Supporting information for

Carbazole and triarylpyrrole synthesis from anilines and cyclohexanones or acetophenones under transition-metal free condition

Jun Wu,[a§] Xiangui Chen,[a§] Yanjun Xie,[a] Yanjun Guo,[a] Qian Zhang[a] and Guo-Jun Deng[a]*

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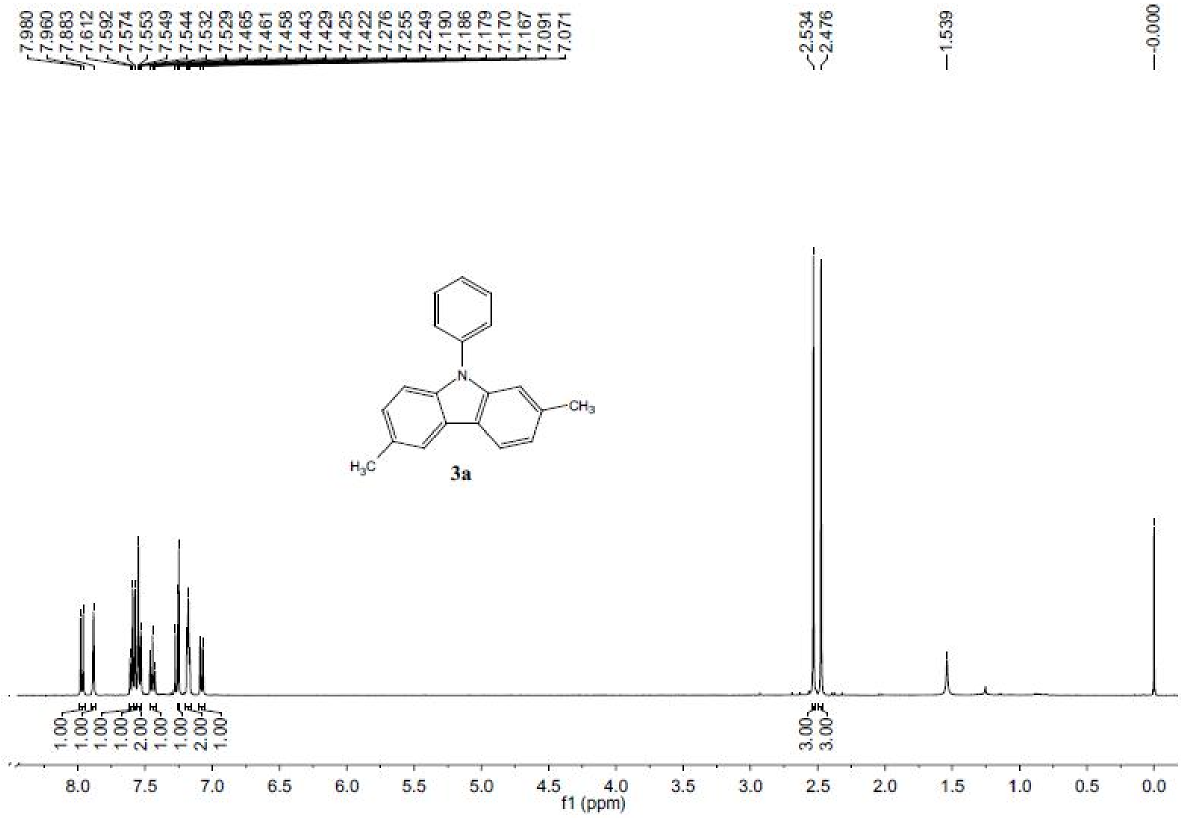
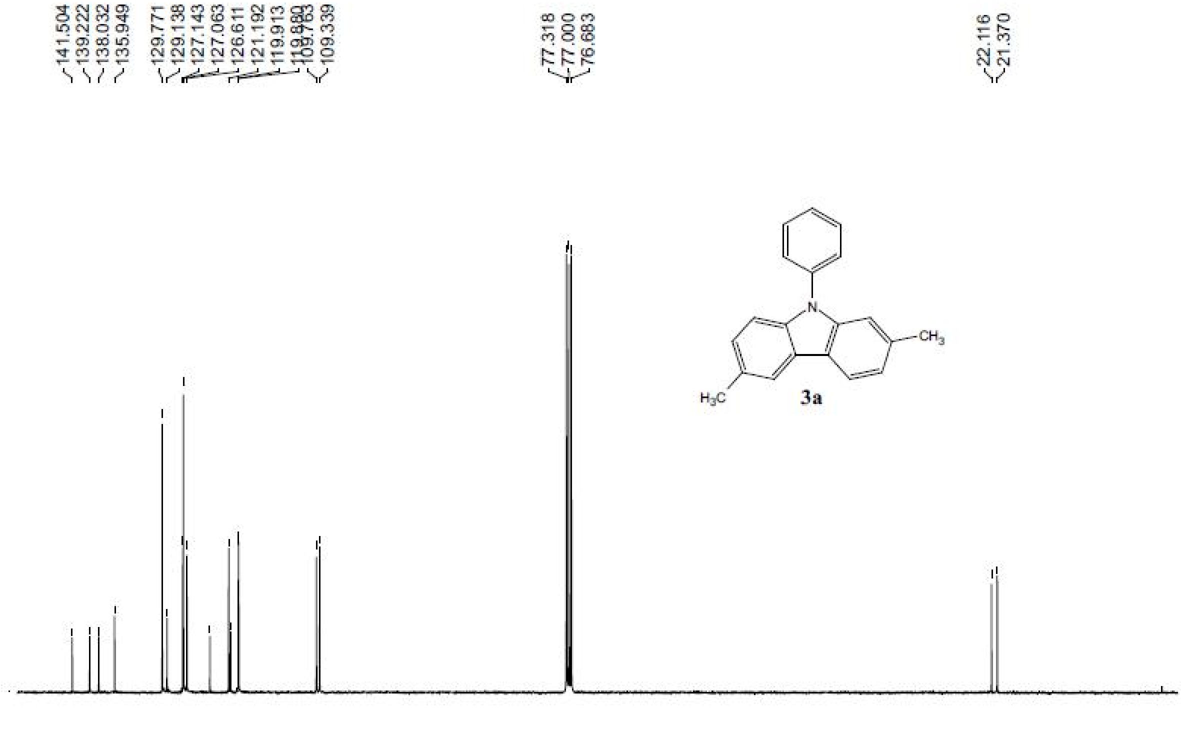
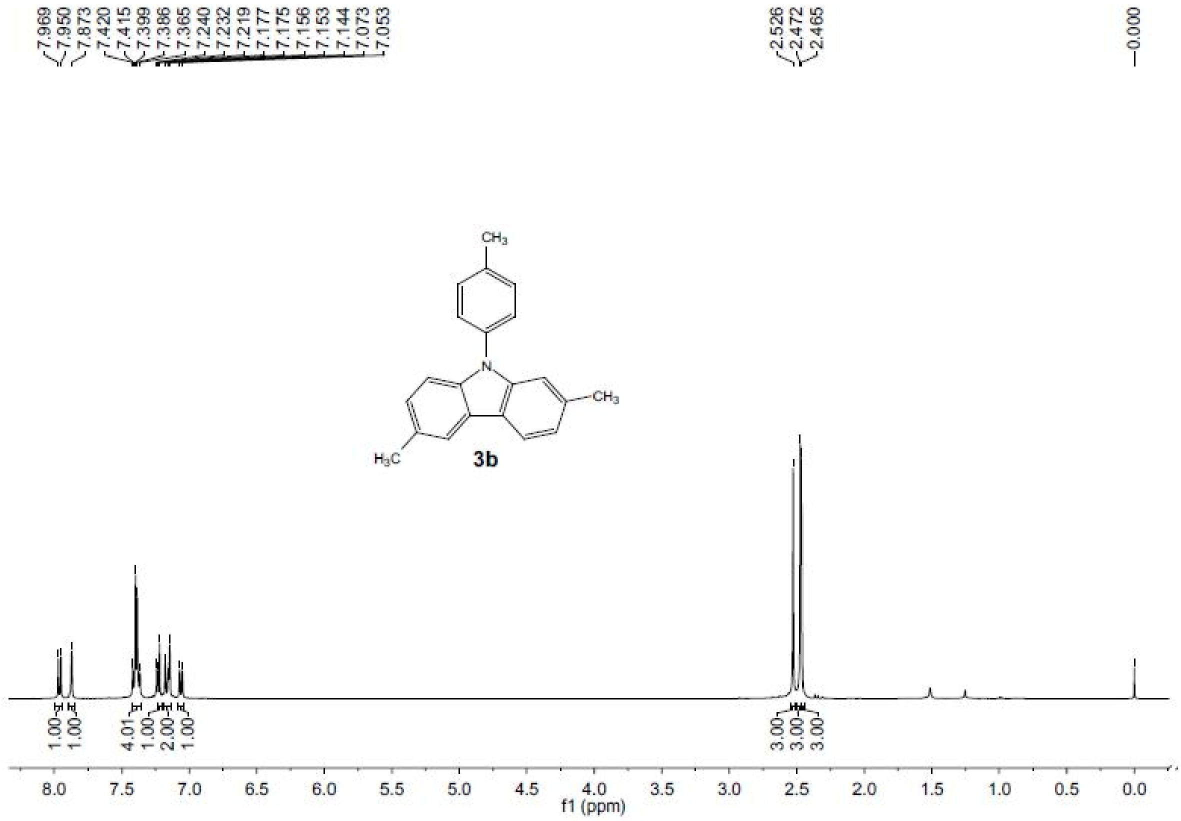
§ Jun Wu and Xiangui Chen contributed equally for this work

^1H NMR and ^{13}C NMR spectra of products



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CH_3
H_3C
3b
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4.01
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2.00
1.00
3.00
3.00
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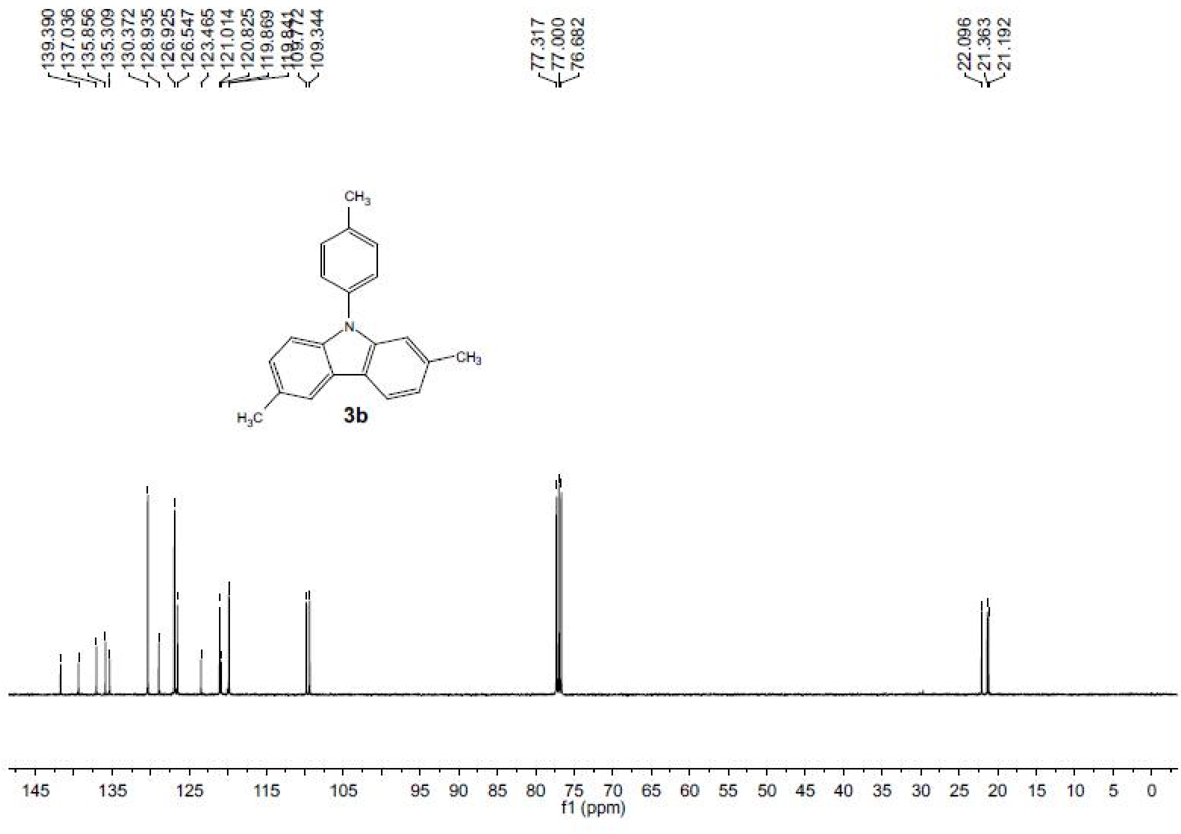
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76.682
22.096
21.363
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CH_3
H_3C
3b
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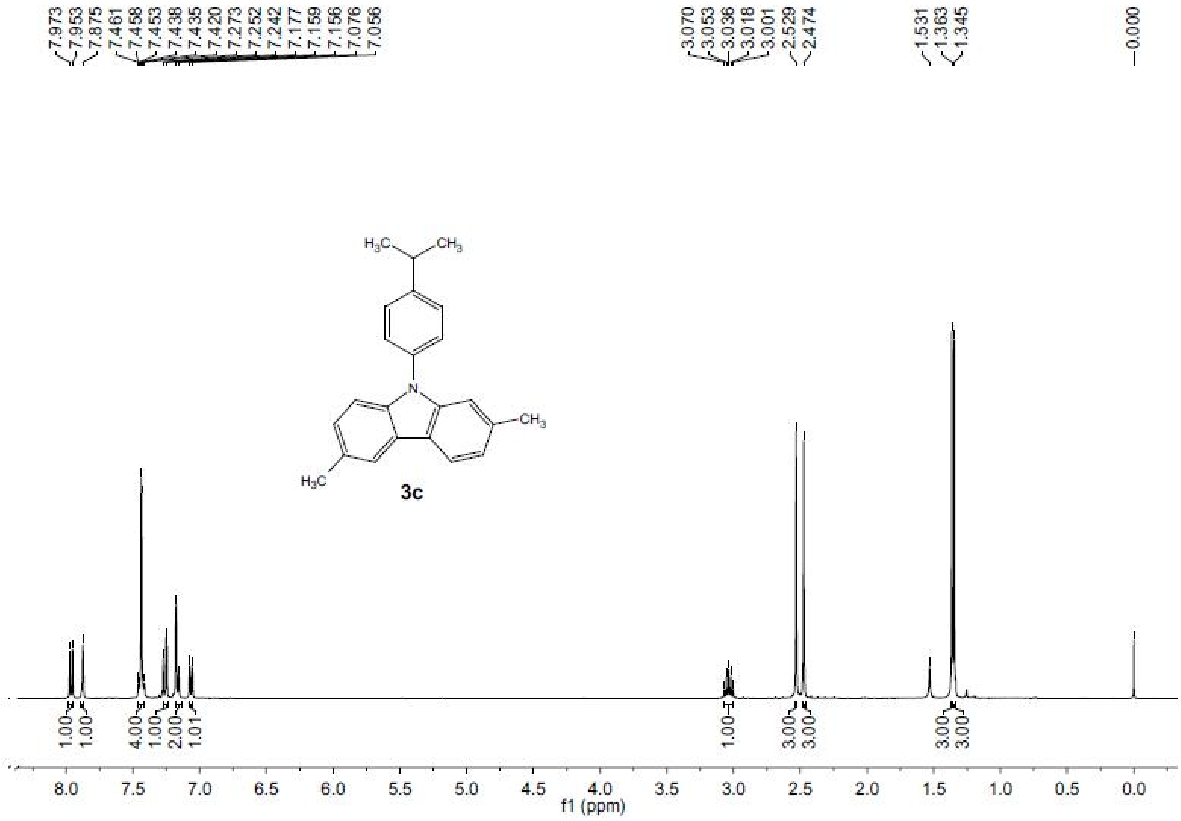
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N
CH_3
H_3C
3c
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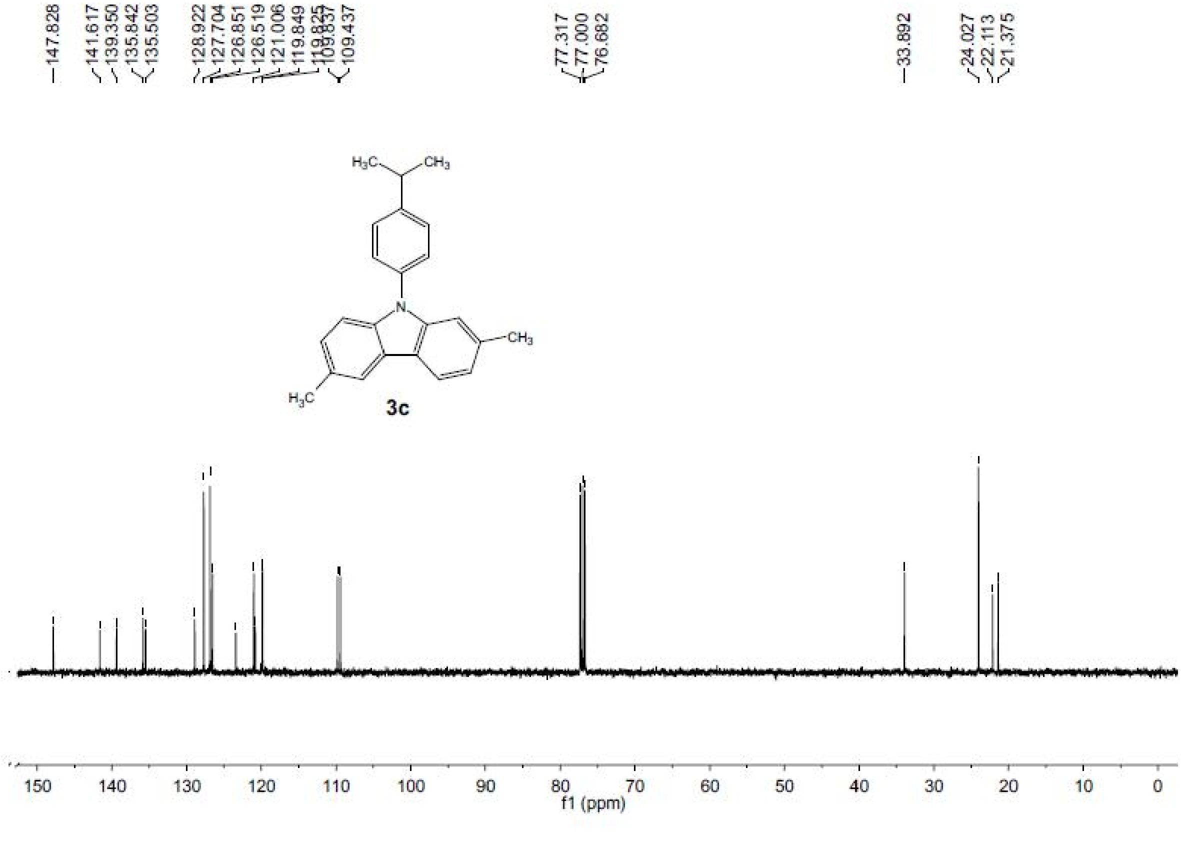
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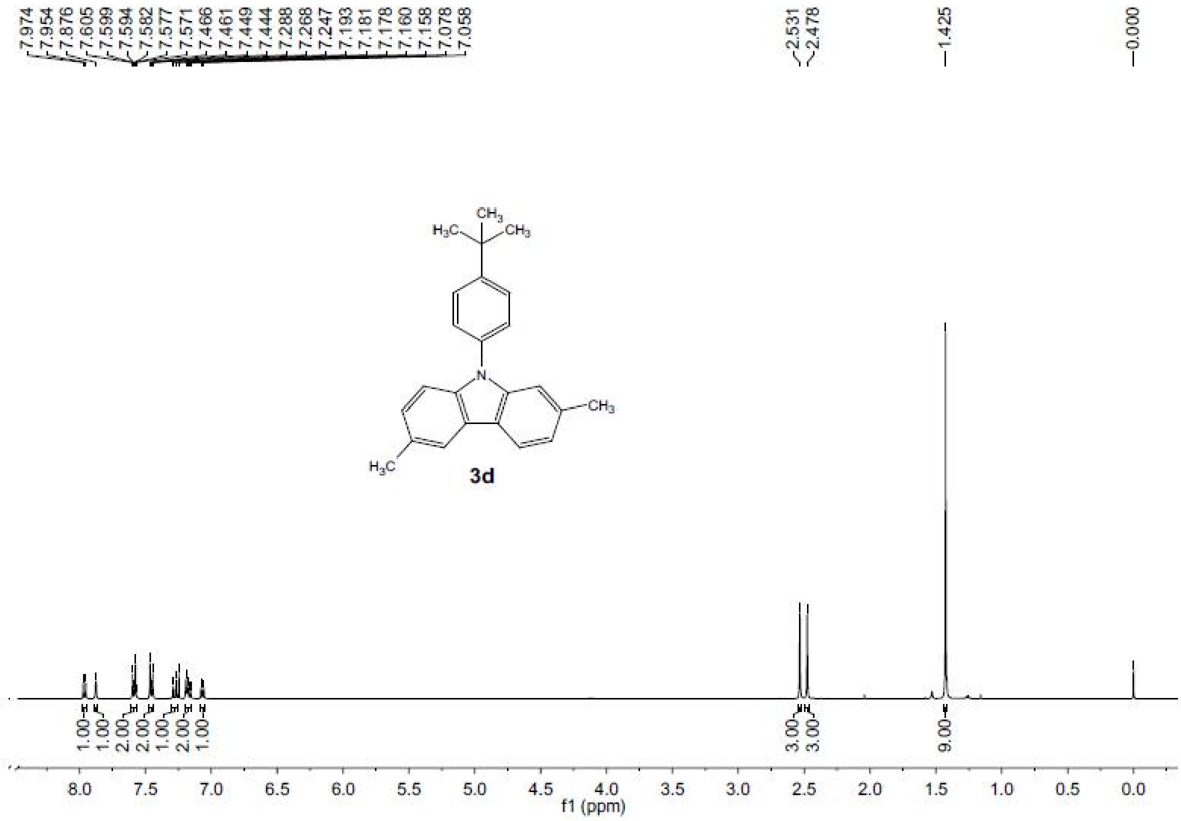
f1 (ppm)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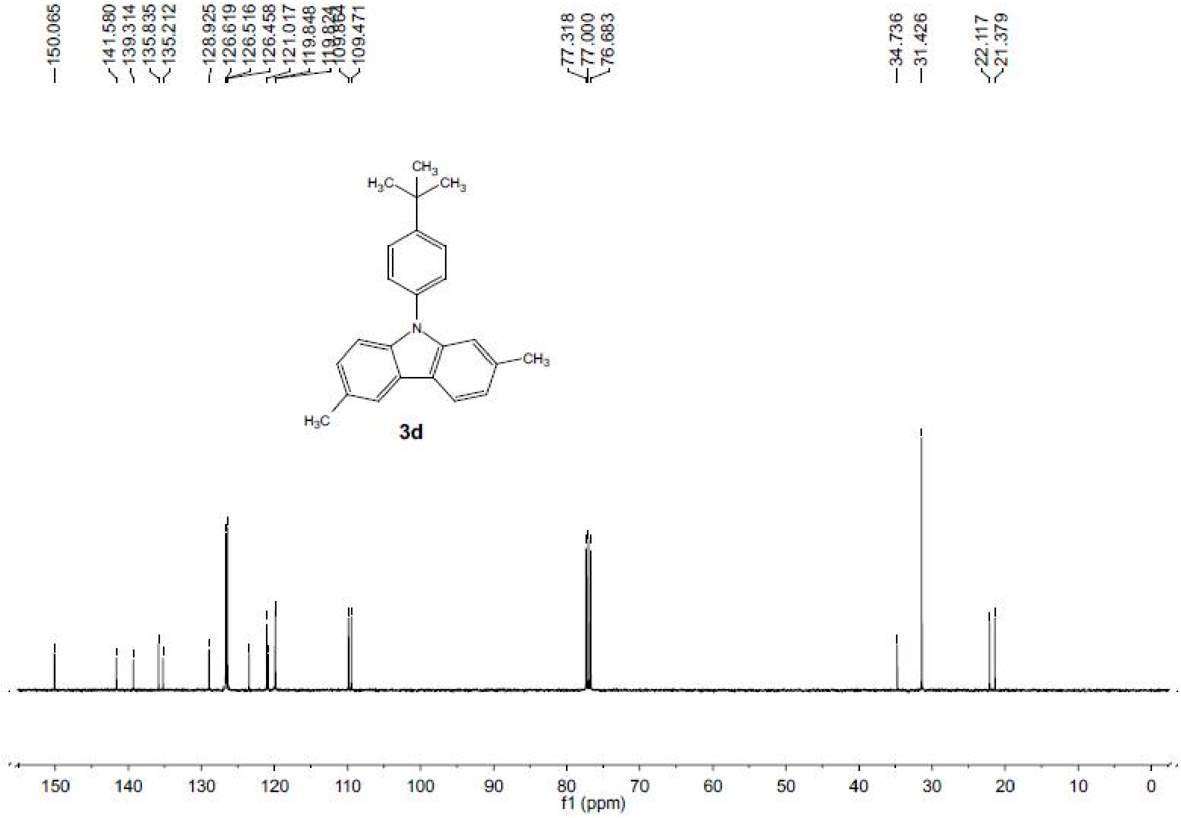
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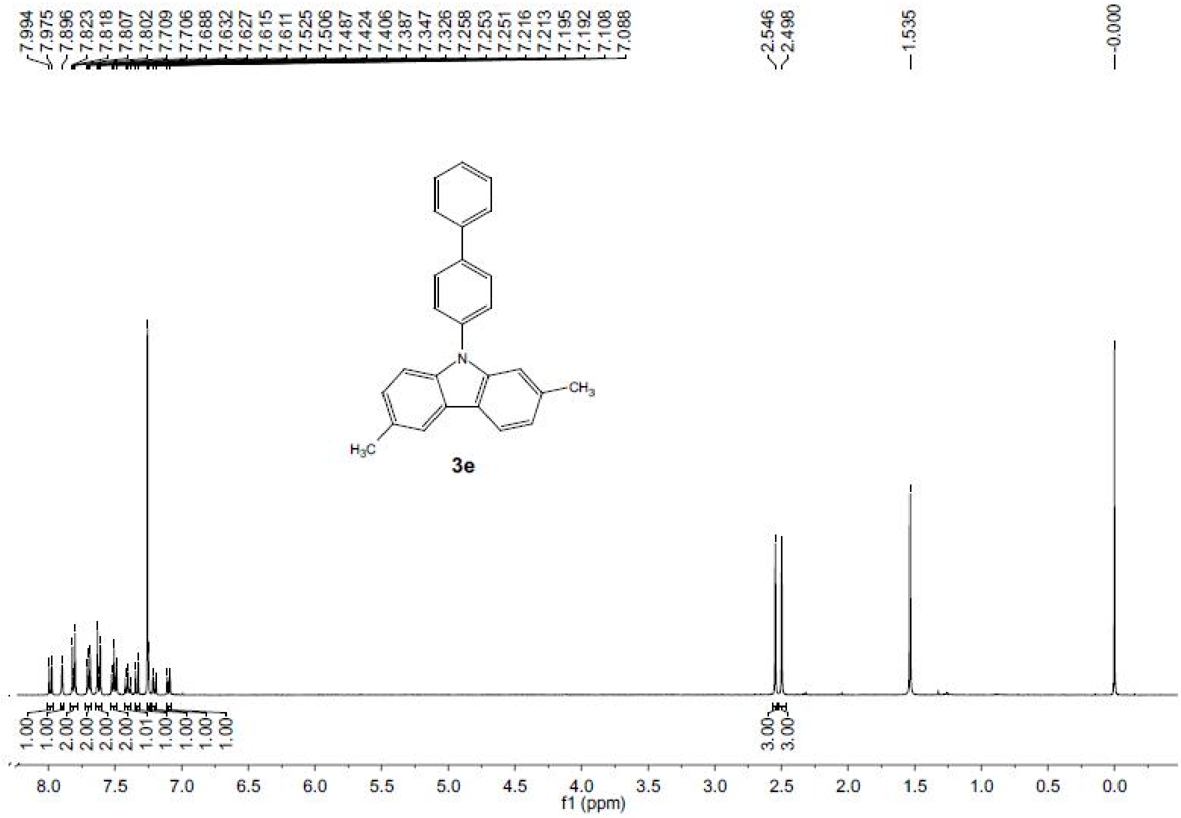
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7.258
7.253
7.251
7.216
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1.00
2.00
2.00
2.00
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1.00
1.00
3.00
3.00
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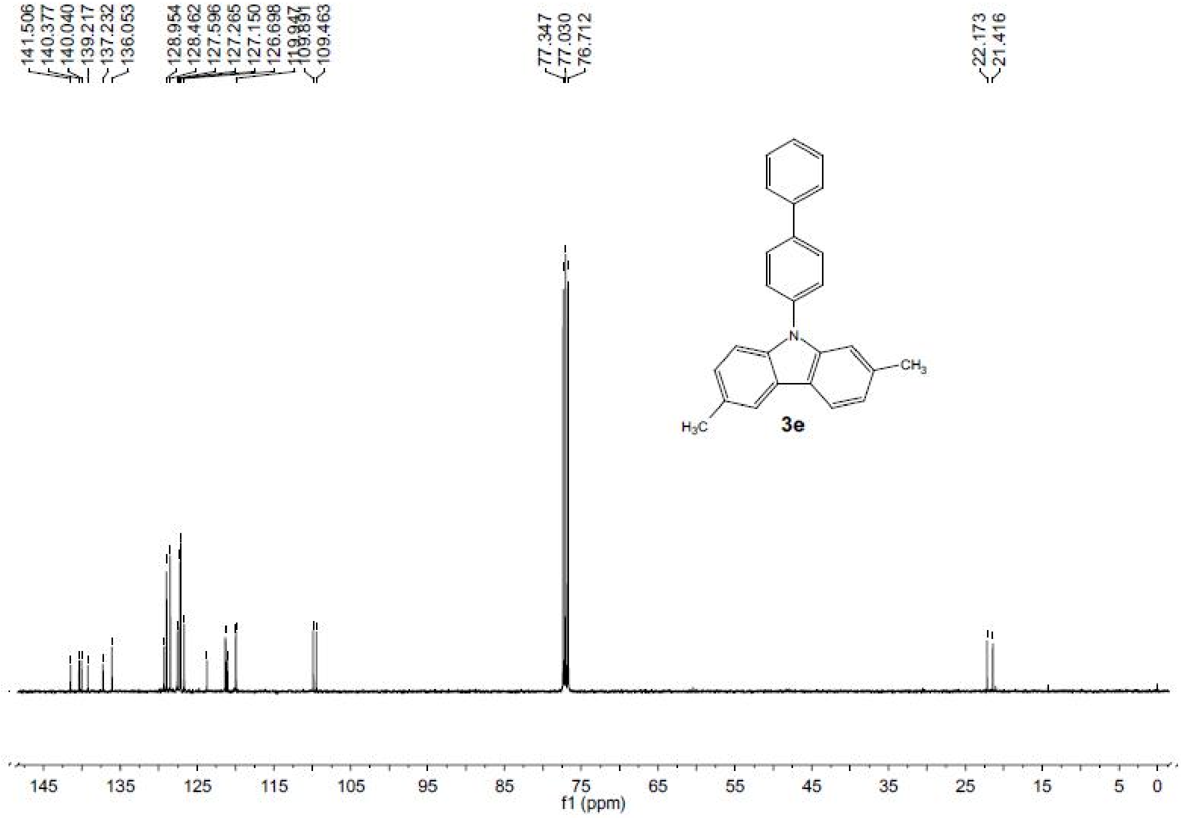
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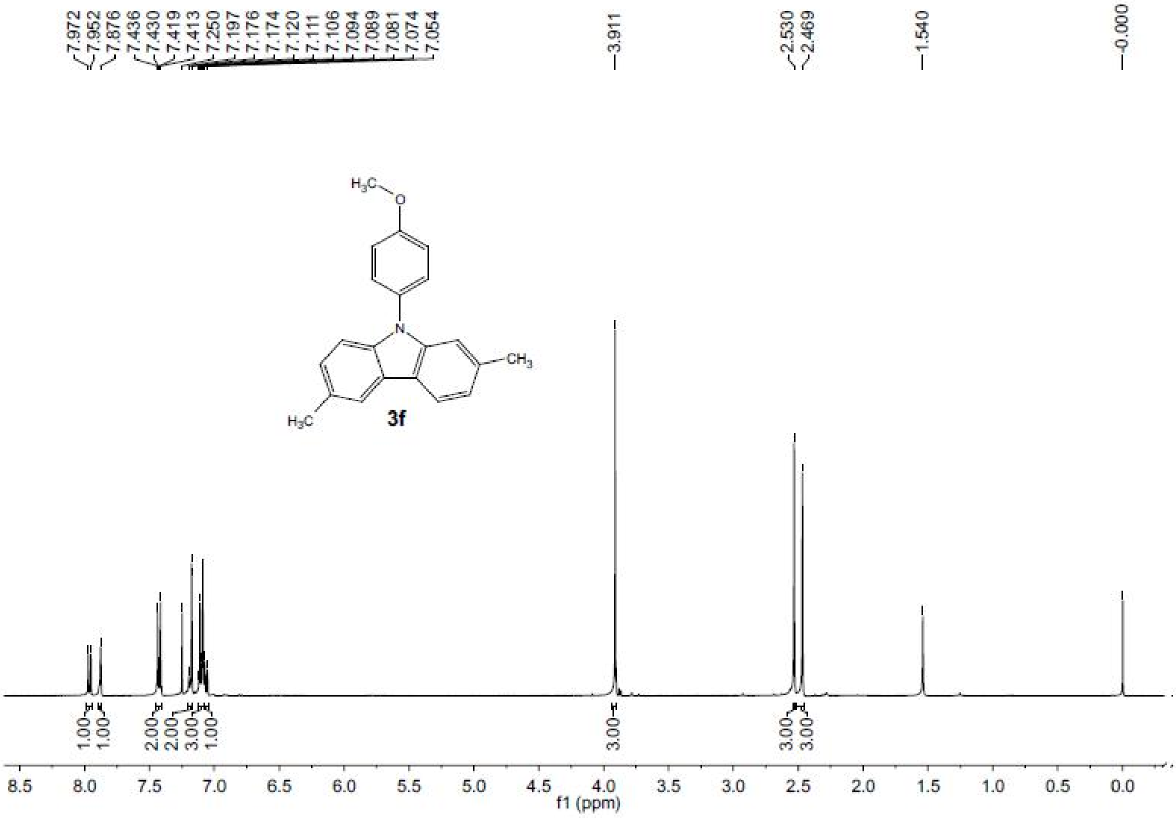
f1 (ppm)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O
N
CH_3
H_3C
3f
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1.00
2.00
2.00
3.00
1.00
3.00
3.00
3.00
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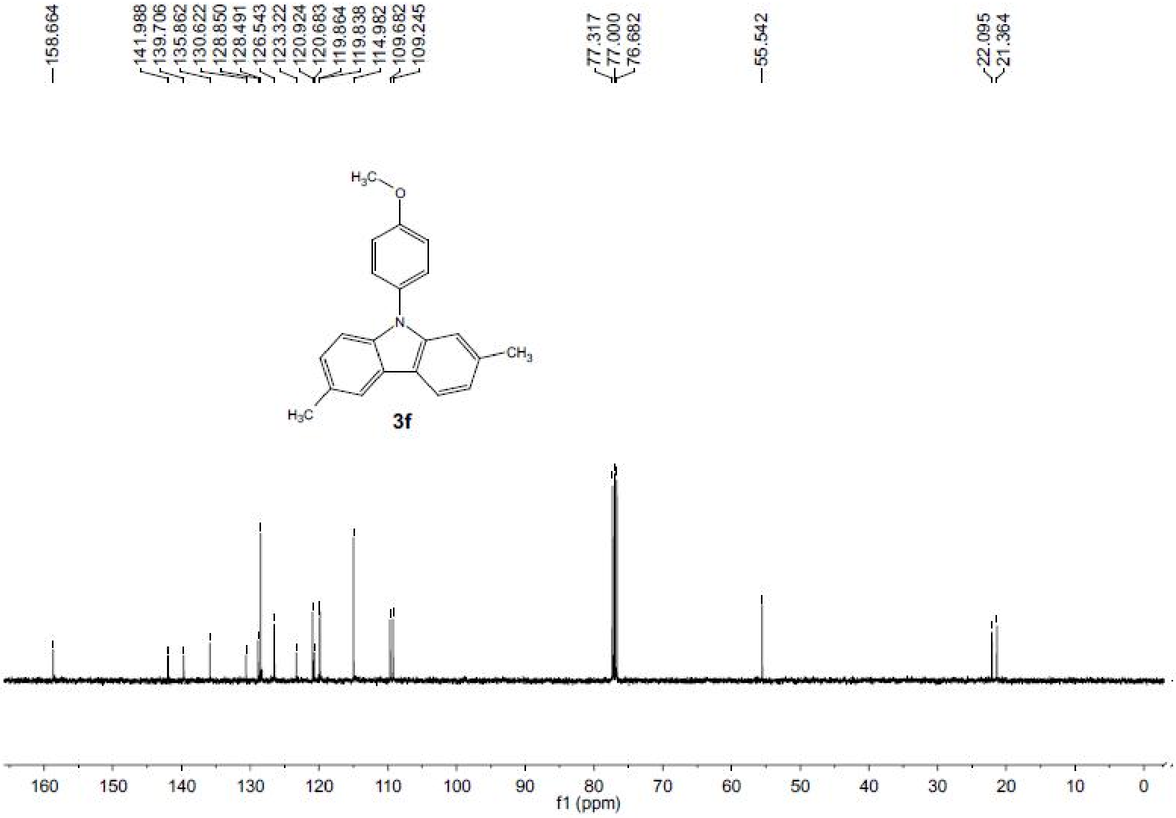
f1 (ppm)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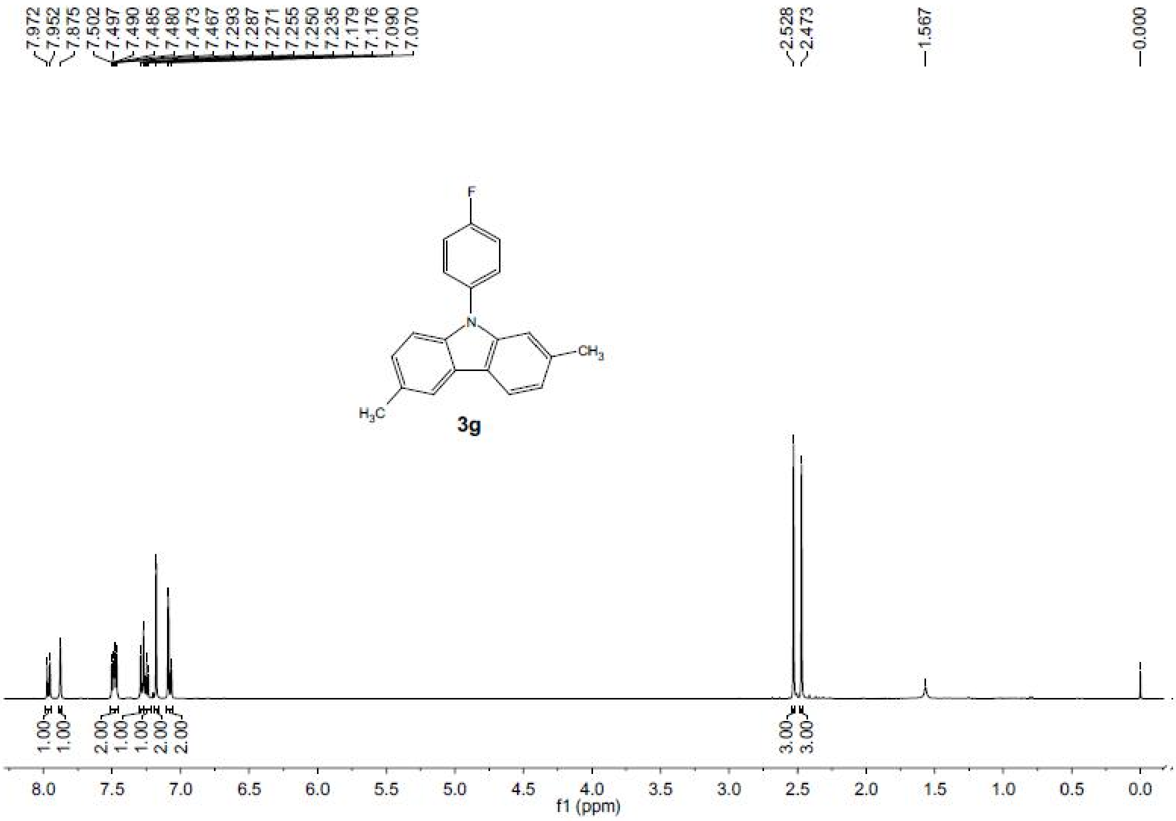
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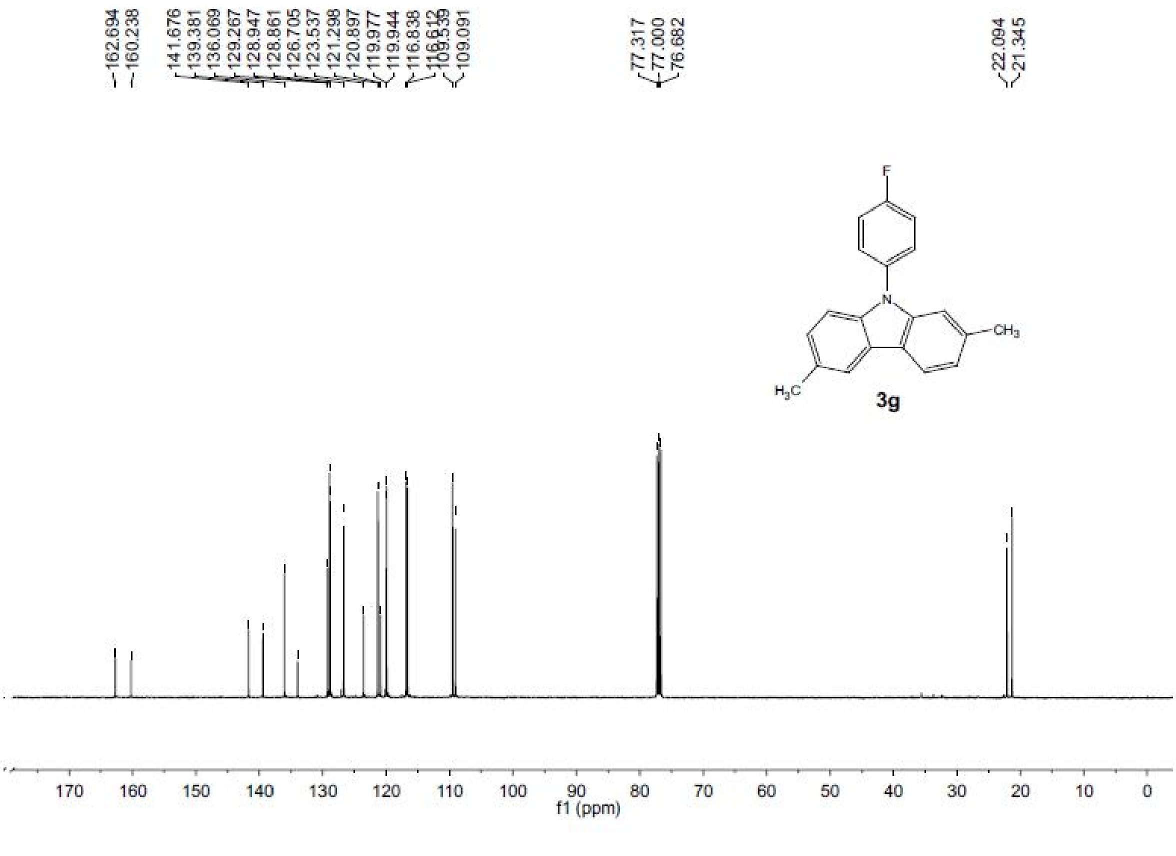
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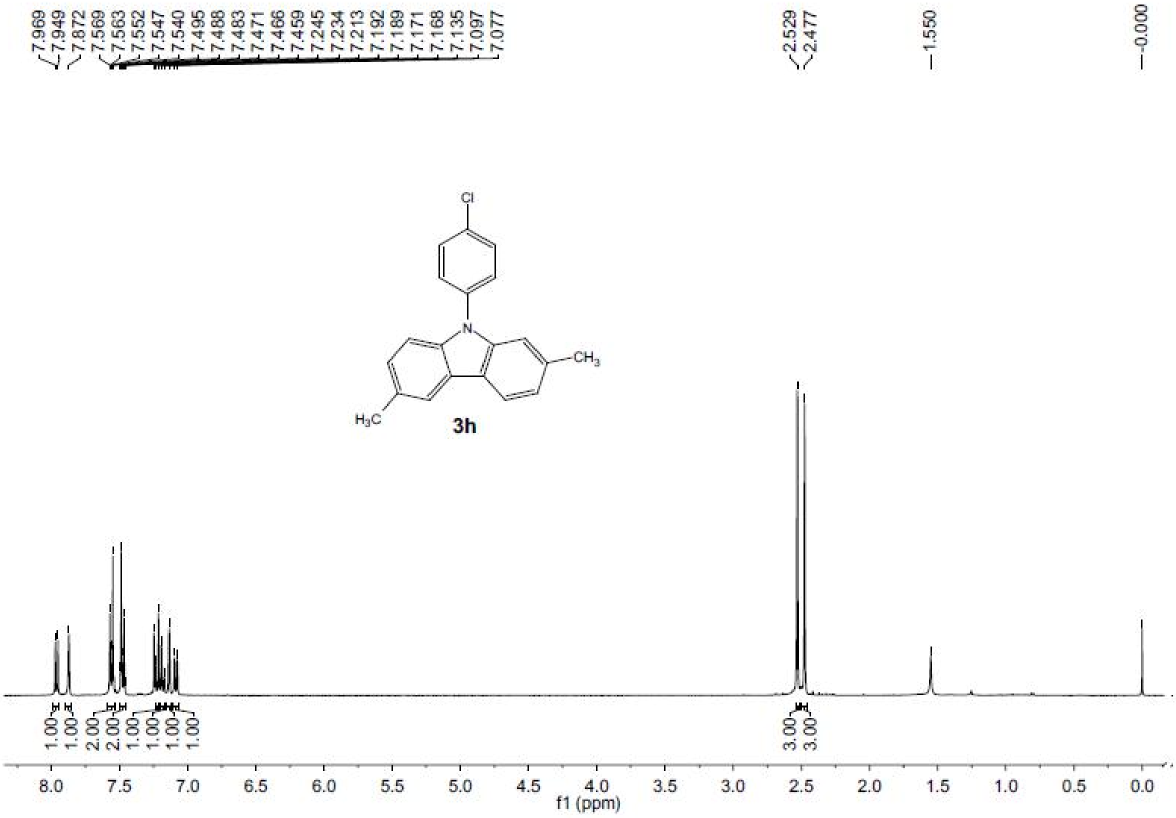
f1 (ppm)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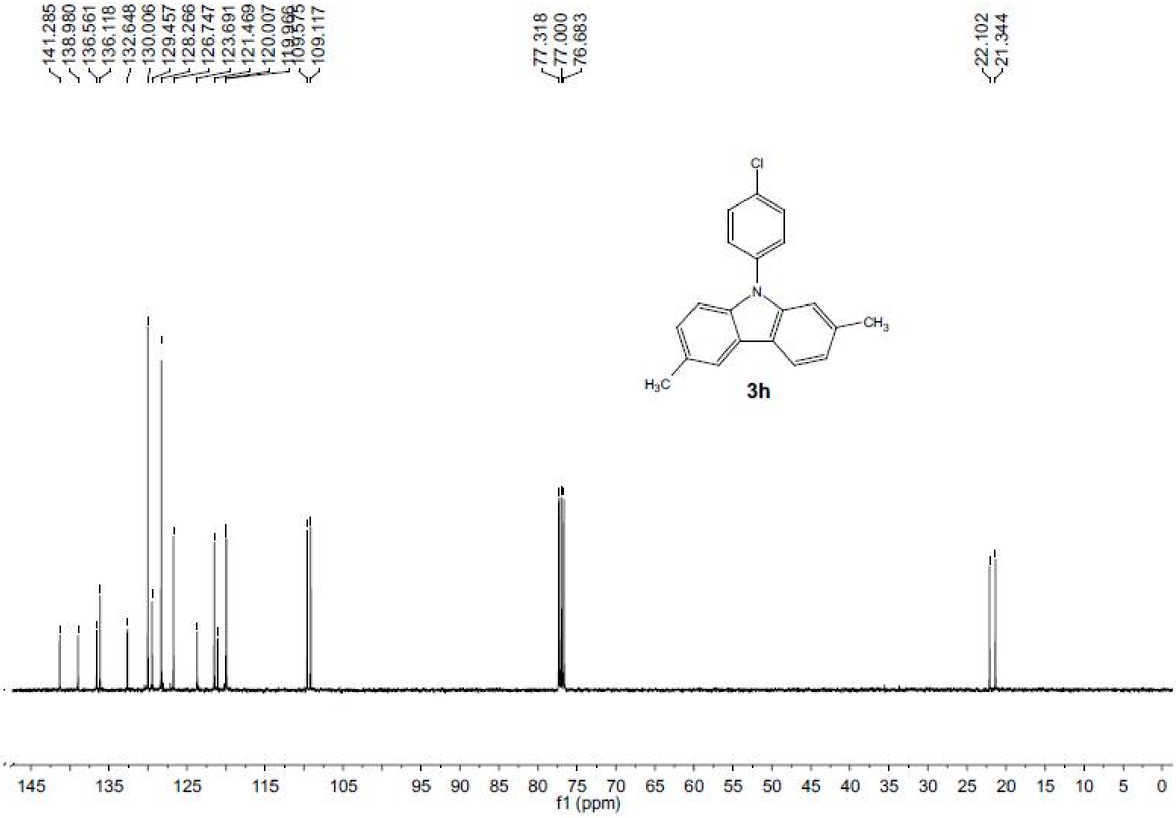
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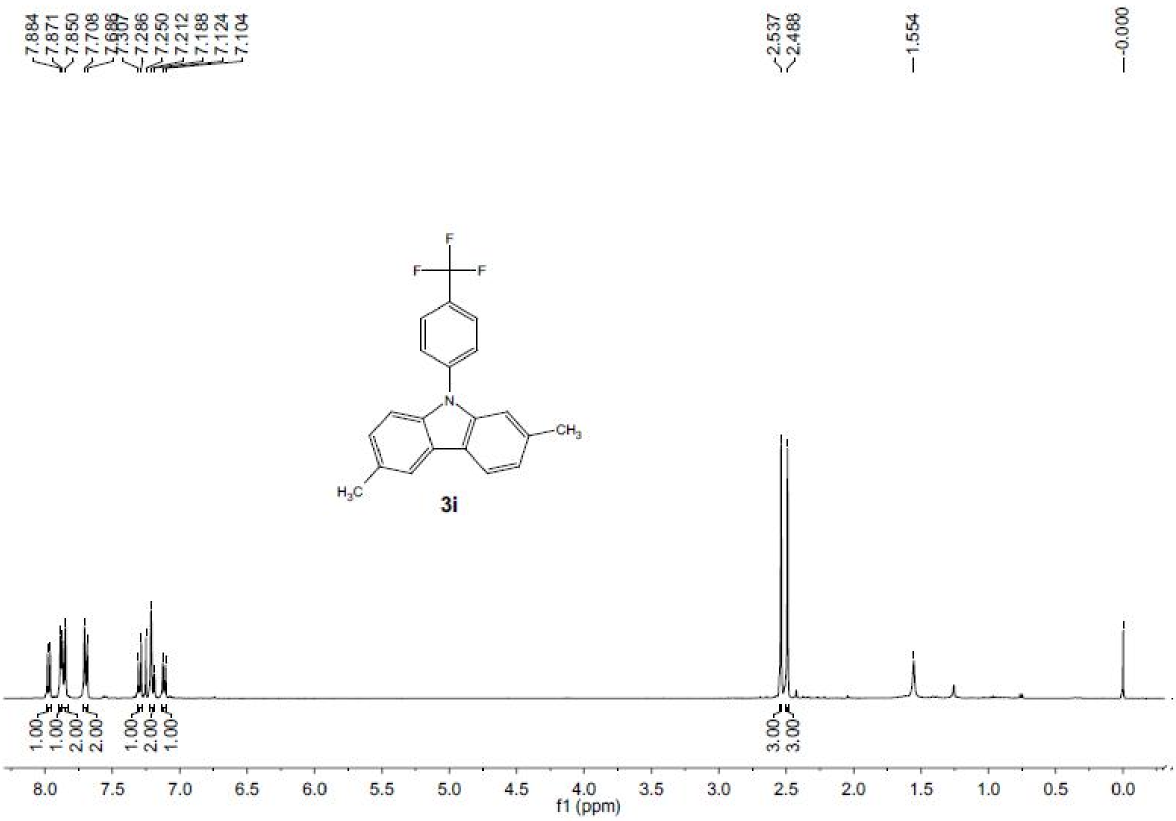

