Supporting Information for

N,*O*-Bidentate ligand-tunable copper(II) complexes as catalyst for Chan-Lam coupling reactions of arylboronic acids with 1*H*-imidazole derivatives

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1. Gerenal experimental information

All coupling reactions were performed under air conditions. Imidazole derivatives and arylboronic Acids were purchased and directly used without purification. The solvents were distilled prior to use. Preparative thin layer chromatography was performed on GF-254 silica gel. The ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker-600 spectrometer using $CDCl_3$ as the solvent at 600 and 150 MHz, respectively. Chemical shifts are given as δ value with $(CH_3)_4Si$ as the internal standard. The coupling constants (*J*) are reported in Hertz (Hz). HRMS data were obtained by ESI on a TOF mass spectrometer.

2. NMR data of the products (3aa-3ak)

1-Phenyl-*1H-benzimidazole (3aa)*.[1, 2] Slightly yellow oil (39.6 mg, 92% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 (s, 1H), 7.93 (dd, *J* = 2.4, 6.6 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 2H),7.55-7.51 (m, 3H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.36-7.34 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 142.21, 136.14, 133.64, 130.13, 128.28, 127.46, 124.16, 123.97, 123.15, 120.43, 110.62.

1-(4-Methylphenyl)-1H-benzimidazole (3ab).[1] Pale yellow solid (43.8 mg, 96% yield); mp: 114-115 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10 (s, 1H), 7.88-7.87 (m, 1H), 7.51-7.49 (m,1H), 7.39-7.35 (m, 4H), 7.33-7.31 (m, 2H), 2.45 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.87, 142.44, 138.17, 133.89, 133.76, 130.59, 124.02, 123.63, 122.73, 120.51, 110.51, 21.14.

1-(4-t-Butylphenyl)-1H-benzimidazole (3ac).[3] Pale yellow solid (50.8 mg, 94% yield); mp: 108-109 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.11 (s, 1H), 7.89 (dd, *J* = 1.8, 6.0 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.54 (dd, *J* = 2.4, 6.6 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.33-7.31(m, 2H), 1.39 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.35, 143.89, 142.45, 133.86, 133.70, 126.94, 123.72, 123.62, 122.74, 120.51, 110.61, 34.80, 31.35.

1-(4-Methoxyphenyl)-1H-benzimidazole (3ad).[2, 4] Pale yellow solid (43 mg, 88% yield); mp: 93-94 °C (lit:[13] 96-97 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.99 (s, 1H), 7.81 (dd, *J* = 1.8, 6.6 Hz, 1H), 7.37-7.36 (m, 1H), 7.33 (d, *J* = 9.0 Hz, 2H), 7.25-7.23(m, 2H), 6.99(d, *J* = 9.0 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.37, 141.44, 133.19, 128.02, 124.73, 122.59, 121.68, 119.39, 114.11, 111.95, 109.37, 54.62.

1-(2-Methylphenyl)-1H-benzimidazole (3ae).[5] Pale yellow solid (39.7 mg, 87% yield); mp: 164-165 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97 (s, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.45-7.42 (m, 2H), 7.38-7.36 (m, 1H), 7.34-7.31 (m, 2H), 7.28-7.26 (m, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 2.11 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.30, 142.98, 135.40, 134.77, 134.72，131.54, 129.35, 127.69, 127.19, 123.53, 122.51, 120.42, 110.52, 17.62.

1-(3-Benzyloxyphenyl)-1H-benzimidazole (3af). Pale yellow solid (62.7 mg, 98% yield); mp: 102-103 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10 (s, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.45-7.44 (m, 2H), 7.43 (d, *J* = 1.8

Hz, 2H), 7.41-7.39 (m, 2H), 7.36-7.35 (m, 1H), 7.32 (dd, *J* = 1.2, 7.8 Hz, 1H), 7.30 (dd, *J* = 1.8, 8.4 Hz, 1H), 7.10-7.05 (m, 3H), 5.13 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.86, 144.01, 142.24, 137.40, 136.30, 133.54, 130.91, 128.79, 128.27, 127.47, 123.76, 122.87, 120.60, 116.27, 114.52, 110.78, 110.64, 70.35. HRMS (ESI) *m*/*z*: calcd for $C_{20}H_{16}N_2O$ $[M + H]^+$ 301.1341 found 301.1335.

1-(4-Fluorophenyl)-1H-benzimidazole (3ag).[3] Slightly yellow oil (45.5 mg, 98% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.89 (dd, *J* = 1.8, 5.4 Hz, 1H), 7.49-7.45 (m, 3H), 7.36-7.33 (m, 2H), 7.27 (dd, *J* = 2.4, 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.86, 161.21, 143.81, 142.33, 133.91, 132.36(*J* = 3.0 Hz), 126.11(*J* = 9.0 Hz), 123.89, 122.96, 120.66, 117.14, 116.99, 110.19.

1-(3-Chlorophenyl)-1H-benzimidazole (3ah). Slightly yellow oil (45.3 mg, 97% yield); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.11 (t, *J* = 2.4 Hz, 1H)，7.89-7.87 (m, 1H), 7.55-7.49(m, 3H), 7.45-7.40(m, 2H), 7.36-7.34 (m, 2H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.01, 141.99, 137.46, 135.75, 133.35, 131.13, 128.21, 124.17, 124.06, 123.16, 122.08, 120.79, 110.32. HRMS (ESI-TOF) *m*/*z*: calcd for $C_{13}H_9N_2Cl$ $[M + H]^+$ 229.0532, found 229.0538.

1-(3-Nitrophenyl)-1H-benzimidazole (3ai).Pale yellow solid (37.3 mg, 72% yield); mp: 172-173 ºC; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.43 (s, 1H), 8.33 (dd, *J* = 1.2, 8.4 Hz, 1H), 8.18 (s, 1H), 7.90-7.89 (m, 2H), 7.81 (t, *J*

= 7.8 Hz, 1H), 7.56 (t, *J* = 4.8 Hz, 1H), 7.39 (t, *J* = 4.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 149.26, 144.17, 141.72, 137.52, 133.08, 131.23, 129.44, 124.49, 123.56, 122.58, 121.07, 118.72, 110.01. HRMS (ESI-TOF) *m*/*z*: calcd for $C_{13}H_9N_3O_2$ $[M + H]^+$ 240.0773, found 240.0768.

1-Naphthyl-1H-benzimidazole (3aj).[6] Pale yellow solid (49.1 mg, 93% yield); mp: 72-73 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.14 (s, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.4Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.62(t, *J* = 7.8 Hz, 1H), 7.59-7.55 (m, 2H), 7.46-7.42 (m, 2H), 7.36(t, *J* = 8.4 Hz, 1H), 7.25(t, *J* = 7.2 Hz, 1H), 7.10 (d, *J* = 8.4Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 143.79, 143.40, 135.67, 134.46, 132.39, 129.82, 129.71, 128.50, 127.58, 127.09, 125.50, 124.96, 123.64, 122.73, 122.59, 120.60, 110.85.

1- Thienyl-1H-benzimidazole (3ak).[7] Pale yellow solid (39.2 mg, 89% yield); mp: 48-49 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.87-7.85 (m, 1H), 7.57-7.55 (m, 1H), 7.37-7.35 (m, 2H), 7.32 (dd, *J* = 1.2, 5.4 Hz, 1H), 7.17 (dd, *J* = 1.2, 3.6 Hz, 1H), 7.12 (dd, *J* = 3.6, 5.4 Hz, 1H); ^{13}C NMR(150 MHz, $CDCl_3$): δ 143.19, 132.33, 130.92, 128.85, 126.44, 124.13, 123.44, 123.20, 121.94, 120.16, 110.53.

3. NMR data of the products (3ba-3ia)

1-Phenyl-1H-imidazole (3ba).[1, 13] Pale yellow solid (27.7 mg, 96% yield); mp: 52-53 °C (lit:[13] 54-55 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88

(s, 1H), 7.49 (t, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.29 (s, 1H), 7.22 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 137.38, 135.65, 130.40, 129.91, 127.54, 121.54, 118.29.

1-Phenyl-4-methyl-1H-imidazole (3ca).[8] Pale yellow solid (26.6 mg, 84% yield); mp: 58-59 °C (lit:[8] 61-63 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 (s, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.36(d, *J* = 7.8 Hz, 2H), 7.33(d, *J* = 7.8 Hz, 1H), 7.01 (s, 1H), 2.30 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.53, 137.51, 134.54, 130.45, 129.83, 127.12, 122.02, 121.11, 114.63, 13.7.

1-Phenyl-4-nitro-1H-imidazole (3da).[9] Pale yellow solid (28.7 mg, 76% yield); mp: 184-185 °C (lit:[9] 187-188 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.73(d, *J* = 7.2 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 2H) , 7.38 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.53, 131.32, 128.86, 127.66, 127.22, 123.37, 121.90, 119.34, 109.34.

1-Phenyl-2-chloromethyl-1H-benzimidazole(3ea).[10] Pale yellow solid (39.2 mg, 81% yield); mp: 98-99 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 2H), 7.53 (dd, *J* = 1.2, 5.4 Hz, 1H), 7.49-7.47 (m, 2H), 7.33-7.30 (m, 1H), 7.28 (dd, *J* = 1.2, 8.4 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 4.58 (s, 2H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.22, 142.29, 136.46, 135.68, 129.77, 128.86, 126.93, 123.63, 122.81, 120.11, 110.58, 66.27, 58.39.

1-Phenyl-2-mercapto-1H-benzimidazole (3fa). Pale yellow solid (42.1 mg, 93% yield); mp: 124-125 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.13(s, 1H), 7.89-7.88 (m, 1H), 7.59 (t, *J* = 8.4 Hz, 2H), 7.56-7.54 (m, 1H), 7.53 (dd, *J* = 1.2, 8.4 Hz, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.36-7.33 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.05，142.31, 136.39, 133.73, 130.08, 128.07, 124.10, 123.72, 122.83, 120.63, 110.48. HRMS (ESI-TOF) *m*/*z*: calcd for $C_{13}H_{10}N_2S$ $[M + H]^+$ 227.0643, found 227.0651.

1-Phenyl-2-acetonitrile-1H-benzimidazole (3ga).[11] Pale yellow solid (34 mg, 73% yield); mp: 115-116 °C (lit:[11] 118-120 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.09(d, *J* = 7.8 Hz, 1H), 7.74 - 7.72 (m, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 1.8, 7.2 Hz, 2H), 7.50-7.48 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.38 (dd, *J* = 0.6, 7.8 Hz, 1H), 4.05 (d, *J* = 7.2 Hz, 2H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 170.14, 145.53, 136.02, 131.32, 129.90, 128.86, 127.66, 127.22, 123.37, 121.90, 119.35, 109.35, 59.38.

1-Phenyl-1H-1,2,4-triazole (3ha).[8, 12] Pale yellow solid (27.9 mg, 96% yield); mp: 42-43 °C (lit:[8] 44-44.5 °C); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.54 (s, 1H), 8.08 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.01, 136.87, 134.53, 130.99, 129.86, 128.48, 127.78, 120.18.

1-Phenyl-1H-benzotriazole (3ia).[8] Pale yellow solid (34.7 mg, 89% yield); mp: 88-89 °C (lit:[8] 85-86 °C) ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08

(d, J = 8.4 Hz, 1H), 7.72 (dd, J = 1.2, 9.0 Hz, 2H), 7.68 (d, J = 8.4 Hz, 1H), 7.55 (t, J = 7.8 Hz, 2H), 7.48 (dt, J = 0.6, 6.6 Hz, 1H), 7.45-7.42 (m, 1H), 7.37 (dt, J = 1.2, 7.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 146.54, 137.04, 132.34, 129.88, 128.68, 128.25, 124.40, 122.91, 120.35, 110.38.

