.94

^{13}C NMR (100 MHz, $\text{CDCl}_3 + \text{DMSO } d_6$)



(3p)



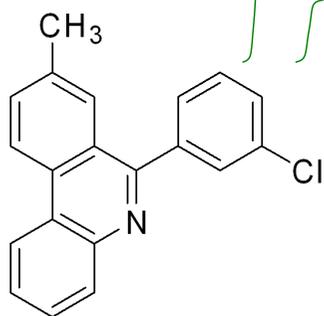
Phenenthridine NMR file
sb-96

8.592
8.576
8.560
8.302
8.283
7.798
7.739
7.712
7.691
7.614
7.602
7.589

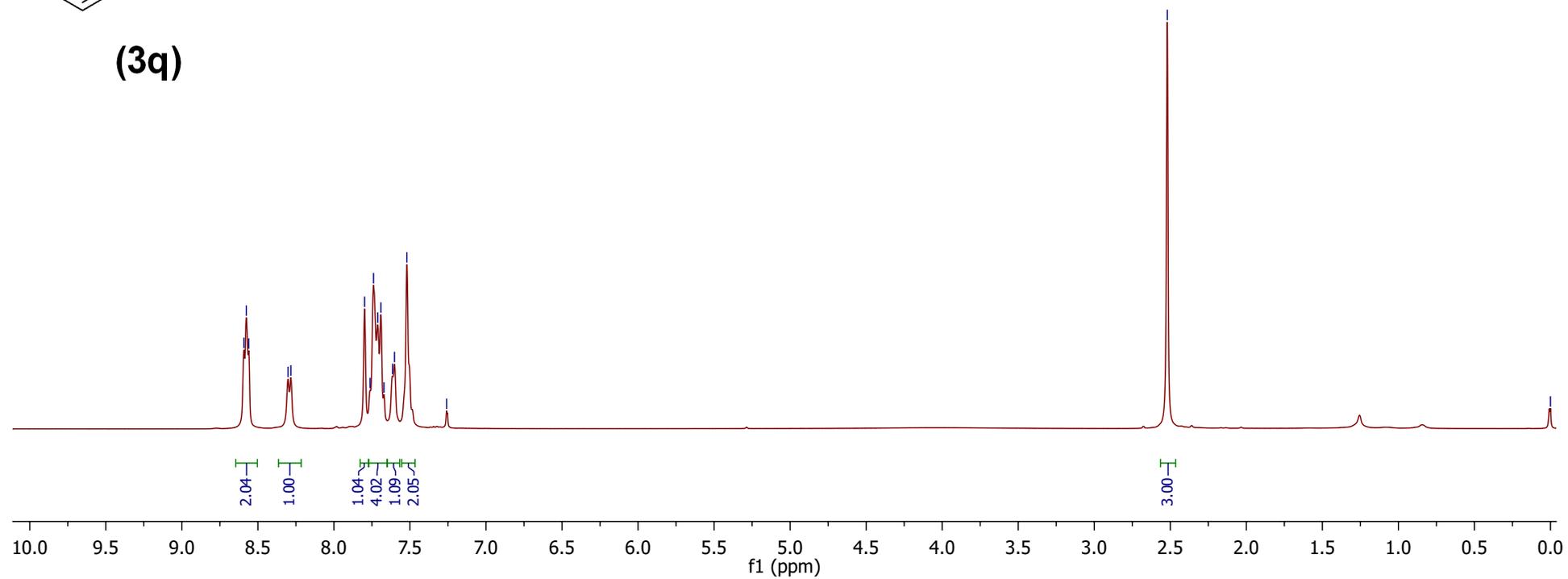
2.520

0.000

^1H NMR (400 MHz, CDCl_3)



(3q)



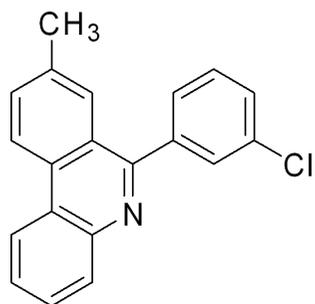
Phenenthridine NMR file
sb-96

159.76
137.57
134.51
132.92
131.47
129.80
129.70
129.02
128.70
127.99
127.92
127.36
124.97
123.94
122.26
121.82

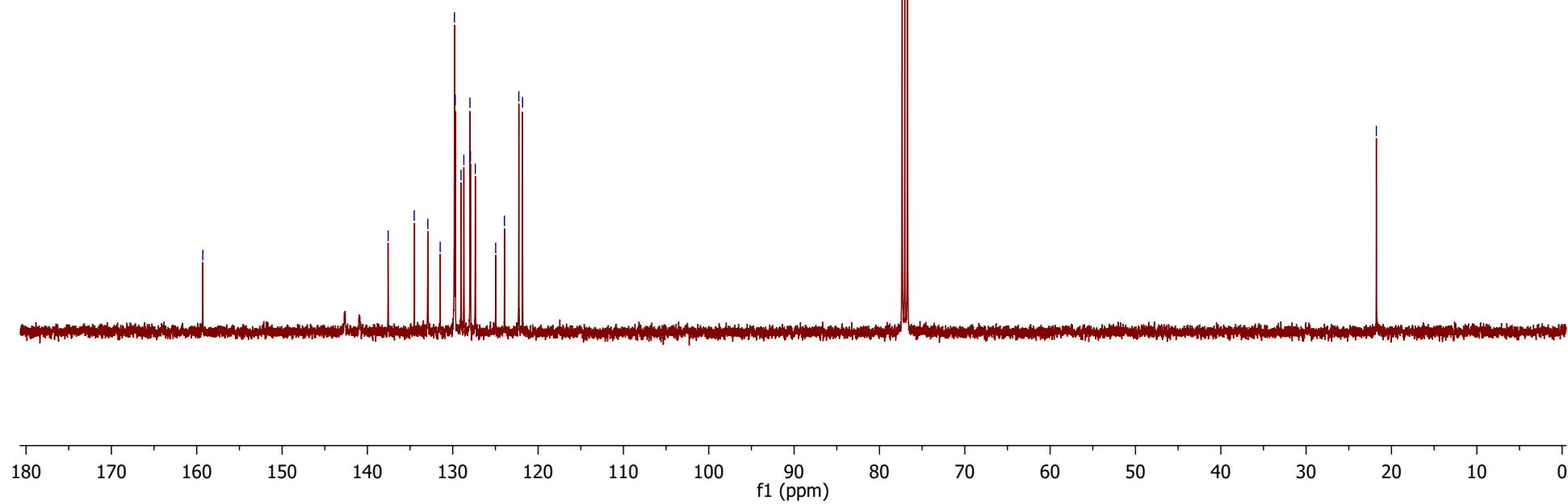
77.35
77.03
76.71

21.77

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



(3q)



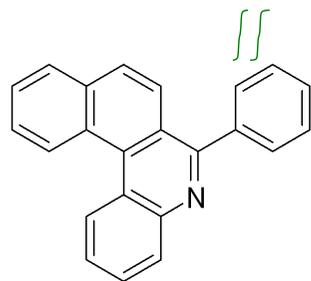
SID105

9.171
9.158
9.067
9.053
8.252
8.250
8.238
8.236
8.190
8.178
8.175
8.073
8.058
7.900
7.885
7.872
7.861
7.850
7.847
7.837
7.836
7.826
7.824
7.812
7.801
7.799
7.714
7.711
7.701
7.699
7.622
7.617
7.614
7.608
7.598
7.595
7.585
7.575
7.572

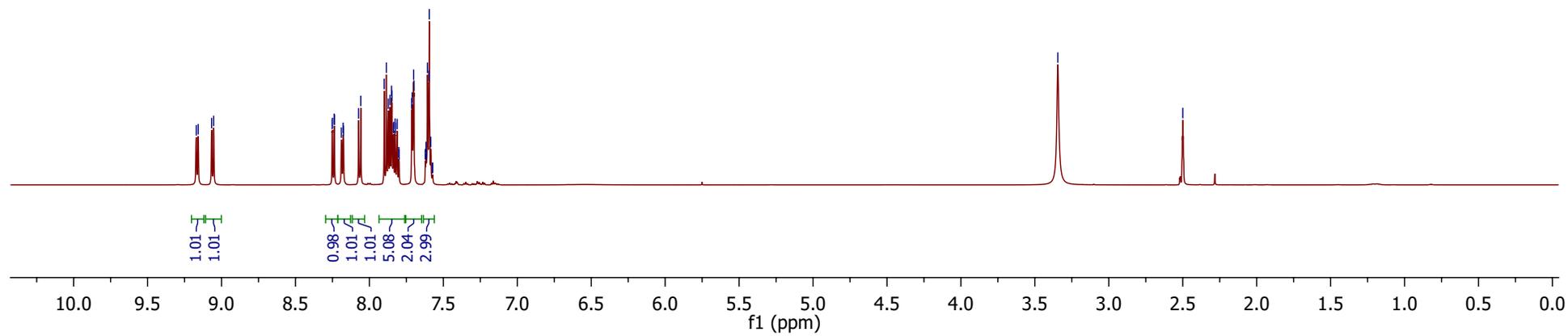
3.345

2.500

¹³C NMR (125 MHz, DMSO-d₆)



(3r)

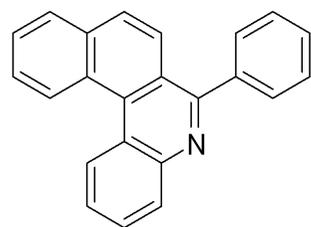


SD105

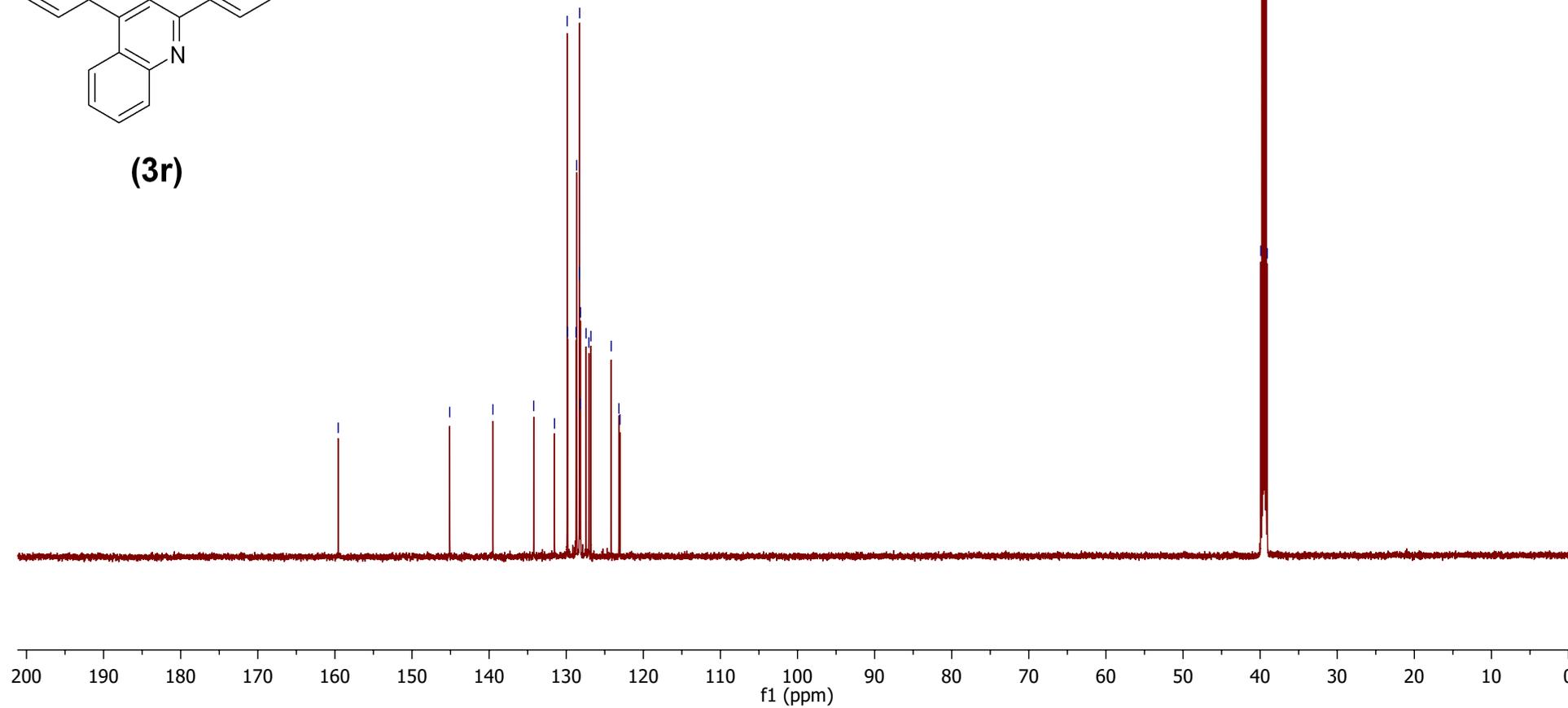
— 159.57
— 145.10
— 139.51
— 134.21
— 131.52
— 129.88
— 129.81
— 128.73
— 128.65
— 128.30
— 128.29
— 128.26
— 128.19
— 128.14
— 127.43
— 127.06
— 126.80
— 124.17
— 123.17
— 123.03

— 39.92
— 39.78
— 39.64
— 39.50
— 39.36
— 39.22
— 39.08

¹H NMR (500 MHz, DMSO-d₆)



(3r)

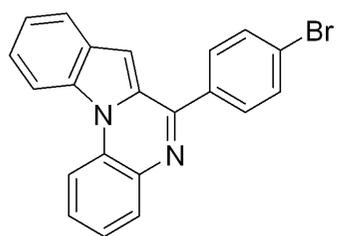
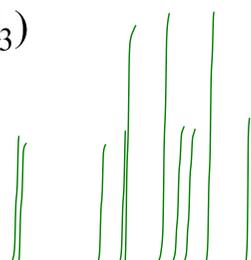


SID-431-021914
SID-431-02192014 1H

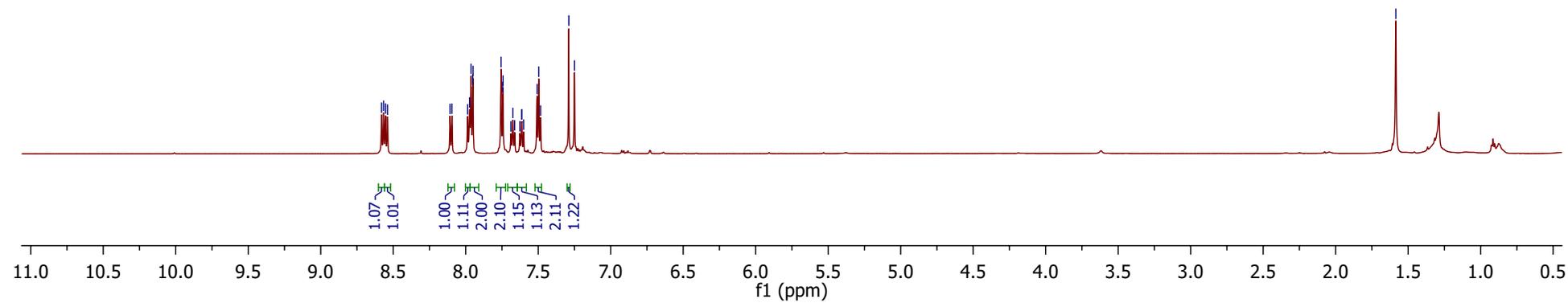
8.580
8.566
8.554
8.539
8.108
8.095
7.987
7.973
7.963
7.952
7.949
7.756
7.745
7.742
7.688
7.675
7.663
7.627
7.615
7.613
7.601
7.508
7.496
7.484
7.289
7.250

1.585

^1H NMR (400 MHz, CDCl_3)



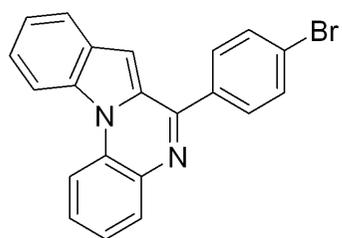
(3s)



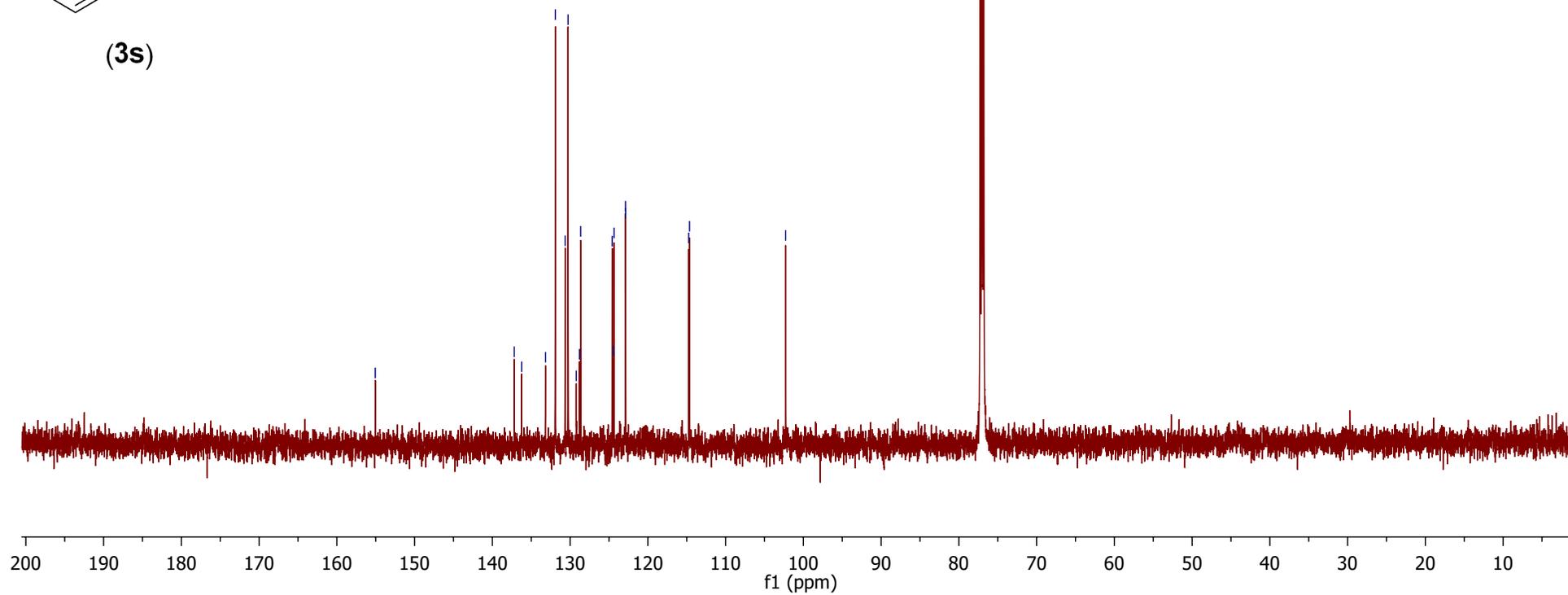
SID-431-021914
SID-431-02192014 1H

155.06
137.19
136.23
133.16
131.90
130.64
130.26
129.21
128.80
128.64
124.59
124.42
124.35
122.88
122.85
114.74
114.64
102.28
77.24
77.03
76.82

