Electronic Supplementary Material (ESI) for Chemical Communications
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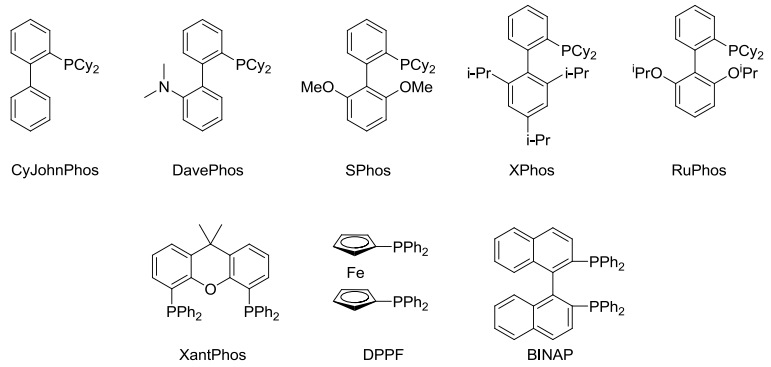
Arylation of 2- Substituted pyridines via Pd-Catalyzed Decarboxylative Cross-Coupling Reactions of 2-Picolinic acid

Supporting Information

1. Abbreviation of various ligands used in Pd-catalyzed cross-coupling reactions
2. General experimental procedures
3. Characterization data of compounds

Various Ligands Used in Pd-catalyzed Cross-coupling Reactions



Scheme 1 Abbreviation of Various Ligands

General Methods. All reactions were performed in dried glass reaction tube equipped with a magnetic stir bar under argon gas atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32-63 μm, standard grade). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25 mm 230-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Solvents were re-distilled prior to use in the reactions. The transformation progress was indicated by GC-MS using Thermo Fisher Scientific DSQⅡ. Melting point were obtained by XT4A micro Melting-point Measurement Instruments , thermometer was unrevised. The high resolution mass spectrum was

received via Agilent Technologies 6540 UHD Accurate-mass Q-Tof LC/MS, with ESI as ion source. NMR spectra were obtained on Bruker DPX 400 systems using $CDCl_3$ (3t, 3u using acetone)as solvent, TMS as internal standard substance, with proton and carbon resonances at 400 and 100 MHz, respectively.

Experimental procedures Section. A dried glass reaction tube equipped with a magnetic stir bar was charged with $PdCl_2$ (5.3 mg, 0.03 mmol, 5 mol %), BINAP (18.7 mg, 0.03 mmol, 5 mol %), K_2CO_3 (248.0 mg, 1.2 mmol, 3 equiv), Cu_2O (51.4 mg, 0.6 mmol, 0.6 equiv), 3Å molecular sieve (200 mg), 2-picolinic acid (73.8 mg, 0.6 mmol, 1.0 equiv) and aryl(heteroaryl, alkyl) bromides (0.9 mmol, 1.5 equiv); anhydrous DMA (3.5 mL) was added and the mixture was charged with argon gas three times. The reaction mixture was then stirred at 150℃ under argon gas until 2-picolinic acid were consumed. The reaction progress was monitored by TLC. The reaction mixture was filtered through a pad of celite, and washed with ethyl acetate after cooling to room temperature. The filtrate was poured into H_2O and extracted with ethyl acetate. The combined organic layer was dried with $MgSO_4$ and filtered. The filtrate was concentrated in vacuo. The residue was purified by silica gel flash chromatography to produce the desired product. The products were characterized by ^{1}H NMR, ^{13}C NMR and GC-MS.

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Characterization data of compounds.

4-(pyridin-2-yl)benzonitrile (**3a**, yield 75%): White solid. m.p. 91-92℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.74(d, *J* = 4.6 Hz, 1H), 8.12 (d, *J* = 8.6Hz, 2H), 7.83(td, *J* = 7.5, 1.7Hz, 1H), 7.77(m, 3H), 7.32(ddd, *J* = 7.3, 4.9, 1.4Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 155.2(s), 150.0(s), 143.4(s), 137.1(s), 132.6(s), 127.5(s) 123.4(s), 120.9(s), 118.8(s),112.4(s).