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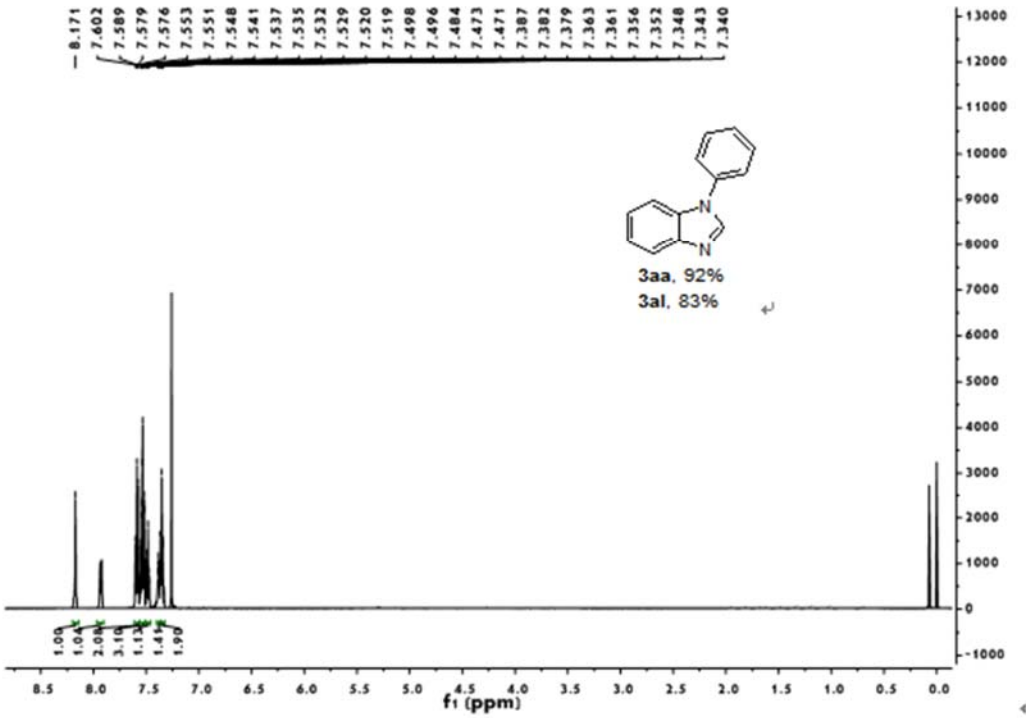
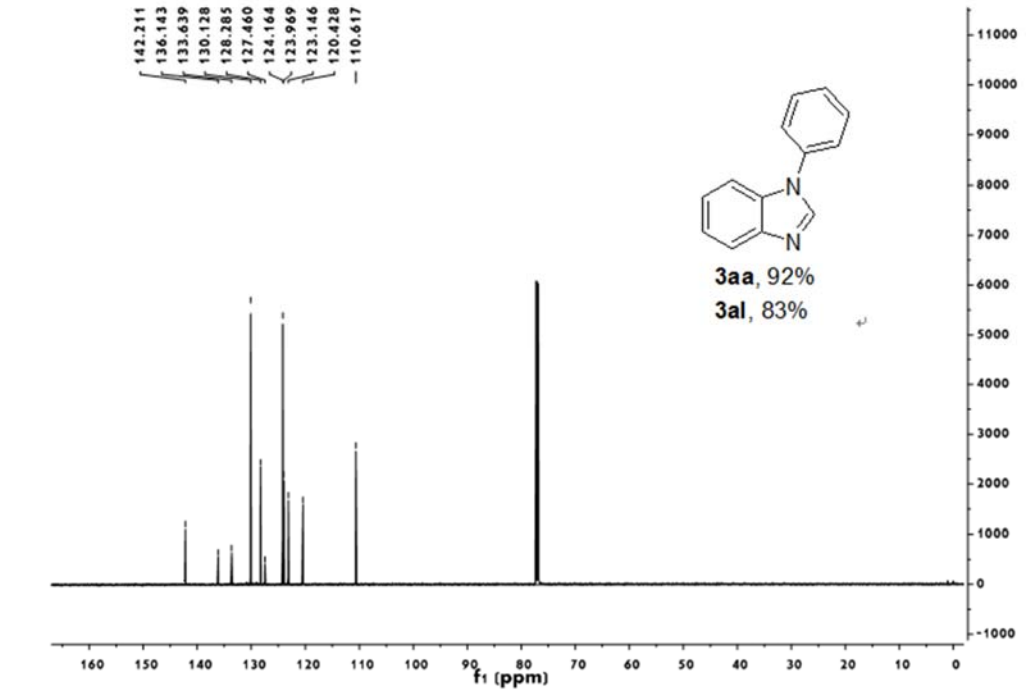
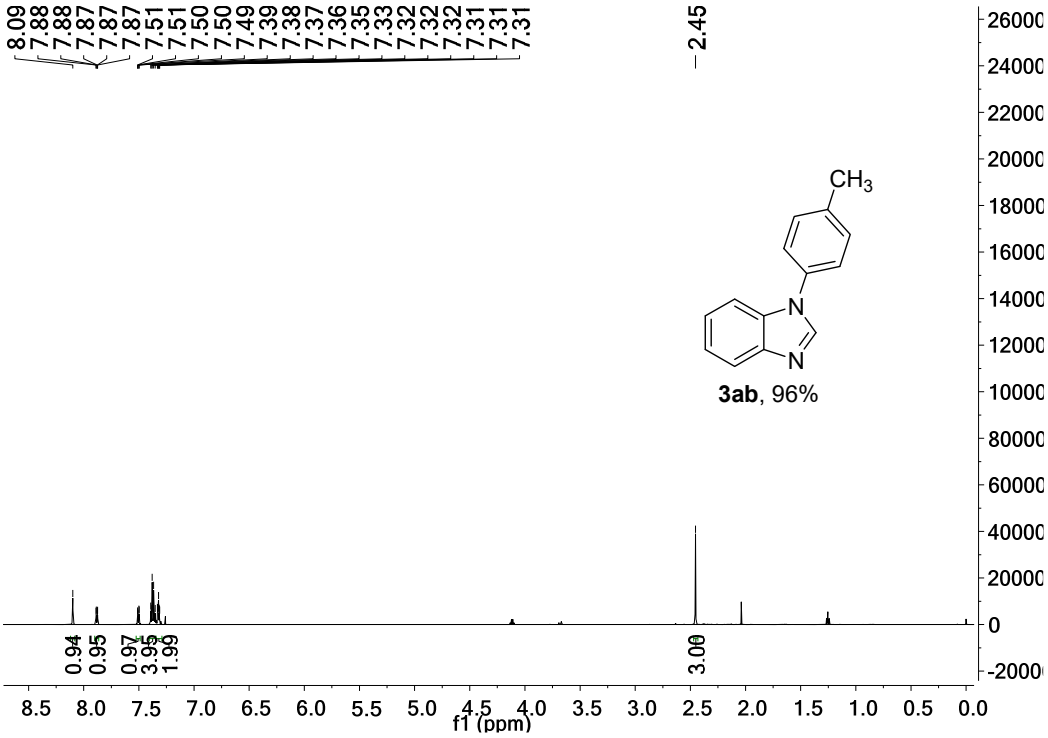
5. NMR Spectral Copies of the products (3aa-3ak)



