Electronic Supplementary Information (ESI)

for

Ligand and Cu free *N*-arylation of indoles, pyrroles and benzylamines with aryl halides catalyzed by a Pd nanocatalyst

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Experimental

General Procedure

The starting materials and all solvents used were purchased from commercial sources. Anhydrous solvents were prepared using standard methods. TLC was performed on pre-coated aluminium plates of silica gel 60 F_{254}. TLC spots were visualized by UV light (254 nm). Photolysis was carried out in an immersion well cooled by chilled water using medium pressure Hg vapour lamp. ^{1}H and ^{13}C-NMR spectra were recorded on Brucker 400 MHz NMR in solution of $CDCl_3$.

General experimental procedure for *N*-arylation

In a 25 mL round bottom flask fitted with a magnetic stirrer bar 1 mmol indole/pyrrole/benzyl amine, 1.1 mmol aryl halides and 2 mmol K_2CO_3 were added and after that in it 10 mL of 1:1 DMSO/DMF was added. Then in the reaction mixture Pd-NP (0.003%) catalyst was added and the whole system was then degassed for 10 minutes with Ar. The reaction mixture was then heated under argon atmosphere at 130 ^{0}C for 24 h. The completion of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was cooled, washed with water and the organic part extracted with ethyl acetate. Then the organic layer dried over anhydrous Na_2SO_4 and concentrated in *vacuo*. The crude product was purified by column chromatography using ethyl acetateandpetroleumbenzeneaseluenttoaffordthedesiredproductwhich wasthencharacterized by standard spectroscopictechniques.

Three Phase Test:

To a 50 mL of round bottomed flask charged with magnetic stirrer bar, Wang Resin (0.625g) was added followed by the addition of anhydrous DCM (7.5 mL). Then the mixture was left to stand for 20 min. to allow it to swell, after which 4-iodobenzoic acid (0.697 g, 2.81 mmol), DCC (0.580 g, 2.81 mmol) and DMAP (0.069 g, 0.565 mmol) was added. The round bottom flask was capped with rubber septum and stirred for 4 days. After TLC indicated the complete disappearance of 4-iodobenzoic acid. Then the solid material was filtered and washed successively three times each with 5 mL of DMF, THF, MeOH, and finally with the CH_2Cl_2. The resin bound material was then dried *in vacuo* for 24 hours. The resin bound acid derivative was then characterized by Solid state NMR spectroscopy.

Compound Characterization

1-*p*-tolyl-*1H*-indole (3a)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.30 (t, *J* = 3.2 Hz, 3H), 7.13-7.23 (m, 2H), 6.66 (d, *J* = 3.2 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 130.1, 129.1, 128.1, 122.2, 121.0, 120.2, 110.5, 103.2, 21.0.

1-phenyl-*1H*-indole (3b)[2]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.7 Hz, 2H), 7.84 (q, *J* = 8.7 Hz, 3H), 7.64-7.71 (m, 3H), 7.40 (d, *J* = 3.3 Hz, 1H), 7.20-7.24 (m, 1H), 6.75 (d, *J* = 4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 130.3, 129.7, 128.0, 127.5, 126.5, 124.4, 122.4, 121.2, 120.4, 110.6, 103.6, 94.5.

1-(4-methoxyphenyl)-1*H*-indole (3c)[3]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.47 (d, *J* = 8.8 Hz, 1H), 7.42 (d, *J* = 9 Hz, 1H), 7.29 (d, *J* = 3.2 Hz, 1H), 7.15-7.24 (m, 2H), 7.04 (d, *J* = 8.9 Hz, 2H), 6.67 (d, *J* = 3.9 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 136.3, 132.9, 129.0, 128.3, 126.0, 122.2, 121.0, 120.1, 114.7, 110.4, 102.9, 55.6.

Methyl-4(*1H*-indol-1-yl) benzoate (3d)[3]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.8 Hz, 2H), 7.59-7.72 (m, 4H), 7.38 (d, *J* = 3.2 Hz, 1H), 7.20-7.30 (m, 2H), 6.74 (d, *J* = 3.2 Hz, 1H), 3.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 143.7, 135.4, 131.2, 129.8, 127.5, 127.4, 123.2, 122.8, 121.4, 120.9, 110.6, 104.9, 52.3.

5-methoxy-1-*p*-tolyl-*1H*-indole (3e)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.8 Hz, 1H), 7.40 (d, *J* = 8 Hz, 2H), 7.33 (s, 1H), 7.31 (d, *J* = 2.8 Hz, 2H), 7.17 (d, *J* = 2.4 Hz, 1H), 6.90 (dd, *J* = 2.4 Hz and *J* = 9.2 Hz, 1H), 6.61 (d, *J* = 3.2 Hz, 1H), 3.90 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 137.4, 136.1, 130.1, 129.7, 128.5, 124.0, 112.4, 111.3, 102.9, 102.7, 55.9, 21.0.

5-cyano-1-*p*-tolyl-*1H*-indole (3f)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 1.2 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.42 (dd, *J* = 3.6 Hz and *J* = 7 Hz, 2H), 7.34 (s, 4H), 6.73 (d, *J* = 3.2 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 136.1, 130.5, 130.4, 128.7, 126.6, 125.0, 124.5, 120.6, 103.8, 103.2, 21.0.

5-bromo-1-*p*-tolyl-*1H*-indole (3g)[4]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 2 Hz, 1H), 7.38-7.44 (m, 2H), 7.36 (d, *J* = 4 Hz, 3H), 7.33 (d, *J* = 2.8 Hz, 2H), 6.63 (d, *J* = 3.2 Hz, 1H), 2.8 (s,

3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 134.8, 130.9, 130.3, 129.3, 125.1, 124.3, 123.5, 113.4, 112.0, 102.7, 21.1.

methyl 4-(5-methoxy-1*H*-indol-1-yl)benzoate (3h)[3]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.4 Hz, 2H), 7.54-7.57 (m, 3H), 7.35 (d, *J* = 3.2 Hz, 1H), 7.16 (d, *J* = 2.4 Hz, 1H), 6.93 (dd, *J* = 2.8 Hz and *J* = 9 Hz, 1H), 6.66 (d, *J* = 3.2 Hz, 1H), 3.97 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 154.9, 143.8, 131.3, 130.5, 127.8, 127.3, 112.8, 111.5, 104.7, 103.1, 55.8, 52.2.

methyl 4-(5-cyano-1*H*-indol-1-yl)benzoate (3i)[3]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.4 Hz, 2H), 8.05 (s, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8 Hz, 2H), 6.98 (d, *J* = 2.4 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 142.5, 137.1, 131.5, 129.9, 129.4, 128.9, 126.8, 125.7, 123.9, 120.2, 111.4, 105.2, 104.1, 52.4.

1-(4-(1H-indol-1-yl)phenyl)ethanone (3j)[2]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.8 Hz, 2H), 7.62-7.71 (m, 4H), 7.39 (d, *J* = 3.2 Hz, 1H), 7.21-7.29 (m, 2H), 6.74 (d, *J* = 3.2 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 143.8, 135.4, 134.6, 130.1, 129.8, 127.4, 123.3, 122.9, 121.4, 121.1, 110.6, 105.1, 26.6.

1-phenyl-1*H*-pyrrole (5a)[5]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.49 (m, 4H), 7.29 (t, *J* = 6.4 Hz, 1H), 7.15 (s, 2H), 6.42 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 129.6, 125.6, 120.6, 119.4, 110.5.

1-*p*-tolyl-1*H*-pyrrole (5b)[6]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8 Hz, 2H), 7.14 (t, *J* = 2 Hz, 2H), 6.42 (t, *J* = 2 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 135.4, 130.1, 120.6, 119.4, 110.1, 20.1.

1-(4-methoxyphenyl)-1*H*-pyrrole (5c)[5]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.31 (m, 2H), 6.98 (t, *J* = 2.2 Hz, 2H), 6.90-6.95 (m, 2H), 6.31 (t, *J* = 2.2 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 134.7, 122.2, 119.7, 114.7, 109.9, 55.6.

methyl 4-(1*H*-pyrrol-1-yl)benzoate (5d)[7]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 2H), 7.17 (t, *J* = 2 Hz, 2H), 6.40 (t, *J* = 2.2 Hz, 2H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 144.0, 131.3, 126.9, 119.3, 119.0, 111.5, 52.1.

1-(4-(1*H*-pyrrol-1-yl)phenyl)ethanone (5e)[5]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 8.8 Hz, 2H), 7.17 (t, *J* = 1.8 Hz, 2H), 6.39 (t, *J* = 1.8 Hz, 2H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 144.0, 134.0, 130.2, 119.3, 119.0, 111.6, 26.5.

***N*-benzylbenzenamine (7a)[8]:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.45 (m, 4H), 7.38 (d, *J* = 6 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 2H), 6.83 (t, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 2H), 4.39 (s, 2H), 4.06 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 139.3, 129.2, 128.5, 127.4, 127.1, 117.5, 112.8, 48.2.

***N*-benzyl-4-methylbenzenamine (7b)[8]:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.38 (m, 6H), 7.0 (t, *J* = 10 Hz, 2H), 6.58 (dd, *J* = 8 Hz and *J* = 12 Hz, 2H), 4.33 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 139.5, 129.6, 128.5, 127.4, 127.0, 126.6, 112.9, 48.5, 20.3.

***N*-benzyl-4-methoxybenzenamine (7c)[8]:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.40 (m, 5H), 6.78-6.82 (m, 2H), 6.62-6.66 (m, 2H), 4.30 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 142.0, 139.4, 128.6, 127.6, 127.2, 114.9, 114.4, 55.8, 49.4.

methyl 4-(benzylamino)benzoate (7d)[9]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8 Hz, 2H), 7.17-7.29 (m, 6H), 6.51 (d, *J* = 8 Hz, 2H), 4.61 (s, 1H), 4.29 (s, 2H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 151.5, 138.2, 131.5, 128.7, 127.5, 127.4, 126.9, 118.6, 111.8, 51.5, 47.7.

References:

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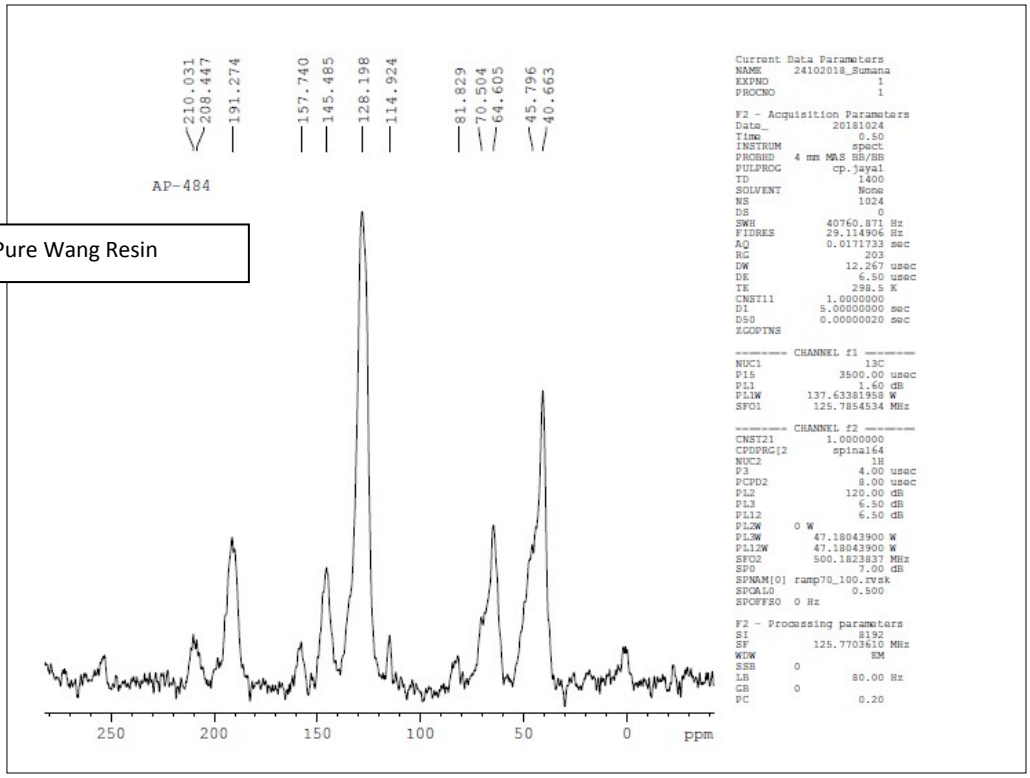
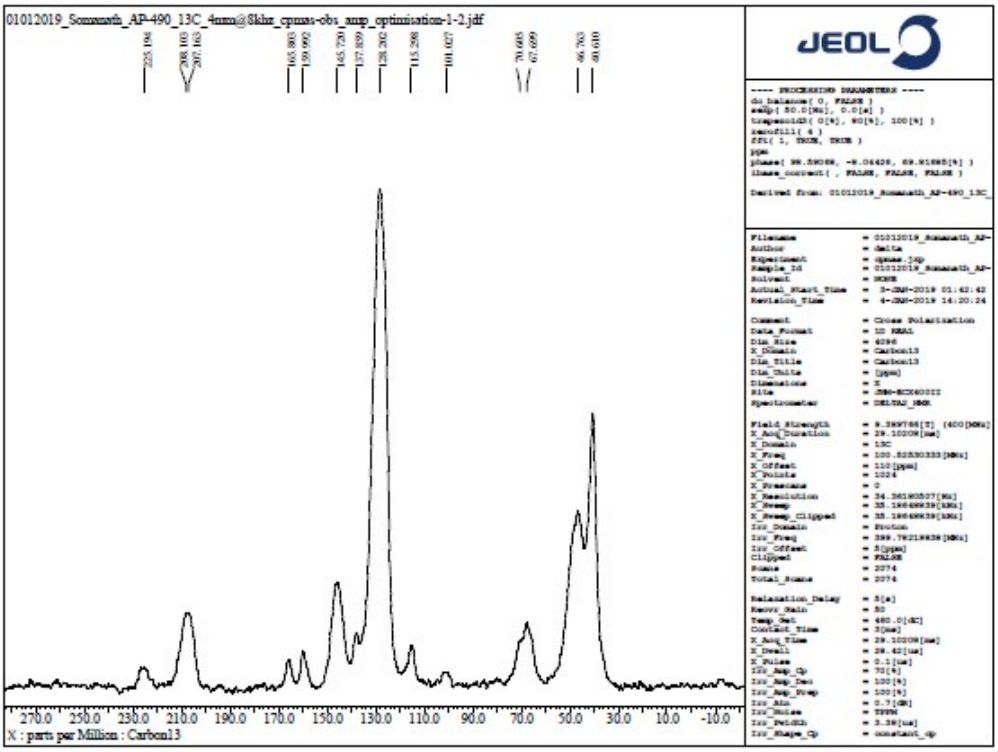
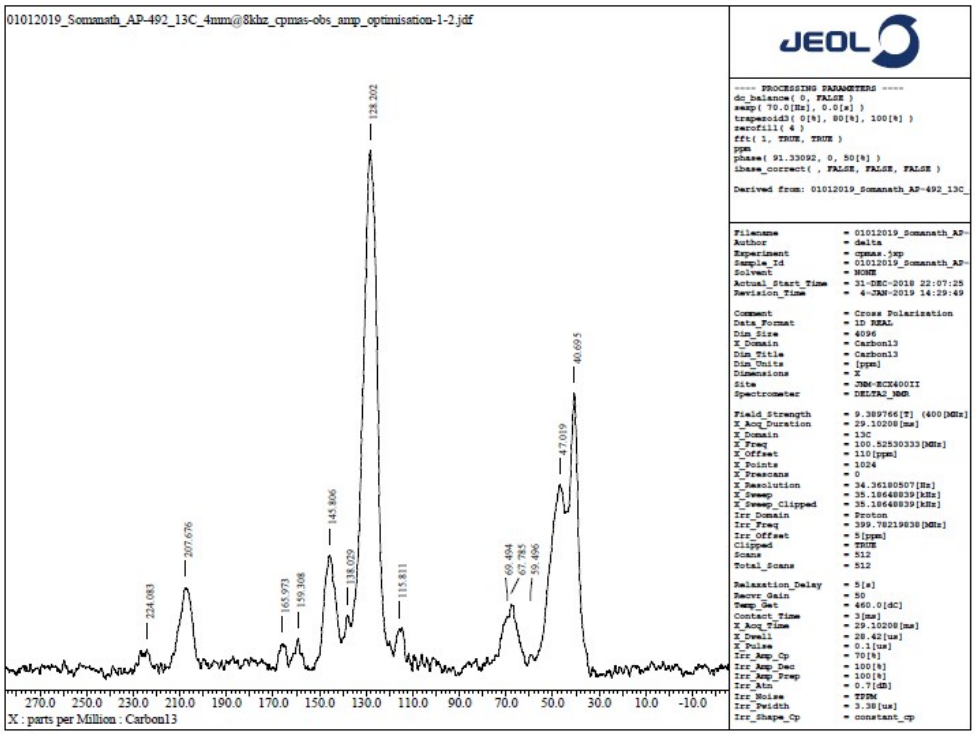


Solid State ^{13}C-NMR spectra of pure Wang Resin.