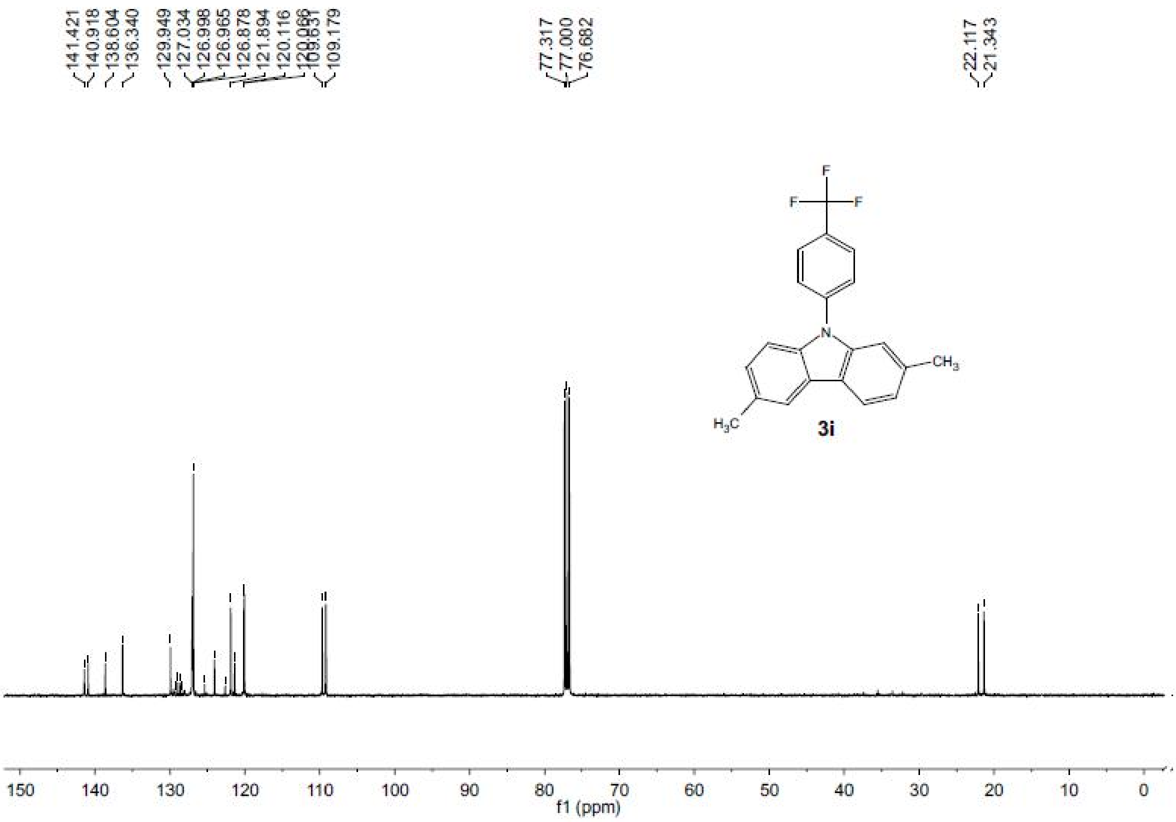

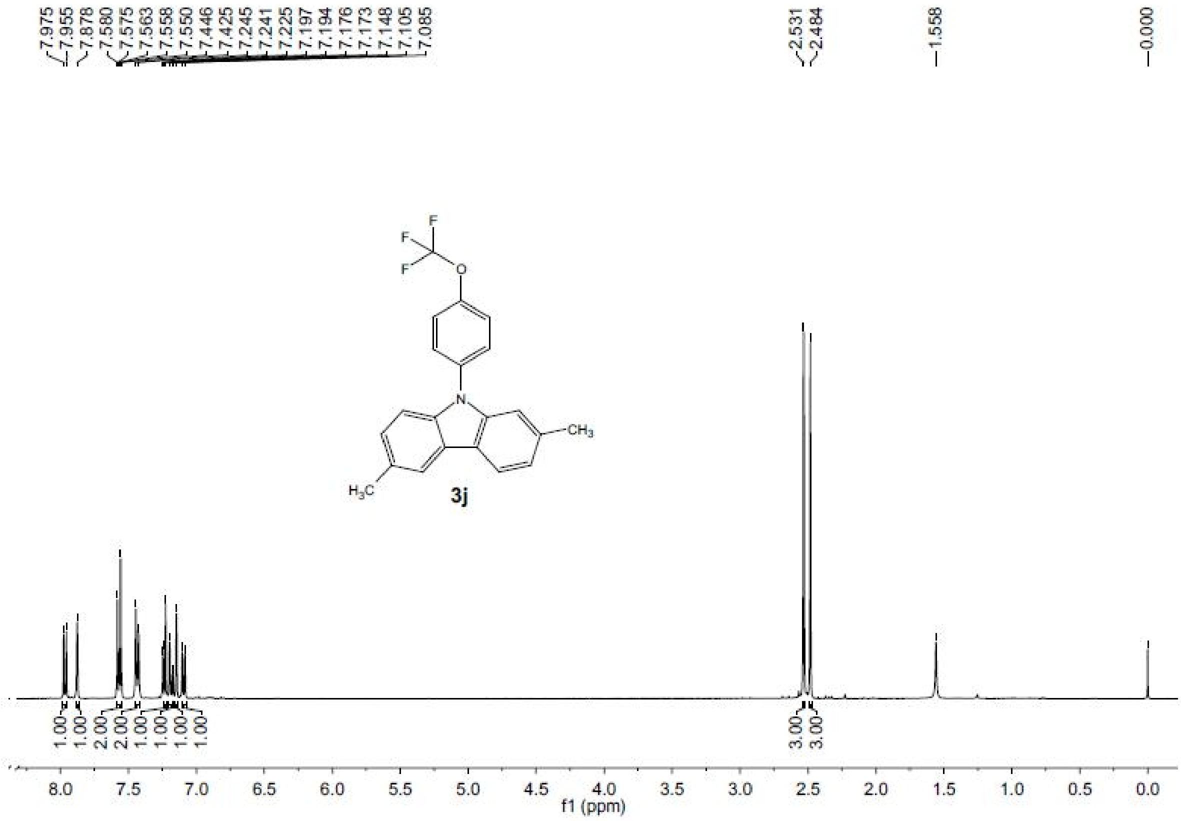
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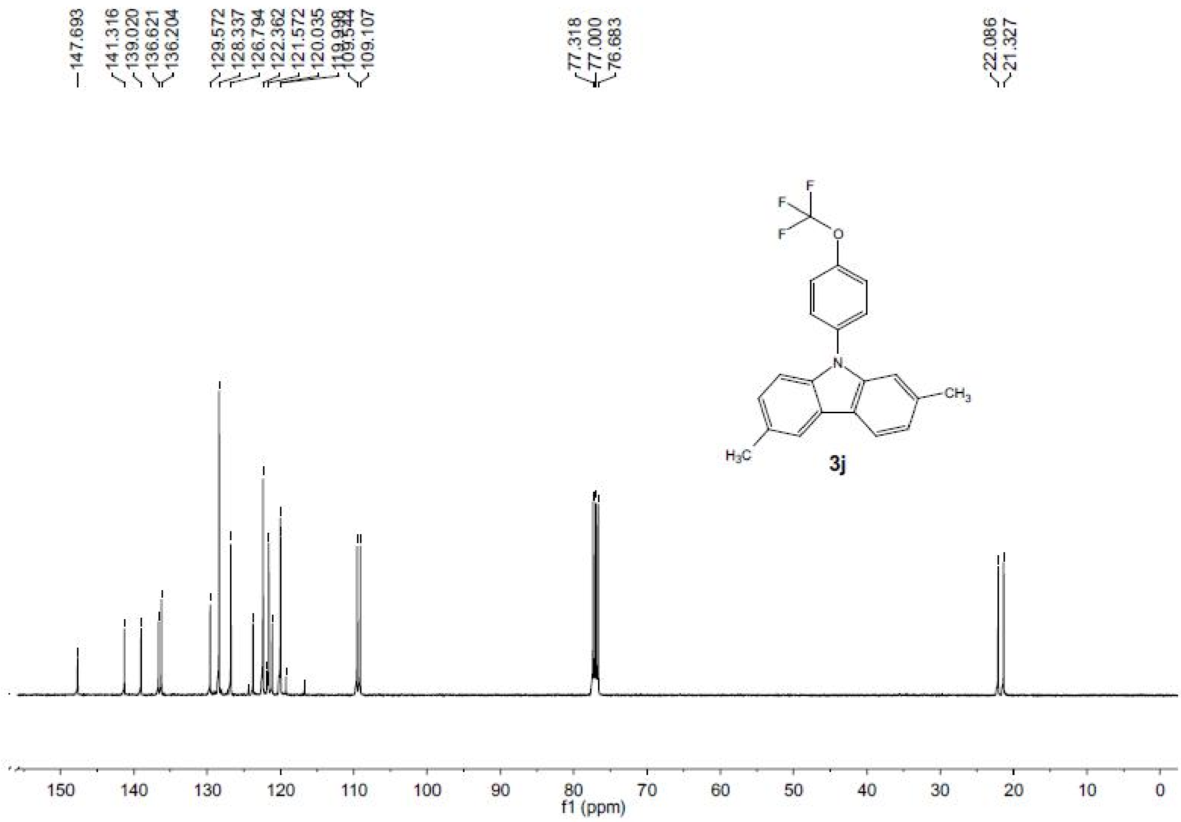
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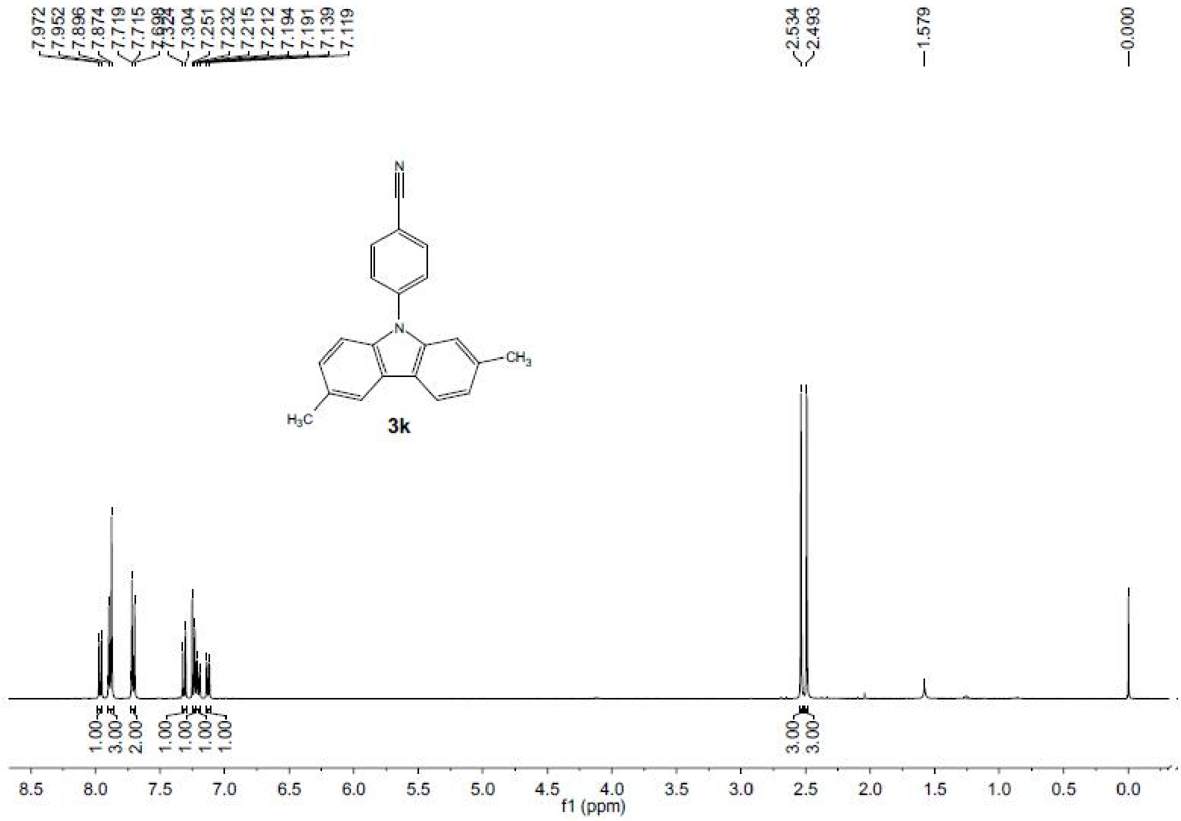
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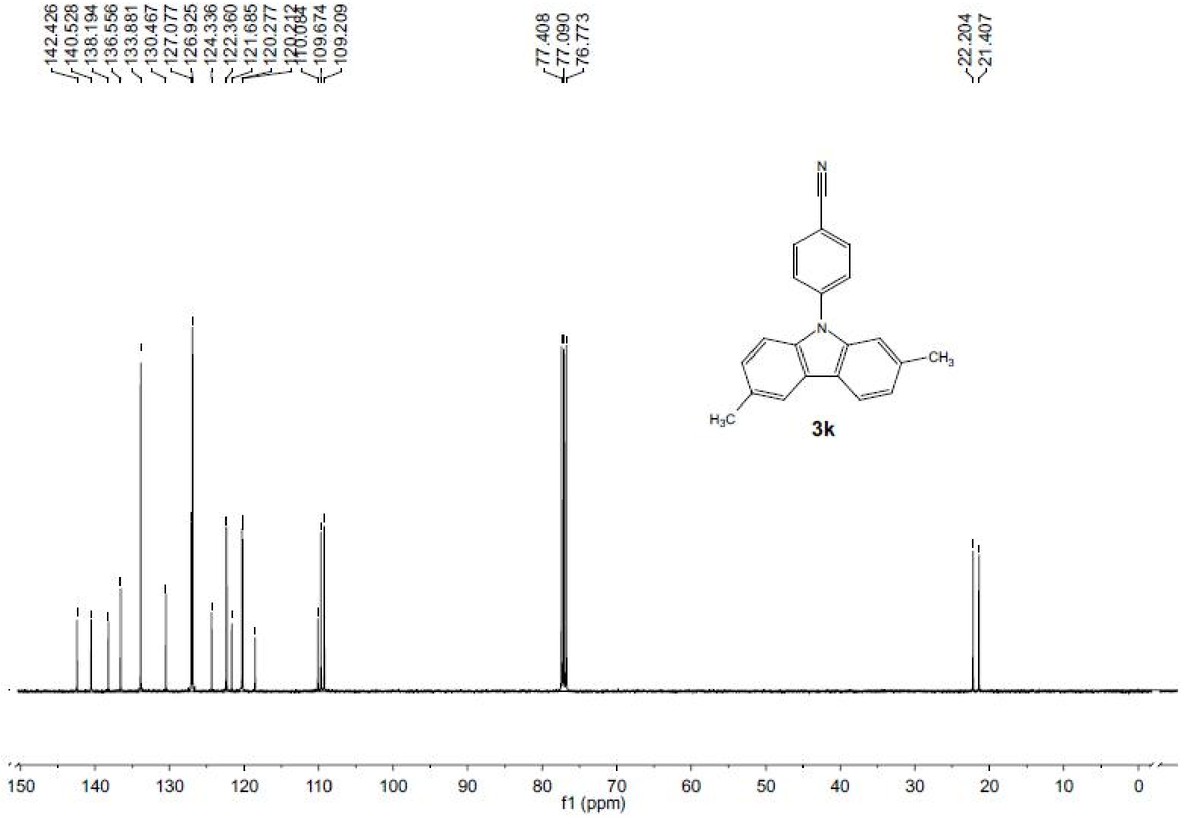
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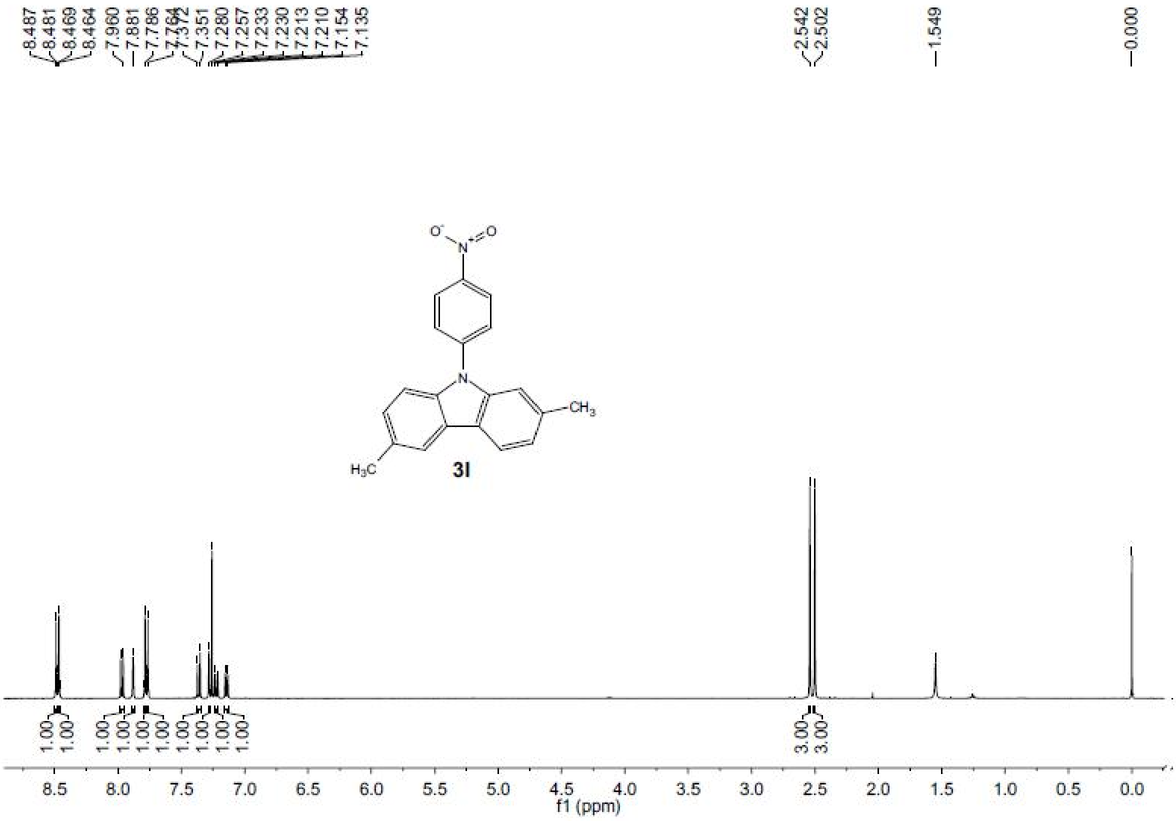
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H_3C
3l
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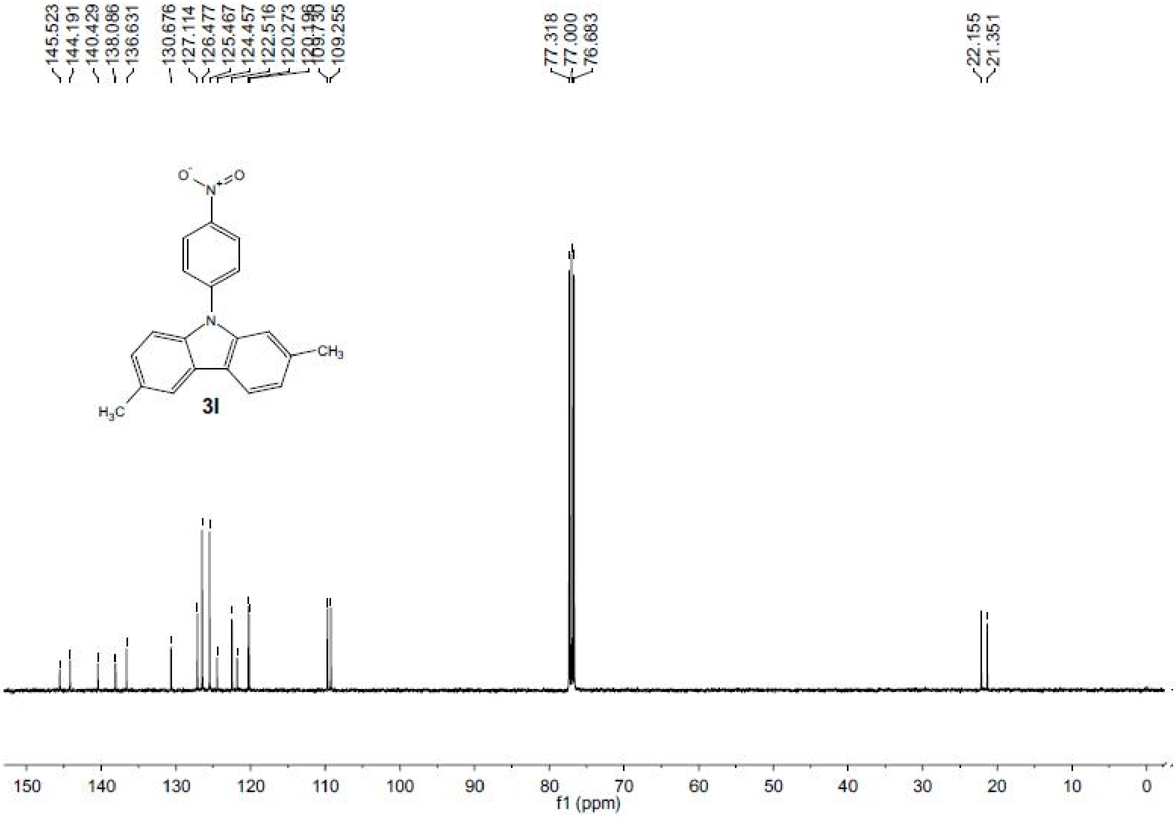
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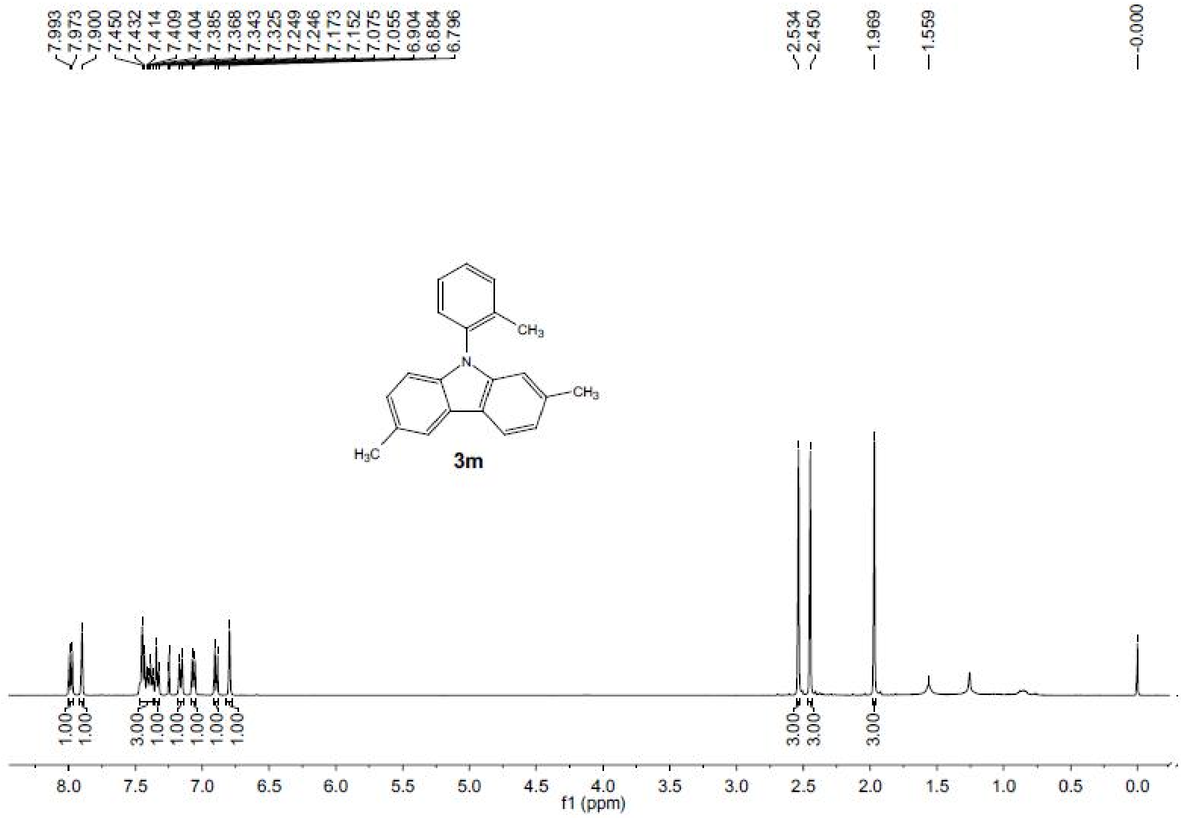