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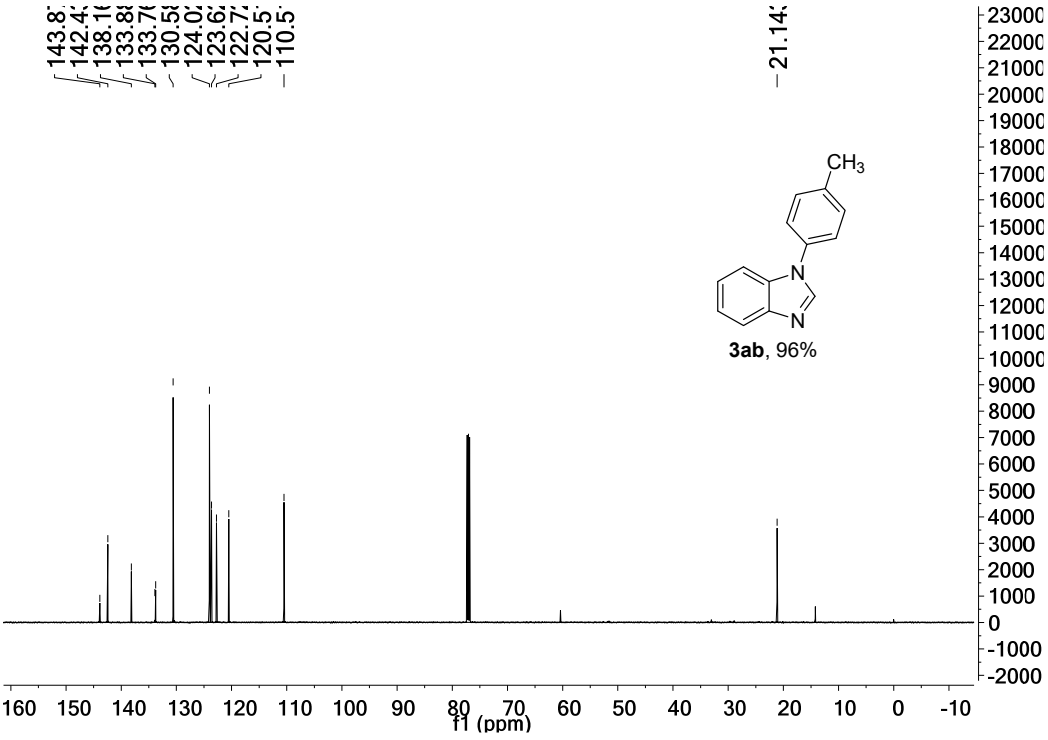
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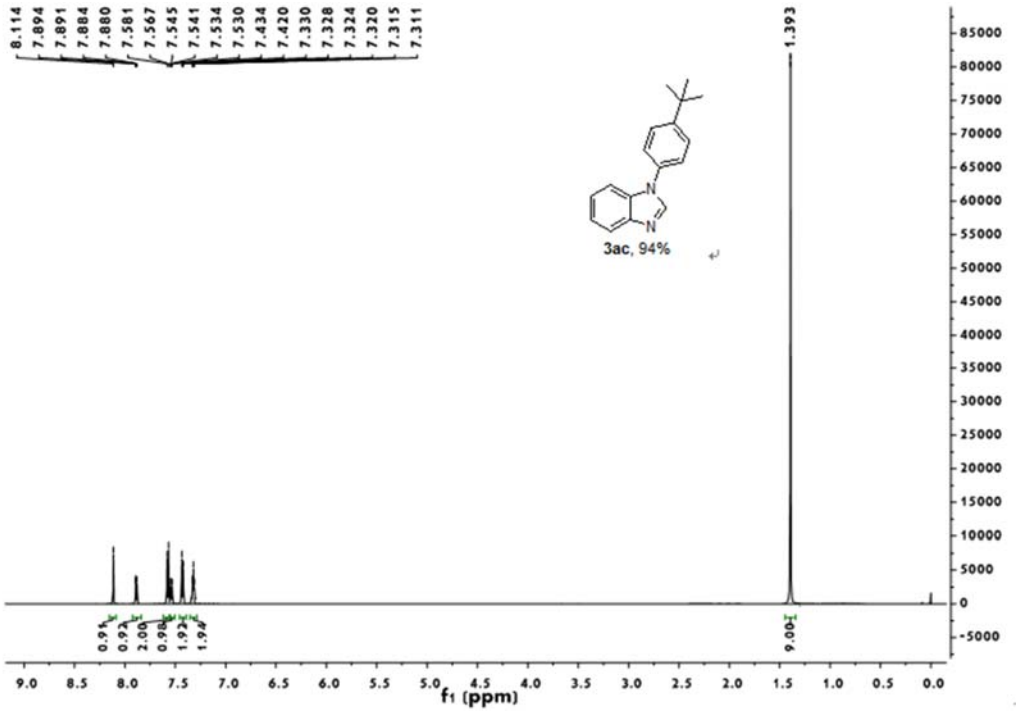
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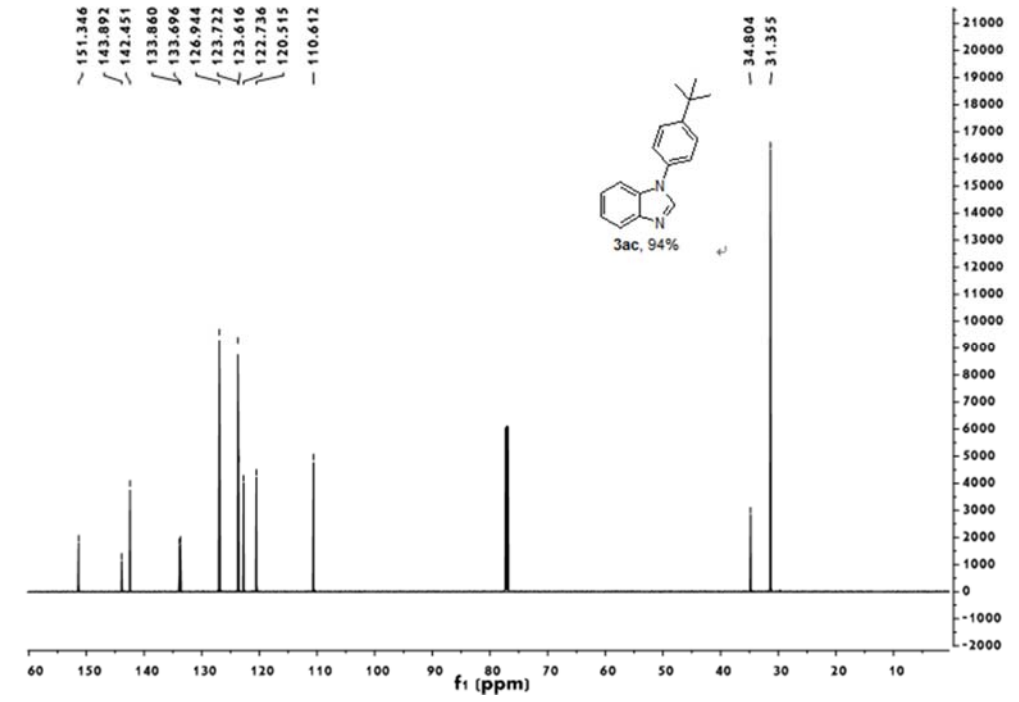
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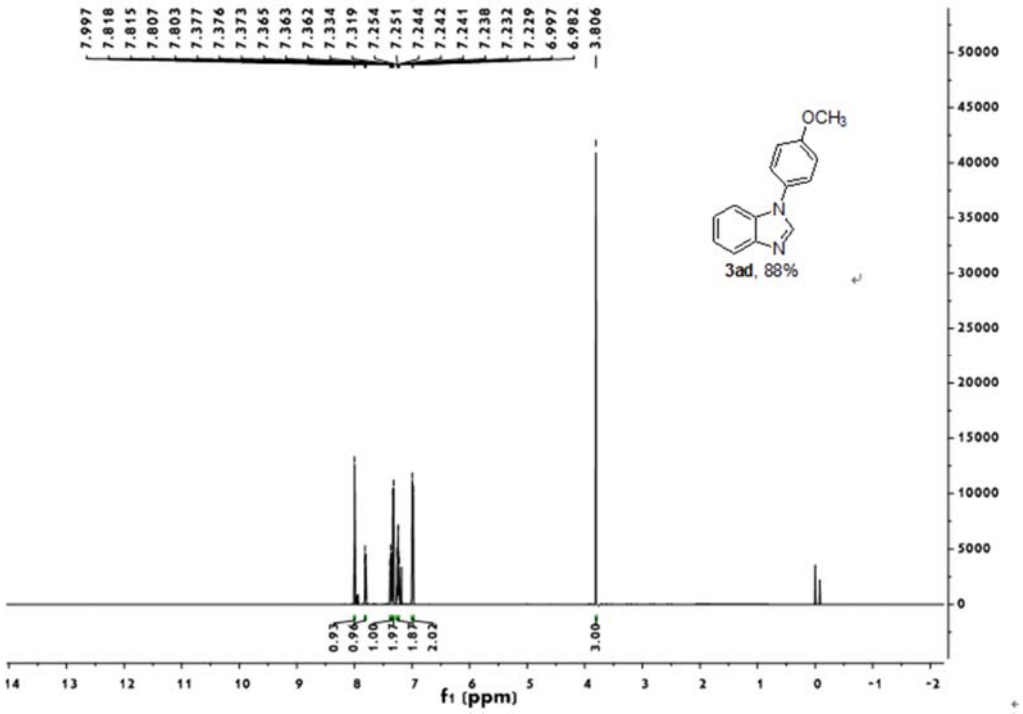
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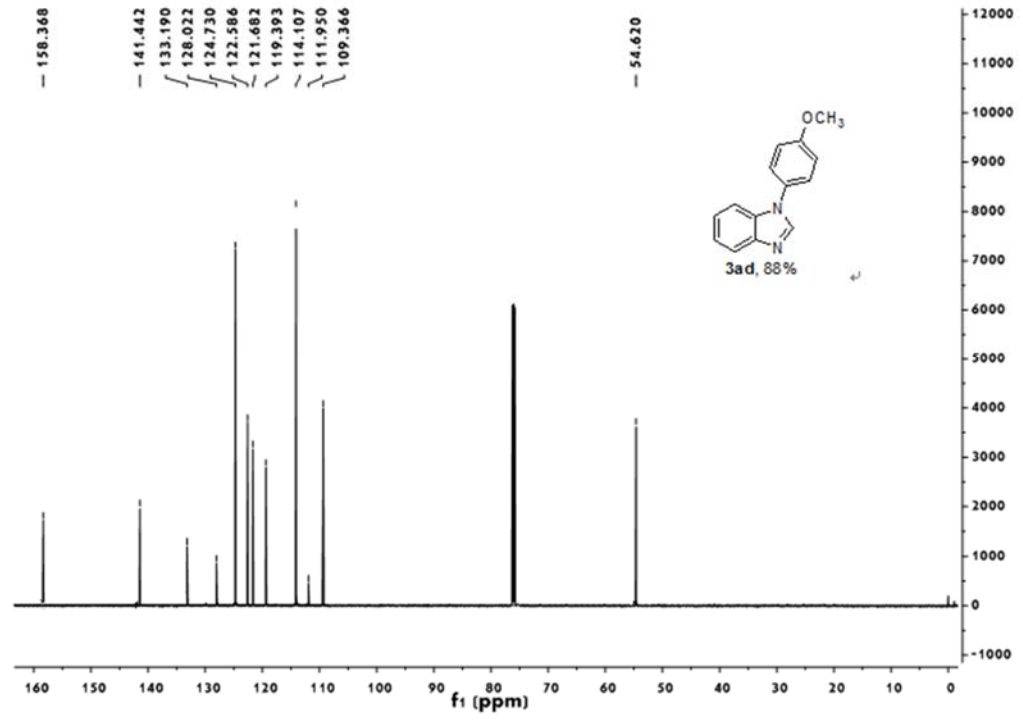
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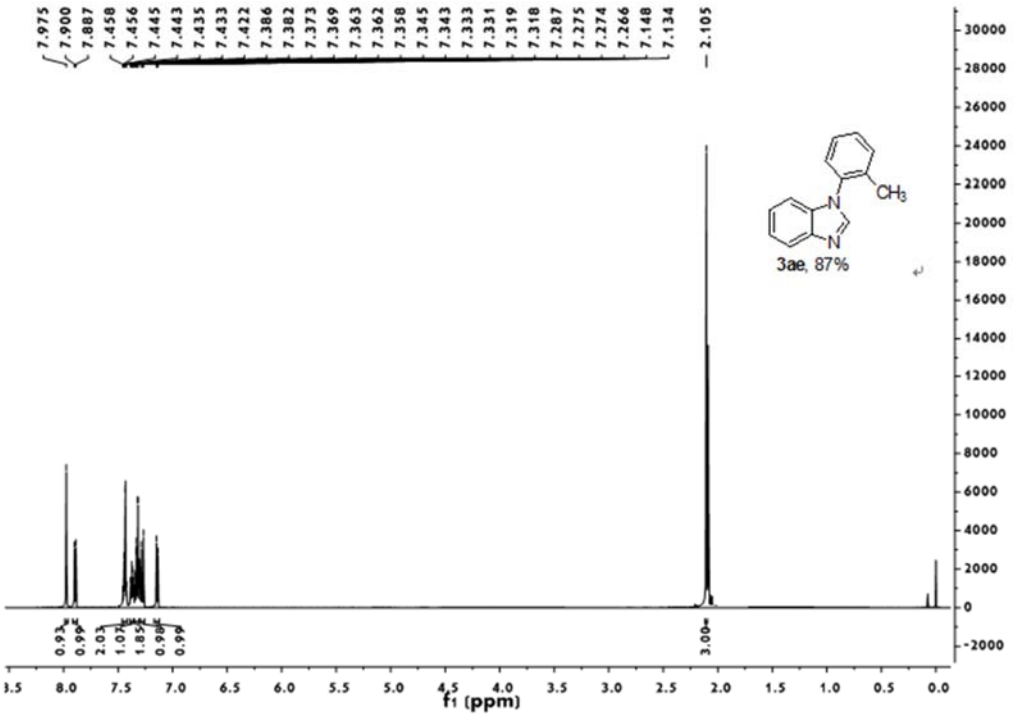
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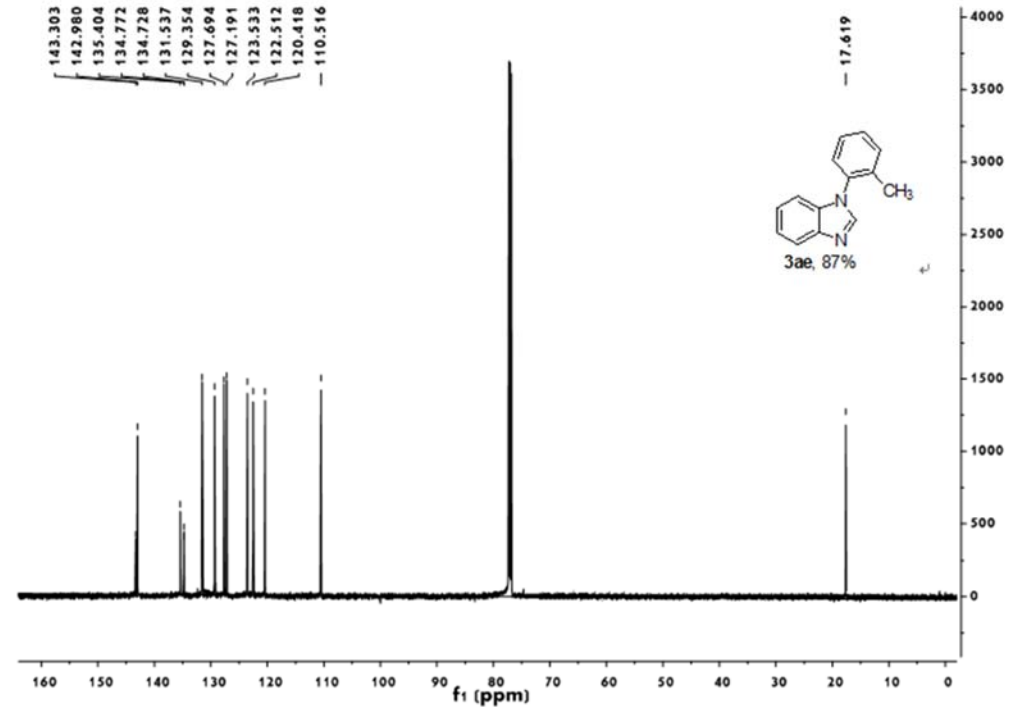
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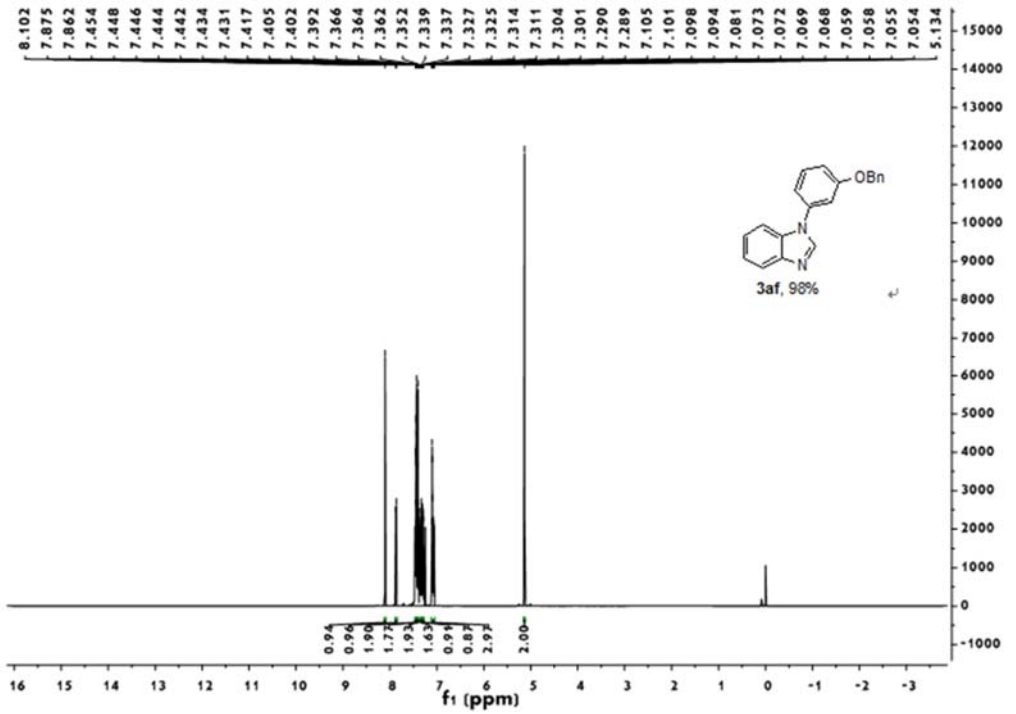
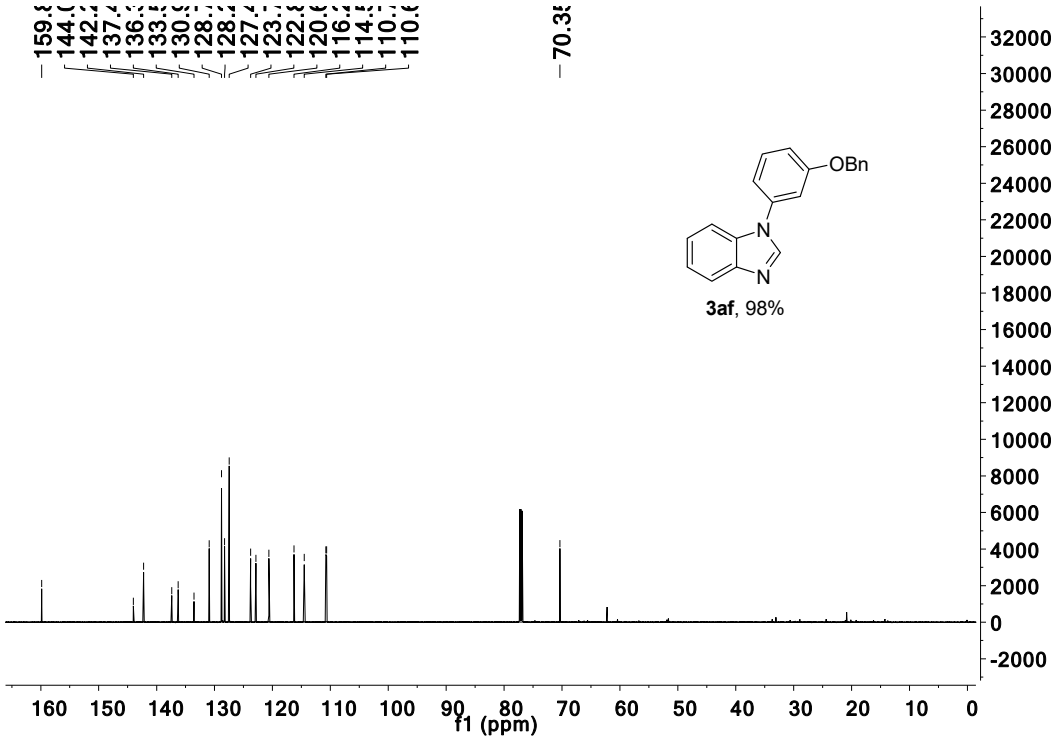
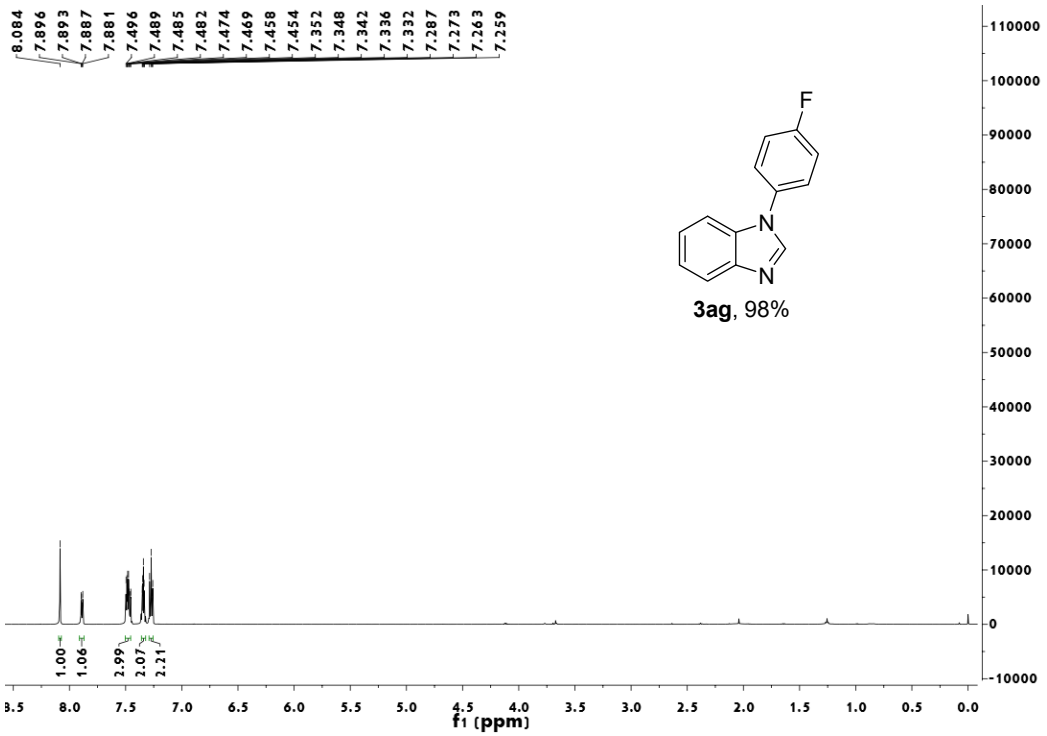
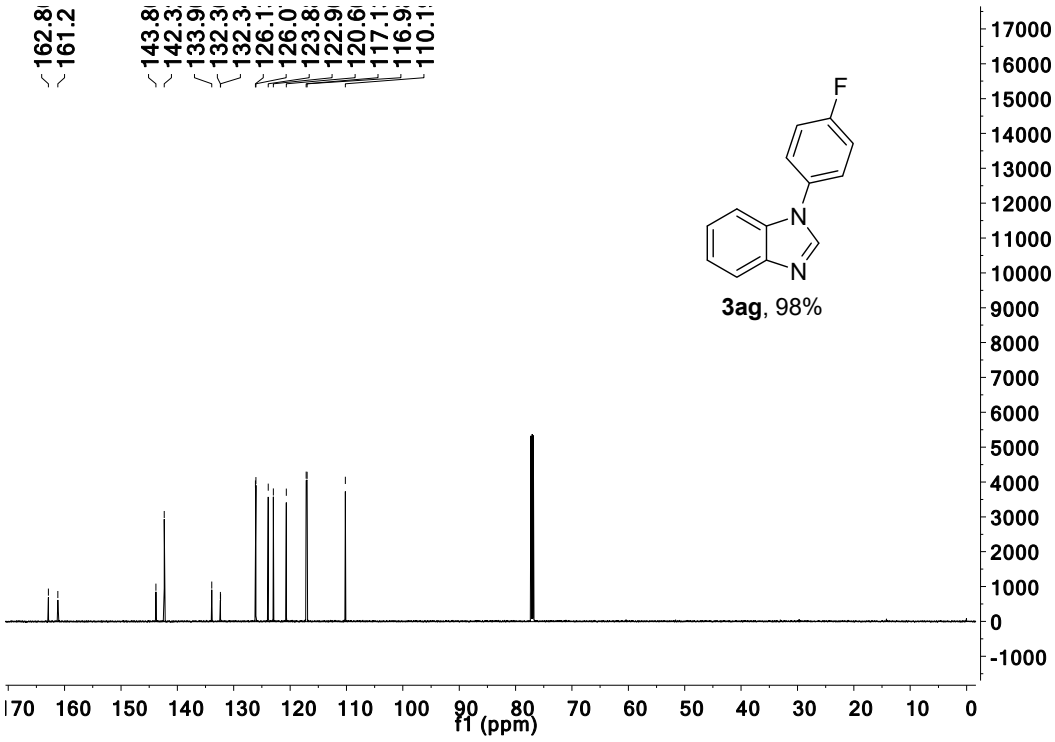
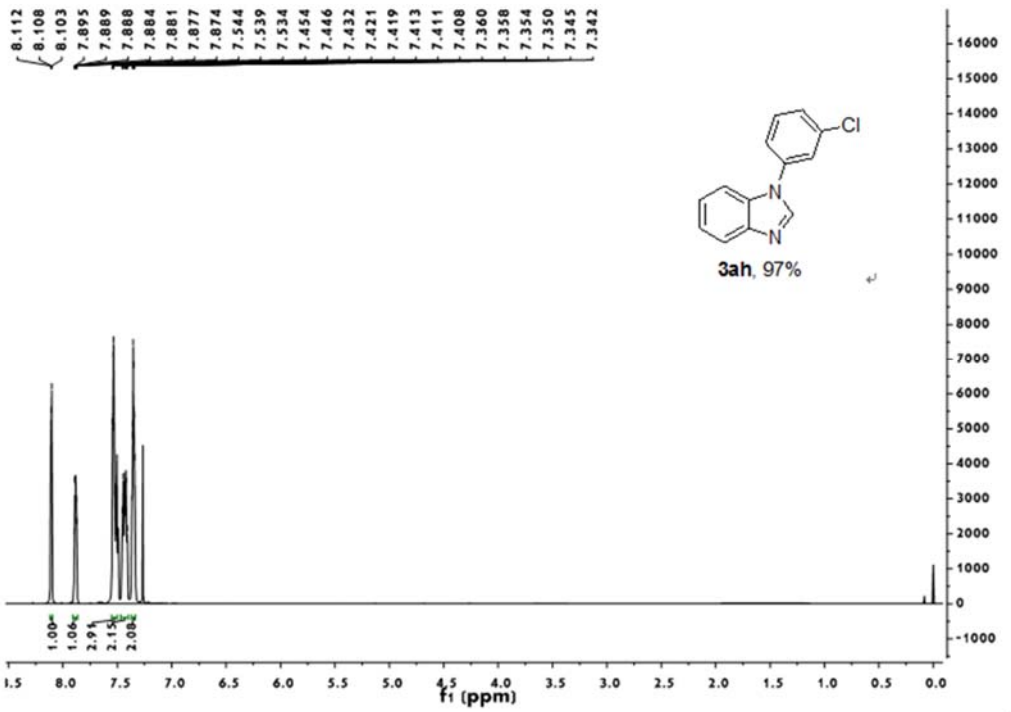
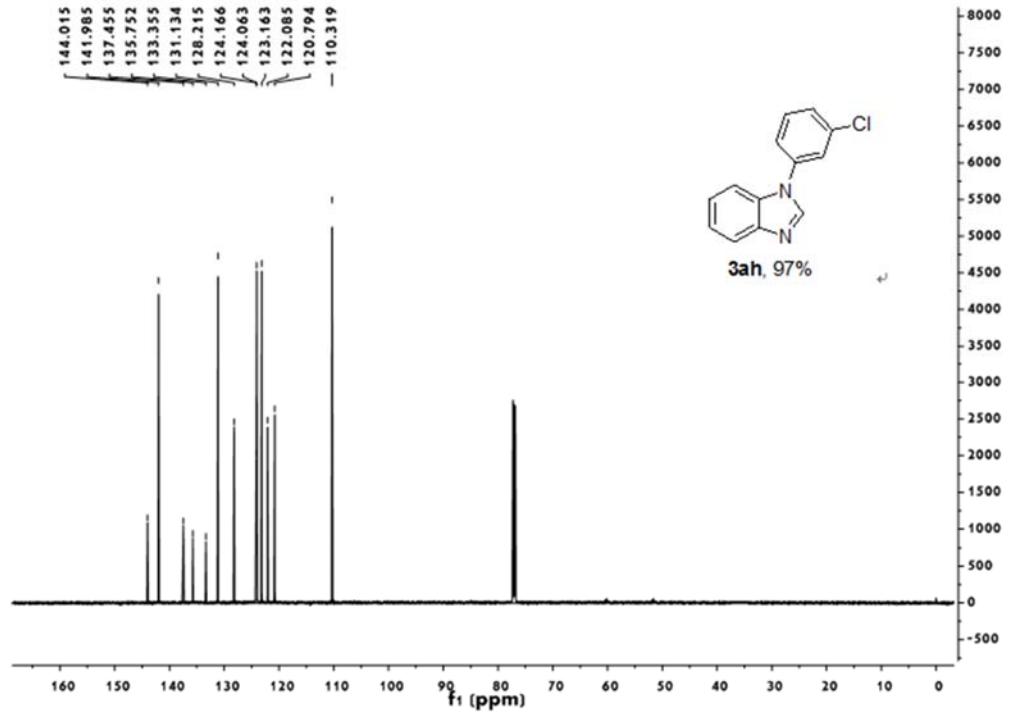