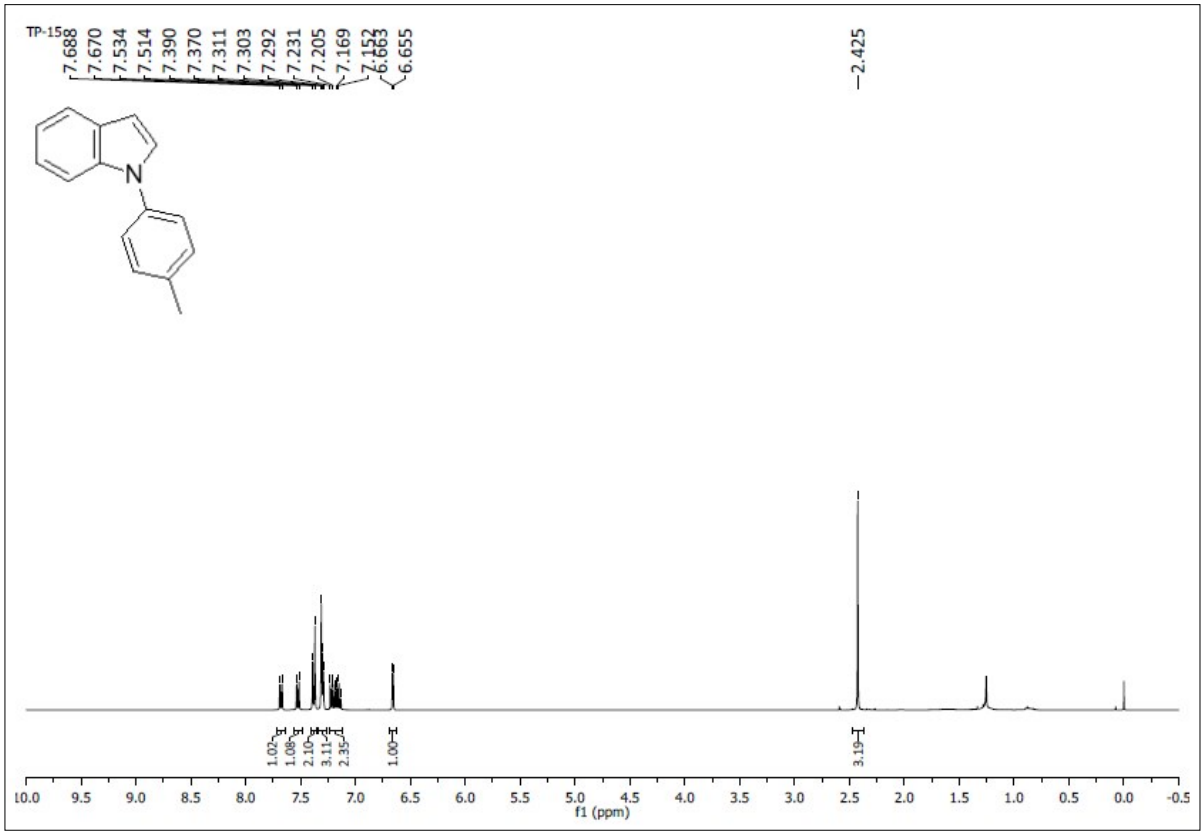


Solid State ^{13}C-NMR spectra of Wang Resin anchored 4-iodobenzoic acid.



Solid State ^{13}C-NMR spectra of Wang Resin anchored 4-iodobenzoic acid after *N*-arylation.