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



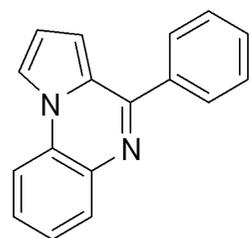
(3s)



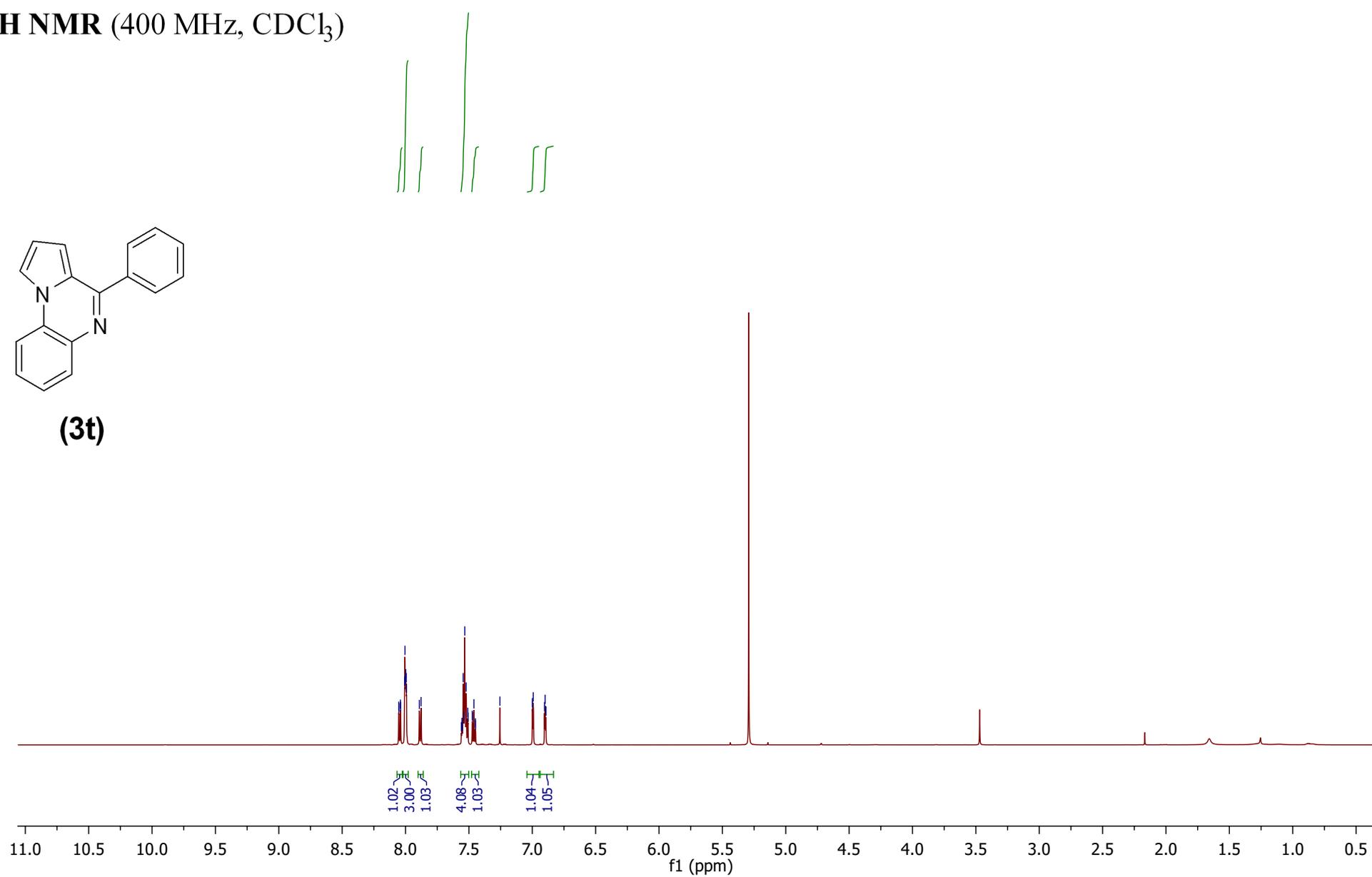
SID-314-121213
SID-314-121313

8.053
8.052
8.040
8.038
8.007
8.004
8.000
7.998
7.994
7.992
7.891
7.877
7.560
7.555
7.552
7.545
7.540
7.533
7.522
7.509
7.507
7.474
7.472
7.461
7.449
7.447
7.256
6.999
6.997
6.992
6.903
6.899

^1H NMR (400 MHz, CDCl_3)

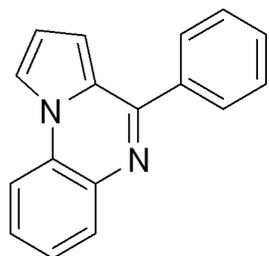


(3t)

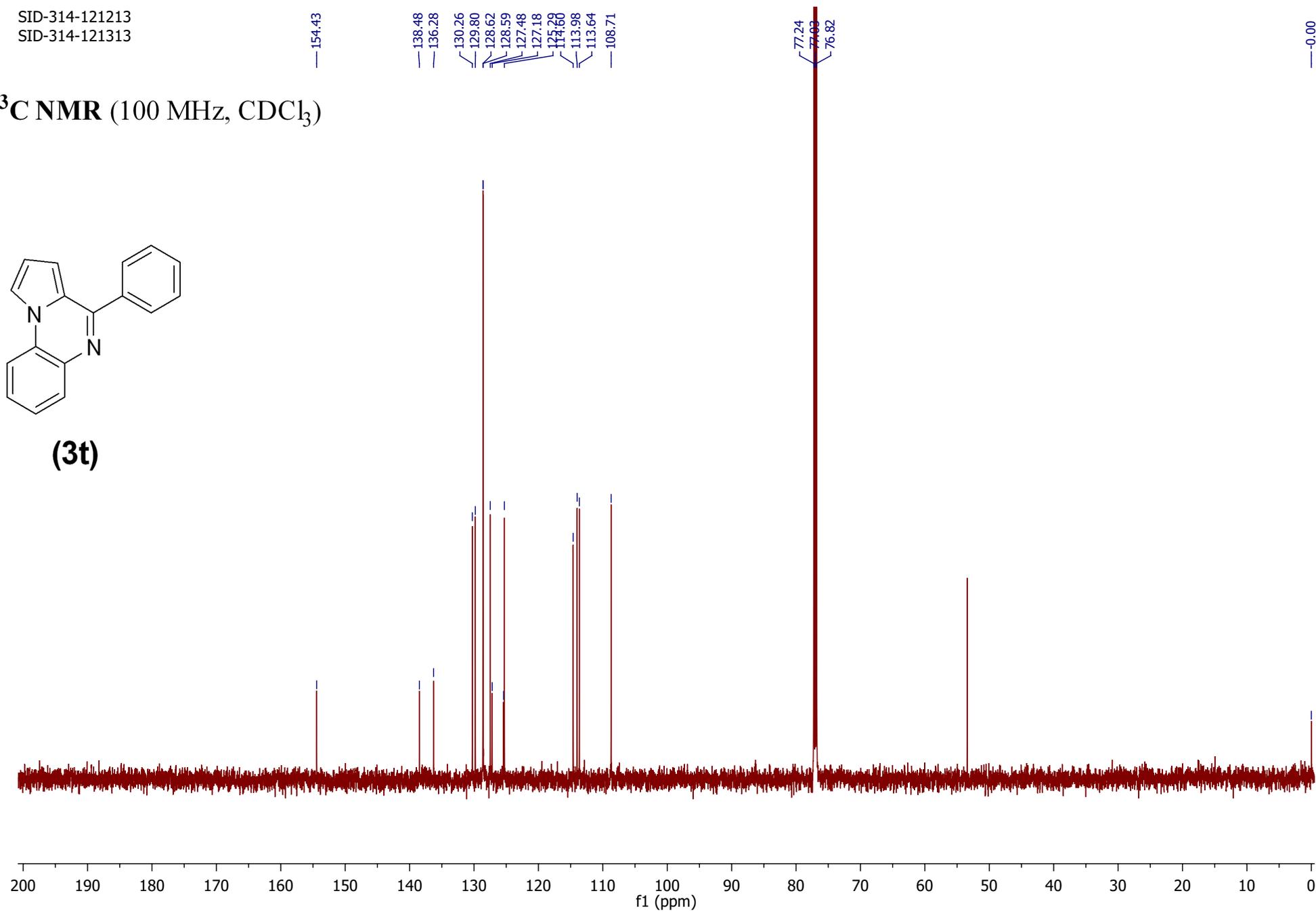


SID-314-121213
SID-314-121313

¹³C NMR (100 MHz, CDCl₃)

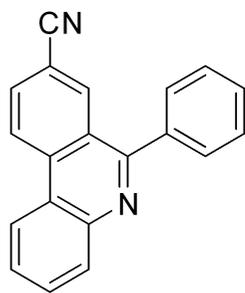


(3t)

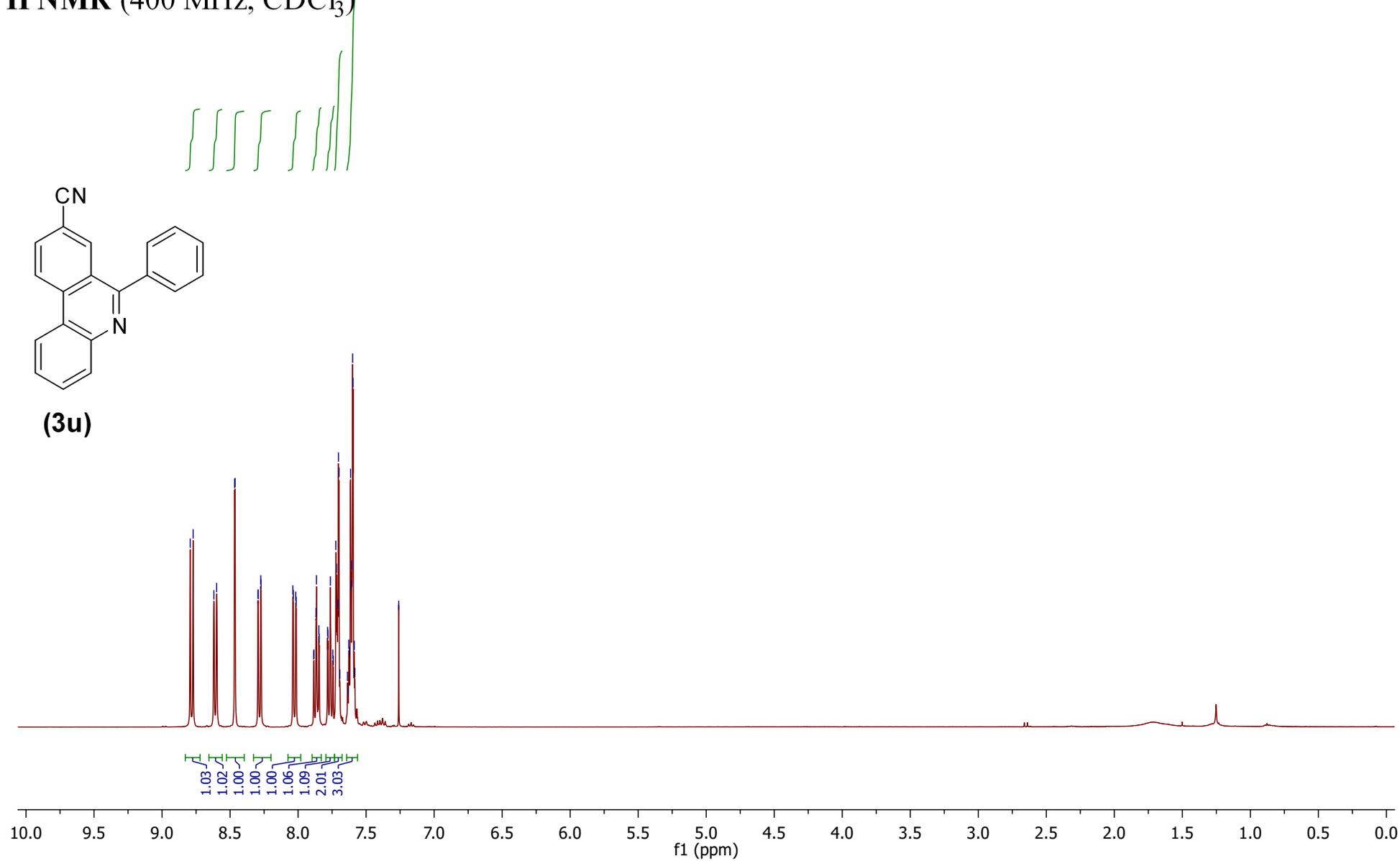


22.0742020
sb 8.779
8.777
8.599
8.463
8.463
8.295
8.292
8.274
8.272
8.039
8.035
7.865
7.762
7.723
7.717
7.703
7.699
7.614
7.610
7.605
7.599
7.586

¹H NMR (400 MHz, CDCl₃)



(3u)



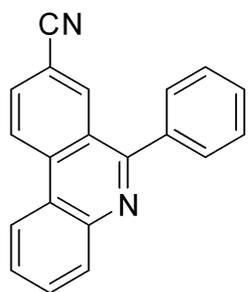
22-07-2020
sb-128

160.43

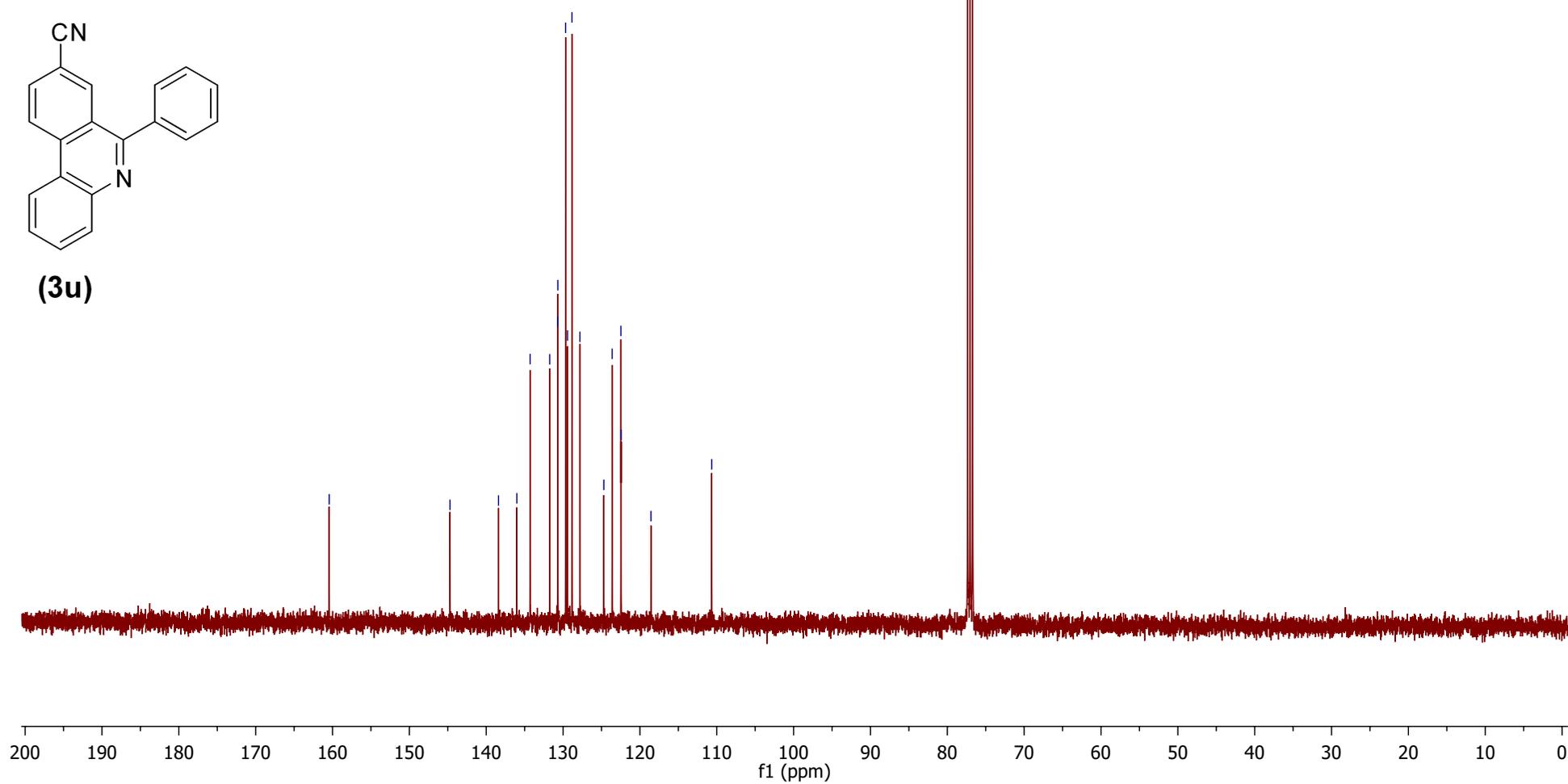
144.71
136.02
134.29
131.74
130.70
130.68
129.67
129.43
128.85
127.81
124.70
123.61
122.47
110.65

77.35
77.03
76.71

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



(3u)



