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Supporting Information

N-Heterocyclic Carbene Palladium-Catalyzed Cascade Annulation/Alkynylation of 2-Alkynylanilines with Terminal Alkynes

Jianxiao Li,‡ Can Li,‡ Lu Ouyang, Chunsheng Li, Wanqing Wu* and Huanfeng Jiang*

Key Laboratory of Functional Molecular Engineering of Guangdong Province, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China

E-mail: cewuwq@scut.edu.cn, jianghf@scut.edu.cn; Fax and Tel.: (+86) 20-87112906

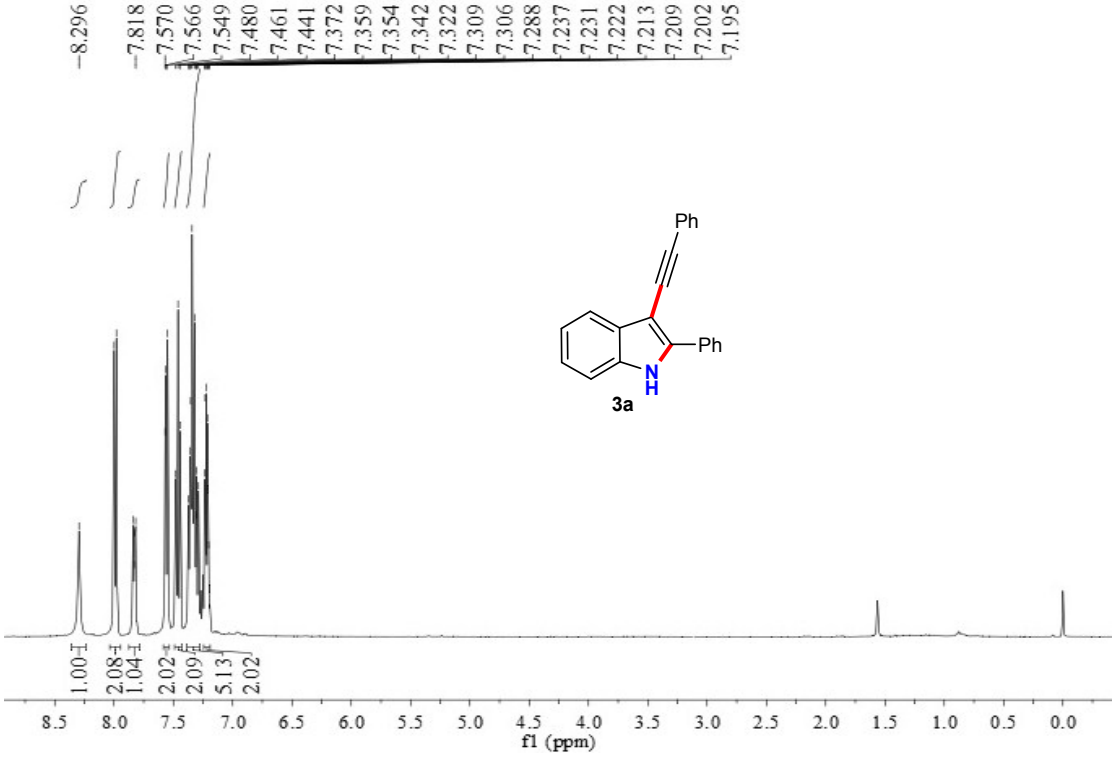
Table of Contents

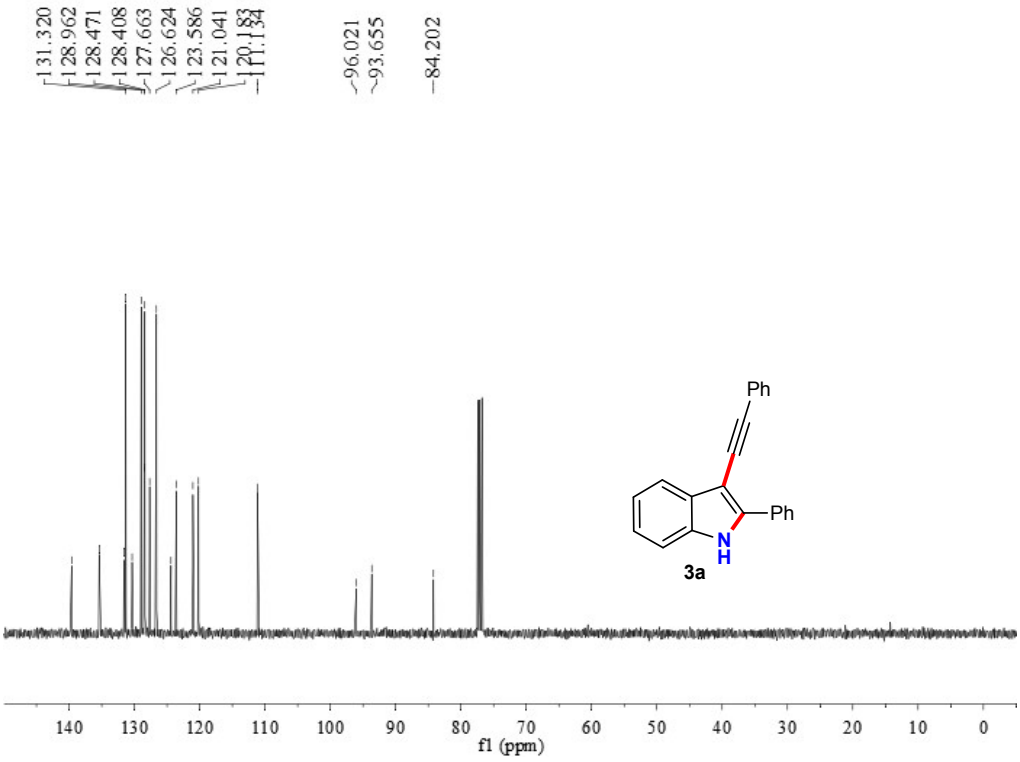
^{1}H and ^{13}C NMR spectra of compounds 3 ..... S2

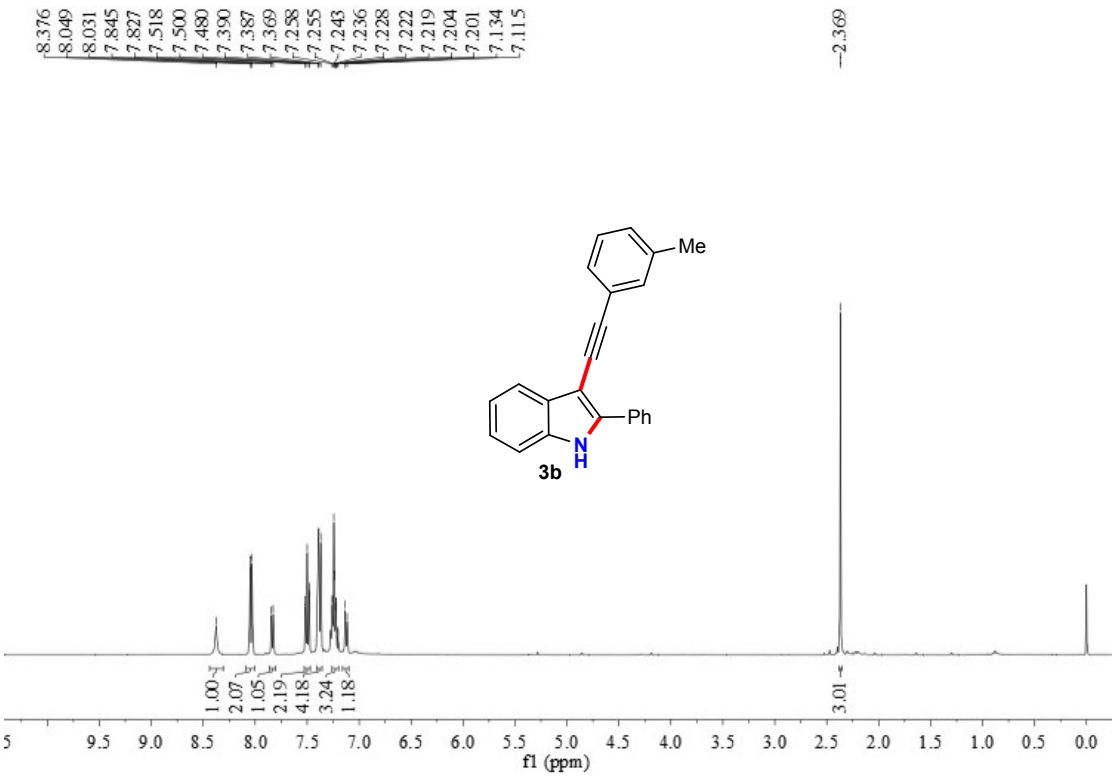
^{1}H and ^{13}C NMR spectra of compounds 4 ..... S28