NMR Spectra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7.231
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7.169
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6.655
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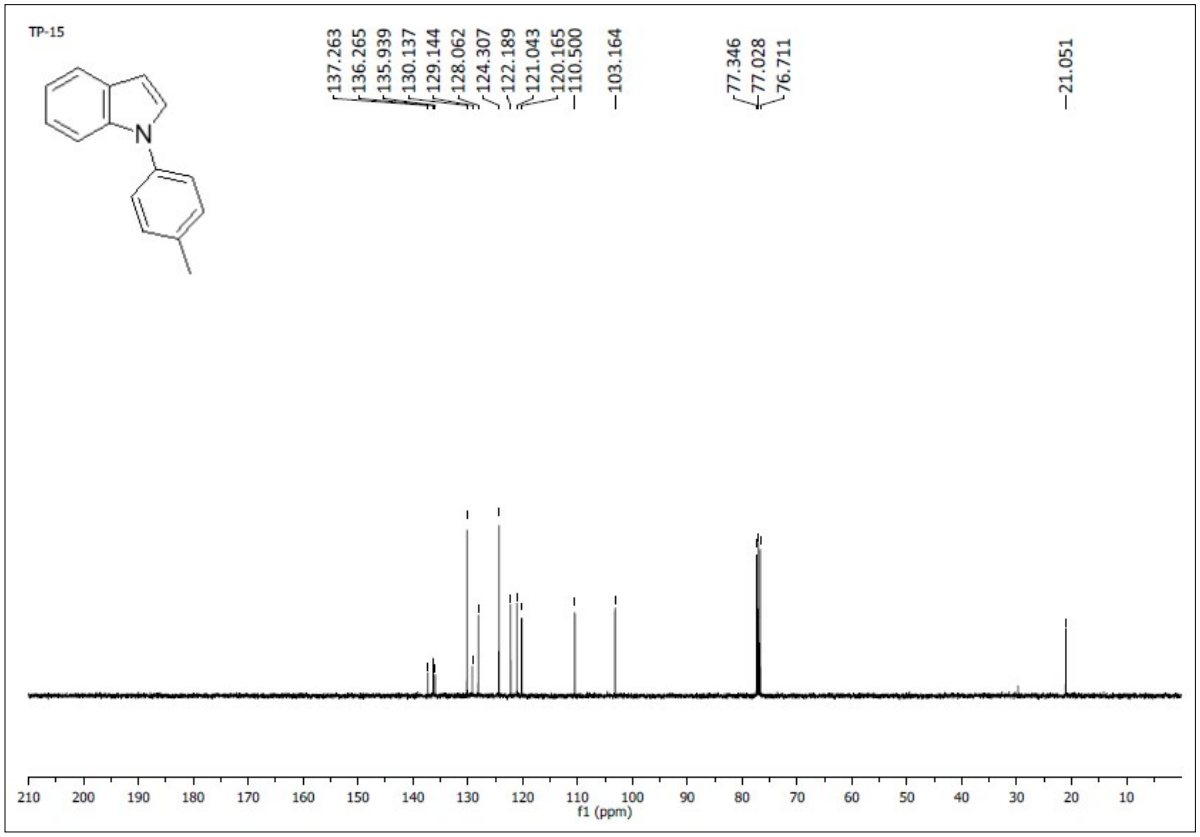
1.08
2.10
3.11
2.35
1.00
3.19
f1 (ppm)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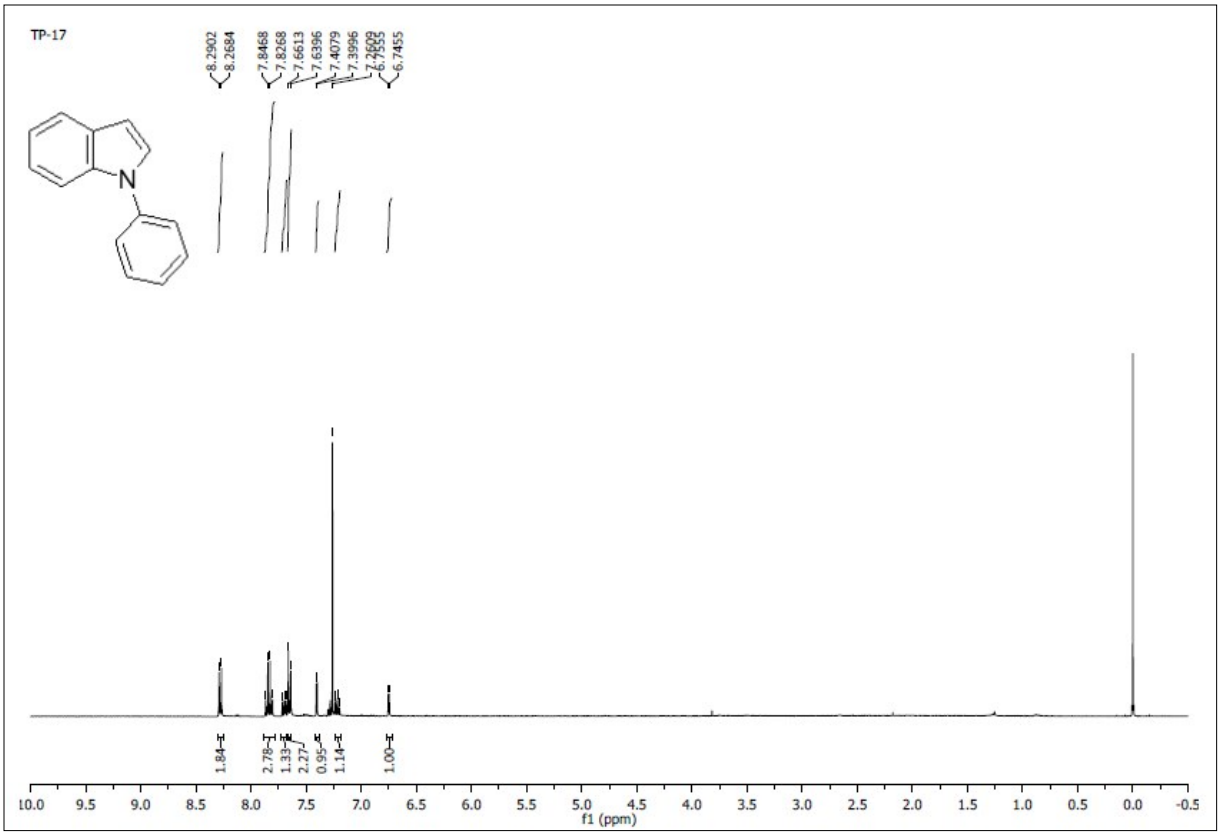
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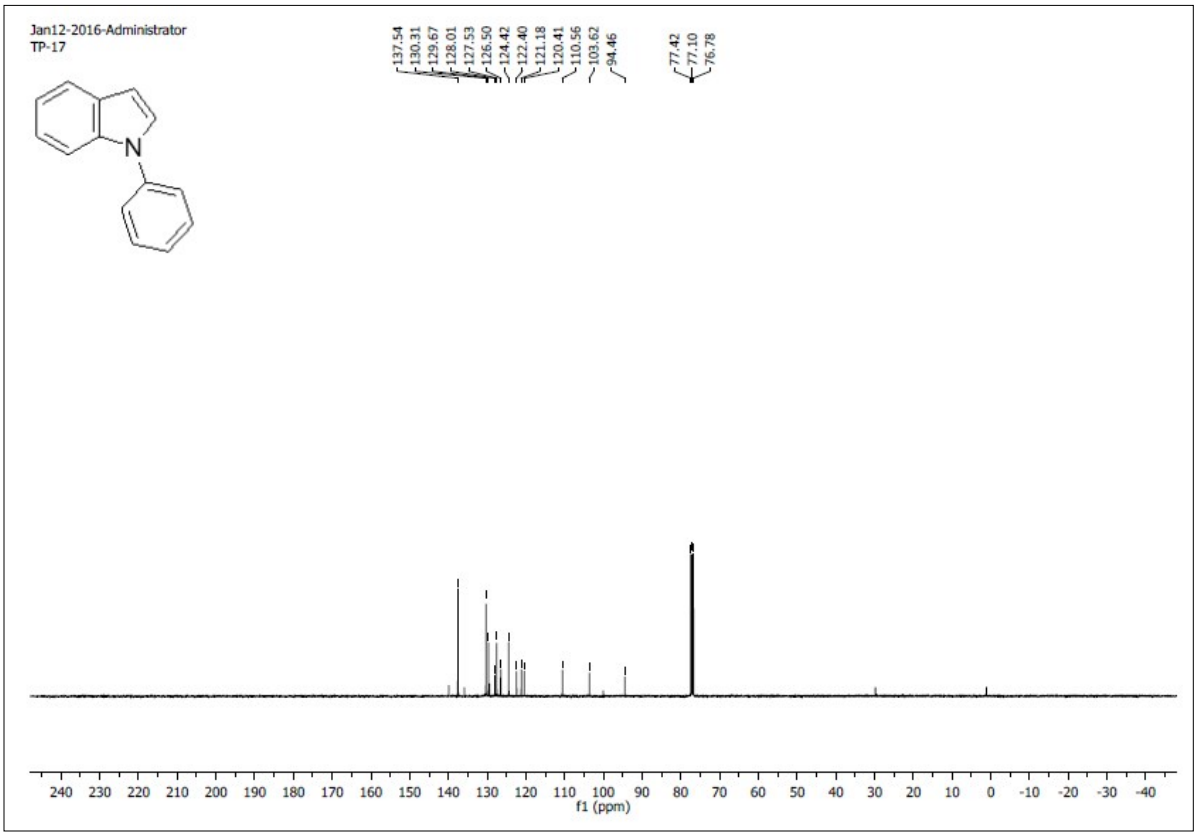
f1 (ppm)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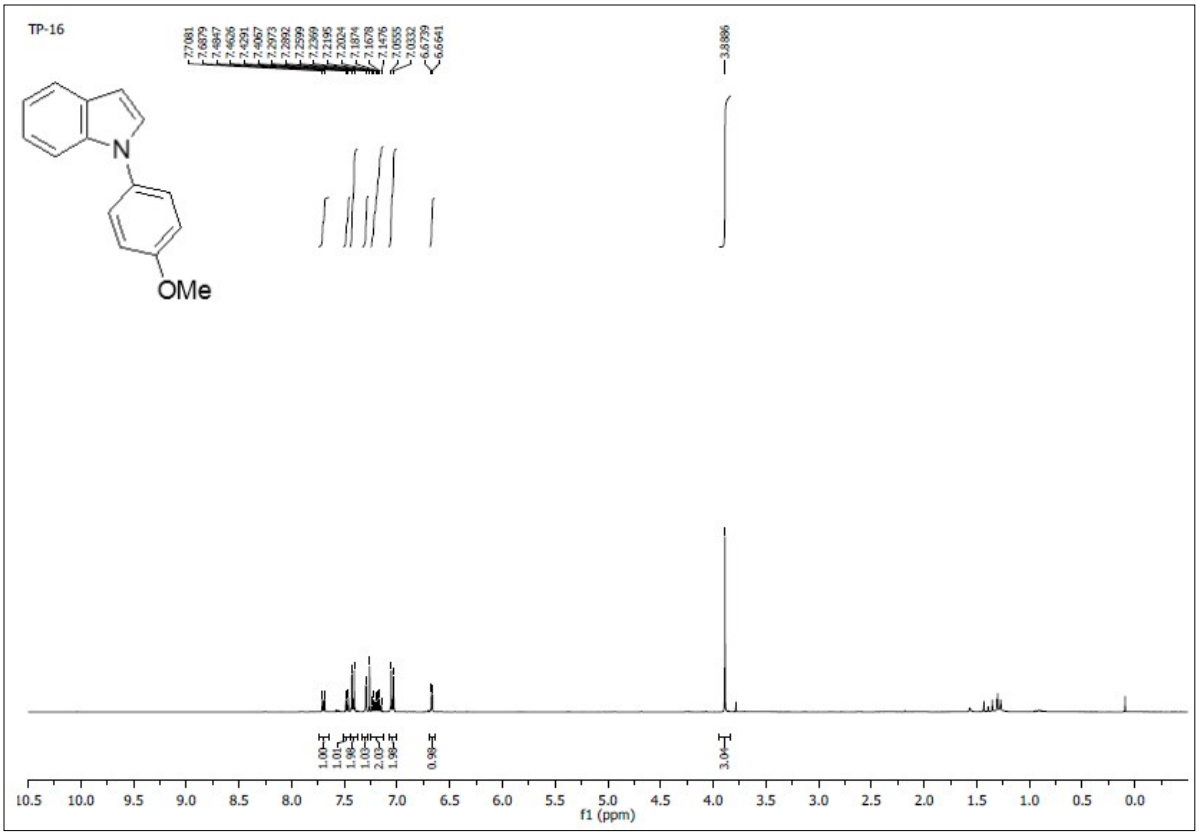
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7.2195
7.2024
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7.1476
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7.0332
6.6739
6.6541
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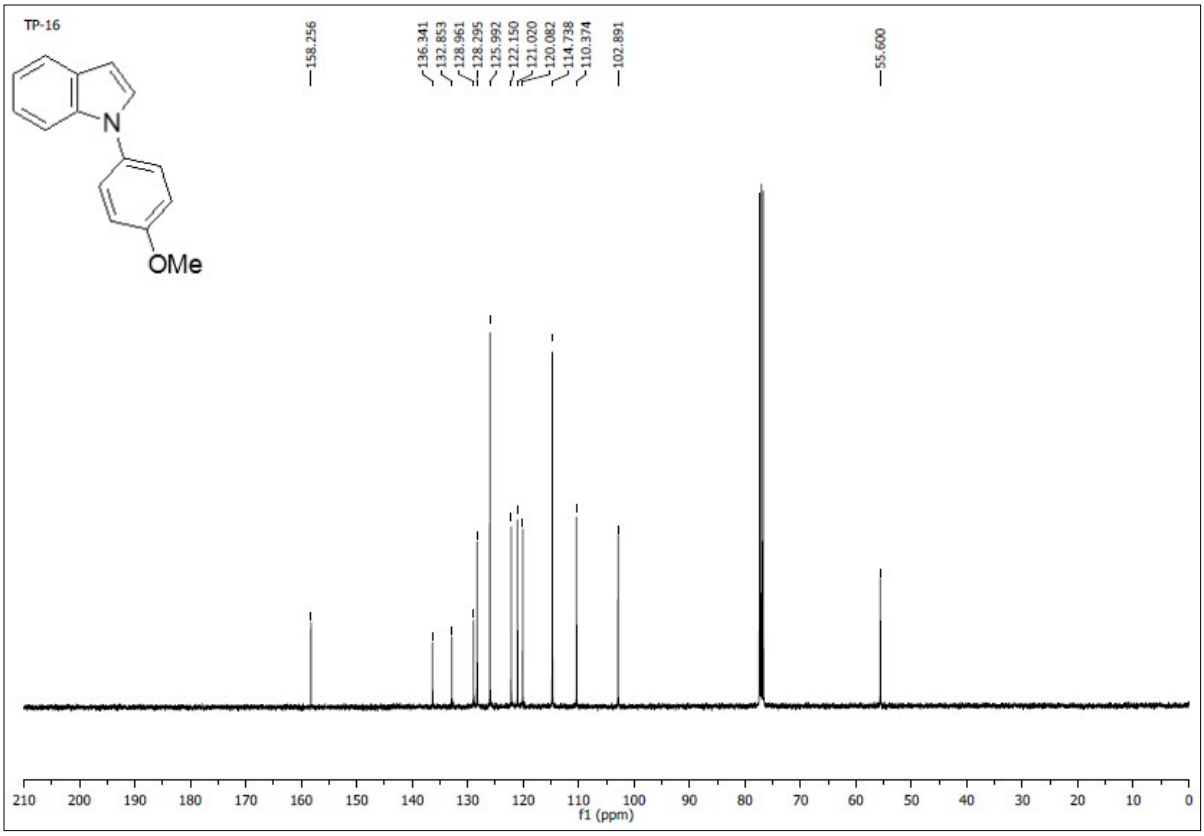
f1 (ppm)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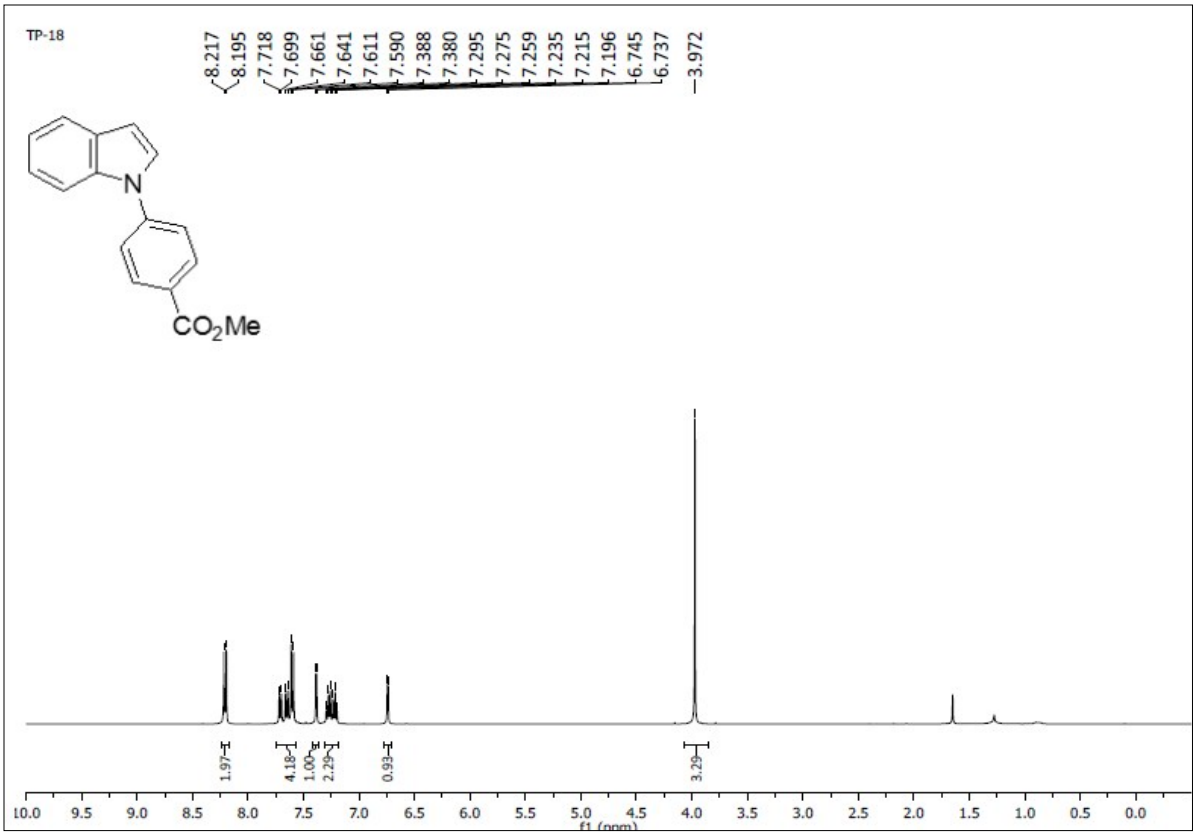
f1 (ppm)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7.235
7.215
7.196
