

SUPPORTING INFORMATION

PROTON NMR AND SELECTED CARBON NMR SPECTRA

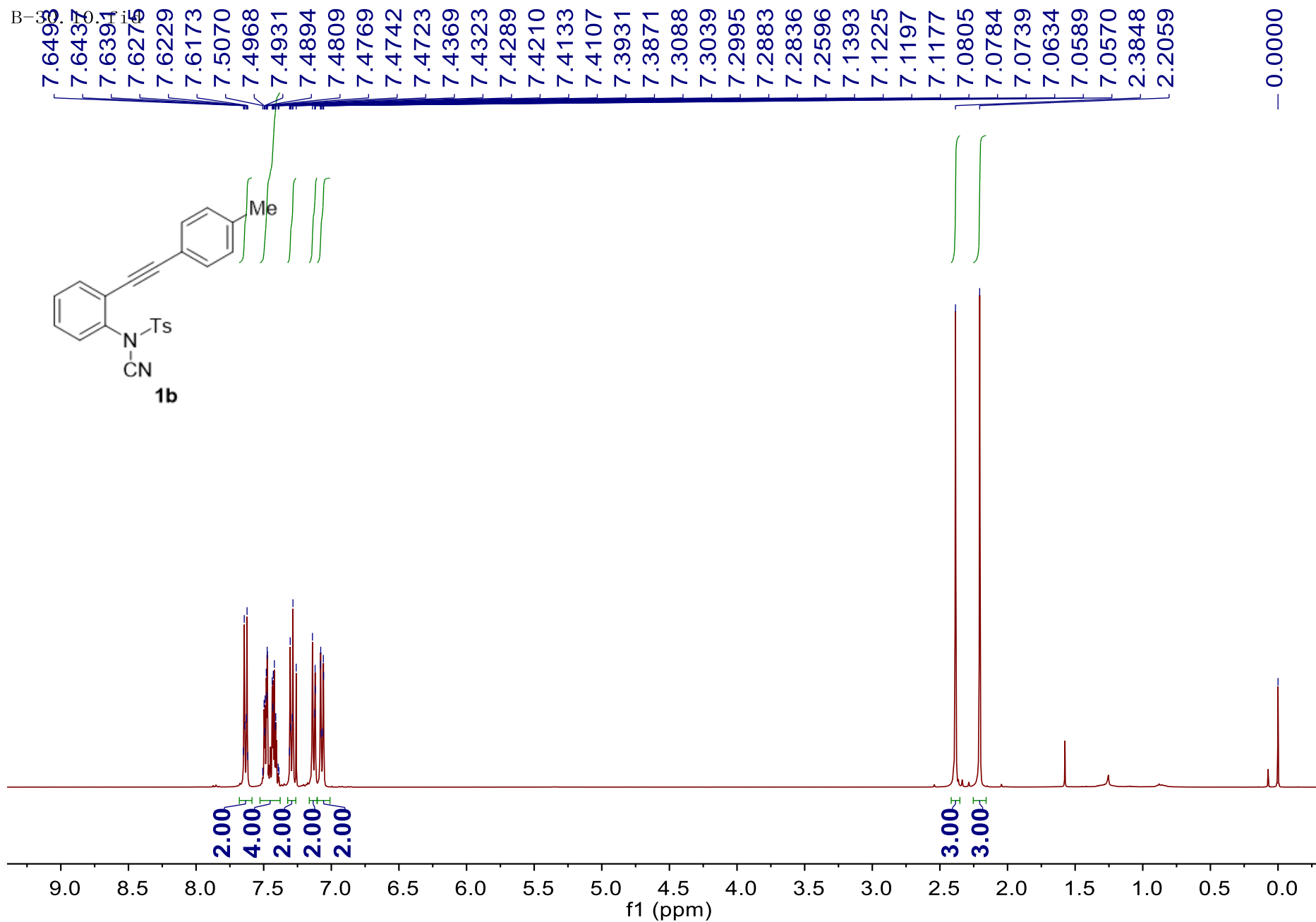
for the
communication
entitled

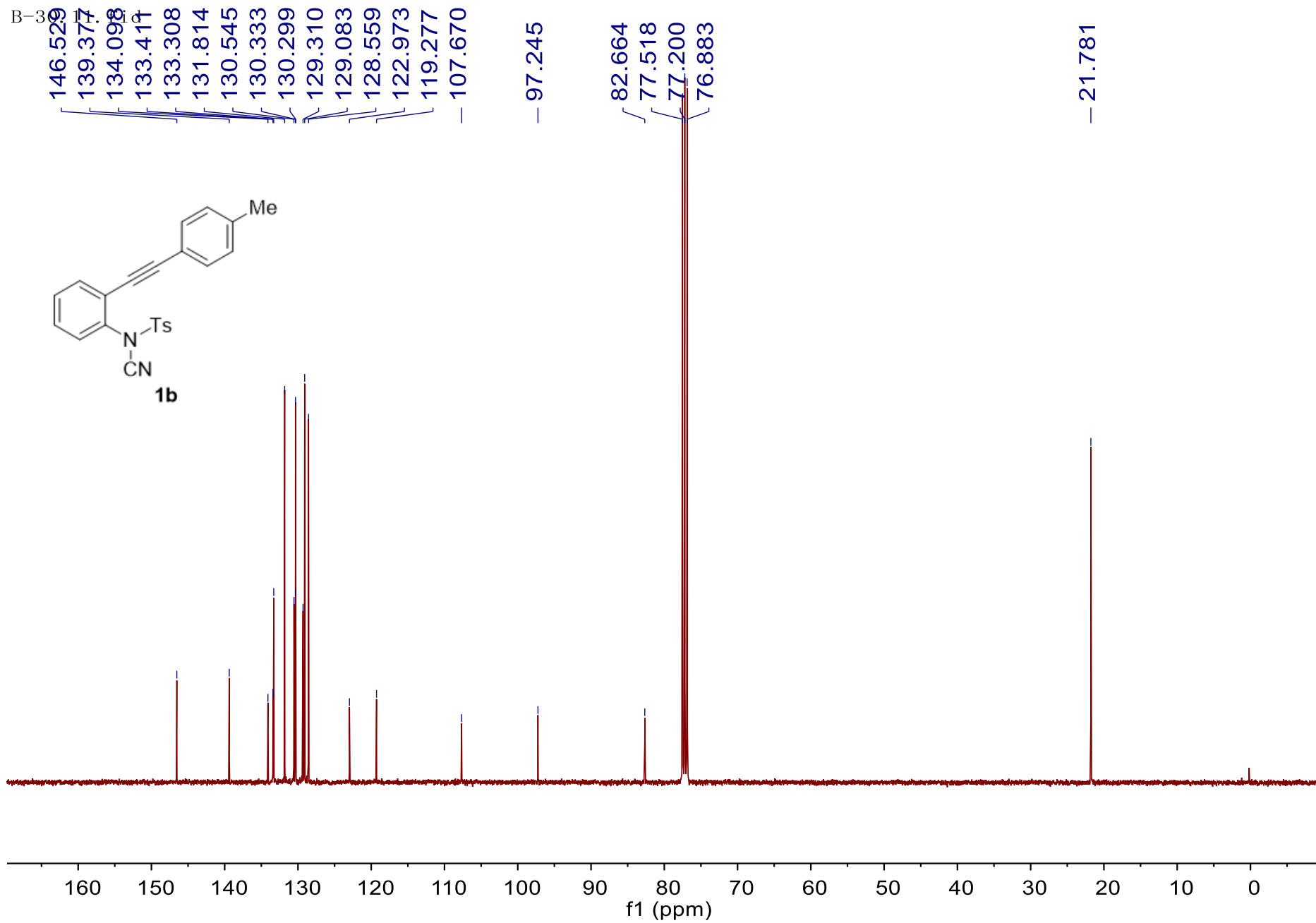
**Synthesis of Amino-Substituted α - and δ -Carbolines via Metal-Free [2 + 2 + 2]
Cycloaddition of Functionalized Alkyne-Nitriles with Ynamides**

authored by

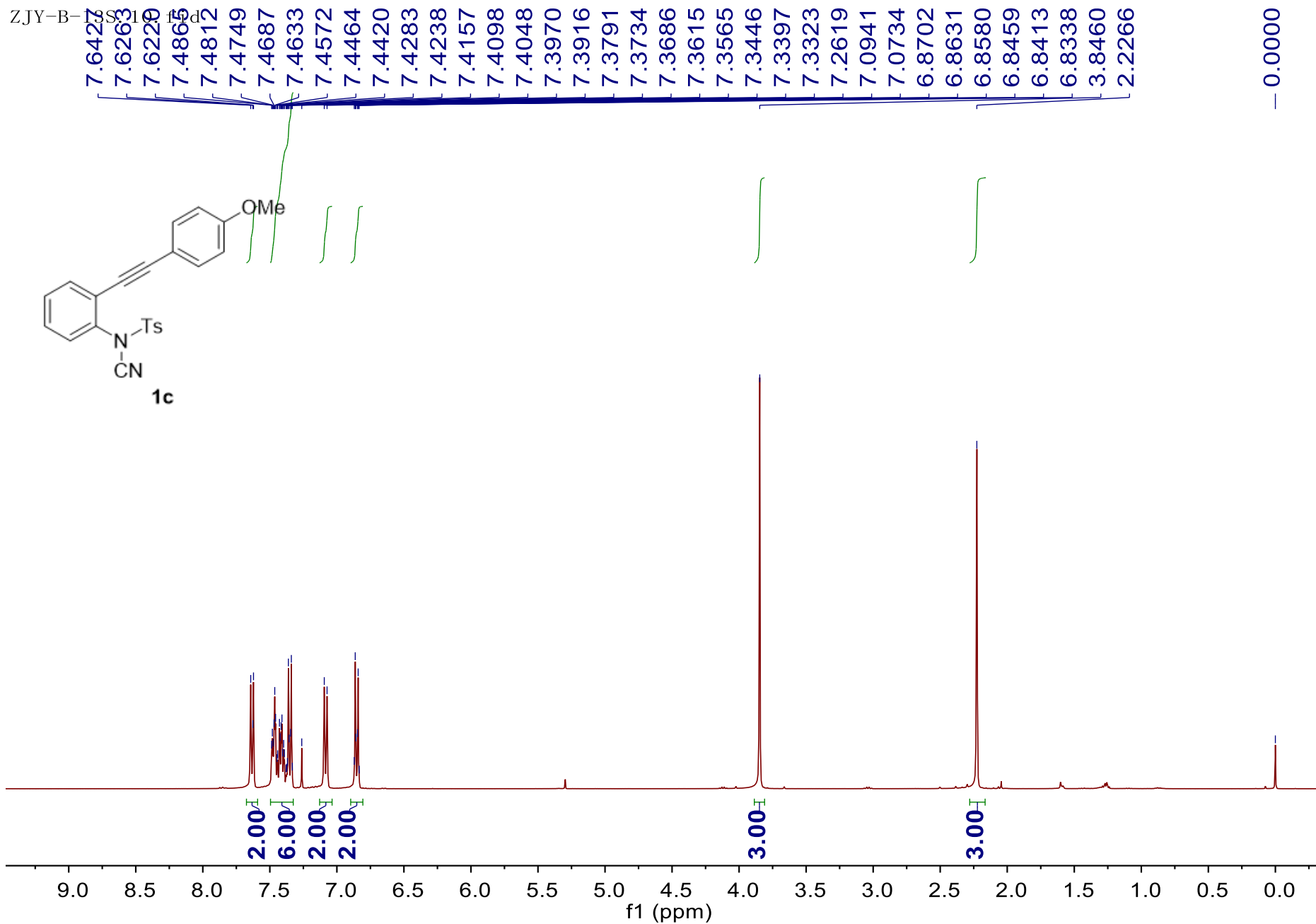
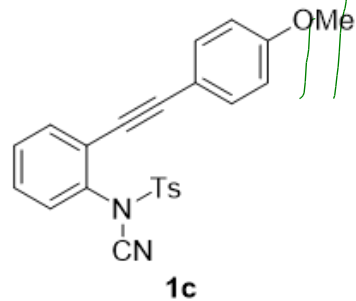
Jingyi Zhang,[†] Meichao Guo,[†] Yajuan Chen, Shuangshuang Zhang, Xiao-Na Wang,* and Junbiao Chang*

Collaborative Innovation Center of New Drug Research and Safety Evaluation, Henan Province, Key Laboratory of Advanced Drug Preparation Technologies, Ministry of Education, School of Pharmaceutical Sciences, and College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou, Henan 450001, P. R. China.





ZJY-B-18811-12d



ZJY-B

160.298

146.525

133.952

133.440

133.123

130.532

130.295

130.235

129.107

128.540

123.099

114.470

113.970

107.709

97.199

82.171

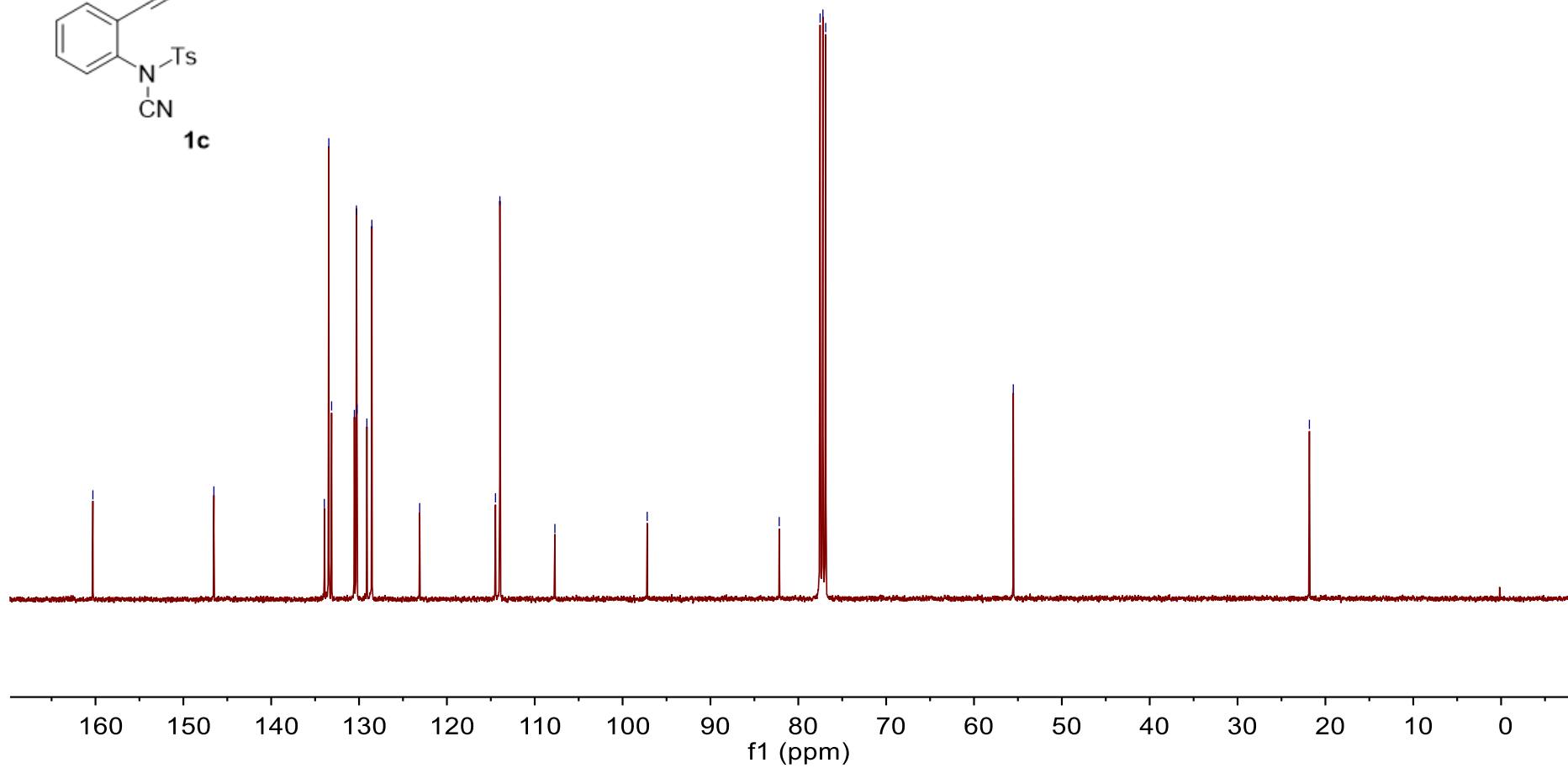
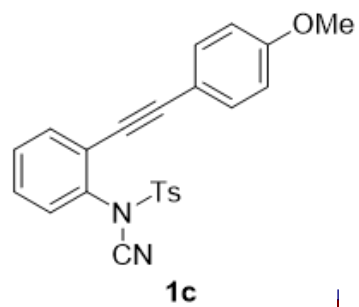
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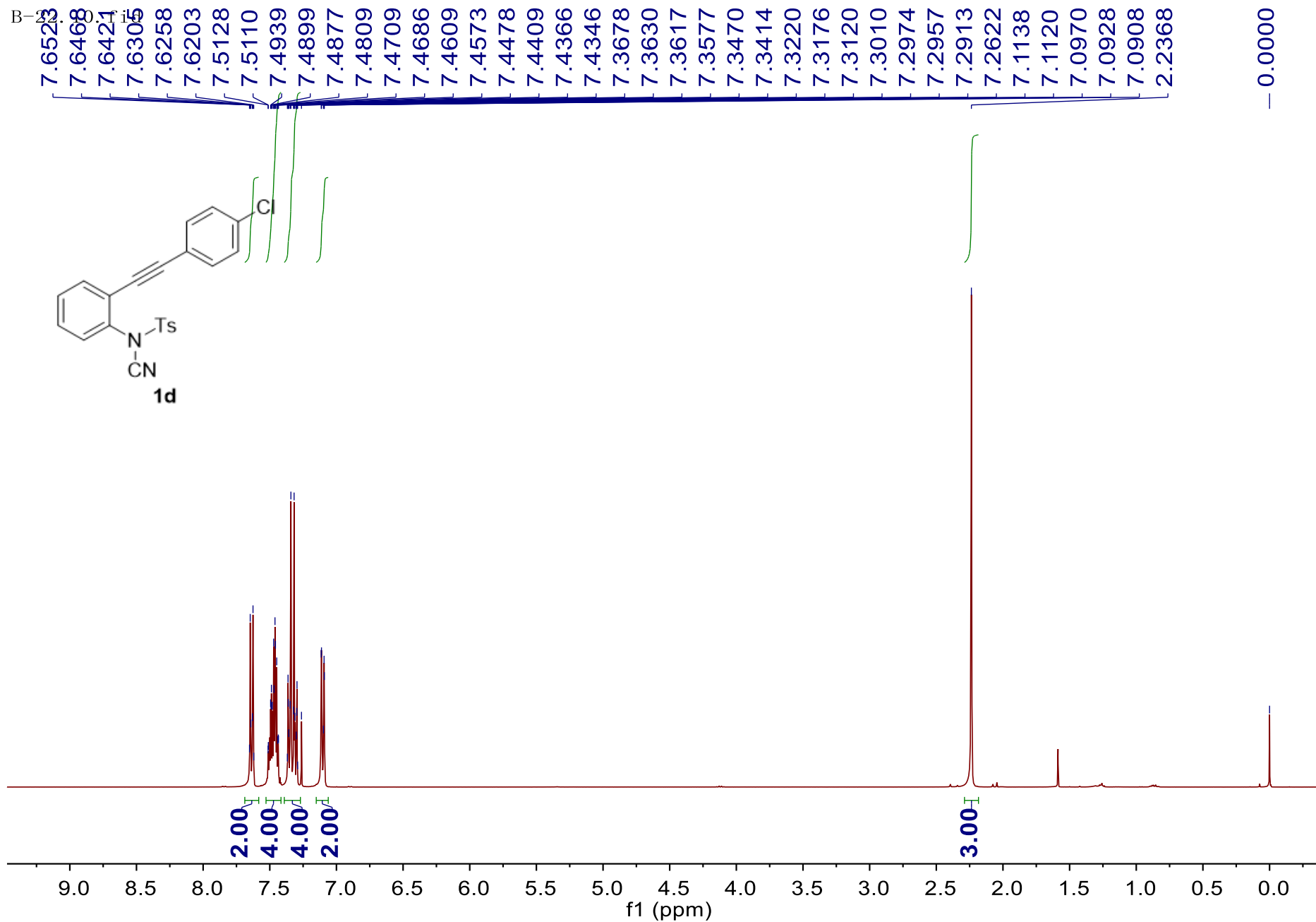
77.200

76.883

55.526

21.820





B-2

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134.294
133.418
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130.354
130.292
129.797
128.720
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122.401
120.799
107.694

— 95.646

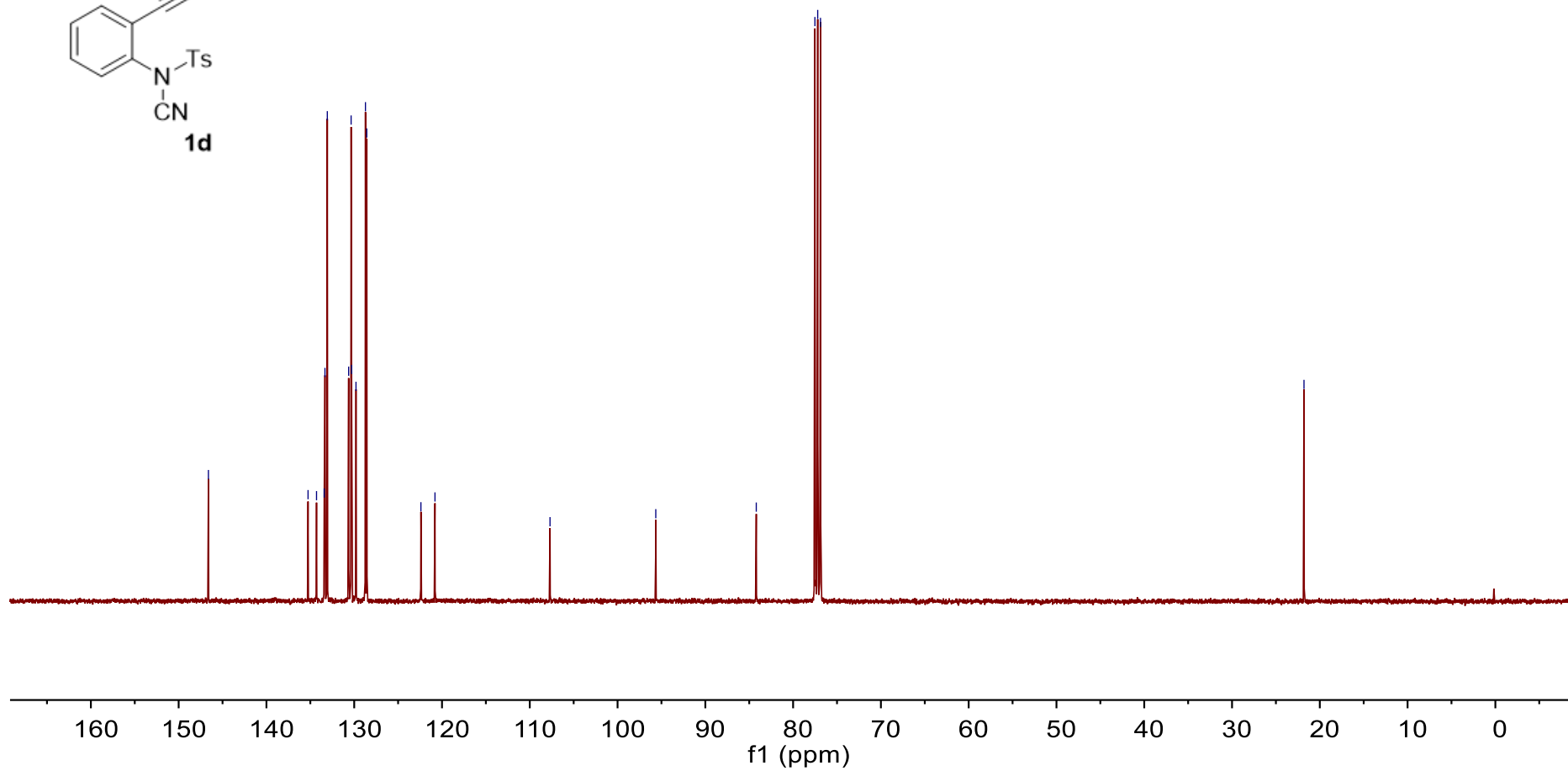
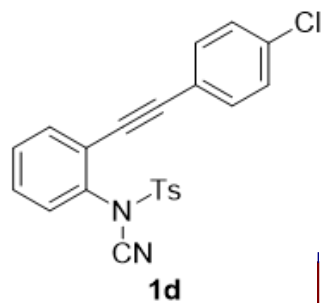
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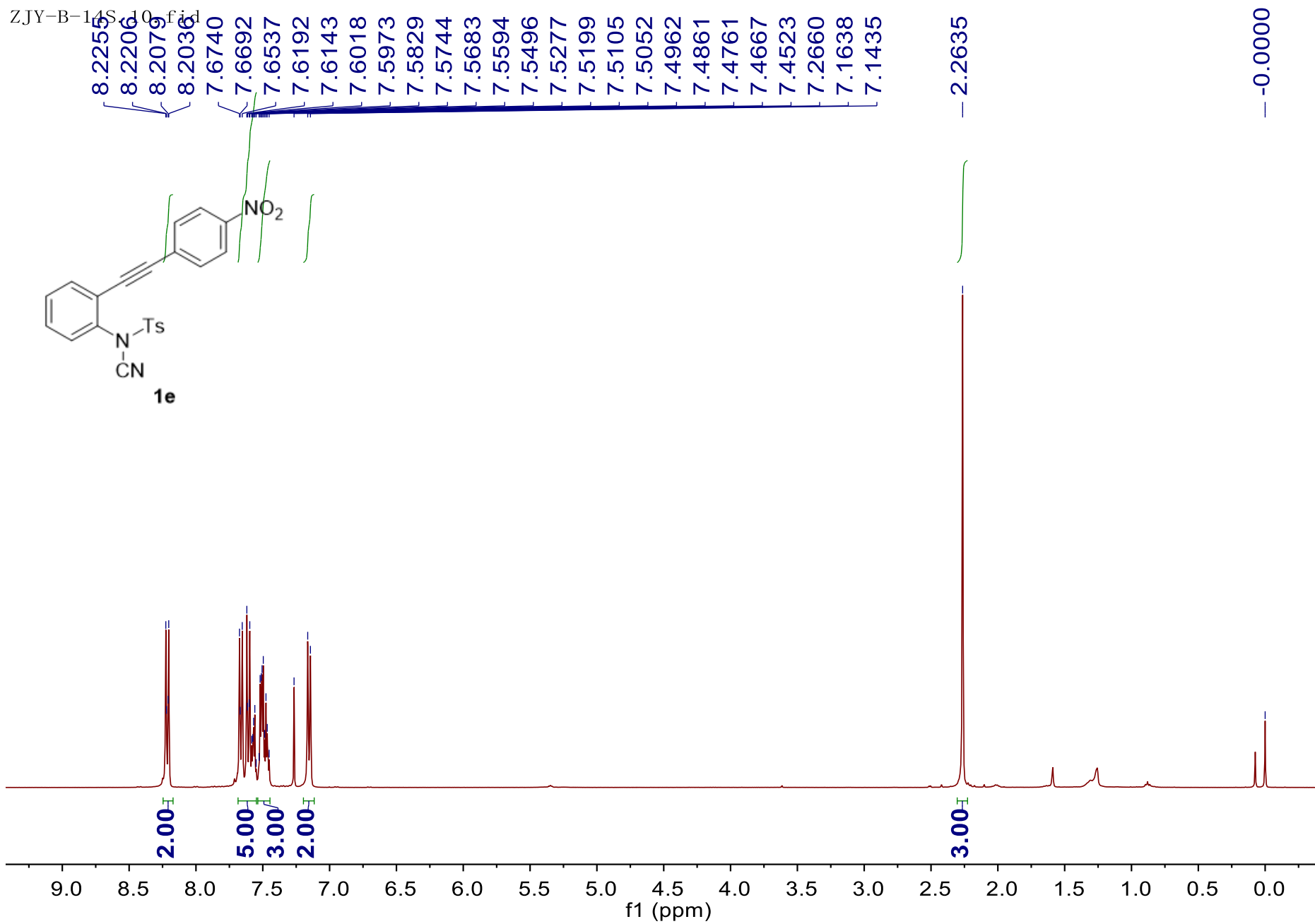
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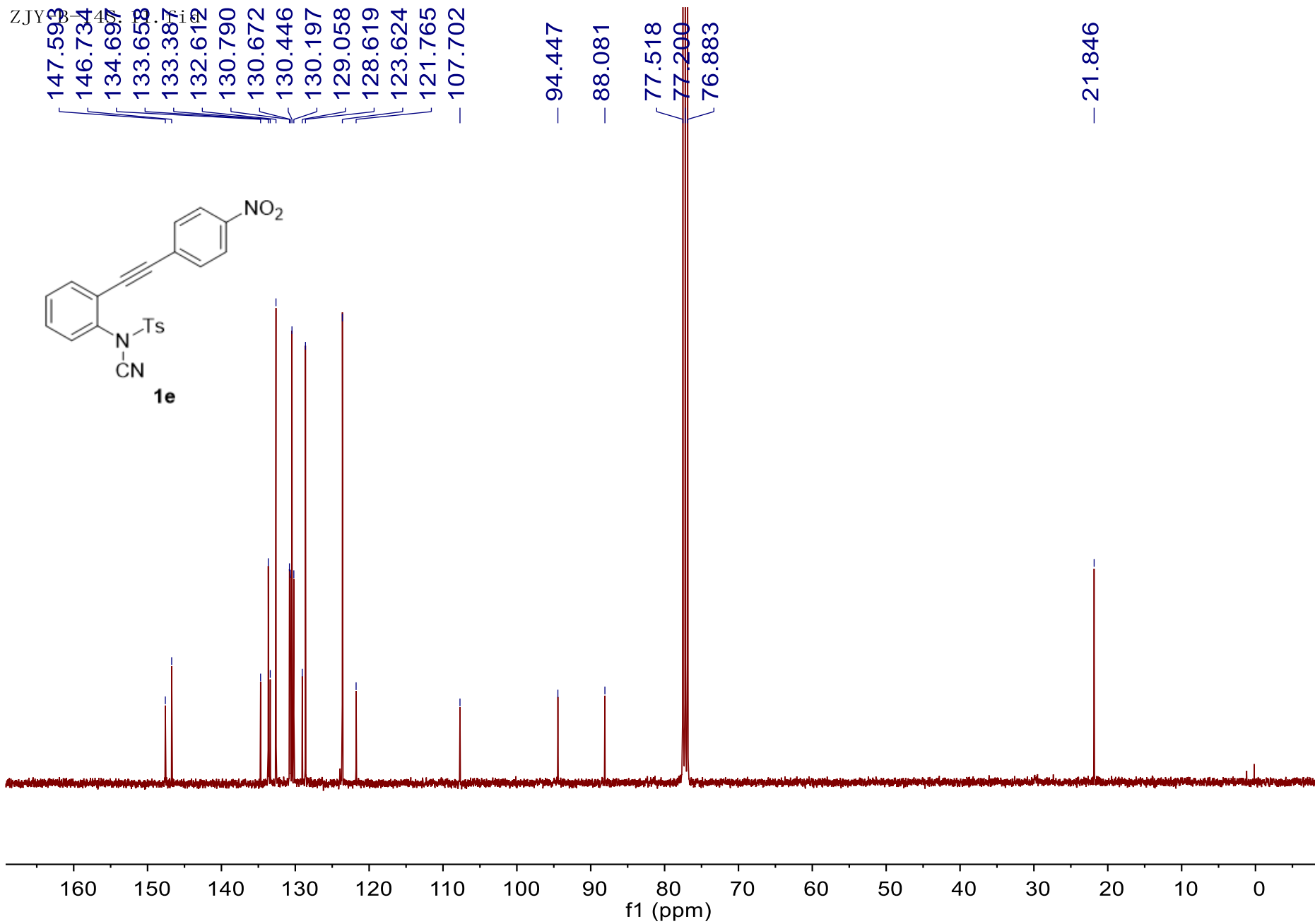
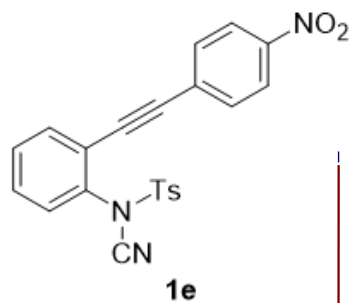


S46

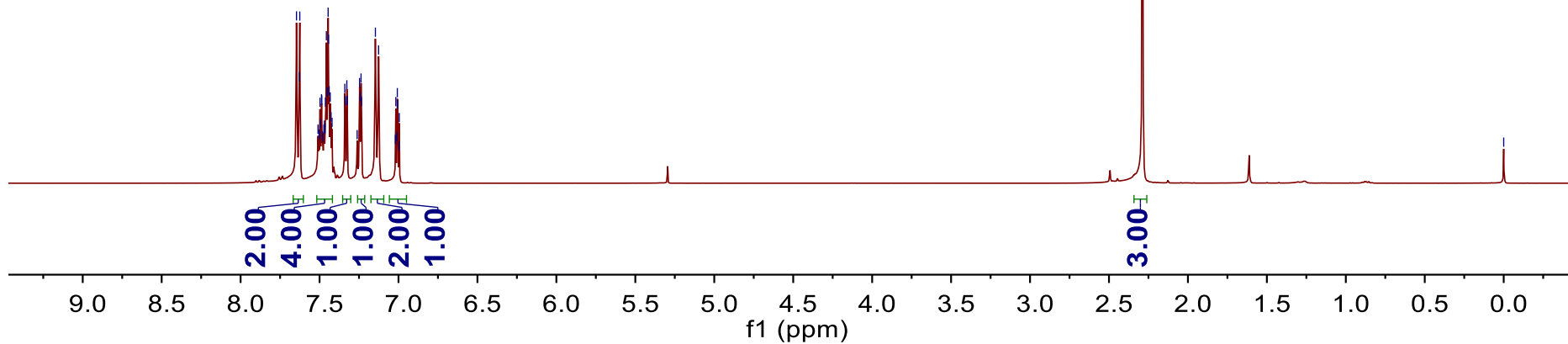
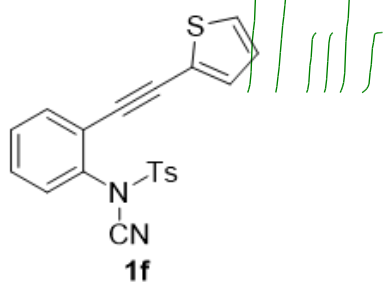
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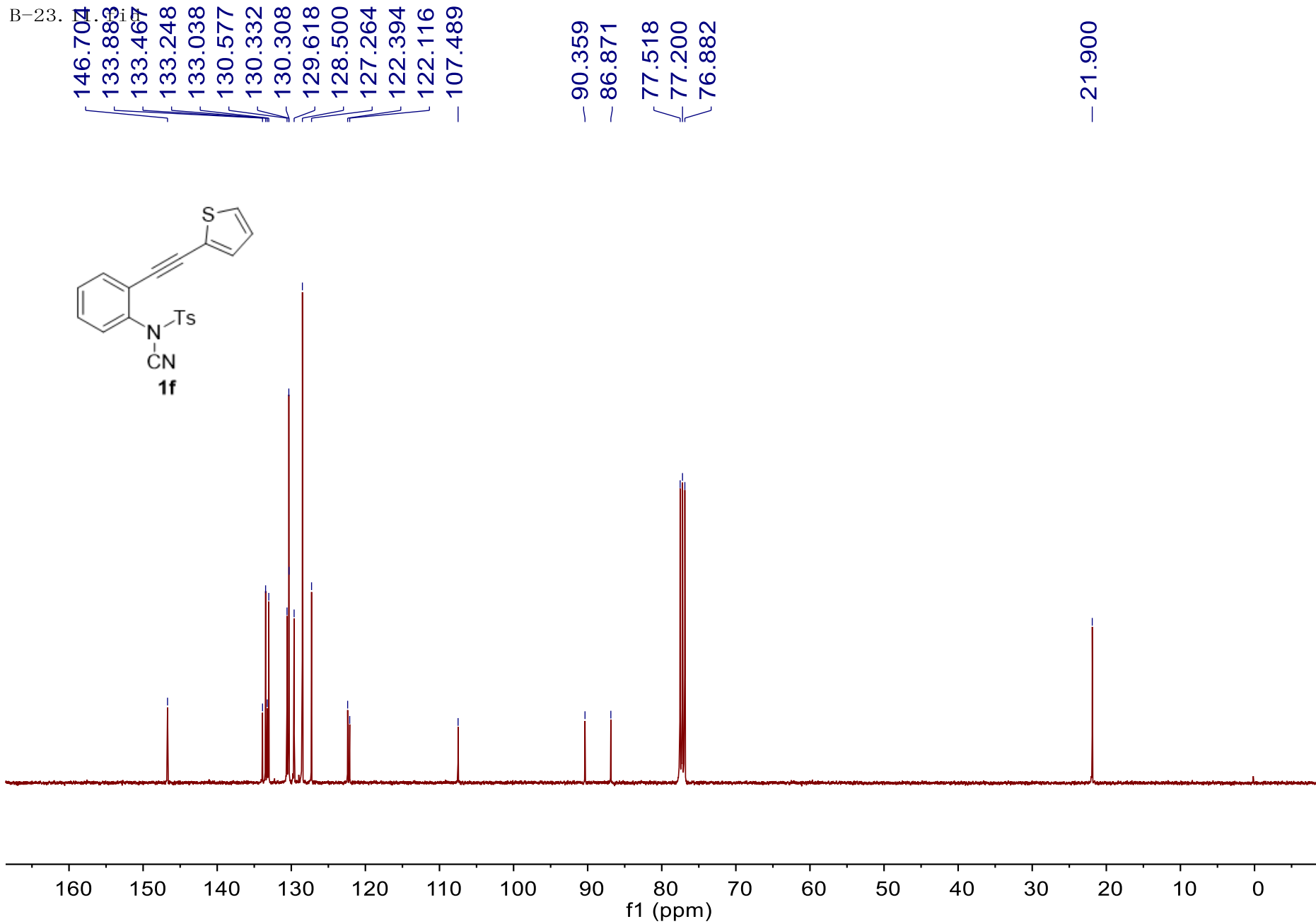
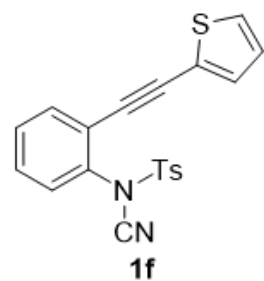
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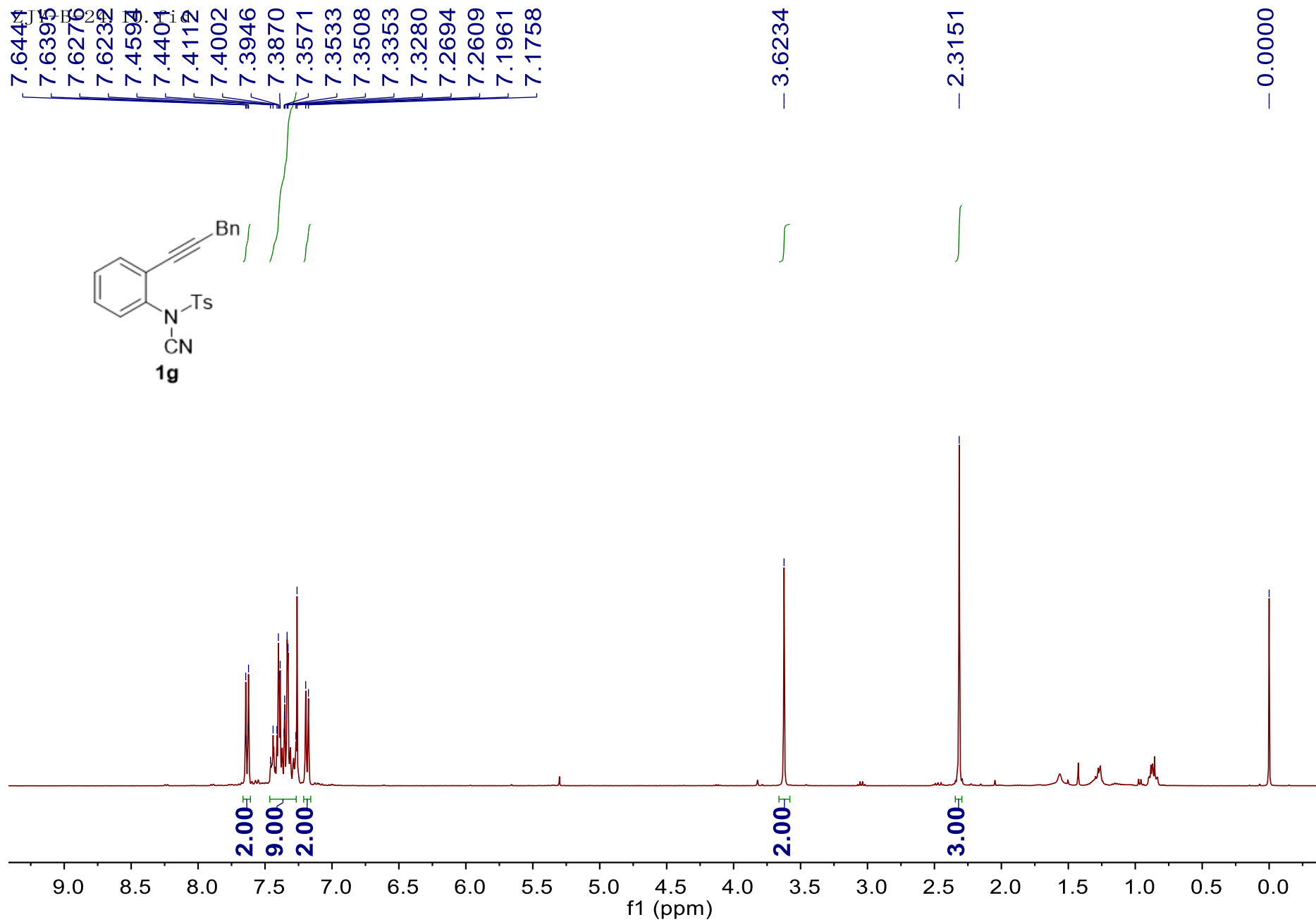


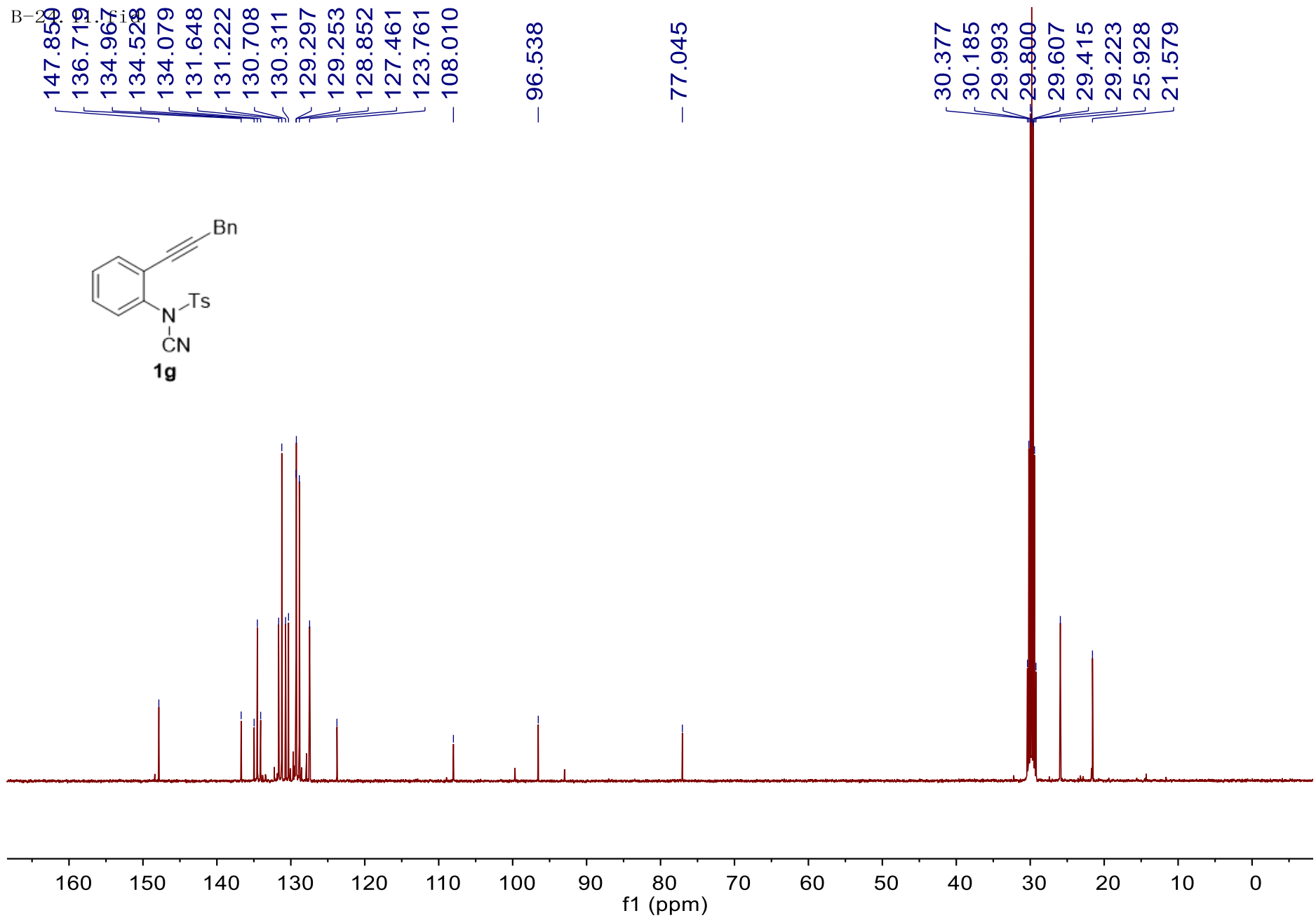
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7.4808
7.4784
7.4725
7.4692
7.4654
7.4626
7.4567
7.4501
7.4457
7.4432
7.4390
7.4324
7.4271
7.4209
7.3400
7.3369
7.3272
7.3242
7.2620
7.2464
7.2433
7.2373
7.2343
7.1463
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7.0039
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0.0000

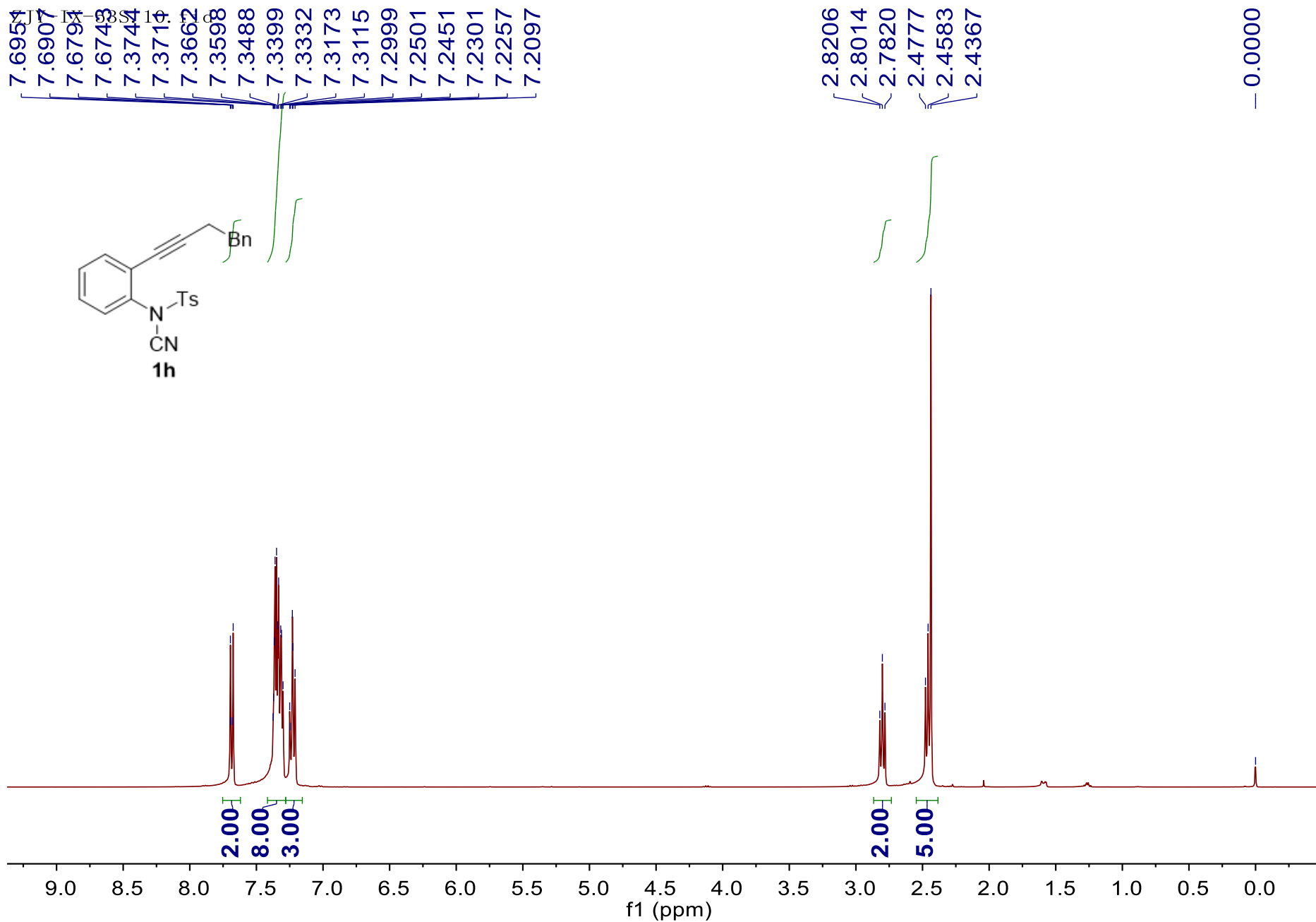


B-23. 1f

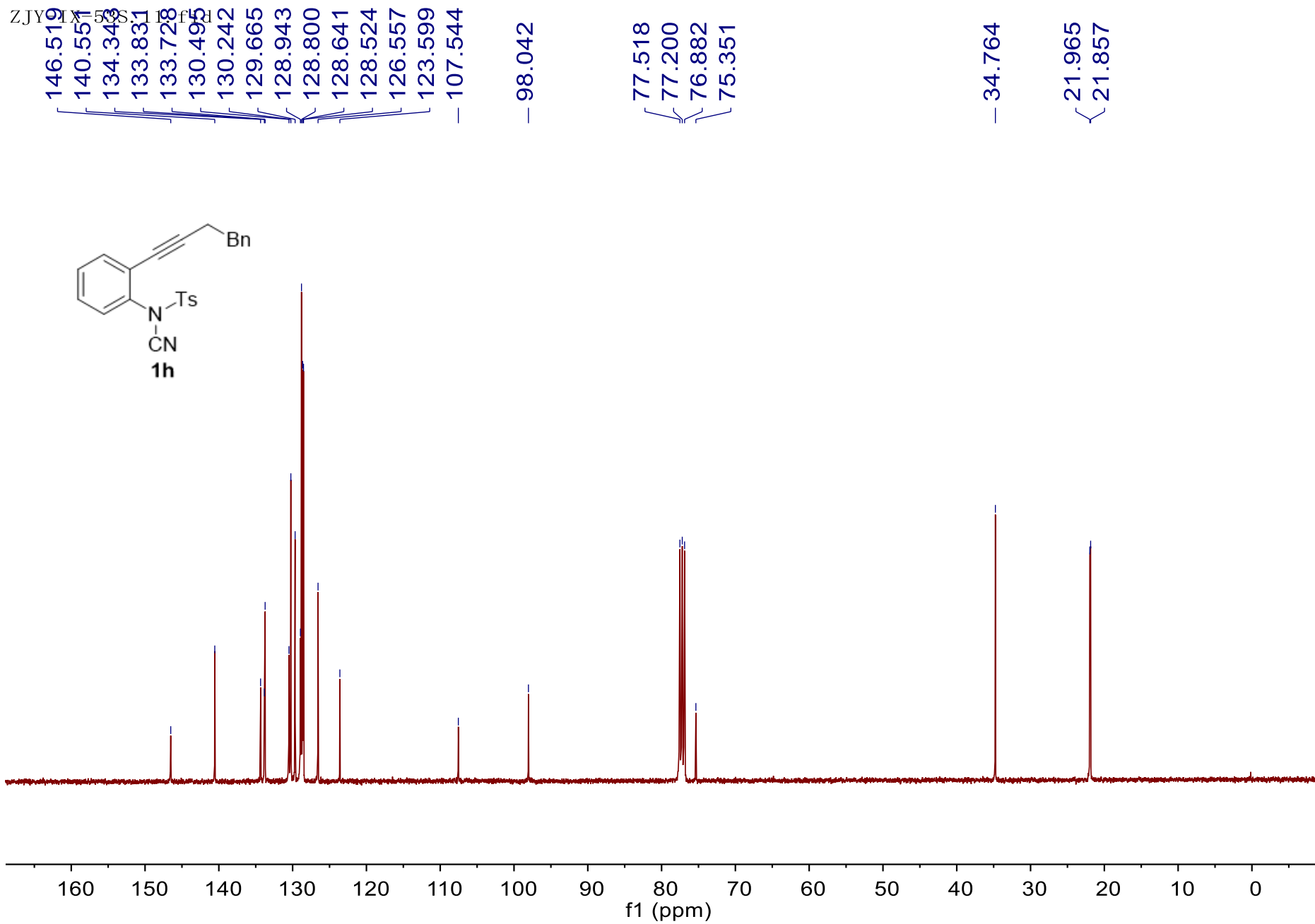
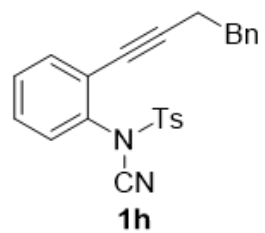




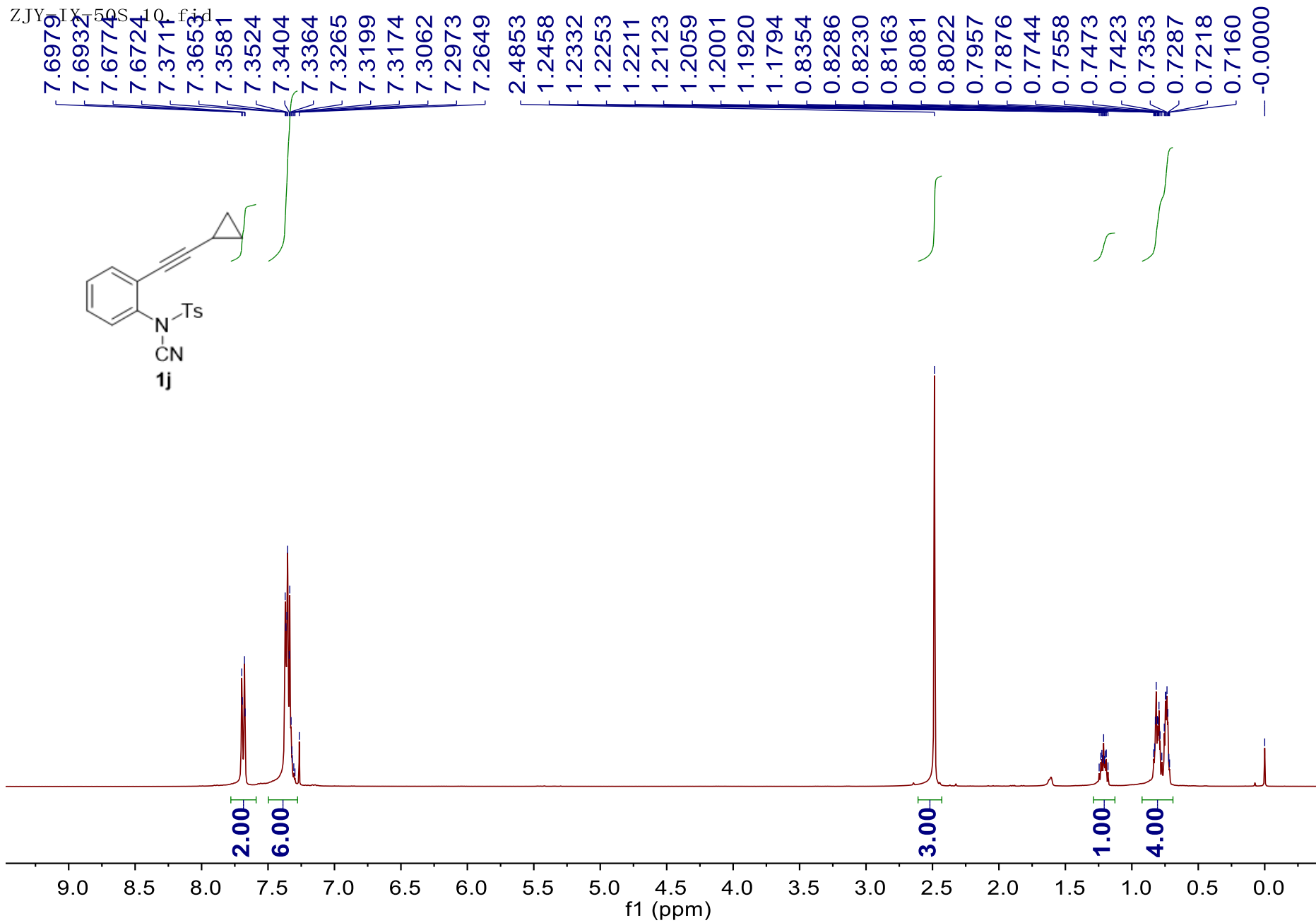




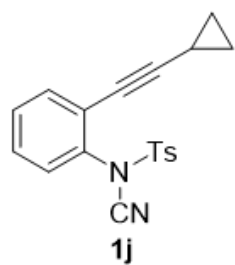
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ZJY-IX-50S. 111f1



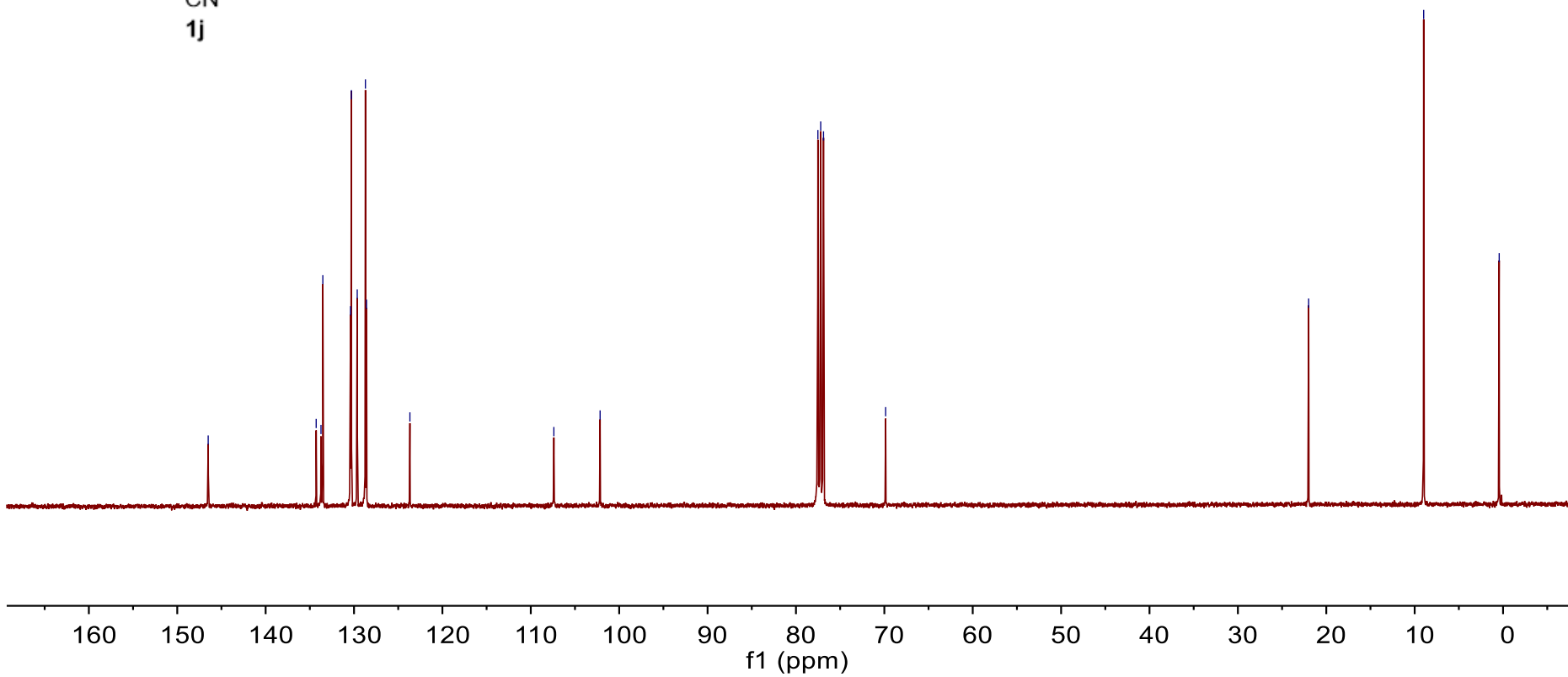
— 146.500
— 134.280
— 133.738
— 133.529
— 130.392
— 130.301
— 129.637
— 128.710
— 128.583
— 123.676
— 107.391
— 102.159

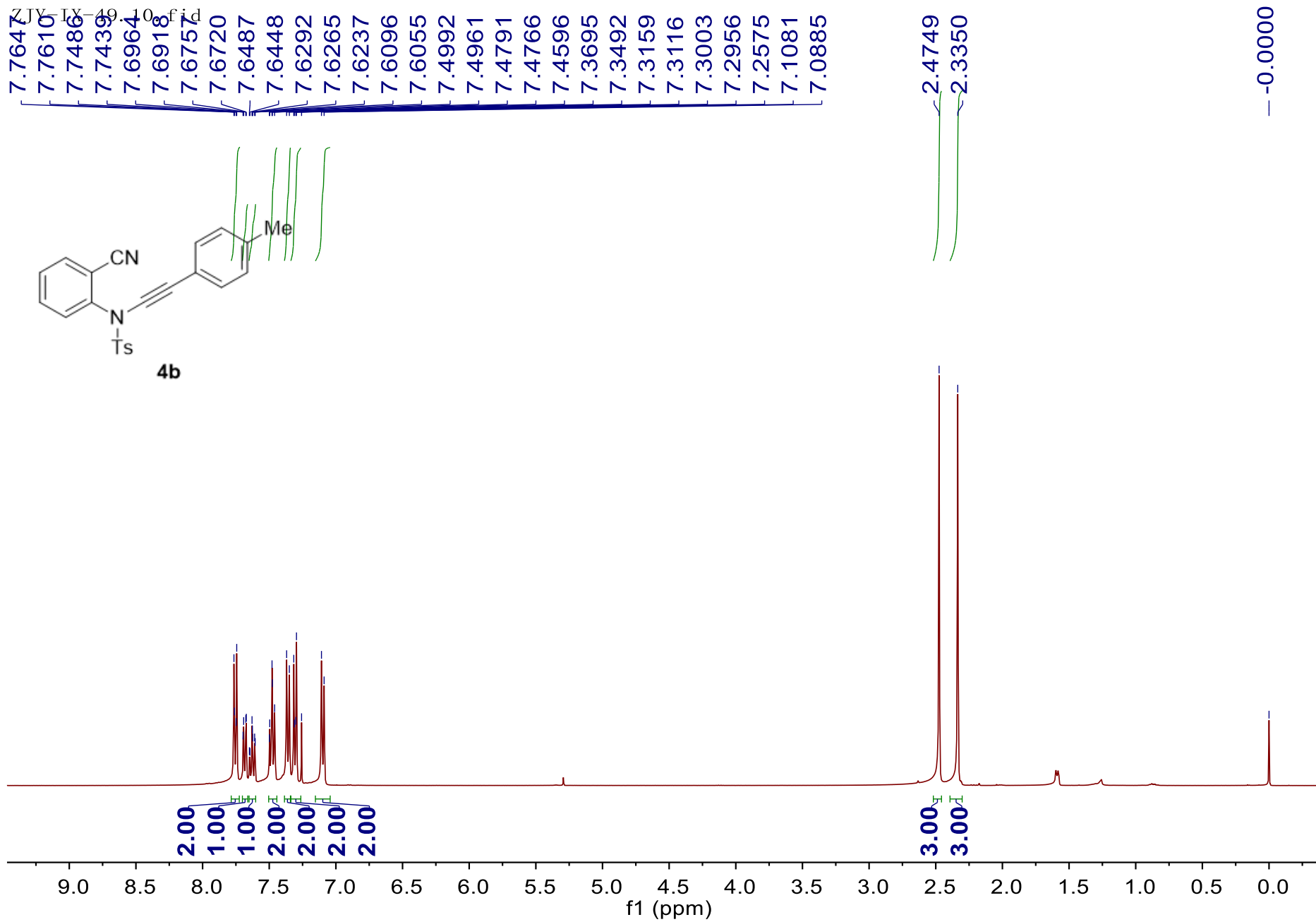
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77.200
76.884
69.854

— 21.996

— 8.980

— 0.437

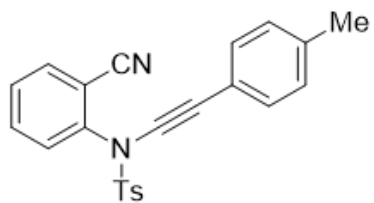




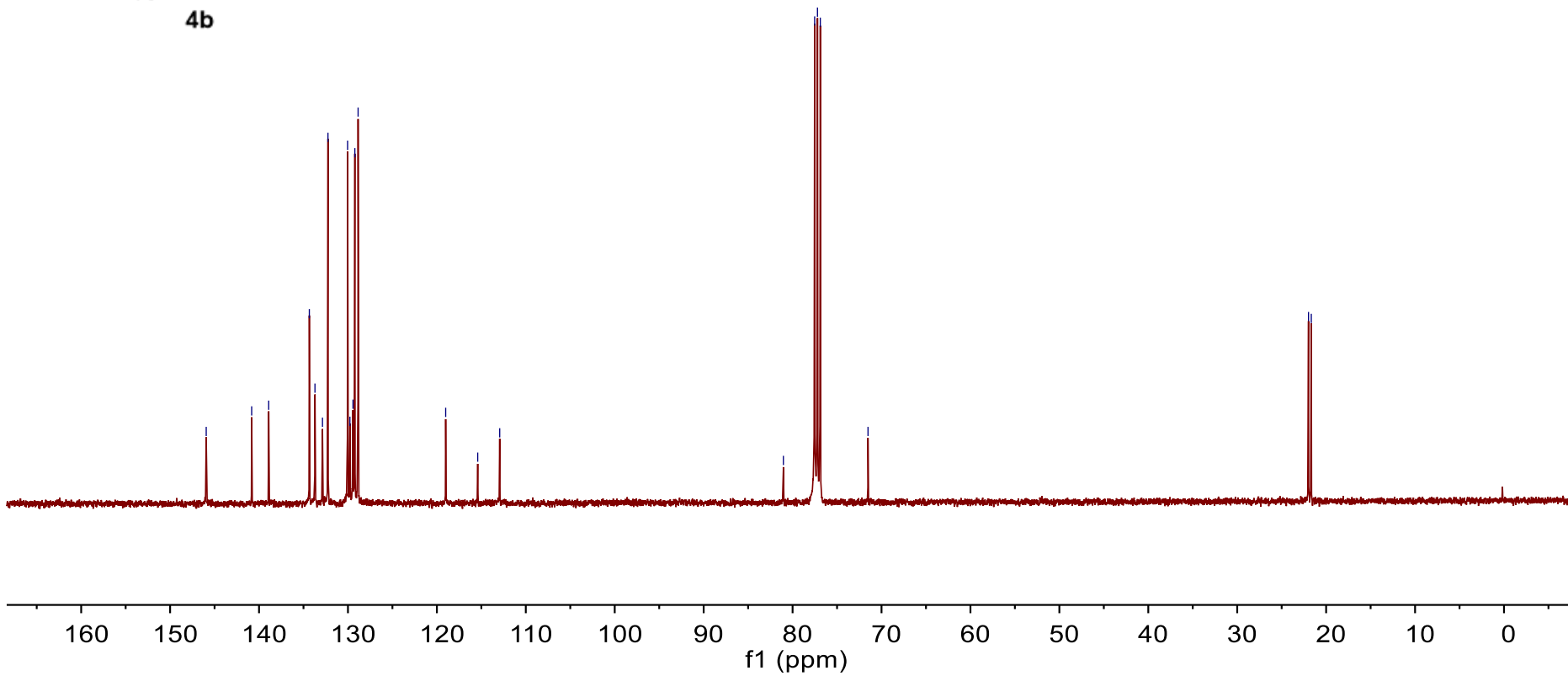
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140.827
138.913
134.343
133.710
132.865
132.248
130.041
129.780
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128.860
~ 119.011
~ 115.409
~ 112.936