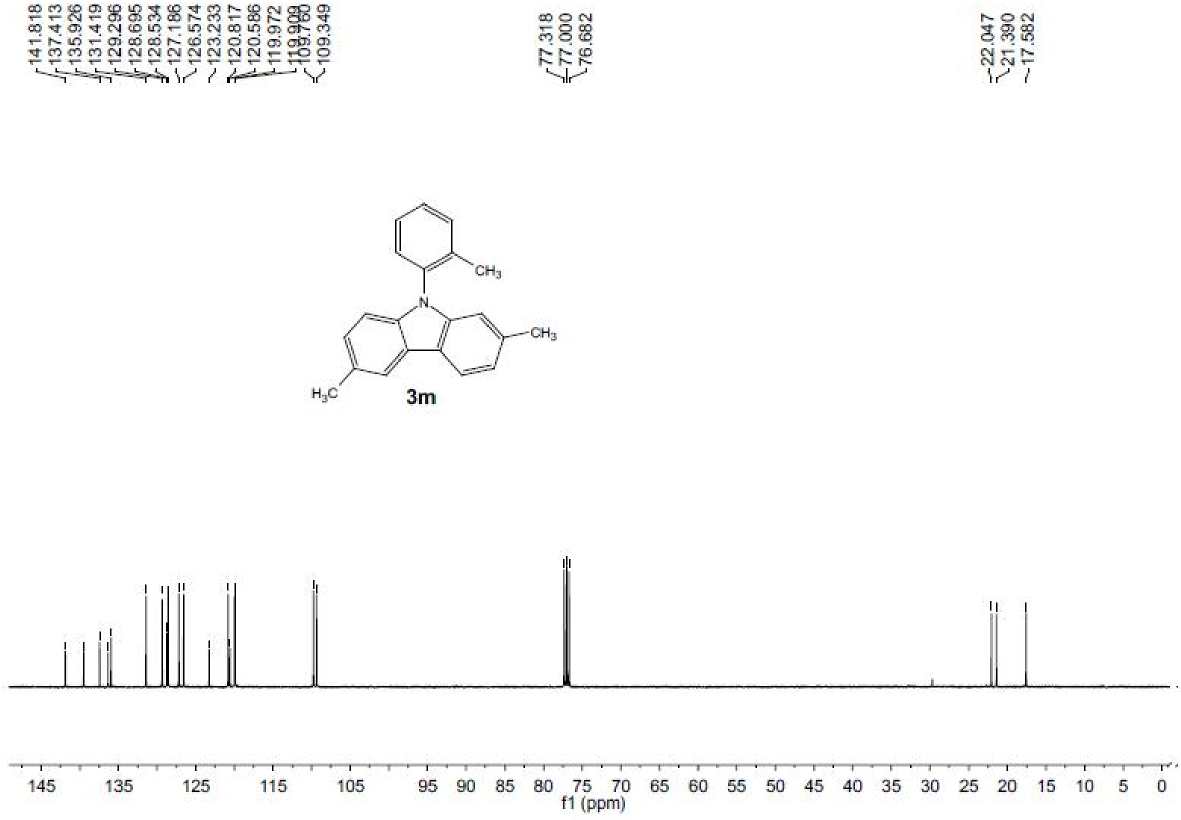

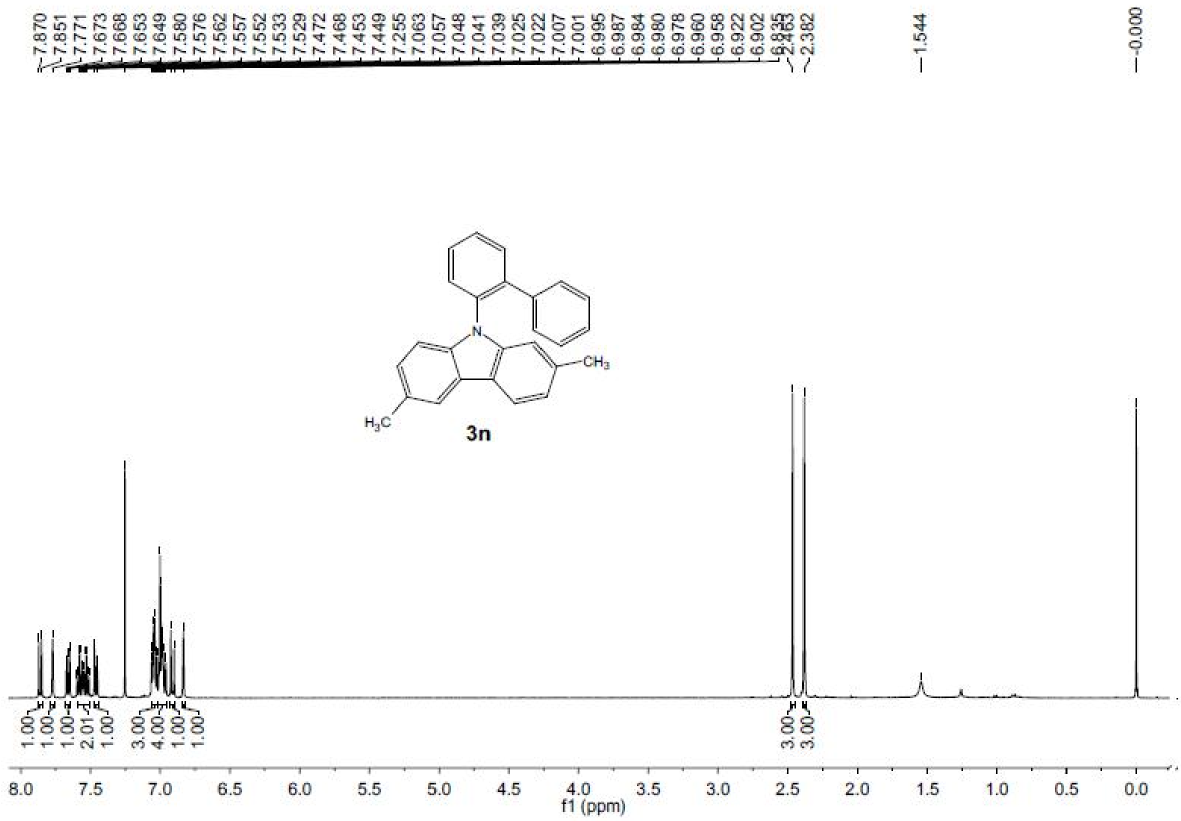
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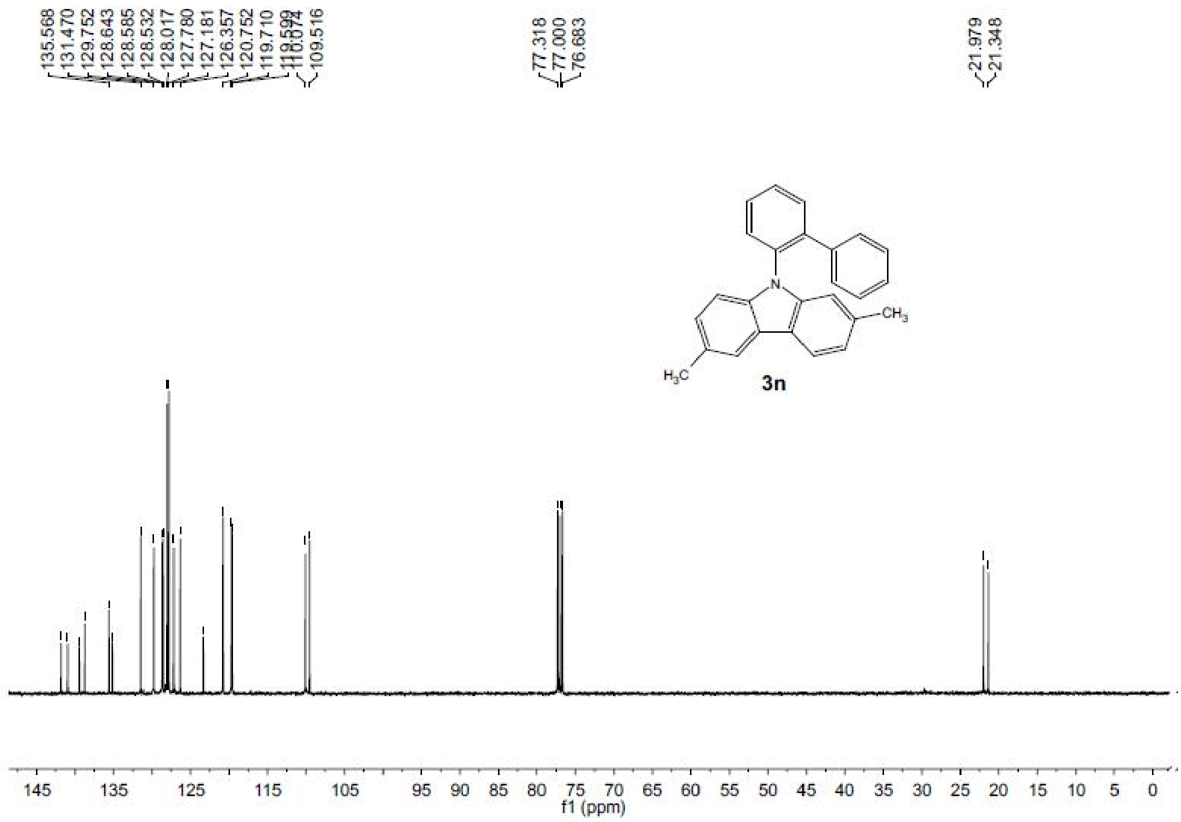
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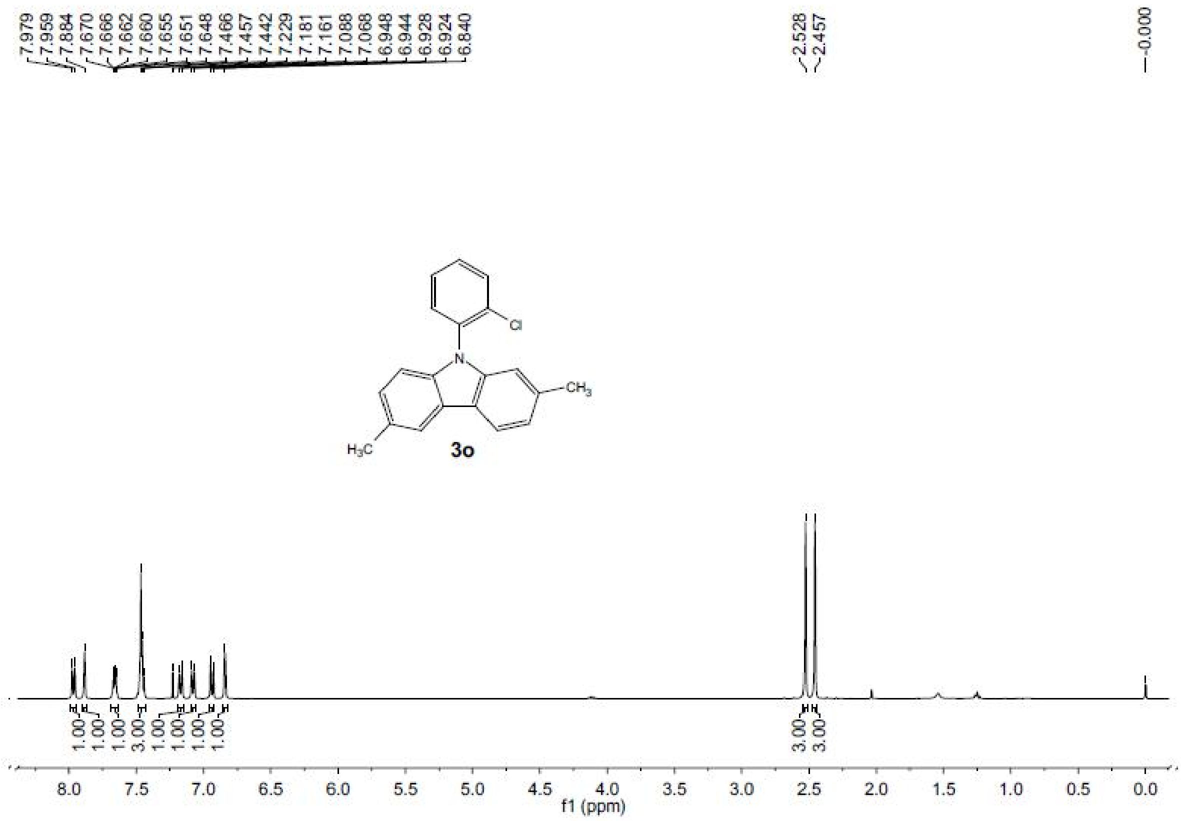

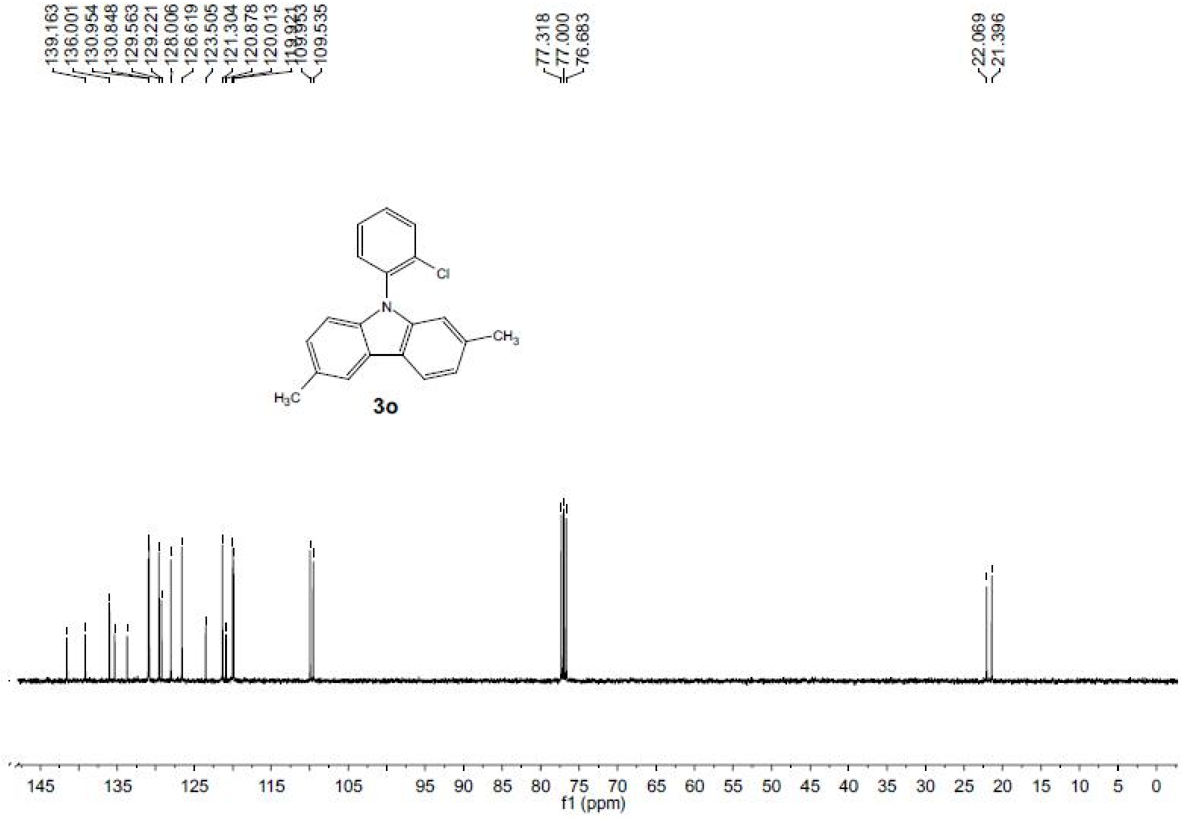

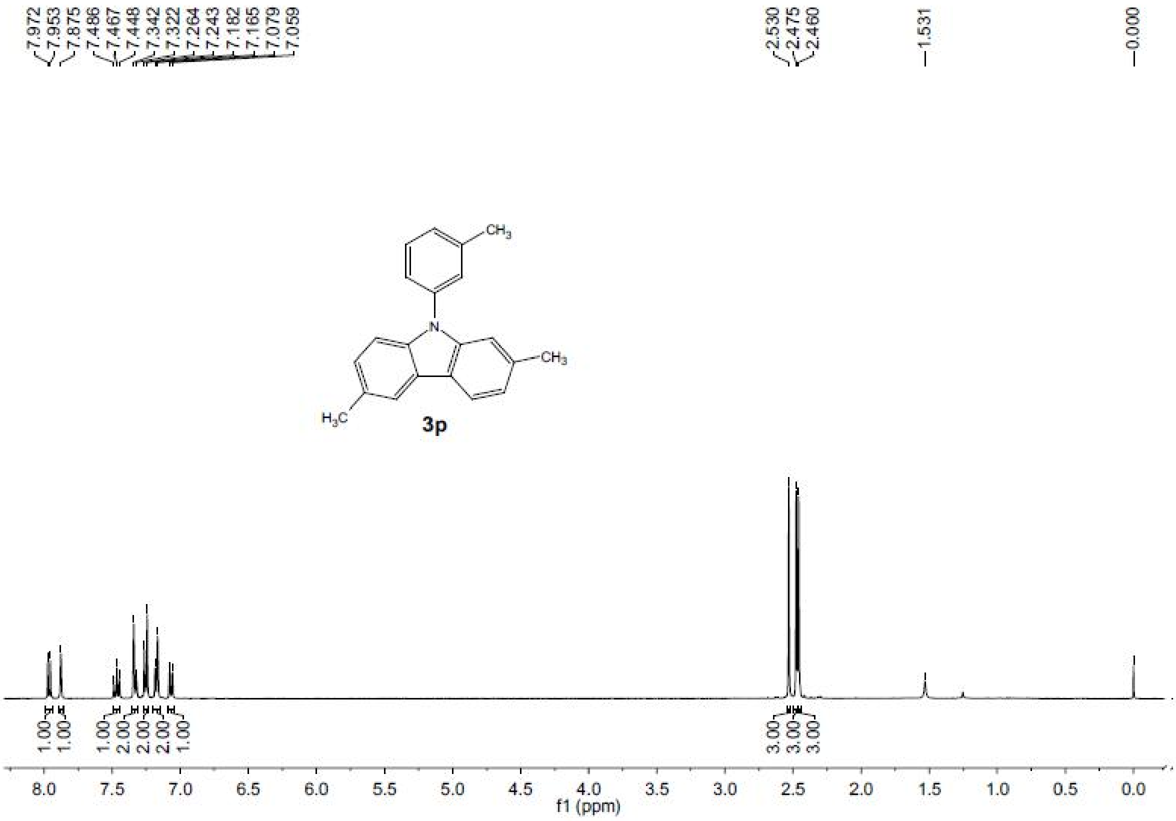
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7.059
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2.475
2.460
1.531
0.000
CH3
CH3
H3C
N
3p
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1.00
1.00
2.00
2.00
2.00
1.00
3.00
3.00
3.00
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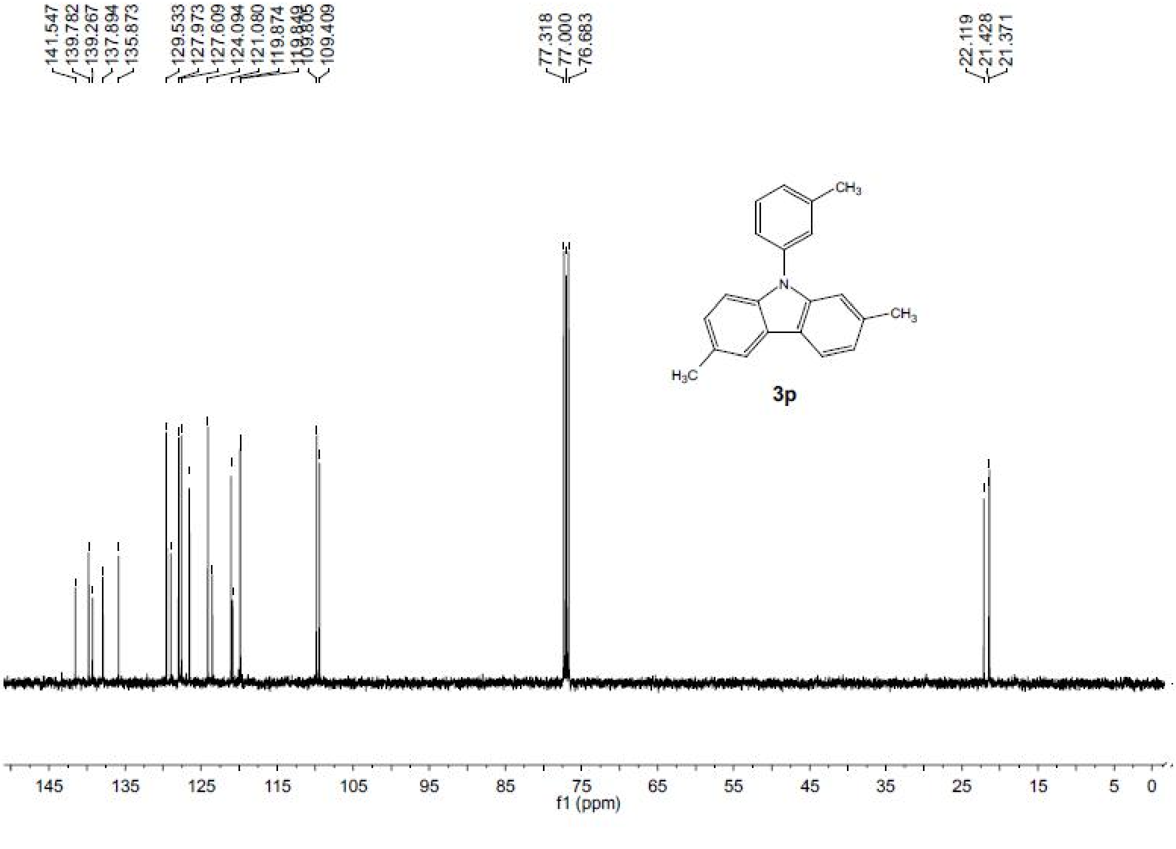
f1 (ppm)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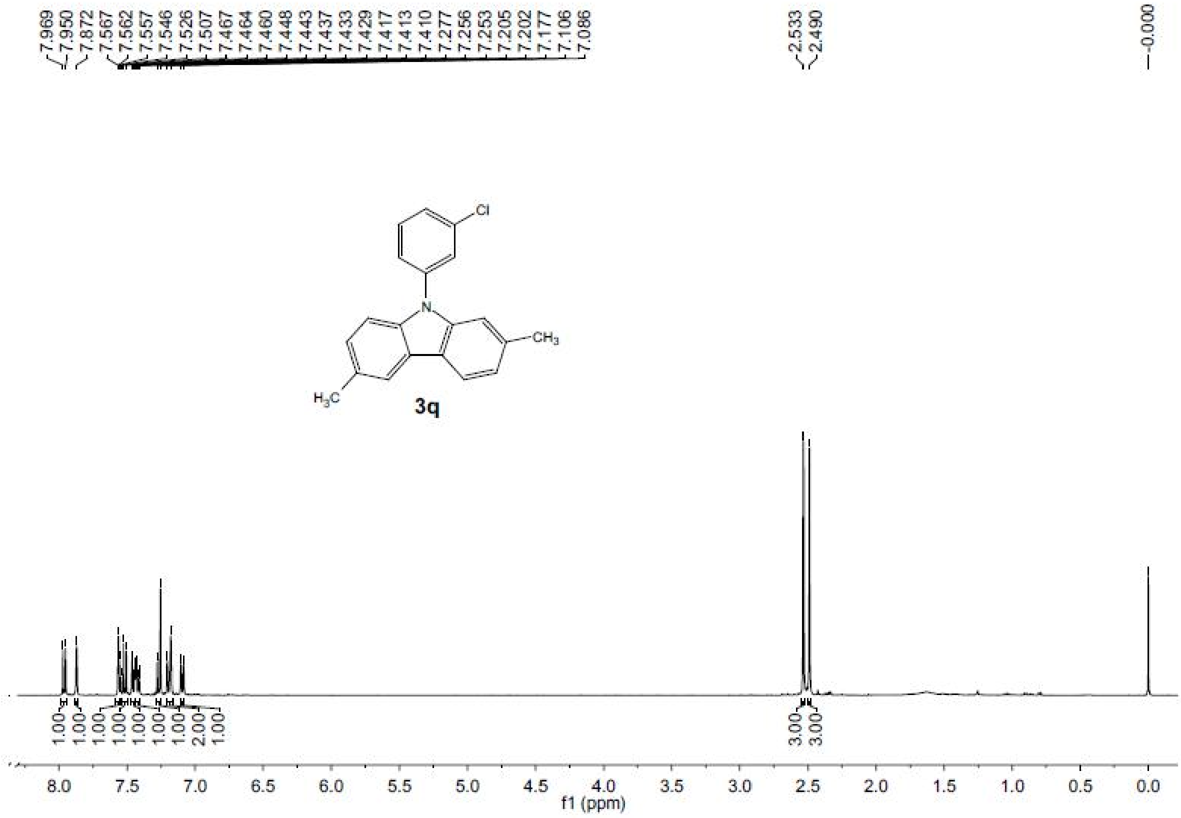