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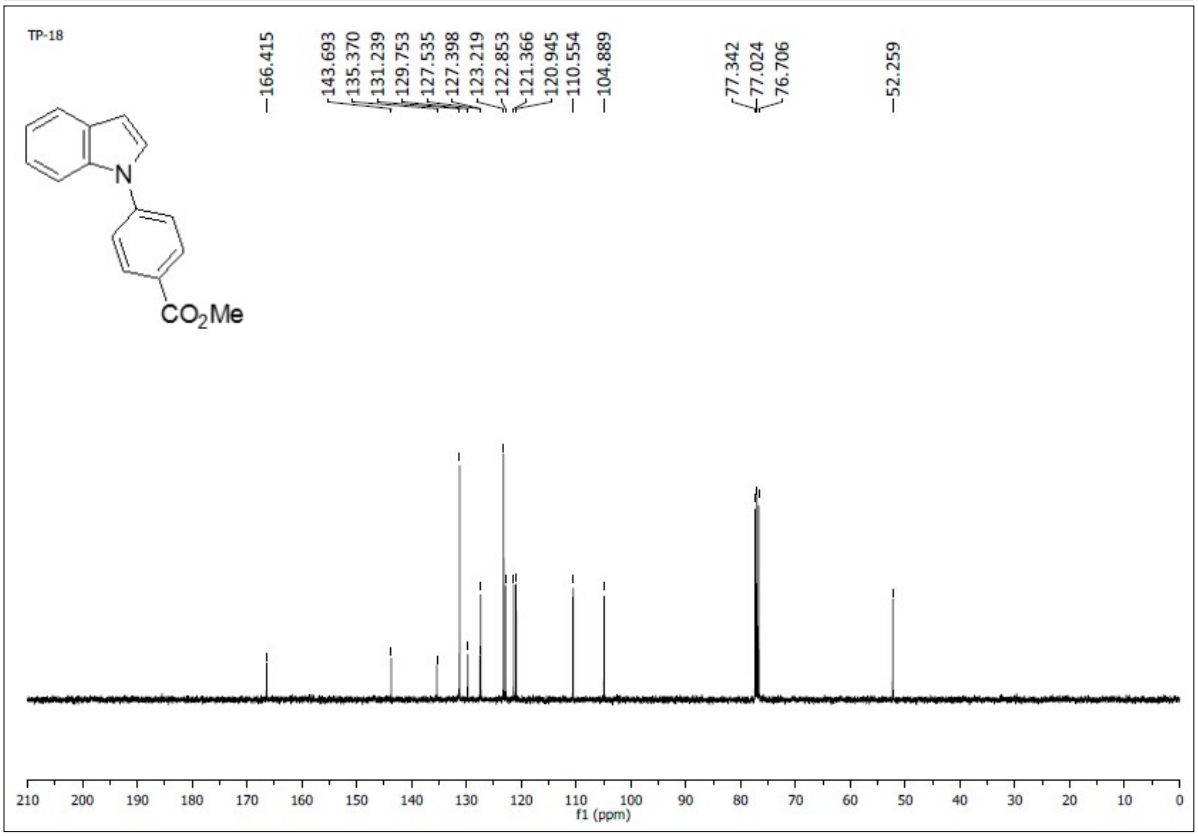
3.29
f1 (ppm)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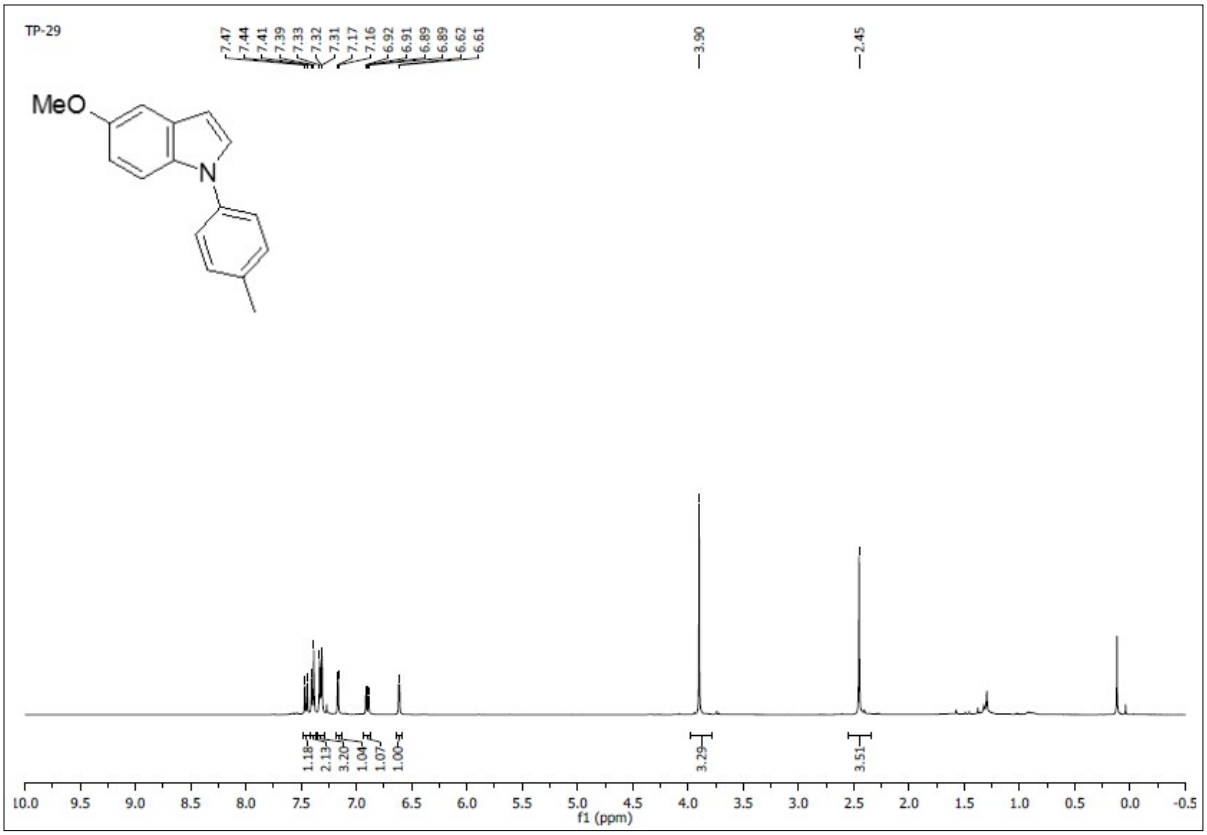
f1 (ppm)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7.32
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7.16
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6.89
6.89
6.62
6.61
3.90
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N
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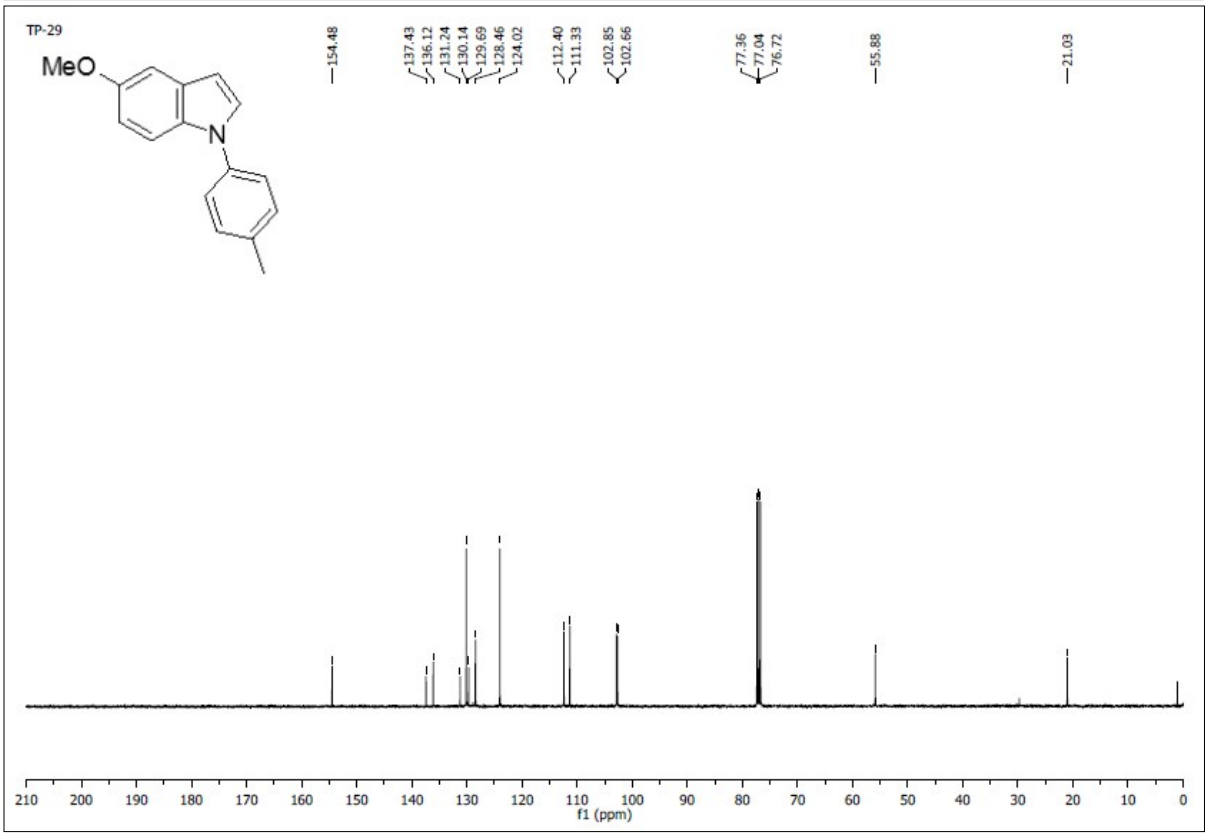
1.00
3.29
3.51
f1 (ppm)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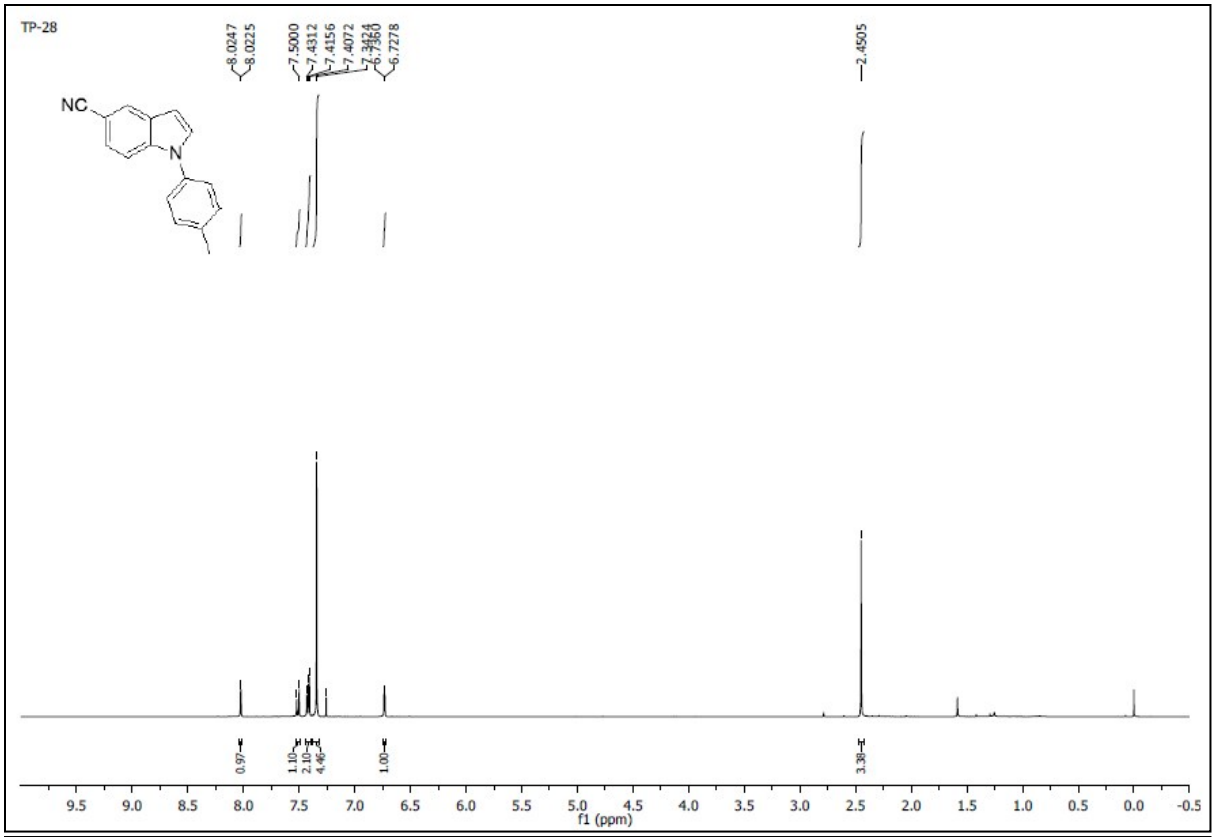
21.03
MeO
N
f1 (ppm)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2.10
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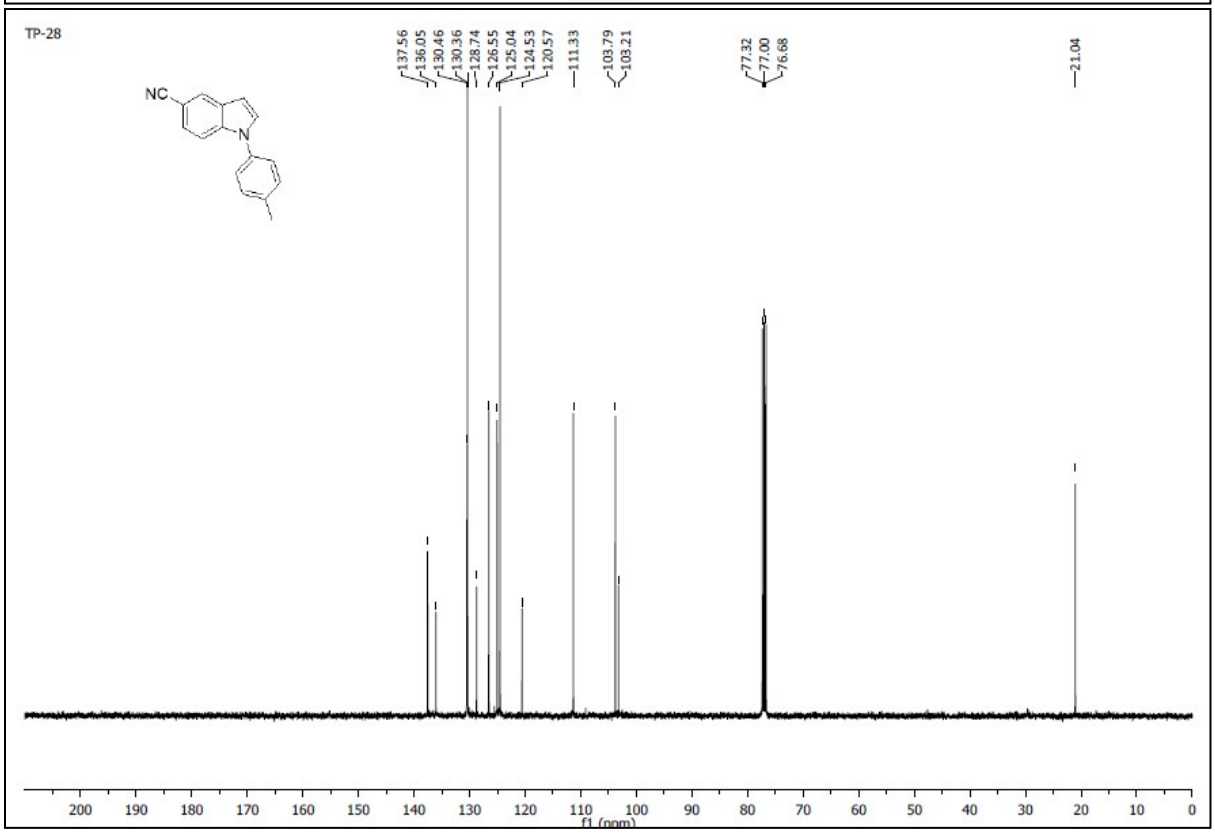
1.00
3.38
f1 (ppm)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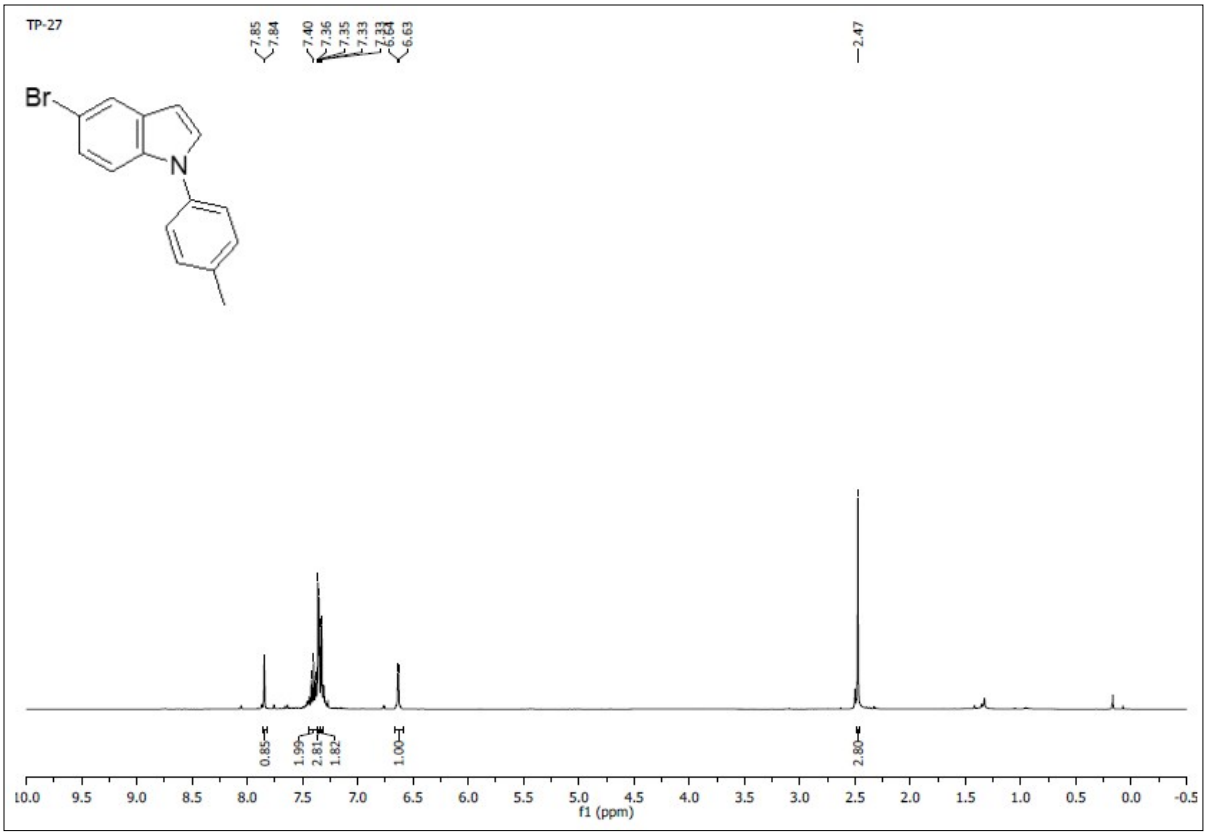
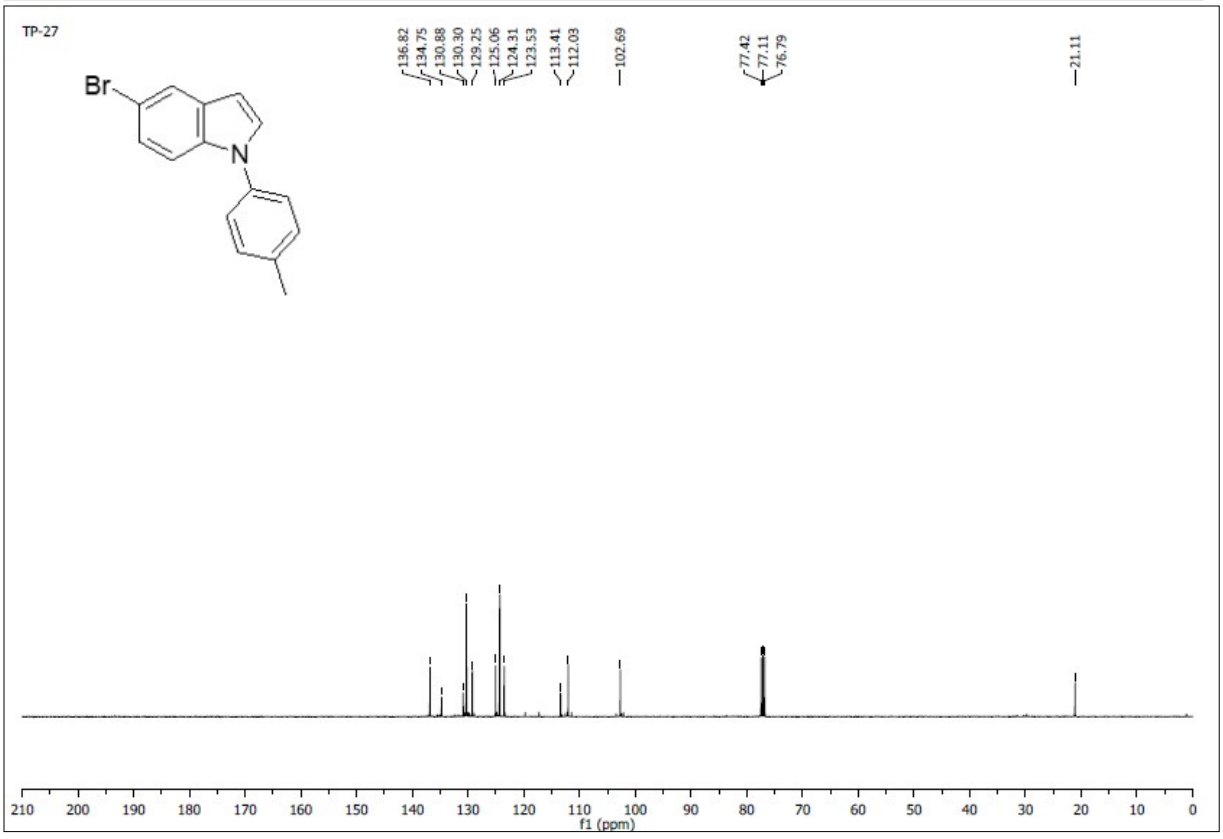
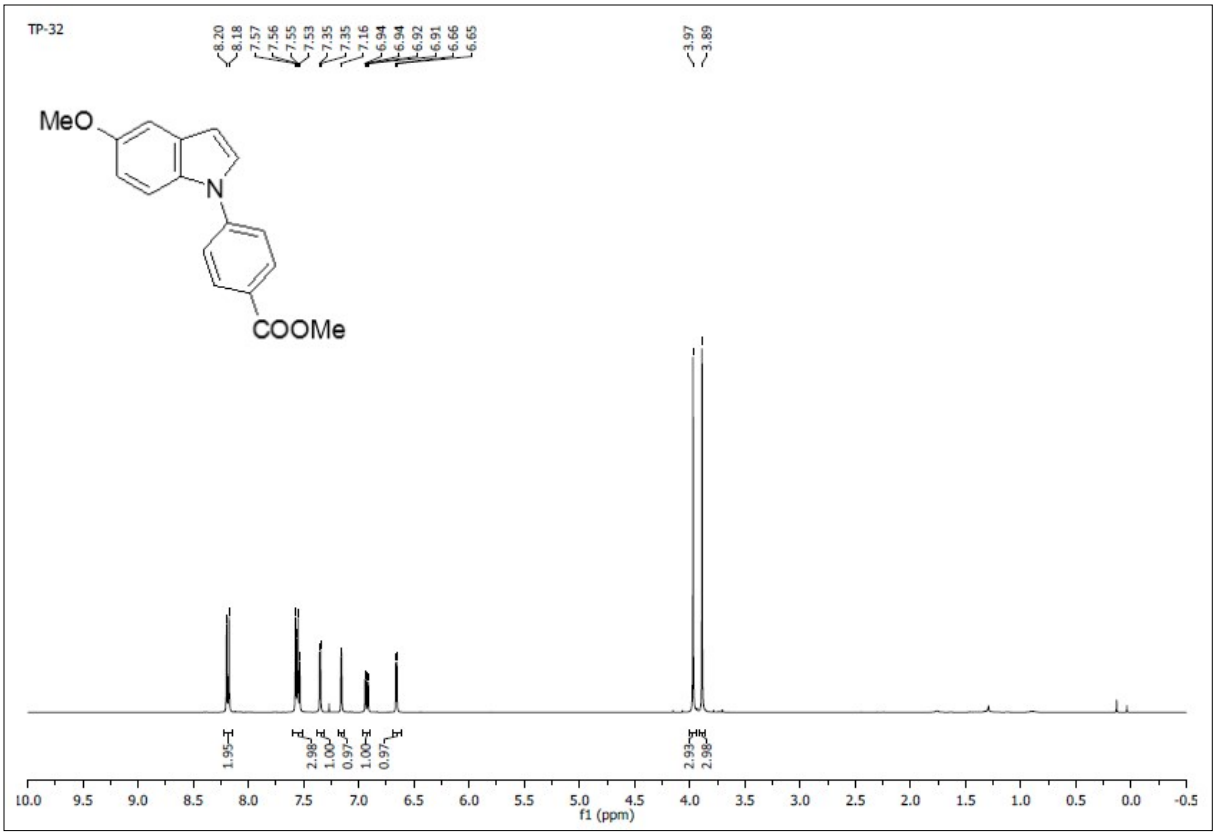
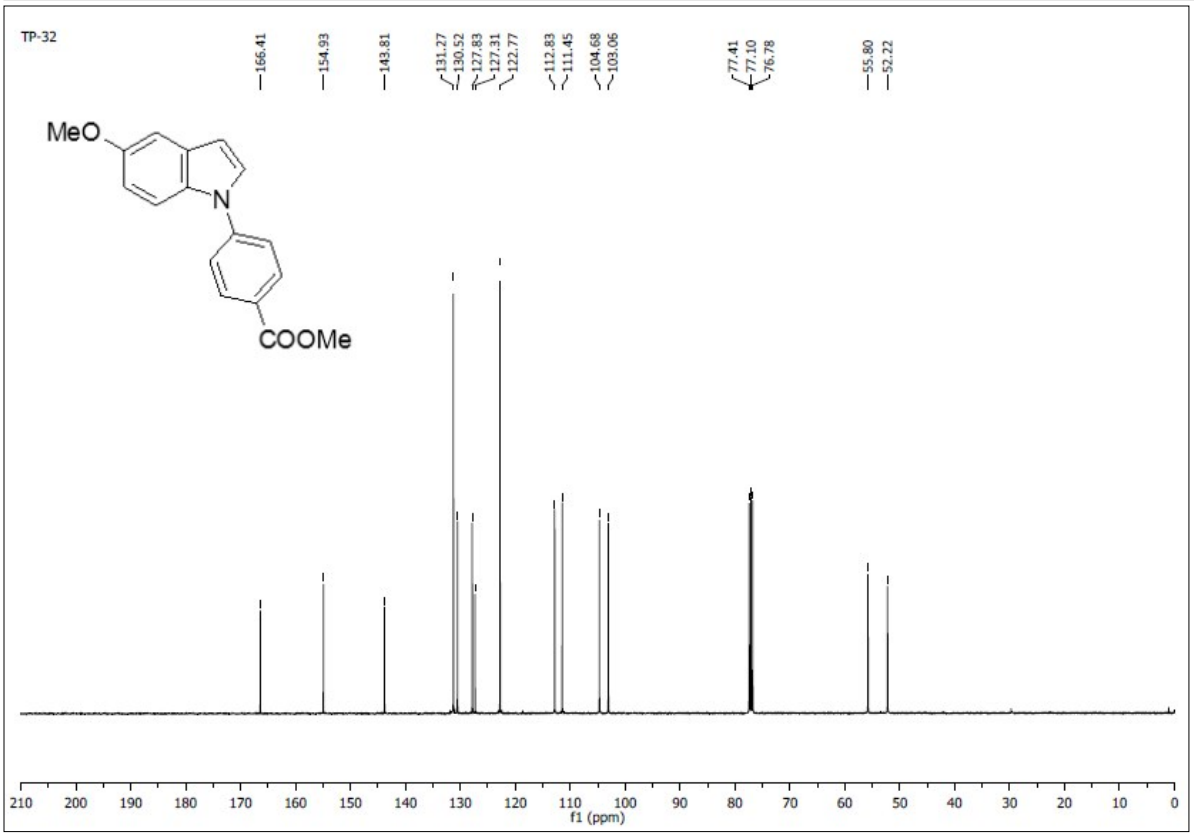
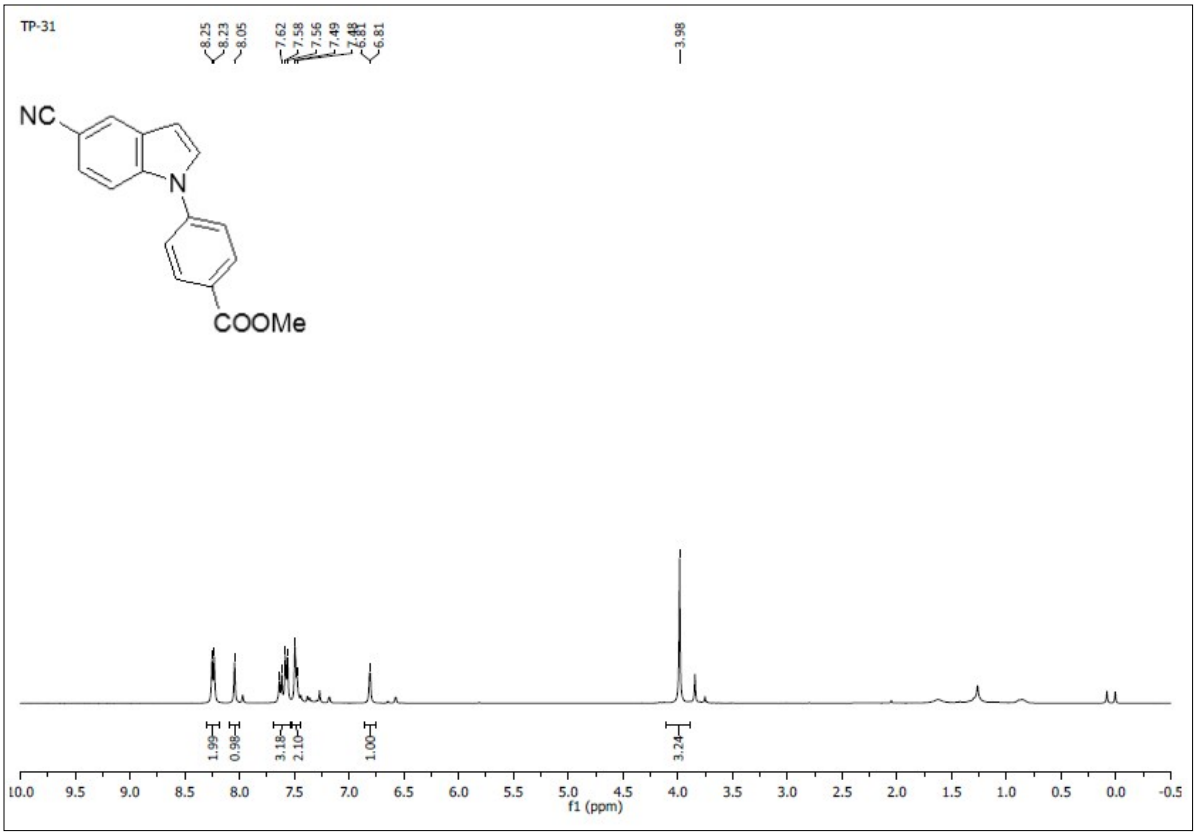
103.79
103.21
77.32
77.00
76.68
21.04
NC
N
f1 (ppm)

