Supporting Information for

Copper-catalyzed synthesis of 1, 2,4-trisubstituted pyrroles via cascade reactions of aryloxy-enynes with amines

Ende Li, Xingcan Cheng, Chengyu Wang, Xia Sun and Yanzhong Li*

Shanghai Key Laboratory of Green Chemistry and Chemical Processes, Department of Chemistry, East China Normal University, Dongchuan Rd. 500, Shanghai, 200241, People's Republic of China

Fax: (+86) 021-54340096, E-mail: yzli@chem.ecnu.edu.cn

Contents:

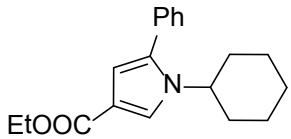
Experimental section

General Methods. All reactions were carried out under nitrogen. THF, Tol. were distilled from sodium/benzophenone. DMF and DMSO were distilled after dried over anhydrous $MgSO_4$. Unless noted, all commercial reagents were used without further purification.

^1H NMR spectra was recorded at 400 MHz, ^{13}C NMR spectra was recorded at 100 MHz, and in $CDCl_3$ (containing 0.03% TMS) solutions. ^1H NMR spectra was recorded with tetramethylsilane (δ = 0.00 ppm) as internal reference; ^{13}C NMR spectra was recorded with $CDCl_3$ (δ = 77.00 ppm) as internal reference.

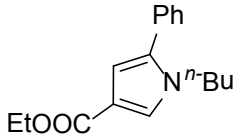
A typical procedure for the Cu-catalyzed synthesis of Ethyl 1-cyclohexyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3a):

(*E*)-ethyl 2-(phenoxymethylene)-4-phenylbut-3-ynoate (88 mg, 0.3 mmol) in DMF (2 mL), CuI (6 mg, 0.03 mmol), cyclohexanamine (0.038 mL, 0.33 mmol), Cs_2CO_3 (196 mg, 0.6 mmol) were added to a Schlenk tube under nitrogen. The resulting solution was stirred at 90 ^oC. After the reaction was complete as monitored by thin-layer chromatography, the mixture was treated with water and extracted with EA. The extract was washed with water and dried over anhydrous Na_2SO_4. The solvent was evaporated under the reduced pressure, and the residue was purified by chromatography on silica gel to afford the 1,2,4-trisubstituted pyrrole derivatives **3a** (71 mg, 80 %) as a yellow oil.



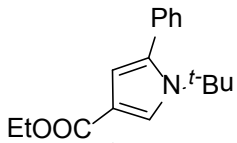
3a

Ethyl 1-cyclohexyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3a) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3a** in 80 % (71 mg) isolated yield as a yellow oil. ^1H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.18-1.29 (m, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.60-1.69 (m, 3H), 1.76-1.84 (m, 2H), 1.97-2.00 (m, 2H), 3.94-4.00 (m, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 6.55 (d, *J* = 1.2 Hz, 1H), 7.32-7.43 (m, 5H), 7.50 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.40, 25.14, 25.61, 34.71, 55.63, 59.53, 109.39, 115.63, 123.51, 127.63, 128.53, 129.32, 132.71, 134.94, 165.11; HRMS (EI) calcd for $C_{19}H_{23}NO_2$ 297.1729, found 297.1730.



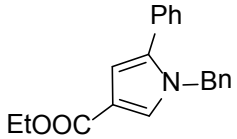
3b

Ethyl 1-butyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3b) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3b** in 68 % (55 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 0.82 (t, *J* = 7.2 Hz, 3H), 1.17-1.23 (m, 2H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.60-1.64 (m, 2H), 3.91 (t, *J* = 7.2 Hz, 2H), 4.29 (q, *J* = 7.2 Hz, 2H), 6.58 (d, *J* = 2 Hz, 1H), 7.35-7.43 (m, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 13.47, 14.47, 19.60, 33.11, 47.31, 59.60, 109.70, 115.40, 126.78, 127.55, 128.44, 129.06, 132.49, 135.19, 164.92; HRMS (EI) calcd for $C_{17}H_{21}NO_2$ 271.1572, found 271.1575.



3c

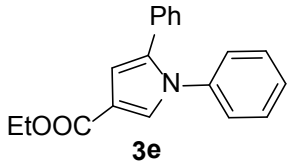
Ethyl 1-*tert*-butyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3c) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3c** in 72 % (58 mg) isolated yield as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$, Me_4Si) δ 1.33 (t, *J* = 7.2 Hz, 3H), 1.43 (s, 9H), 4.28 (q, *J* = 7.2 Hz, 2H), 6.44 (d, *J* = 2 Hz, 1H), 7.35-7.38 (m, 5H), 7.56 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.51, 31.52, 58.19, 59.52, 112.85, 113.36, 124.32, 127.50, 128.03, 131.81, 135.00, 135.81, 165.11; HRMS (EI) calcd for $C_{17}H_{21}NO_2$ 271.1572, found 271.1578.



3d

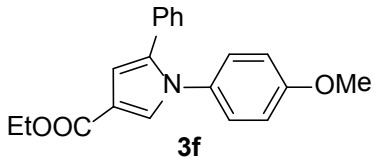
Ethyl 1-benzyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3d) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3d** in 78 % (72 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.33 (t, *J* = 7.2 Hz, 3H), 4.28 (q, *J* = 7.2 Hz, 2H), 5.10 (s, 2H), 6.68 (d, *J* = 2 Hz, 1H), 6.98-7.00 (m, 2H), 7.24-7.36 (m, 8H), 7.37 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (100.6 MHz,

$CDCl_3$, Me_4Si) δ 14.43, 51.07, 59.67, 109.87, 116.10, 126.58, 127.52, 127.67, 127.70, 128.44, 128.75, 129.05, 132.02, 135.74, 137.36, 164.77; HRMS (EI) calcd for $C_{20}H_{19}NO_2$ 305.1416, found 305.1417.



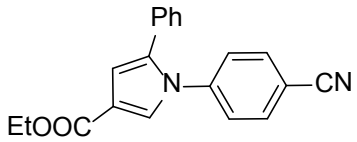
3e

Ethyl 1, 5-diphenyl-1*H*-pyrrole-3-carboxylate (3e) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3e** in 43 % (38 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.36 (t, *J* = 7.6 Hz, 3H), 4.33 (q, *J* = 7.2 Hz, 2H), 6.84 (d, *J* = 2 Hz, 1H), 7.10-7.21 (m, 7H), 7.31-7.34 (m, 3H), 7.55 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.46, 59.84, 110.96, 116.91, 125.65, 126.96, 127.50, 128.13, 128.35, 128.66, 129.14, 131.81, 134.77, 139.48, 164.72; HRMS (EI) calcd for $C_{19}H_{17}NO_2$ 291.1259, found 291.1262.



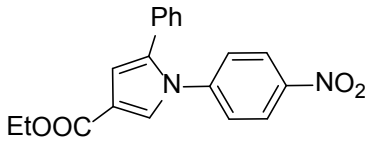
3f

Ethyl 1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3f) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3f** in 42 % (40 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.36 (t, *J* = 7.2 Hz, 3H), 3.81 (s, 3H), 4.32 (q, *J* = 6.8 Hz, 2H), 6.82 (d, *J* = 1.6 Hz, 1H), 6.84-6.86 (m, 2H), 7.07-7.13 (m, 4H), 7.19-7.26 (m, 3H), 7.49 (d, *J* = 2 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.49, 55.44, 59.82, 110.54, 114.25, 116.56, 126.88, 126.90, 128.14, 128.34, 128.83, 131.92, 132.59, 134.91, 158.76, 164.81; HRMS (EI) calcd for $C_{20}H_{19}NO_3$ 321.1365, found 321.1364.



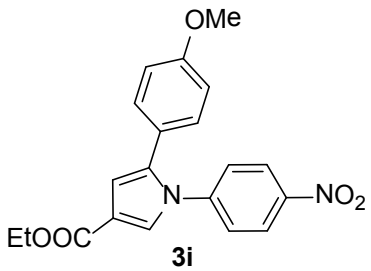
3g

Ethyl 1-(4-cyanophenyl)-5-phenyl-1H-pyrrole-3-carboxylate (3g) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3g** in 68 % (65 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.28 (t, *J* = 7.2 Hz, 3H), 4.25 (q, *J* = 6.8 Hz, 2H), 6.77 (d, *J* = 1.2 Hz, 1H), 7.01-7.02 (m, 2H), 7.17-7.19 (m, 5H), 7.49 (d, *J* = 1.2 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.09, 59.98, 111.21, 112.31, 118.07, 118.41, 126.12, 127.82, 128.23, 128.72, 131.37, 133.44, 135.01, 143.26, 164.64; HRMS (ESI) calcd for $C_{20}H_{17}N_2O_2$ 317.1290, found 317.1296 .



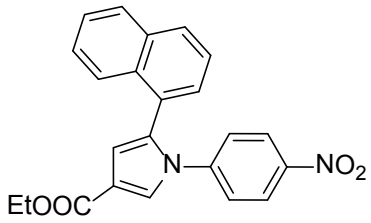
3h

Ethyl 1-(4-nitrophenyl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3h) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3h** in 79 % (80 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.37 (t, *J* = 7.2 Hz, 3H), 4.34 (q, *J* = 7.2 Hz, 2H), 6.86 (d, *J* = 1.6 Hz, 1H), 7.01-7.12 (m, 2H), 7.27-7.32 (m, 5H), 7.60 (d, *J* = 1.6 Hz, 1H), 8.20-8.22 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.40, 60.12, 112.37, 118.41, 124.74, 125.72, 127.68, 128.02, 128.52, 128.54, 131.06, 134.86, 144.52, 146.20, 164.19; HRMS (EI) calcd for $C_{19}H_{16}N_2O_4$ 336.1110, found 336.1106.



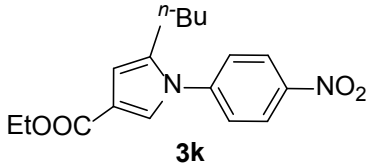
3i

Ethyl 5-(4-methoxyphenyl)-1-(4-nitrophenyl)-1*H*-pyrrole-3-carboxylate (3i) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3i** in 80 % (88 mg) isolated yield as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.37 (t, *J* = 7.2 Hz, 3H), 3.80 (s, 3H), 4.34 (q, *J* = 6.8 Hz, 2H), 6.79 (d, *J* = 2.8 Hz, 2H), 6.82 (s, 1H), 7.03 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 0.8 Hz, 1H), 8.22 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.30, 55.14, 60.02, 111.65, 114.07, 118.36, 123.63, 124.74, 125.80, 127.52, 130.00, 134.87, 144.75, 146.29, 159.32, 164.37; HRMS (EI) calcd for $C_{20}H_{18}N_2O_5$ 366.1216, found 366.1219.



3j

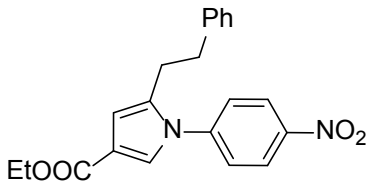
Ethyl 5-(naphthalen-1-yl)-1-(4-nitrophenyl)-1*H*-pyrrole-3-carboxylate (3j) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3j** in 89 % (103 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.39 (t, *J* = 7.2 Hz, 3H), 4.37 (q, *J* = 7.2 Hz, 2H), 6.94 (d, *J* = 2 Hz, 1H), 7.15-7.27 (m, 3H), 7.36-7.47 (m, 3H), 7.75-7.84 (m, 4H), 7.97-8.00 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.44, 60.18, 114.28, 118.42, 124.53, 124.68, 125.05, 125.23, 126.21, 126.72, 127.03, 128.38, 128.82, 129.07, 129.15, 132.18, 132.57, 133.57, 144.43, 145.88, 164.32; HRMS (EI) calcd for $C_{23}H_{18}N_2O_4$ 386.1267, found 386.1266.



3k

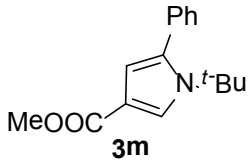
Ethyl 5-butyl-1-(4-nitrophenyl)-1*H*-pyrrole-3-carboxylate (3k) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the

title product **3k** in 65 % (62 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 0.85 (t, *J* = 7.2 Hz, 3H), 1.25-1.33 (m, 2H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.47-1.53 (m, 2H), 2.53 (t, *J* = 7.2 Hz, 2H), 4.30 (q, *J* = 7.2 Hz, 2H), 6.54 (m, 1H), 7.39 (d, *J* = 2 Hz, 1H), 7.49-7.51 (m, 2H), 8.36-8.38 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 13.44, 14.15, 21.94, 26.15, 30.61, 59.84, 109.39, 117.59, 125.17, 126.33, 126.55, 135.48, 144.99, 147.09, 164.95; HRMS (EI) calcd for $C_{17}H_{20}N_2O_4$ 316.1423, found 316.1425.



3l

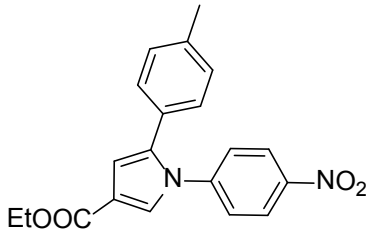
Ethyl 1-(4-nitrophenyl)-5-phenethyl-1*H*-pyrrole-3-carboxylate (3l) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3l** in 74 % (81 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.36 (t, *J* = 7.2 Hz, 3H), 2.84 (brs, , 4H), 4.31 (q, *J* = 6.8 Hz, 2H), 6.64 (s, 1H), 7.01-7.03 (m, 2H), 7.18-7.26 (m, 3H), 7.31-7.37 (m, 3H), 8.27-8.30 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.13, 28.40, 35.33, 59.89, 109.71, 117.67, 125.08, 126.45, 126.53, 126.65, 128.51, 128.71, 134.57, 140.81, 144.68, 147.08, 164.89; HRMS (EI) calcd for $C_{21}H_{20}N_2O_4$ 364.1423, found 364.1421.