OBn
N
N
3af, 98%
f1 (ppm)

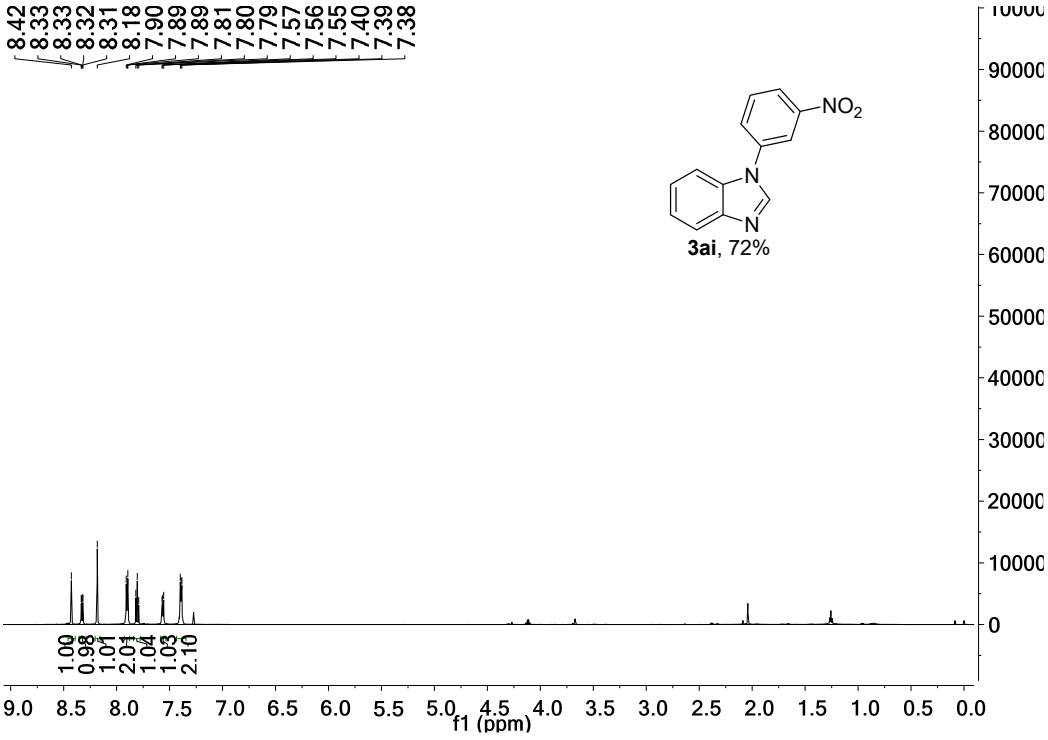

OBn
N
N
3af, 98%
f1 (ppm)