2-(4-methoxyphenyl)pyridine (**3b**, yield 47%): White solid. m.p. 53-55℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.65(d, *J* = 4.8 Hz, 1H), 7.95(d, *J* = 8.8 Hz, 2H), 7.70(td, *J* = 7.7, 2.0 Hz, 1H), 7.66(d, *J* = 7.4 Hz, 1H), 7.16(m, 1H), 6.99(d, *J* = 8.8 Hz, 2H), 3.86(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 160.4(s), 157.1(s), 149.5(s), 136.6(s), 132.0(s), 128.1(s), 121.4(s), 119.8(s), 114.1(s), 55.3(s).

2-phenylpyridine (**3c**, yield 43%): colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.70(d, *J* = 5.0 Hz, 1H), 7.99(m, 2H), 7.74(m, 2H), 7.48(m, 2H), 7.23(m, 1H), 7.42(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 157.5(s), 149.6(s), 139.4(s), 136.7(s), 128.9(s) , 128.7(s), 126.9(s), 122.1(s), 120.6(s).

1-(4-(pyridin-2-yl)phenyl)ethanone (**3d**, yield 27%): White solid. m.p. 83-85℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.73(d, *J* = 4.8Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 2H), 8.06 (d, *J* = 8.5 Hz, 2H), 7.80 (d, *J* =4.0 Hz, 2H), 7.3(m, 1H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.8(s), 155.0(s), 148.9(s), 142.5(s), 136.1(s), 135.9(s), 127.8(s), 126.0(s), 121.9(s), 120.0(s), 25.7(s).

phenyl(4-(pyridin-2-yl)phenyl)methanone (**3e**, yield 47%): White solid. m.p. 89-90℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.73(d, *J* = 5.0 Hz, 1H), 8.11(d, *J* = 8.5Hz, 2H), 7.91(d, *J* = 8.5 Hz, 2H), 7.81(m, 4H), 7.60(t, *J* = 7.3 Hz, 1H), 7.49(t, *J* = 7.5Hz, 2H) , 7.29(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 196.3(s), 156.2(s), 149.9(s), 143.0(s), 137.6(s), 137.6(s), 136.9(s), 132.5(s), 130.6(s), 130.0(s), 128.3(s), 126.7(s), 122.9(s), 121.0(s).

2-(4-(trifluoromethyl)phenyl)pyridine (**3f**, yield 40%): white solid. m.p. 69-70℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.72(d, *J* = 5.0 Hz, 1H), 8.10(d, *J* = 8.4 Hz, 2H), 7.78(m, 2H) , 7.72(d, *J* = 8.4 Hz, 2H) , 7.28(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 155.8(s), 149.9(s), 142.6(s), 136.9(s), 130.9(s), 130.6(s), 127.1(s), 125.6(s),

125.6(s), 122.9(s), 120.8(s).

methyl 4-(pyridin-2-yl)benzoate (**3g**, yield 57%): White solid. m.p. 97-98℃. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.73(d, *J* = 4.2 Hz, 1H), 8.11(dd, *J* = 15.0, 10.1Hz, 4H), 7.79(d, *J* = 3.5 Hz, 2H), 7.28(q, *J* = 4.5 Hz, 1H), 3.94(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 166.9(s), 156.2(s), 149.9(s), 143.5(s), 136.9(s),130.3(s), 126.8(s), 122.8(s), 121.0(s), 52.2(s).

2-(4-nitrophenyl)pyridine (**3h**, yield 30%): Yellow solid. m.p. 129-131℃. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.75 (d, *J* = 4.7 Hz, 1H), 8.33(d, *J* = 8.7Hz, 2H), 8.18(d, *J* = 8.7 Hz, 2H), 7.82(m, 2H), 7.34(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 154.8(s), 150.1(s), 148.1(s), 145.2(s), 137.1(s), 127.6(s), 124.0(s), 123.5(s), 121.2(s).

2-p-tolylpyridine (**3i**, yield 50%): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.67(d, *J* = 4.8 Hz, 1H), 7.89(d, *J* =8.4 Hz, 2H), 7.71(dd, *J* = 6.1, 2.2Hz, 2H), 7.28(d, *J* = 8.4 Hz, 2H), 7.19(m, 1H), 2.4(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 157.4(s), 49.6(s), 138.9(s), 136.6(s), 136.6(s), 129.4(s), 126.7(s), 121.8(s), 120.2(s), 21.2(s).