3m

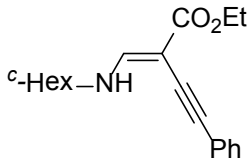
Methyl 1-*tert*-butyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3m) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3m** in 78 % (60 mg) isolated yield as a yellow solid. M.p. 105-106°C. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.43 (s, 9H), 3.80 (s, 3H), 6.43 (s, 1H), 7.36-3.38 (m, 5H), 7.56 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 31.50,

50.89, 58.23, 112.94, 113.12, 124.54, 127.59, 128.15, 131.90, 135.21, 135.91, 165.65; HRMS (EI) calcd for $C_{16}H_{19}NO_2$ 257.1416, found 257.1418.



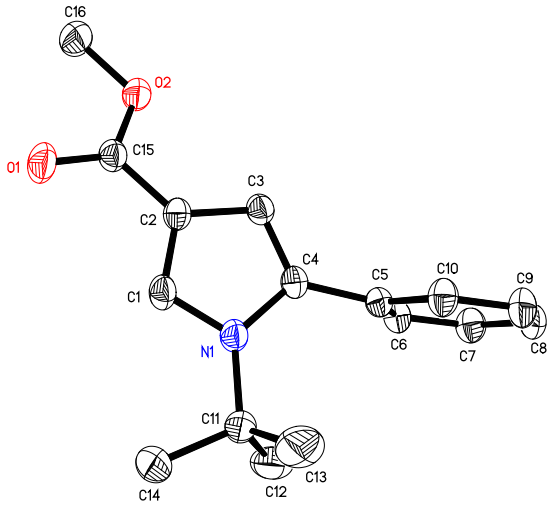
3n

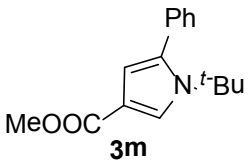
Ethyl 1-(4-nitrophenyl)-5-*p*-tolyl-1*H*-pyrrole-3-carboxylate (3n) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **3n** in 90 % (95 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.37 (t, *J* = 7.2 Hz, 3H), 2.33 (s, 3H), 4.33 (q, *J* = 7.6 Hz, 2H), 6.81-6.83 (m, 1H), 6.98-7.01 (m, 2H), 7.06-7.09 (m, 2H), 7.26-7.32 (m, 2H), 7.58 (s, 1H), 8.19-8.22 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.44, 21.15, 60.13, 112.00, 118.38, 124.74, 125.75, 127.77, 128.22, 128.50, 129.29, 135.04, 137.69, 144.68, 146.21, 164.30; HRMS (EI) calcd for $C_{20}H_{18}N_2O_4$ 350.1267, found 350.1263.



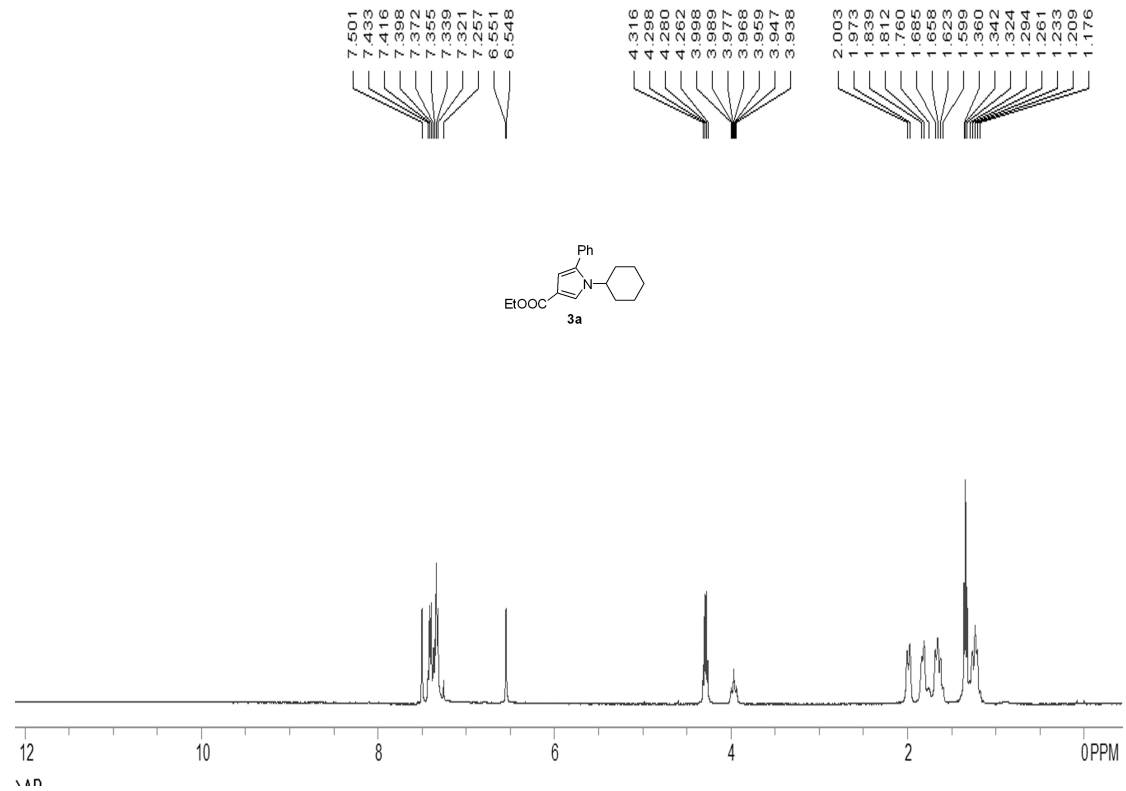
4

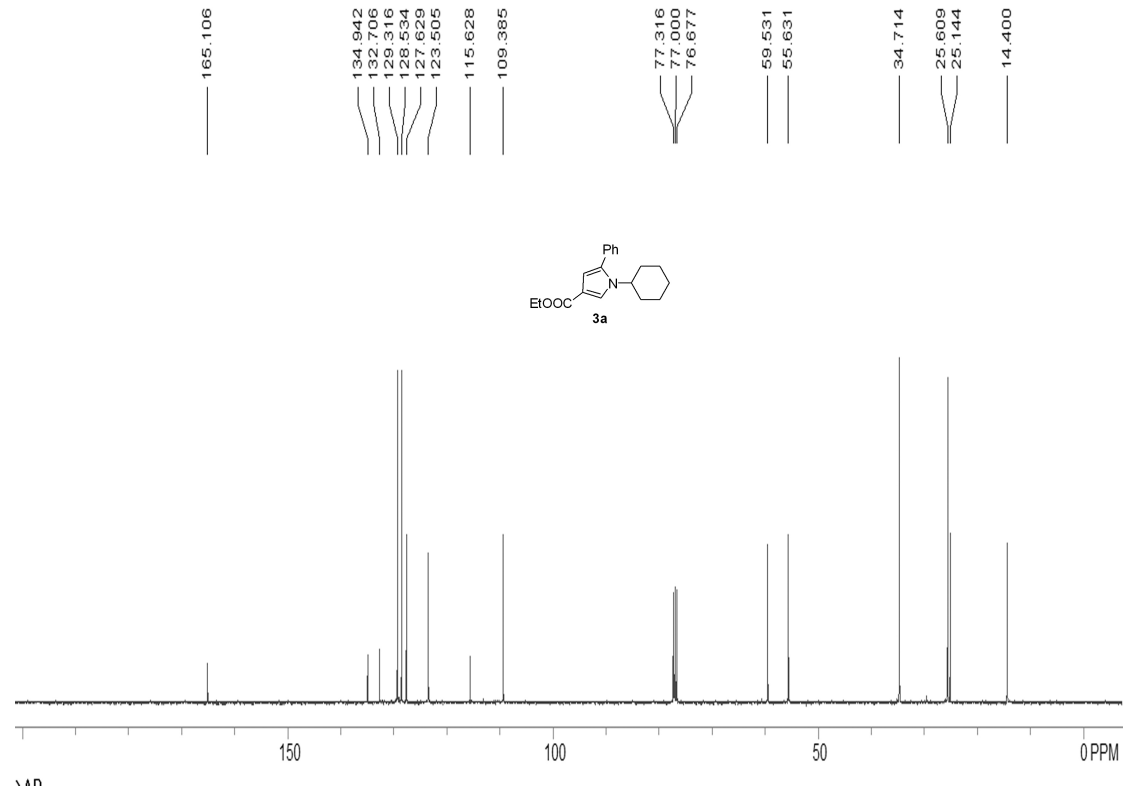
(*E*)-Ethyl 2-((cyclohexylamino)methylene)-4-phenylbut-3-ynoate (4) Column chromatography on silica gel (eluent: n-hexane / ethyl acetate = 50:1) afforded the title product **4** in 82 % (73 mg) isolated yield as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 1.18-1.25 (m, 8H), 1.54-1.57 (m, 1H), 1.69-1.75 (m, 2H), 1.89-1.90 (m, 2H), 3.14 (s, br, 1H), 4.14 (q, *J* = 6.8 Hz, 2H), 5.38-5.43 (m, 1H), 7.19-7.25 (m, 3H), 7.37-7.39 (m, 2H), 7.76 (d, *J* = 14.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$, Me_4Si) δ 14.43, 24.47, 24.99, 34.05, 56.54, 59.88, 82.43, 82.94, 96.89, 124.09, 127.47, 128.22, 131.09, 152.26, 167.54; HRMS (ESI) calcd for $C_{19}H_{24}NO_2$ ($M+H^+$) 298.1807, found 298.1803.