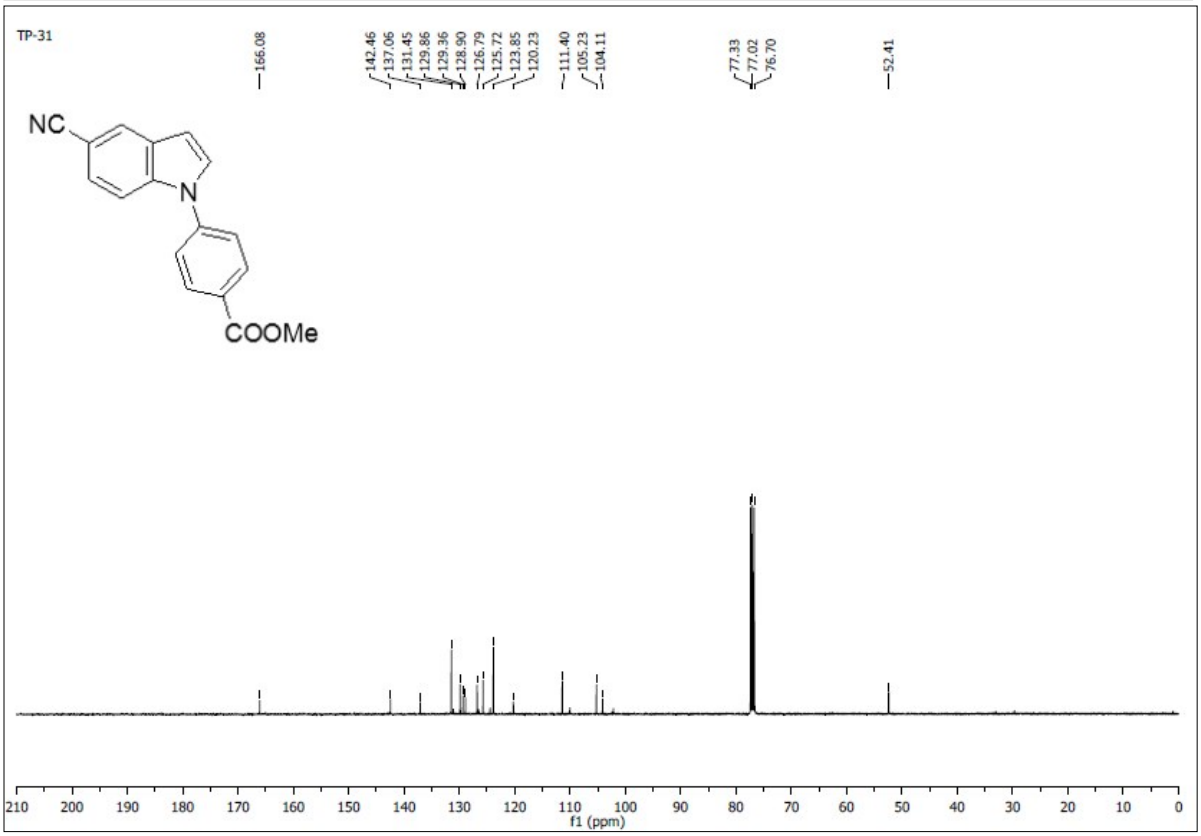

TP-27
7.85
7.84
7.40
7.36
7.35
7.33
7.33
6.64
6.63
2.47
Br
N
0.85
1.99
2.81
1.82
1.00
2.80
f1 (ppm)

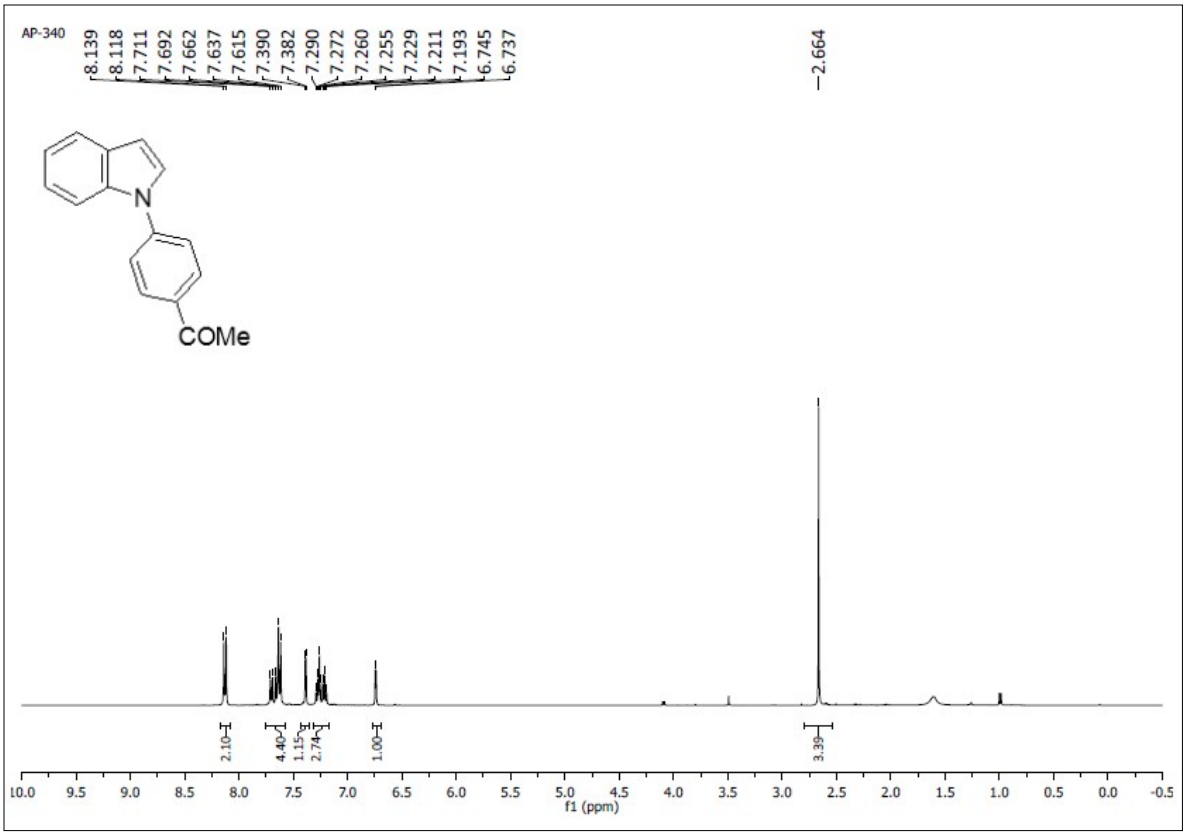

TP-27
136.82
134.75
130.88
130.30
129.25
125.06
124.31
123.53
113.41
112.03
102.69
77.42
77.11
76.79
21.11
Br
N
f1 (ppm)

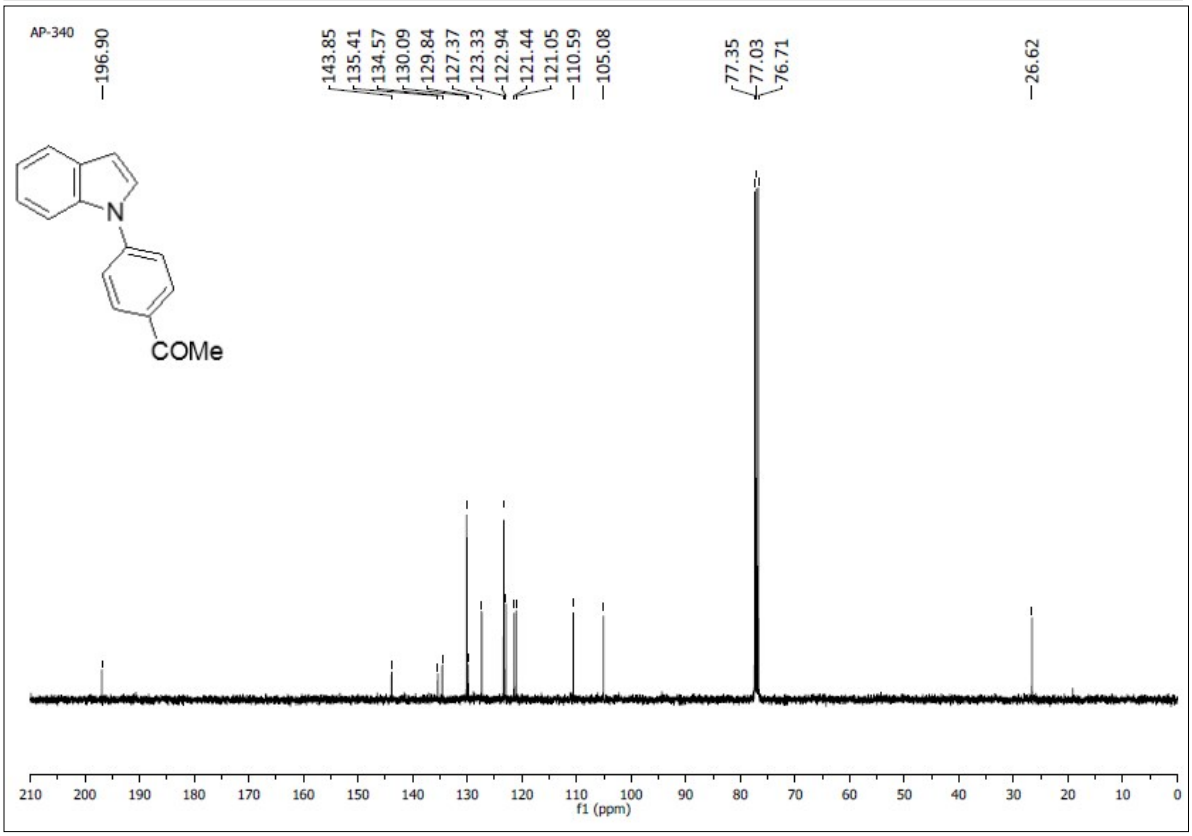

TP-32
8.20
8.18
7.57
7.56
7.55
7.53
7.35
7.35
7.16
6.94
6.94
6.92
6.91
6.66
6.65
3.97
3.89
MeO
N
COOMe
1.95
2.98
1.00
0.97
1.00
0.97
2.93
2.98
f1 (ppm)

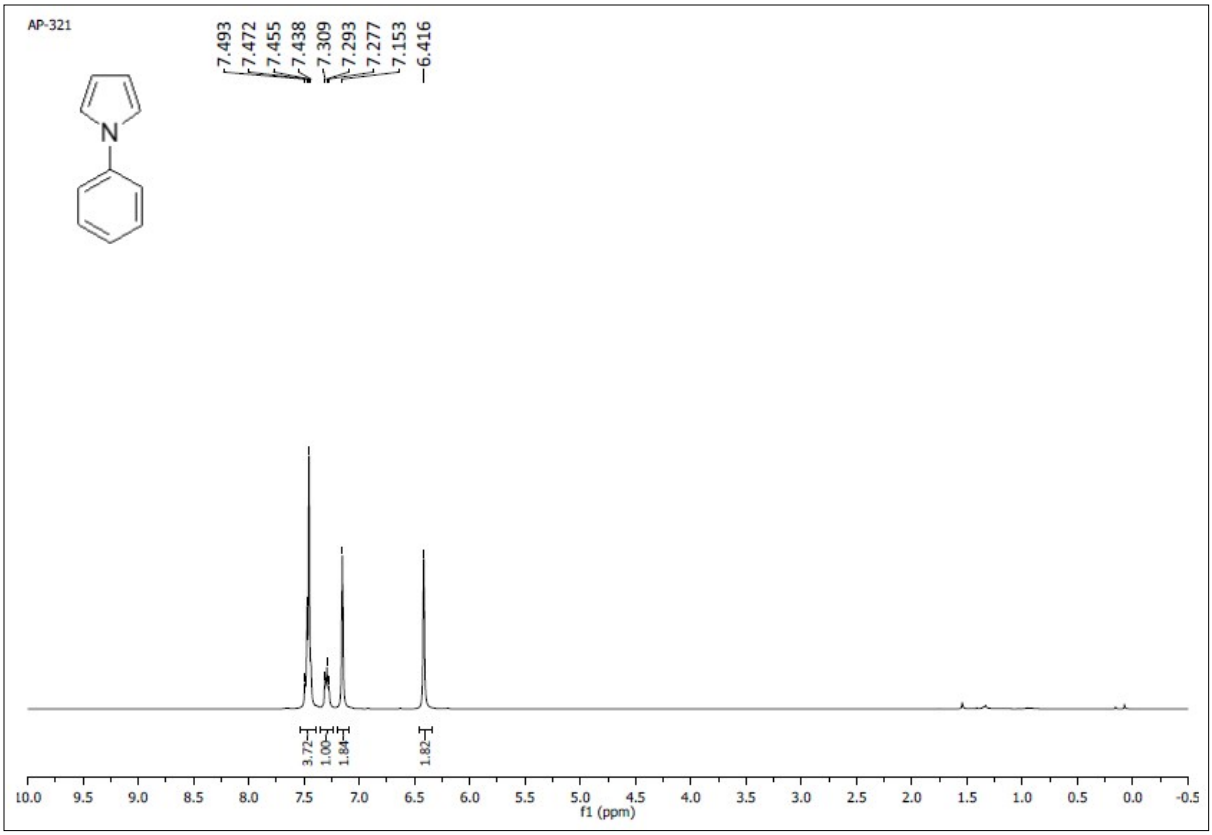

TP-32
166.41
154.93
143.81
131.27
130.52
127.83
127.31
122.77
112.83
111.45
104.68
103.06
77.41
77.10
76.78
55.80
52.22
MeO
N
COOMe
f1 (ppm)

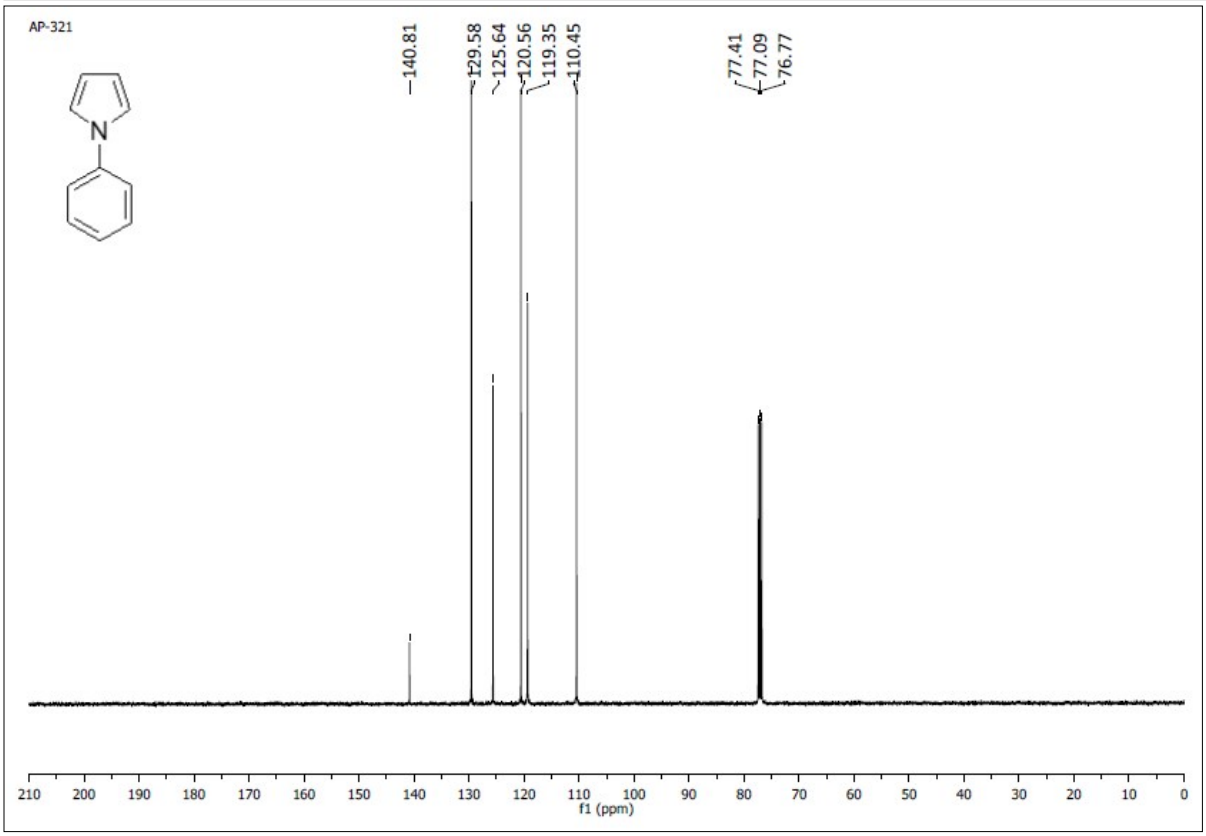

TP-31
8.25
8.23
8.05
7.62
7.58
7.56
7.49
7.48
6.81
6.81
3.98
NC
N
COOMe
1.99
0.98
3.18
2.10
1.00
3.24
f1 (ppm)