^{1}H and ^{13}C NMR spectra of compounds 5 ..... S42

^{1}H and ^{13}C NMR spectra of compounds 3



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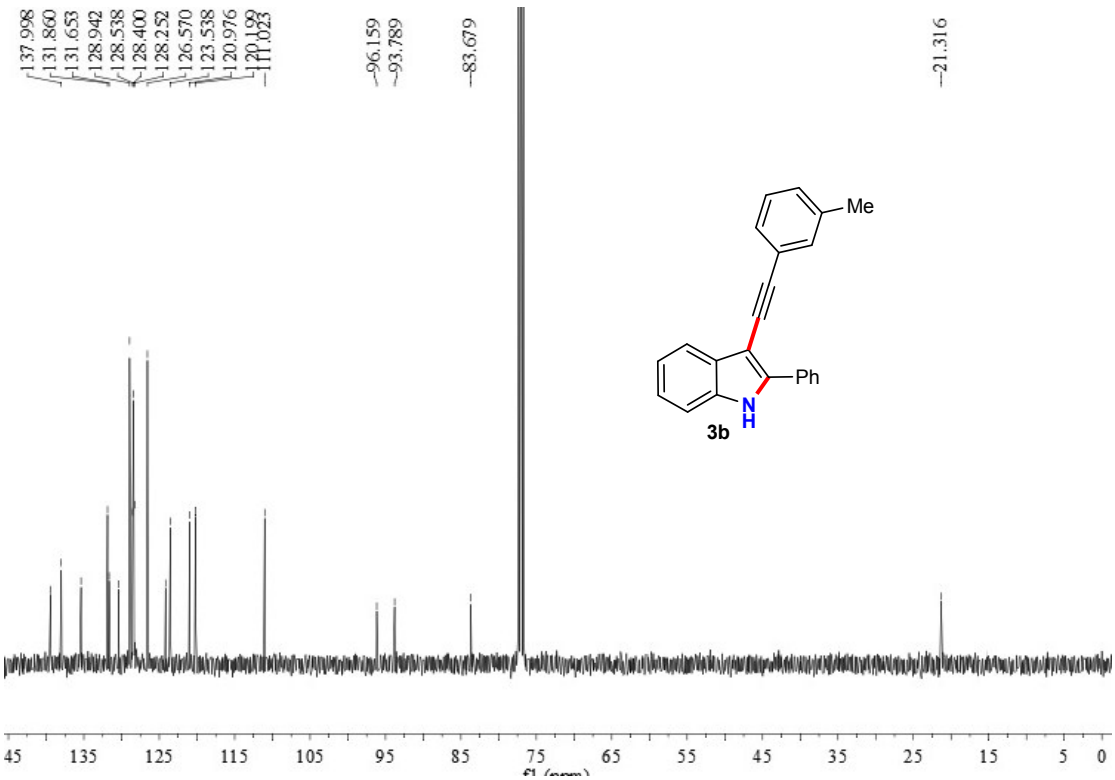
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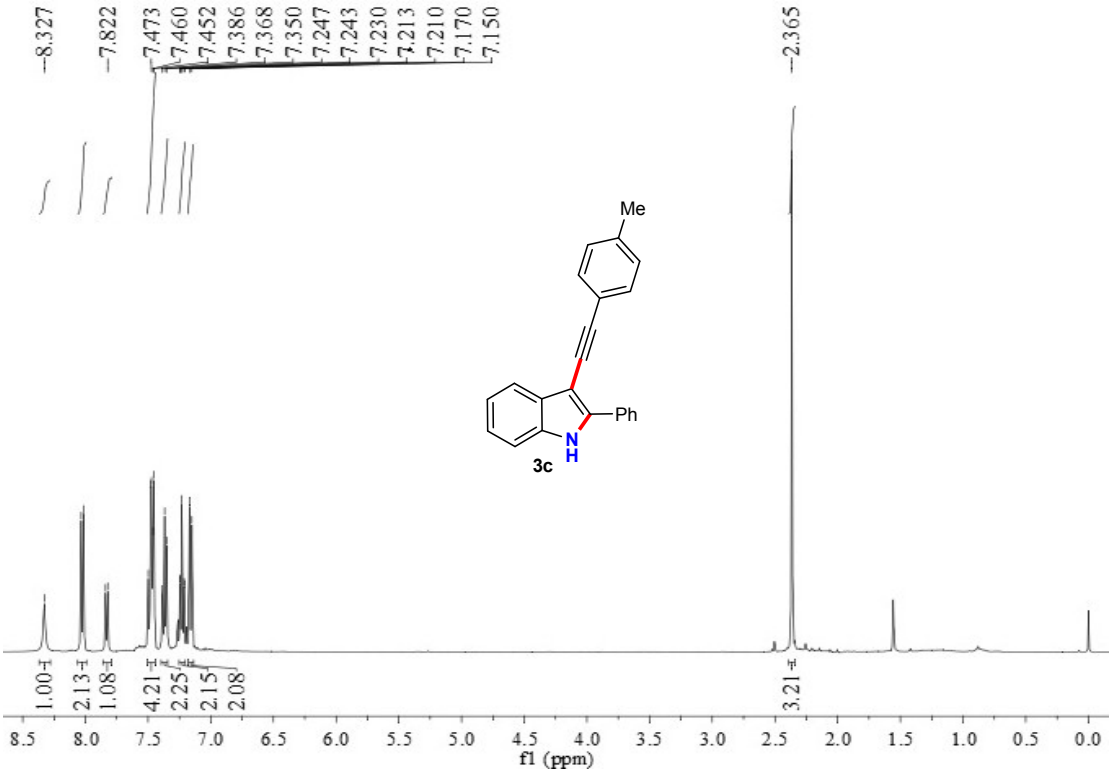
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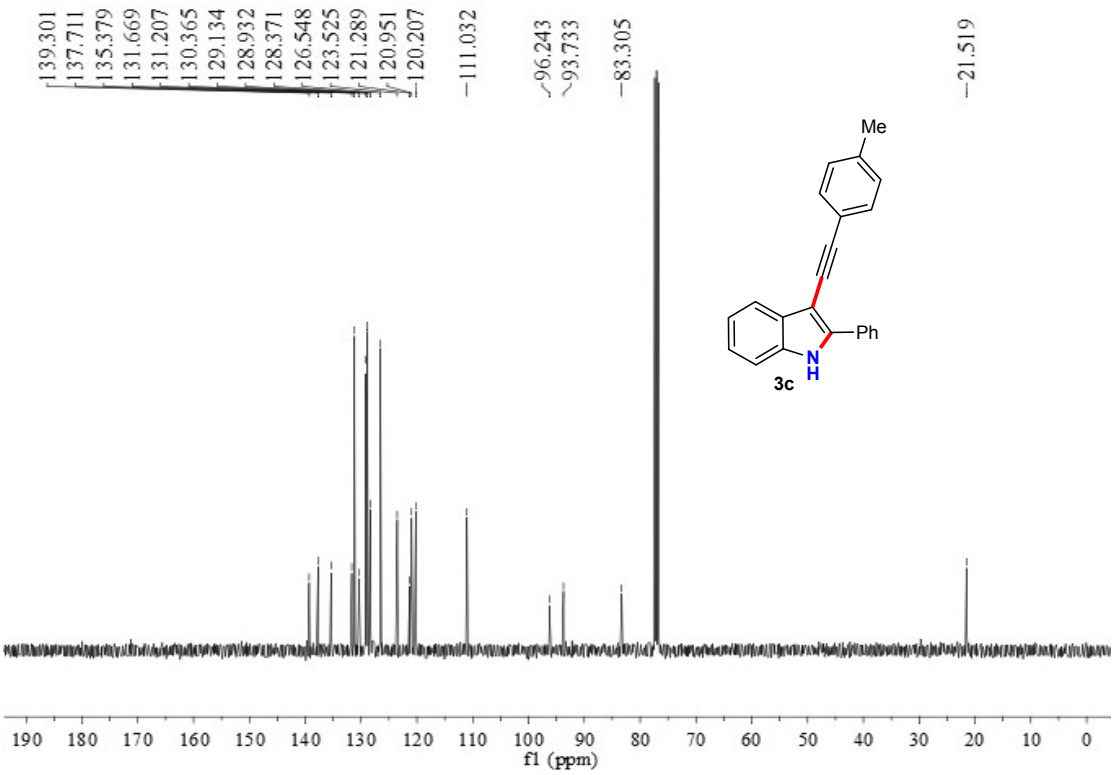
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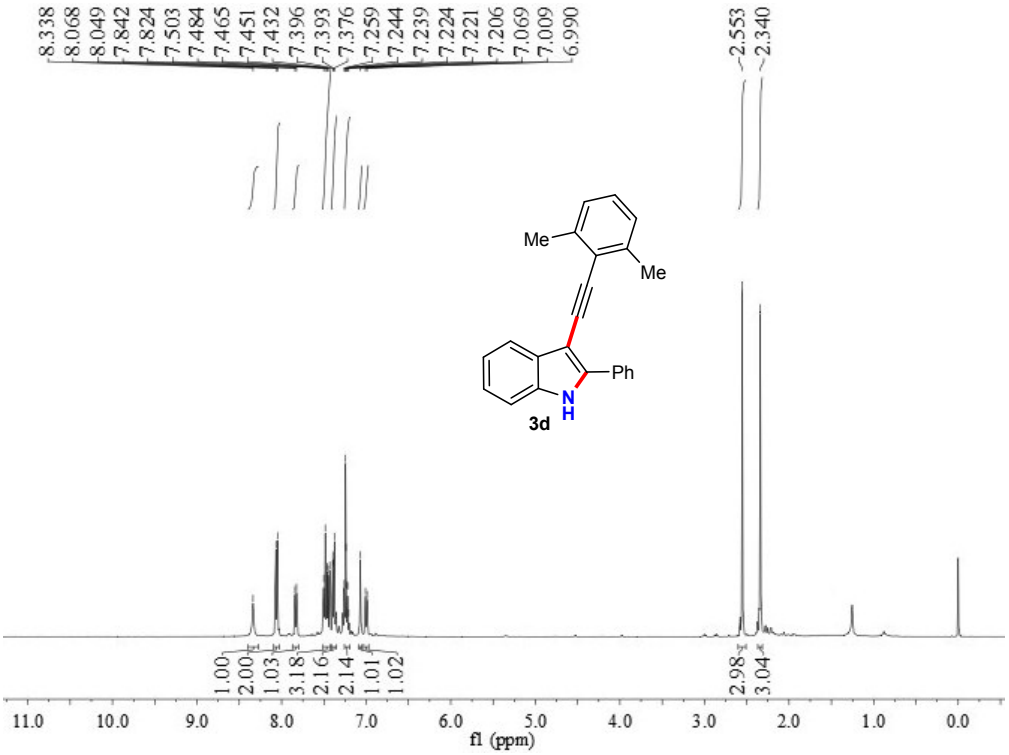
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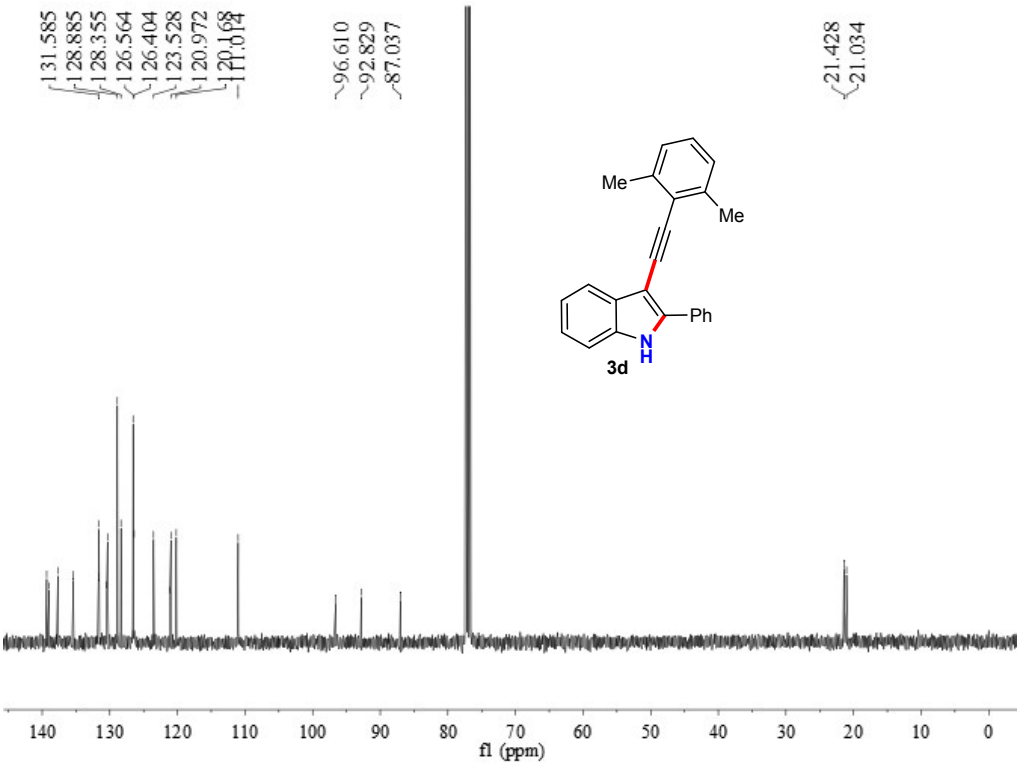
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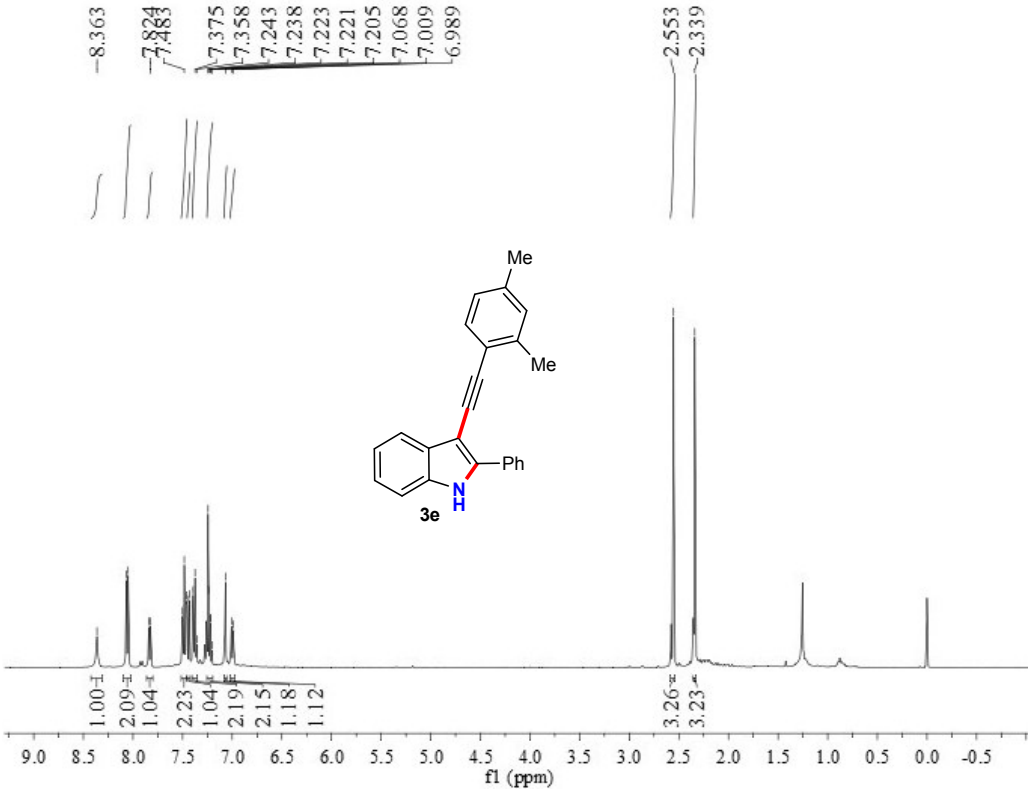
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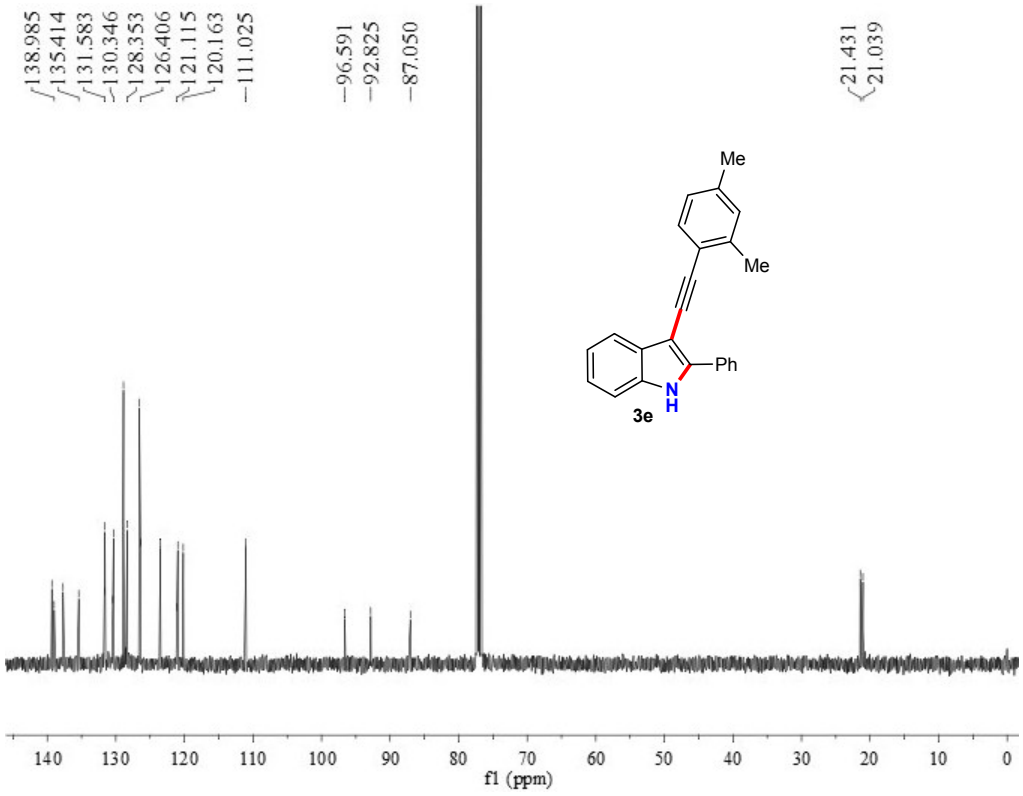
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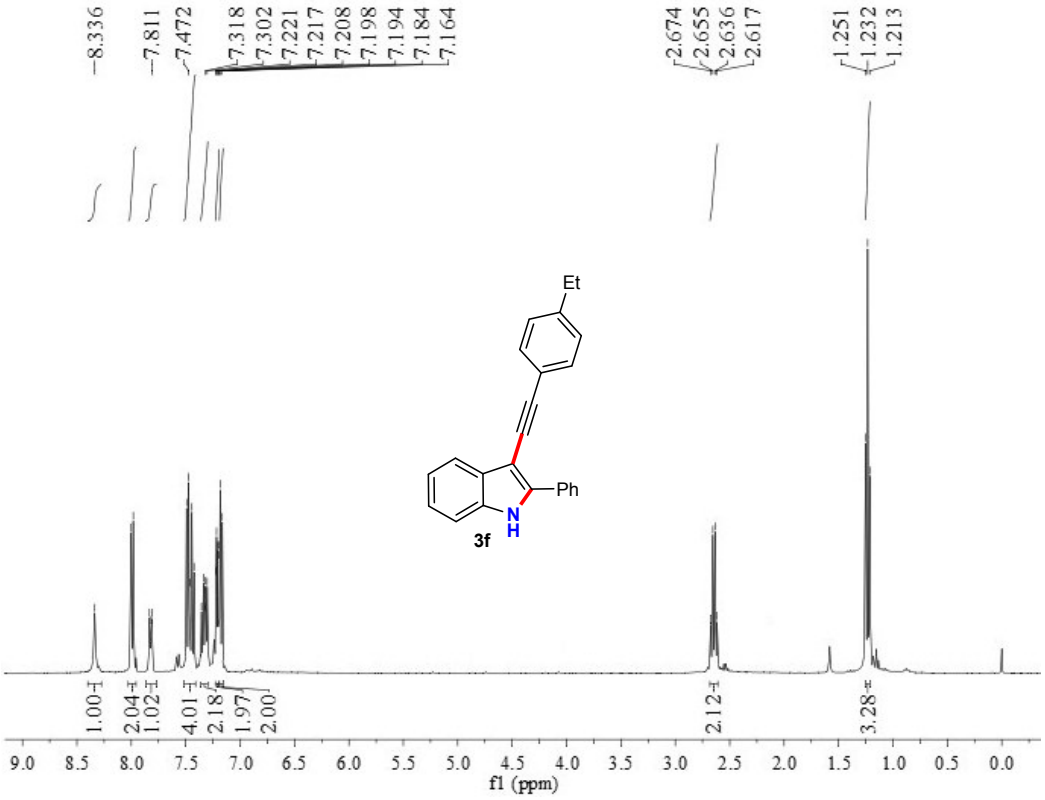
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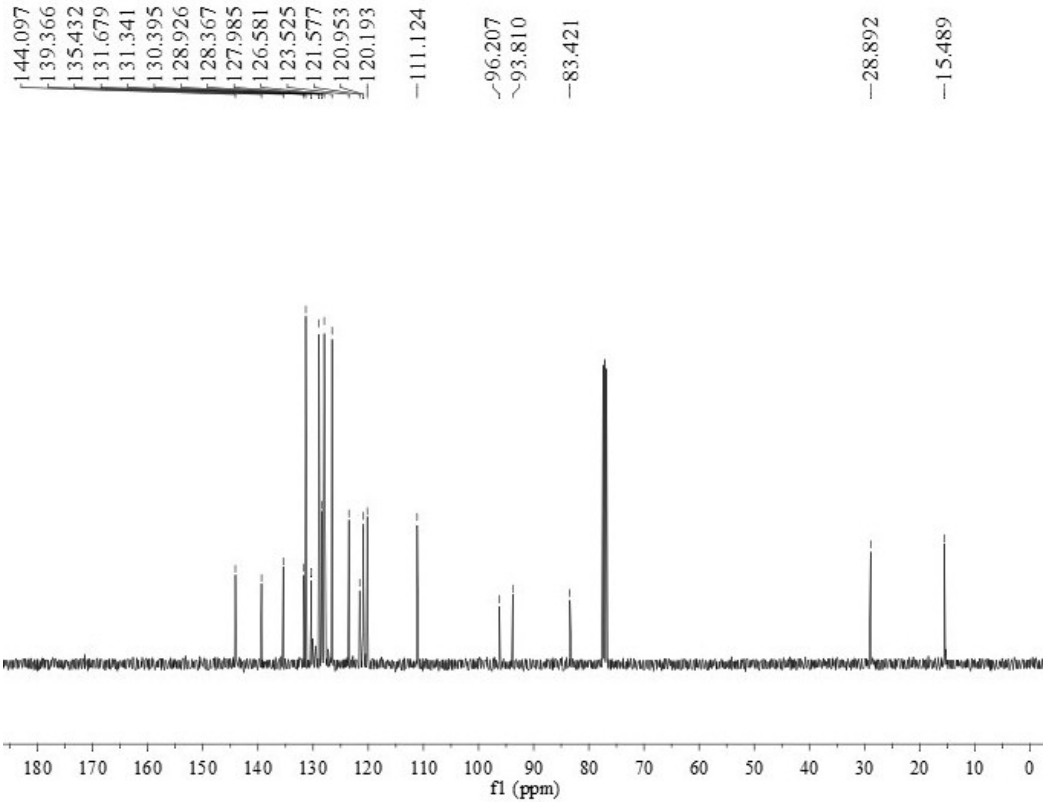
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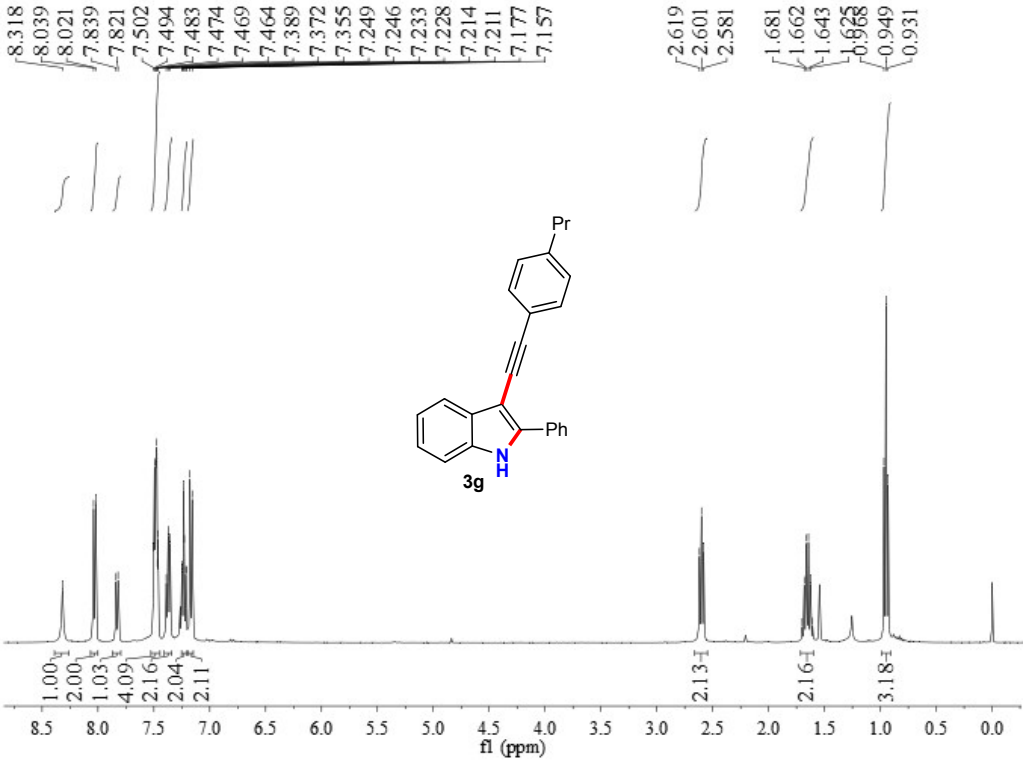
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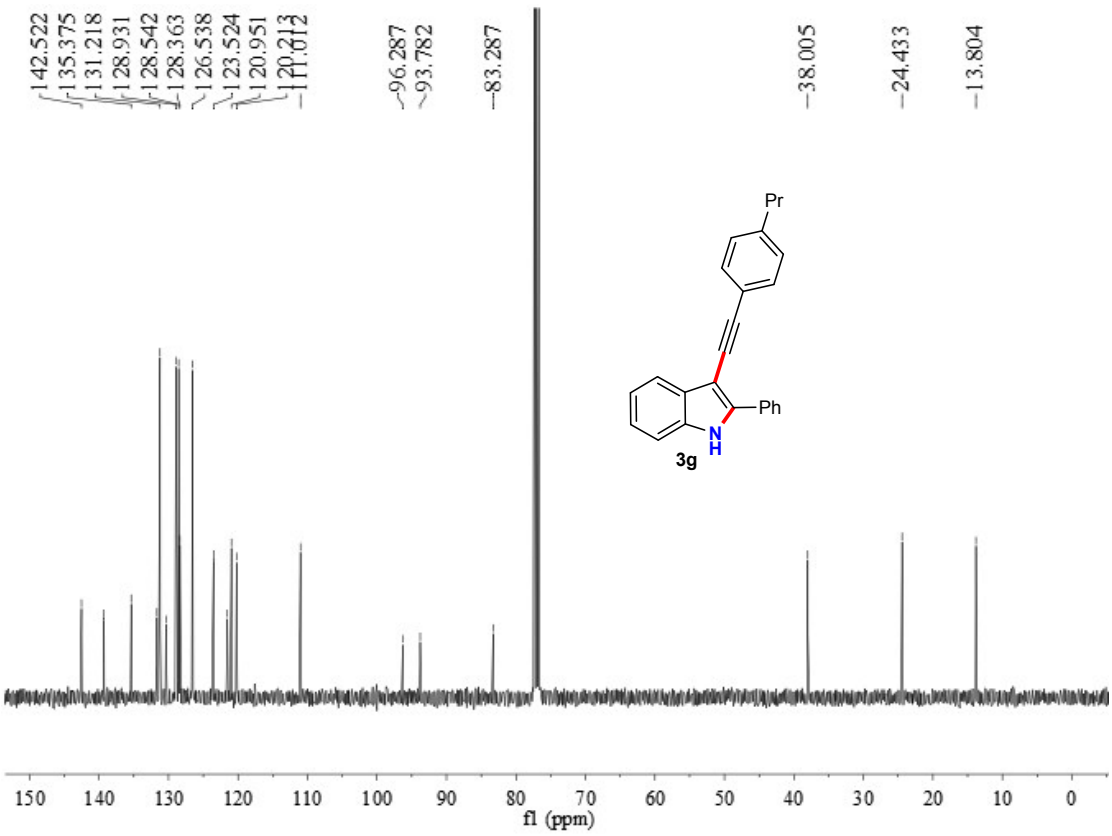
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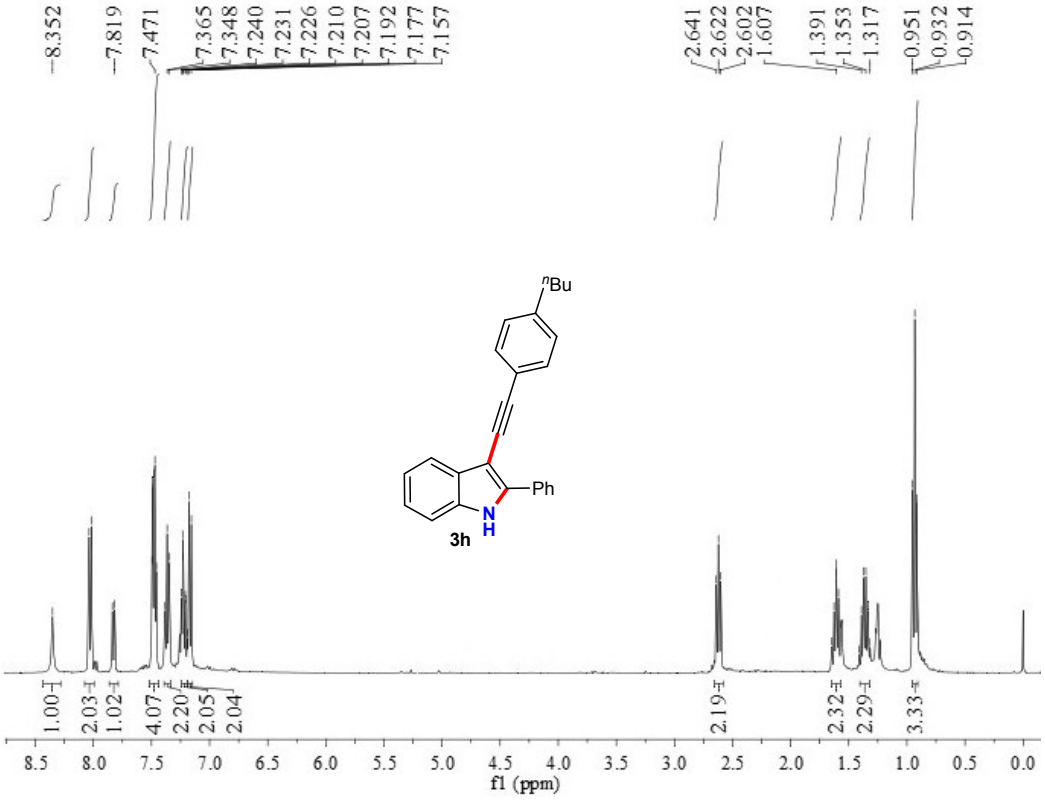
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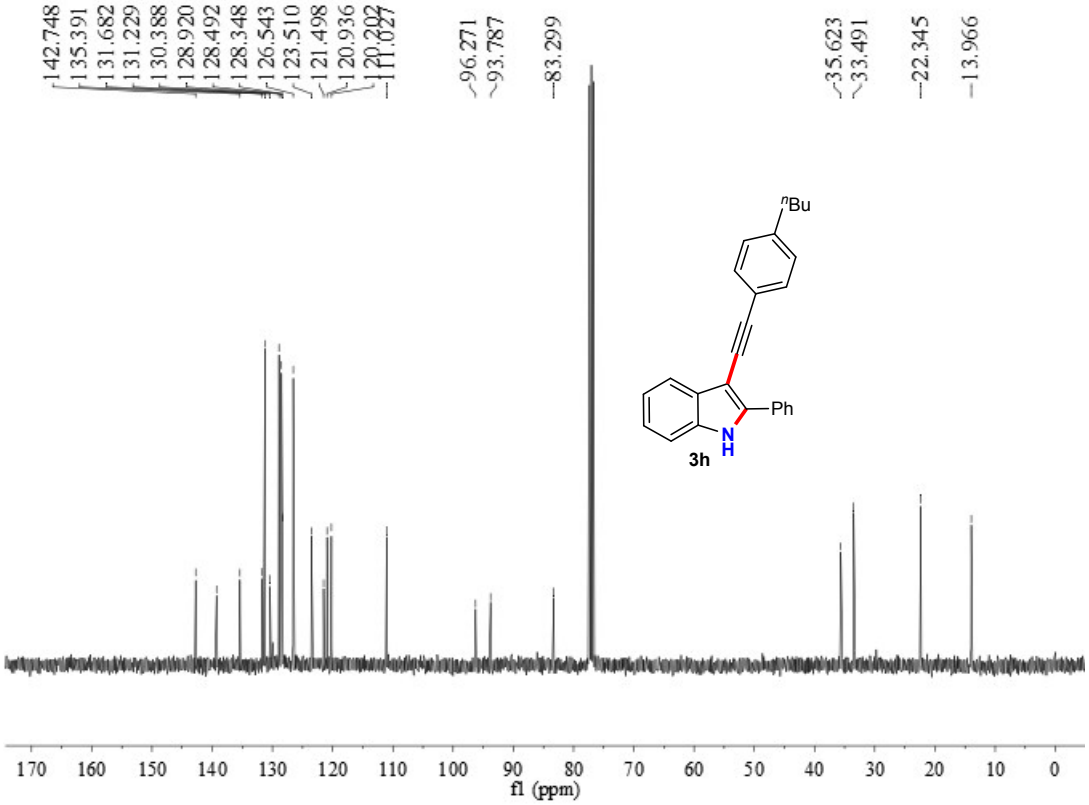
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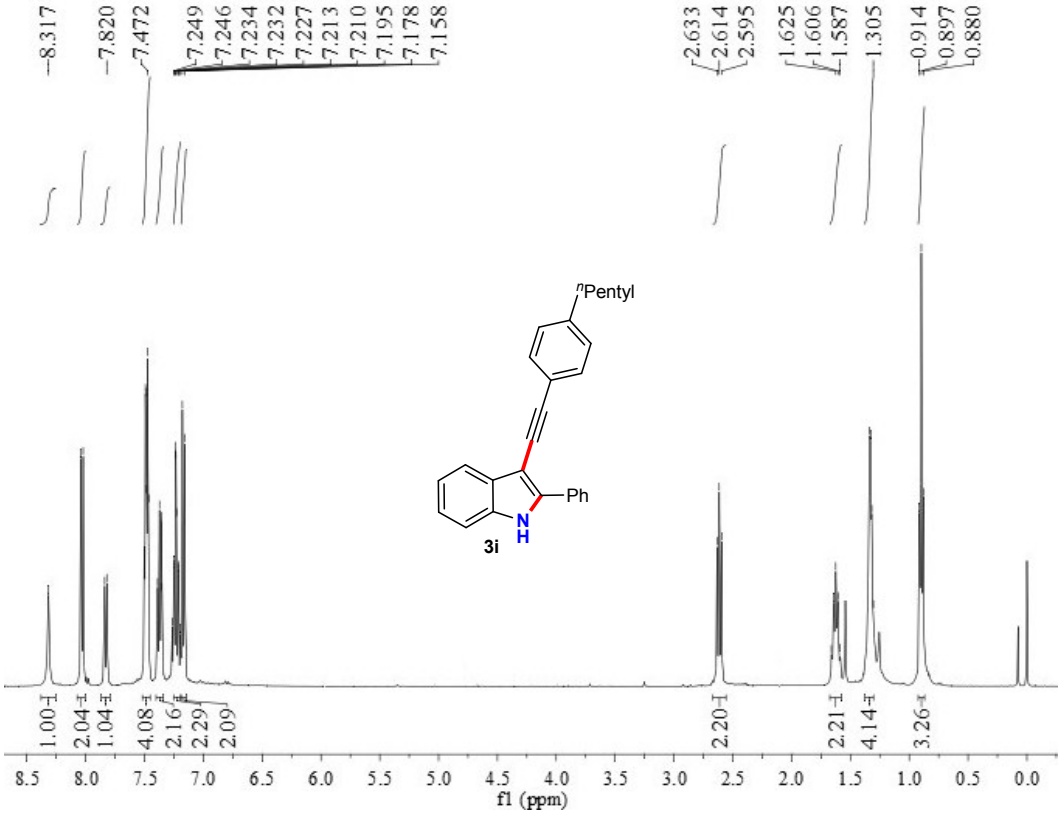
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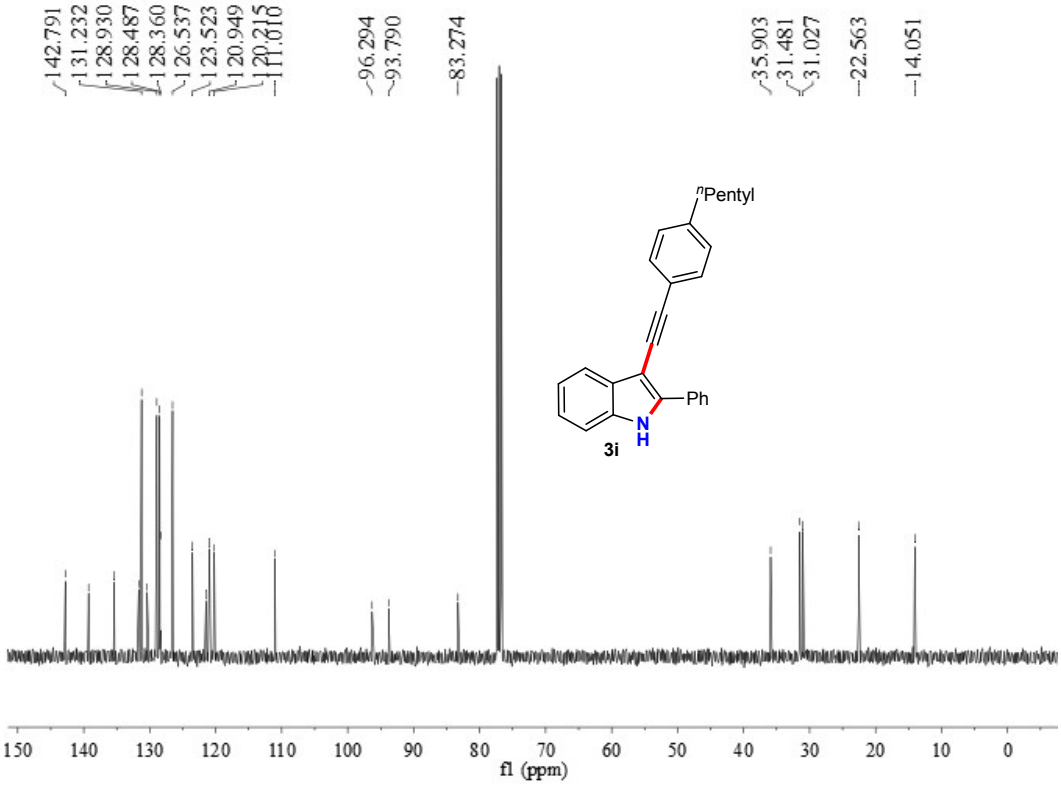
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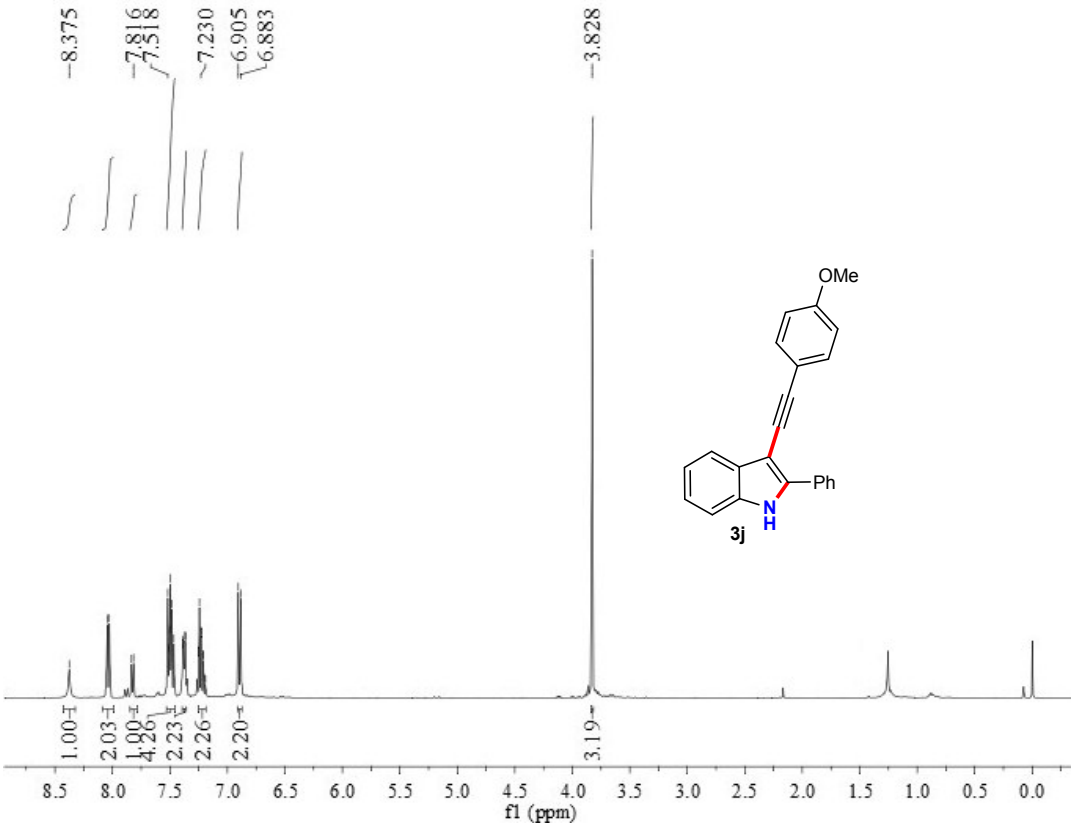
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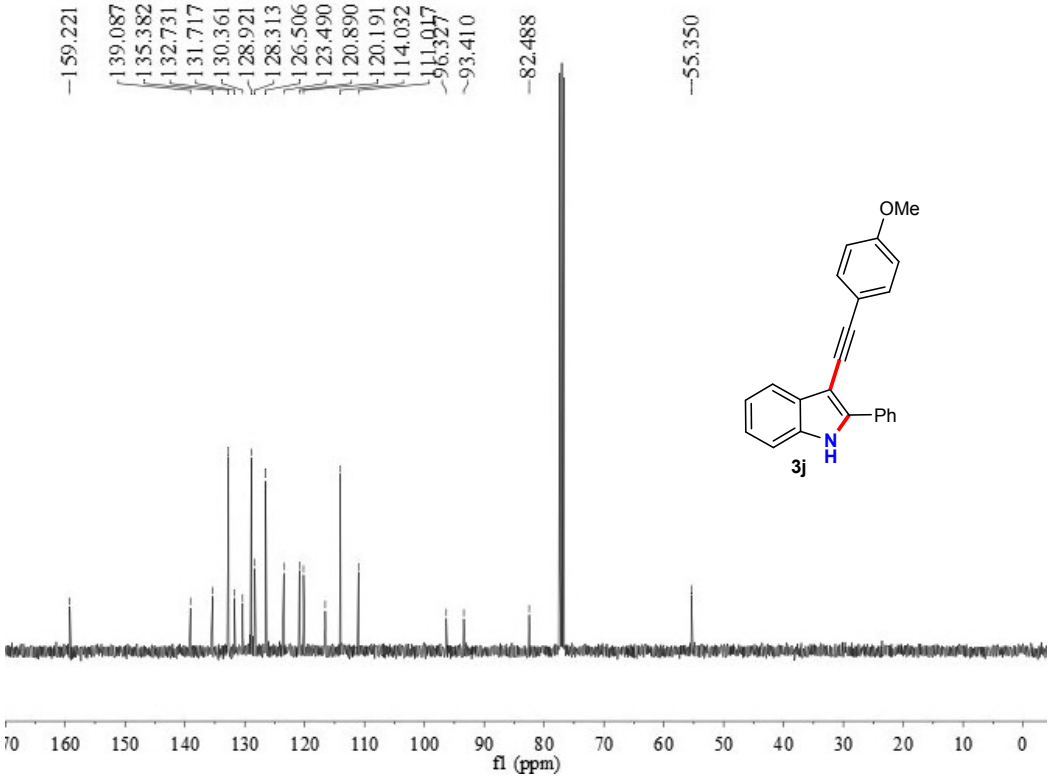
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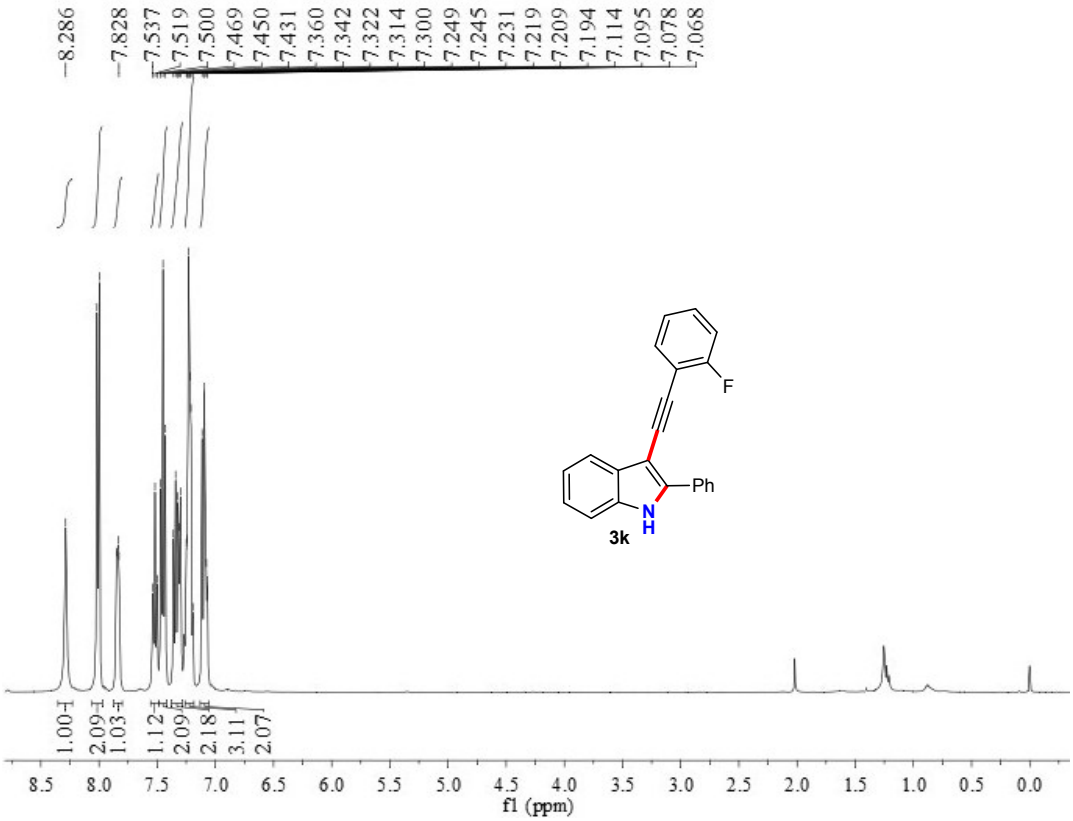
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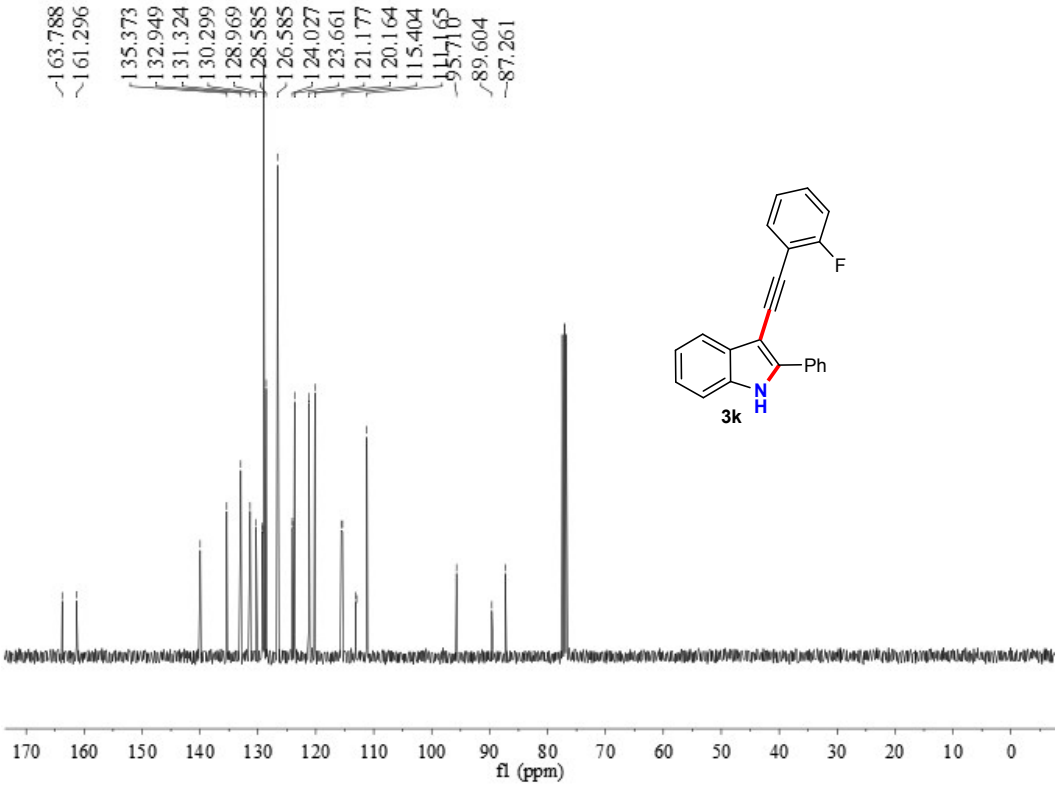
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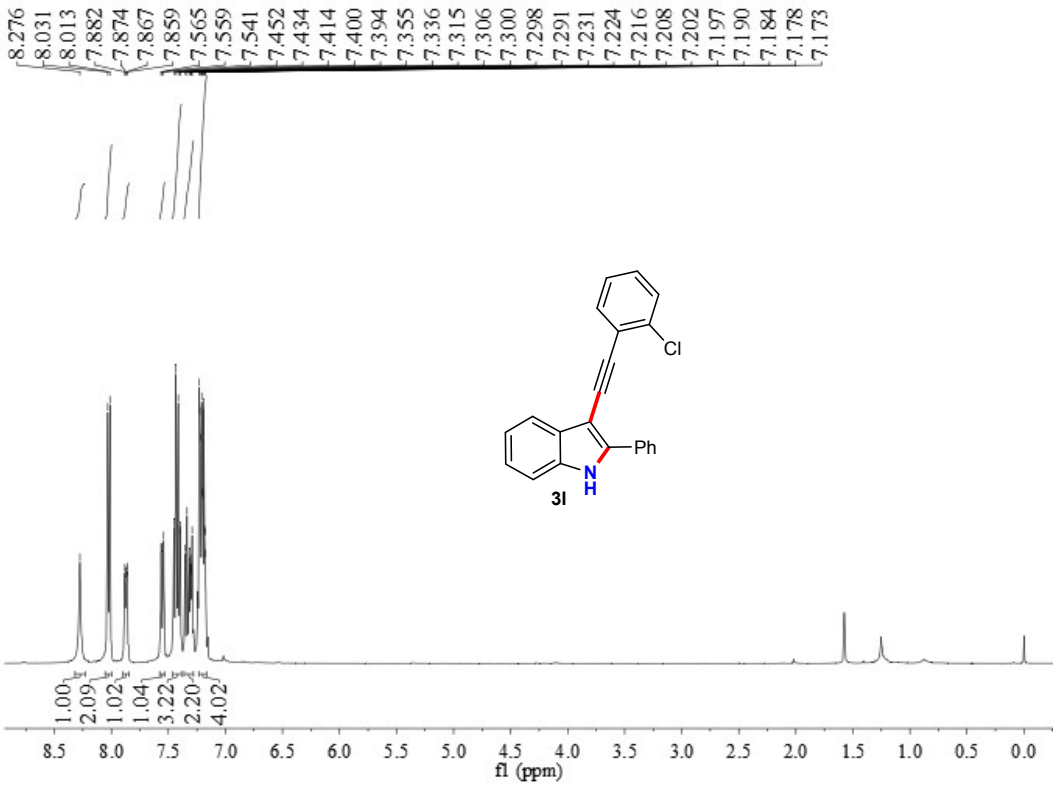
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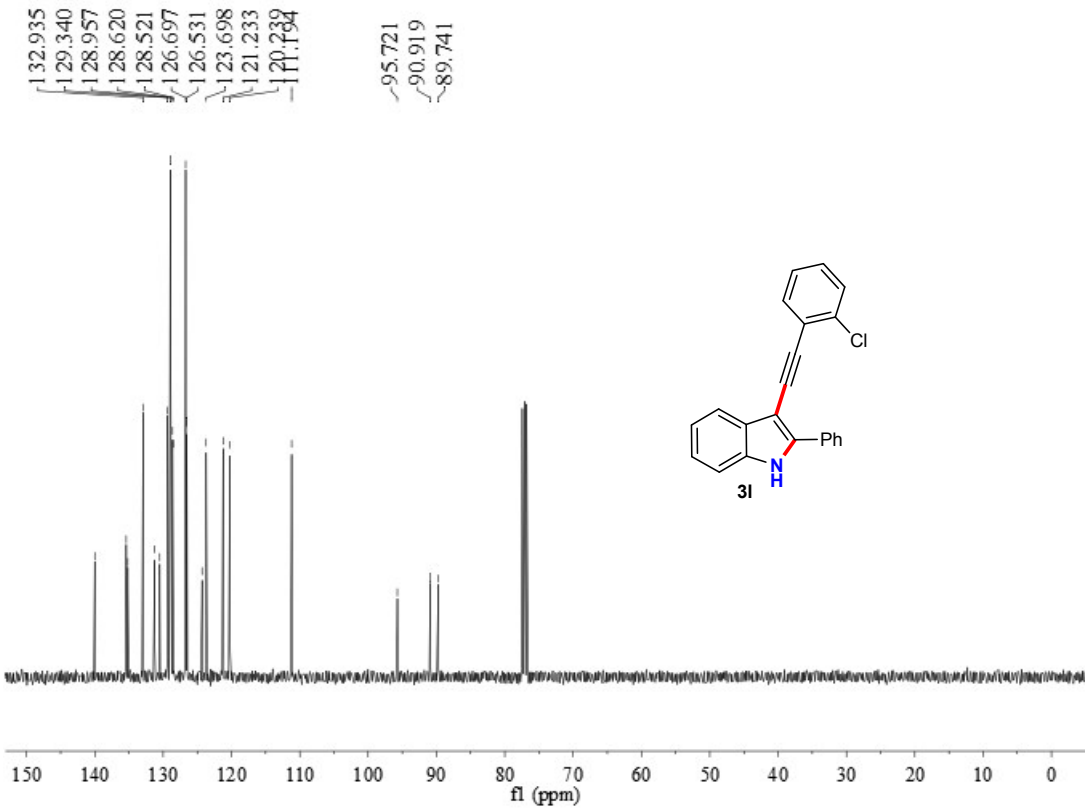
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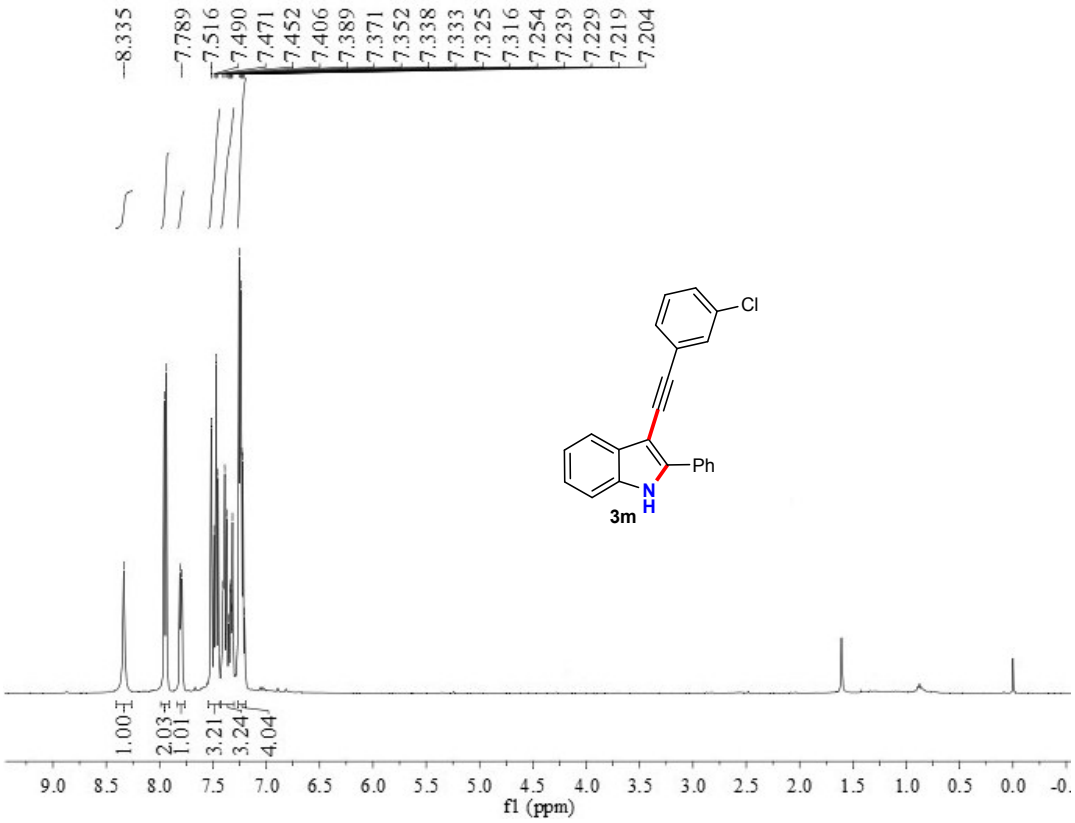
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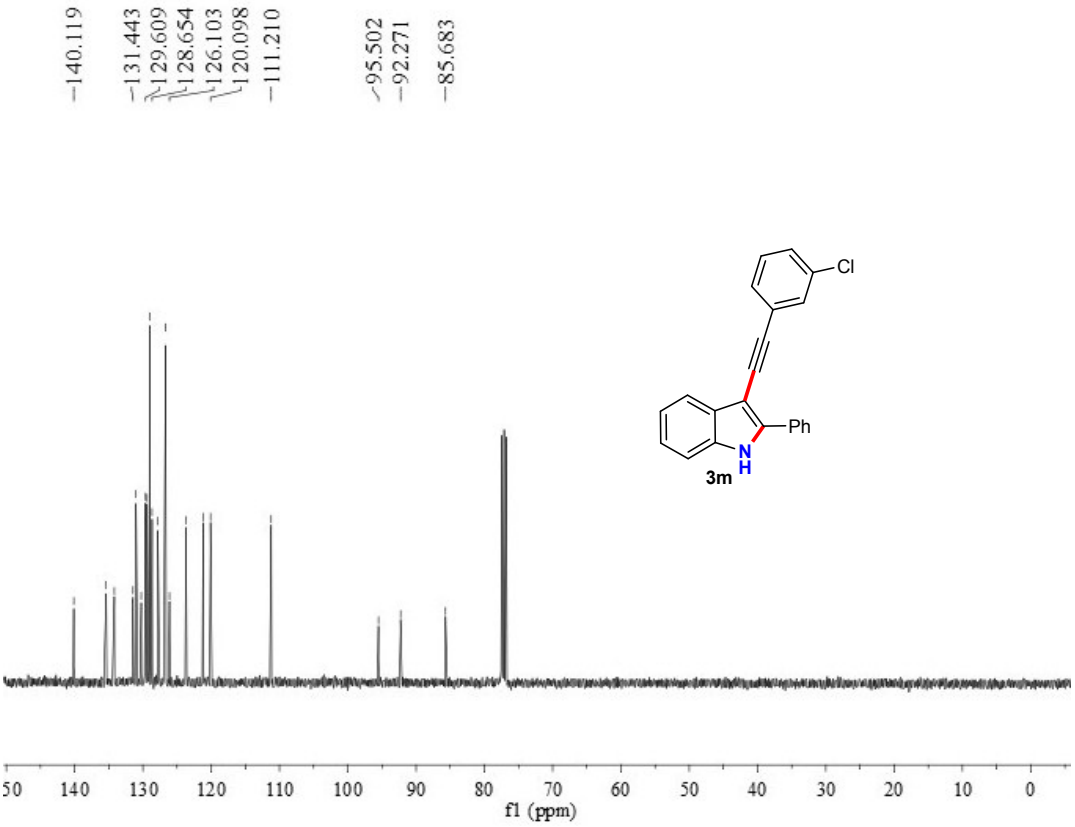
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.609
128.654
126.103
120.098
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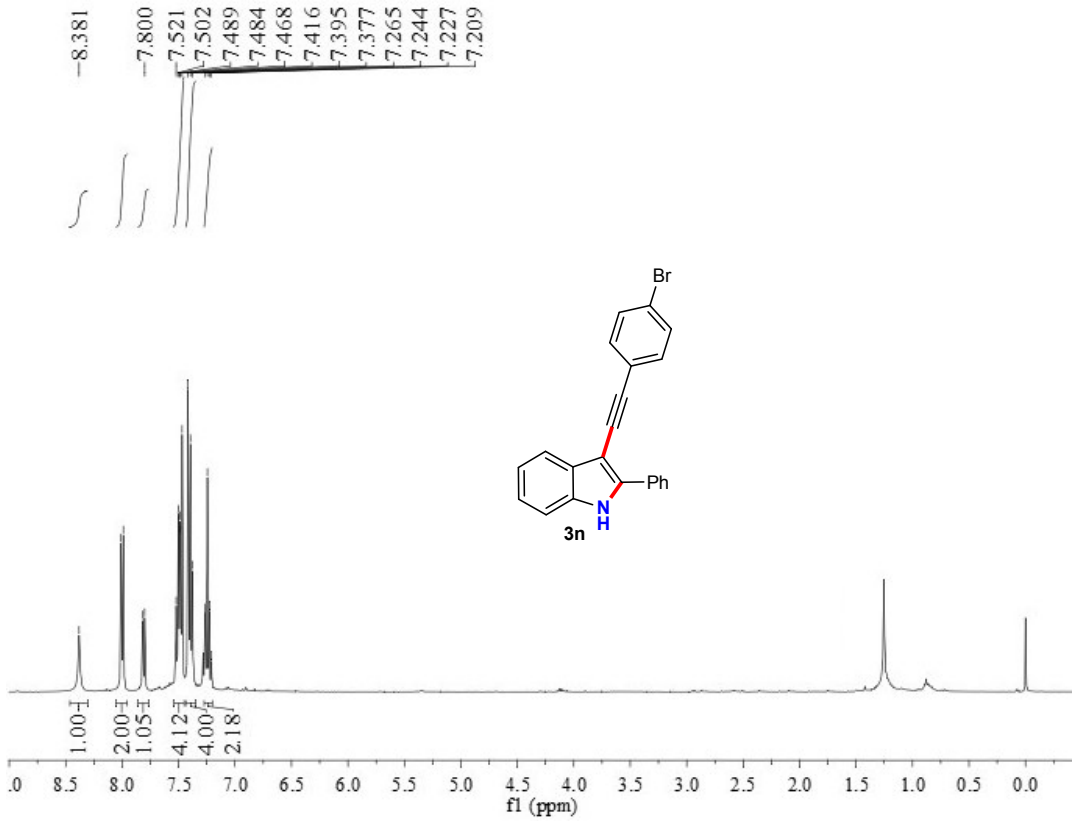
95.502
92.271
85.683
Cl
Ph
N
H
3m
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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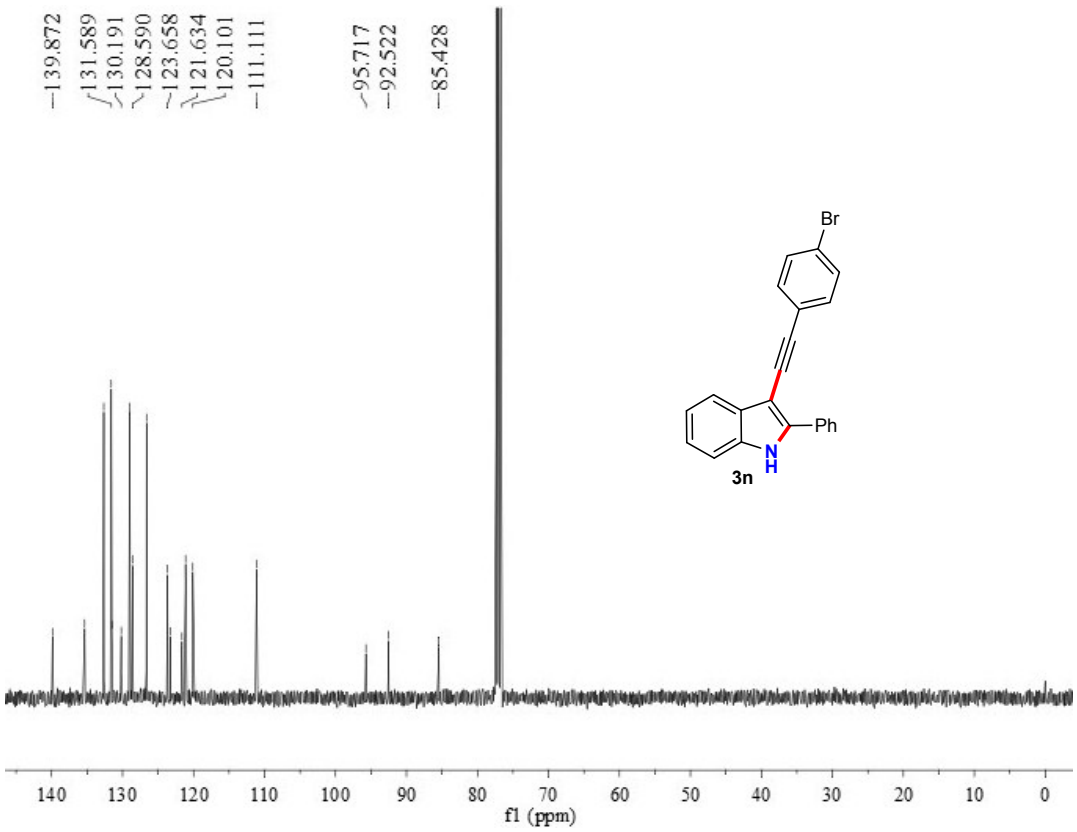
7.521
7.502
7.489
7.484
7.468
7.416
7.395
7.377
7.265
7.244
7.227
7.209
Br
Ph
N
H
3n
1.00
2.00
1.05
4.12
4.00
2.18
f1 (ppm)