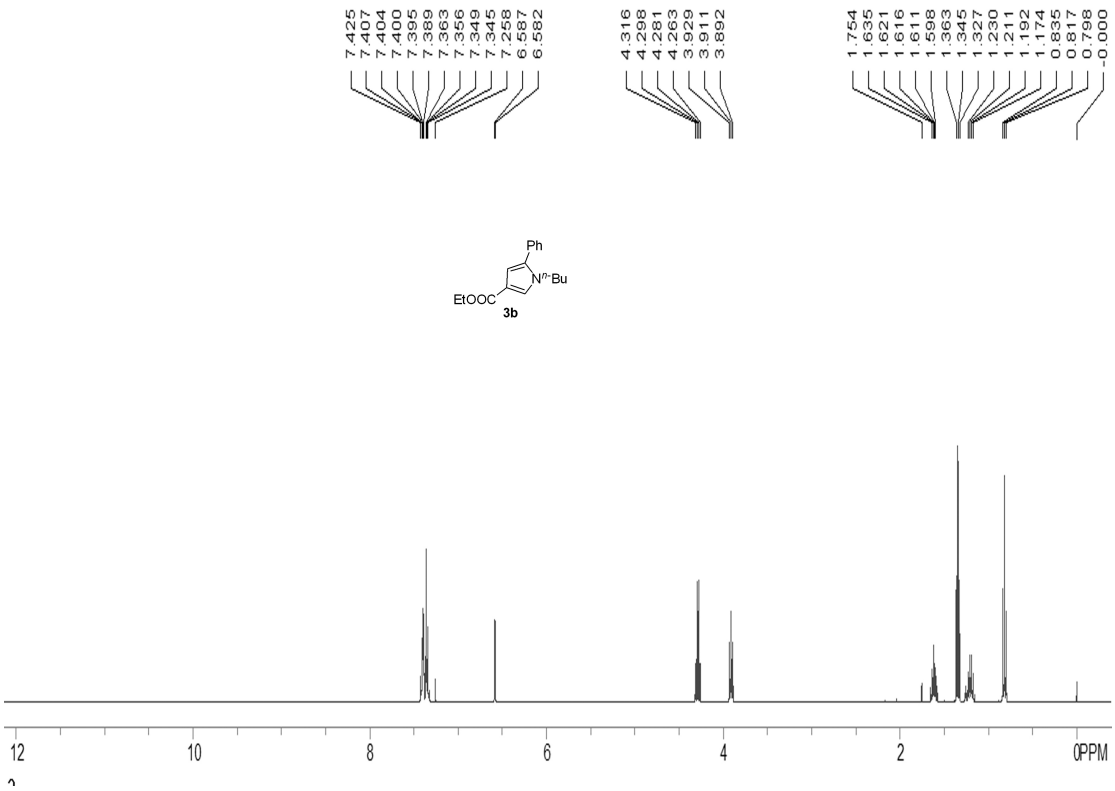


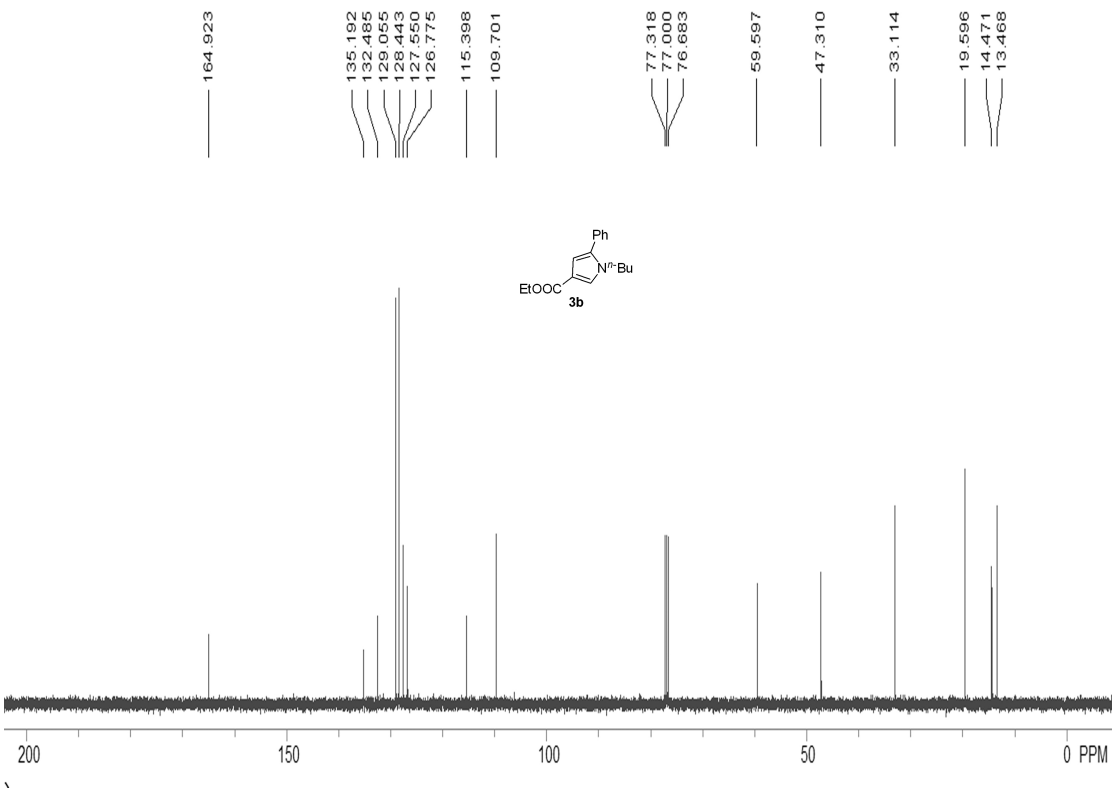


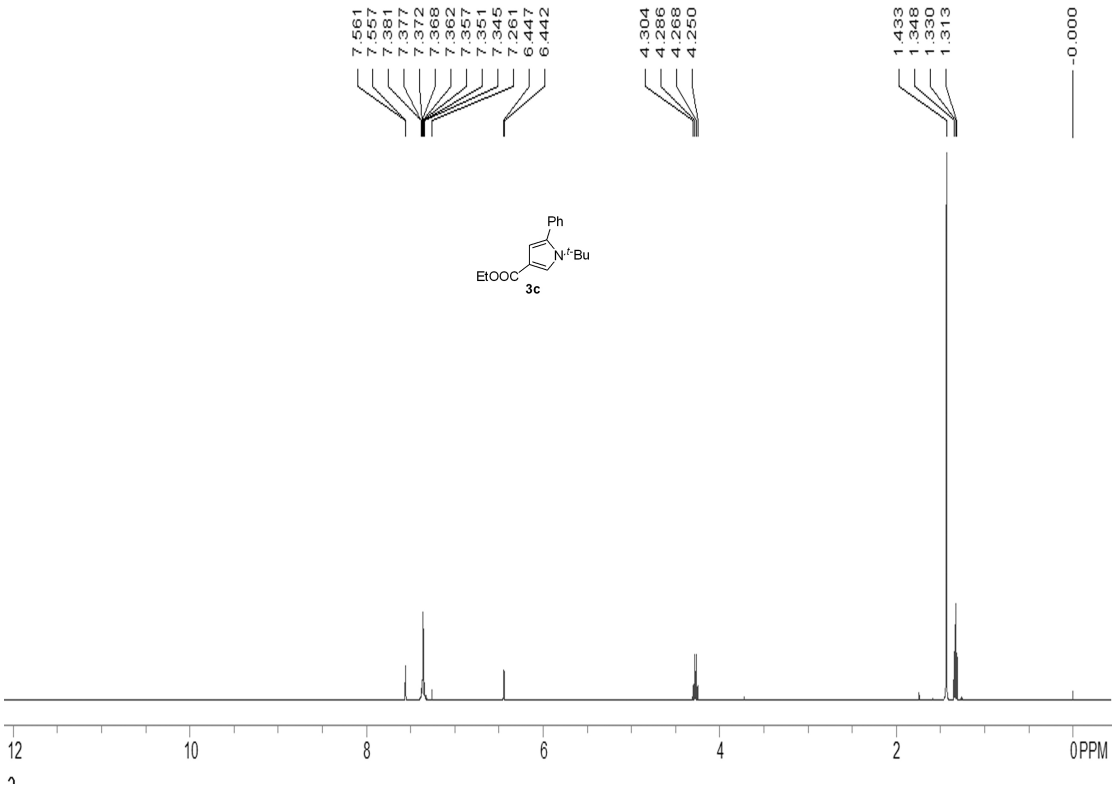
3m

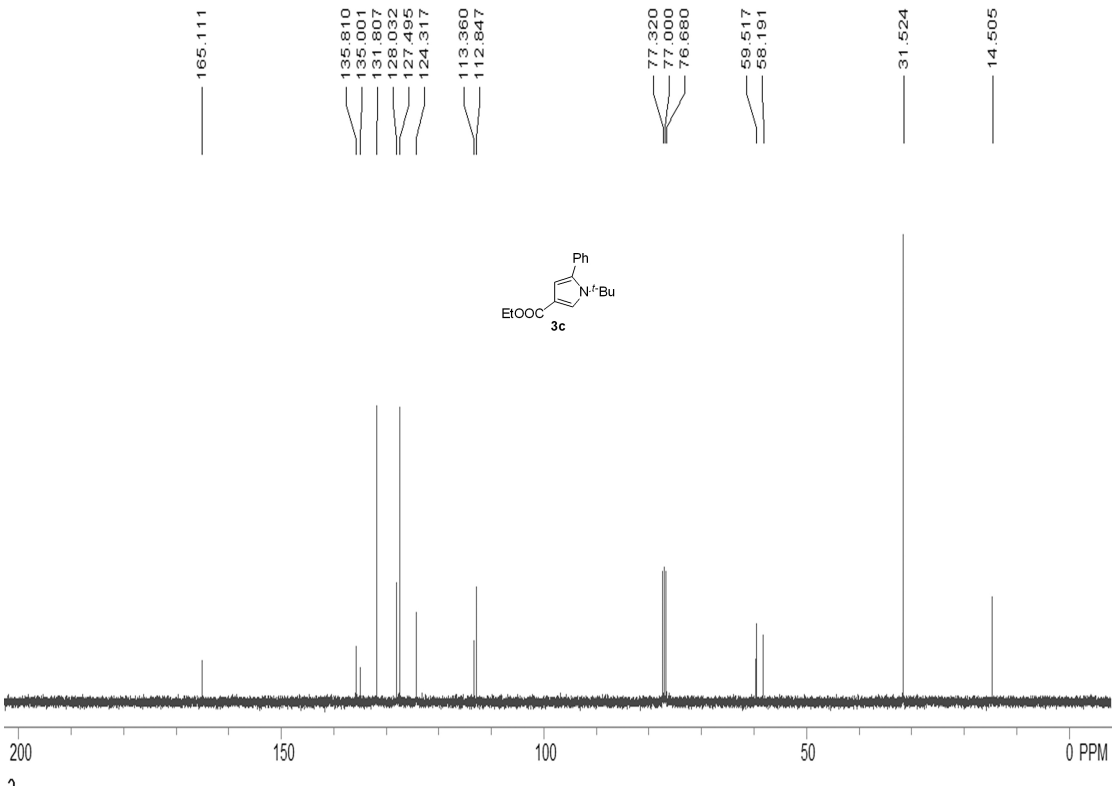

7.501
7.433
7.416
7.398
7.372
7.355
7.339
7.321
7.257
6.551
6.548
4.316
4.298
4.280
4.262
3.998
3.989
3.977
3.968
3.959
3.947
3.938
2.003
1.973
1.839
1.812
1.760
1.685
1.658
1.623
1.599
1.360
1.342
1.324
1.294
1.261
1.233
1.209
1.176
Ph
N
EtOOC
3a
12
10
8
6
4
2
0 PPM

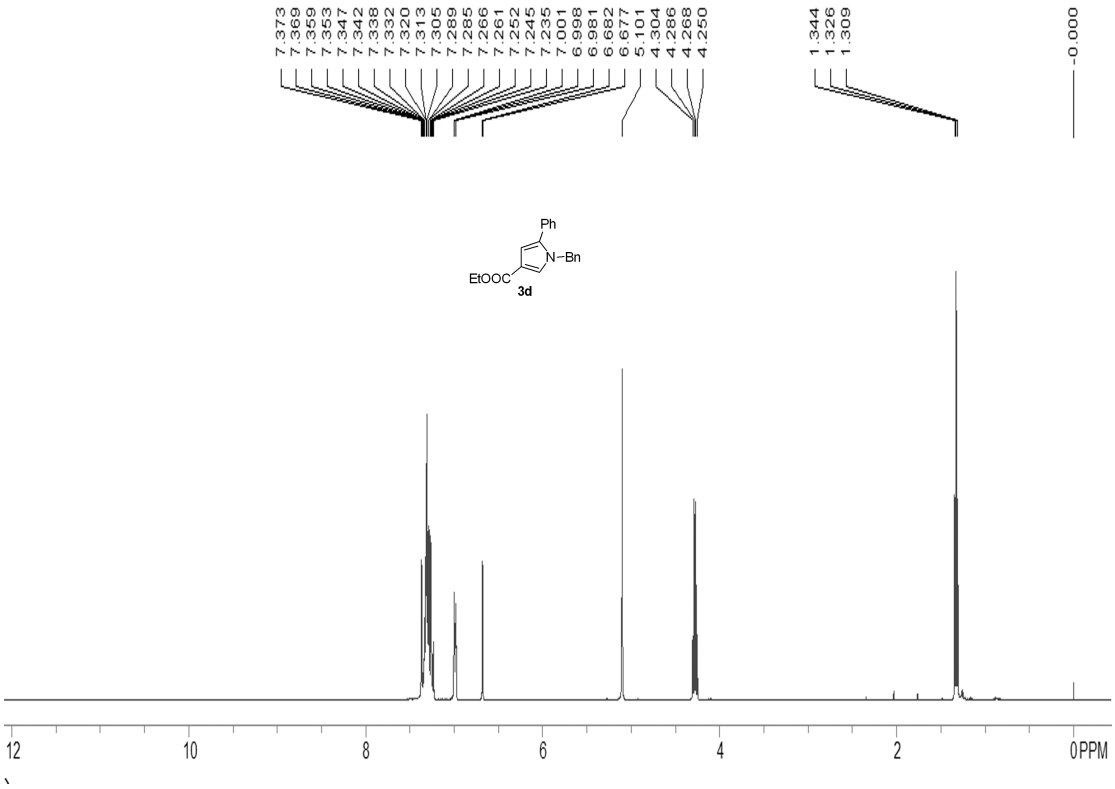

165.106
134.942
132.706
129.316
128.534
127.629
123.505
115.628
109.385
77.316
77.000
76.677
59.531
55.631
34.714
25.609
25.144
14.400
Ph
N
EtOOC
3a
150
100
50
0 PPM

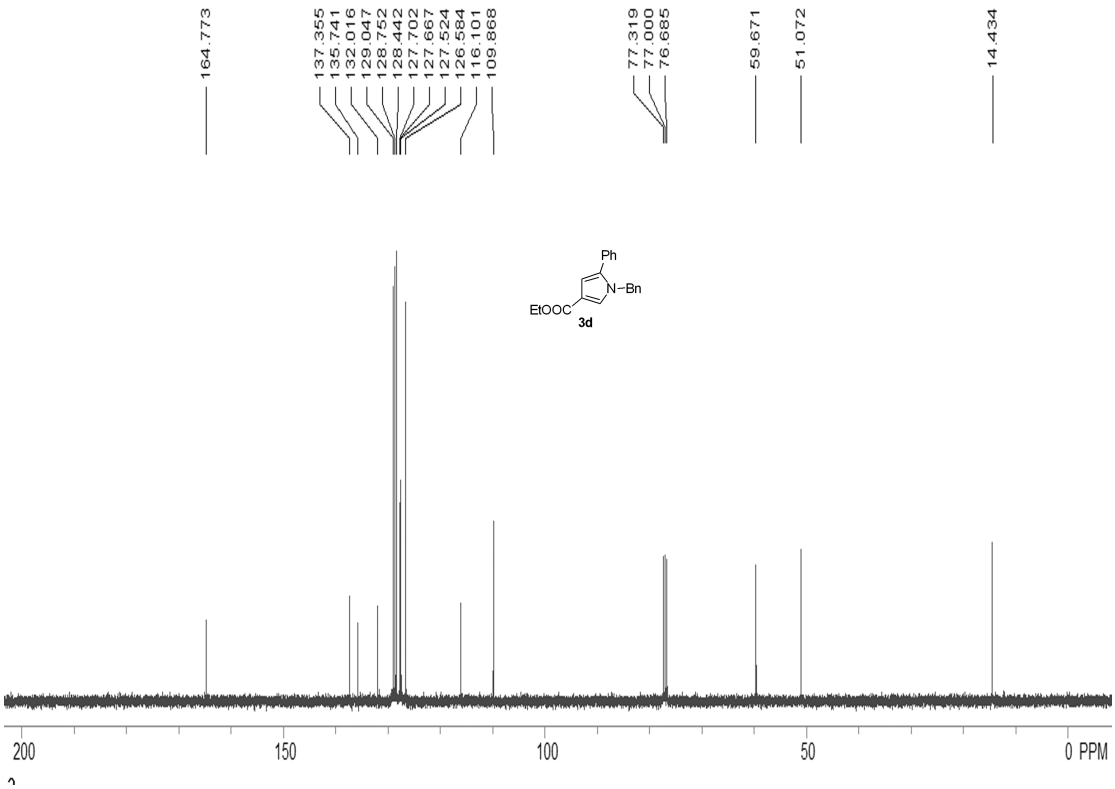

7.425
7.407
7.404
7.400
7.395
7.389
7.363
7.356
7.349
7.345
7.258
6.587
6.582
4.316
4.298
4.281
4.263
3.929
3.911
3.892
1.754
1.635
1.621
1.616
1.611
1.598
1.363
1.345
1.327
1.230
1.211
1.192
1.174
0.835
0.817
0.798
-0.000
Ph
N n-Bu
EtOOC
3b
12
10
8
6
4
2
0PPM