81.033
77.518
77.200
76.883
71.519

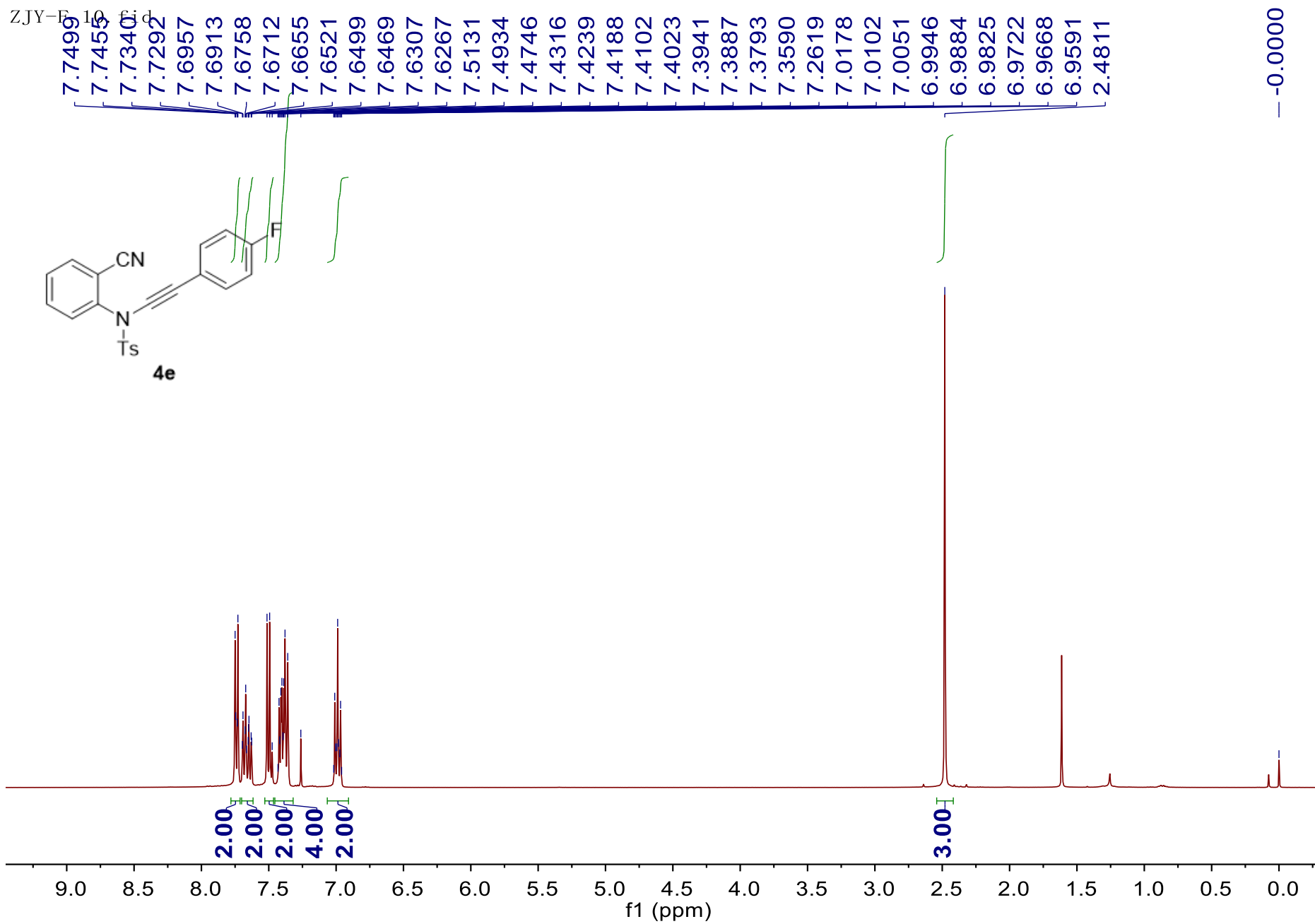
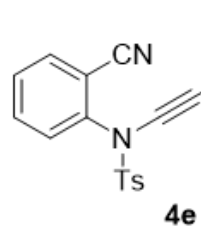
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21.670



4b



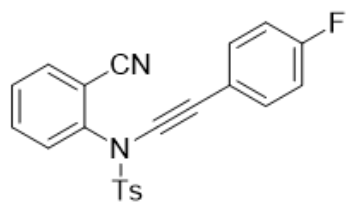
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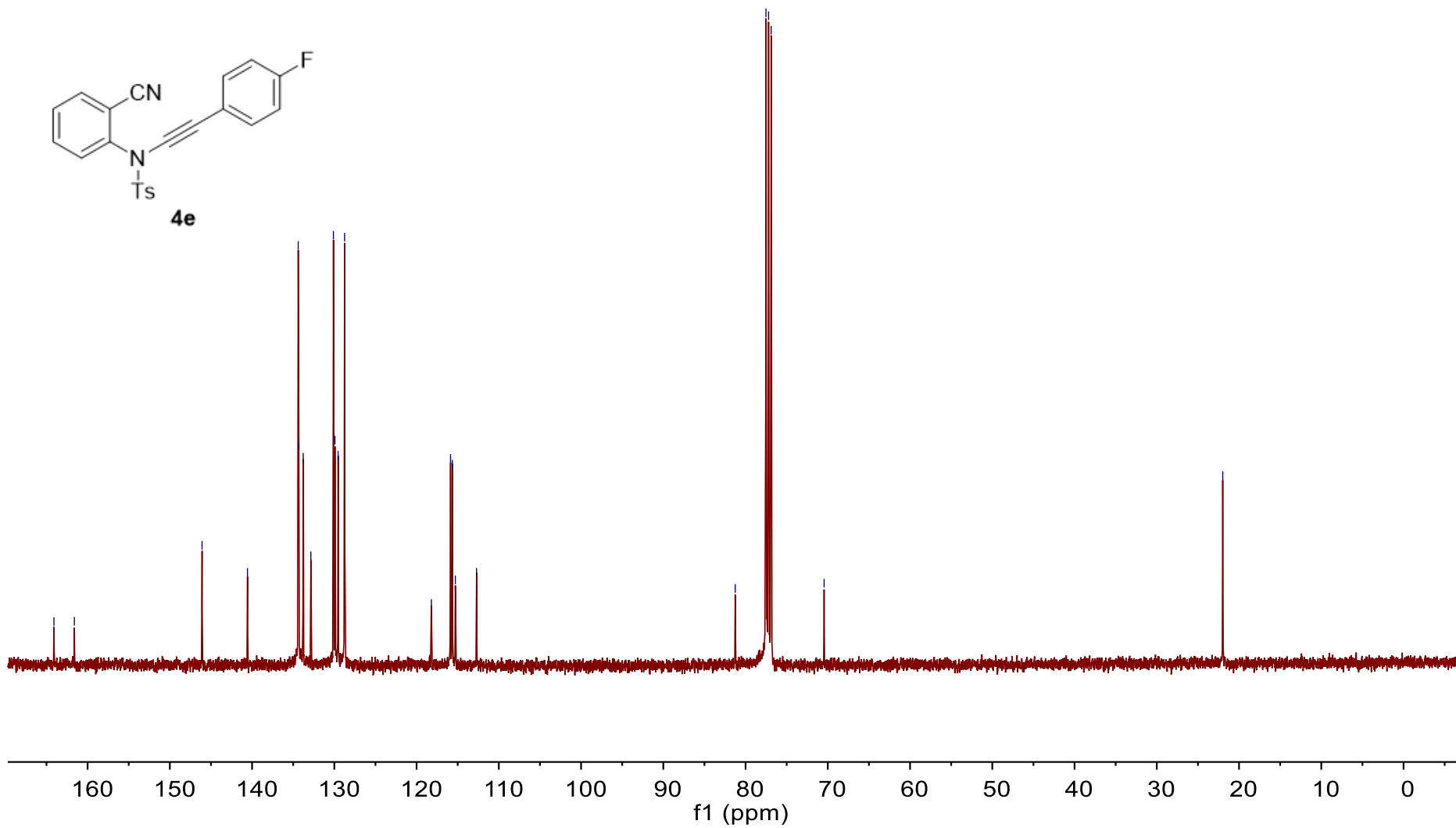
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115.654
115.286
112.709

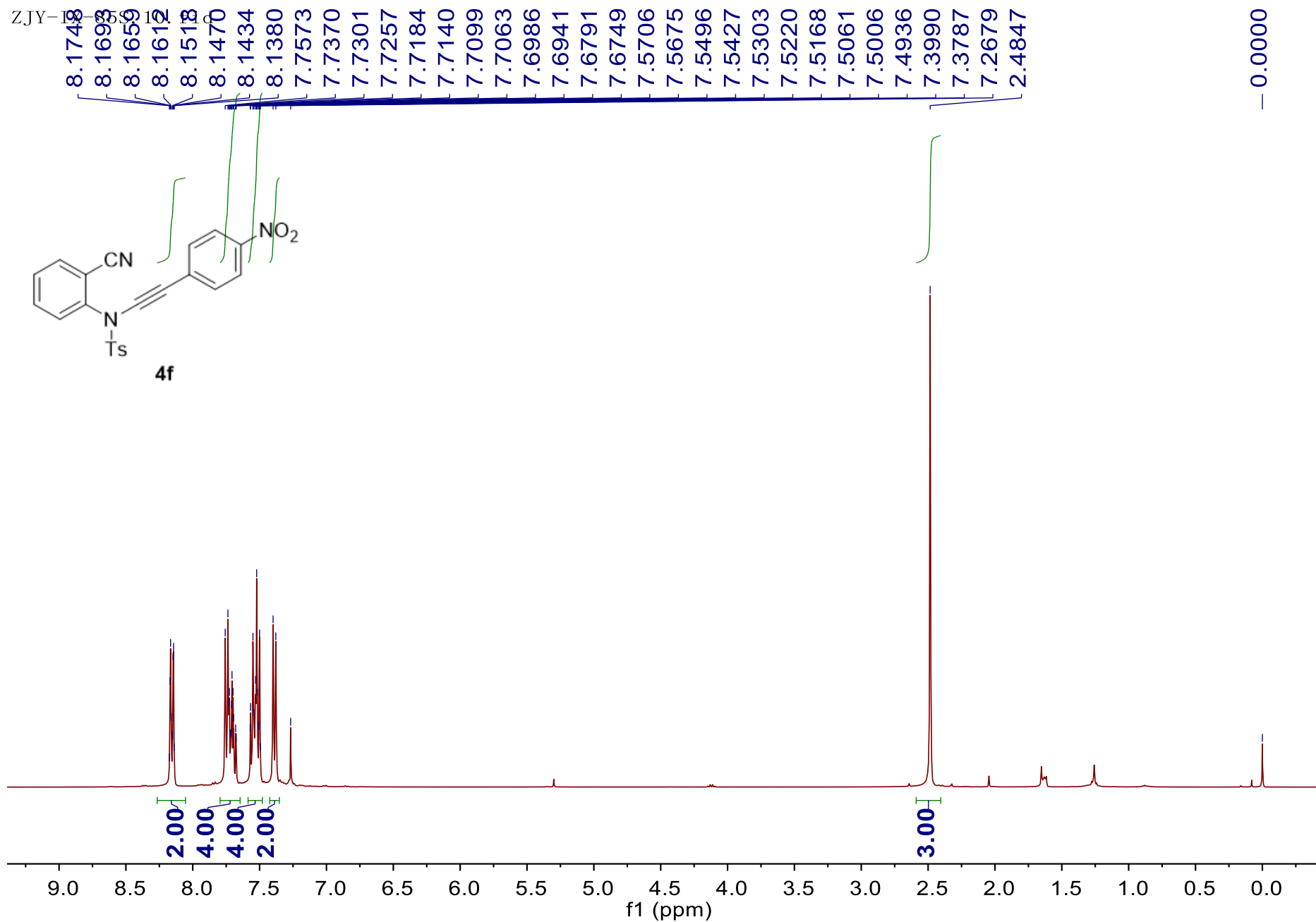
81.256
77.518
77.200
76.883
70.450

21.978



4e





146.924
146.530
139.814
134.486
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132.719
131.853
130.304
130.041
129.952
129.550
128.711
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115.038
112.627

86.805

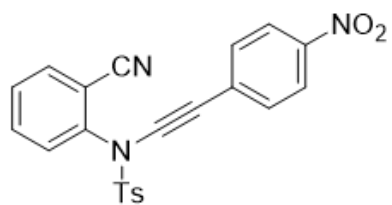
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77.200

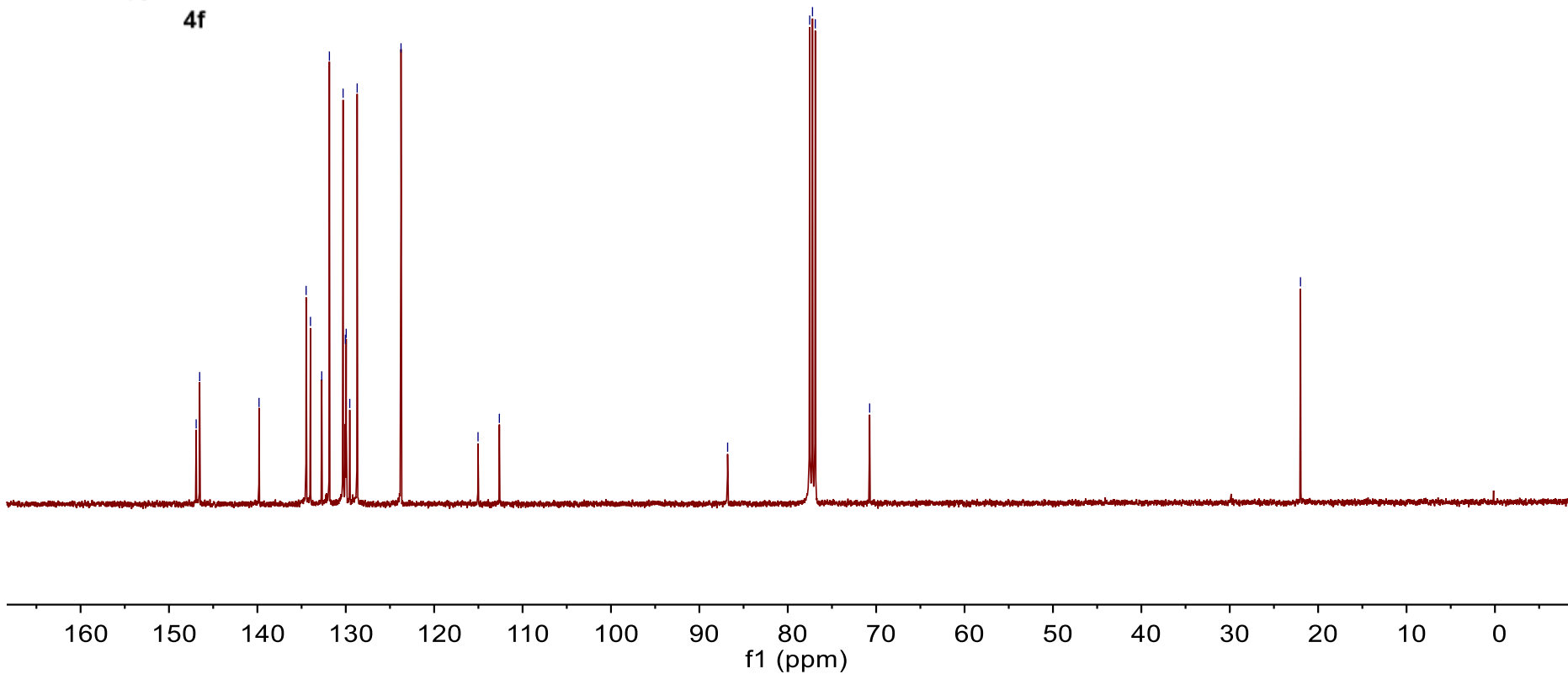
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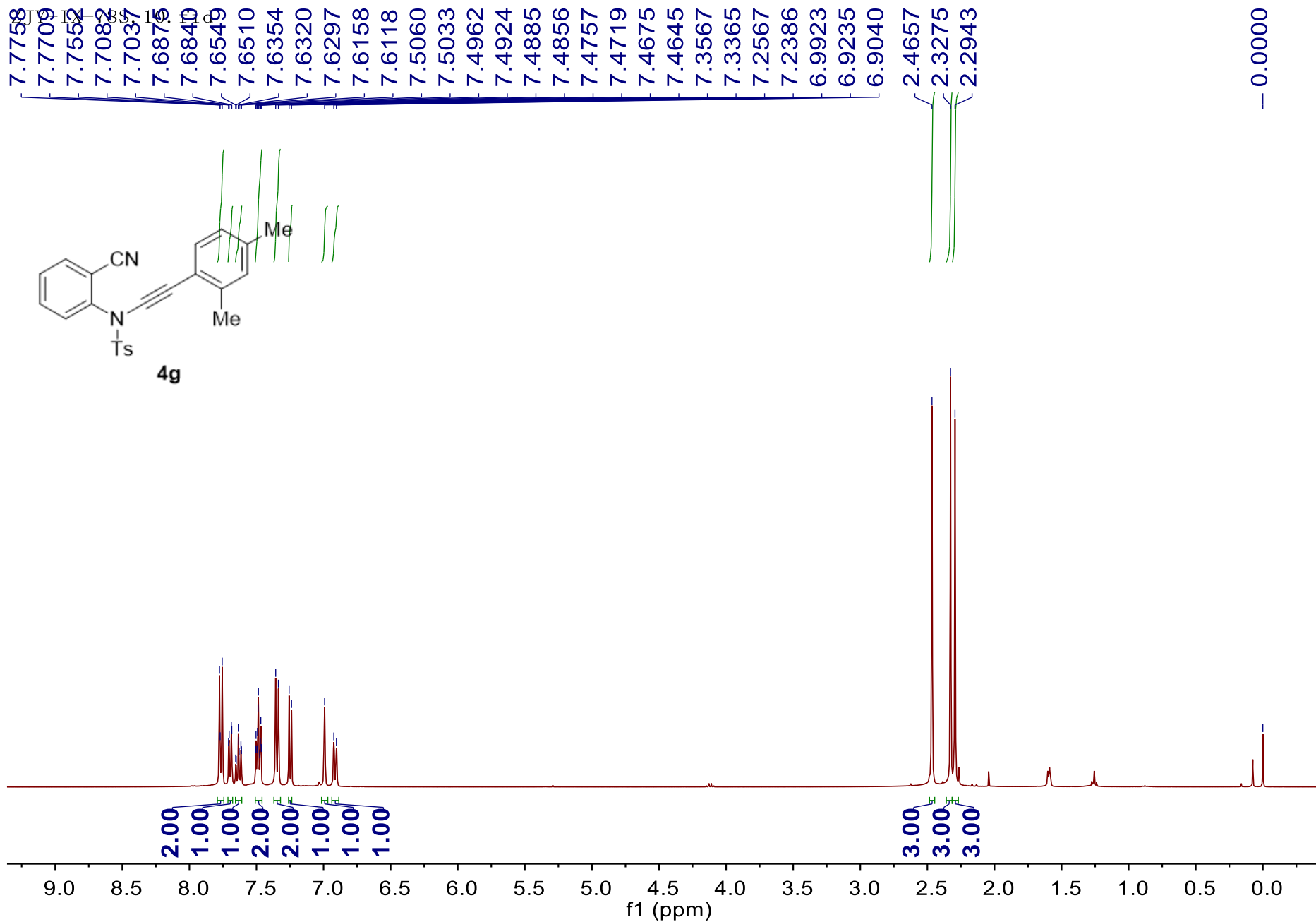
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21.996

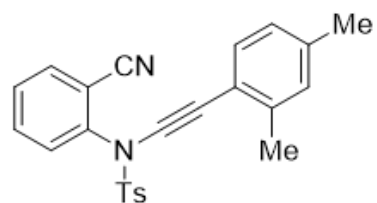


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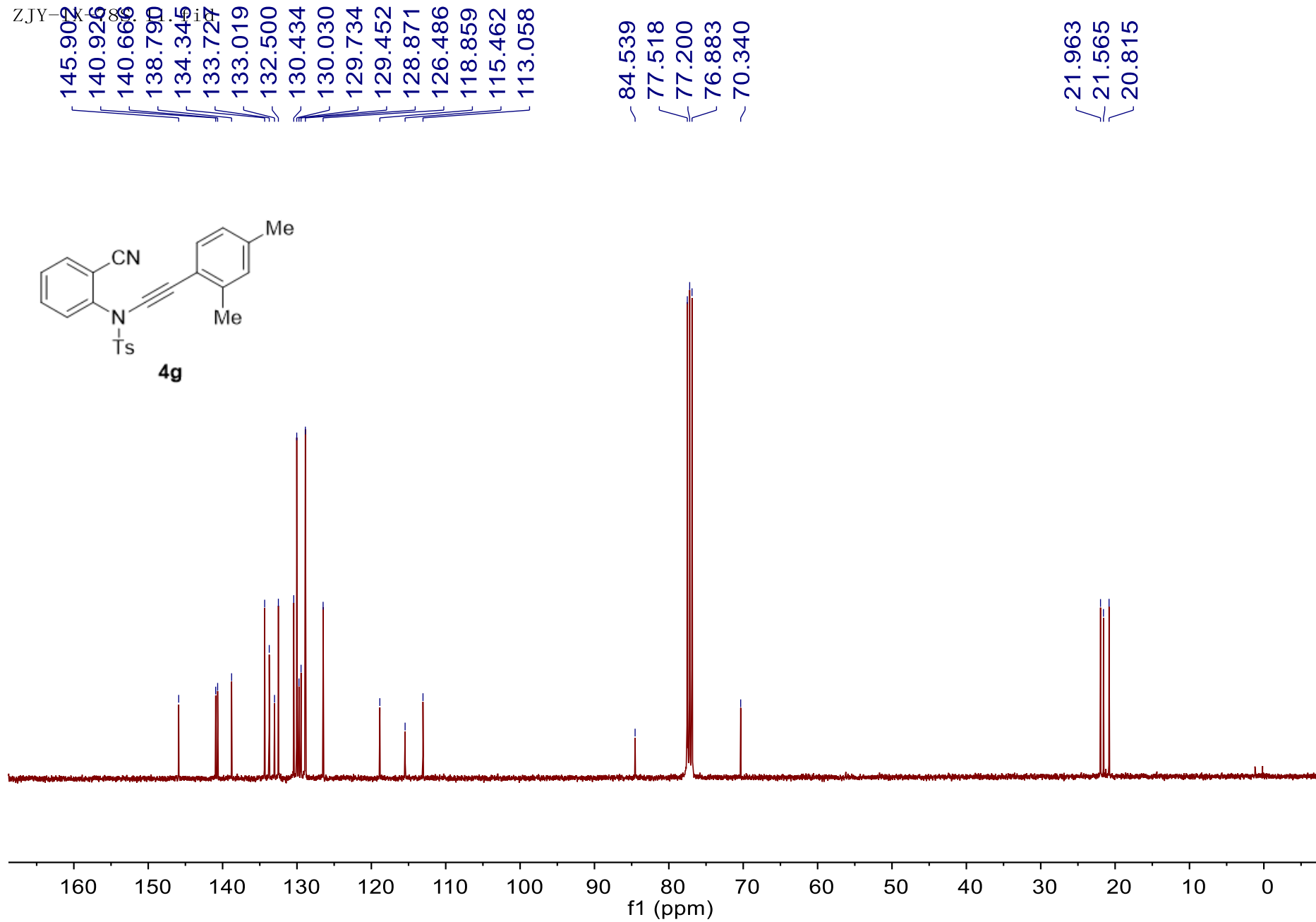


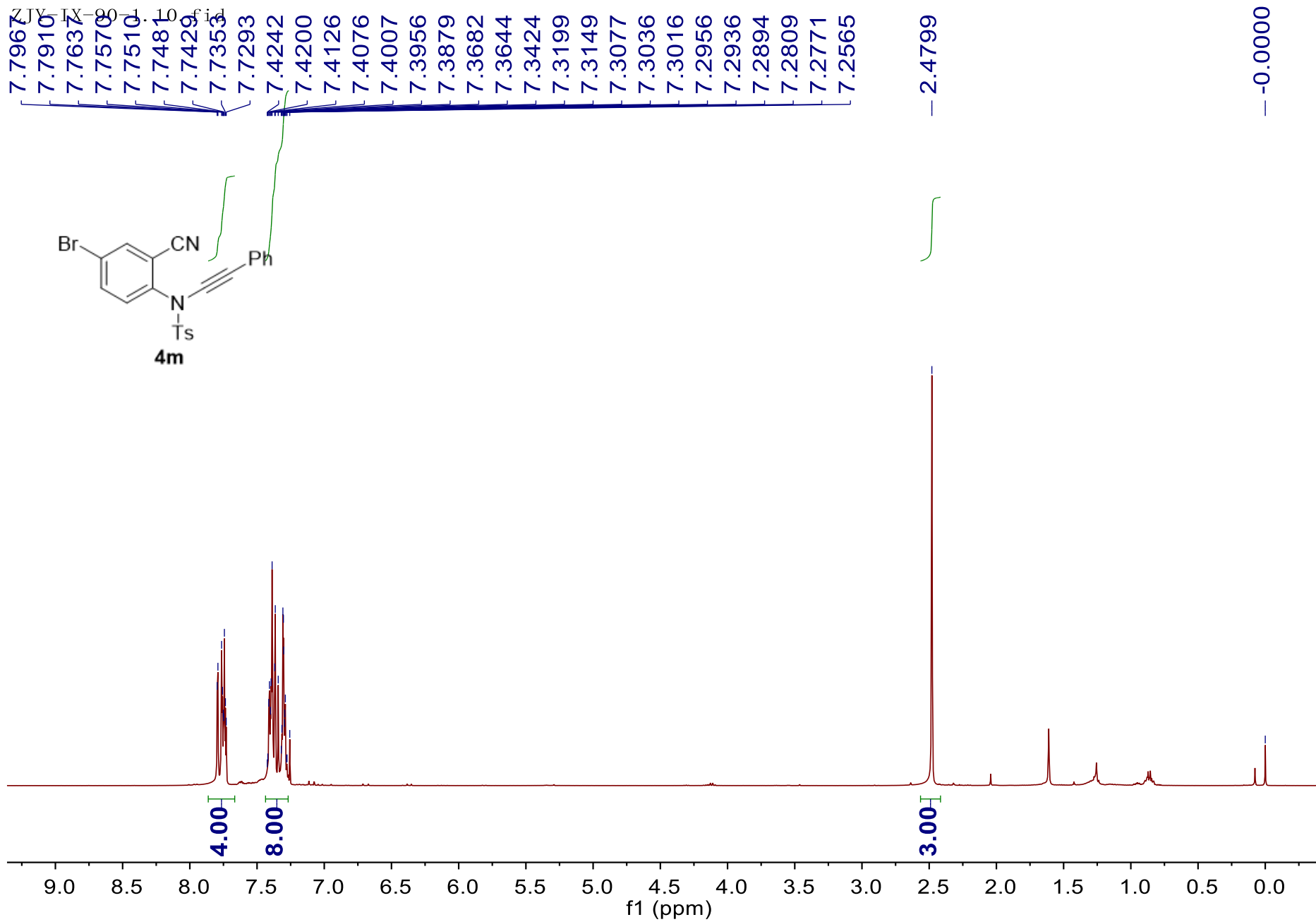


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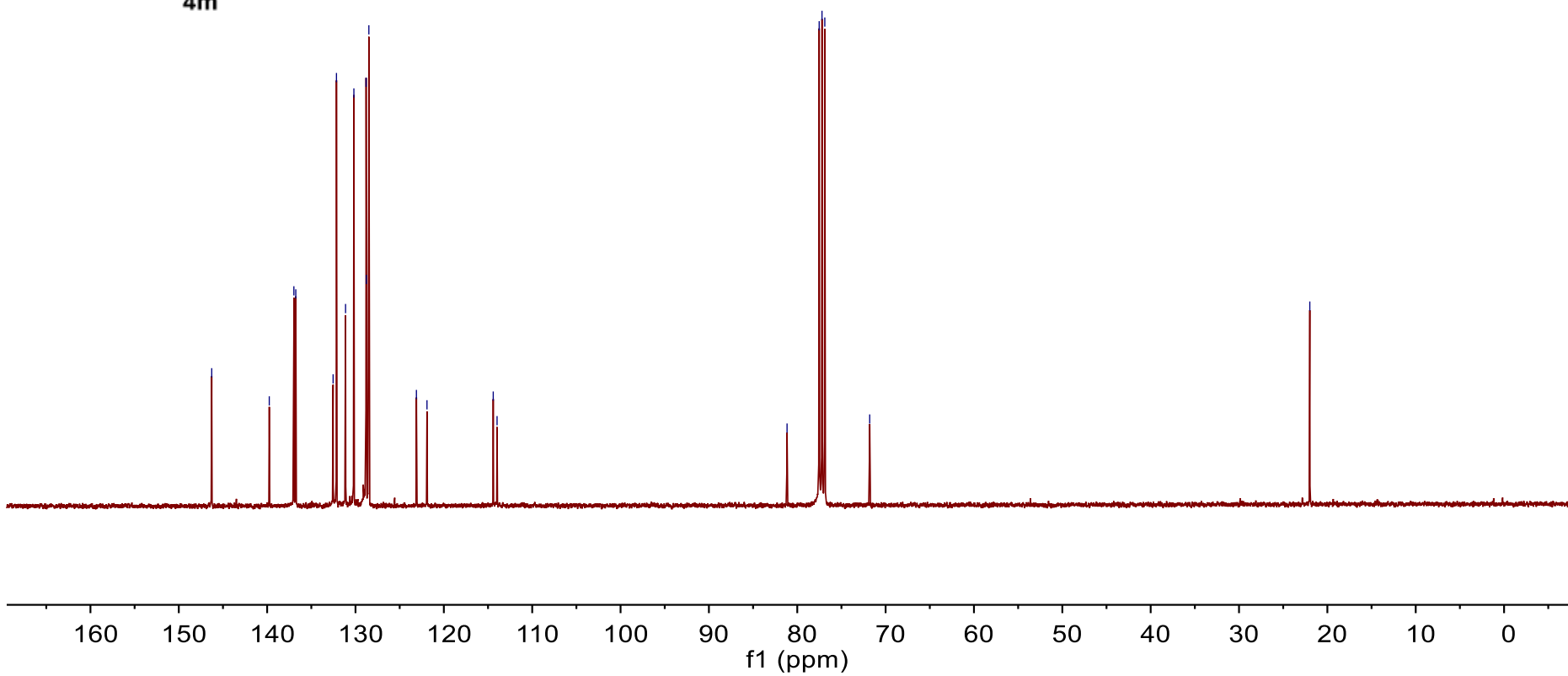
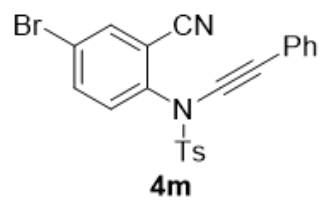


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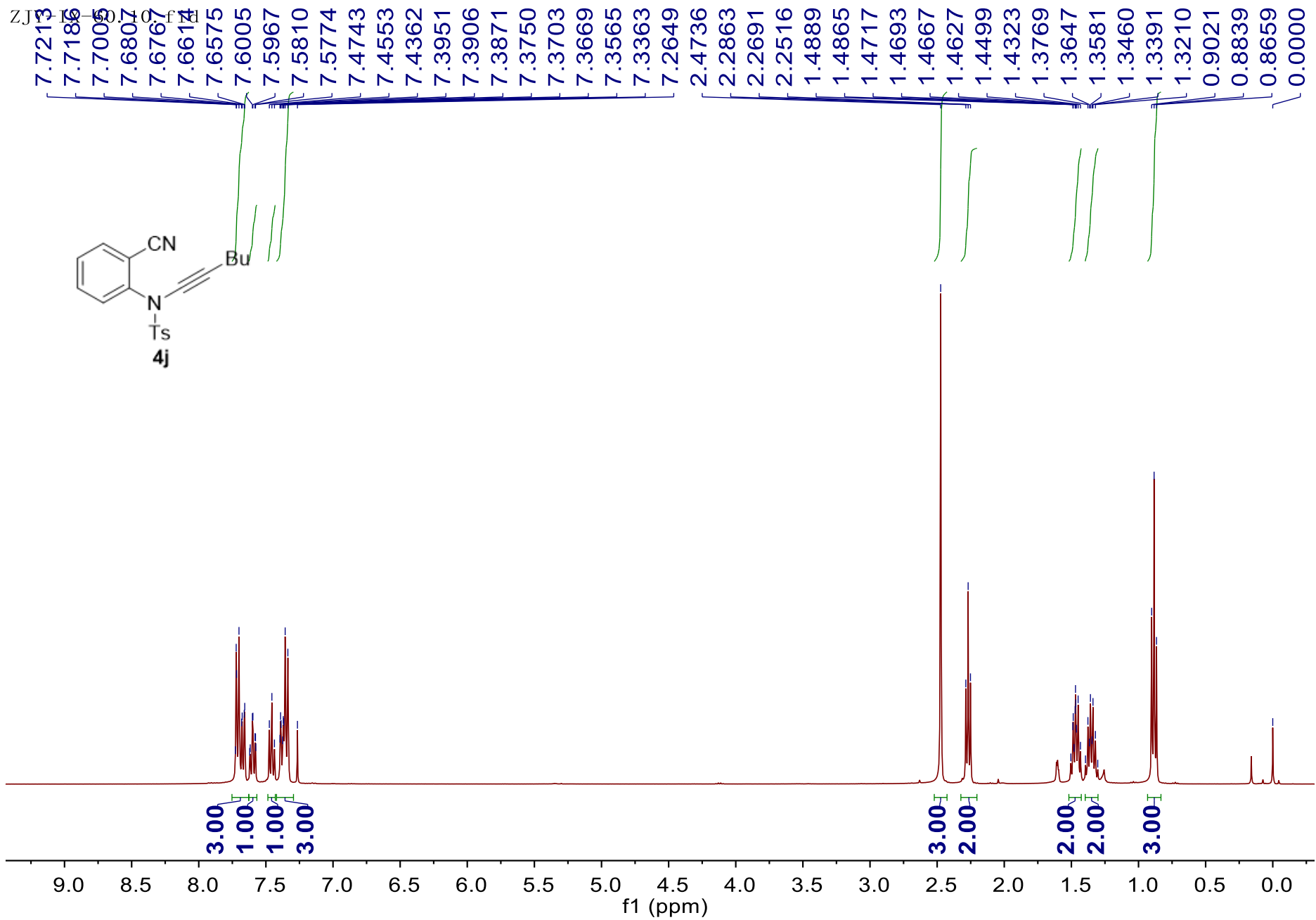




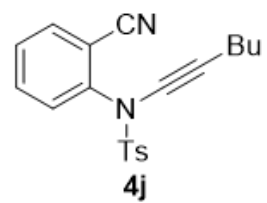
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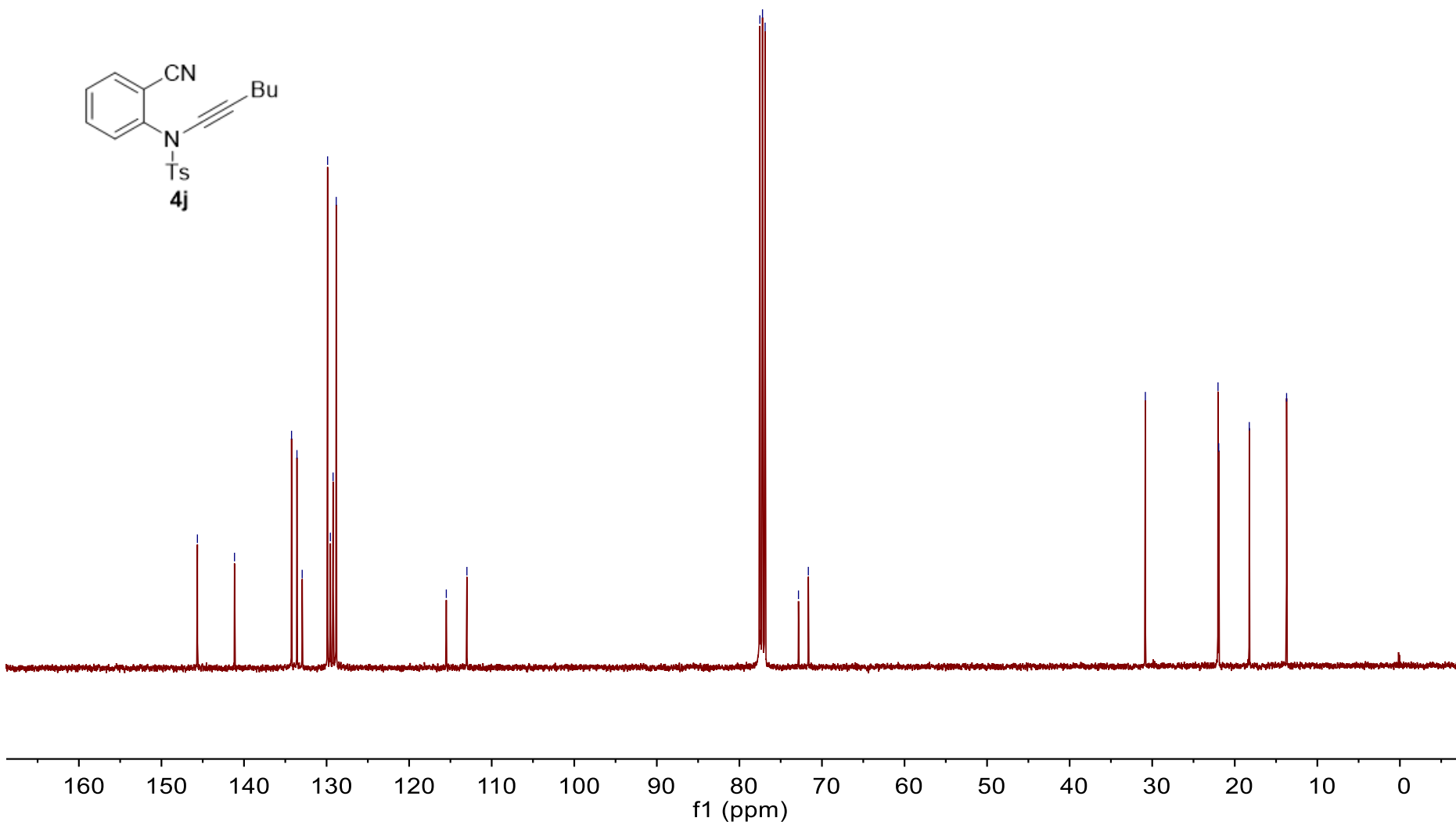
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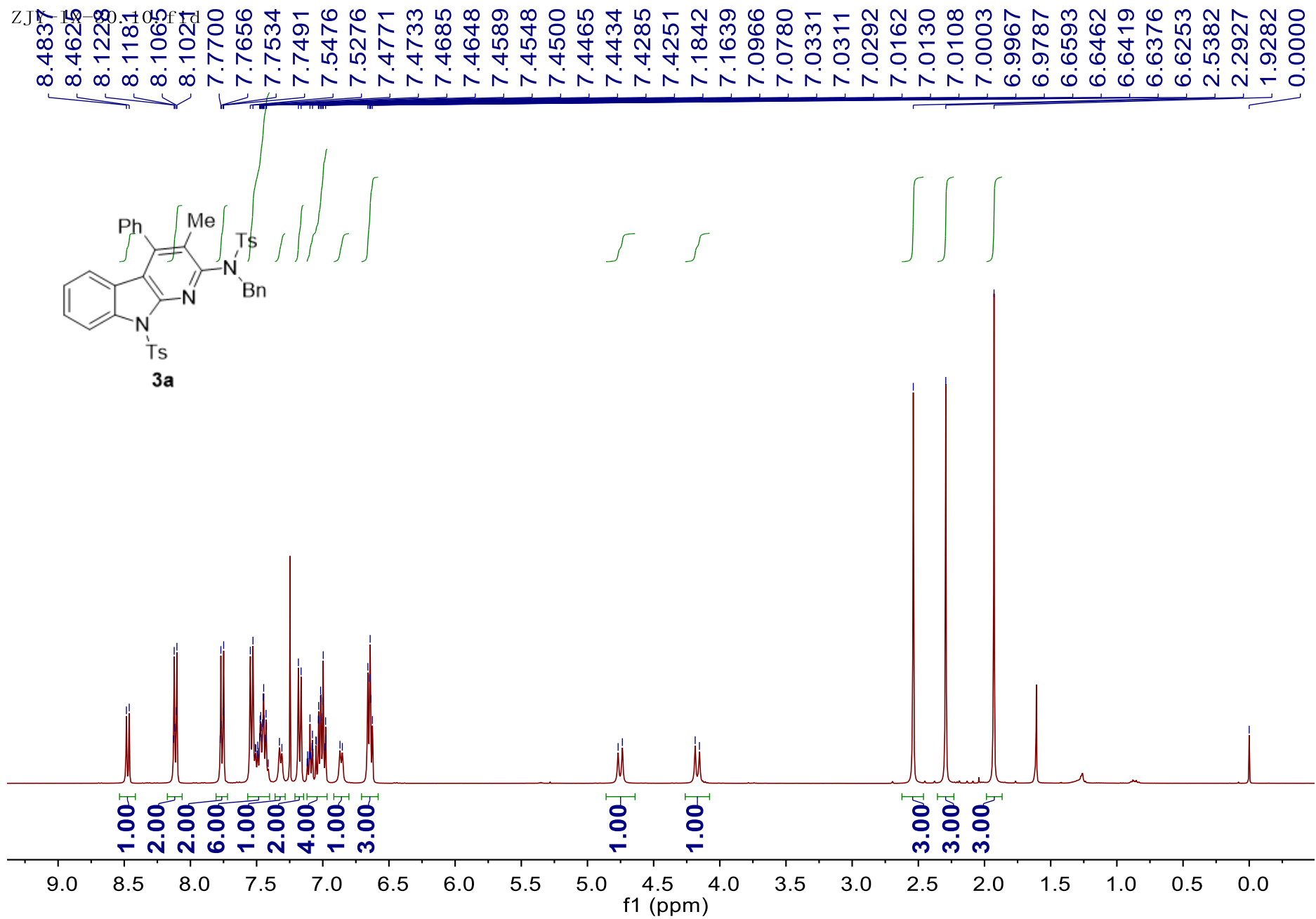


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134.242
133.587
132.953
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129.540
129.210
128.828
~ 115.498
~ 113.001

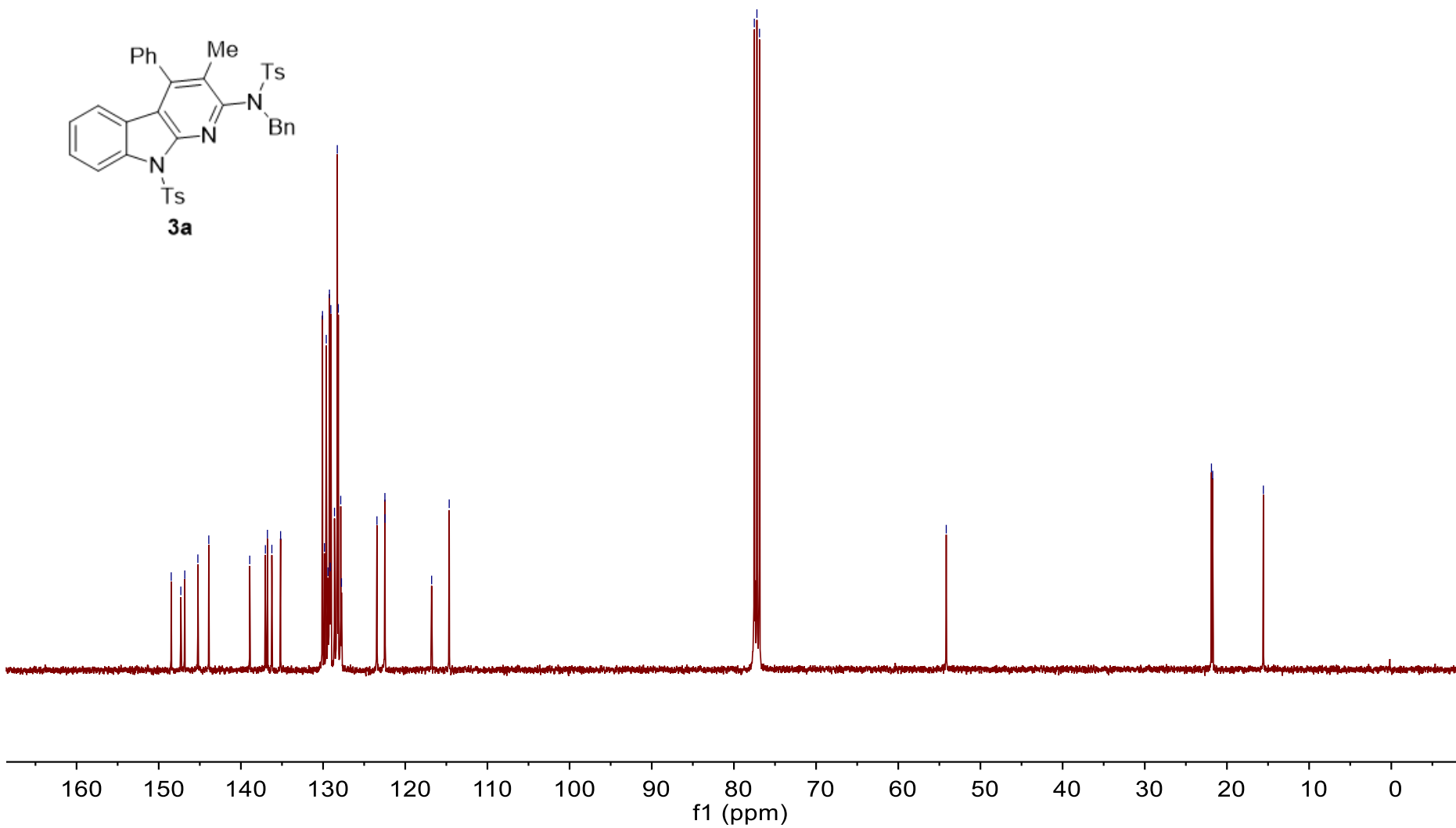
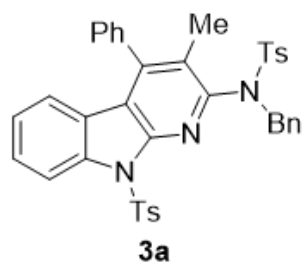
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77.200
76.883
72.841
71.648

— 30.829
22.030
21.942
18.241
13.723

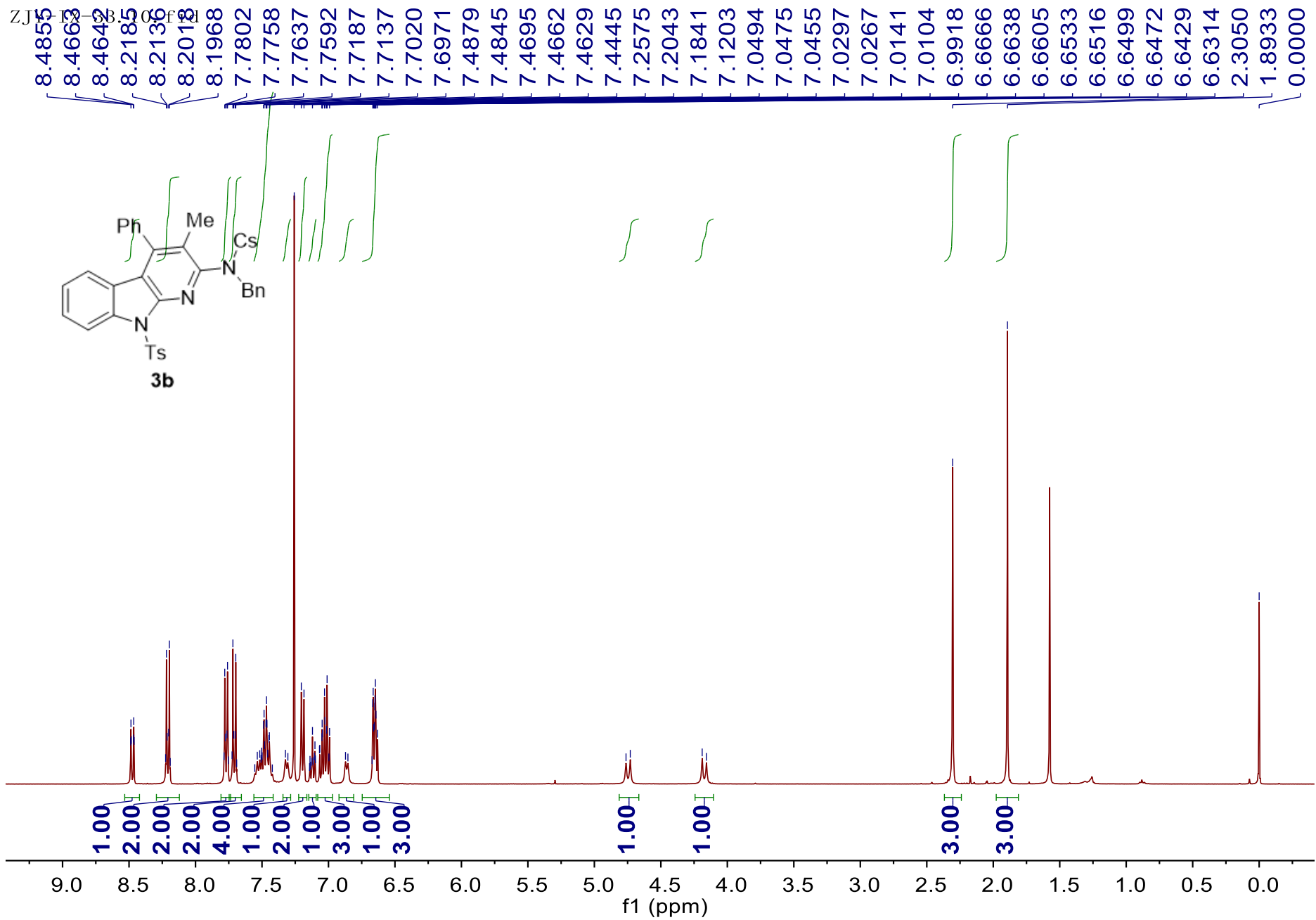




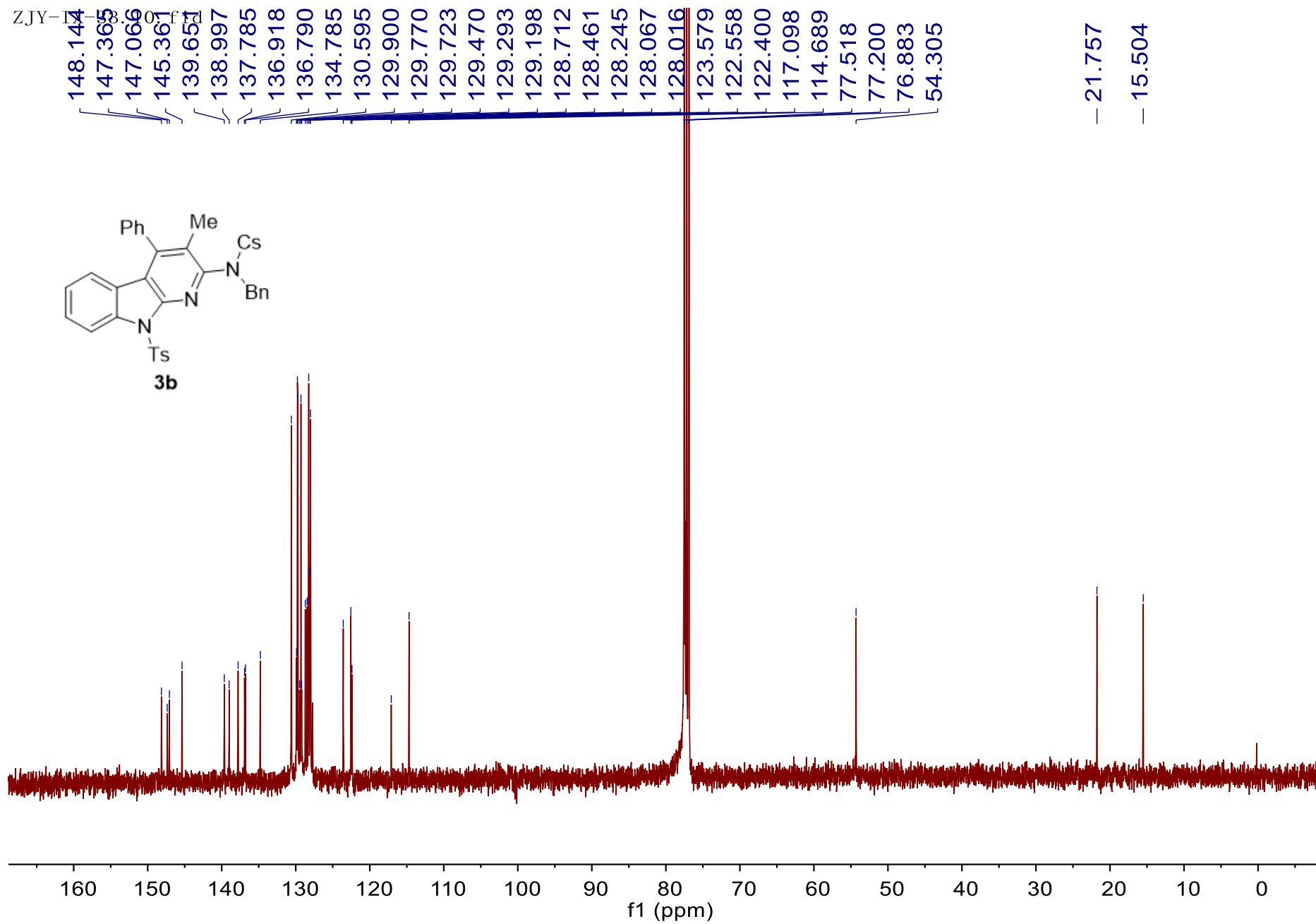
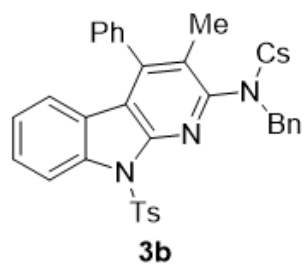
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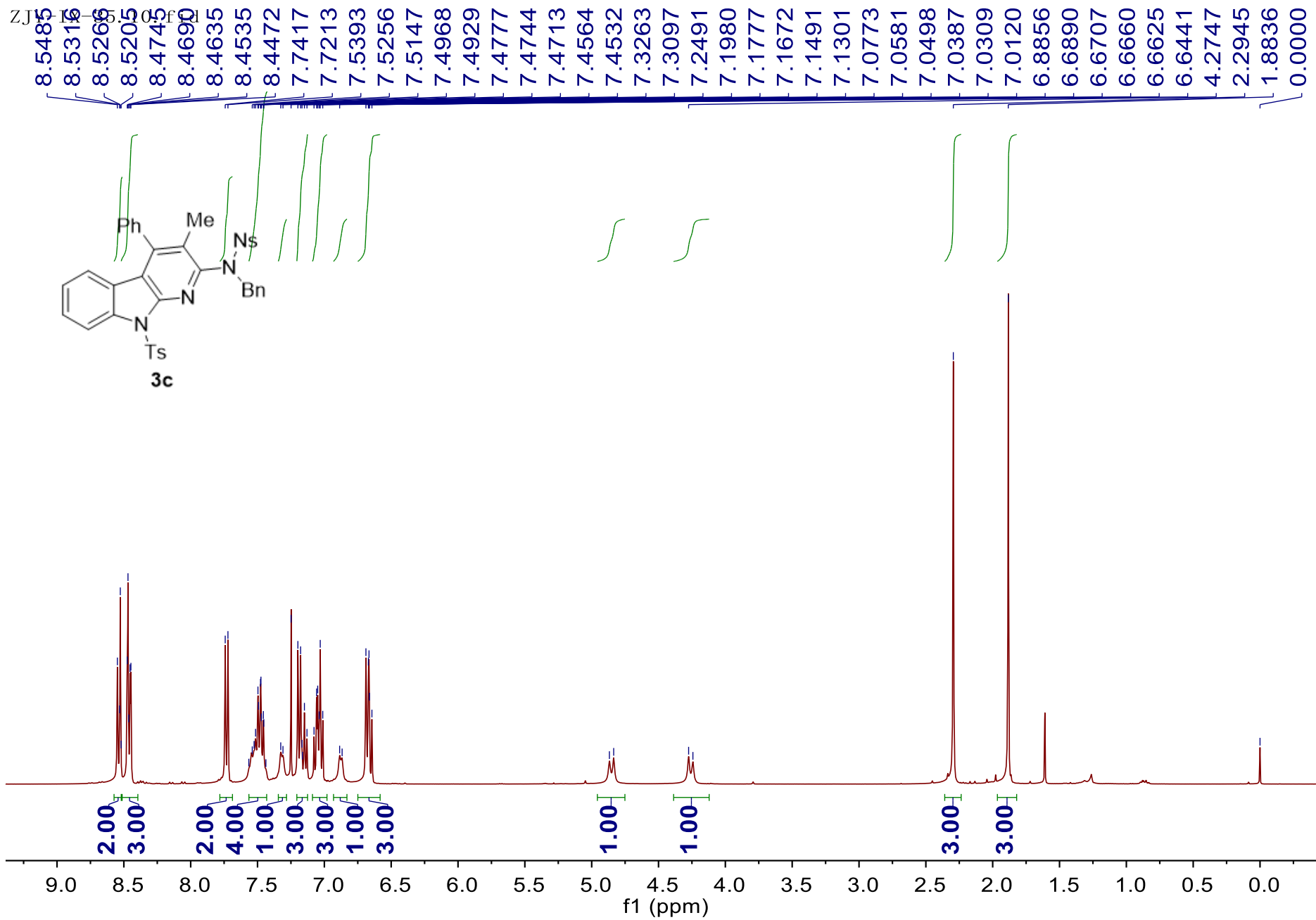


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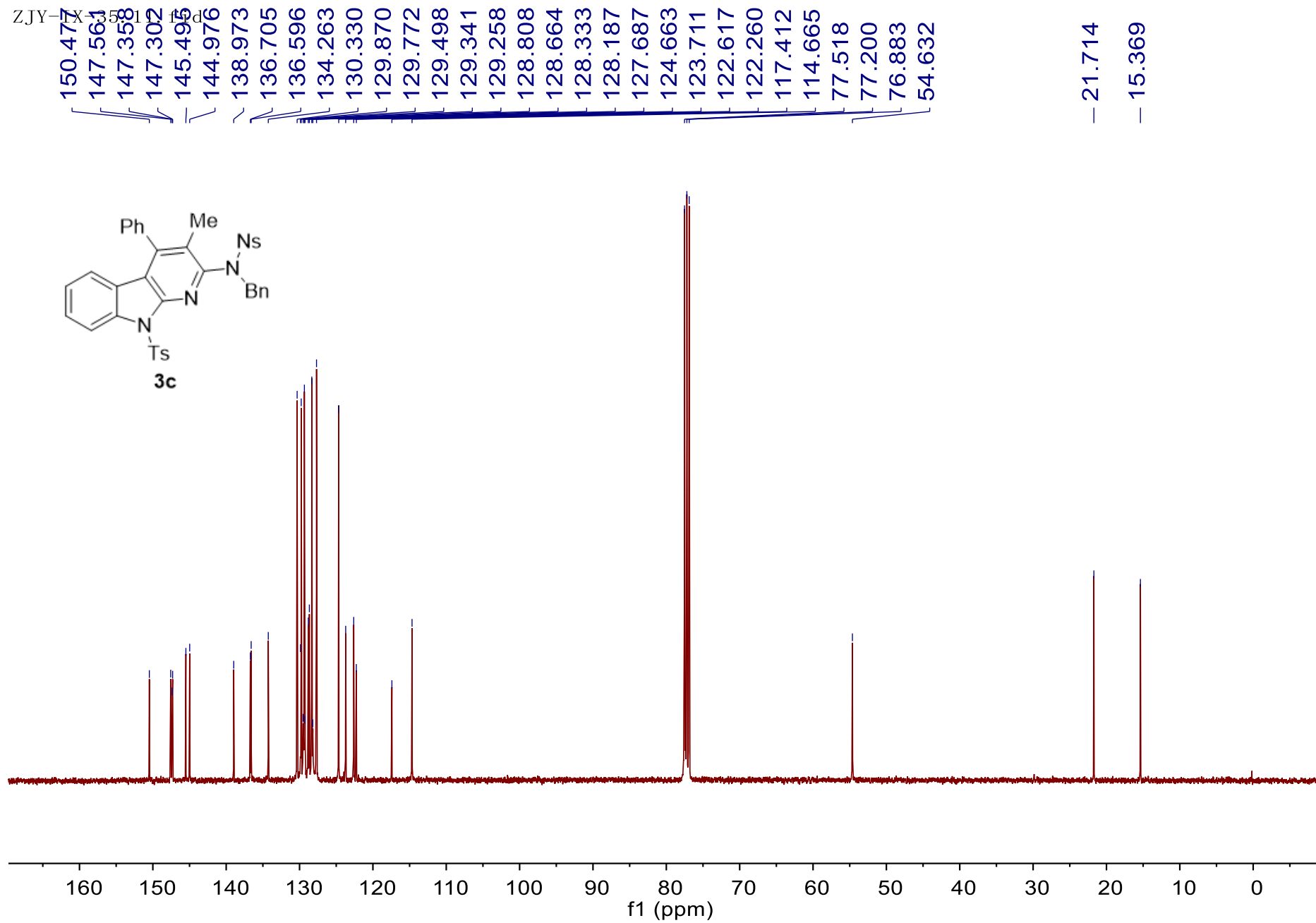
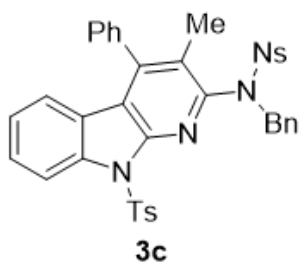


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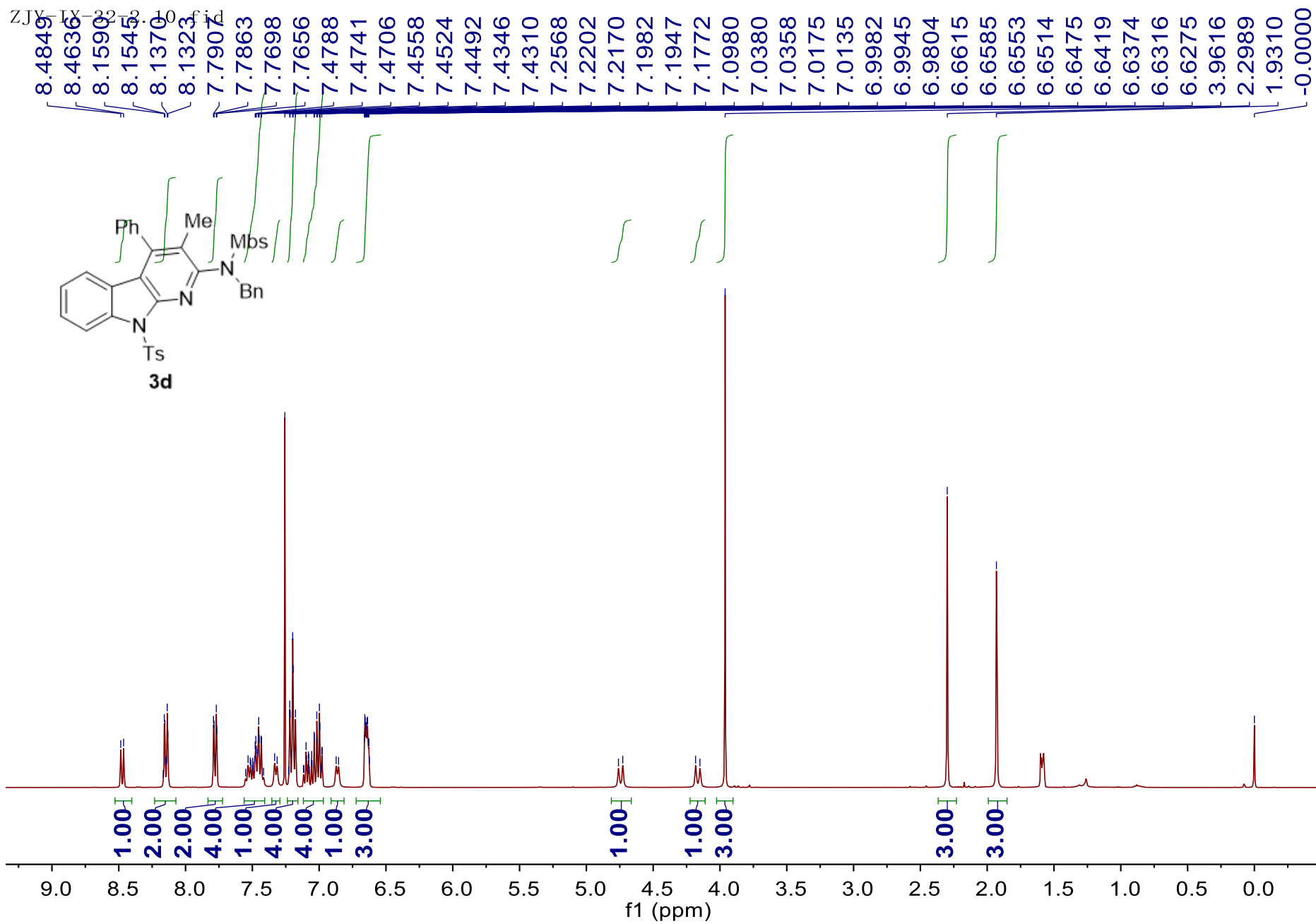


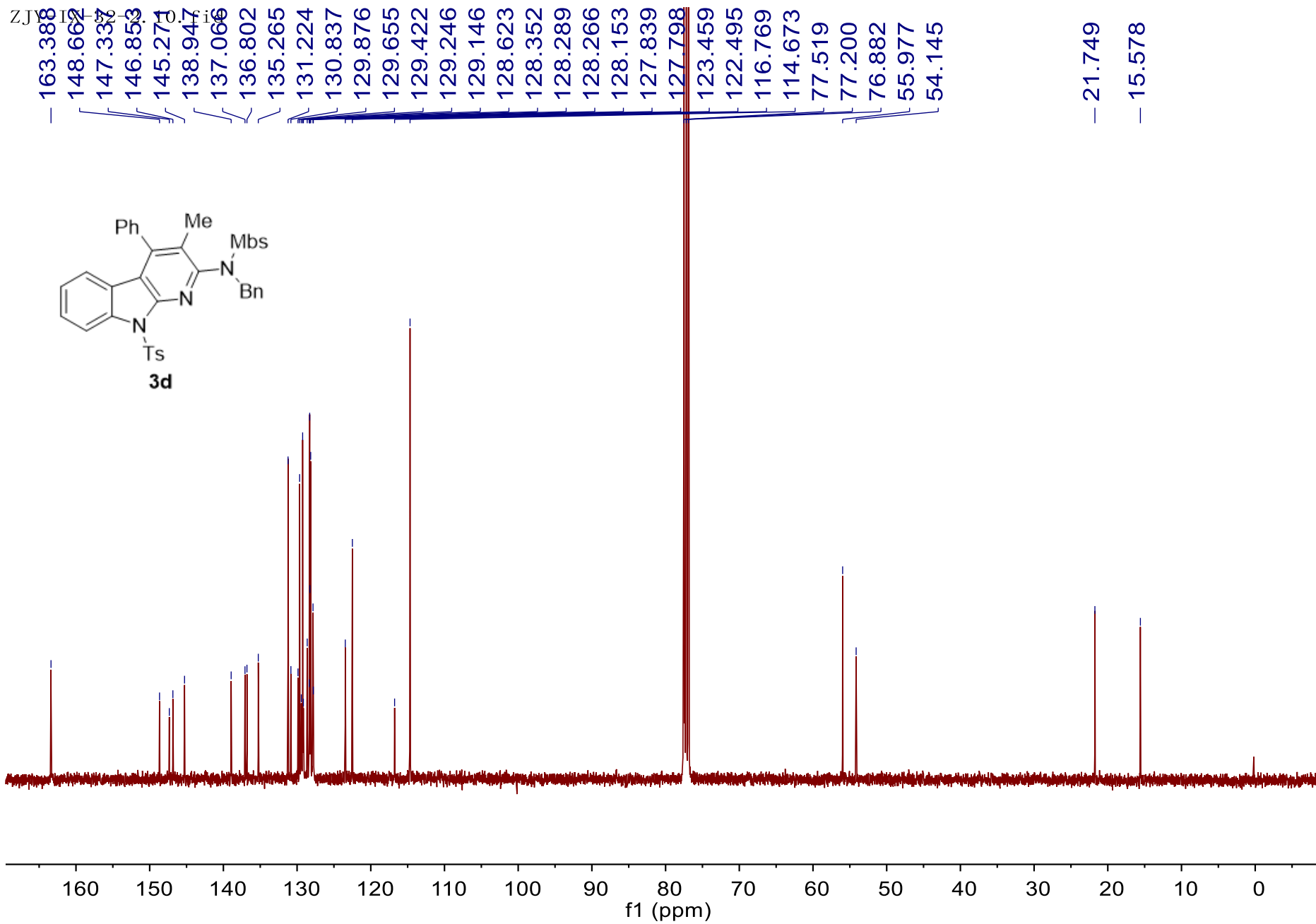


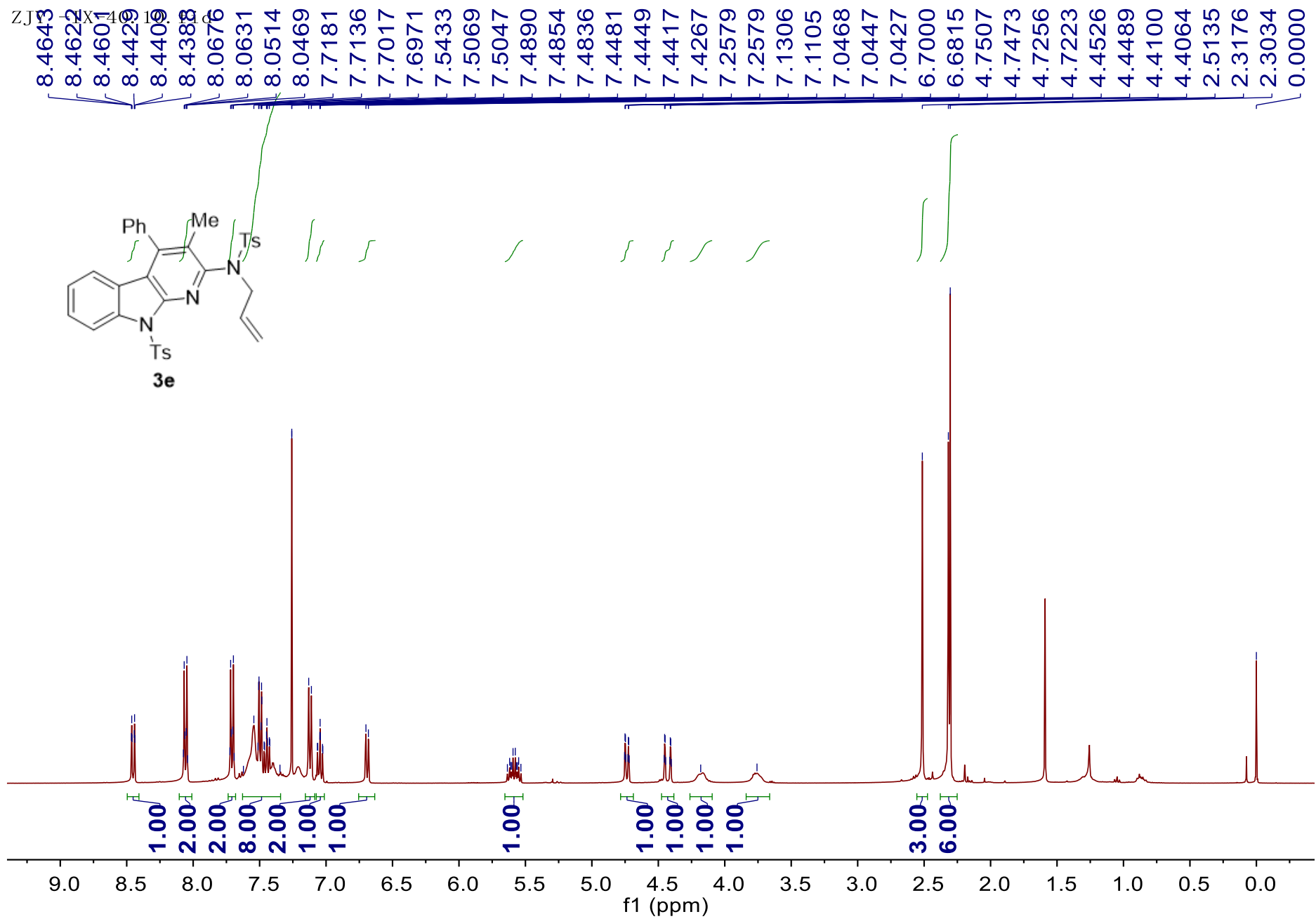
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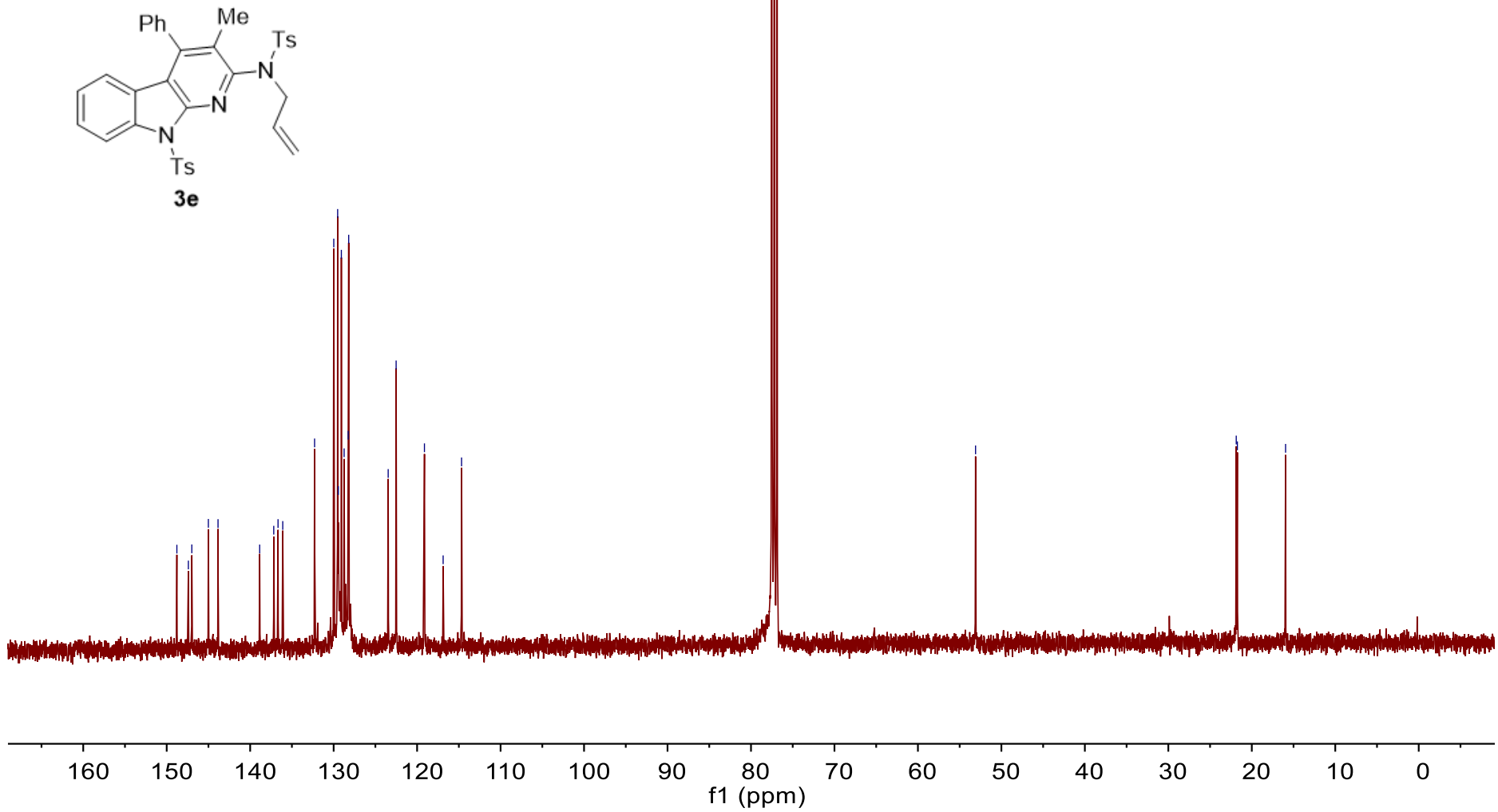
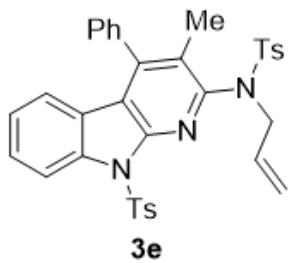