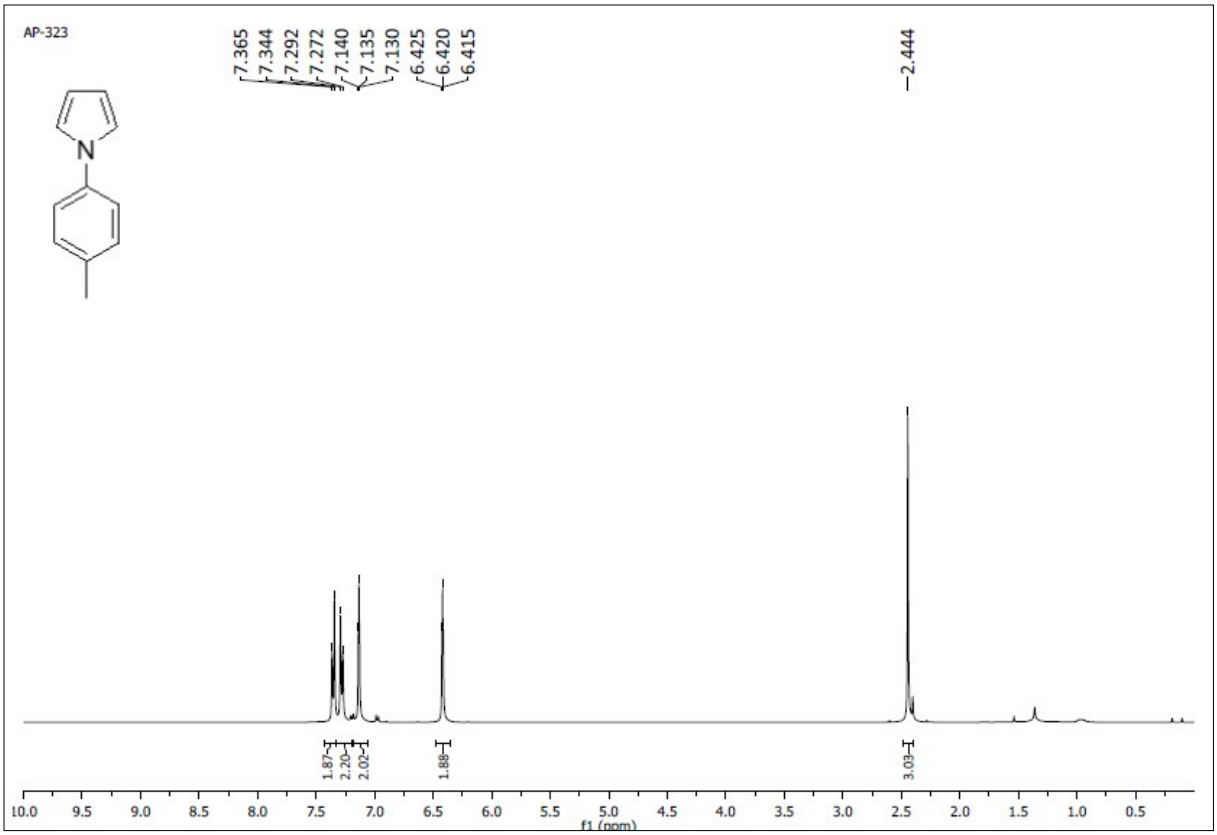

TP-31
166.08
142.46
137.06
131.45
129.86
129.36
128.90
126.79
125.72
123.85
120.23
111.40
105.23
104.11
77.33
77.02
76.70
52.41
NC
N
COOMe
f1 (ppm)

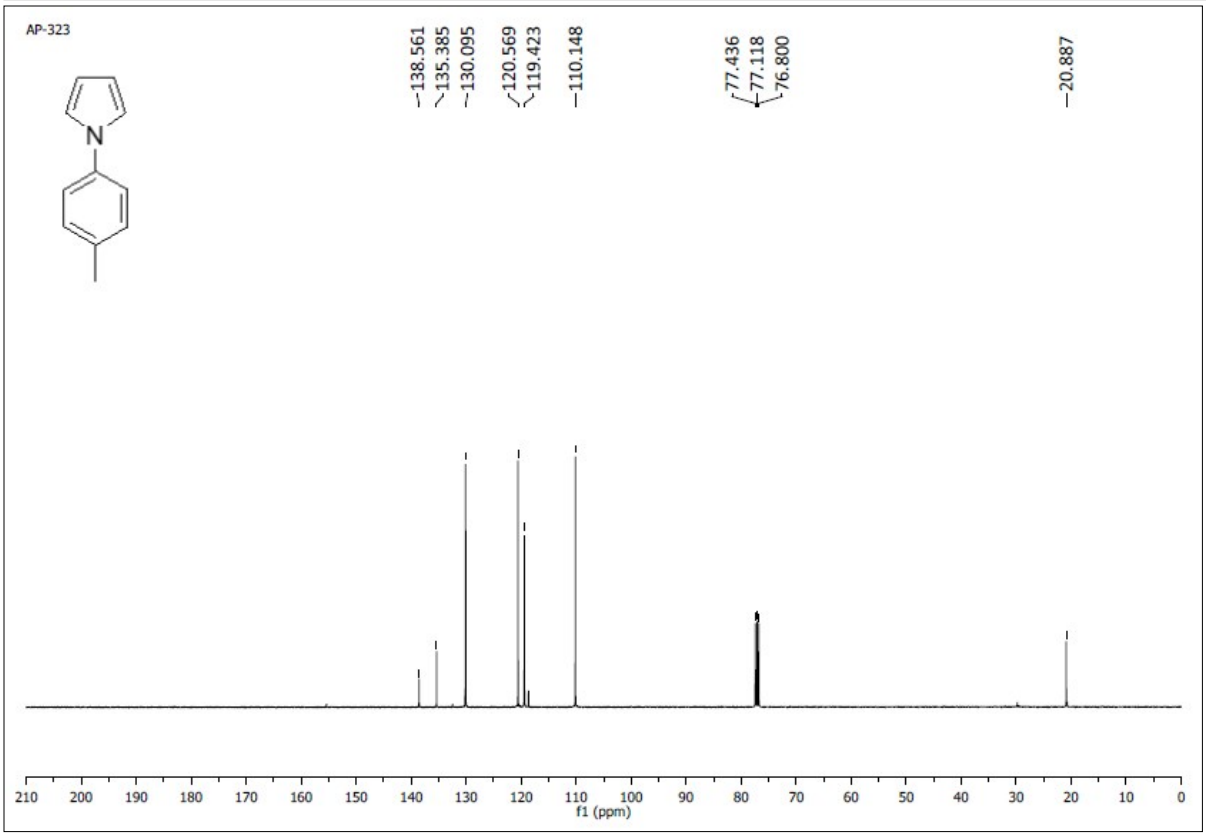

AP-340
8.139
8.118
7.711
7.692
7.662
7.637
7.615
7.390
7.382
7.290
7.272
7.260
7.255
7.229
7.211
7.193
6.745
6.737
2.664
N
COMe
2.10
4.40
1.15
2.74
1.00
3.39
f1 (ppm)

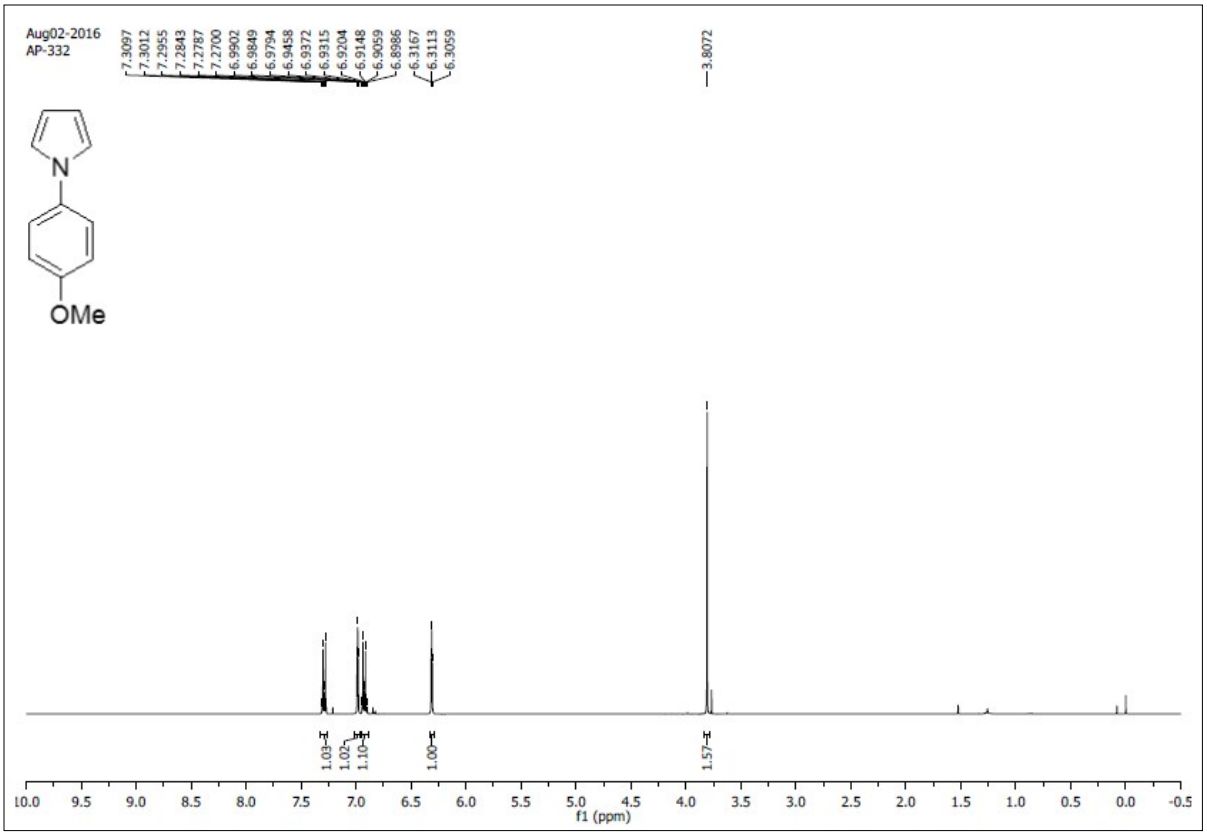

AP-340
196.90
143.85
135.41
134.57
130.09
129.84
127.37
123.33
122.94
121.44
121.05
110.59
105.08
77.35
77.03
76.71
26.62
N
COMe
f1 (ppm)

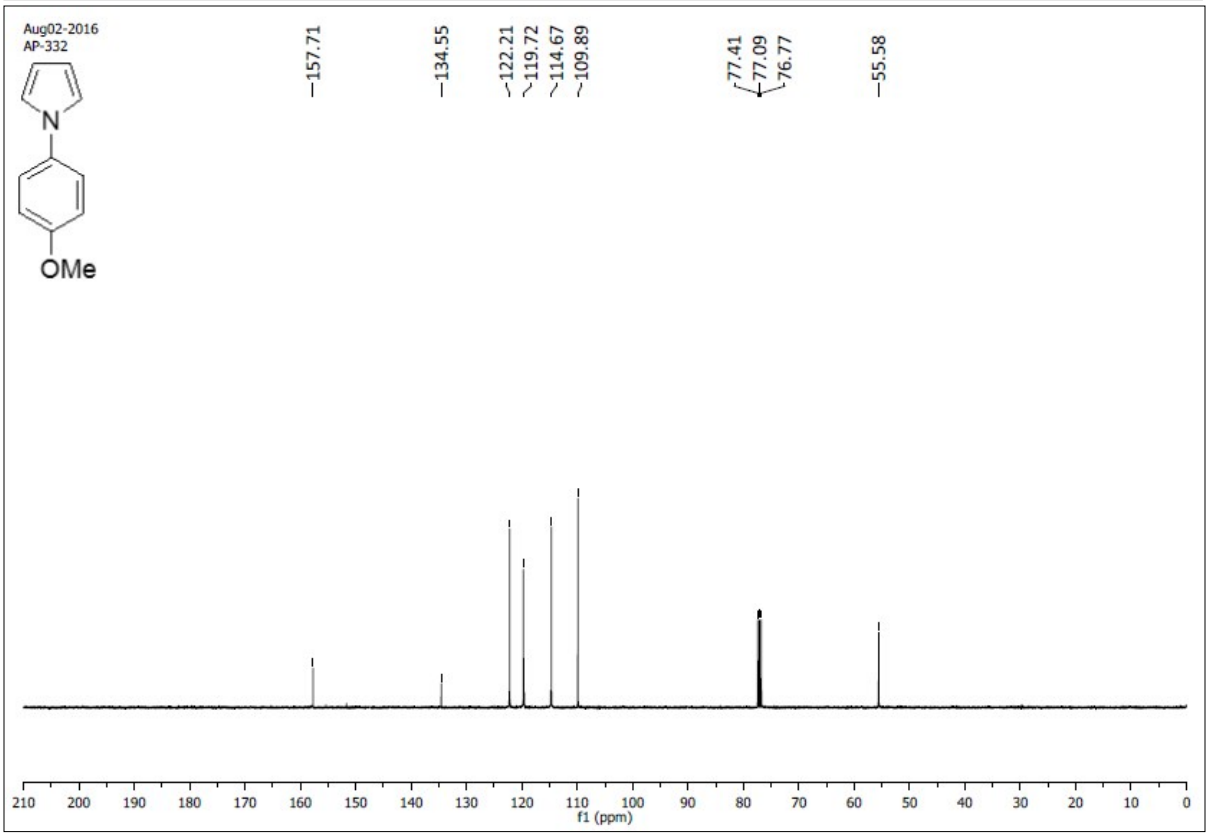

AP-321
7.493
7.472
7.455
7.438
7.309
7.293
7.277
7.153
6.416
N
3.72
1.00
1.84
1.82
f1 (ppm)

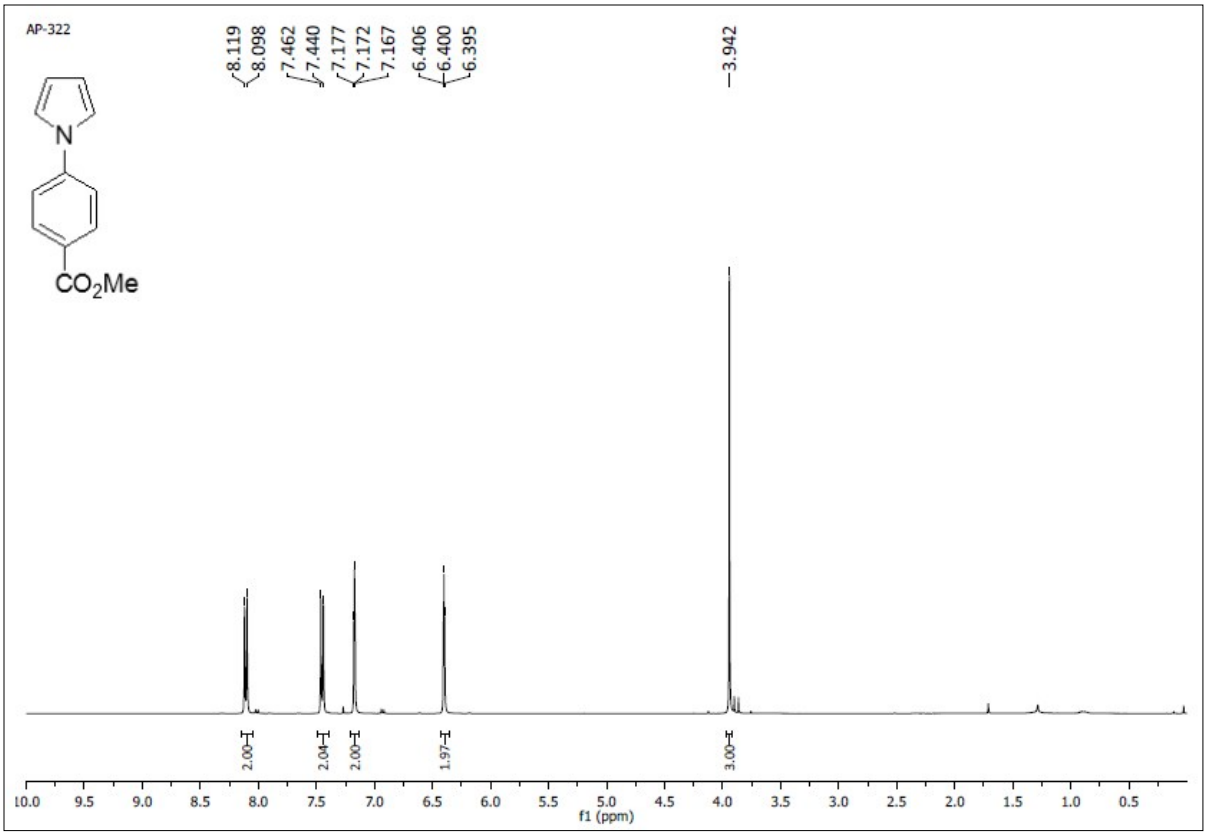

AP-321
140.81
129.58
125.64
120.56
119.35
110.45
77.41
77.09
76.77
N
f1 (ppm)

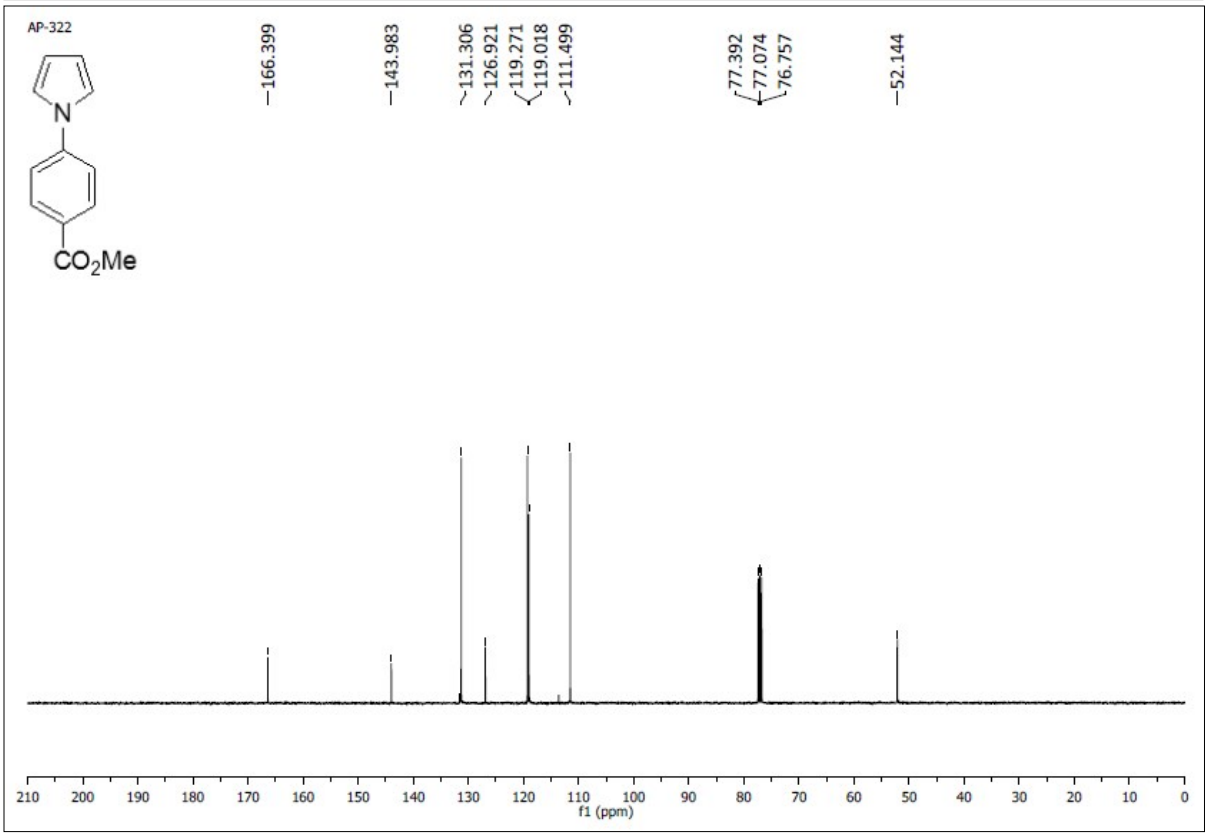

AP-323
7.365
7.344
7.292
7.272
7.140
7.135
7.130
6.425
6.420
6.415
2.444
1.87
2.20
2.02
1.88
3.03
f1 (ppm)