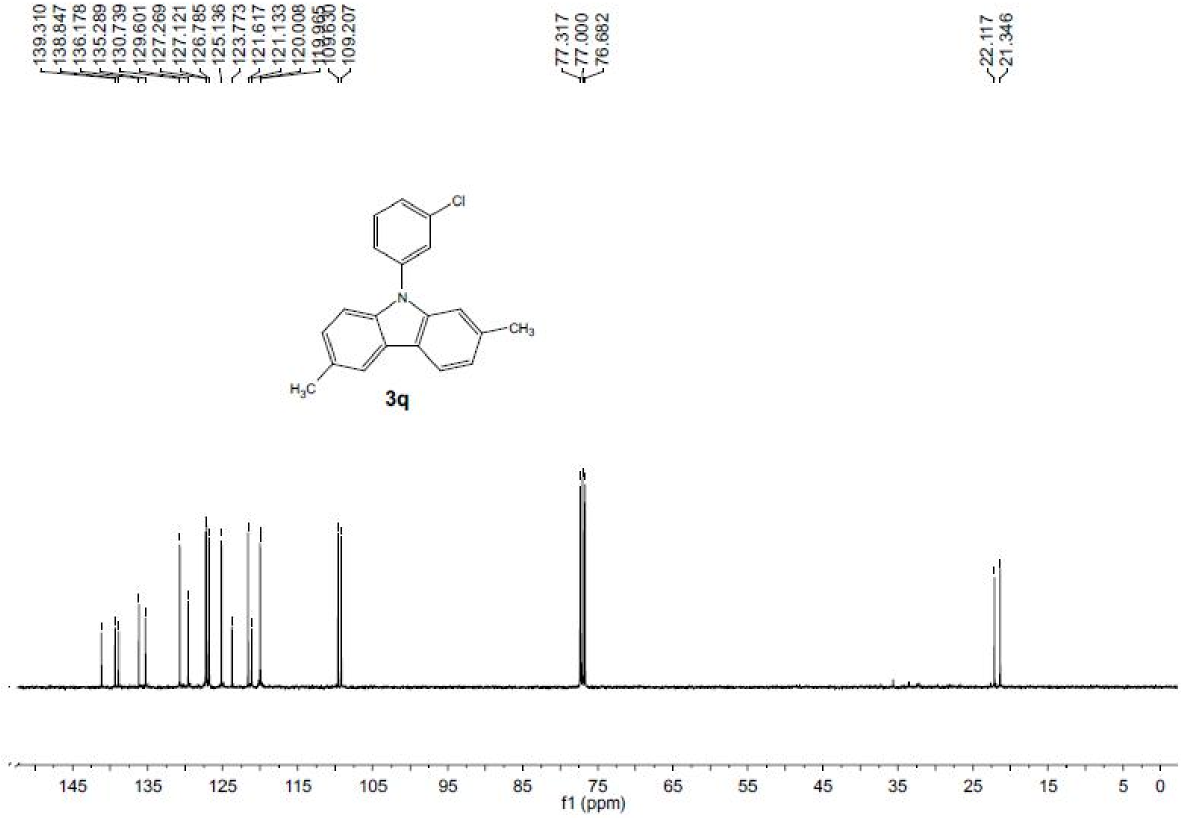

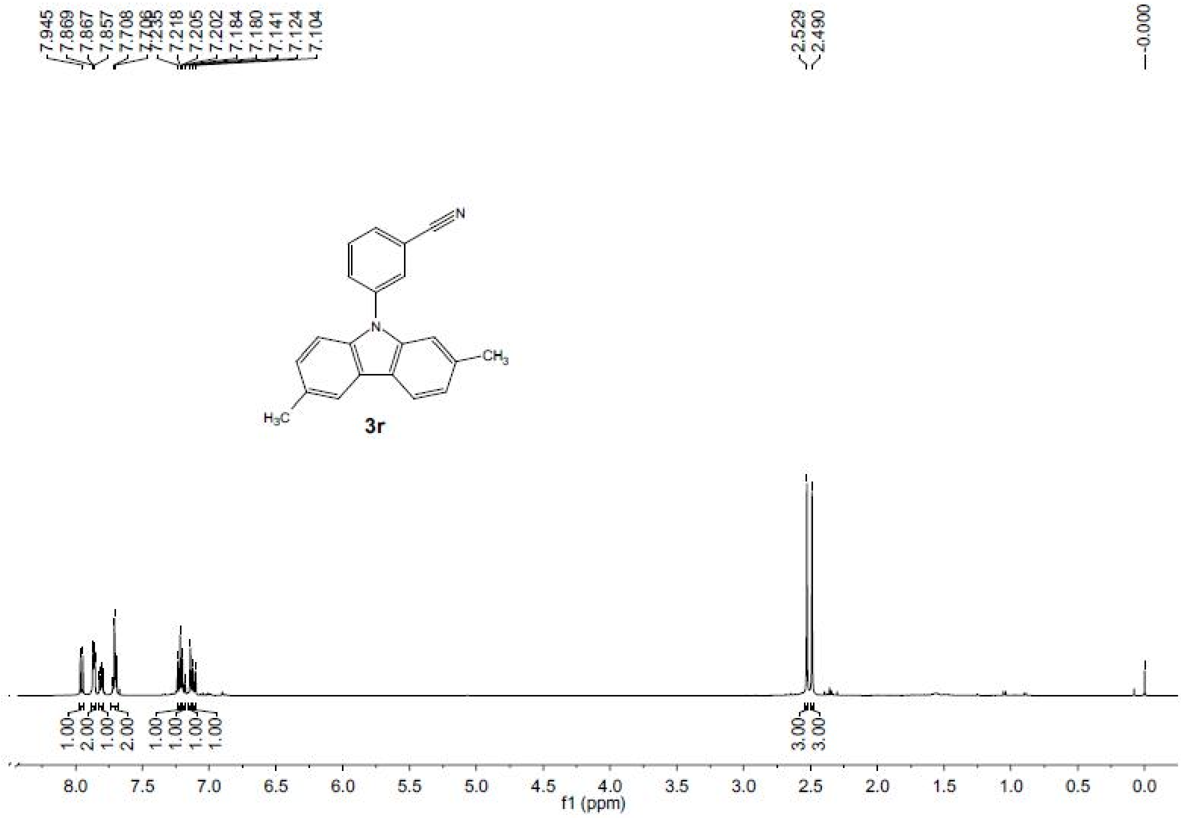
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7.867
7.857
7.708
7.706
7.235
7.218
7.205
7.202
7.184
7.180
7.141
7.124
7.104
2.529
2.490
0.000
N
CH3
H3C
3r
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
3.00
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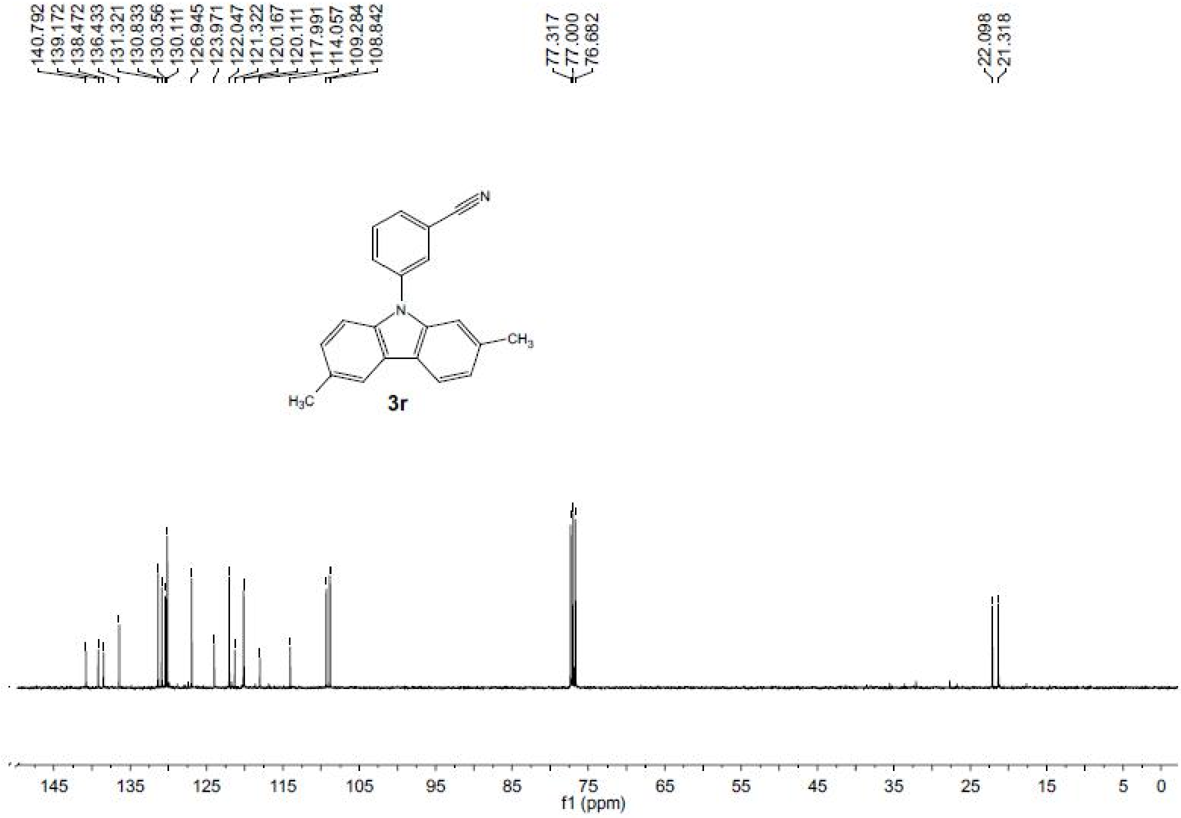
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120.167
120.111
117.991
114.057
109.284
108.842
77.317
77.000
76.682
22.098
21.318
N
CH3
H3C
3r
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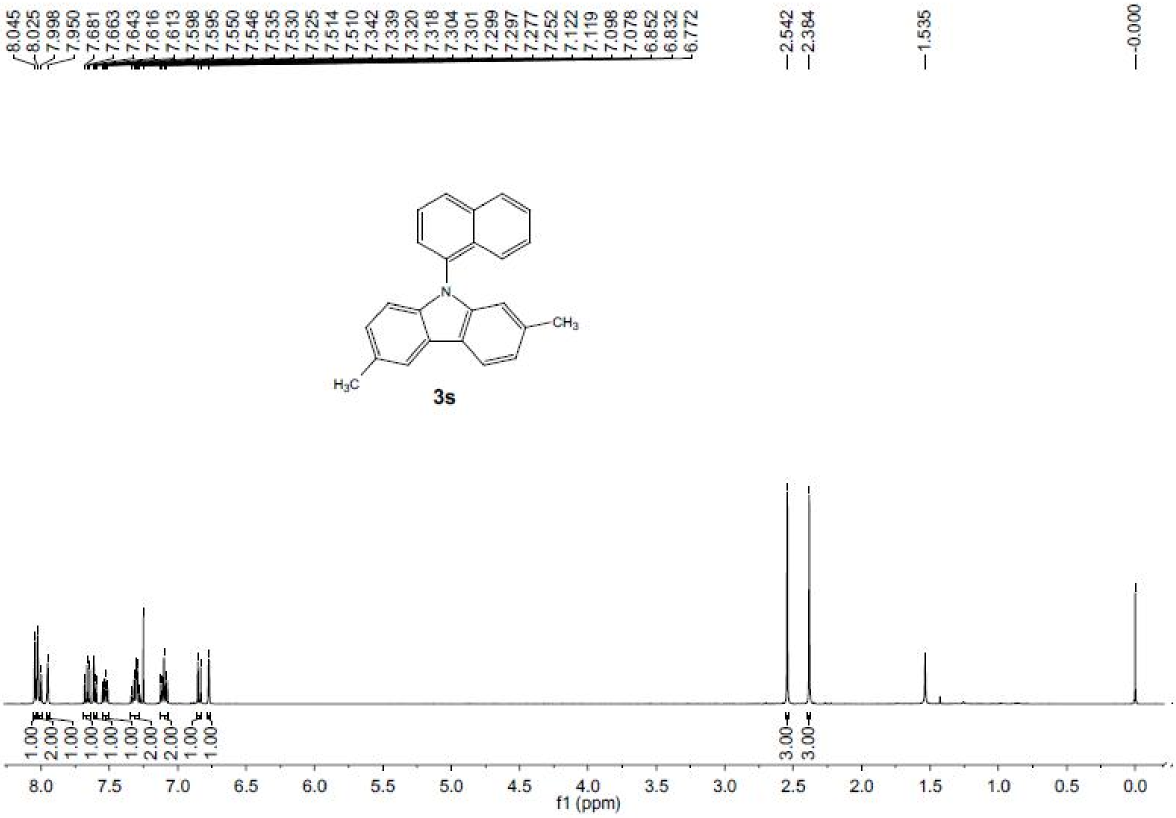
f1 (ppm)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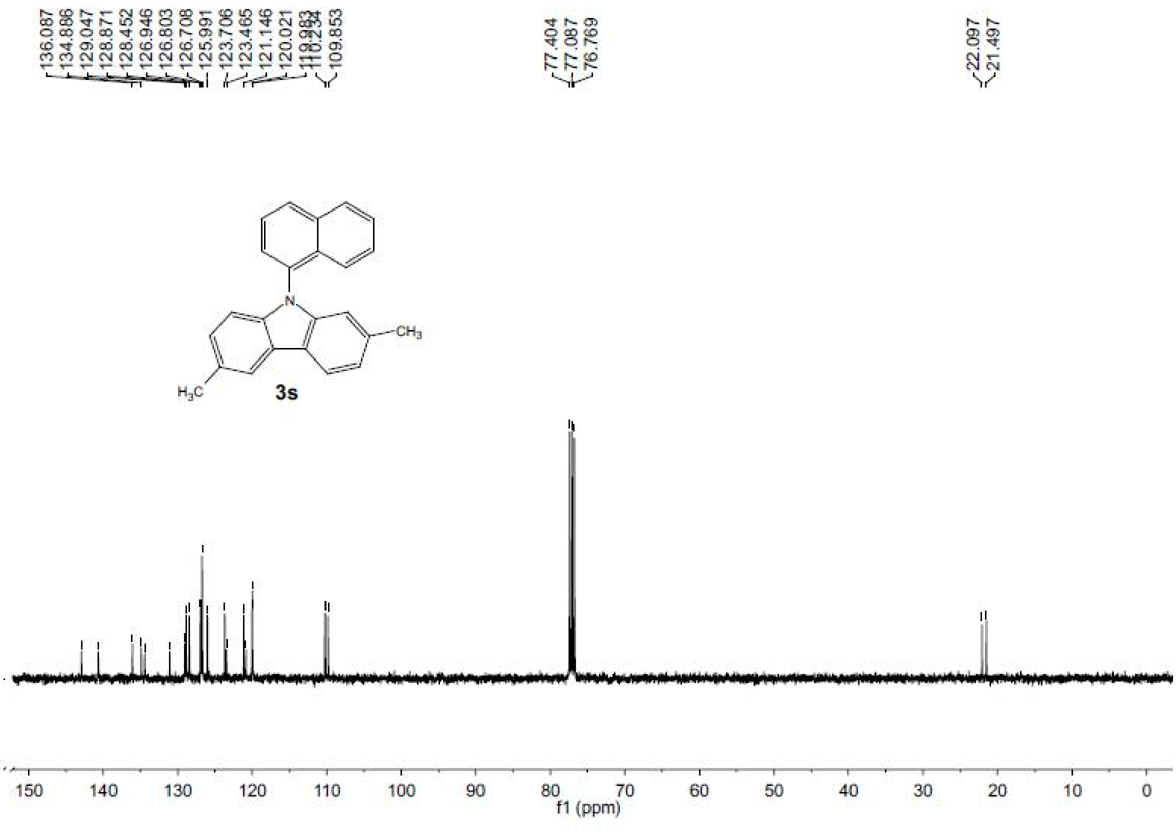
7.535
7.530
7.525
7.514
7.510
7.342
7.339
7.320
7.318
7.304
7.301
7.299
7.297
7.277
7.252
7.122
7.119
7.098
7.078
6.852
6.832
6.772
2.542
2.384
1.535
0.000
CH3
H3C
3s
1.00
2.00
1.00
1.00
1.00
1.00
2.00
2.00
1.00
1.00
3.00
3.00
f1 (ppm)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126.708
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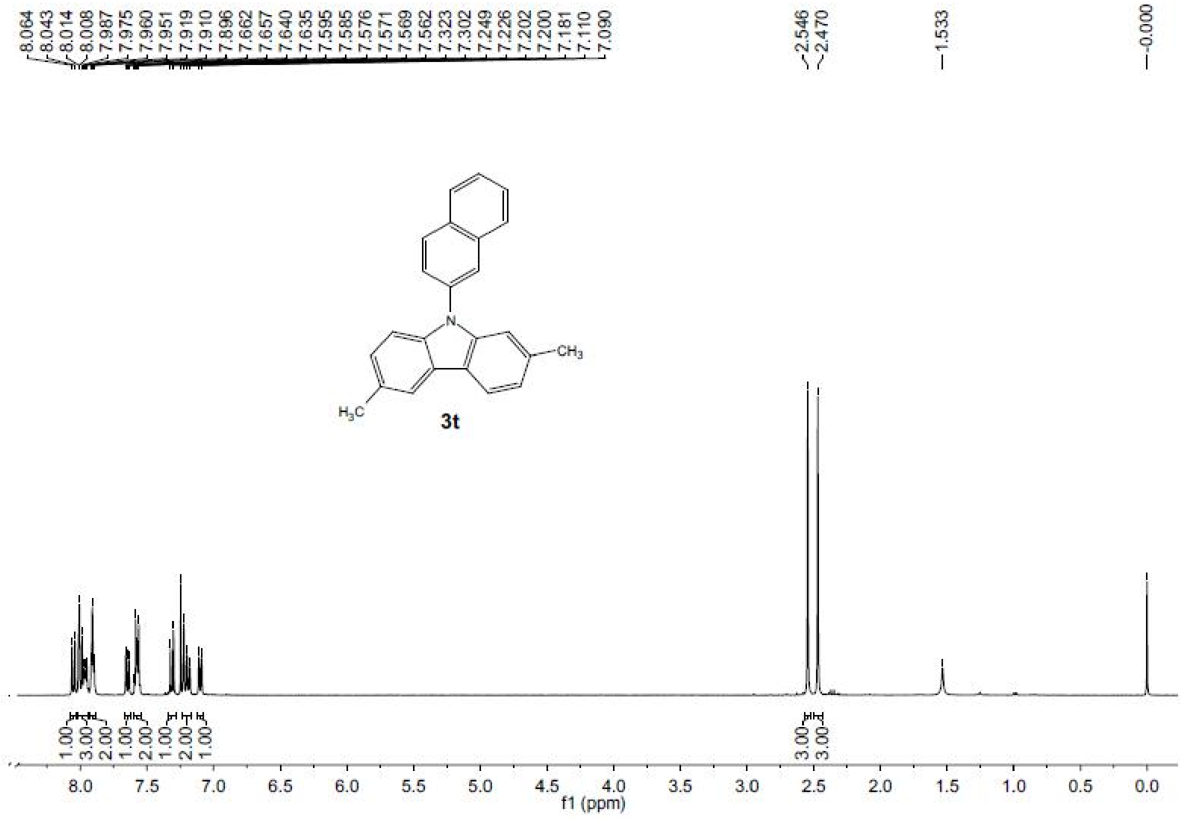
H3C
3s
f1 (ppm)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7.640
7.635
7.595
7.585
7.576
7.571
7.569
7.562
7.323
7.302
7.249
7.226
7.202
7.200
7.181
7.110
7.090
2.546
2.470
1.533
-0.000
CH3
H3C
3t
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3.00
2.00
1.00
2.00
1.00
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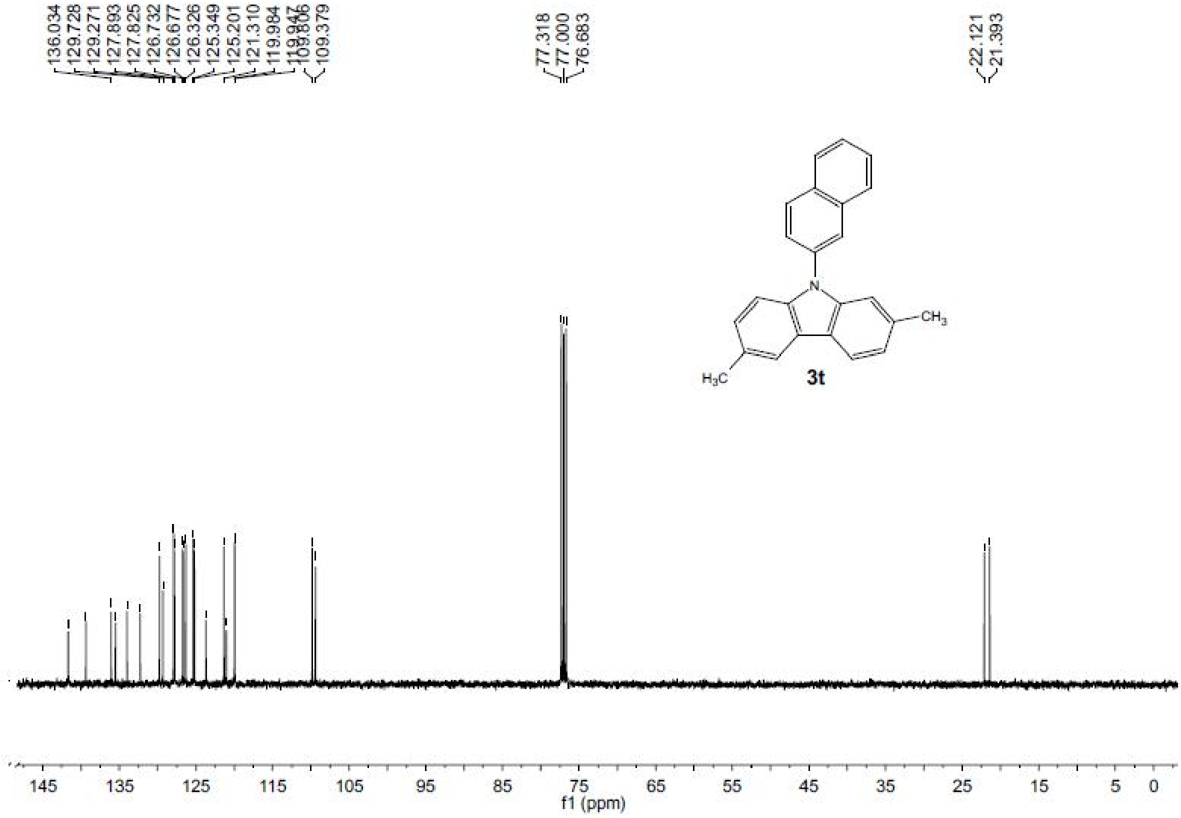
1.00
3.00
3.00
f1 (ppm)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125.201
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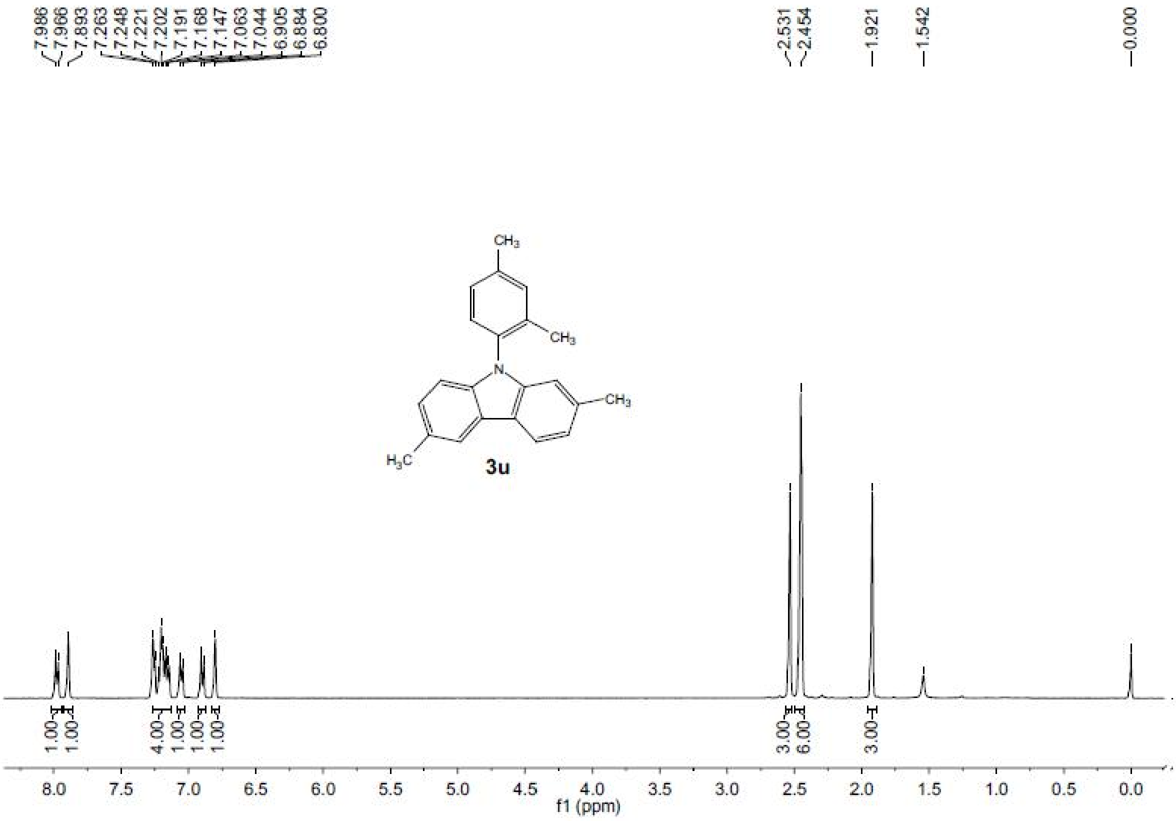
H3C
3t
f1 (ppm)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6.905
6.884
6.800
2.531
2.454
1.921
1.542
0.000
CH3
CH3
CH3
H3C
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1.00
4.00
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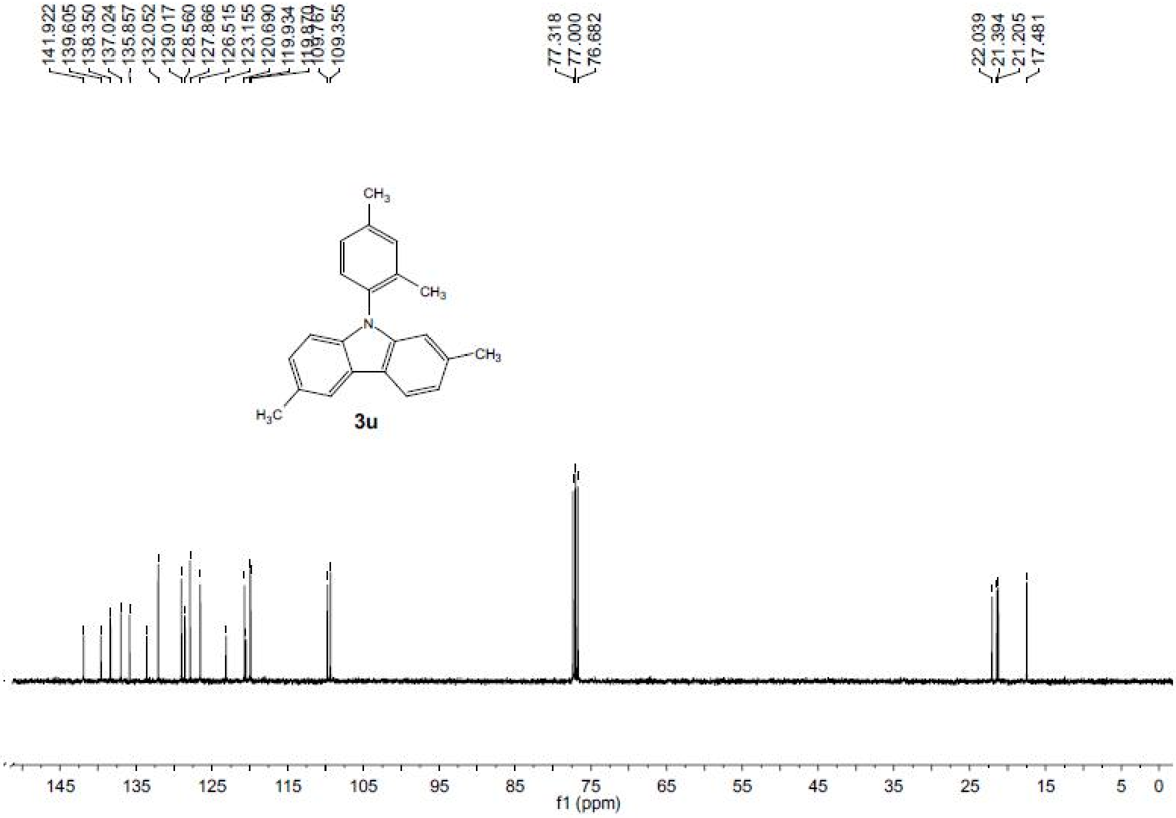
3.00
6.00
3.00
f1 (ppm)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119.934
119.870
109.767
109.355
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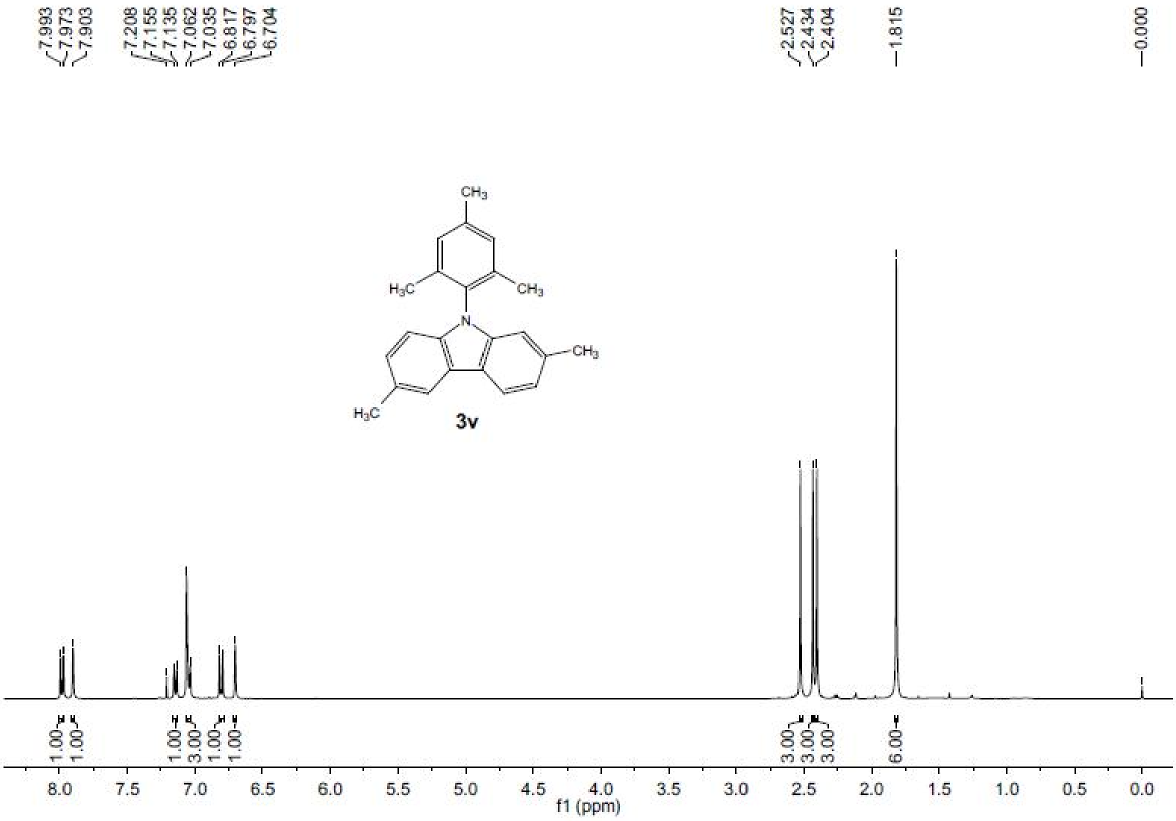
CH3
CH3
CH3
H3C
3u
f1 (ppm)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7.135
7.062
7.035
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6.797
6.704
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2.434
2.404
1.815
0.000
CH3
H3C
CH3
N
CH3
H3C
3v
1.00
1.00
1.00
3.00
1.00
1.00
3.00
3.00
3.00
6.00
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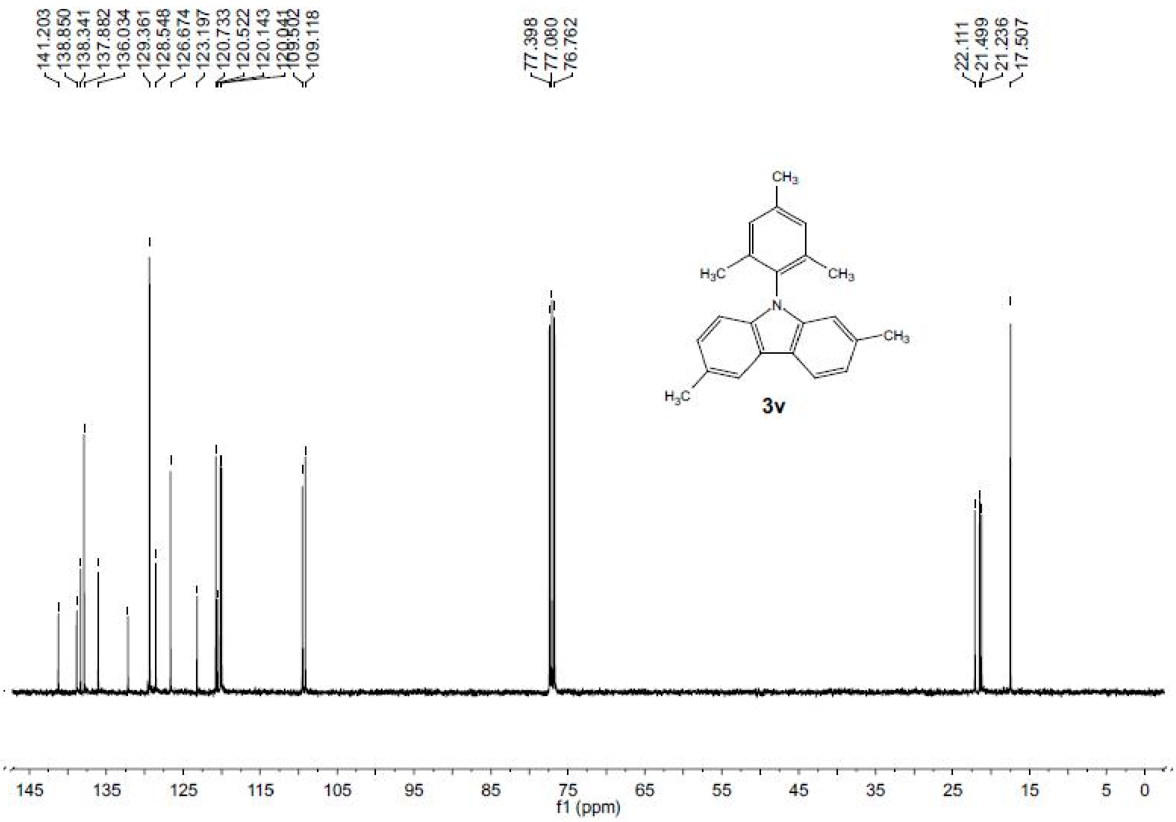
f1 (ppm)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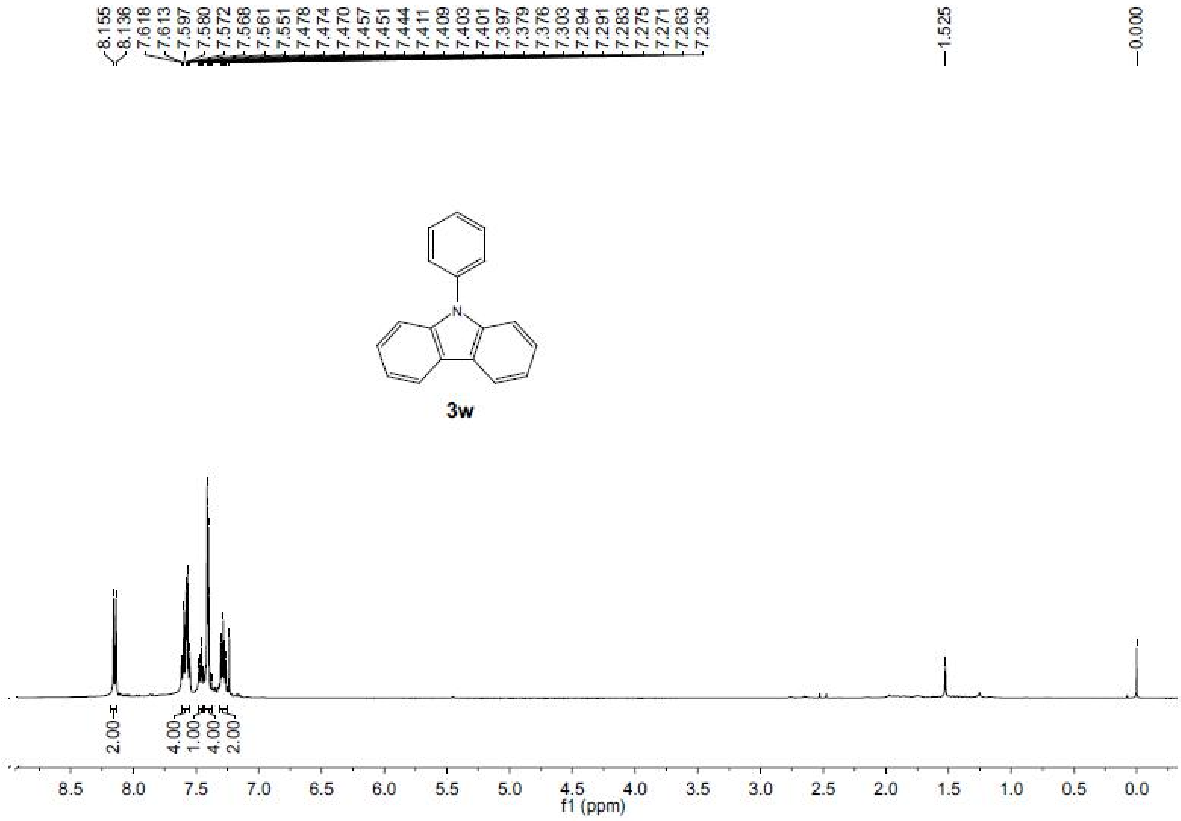
109.502
109.118
77.398
77.080
76.762
22.111
21.499
21.236
17.507
CH3
H3C
CH3
N
CH3
H3C
3v
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)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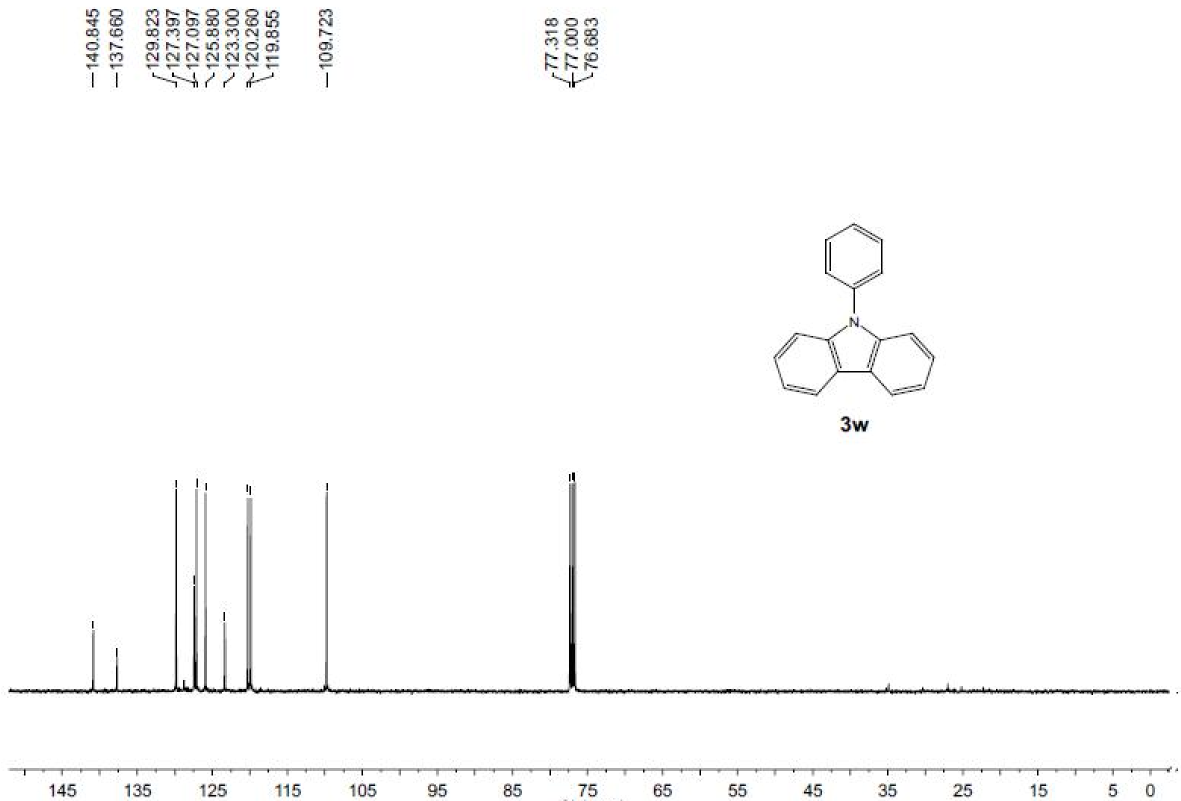
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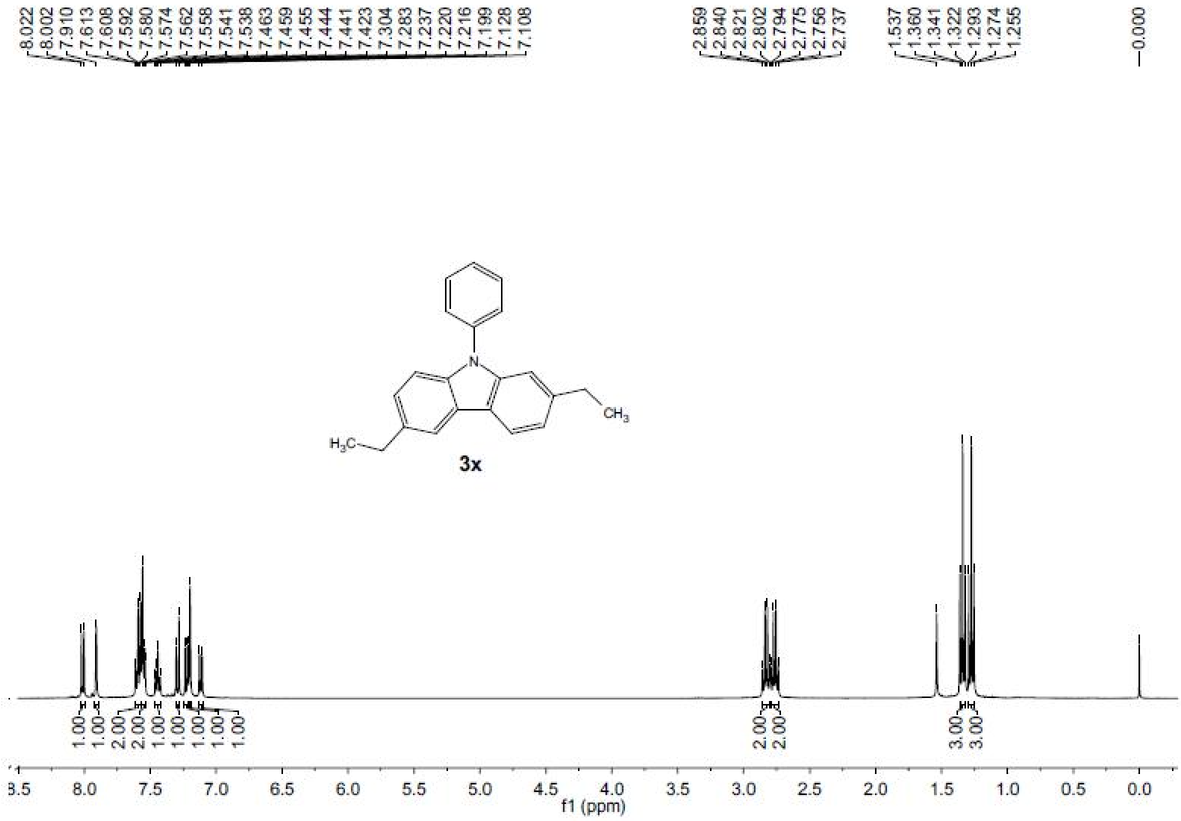