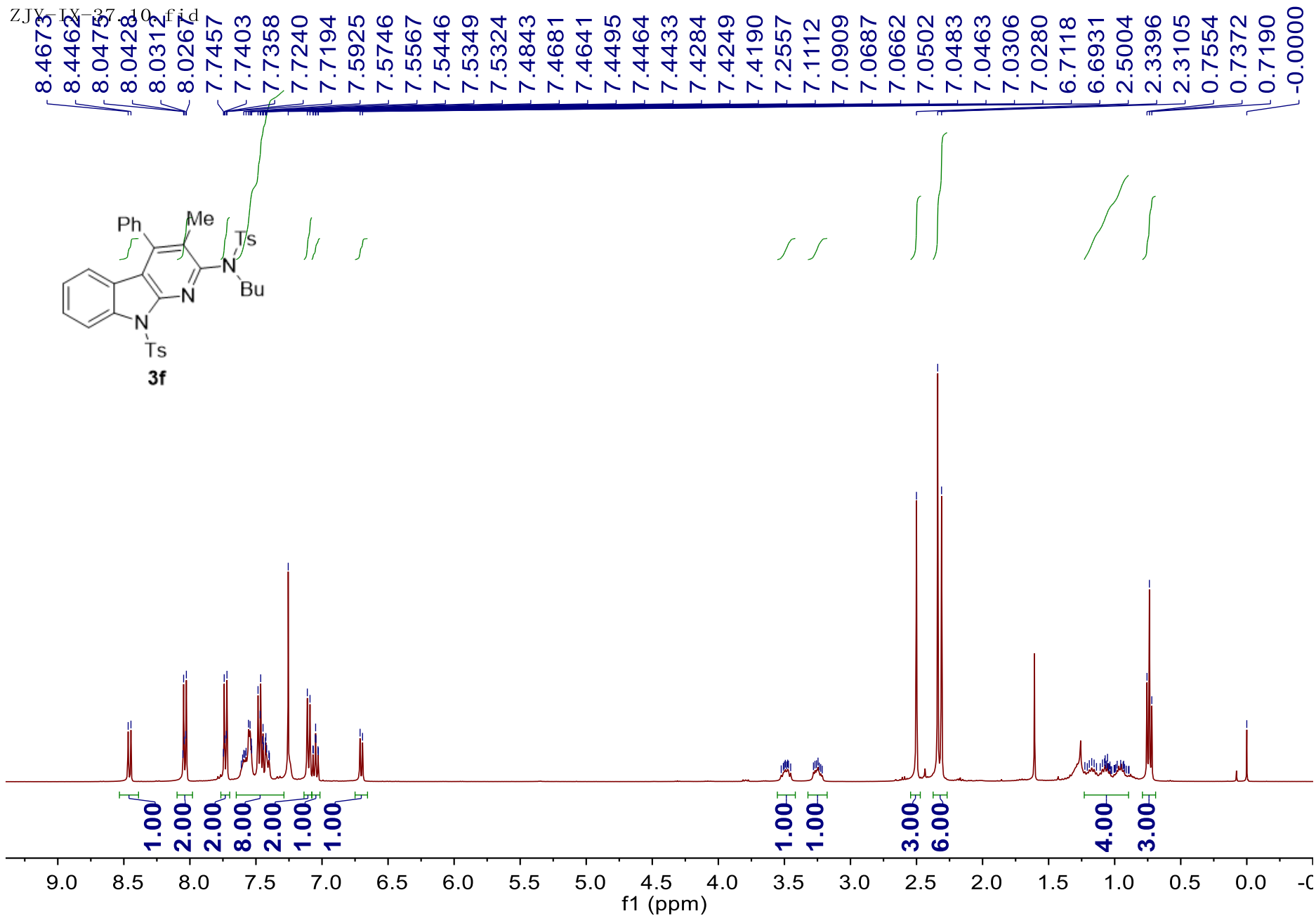
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129.443
129.076
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114.673
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77.200
76.882

53.093

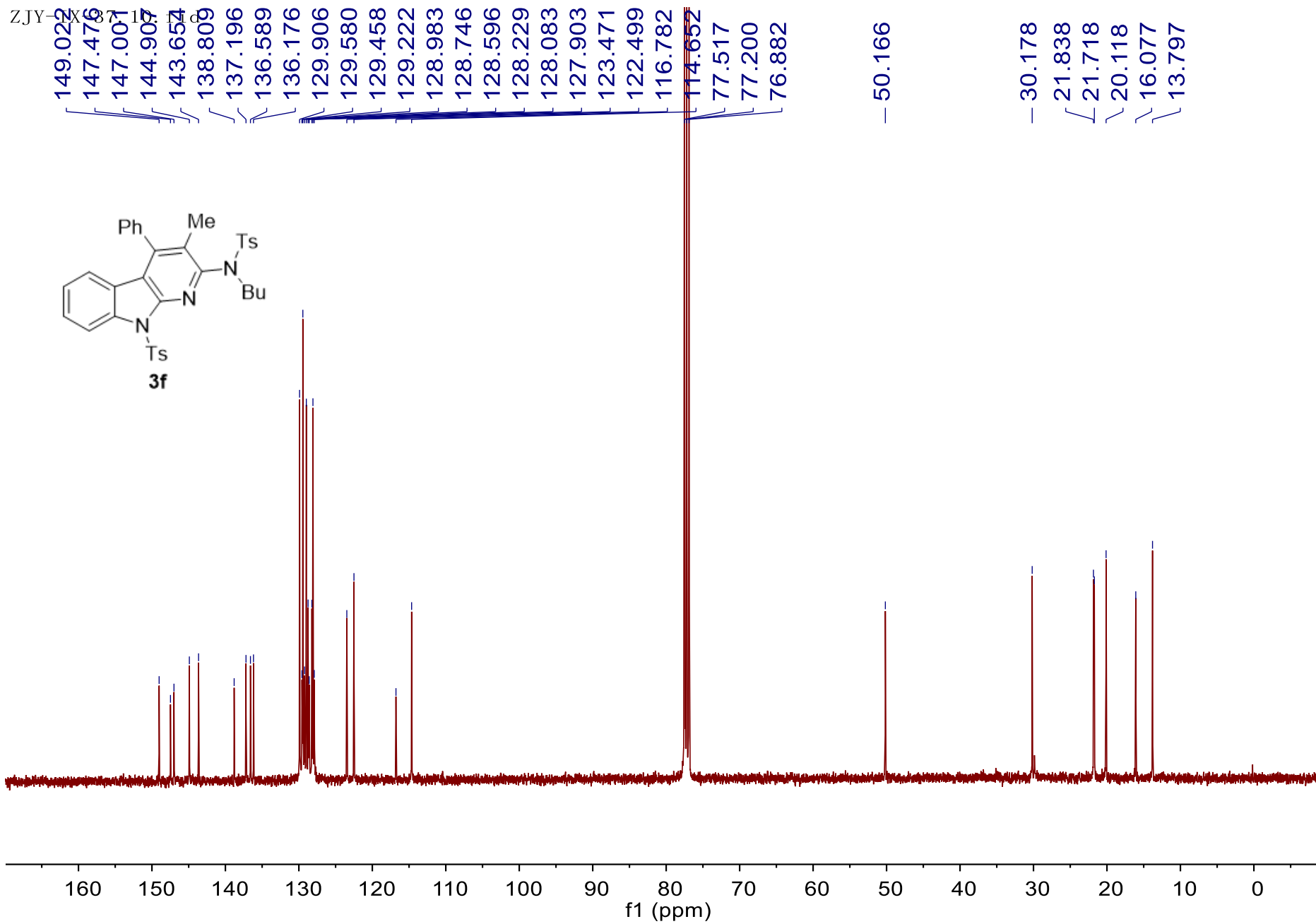
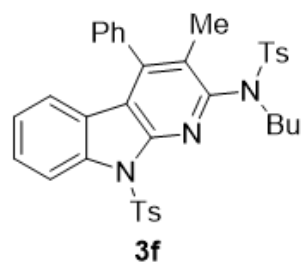
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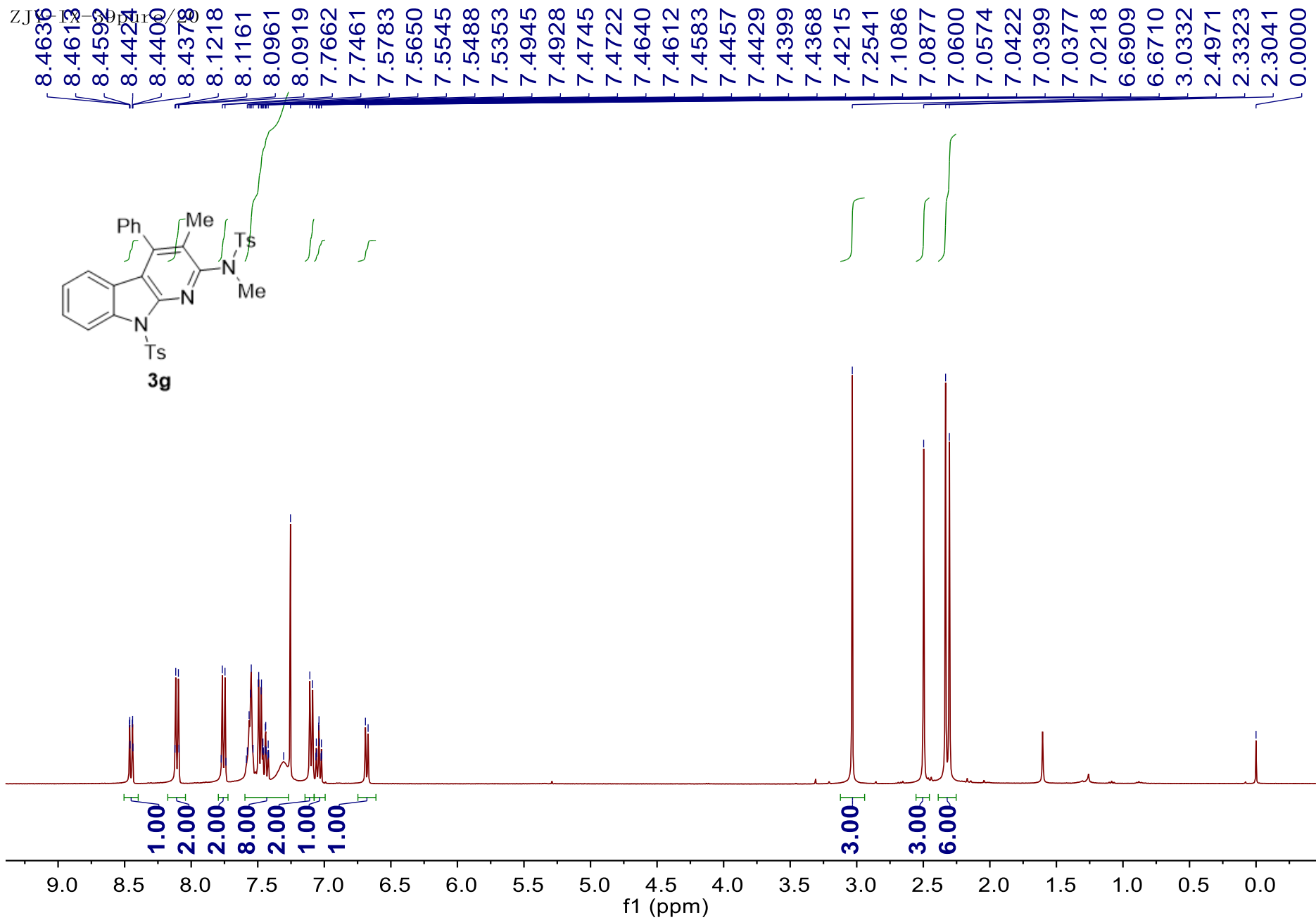
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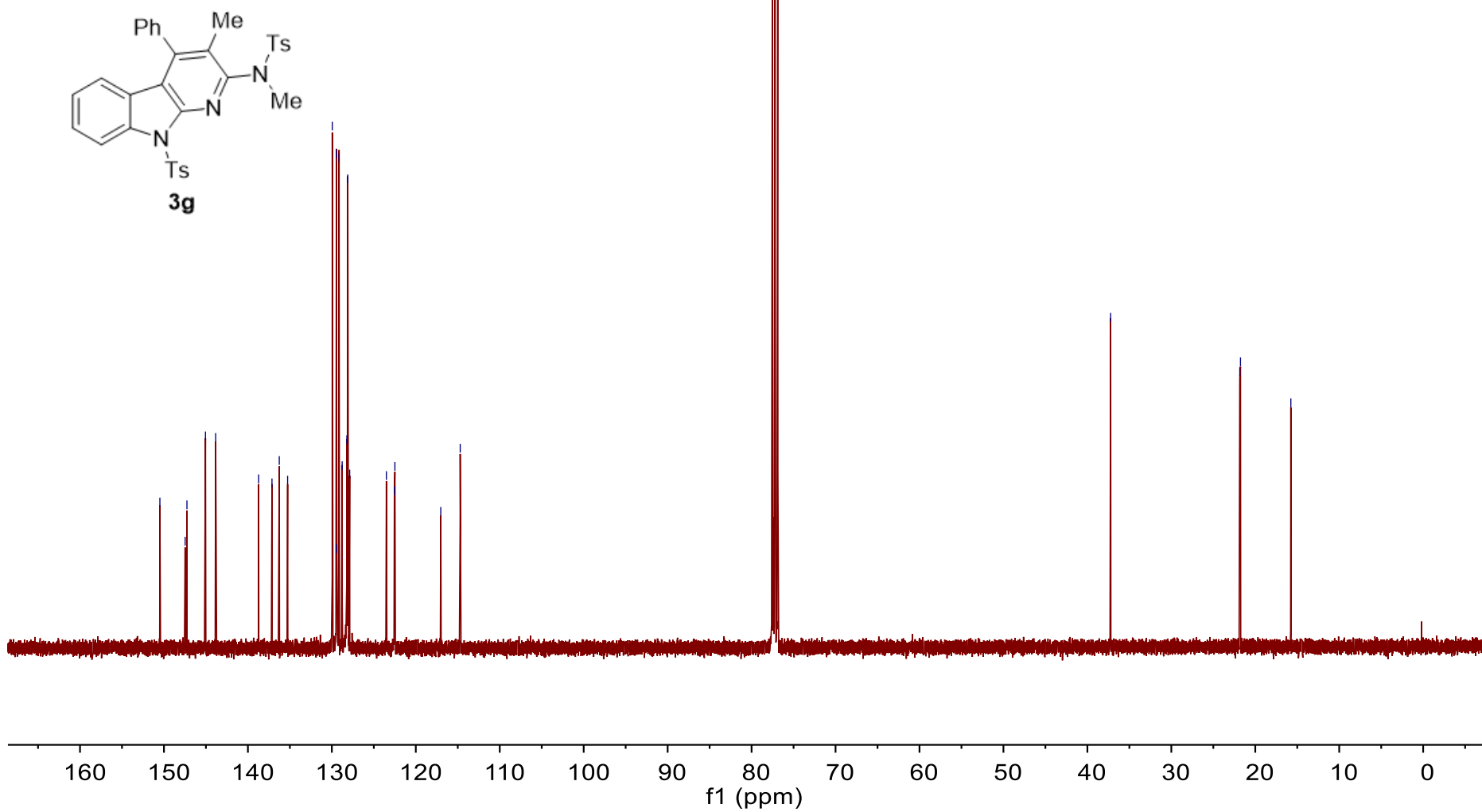
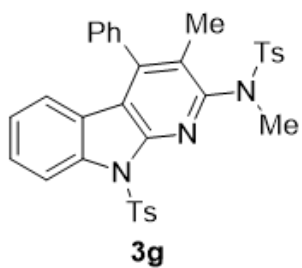
S80



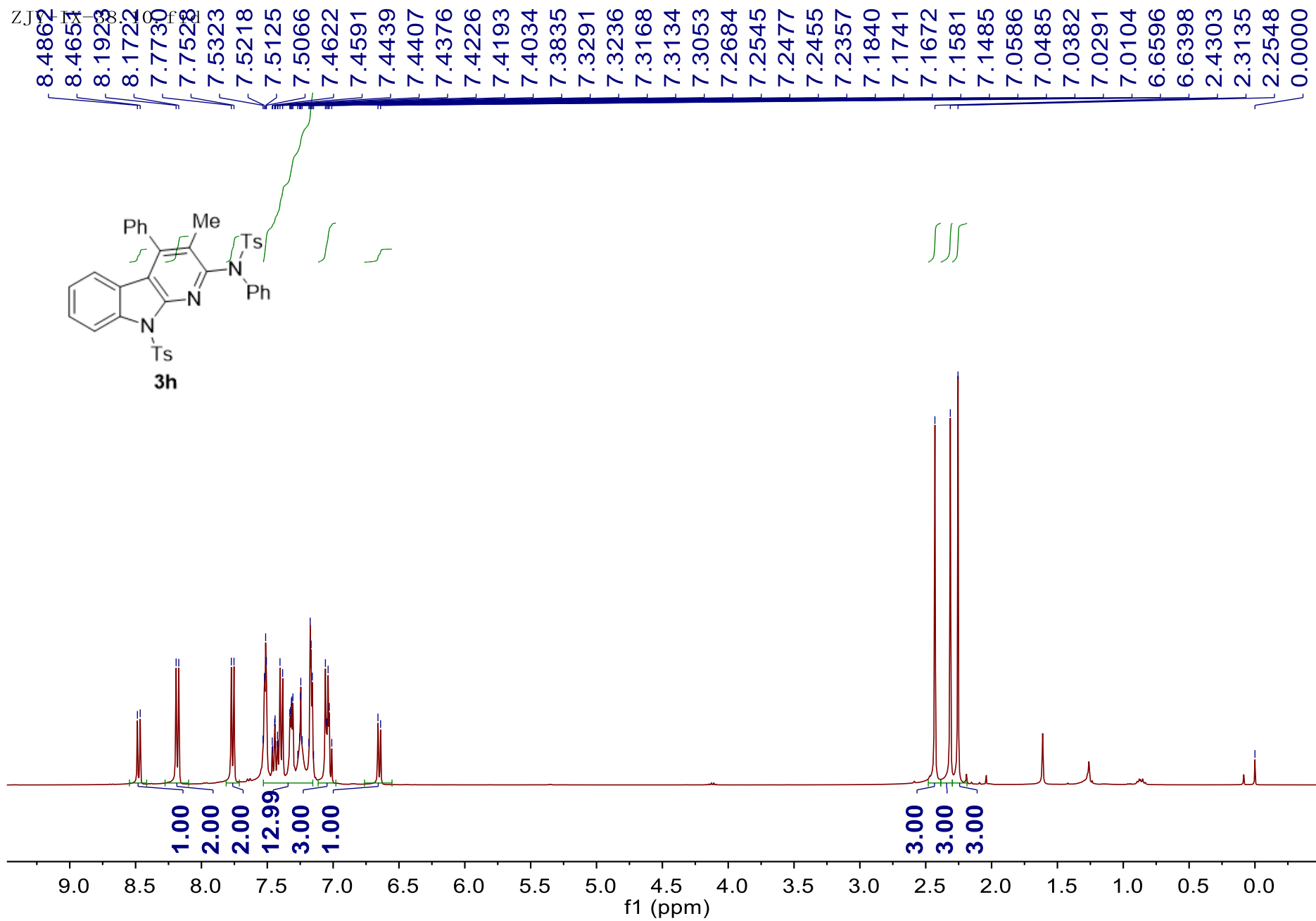
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128.770
128.216
128.106
127.876
123.501
122.550
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117.024
114.709
77.518
77.200
76.883

— 37.229

21.846
21.762
~ 15.762

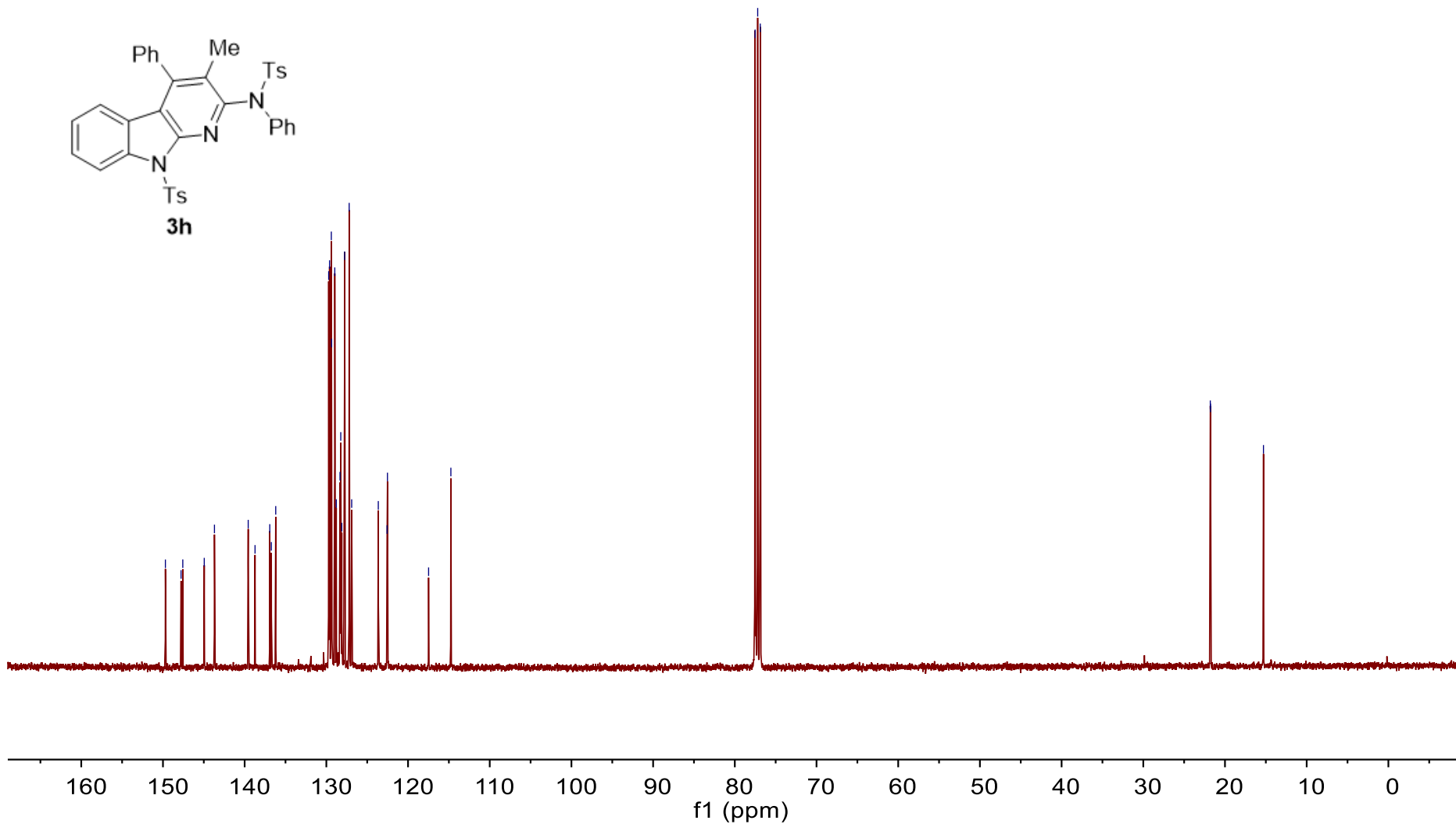
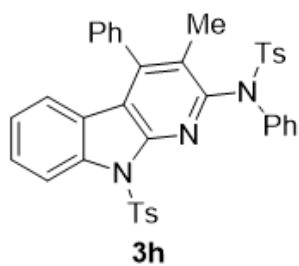


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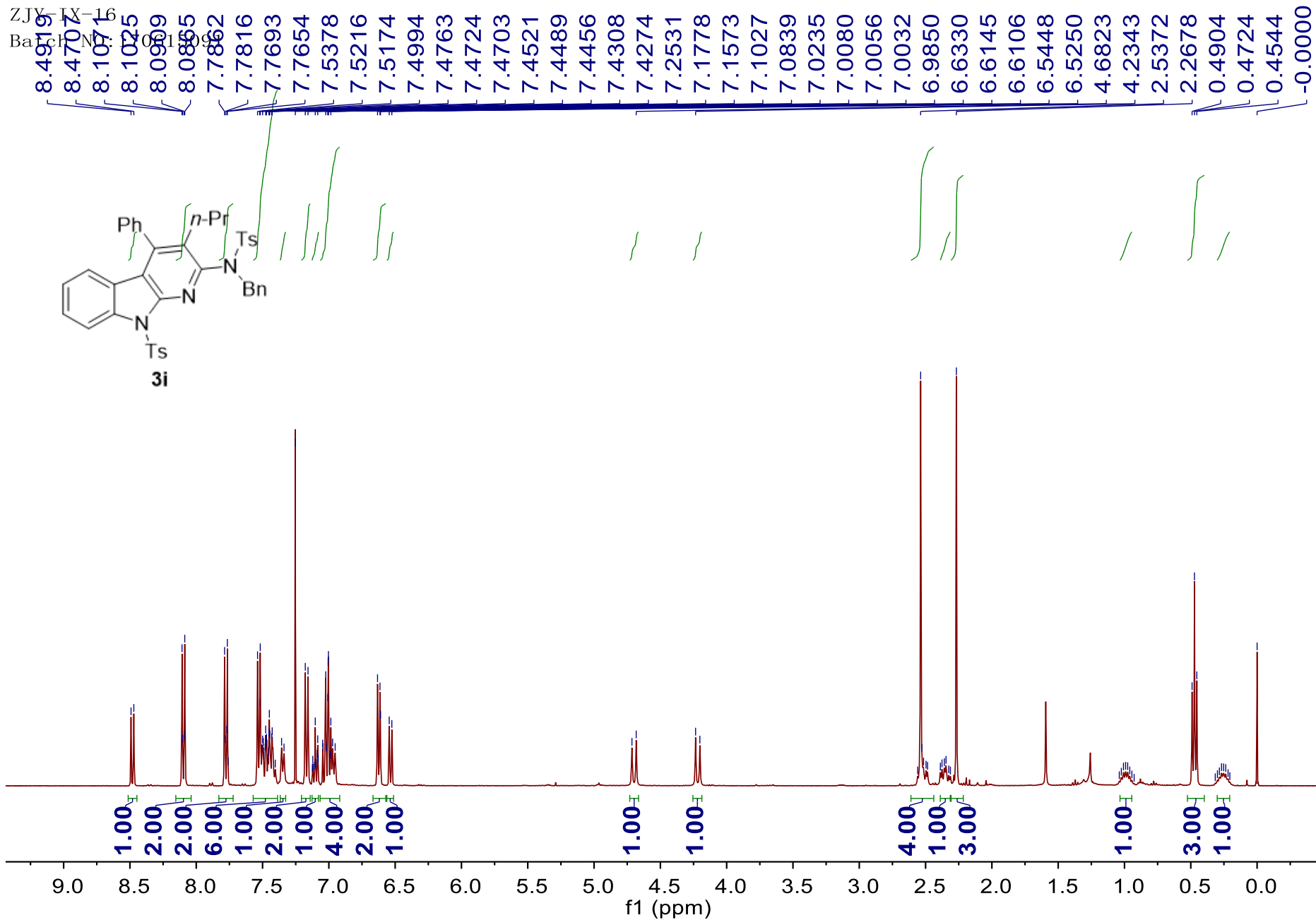
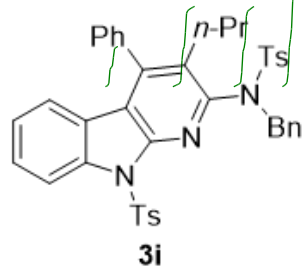


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147.783
147.572
144.945
143.696
139.563
138.722
136.926
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136.195
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129.610
129.392
129.350
128.967
128.785
128.328
128.234
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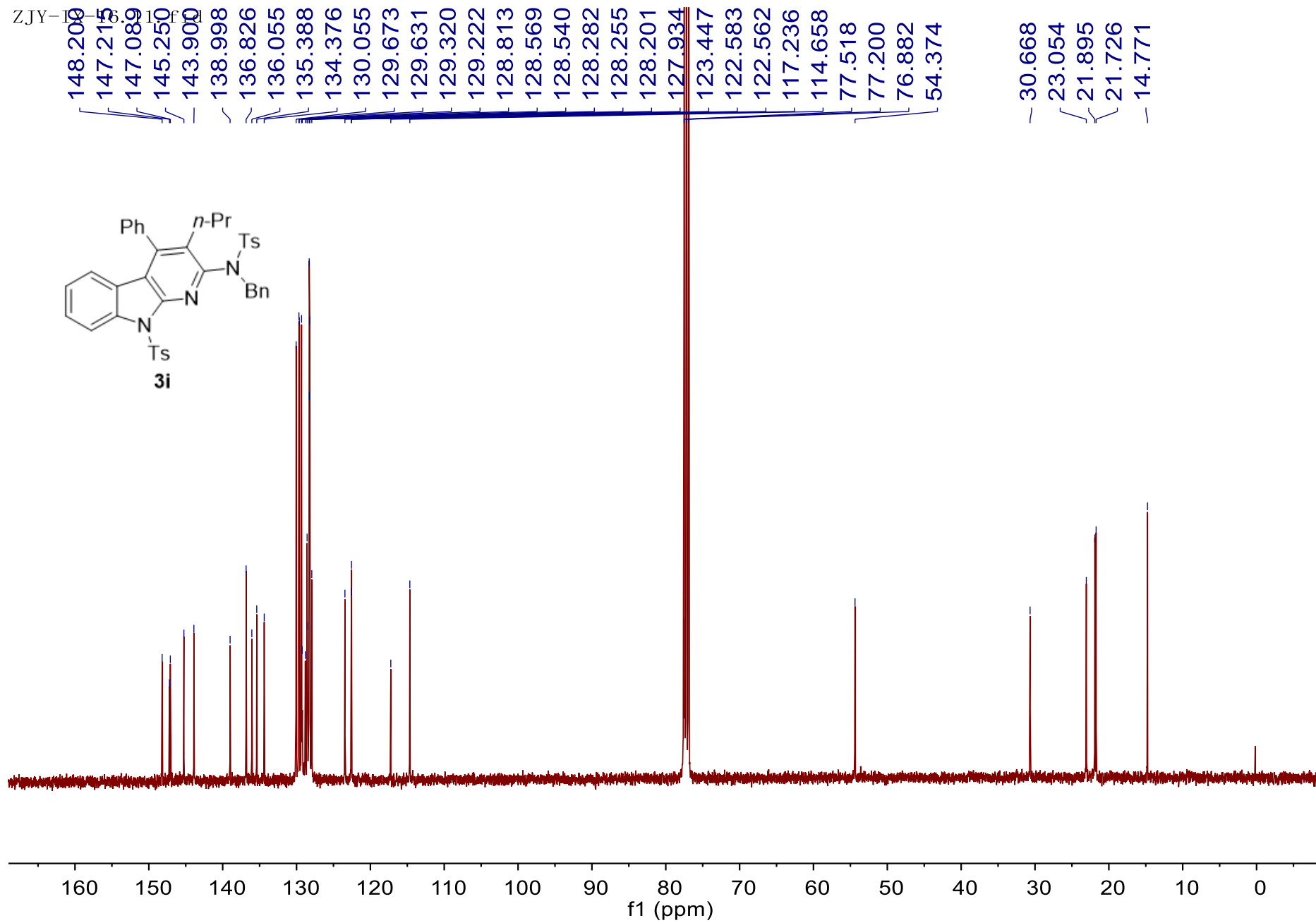
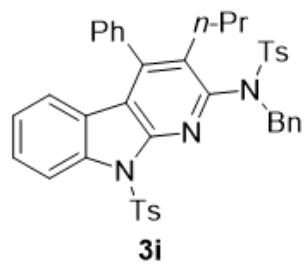
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21.774
~ 15.289



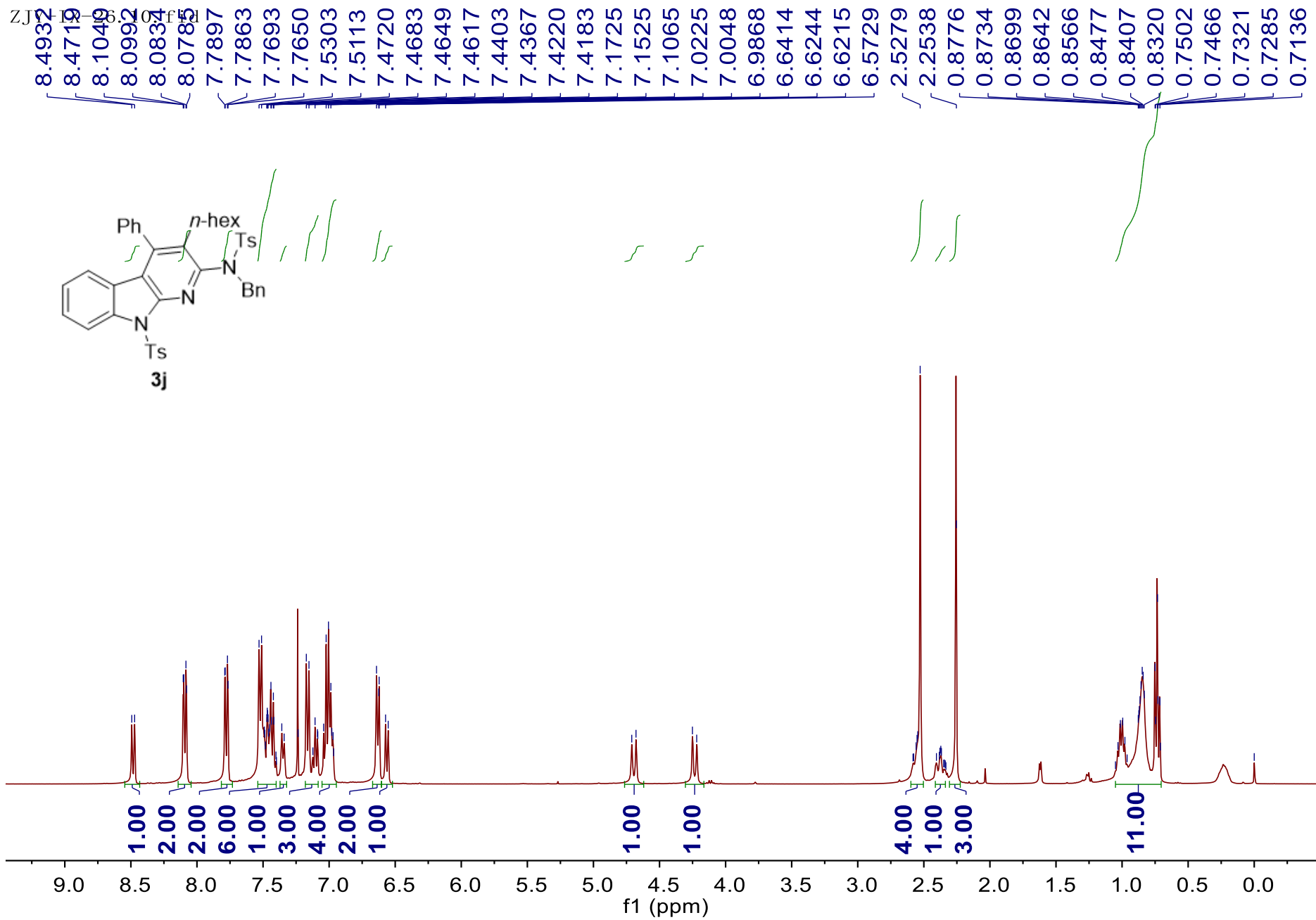
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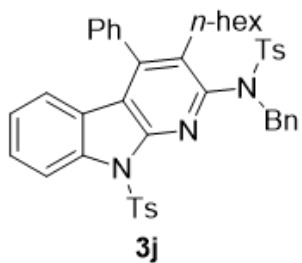
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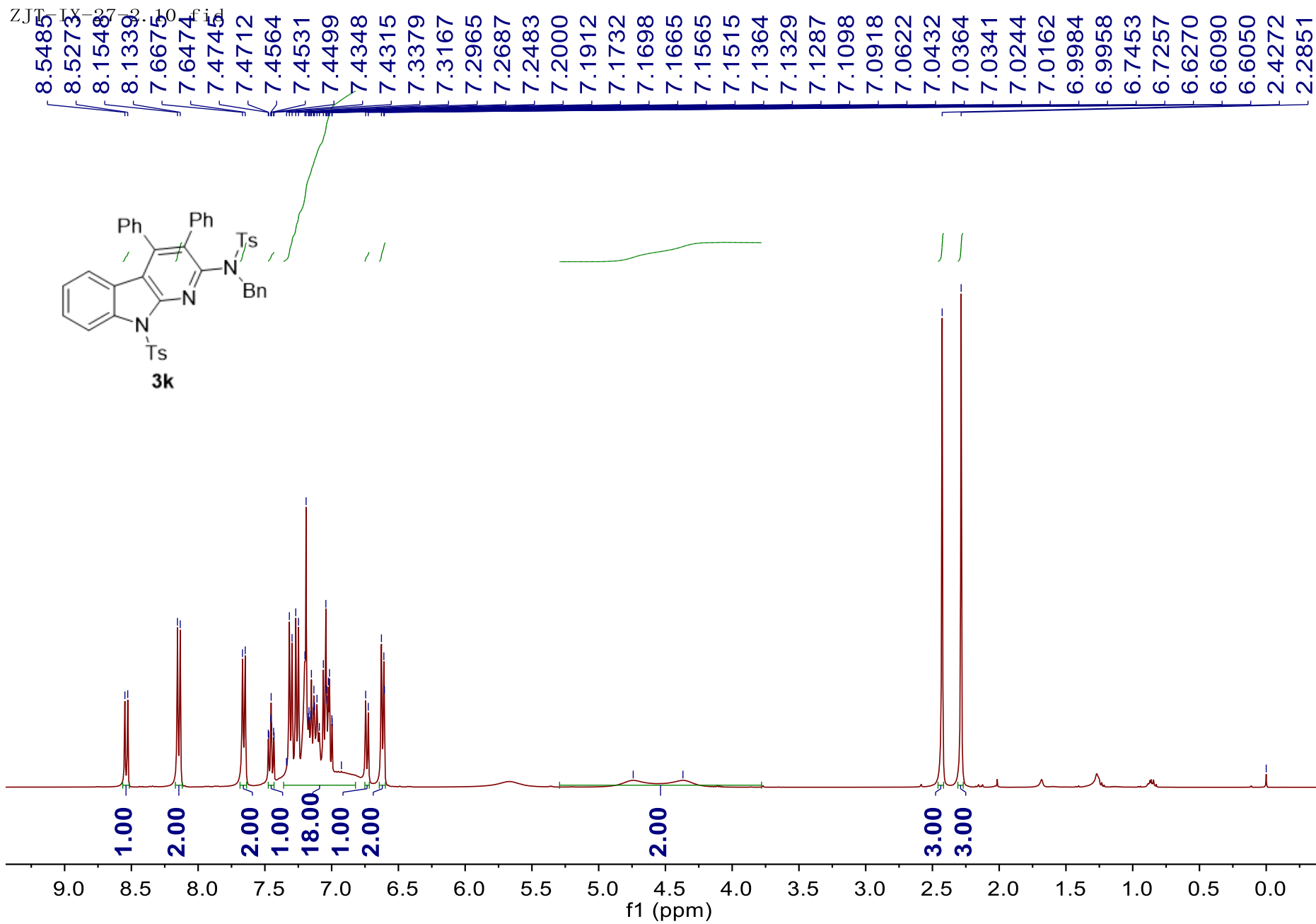
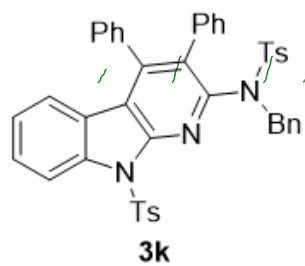
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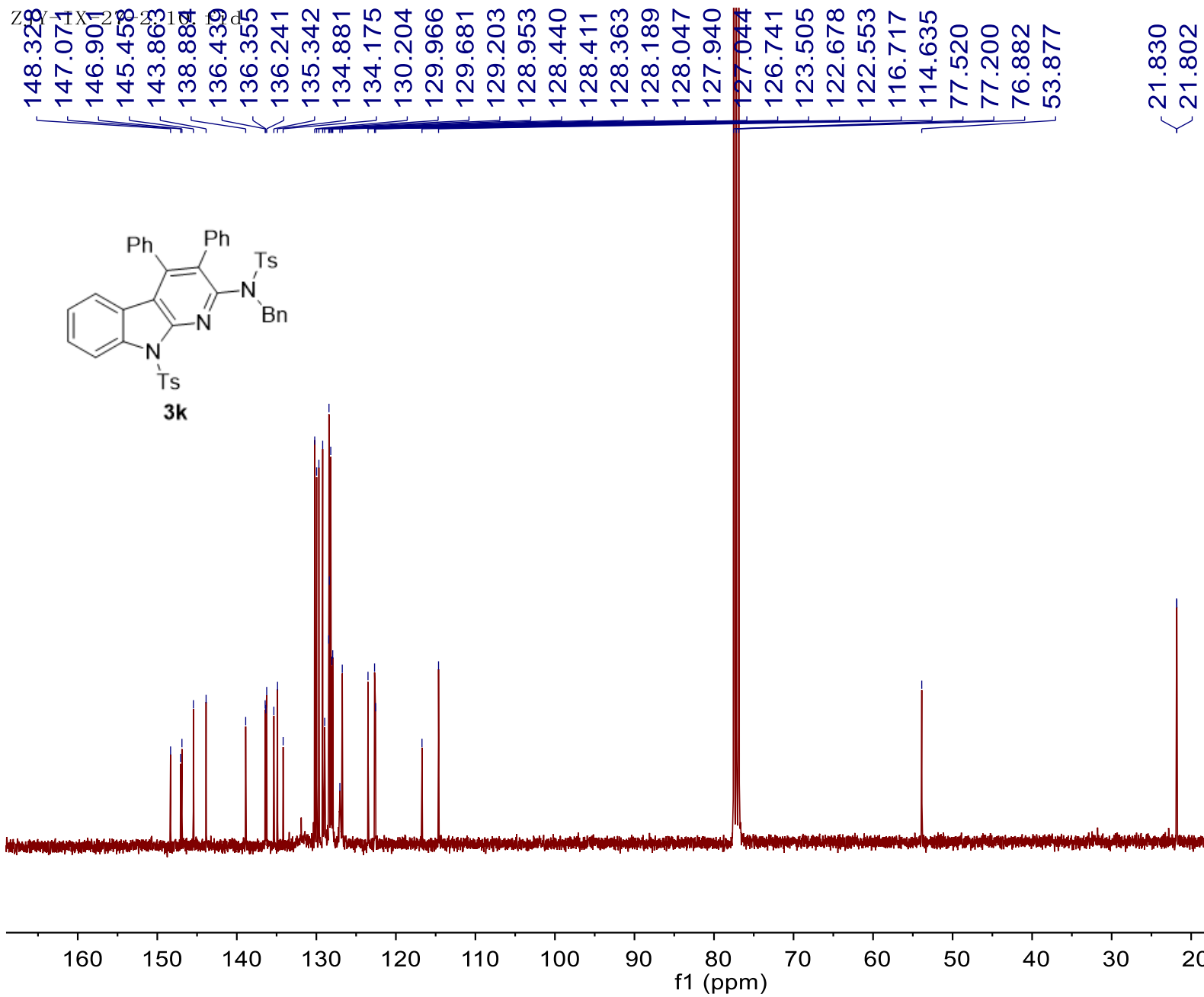


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 147.051
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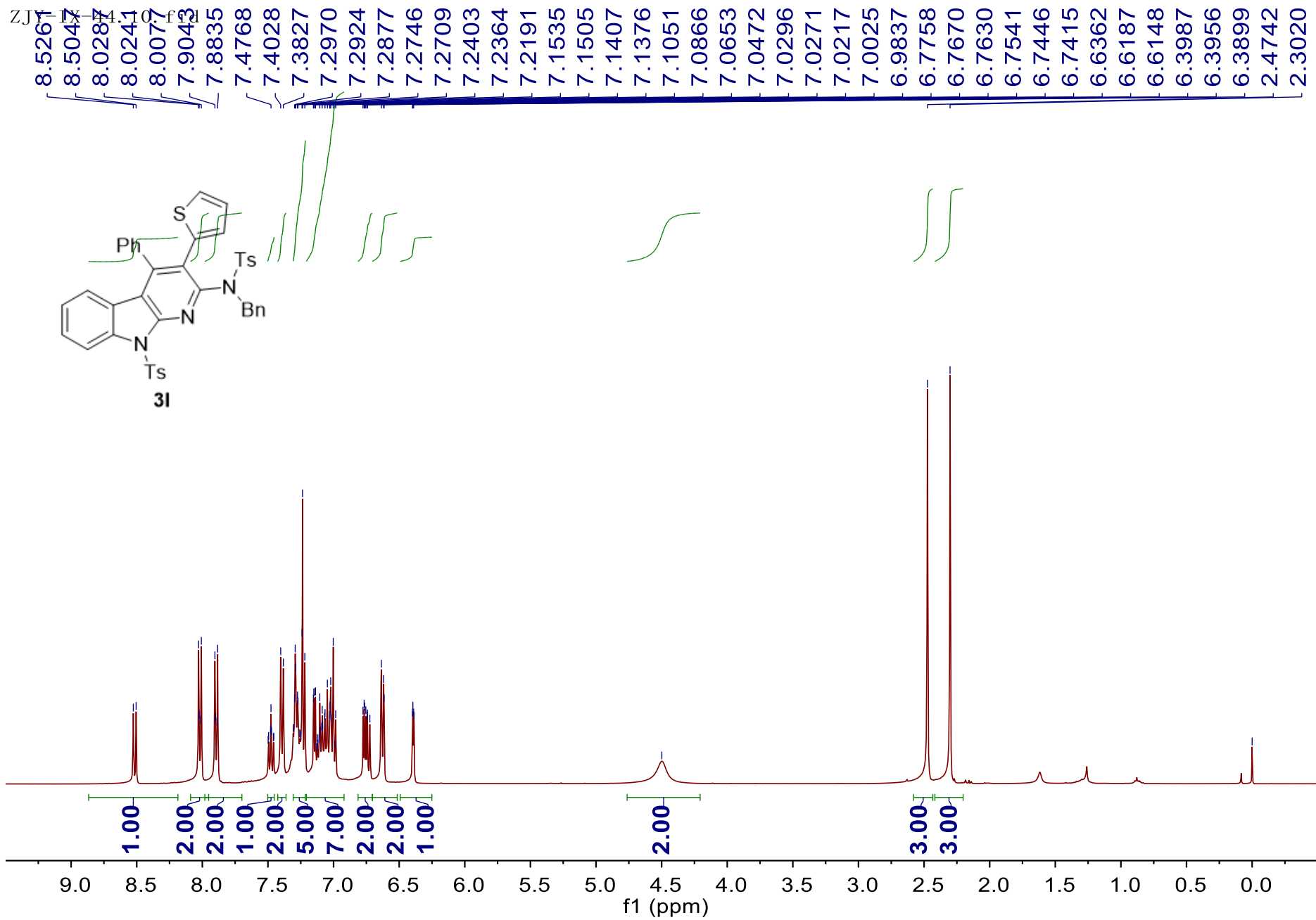


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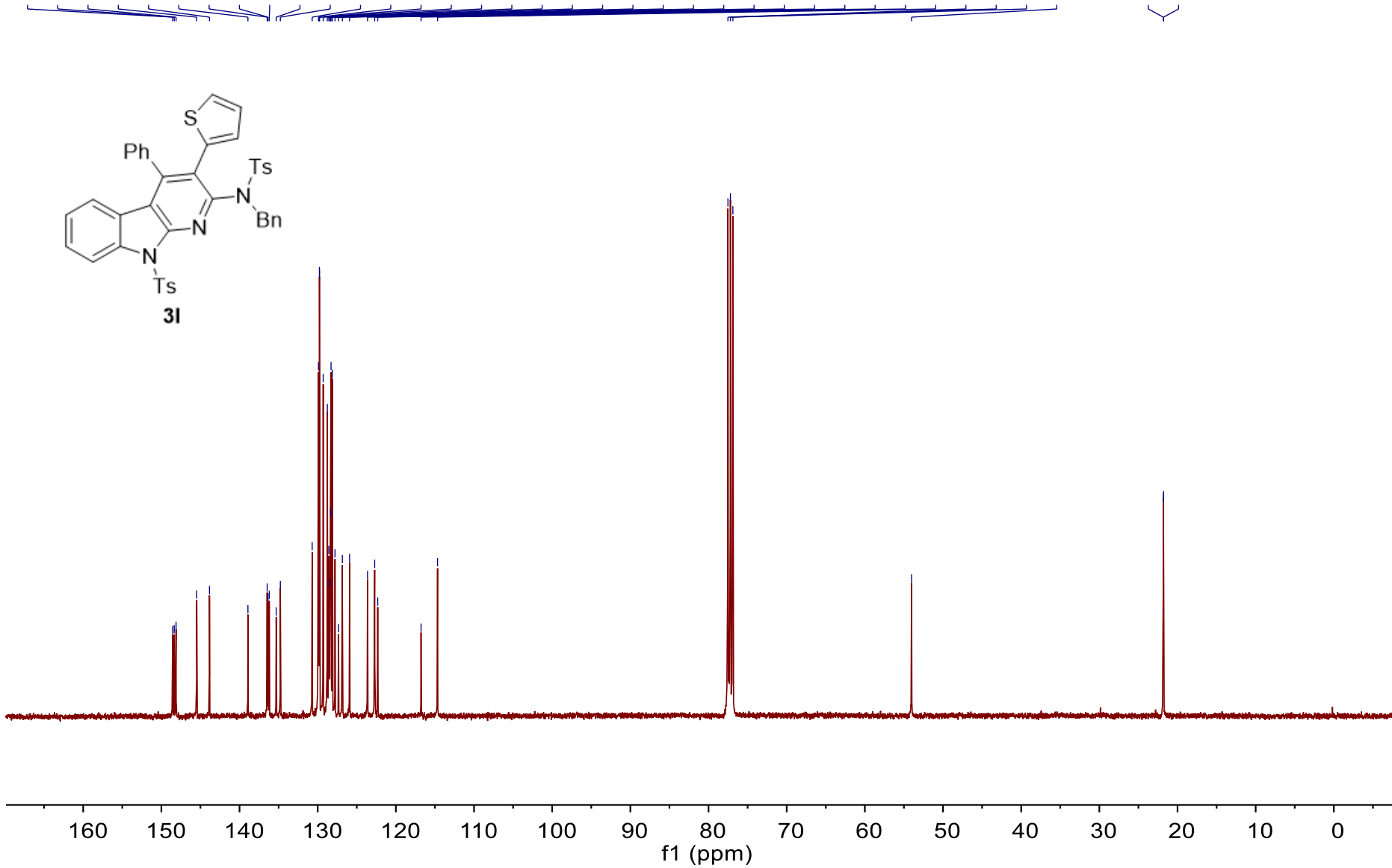
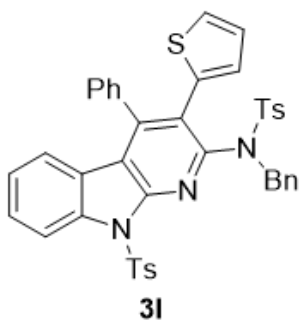


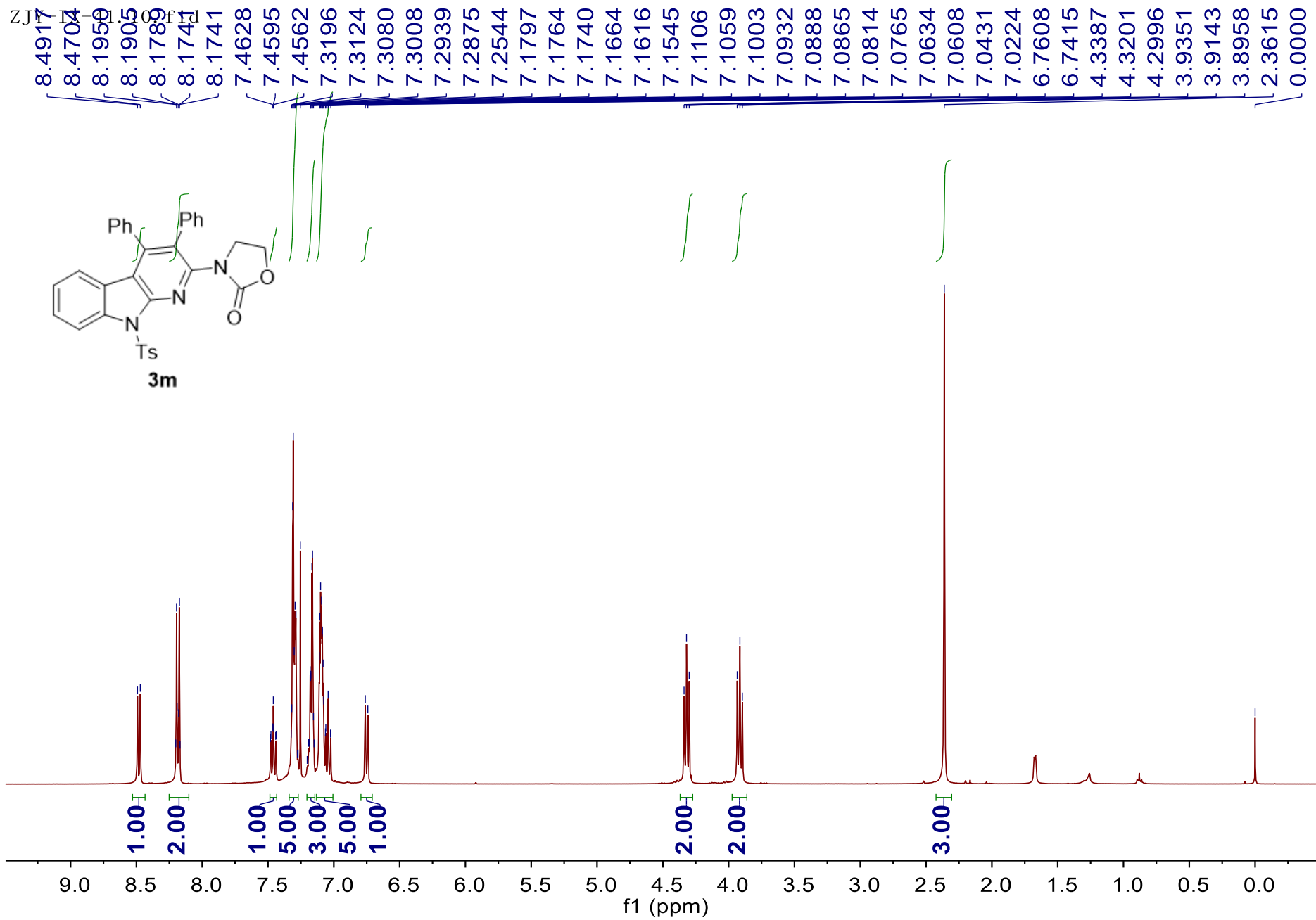


S90

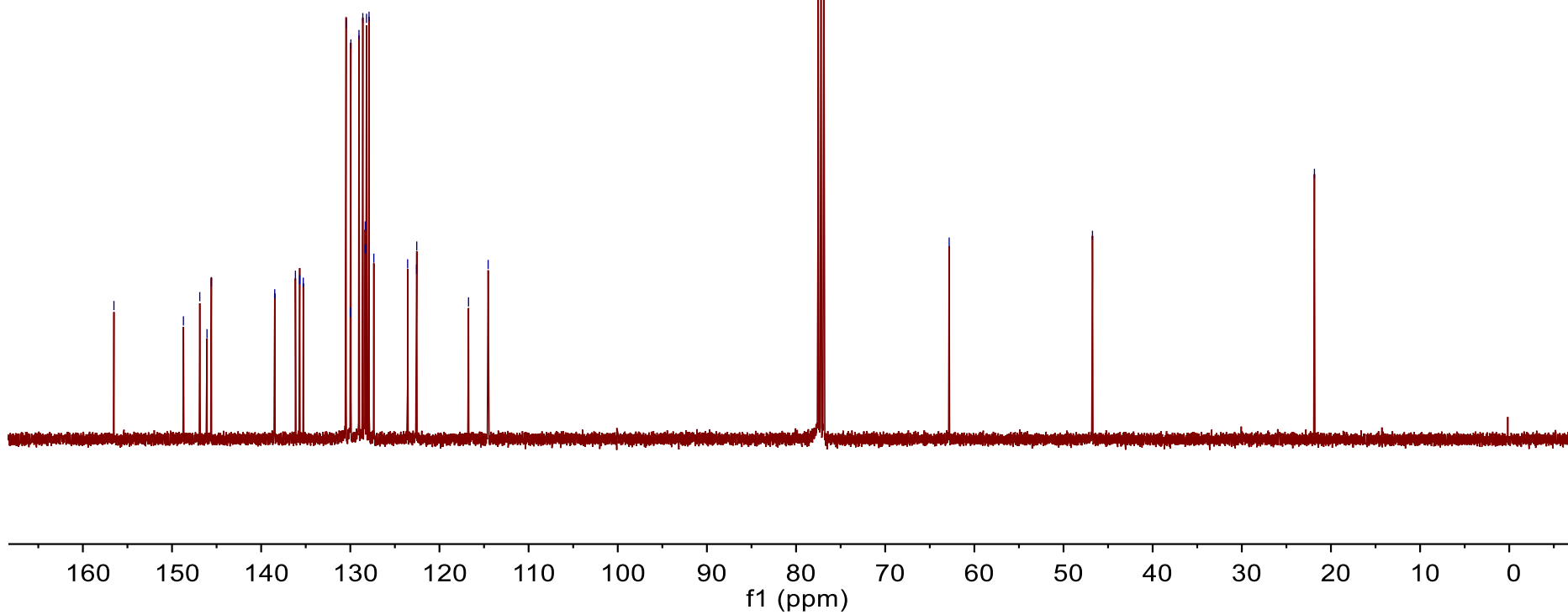
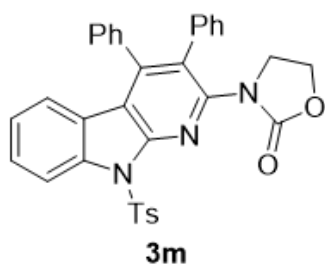


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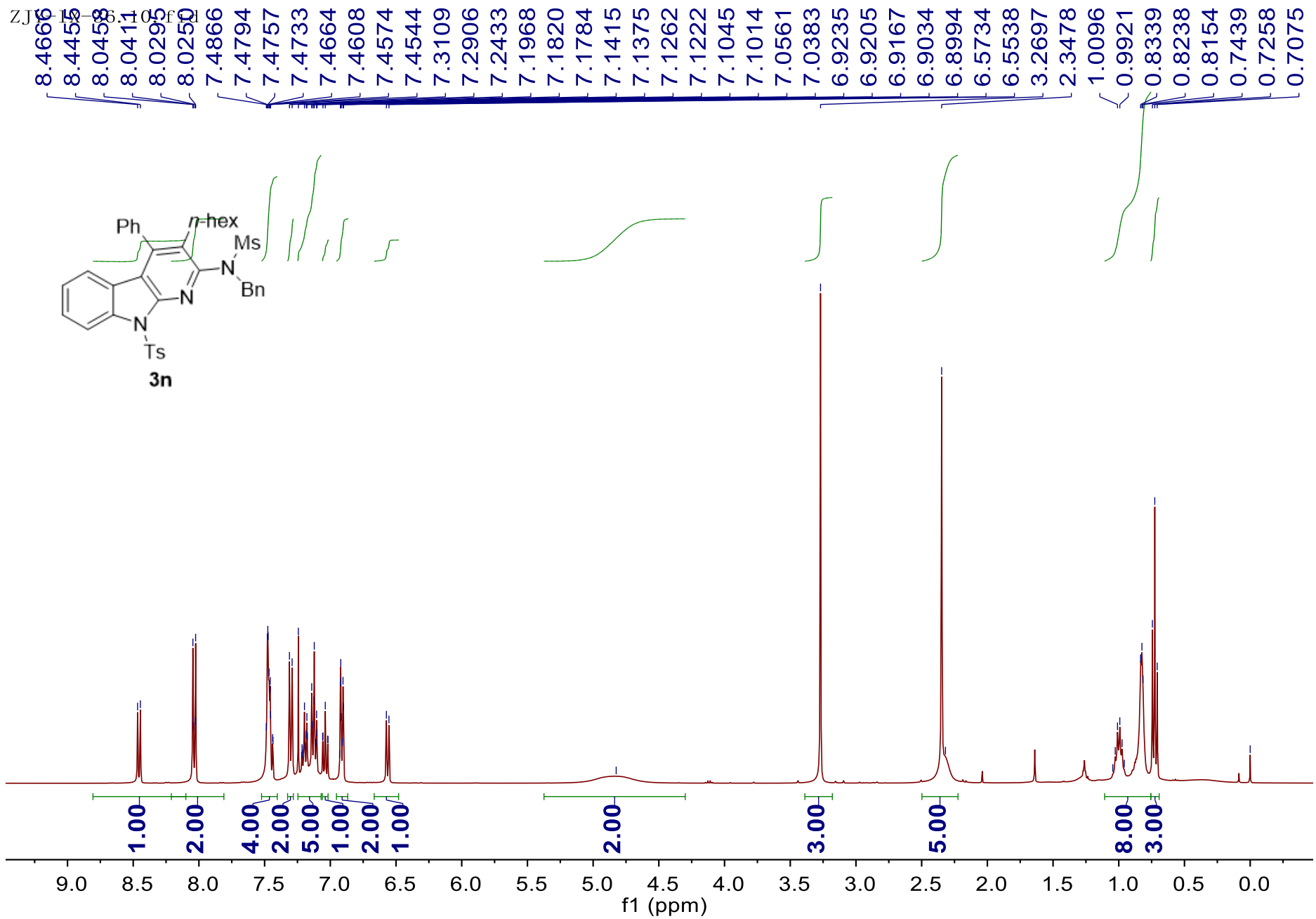




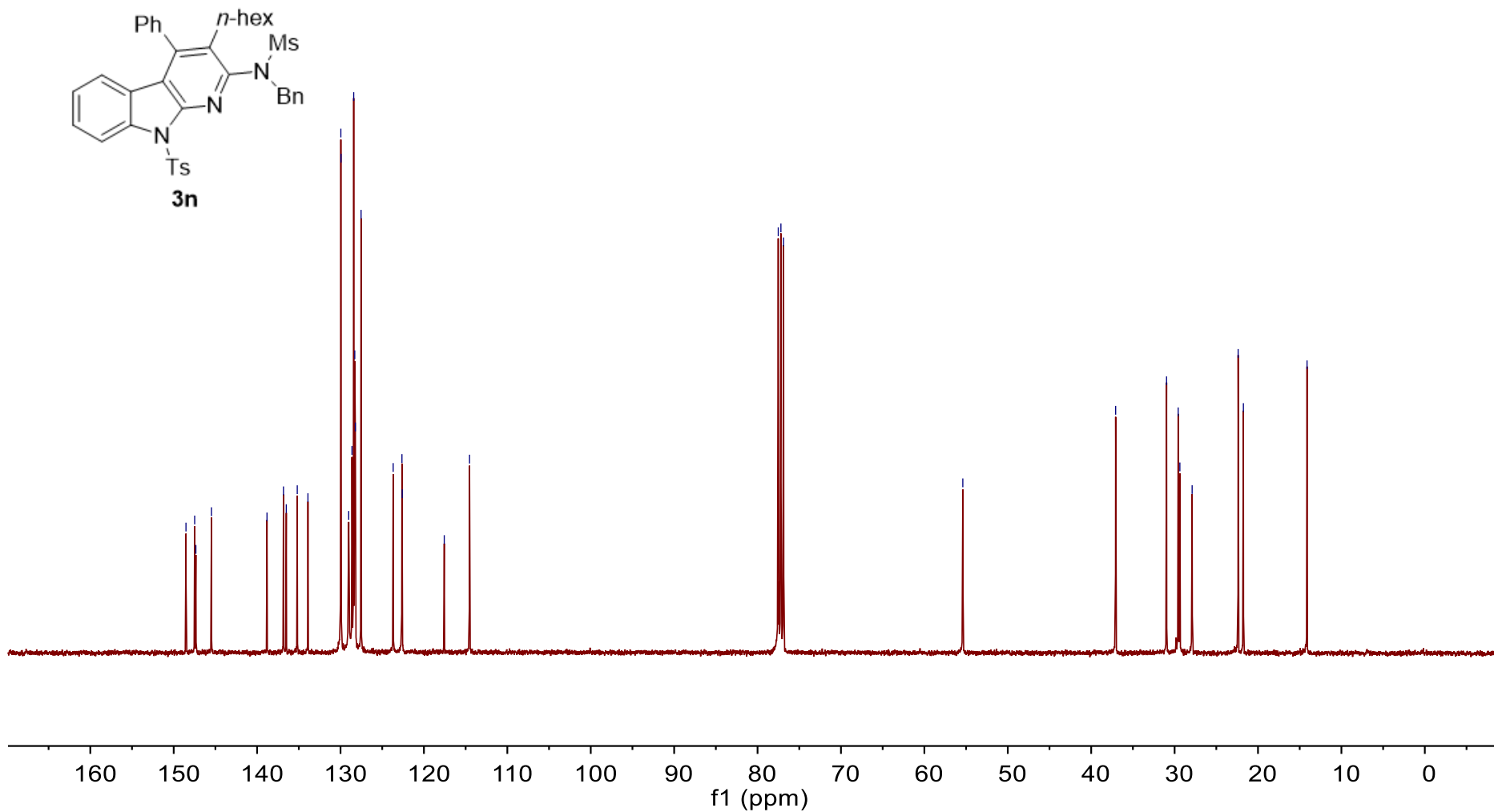
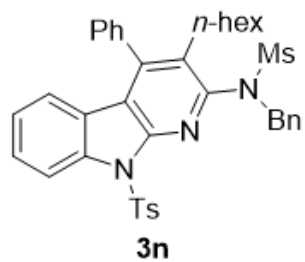
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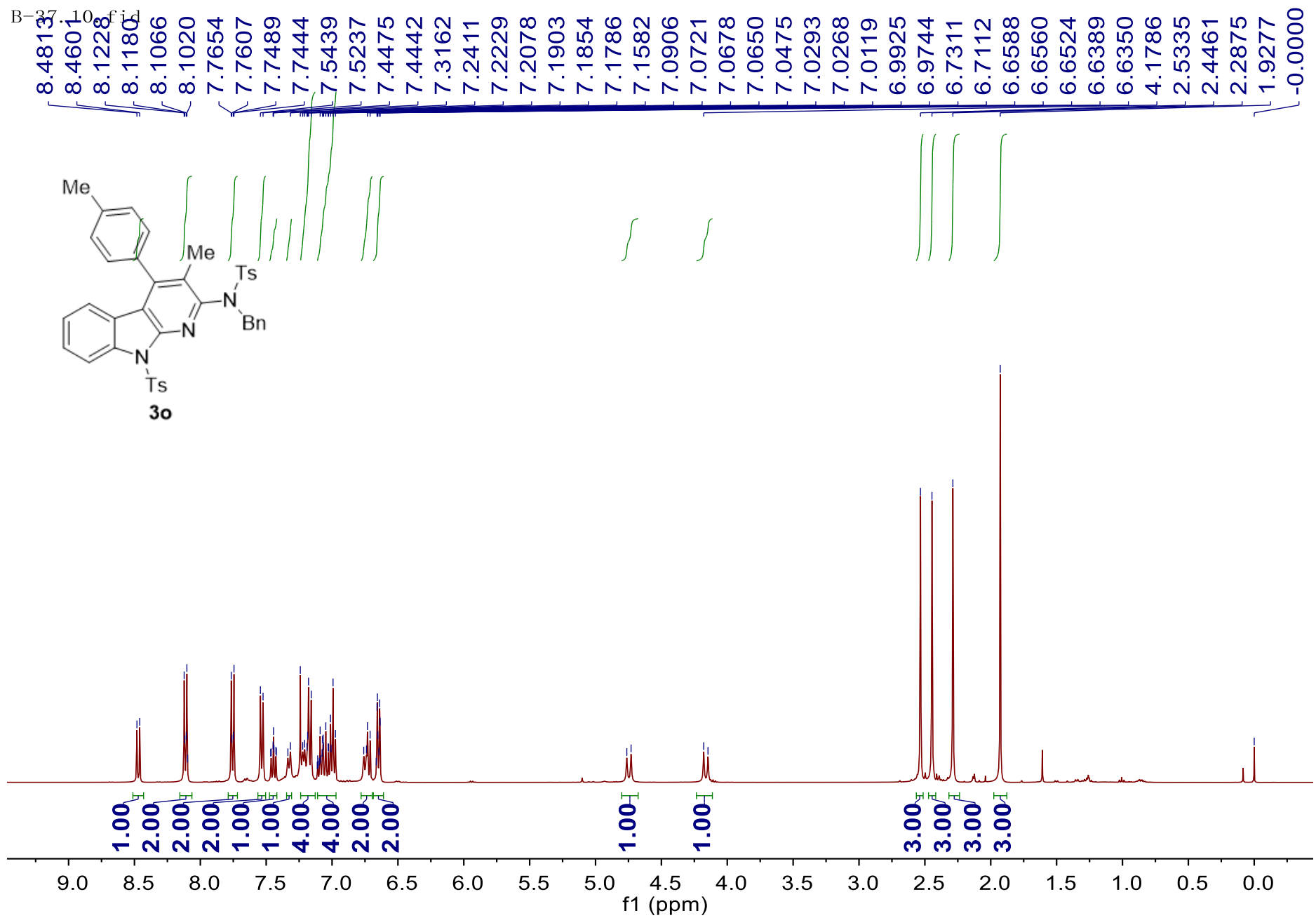