139.872
131.589
130.191
128.590
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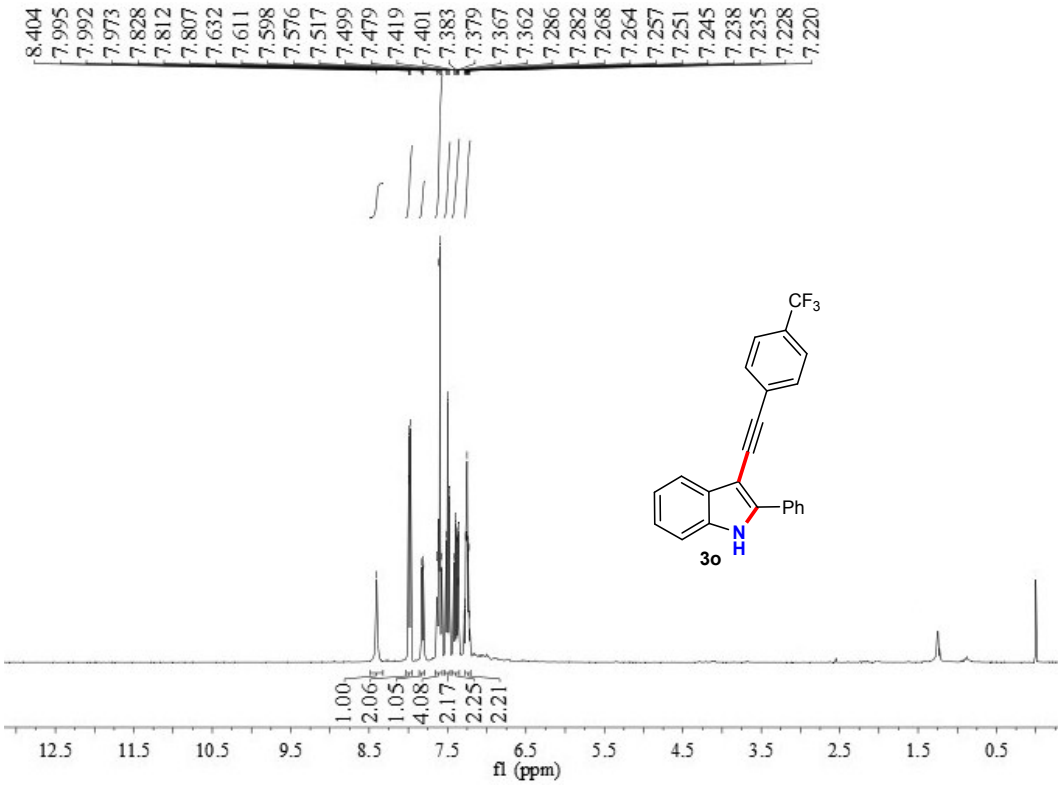
120.101
111.111
95.717
92.522
85.428
Br
Ph
N
H
3n
f1 (ppm)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7.992
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7.632
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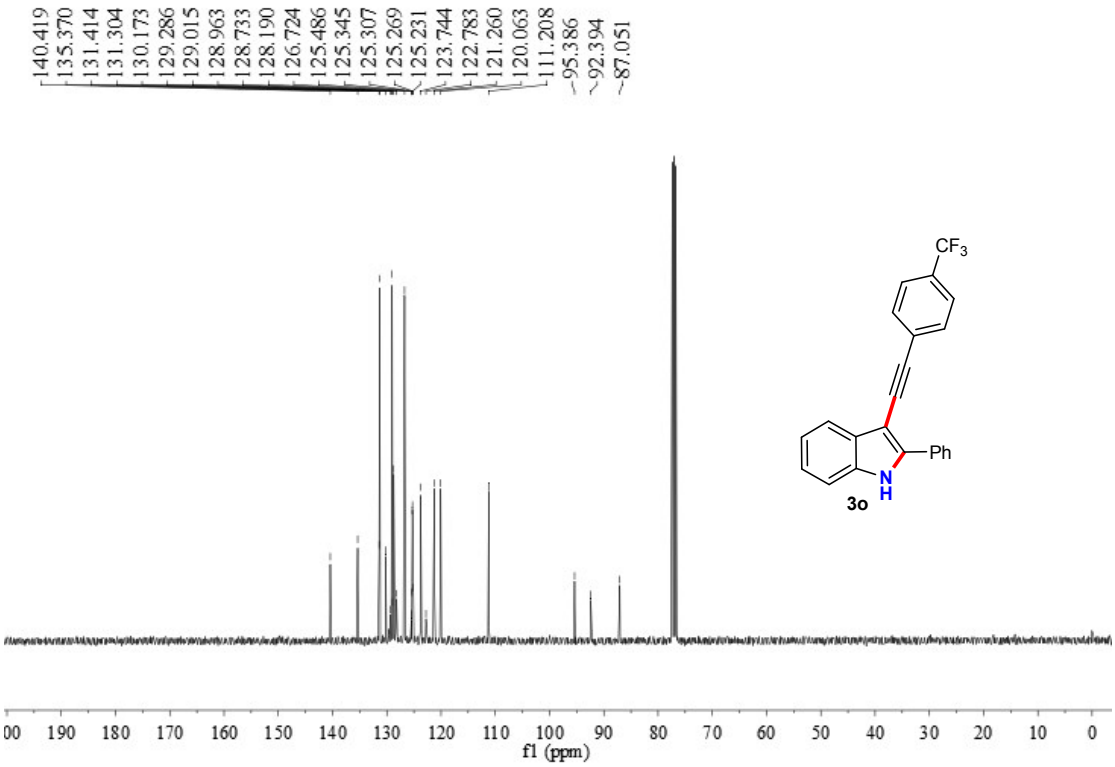
7.598
7.576
7.517
7.499
7.479
7.419
7.401
7.383
7.379
7.367
7.362
7.286
7.282
7.268
7.264
7.257
7.251
7.245
7.238
7.235
7.228
7.220
CF3
Ph
N
H
3o
1.00
2.06
1.05
4.08
2.17
2.25
2.21
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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131.304
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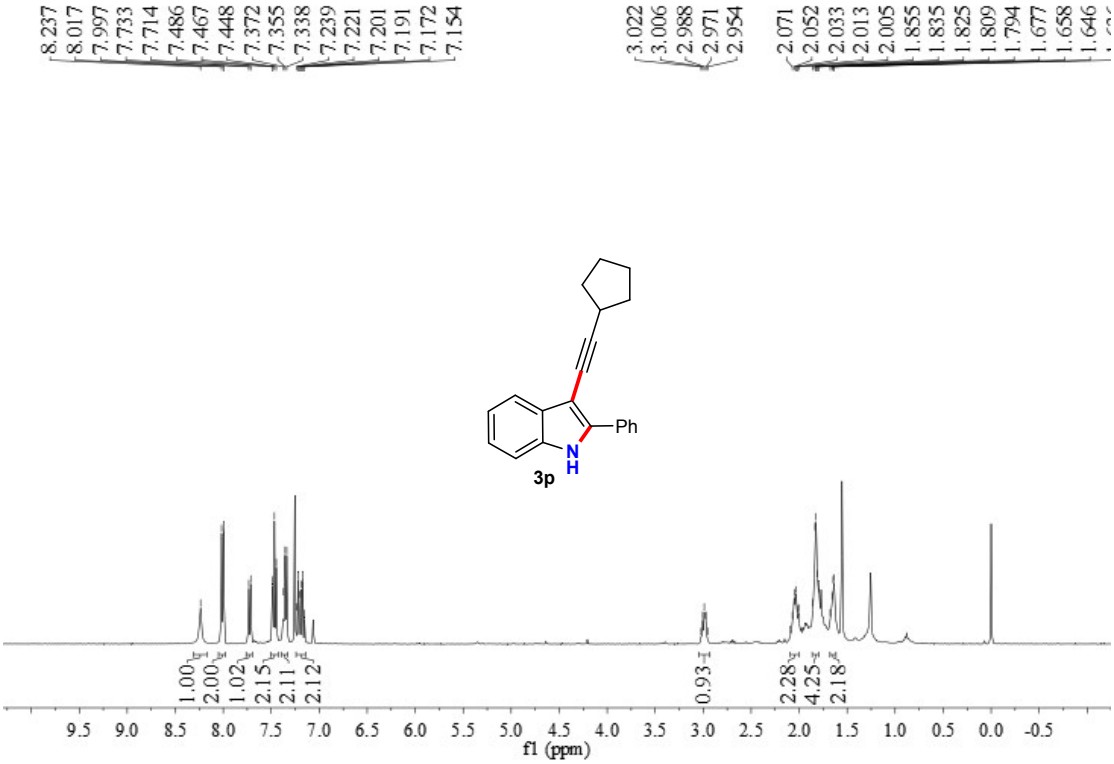
129.286
129.015
128.963
128.733
128.190
126.724
125.486
125.345
125.307
125.269
125.231
123.744
122.783
121.260
120.063
111.208
95.386
92.394
87.051
CF3
Ph
N
H
3o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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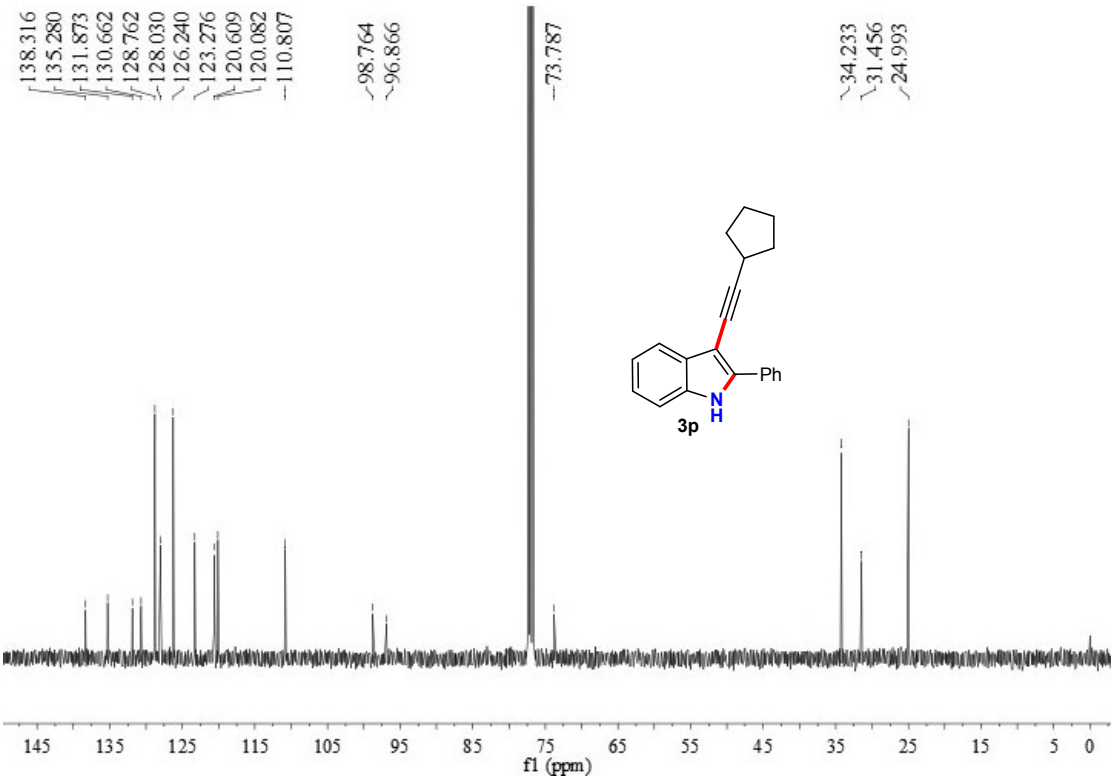
7.733
7.714
7.486
7.467
7.448
7.372
7.355
7.338
7.239
7.221
7.201
7.191
7.172
7.154
3.022
3.006
2.988
2.971
2.954
2.071
2.052
2.033
2.013
2.005
1.855
1.835
1.825
1.809
1.794
1.677
1.658
1.646
Ph
N
H
3p
1.00
2.00
1.02
2.15
2.11
2.12
0.93
2.28
4.25
2.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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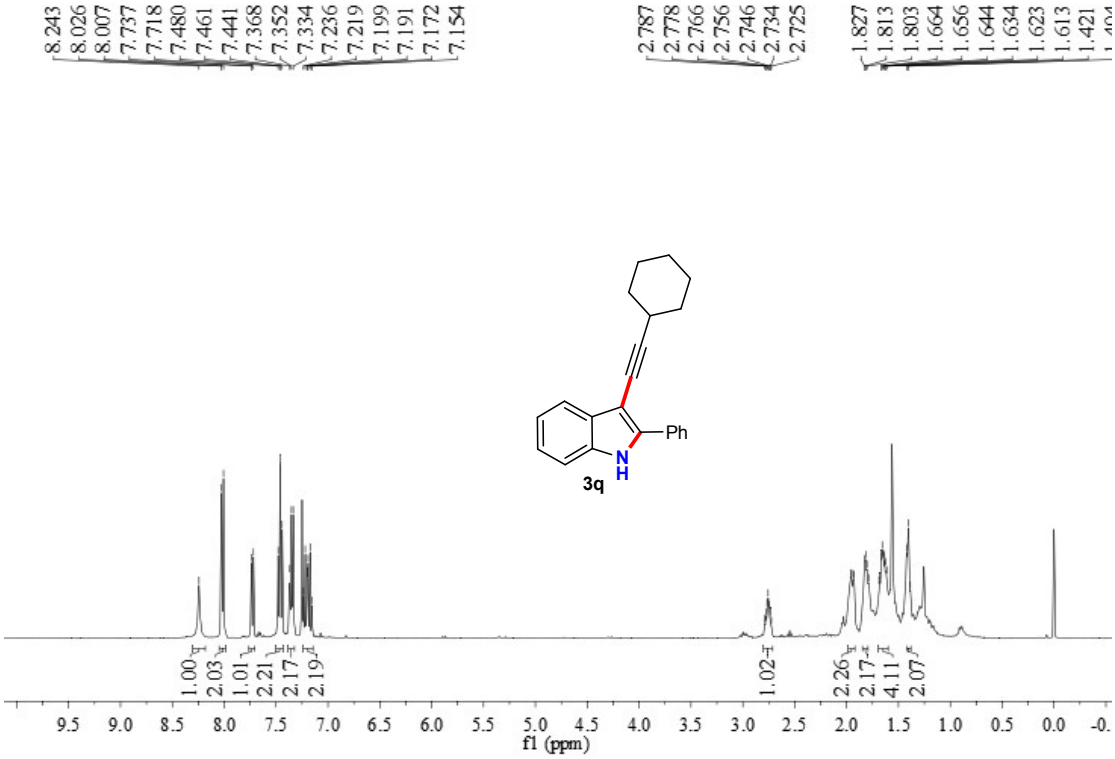
128.030
126.240
123.276
120.609
120.082
110.807
98.764
96.866
73.787
34.233
31.456
24.993
Ph
N
H
3p
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)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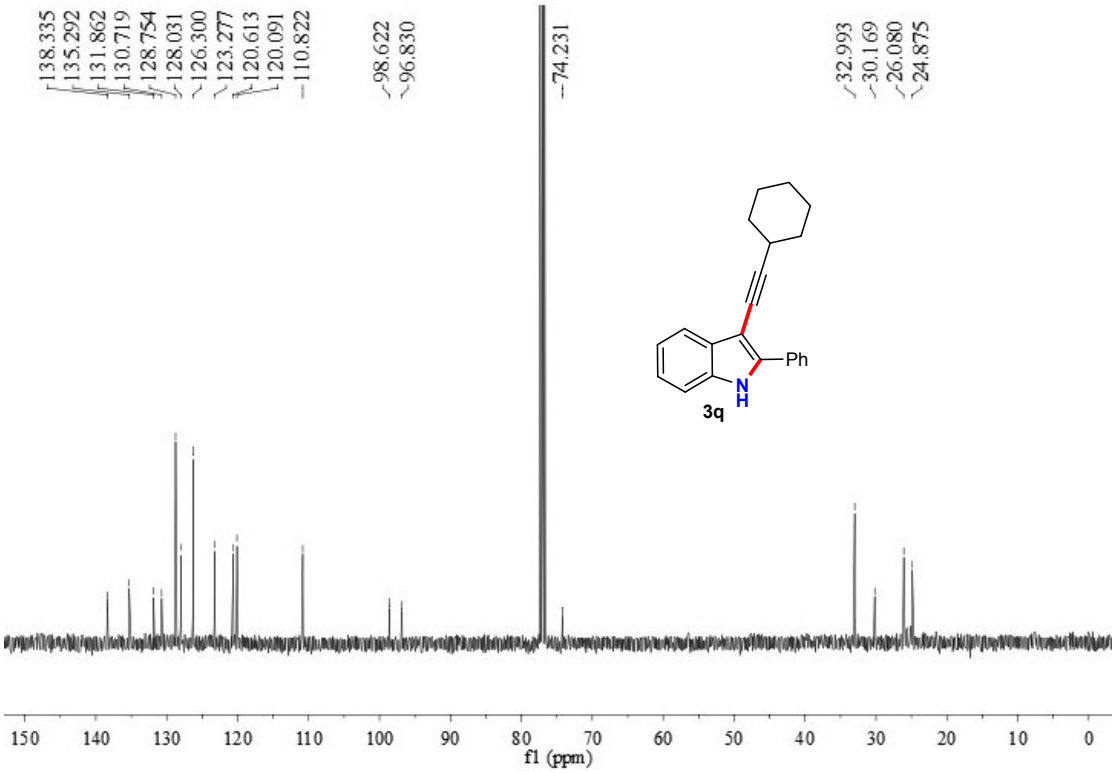
8.026
8.007
7.737
7.718
7.480
7.461
7.441
7.368
7.352
7.334
7.236
7.219
7.199
7.191
7.172
7.154
2.787
2.778
2.766
2.756
2.746
2.734
2.725
1.827
1.813
1.803
1.664
1.656
1.644
1.634
1.623
1.613
1.421
Ph
N
H
3q
1.00
2.03
1.01
2.21
2.17
2.19
1.02
2.26
2.17
4.11
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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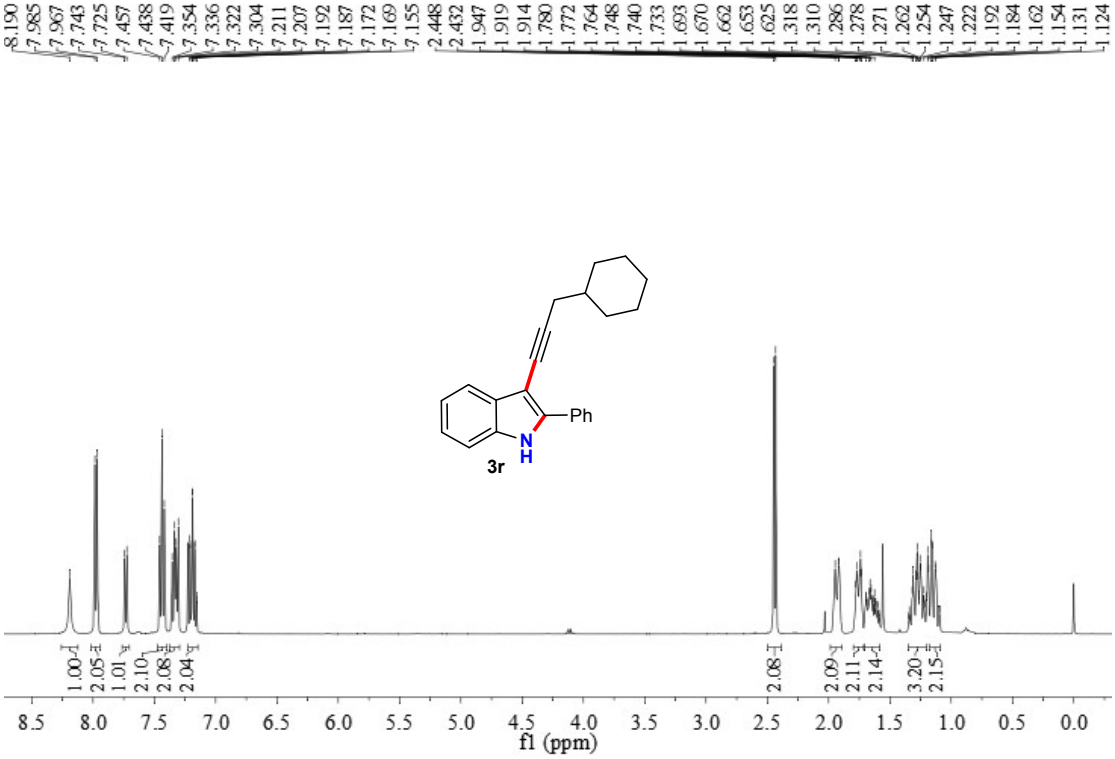
130.719
128.754
128.031
126.300
123.277
120.613
120.091
110.822
98.622
96.830
74.231
32.993
30.169
26.080
24.875
Ph
N
H
3q
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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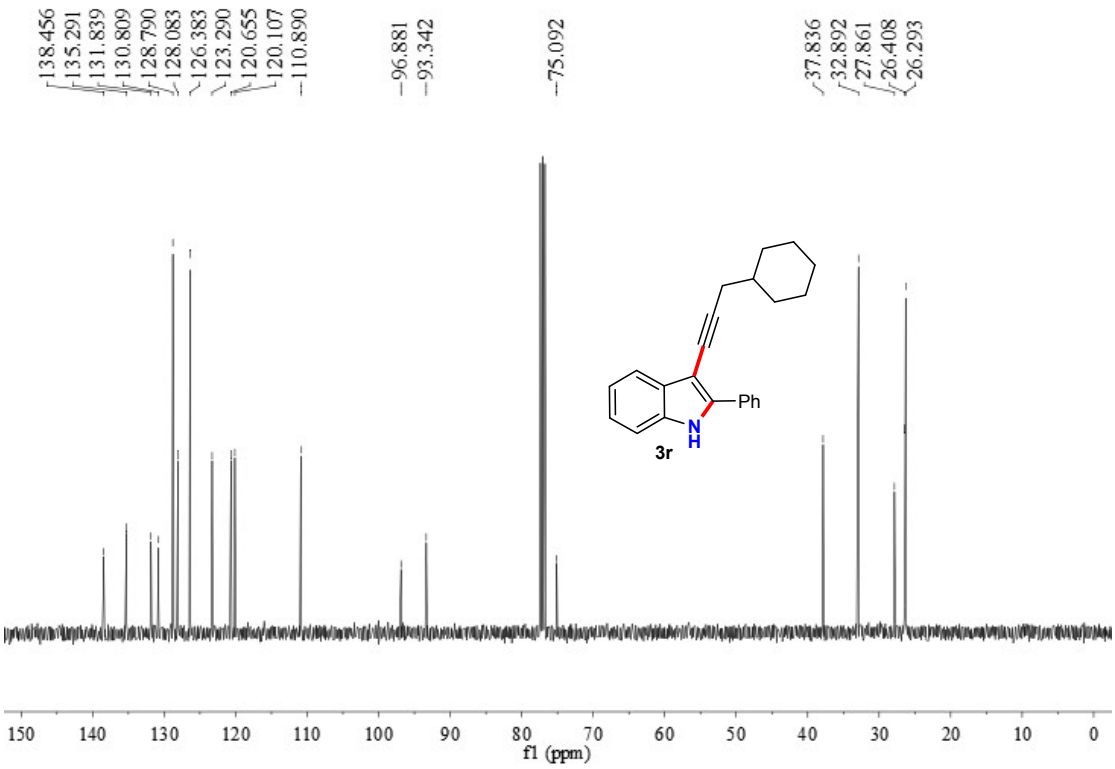
7.967
7.743
7.725
7.457
7.438
7.419
7.354
7.336
7.322
7.304
7.211
7.207
7.192
7.187
7.172
7.169
7.155
2.448
2.432
1.947
1.919
1.914
1.780
1.772
1.764
1.748
1.740
1.733
1.693
1.670
1.662
1.653
1.625
1.318
1.310
1.286
1.278
1.271
1.262
1.254
1.247
1.222
1.192
1.184
1.162
1.154
1.131
1.124
Ph
N
H
3r
1.00
2.05
1.01
2.10
2.08
2.04
2.08
2.09
2.11
2.14
3.20
2.15
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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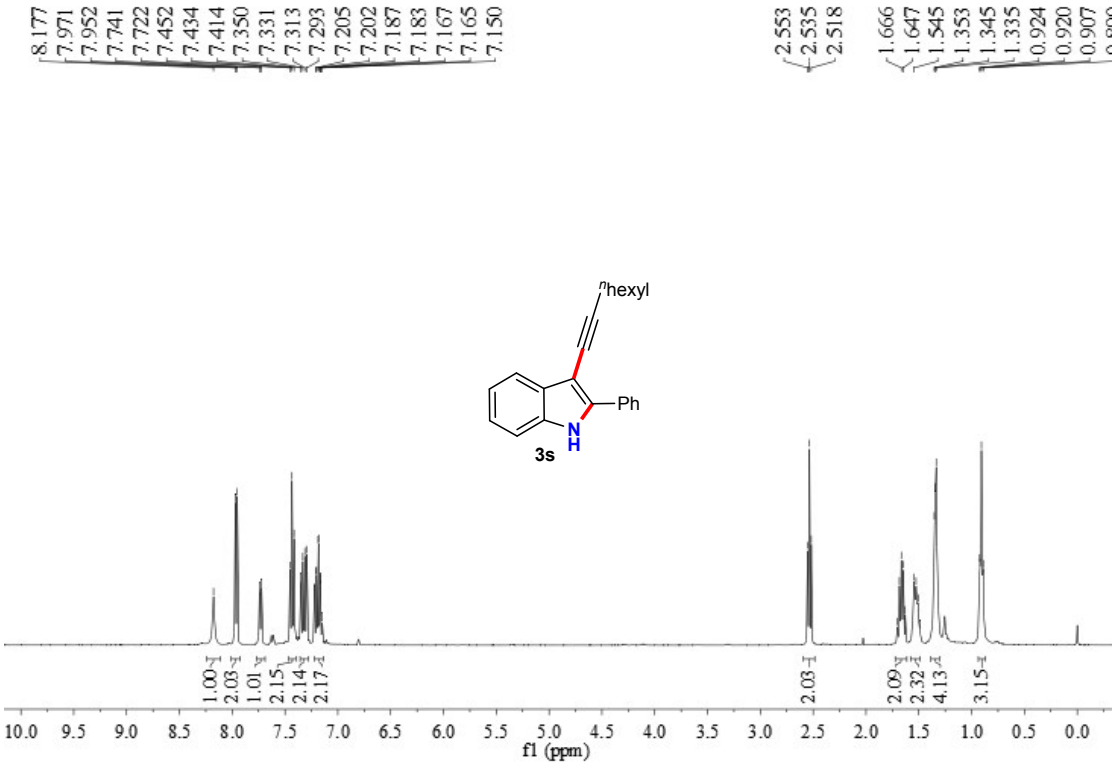
96.881
93.342
75.092
37.836
32.892
27.861
26.408
26.293
Ph
N
H
3r
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.741
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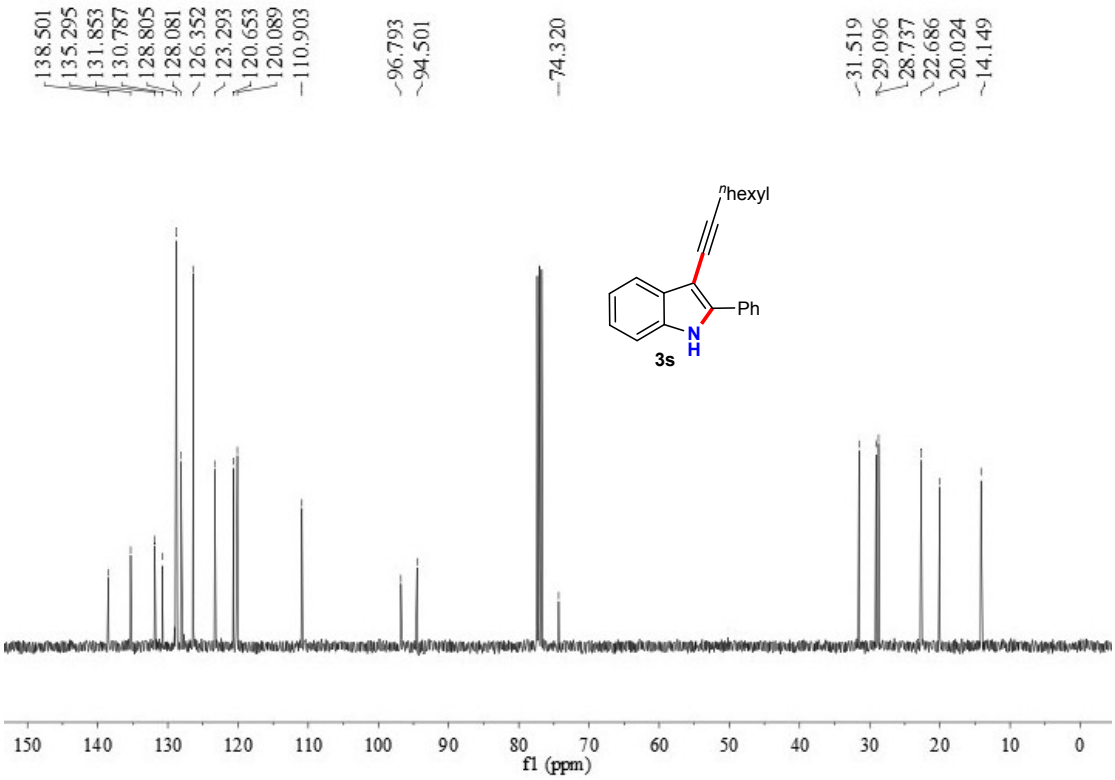
7.452
7.434
7.414
7.350
7.331
7.313
7.293
7.205
7.202
7.187
7.183
7.167
7.165
7.150
2.553
2.535
2.518
1.666
1.647
1.545
1.353
1.345
1.335
0.924
0.920
0.907
nhexyl
Ph
N
H
3s
1.00
2.03
1.01
2.15
2.14
2.17
2.03
2.09
2.32
4.13
3.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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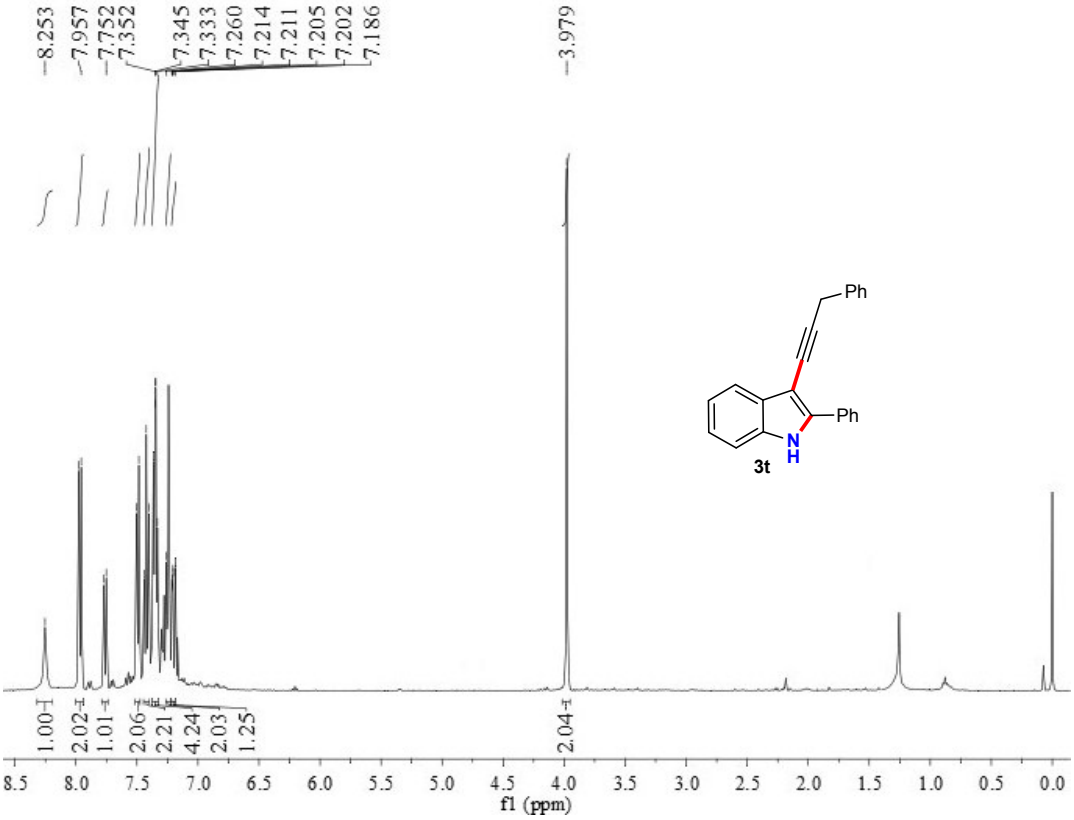
130.787
128.805
128.081
126.352
123.293
120.653
120.089
110.903
96.793
94.501
74.320
31.519
29.096
28.737
22.686
20.024
14.149
nhexyl
Ph
N
H
3s
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.352
7.345
7.333
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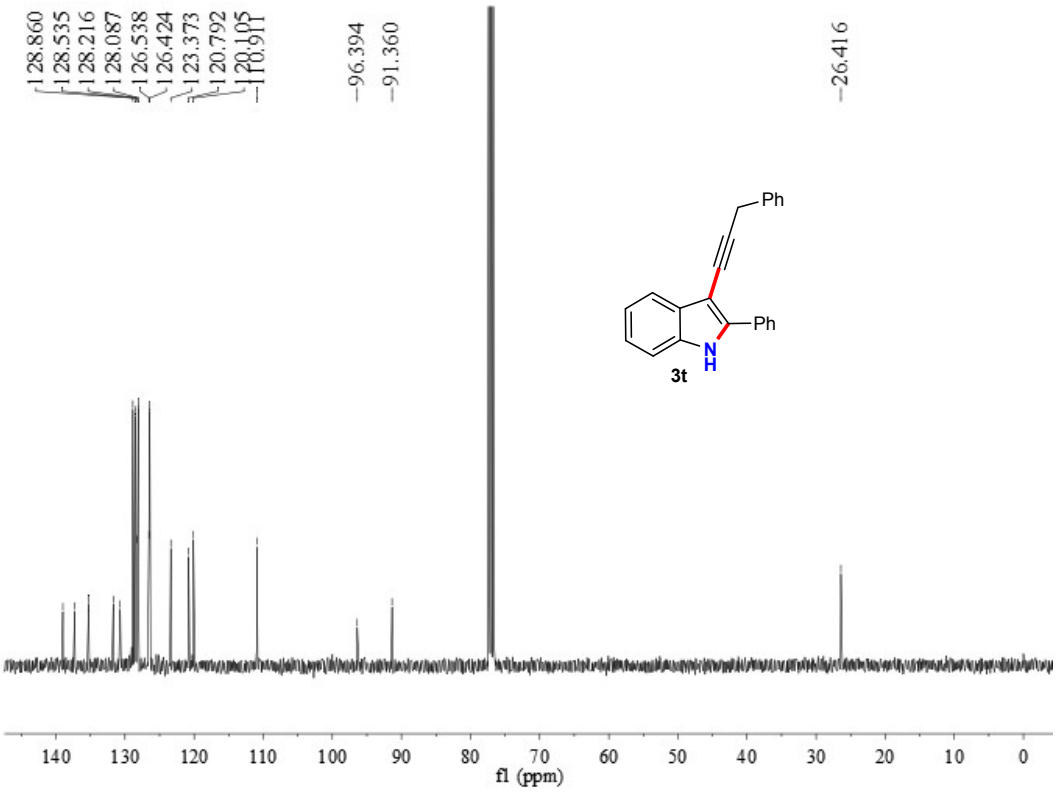
7.214
7.211
7.205
7.202
7.186
3.979
1.00
2.02
1.01
2.06
2.21
4.24
2.03
1.25
2.04
Ph
Ph
N
H
3t
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