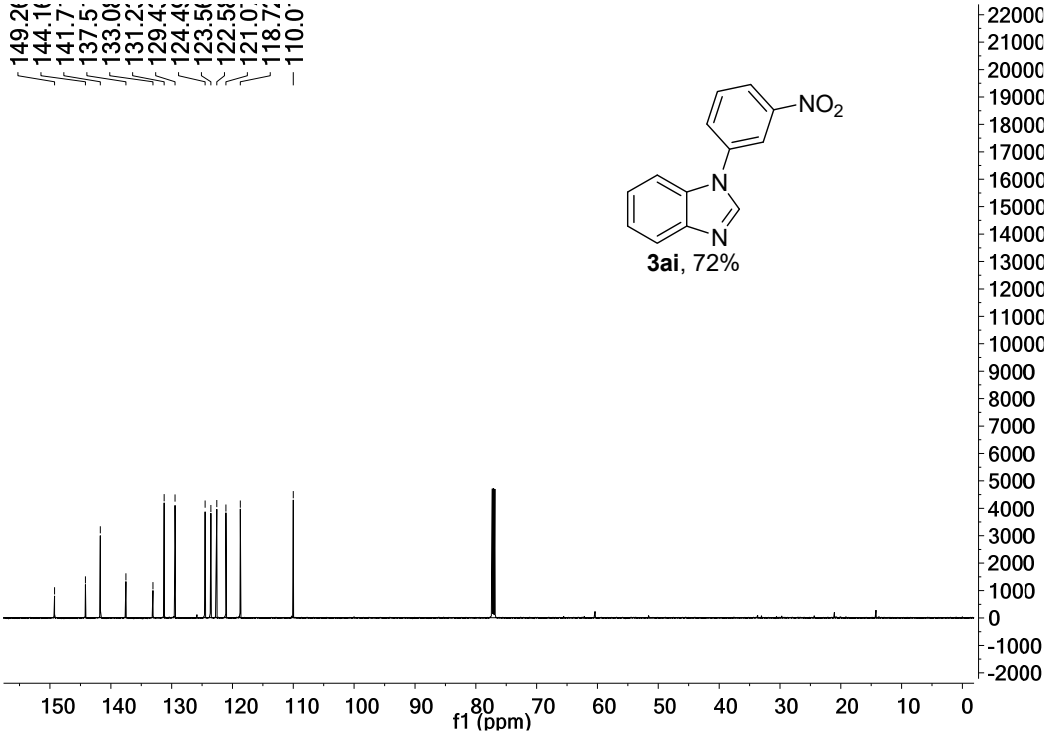

8.084
7.896
7.893
7.887
7.881
7.496
7.489
7.485
7.482
7.474
7.469
7.458
7.454
7.352
7.348
7.342
7.336
7.332
7.287
7.273
7.263
7.259
F
N
N
3ag, 98%
1.00
1.06
2.99
2.07
2.21
f1 (ppm)

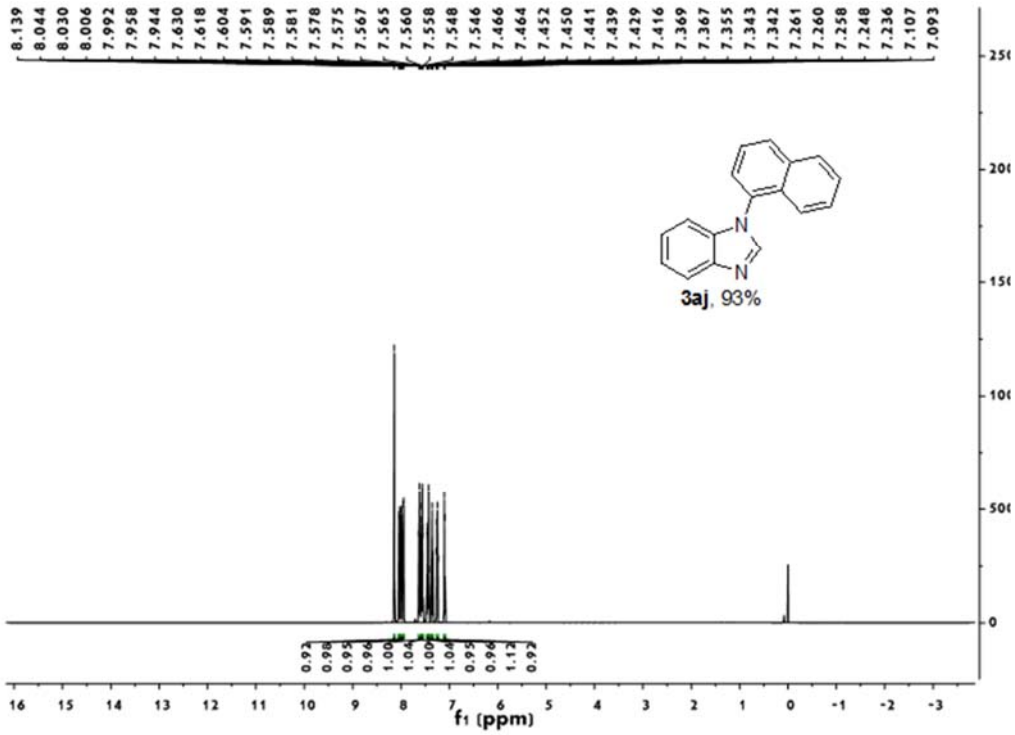

162.8
161.2
143.8
142.3
133.9
132.3
132.3
126.1
126.0
123.8
122.9
120.6
117.1
116.9
110.1
F
N
N
3ag, 98%
f1 (ppm)

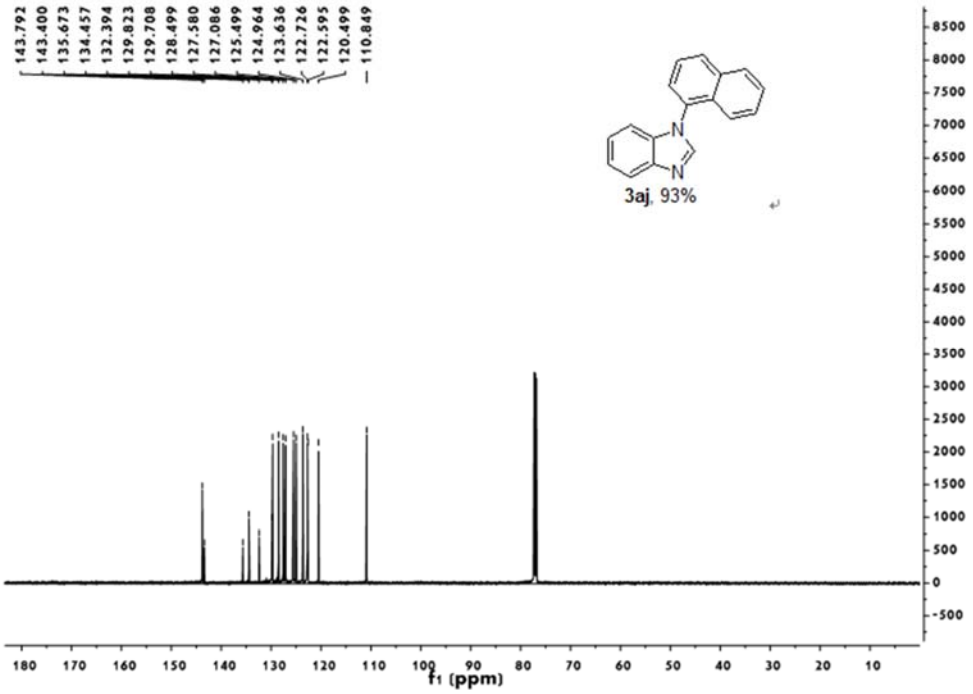

8.112
8.108
8.103
7.895
7.889
7.888
7.884
7.881
7.877
7.874
7.544
7.539
7.534
7.454
7.446
7.432
7.421
7.419
7.413
7.411
7.408
7.360
7.358
7.354
7.350
7.345
7.342
Cl
N
N
3ah, 97%
1.00
1.06
2.91
2.15
2.08
f1 (ppm)

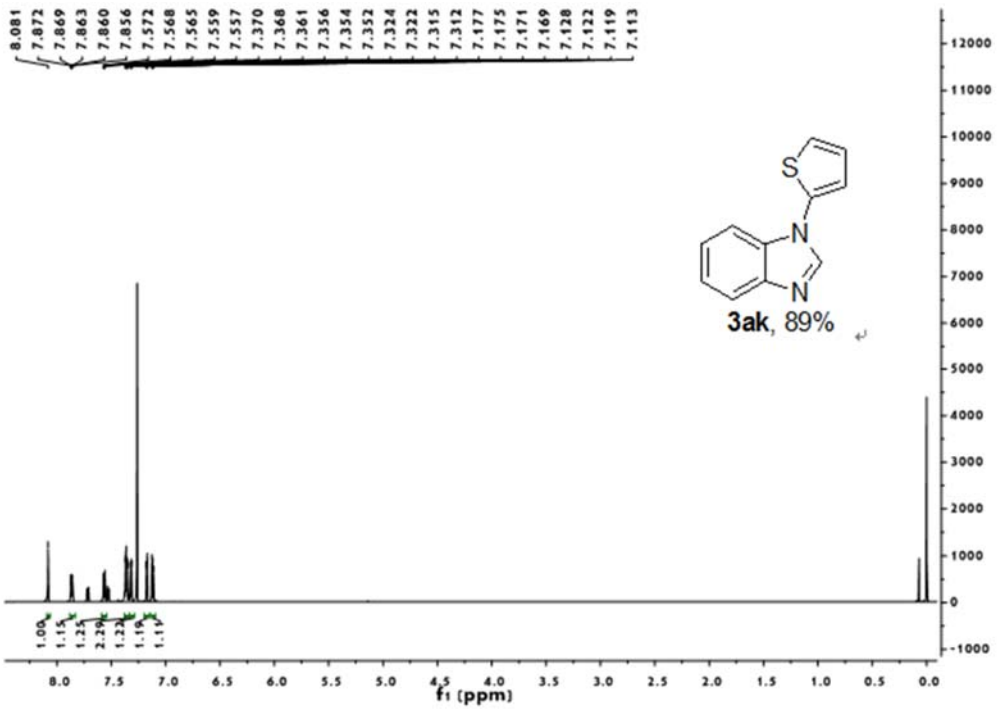

144.015
141.985
137.455
135.752
133.355
131.134
128.215
124.166
124.063
123.163
122.085
120.794
110.319
Cl
N
N
3ah, 97%
f1 (ppm)

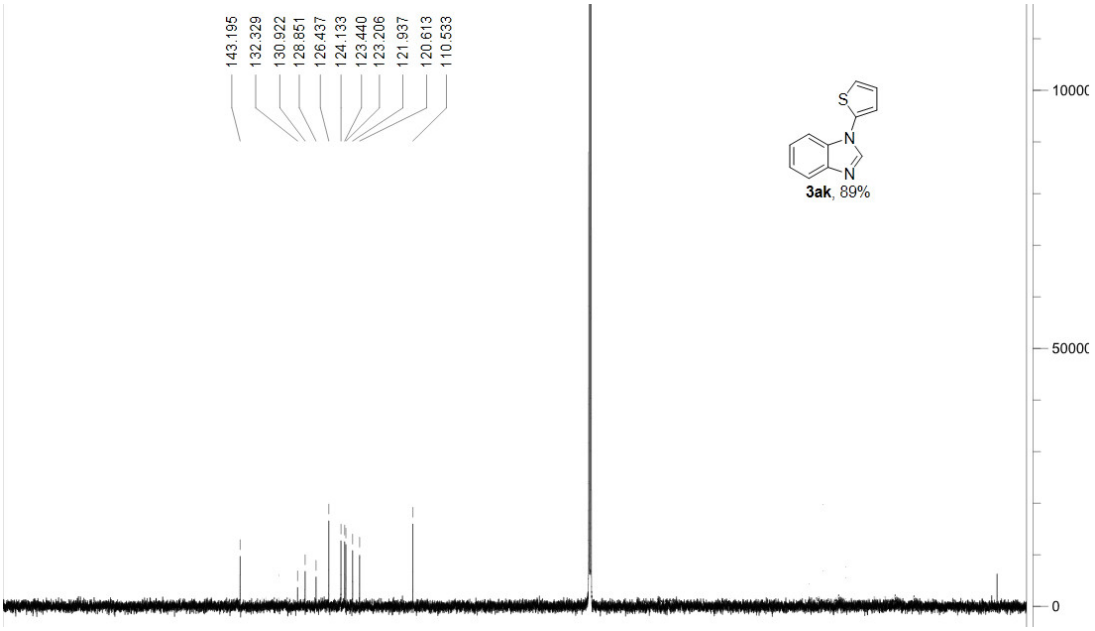

8.42
8.33
8.33
8.32
8.31
8.18
7.90
7.89
7.89
7.81
7.80
7.79
7.57
7.56
7.55
7.40
7.39
7.38
NO2
N
N
3ai, 72%
1.00
0.98
1.01
2.01
1.04
1.03
2.10
f1 (ppm)


NO2
N
N
3ai, 72%
f1 (ppm)