Amide NMR
sid-bk-204

7.701
7.681

7.272

6.909
6.890

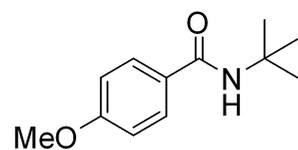
5.911

3.839

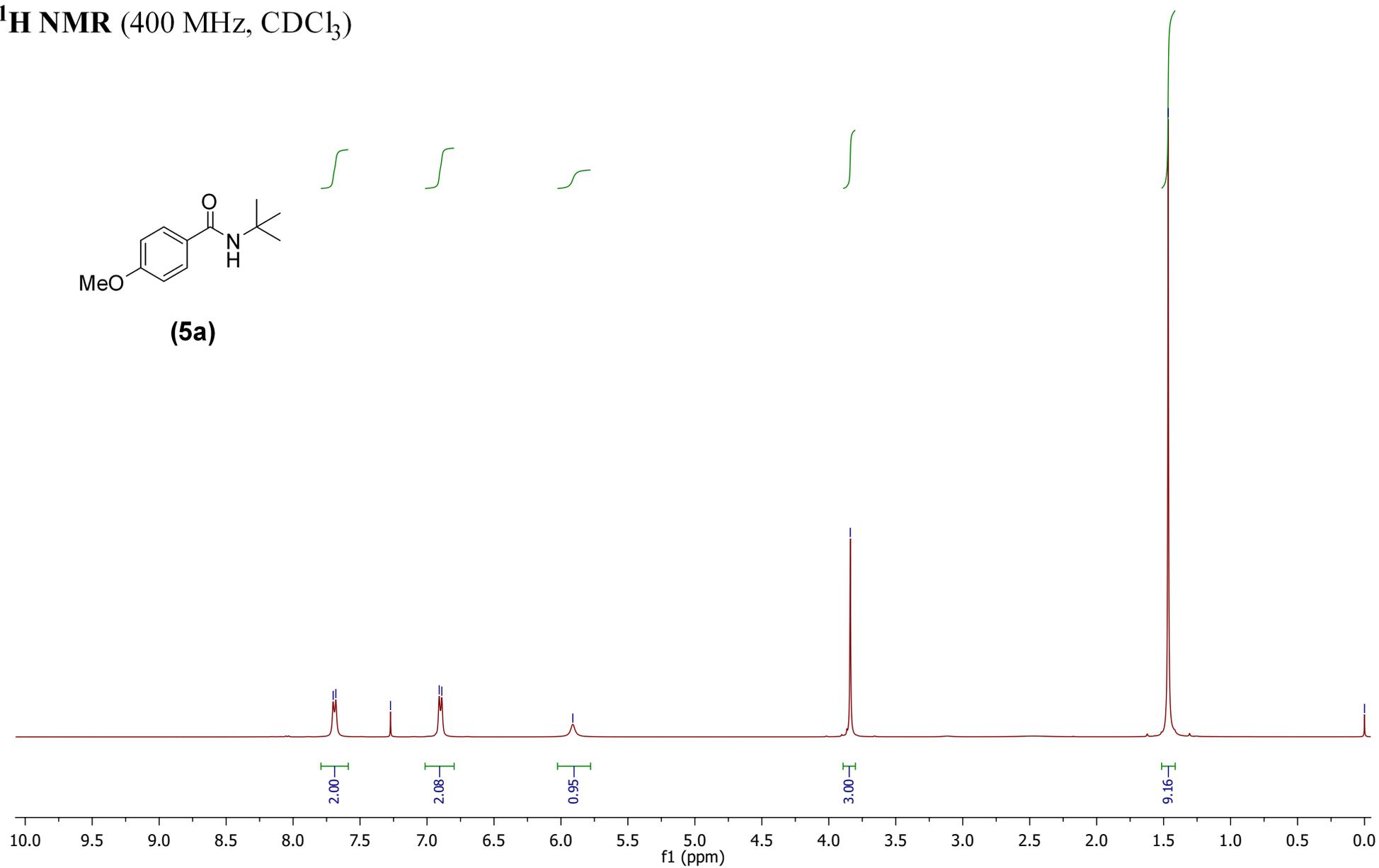
1.466

0.000

^1H NMR (400 MHz, CDCl_3)



(5a)



Amide NMR
sid-bk-204

—166.42
—161.77

—128.42
—128.05

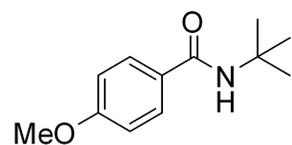
—113.55

—77.32
—77.00
—76.68

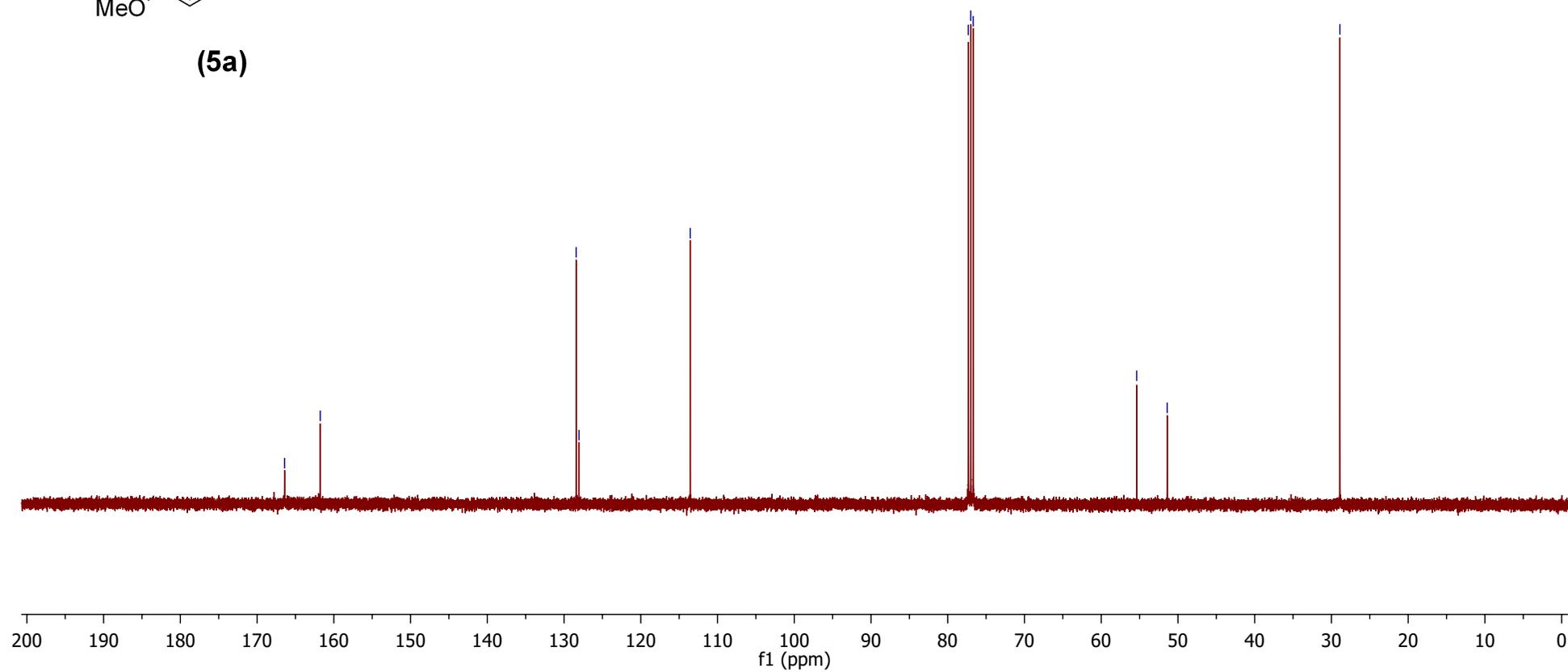
—55.38
—51.41

—28.89

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

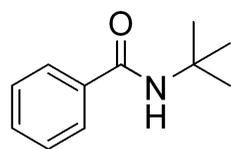


(5a)

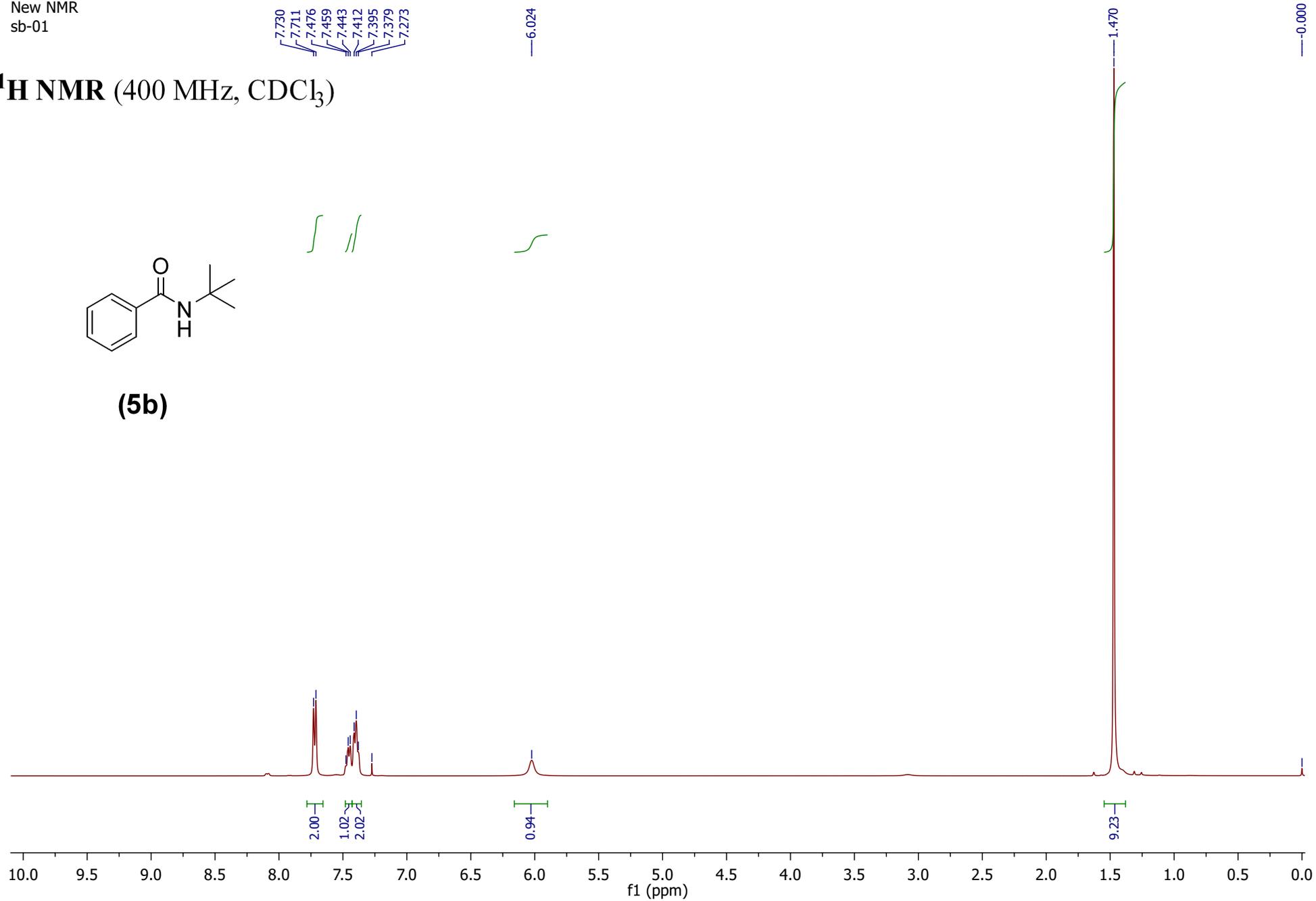


New NMR
sb-01

^1H NMR (400 MHz, CDCl_3)



(5b)



New NMR
sb-01

—166.91

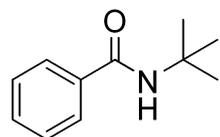
—135.80
—131.01
—128.40
—126.66

—77.35
—77.03
—76.71

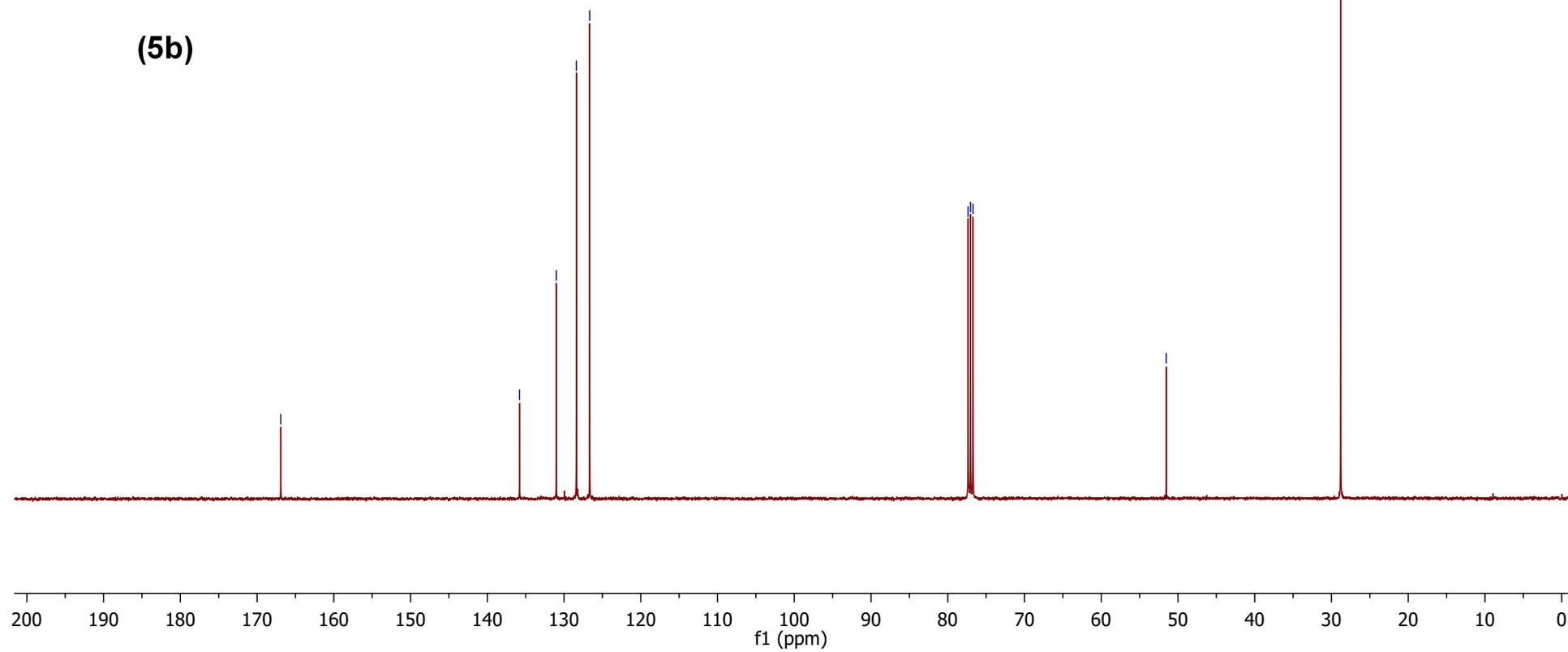
—51.54

—28.80

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



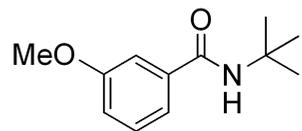
(5b)



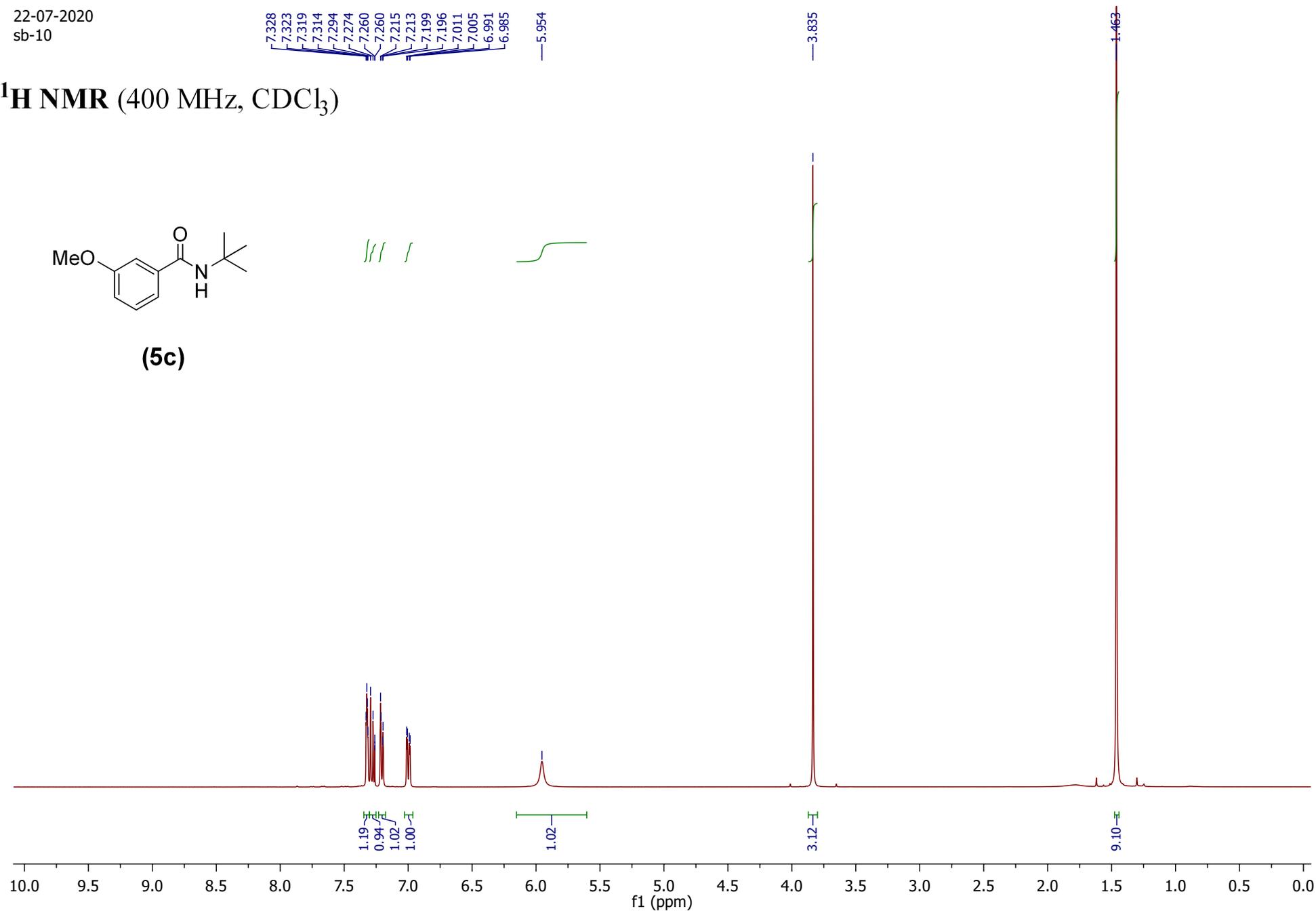
22-07-2020
sb-10

7.328
7.323
7.319
7.314
7.294
7.274
7.260
7.260
7.215
7.213
7.199
7.196
7.011
7.005
6.991
6.985
5.954