128.860
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128.216
128.087
126.538
126.424
123.373
120.792
120.105
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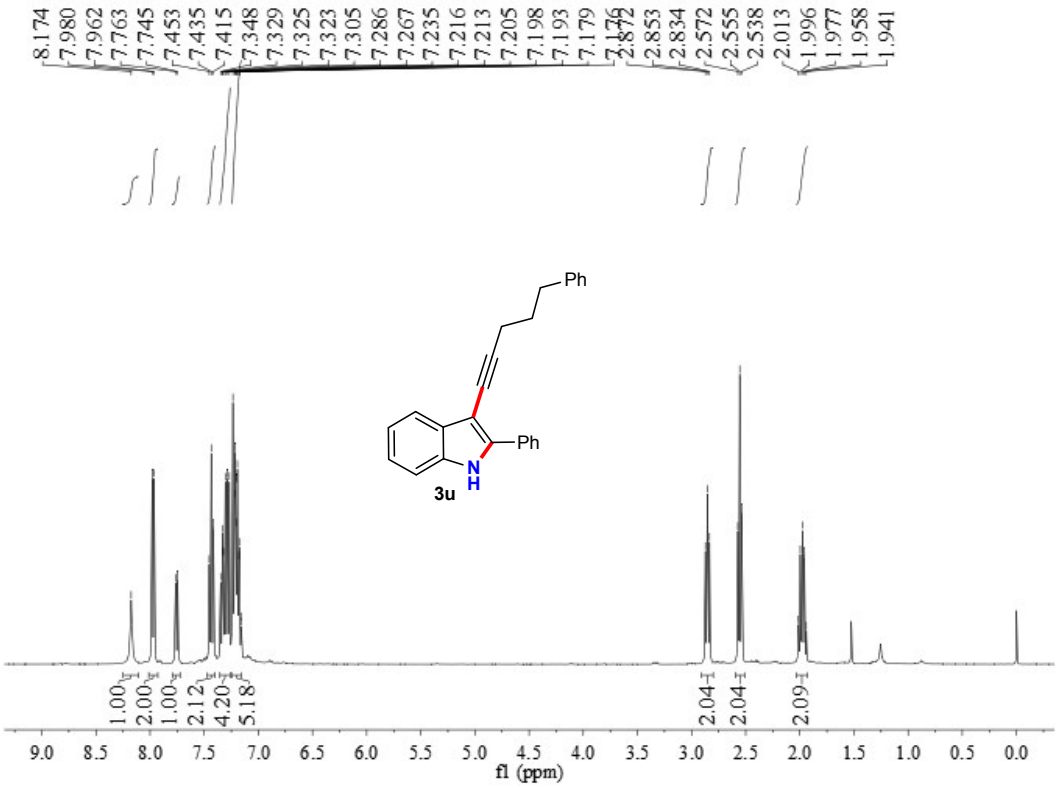
96.394
91.360
26.416
Ph
Ph
N
H
3t
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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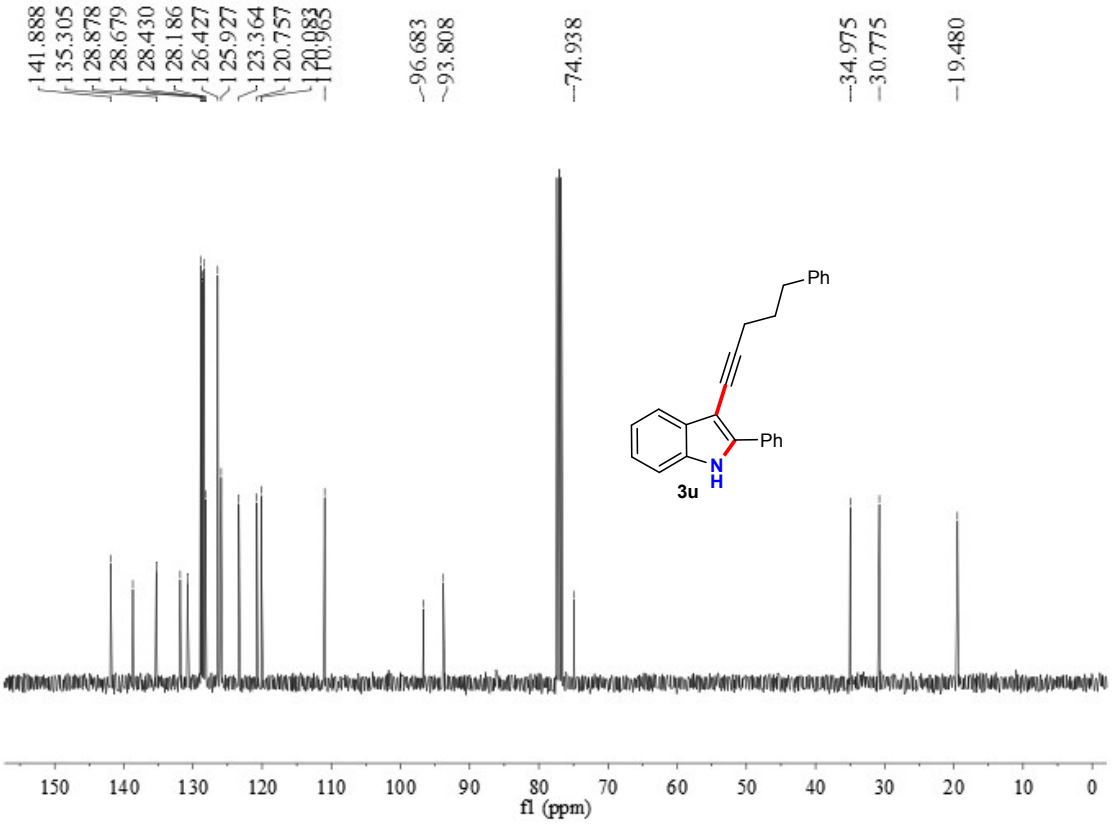
7.323
7.305
7.286
7.267
7.235
7.216
7.213
7.205
7.198
7.193
7.179
2.853
2.834
2.572
2.555
2.538
2.013
1.996
1.977
1.958
1.941
Ph
Ph
N
H
3u
1.00
2.00
1.00
2.12
4.20
5.18
2.04
2.04
2.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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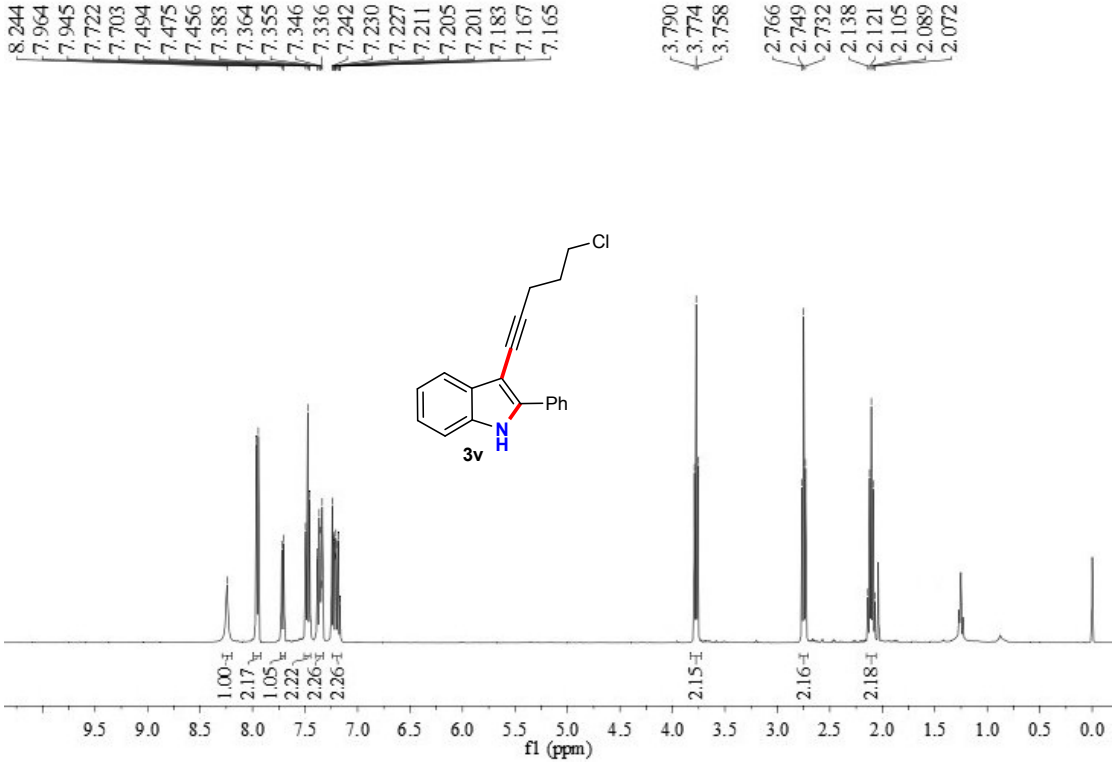
128.430
128.186
126.427
125.927
123.364
120.757
96.683
93.808
74.938
34.975
30.775
19.480
Ph
Ph
N
H
3u
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.722
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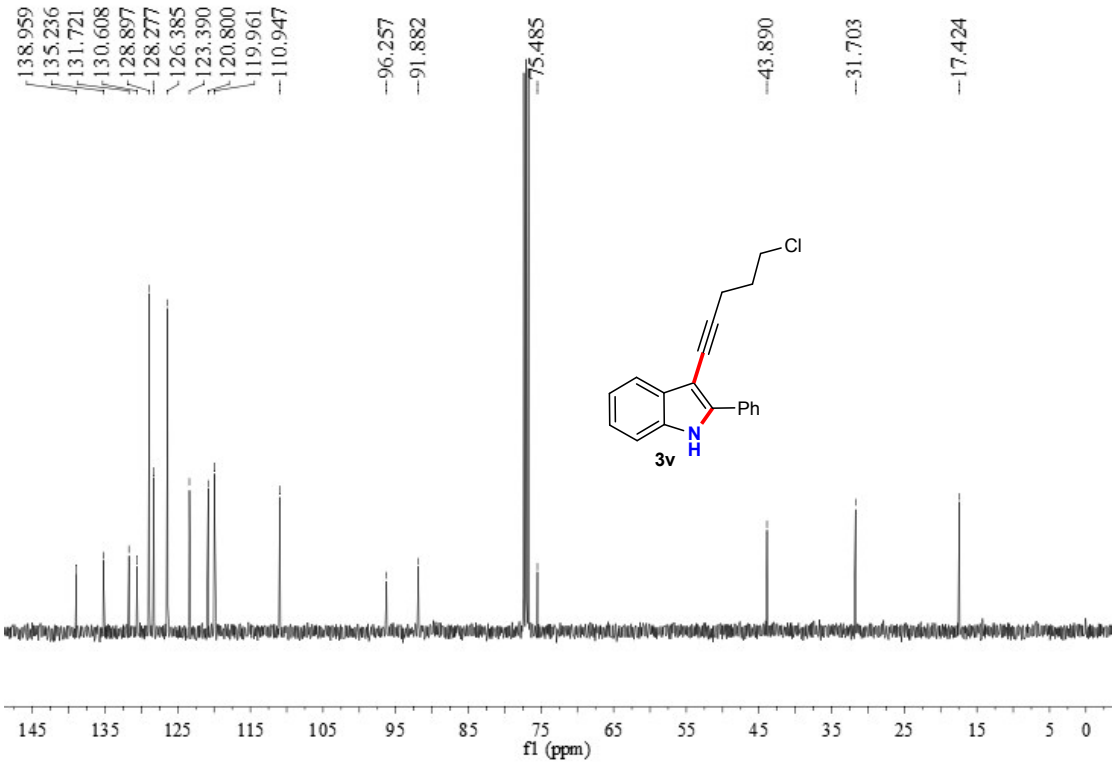
7.475
7.456
7.383
7.364
7.355
7.346
7.336
7.242
7.230
7.227
7.211
7.205
7.201
7.183
7.167
7.165
3.790
3.774
3.758
2.766
2.749
2.732
2.138
2.121
2.105
2.089
2.072
Cl
Ph
N
H
3v
1.00
2.17
1.05
2.22
2.26
2.26
2.15
2.16
2.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.390
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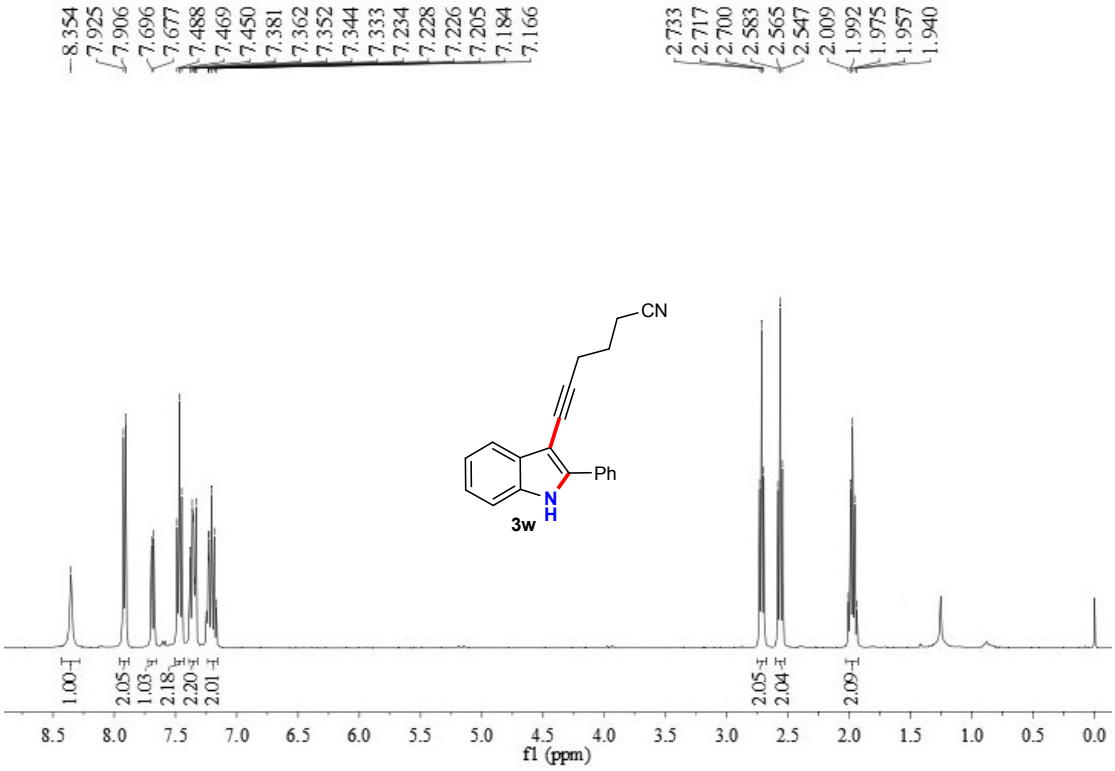
96.257
91.882
75.485
43.890
31.703
17.424
Cl
Ph
N
H
3v
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)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7.234
7.228
7.226
7.205
7.184
7.166
2.733
2.717
2.700
2.583
2.565
2.547
2.009
1.992
1.975
1.957
1.940
CN
Ph
N
H
3w
1.00
2.05
1.03
2.18
2.20
2.01
2.05
2.04
2.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
2.0
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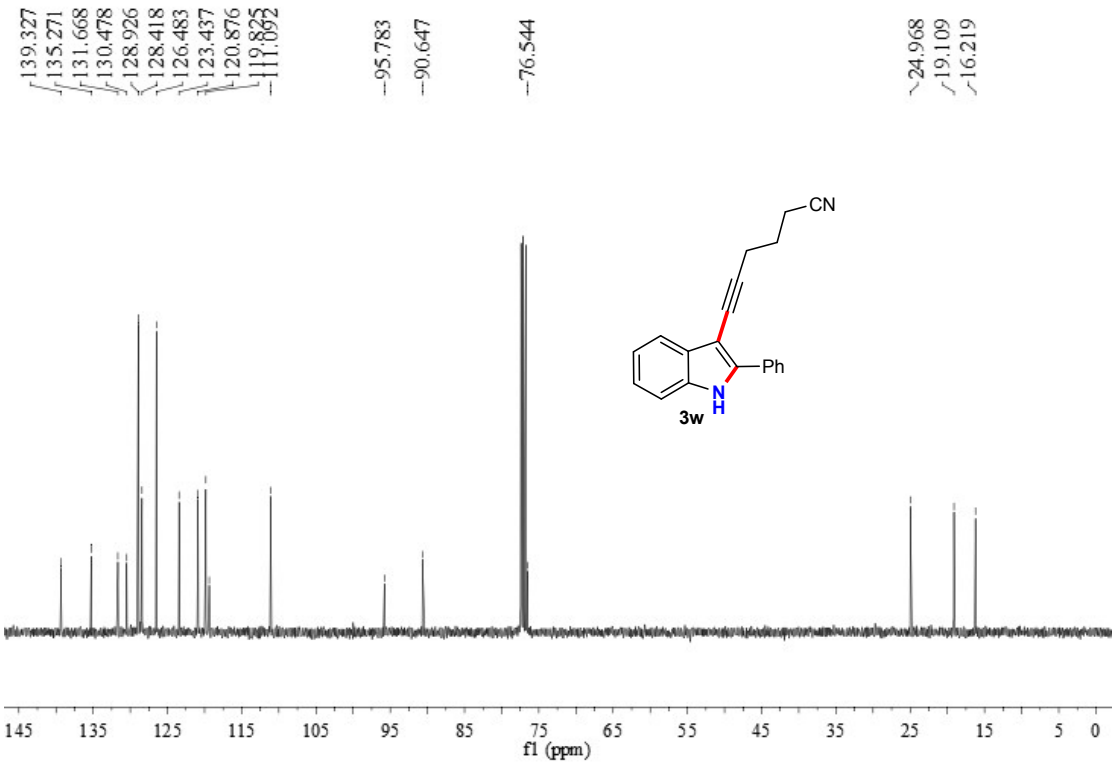
f1 (ppm)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123.437
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119.825
111.092
95.783
90.647
76.544
24.968
19.109
16.219
CN
Ph
N
H
3w
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105
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85
75
65
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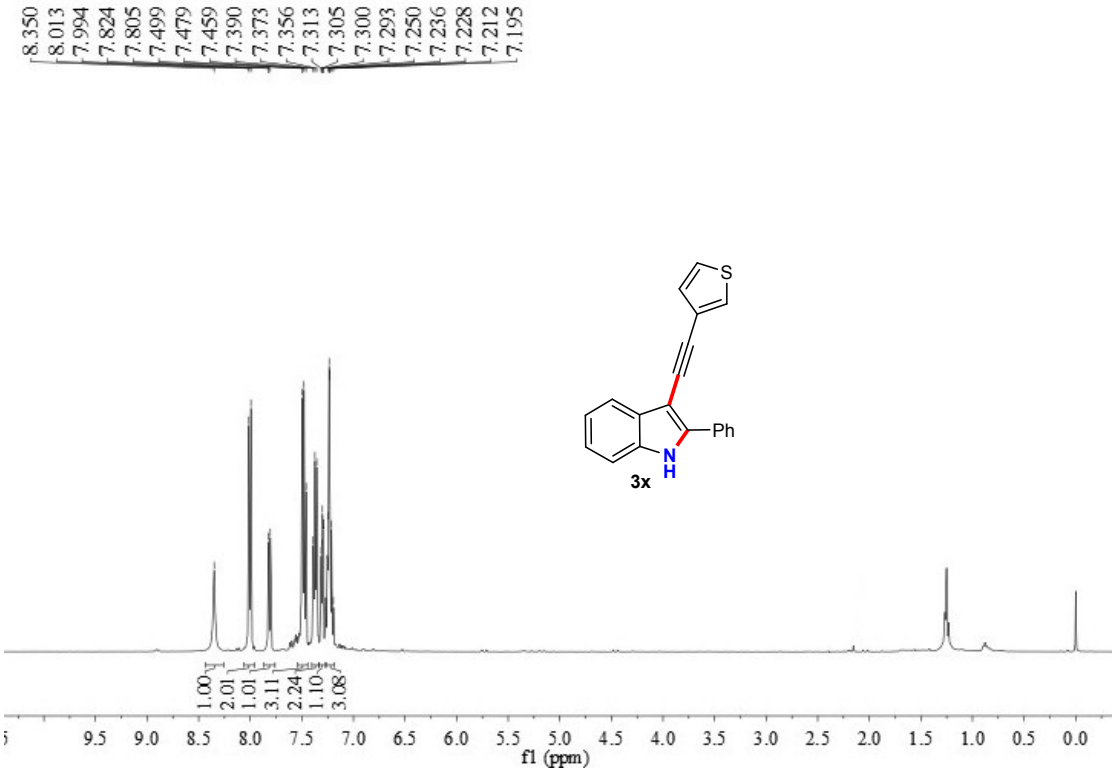
0
f1 (ppm)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7.459
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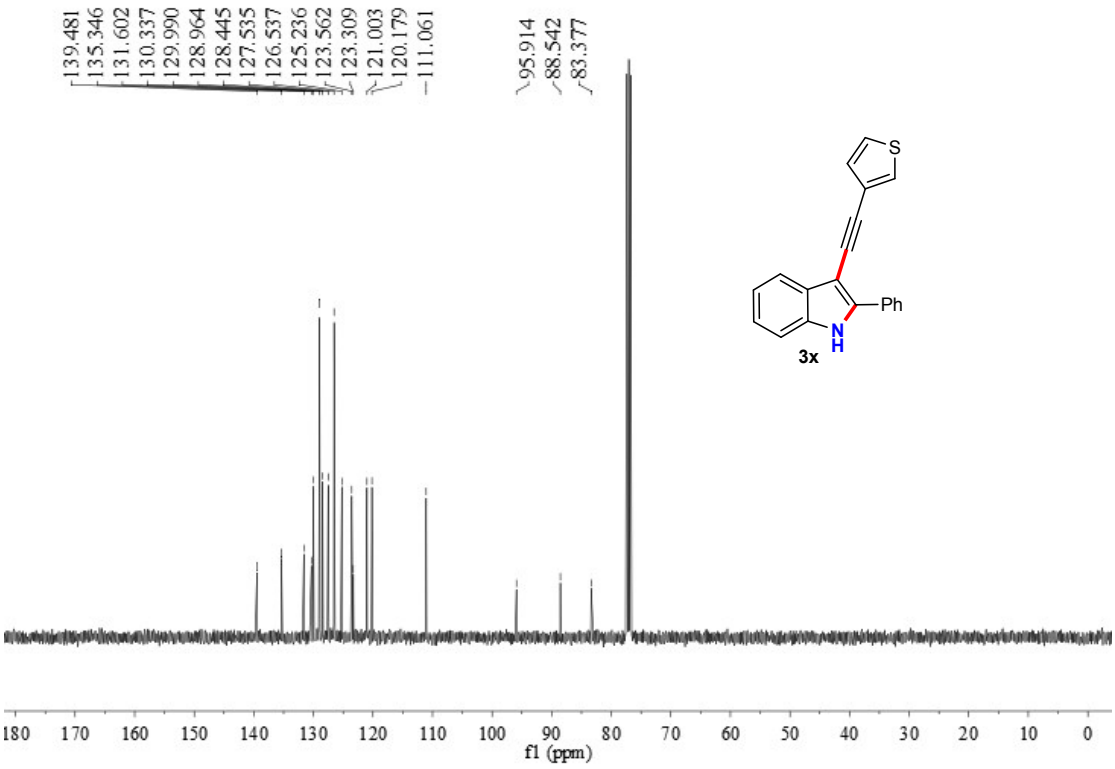
7.305
7.300
7.293
7.250
7.236
7.228
7.212
7.195
S
Ph
N
H
3x
1.00
2.01
1.01
3.11
2.24
1.10
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.562
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120.179
111.061
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83.377
S
Ph
N
H
3x
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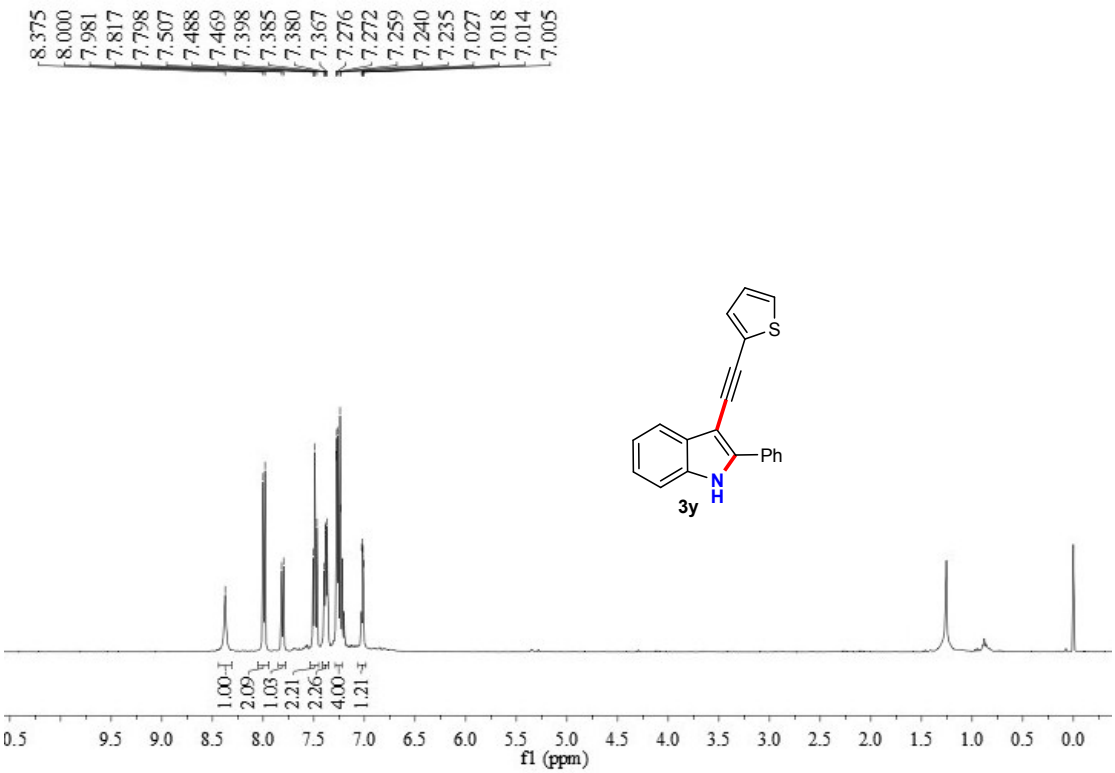
f1 (ppm)


8.375
8.000
7.981
7.817
7.798
7.507
7.488
7.469
7.398
7.385
7.380
7.367
7.276
7.272
7.259
7.240
7.235
7.027
7.018
7.014
7.005
S
Ph
N
H
3y
1.00
2.09
1.03
2.21
2.26
4.00
1.21
0.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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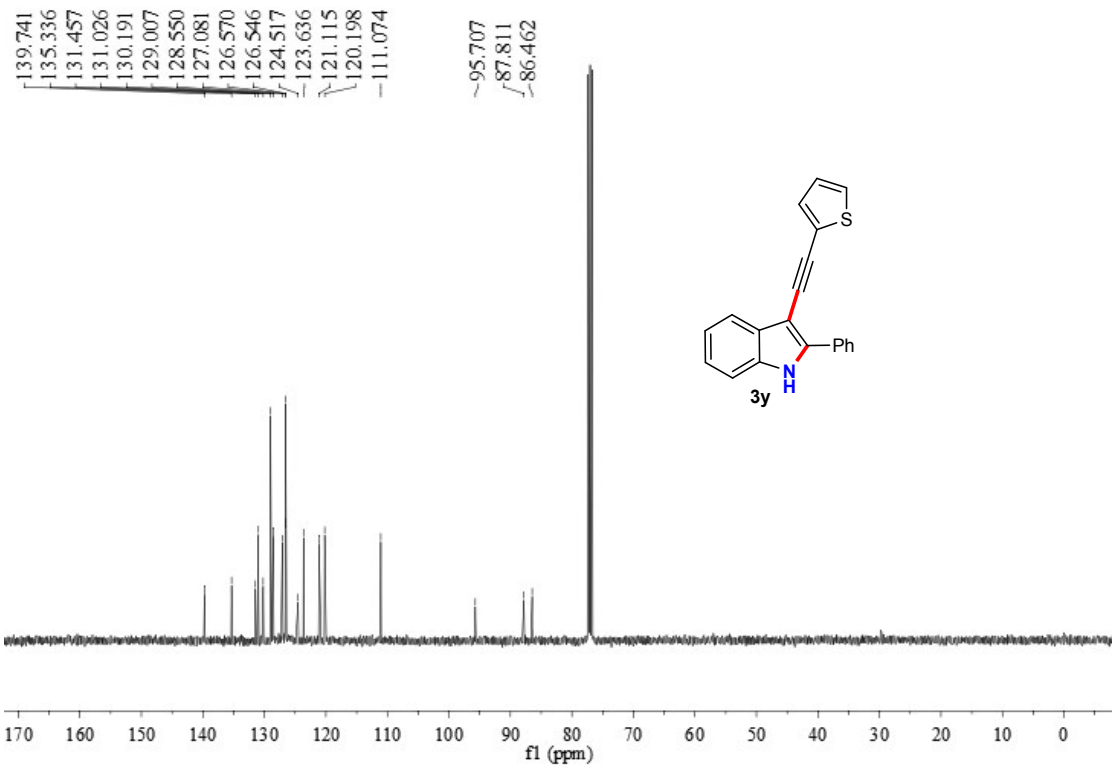
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.457
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127.081
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126.546
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123.636
121.115
120.198
111.074
95.707
87.811
86.462
S
Ph
N
H
3y
170
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130
120
110
100
90
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50
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10
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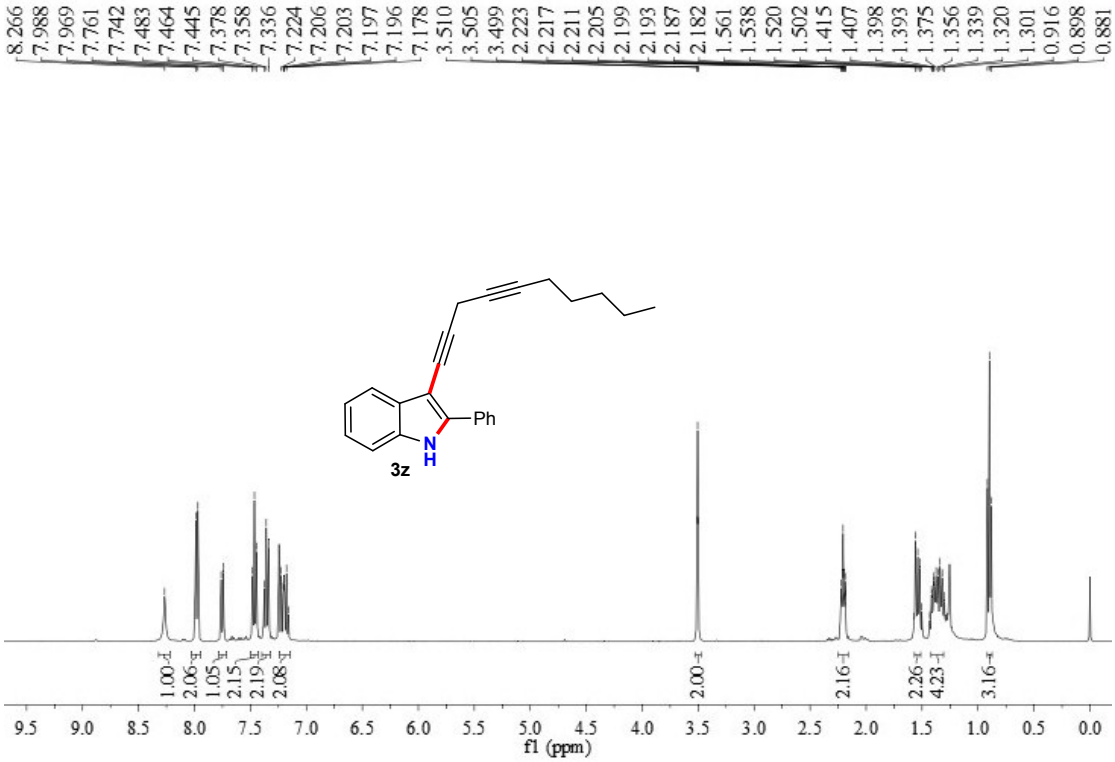
f1 (ppm)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7.445
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7.358
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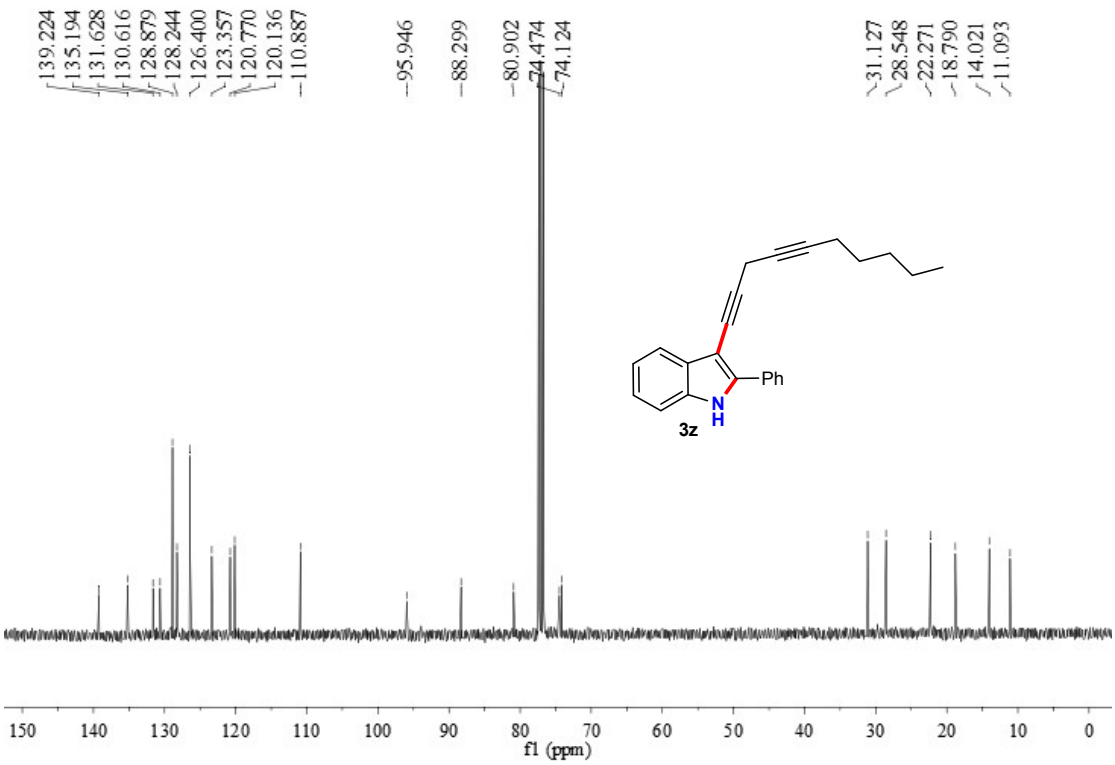
7.206
7.203
7.197
7.196
7.178
3.510
3.505
3.499
2.223
2.217
2.211
2.205
2.199
2.193
2.187
2.182
1.561
1.538
1.520
1.502
1.415
1.407
1.398
1.393
1.375
1.356
1.339
1.320
1.301
0.916
0.898
0.881
Ph
N
H
3z
1.00
2.06
1.05
2.15
2.19
2.08
2.00
2.16
2.26
4.23
3.16
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.194
131.628
130.616
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128.244
126.400
123.357
120.770
120.136
110.887
95.946
88.299
80.902
74.474
74.124
31.127
28.548
22.271
18.790
14.021
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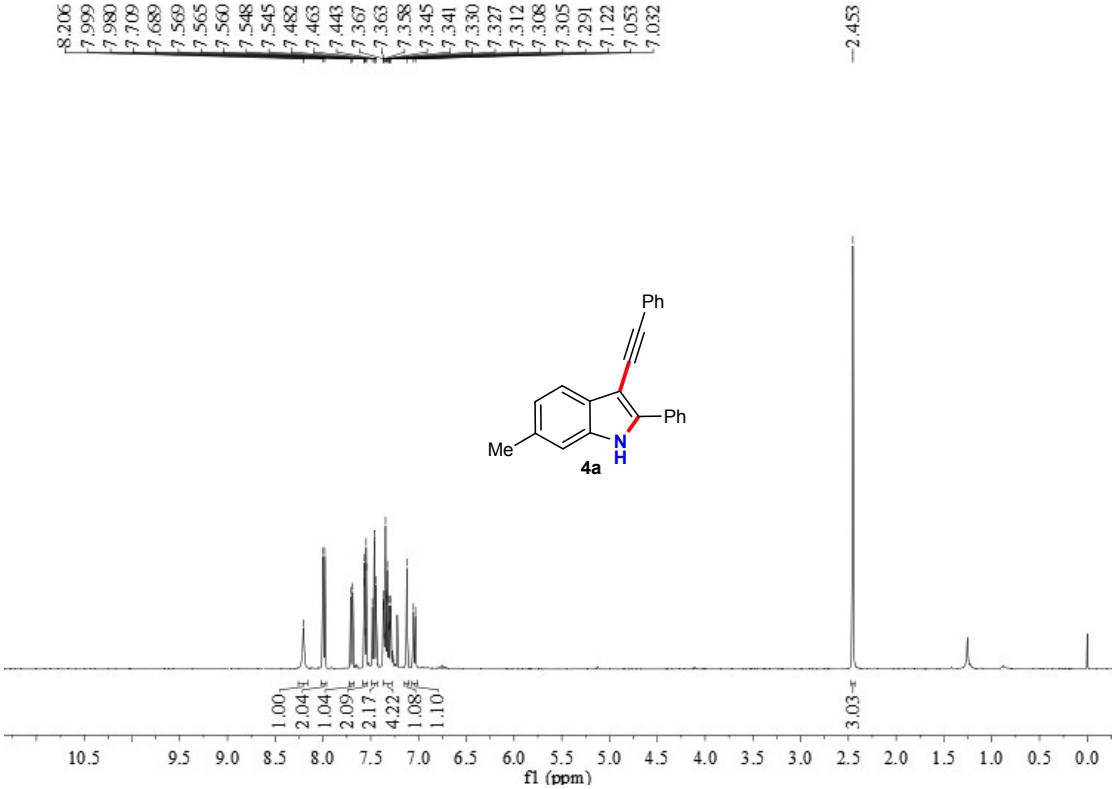
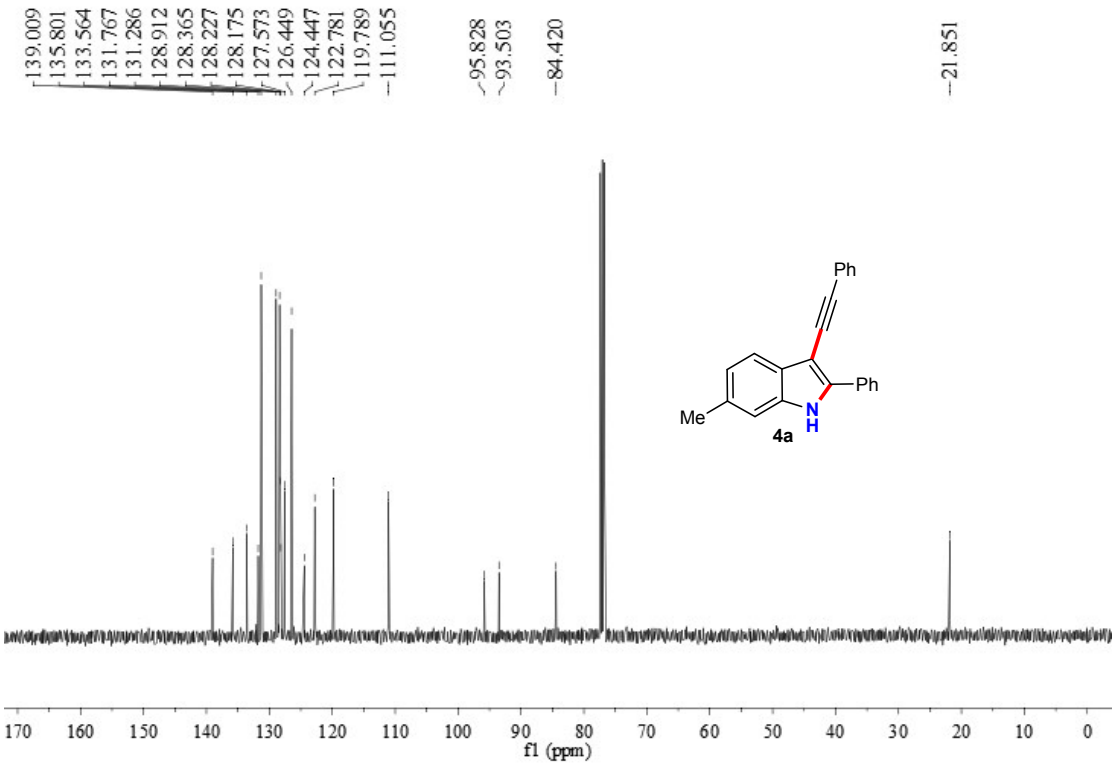
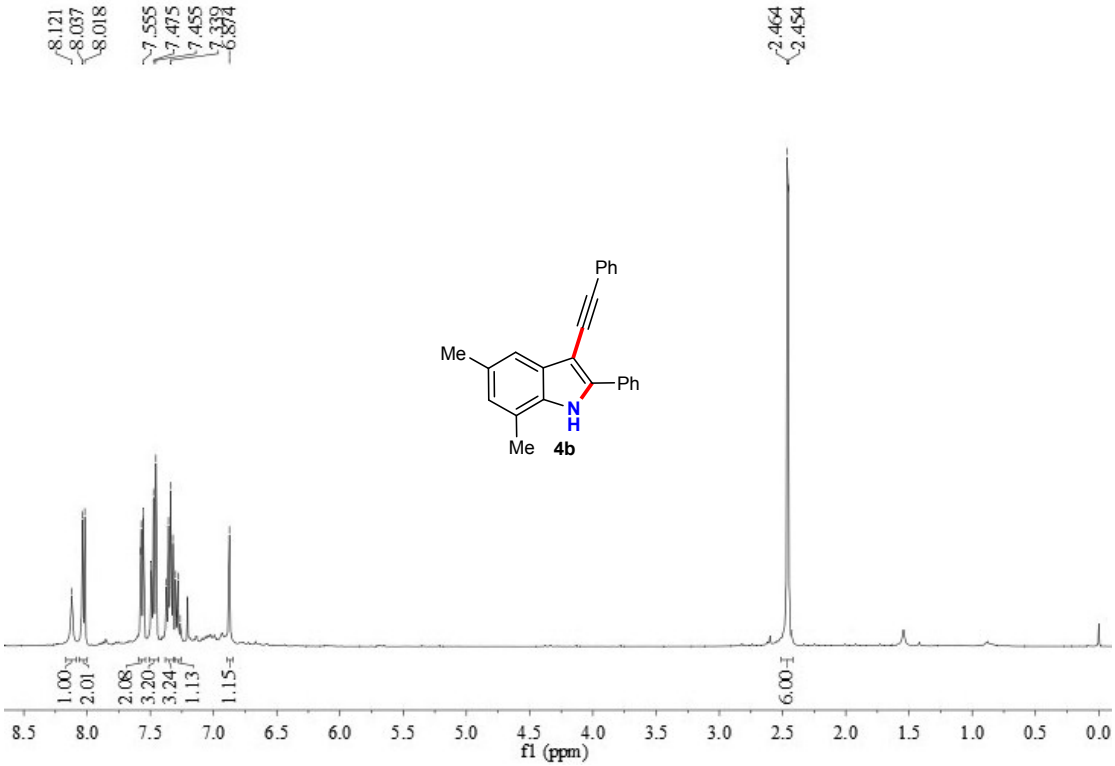
Ph
N
H
3z
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compounds 4