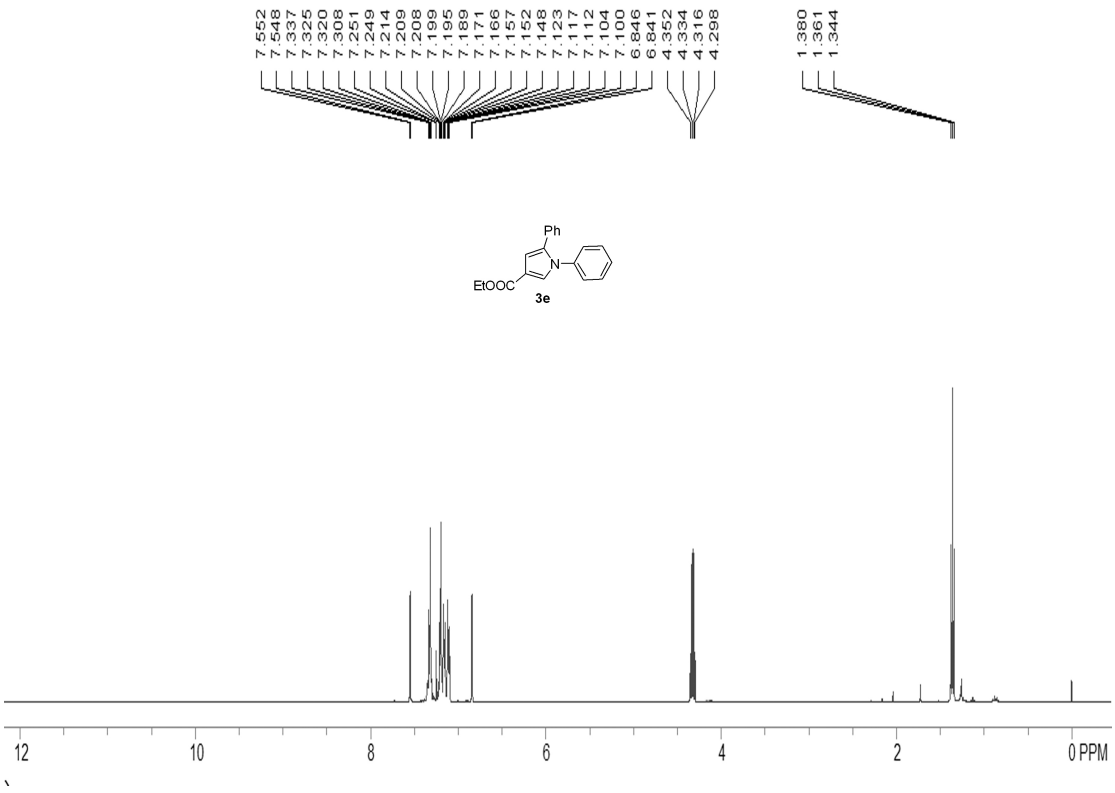

164.923
135.192
132.485
129.055
128.443
127.550
126.775
115.398
109.701
77.318
77.000
76.683
59.597
47.310
33.114
19.596
14.471
13.468
Ph
N n-Bu
EtOOC
3b
200
150
100
50
0 PPM

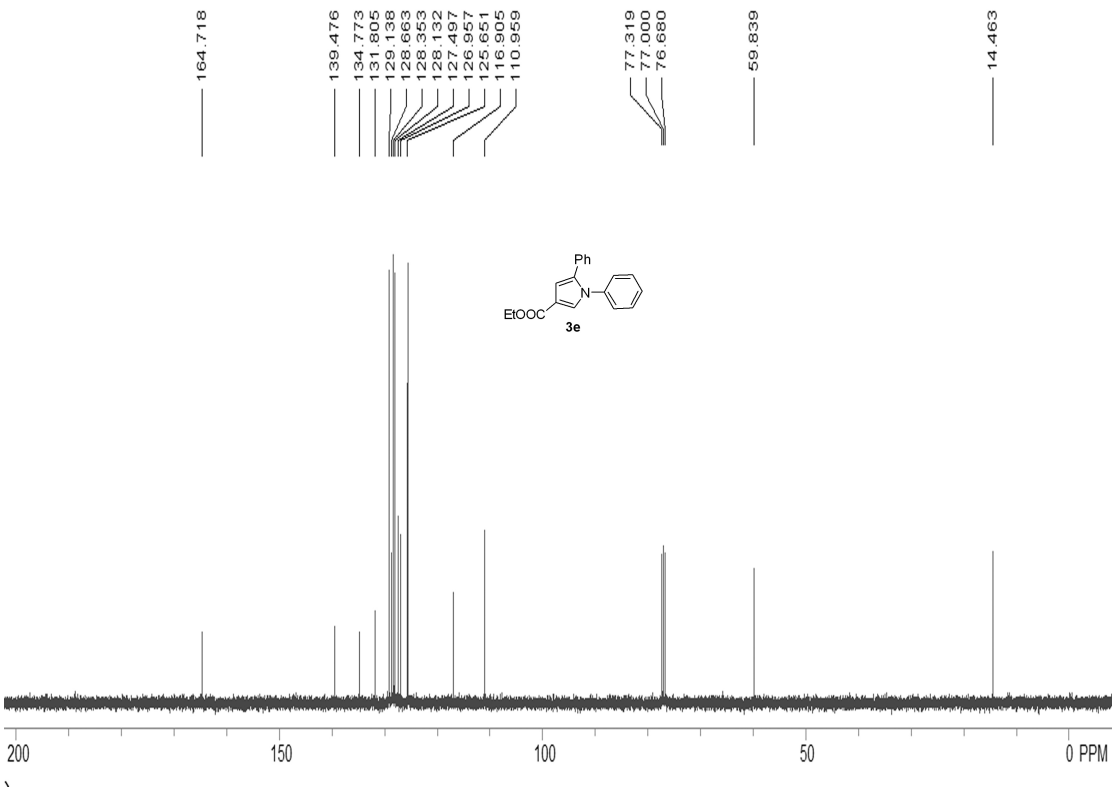

7.561
7.557
7.381
7.377
7.372
7.368
7.362
7.357
7.351
7.345
7.261
6.447
6.442
4.304
4.286
4.268
4.250
1.433
1.348
1.330
1.313
0.000
Ph
N-t-Bu
EtOOC
3c
12
10
8
6
4
2
0 PPM

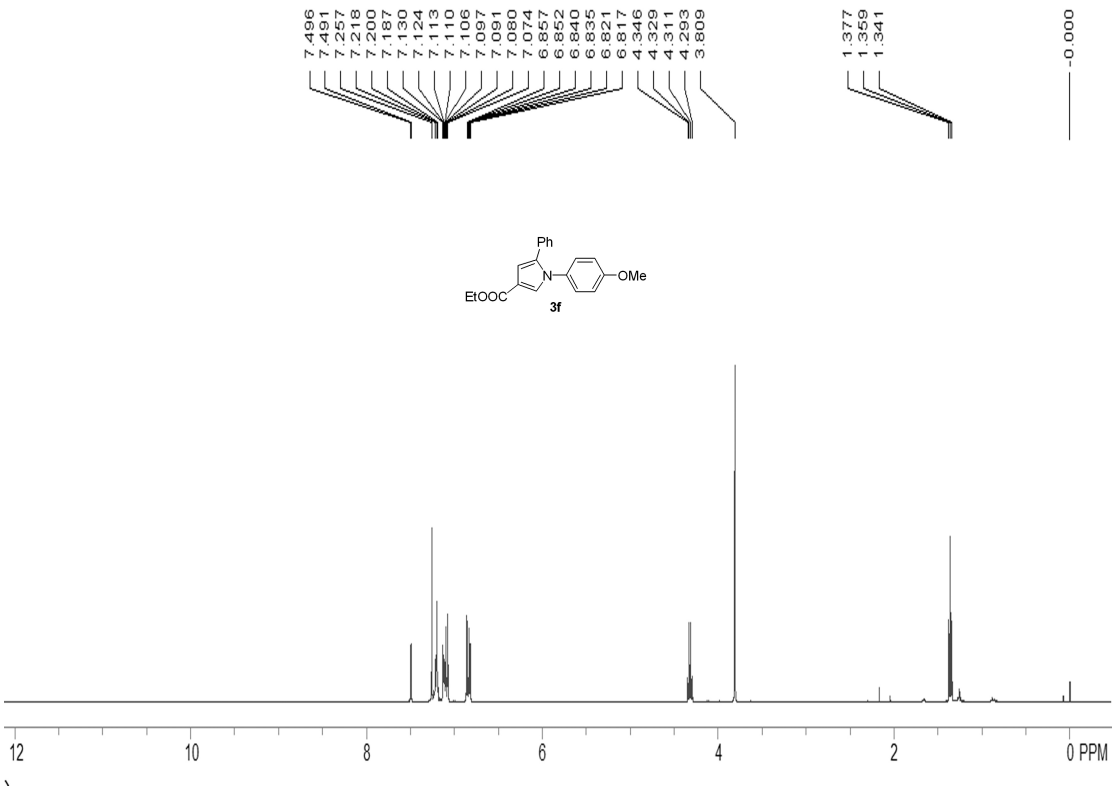

165.111
135.810
135.001
131.807
128.032
127.495
124.317
113.360
112.847
77.320
77.000
76.680
59.517
58.191
31.524
14.505
Ph
N-t-Bu
EtOOC
3c
200
150
100
50
0 PPM

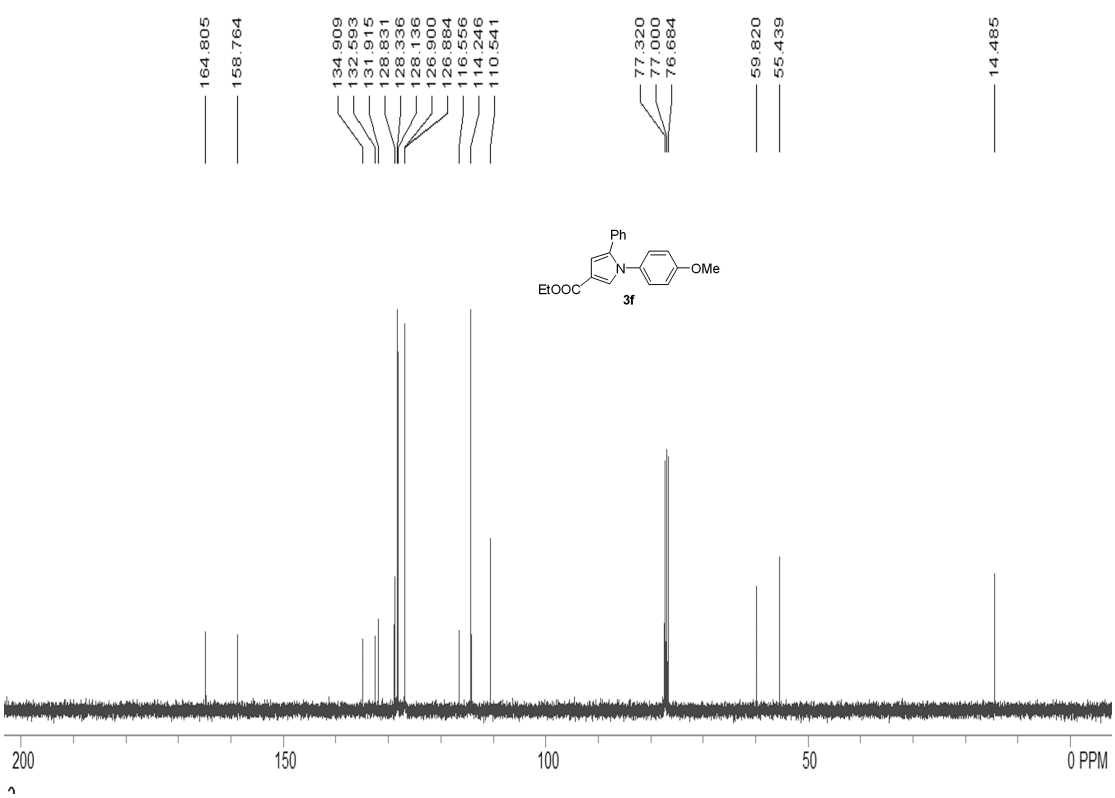

7.373
7.369
7.359
7.353
7.347
7.342
7.338
7.332
7.320
7.313
7.305
7.289
7.285
7.266
7.261
7.252
7.245
7.235
7.001
6.998
6.981
6.682
6.677
5.101
4.304
4.286
4.268
4.250
1.344
1.326
1.309
0.000
Ph
N–Bn
EtOOC
3d
12
10
8
6
4
2
0 PPM