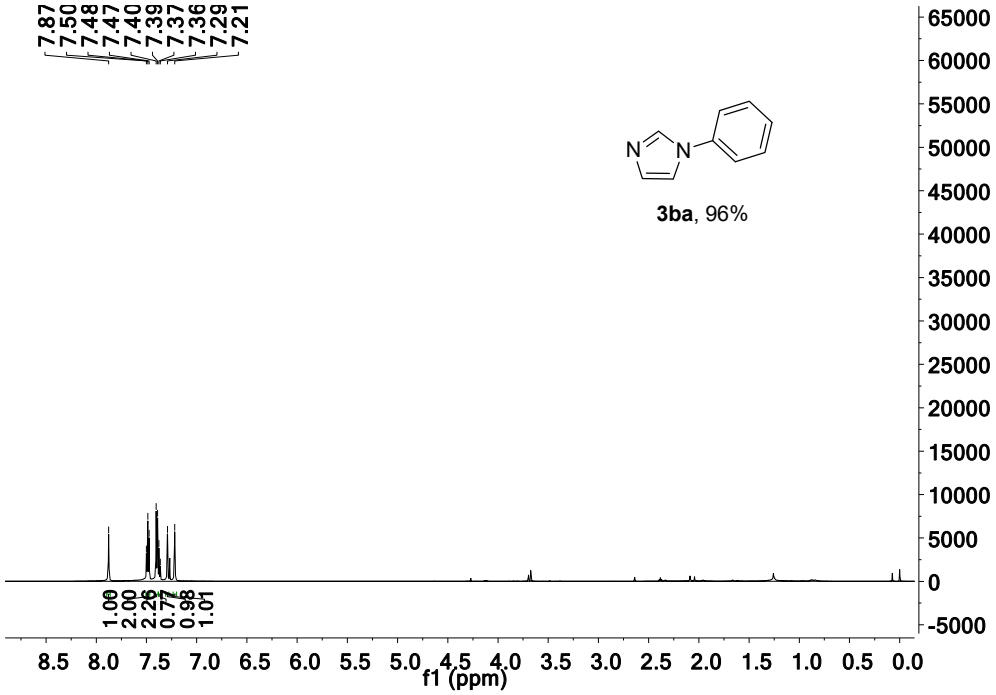

8.139
8.044
8.030
8.006
7.992
7.958
7.944
7.630
7.618
7.604
7.591
7.589
7.581
7.578
7.575
7.567
7.565
7.560
7.558
7.548
7.546
7.466
7.464
7.452
7.450
7.441
7.439
7.429
7.416
7.369
7.367
7.355
7.343
7.342
7.261
7.260
7.258
7.248
7.236
7.107
7.093
3aj, 93%
0.92
0.98
0.95
0.96
1.00
1.04
1.00
1.04
0.95
0.96
1.12
0.92
f1 (ppm)

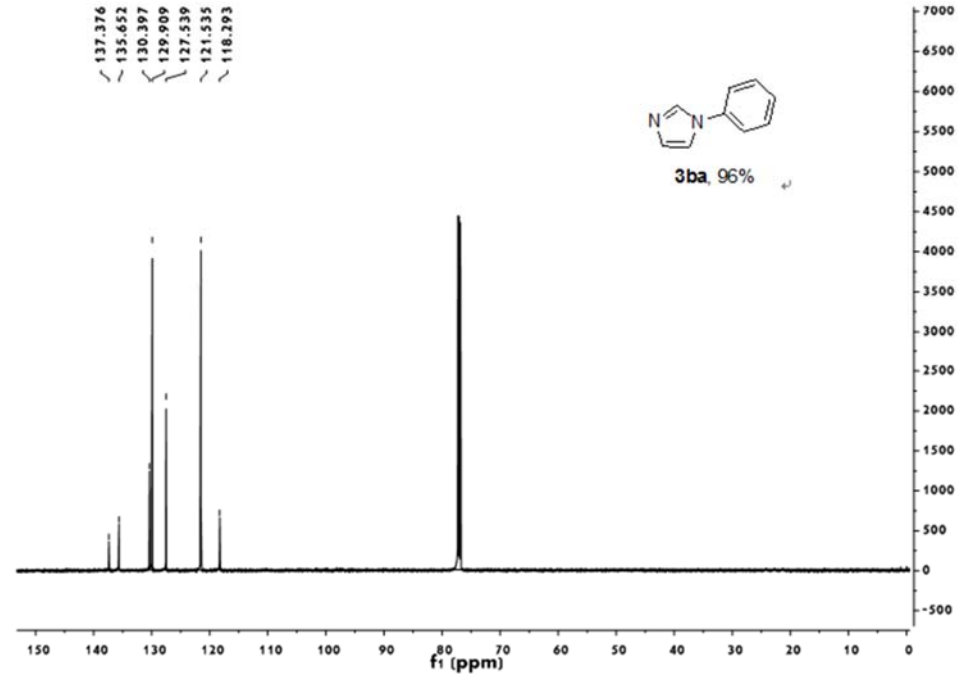

143.792
143.400
135.673
134.457
132.394
129.823
129.708
128.499
127.580
127.086
125.499
124.964
123.636
122.726
122.595
120.499
110.849
3aj, 93%
f1 (ppm)

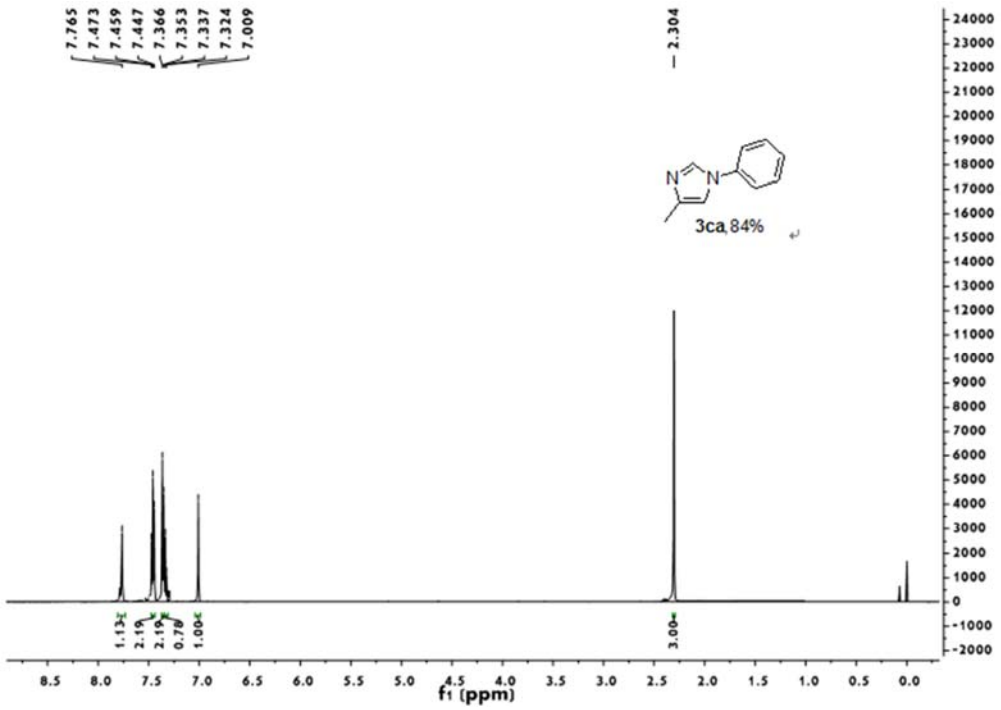

8.081
7.872
7.869
7.863
7.860
7.856
7.572
7.568
7.565
7.559
7.557
7.370
7.368
7.361
7.356
7.354
7.352
7.324
7.322
7.315
7.312
7.177
7.175
7.171
7.169
7.128
7.122
7.119
7.113
3ak, 89%
f1 (ppm)

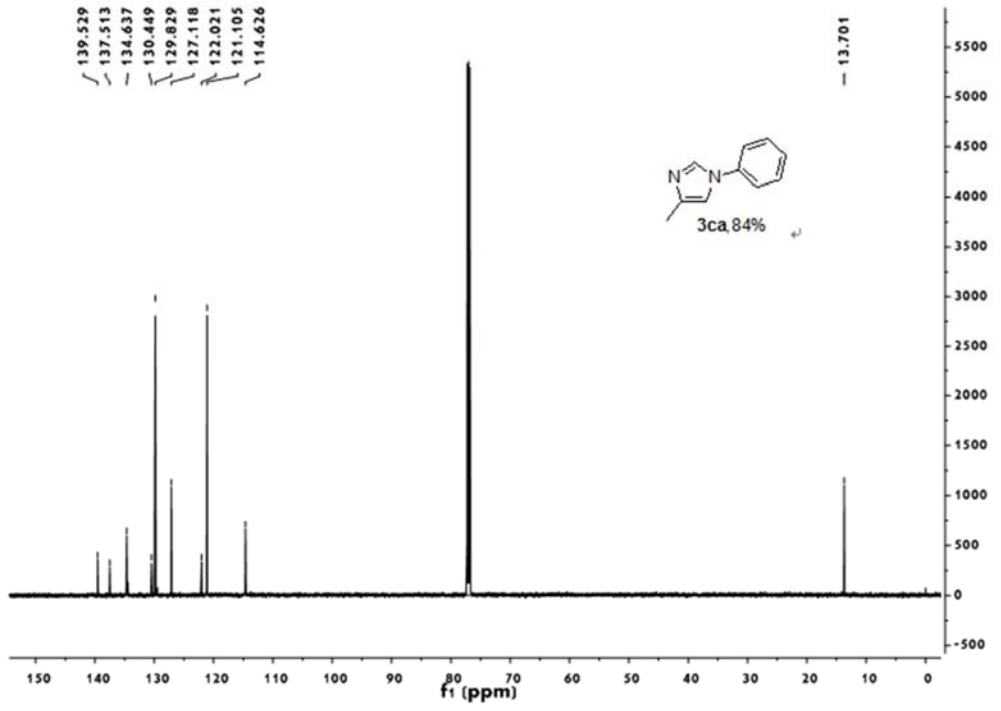

143.195
132.329
130.922
128.851
126.437
124.133
123.440
123.206
121.937
120.613
110.533
3ak, 89%

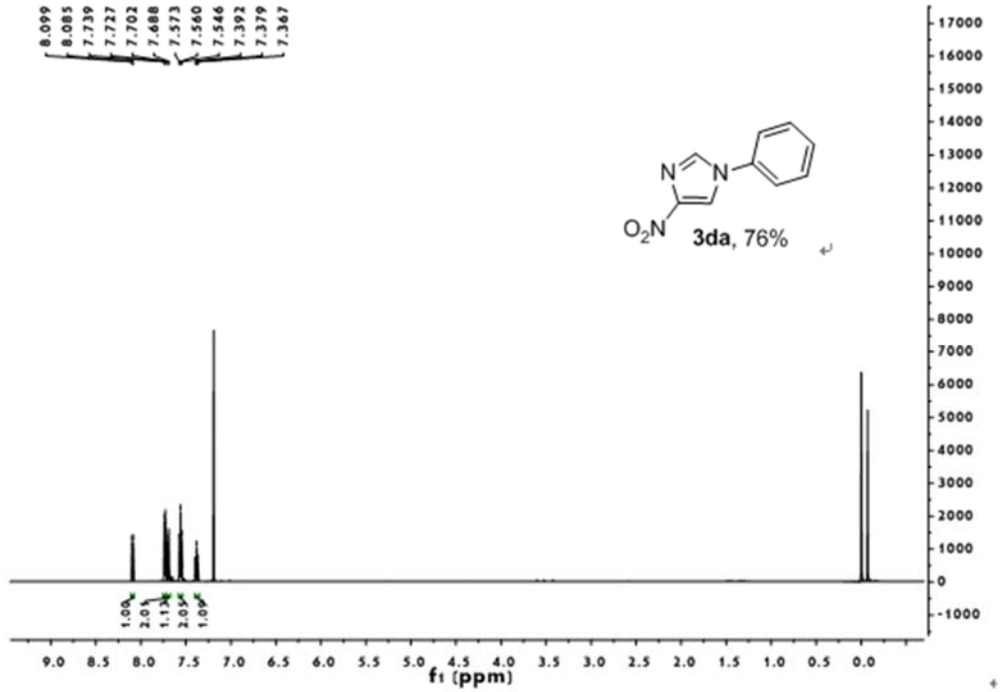
6. NMR Spectral Copies of the products (3ba-3ia)