2-o-tolylpyridine (**3j**, yield 48%): Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.69(d, *J* = 5.0 Hz, 1H), 7.73(td, *J* = 7.7, 1.9Hz, 1H), 7.39(d, *J* = 7.3 Hz, 2H), 7.26(m, 4H), 2.36(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 160.0(s), 149.2(s), 140.4(s), 136.1(s), 135.7(s), 130.7(s), 129.6(s), 128.2(s), 125.8(s), 124.1(s), 121.6(s), 20.2(s).

2-(3-methoxyphenyl)pyridine (**3l**, yield 64%): Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.69(d, *J* = 4.8 Hz, 1H), 7.72(m, 2H), 7.60(s, 1H), 7.55(d, *J* = 7.7Hz, 1H), 7.38(t, *J* = 8.2Hz, 1H), 7.22(m, 1H), 6.97(dd, *J* = 7.7, 2.4Hz, 1H), 3.89(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 160.0(s), 157.2(s), 149.6(s), 140.9(s), 136.7(s), 129.7(s), 122.2(s), 120.7(s), 119.3(s), 115.0(s), 112.0(s), 55.3(s).

2-(pyridin-2-yl)benzonitrile (**3m**, yield 42%): Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.78(d, *J* = 4.1 Hz, 1H), 7.58(m, 2H), 7.78(m, 1H), 7.69(td, *J* =7.6, 1.4Hz, 1H), 7.51(td, *J* = 7.5, 1.1Hz, 1H), 7.36(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 155.2(s), 149.9(s), 143.5(s), 136.8(s), 134.1(s), 132.8(s),

129.9(s), 128.7(s), 123.3(s), 123.2(s), 118.7(s), 111.0(s).

1-(3-(pyridin-2-yl)phenyl)ethanone (**3n**, yield 36%): Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.72(d, *J* = 5.1 Hz, 1H), 8.58(s, 1H), 8.22(d, *J* = 6.5 Hz, 1H), 8.01(d, *J* = 7.3Hz, 1H), 7.79(d, *J* = 4.0 Hz, 2H), 7.58(t, *J* = 7.8 Hz, 1H), 7.28(m, 1H), 2.69(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 198.0(s), 156.4(s), 149.8(s), 139.9(s), 137.6(s), 136.9(s), 131.4(s), 129.0(s), 128.6(s), 126.8(s), 122.6(s), 120.6(s), 26.8(s).

methyl 4-methyl-3-(pyridin-2-yl)benzoate (**3o**, yield 46%): colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.70(d, *J* = 4.8 Hz, 1H), 8.09(d, *J* = 1.8 Hz, 1H), 7.96(dd, *J* = 8.0, 1.7 Hz, 1H), 7.77(td, *J* = 7.9, 1.8 Hz, 1H), 7.42(d, *J* = 7.9 Hz, 1H), 7.35(d, *J* = 8.0 Hz, 1H), 7.27(ddd, *J* = 7.4, 4.9, 1.0Hz, 1H), 3.90(s, 3H), 2.4(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 166.9(s), 159.0(s), 149.2(s), 141.5(s), 140.5(s), 136.3(s), 130.9(s), 130.8(s), 129.2(s), 127.9(s), 124.0(s) 122.0(s), 52.0(s), 20.5(s). HRMS (ESI$^+$) calcd for $C_{14}H_{14}NO_2$ $(M + H)^+$ 228.1025, found 228.1012.

2-(naphthalen-2-yl)pyridine (**3p**, yield 78%): Yellow solid. m.p. 77-79℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.75(d, *J* = 4.5 Hz, 1H), 8.49(s, 1H), 8.14(dd, *J* = 8.7, 1.9Hz, 1H), 7.95(d, *J* = 8.0Hz, 2H), 7.88(d, *J* = 7.0Hz, 2H), 7.79(td, *J* = 7.5, 1.8Hz, 1H), 7.51(q, *J* = 3.2Hz, 2H), 7.26(m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 157.3(s), 149.8(s), 136.8(s), 136.6(s), 133.6(s), 133.5(s), 128.7(s), 127.6(s), 126.5(s), 126.3(s), 126.3(s), 124.5(s), 122.1(s), 120.8(s).