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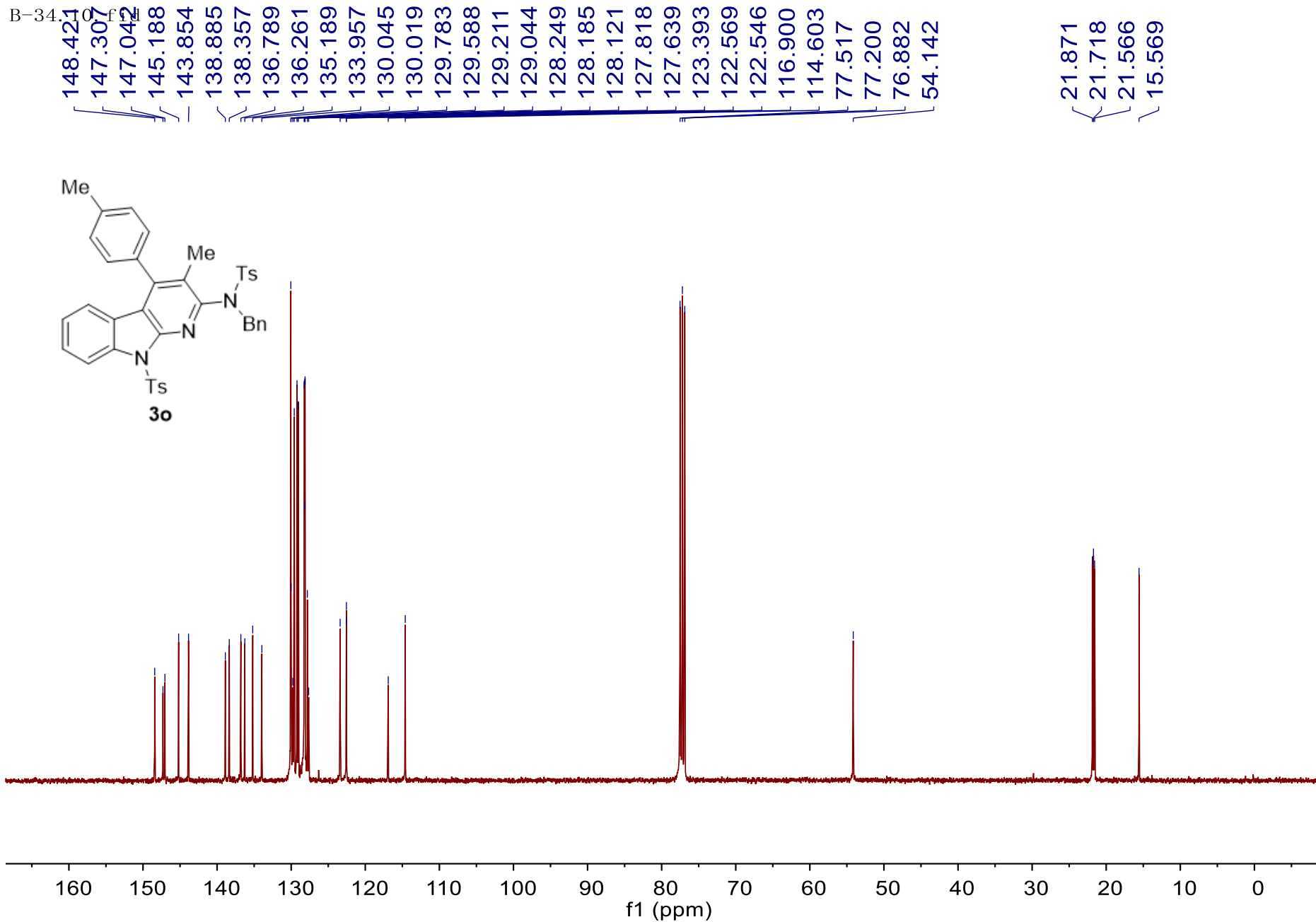
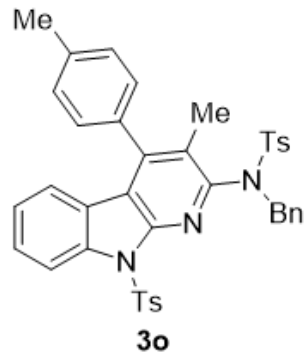


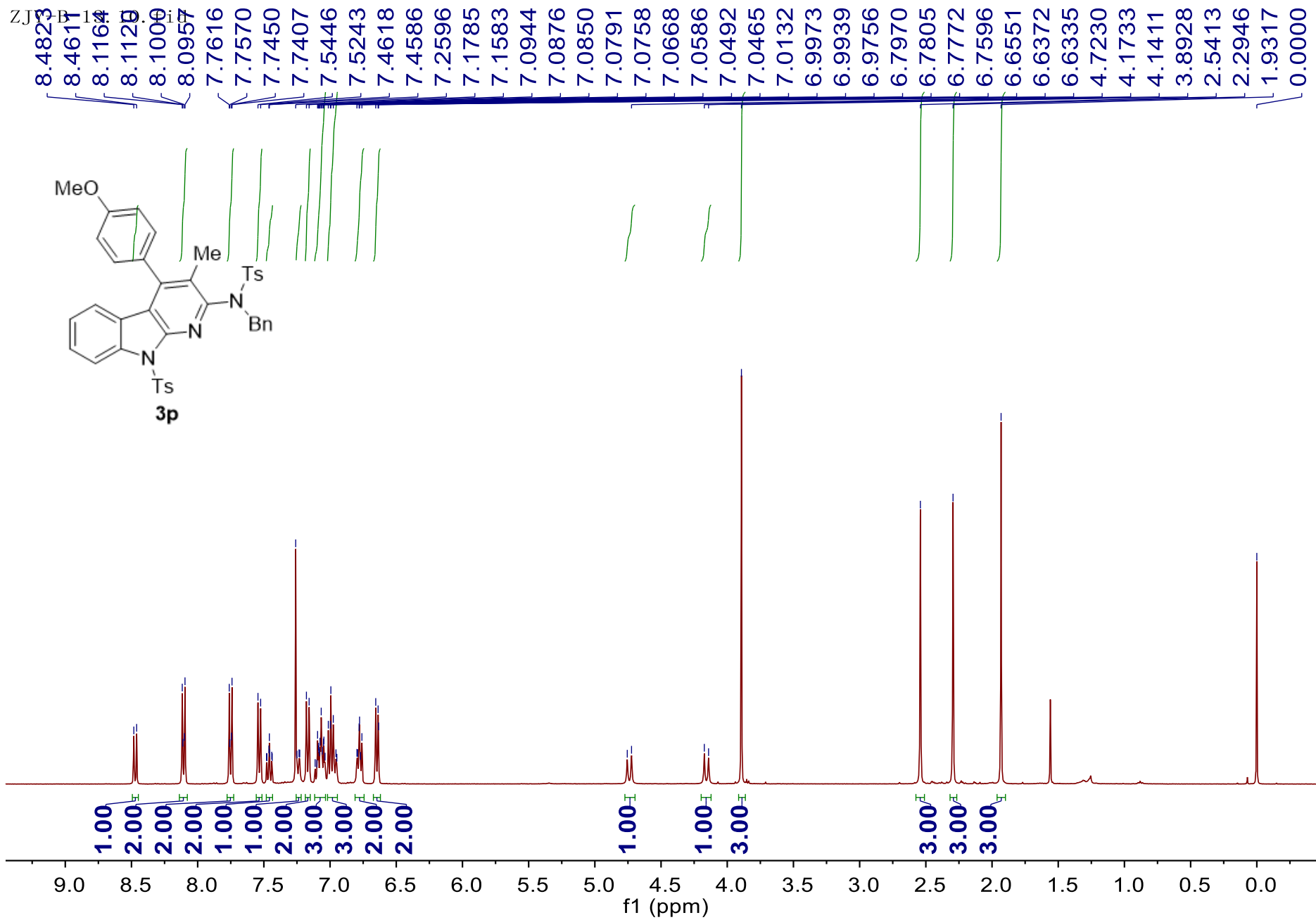
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 127.535
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 122.634
 122.601
 117.564
 114.533
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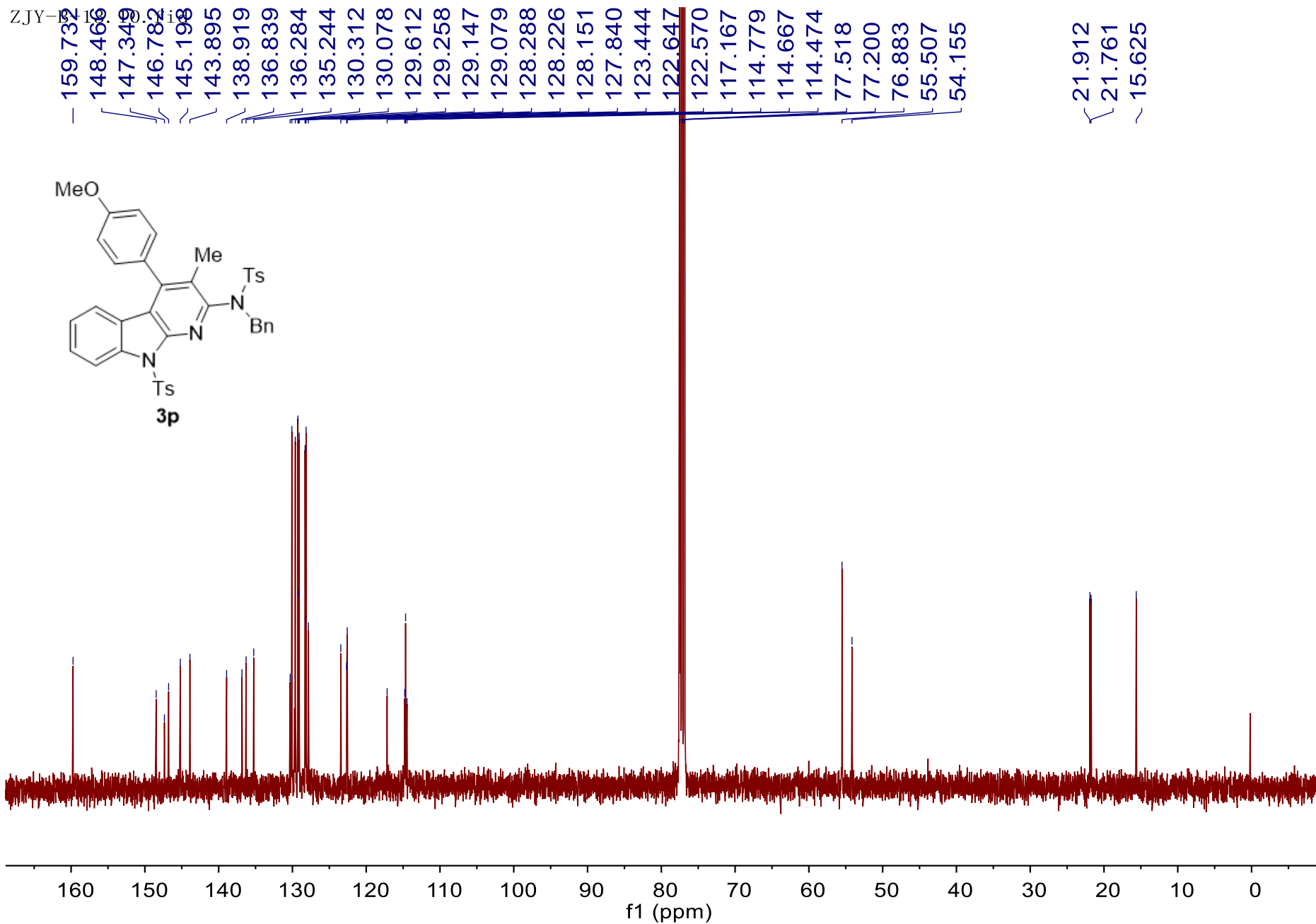
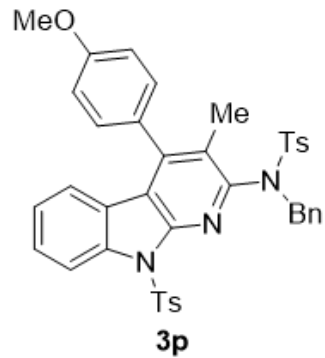


B-34.



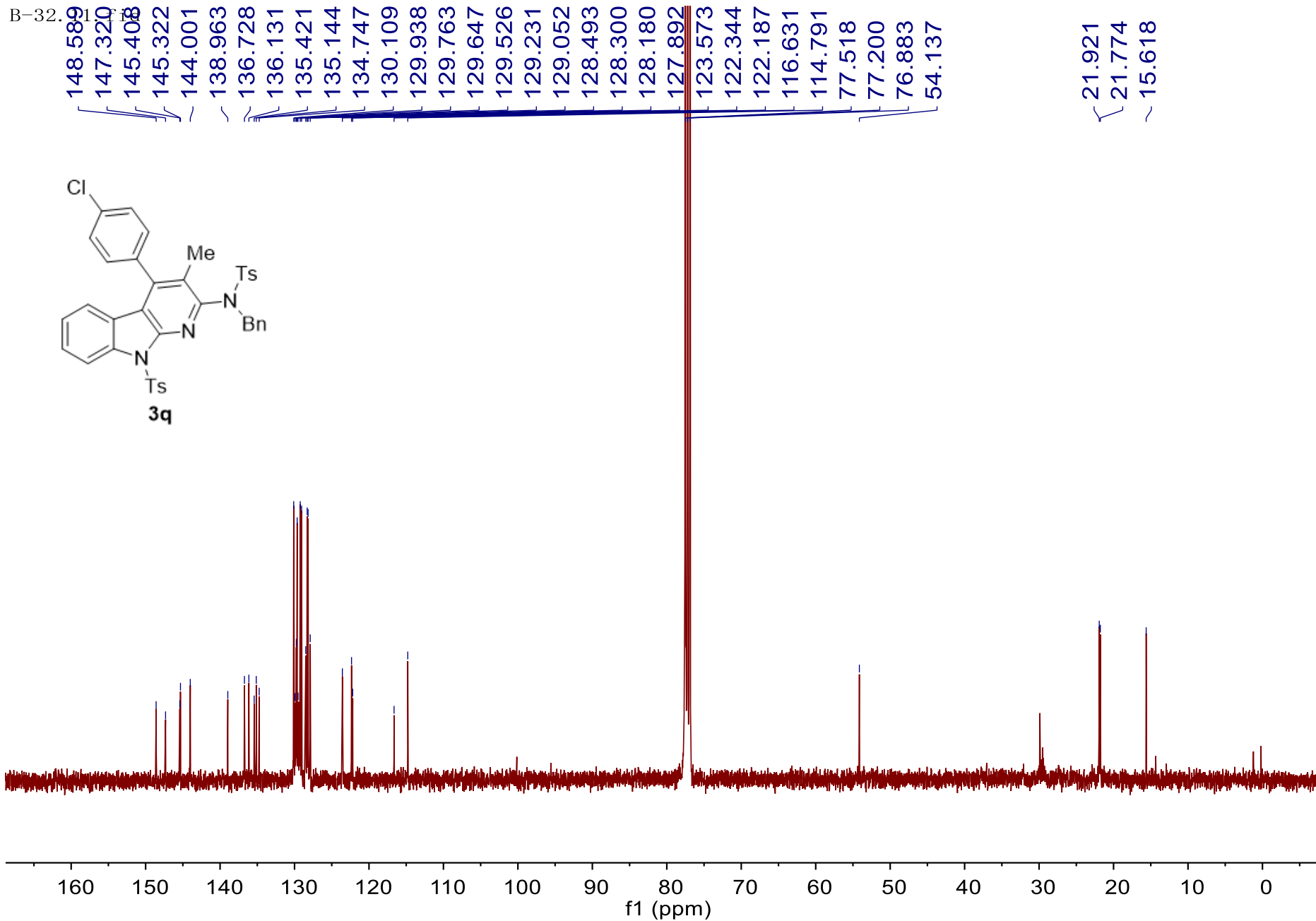
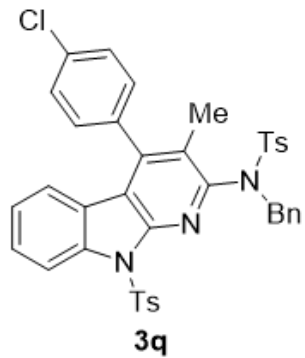


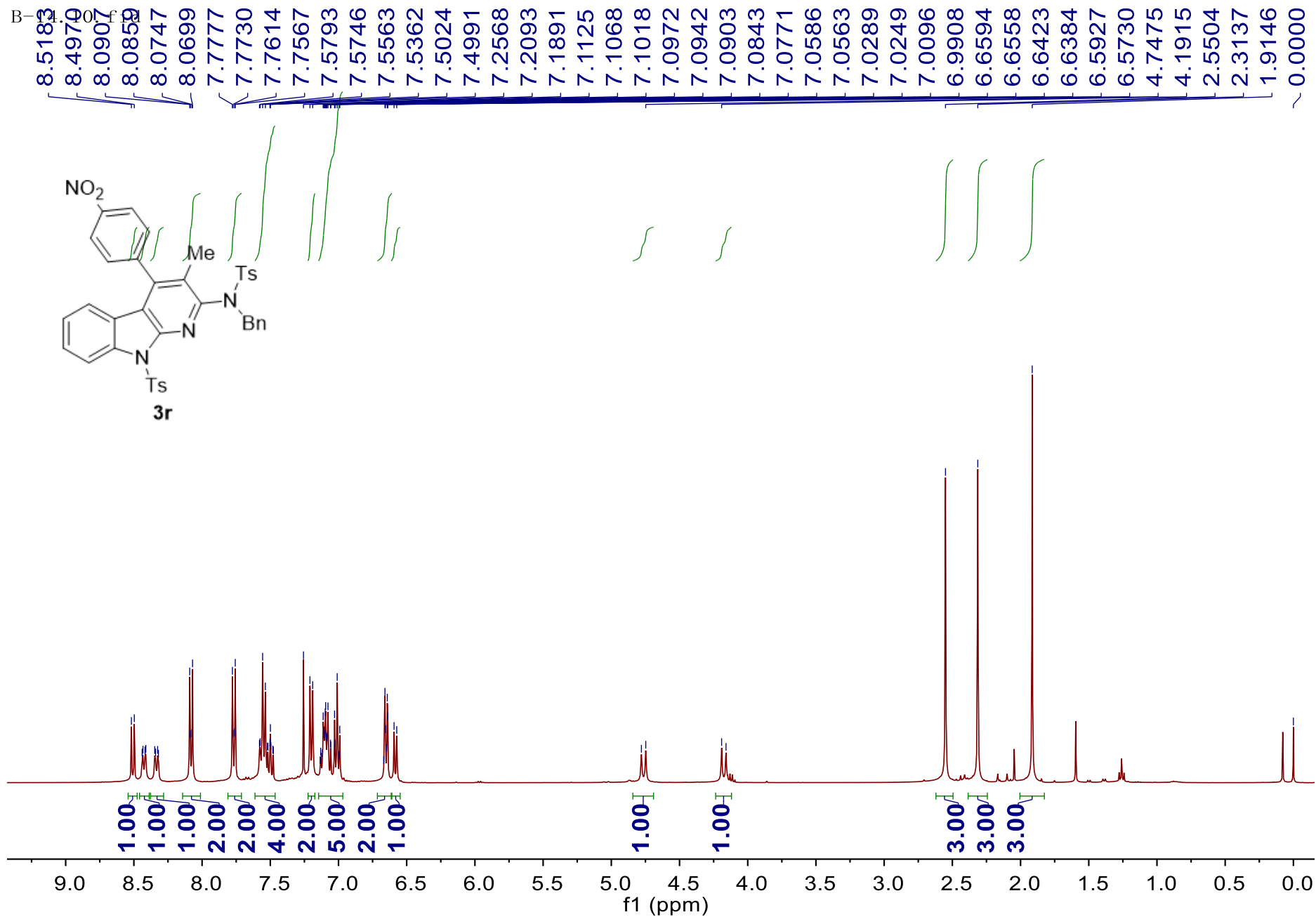
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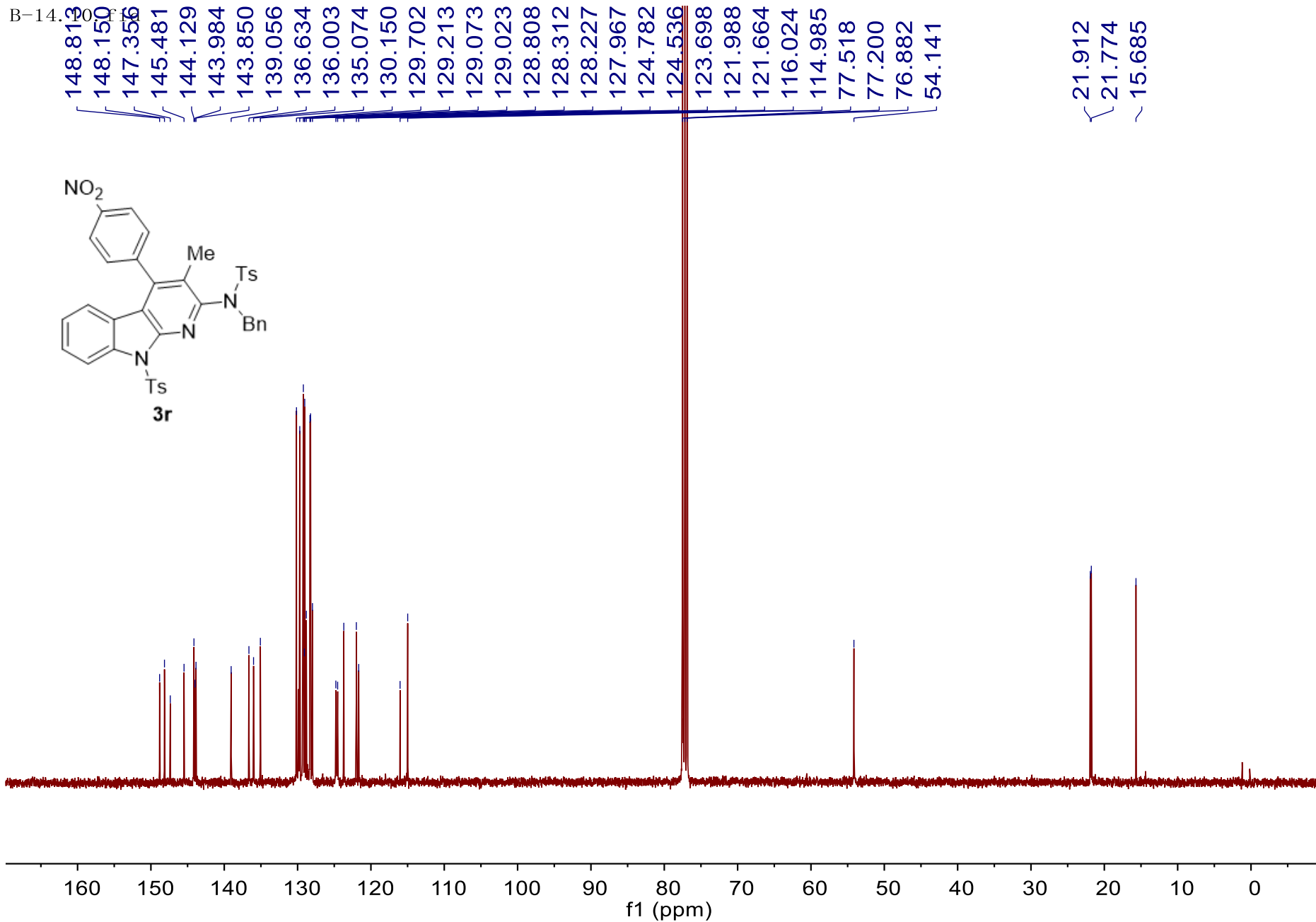
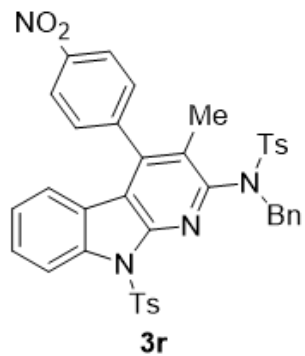
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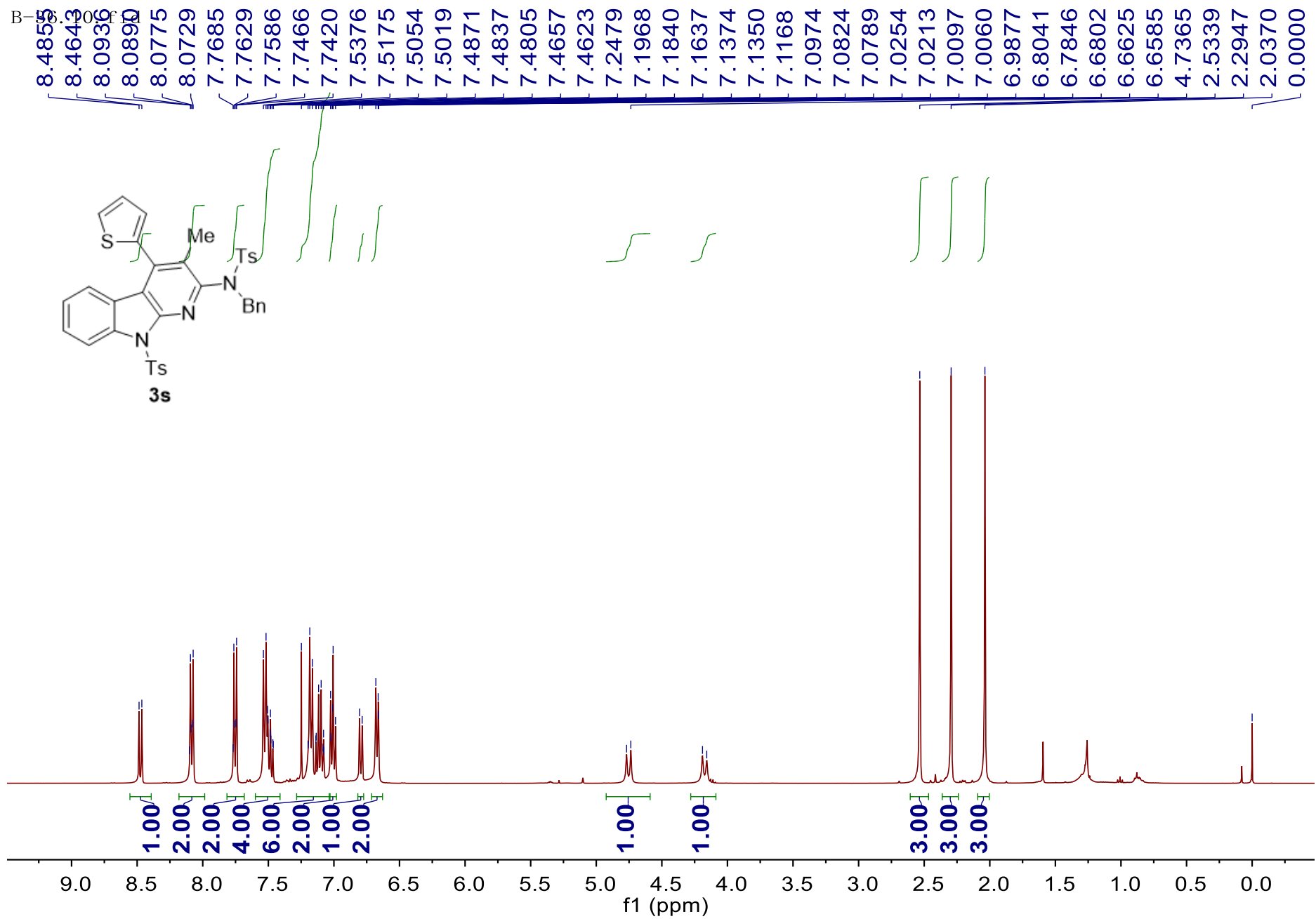


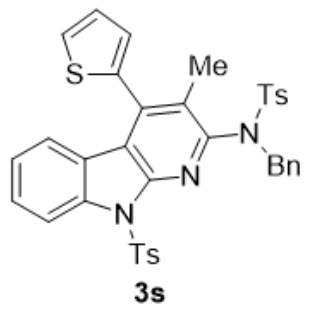
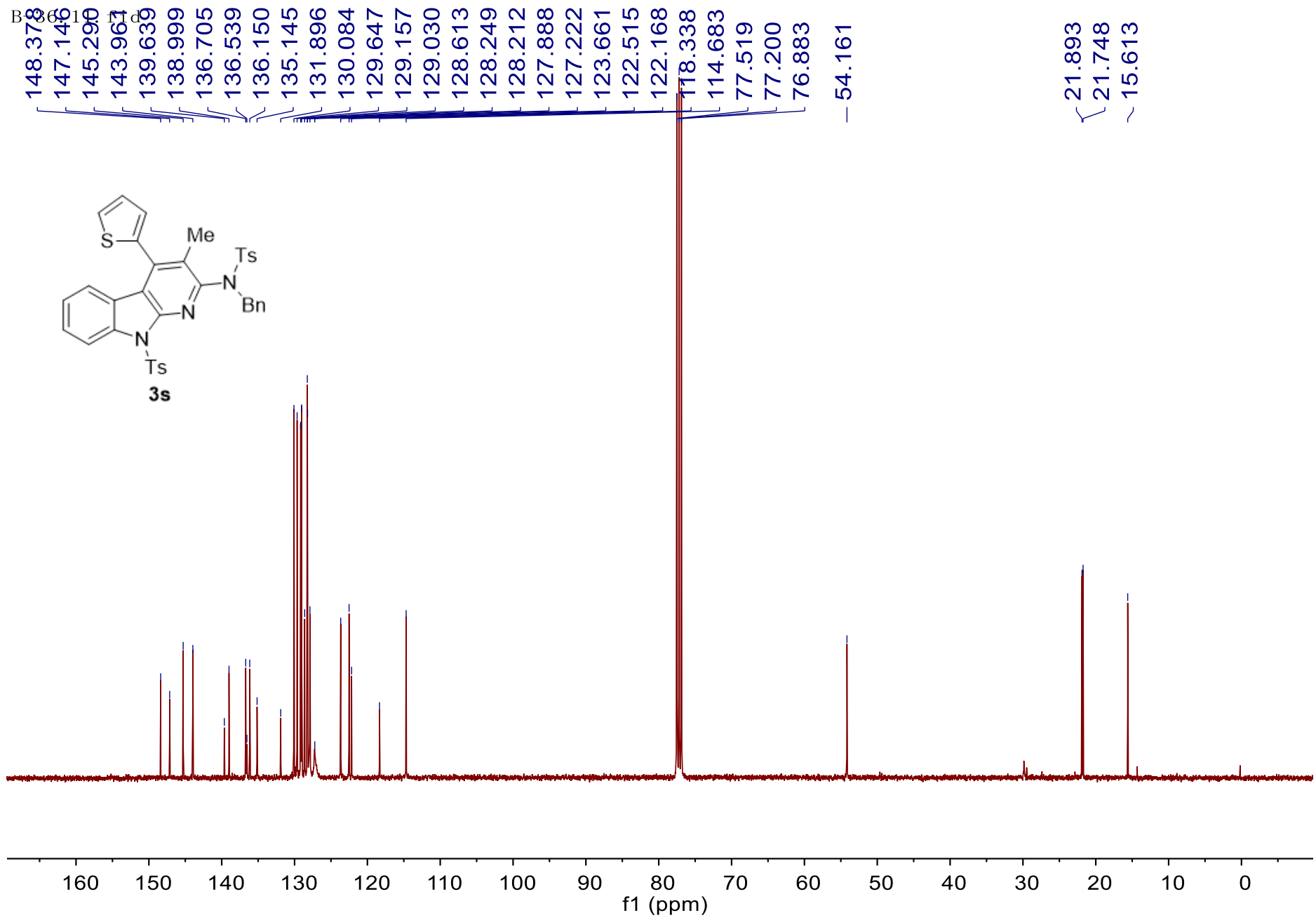


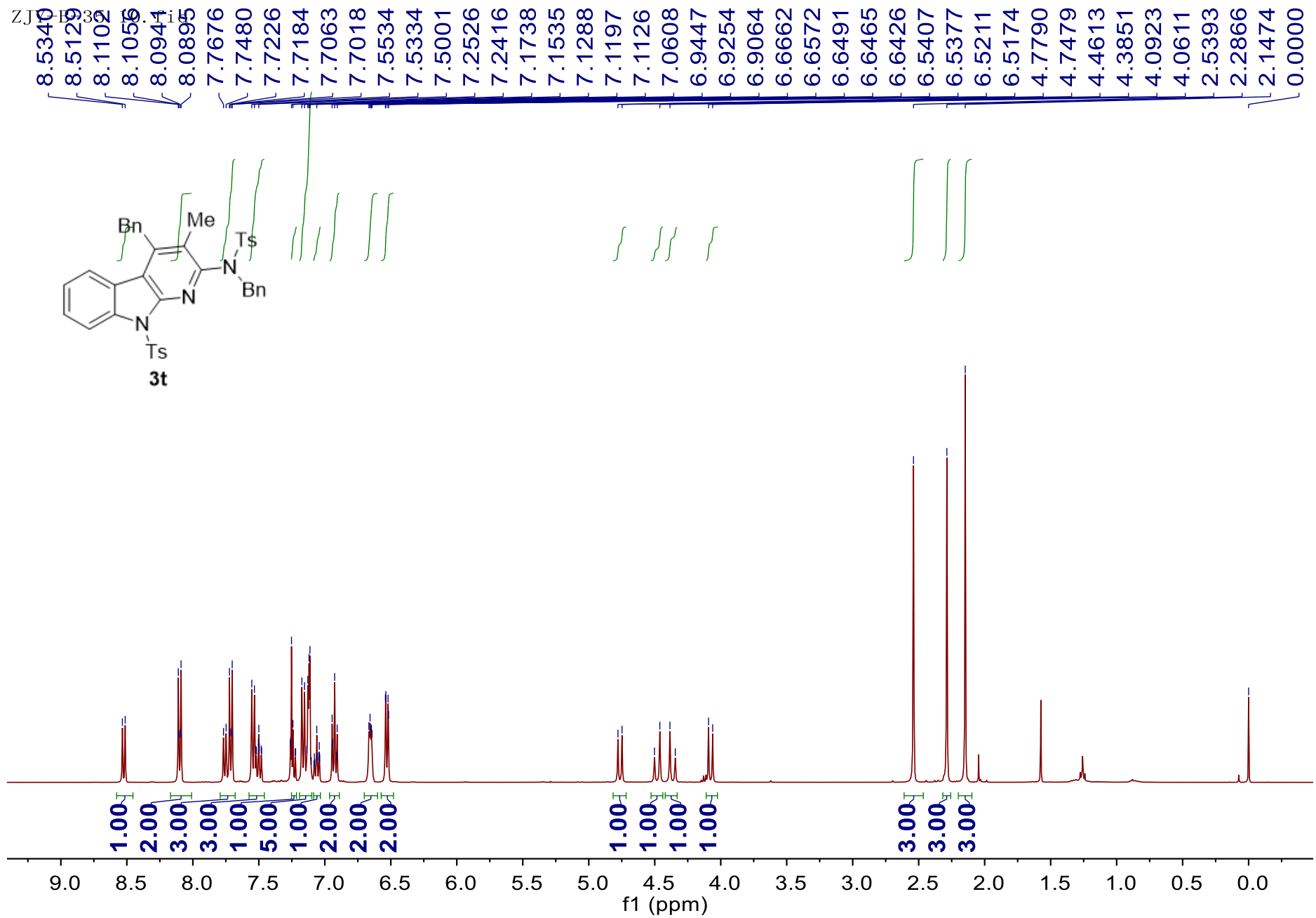
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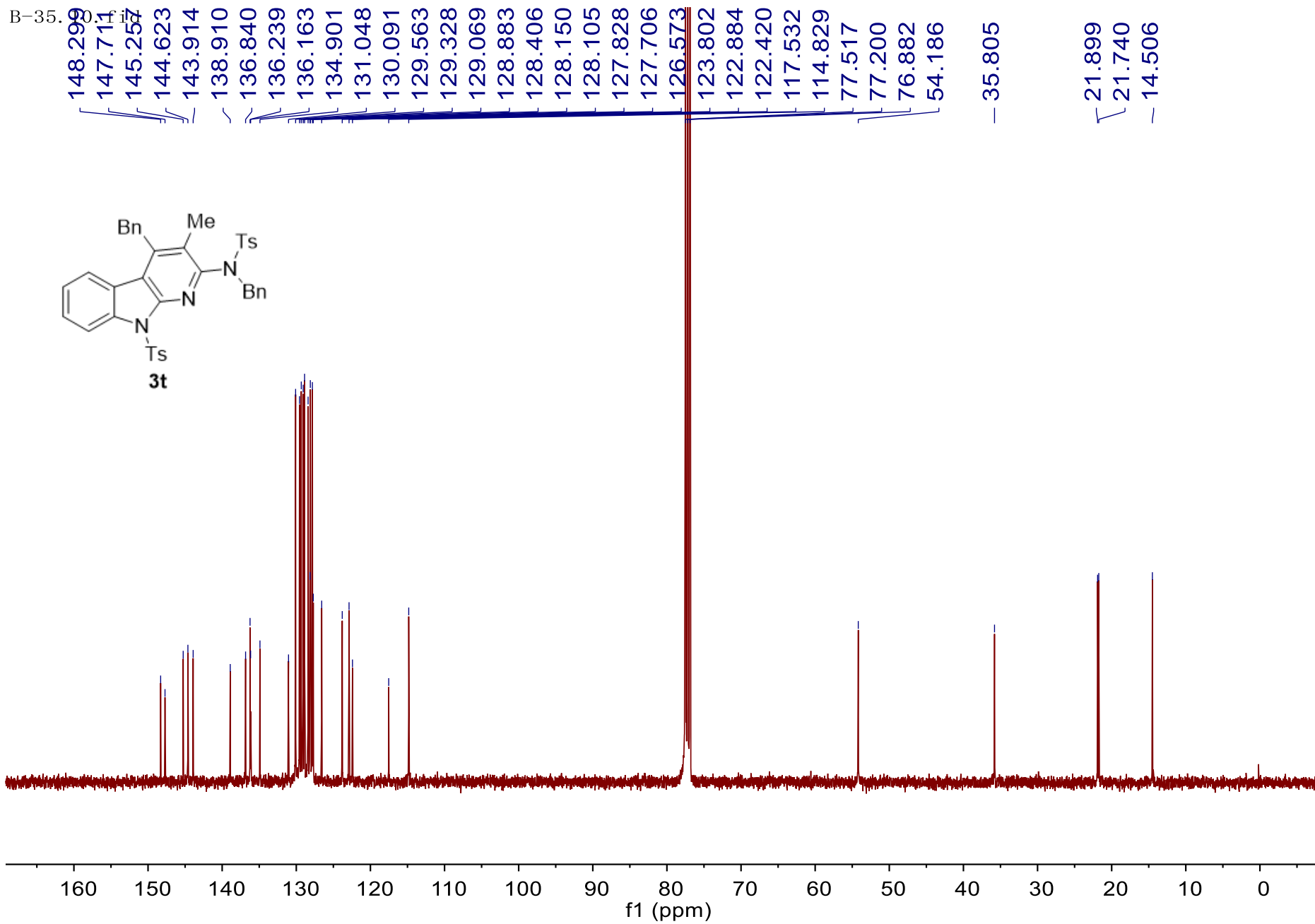
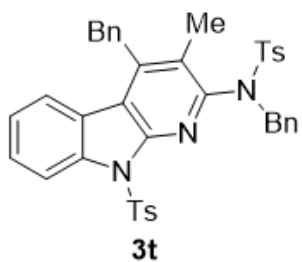
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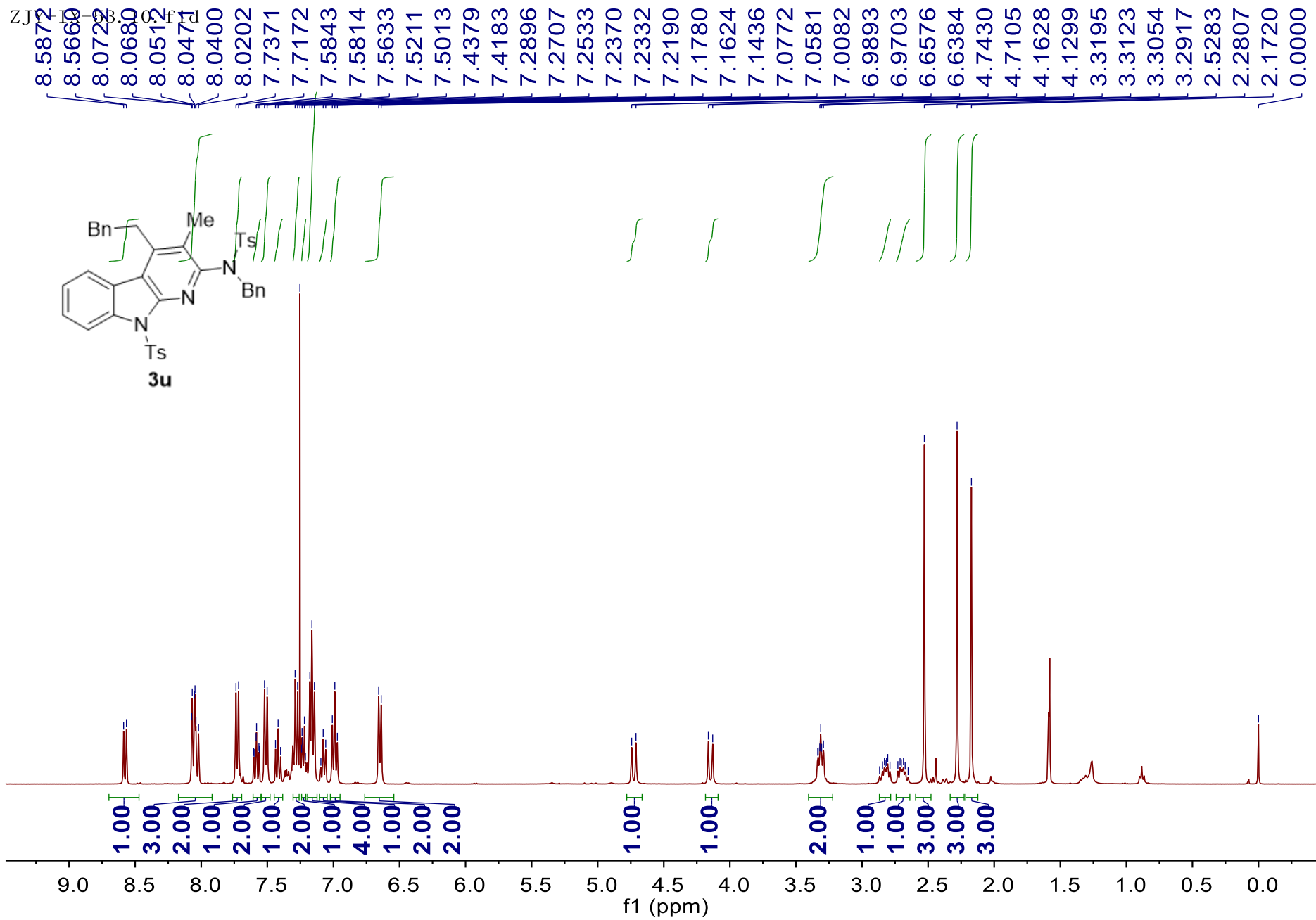




B-35. 0. f1



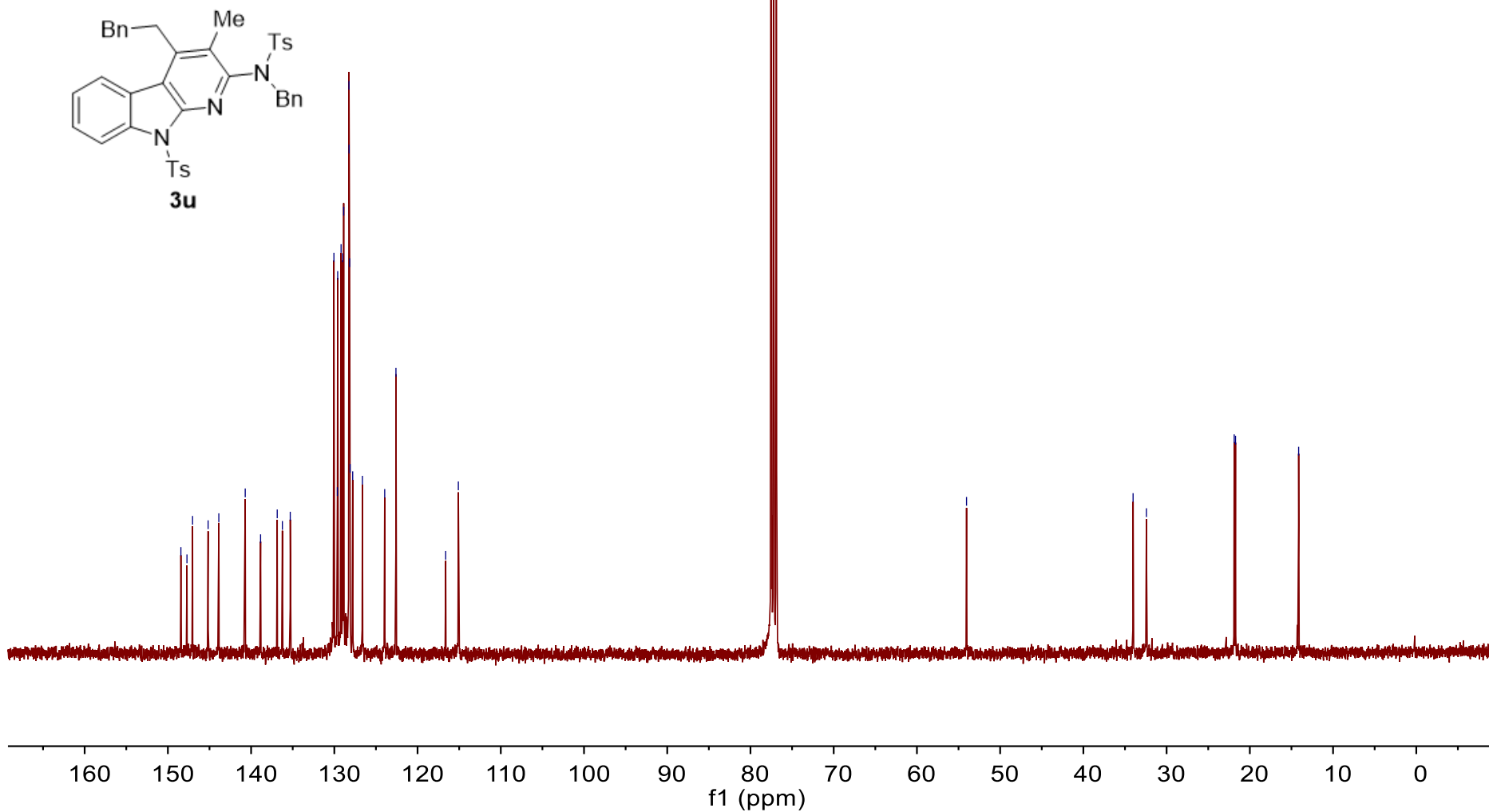
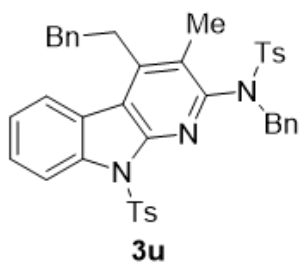
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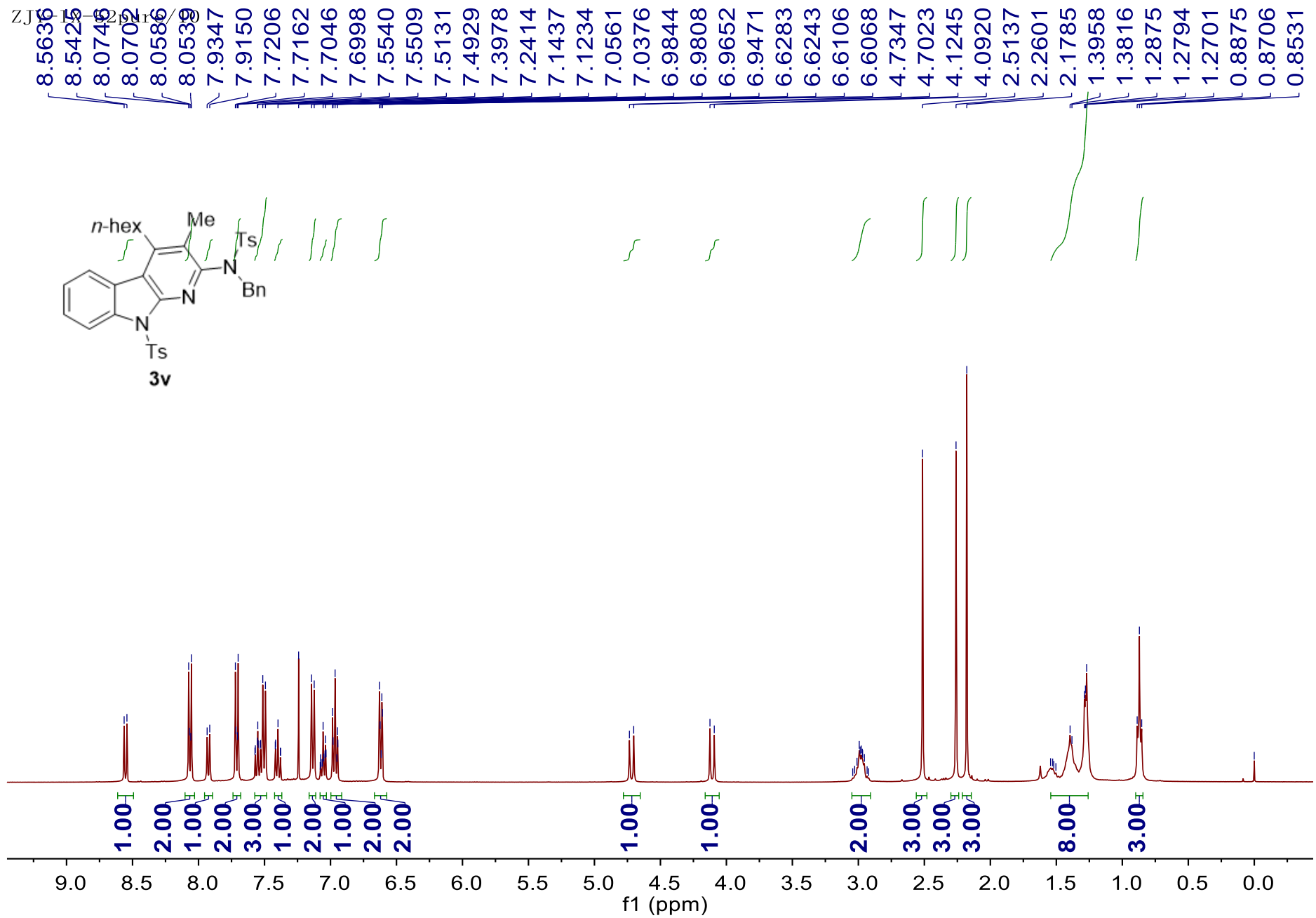


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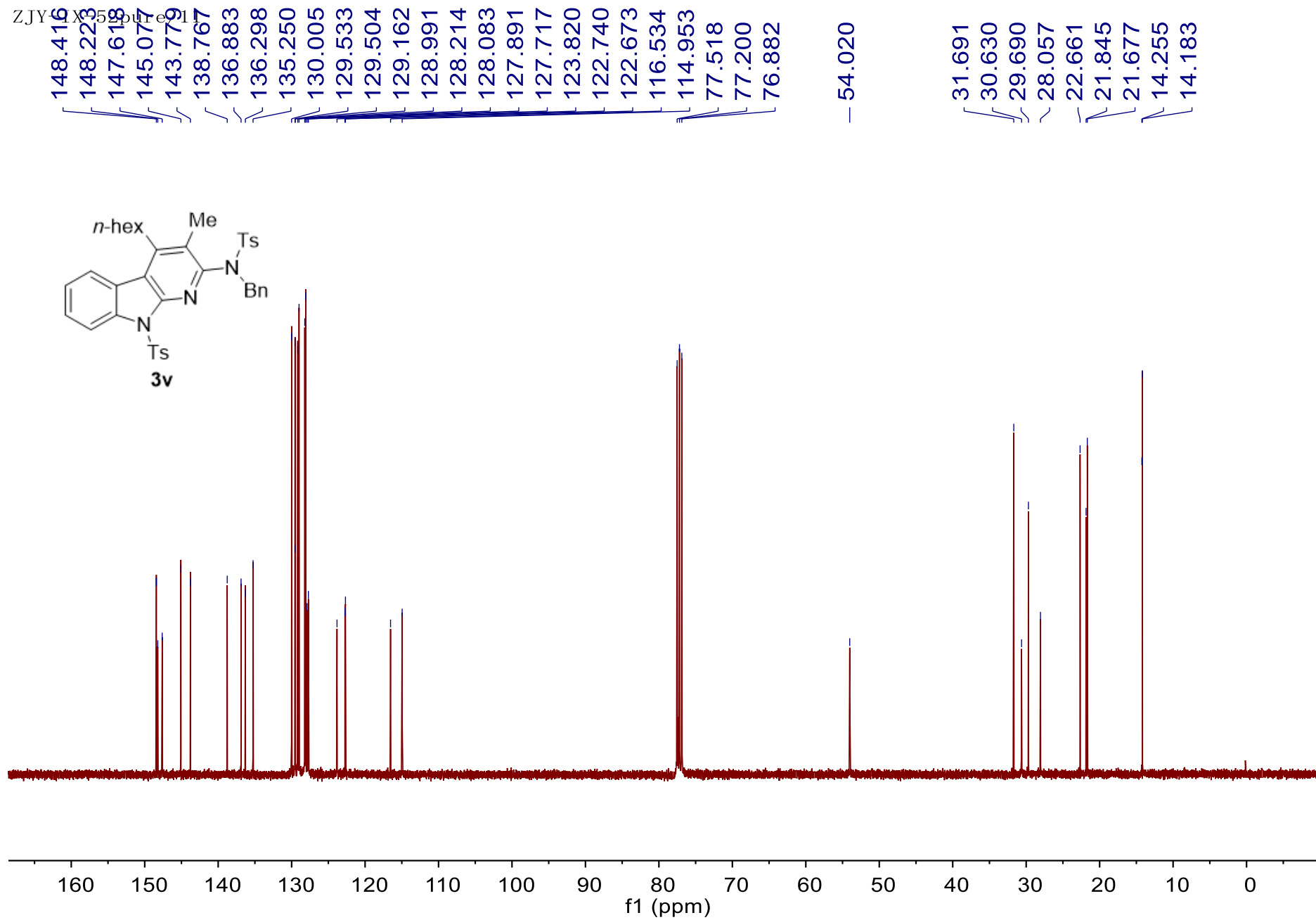
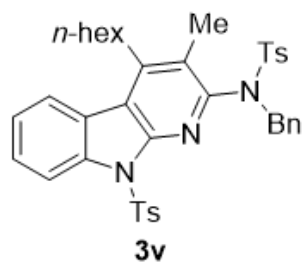
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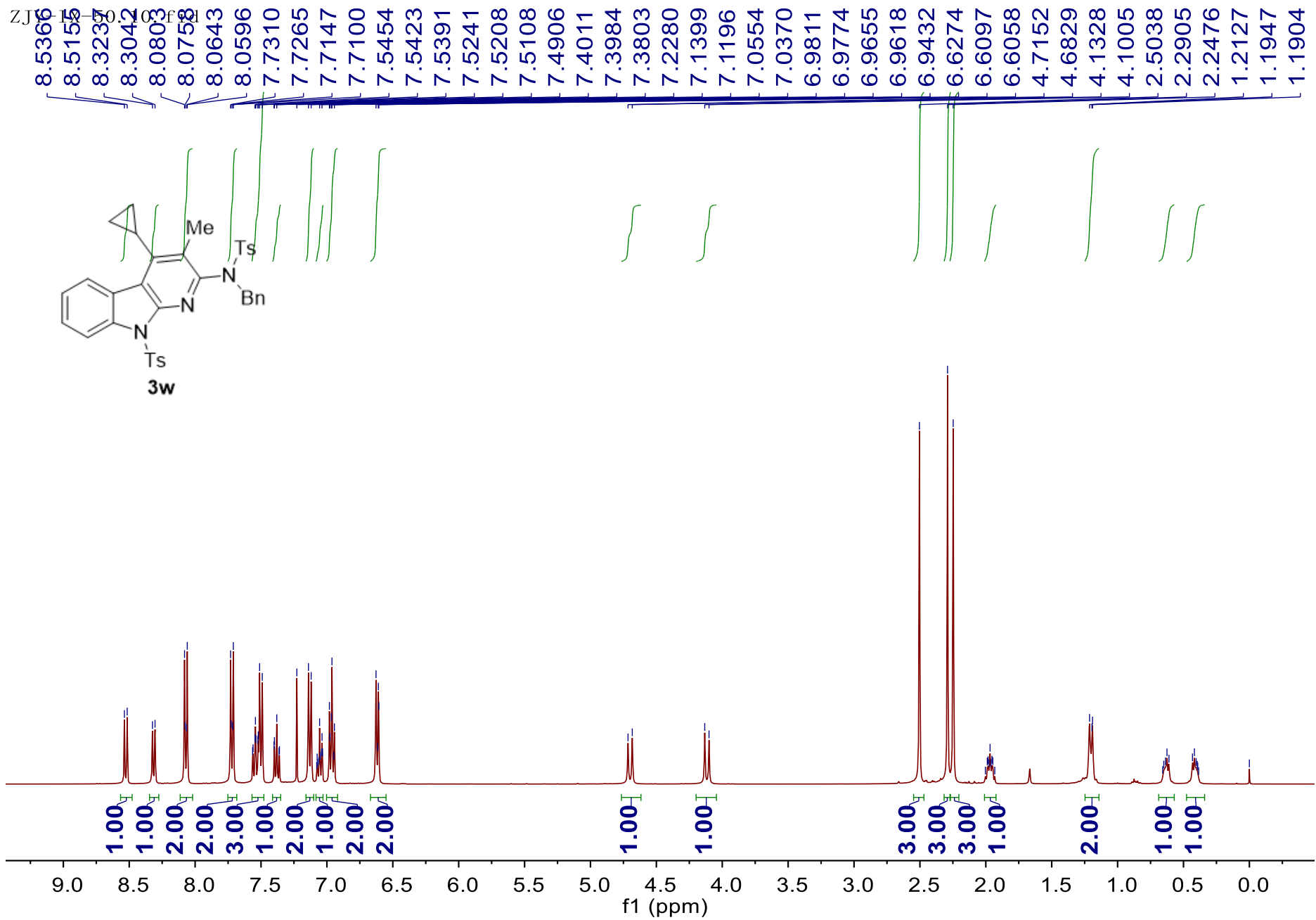




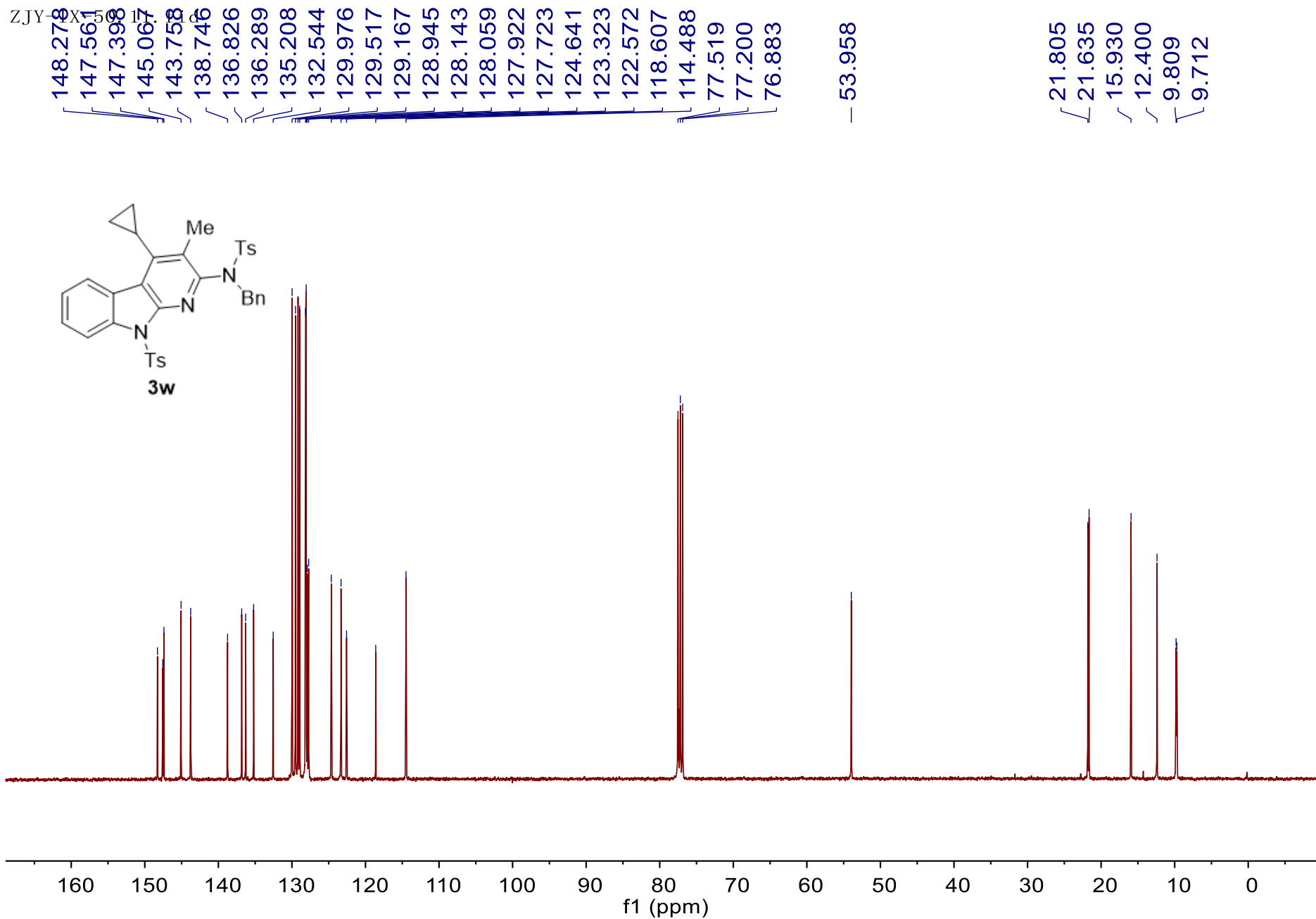
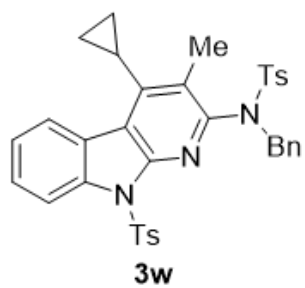
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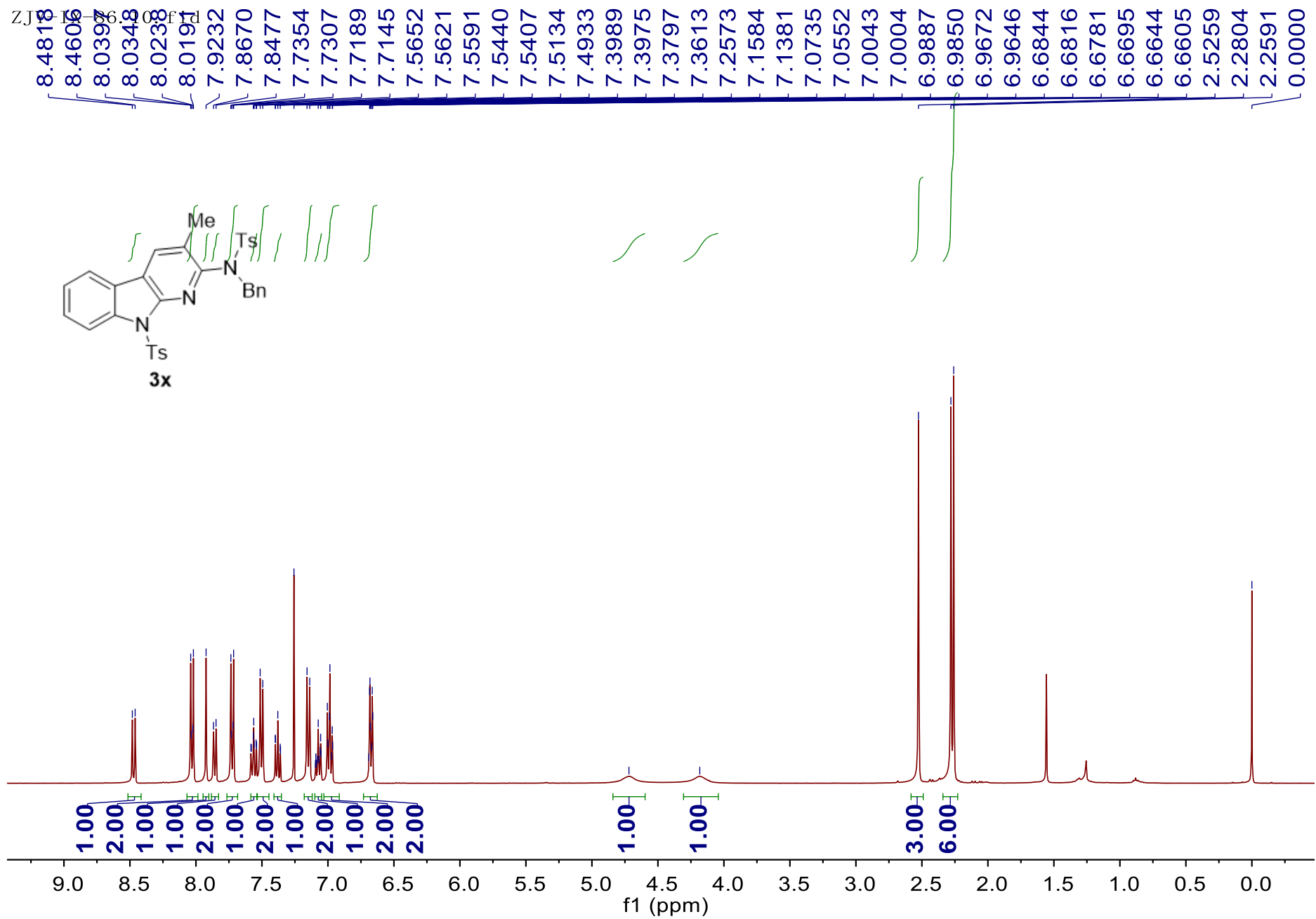