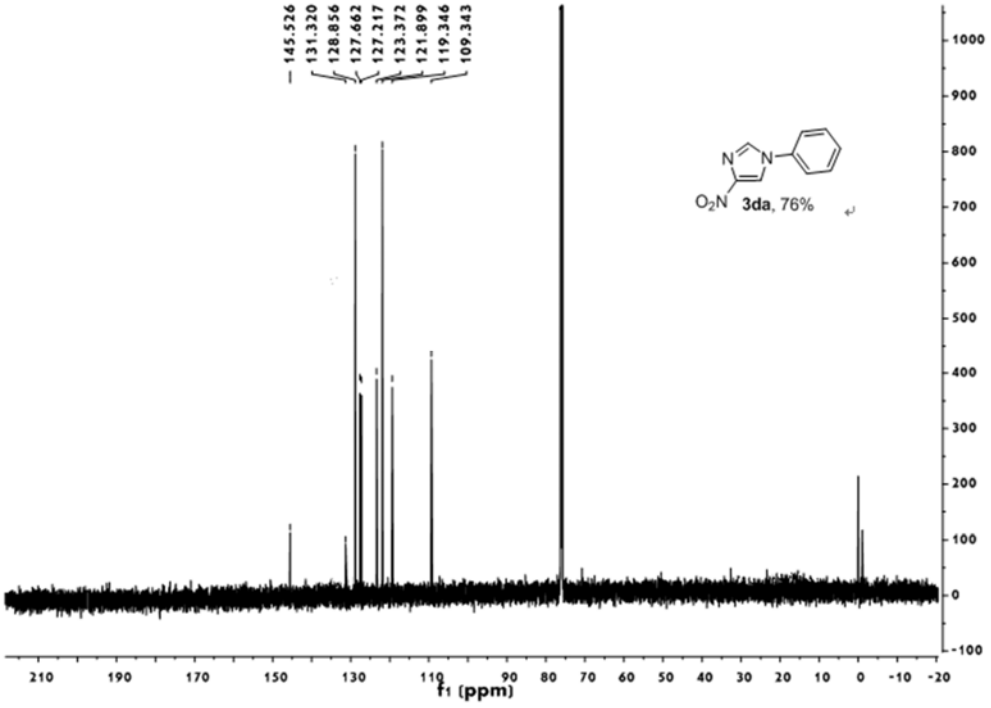


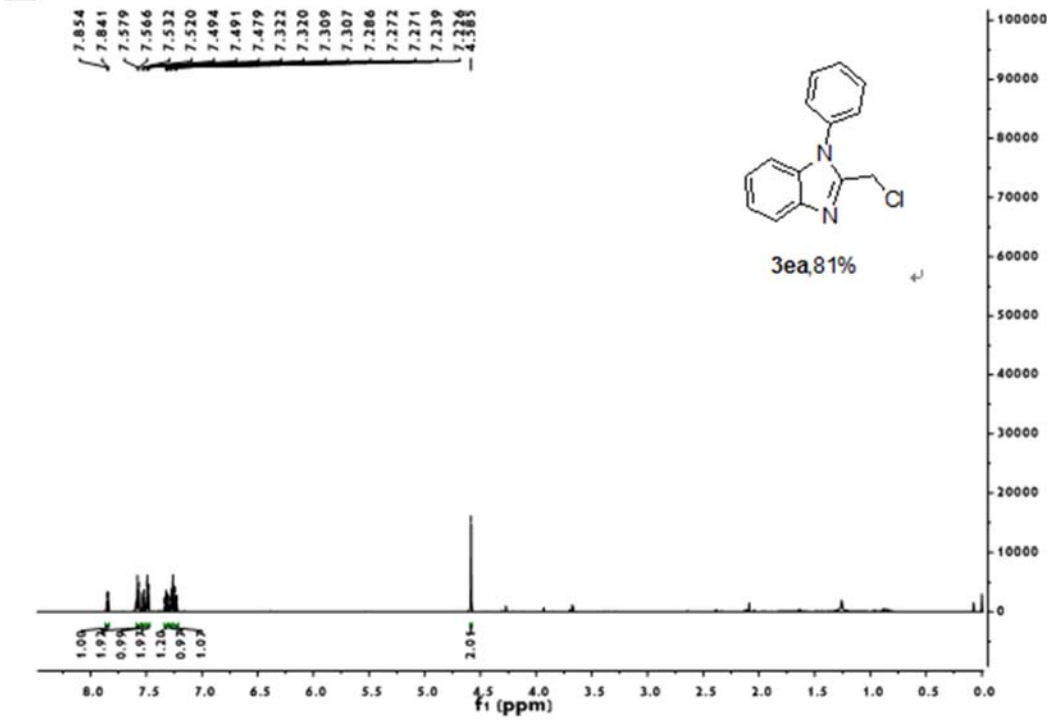


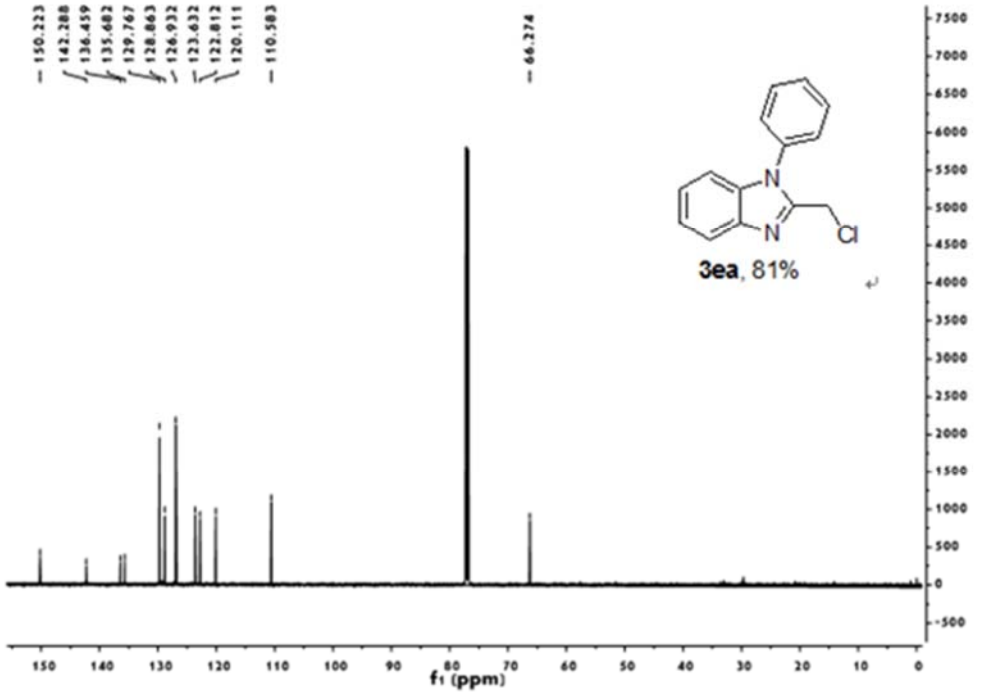

7.765
7.473
7.459
7.447
7.366
7.353
7.337
7.324
7.009
2.304
3ca,84%
1.13
2.19
2.19
0.78
1.00
3.00
f1 (ppm)

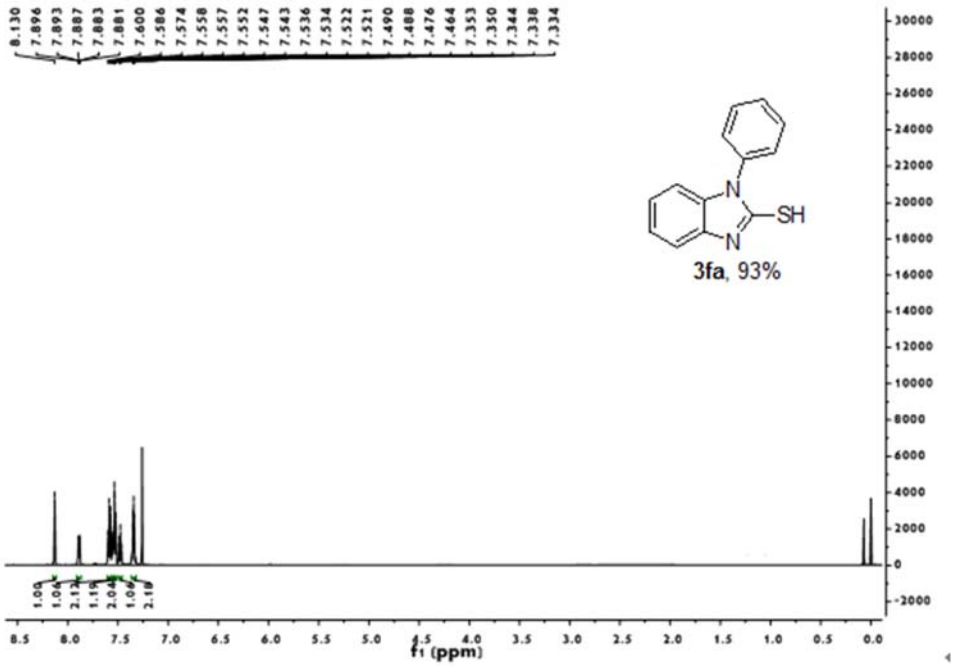

139.529
137.513
134.637
130.449
129.829
127.118
122.021
121.105
114.626
13.701
3ca,84%
f1 (ppm)

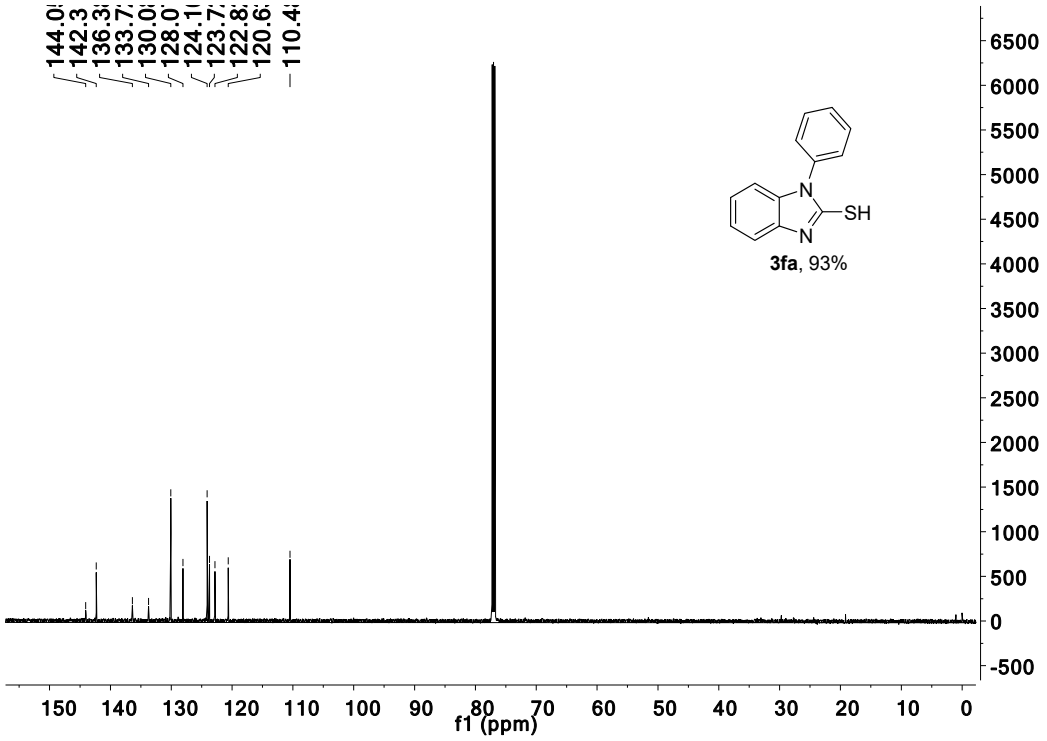

8.099
8.085
7.739
7.727
7.702
7.688
7.573
7.560
7.546
7.392
7.379
7.367
3da, 76%
f1 (ppm)

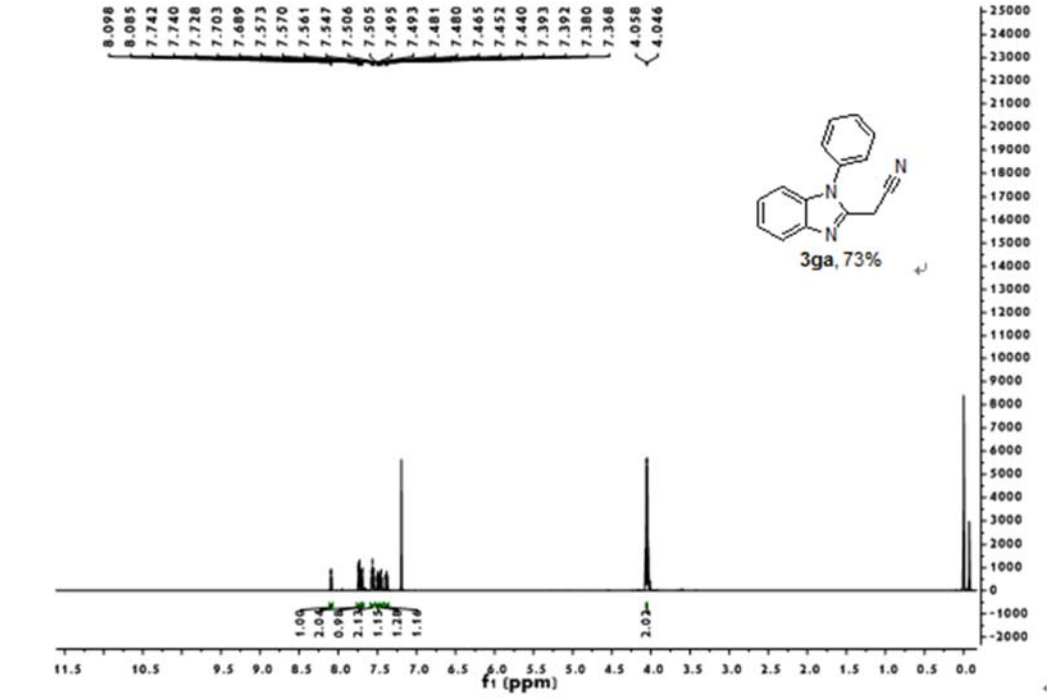

145.526
131.320
128.856
127.662
127.217
123.372
121.899
119.346
109.343
3da, 76%
f1 (ppm)