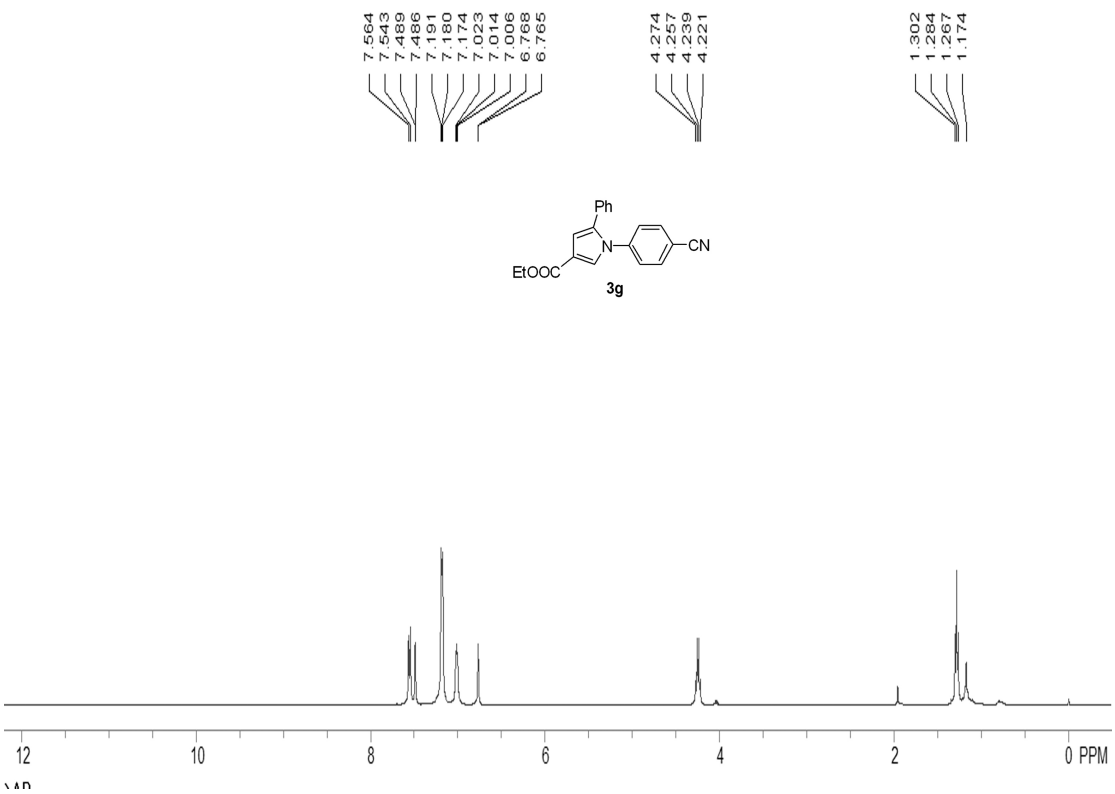

164.773
137.355
135.741
132.016
129.047
128.752
128.442
127.702
127.667
127.524
126.584
116.101
109.868
77.319
77.000
76.685
59.671
51.072
14.434
Ph
N–Bn
EtOOC
3d
200
150
100
50
0 PPM

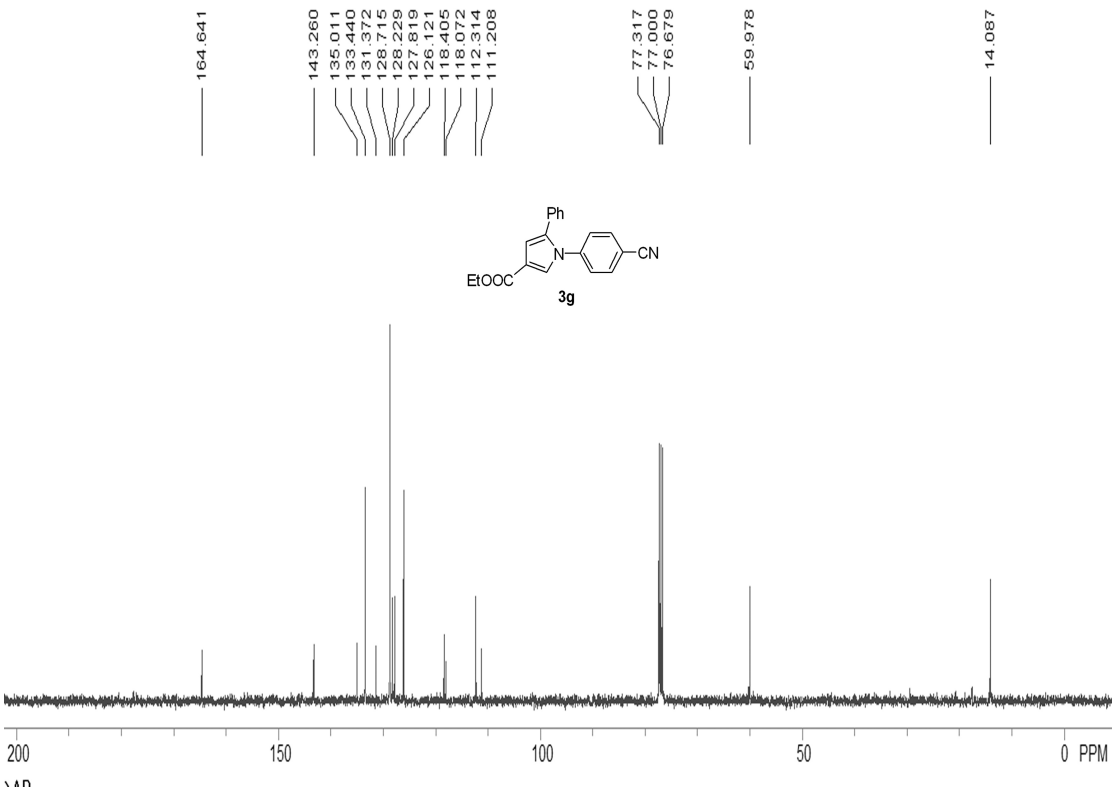

7.552
7.548
7.337
7.325
7.320
7.308
7.251
7.249
7.214
7.209
7.208
7.199
7.195
7.189
7.171
7.166
7.157
7.152
7.148
7.123
7.117
7.112
7.104
7.100
6.846
6.841
4.352
4.334
4.316
4.298
1.380
1.361
1.344
Ph
N
EtOOC
3e
12
10
8
6
4
2
0 PPM

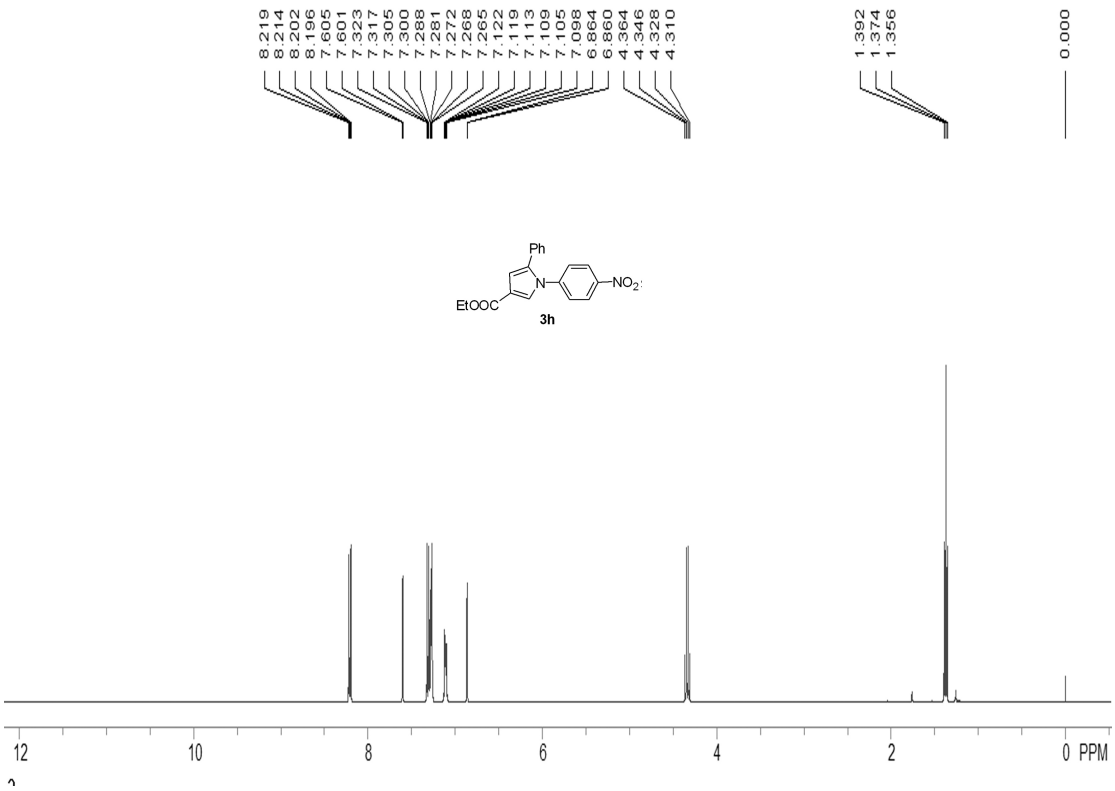

164.718
139.476
134.773
131.805
129.138
128.663
128.353
128.132
127.497
126.957
125.651
116.905
110.959
77.319
77.000
76.680
59.839
14.463
Ph
N
EtOOC
3e
200
150
100
50
0 PPM