2-(naphthalen-1-yl)pyridine (**3q**, yield 66%): Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.80(d, *J* = 4.0Hz, 1H), 8.01(d, *J* = 7.6Hz, 1H), 7.92(d, *J* = 8.2Hz, 2H), 7.82(td, *J* = 8.0, 1.7Hz, 1H), 7.59(m, 3H), 7.49(m, 2H), 7.33(m, 1H),. ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 159.2(s), 149.5 (s), 138.5(s), 136.4(s), 133.9(s), 131.1(s), 128.9(s), 128.3(s), 127.4(s), 126.4(s), 125.8(s), 125.6(s), 125.3(s), 125.0(s), 122.0(s).

2,2'-bipyridine (**3r**, yield 46%): White solid. m.p. 68-70℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.67(s, 2H), 8.39(d, *J* = 8.2 Hz, 2H), 7.80(td, *J* = 7.8, 1.7Hz, 2H), 7.29(m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 156.1(s), 149.1(s), 136.9(s), 123.7(s), 121.0(s).

2,3'-bipyridine (**3s**, yield 35%): colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.33(s, 1H), 8.70(m, 2H), 8.46(d, *J* = 7.9 Hz, 1H), 8.02(d, *J* = 7.9 Hz, 1H), 7.94(td, *J* = 7.6, 1.8 Hz, 1H), 7.53(m, 1H), 7.41(ddd, *J* =7.6, 4.7, 1.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 155.3(s), 150.8(s), 150.6(s), 148.8(s), 138.1(s), 134.8(s), 124.0(s), 121.4(s).

2,4'-bipyridine (**3t**, yield 45%): white solid. m.p. 59-60℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.75(m, 3H), 8.09(d, *J* = 7.7 Hz, 3H), 7.97(td, *J* = 7.4, 1.9 Hz, 1H), 7.48(ddd, *J* =7.6, 4.7, 0.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δδ 154.9(s), 151.1(s), 150.9(s), 147.0(s), 138.3(s), 125.0(s), 121.8(s).

2-(pyridin-2-yl)quinoline (**3u**, yield 46%): Yellow solid. m.p. 96-97℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.74(d, *J* = 4.5Hz, 1H), 8.65(d, *J* = 7.9 Hz, 1H), 8.56(d, *J* = 8.7Hz, 1H), 8.28(d, *J* = 8.6Hz, 1H), 8.18(d, *J* = 8.4Hz, 1H), 7.87(m, 2H), 7.74(m,1H), 7.55(t, *J* = 7.3Hz, 1H), 7.36(ddd, *J* = 7.2, 4.7, 1.0Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 156.3(s), 156.1(s), 149.1(s), 147.9(s), 136.9(s), 136.8(s), 129.8(s), 129.5(s), 128.2(s), 127.6(s), 126.7(s), 124.0(s), 121.8(s), 118.9(s).

3-(pyridin-2-yl)quinoline (**3v**, yield 59%): Yellow solid. m.p. 97-99℃.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.53(s, 1H), 8.76(s, 2H), 8.14(d, *J* = 8.5 Hz, 1H), 7.9(m, 2H), 7.82(td, *J* = 8.0, 1.7Hz, 1H), 7.73(t, *J* = 7.89 Hz, 1H), 7.57(t, *J* = 7.4 Hz, 1H), 7.30(ddd, *J* = 7.5, 4.8, 1.1Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 154.8(s), 150.1(s), 149.2(s), 148.2(s), 137.0(s), 133.8(s), 129.9(s), 129.2(s), 128.5(s), 127.0(s), 122.8(s), 120.8(s).