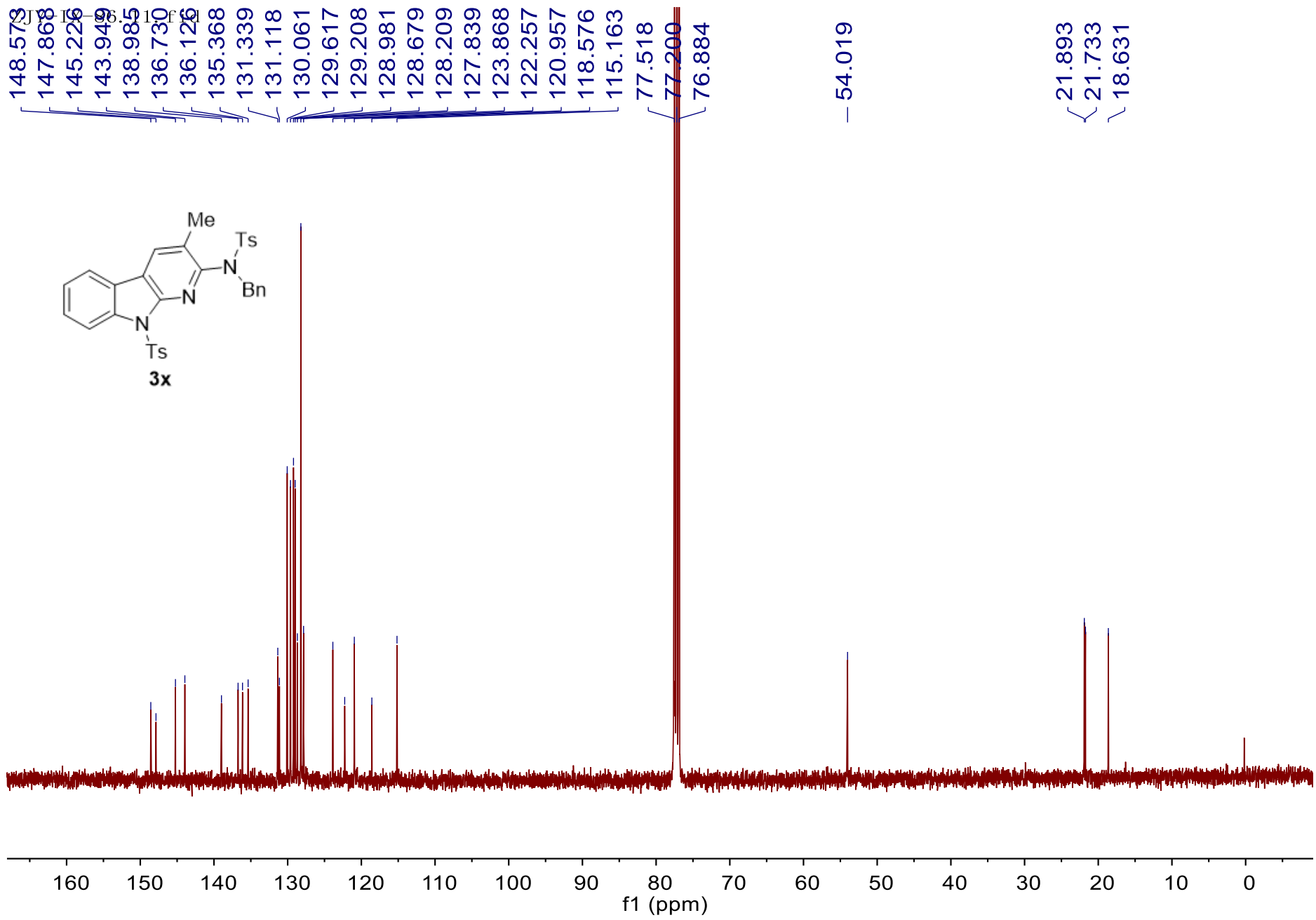
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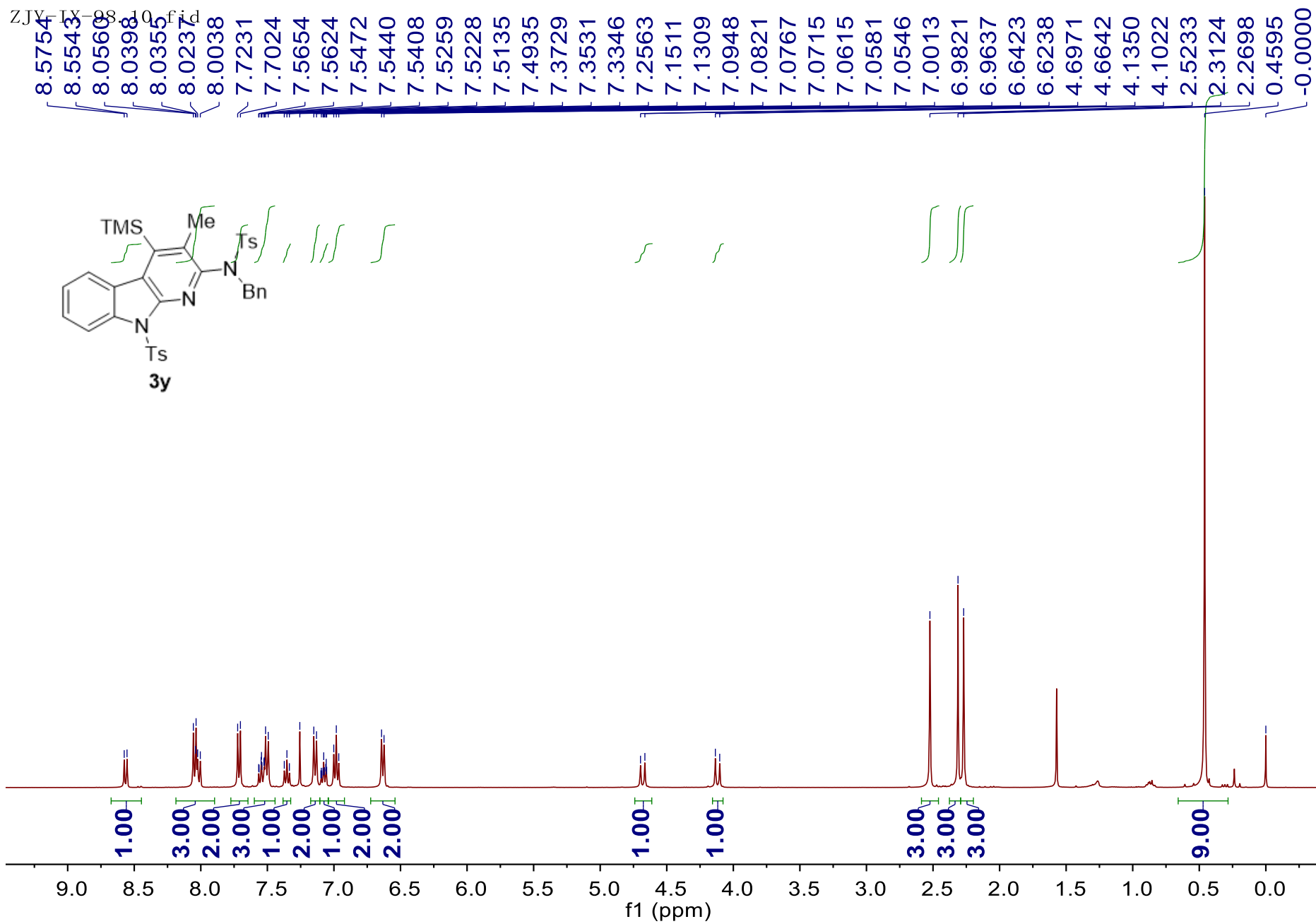
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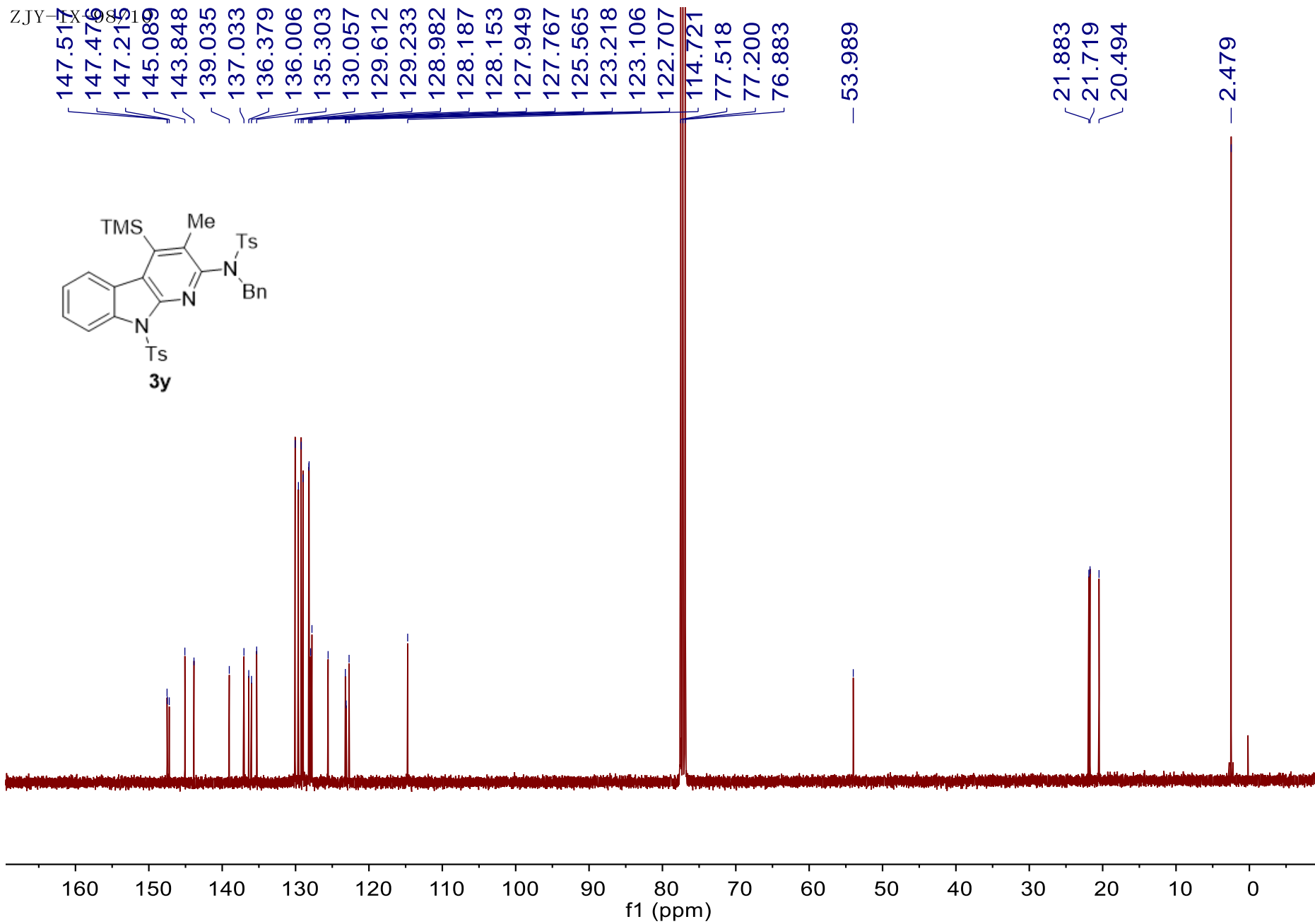
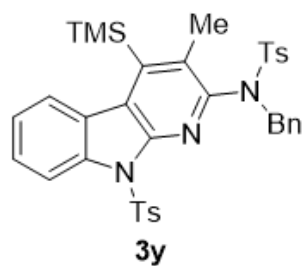




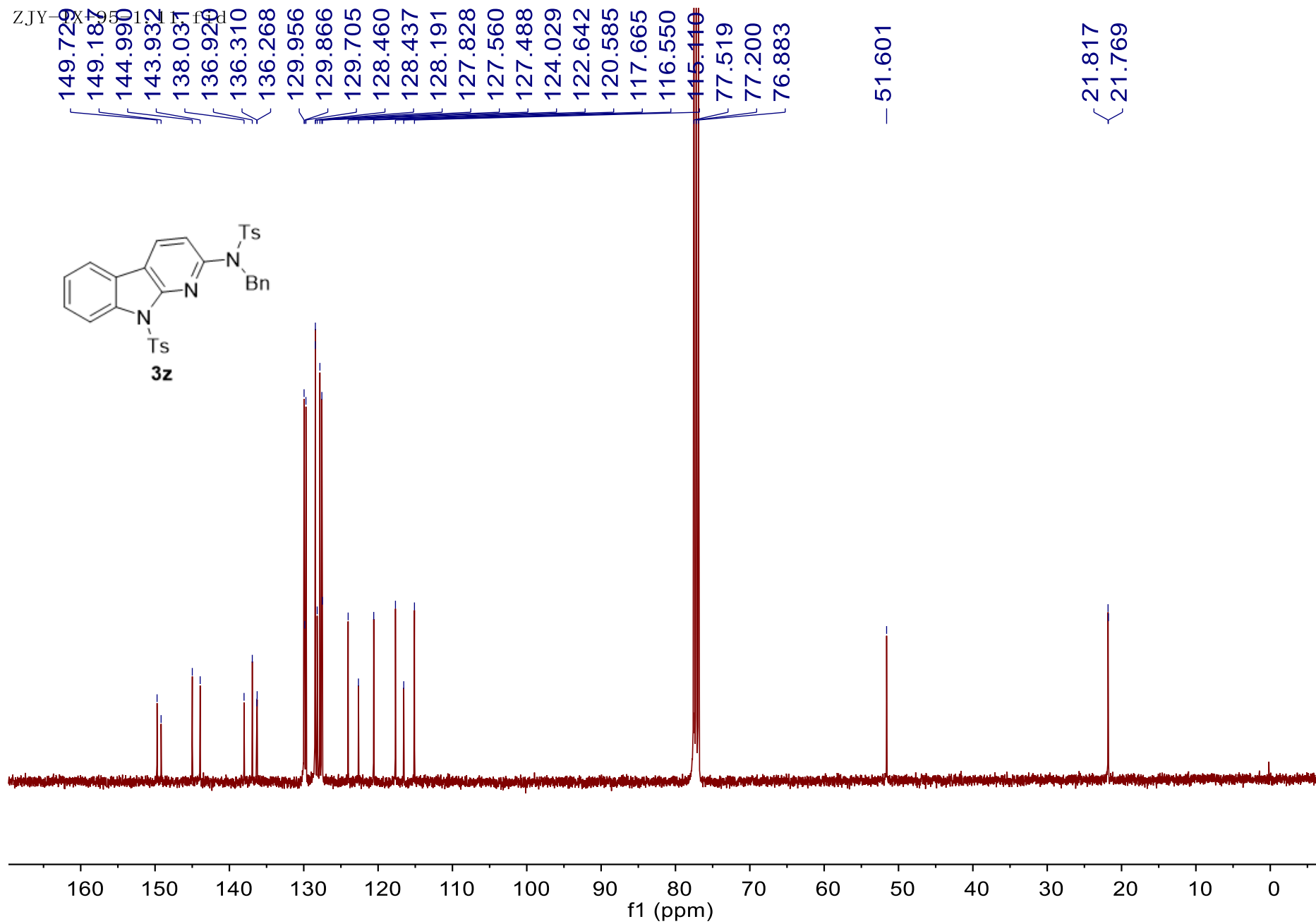
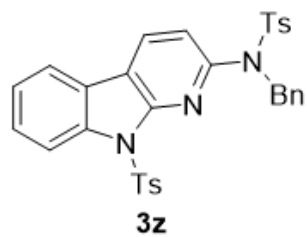
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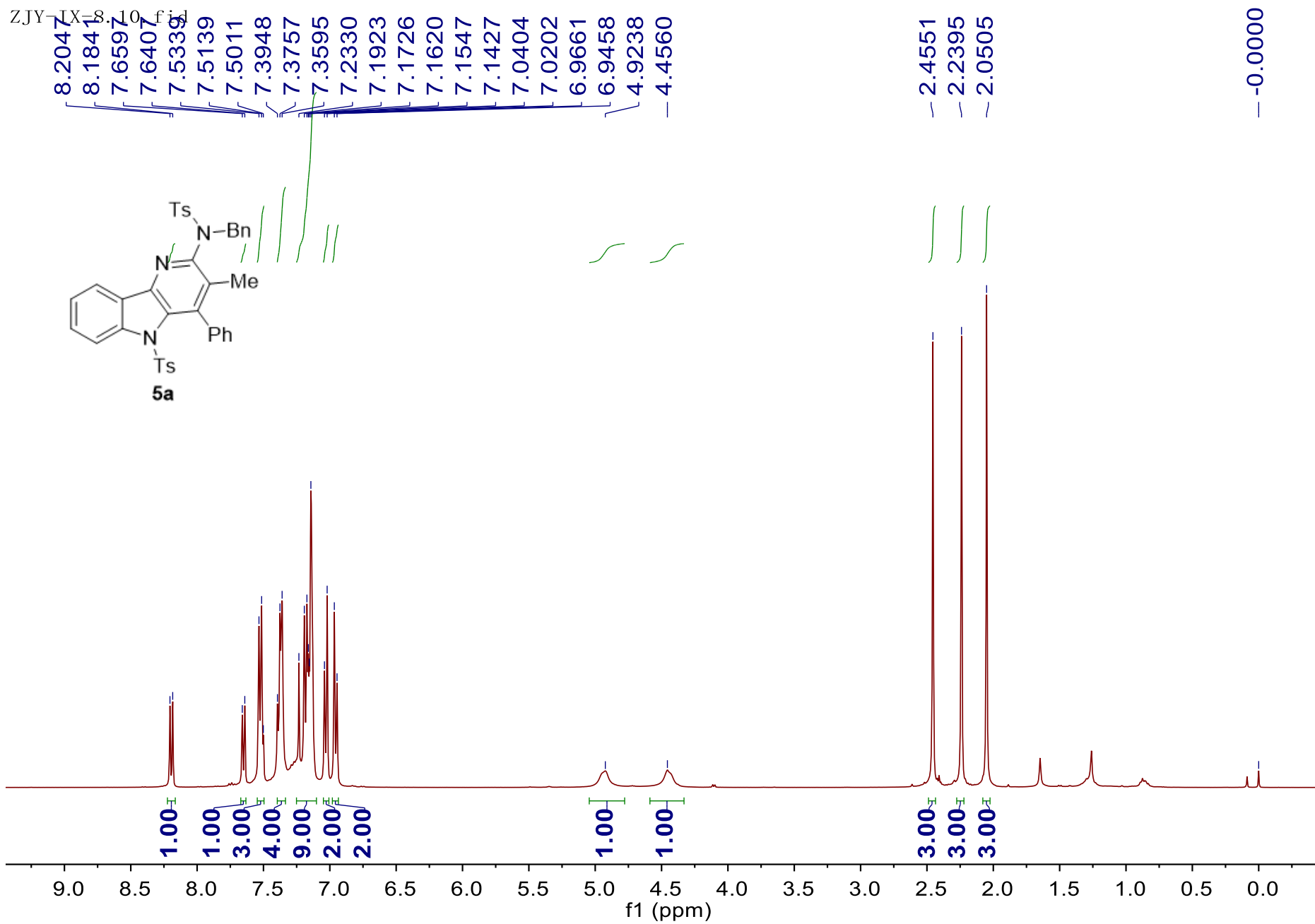


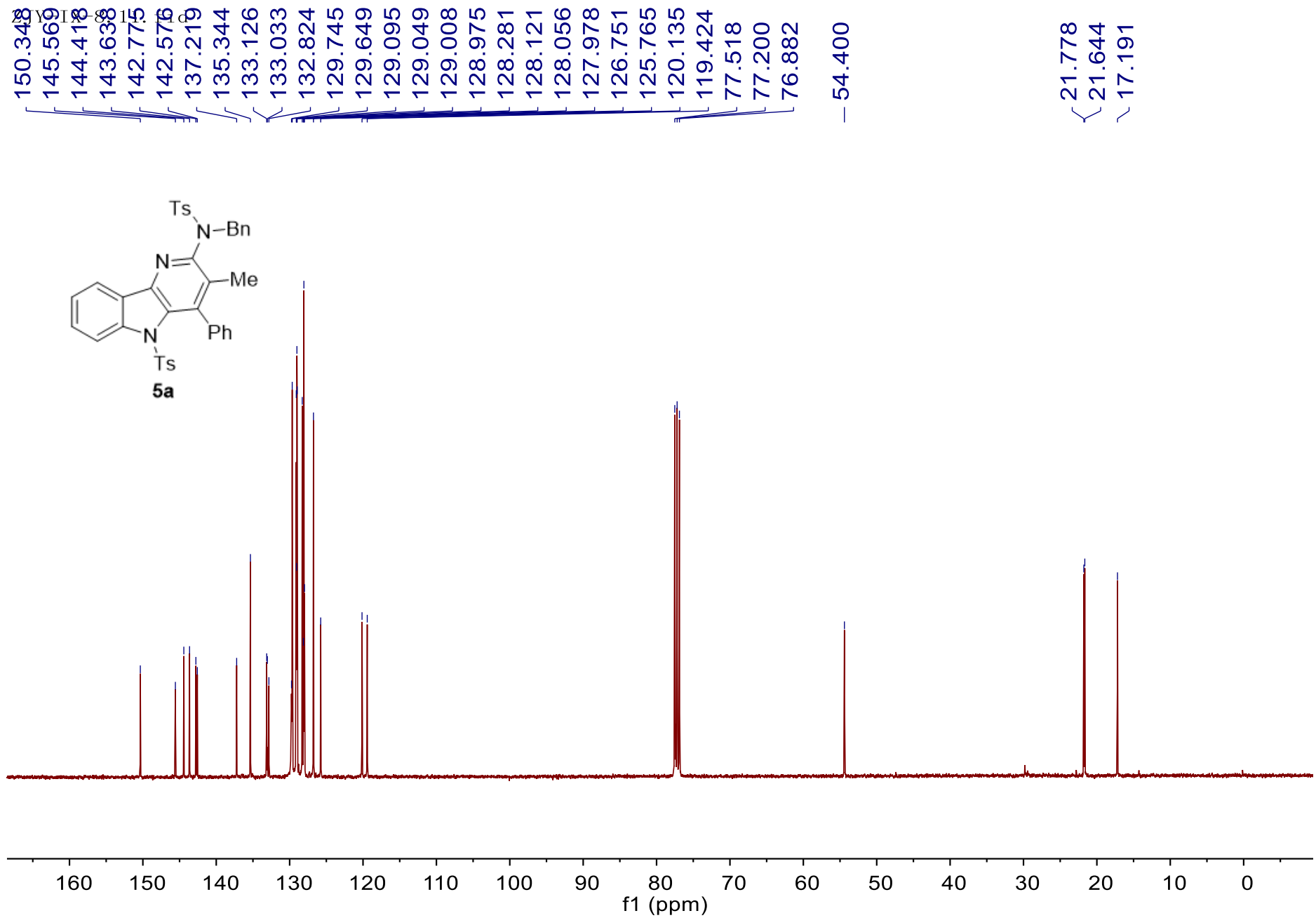
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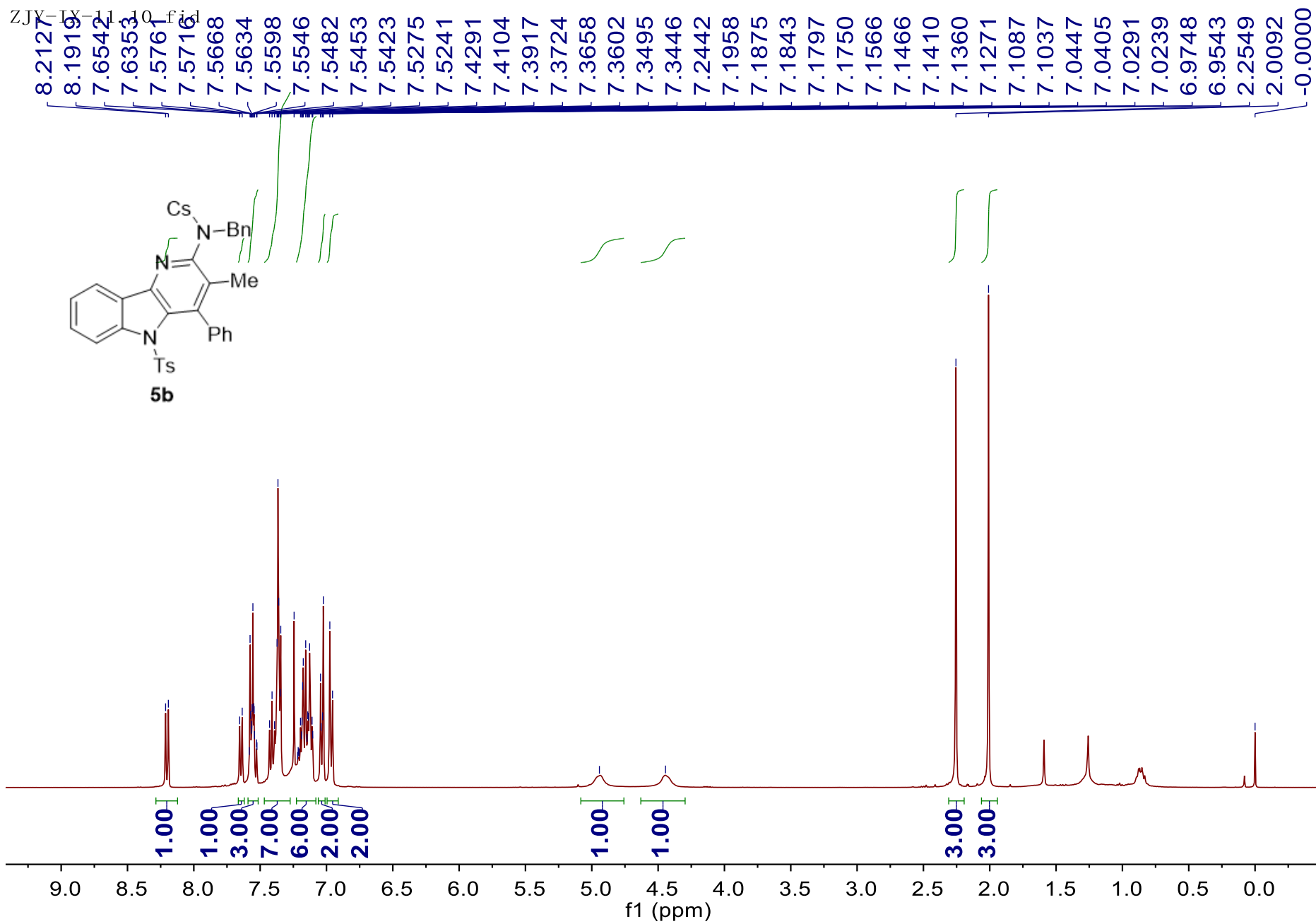
S120

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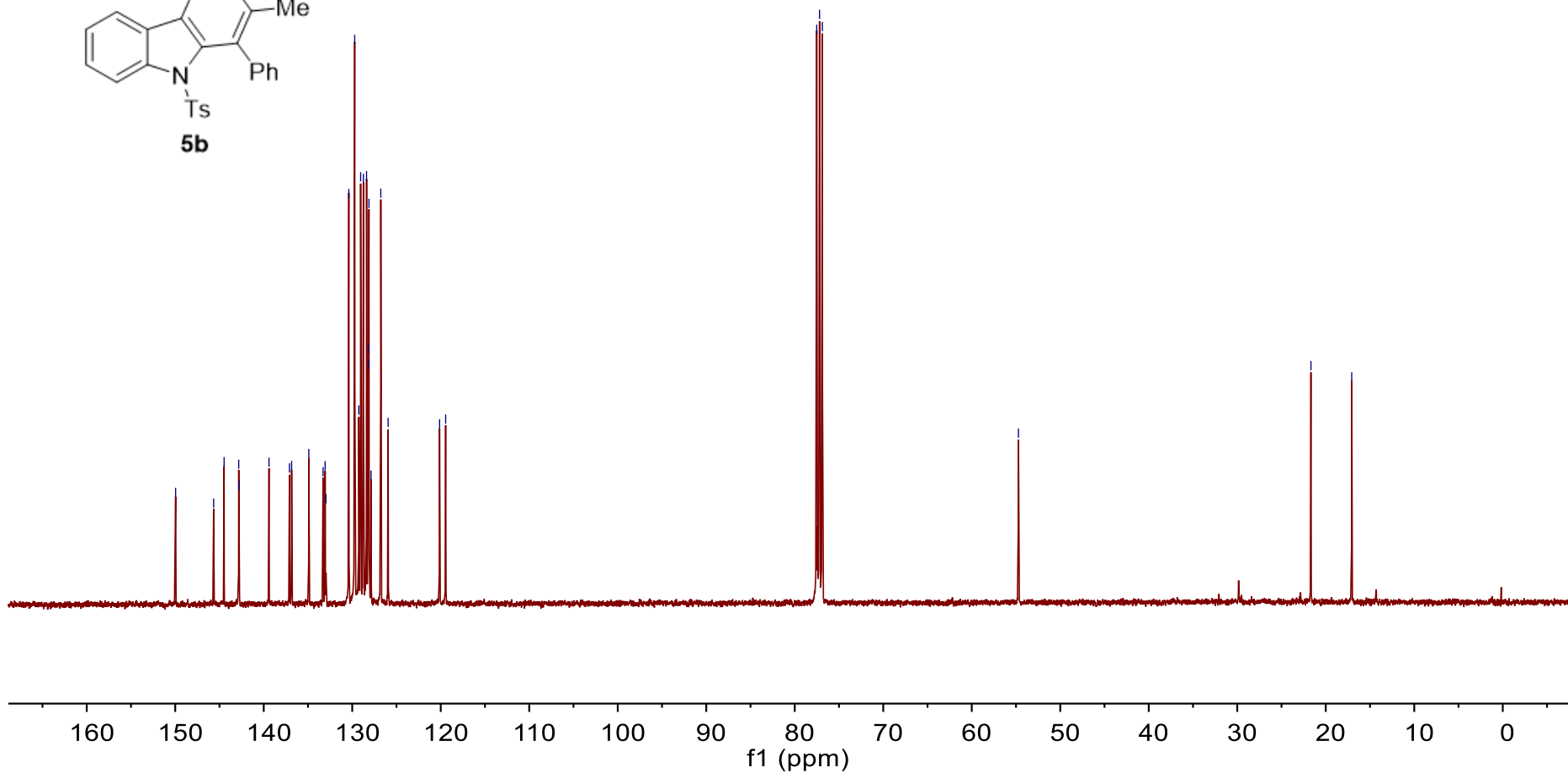
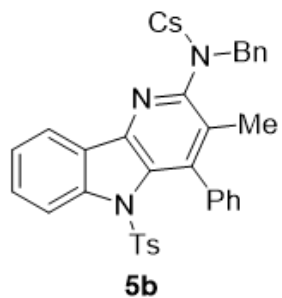


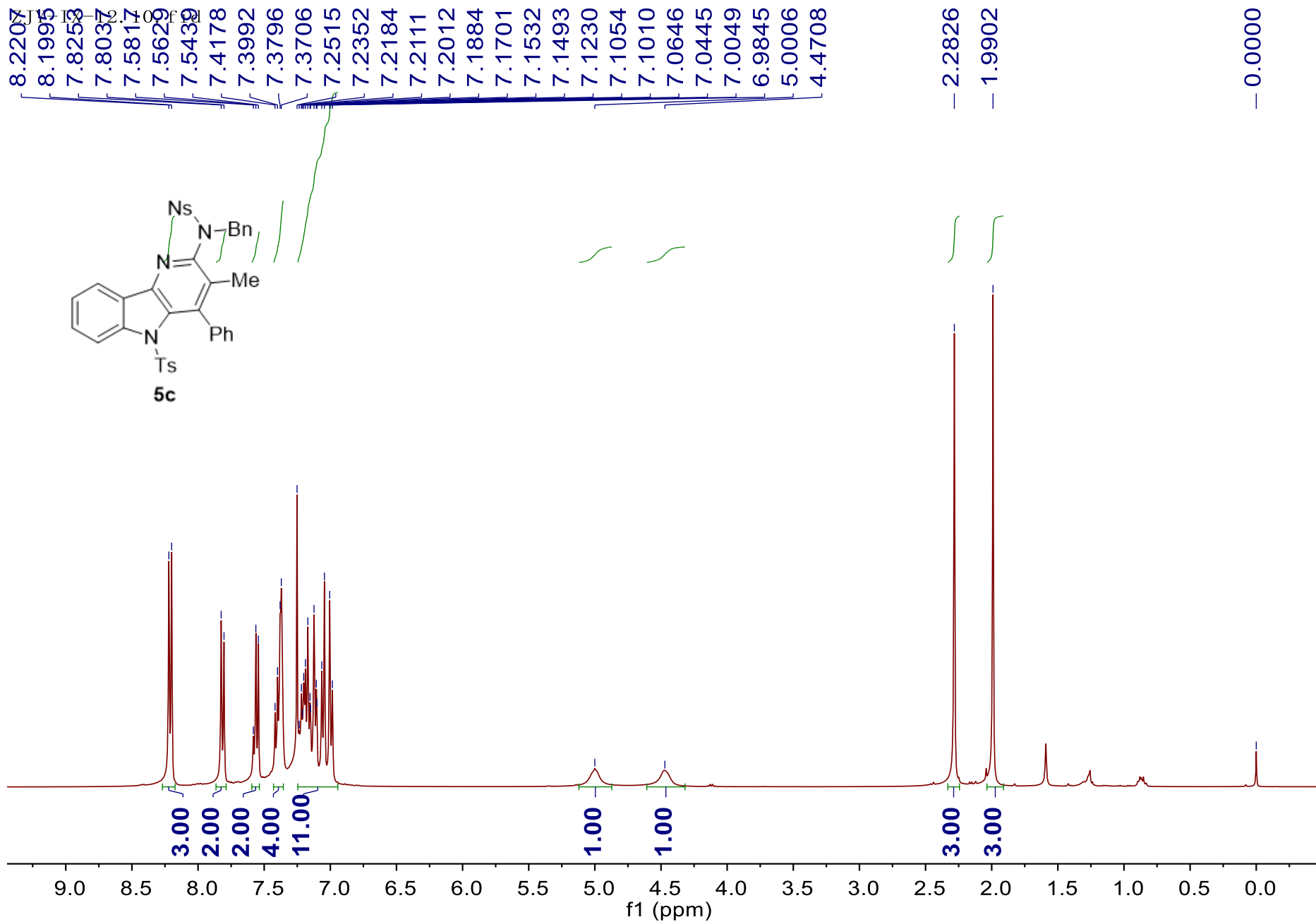
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129.050
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128.382
128.186
128.161
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54.722

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17.068

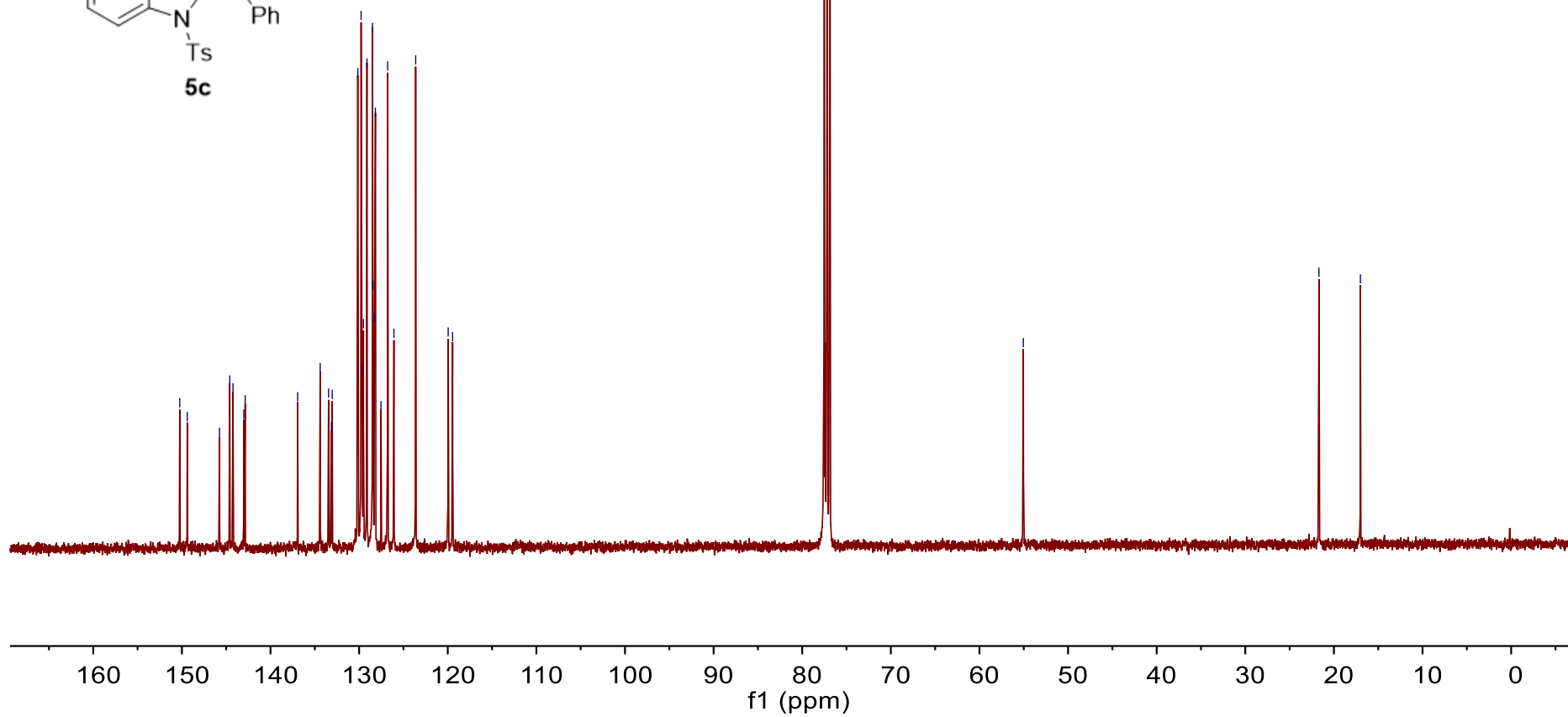
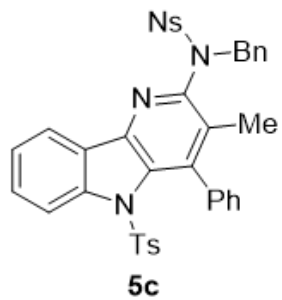




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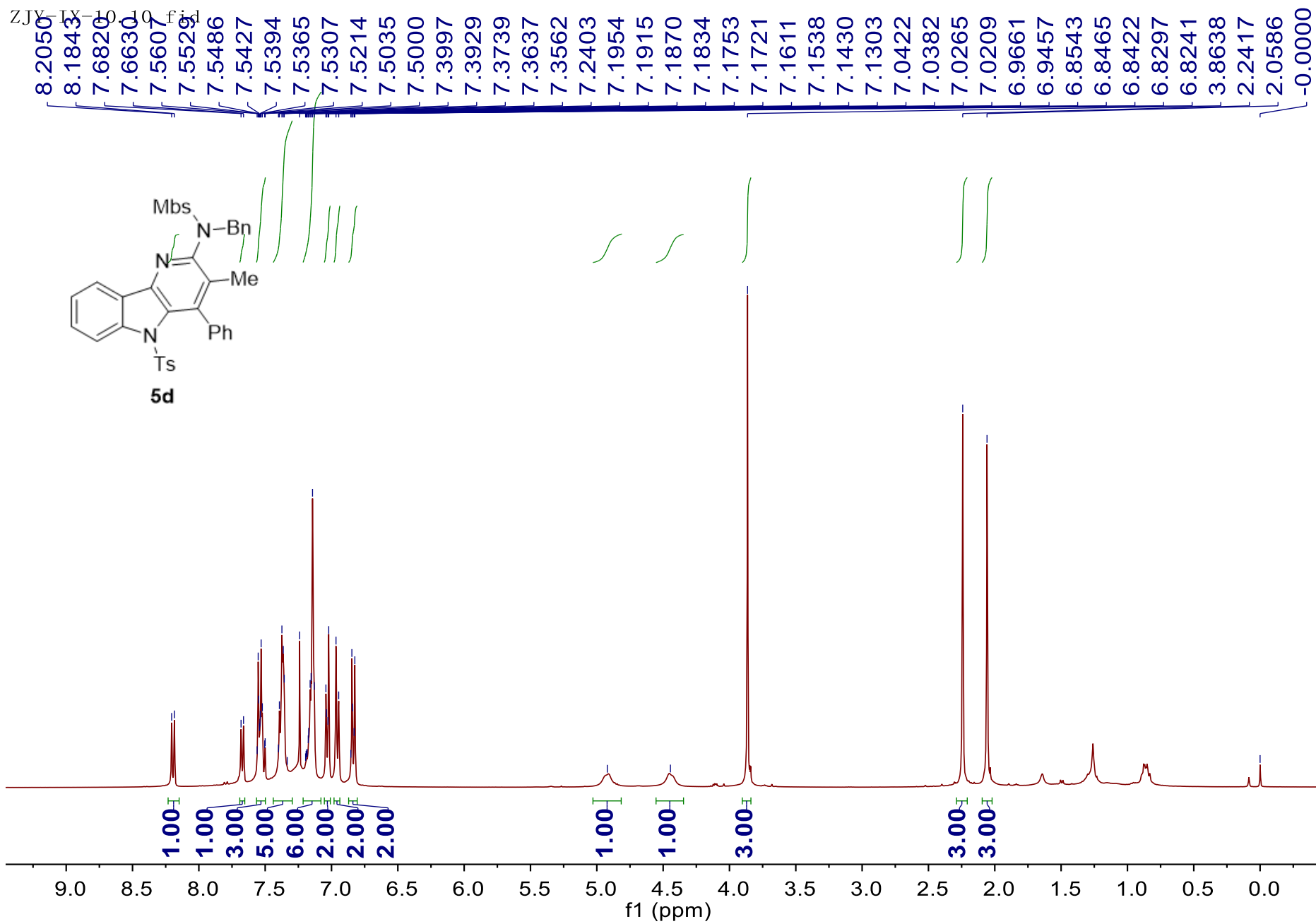
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128.490
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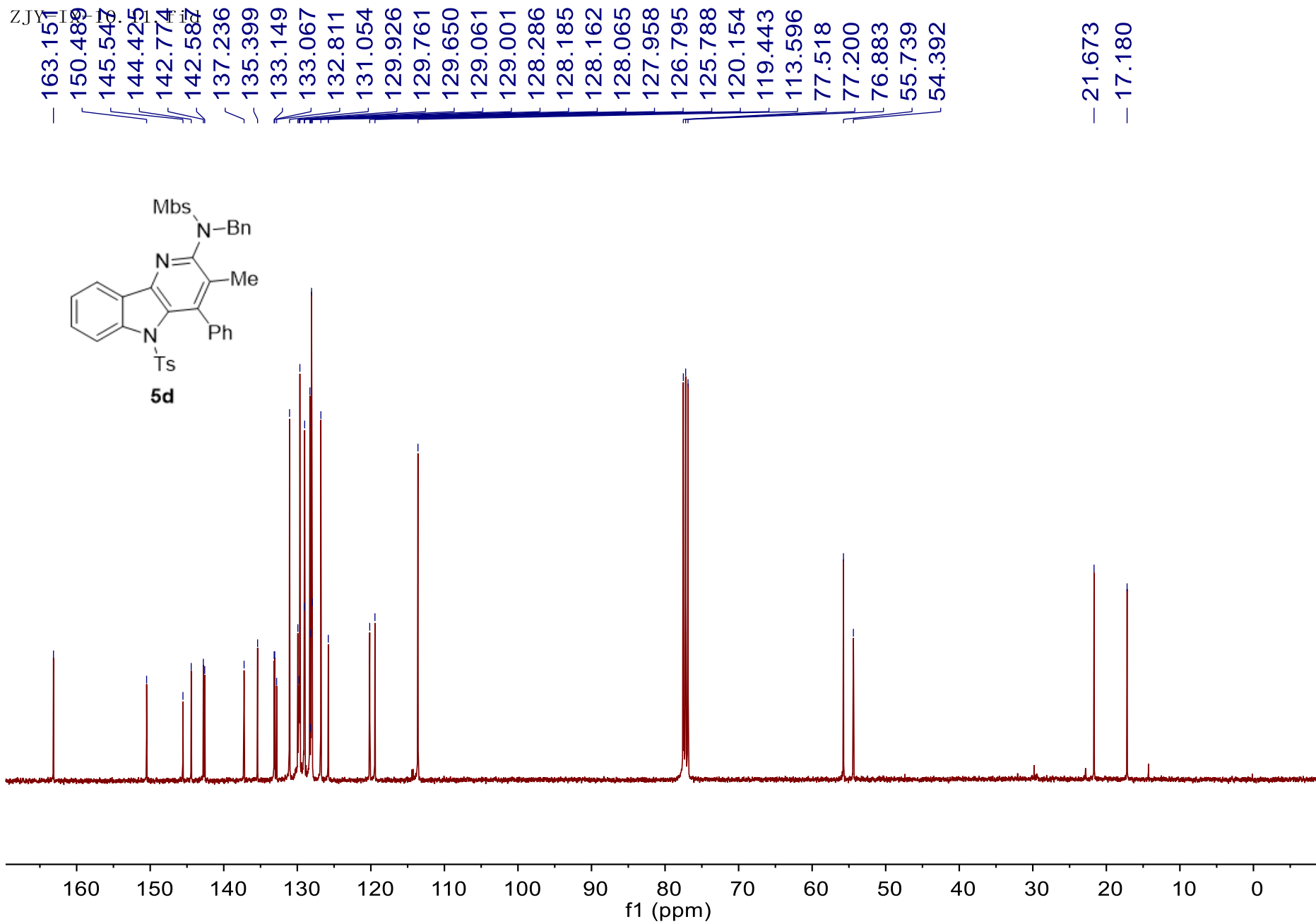
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- 17.013



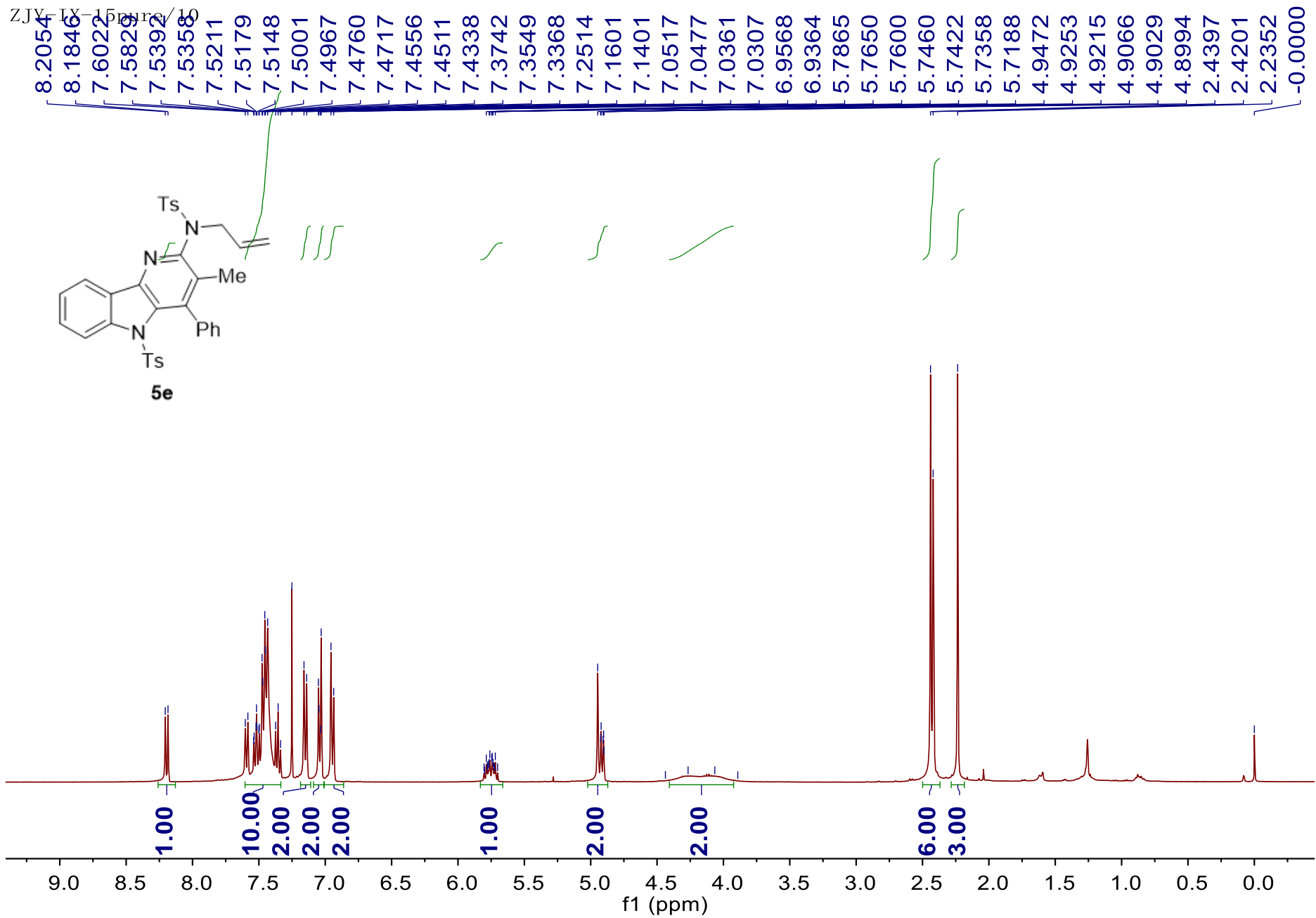
S126

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ZJY-IX-15pure/10

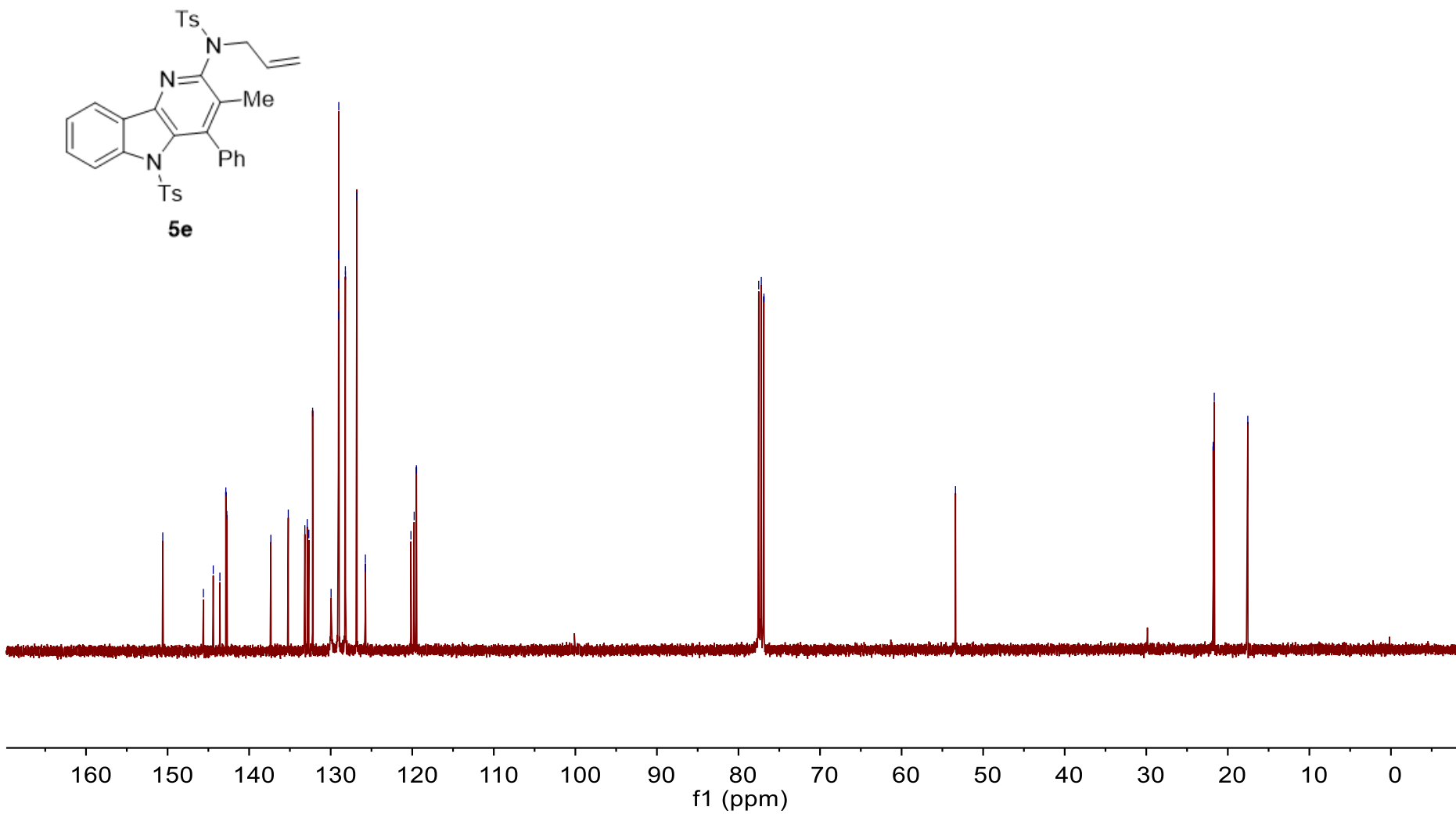
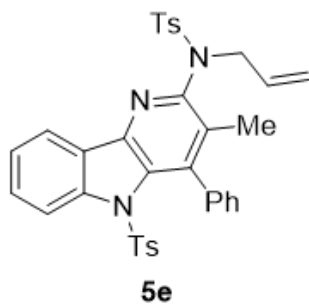


Zy-X1 source

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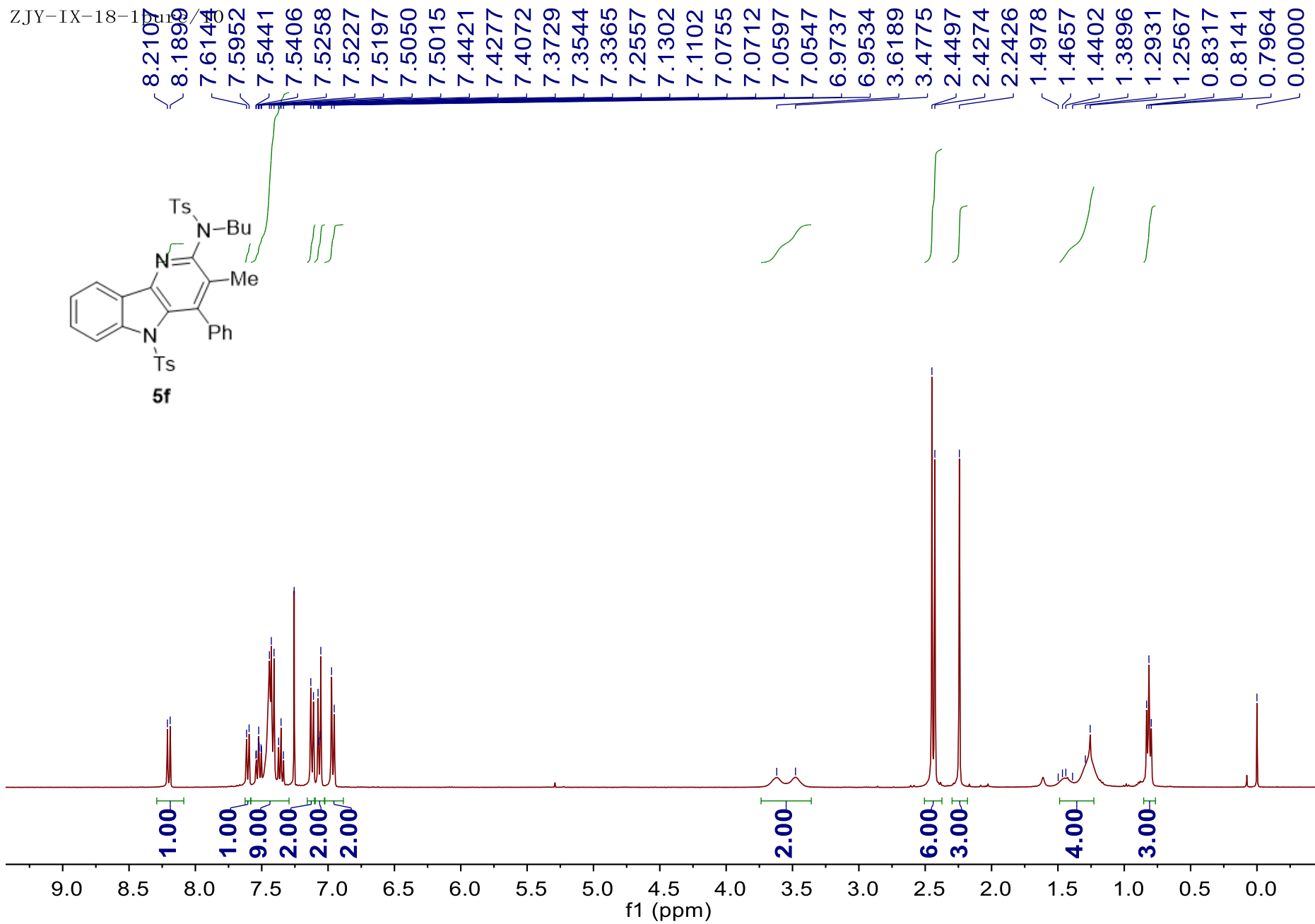
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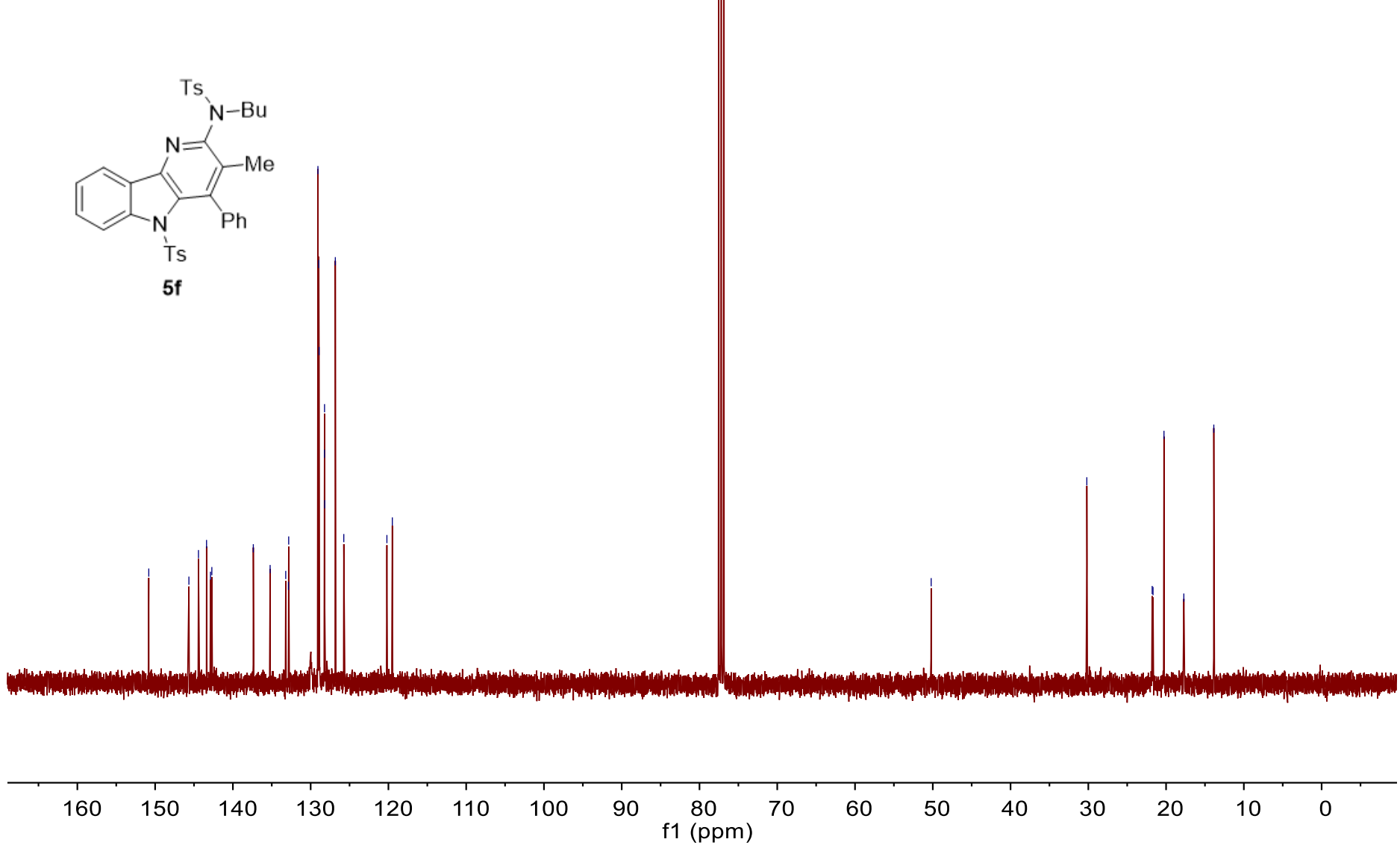
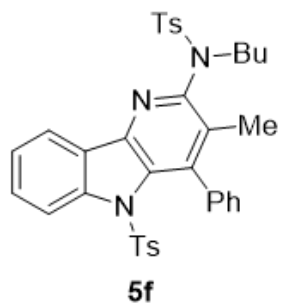


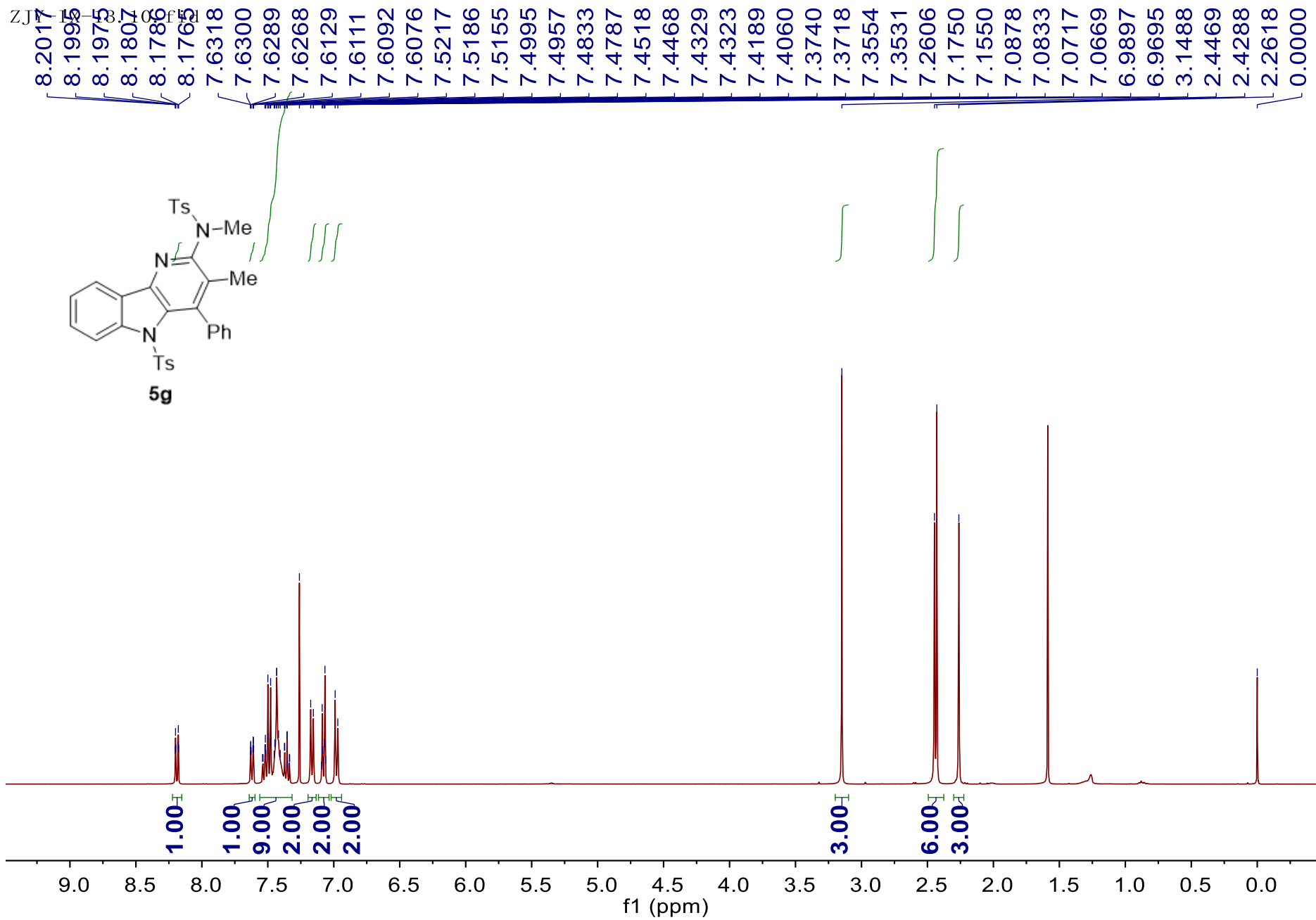
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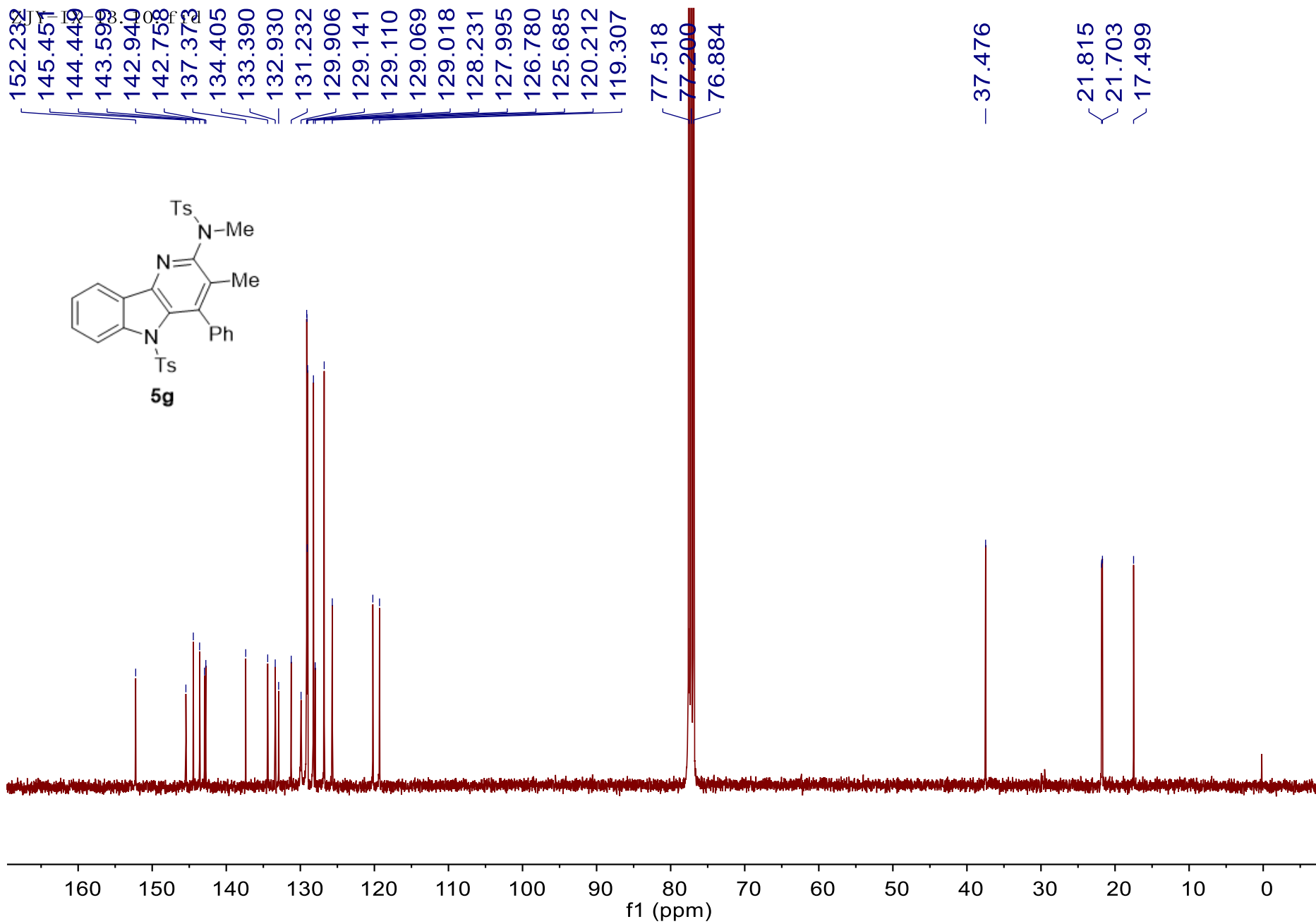
ZJY-IX-18-10113



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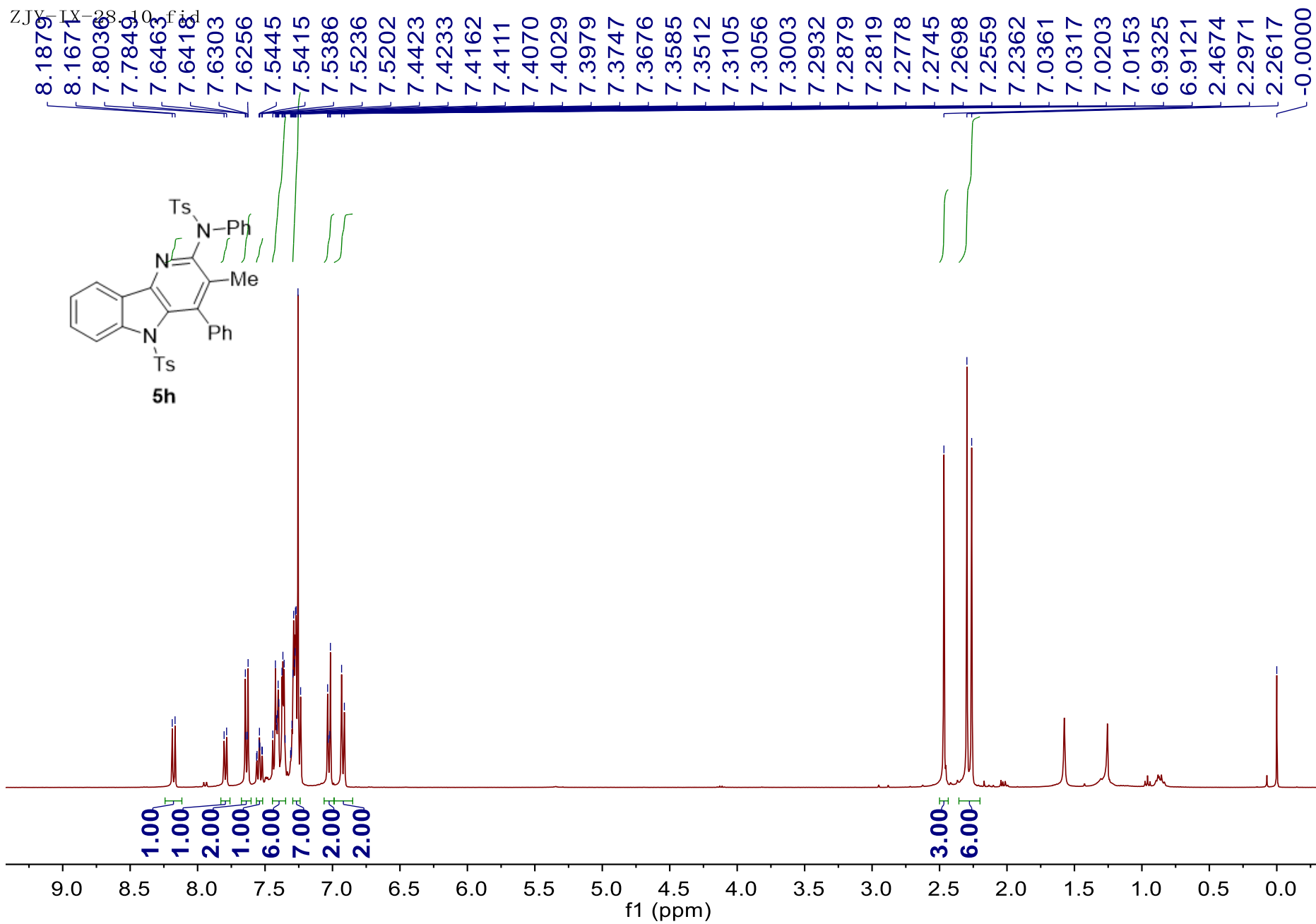