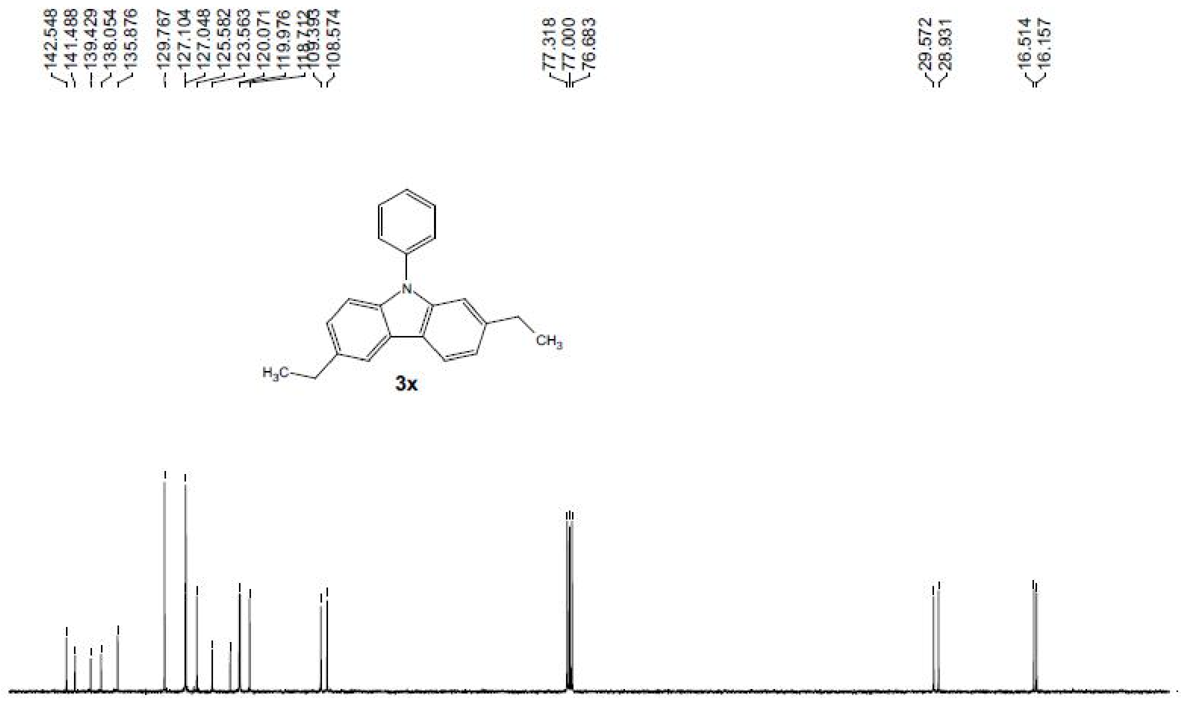

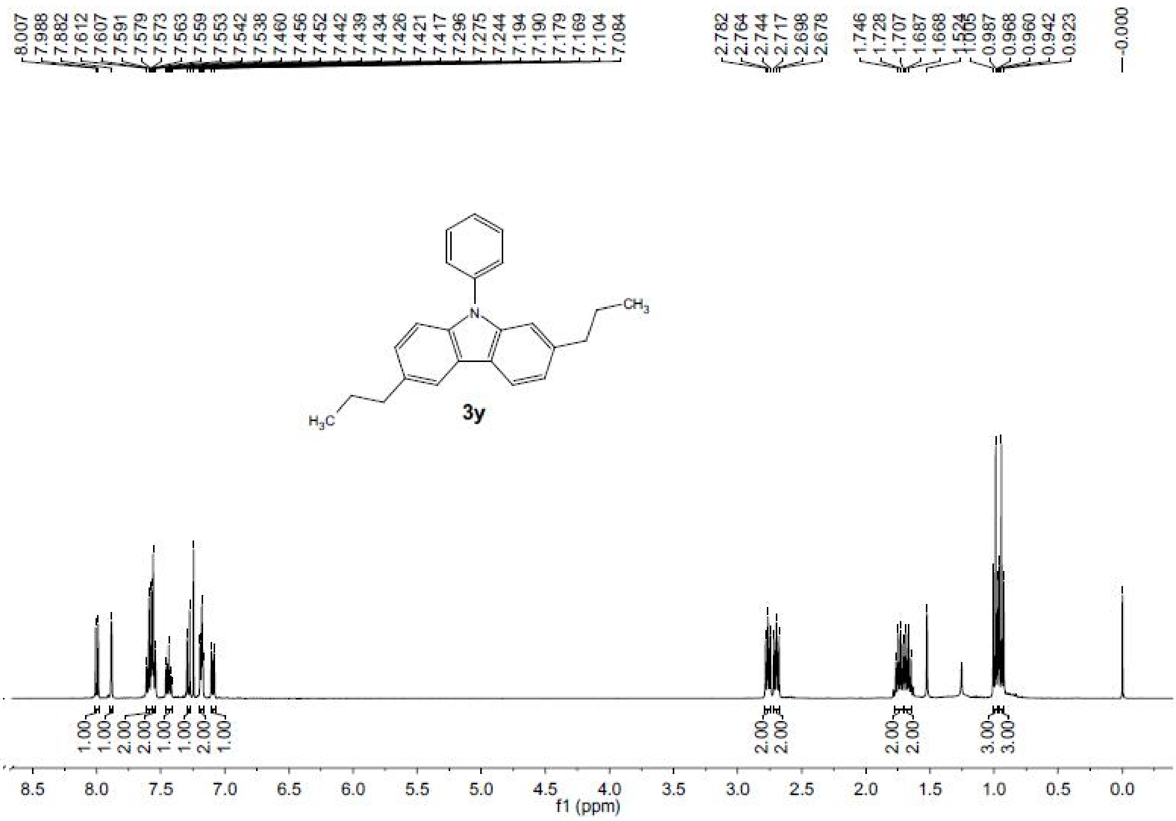
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7.559
7.553
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7.538
7.460
7.456
7.452
7.442
7.439
7.434
7.426
7.421
7.417
7.296
7.275
7.244
7.194
7.190
7.179
7.169
7.104
7.084
2.782
2.764
2.744
2.717
2.698
2.678
1.746
1.728
1.707
1.687
1.668
1.524
1.005
0.987
0.968
0.960
0.942
0.923
-0.000
CH3
H3C
3y
1.00
1.00
2.00
2.00
1.00
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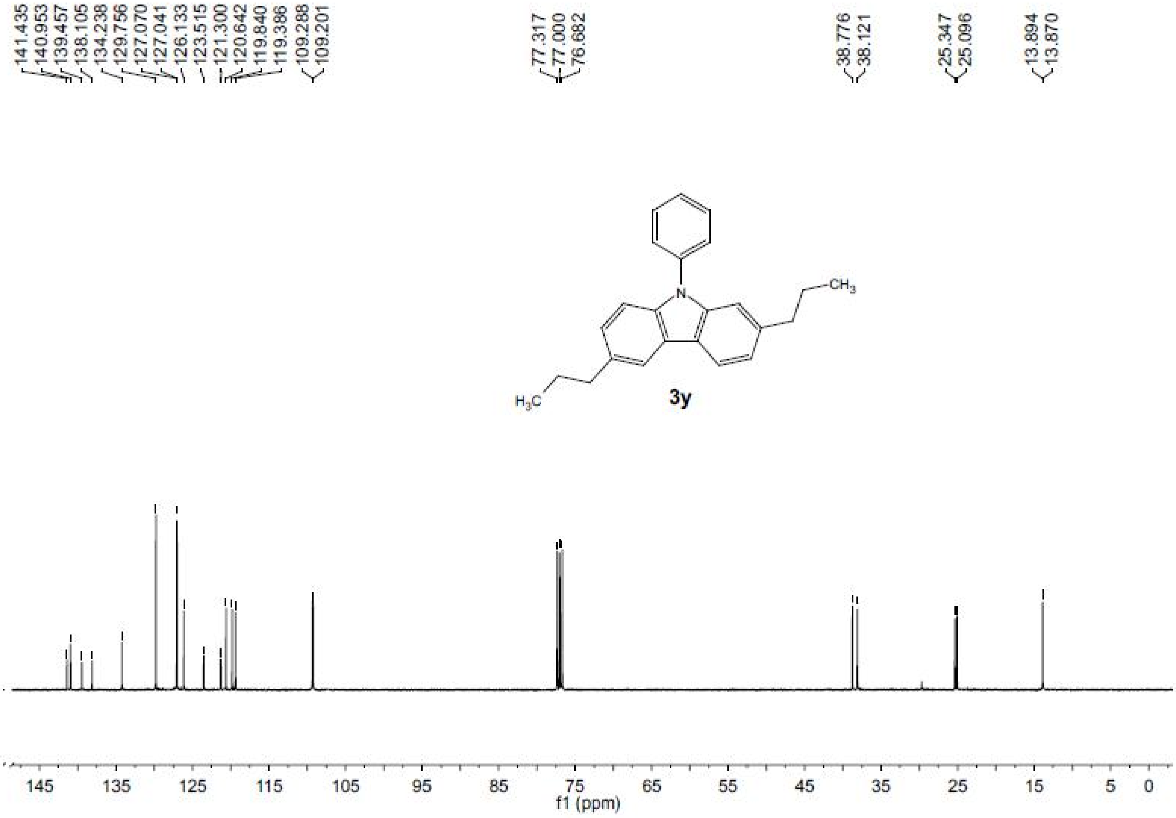
2.00
1.00
2.00
2.00
2.00
2.00
3.00
3.00
f1 (ppm)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123.515
121.300
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119.840
119.386
109.288
109.201
77.317
77.000
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38.121
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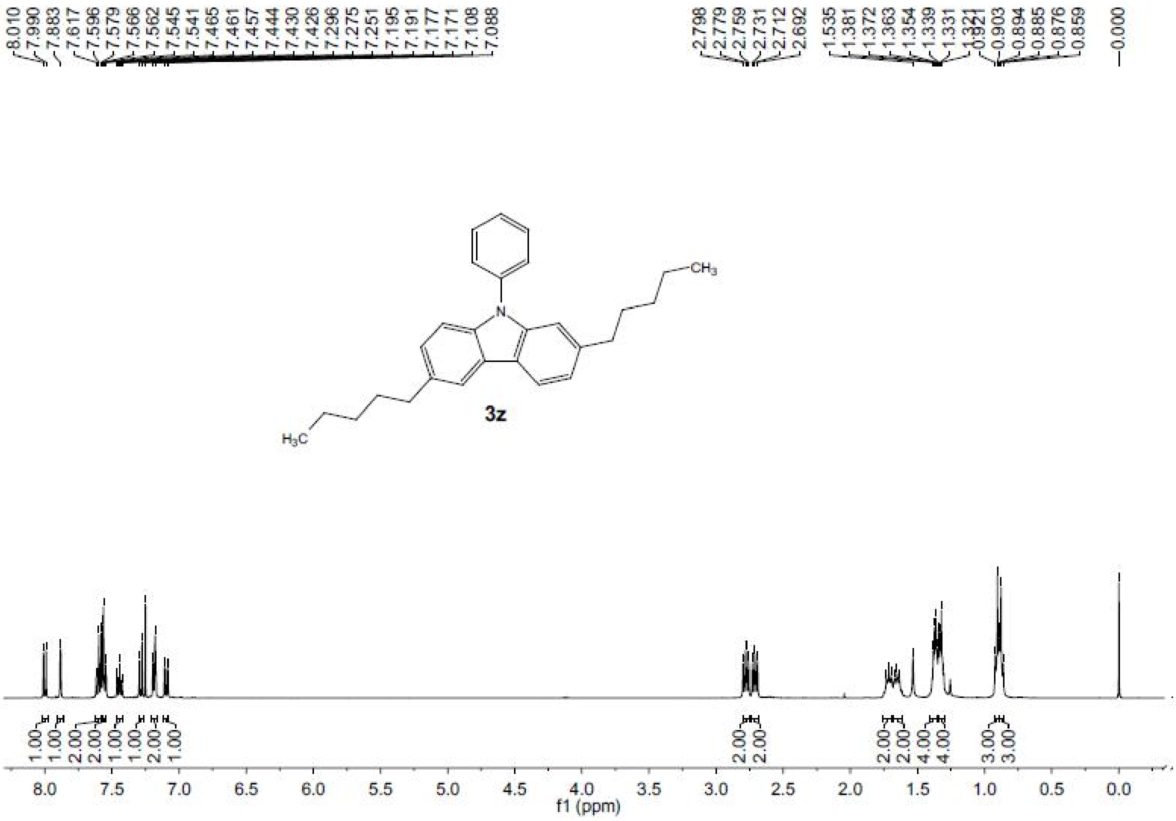
25.096
13.894
13.870
CH3
H3C
3y
f1 (ppm)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7.562
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7.461
7.457
7.444
7.430
7.426
7.296
7.275
7.251
7.195
7.191
7.177
7.171
7.108
7.088
2.798
2.779
2.759
2.731
2.712
2.692
1.535
1.381
1.372
1.363
1.354
1.339
1.331
1.321
0.921
0.903
0.894
0.885
0.876
0.859
0.000
CH3
H3C
3z
1.00
1.00
2.00
2.00
1.00
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2.00
2.00
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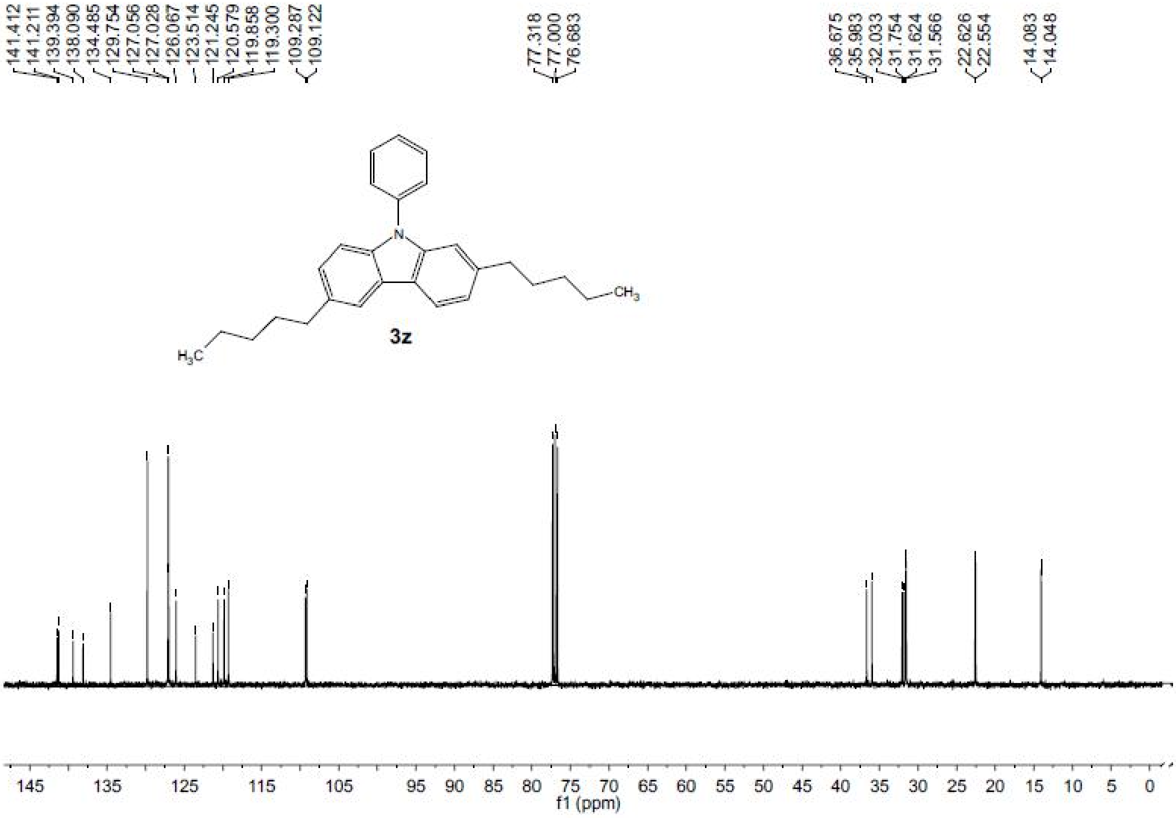
f1 (ppm)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123.514
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120.579
119.858
119.300
109.287
109.122
77.318
77.000
76.683
36.675
35.983
32.033
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31.566
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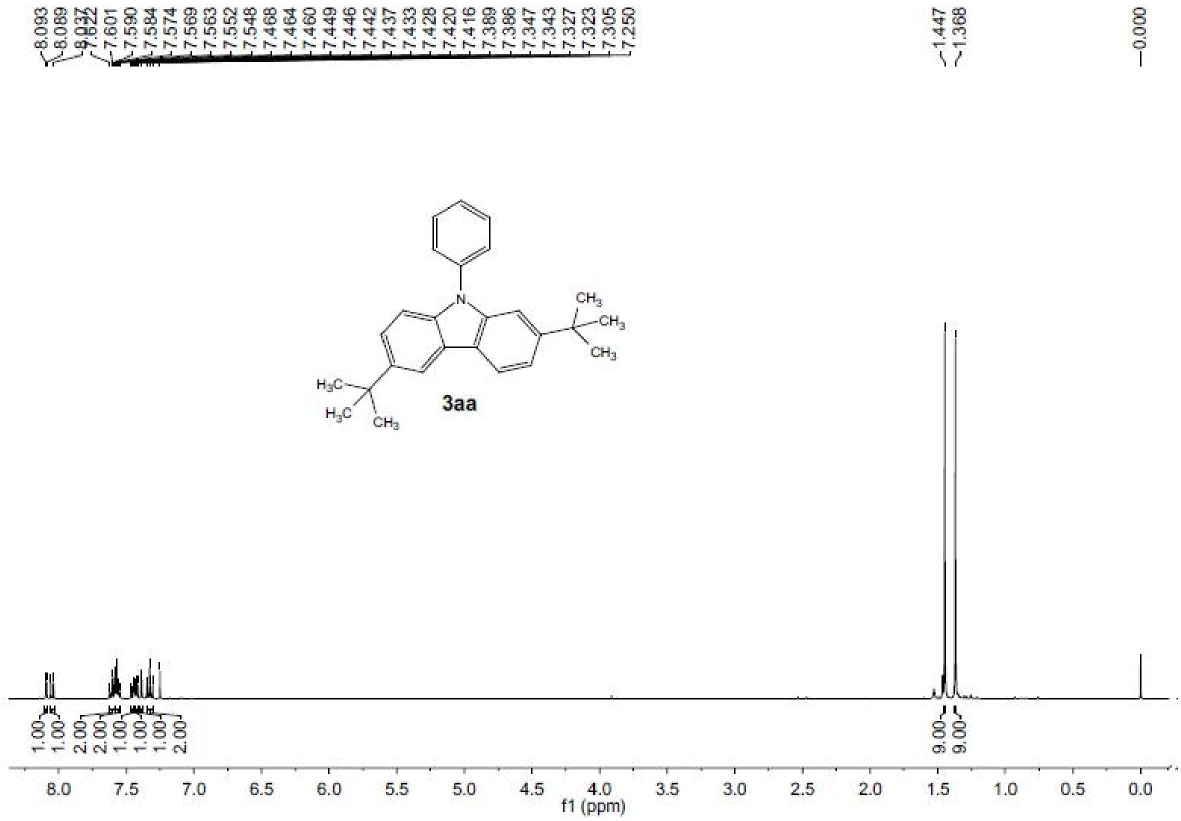
22.554
14.083
14.048
CH3
H3C
3z
f1 (ppm)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7.468
7.464
7.460
7.449
7.446
7.442
7.437
7.433
7.428
7.420
7.416
7.389
7.386
7.347
7.343
7.327
7.323
7.305
7.250
1.447
1.368
0.000
3aa
1.00
1.00
2.00
2.00
1.00
1.00
1.00
2.00
9.00
9.00
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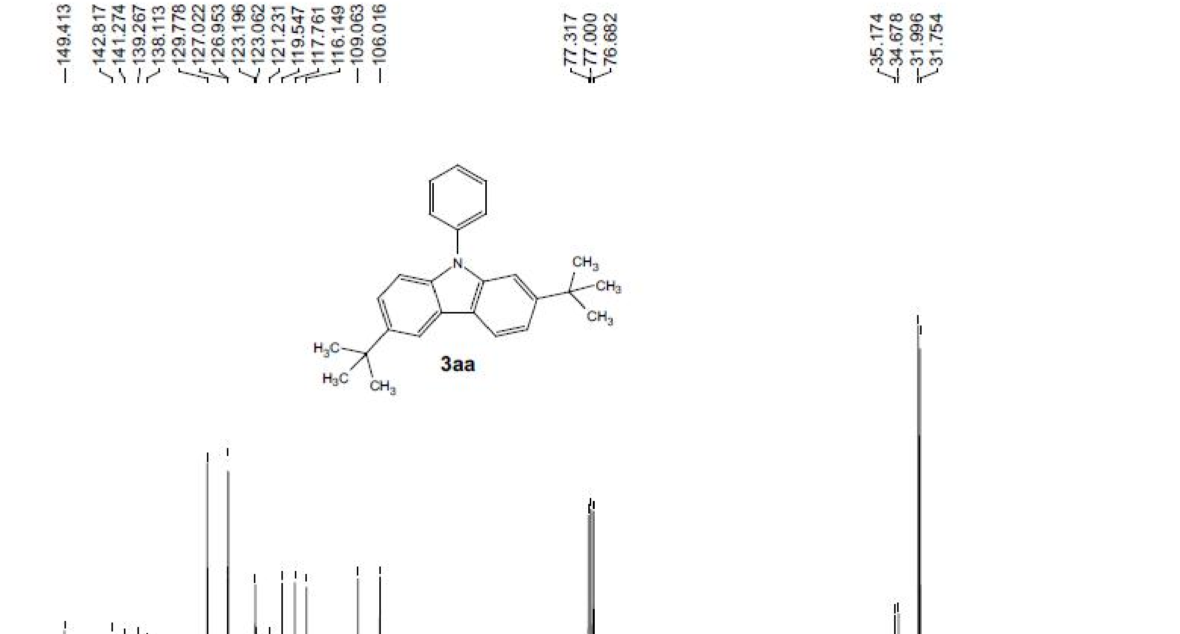
f1 (ppm)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117.761
116.149
109.063
106.016
77.317
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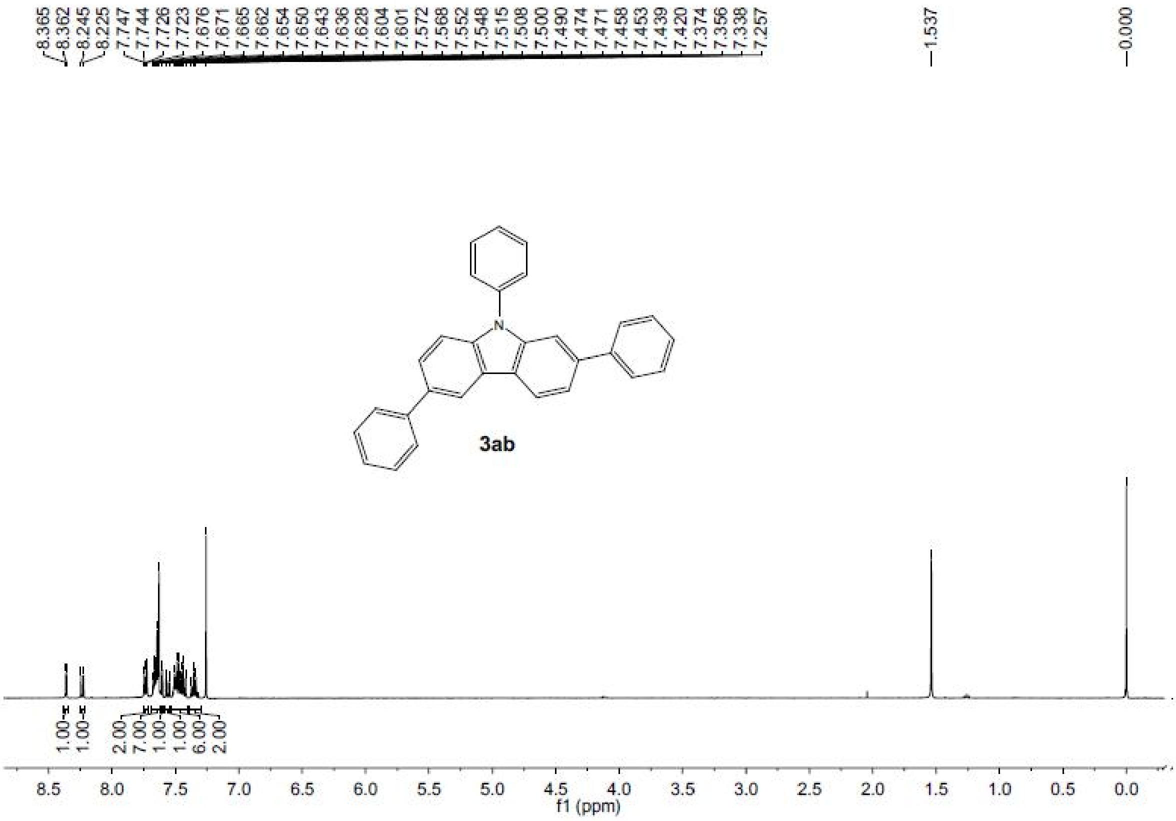
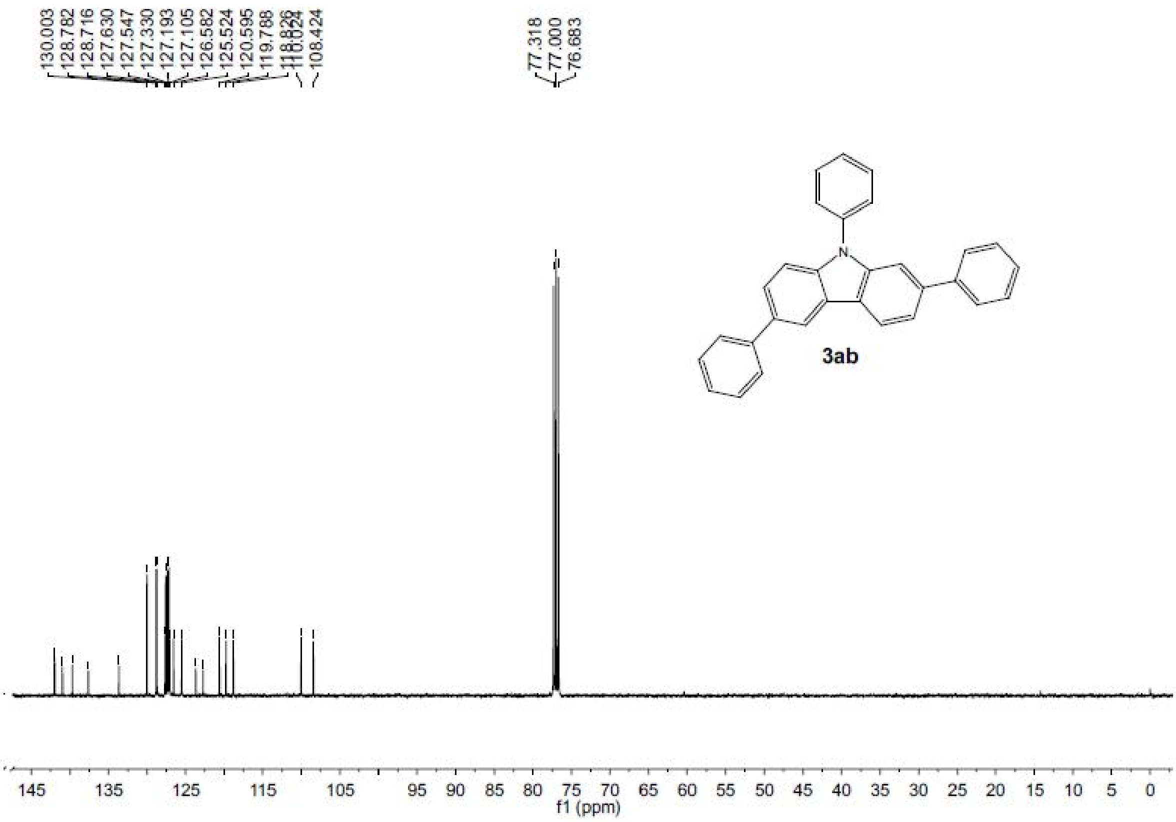
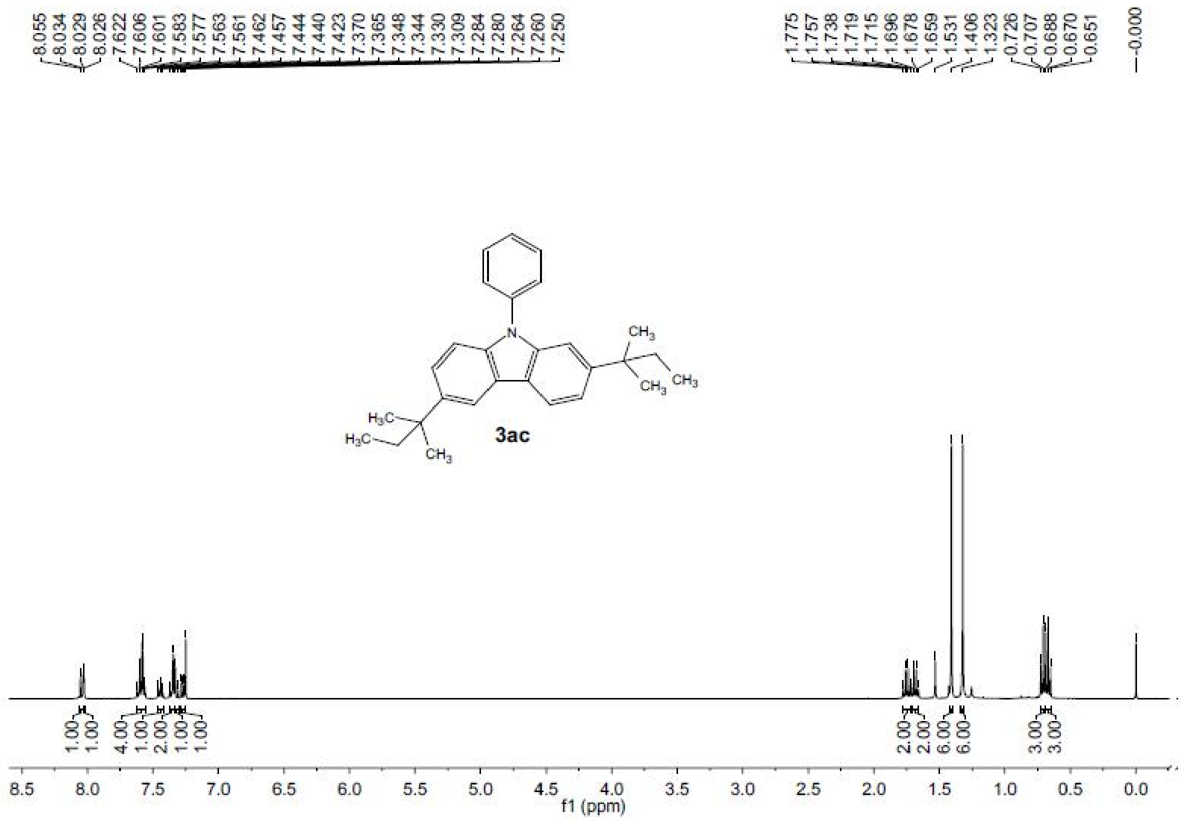
f1 (ppm)