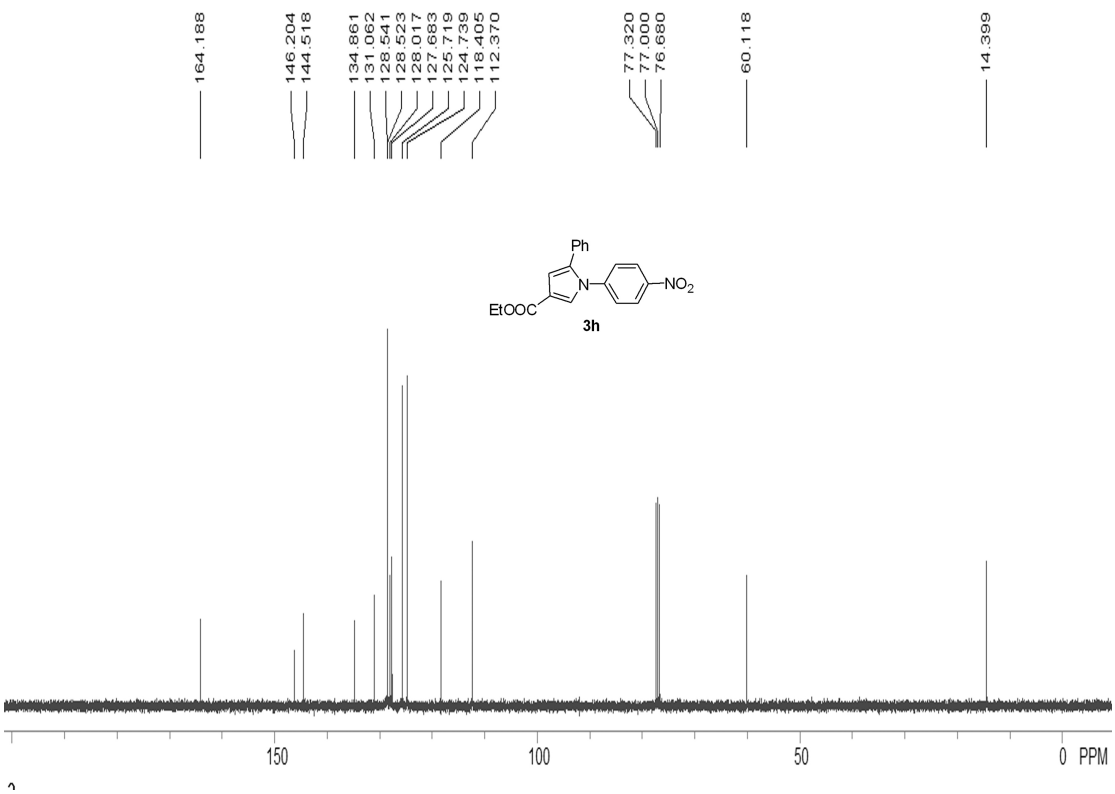


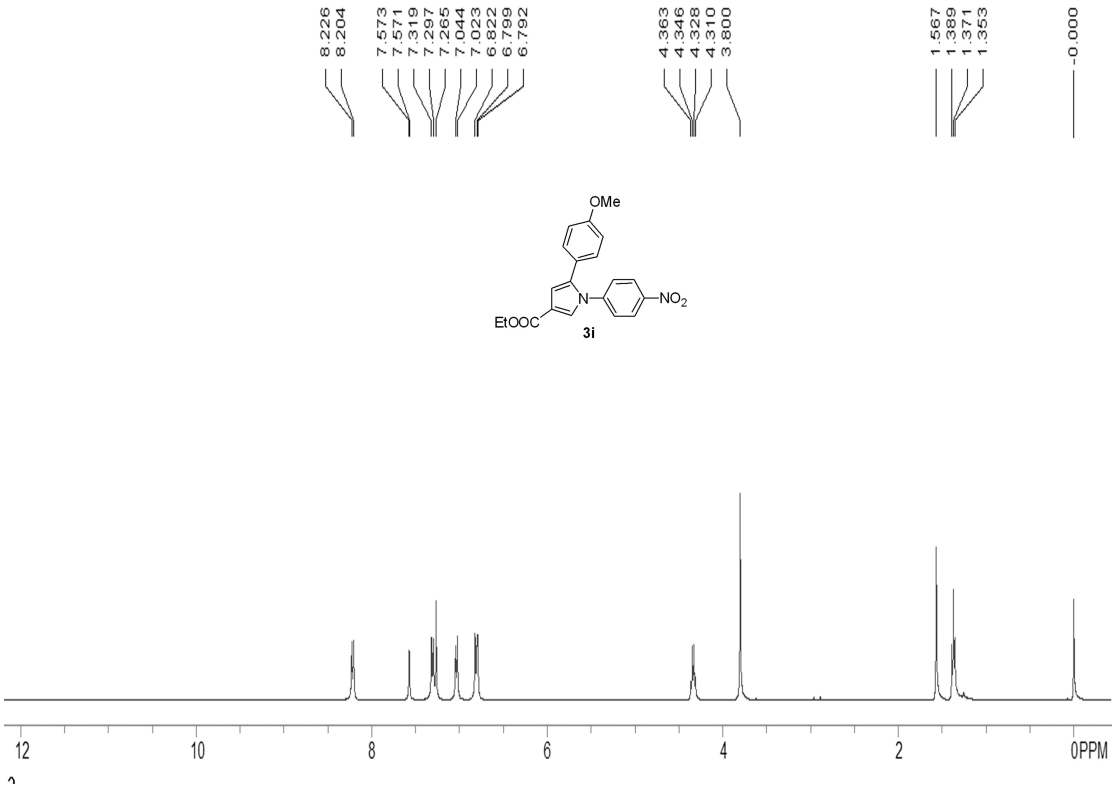


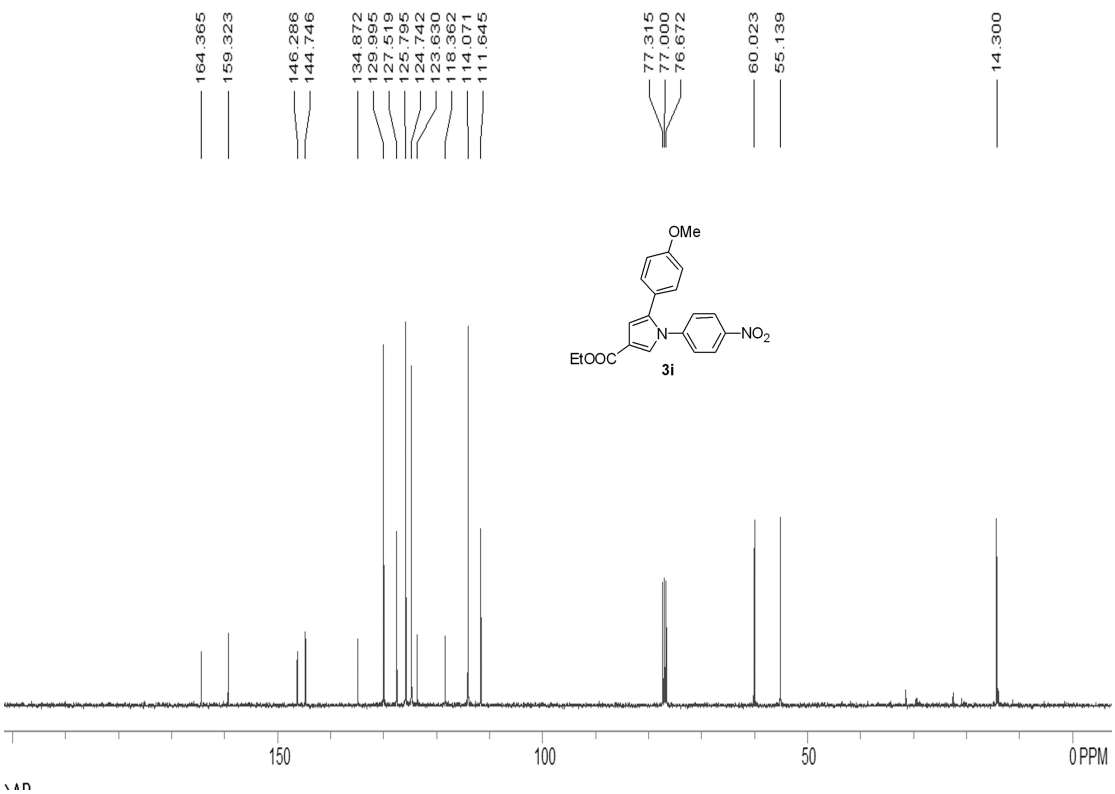

7.564
7.543
7.489
7.486
7.191
7.180
7.174
7.023
7.014
7.006
6.768
6.765
4.274
4.257
4.239
4.221
1.302
1.284
1.267
1.174
Ph
N
CN
EtOOC
3g
12
10
8
6
4
2
0 PPM

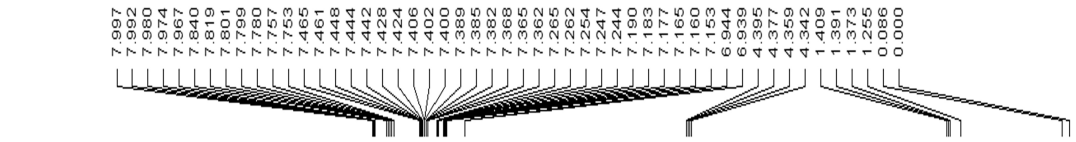

164.641
143.260
135.011
133.440
131.372
128.715
128.229
127.819
126.121
118.405
118.072
112.314
111.208
77.317
77.000
76.679
59.978
14.087
Ph
N
CN
EtOOC
3g
200
150
100
50
0 PPM

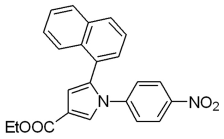

8.219
8.214
8.202
8.196
7.605
7.601
7.323
7.317
7.305
7.300
7.288
7.281
7.272
7.268
7.265
7.122
7.119
7.113
7.109
7.105
7.098
6.864
6.860
4.364
4.346
4.328
4.310
1.392
1.374
1.356
0.000
Ph
N
NO2
EtOOC
3h
12
10
8
6
4
2
0 PPM


164.188
146.204
144.518
134.861
131.062
128.541
128.523
128.017
127.683
125.719
124.739
118.405
112.370
77.320
77.000
76.680
60.118
14.399
Ph
N
NO2
EtOOC
3h
150
100
50
0 PPM

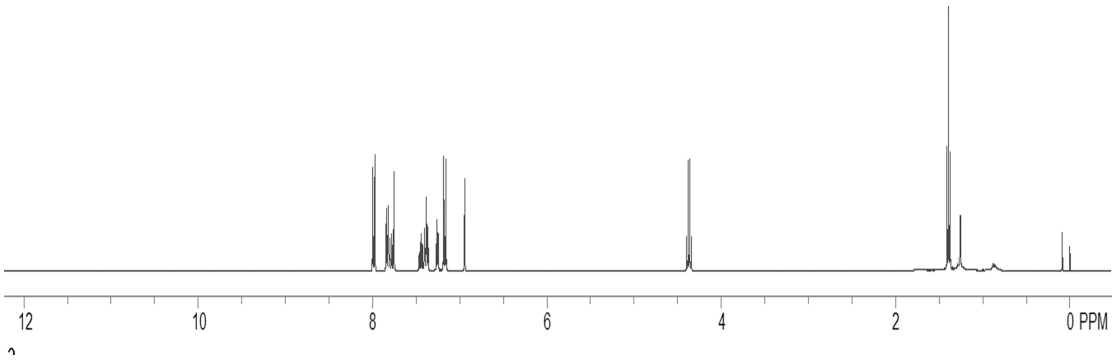

8.226
8.204
7.573
7.571
7.319
7.297
7.265
7.044
7.023
6.822
6.799
6.792
4.363
4.346
4.328
4.310
3.800
1.567
1.389
1.371
1.353
0.000
OMe
NO2
EtOOC
3i
12
10
8
6
4
2
0PPM

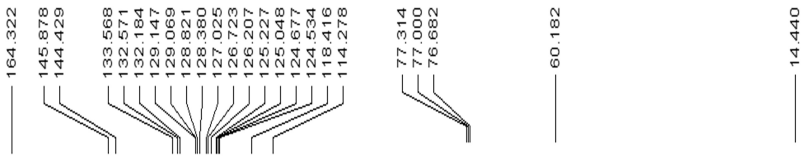

164.365
159.323
146.286
144.746
134.872
129.995
127.519
125.795
124.742
123.630
118.362
114.071
111.645
77.315
77.000
76.672
60.023
55.139
14.300
OMe
NO2
EtOOC
3i
150
100
50
0 PPM

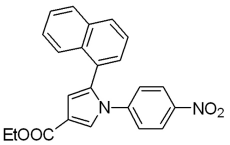

7.997
7.992
7.980
7.974
7.967
7.840
7.819
7.801
7.799
7.780
7.757
7.753
7.465
7.461
7.448
7.444
7.442
7.428
7.424
7.406
7.402
7.400
7.389
7.385
7.382
7.368
7.365
7.362
7.265
7.262
7.254
7.247
7.244
7.190
7.183
7.177
7.165
7.160
7.153
6.944
6.939
4.395
4.377
4.359
4.342
1.409
1.391
1.373
1.255
0.086
0.000


N
NO2
EtOOC

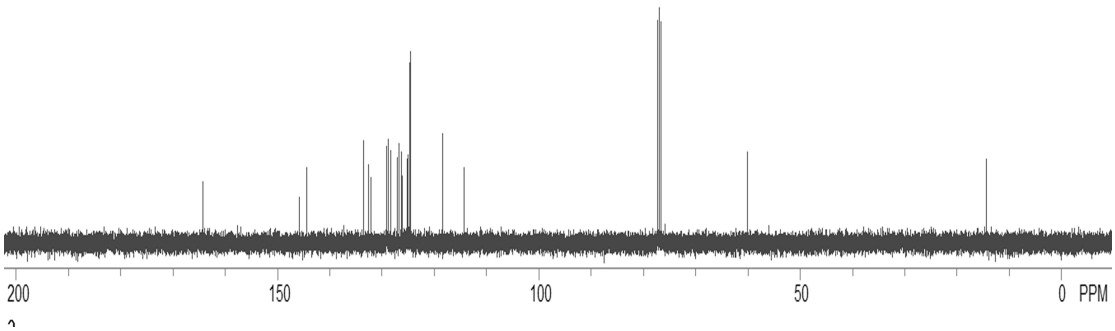
3j

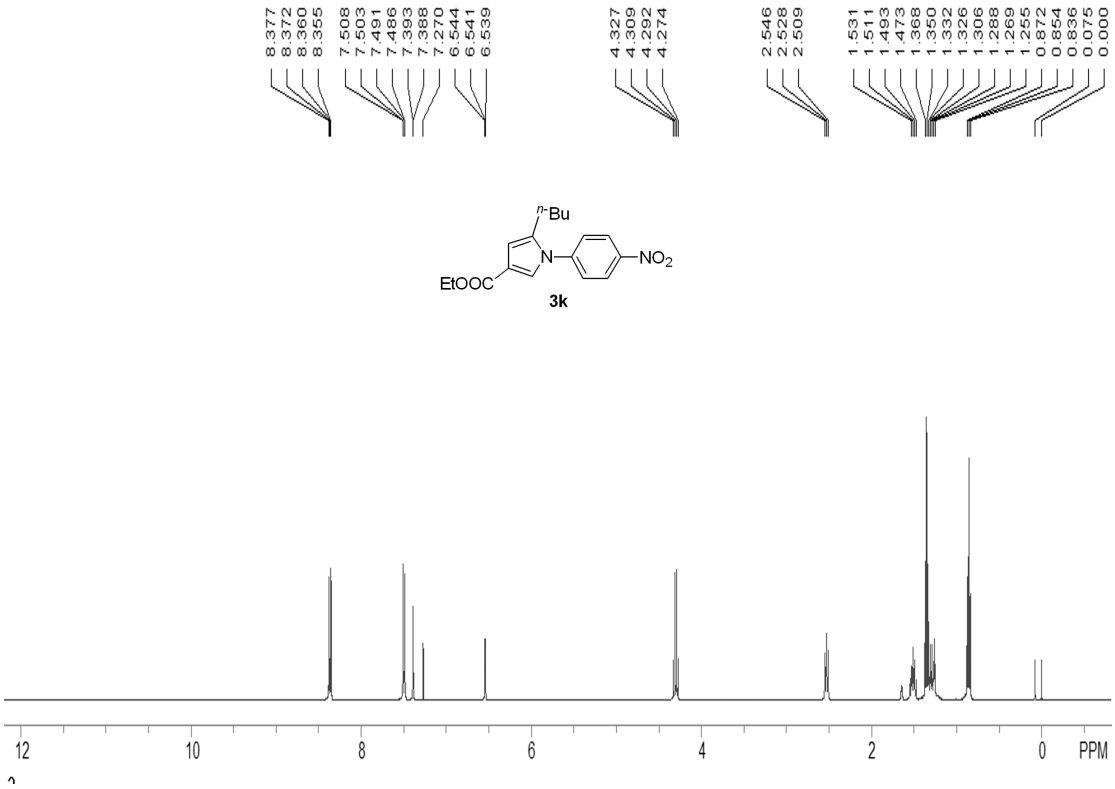

12
10
8
6
4
2
0 PPM

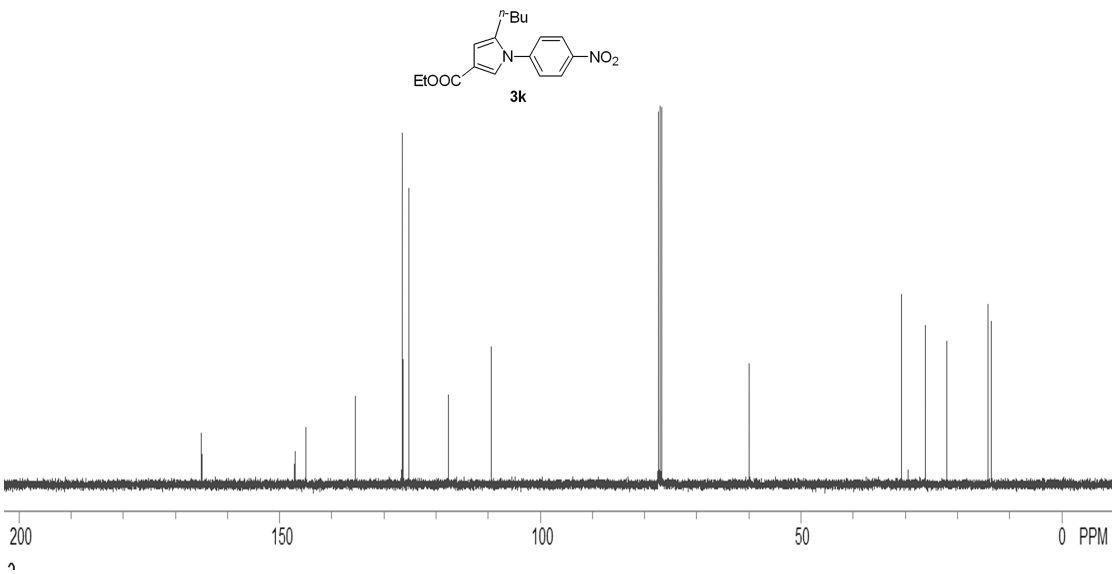

164.322
145.878
144.429
133.568
132.571
132.184
129.147
129.069
128.821
128.380
127.025
126.723
126.207
125.227
125.048
124.677
124.534
118.416
114.278
77.314
77.000
76.682
60.182
14.440