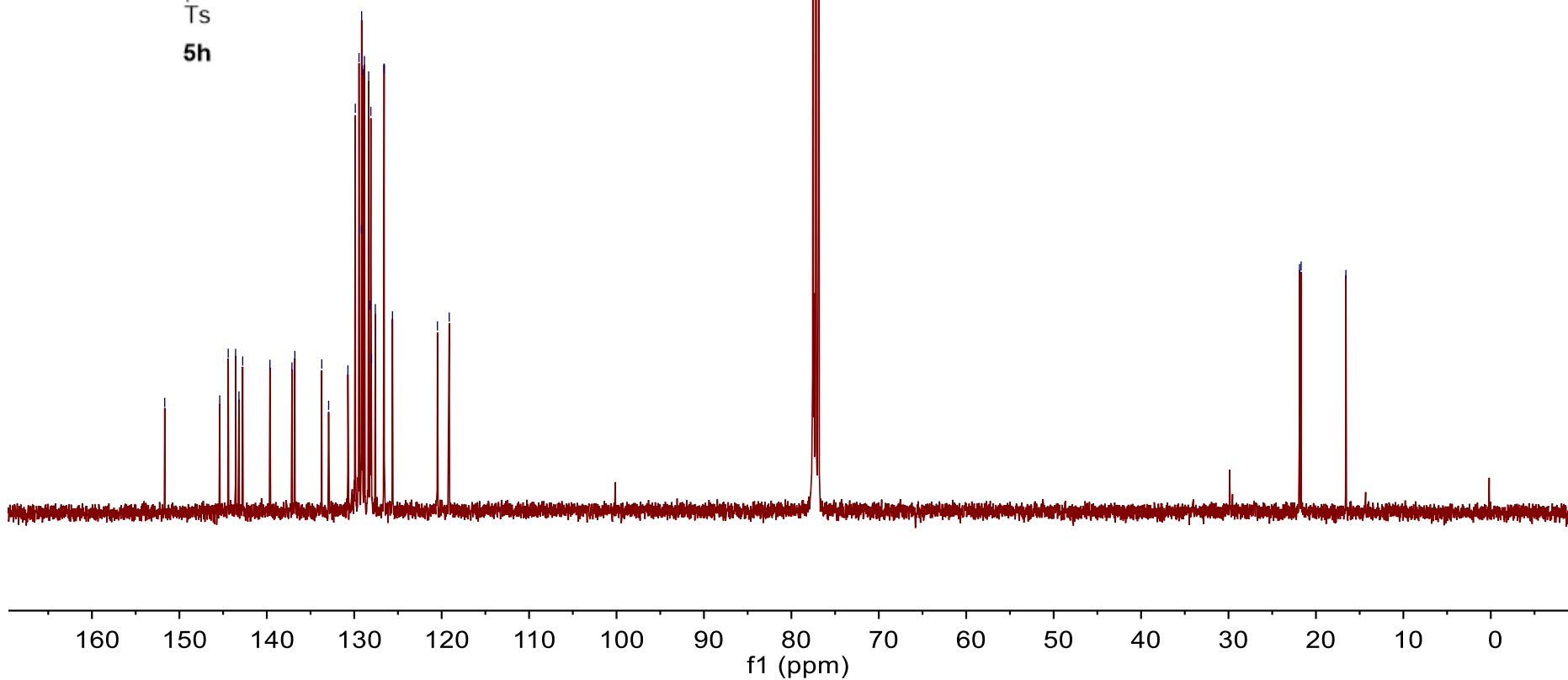
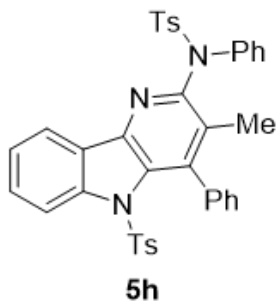
S134

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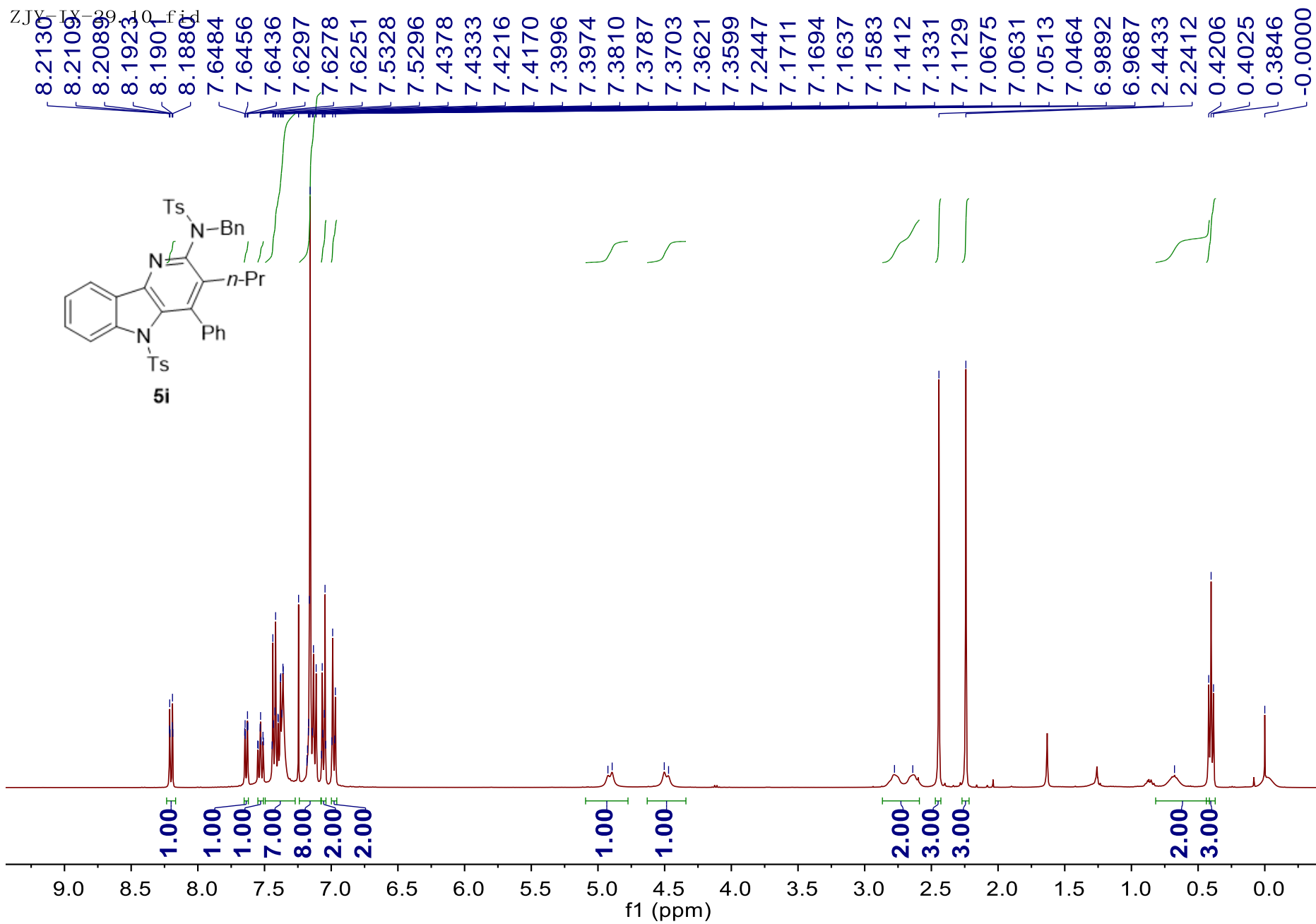
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128.352
128.192
128.102
128.018
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120.483
119.134
77.518
77.200
76.883

21.871
21.696
16.571



S136

ZJY-IX-39-10.fid



ZJY-K-1911-fd

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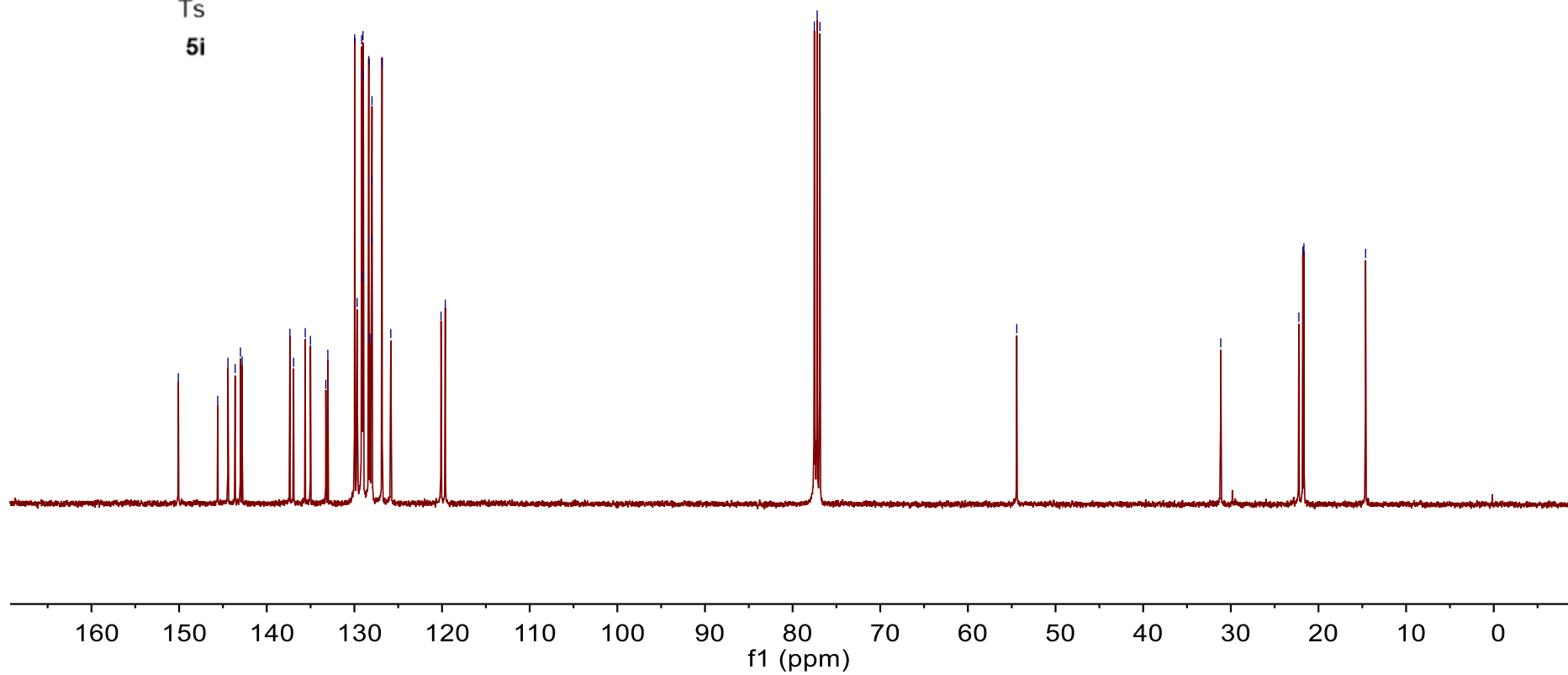
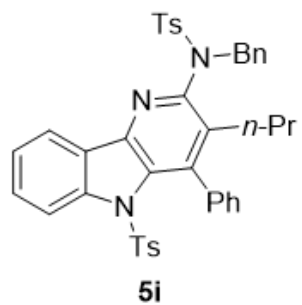
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22.236

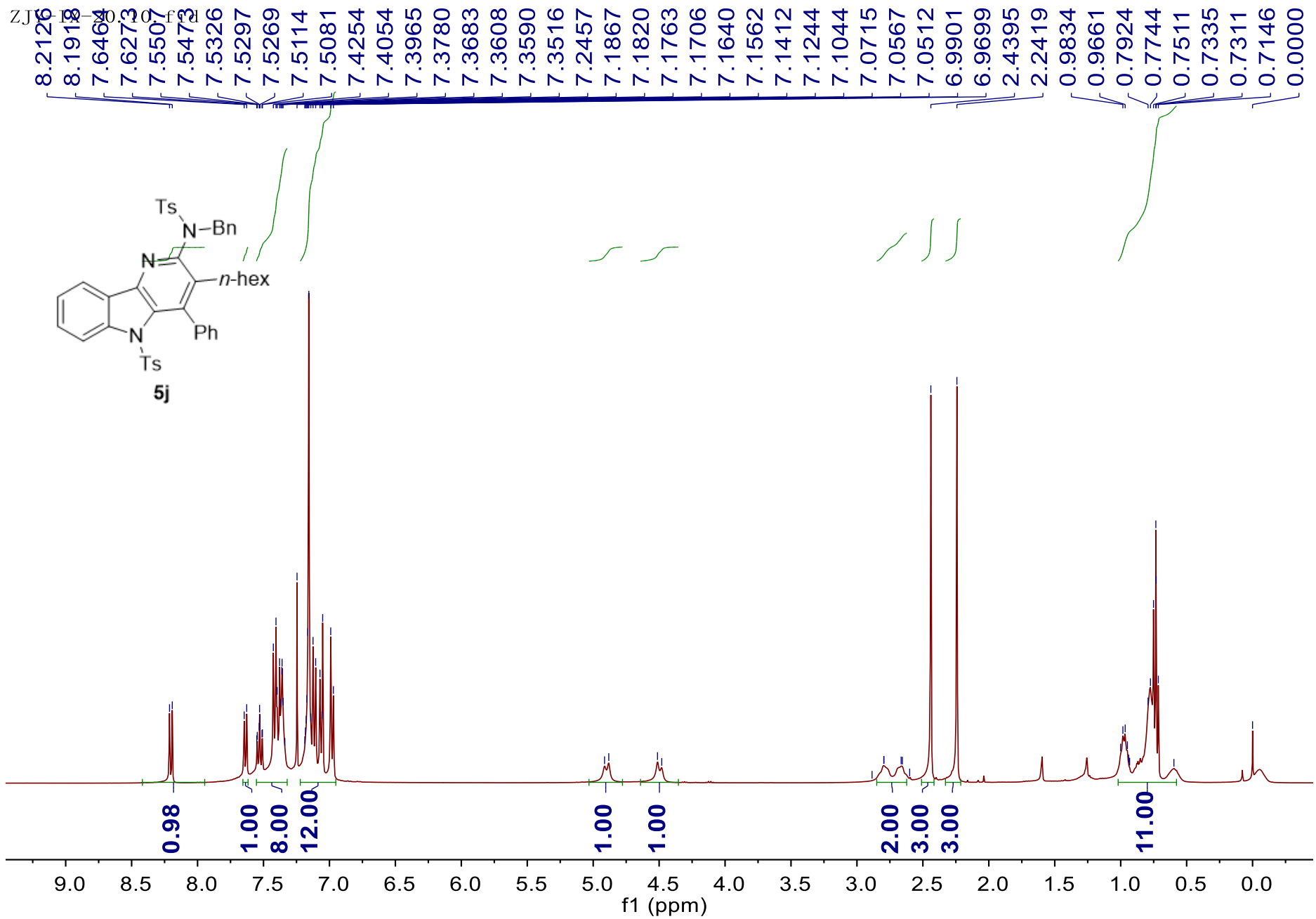
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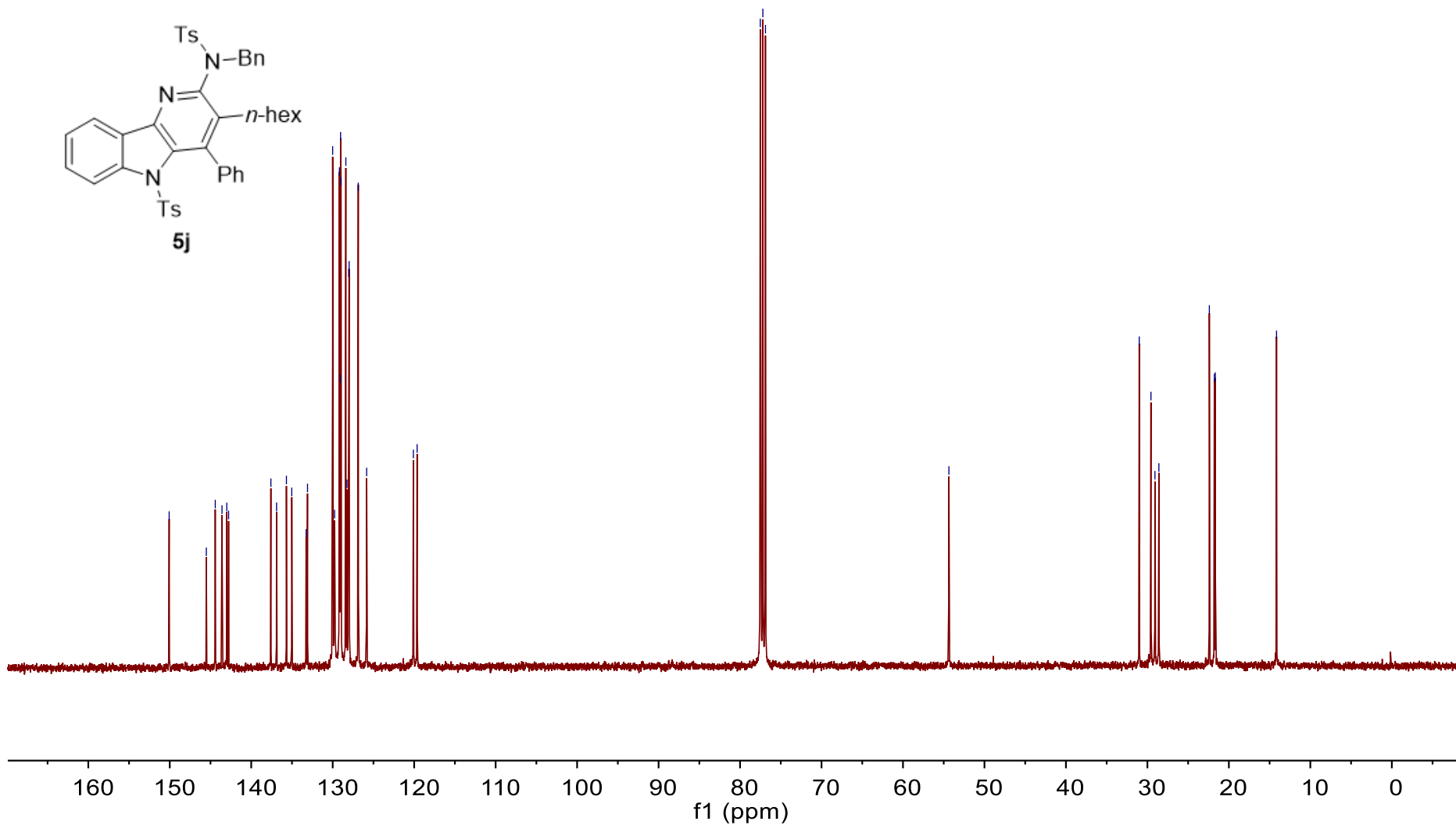
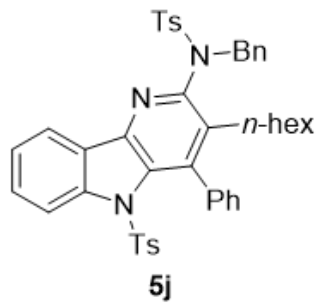
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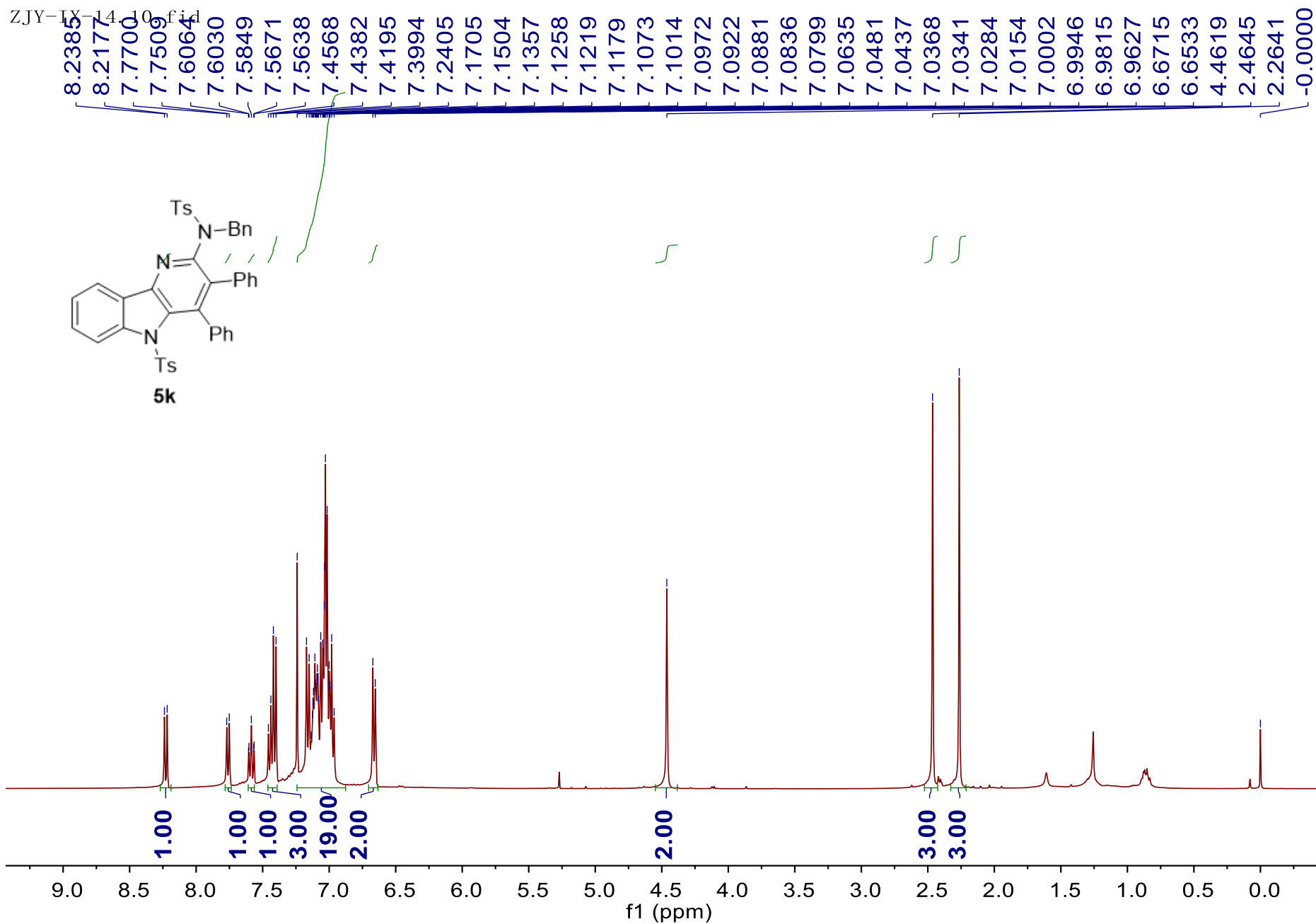
ZJ-13-2010-f1a



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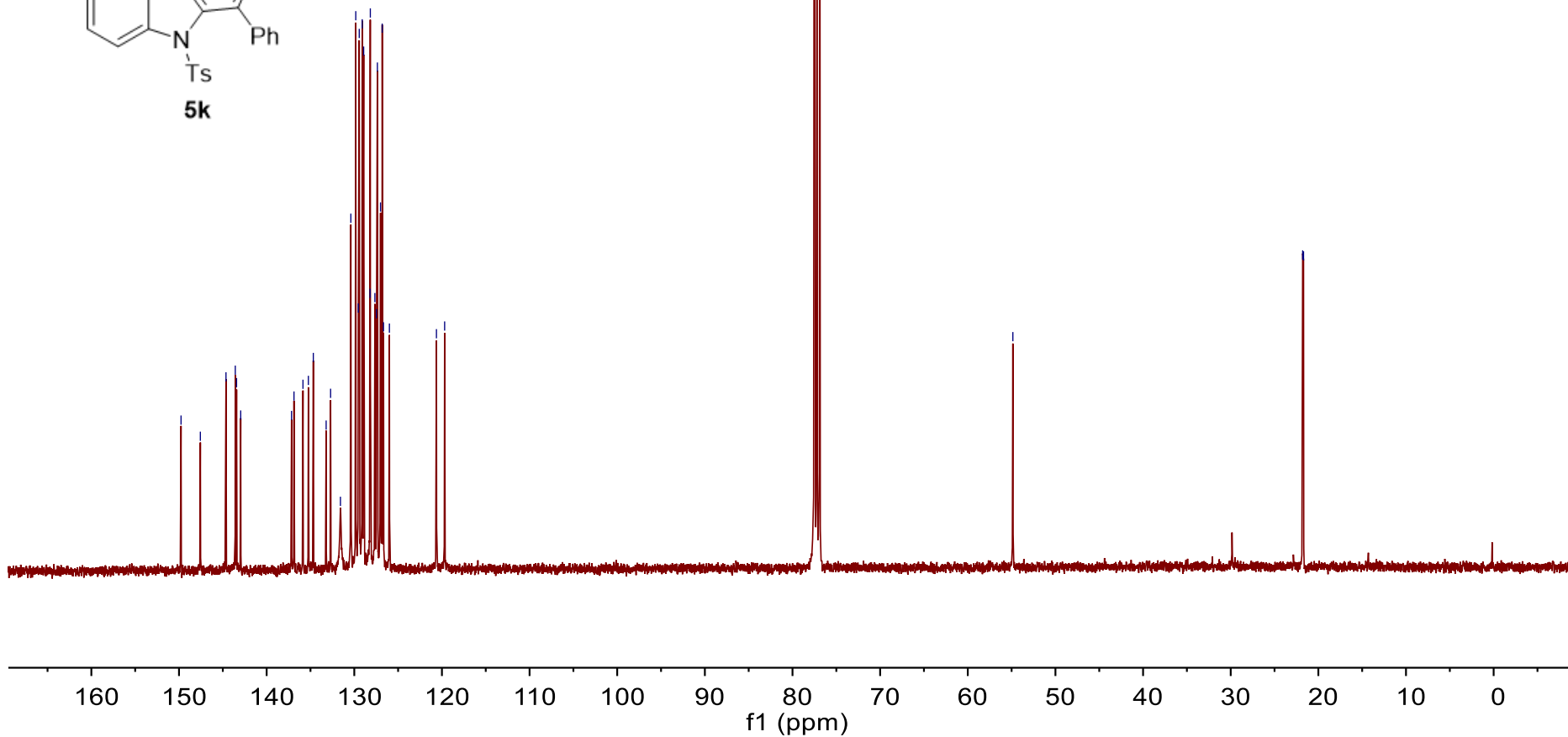
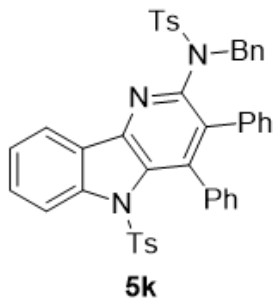


ZJY-IX-14-10.fid

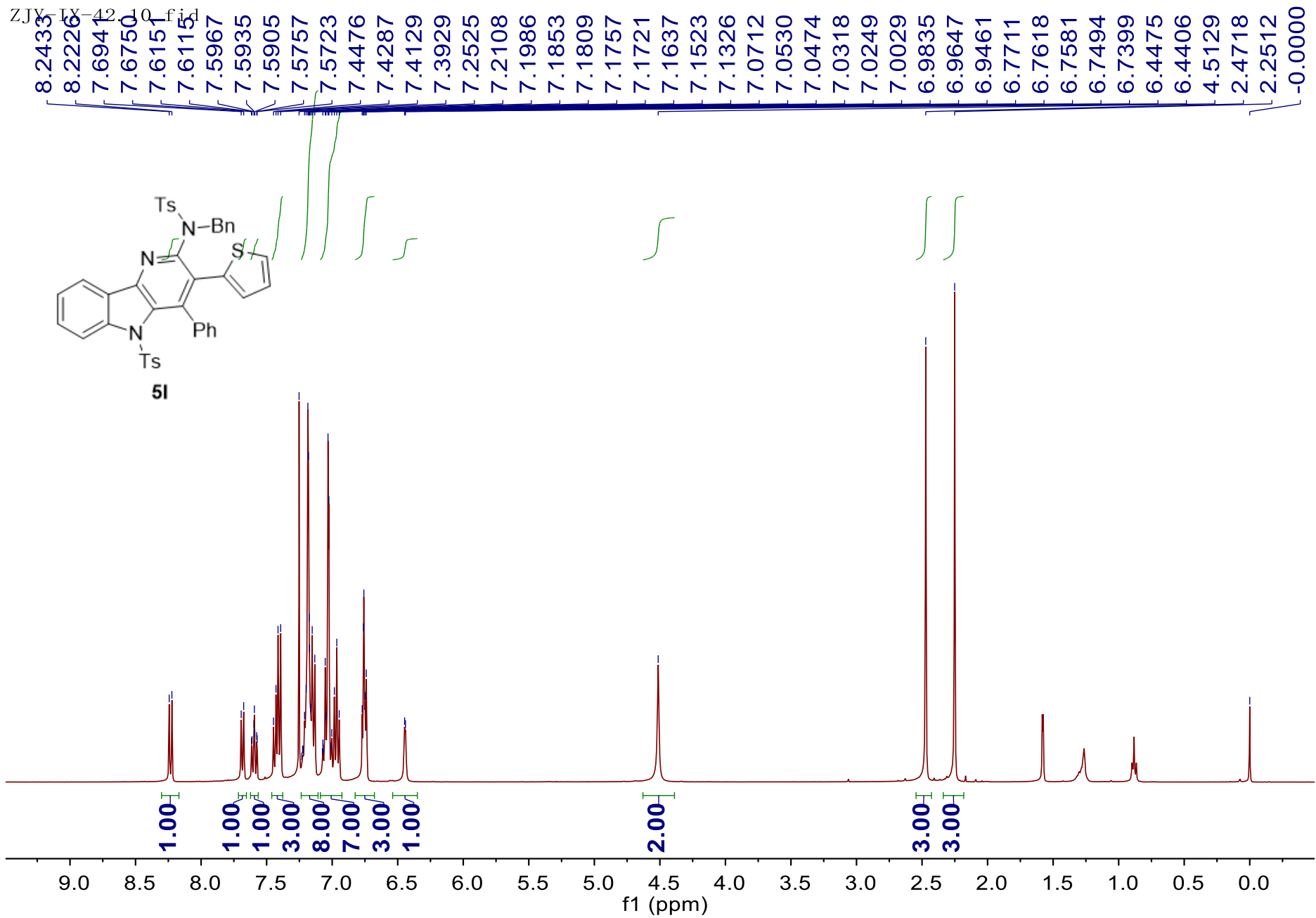


149.767
147.564
144.640
143.578
143.432
142.959
137.159
136.881
135.855
135.237
134.675
133.210
132.704
131.579
130.392
129.831
129.541
129.434
129.097
128.930
128.199
128.170
127.650
127.466
127.364
127.008
126.815
126.667
125.993
120.627
119.690
77.518
77.200
76.883
54.856

21.790
21.690

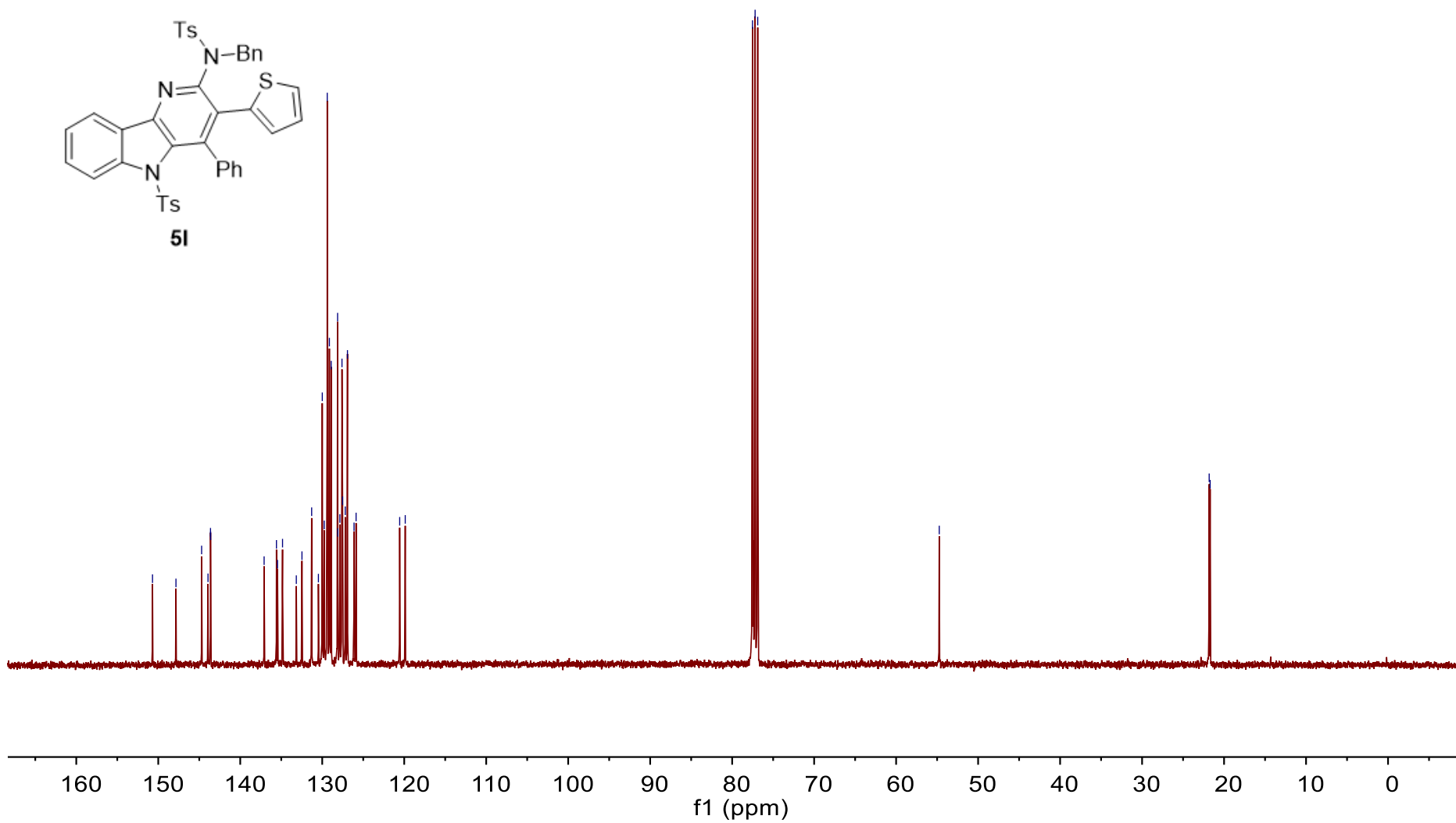
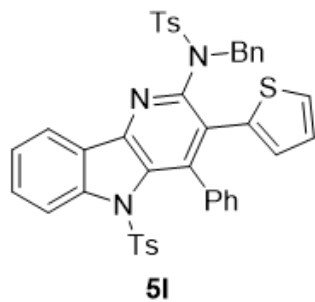


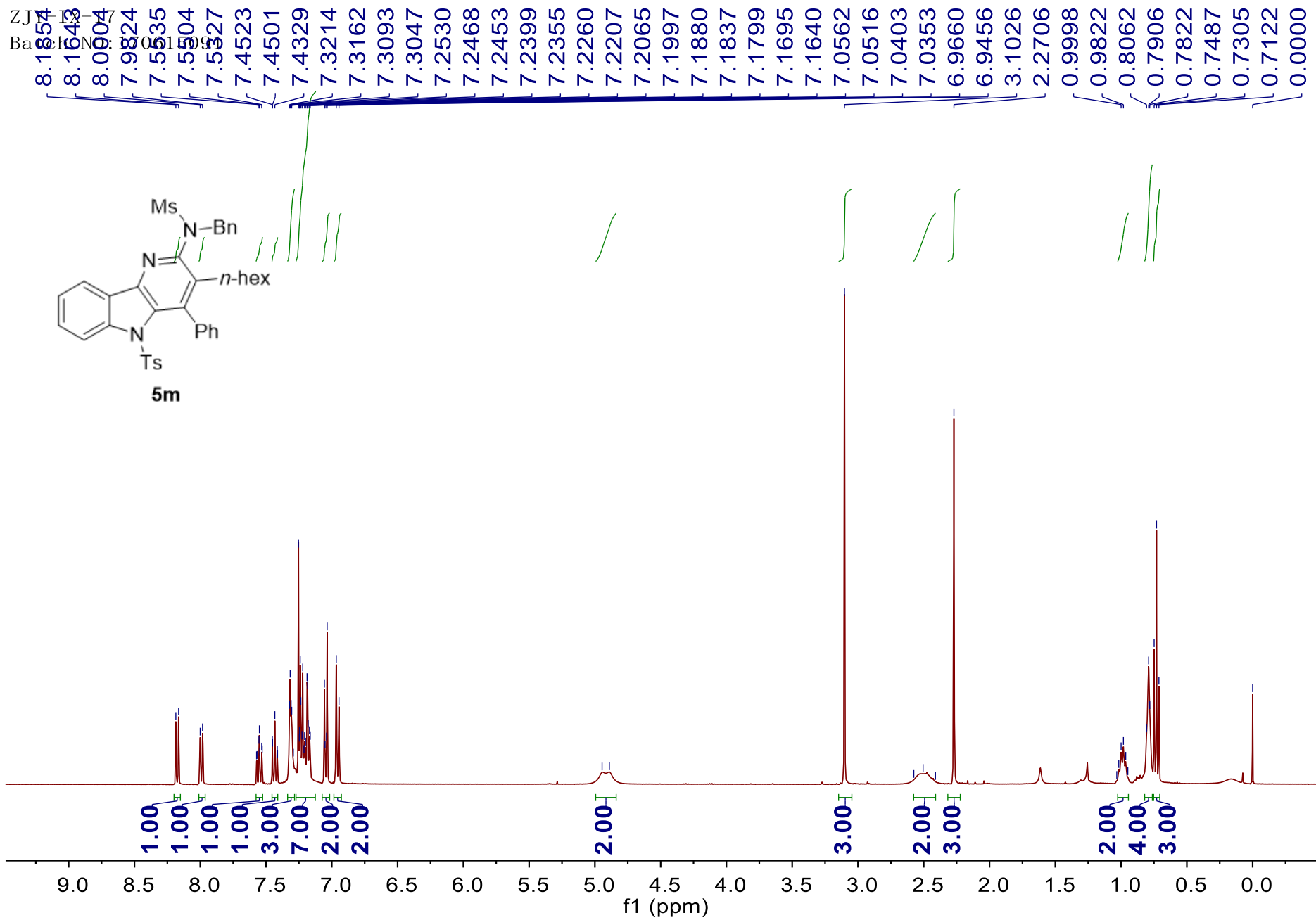
ZJY-IX-42-10.fid



150.702
147.841
144.710
143.932
143.627
143.613
137.087
135.582
135.455
134.841
133.161
132.471
131.288
130.467
129.994
129.755
129.387
129.126
128.908
128.123
128.095
127.850
127.591
127.515
127.190
126.922
126.119
125.870
120.552
119.874
77.518
77.200
76.882
54.739

21.816
21.699



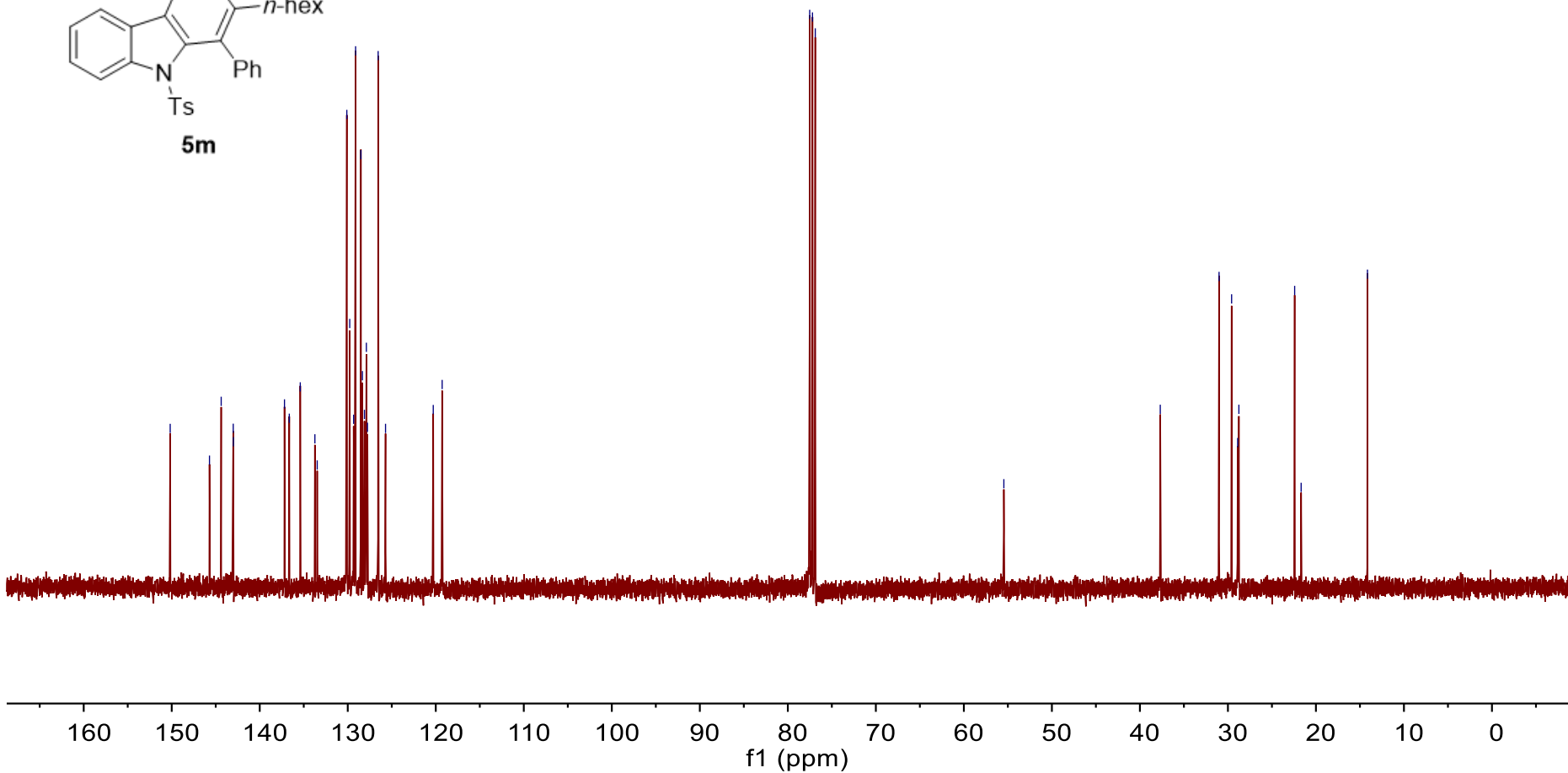
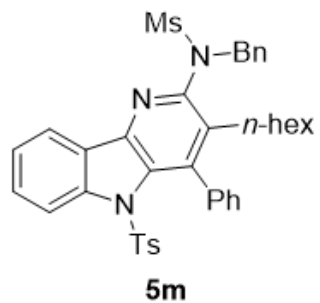


ZJY-LX-100ppm
Gradient Spinning

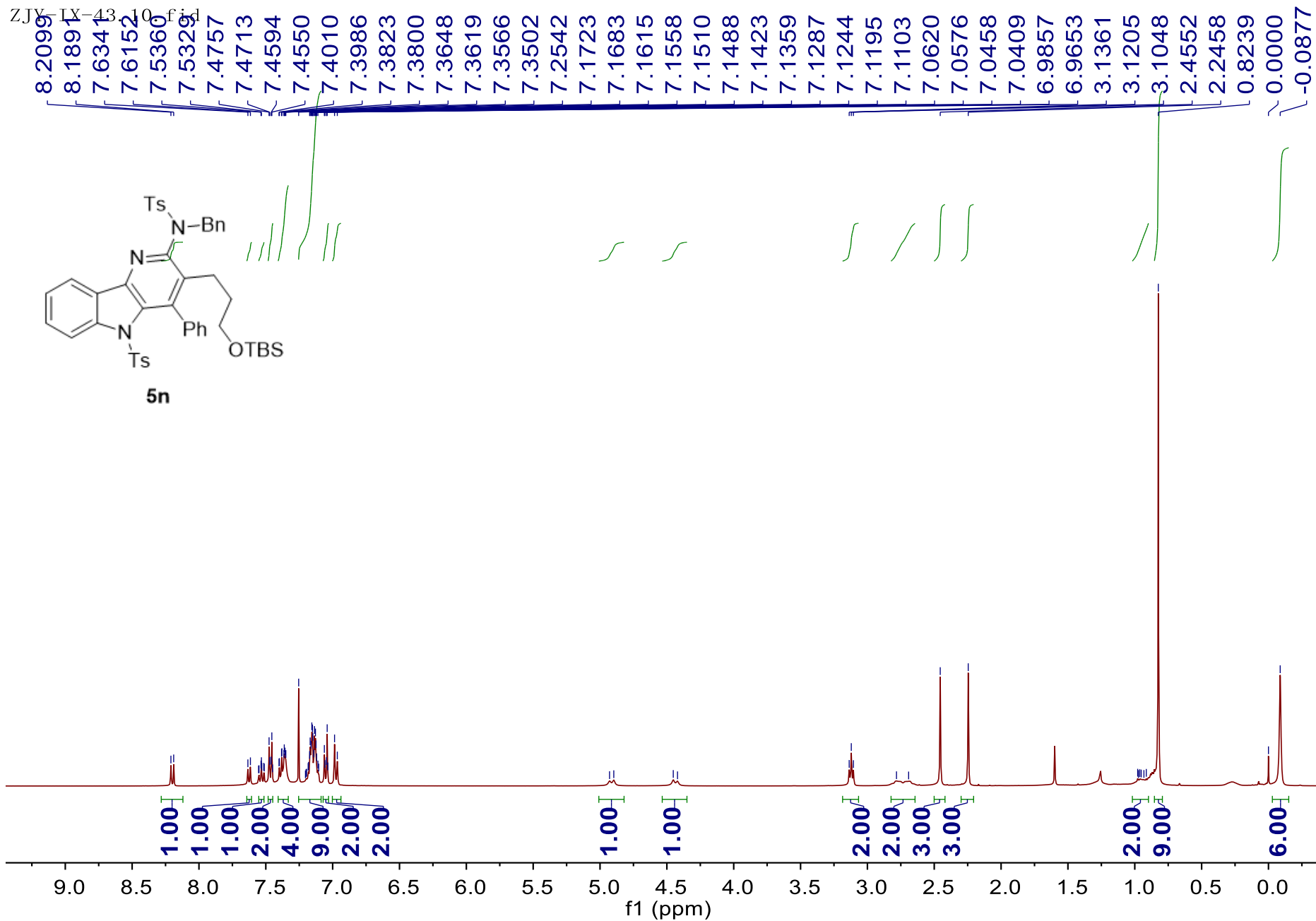
150.174
145.711
144.580
143.610
142.992
137.189
136.644
135.395
133.732
133.471
130.106
129.776
129.332
129.108
128.509
128.338
128.105
127.886
127.761
126.547
125.709
120.287
119.276
77.518
77.200
76.882

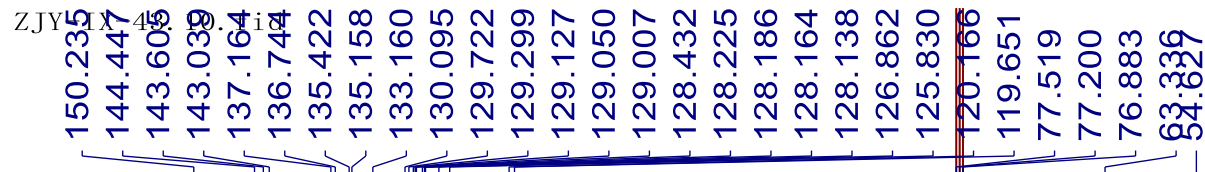
— 55.457

37.686
31.005
29.580
28.891
28.753
22.416
21.680
14.146

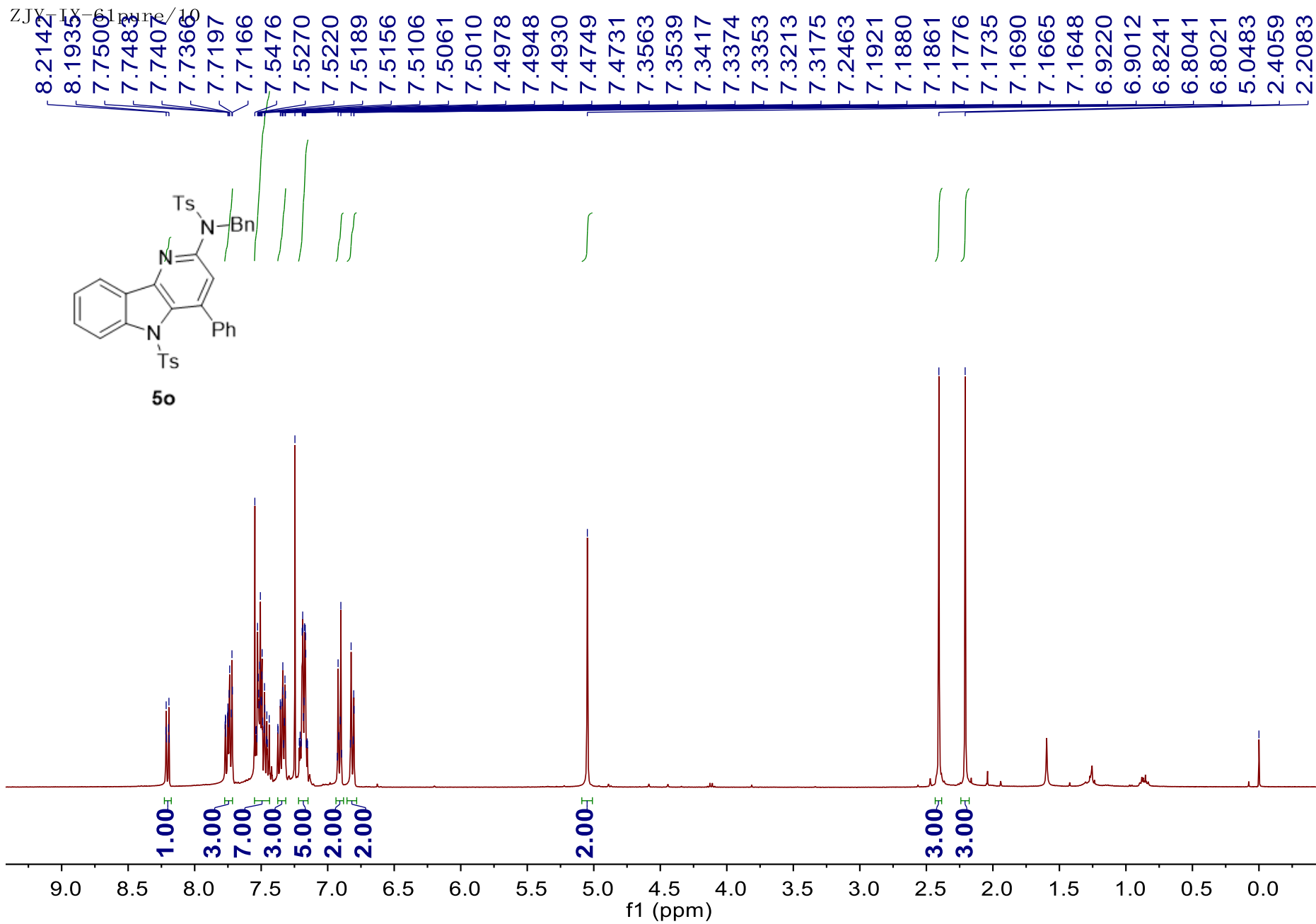


ZJY-LX-43-10.fid



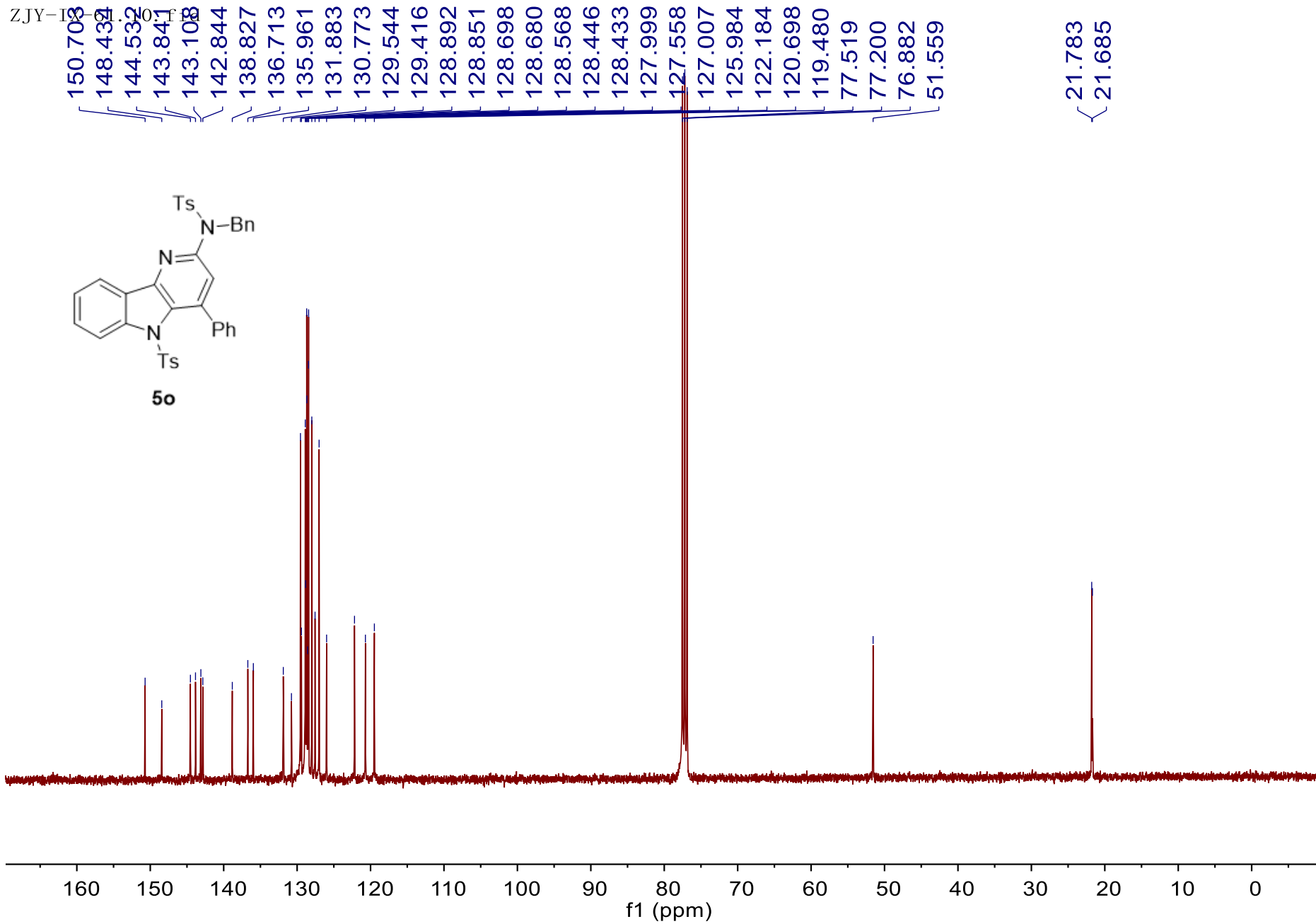
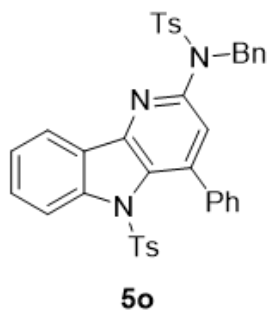


ZJY-IX-61pure/10



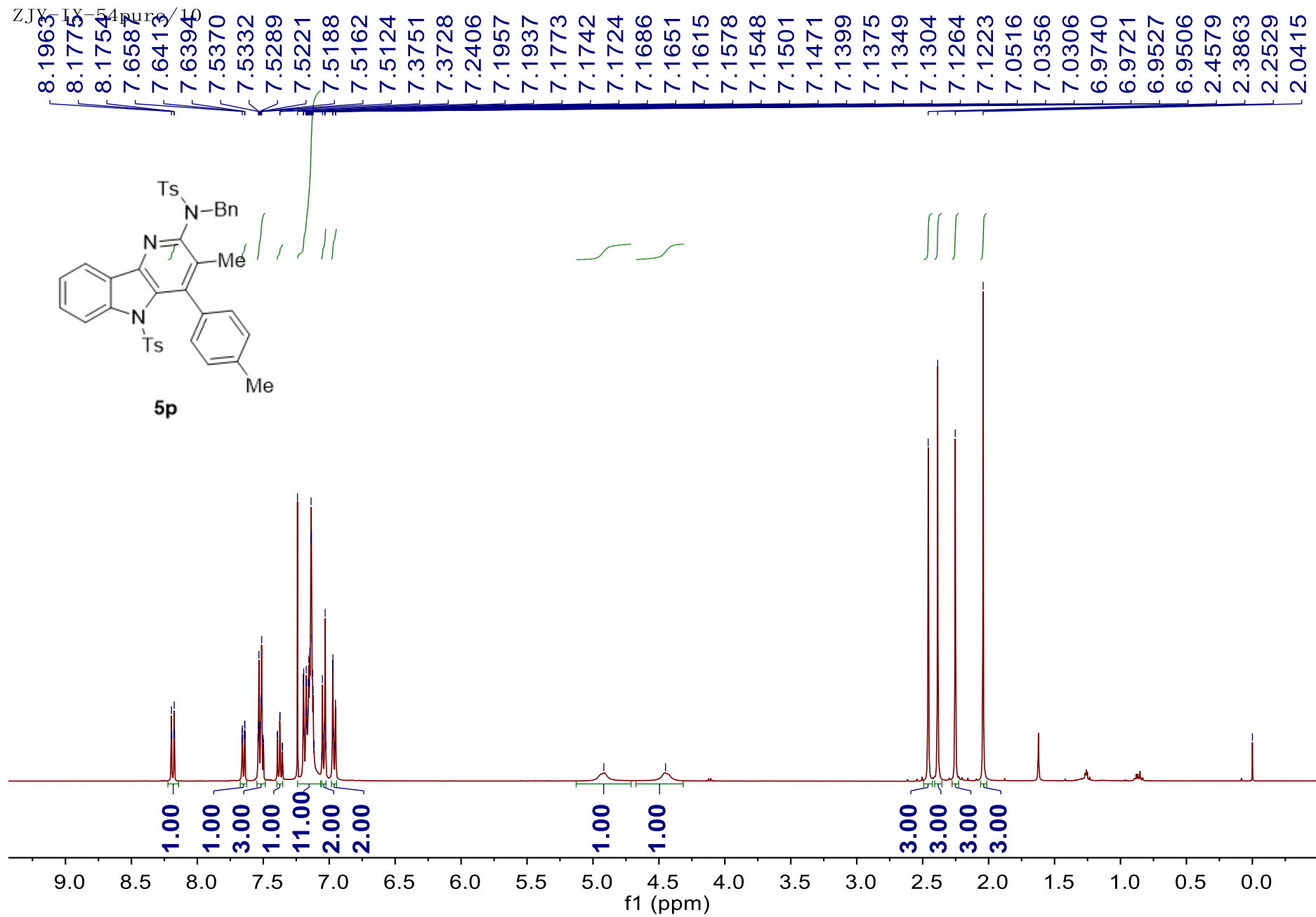
S149

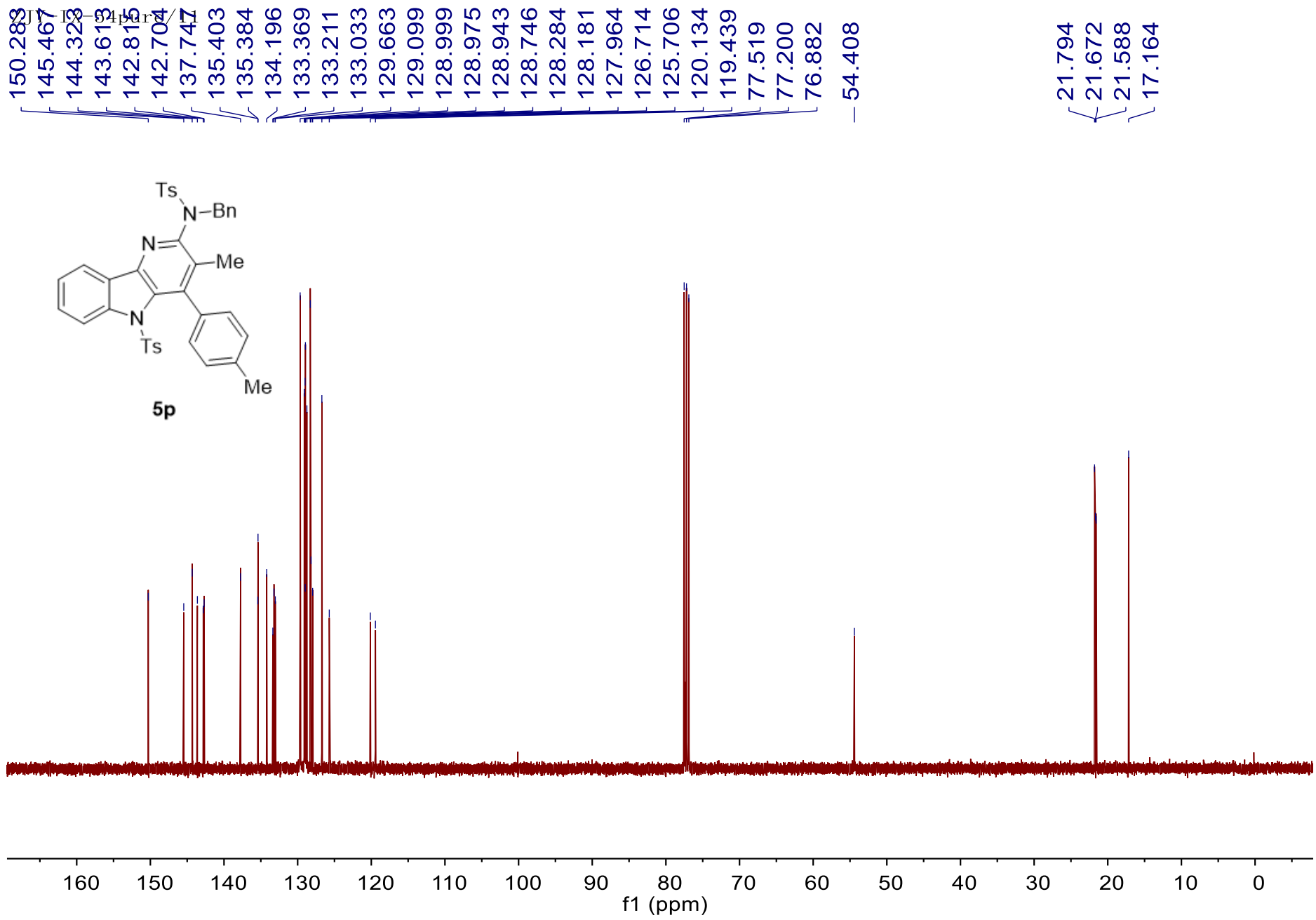
ZJY-13-01-001



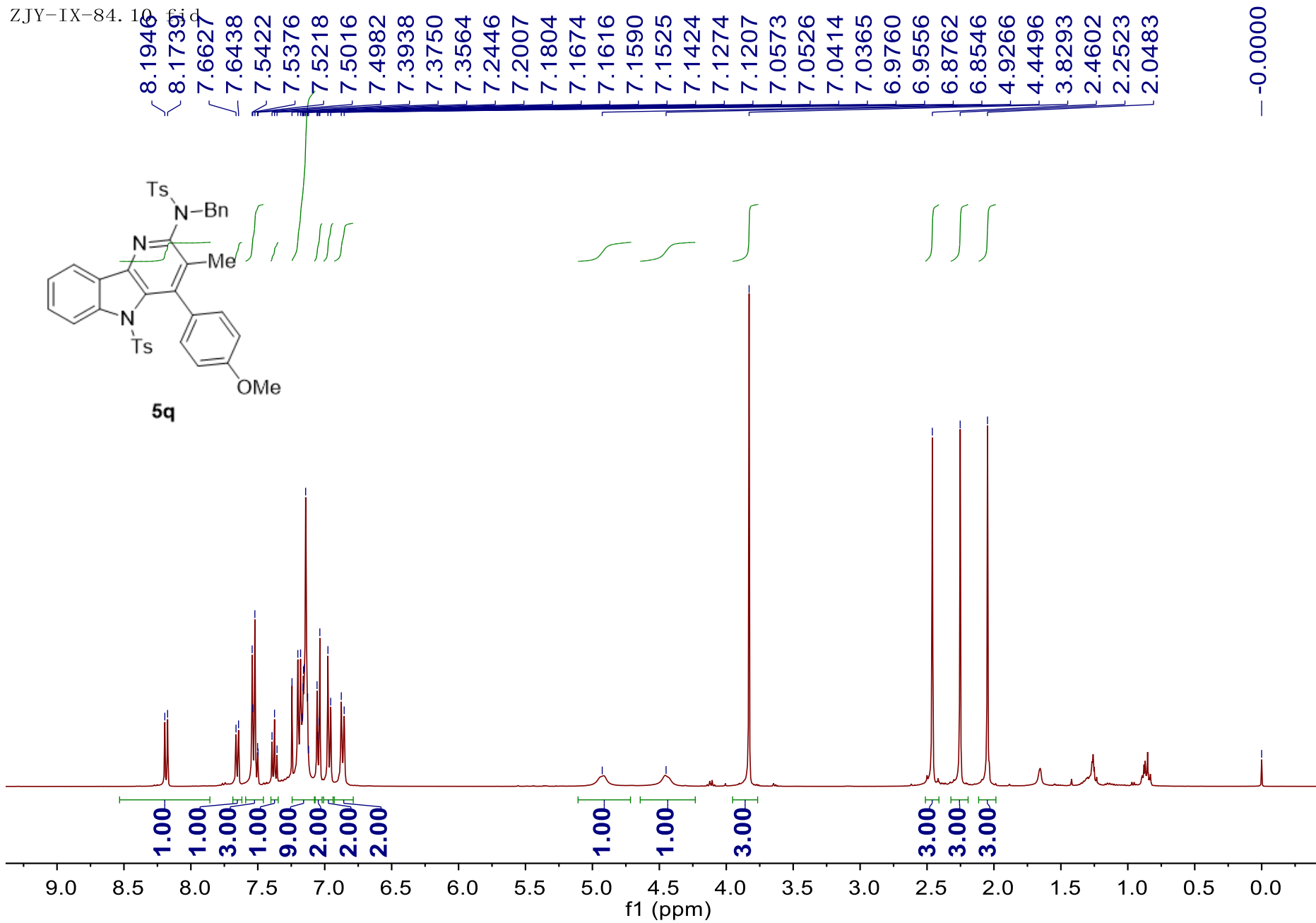
S150

ZJY-IX-54pure/10

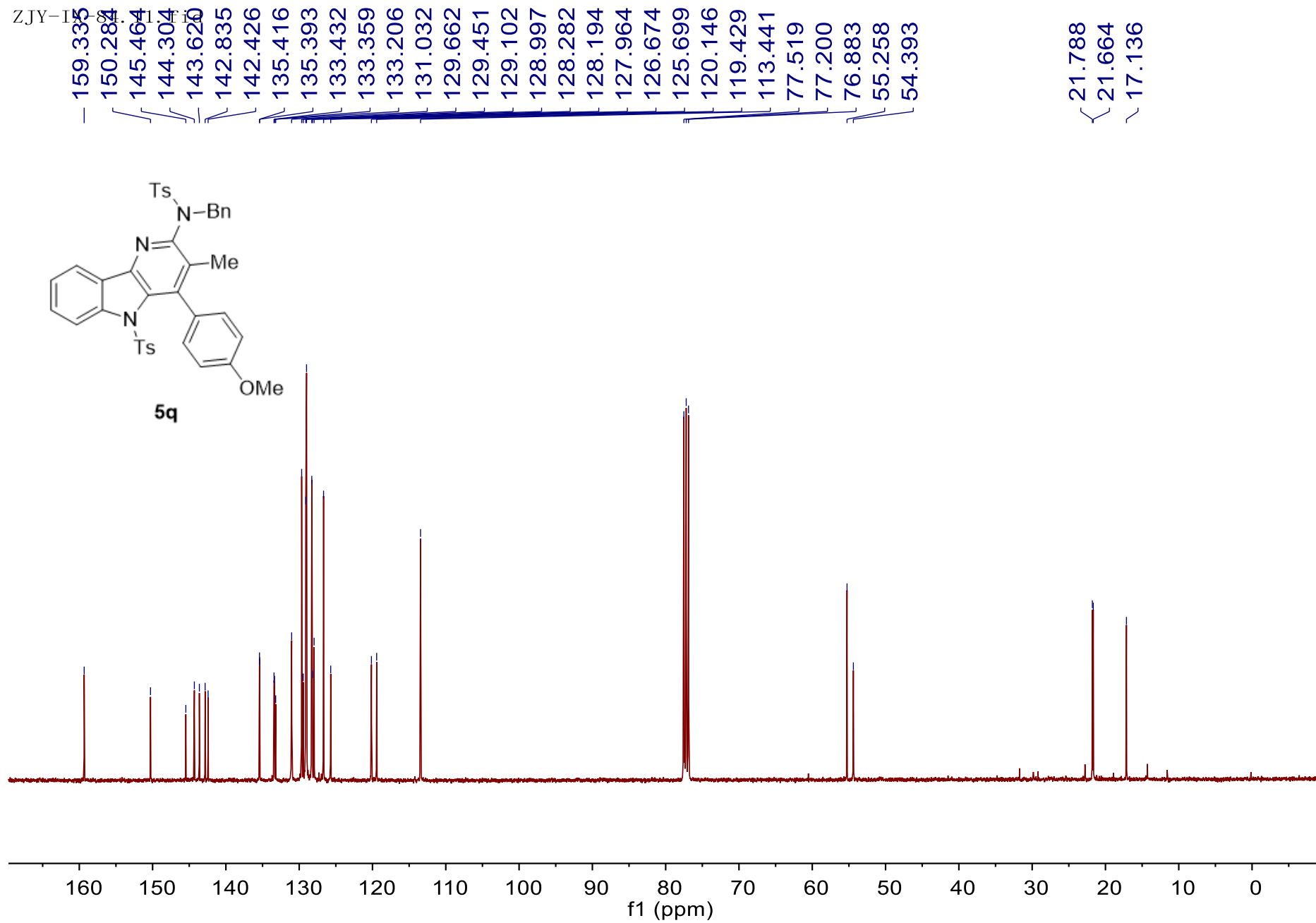
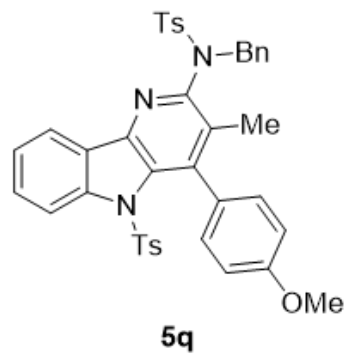