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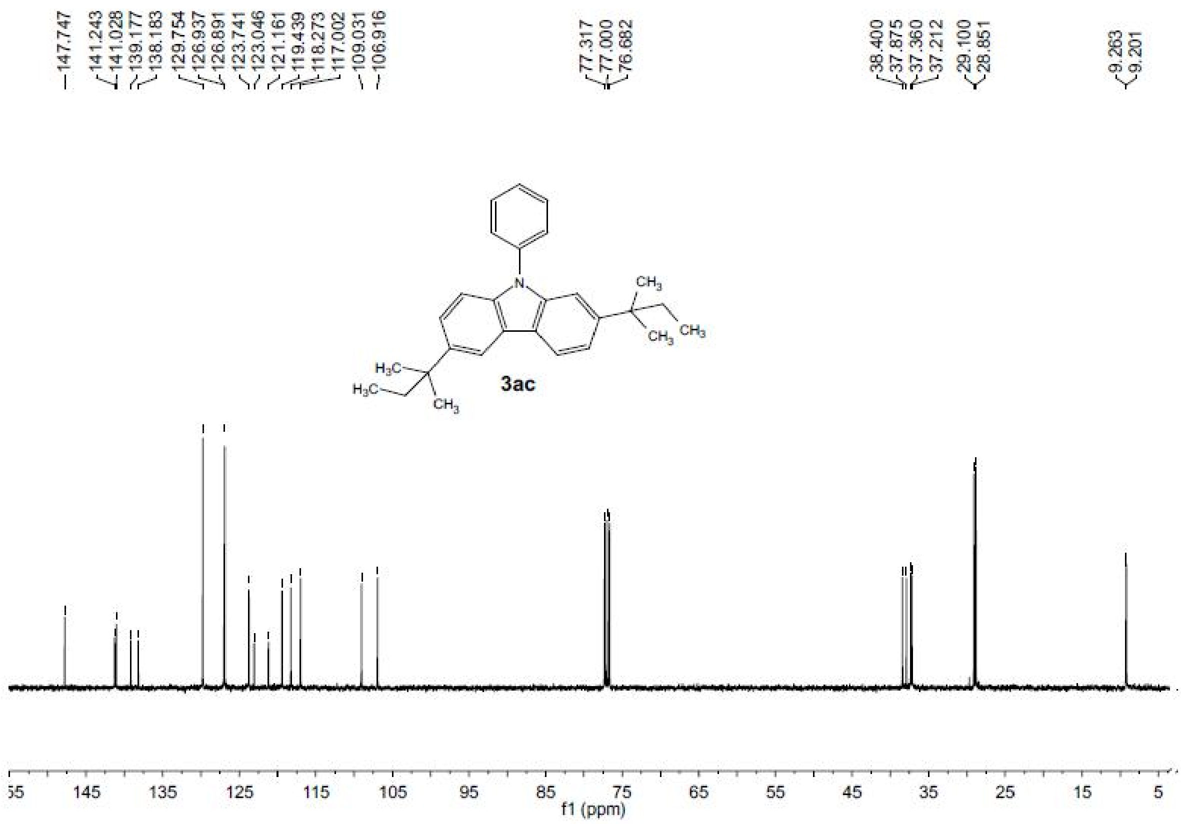
1.775 1.757 1.738 1.719 1.715 1.696 1.678 1.659 1.531 1.406 1.323 0.726 0.707 0.688 0.670 0.651
0.000
CH3
CH3 CH3
H3C
H3C
CH3
N
3ac
1.00 1.00 4.00 1.00 2.00 1.00 1.00
2.00 2.00 6.00 6.00 3.00 3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.317 77.000 76.682
38.400 37.875 37.360 37.212 29.100 28.851
9.263 9.201
CH3
CH3 CH3
H3C
H3C
CH3
N
3ac
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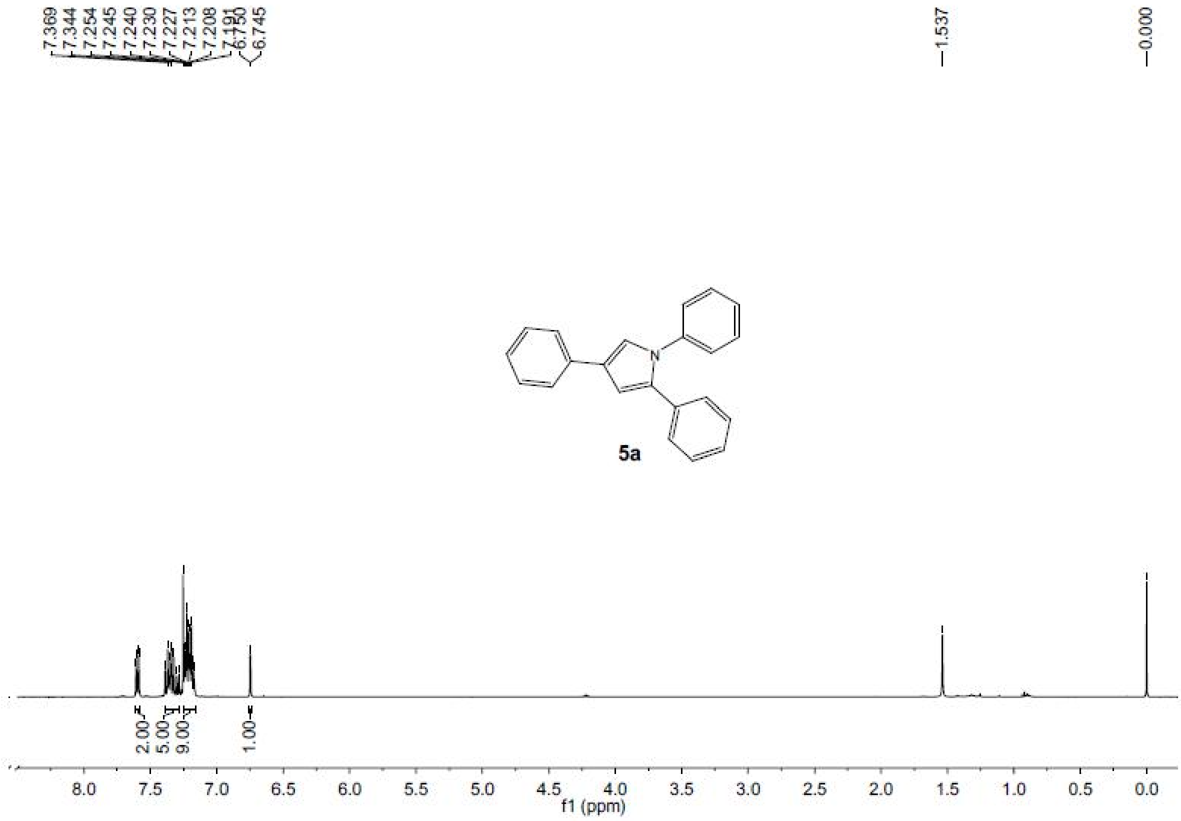
f1 (ppm)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0.000
N
5a
2.00
5.00
9.00
1.00
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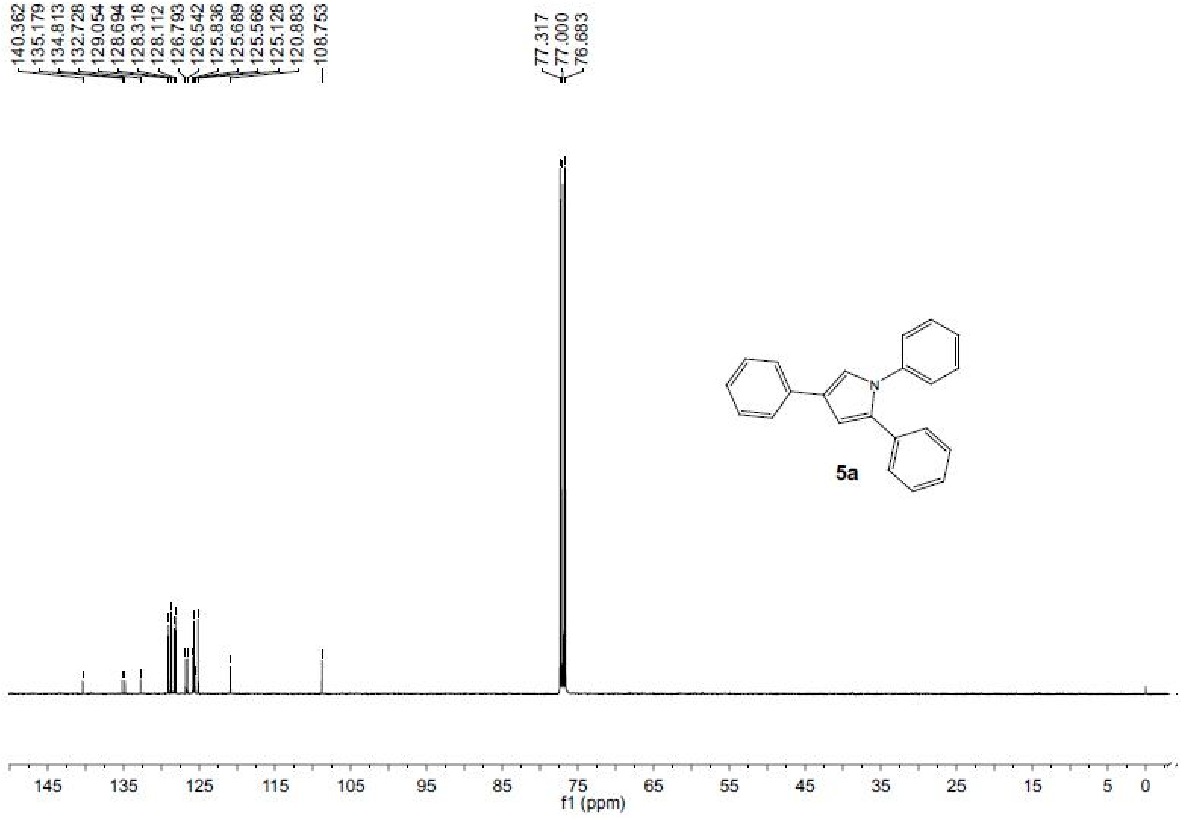
f1 (ppm)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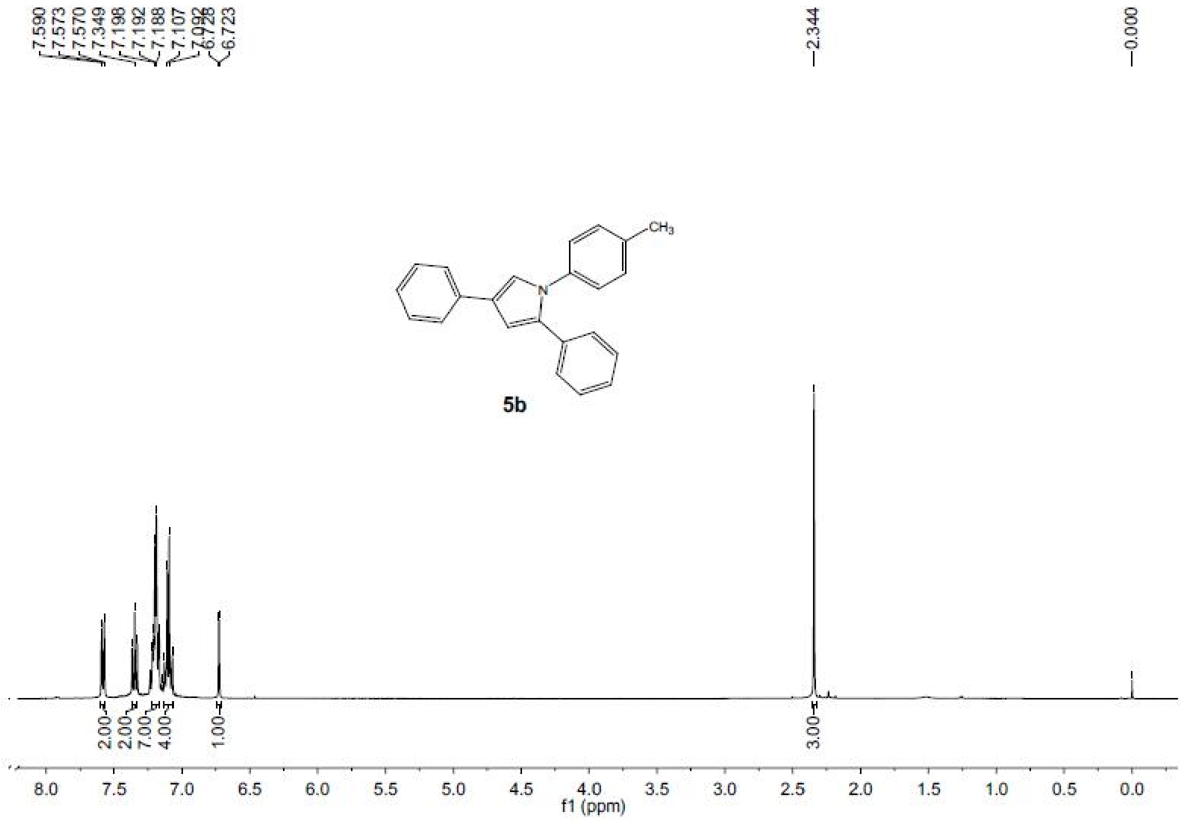
77.000
76.683
N
5a
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)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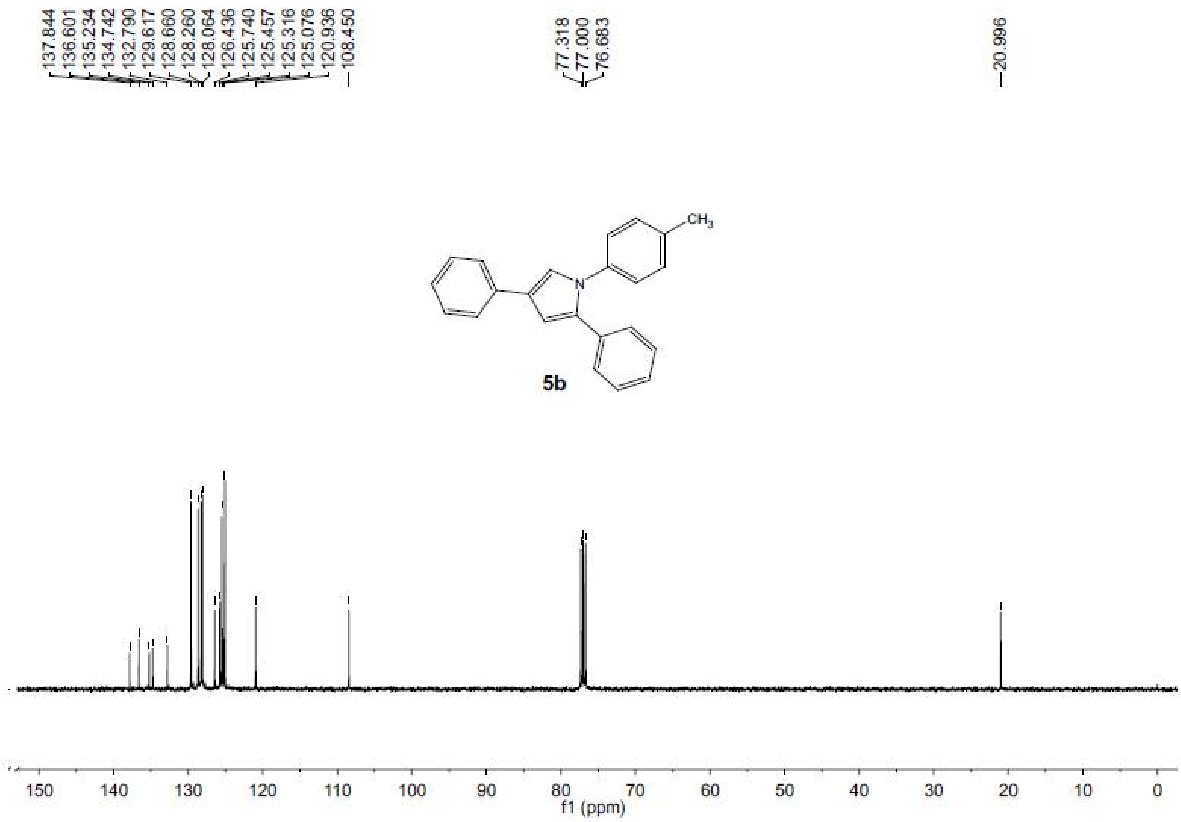
2.344
0.000
CH3
N
5b
2.00
2.00
7.00
4.00
1.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.076
120.936
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76.683
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CH3
N
5b
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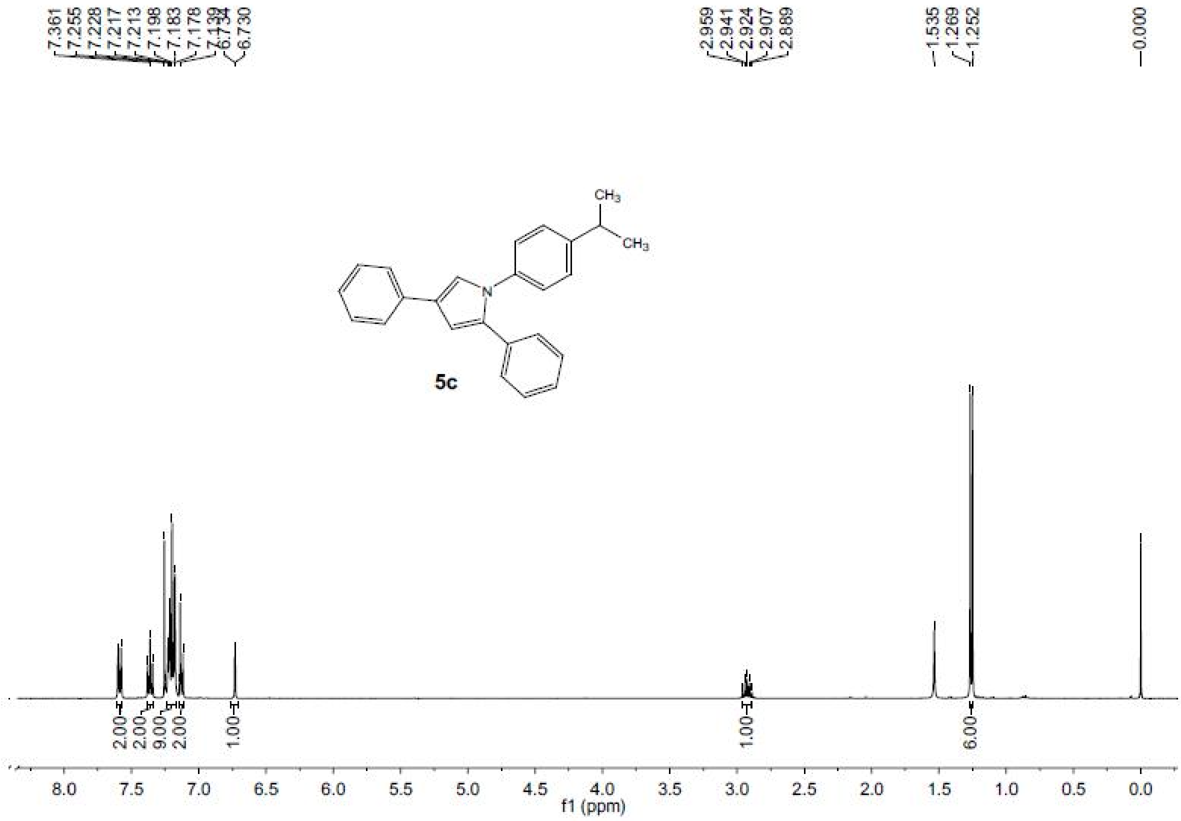
f1 (ppm)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2.889
1.535
1.269
1.252
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CH3
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5c
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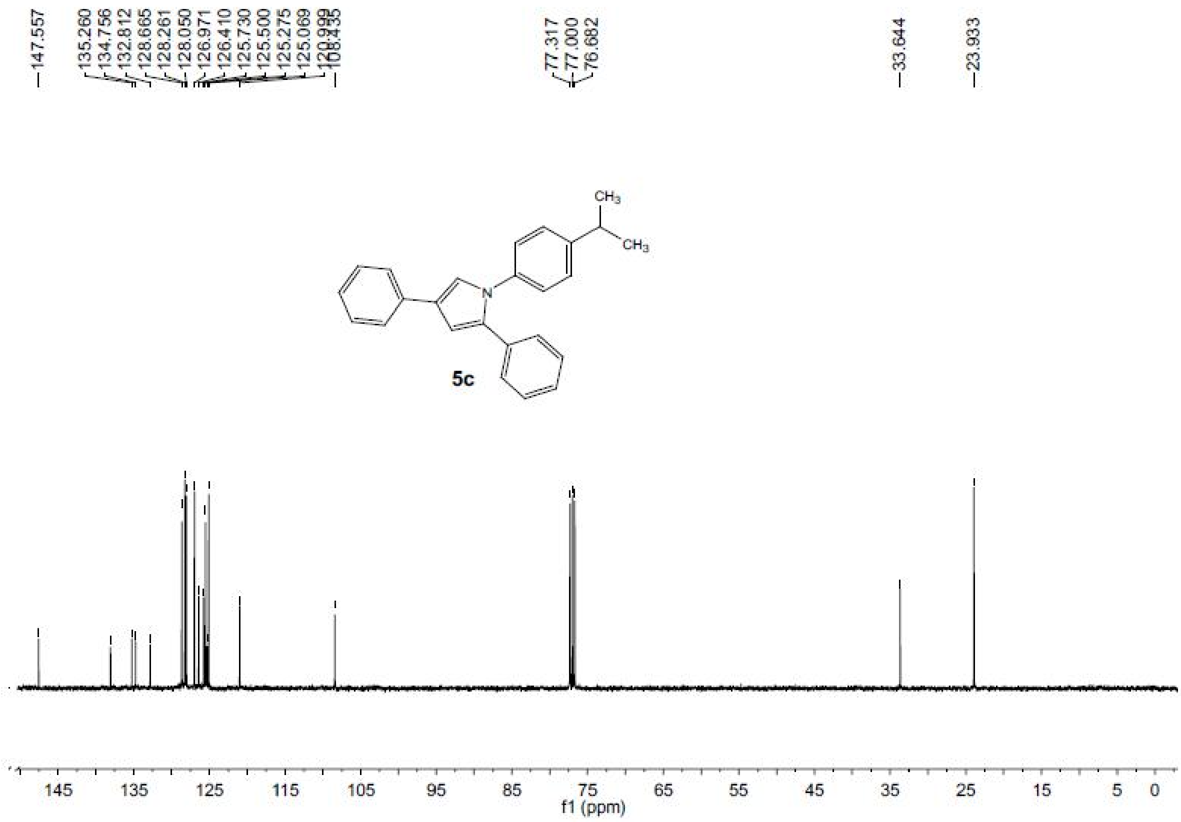
2.00
9.00
2.00
1.00
1.00
6.00
f1 (ppm)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77.000
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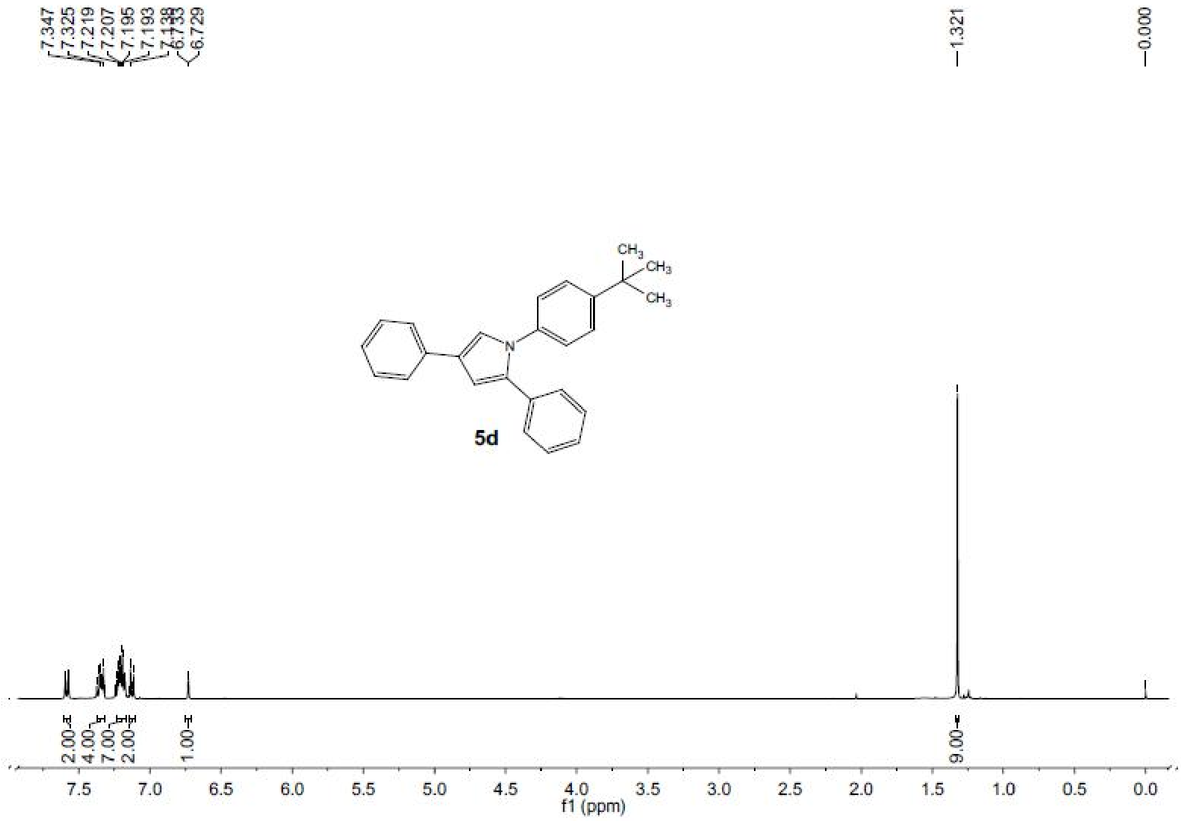
CH3
CH3
N
5c
f1 (ppm)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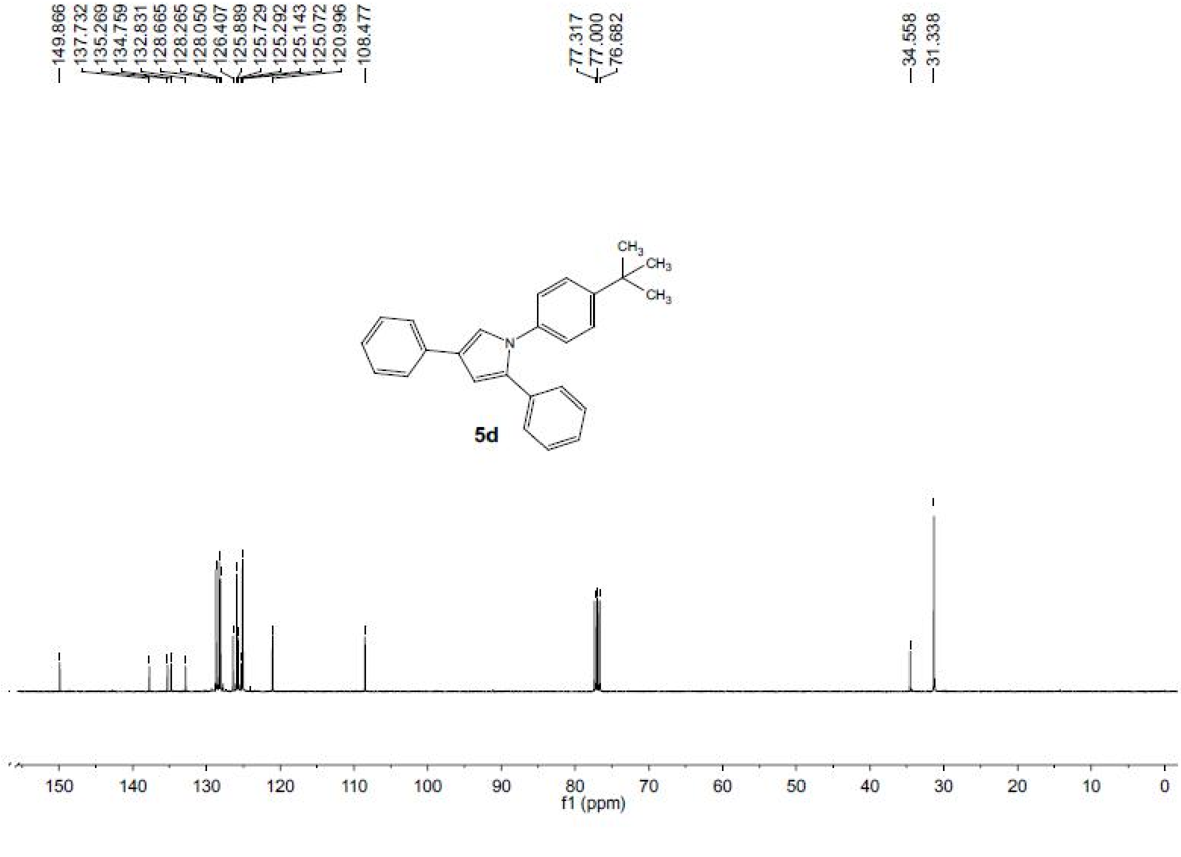
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125.072
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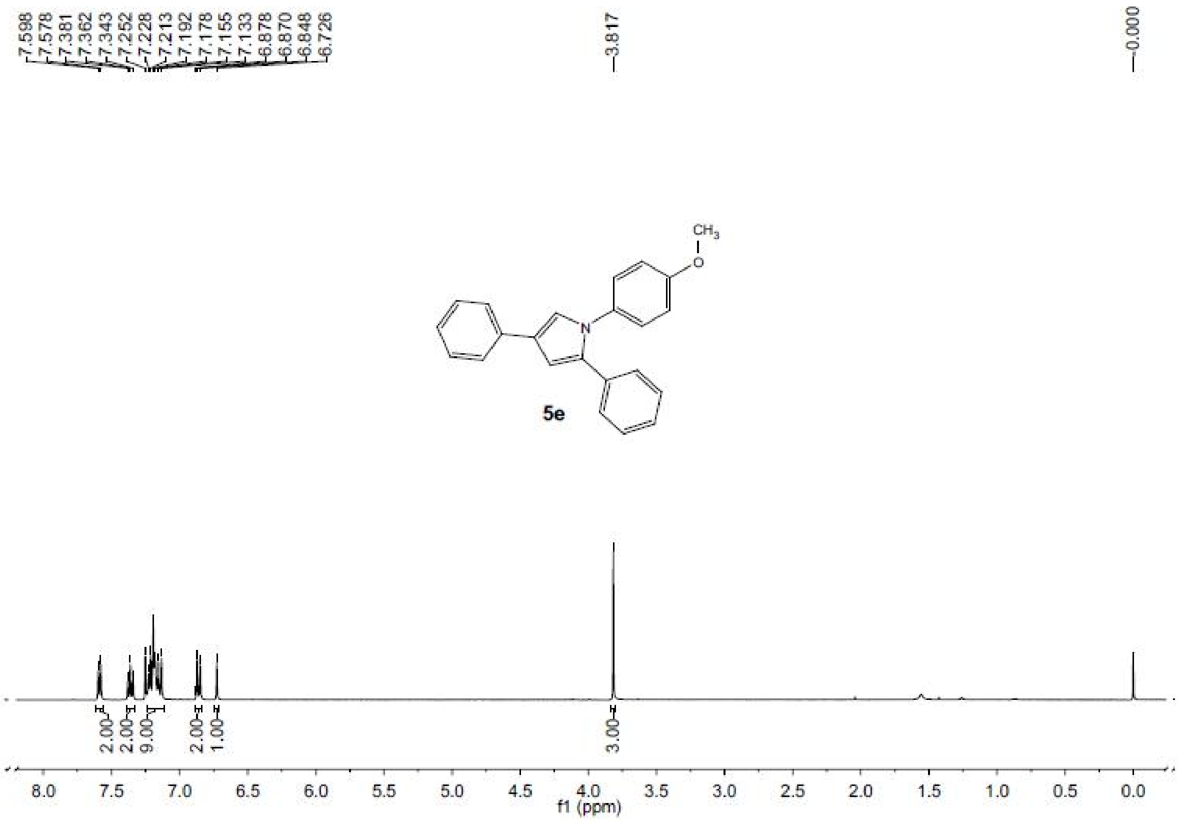
CH3
N
5d
f1 (ppm)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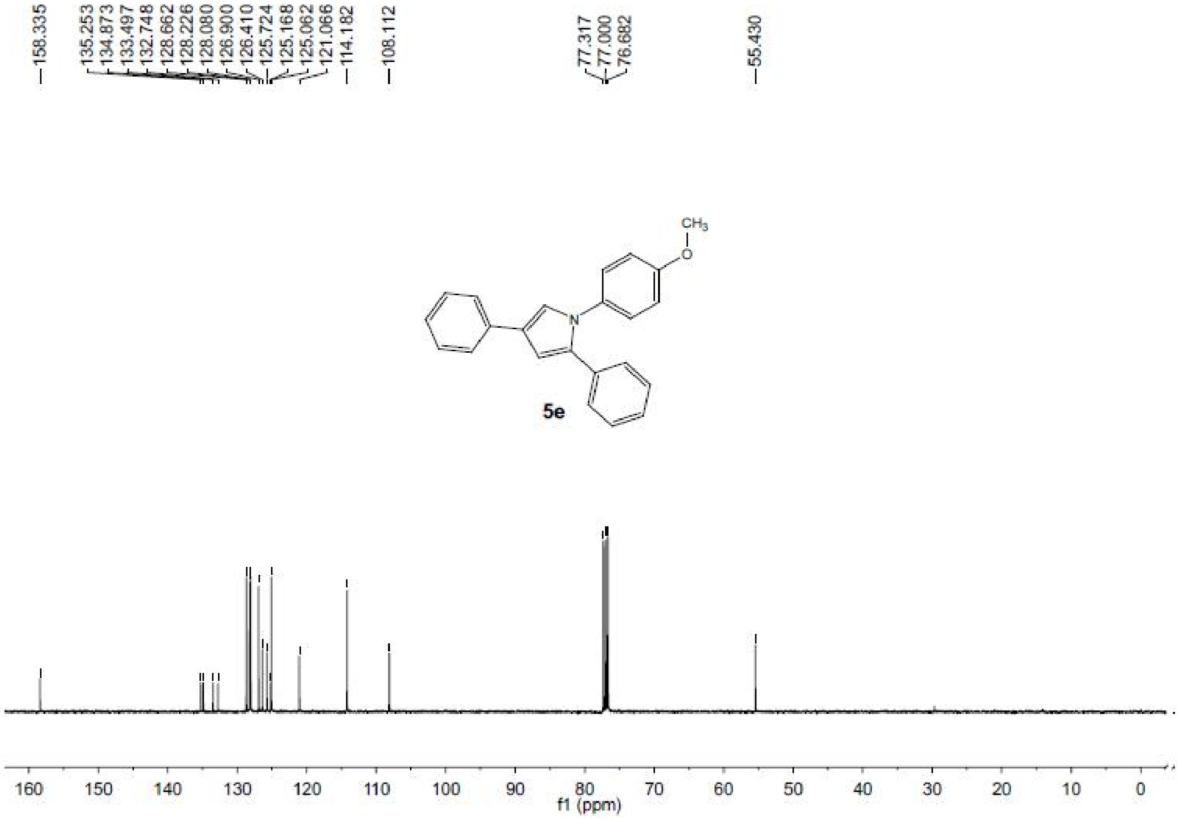
7.192
7.178
7.155
7.133
6.878
6.870
6.848
6.726
3.817
0.000
CH3
O
N
5e
2.00
2.00
9.00
2.00
1.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.748
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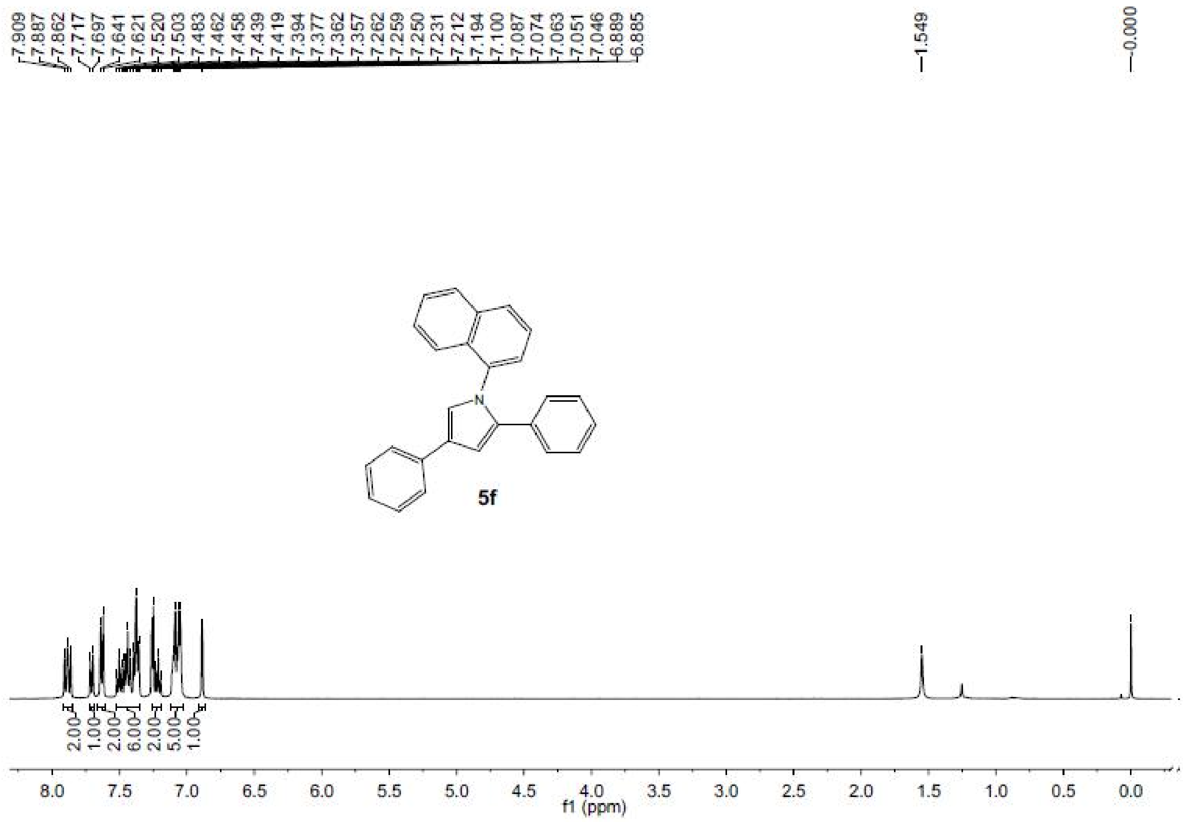
128.226
128.080
126.900
126.410
125.724
125.168
125.062
121.066
114.182
108.112
77.317
77.000
76.682
55.430
CH3
O
N
5e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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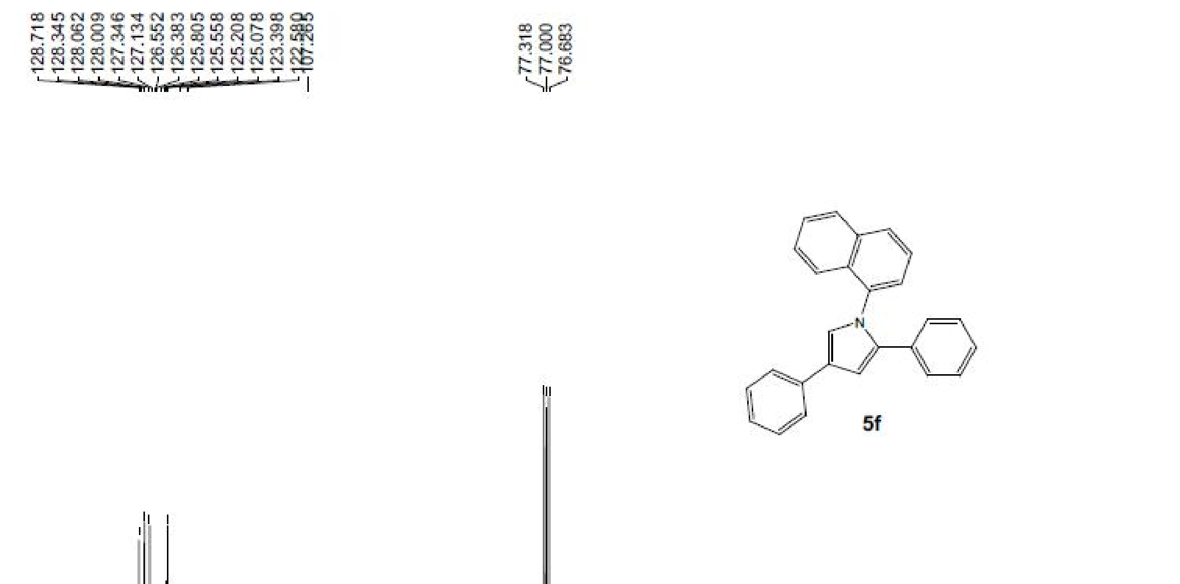
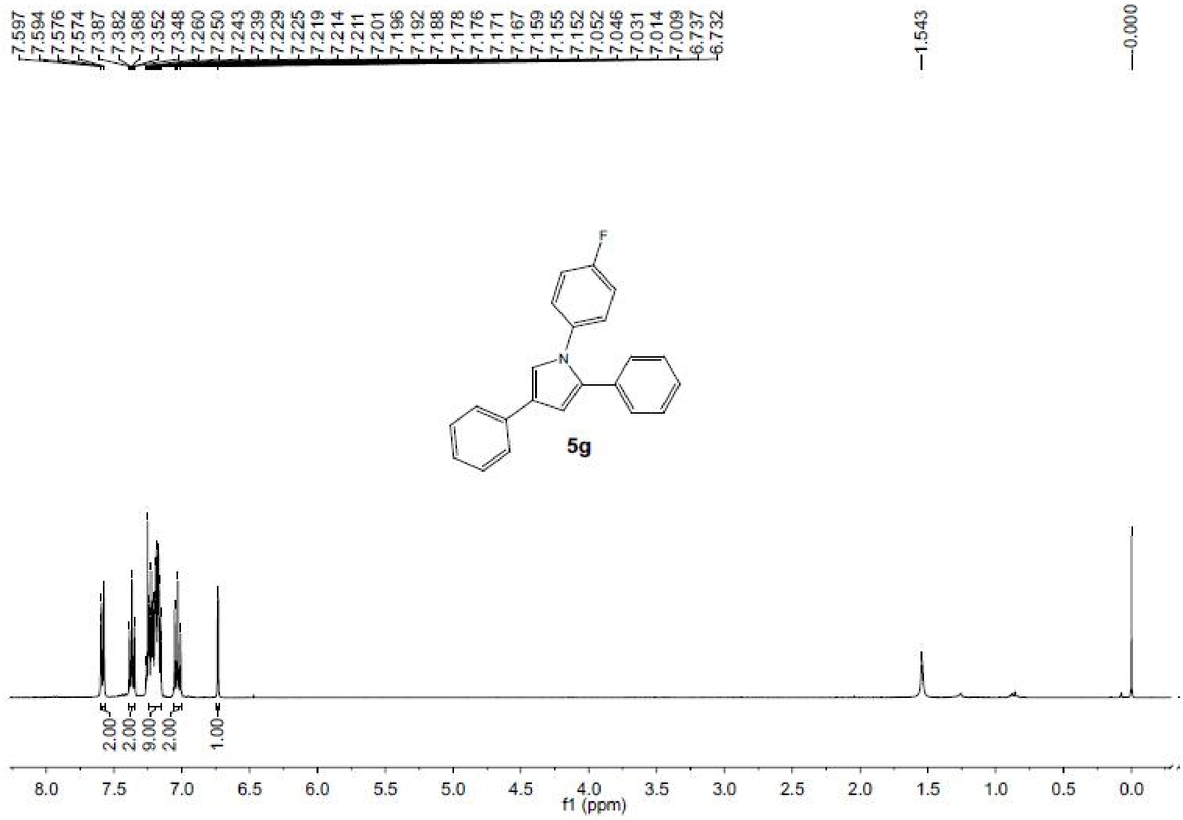
7.862
7.717
7.697
7.641
7.621
7.520
7.503
7.483
7.462
7.458
7.439
7.419
7.394
7.377
7.362
7.357
7.262
7.259
7.250
7.231
7.212
7.194
7.100
7.087
7.074
7.063
7.051
7.046
6.889
6.885
1.549
0.000
N
5f
2.00
1.00
2.00
6.00
2.00
5.00
1.00
f1 (ppm)