^1H NMR (400 MHz, CDCl_3)



(5c)



22-07-2020
sb-10

—166.71

—159.80

—137.41

—129.40

118.38

117.34

—112.12

77.35

77.03

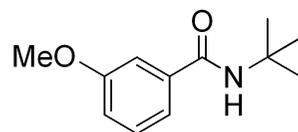
76.71

—55.42

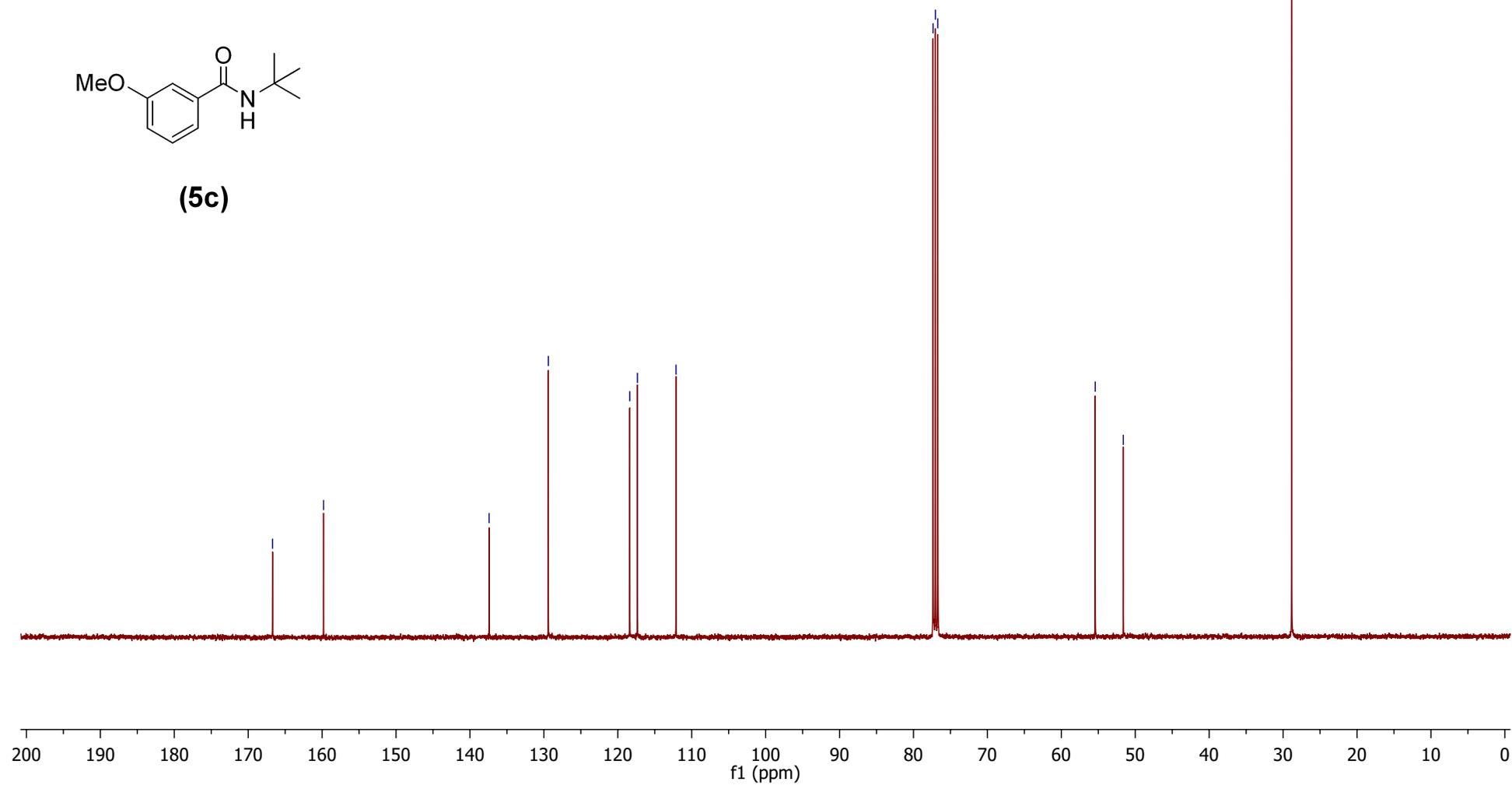
—51.62

—28.84

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



(5c)



New NMR
sb-15

7.545
7.504
7.497
7.493
7.491
7.488
7.483
7.478
7.306
7.287
7.273
7.272

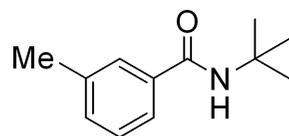
5.972

2.382

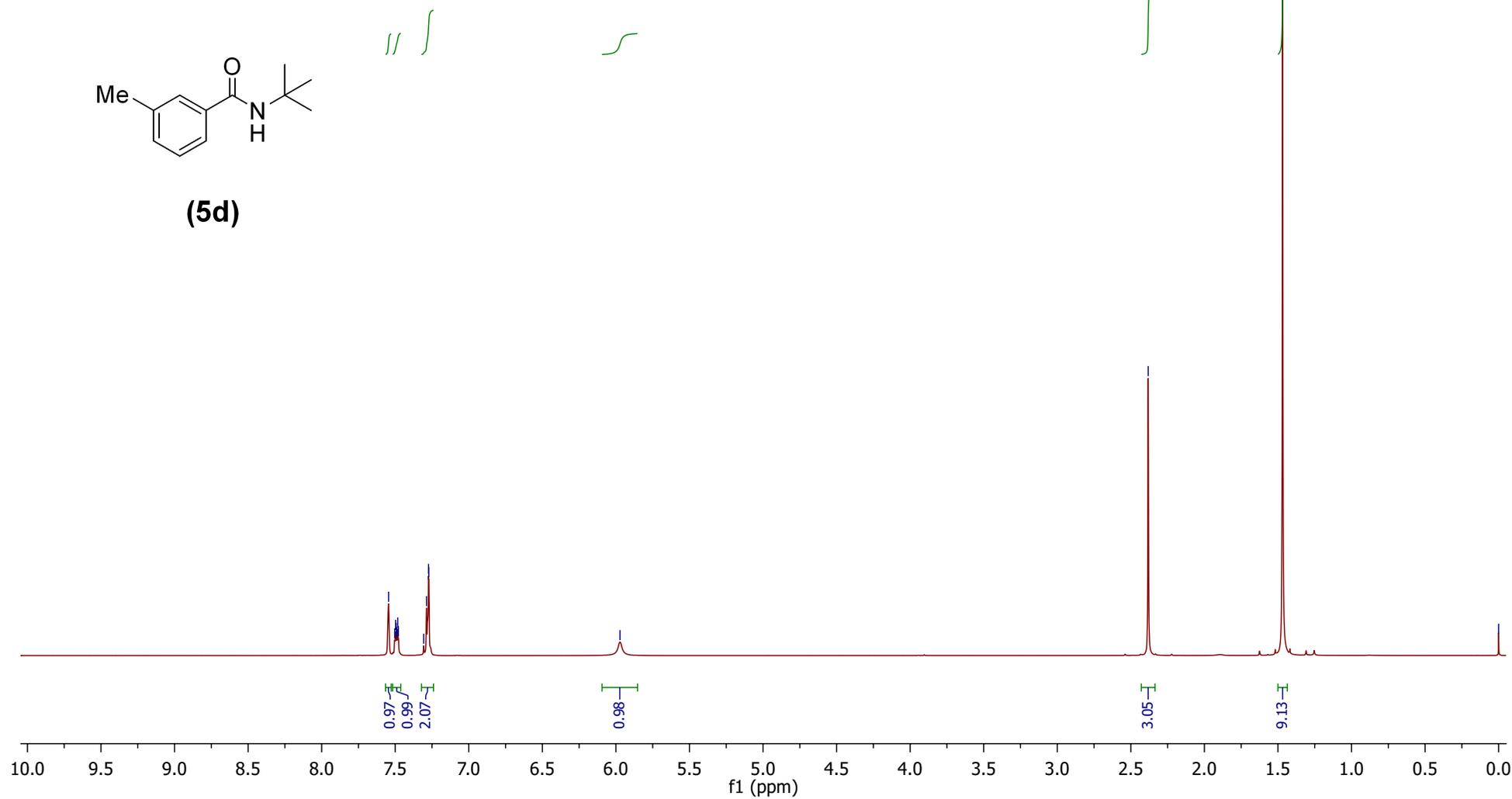
1.469

0.000

^1H NMR (400 MHz, CDCl_3)



(5d)



New NMR
sb-15

—167.06

138.25
135.82
131.75
128.29
127.45
123.61

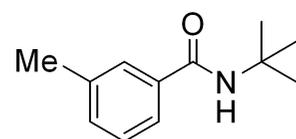
77.35
77.03
76.71

—51.51

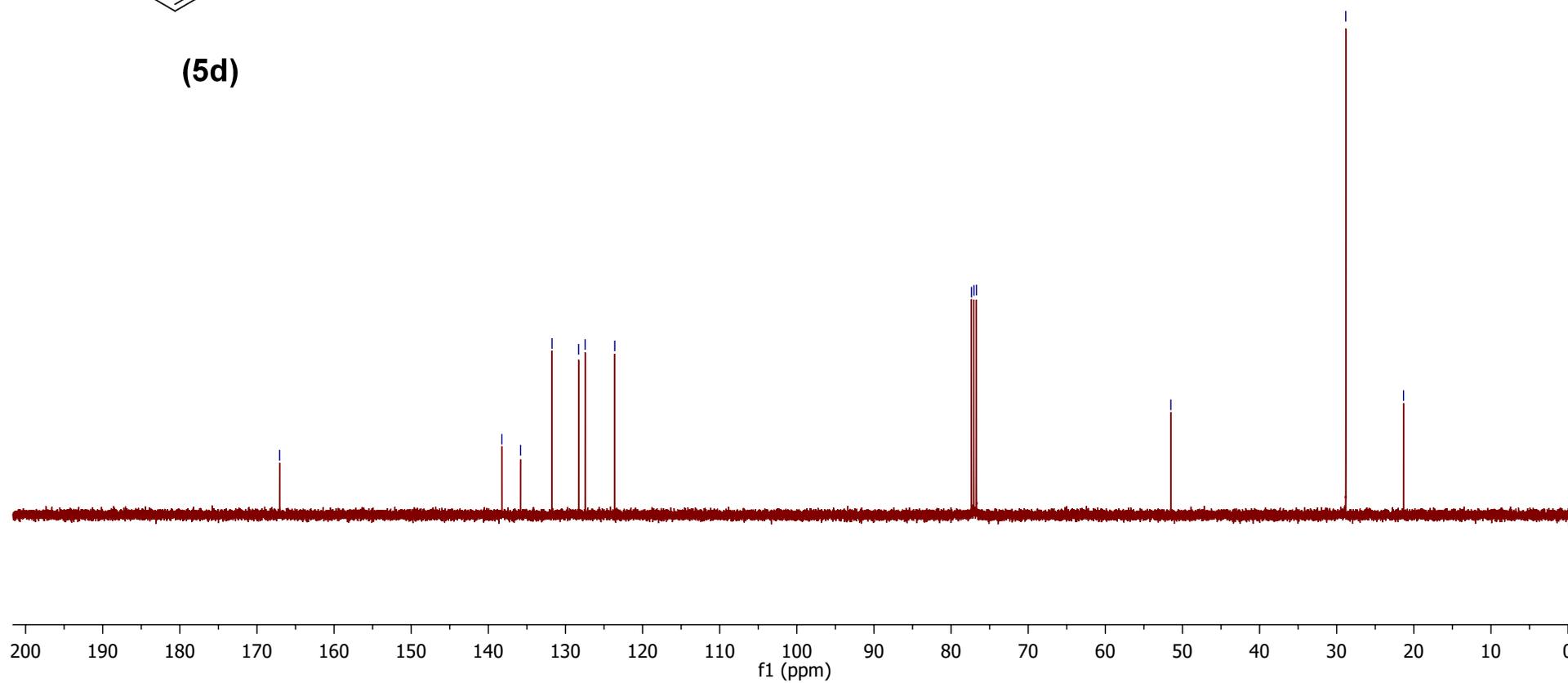
—28.82

—21.33

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



(5d)



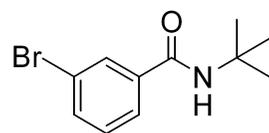
New NMR
sb-11

7.851
7.847
7.842
7.648
7.628
7.604
7.602
7.599
7.584
7.582
7.579
7.305
7.285
7.270
7.266

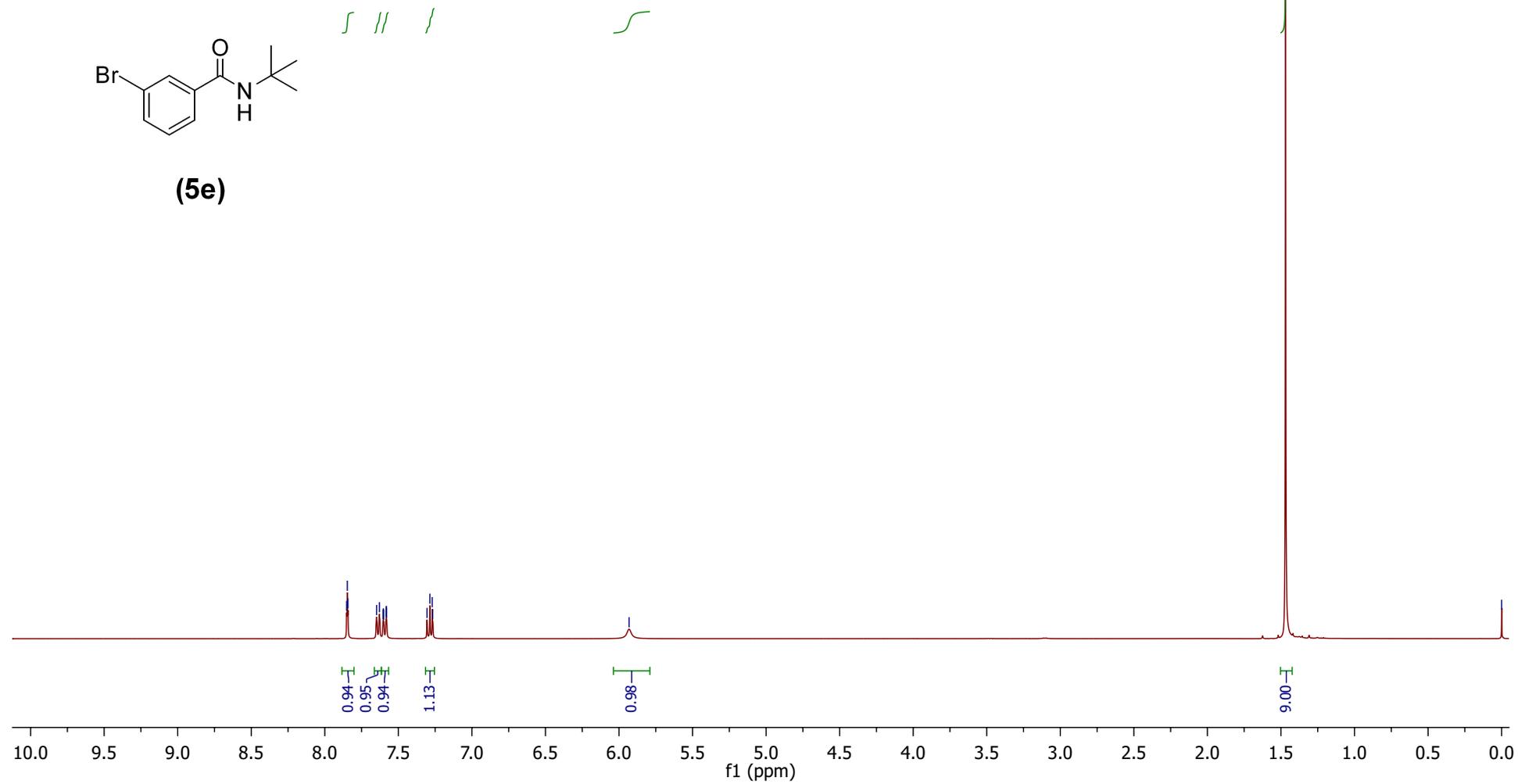
5.931

1.469
0.000

^1H NMR (400 MHz, CDCl_3)



(5e)