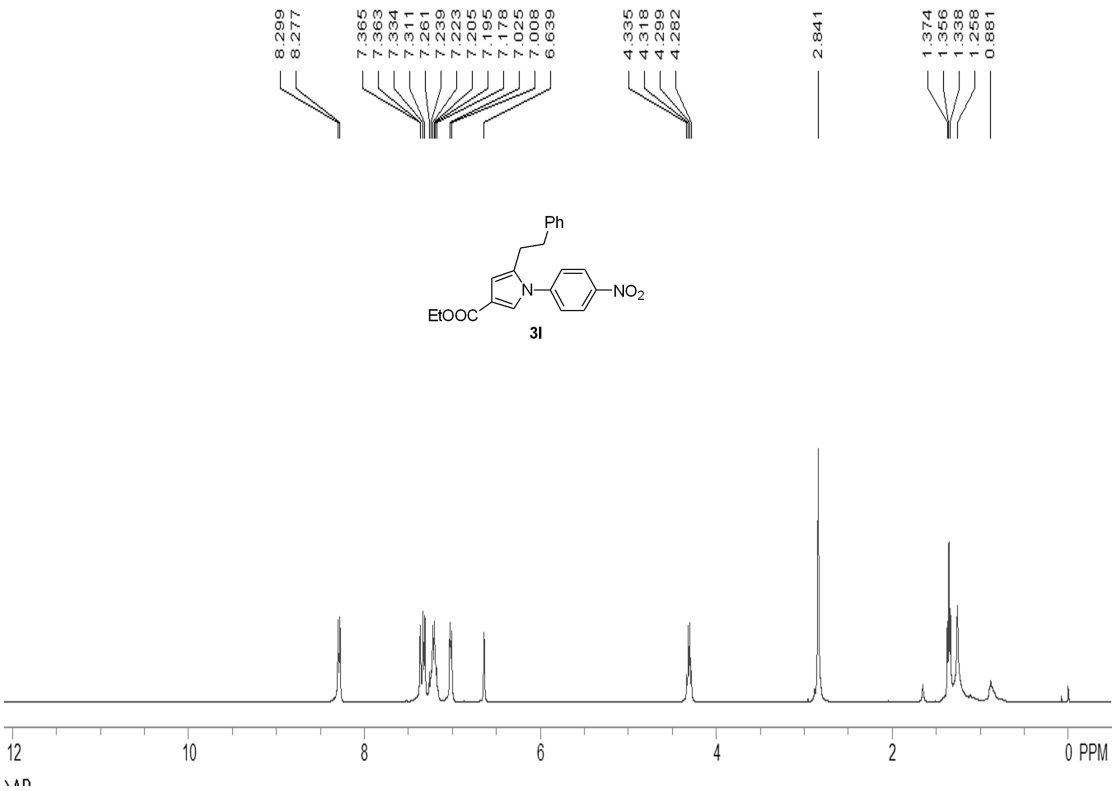

N
NO2
EtOOC

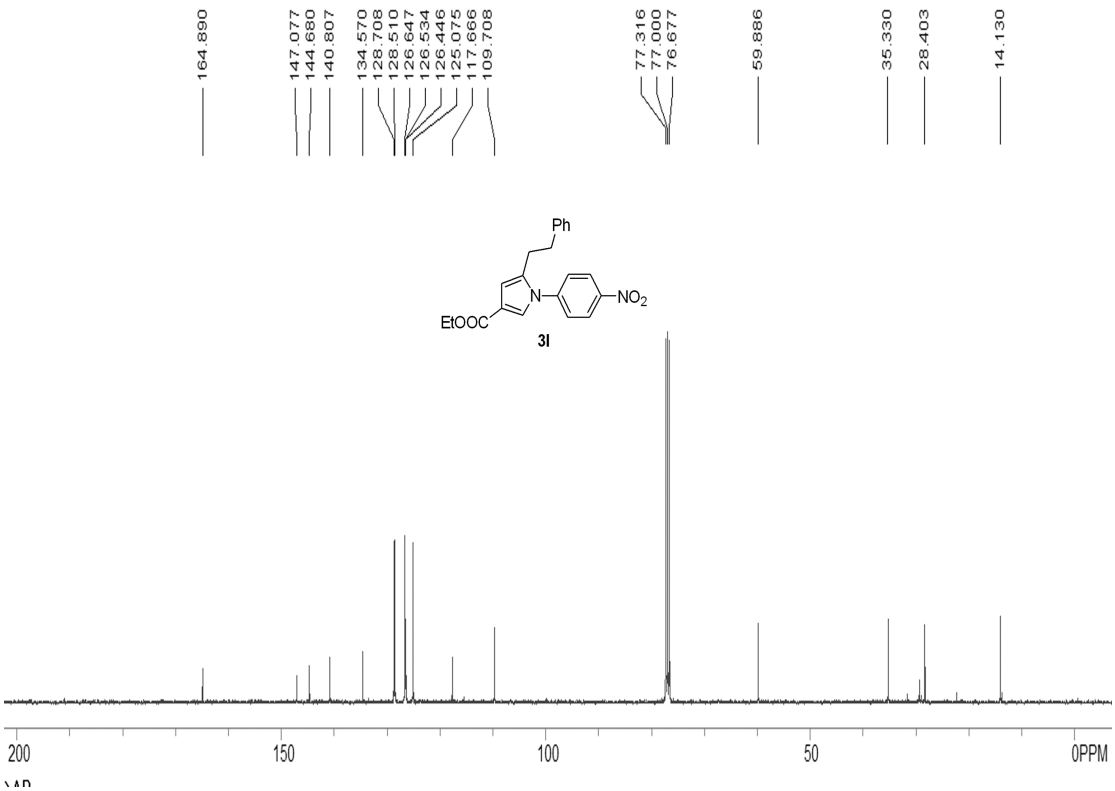
3j

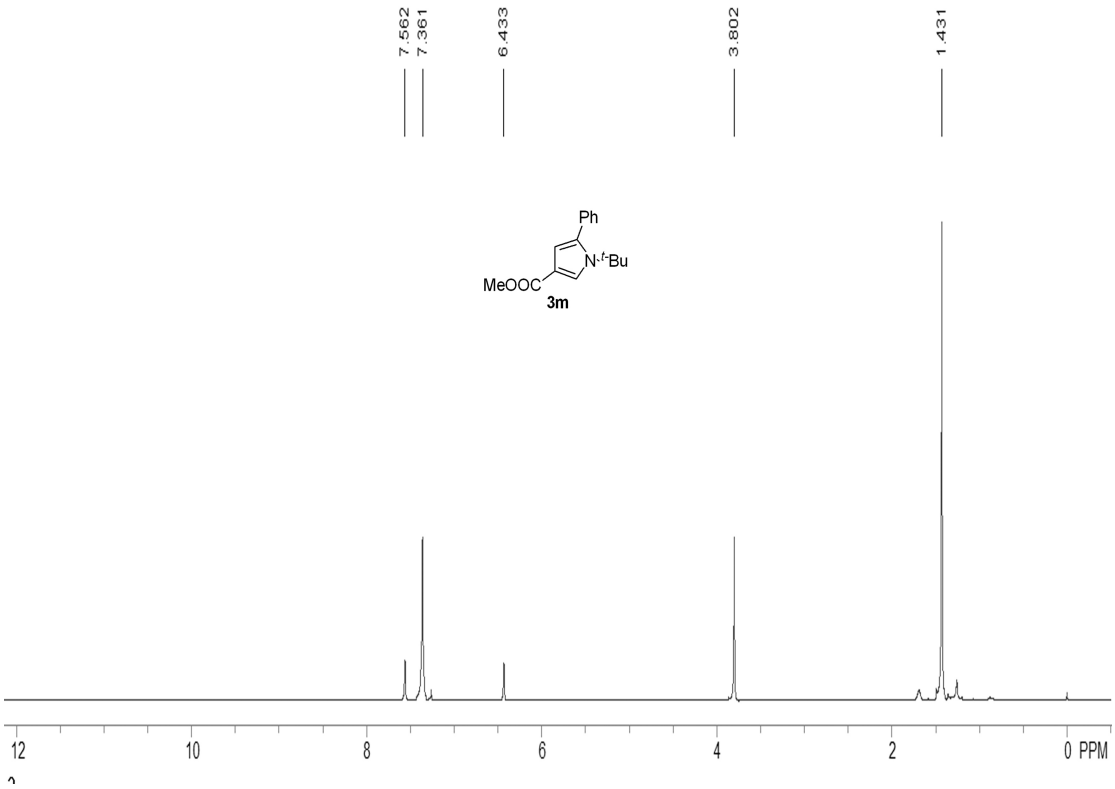

200
150
100
50
0 PPM

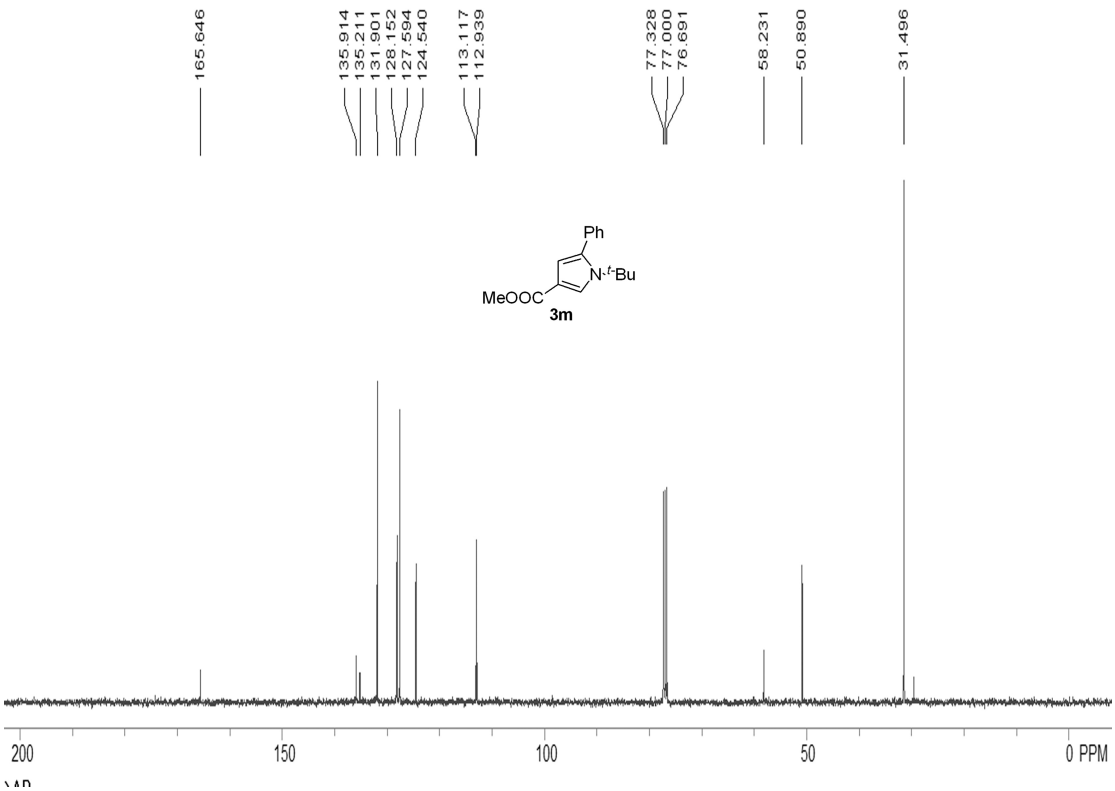

8.377
8.372
8.360
8.355
7.508
7.503
7.491
7.486
7.393
7.388
7.270
6.544
6.541
6.539
4.327
4.309
4.292
4.274
2.546
2.528
2.509
1.531
1.511
1.493
1.473
1.368
1.350
1.332
1.326
1.306
1.288
1.269
1.255
0.872
0.854
0.836
0.075
0.000
n-Bu
N
NO2
EtOOC
3k
12
10
8
6
4
2
0
PPM