128.718
128.345
128.062
128.009
127.346
127.134
126.552
126.383
125.805
125.558
125.208
125.078
123.398
107.265
77.318
77.000
76.683
N
5f
f1 (ppm)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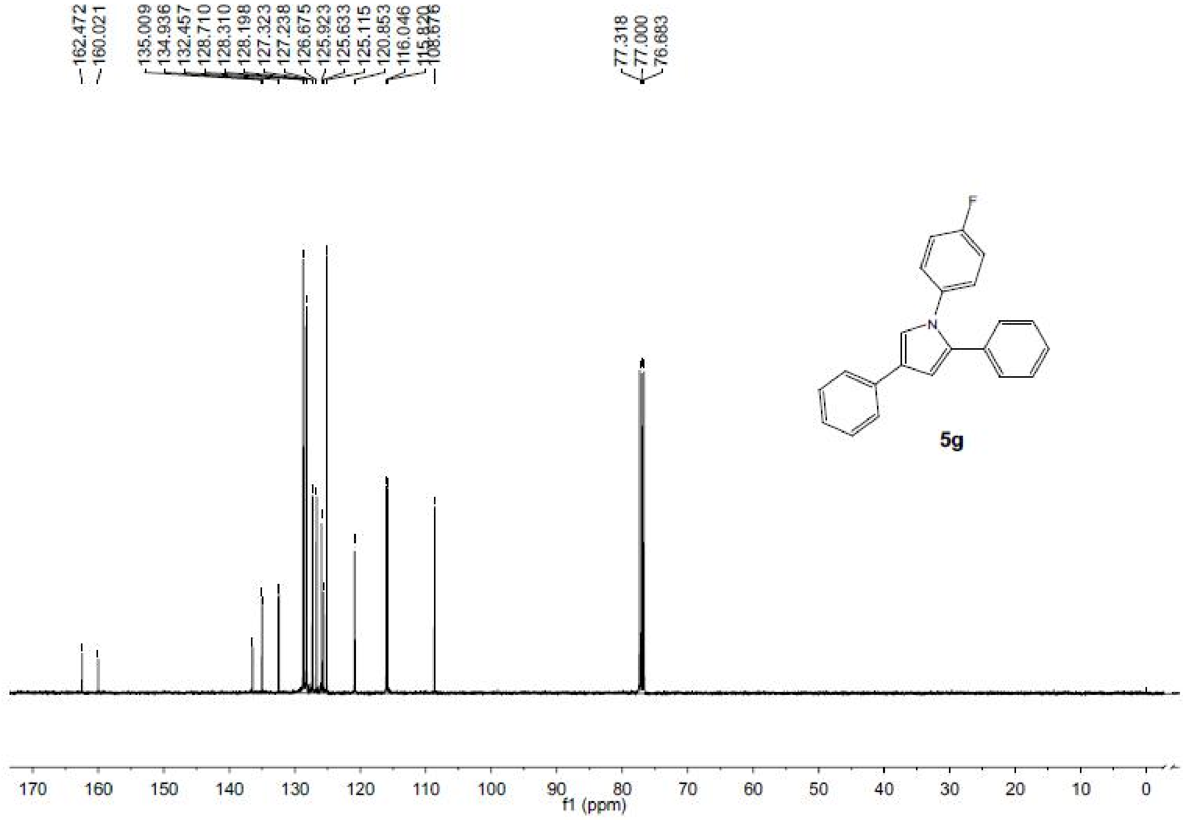
7.594
7.576
7.574
7.387
7.382
7.368
7.352
7.348
7.260
7.250
7.243
7.239
7.229
7.225
7.219
7.214
7.211
7.201
7.196
7.192
7.188
7.178
7.176
7.171
7.167
7.159
7.155
7.152
7.052
7.046
7.031
7.014
7.009
6.737
6.732
1.543
0.000
F
N
5g
2.00
2.00
9.00
2.00
1.00
f1 (ppm)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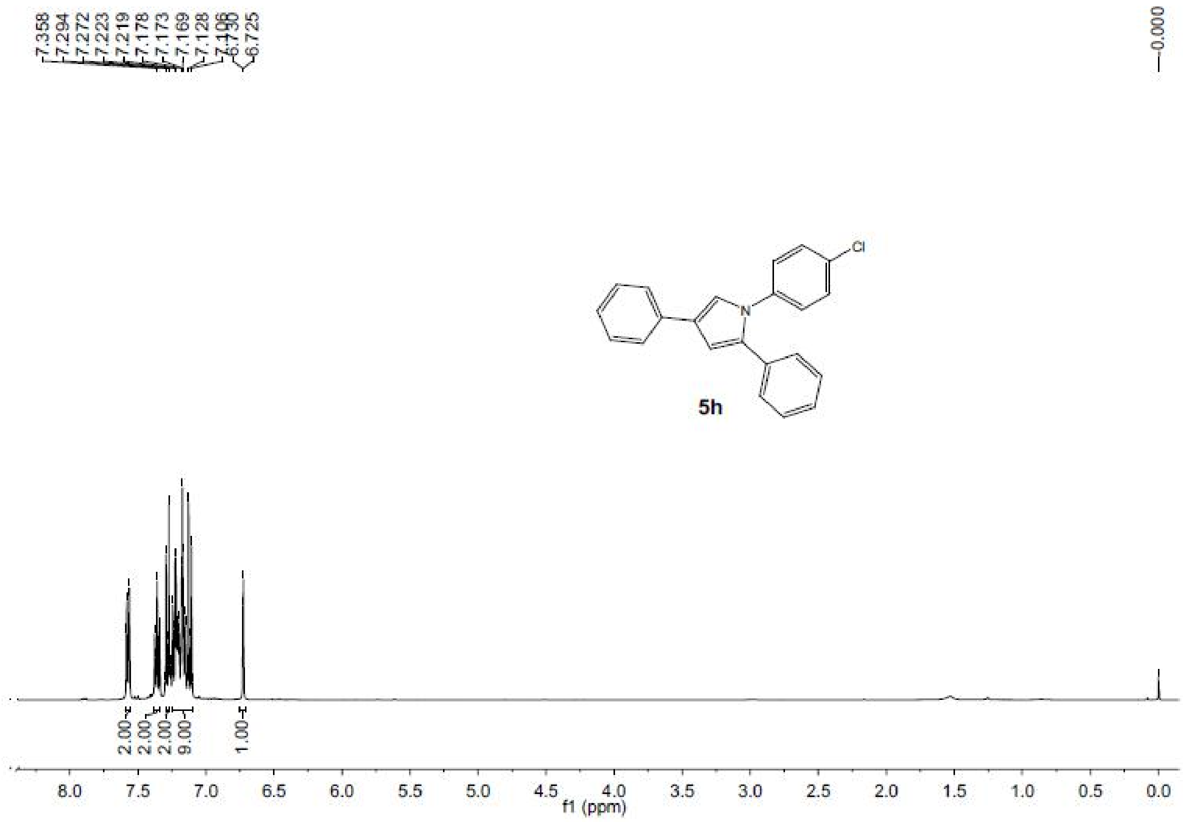
160.021
135.009
134.936
132.457
128.710
128.310
128.198
127.323
127.238
126.675
125.923
125.633
125.115
120.853
116.046
115.820
108.676
77.318
77.000
76.683
F
N
5g
f1 (ppm)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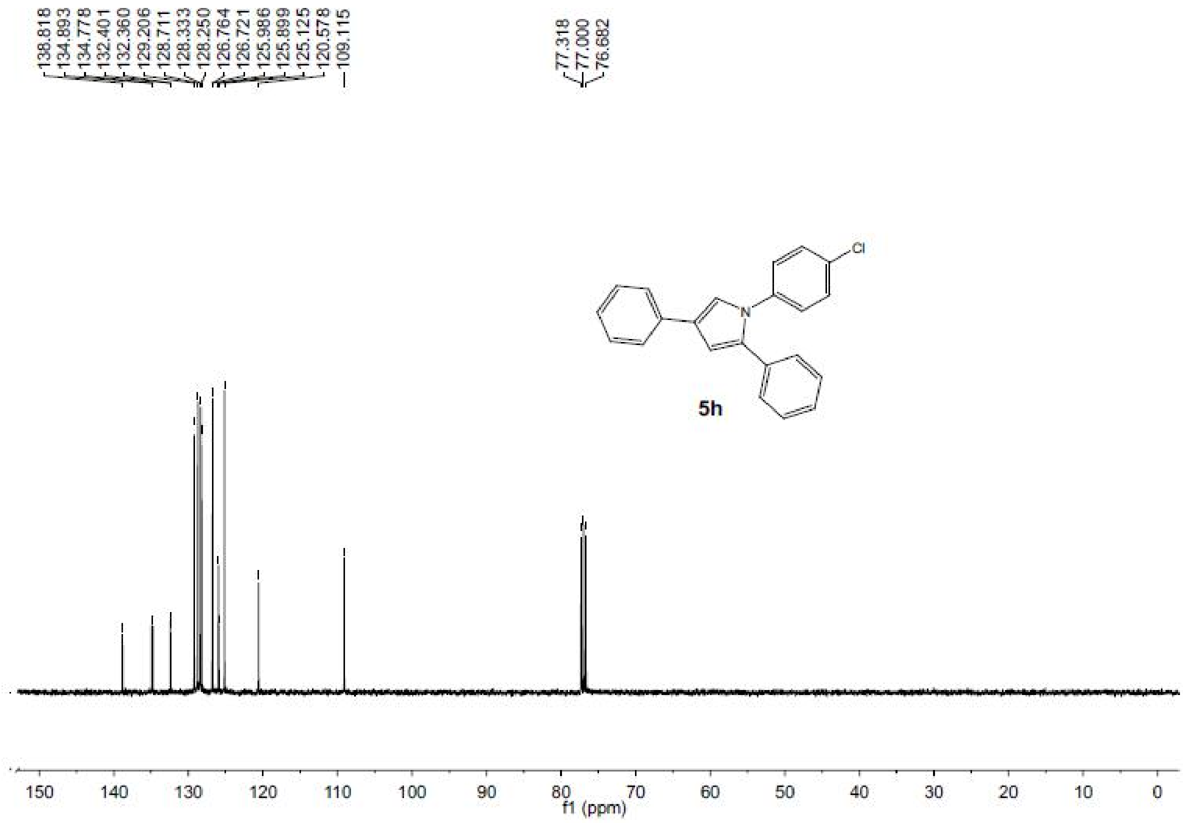
7.294
7.272
7.223
7.219
7.178
7.173
7.169
7.128
7.106
6.730
6.725
0.000
Cl
N
5h
2.00
2.00
2.00
9.00
1.00
f1 (ppm)


138.818
134.893
134.778
132.401
132.360
129.206
128.711
128.333
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126.764
126.721
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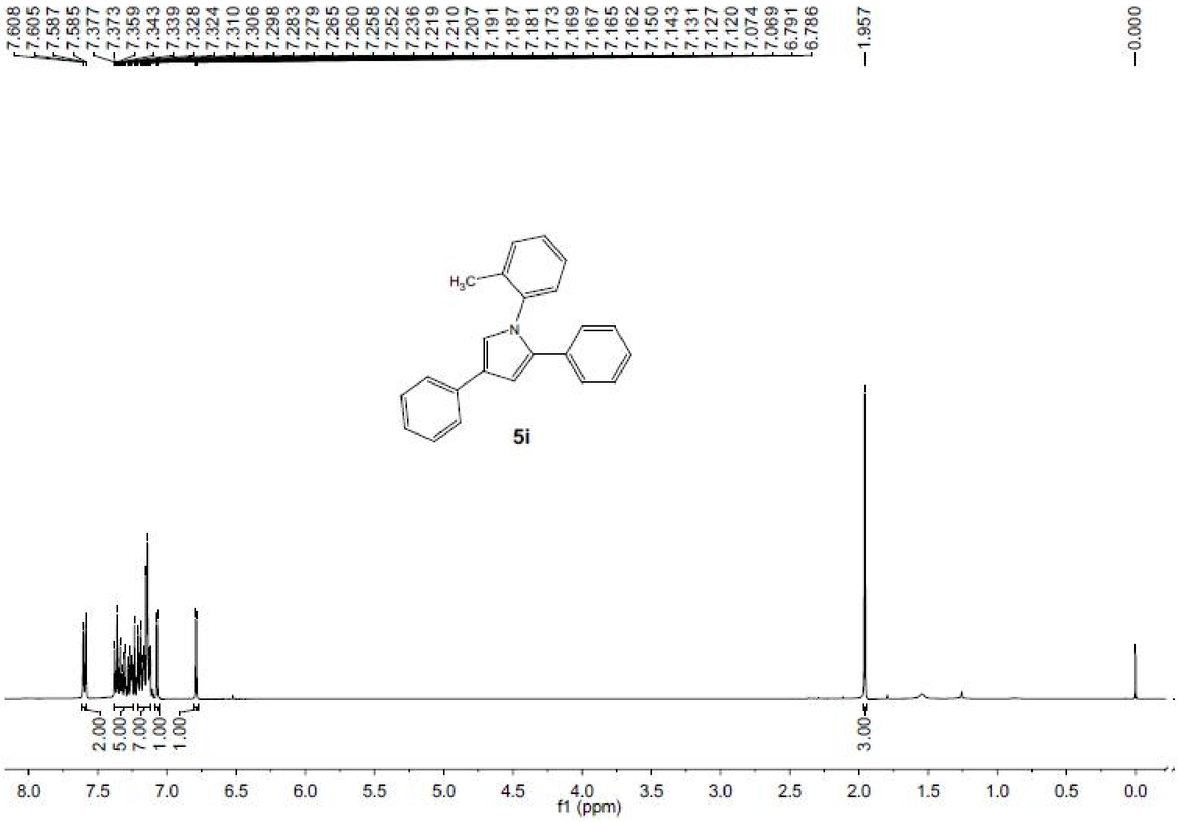
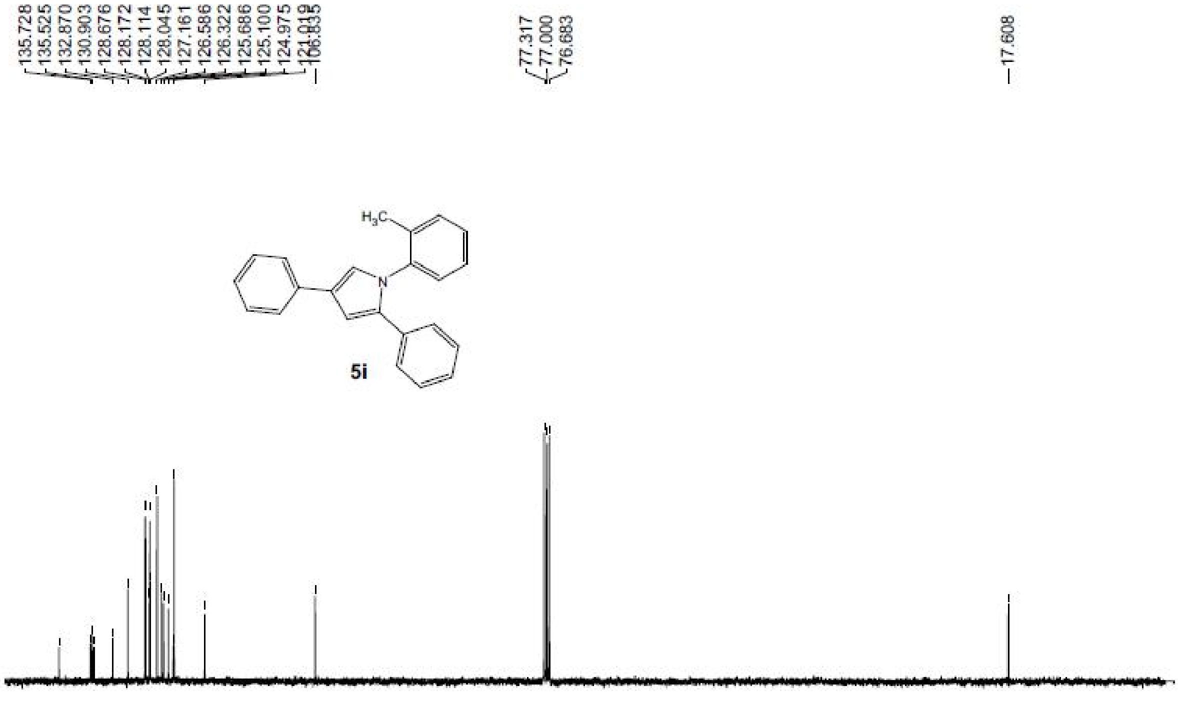
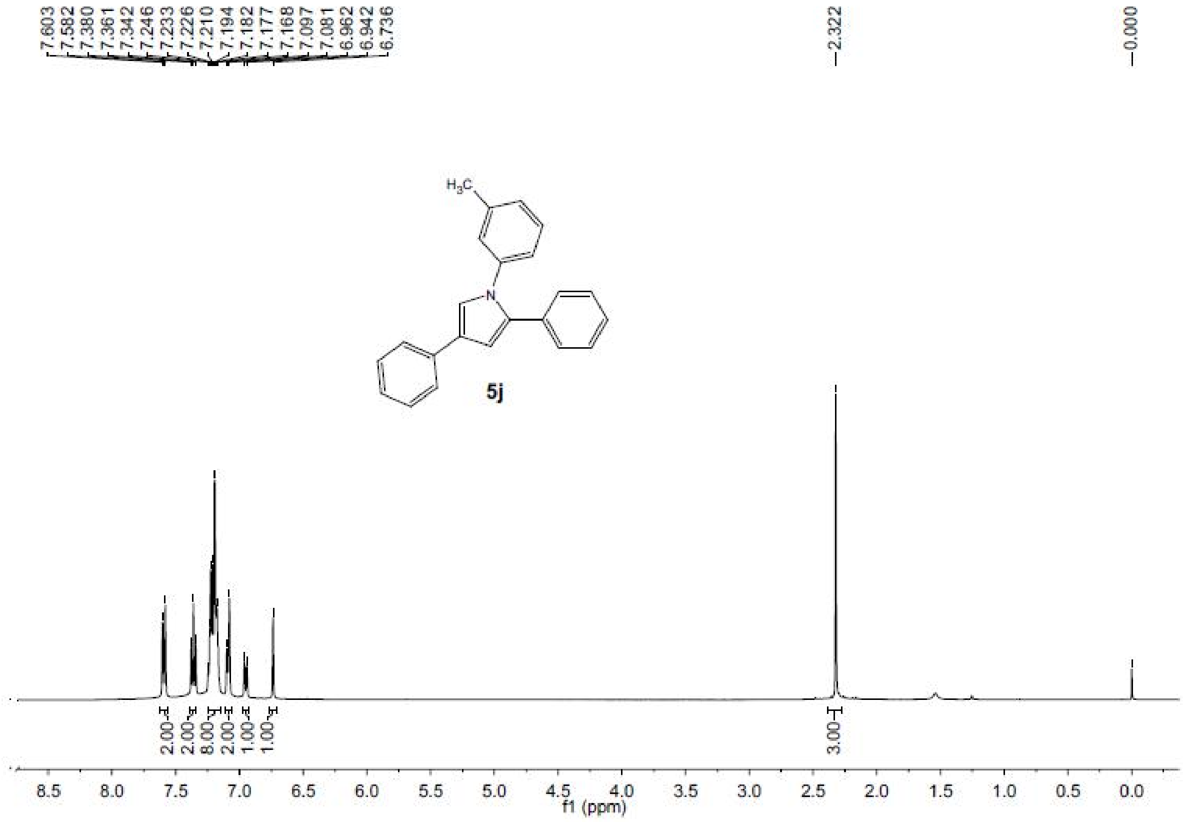
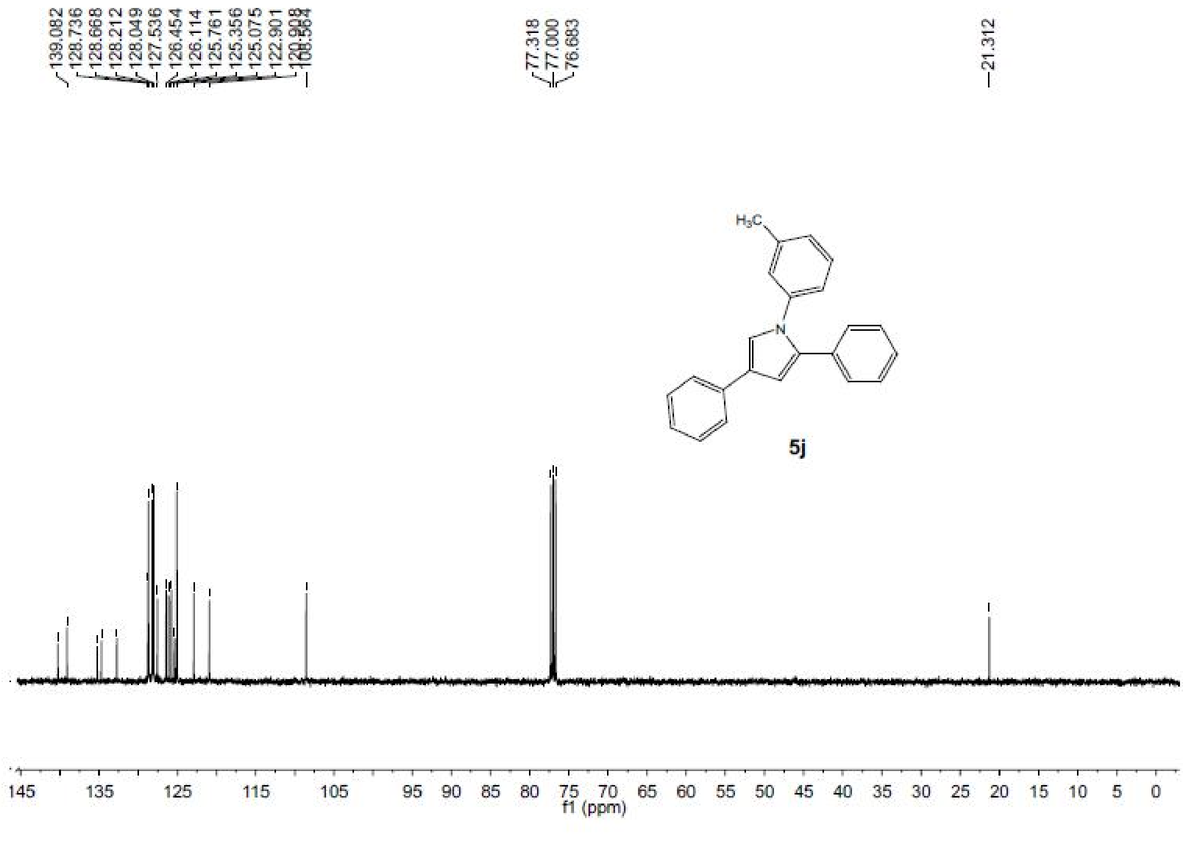
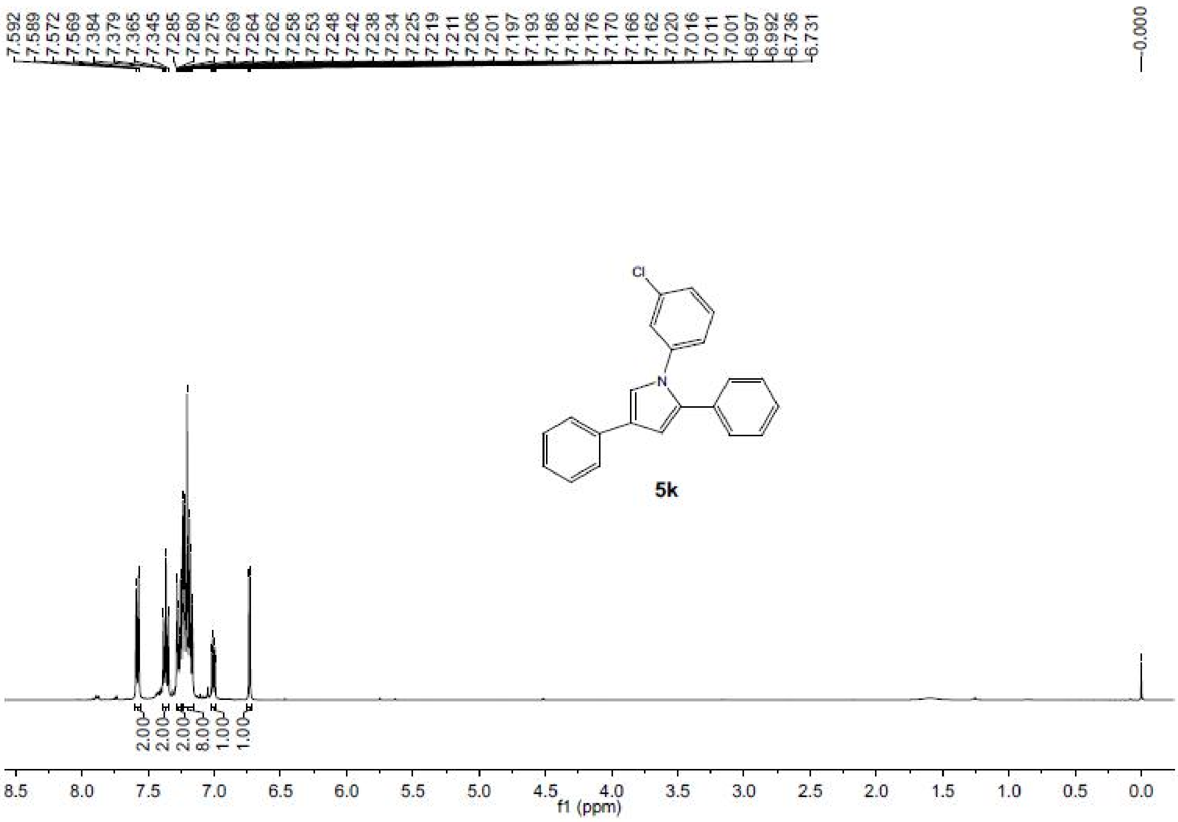
125.899
125.125
120.578
109.115
77.318
77.000
76.682
Cl
N
5h
f1 (ppm)