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7.455
7.339
6.874
2.464
2.454
Ph
Me
Ph
N
H
Me
4b
1.00
2.01
2.08
3.20
3.24
1.13
1.15
6.00
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
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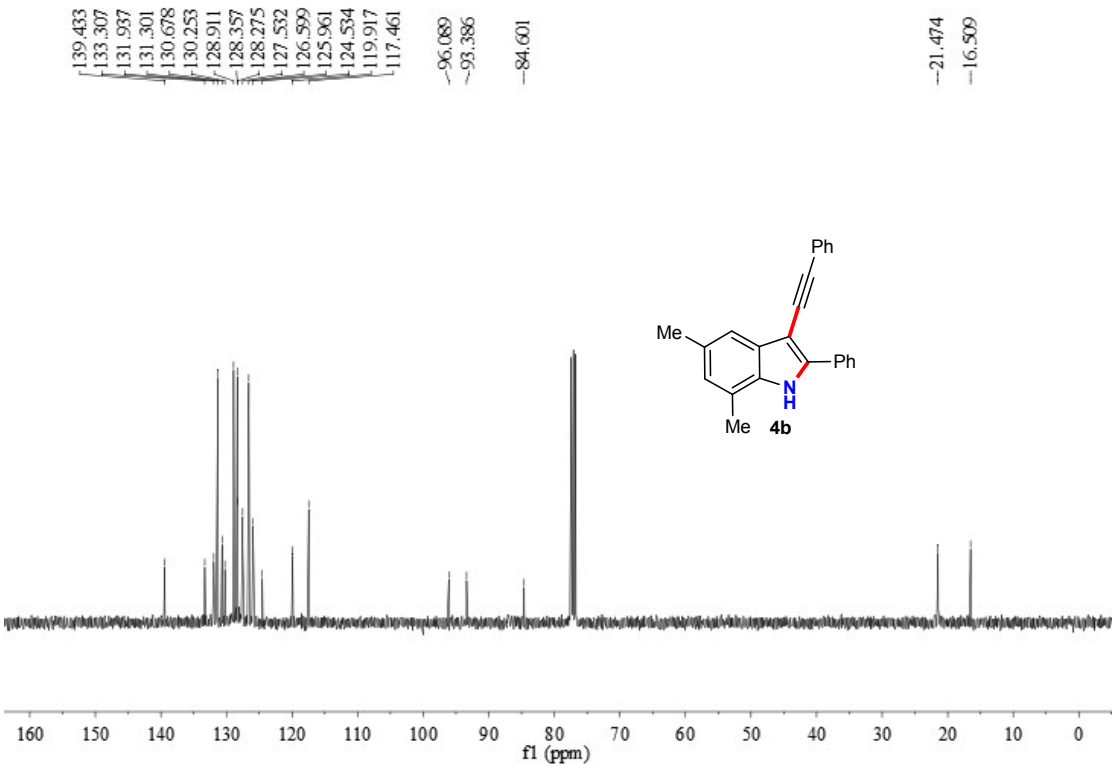
f1 (ppm)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128.357
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127.532
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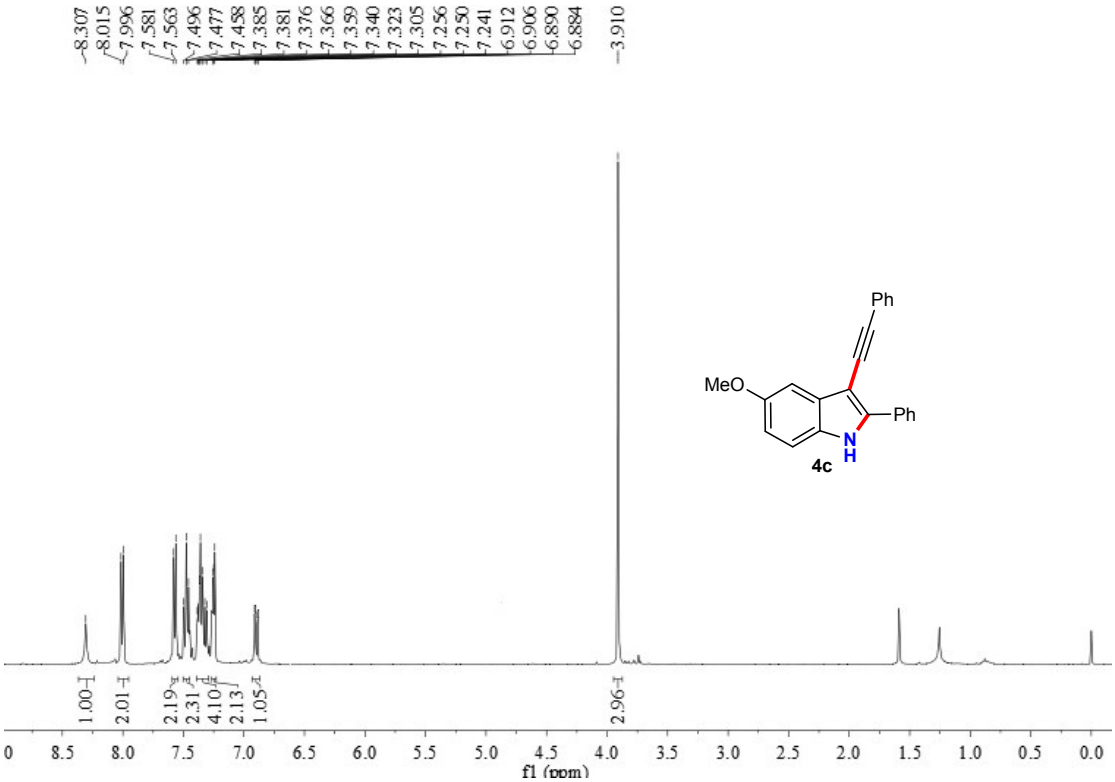
125.961
124.534
119.917
117.461
96.089
93.386
84.601
21.474
16.509
Ph
Me
Ph
N
H
Me
4b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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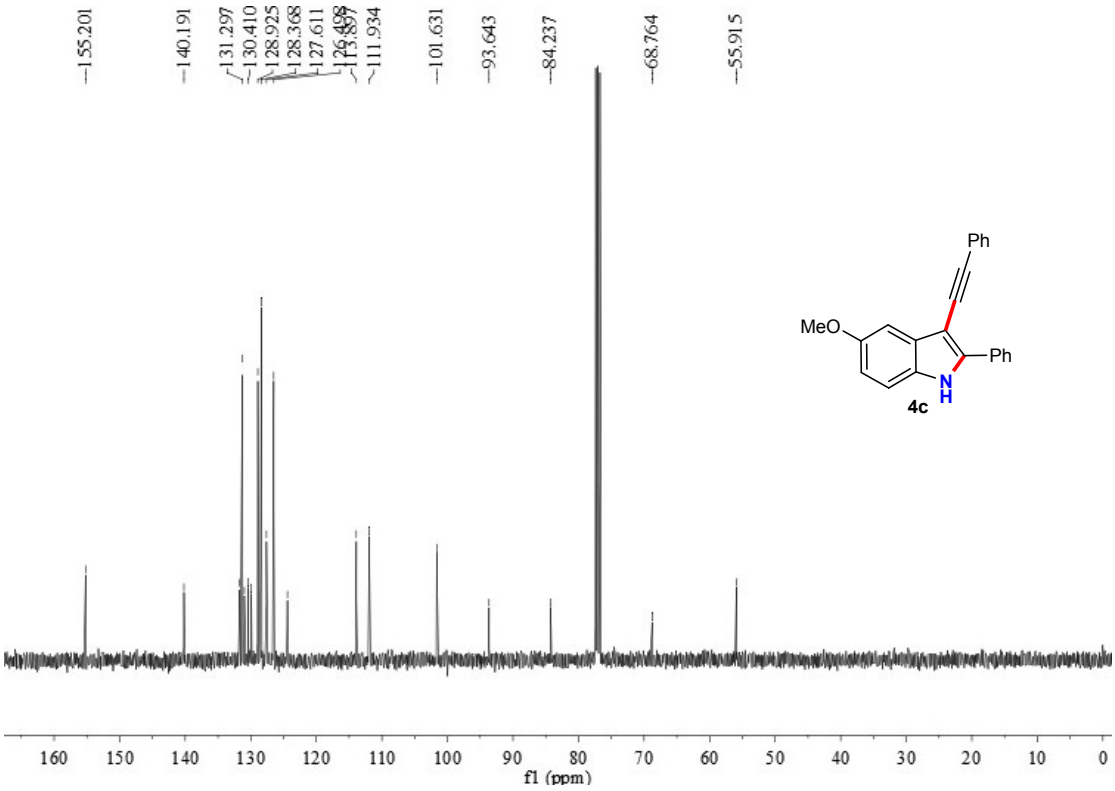
8.015
7.996
7.581
7.563
7.496
7.477
7.458
7.385
7.381
7.376
7.366
7.359
7.340
7.323
7.305
7.256
7.250
7.241
6.912
6.906
6.890
6.884
3.910
1.00
2.01
2.19
2.31
4.10
2.13
1.05
2.96
Ph
MeO
Ph
N
H
4c
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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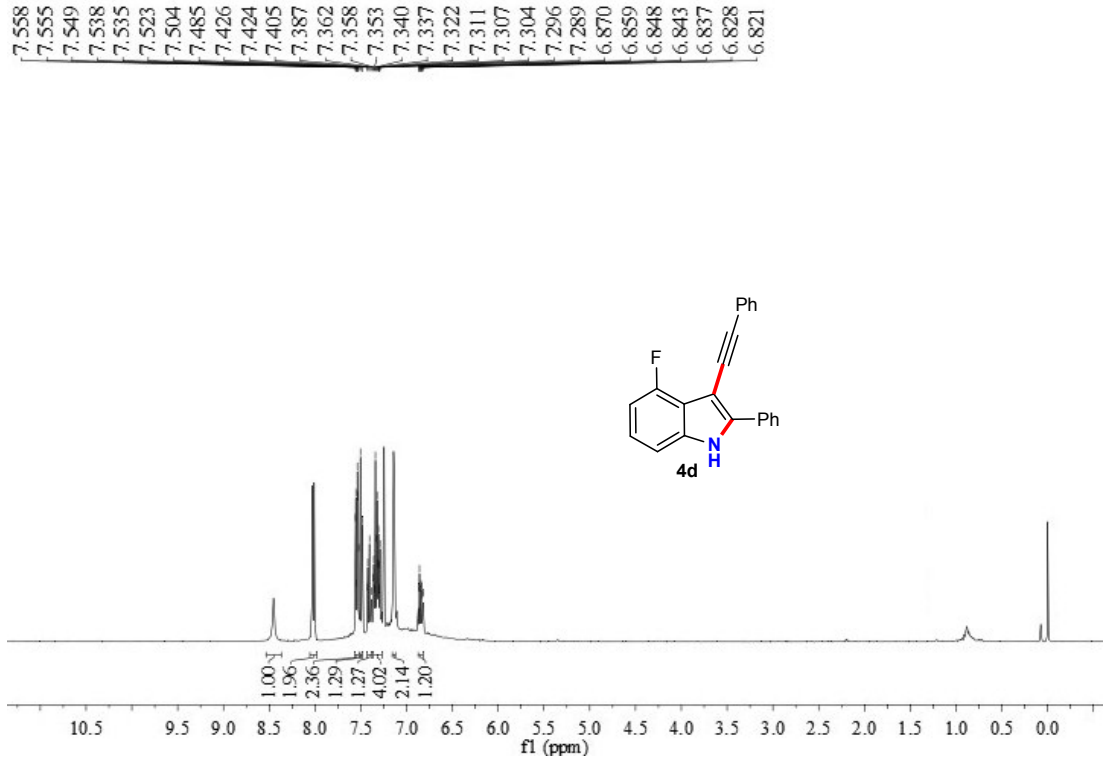
140.191
131.297
130.410
128.925
128.368
127.611
111.934
101.631
93.643
84.237
68.764
55.915
Ph
MeO
Ph
N
H
4c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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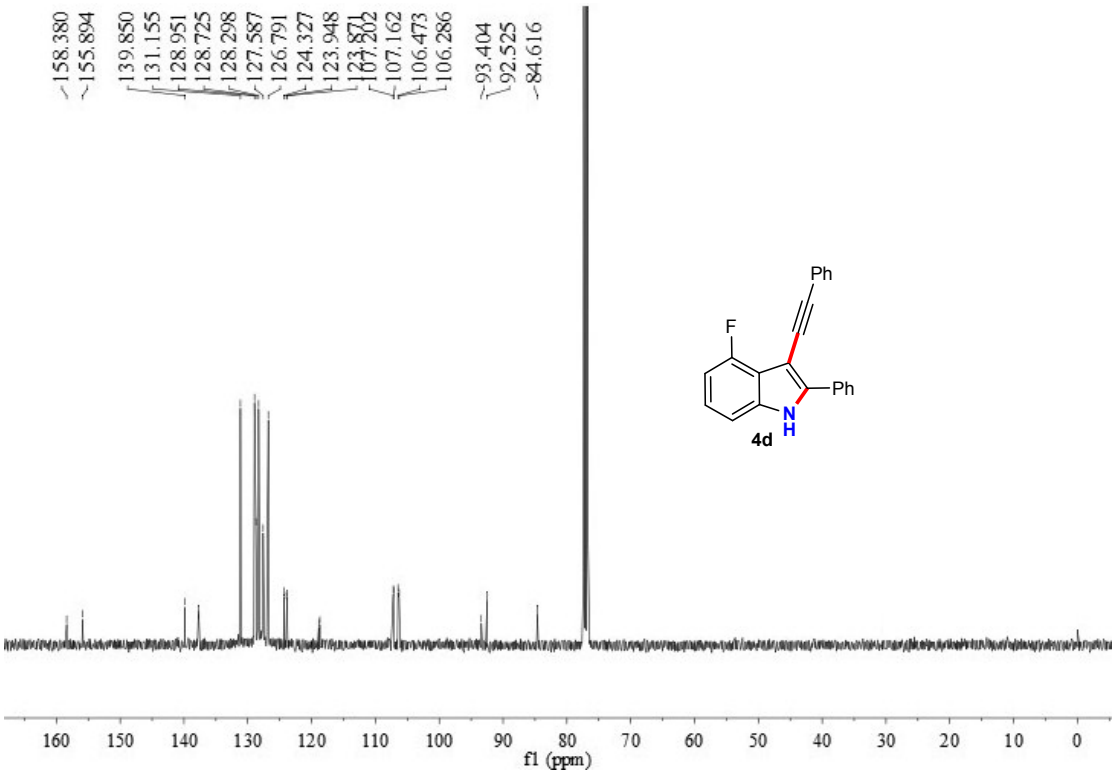
7.555
7.549
7.538
7.535
7.523
7.504
7.485
7.426
7.424
7.405
7.387
7.362
7.358
7.353
7.340
7.337
7.322
7.311
7.307
7.304
7.296
7.289
6.870
6.859
6.848
6.843
6.837
6.828
6.821
Ph
F
Ph
N
H
4d
1.00
1.96
2.36
1.29
1.27
4.02
2.14
1.20
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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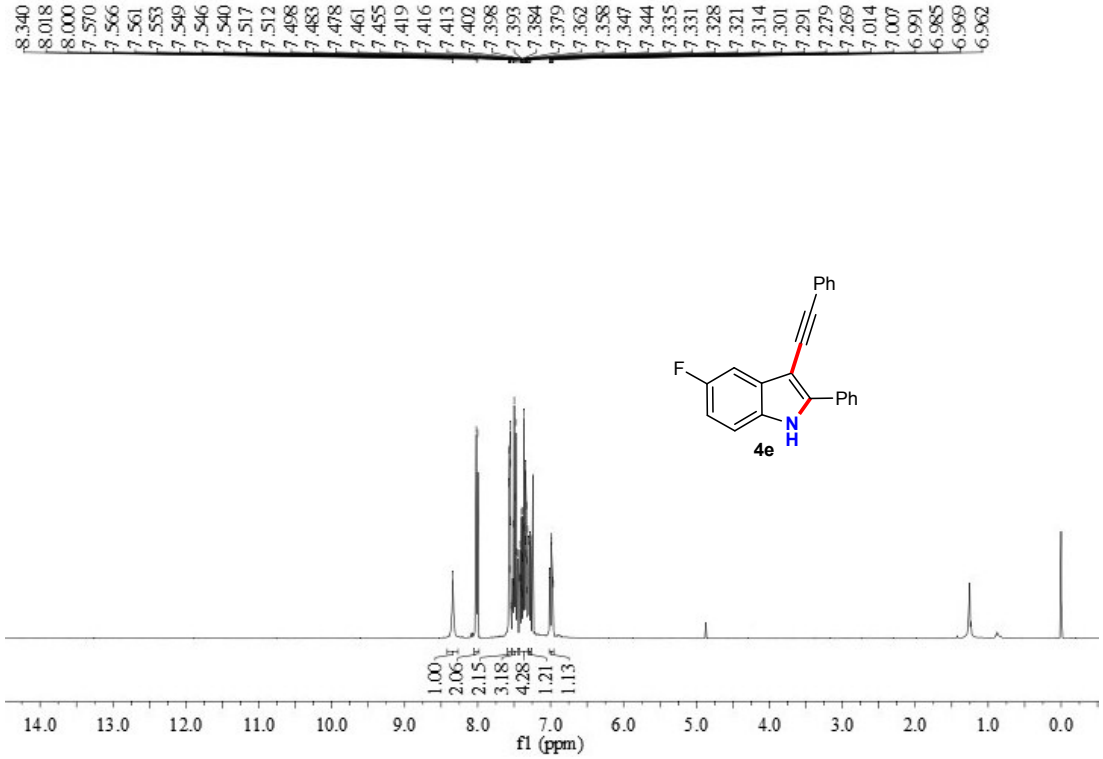
139.850
131.155
128.951
128.725
128.298
127.587
126.791
124.327
123.948
123.871
107.202
107.162
106.473
106.286
93.404
92.525
84.616
Ph
F
Ph
N
H
4d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.561
7.553
7.549
7.546
7.540
7.517
7.512
7.498
7.483
7.478
7.461
7.455
7.419
7.416
7.413
7.402
7.398
7.393
7.384
7.379
7.362
7.358
7.347
7.344
7.335
7.331
7.328
7.321
7.314
7.301
7.291
7.279
7.269
7.014
7.007
6.991
6.985
6.969
6.962
Ph
F
Ph
N
H
4e
1.00
2.06
2.15
3.18
4.28
1.21
1.13
14.0
13.0
12.0
11.0
10.0
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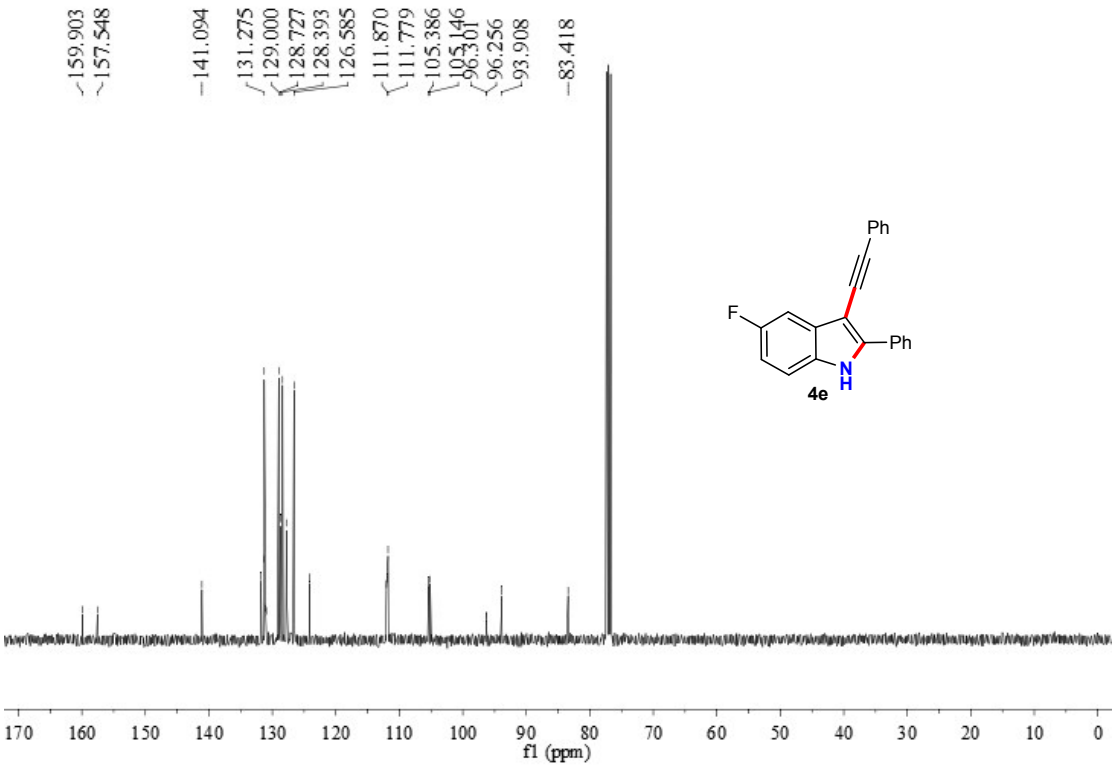
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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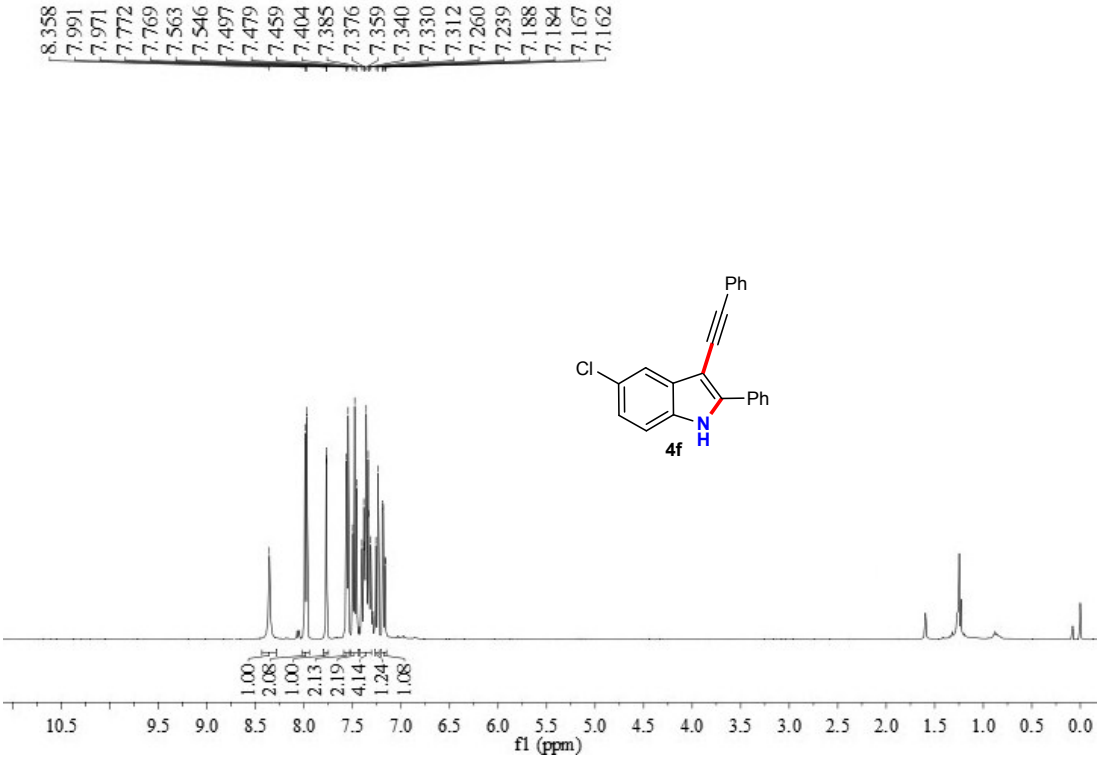
128.727
128.393
126.585
111.870
111.779
105.386
105.146
96.301
96.256
93.908
83.418
Ph
F
Ph
N
H
4e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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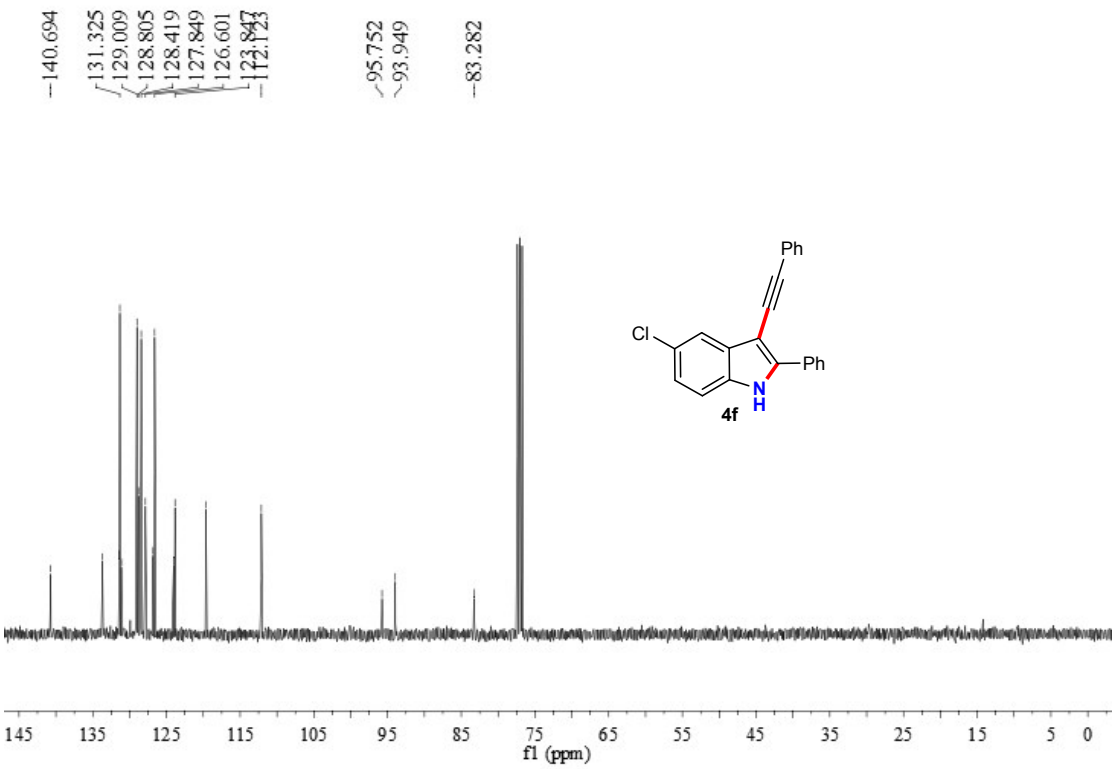
7.459
7.404
7.385
7.376
7.359
7.340
7.330
7.312
7.260
7.239
7.188
7.184
7.167
7.162
Ph
Cl
Ph
N
H
4f
1.00
2.08
1.00
2.13
2.19
4.14
1.24
1.08
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.849
126.601
95.752
93.949
83.282
Ph
Cl
Ph
N
H
4f
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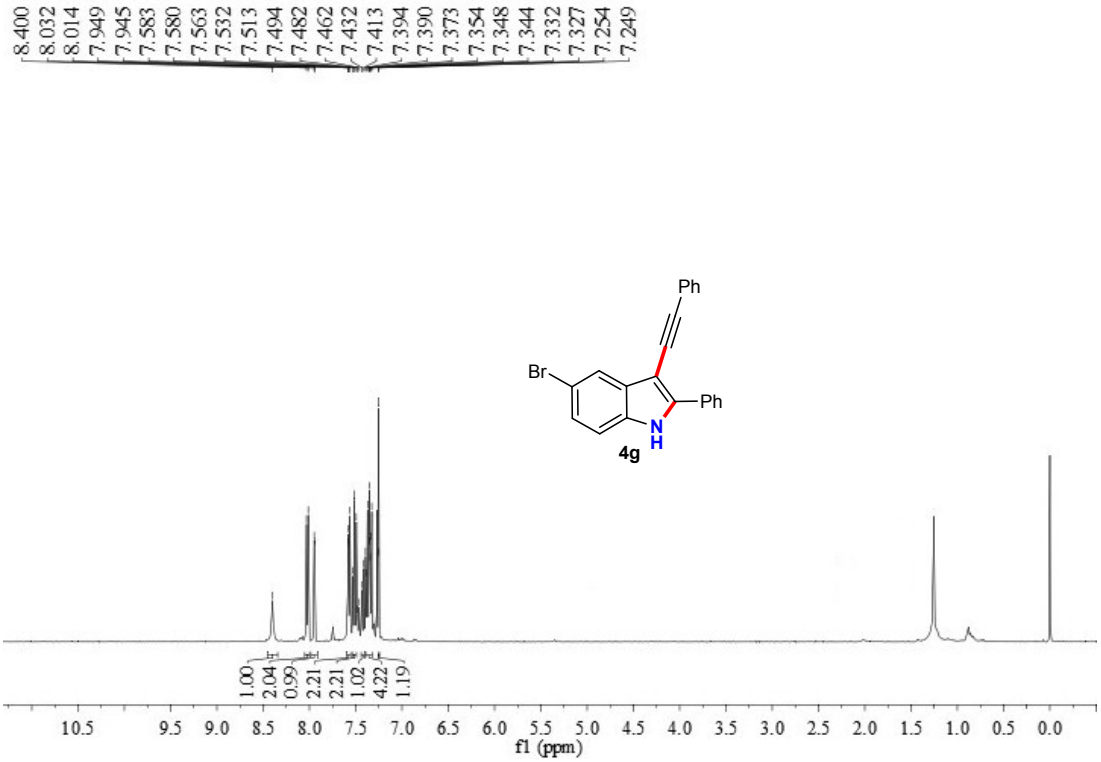
125
115
105
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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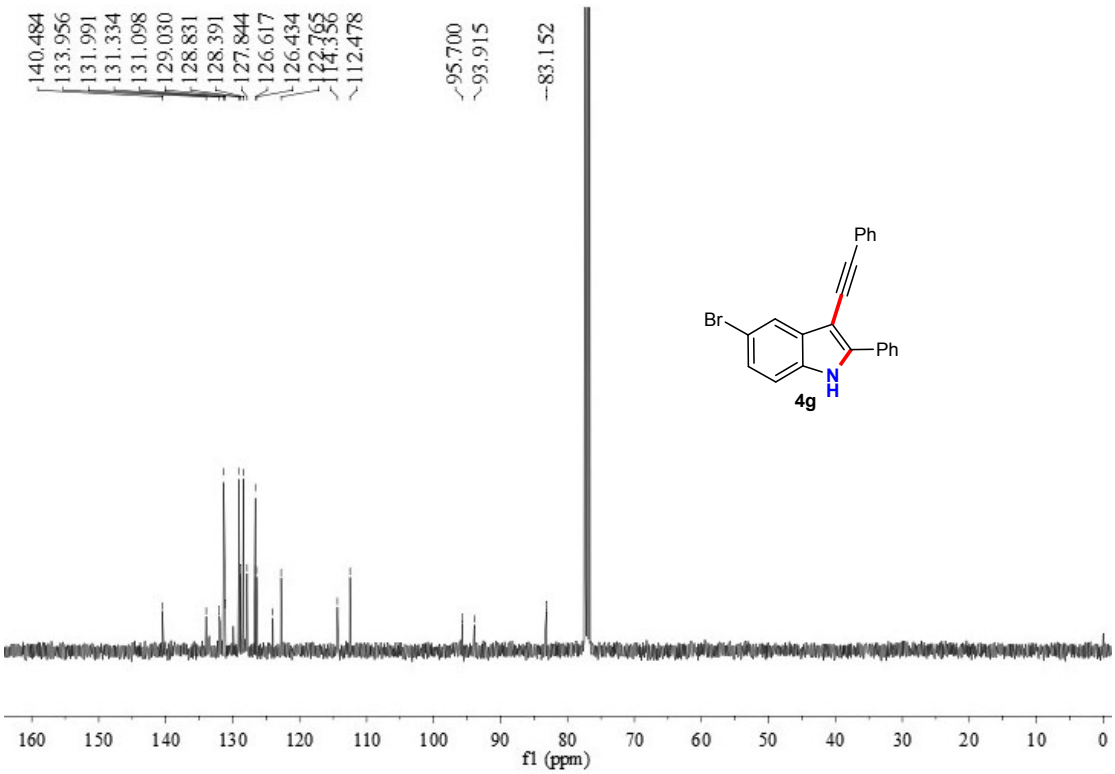
7.580
7.563
7.532
7.513
7.494
7.482
7.462
7.432
7.413
7.394
7.390
7.373
7.354
7.348
7.344
7.332
7.327
7.254
7.249
Ph
Br
Ph
N
H
4g
1.00
2.04
0.99
2.21
2.21
1.02
4.22
1.19
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.334
131.098
129.030
128.831
128.391
127.844
126.617
126.434
122.765
114.356
112.478
95.700
93.915
83.152
Ph
Br
Ph
N
H
4g
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150
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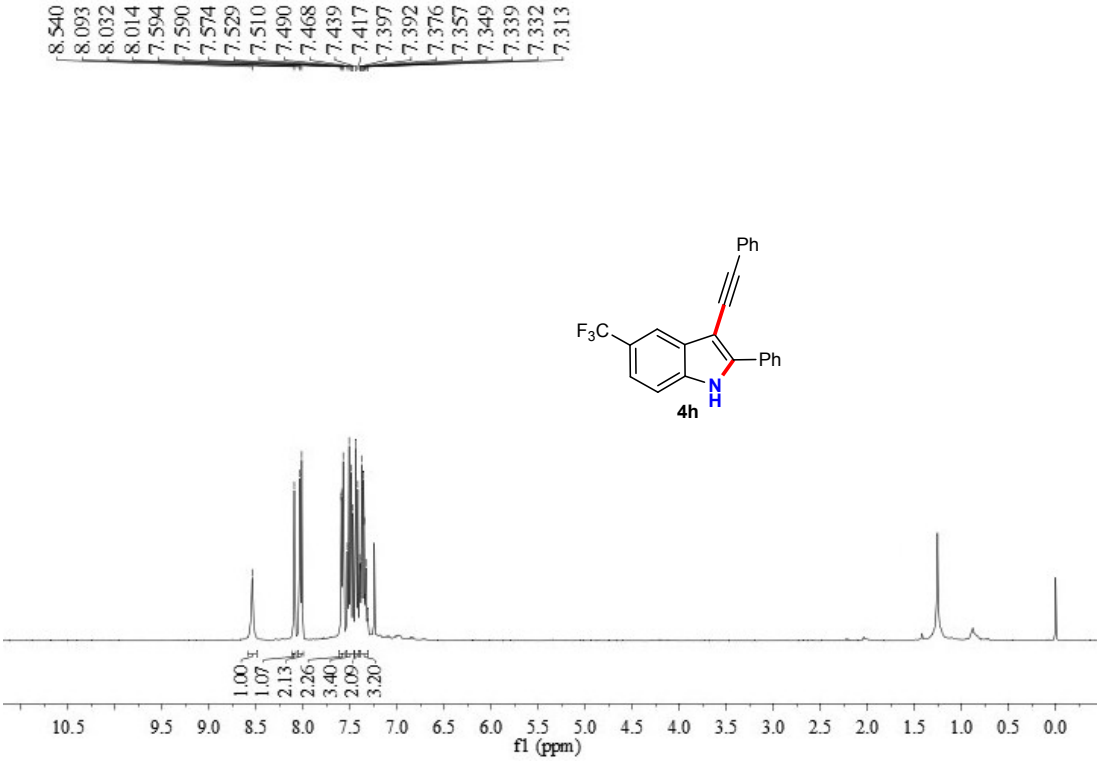
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.590
7.574
7.529
7.510
7.490
7.468
7.439
7.417
7.397
7.392
7.376
7.357
7.349
7.339
7.332
7.313
Ph
F3C
Ph
N
H
4h
1.00
1.07
2.13
2.26
3.40
2.09
3.20
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
1.5
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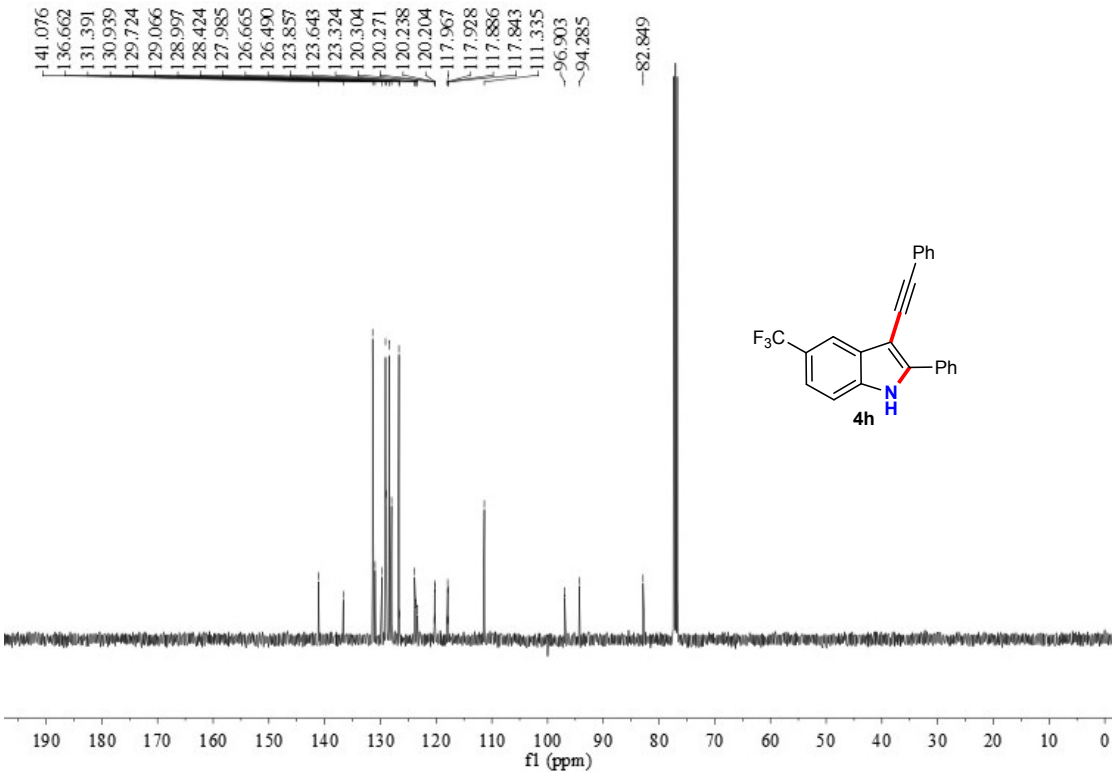
0.0
f1 (ppm)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128.424
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126.490
123.857
123.643
123.324
120.304
120.271
120.238
120.204
117.967
117.928
117.886
117.843