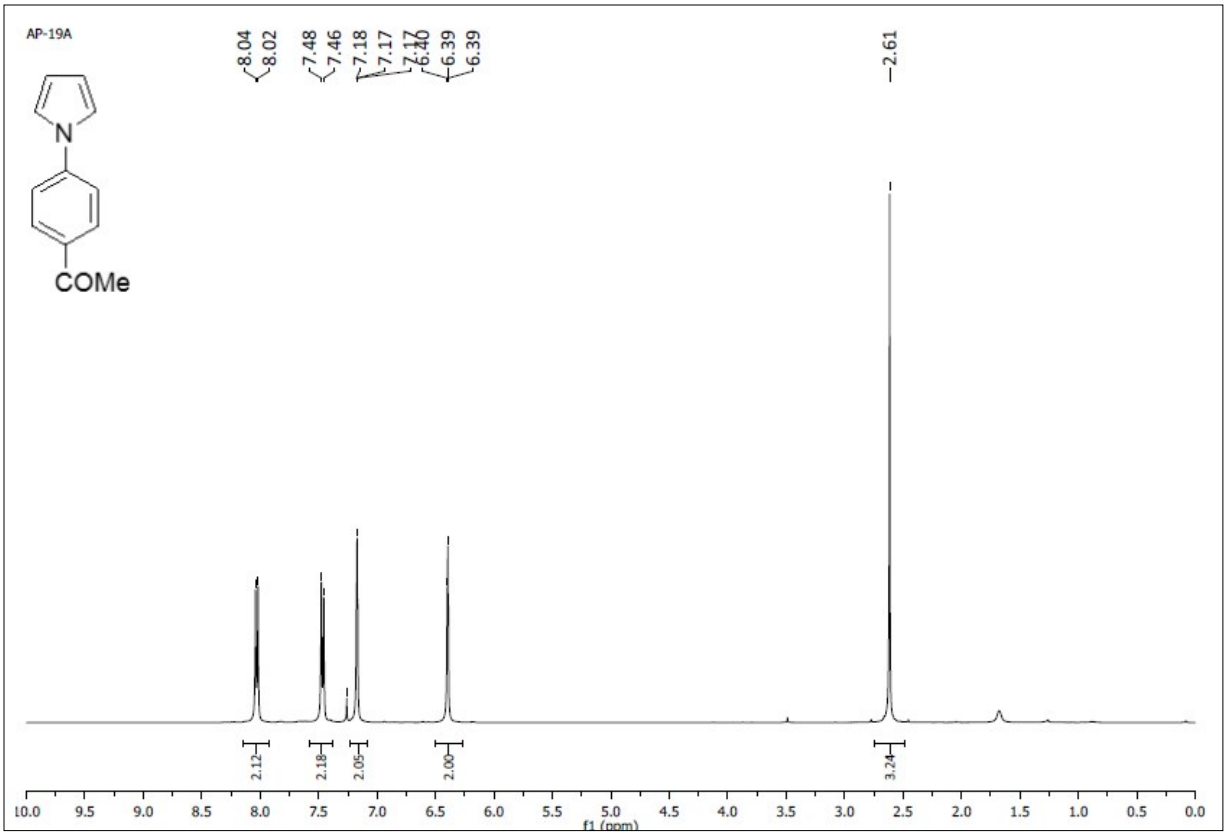

AP-323
138.561
135.385
130.095
120.569
119.423
110.148
77.436
77.118
76.800
20.887
f1 (ppm)

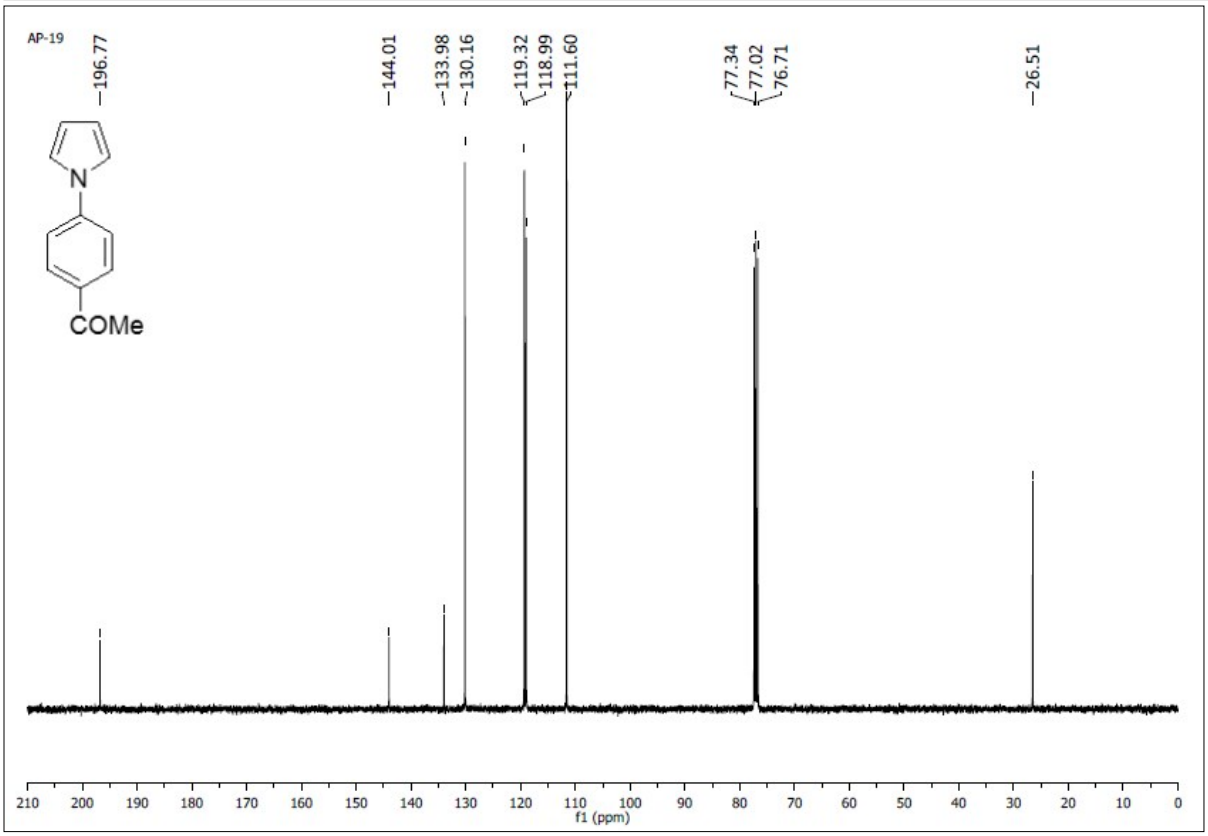

Aug02-2016
AP-332
7.3097
7.3012
7.2955
7.2843
7.2787
7.2700
6.9902
6.9849
6.9794
6.9458
6.9372
6.9315
6.9204
6.9148
6.9059
6.8886
6.3167
6.3113
6.3059
3.8072
N
OMe
1.03
1.02
1.10
1.00
1.57
f1 (ppm)

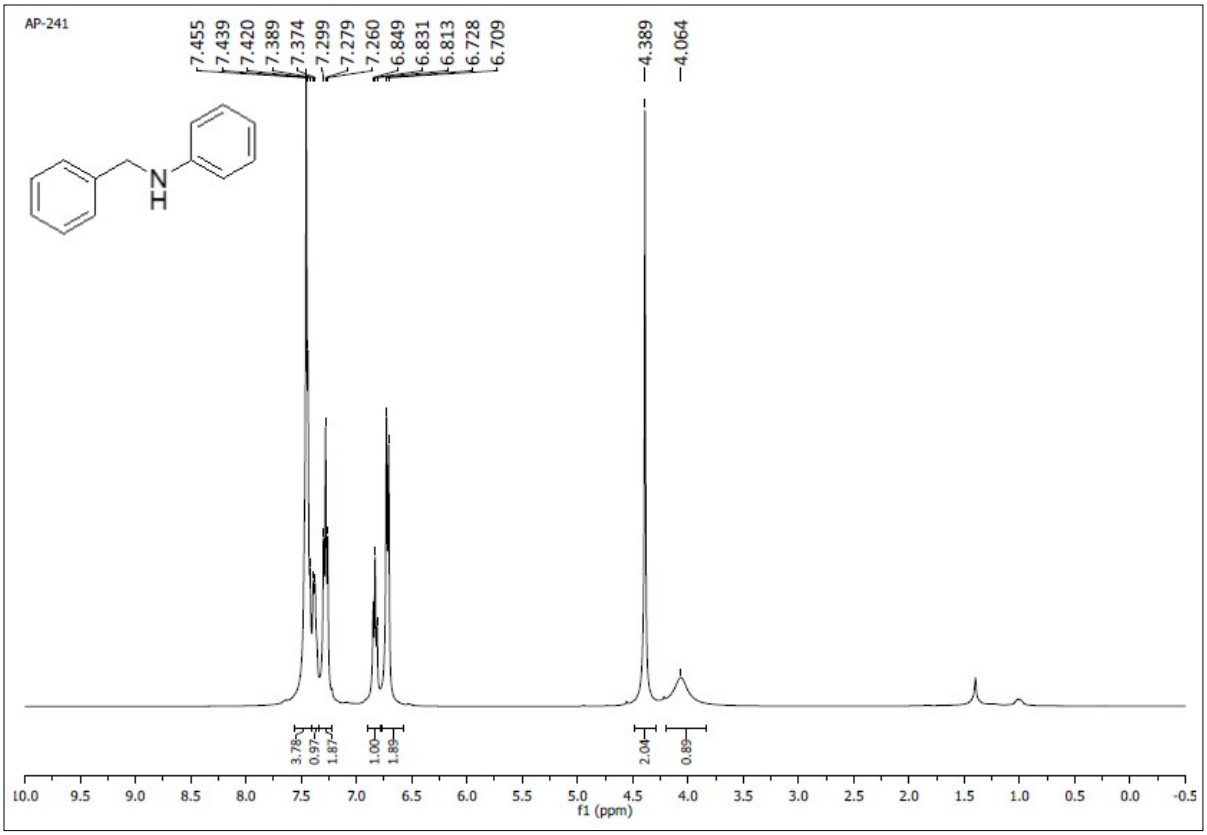

Aug02-2016
AP-332
157.71
134.55
122.21
119.72
114.67
109.89
77.41
77.09
76.77
55.58
N
OMe
f1 (ppm)

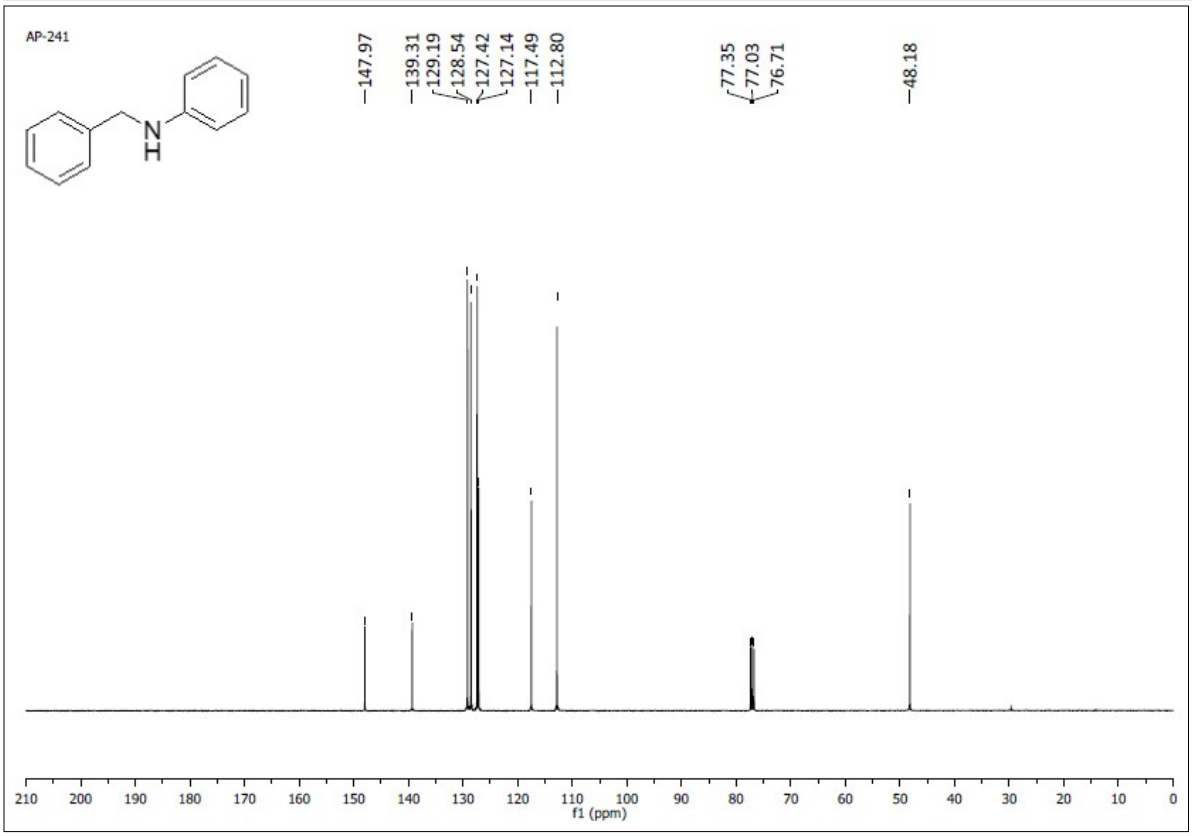

AP-322
8.119
8.098
7.462
7.440
7.177
7.172
7.167
6.406
6.400
6.395
3.942
N
CO2Me
2.00
2.04
2.00
1.97
3.00
f1 (ppm)

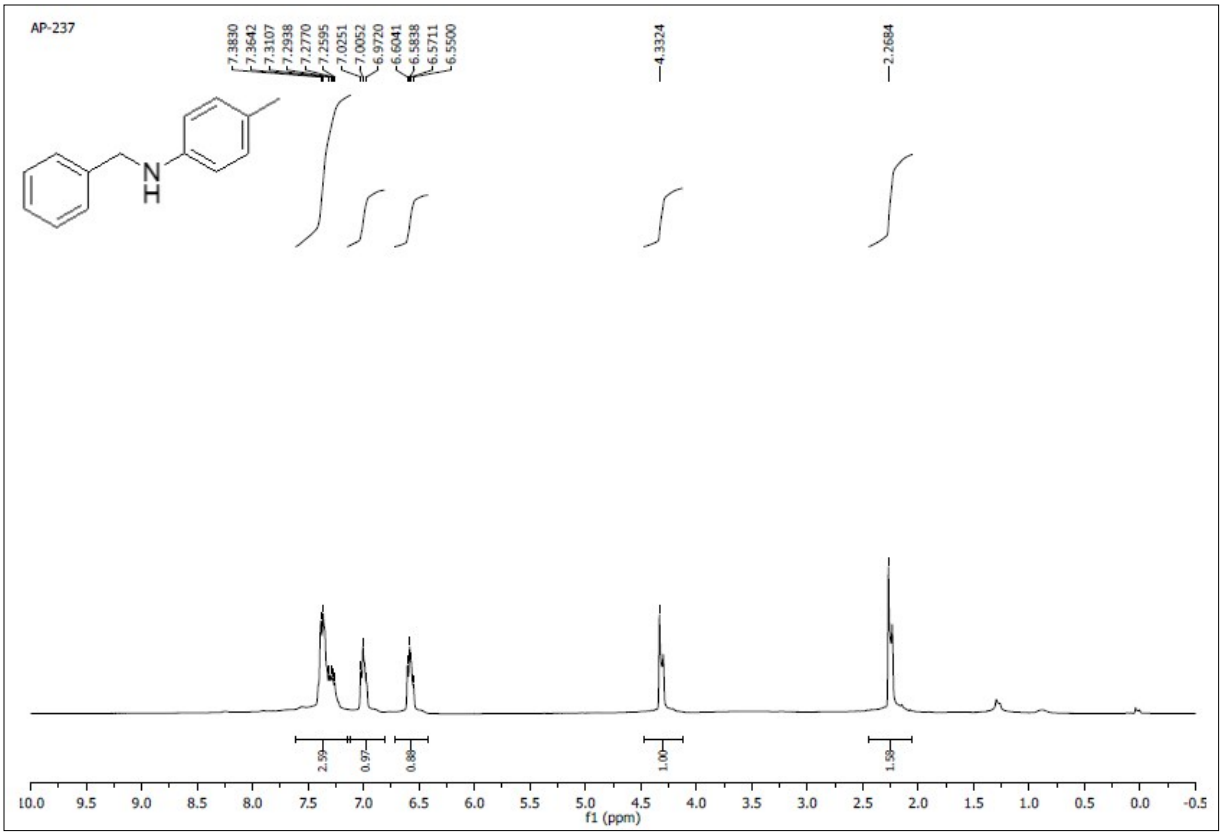

AP-322
166.399
143.983
131.306
126.921
119.271
119.018
111.499
77.392
77.074
76.757
52.144
N
CO2Me
f1 (ppm)