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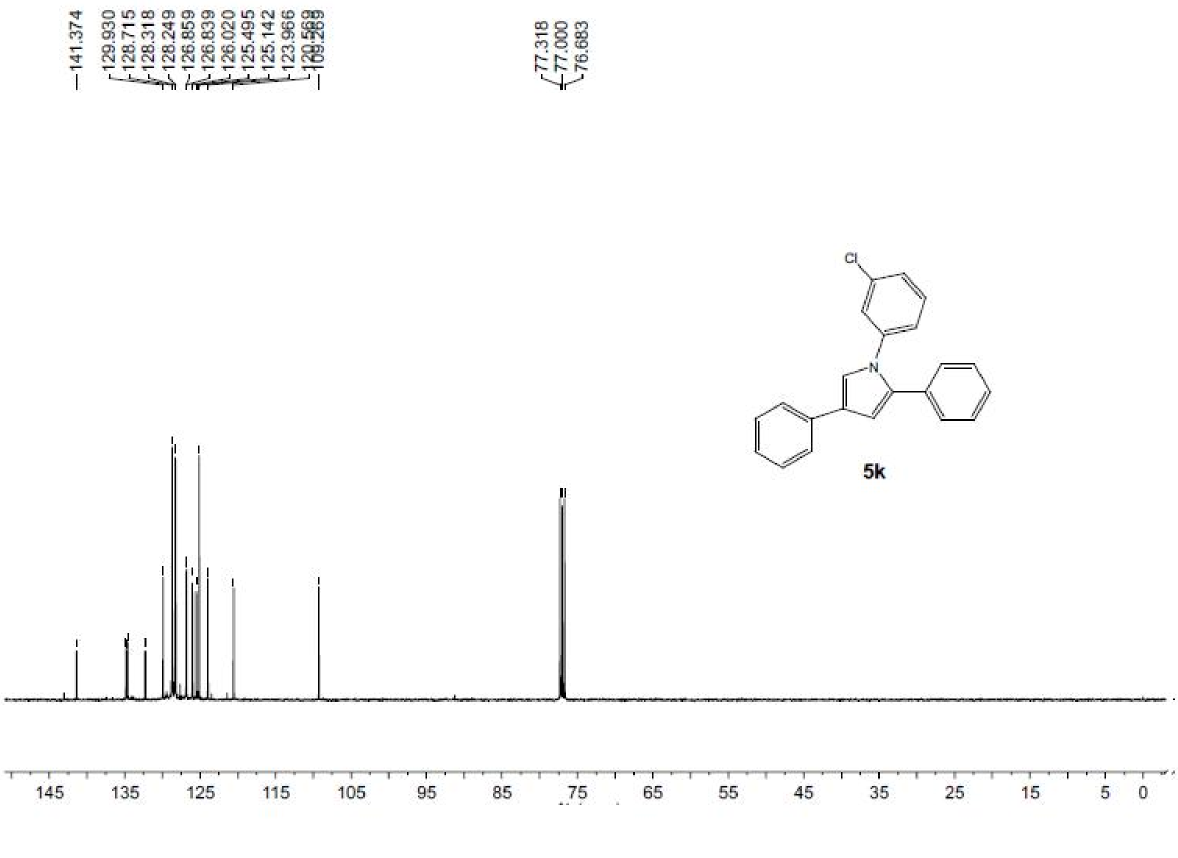
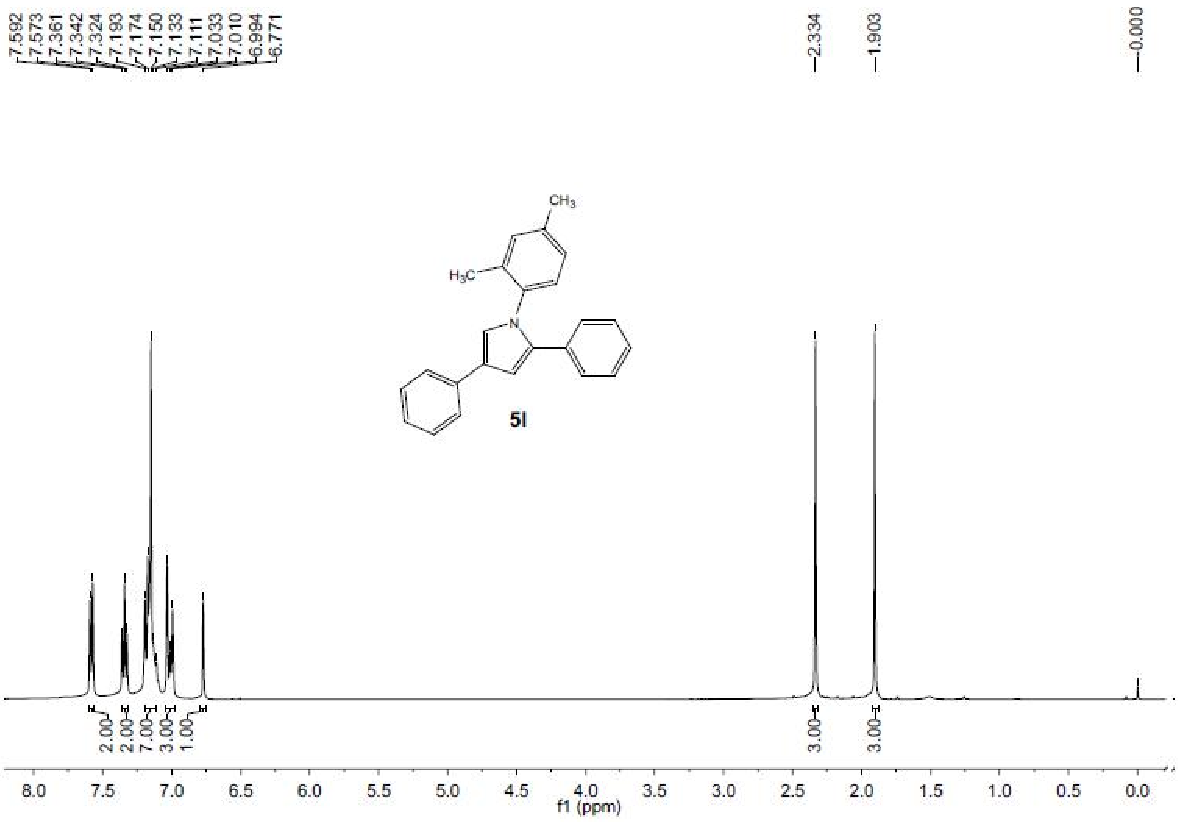
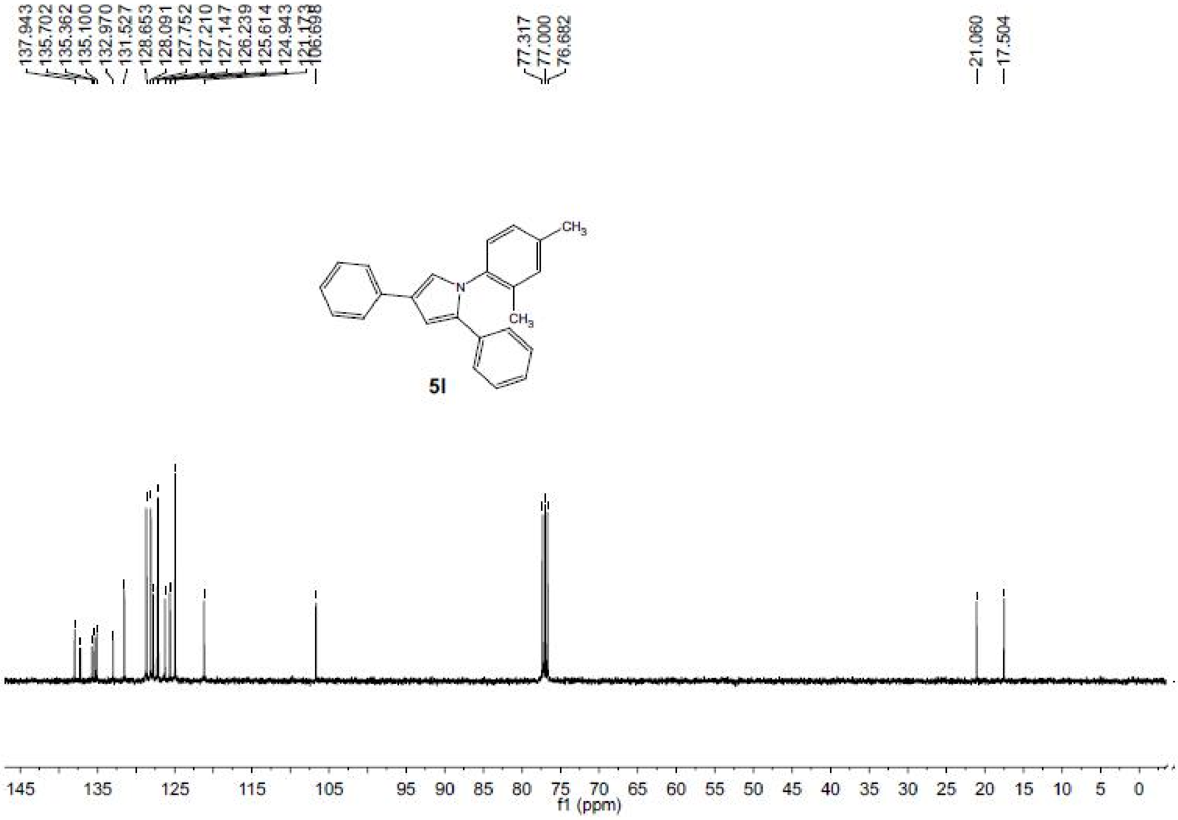
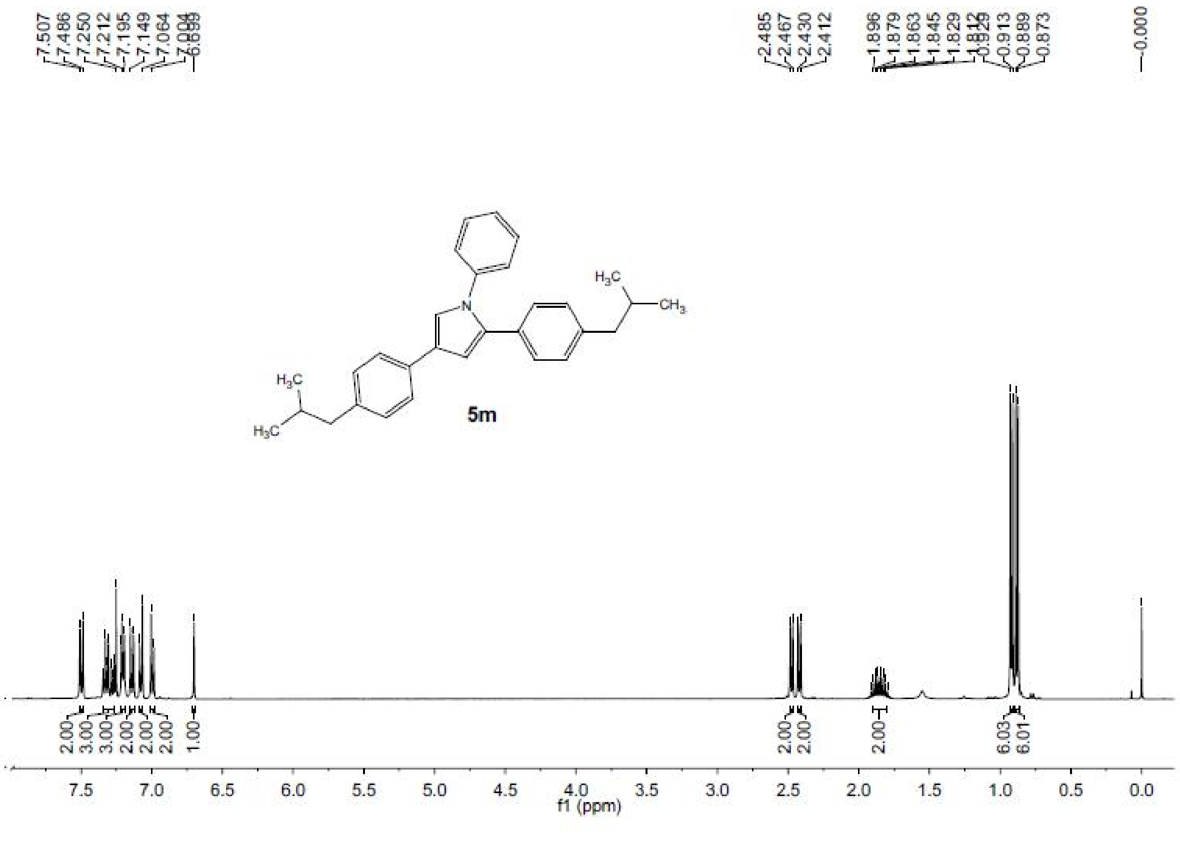
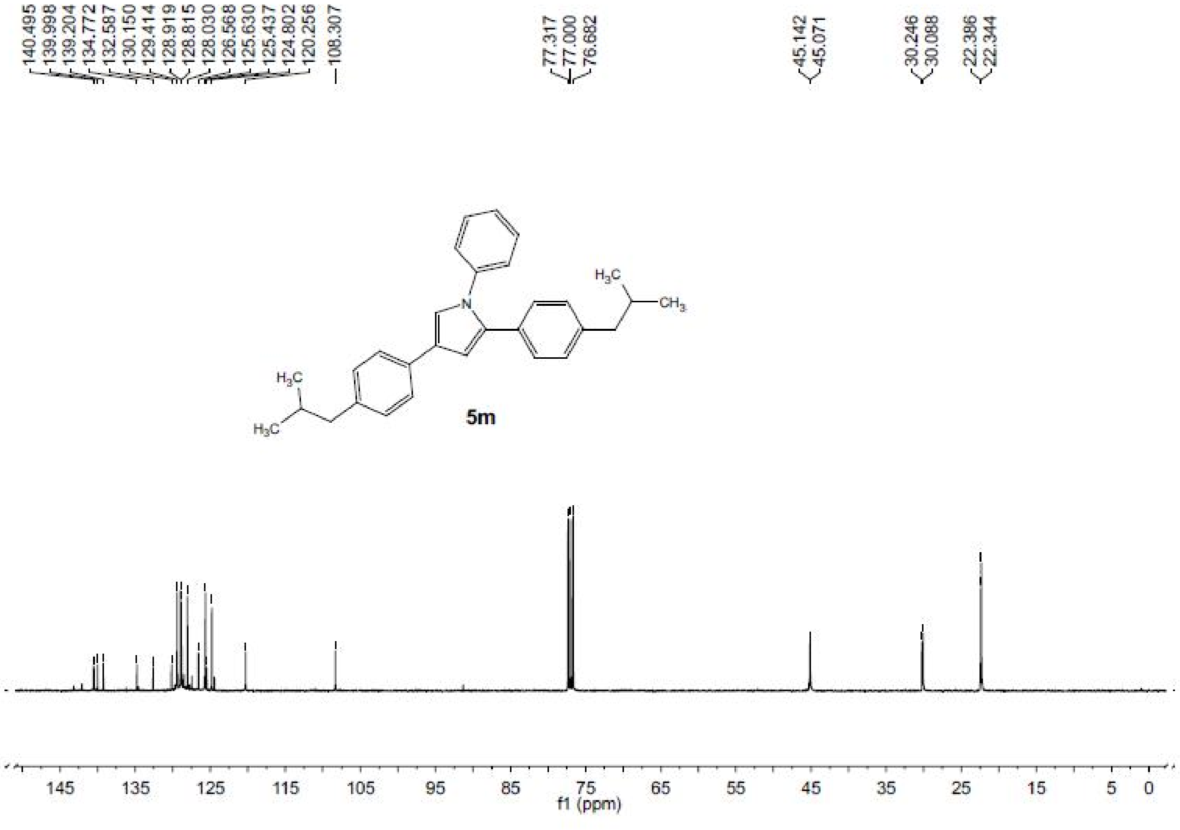
7.569
7.384
7.379
7.365
7.345
7.285
7.280
7.275
7.269
7.264
7.262
7.258
7.253
7.248
7.242
7.238
7.234
7.225
7.219
7.211
7.206
7.201
7.197
7.193
7.186
7.182
7.176
7.170
7.166
7.162
7.020
7.016
7.011
7.001
6.997
6.992
6.736
6.731
0.000
Cl
N
5k
2.00
2.00
2.00
8.00
1.00
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


141.374
129.930
128.715
128.318
128.249
126.859
126.839
126.020
125.495
125.142
123.966
77.318
77.000
76.683
Cl
N
5k
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0






7.507
7.486
7.250
7.212
7.195
7.149
7.064
7.004
6.999
2.485
2.467
2.430
2.412
1.896
1.879
1.863
1.845
1.829
1.812
0.925
0.913
0.889
0.873
0.000
H_3C
CH_3
N
5m
2.00
3.00
3.00
2.00
2.00
2.00
1.00
2.00
2.00
2.00
6.03
6.01
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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139.204
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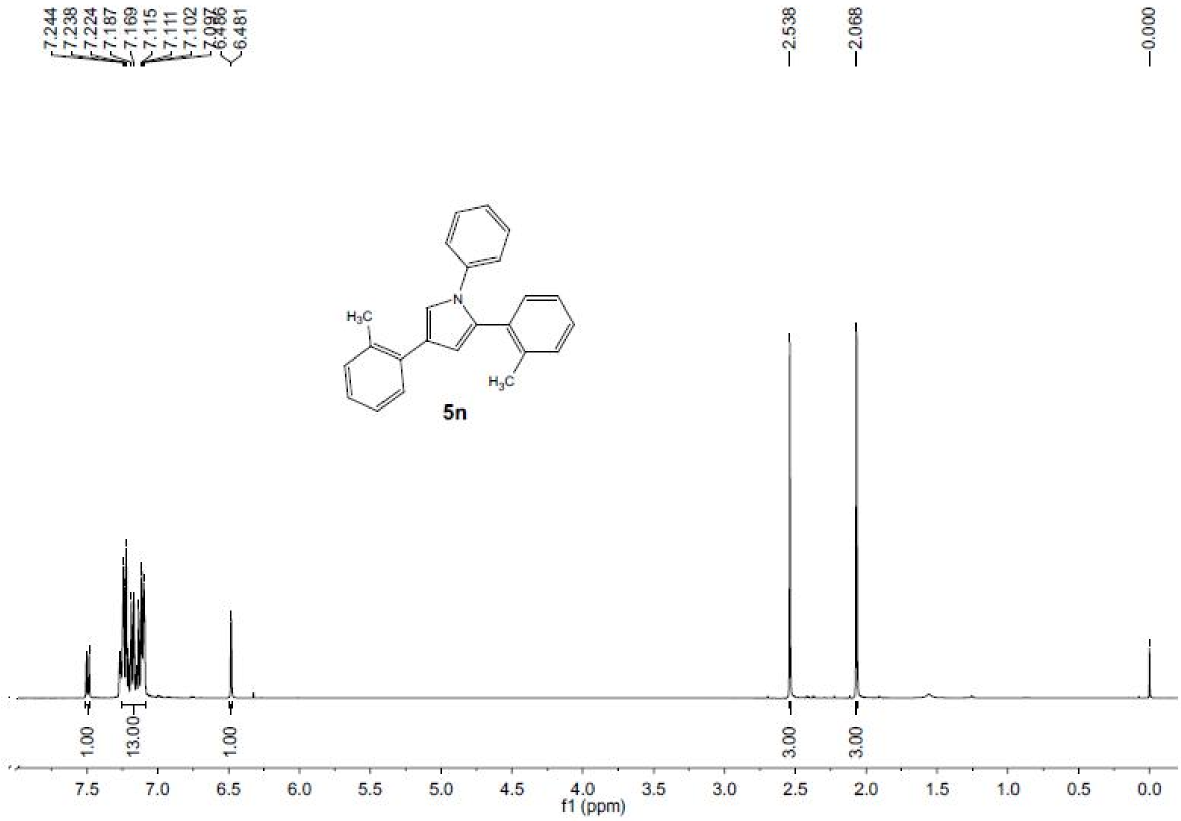
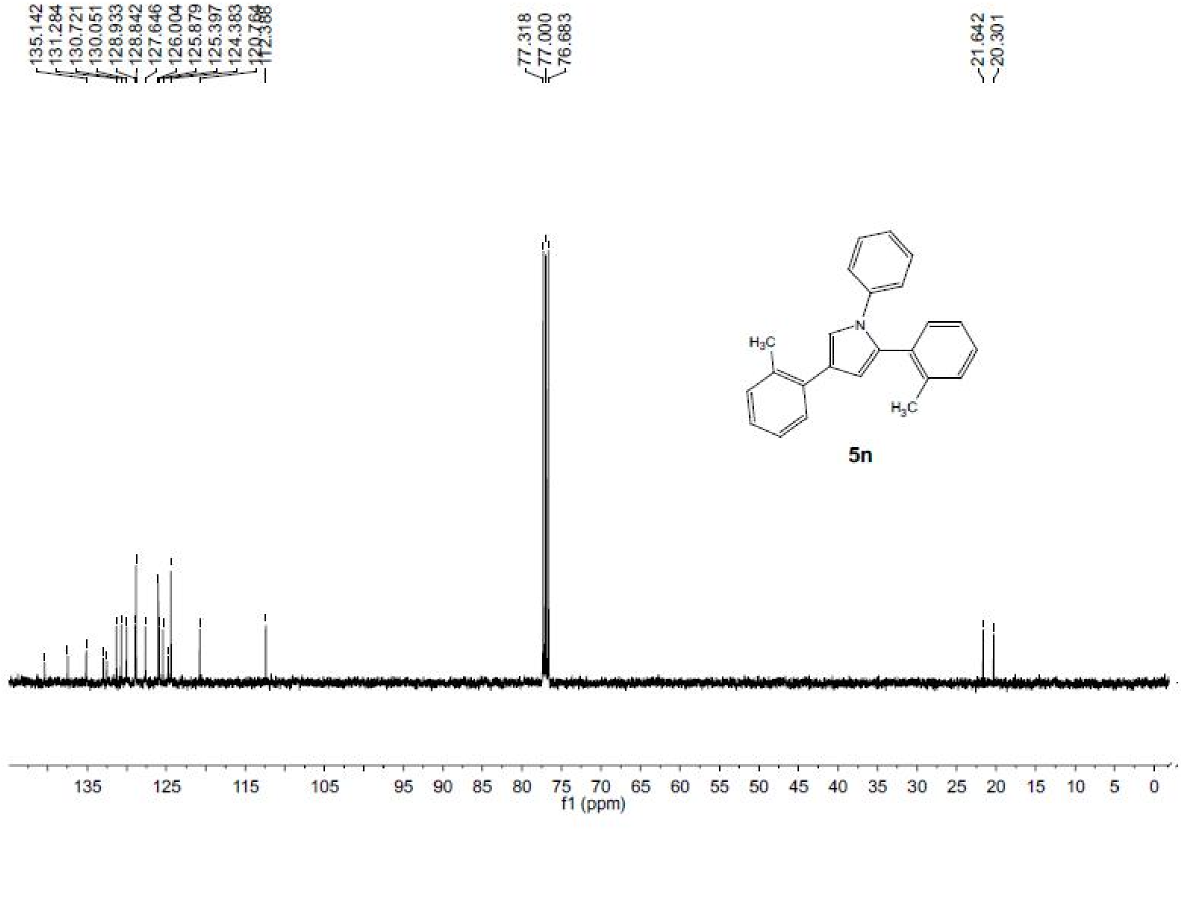
130.150
129.414
128.919
128.815
128.030
126.568
125.630
125.437
124.802
120.256
108.307
77.317
77.000
76.682
45.142
45.071
30.246
30.088
22.386
22.344
H_3C
CH_3
N
5m
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)


7.244
7.238
7.224
7.187
7.169
7.115
7.111
7.102
7.097
6.481
2.538
2.068
0.000
H_3C
N
H_3C
5n
1.00
13.00
1.00
3.00
3.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


135.142
131.284
130.721
130.051
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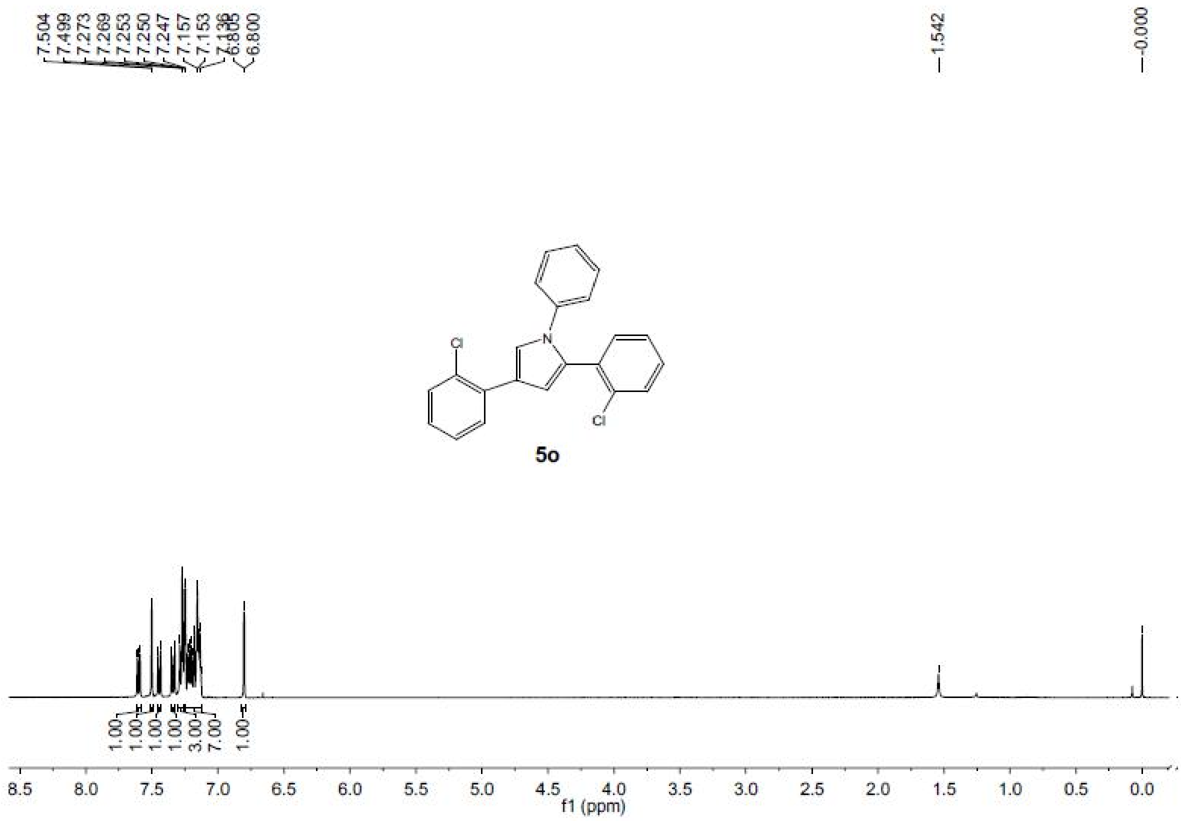
128.842
127.646
126.004
125.879
125.397
124.383
112.388
77.318
77.000
76.683
21.642
20.301
H_3C
N
H_3C
5n
135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.269
7.253
7.250
7.247
7.157
7.153
6.805
6.800
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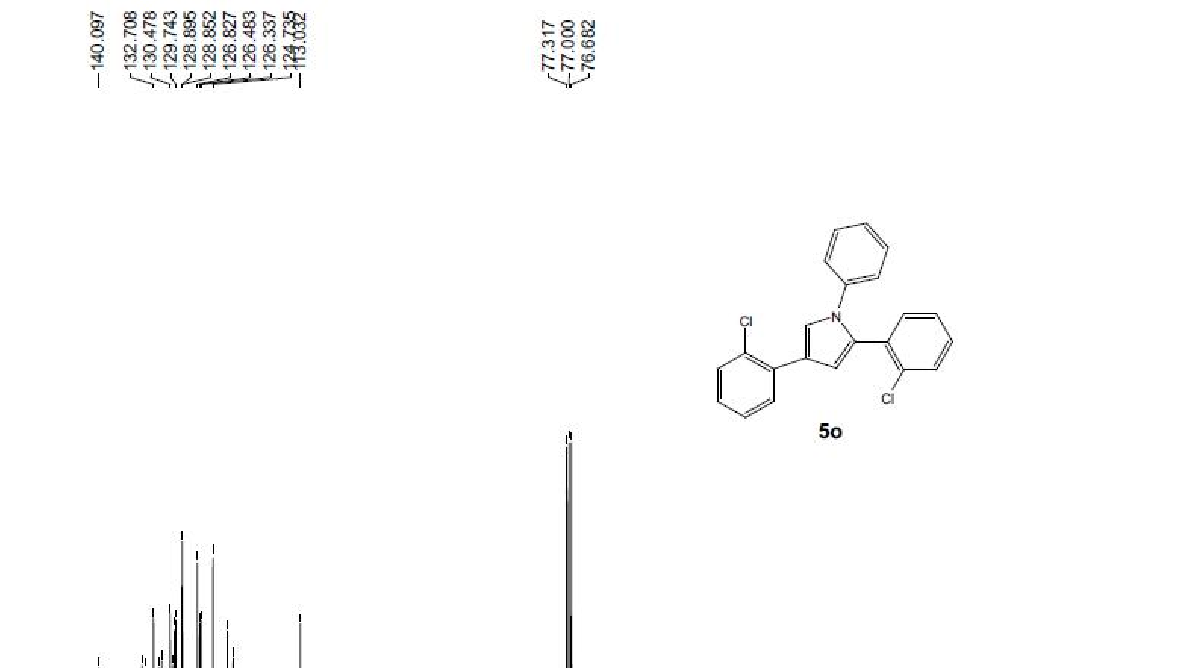
0.000
Cl
N
Cl
5o
1.00
1.00
1.00
3.00
7.00
1.00
f1 (ppm)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132.708
130.478
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126.827
126.483
126.337
113.032
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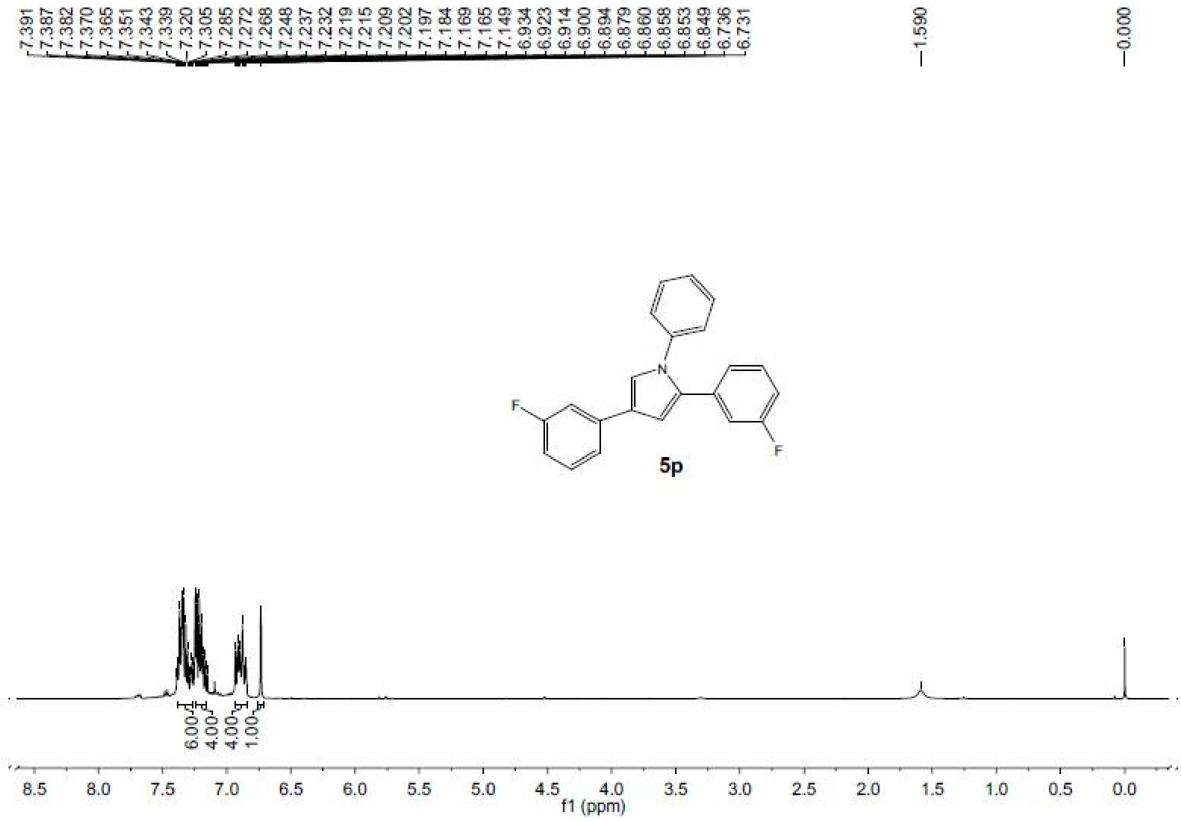
77.000
76.682
Cl
N
Cl
5o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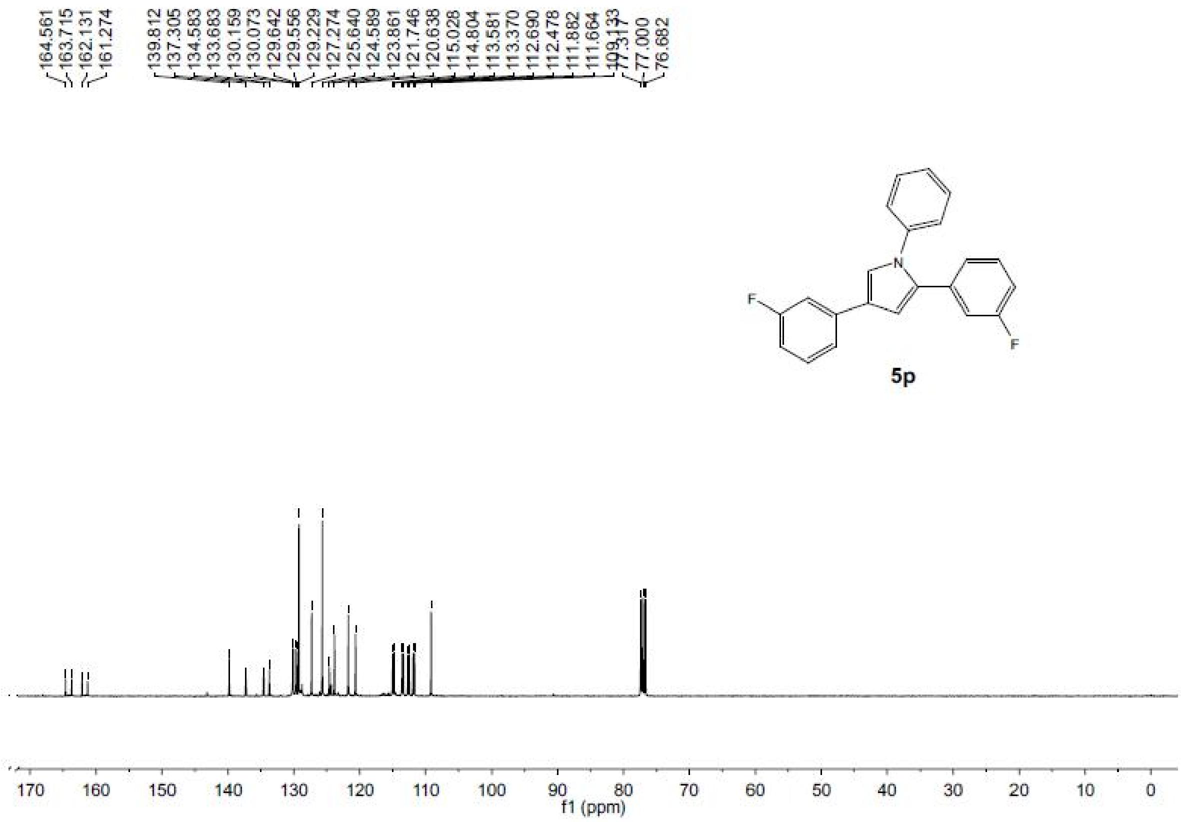
7.305
7.285
7.272
7.268
7.248
7.237
7.232
7.219
7.215
7.209
7.202
7.197
7.184
7.169
7.165
7.149
6.934
6.923
6.914
6.900
6.894
6.879
6.860
6.858
6.853
6.849
6.736
6.731
1.590
0.000
F
N
F
5p
6.00
4.00
4.00
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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161.274
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133.683
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130.073
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129.556
129.229
127.274
125.640
124.589
123.861
121.746
120.638
115.028
114.804
113.581
113.370
112.690
112.478
111.882
111.664
109.133
77.317
77.000
76.682
F
N
F
5p
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)