New NMR
sb-11

165.41

137.88

134.01

130.06

129.93

125.35

122.62

77.34

77.02

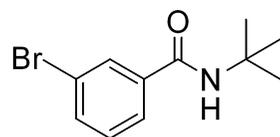
76.71

51.88

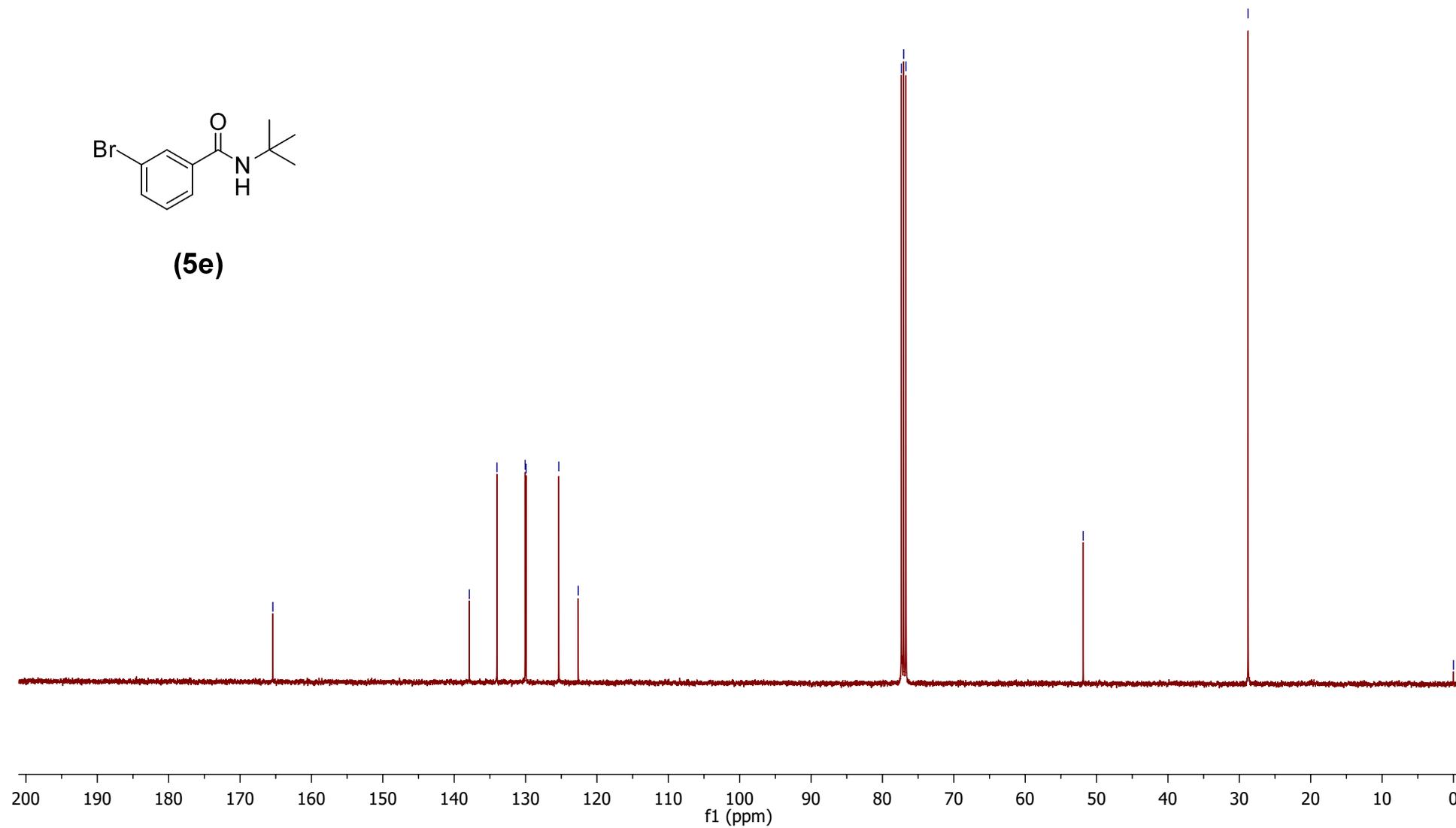
28.78

-0.00

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



(5e)



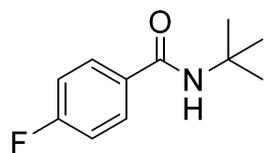
22-07-2020
sb-14

7.737
7.730
7.725
7.717
7.713
7.708
7.700
7.695
7.688
7.260
7.083
7.062
7.040

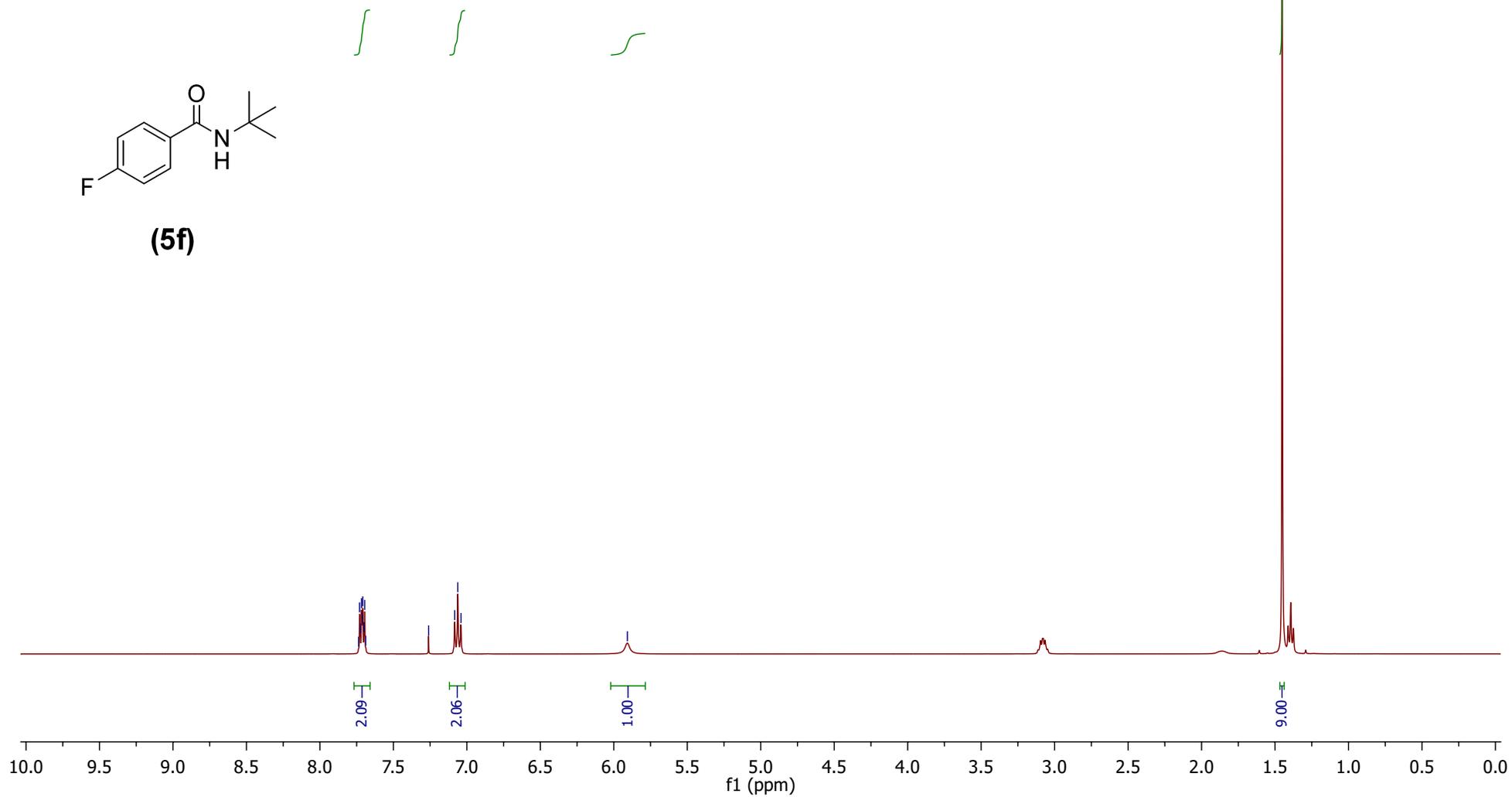
5.907

1.451

^1H NMR (400 MHz, CDCl_3)



(5f)



22-07-2020
sb-14

165.85
165.69
163.19

132.08
132.05
129.02
128.93

115.50
115.28

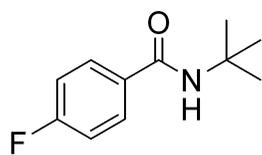
77.35
77.03
76.71

51.70
45.79

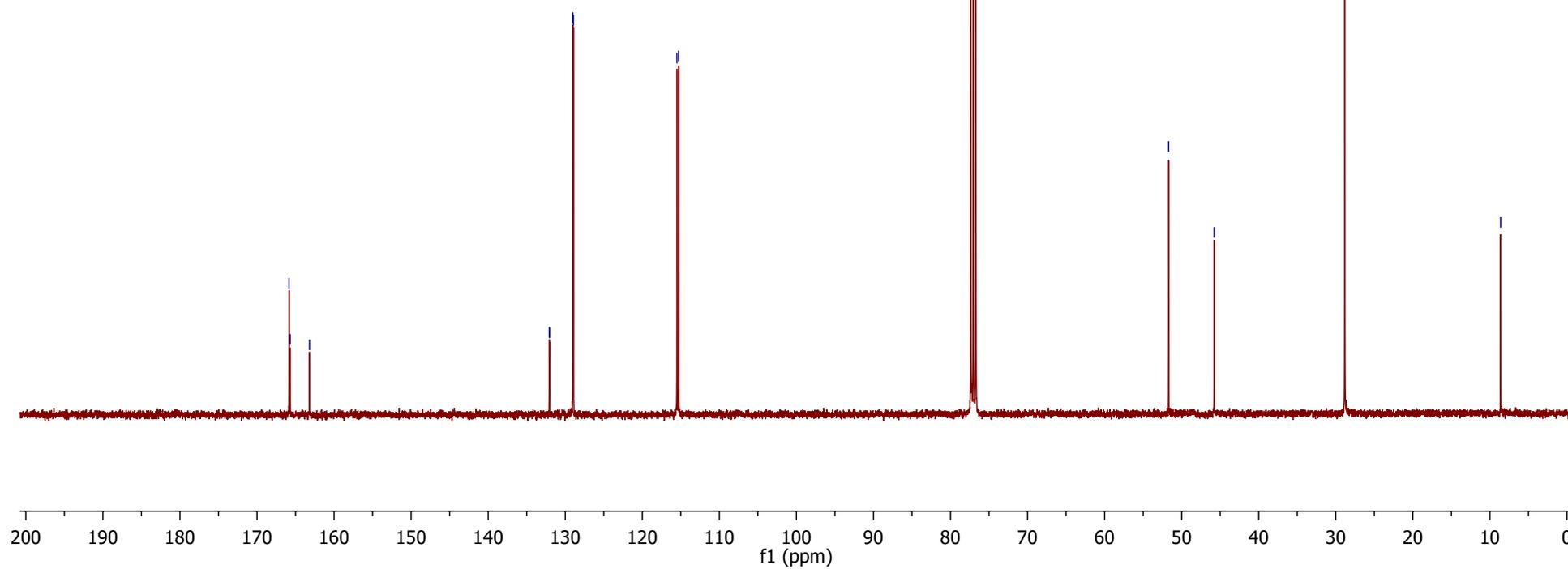
28.84

8.61

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



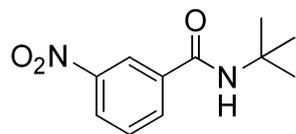
(5f)



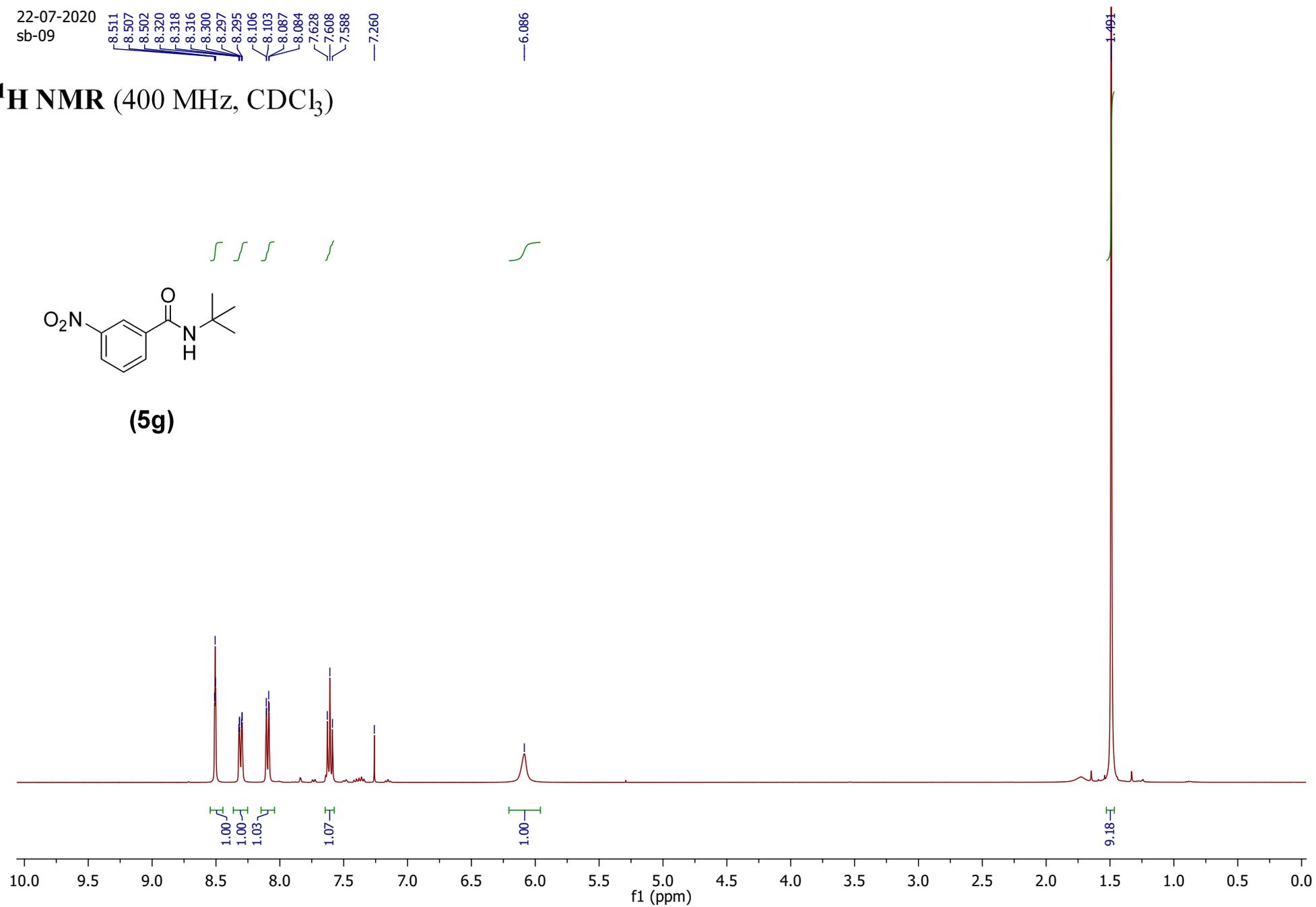
22-07-2020
sb-09

8.511
8.507
8.502
8.320
8.318
8.316
8.300
8.297
8.295
8.106
8.103
8.087
8.084
7.628
7.608
7.588
7.260
6.086

^1H NMR (400 MHz, CDCl_3)



(5g)



22-07-2020
sb-09

—164.44

—148.07

—137.52

—133.09

—129.74

—125.68

—121.53

—77.35

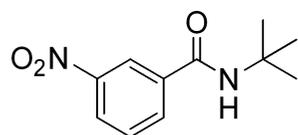
—77.03

—76.71

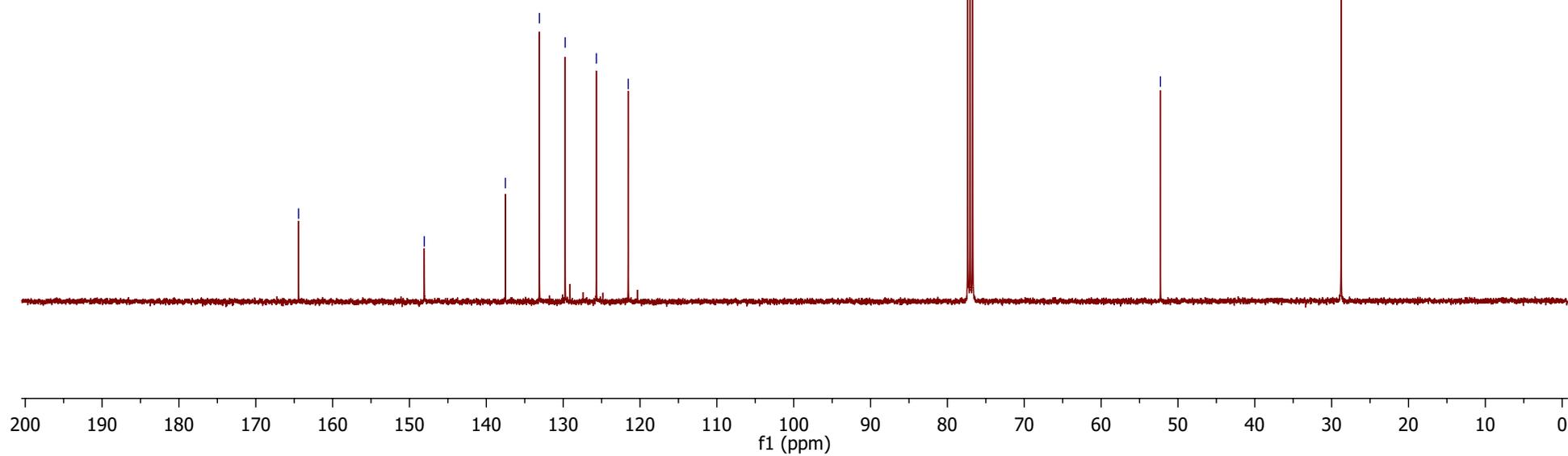
—52.28

—28.76

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

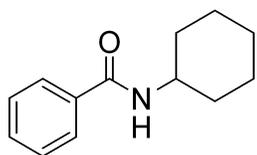


(5g)