111.335
96.903
94.285
82.849
Ph
F3C
Ph
N
H
4h
190
180
170
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150
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130
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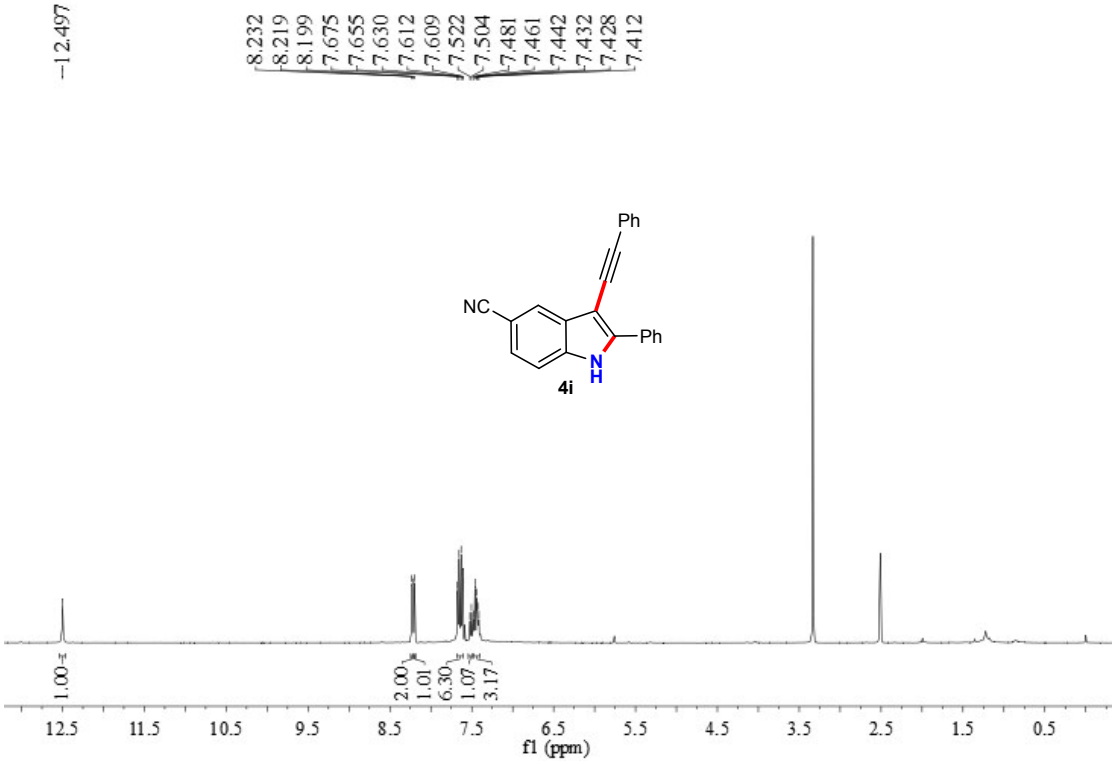
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.612
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7.522
7.504
7.481
7.461
7.442
7.432
7.428
7.412
Ph
NC
Ph
N
H
4i
1.00
2.00
1.01
6.30
1.07
3.17
12.5
11.5
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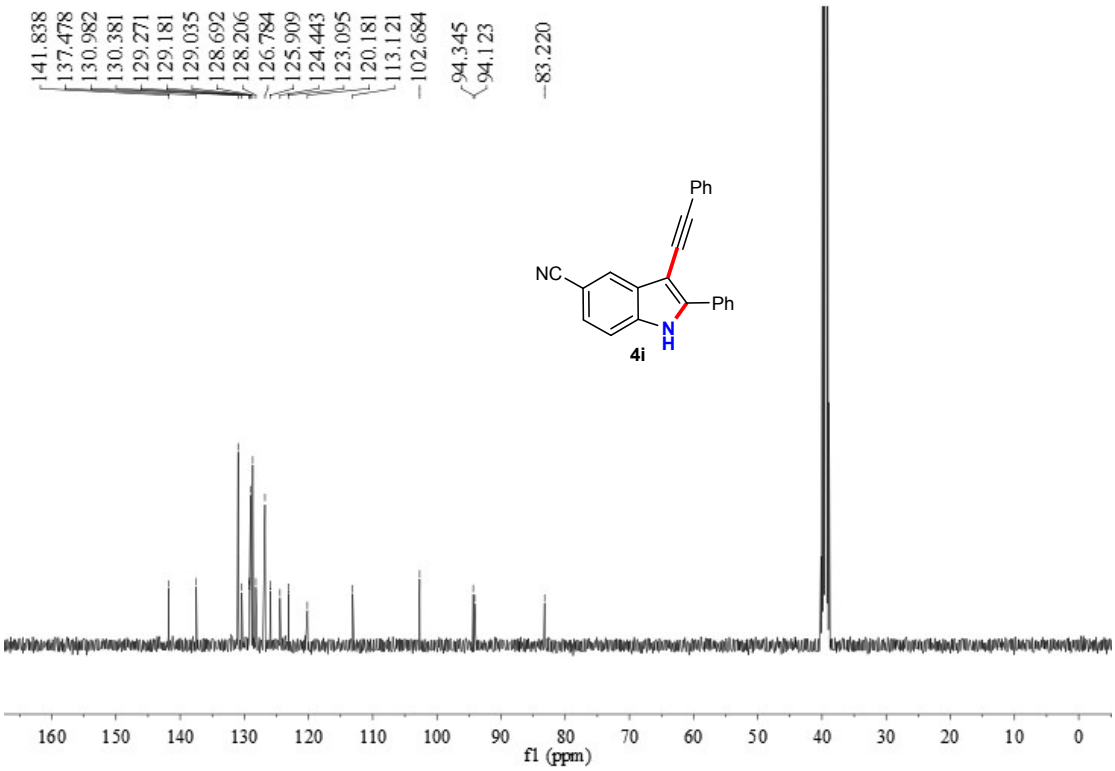
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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128.692
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124.443
123.095
120.181
113.121
102.684
94.345
94.123
83.220
Ph
NC
Ph
N
H
4i
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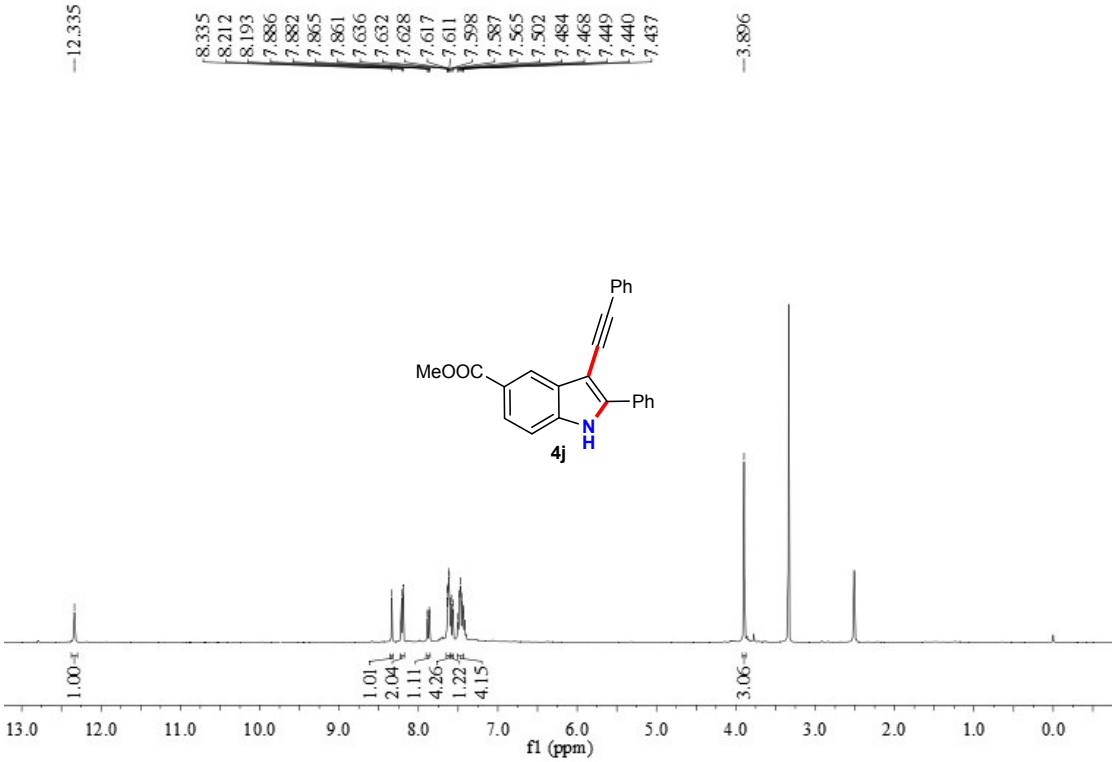
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.611
7.598
7.587
7.565
7.502
7.484
7.468
7.449
7.440
7.437
3.896
Ph
MeOOC
Ph
N
H
4j
1.00
1.01
2.04
1.11
4.26
1.22
4.15
3.06
13.0
12.0
11.0
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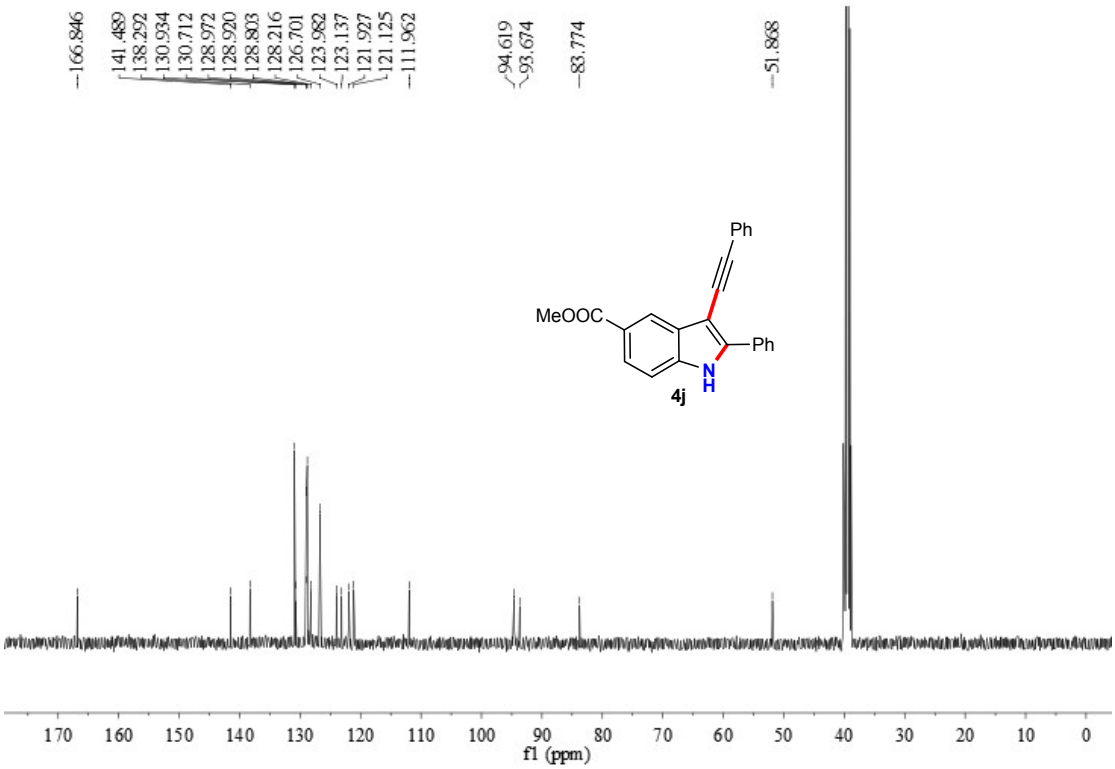
2.0
1.0
0.0
f1 (ppm)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128.803
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123.137
121.927
121.125
111.962
94.619
93.674
83.774
51.868
Ph
MeOOC
Ph
N
H
4j
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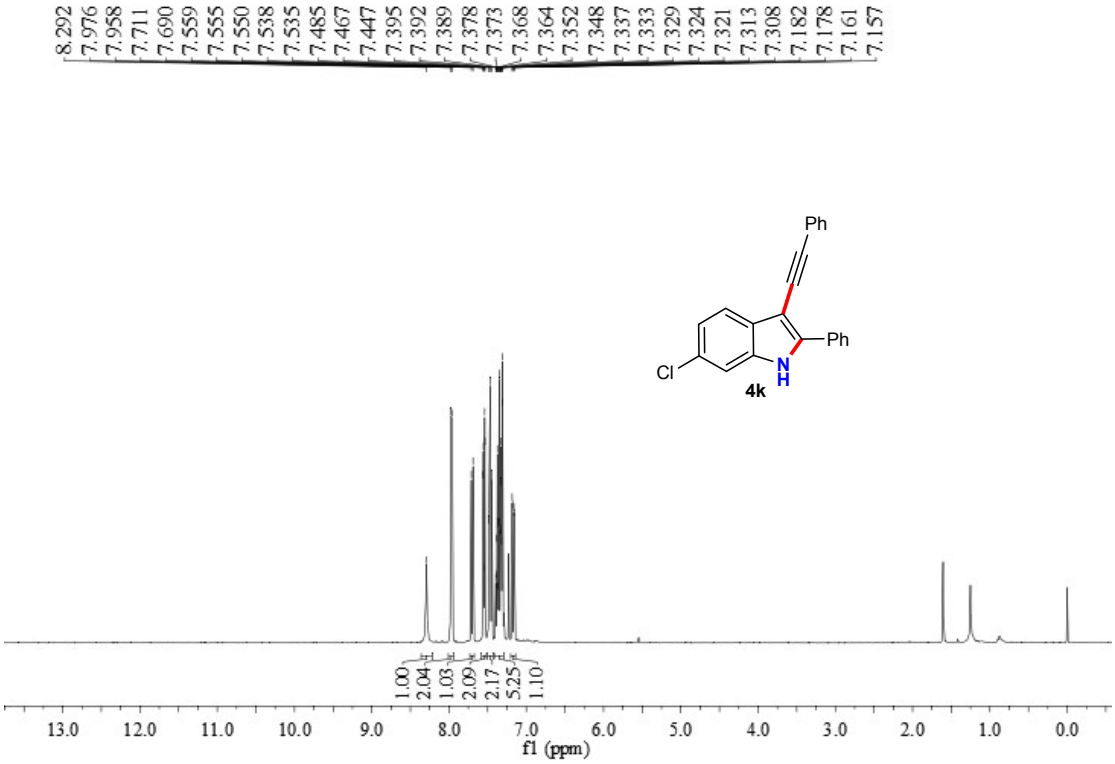
f1 (ppm)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7.389
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7.324
7.321
7.313
7.308
7.182
7.178
7.161
7.157
Ph
Ph
Cl
N
H
4k
1.00
2.04
1.03
2.09
2.17
5.25
1.10
13.0
12.0
11.0
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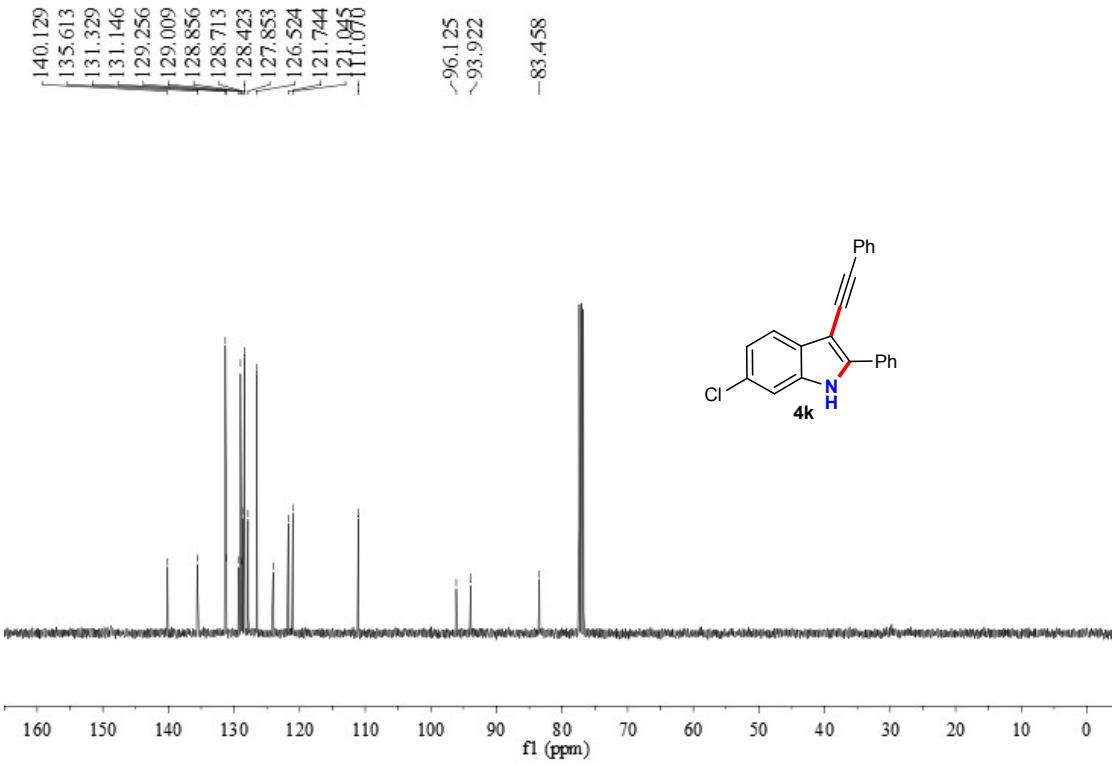
f1 (ppm)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96.125
93.922
83.458
Ph
Ph
Cl
N
H
4k
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50
40
30
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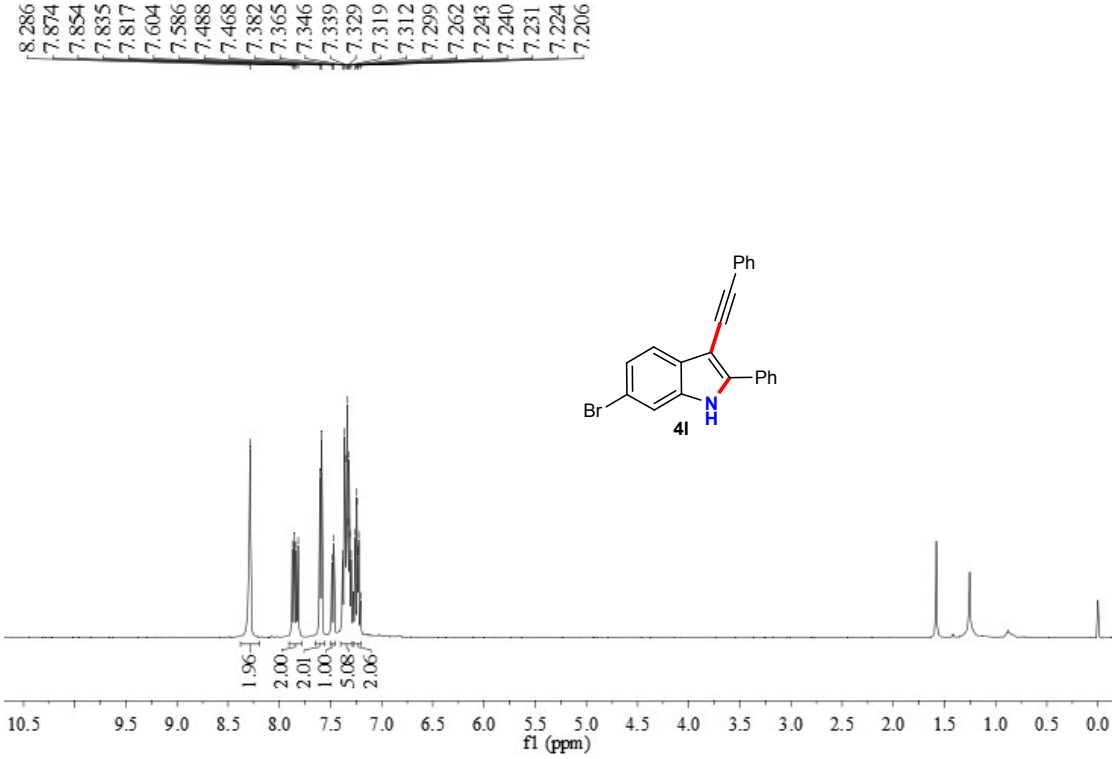
f1 (ppm)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7.488
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7.339
7.329
7.319
7.312
7.299
7.262
7.243
7.240
7.231
7.224
7.206
Ph
Ph
Br
N
H
4l
1.96
2.00
2.01
1.00
5.08
2.06
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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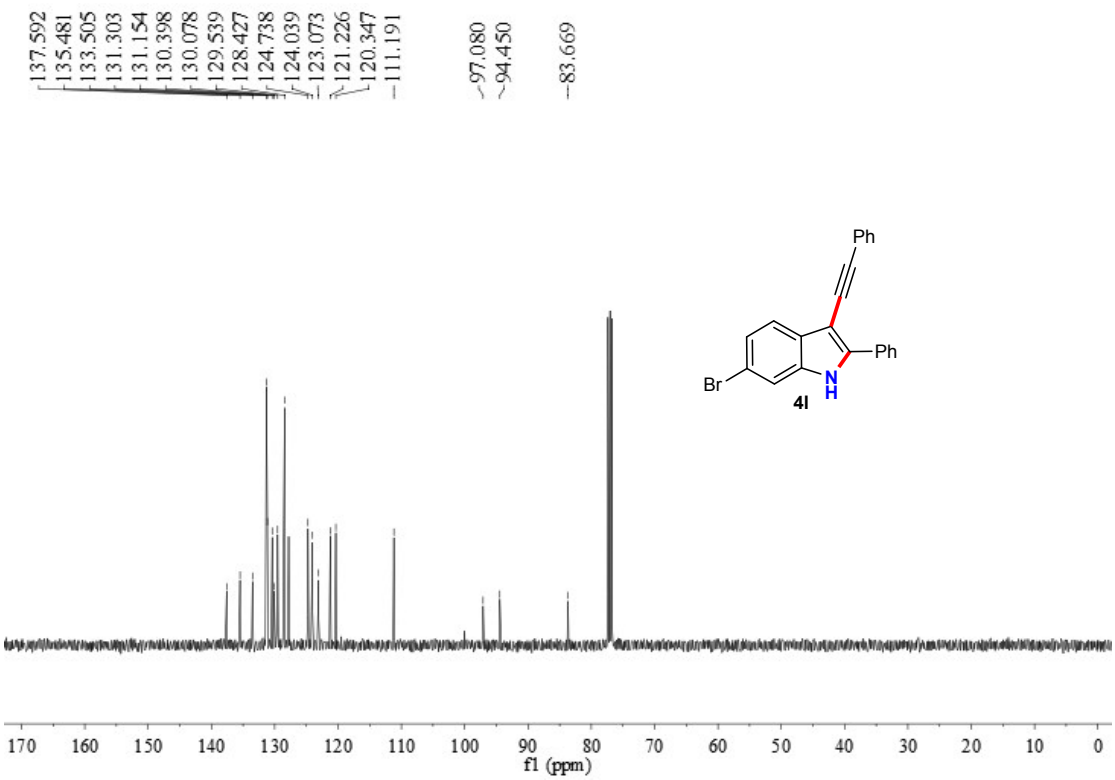
0.0
f1 (ppm)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129.539
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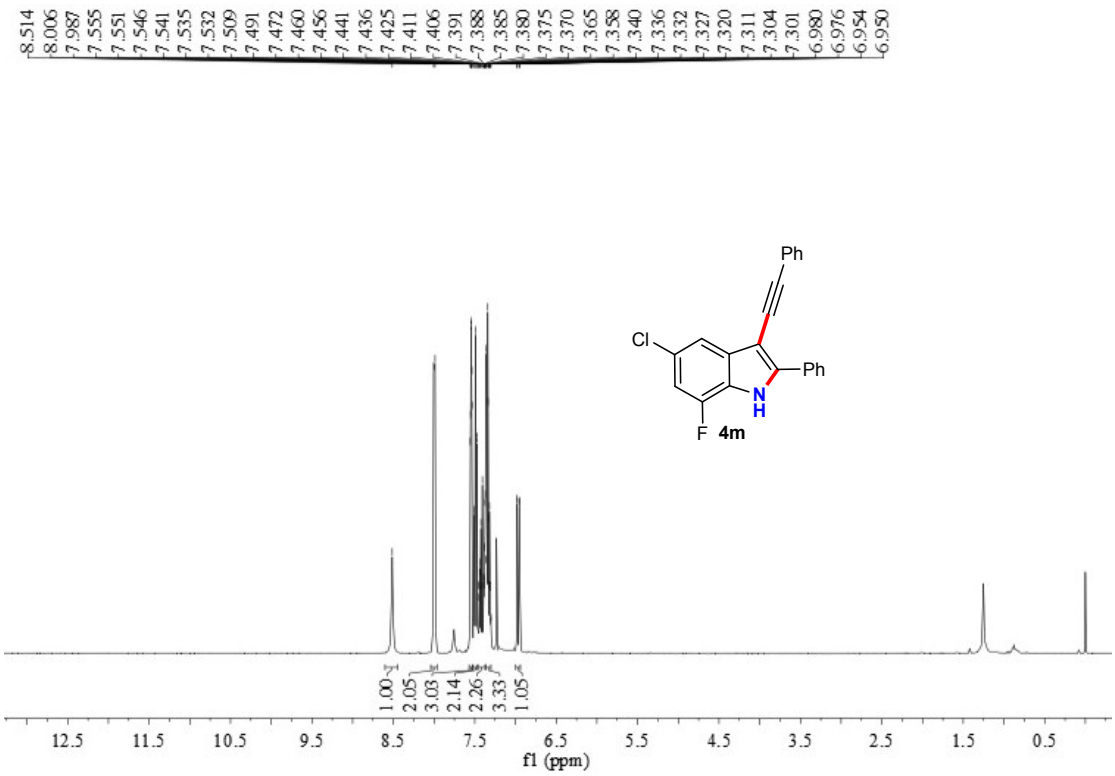
124.039
123.073
121.226
120.347
111.191
97.080
94.450
83.669
Ph
Ph
Br
N
H
4l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.551
7.546
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7.535
7.532
7.509
7.491
7.472
7.460
7.456
7.441
7.436
7.425
7.411
7.406
7.391
7.388
7.385
7.380
7.375
7.370
7.365
7.358
7.340
7.336
7.332
7.327
7.320
7.311
7.304
7.301
6.980
6.976
6.954
6.950
Ph
Cl
Ph
N
H
F
4m
1.00
2.05
3.03
2.14
2.26
3.33
1.05
12.5
11.5
10.5
9.5
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7.5
6.5
5.5
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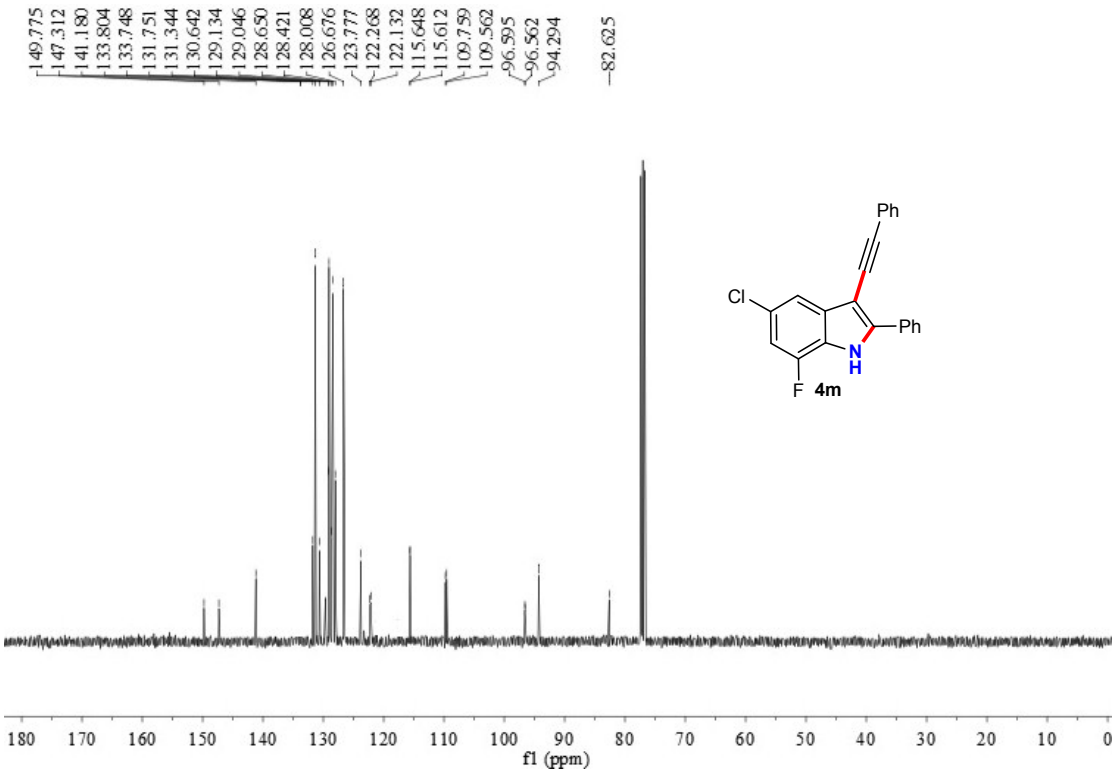
3.5
2.5
1.5
0.5
f1 (ppm)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130.642
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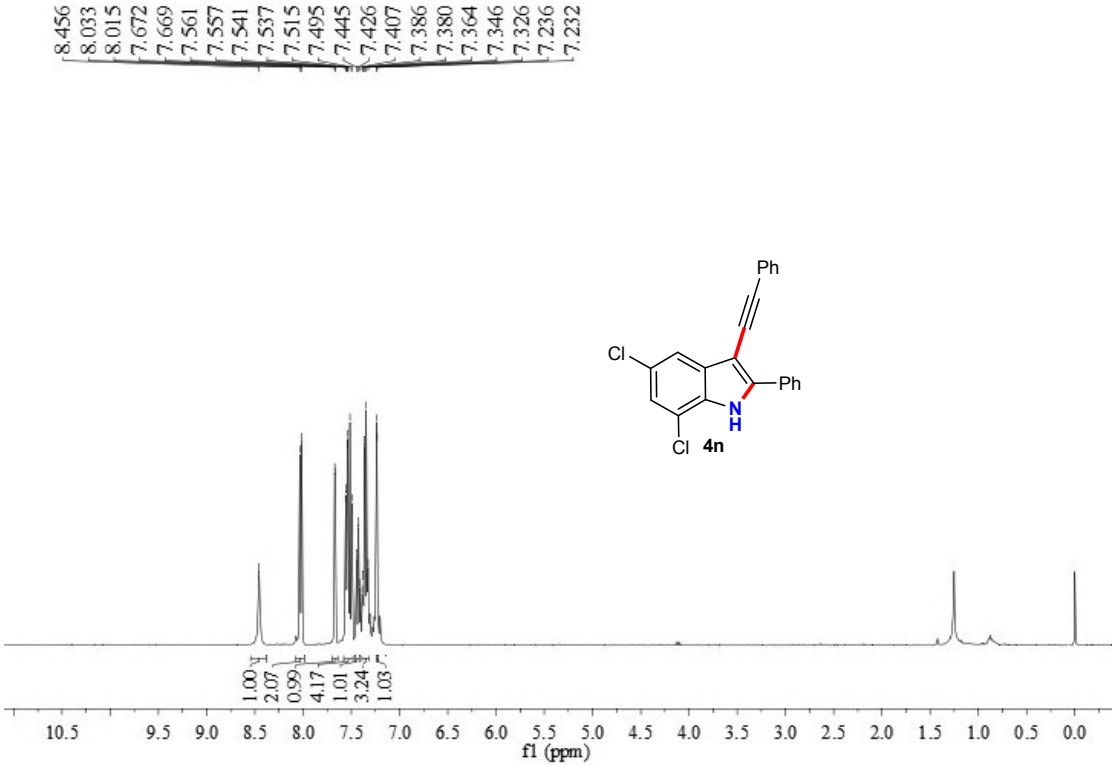
128.650
128.421
128.008
126.676
123.777
122.268
122.132
115.648
115.612
109.759
109.562
96.595
96.562
94.294
82.625
Ph
Cl
Ph
N
H
F
4m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.033
8.015
7.672
7.669
7.561
7.557
7.541
7.537
7.515
7.495
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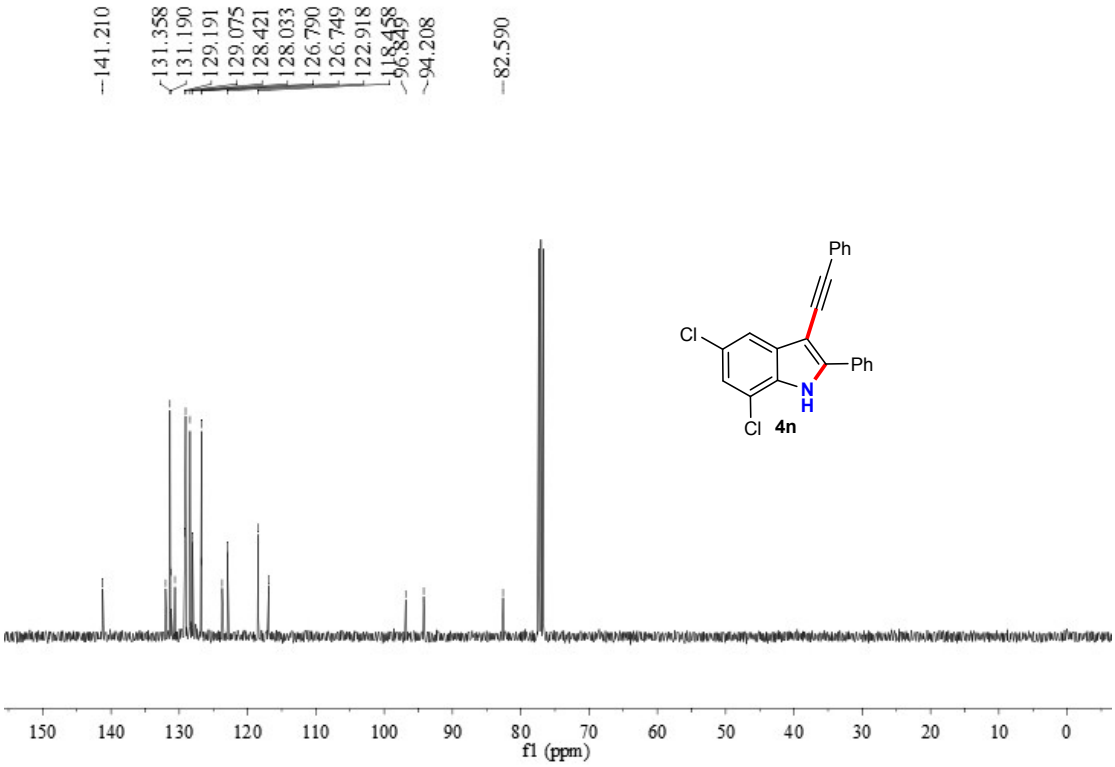
7.426
7.407
7.386
7.380
7.364
7.346
7.326
7.236
7.232
Ph
Cl
Ph
N
H
Cl
4n
1.00
2.07
0.99
4.17
1.01
3.24
1.03
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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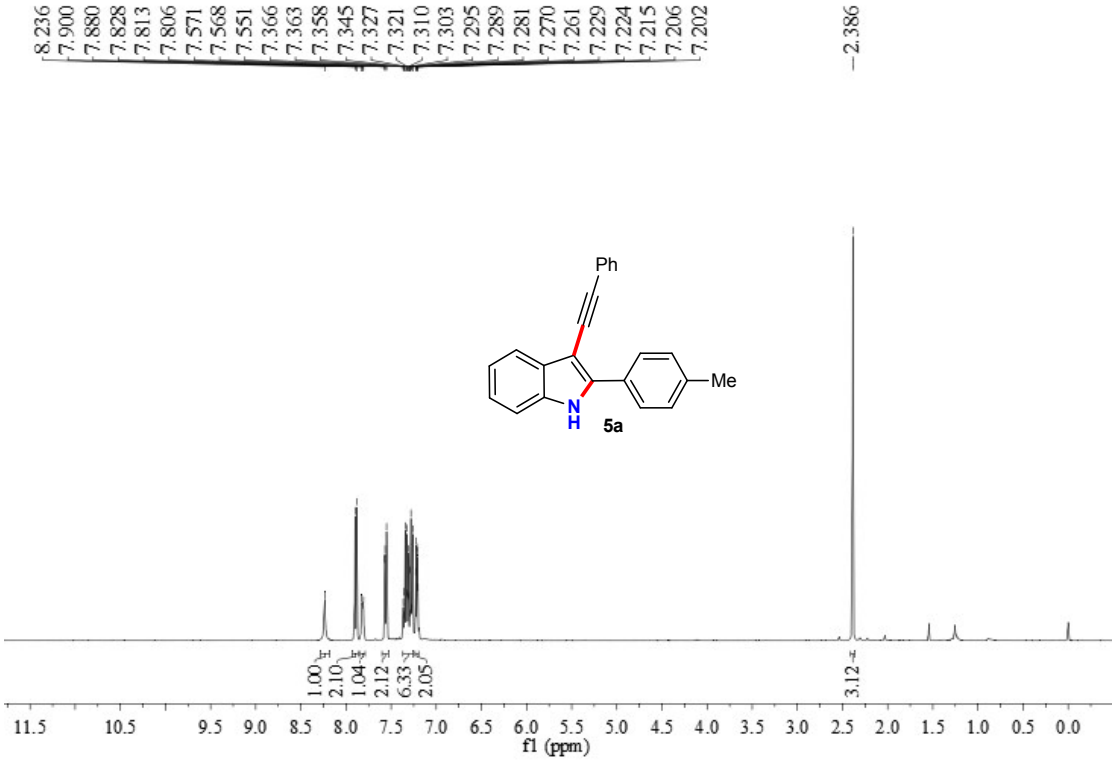
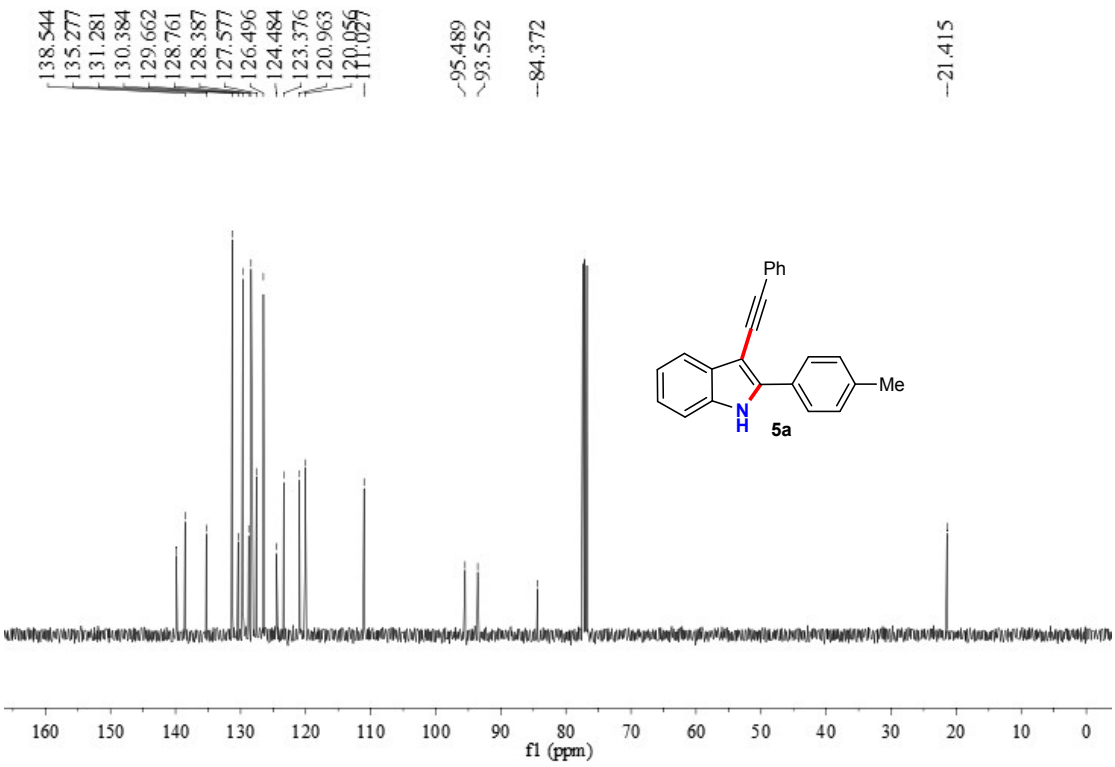
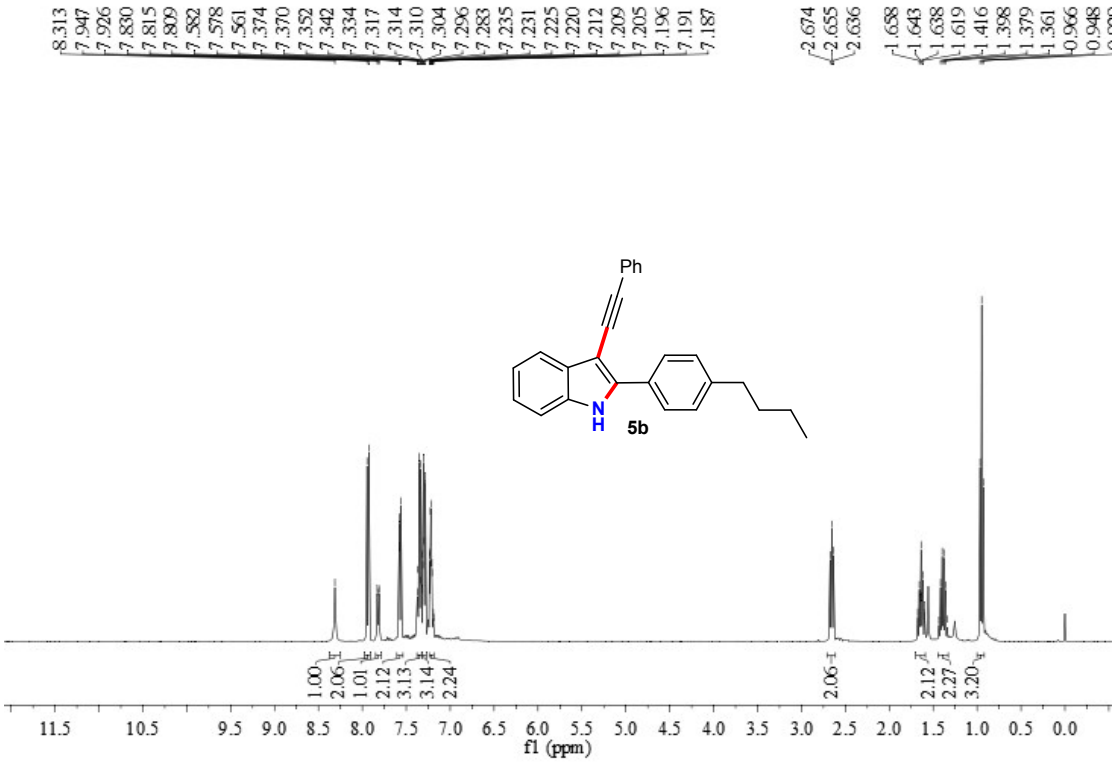
131.190
129.191
129.075
128.421
128.033
126.790
126.749
122.918
118.458
96.849
94.208
82.590
Ph
Cl
Ph
N
H
Cl
4n
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compounds 5