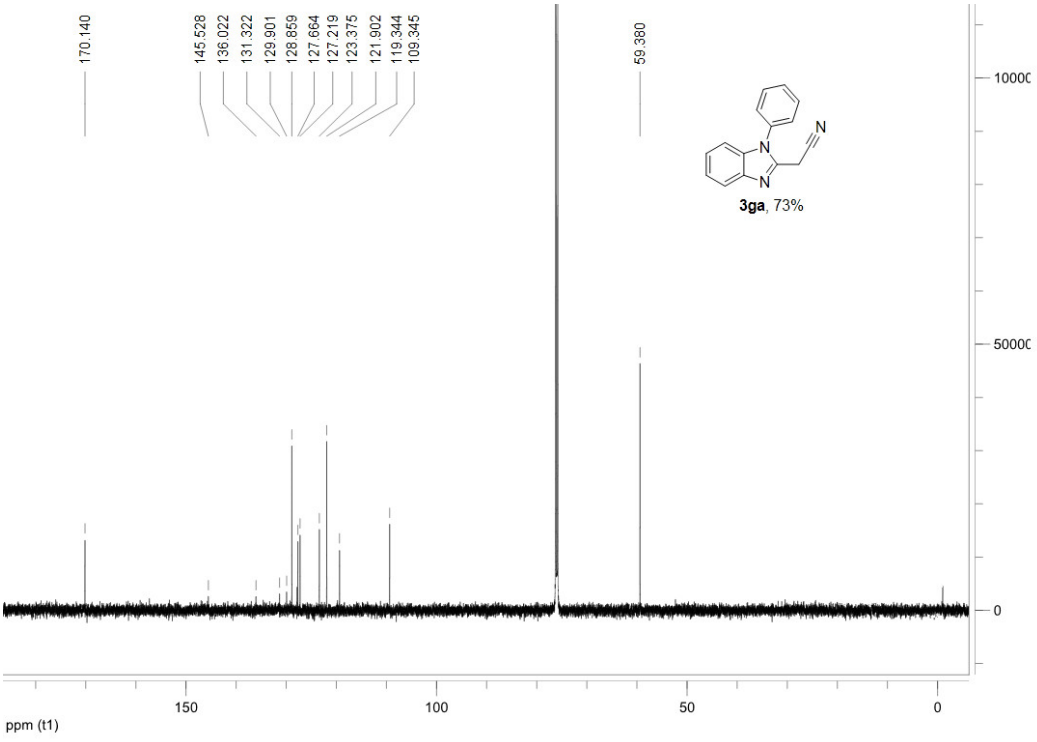

7.854
7.841
7.579
7.566
7.532
7.520
7.494
7.491
7.479
7.322
7.320
7.309
7.307
7.286
7.272
7.271
7.239
4.383
1.00
1.94
0.99
1.92
1.20
0.93
1.07
2.01
f1 (ppm)
3ea,81%

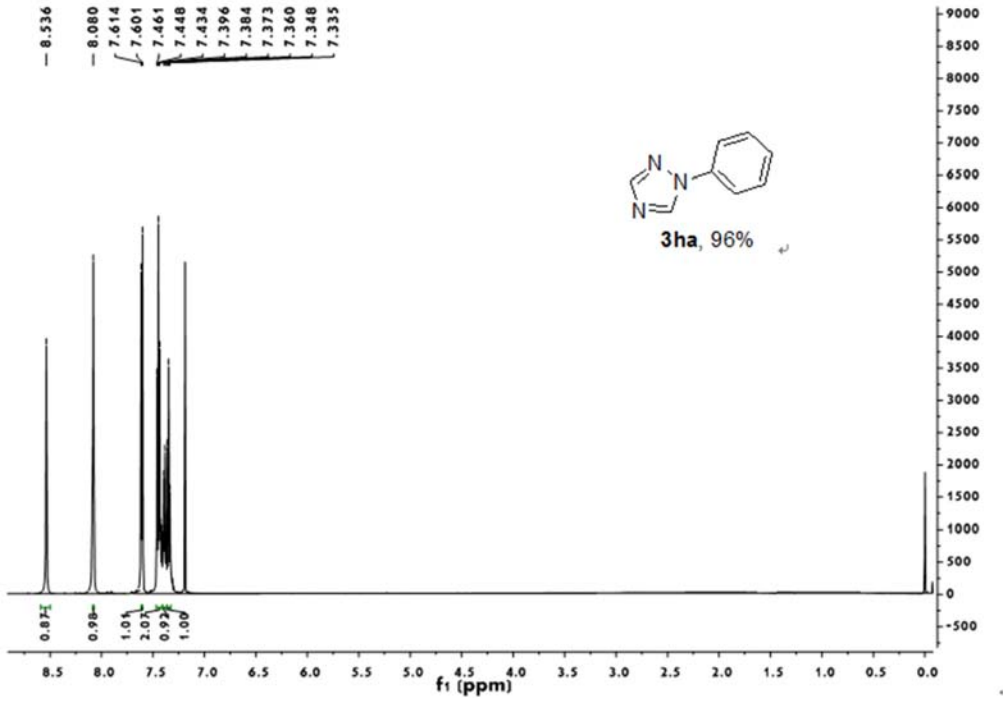

150.223
142.288
136.459
135.682
129.767
128.863
126.932
123.632
122.812
120.111
110.583
66.274
f1 (ppm)
3ea, 81%

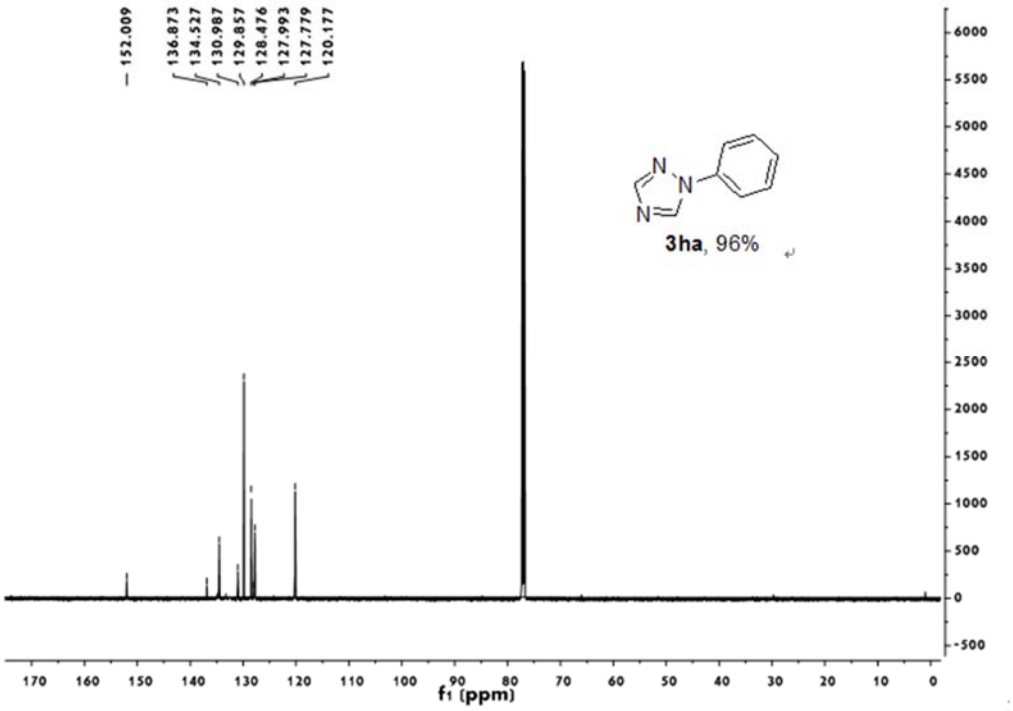

8.130
7.896
7.893
7.887
7.883
7.881
7.600
7.586
7.574
7.558
7.557
7.552
7.547
7.543
7.536
7.534
7.522
7.521
7.490
7.488
7.476
7.464
7.353
7.350
7.344
7.338
7.334
SH
N
N
3fa, 93%
f1 (ppm)

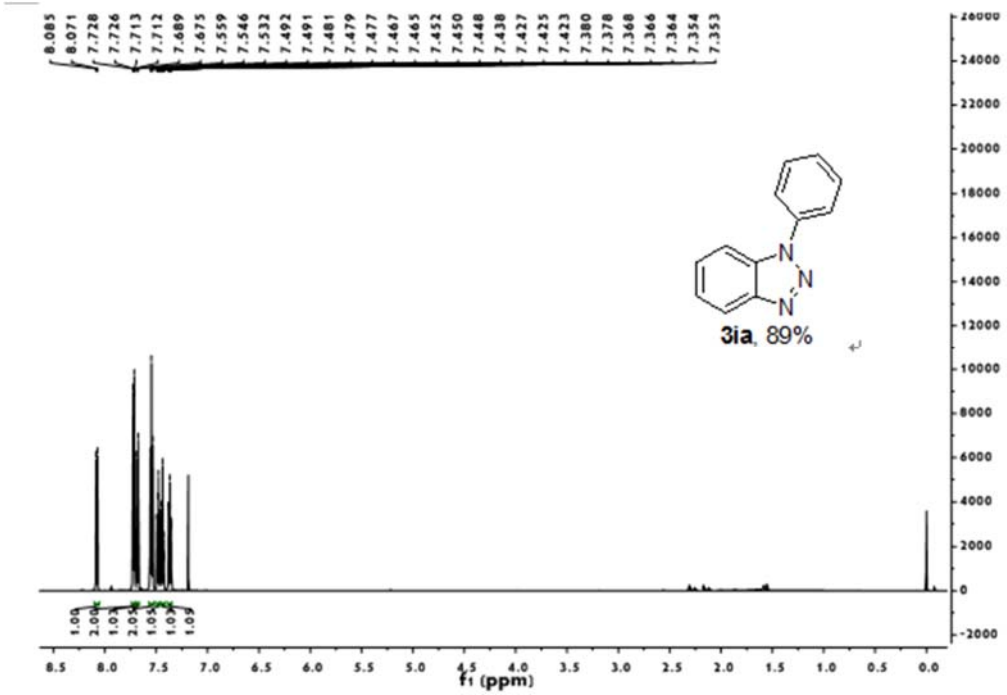

144.0
142.3
136.3
133.7
130.0
128.0
124.1
123.7
122.8
120.6
110.4
SH
N
N
3fa, 93%
f1 (ppm)

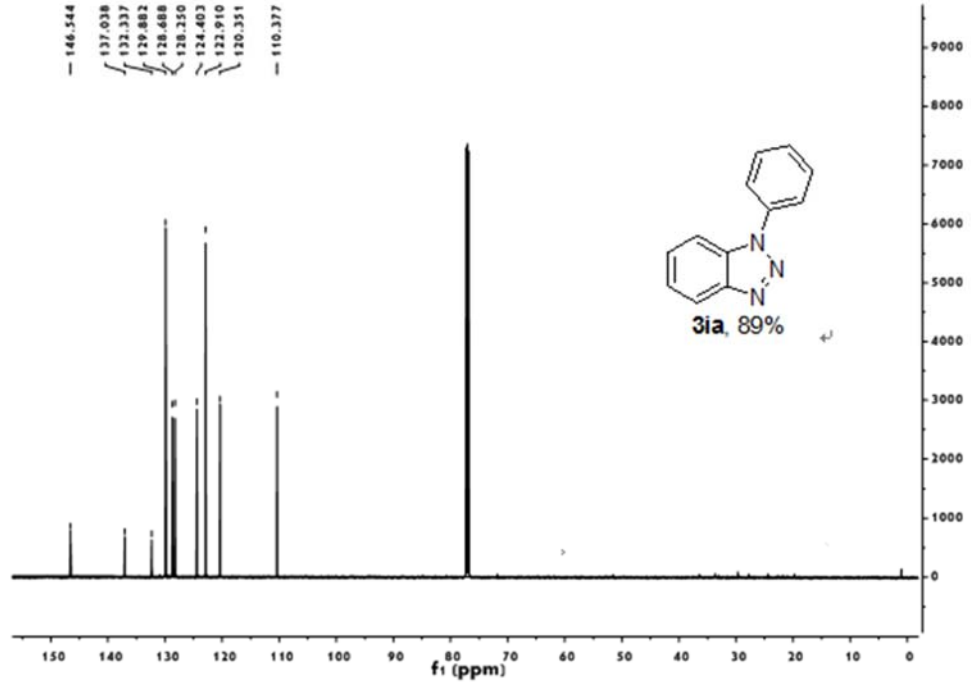

8.098
8.085
7.742
7.740
7.728
7.703
7.689
7.573
7.570
7.561
7.547
7.506
7.505
7.495
7.493
7.481
7.480
7.465
7.452
7.440
7.393
7.392
7.380
7.368
4.058
4.046
N
N
N
3ga, 73%
1.00
2.04
0.98
2.13
1.15
1.28
1.11
2.01
f1 (ppm)


170.140
145.528
136.022
131.322
129.901
128.859
127.664
127.219
123.375
121.902
119.344
109.345
59.380
N
N
N
3ga, 73%
ppm (t1)


8.536
8.080
7.614
7.601
7.461
7.448
7.434
7.396
7.384
7.373
7.360
7.348
7.335
0.87
0.98
1.01
2.01
0.93
1.00
3ha, 96%
f1 (ppm)


152.009
136.873
134.527
130.987
129.857
128.476
127.993
127.779
120.177
3ha, 96%
f1 (ppm)


8.085
8.071
7.728
7.726
7.713
7.712
7.689
7.675
7.559
7.546
7.532
7.492
7.491
7.481
7.479
7.477
7.467
7.465
7.452
7.450
7.448
7.438
7.427
7.425
7.423
7.380
7.378
7.368
7.366
7.364
7.354
7.353
1.00
2.00
1.03
2.03
1.03
1.03
1.07
3ia, 89%
f1 (ppm)


146.544
137.038
132.337
129.882
128.688
128.350
124.403
122.910
120.351
110.377
3ia, 89%
f1 (ppm)