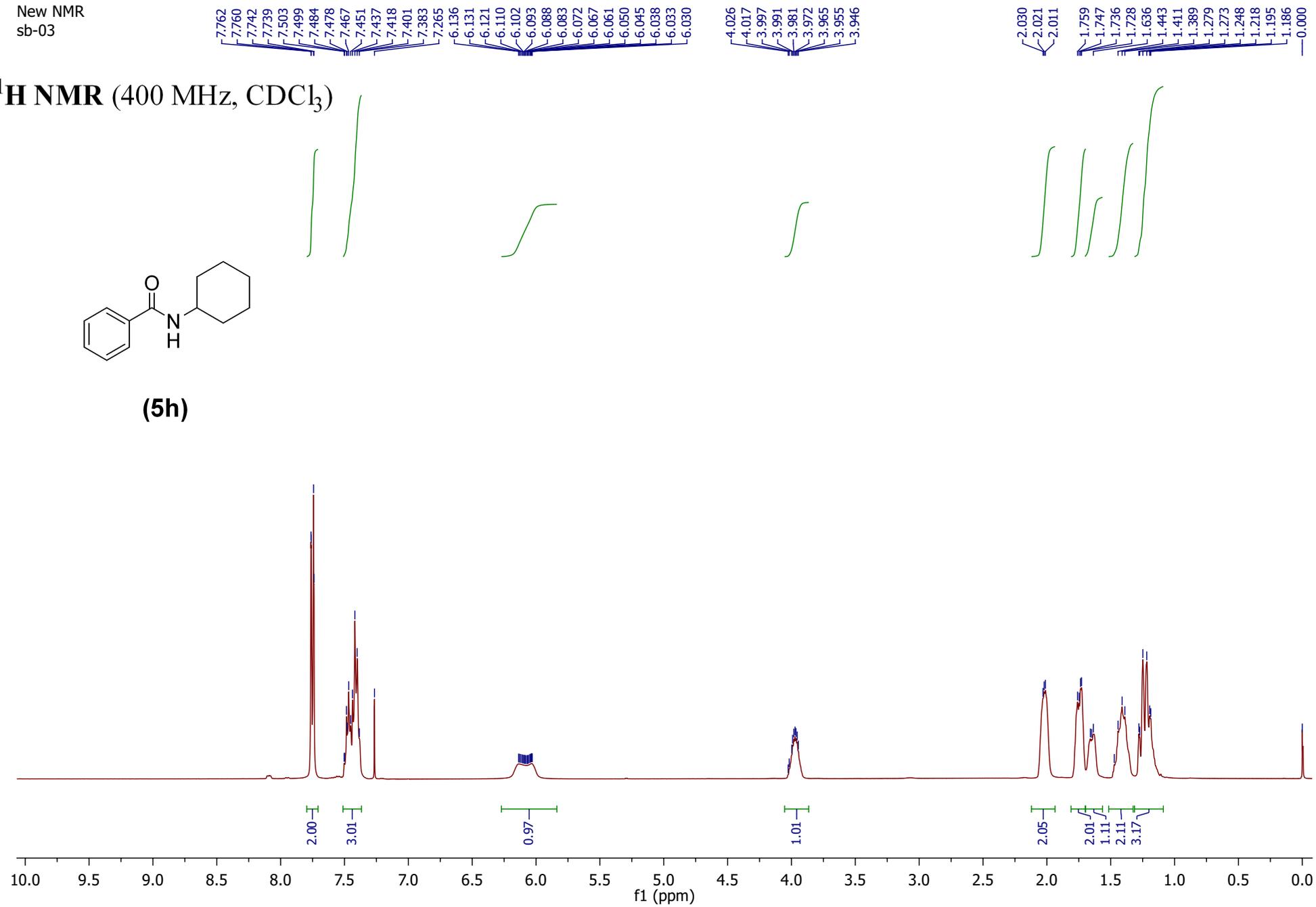


New NMR
sb-03

^1H NMR (400 MHz, CDCl_3)



(5h)



New NMR
sb-03

—166.66

—135.05
—131.21
—128.50
—128.47
—126.85

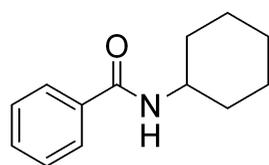
—77.35
—77.03
—76.71

—48.68

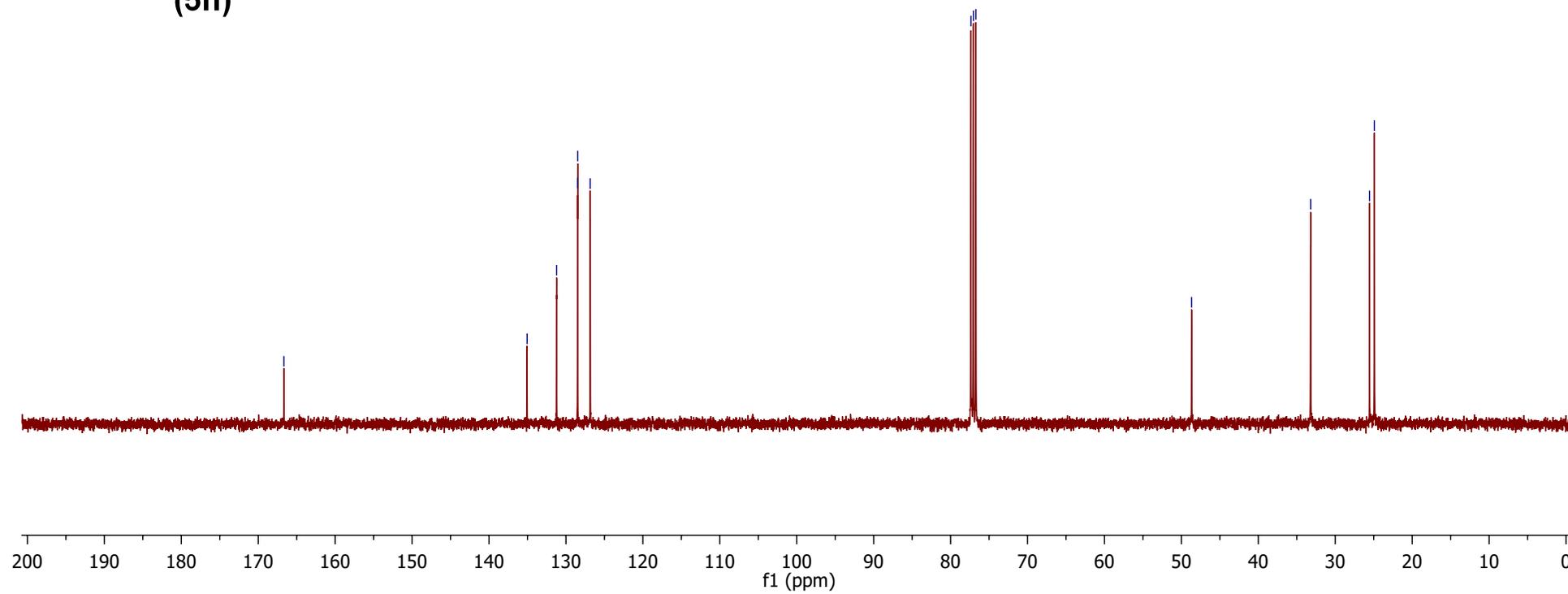
—33.19

—25.54
—24.92

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



(5h)



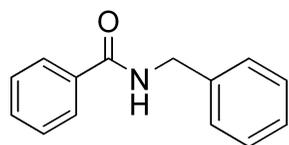
New NMR
sb-04

7.805
7.800
7.797
7.784
7.780
7.776
7.492
7.473
7.430
7.413
7.409
7.349
7.338
6.580

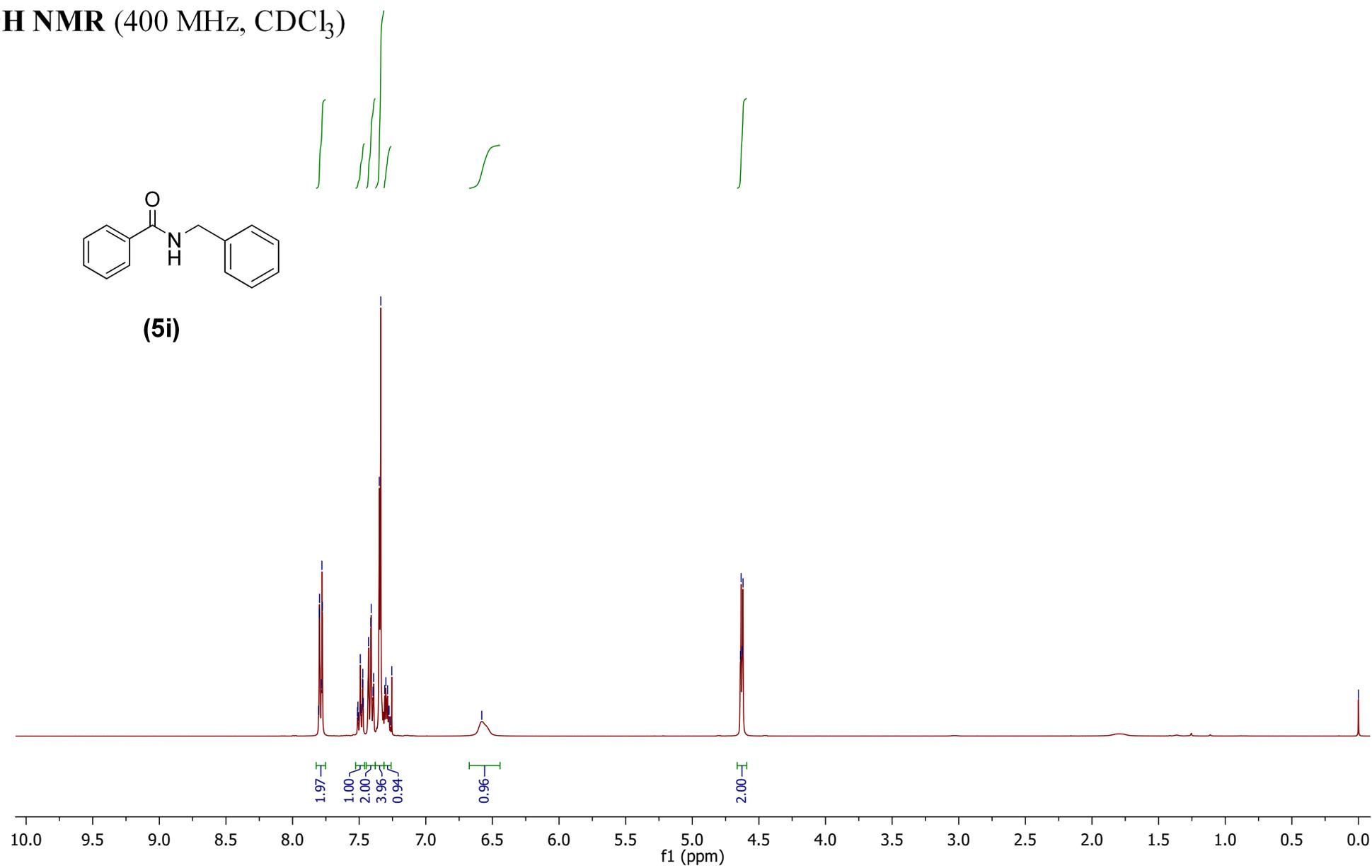
4.639
4.634
4.625
4.619

-0.000

^1H NMR (400 MHz, CDCl_3)



(5i)



New NMR
sb-04

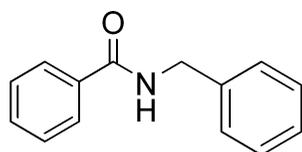
—167.38

138.17
134.33
131.53
128.76
128.57
127.89
127.58
126.96

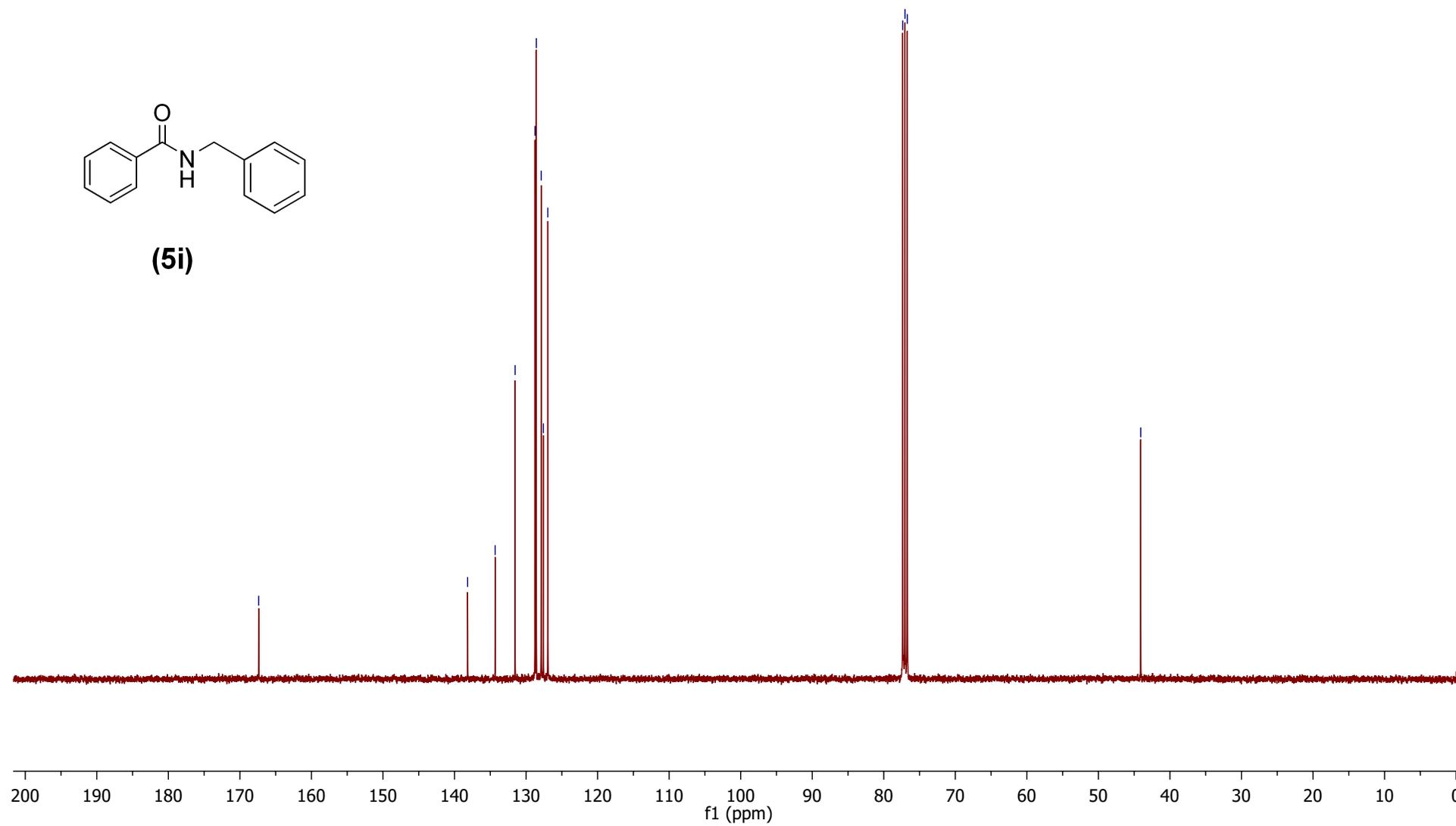
77.35
77.03
76.71

—44.08

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



(5i)



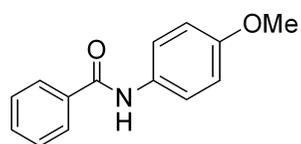
New NMR
sb-05

7.868
7.851
7.847
7.819
7.553
7.531
7.469
7.391
6.913
6.907
6.896
6.890
6.882

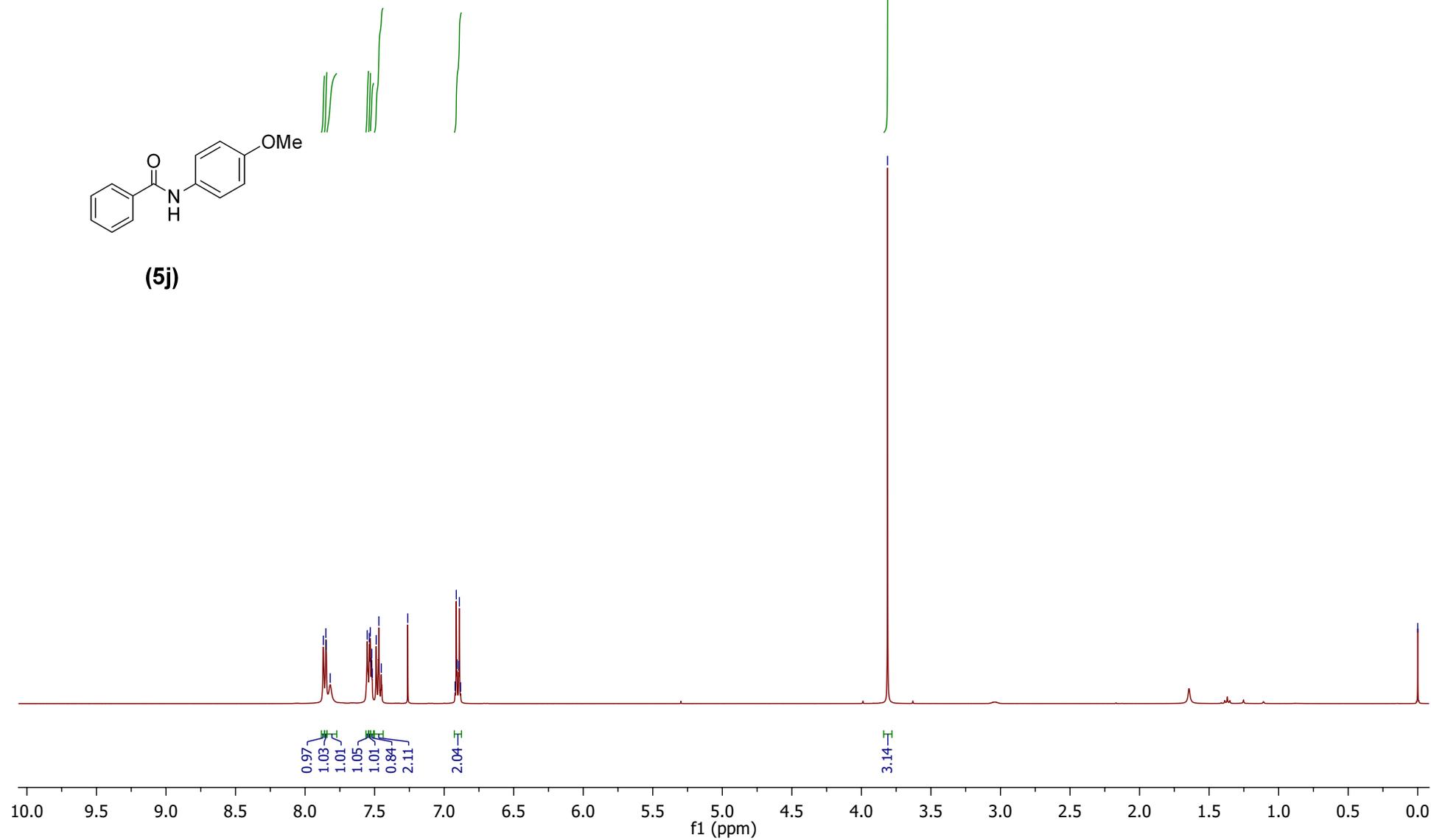
3.812

0.000

^1H NMR (400 MHz, CDCl_3)