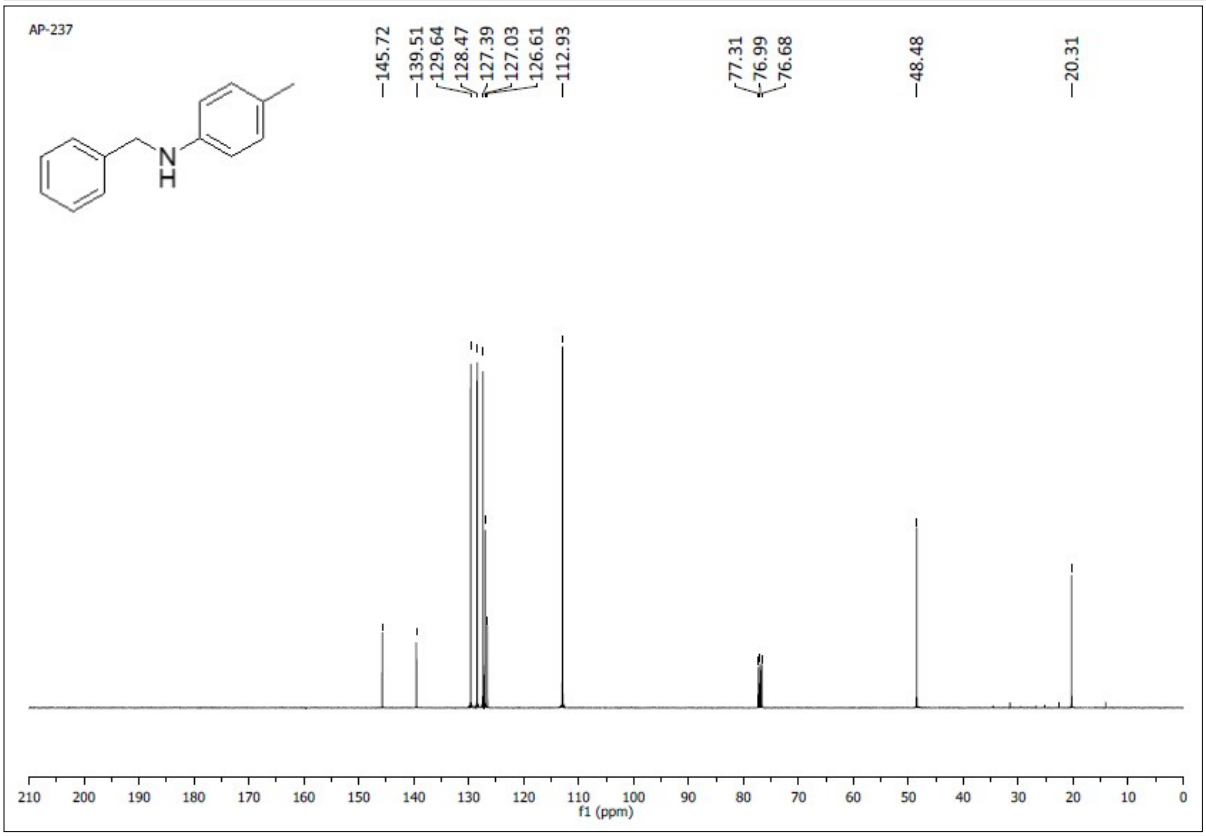

AP-19A
8.04
8.02
7.48
7.46
7.18
7.17
7.17
6.40
6.39
6.39
2.61
N
COMe
2.12
2.18
2.05
2.00
3.24
f1 (ppm)

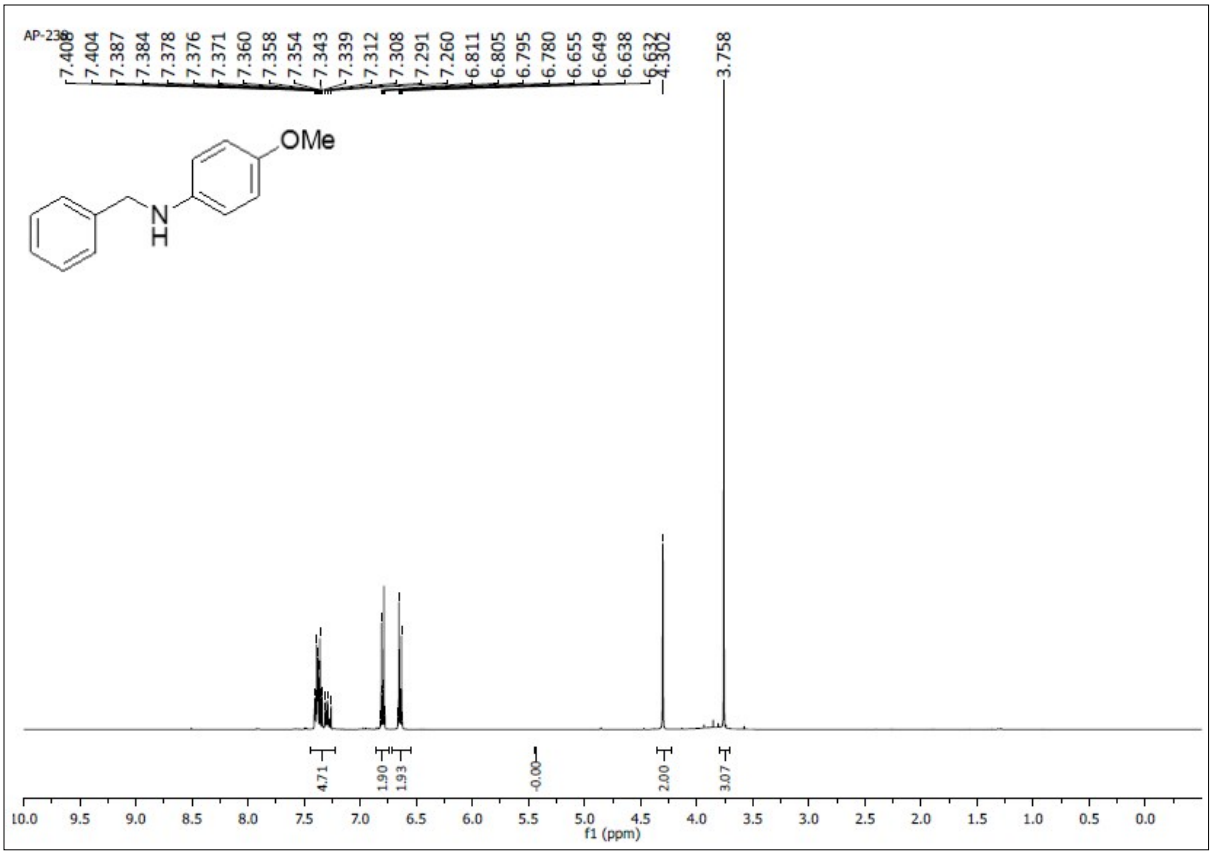

AP-19
196.77
144.01
133.98
130.16
119.32
118.99
111.60
77.34
77.02
76.71
26.51
N
COMe
f1 (ppm)

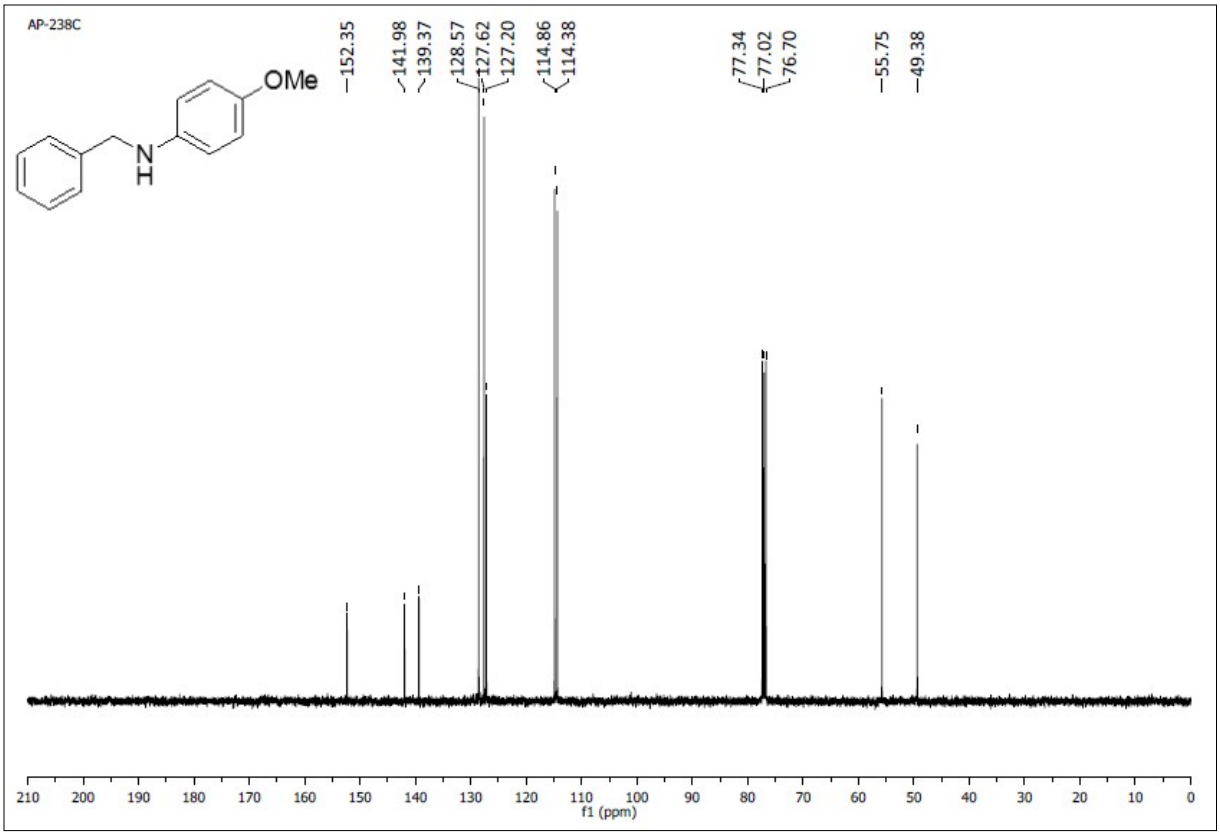

AP-241
7.455
7.439
7.420
7.389
7.374
7.299
7.279
7.260
6.849
6.831
6.813
6.728
6.709
4.389
4.064
3.78
0.97
1.87
1.00
1.89
2.04
0.89
f1 (ppm)

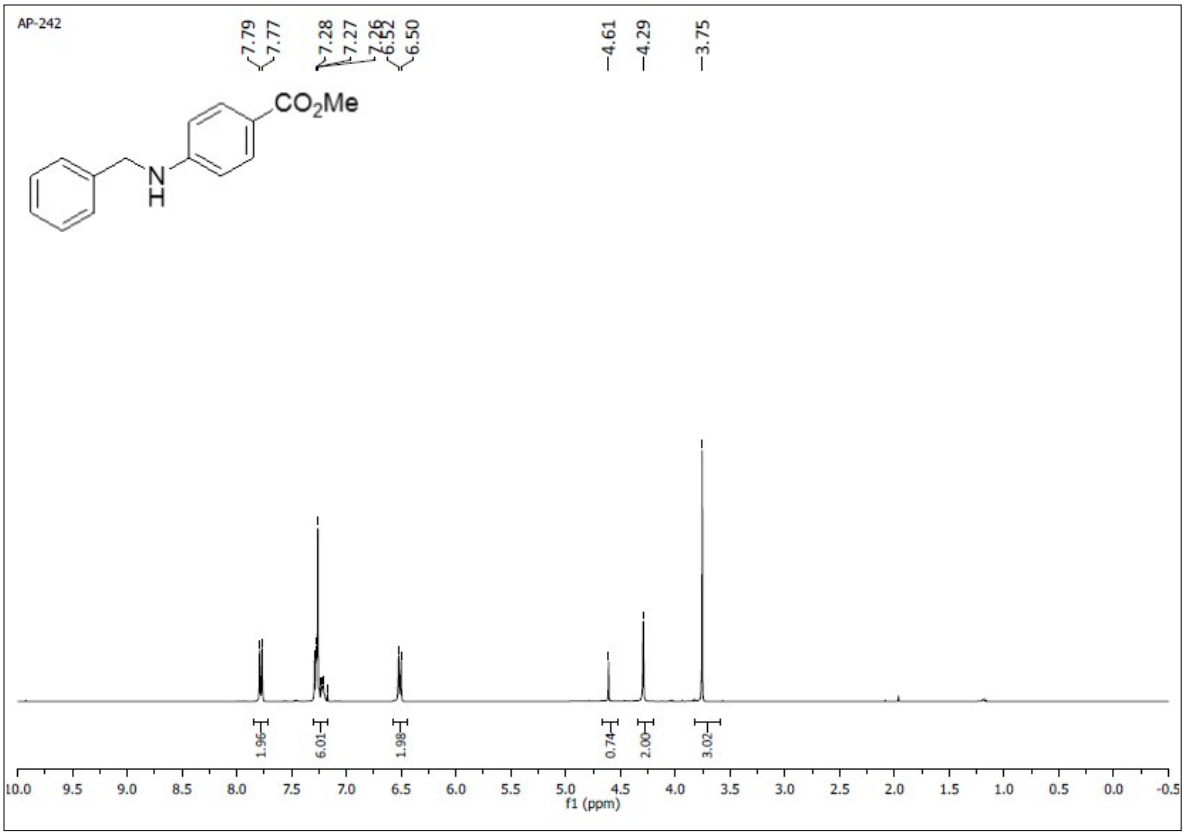

AP-241
147.97
139.31
129.19
128.54
127.42
127.14
117.49
112.80
77.35
77.03
76.71
48.18
f1 (ppm)

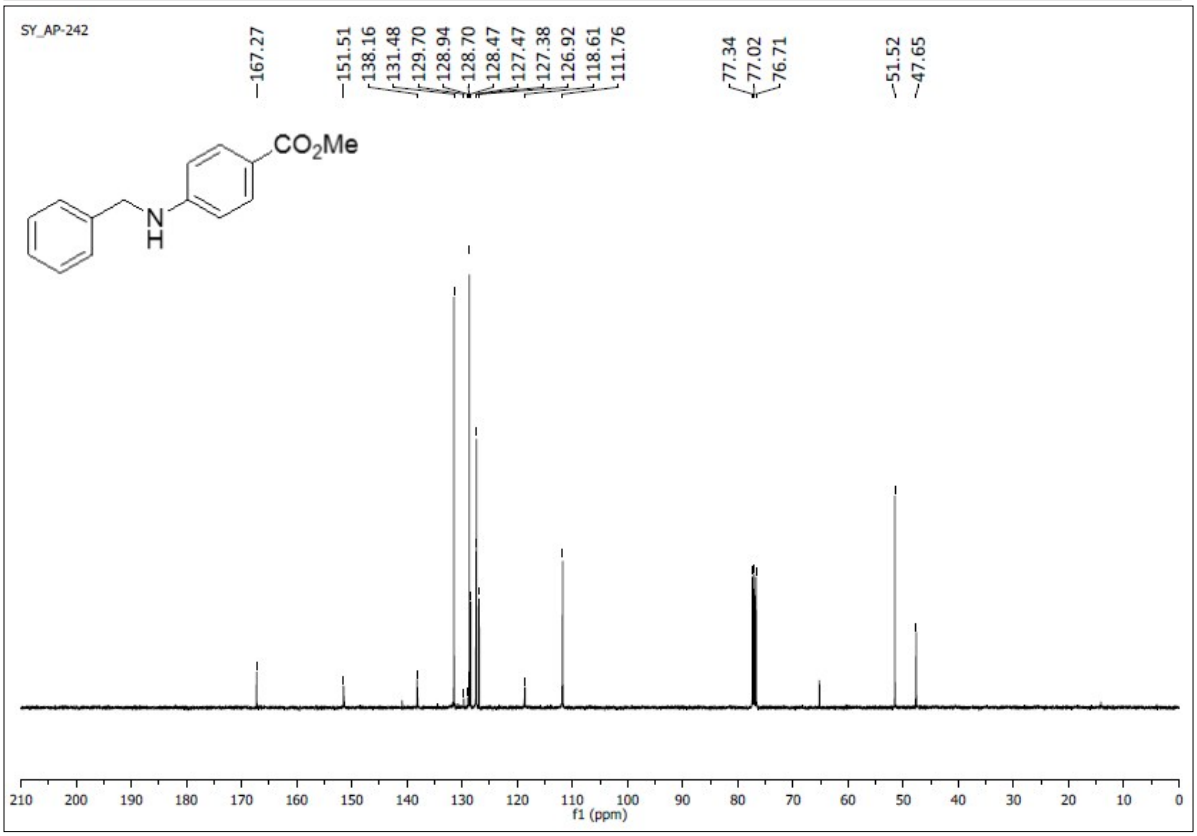

AP-237
7.3830
7.3642
7.3107
7.2938
7.2770
7.2595
7.0251
7.0052
6.9720
6.6041
6.5838
6.5711
6.5500
4.3324
2.2684
2.99
0.97
0.88
1.00
1.59
f1 (ppm)


AP-237
145.72
139.51
129.64
128.47
127.39
127.03
126.61
112.93
77.31
76.99
76.68
48.48
20.31
f1 (ppm)


AP-238
7.408
7.404
7.387
7.384
7.378
7.376
7.371
7.360
7.358
7.354
7.343
7.339
7.312
7.308
7.291
7.260
6.811
6.805
6.795
6.780
6.655
6.649
6.638
6.632
4.302
3.758
OMe
N
H
4.71
1.90
1.93
0.00
2.00
3.07
f1 (ppm)


AP-238C
152.35
141.98
139.37
128.57
127.62
127.20
114.86
114.38
77.34
77.02
76.70
55.75
49.38
OMe
N
H
f1 (ppm)


AP-242
7.79
7.77
7.28
7.27
6.52
6.50
4.61
4.29
3.75
CO2Me
N
H
1.96
6.01
1.98
0.74
2.00
3.02
f1 (ppm)


SY_AP-242
167.27
151.51
138.16
131.48
129.70
128.94
128.70
128.47
127.47
127.38
126.92
118.61
111.76
77.34
77.02
76.71
51.52
47.65
CO2Me
N
H
f1 (ppm)