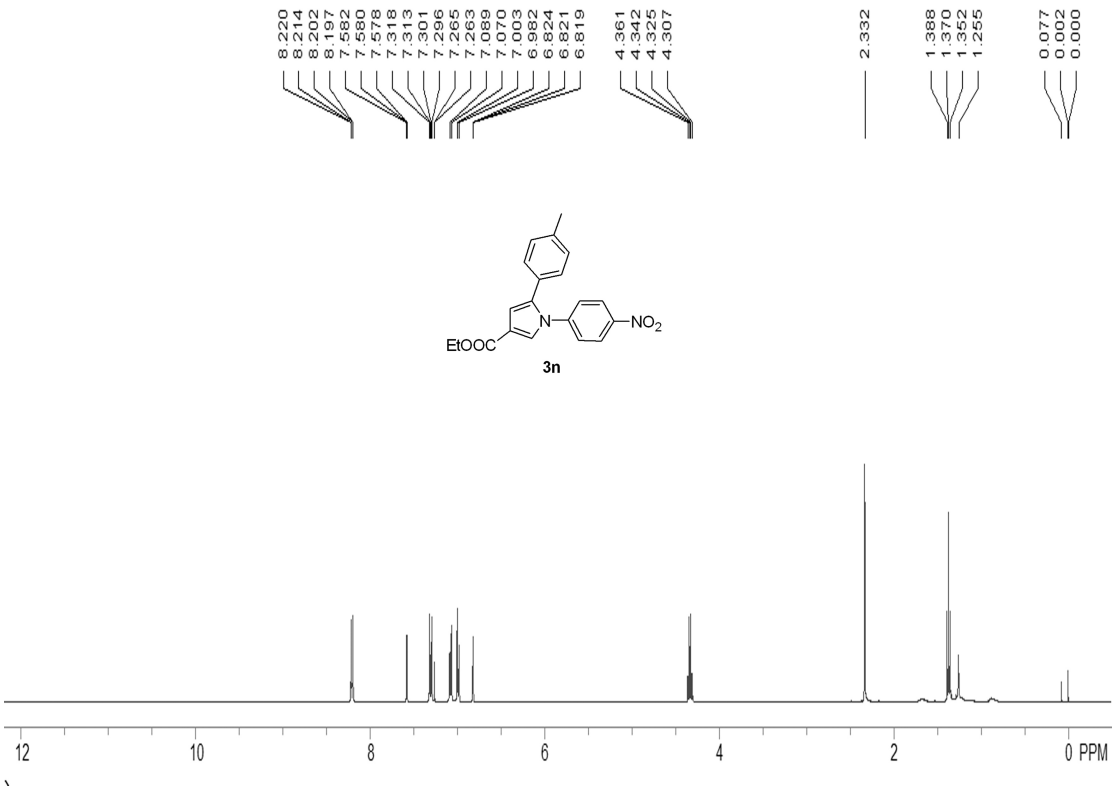

164.946
147.091
144.993
135.480
126.545
126.327
125.168
117.588
109.389
77.323
77.000
76.684
59.840
30.606
26.146
21.939
14.146
13.438
n-Bu
N
NO2
EtOOC
3k
200
150
100
50
0
PPM

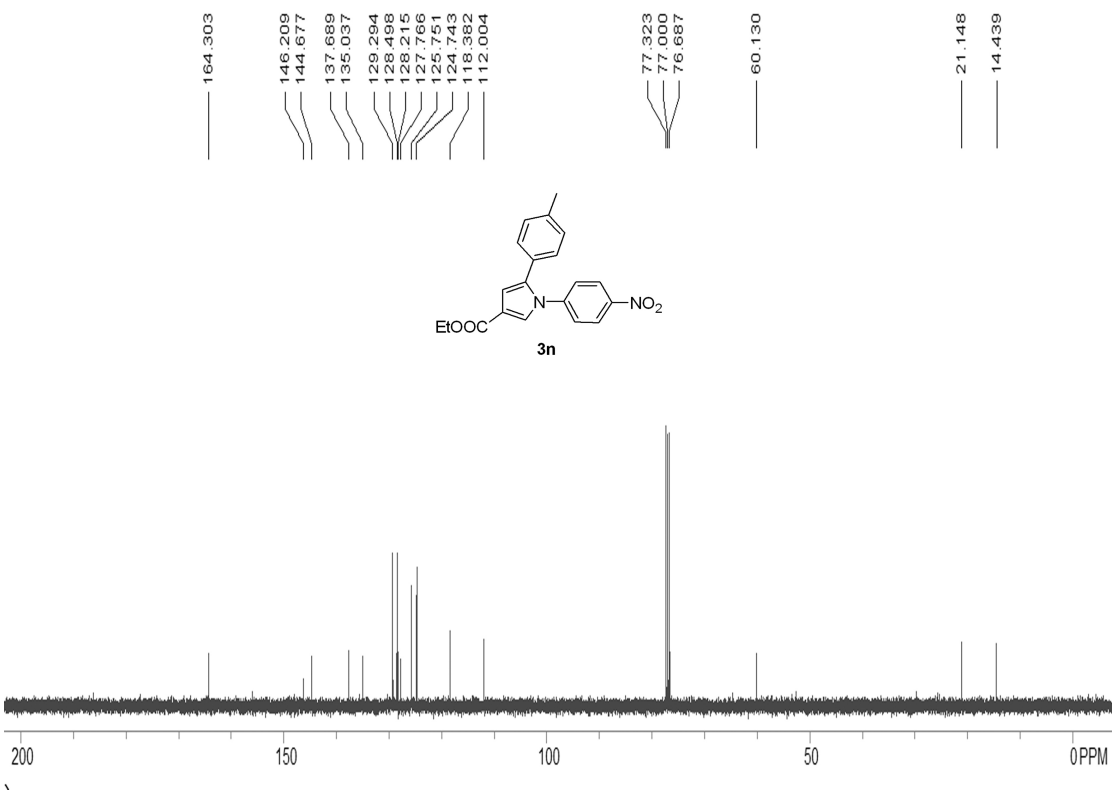

8.299
8.277
7.365
7.363
7.334
7.311
7.261
7.239
7.223
7.205
7.195
7.178
7.025
7.008
6.639
4.335
4.318
4.299
4.282
2.841
1.374
1.356
1.338
1.258
0.881
Ph
N
NO2
EtOOC
3l
12
10
8
6
4
2
0 PPM

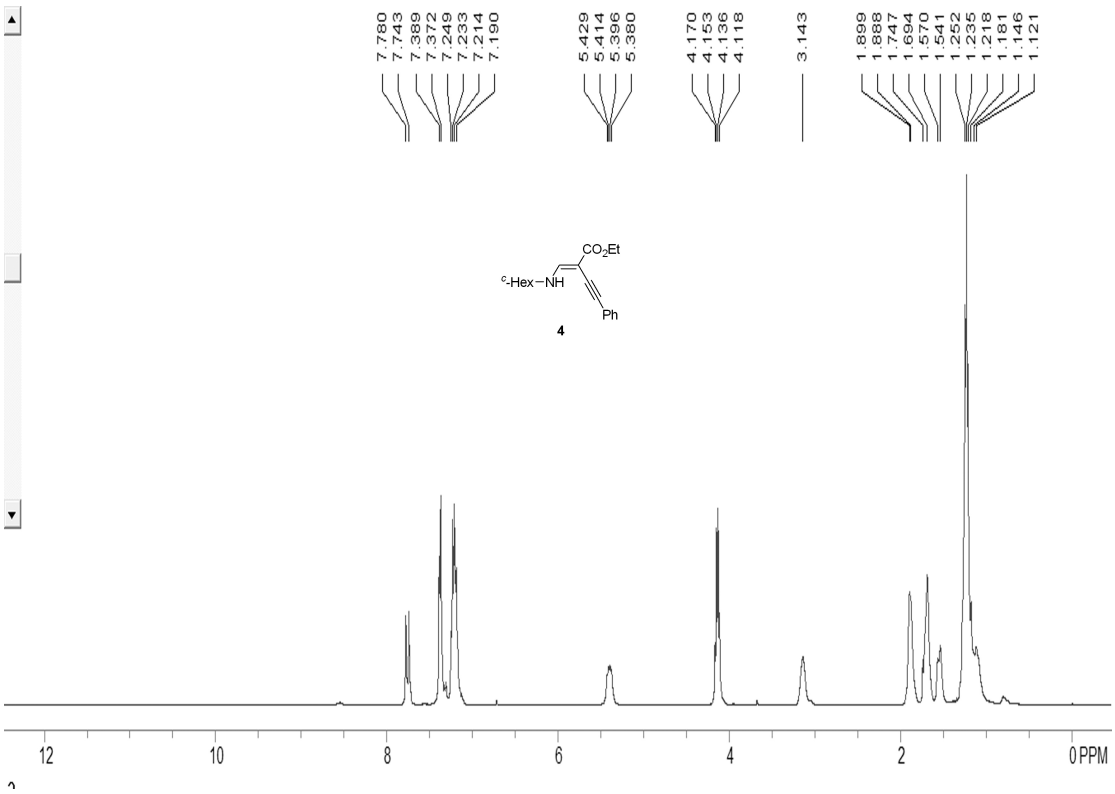

164.890
147.077
144.680
140.807
134.570
128.708
128.510
126.647
126.534
126.446
125.075
117.666
109.708
77.316
77.000
76.677
59.886
35.330
28.403
14.130
Ph
N
NO2
EtOOC
3l
200
150
100
50
0PPM

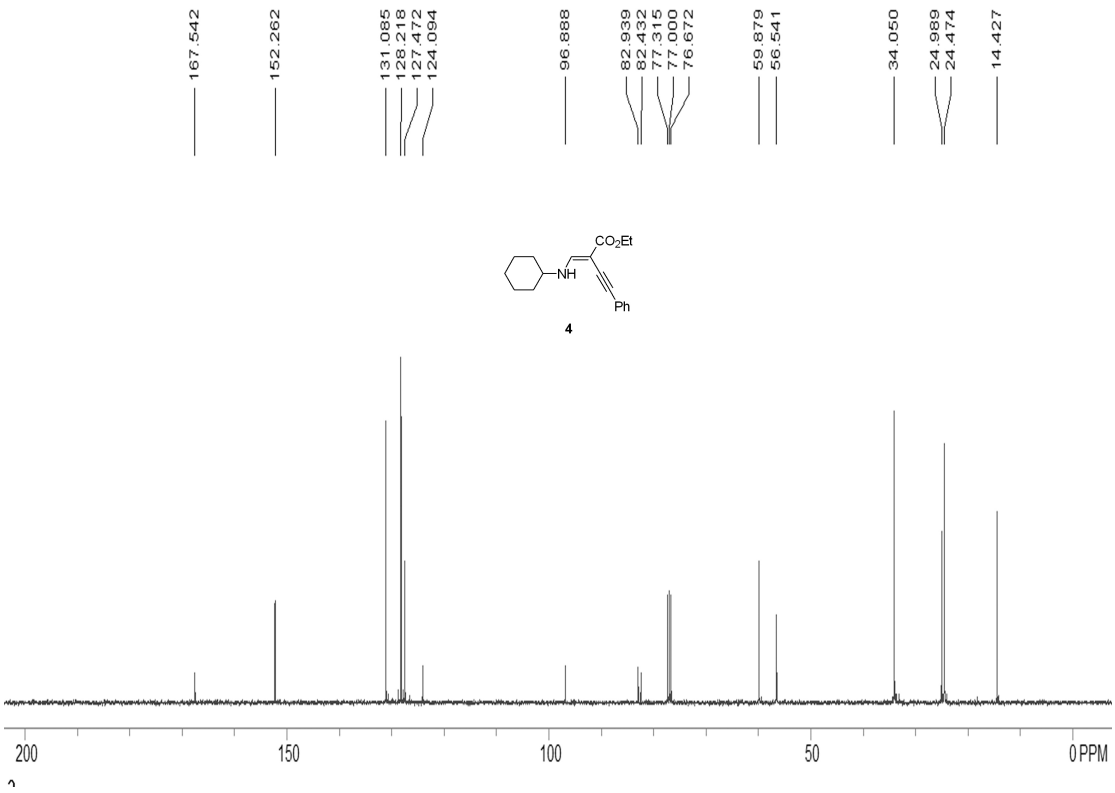

7.562
7.361
6.433
3.802
1.431
Ph
N-t-Bu
MeOOC
3m
12
10
8
6
4
2
0 PPM


165.646
135.914
135.211
131.901
128.152
127.594
124.540
113.117
112.939
77.328
77.000
76.691
58.231
50.890
31.496
Ph
N-t-Bu
MeOOC
3m
200
150
100
50
0 PPM


8.220
8.214
8.202
8.197
7.582
7.580
7.578
7.318
7.313
7.301
7.296
7.265
7.263
7.089
7.070
7.003
6.982
6.824
6.821
6.819
4.361
4.342
4.325
4.307
2.332
1.388
1.370
1.352
1.255
0.077
0.002
0.000
EtOOC
N
NO2
3n
12
10
8
6
4
2
0 PPM


164.303
146.209
144.677
137.689
135.037
129.294
128.498
128.215
127.766
125.751
124.743
118.382
112.004
77.323
77.000
76.687
60.130
21.148
14.439
EtOOC
N
NO2
3n
200
150
100
50
0 PPM


7.780
7.743
7.389
7.372
7.249
7.233
7.214
7.190
5.429
5.414
5.396
5.380
4.170
4.153
4.136
4.118
3.143
1.899
1.888
1.747
1.694
1.570
1.541
1.252
1.235
1.218
1.181
1.146
1.121
CO2Et
c-Hex–NH
Ph
4
12
10
8
6
4
2
0 PPM


167.542
152.262
131.085
128.218
127.472
124.094
96.888
82.939
82.432
77.315
77.000
76.672
59.879
56.541
34.050
24.989
24.474
14.427
CO2Et
NH
Ph
4
200
150
100
50
0 PPM