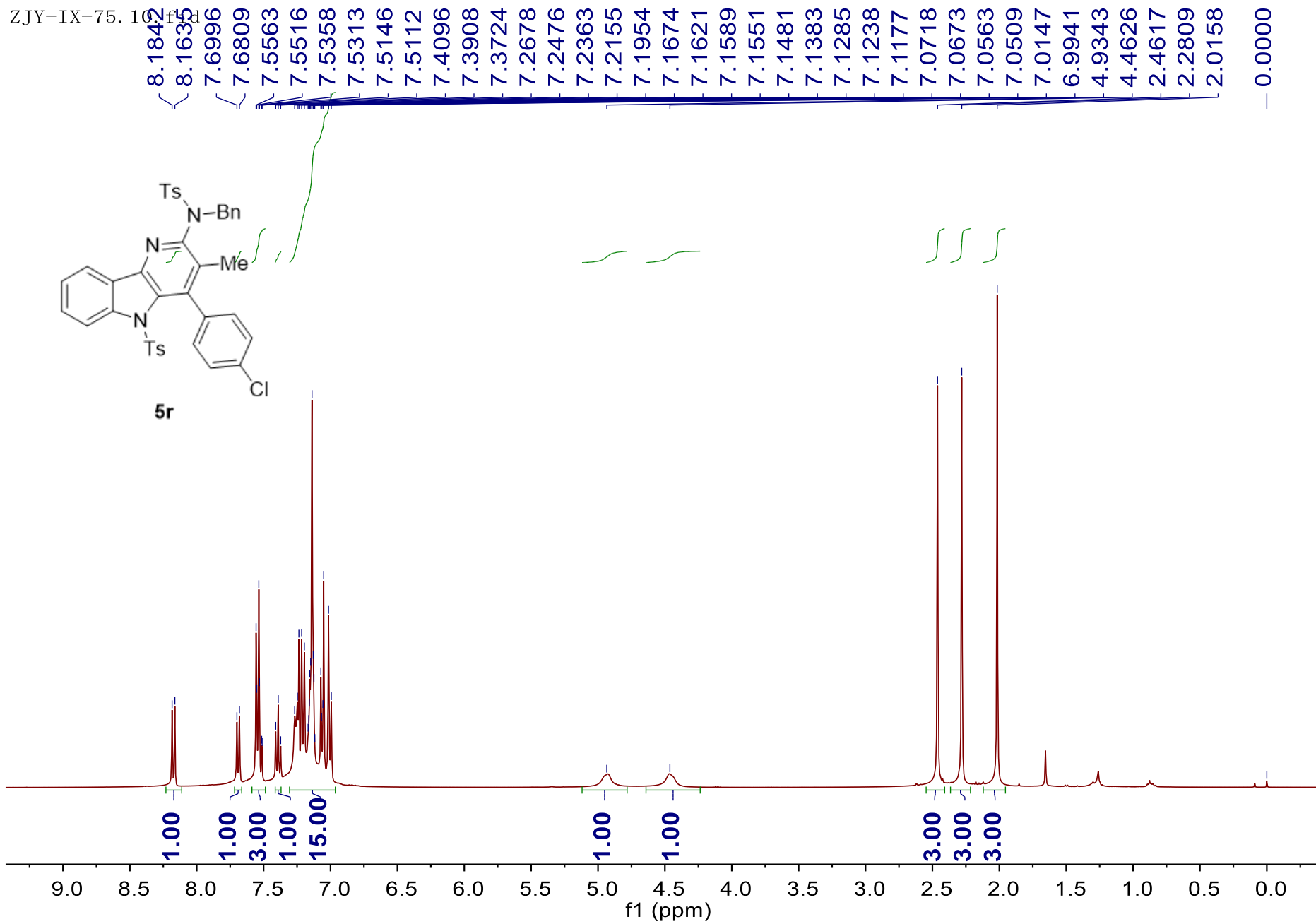
ZJY-IX-84.10.fid

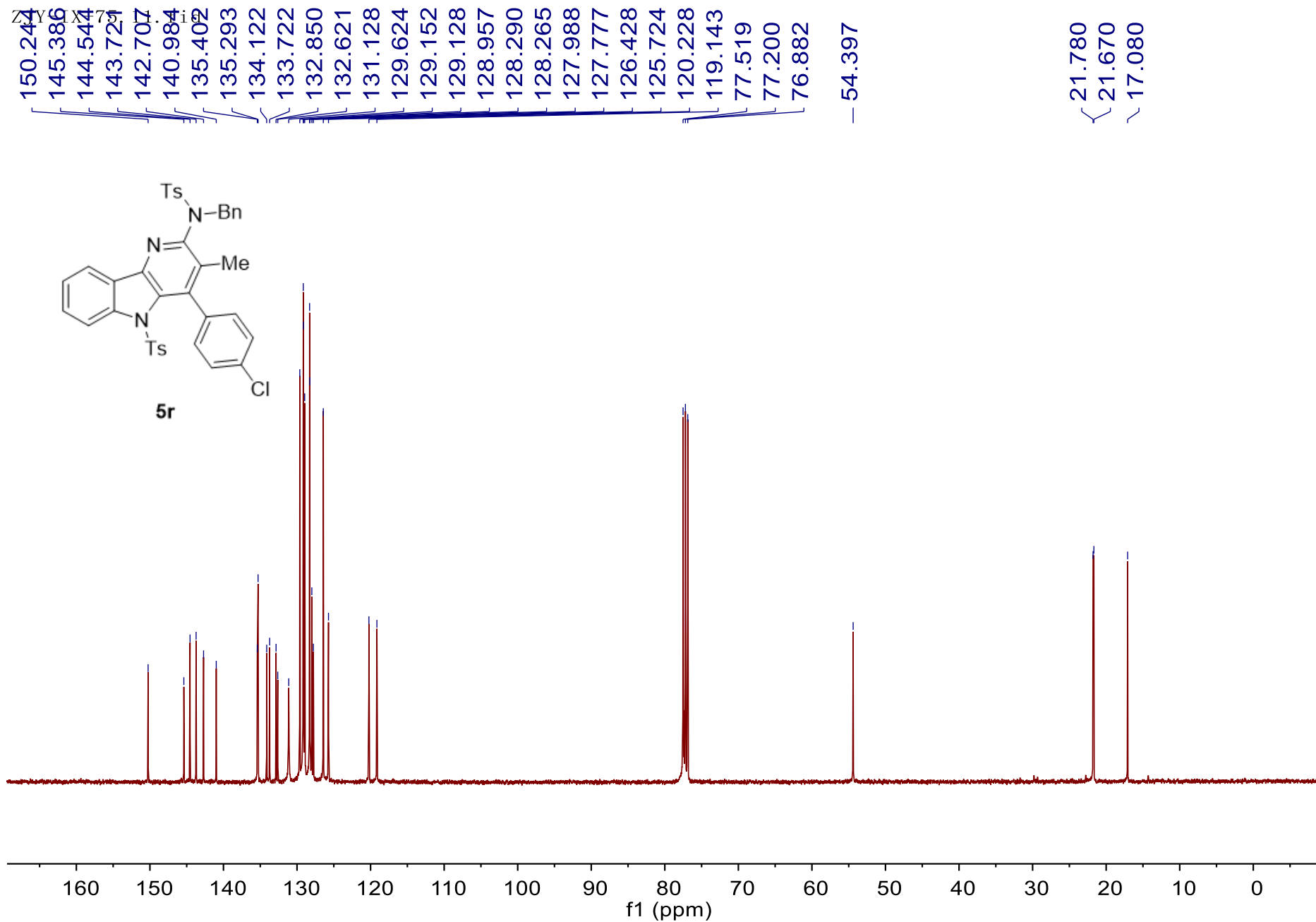


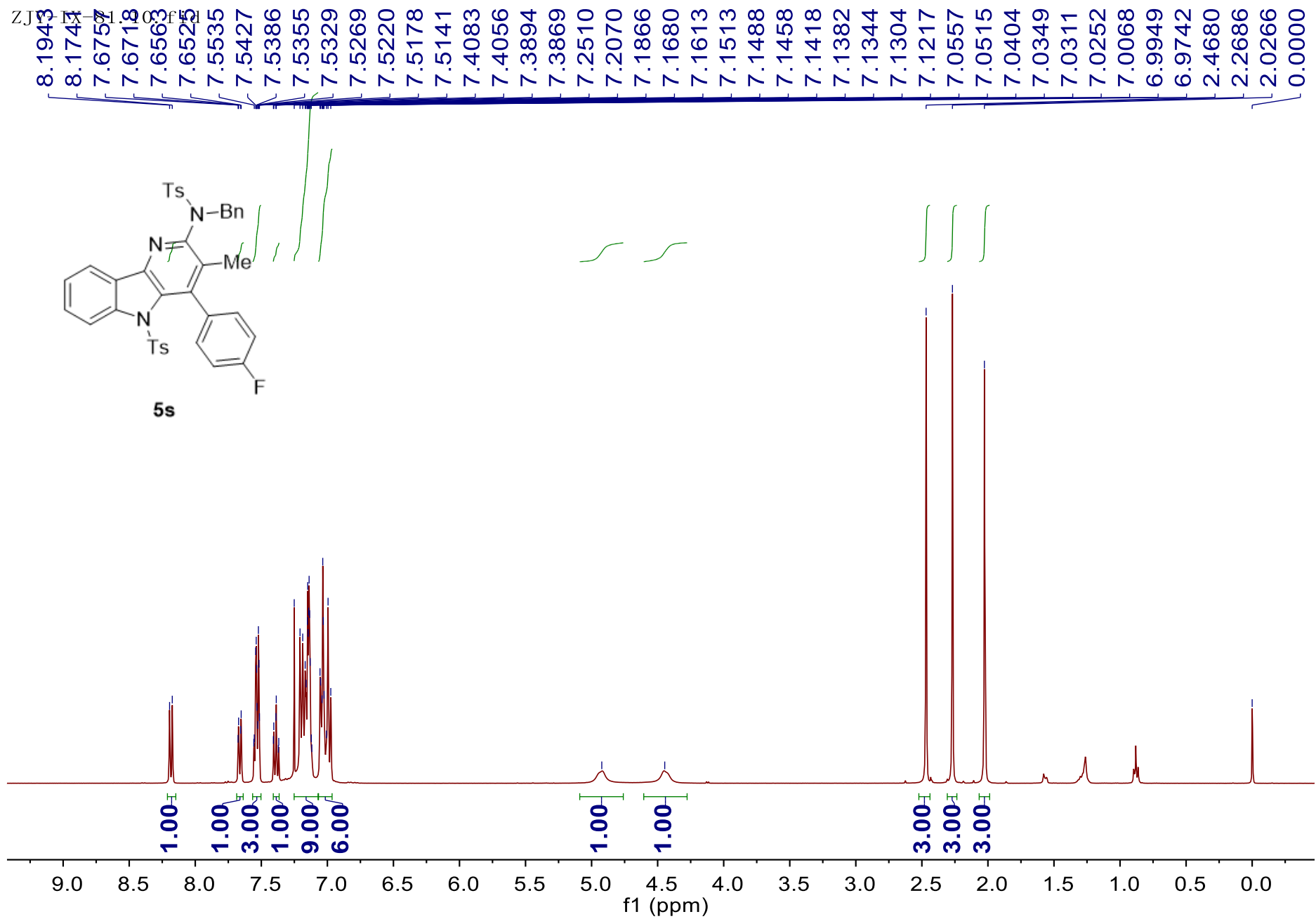
ZJY-15-84-11-11

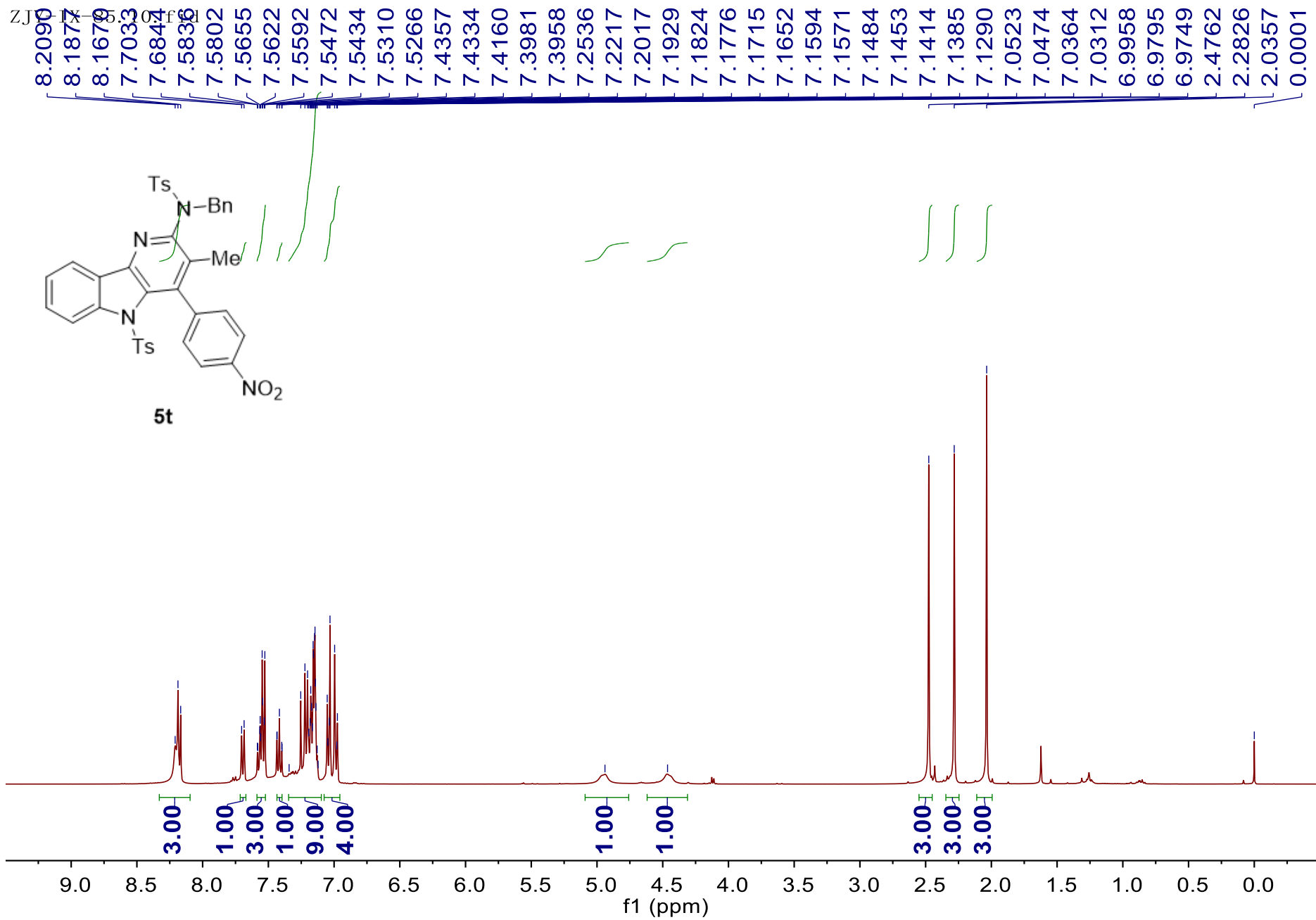


ZJY-IX-75.10 f1d





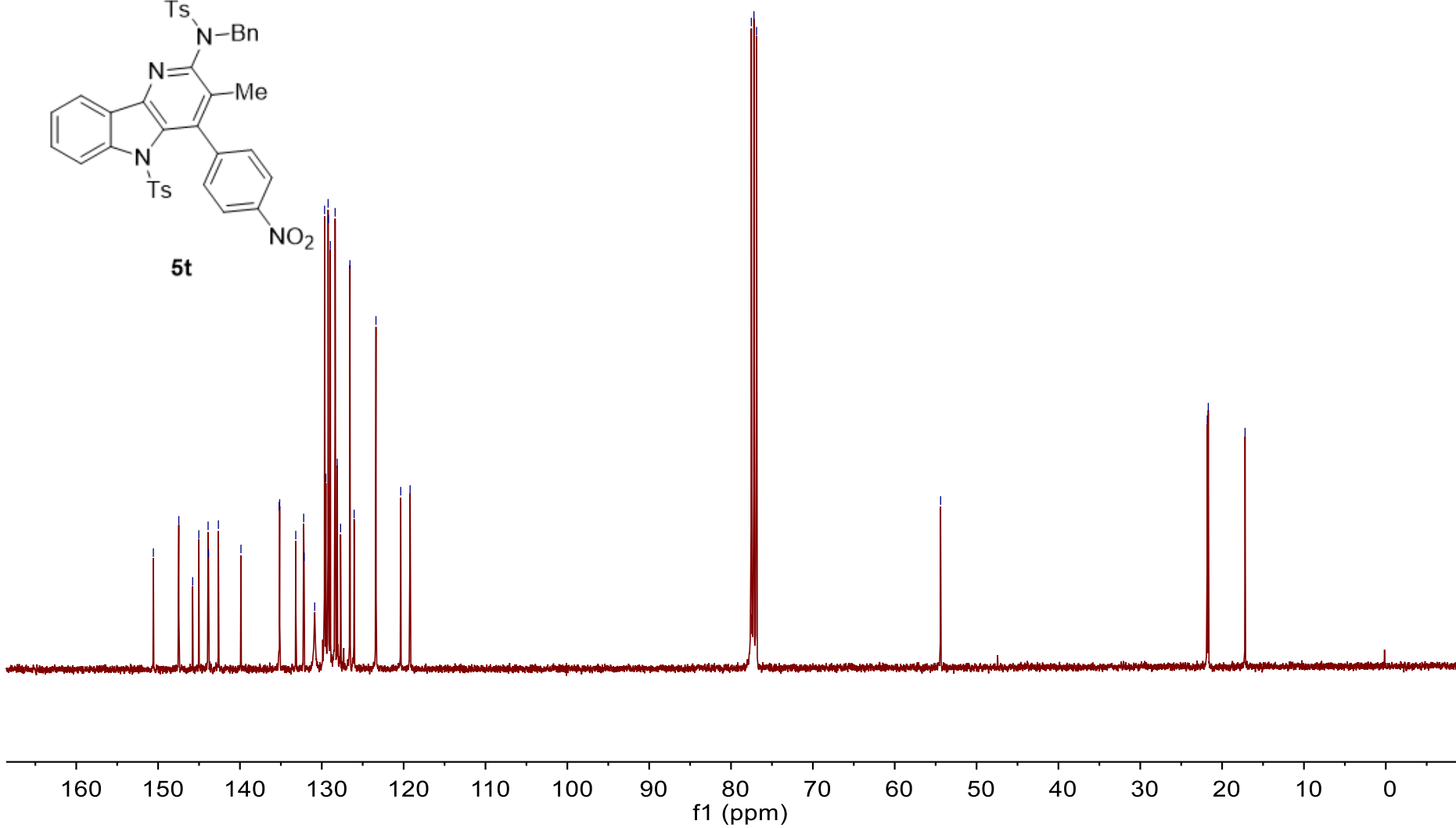
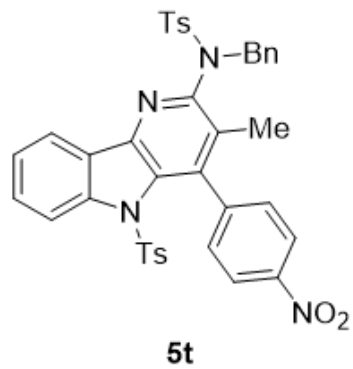




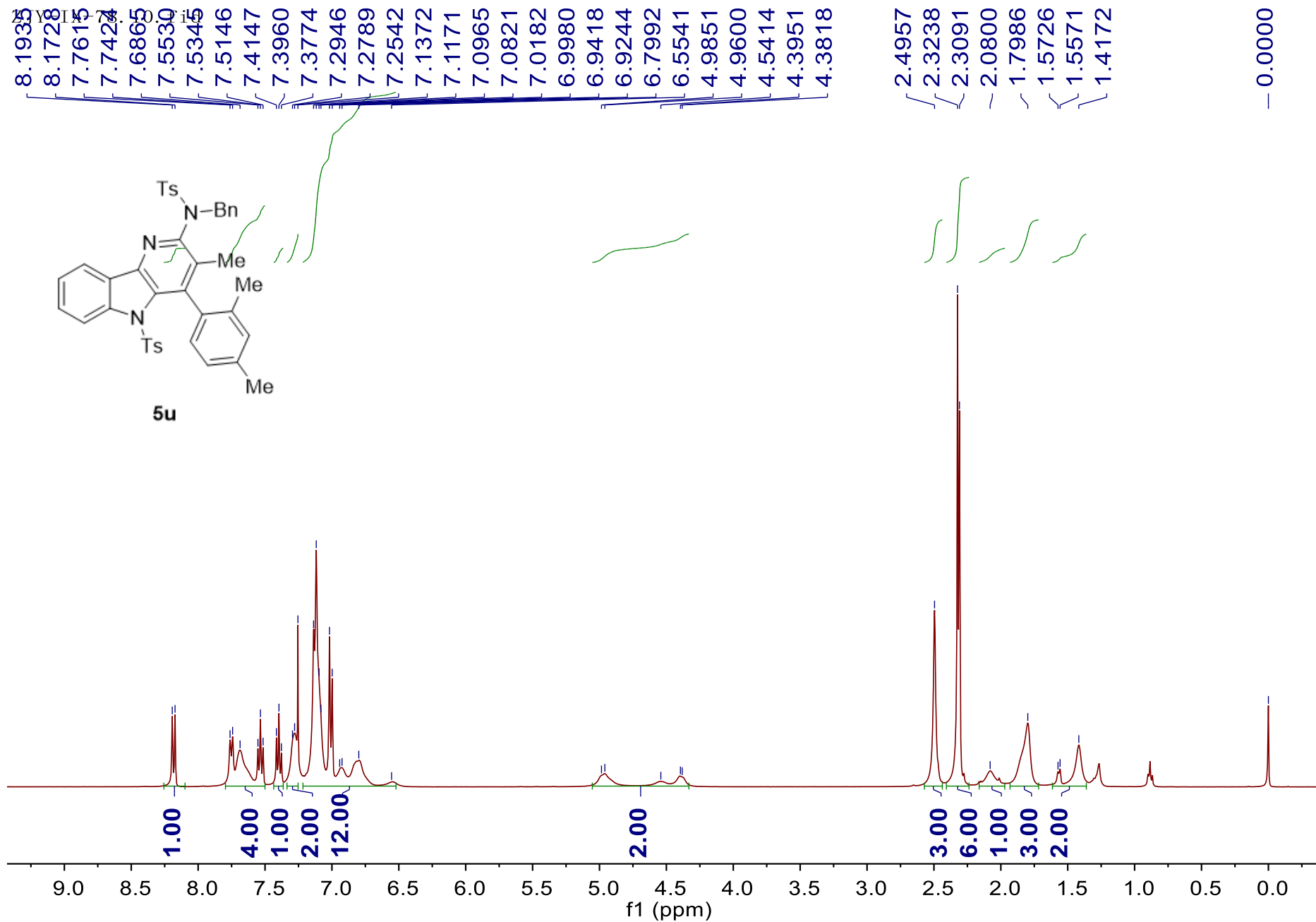
ZJY-EX-88-11c

150.578
147.470
145.778
145.023
143.891
143.844
142.634
139.874
135.211
135.147
133.181
132.212
132.163
130.867
129.660
129.505
129.226
129.194
128.960
128.370
128.108
127.706
126.559
126.049
123.379
120.354
119.211
77.518
77.200
76.882
54.396

21.814
21.687
17.196

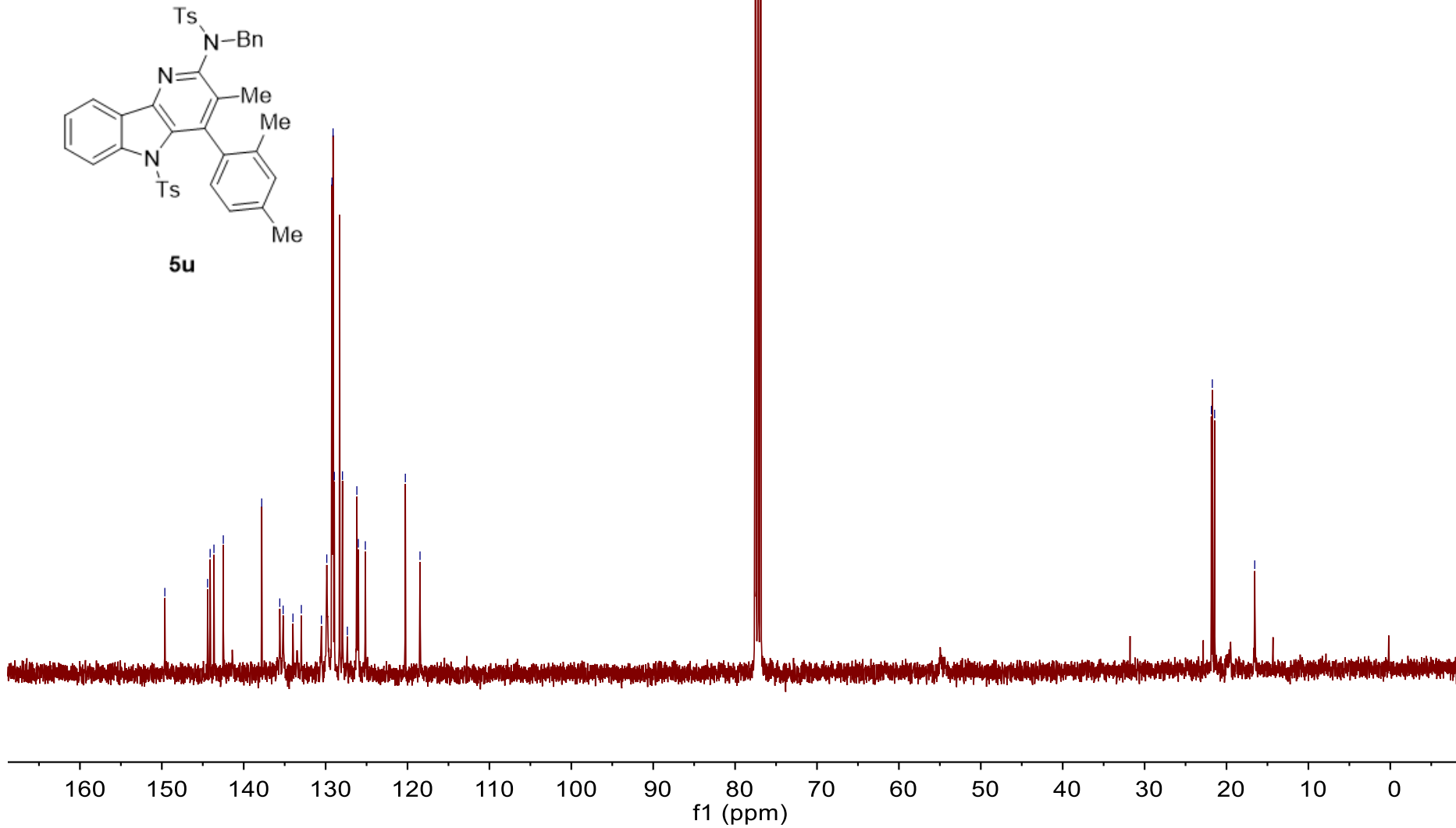
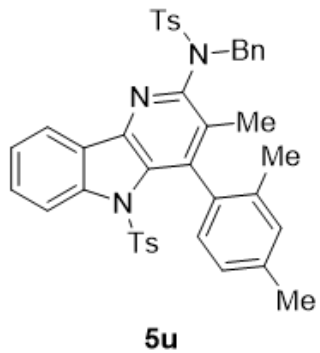


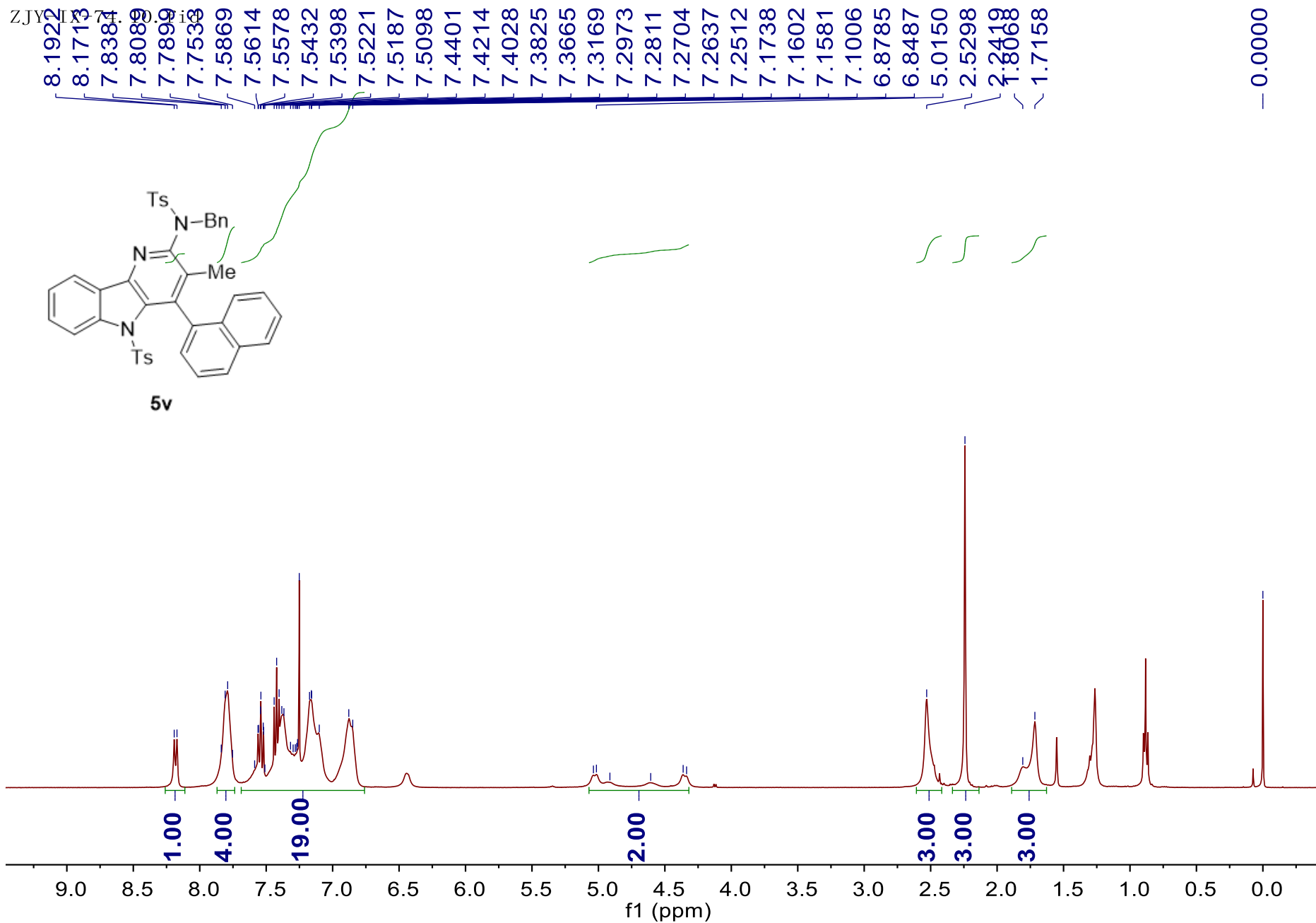
S160



149.632
144.409
144.101
143.635
142.495
137.802
135.593
135.189
133.990
132.966
130.515
129.856
129.226
129.092
128.937
127.941
127.344
126.186
126.010
125.152
120.266
118.474
77.518
77.200
76.883

21.848
21.731
21.450
16.554



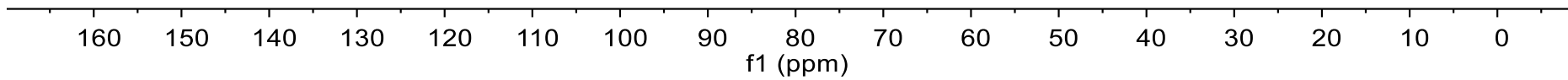
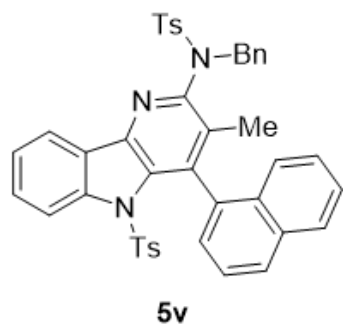


ZJY-IX-74.13

149.713
143.746
142.573
129.275
129.134
129.031
128.837
128.641
128.356
127.988

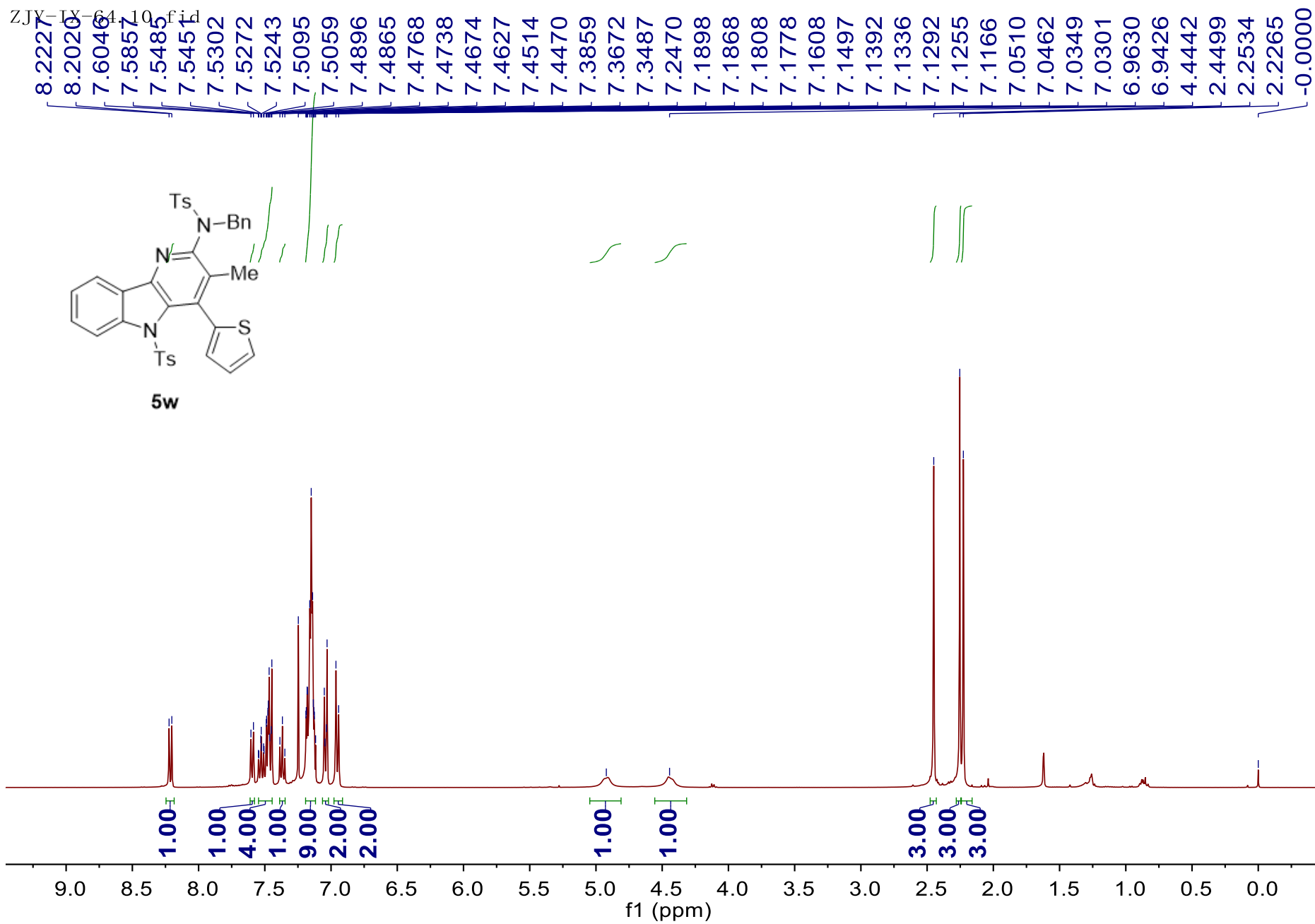
77.518
77.200
76.883

21.881
21.670

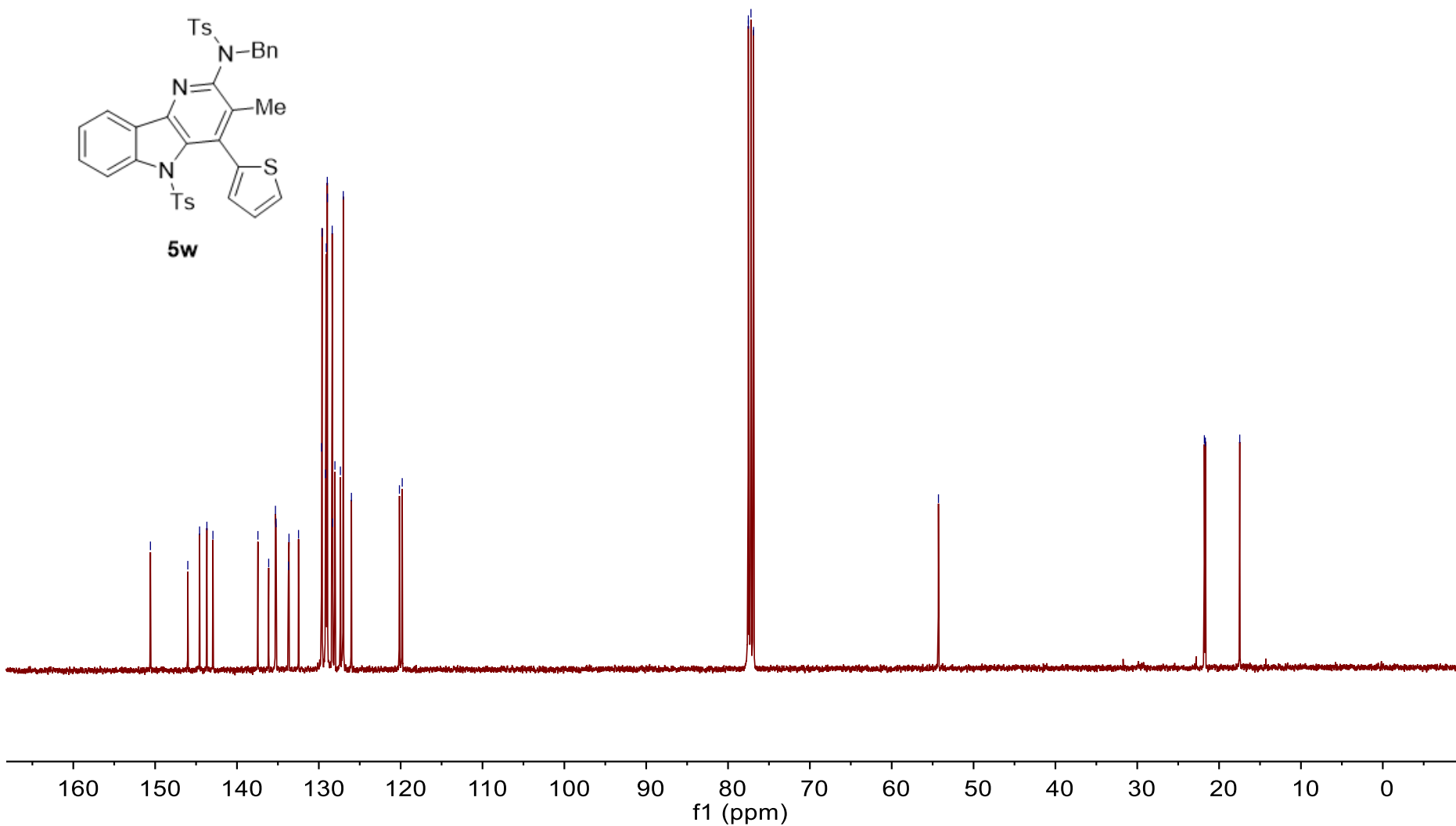
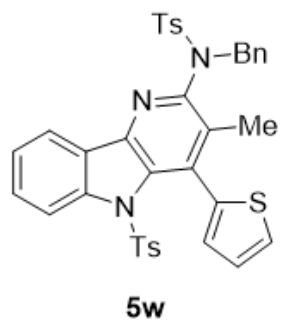


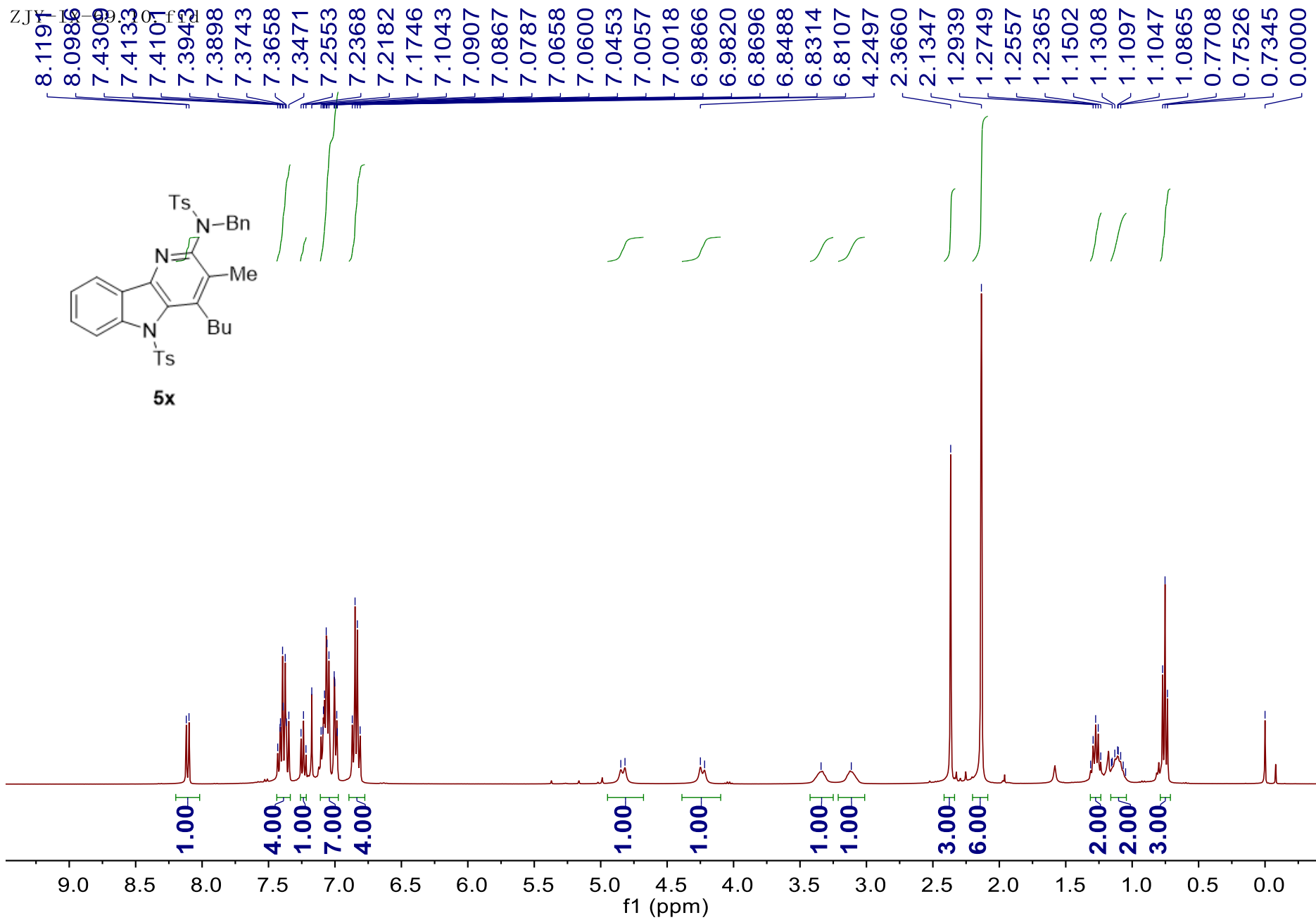
S164

ZJY-IX-64_10.fid

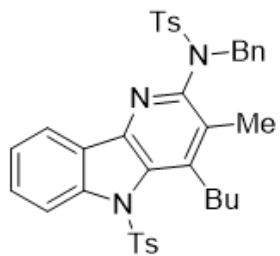


ZJY-LX669

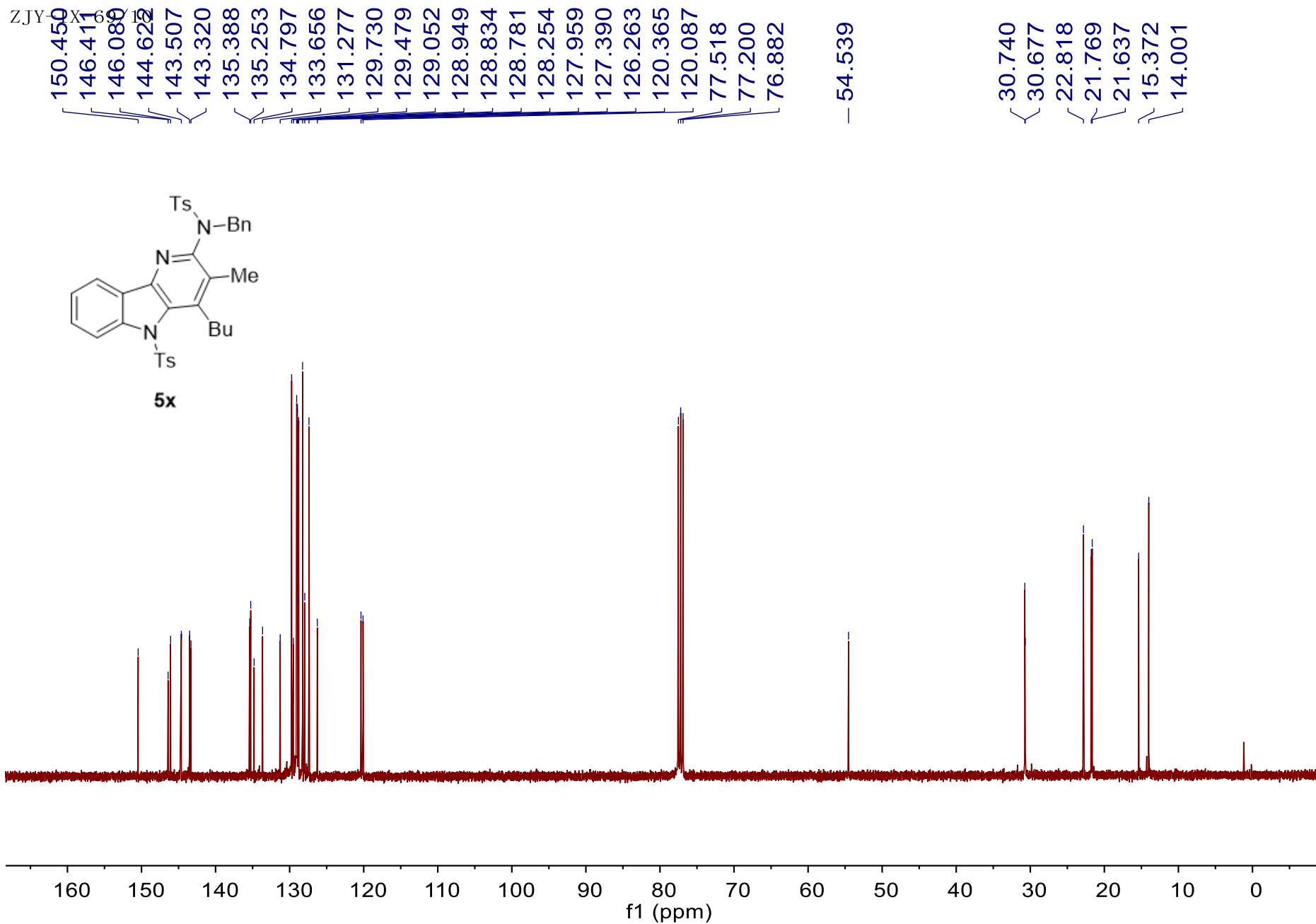




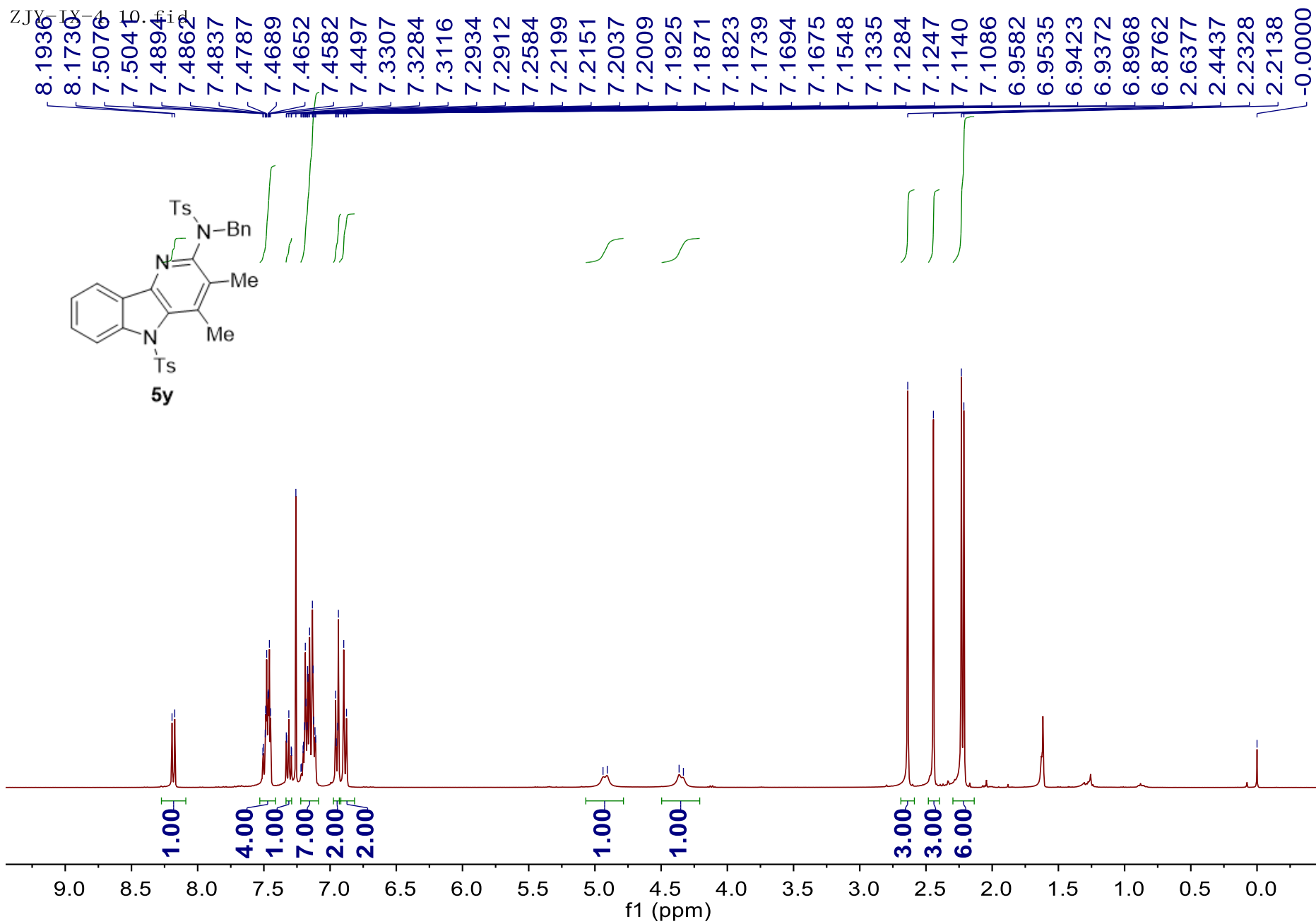
ZJY-6912



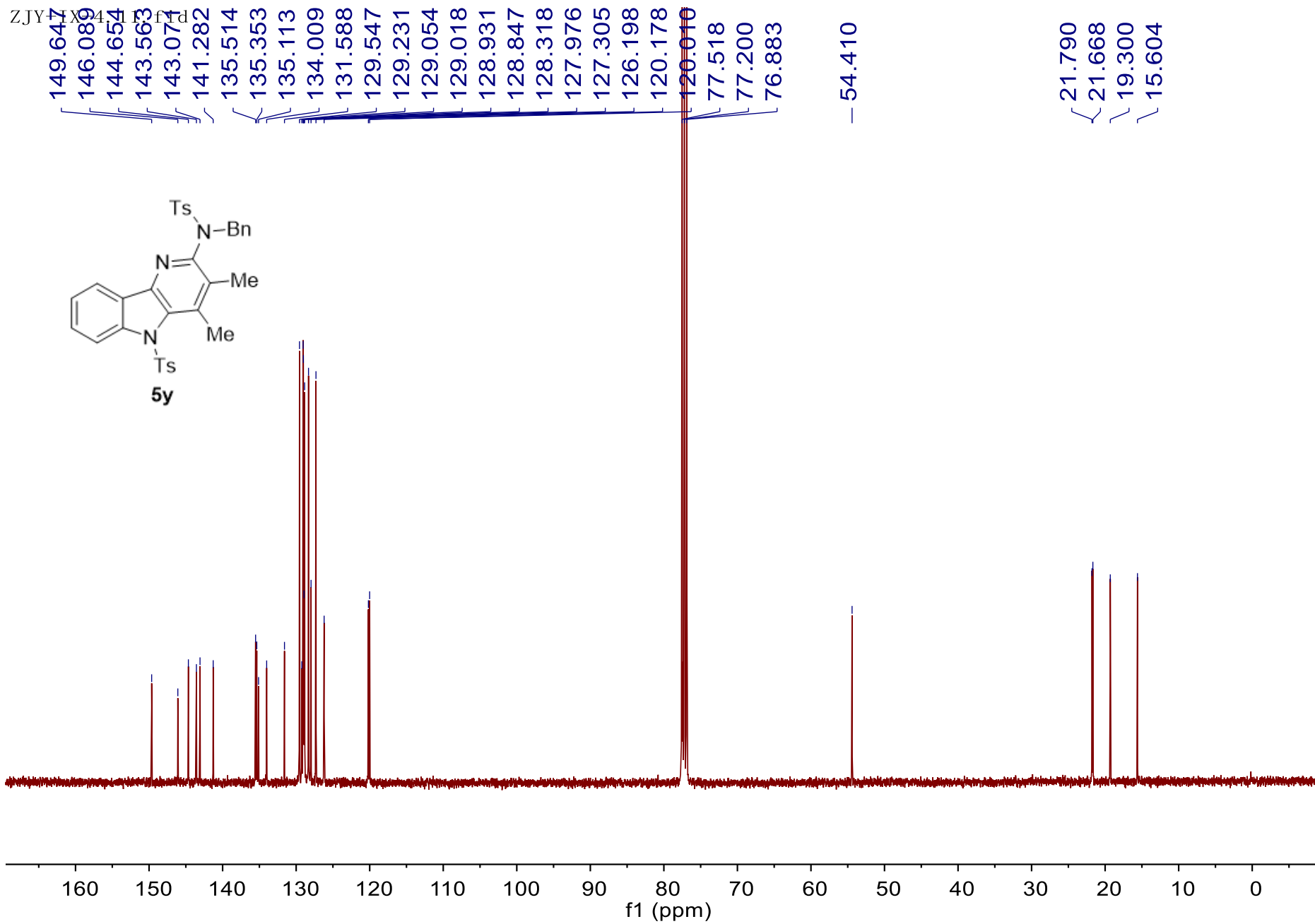
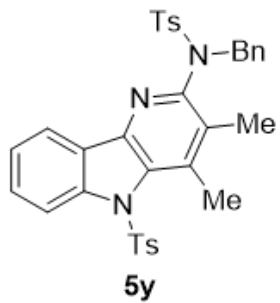
5x



ZJY-IX-4 10.fid

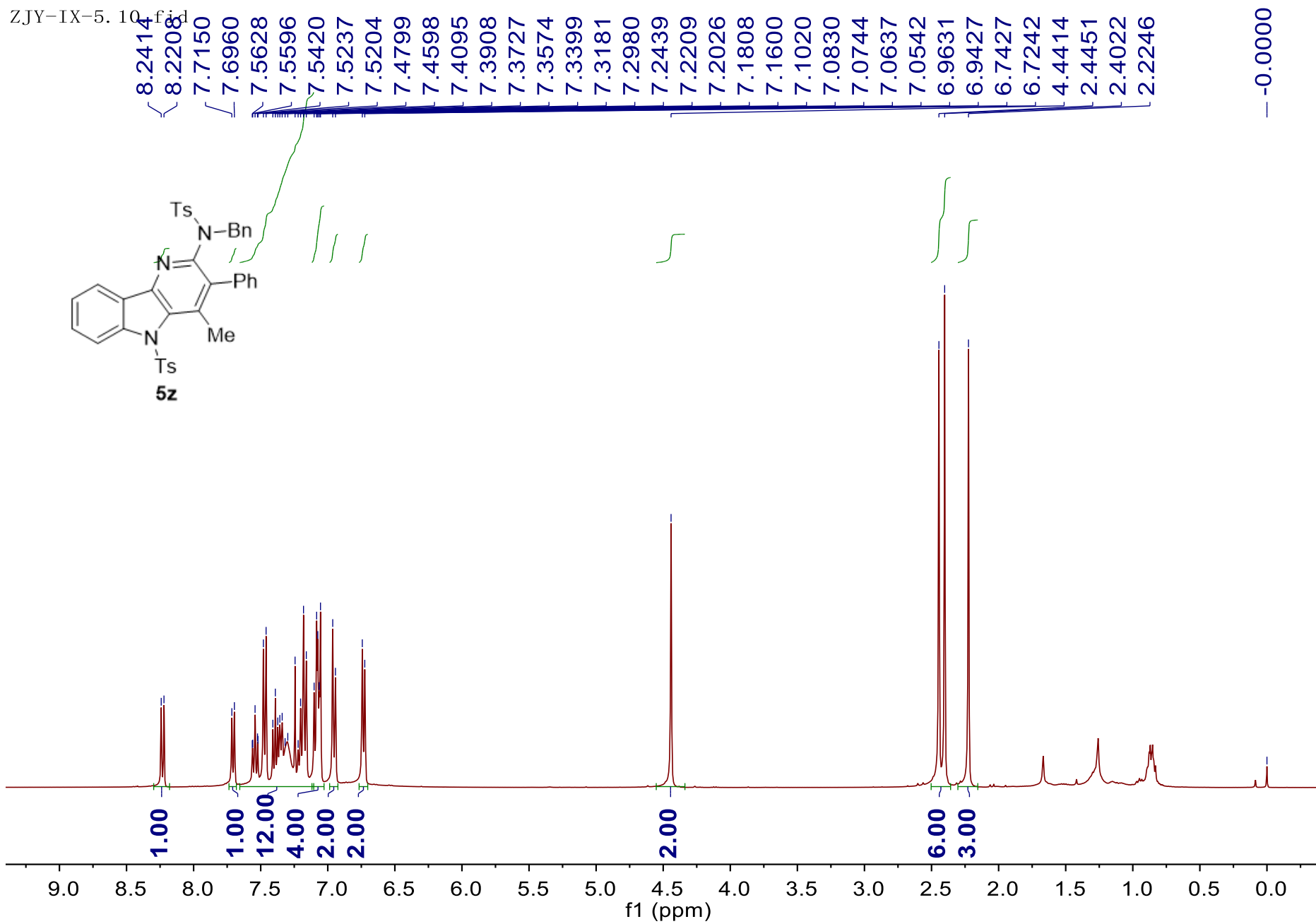


ZJY-EX411.f1d

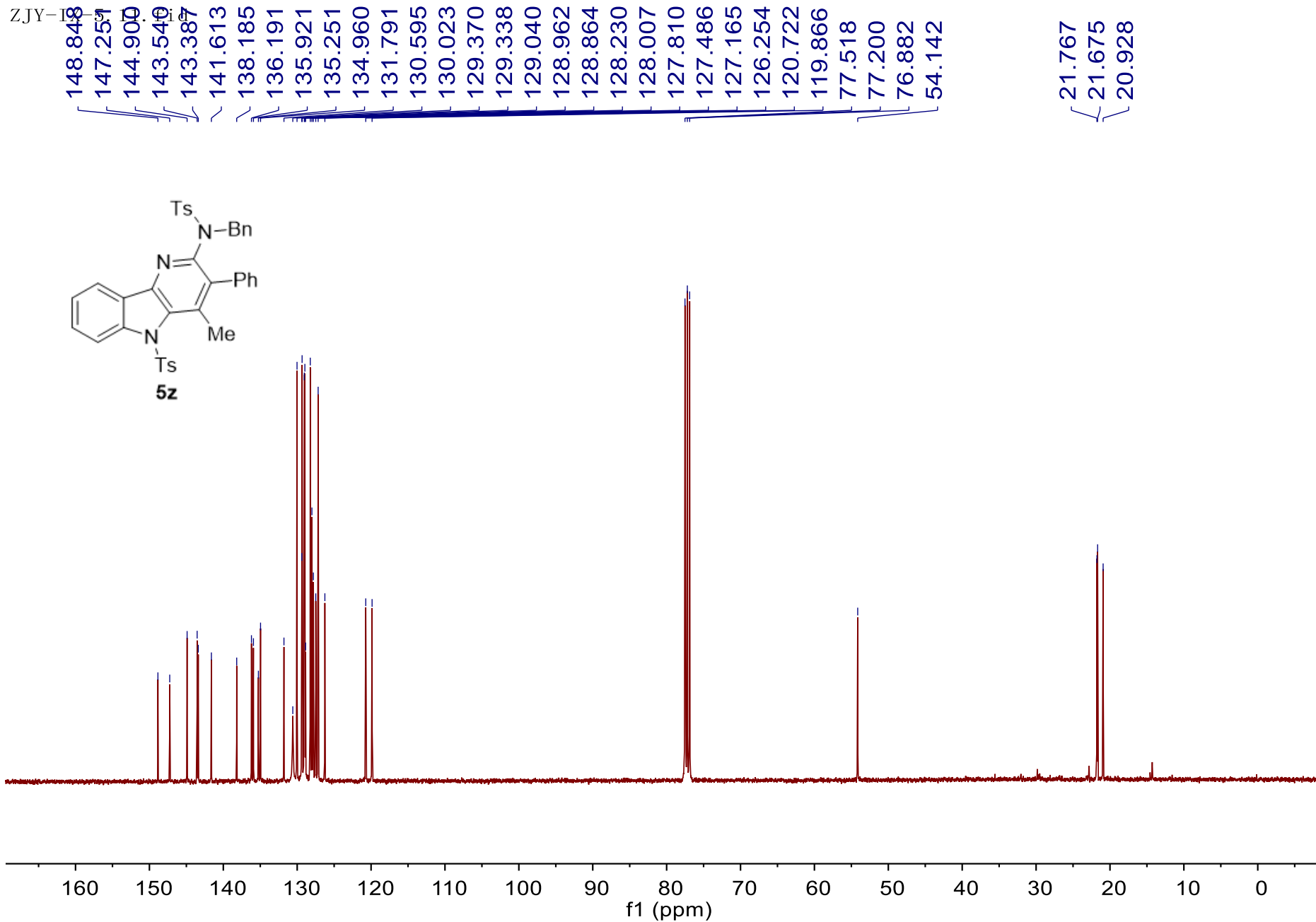
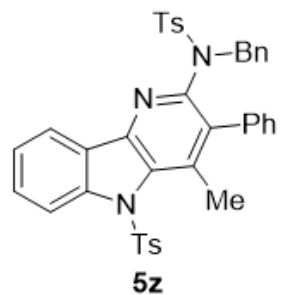


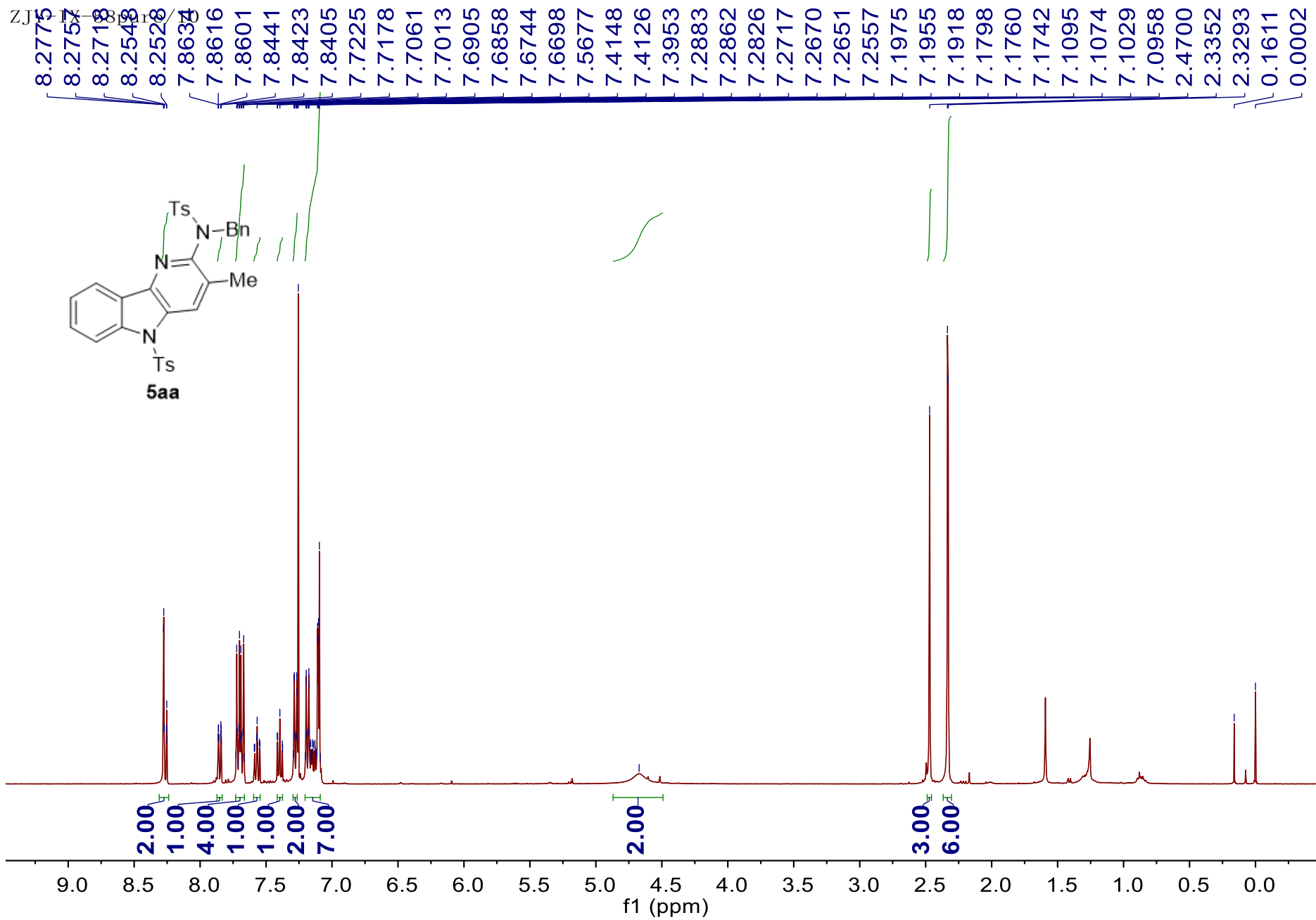
S170

ZJY-IX-5.10.fid

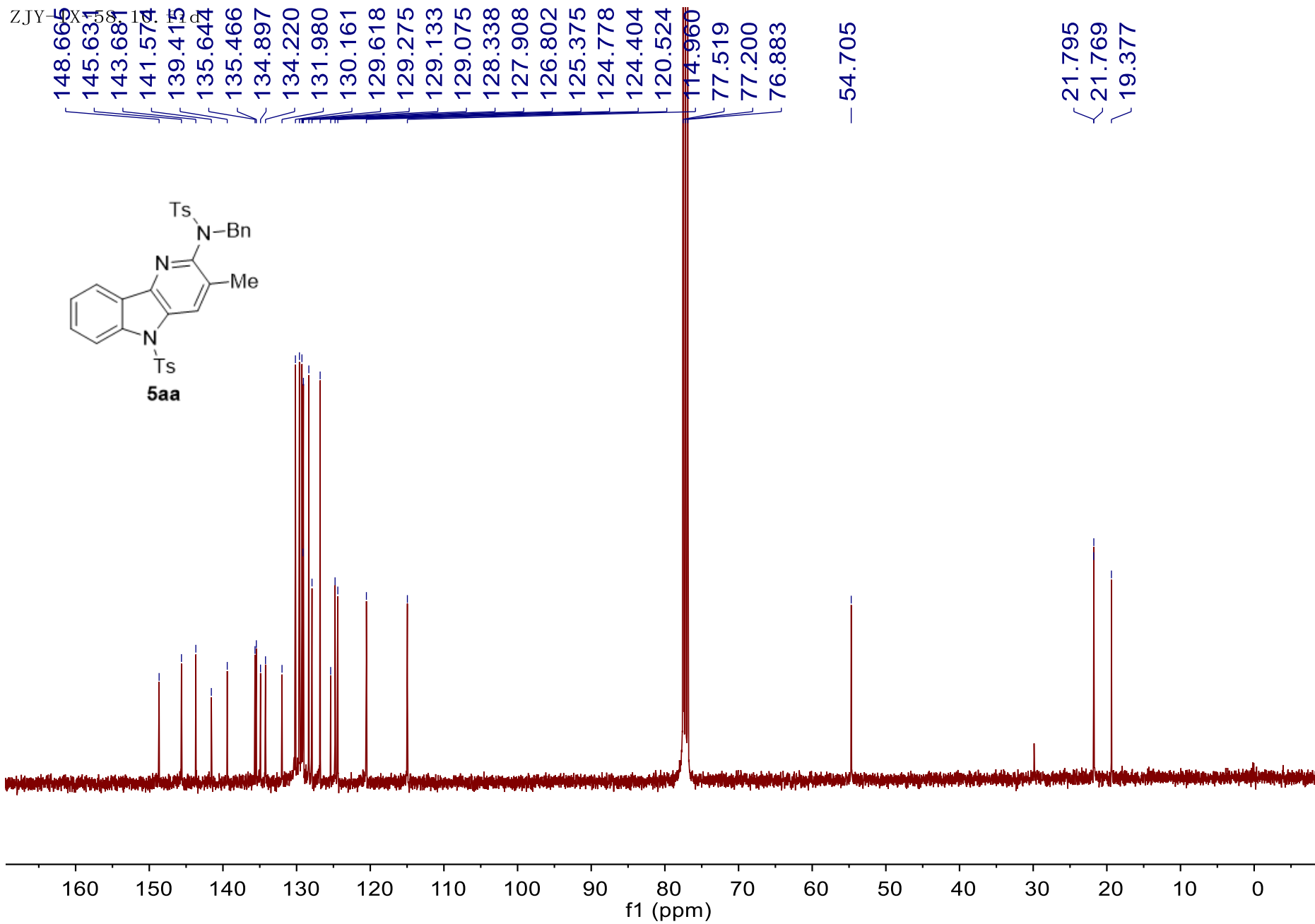
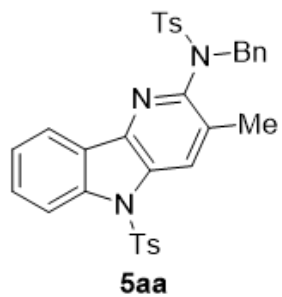