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7.561
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7.352
7.342
7.334
7.317
7.314
7.310
7.304
7.296
7.283
7.235
7.231
7.225
7.220
7.212
7.209
7.205
7.196
7.191
7.187
2.674
2.655
2.636
1.658
1.643
1.638
1.619
1.416
1.398
1.379
1.361
0.966
0.948
Ph
N
H
5b
1.00
2.06
1.01
2.12
3.13
3.14
2.24
2.06
2.12
2.27
3.20
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
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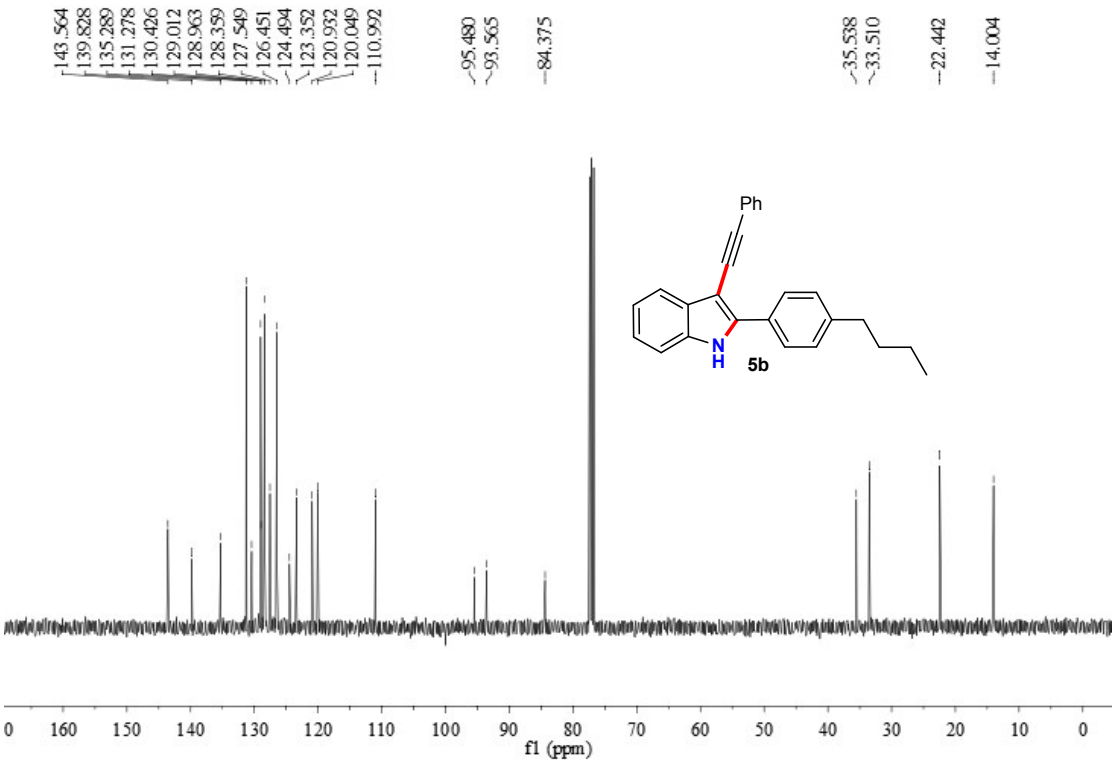
1.5
1.0
0.5
0.0
f1 (ppm)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127.549
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120.932
120.049
110.992
95.480
93.565
84.375
35.538
33.510
22.442
14.004
Ph
N
H
5b
0
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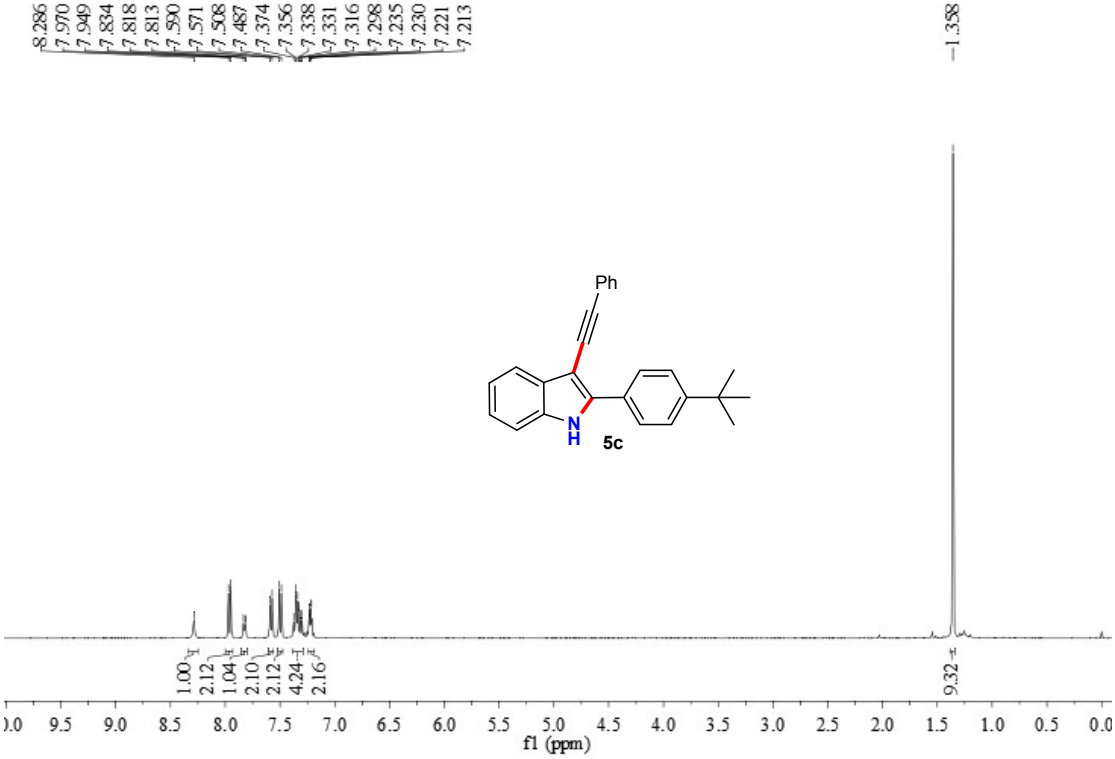
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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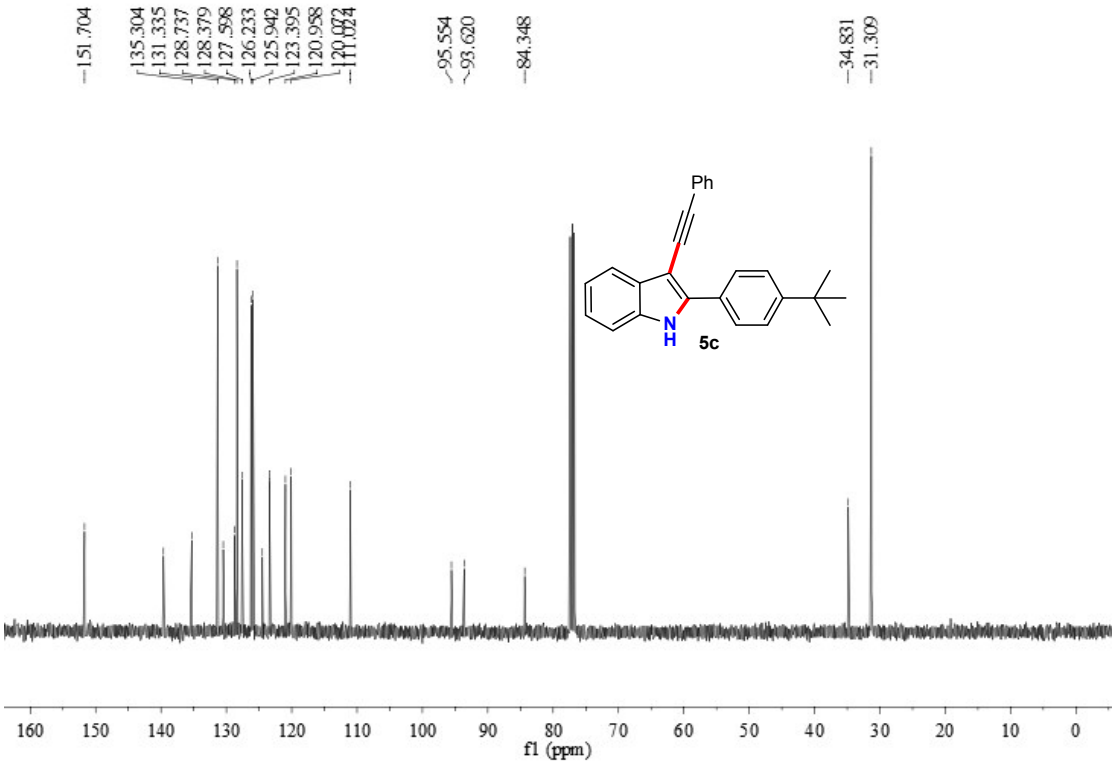
7.590
7.571
7.508
7.487
7.374
7.356
7.338
7.331
7.316
7.298
7.235
7.230
7.221
7.213
1.358
Ph
N
H
5c
1.00
2.12
1.04
2.10
2.12
4.24
2.16
9.32
f1 (ppm)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128.379
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126.233
125.942
123.395
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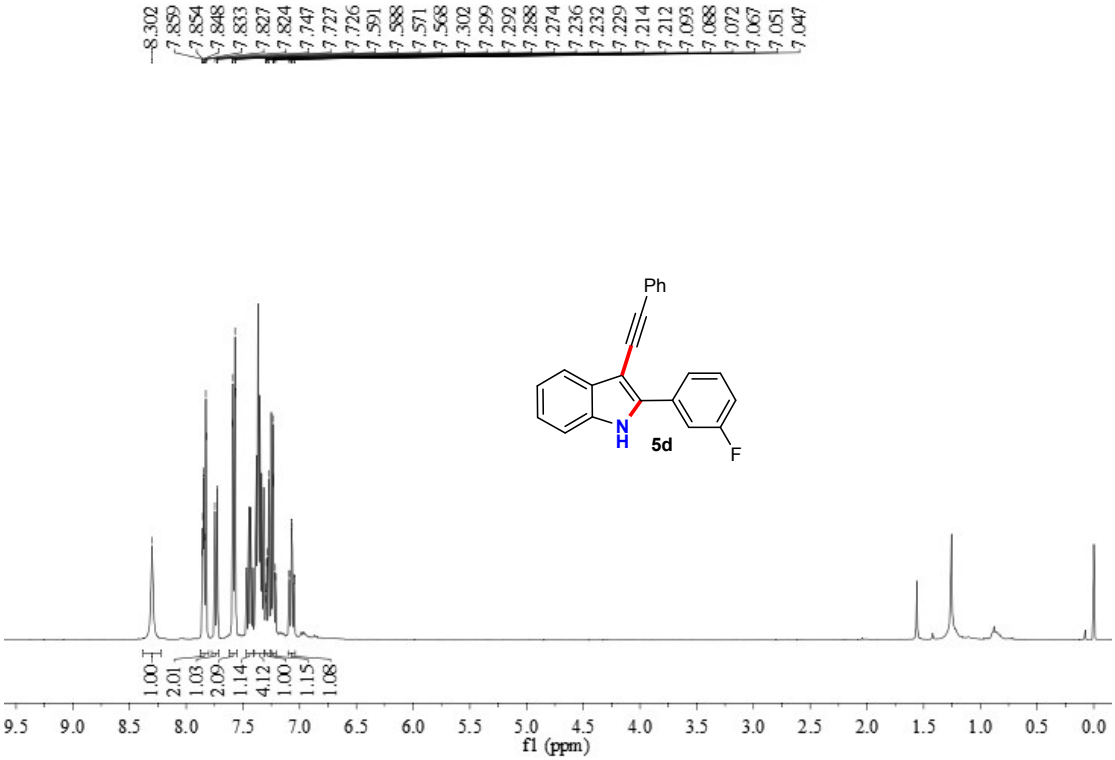
95.554
93.620
84.348
34.831
31.309
Ph
N
H
5c
f1 (ppm)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7.833
7.827
7.824
7.747
7.727
7.726
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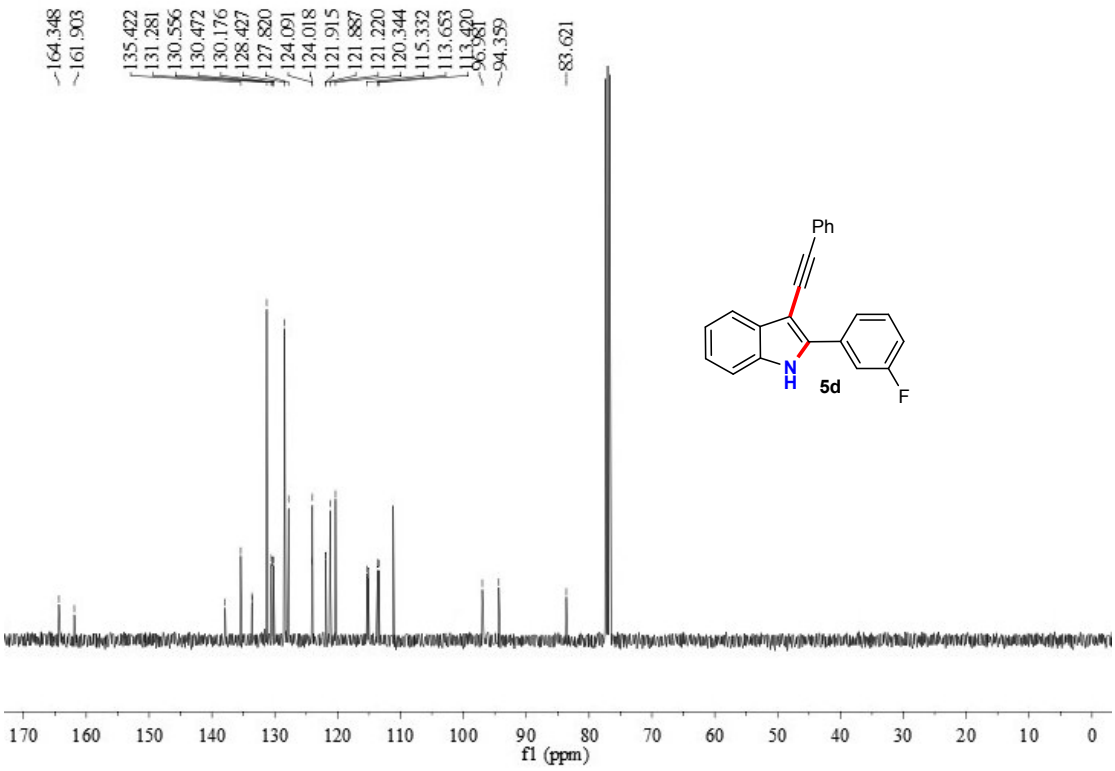
7.588
7.571
7.568
7.302
7.299
7.292
7.288
7.274
7.236
7.232
7.229
7.214
7.212
7.093
7.088
7.072
7.067
7.051
7.047
Ph
N
H
5d
F
1.00
2.01
1.03
2.09
1.14
4.12
1.00
1.15
1.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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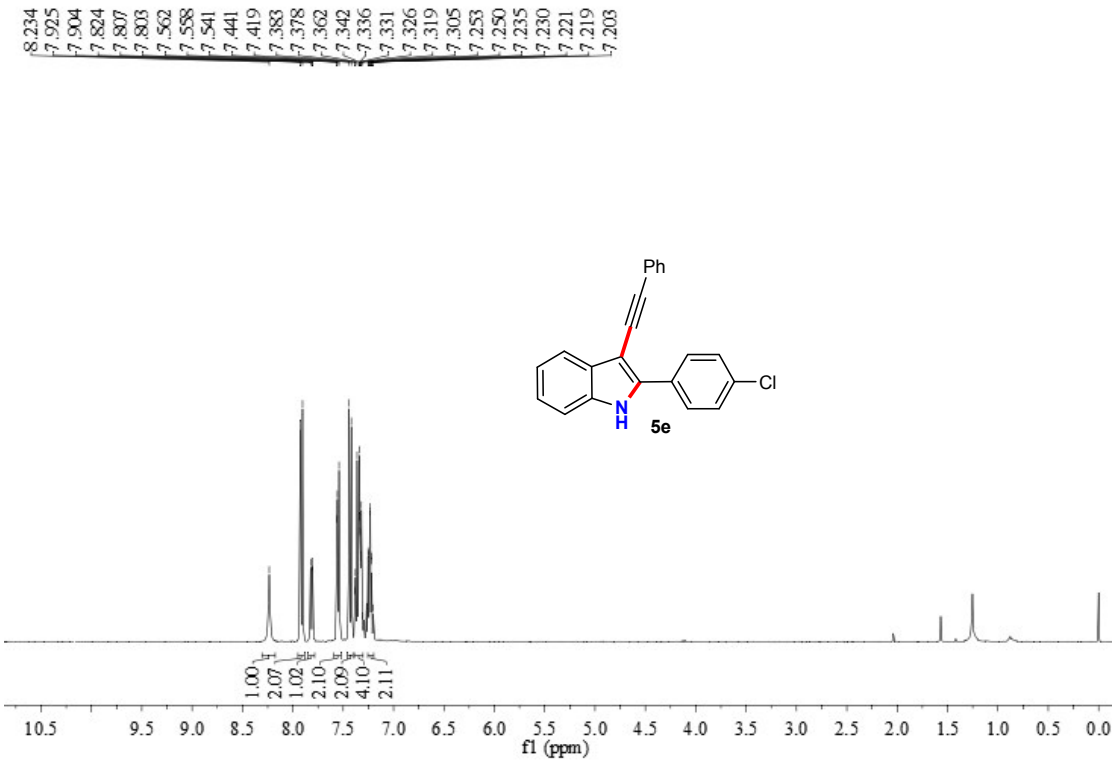
127.820
124.091
124.018
121.915
121.887
121.220
120.344
115.332
113.653
113.420
96.981
94.359
83.621
Ph
N
H
5d
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.441
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7.383
7.378
7.362
7.342
7.336
7.331
7.326
7.319
7.305
7.253
7.250
7.235
7.230
7.221
7.219
7.203
Ph
Cl
N
H
5e
1.00
2.07
1.02
2.10
2.09
4.10
2.11
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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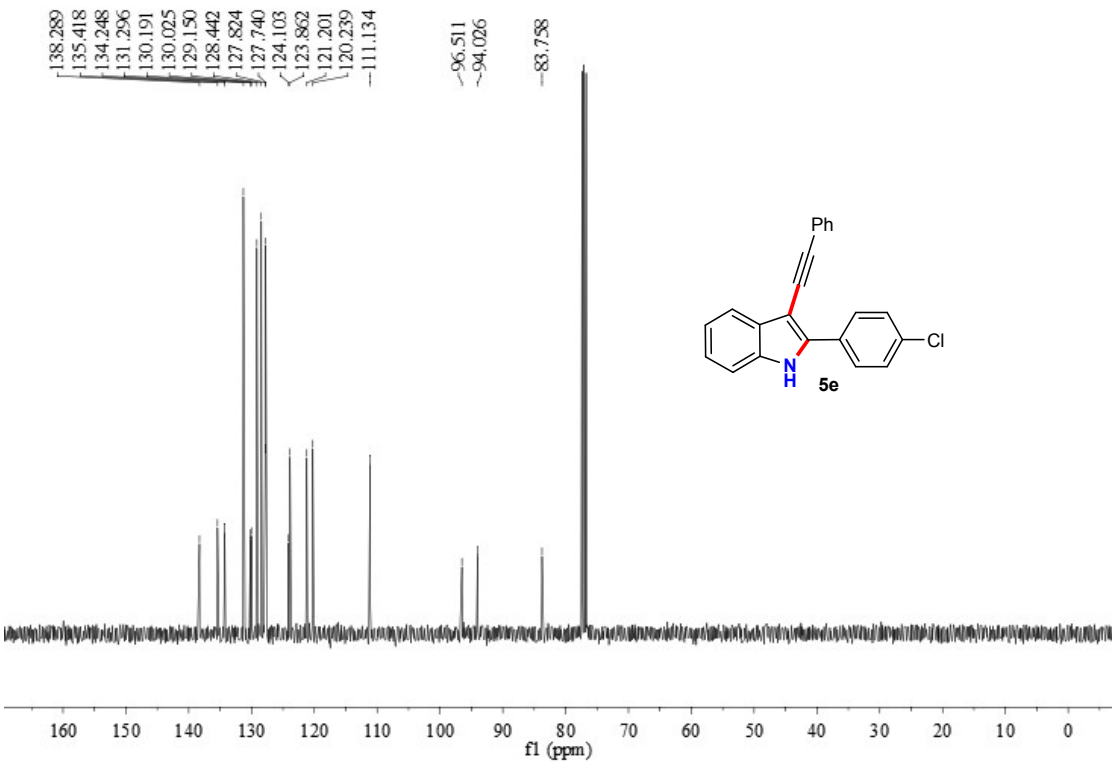
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.824
127.740
124.103
123.862
121.201
120.239
111.134
96.511
94.026
83.758
Ph
Cl
N
H
5e
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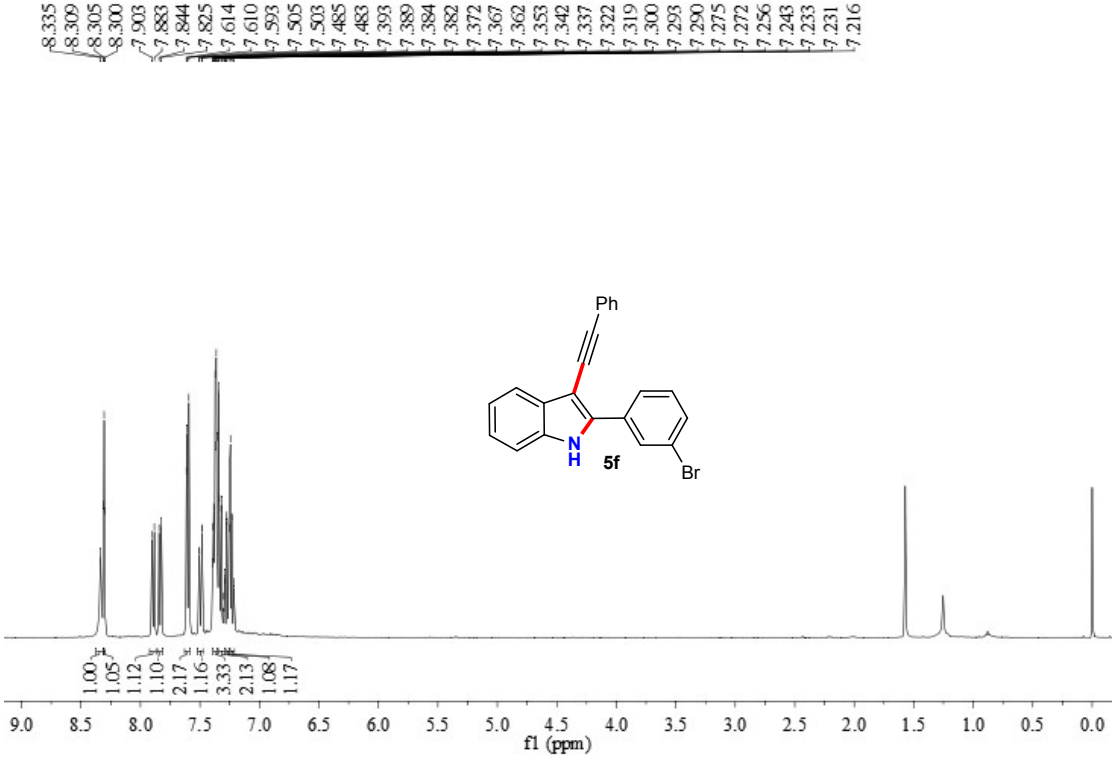
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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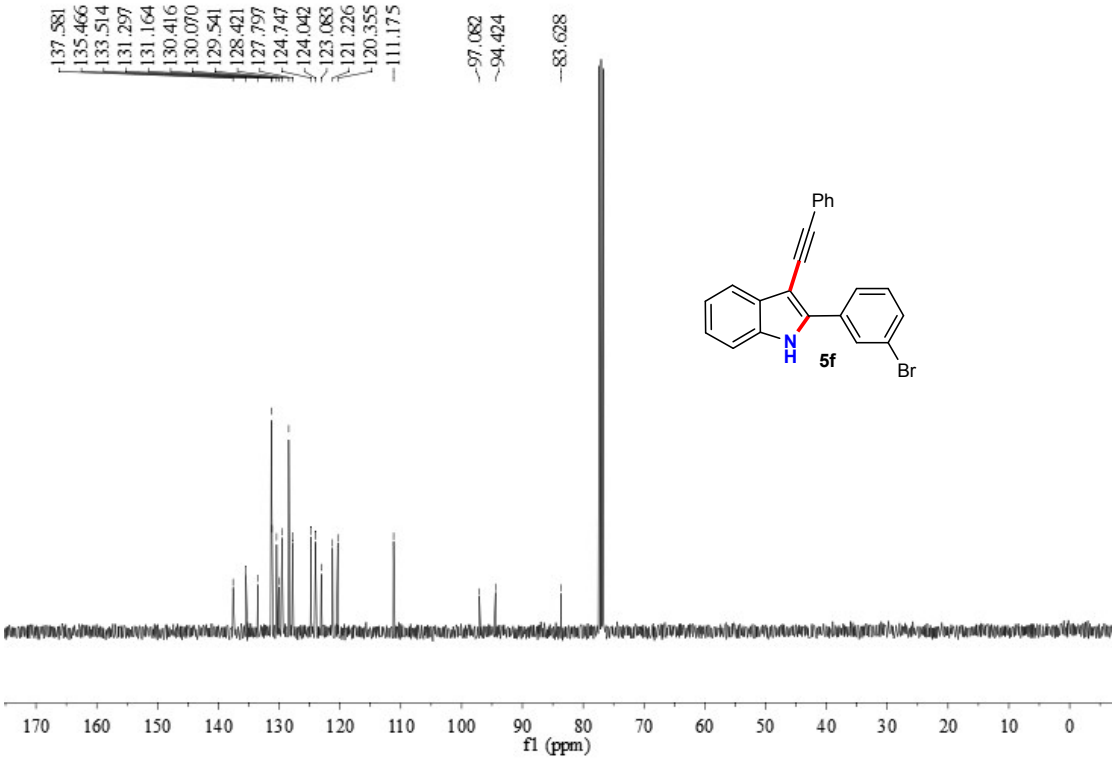
7.503
7.485
7.483
7.393
7.389
7.384
7.382
7.372
7.367
7.362
7.353
7.342
7.337
7.322
7.319
7.300
7.293
7.290
7.275
7.272
7.256
7.243
7.233
7.231
7.216
Ph
N
H
5f
Br
1.00
1.05
1.12
1.10
2.17
1.16
3.33
2.13
1.08
1.17
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.541
128.421
127.797
124.747
124.042
123.083
121.226
120.355
111.175
97.082
94.424
83.628
Ph
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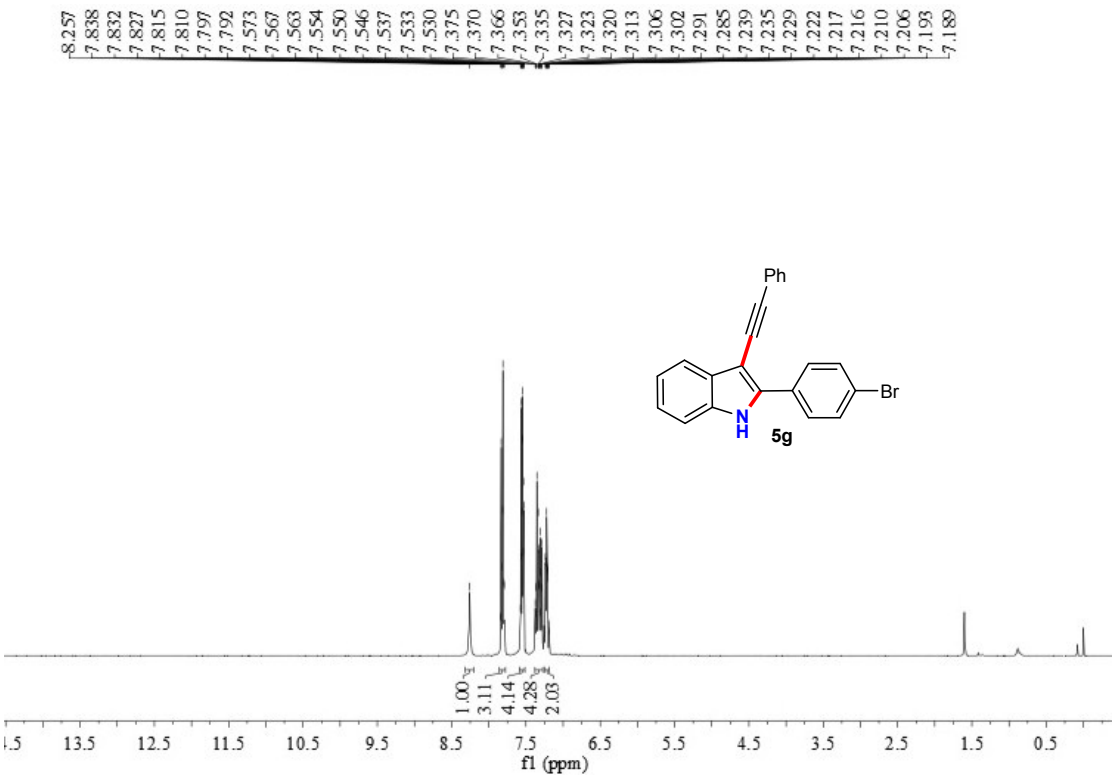
H
5f
Br
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.550
7.546
7.537
7.533
7.530
7.375
7.370
7.366
7.353
7.335
7.327
7.323
7.320
7.313
7.306
7.302
7.291
7.285
7.239
7.235
7.229
7.222
7.217
7.216
7.210
7.206
7.193
7.189
Ph
Br
N
H
5g
1.00
3.11
4.14
4.28
2.03
13.5
12.5
11.5
10.5
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6.5
5.5
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1.5
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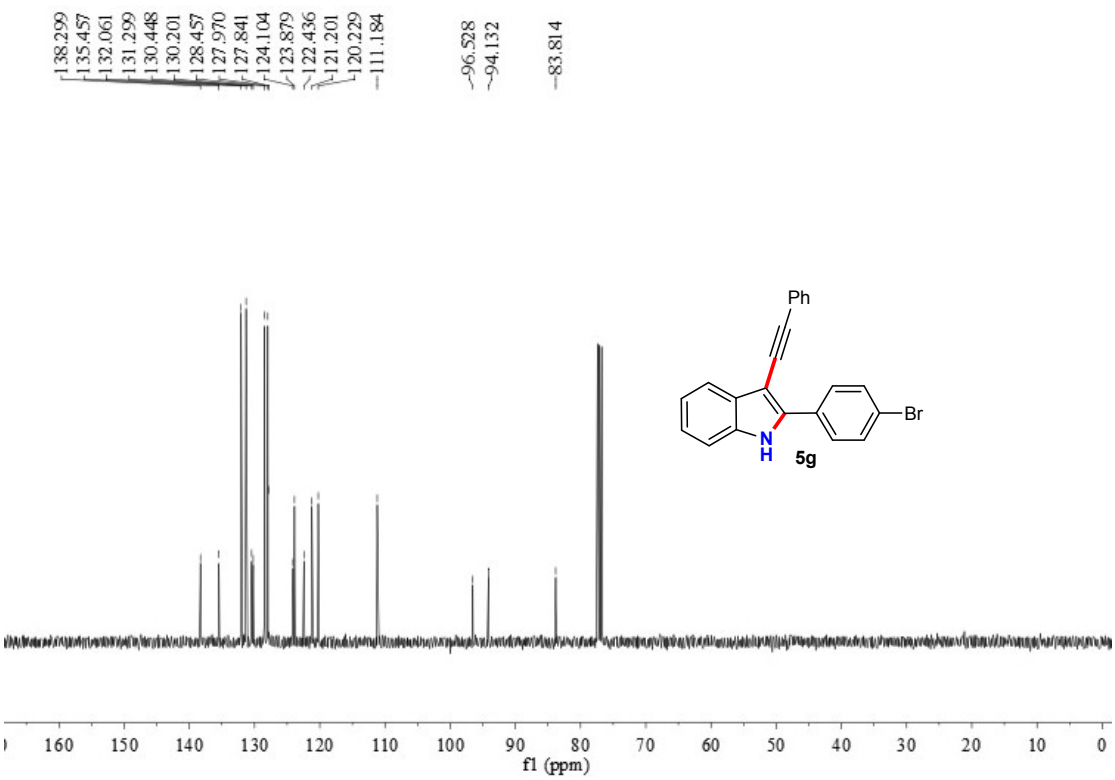
f1 (ppm)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130.448
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128.457
127.970
127.841
124.104
123.879
122.436
121.201
120.229
111.184
96.528
94.132
83.814
Ph
Br
N
H
5g
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130
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110
100
90
80
70
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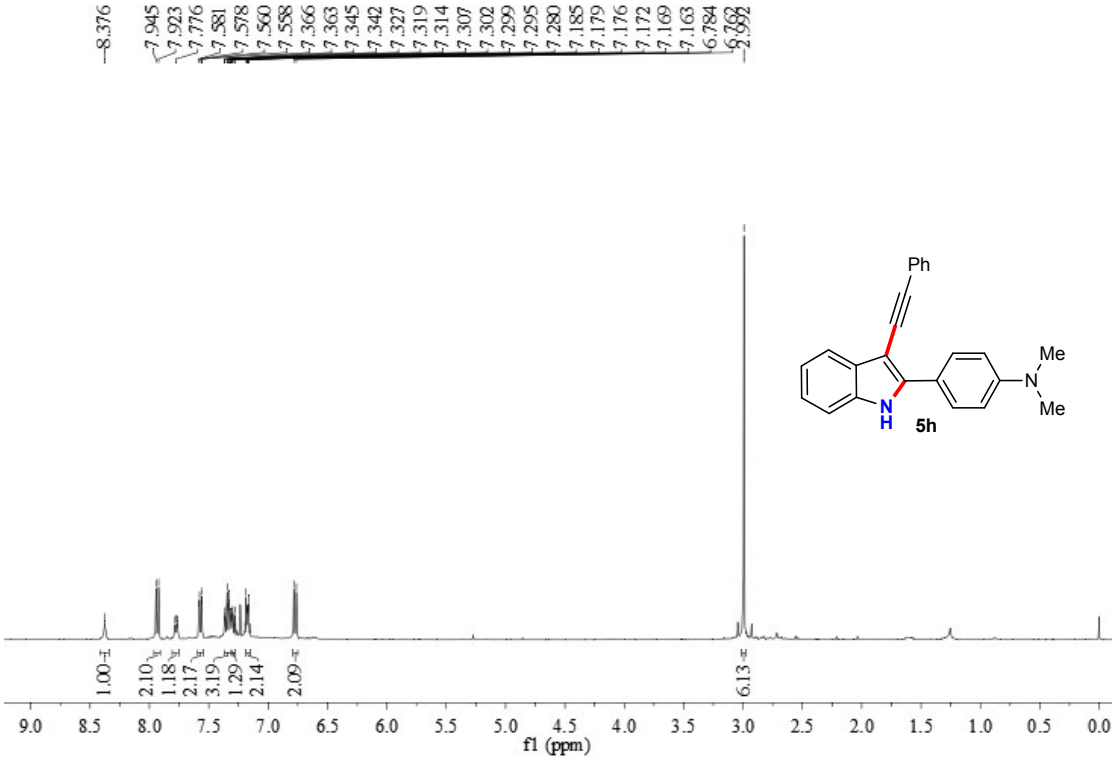
50
40
30
20
10
0
f1 (ppm)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7.327
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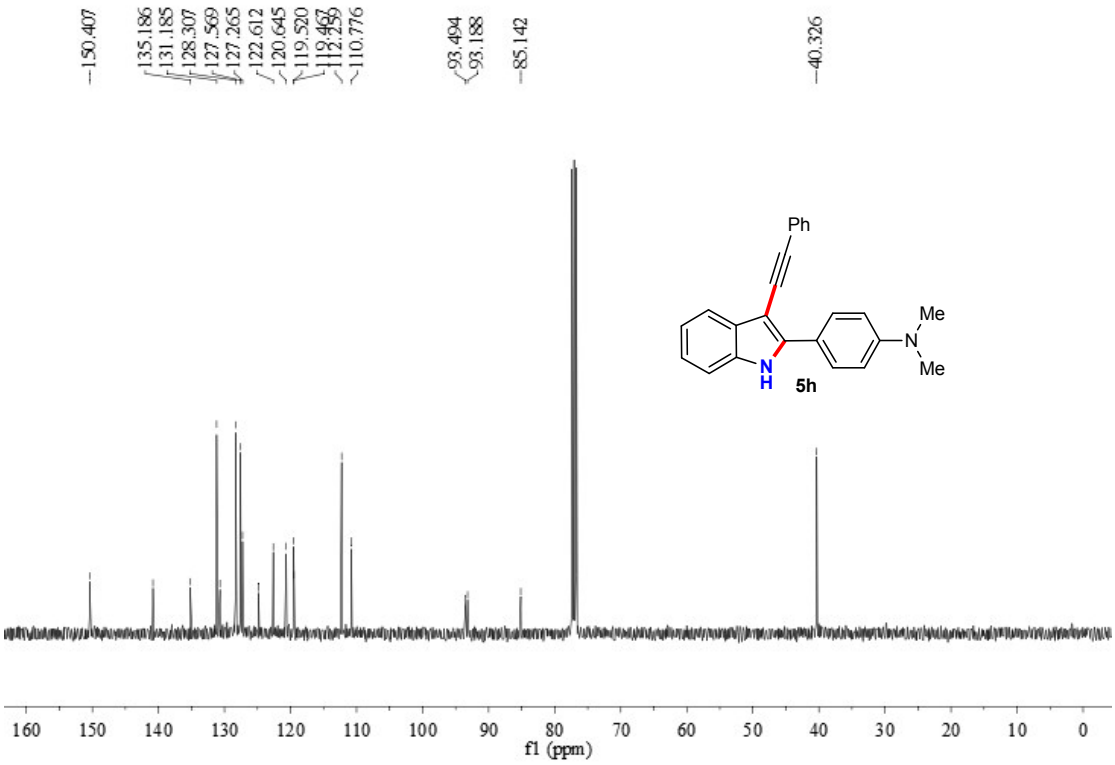