(5j)



New NMR
sb-05

— 165.65

— 156.60

— 135.01

— 131.71

— 130.98

— 128.74

— 126.98

— 122.11

— 114.22

— 77.34

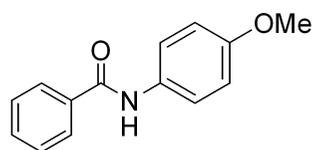
— 77.03

— 76.71

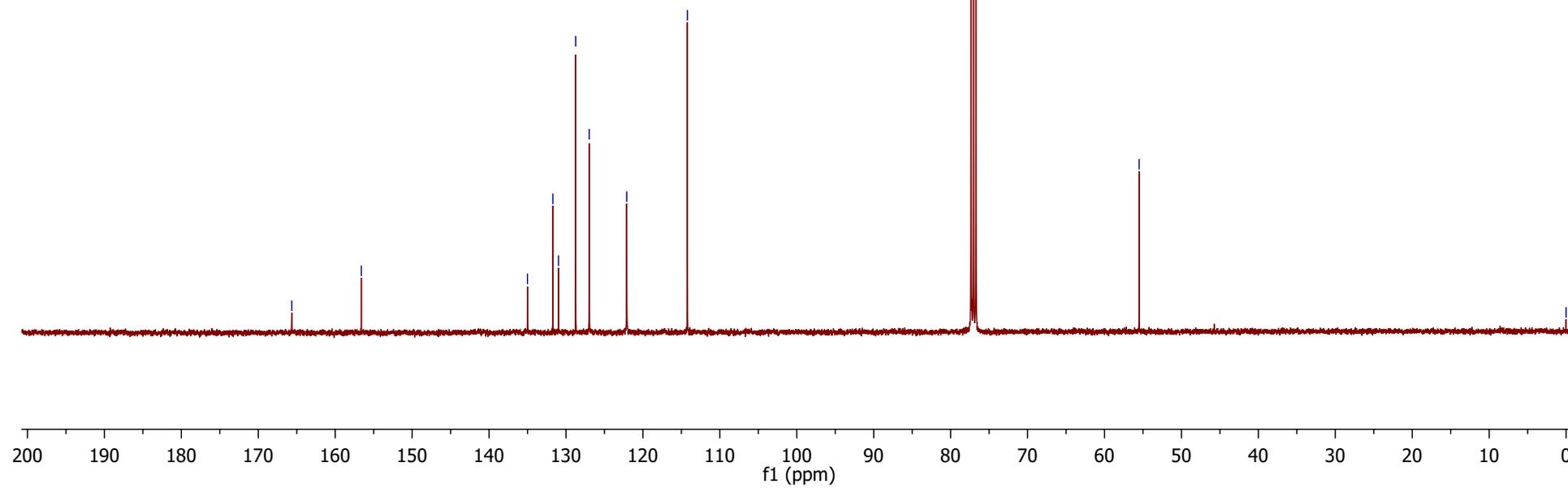
— 55.50

— 0.00

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



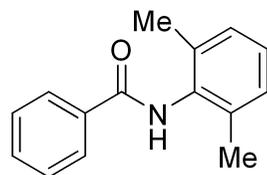
(5j)



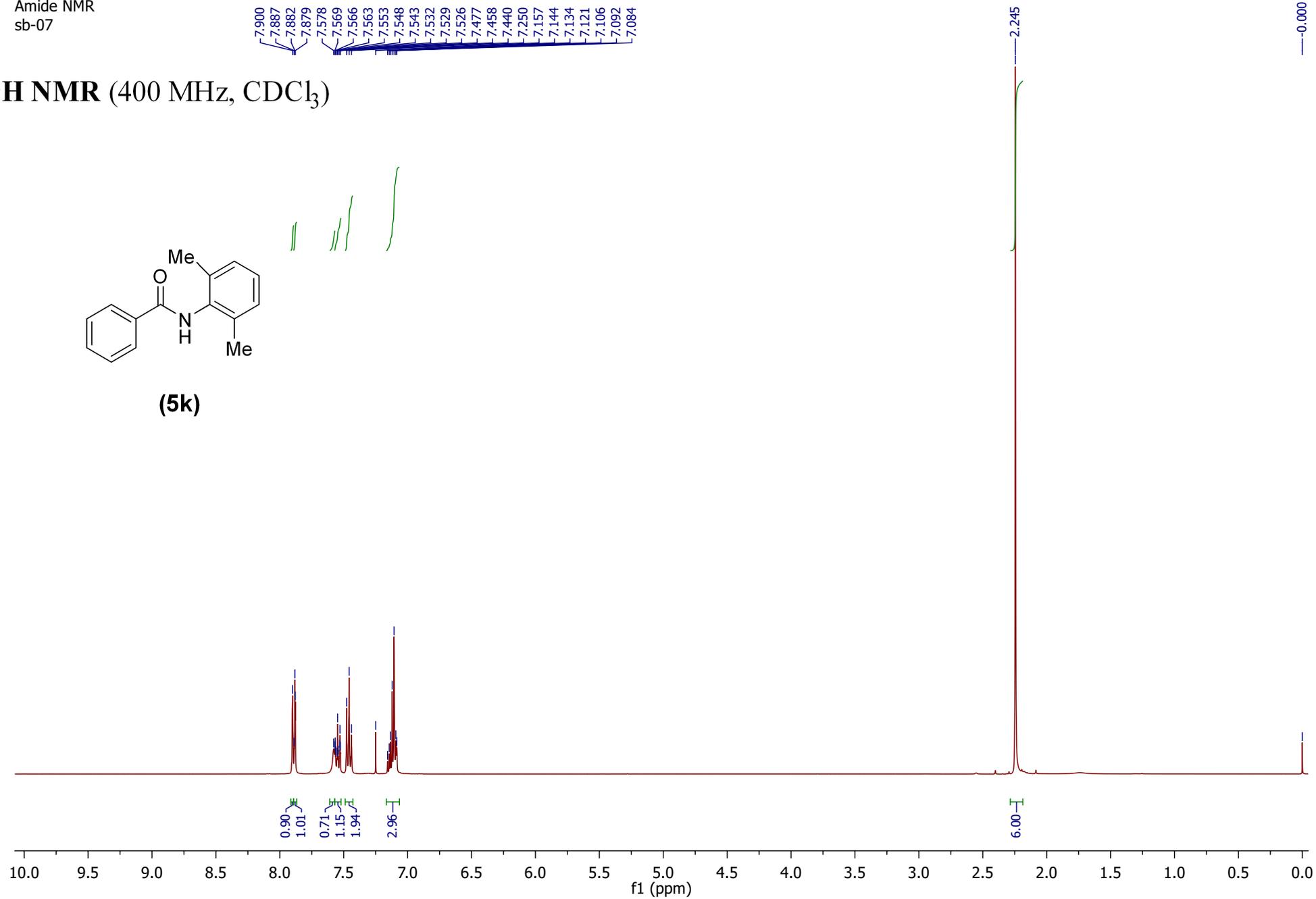
Amide NMR
sb-07

7.900
7.887
7.882
7.879
7.578
7.569
7.566
7.563
7.553
7.548
7.543
7.532
7.529
7.526
7.477
7.458
7.440
7.250
7.157
7.144
7.134
7.121
7.106
7.092
7.084

^1H NMR (400 MHz, CDCl_3)



(5k)



Amide NMR
sb-07

165.93

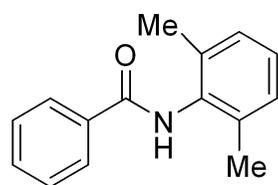
135.57
134.38
133.87
131.74
128.69
128.23
127.38
127.22

77.35
77.03
76.71

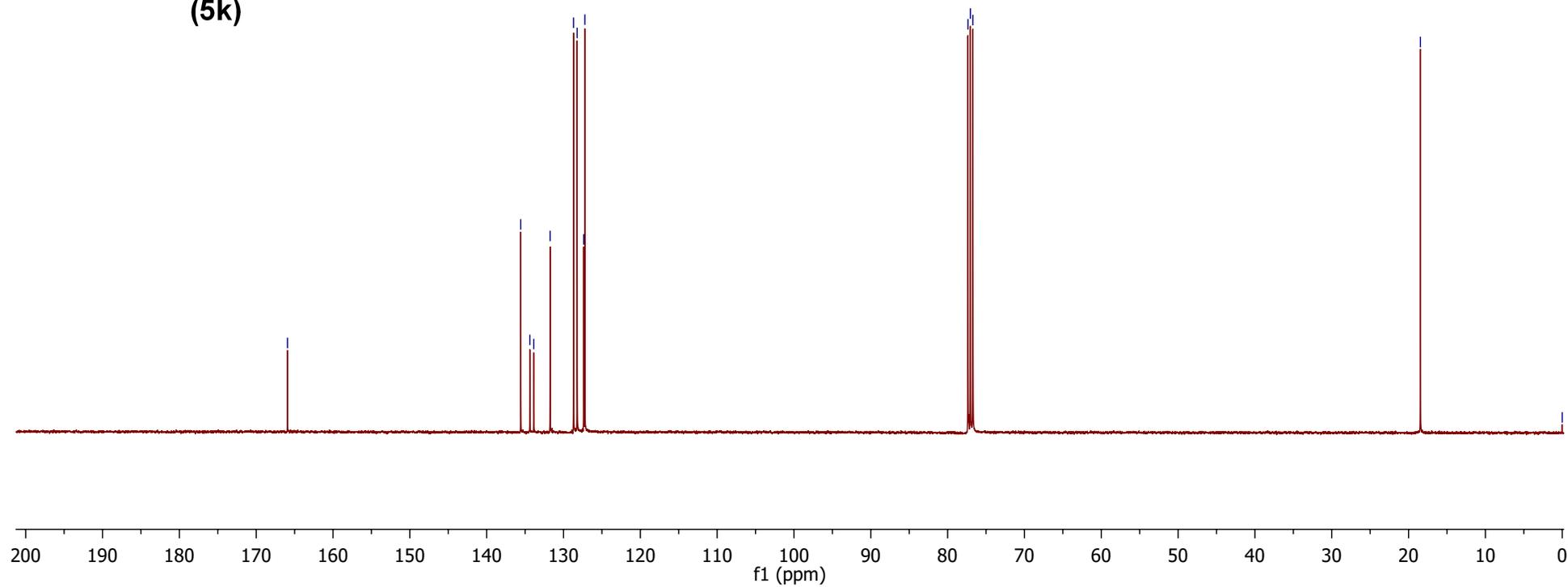
18.46

0.00

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



(5k)



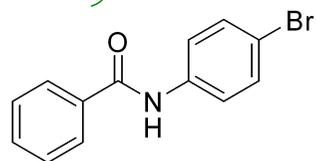
Amide NMR
sb-08

9.157

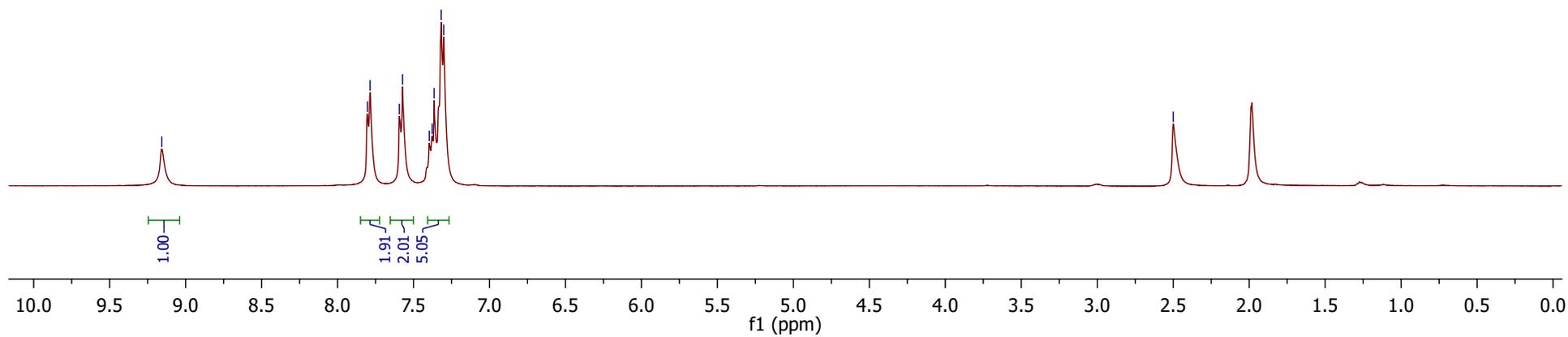
7.804
7.786
7.593
7.572
7.396
7.377
7.364
7.318
7.301

2.500

^1H NMR (400 MHz, $\text{CDCl}_3 + \text{DMSO } d_6$)



(51)



Amide NMR
sb-08

166.23

138.18

135.06

131.81

128.58

127.56

122.10

116.55

77.93

77.61

77.29

30.69

30.50

30.30

30.11

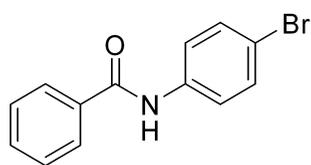
29.92

29.72

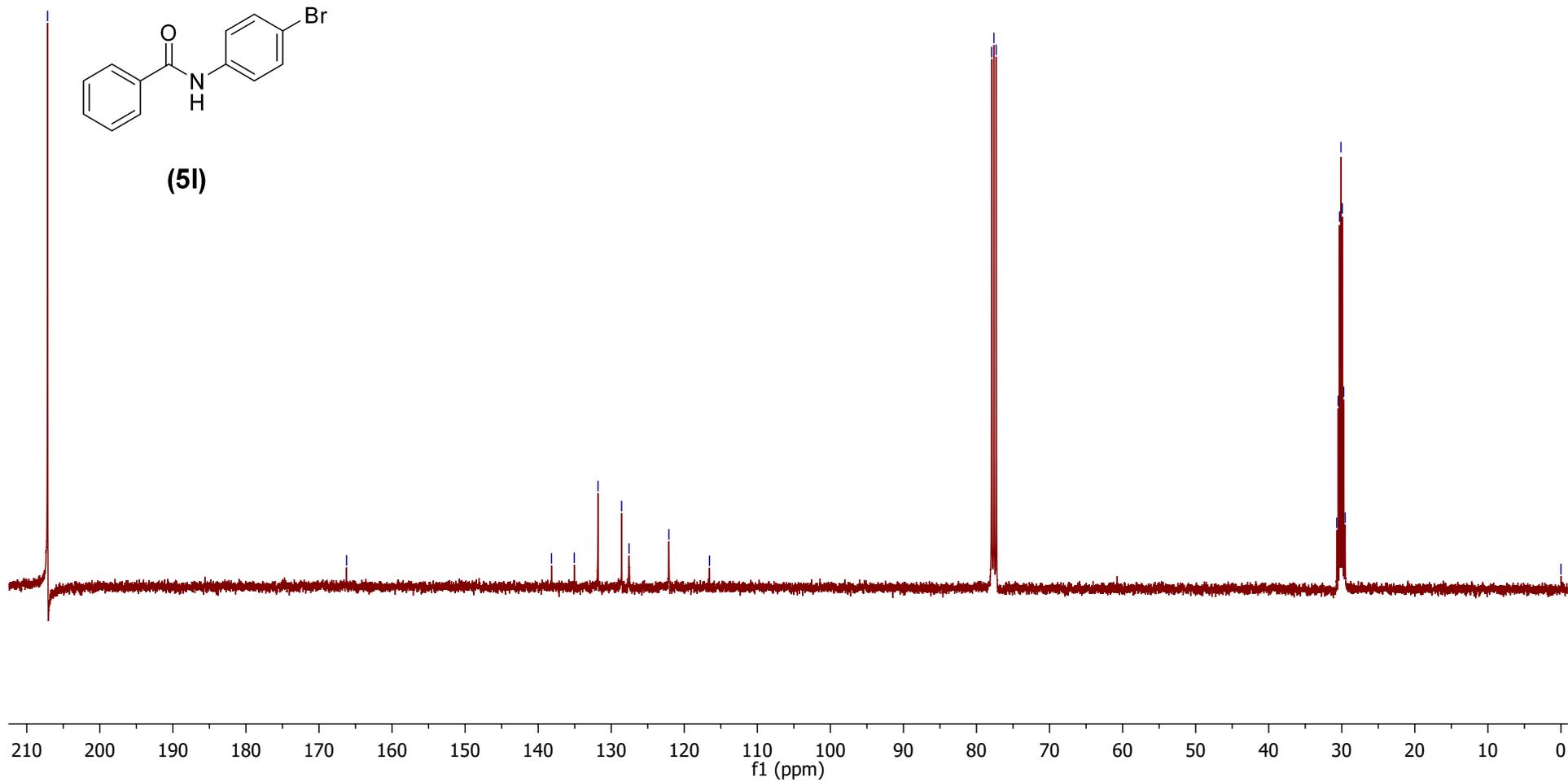
29.53

-0.00

^{13}C NMR (100 MHz, $\text{CDCl}_3 + \text{DMSO } d_6$)



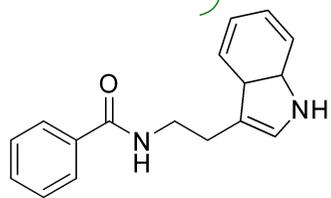
(5I)