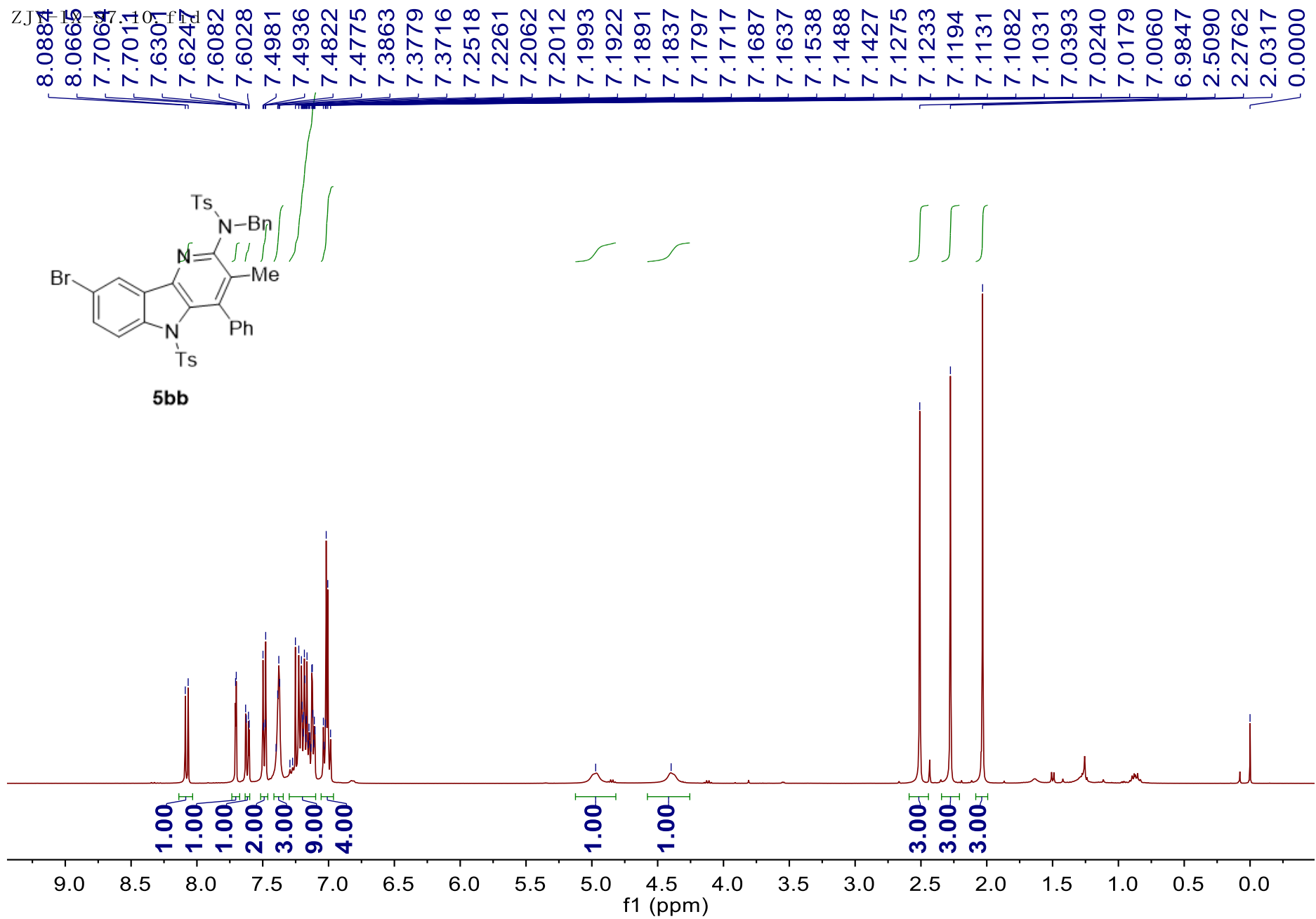
ZJY-19

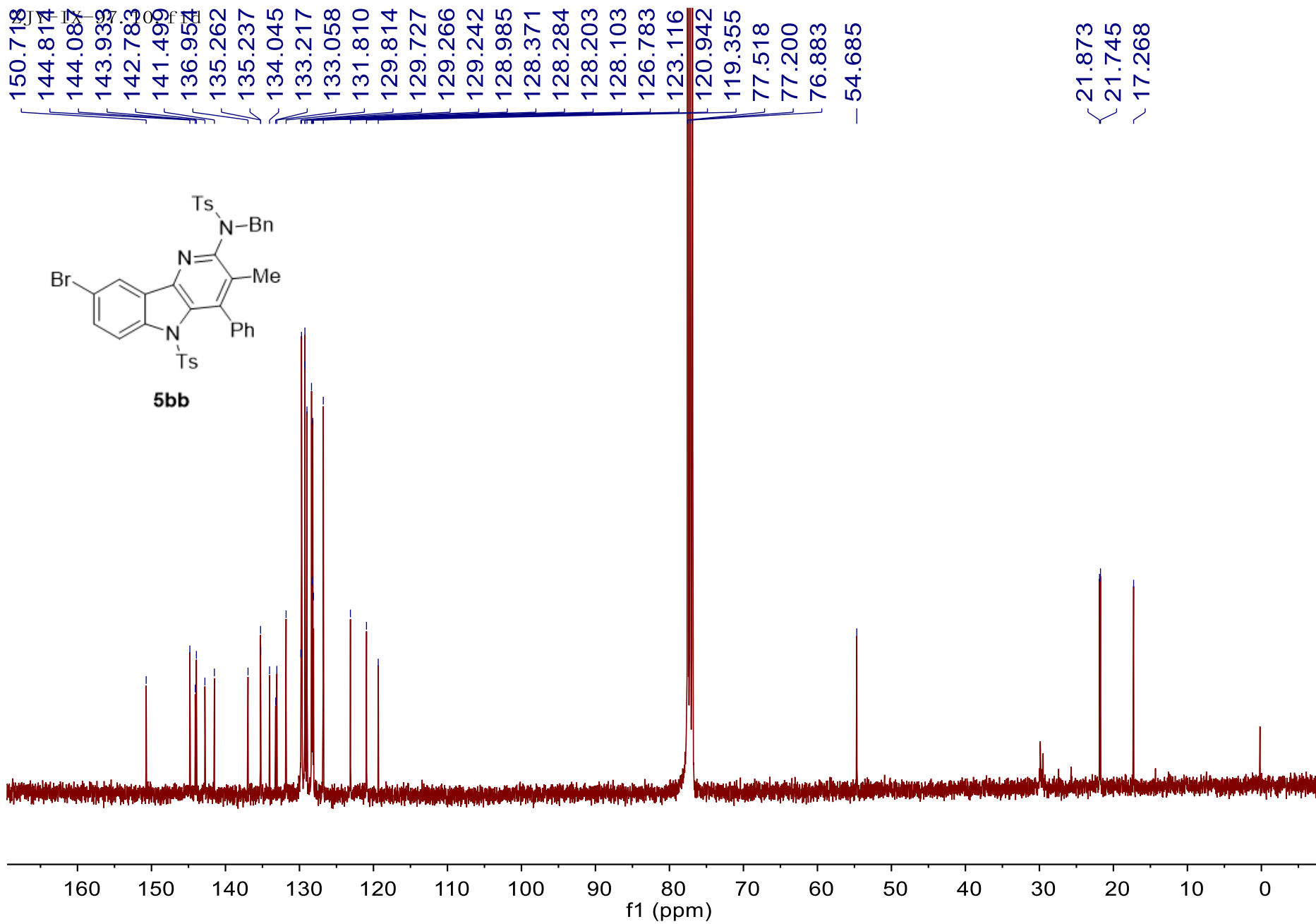


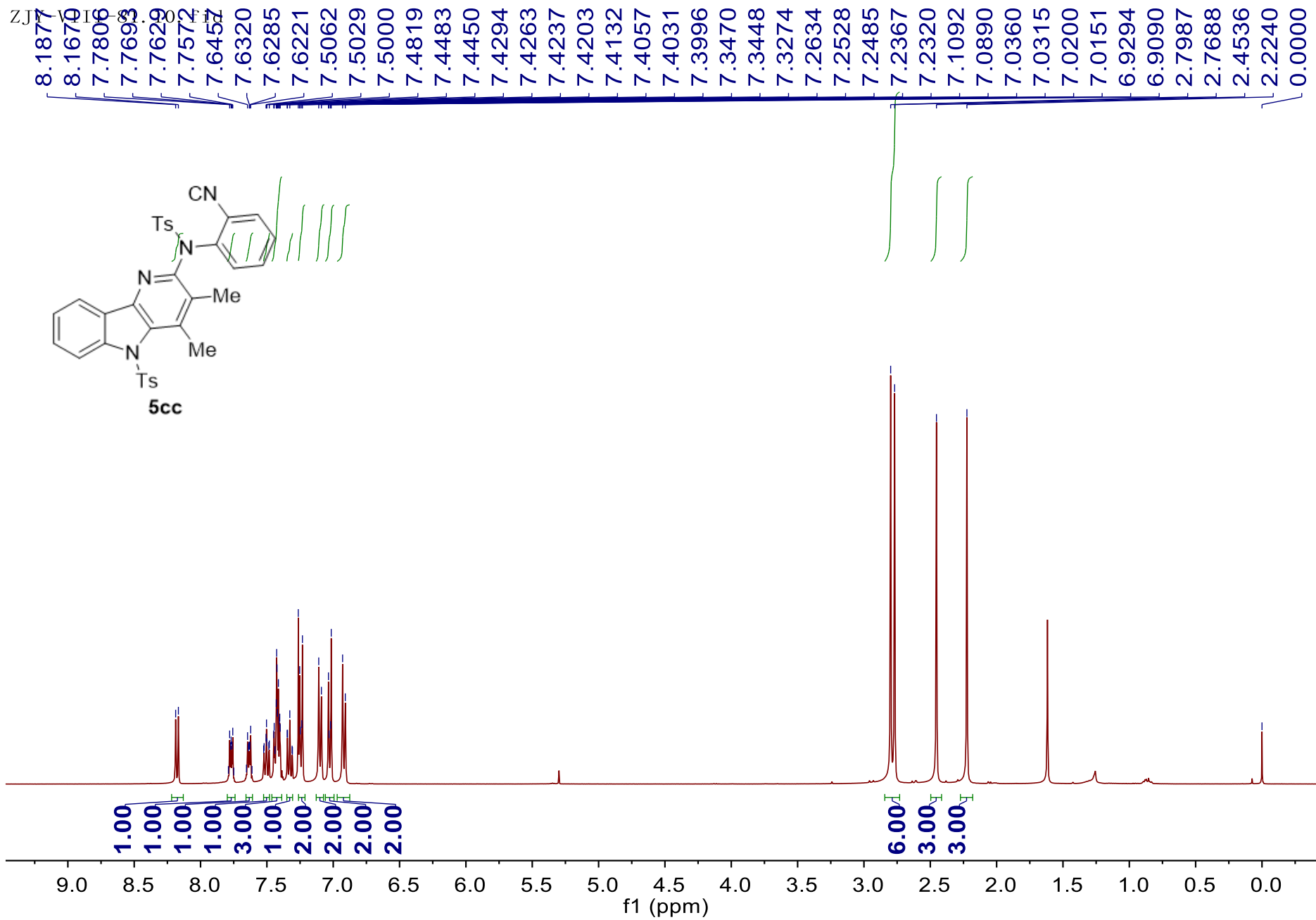


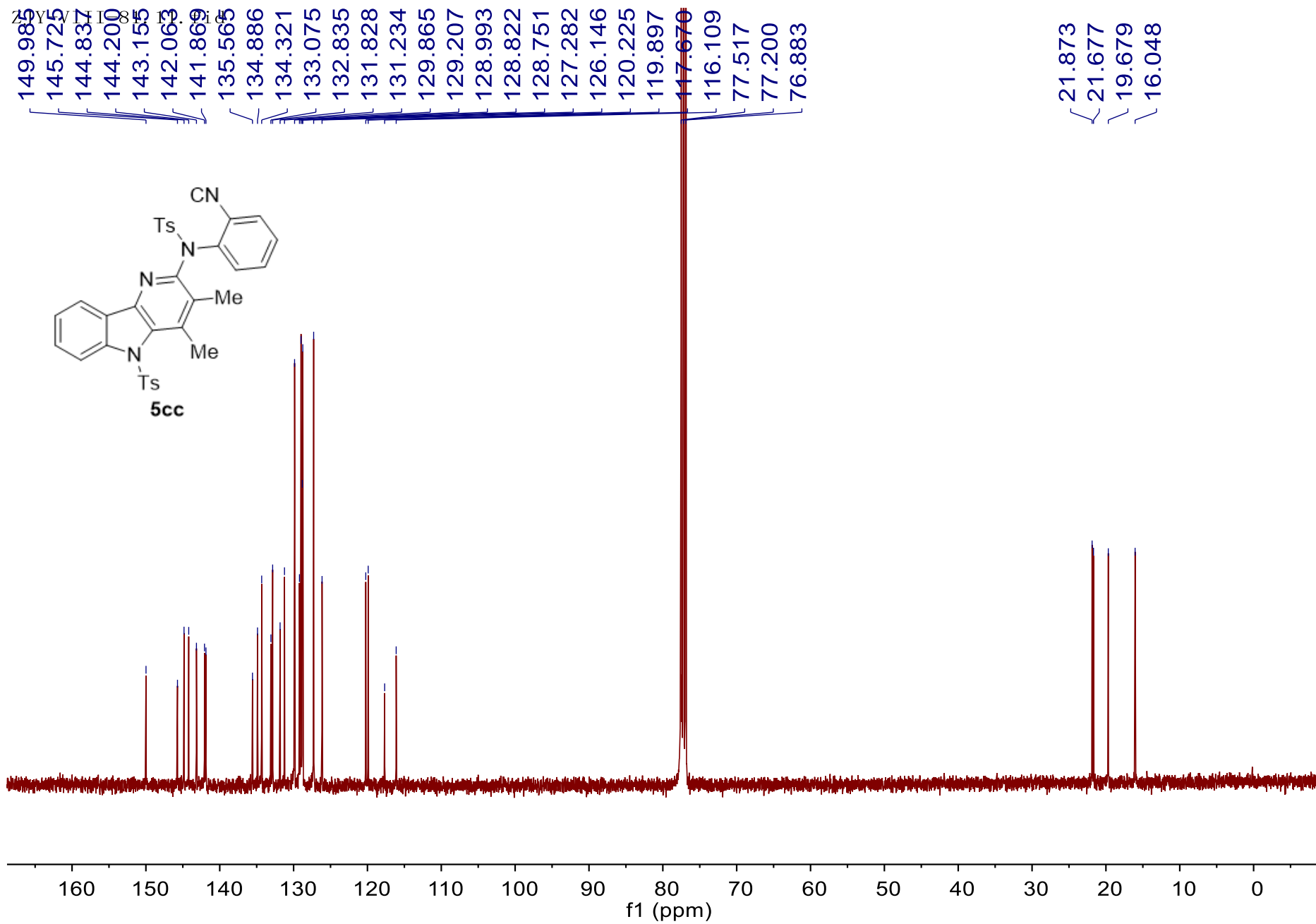
ZJY-X-58-1-14d



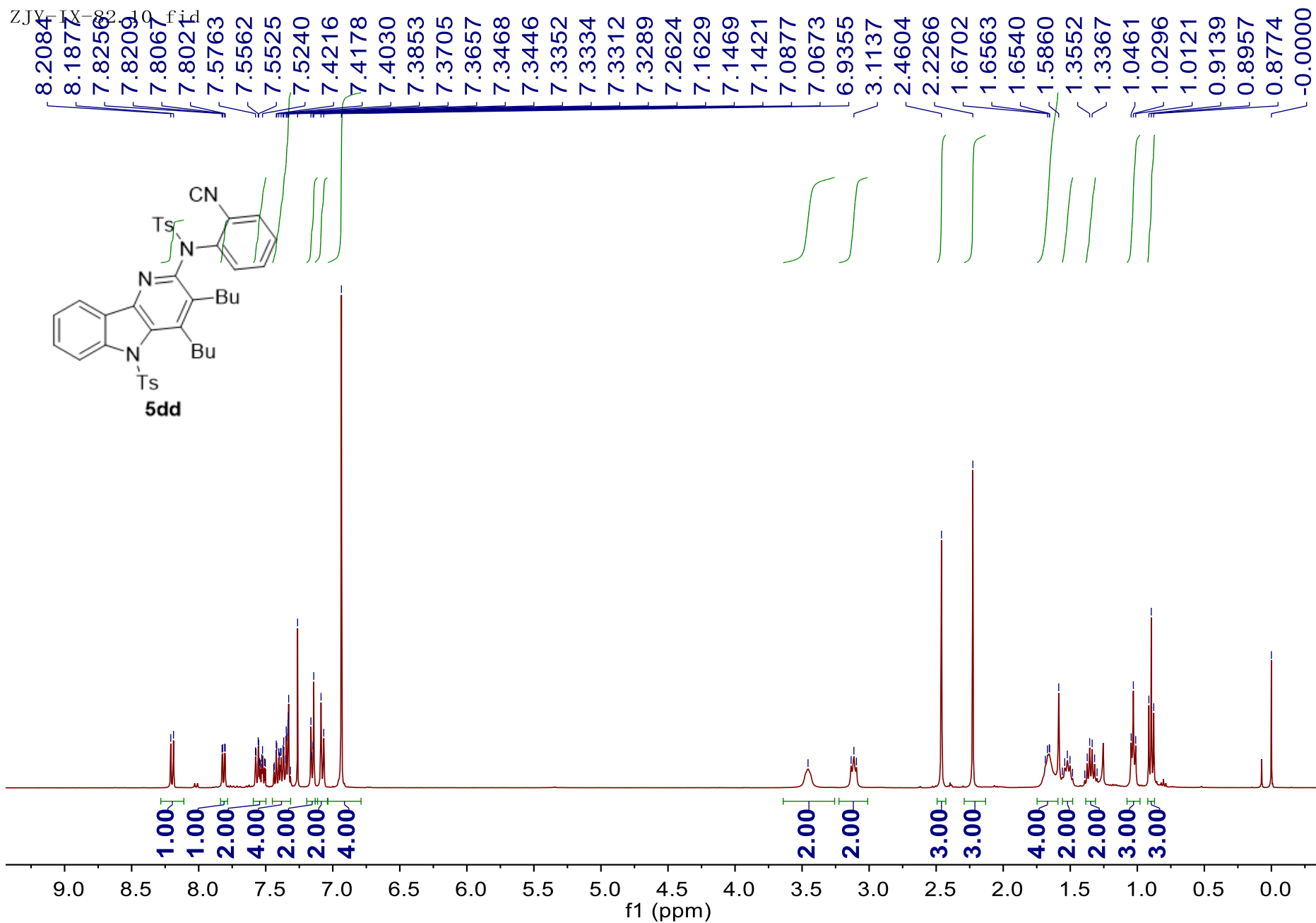


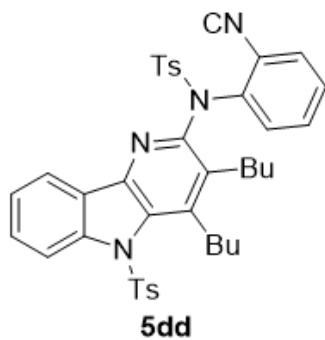
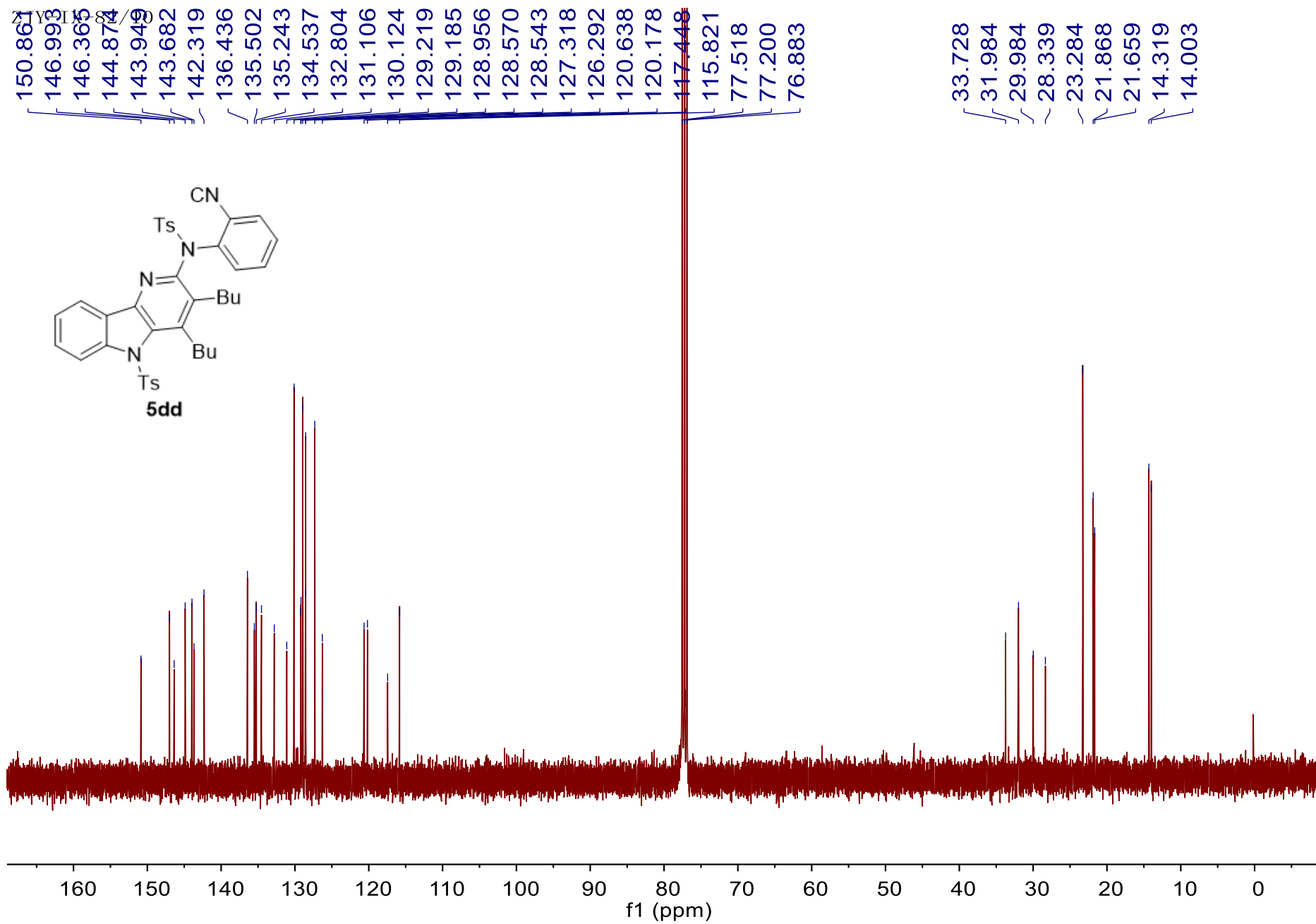






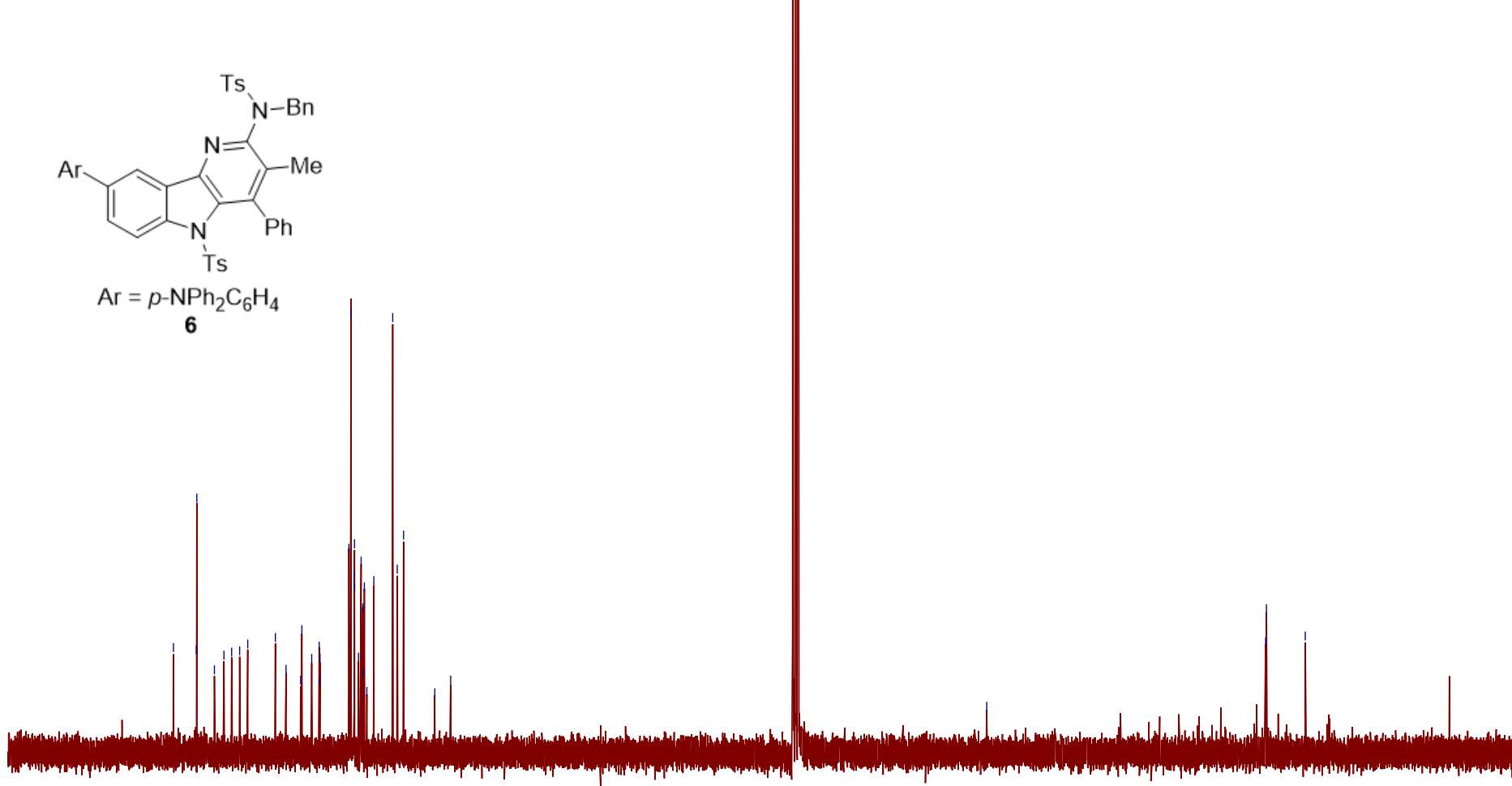
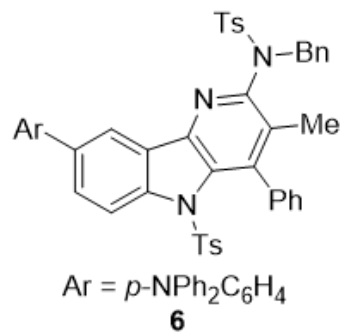
ZJY-IX-82-10.fid





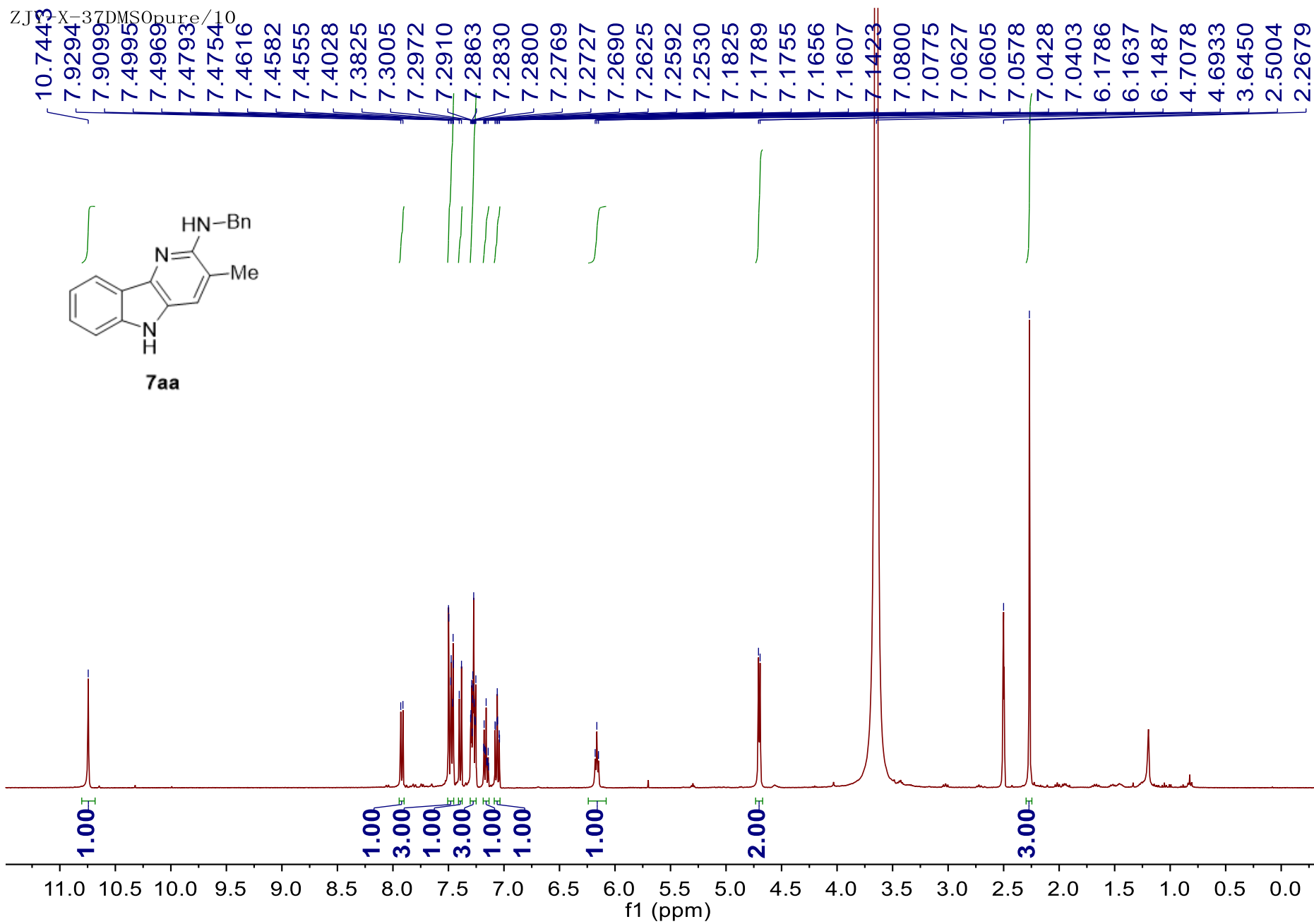
S180

150.451
 147.760
 147.699
 145.628
 144.505
 143.597
 142.654
 141.702
 138.447
 137.194
 135.470
 135.330
 134.171
 133.285
 133.227
 133.191
 129.791
 129.535
 129.164
 129.129
 129.117
 128.659
 128.349
 128.146
 128.087
 127.968
 127.677
 126.855
 124.628
 124.095
 123.352
 119.680
 117.806
 77.517
 77.200
 76.882
 54.676
 21.832
 21.733
 17.163

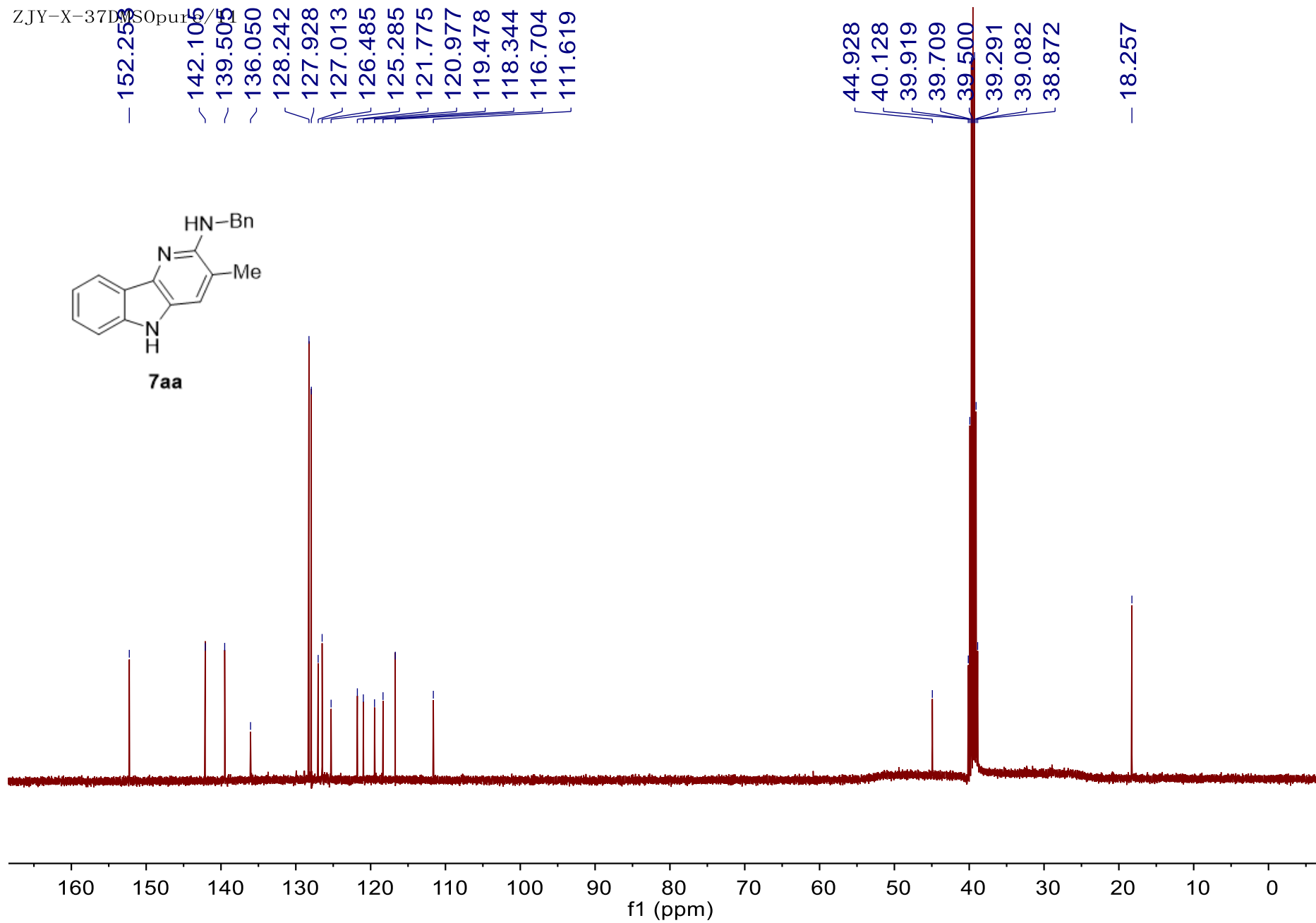
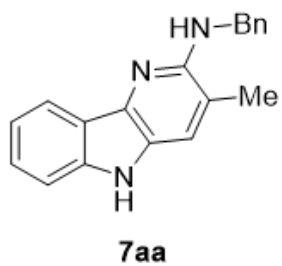


160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
 f1 (ppm)

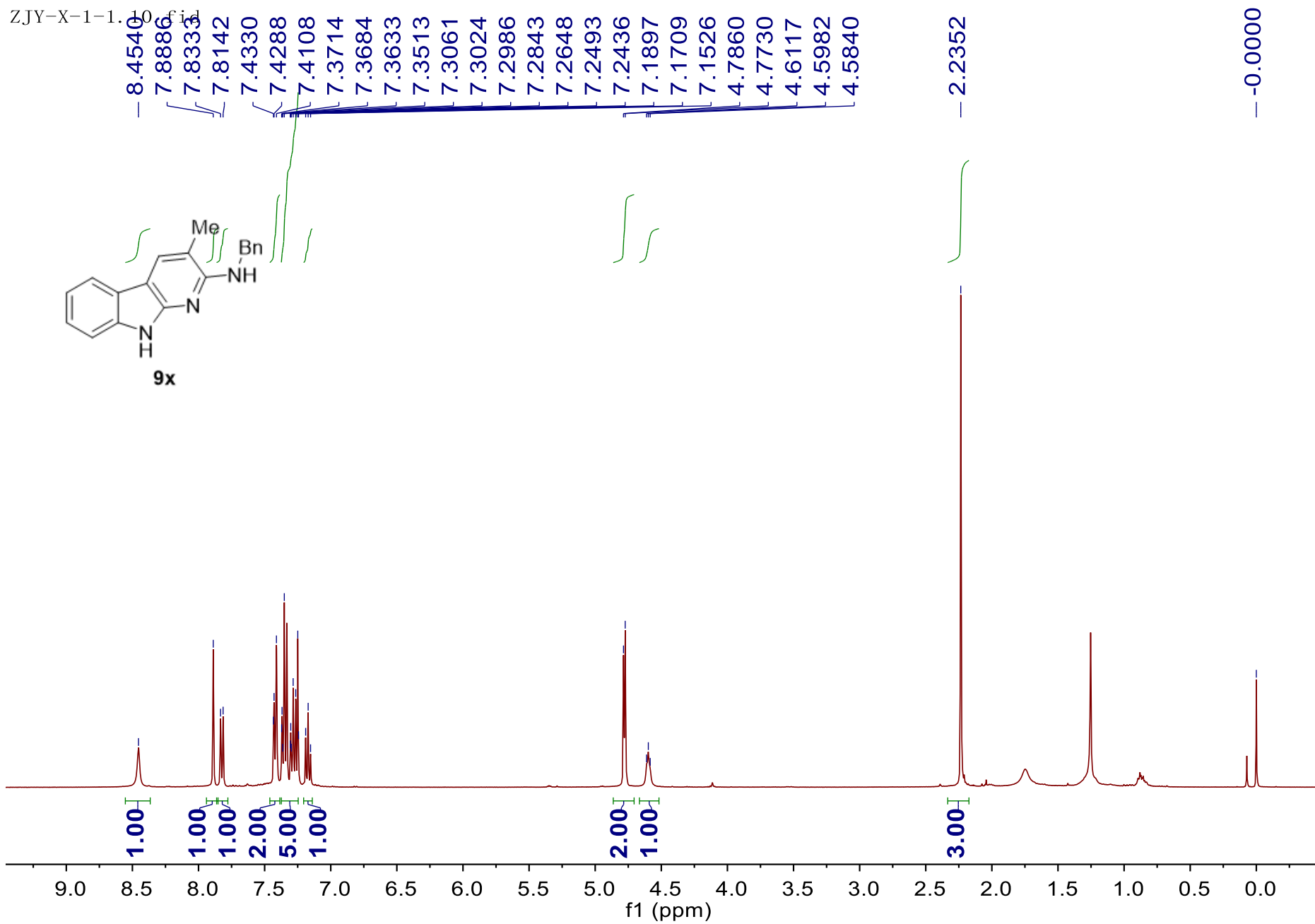
ZJ-X-37DMSO pure/10



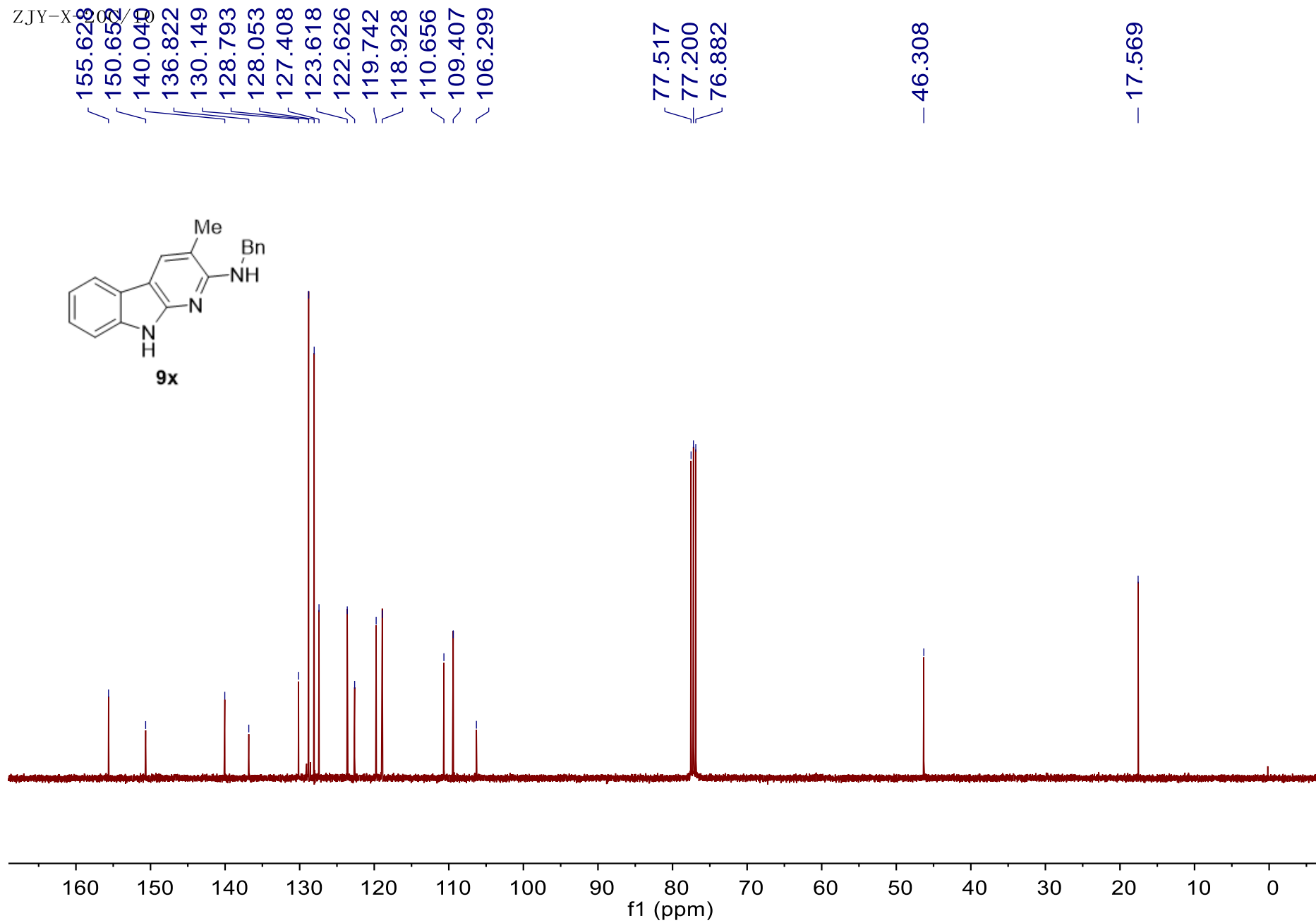
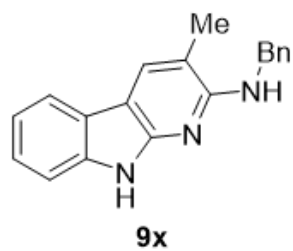
ZJY-X-37DMSOpur

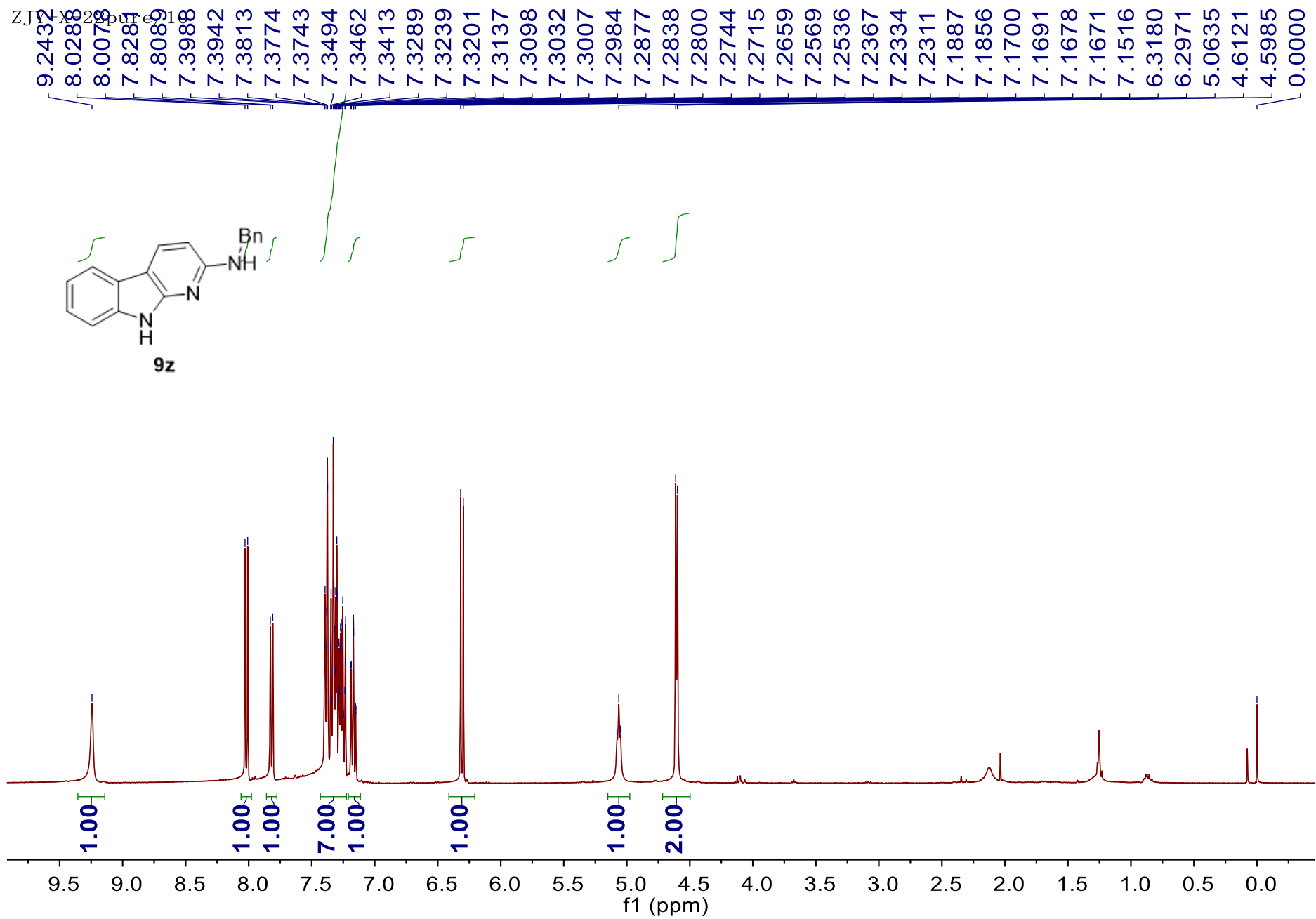


ZJY-X-1-1-10.fid

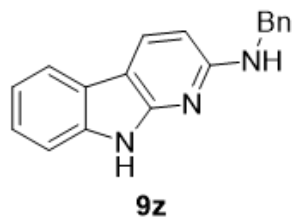


ZJY-X-102





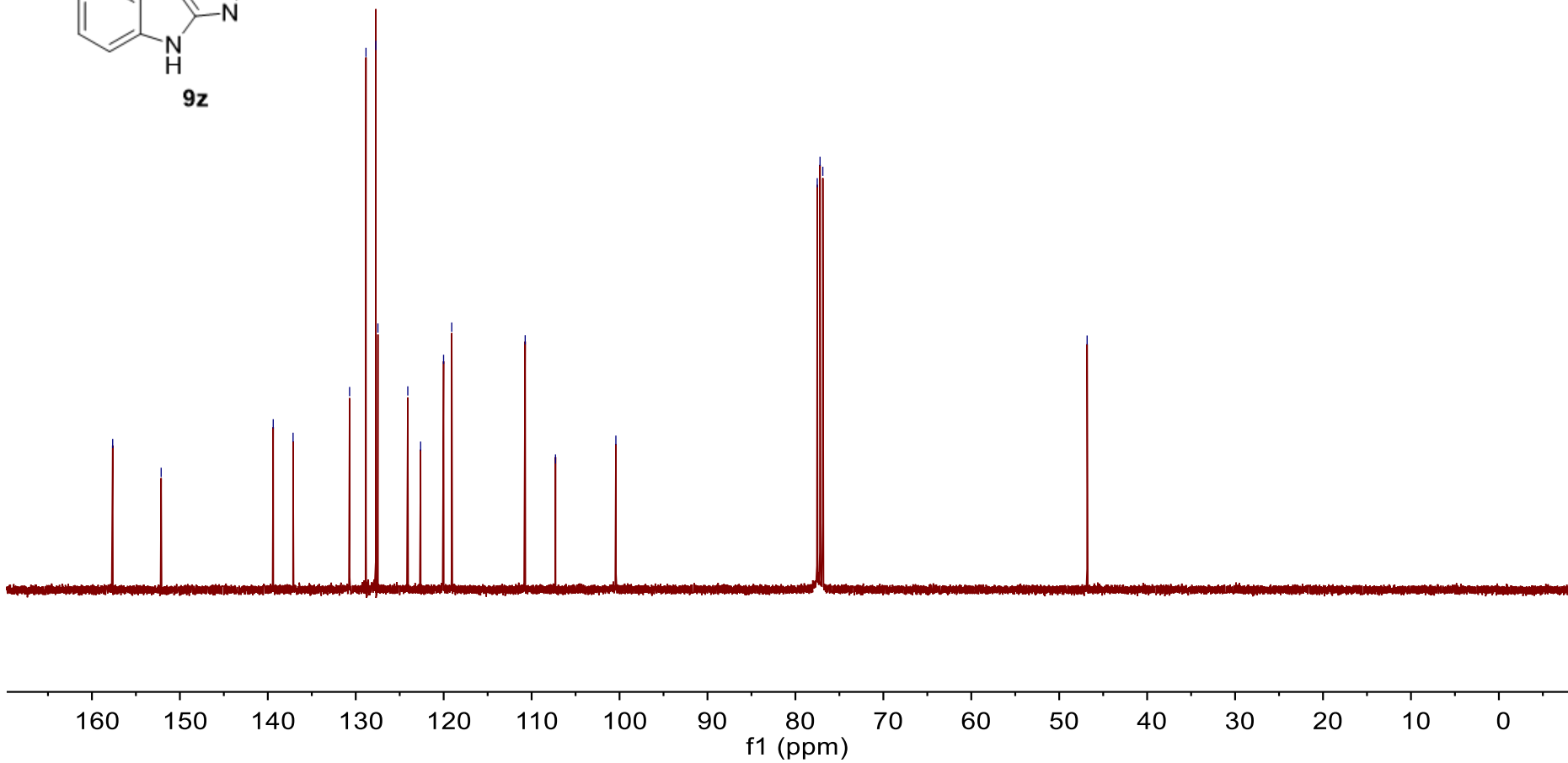
ZJY-X-2 pure 1



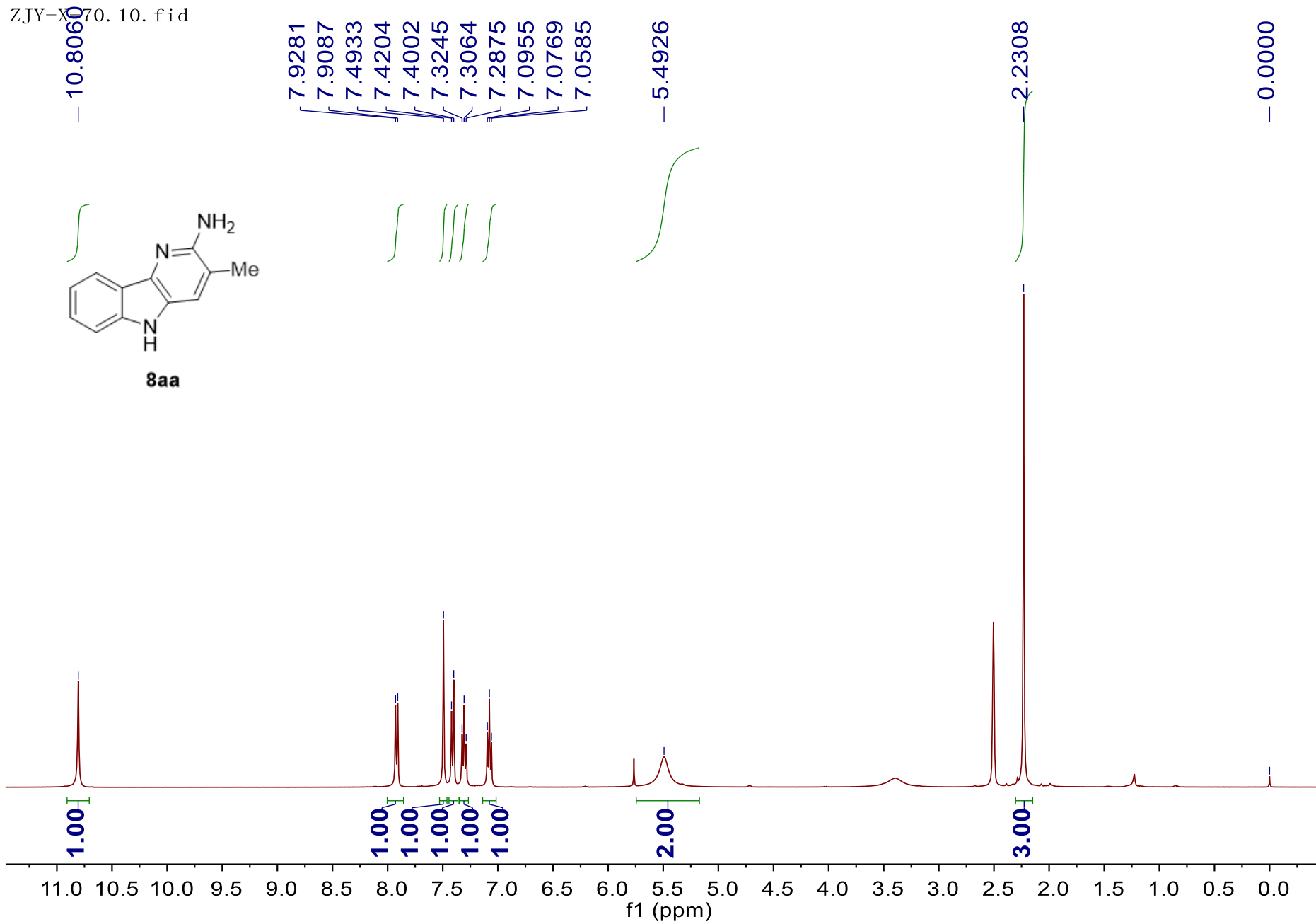
157.649
152.128
139.384
137.128
130.697
128.835
127.717
127.479
124.081
122.623
120.009
119.084
110.728
107.281
100.416

77.517
77.200
76.882

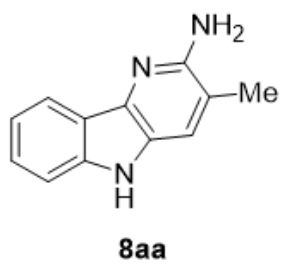
46.827



ZJY-X070.10.fid



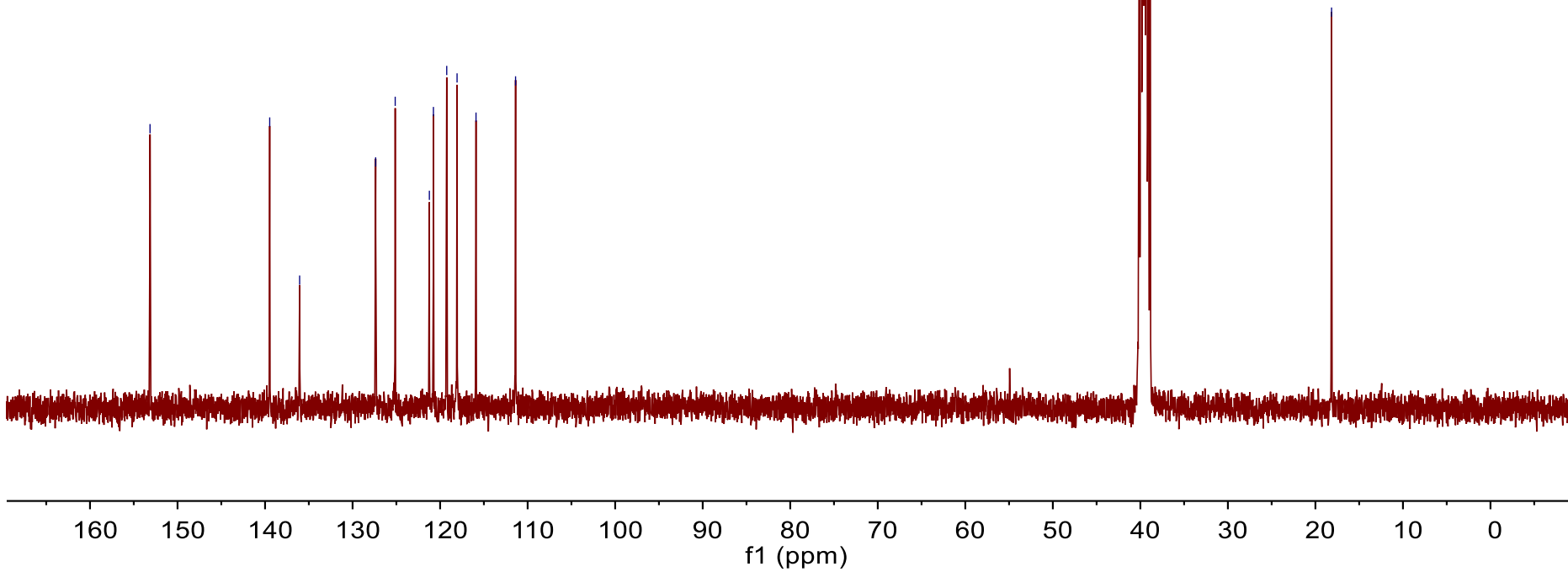
ZJY-X-70.0.fid



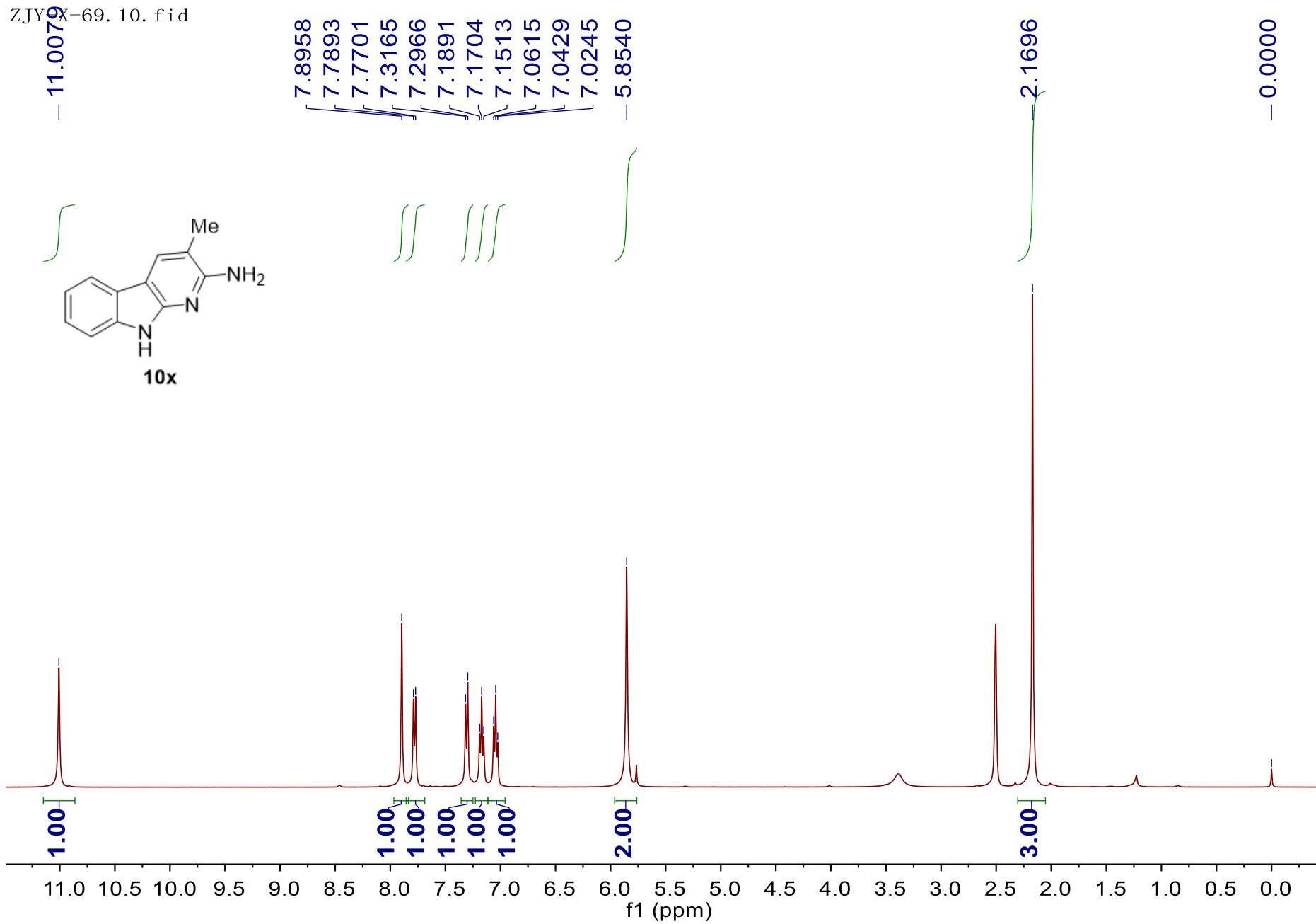
153.142
139.469
136.050
127.365
125.132
121.228
120.766
119.245
118.064
115.899
111.381

40.126
39.918
39.709
39.500
39.293
39.083
38.874

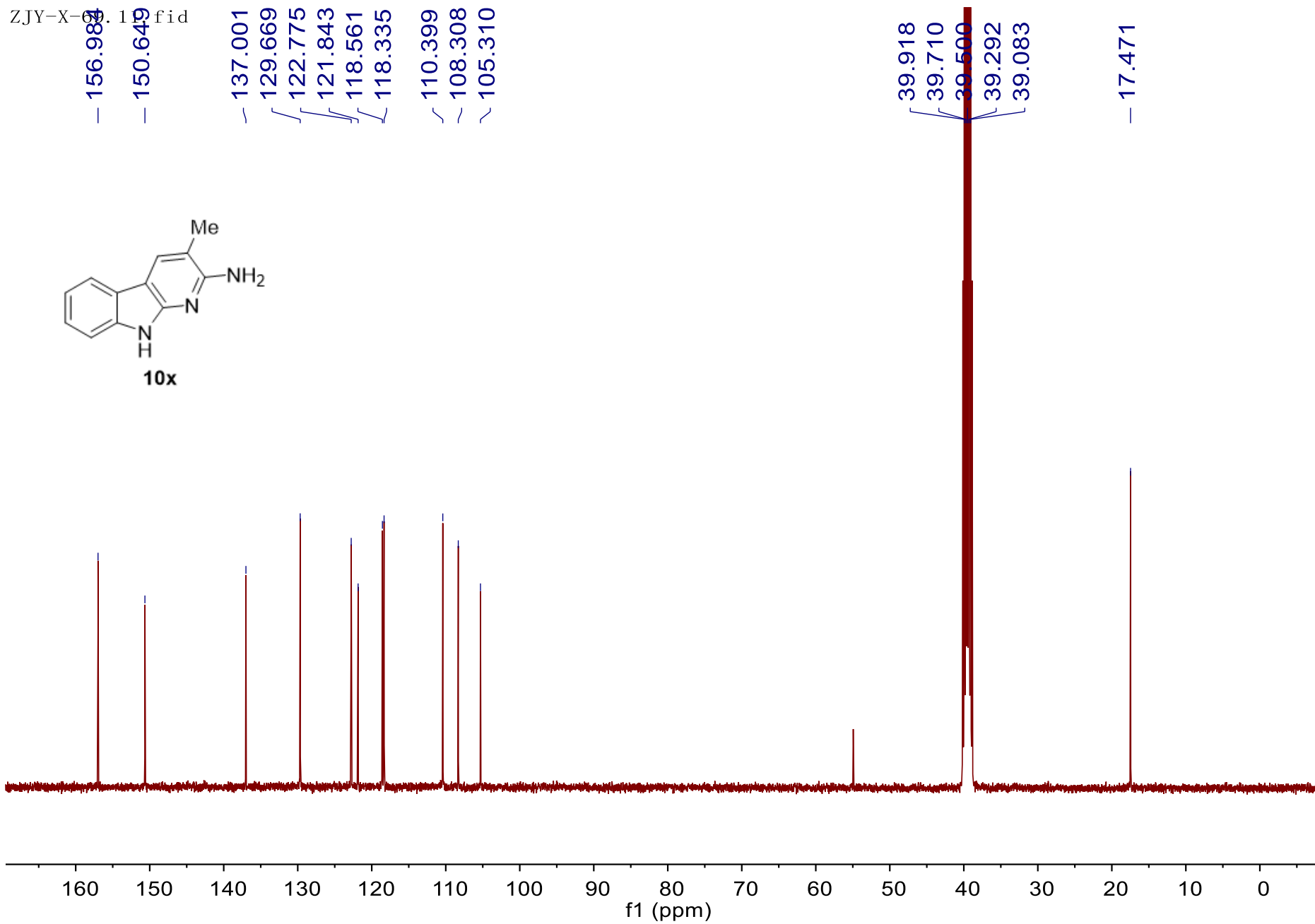
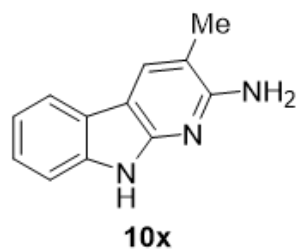
18.155



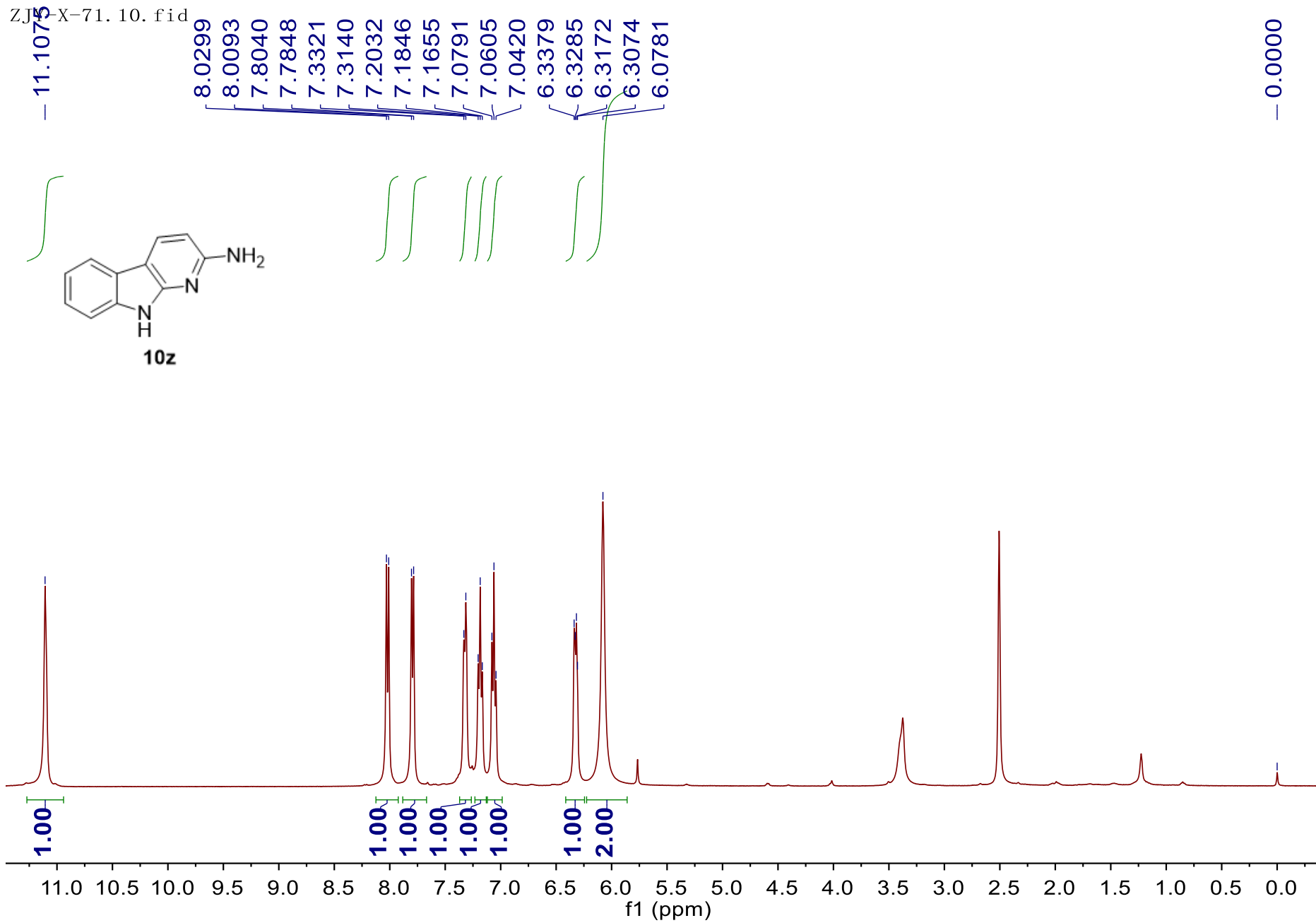
ZJYX-69.10.fid



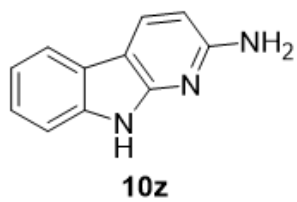
ZJY-X-69.1.fid



ZJ5-X-71.10.fid



ZJY-X-1.fid



158.673
152.049
136.953
129.912
122.924
122.046
118.819
118.349
110.470
104.770
101.134

39.918
39.710
39.500
39.292
39.083