7.299
7.295
7.280
7.185
7.179
7.176
7.172
7.169
7.163
6.784
6.762
2.992
1.00
2.10
1.18
2.17
3.19
1.29
2.14
2.09
6.13
Ph
Me
N
Me
N
H
5h
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.186
131.185
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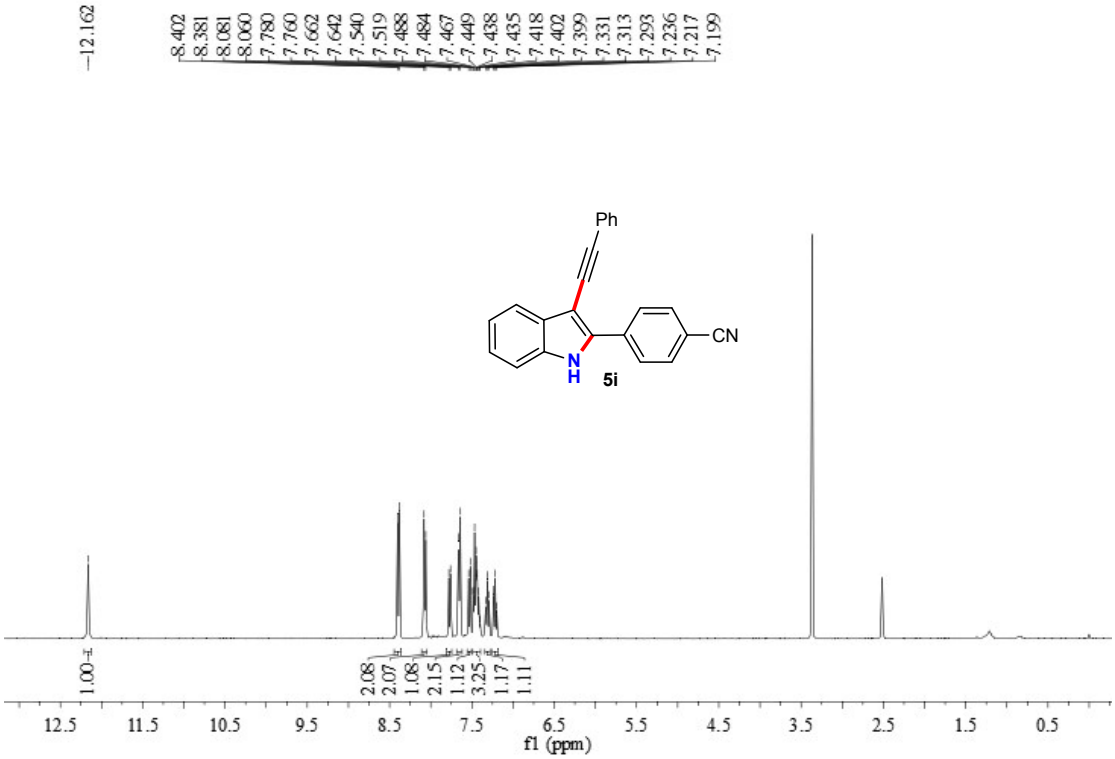
127.569
127.265
122.612
120.645
119.520
110.776
93.494
93.188
85.142
40.326
Ph
Me
N
Me
N
H
5h
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.381
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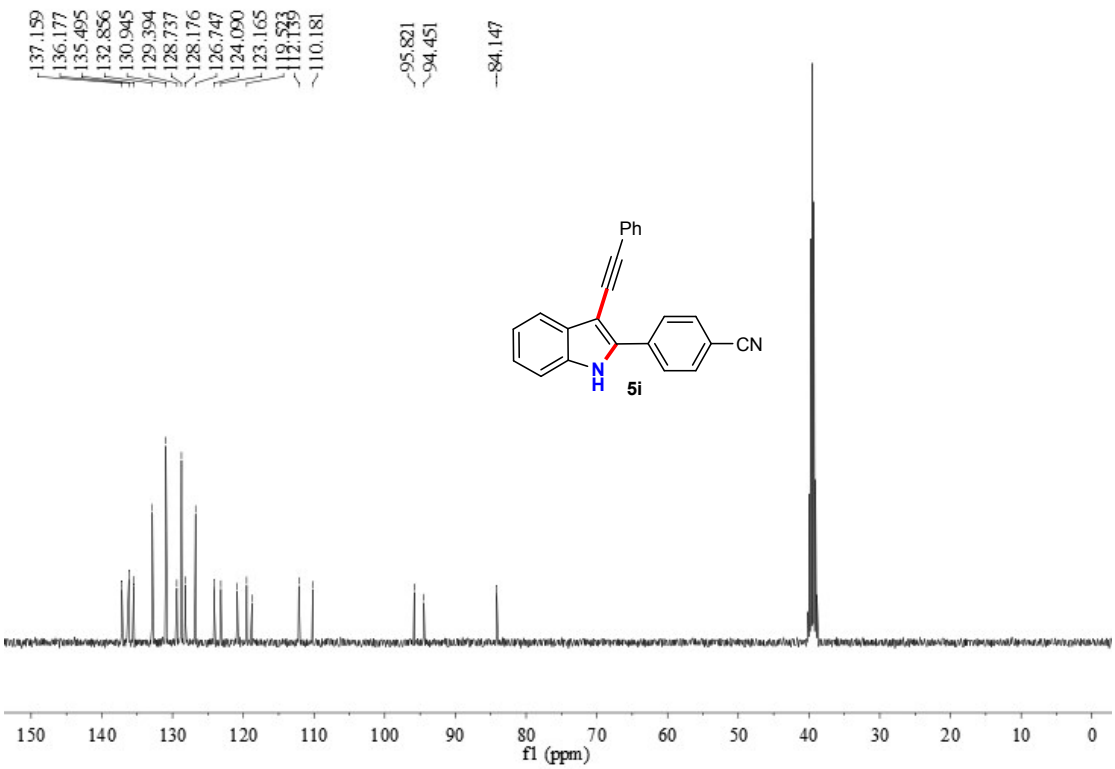
8.060
7.780
7.760
7.662
7.642
7.540
7.519
7.488
7.484
7.467
7.449
7.438
7.435
7.418
7.402
7.399
7.331
7.313
7.293
7.236
7.217
7.199
Ph
CN
N
H
5i
1.00
2.08
2.07
1.08
2.15
1.12
3.25
1.17
1.11
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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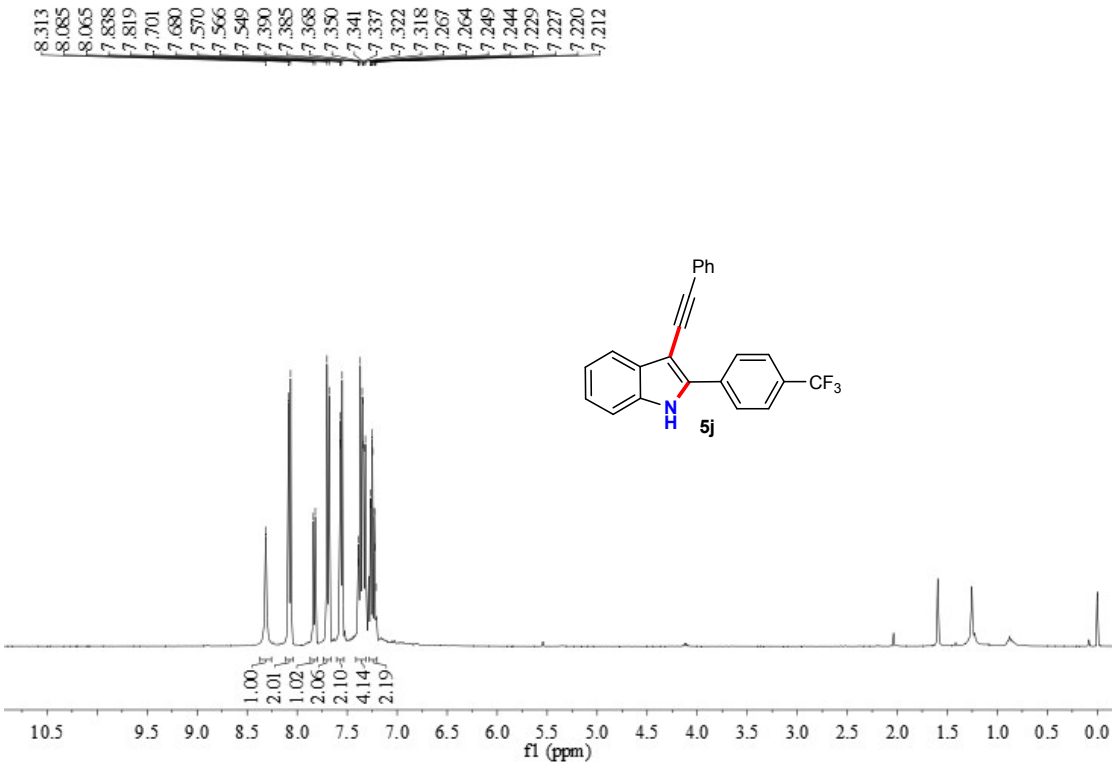
136.177
135.495
132.856
130.945
129.394
128.737
128.176
126.747
124.030
123.165
119.523
112.139
110.181
95.821
94.451
84.147
Ph
CN
N
H
5i
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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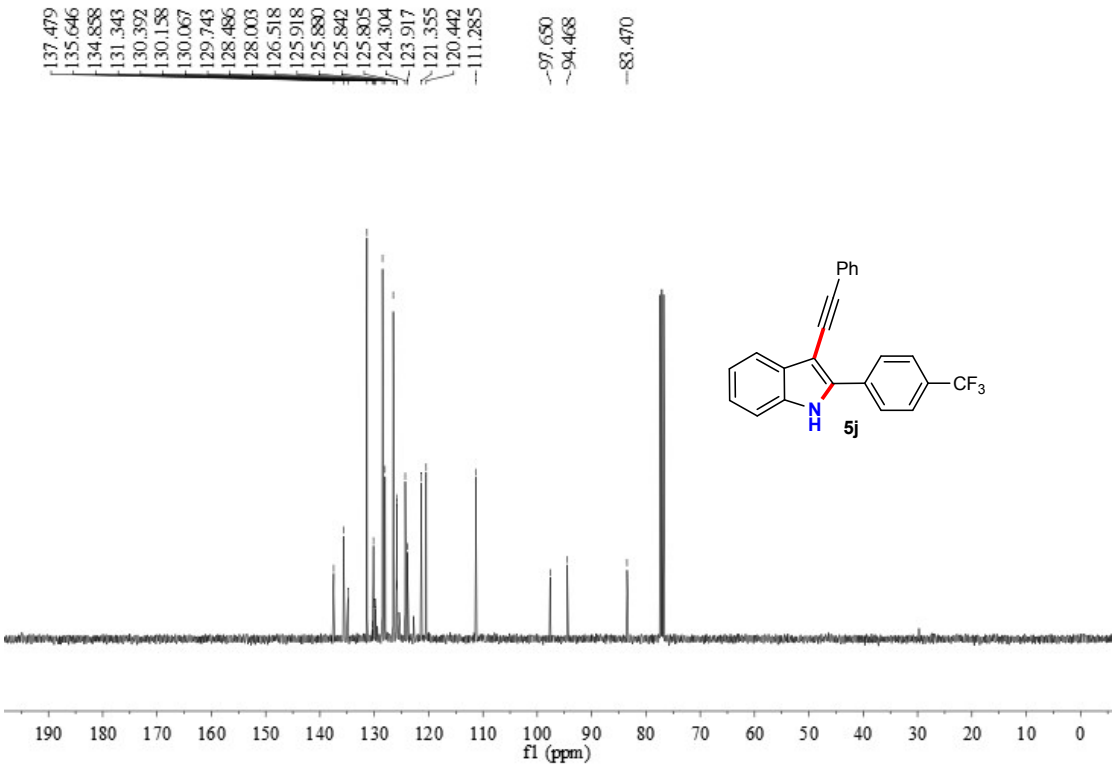
8.085
8.065
7.838
7.819
7.701
7.680
7.570
7.566
7.549
7.390
7.385
7.368
7.350
7.341
7.337
7.322
7.318
7.267
7.264
7.249
7.244
7.229
7.227
7.220
7.212
Ph
CF3
N
H
5j
1.00
2.01
1.02
2.06
2.10
4.14
2.19
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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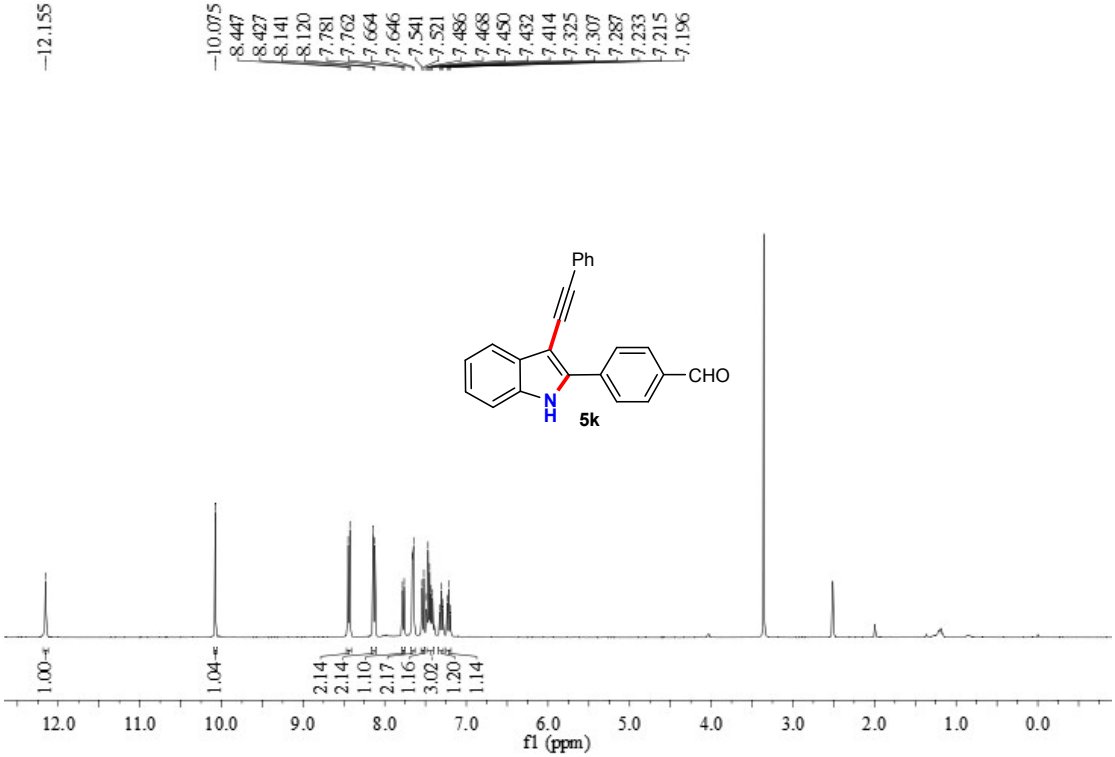
135.646
134.858
131.343
130.392
130.158
130.067
129.743
128.486
128.003
126.518
125.918
125.880
125.842
125.805
124.304
123.917
121.355
120.442
111.285
97.650
94.468
83.470
Ph
CF3
N
H
5j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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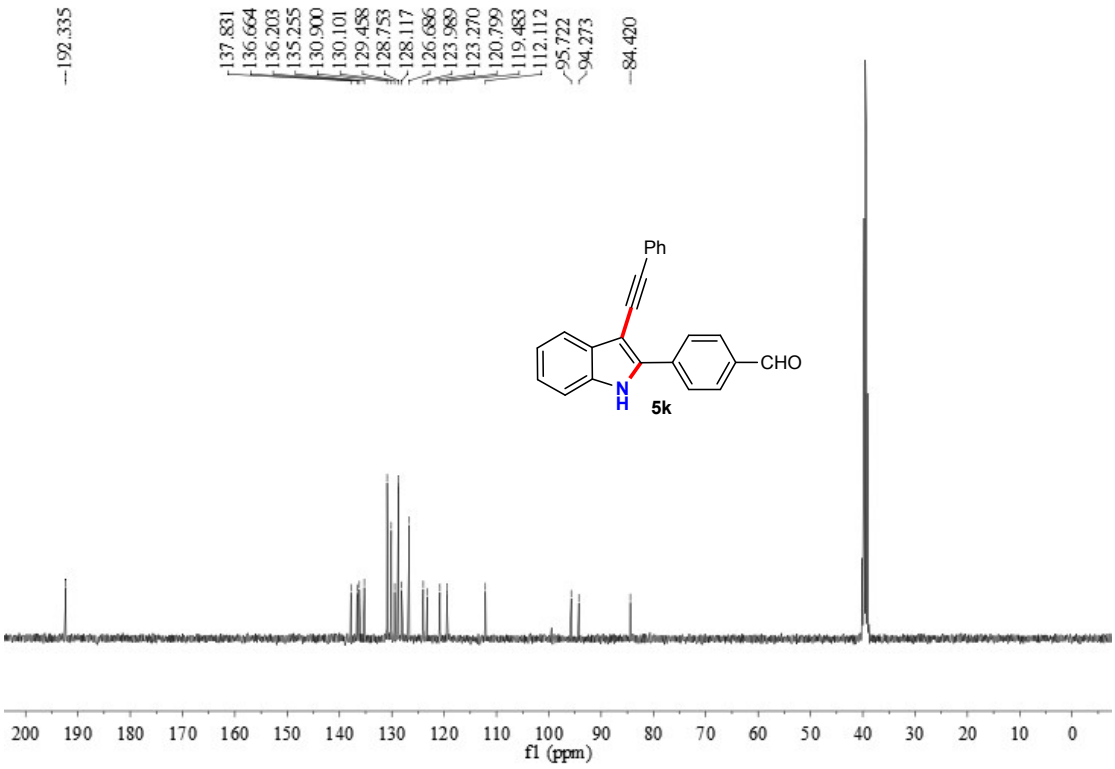
10.075
8.447
8.427
8.141
8.120
7.781
7.762
7.664
7.646
7.541
7.521
7.486
7.468
7.450
7.432
7.414
7.325
7.307
7.287
7.233
7.215
7.196
Ph
CHO
N
H
5k
1.00
1.04
2.14
2.14
1.10
2.17
1.16
3.02
1.20
1.14
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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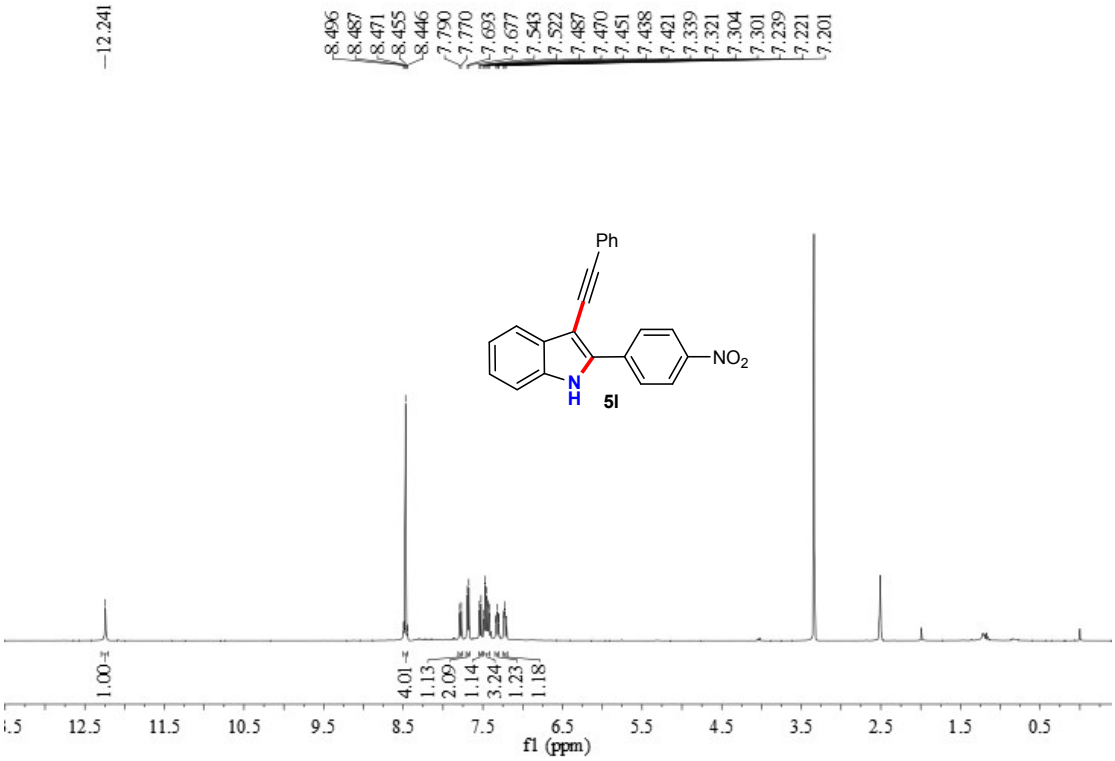
137.831
136.664
136.203
135.255
130.900
130.101
129.458
128.753
128.117
126.686
123.989
123.270
120.799
119.483
112.112
95.722
94.273
84.420
Ph
CHO
N
H
5k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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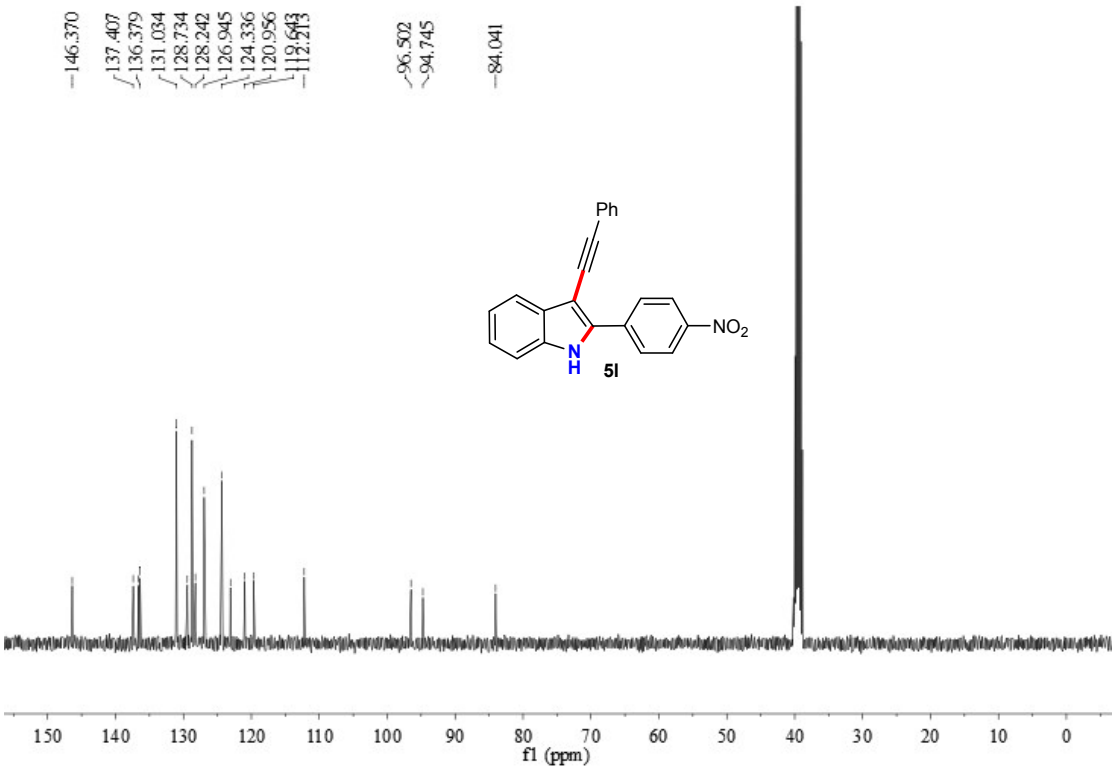
8.487
8.471
8.455
8.446
7.790
7.770
7.693
7.677
7.543
7.522
7.487
7.470
7.451
7.438
7.421
7.339
7.321
7.304
7.301
7.239
7.221
7.201
Ph
NO2
N
H
5l
1.00
4.01
1.13
2.09
1.14
3.24
1.23
1.18
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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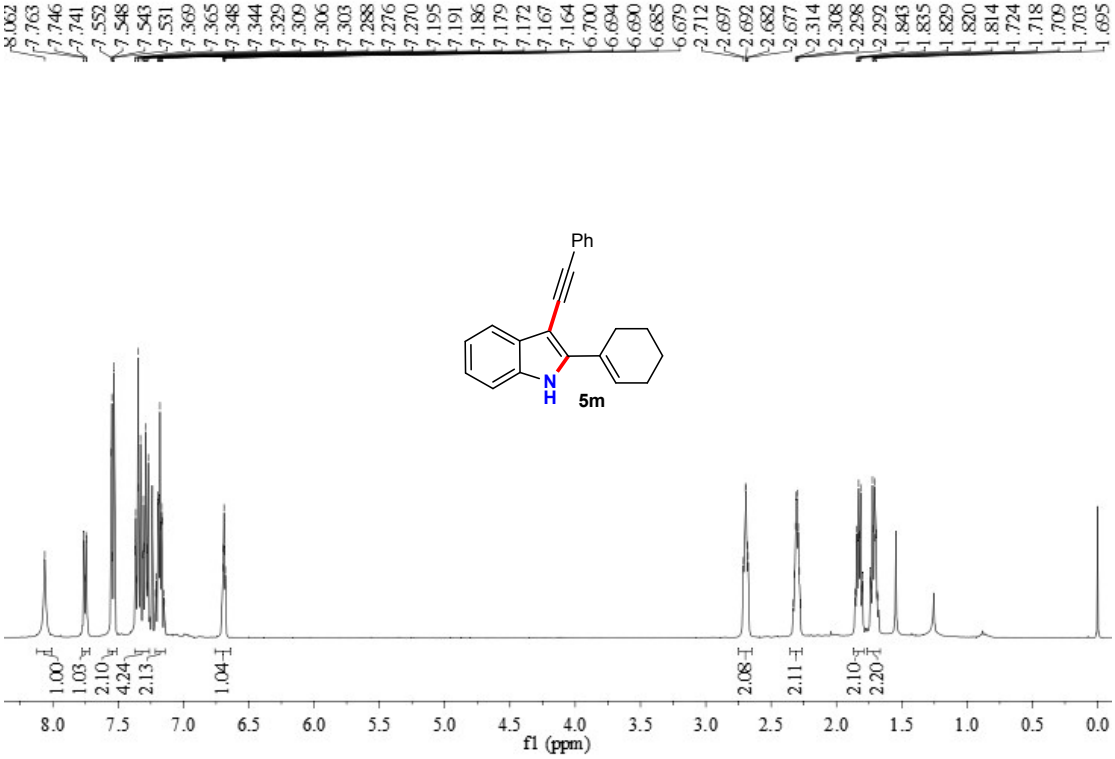
136.379
131.034
128.734
128.242
126.945
124.336
120.956
96.502
94.745
84.041
Ph
NO2
N
H
5l
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.741
7.552
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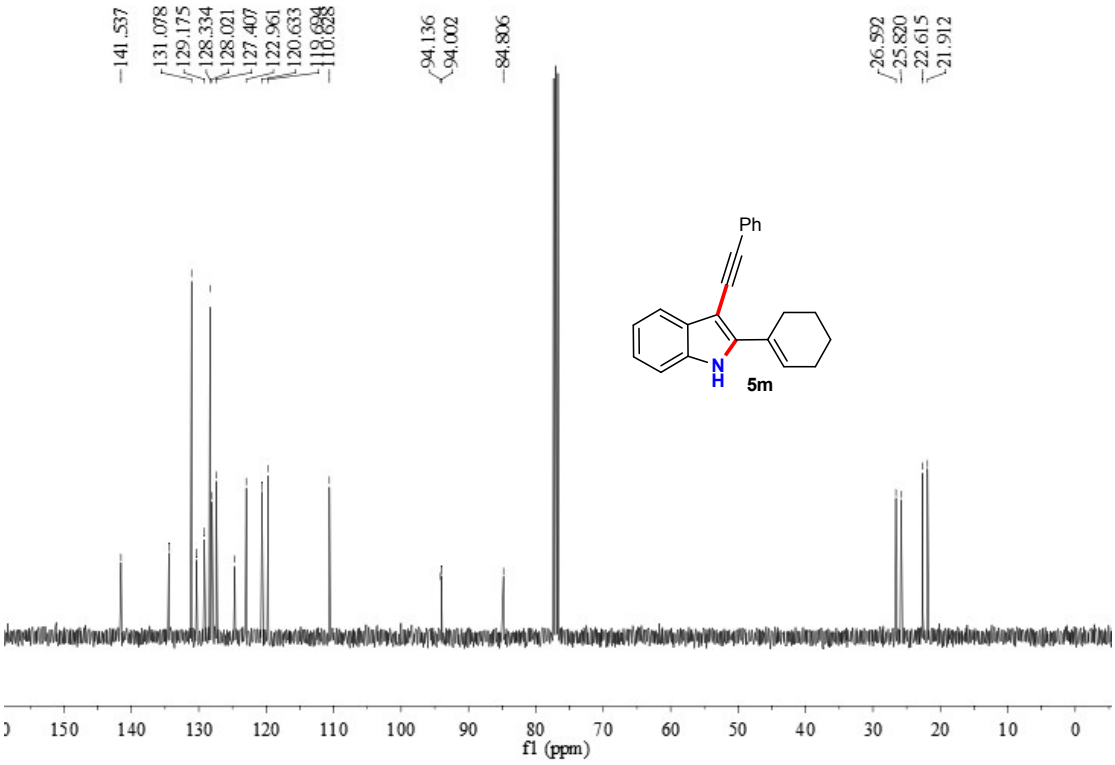
7.531
7.369
7.365
7.348
7.344
7.329
7.309
7.306
7.303
7.288
7.276
7.270
7.195
7.191
7.186
7.179
7.172
7.167
7.164
6.700
6.694
6.690
6.685
6.679
2.712
2.697
2.692
2.682
2.677
2.314
2.308
2.298
2.292
1.843
1.835
1.829
1.820
1.814
1.724
1.718
1.709
1.703
1.695
Ph
N
H
5m
1.00
1.03
2.10
4.24
2.13
1.04
2.08
2.11
2.10
2.20
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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129.175
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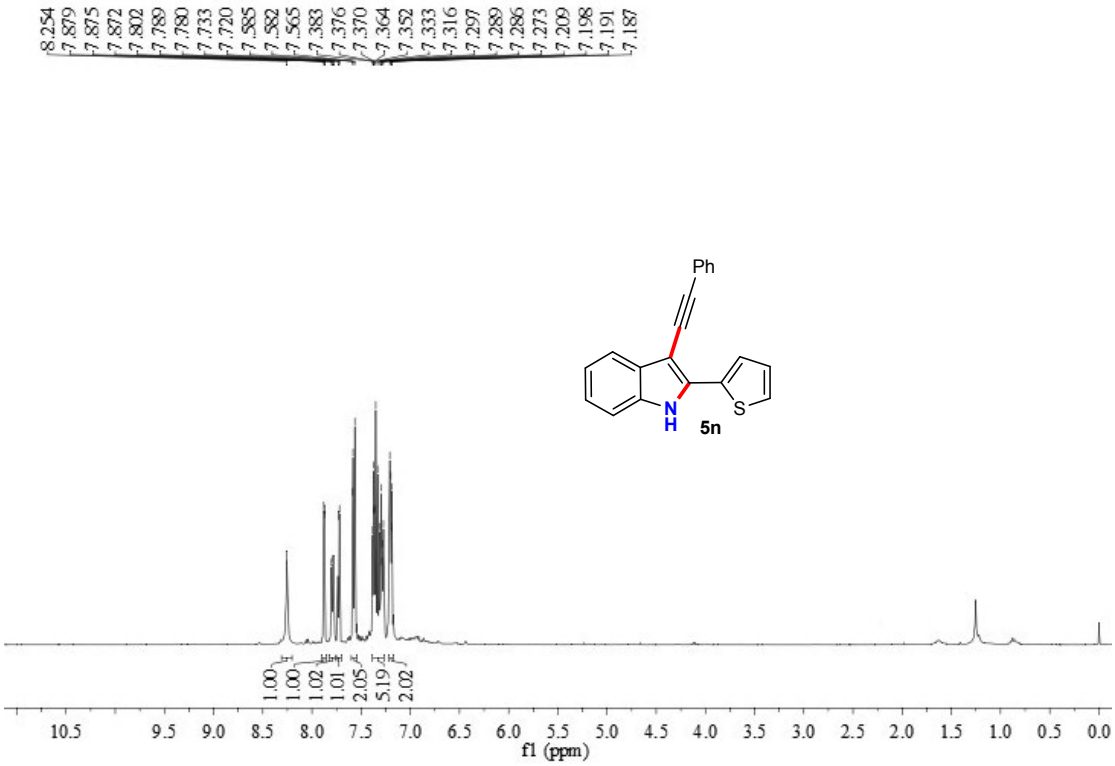
128.021
127.407
122.961
120.633
119.694
110.628
94.136
94.002
84.806
26.592
25.820
22.615
21.912
Ph
N
H
5m
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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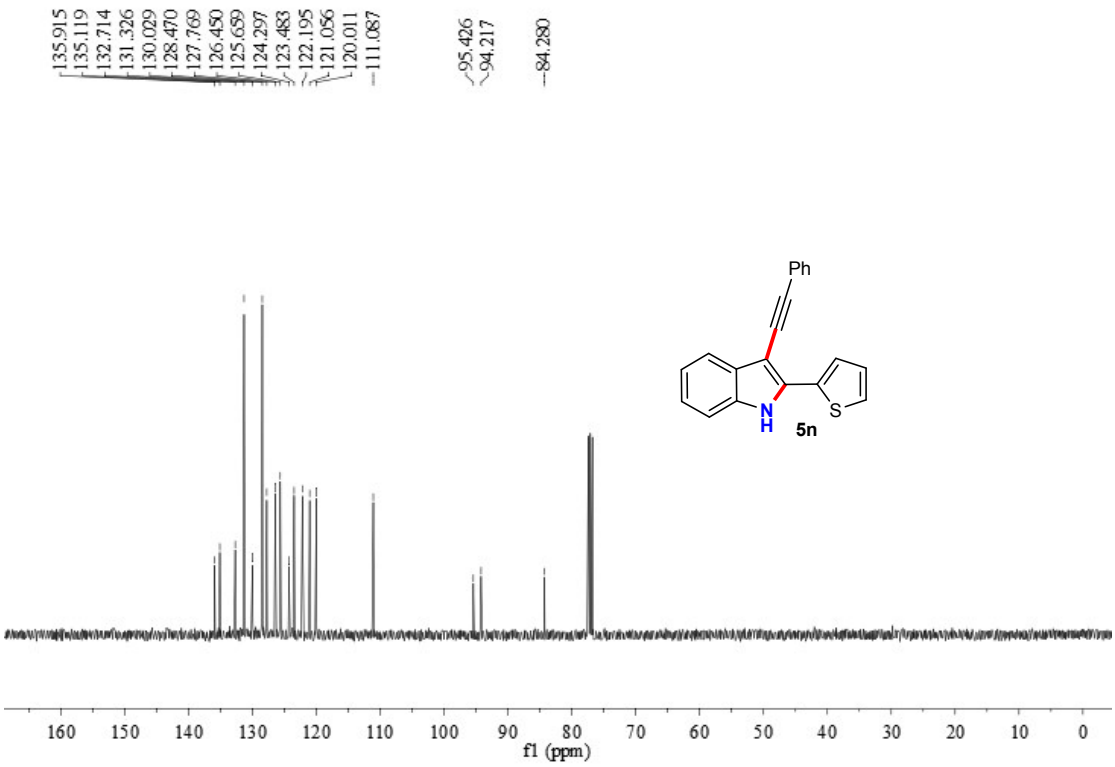
7.733
7.720
7.585
7.582
7.565
7.383
7.376
7.370
7.364
7.352
7.333
7.316
7.297
7.289
7.286
7.273
7.209
7.198
7.191
7.187
Ph
N
H
S
5n
1.00
1.00
1.02
1.01
2.05
5.19
2.02
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


135.915
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132.714
131.326
130.029
128.470
127.769
126.450
125.659
124.297
123.483
122.195
121.056
120.011
111.087
95.426
94.217
84.280
Ph
N
H
S
5n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)