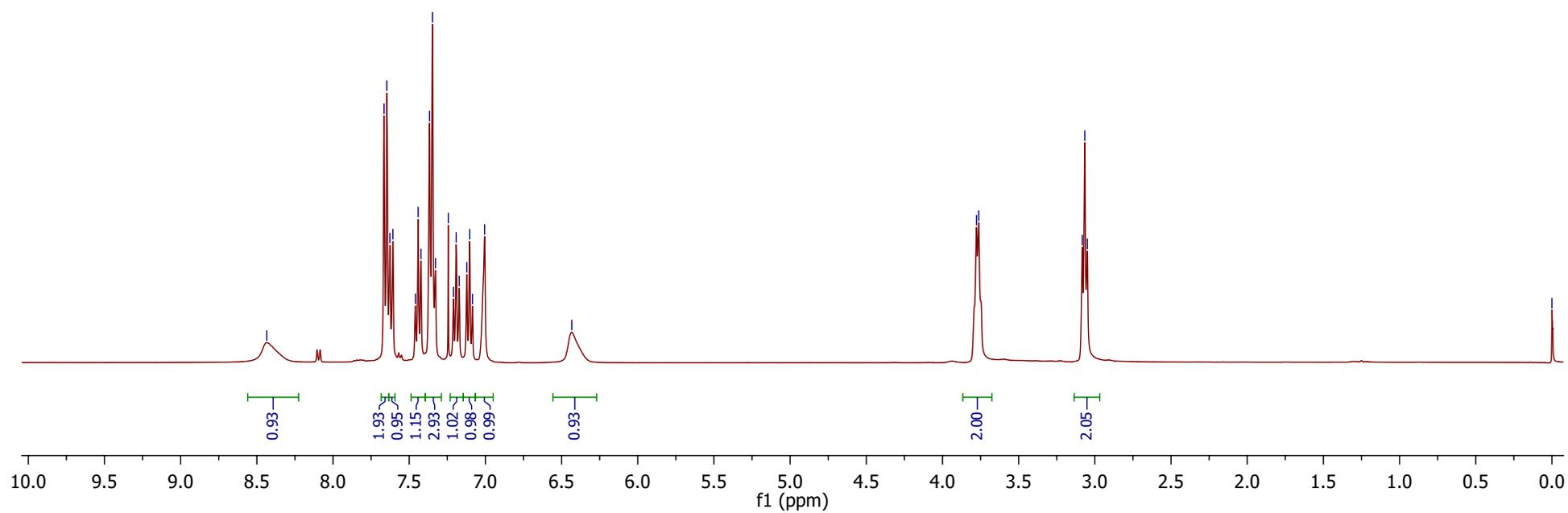
Amide NMR
sb-06

8.435
7.665
7.647
7.627
7.607
7.441
7.423
7.366
7.347
7.327
7.243
7.192
7.172
7.122
7.103
6.995
3.776
3.762
3.082
3.066
3.049
-0.000

^1H NMR (400 MHz, CDCl_3)



(5m)



Amide NMR
sb-06

—167.73

136.42
134.39
131.44
128.52
127.23
126.87
122.24
122.13
119.41
118.66
112.67
111.39

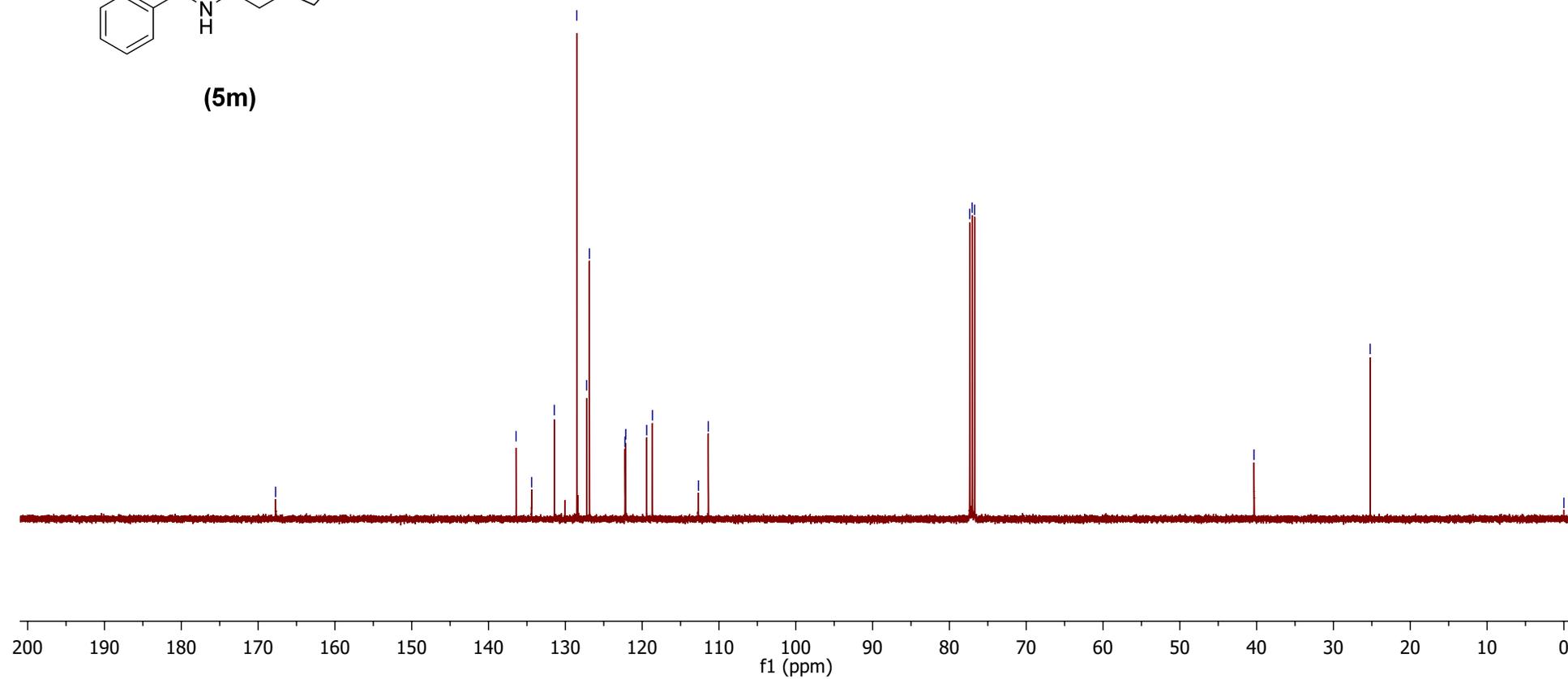
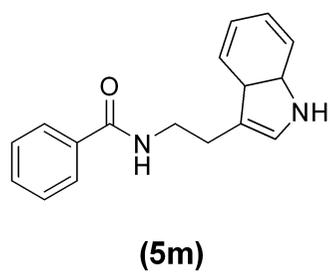
77.36
77.04
76.72

—40.35

—25.22

—0.00

¹³C NMR (100 MHz, CDCl₃)



NJC
bb-38

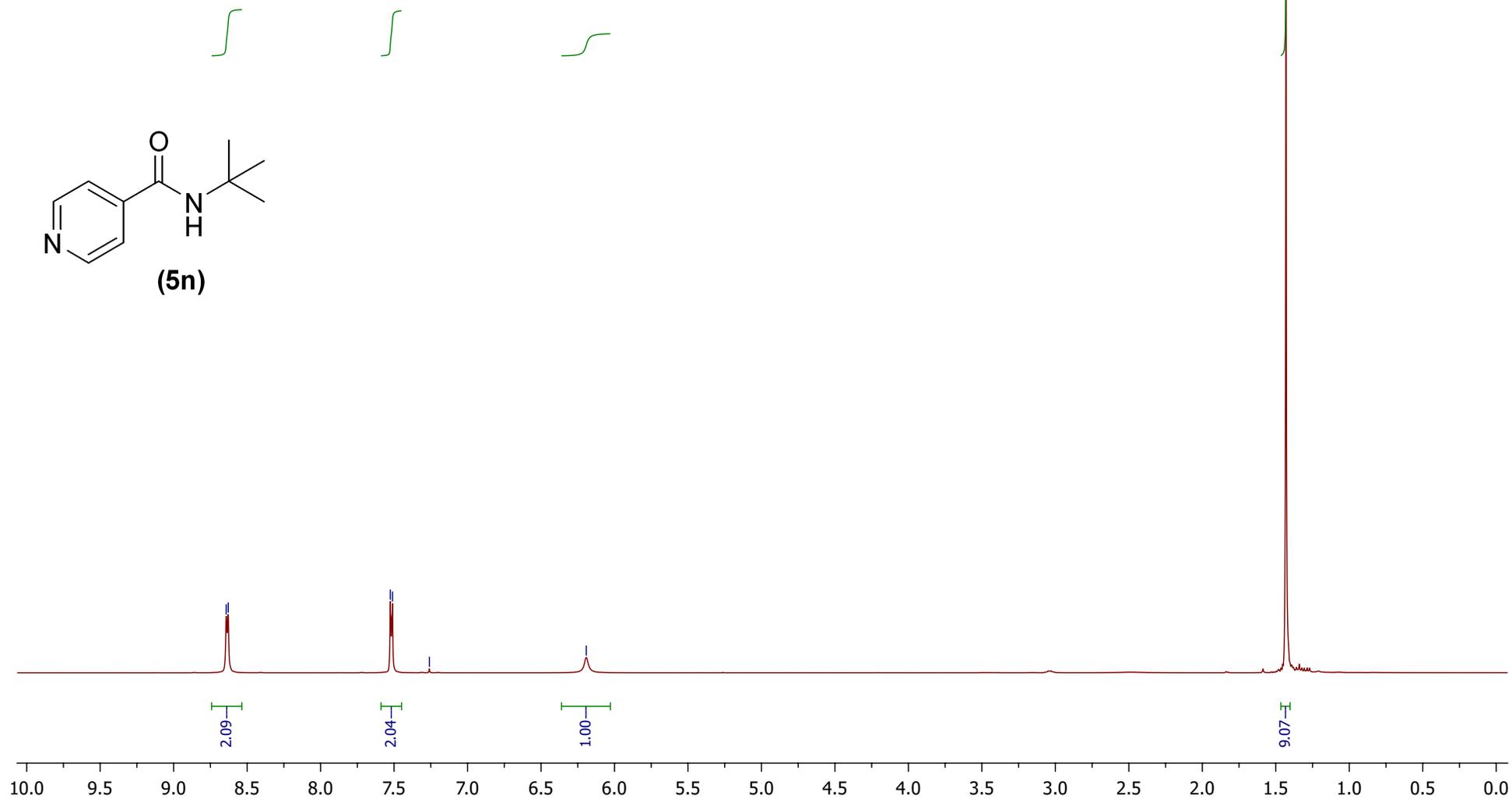
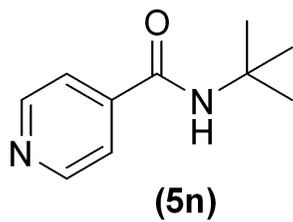
8.643
8.629

7.526
7.511
7.260

6.192

1.430

^1H NMR (400 MHz, CDCl_3)



NJC
bb-38

— 164.83

— 150.29

— 142.82

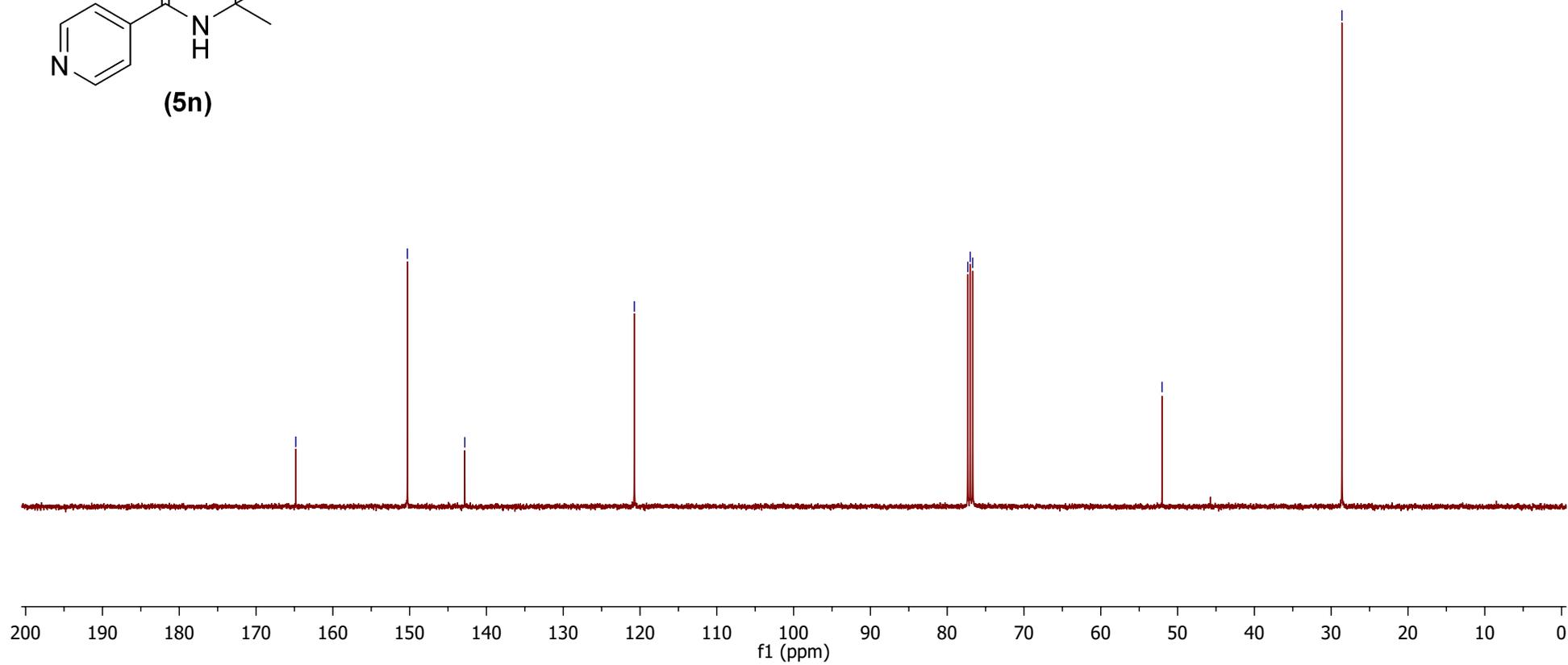
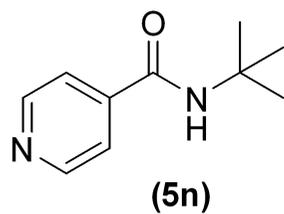
— 120.74

77.32
77.00
76.68

— 52.03

— 28.59

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



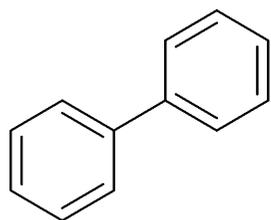
NMR July 2019
sb-47

7.512
7.509
7.504
7.493
7.491
7.488
7.482
7.326
7.324
7.319
7.306
7.302
7.290
7.287
7.281
7.262
7.249
7.246
7.242
7.232
7.227
7.222
7.212
7.209
7.206

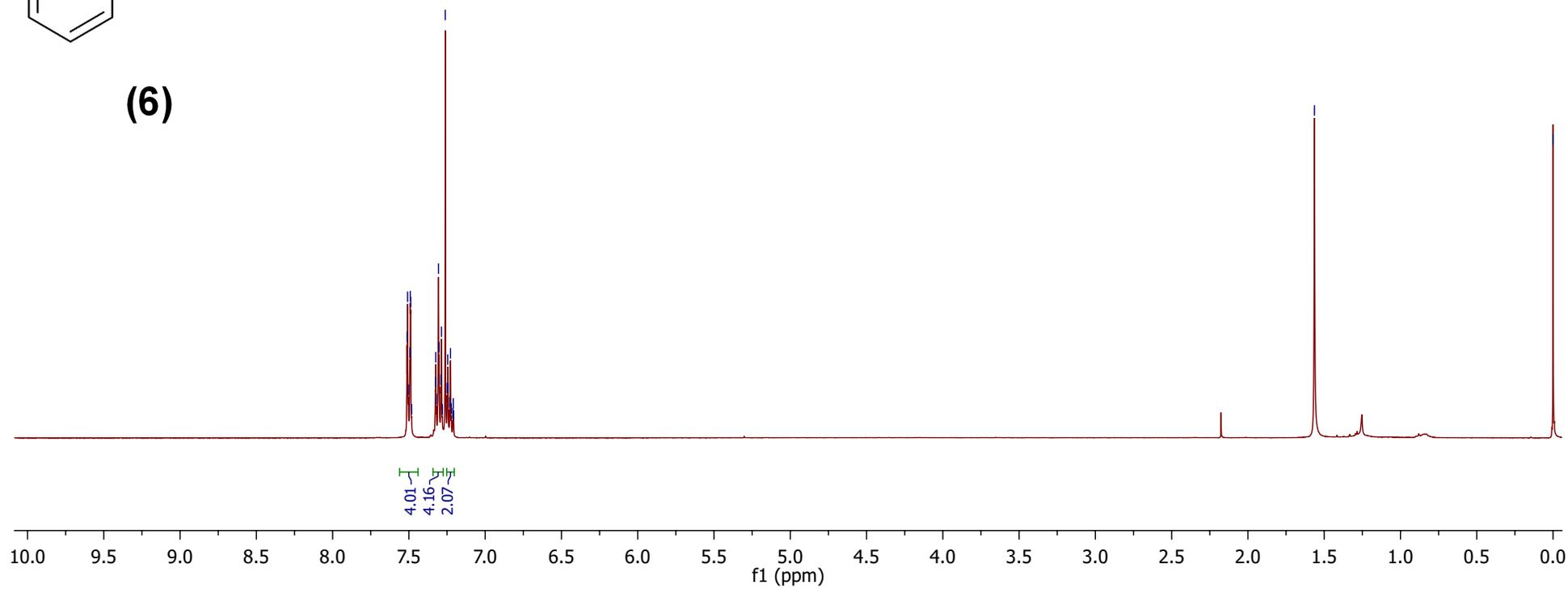
1.564

0.000

^1H NMR (400 MHz, CDCl_3)



(6)



NMR july 2019
sb-47

136.99

129.05

127.46

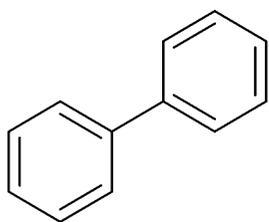
127.13

77.32

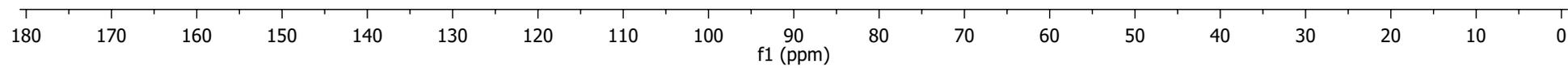
77.00

76.68

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



(6)



SID-56-A 17 (0.304) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (17:20)

TOF MS ES+
1.58e7