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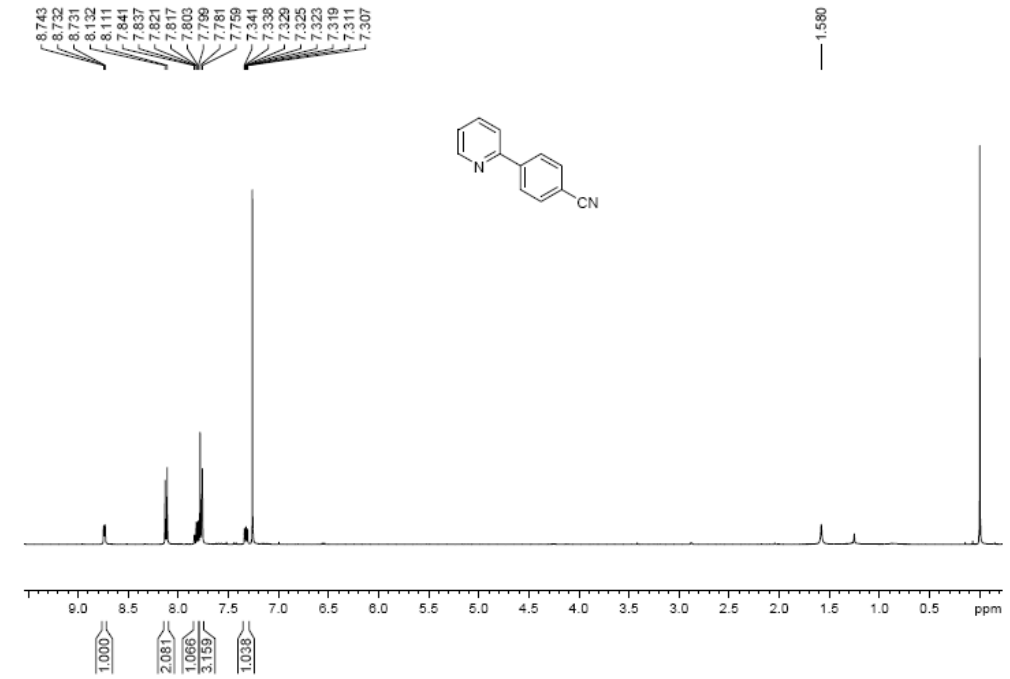
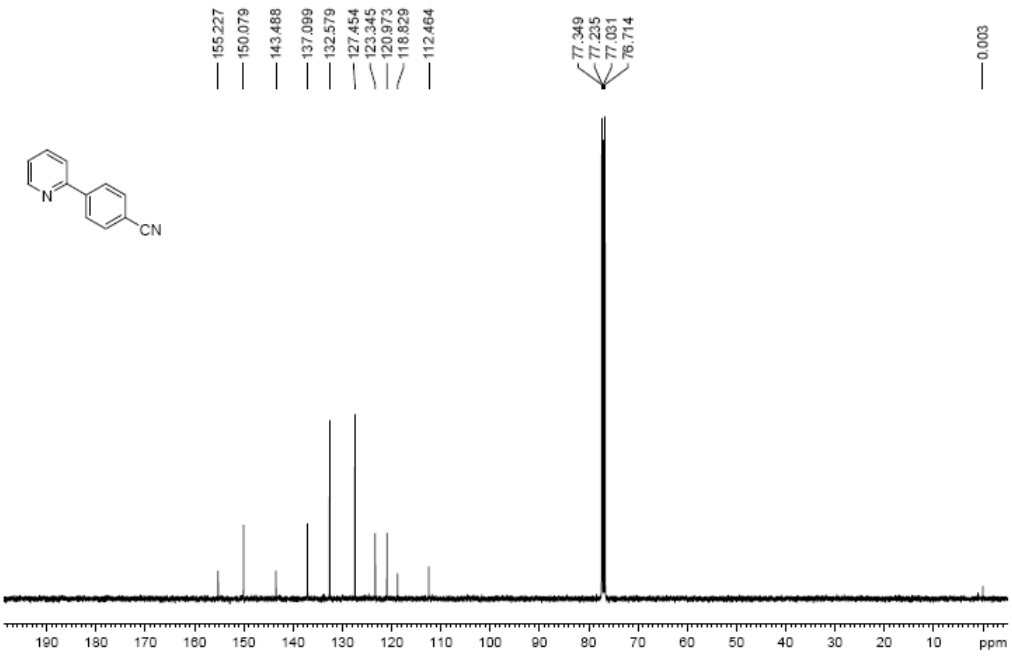
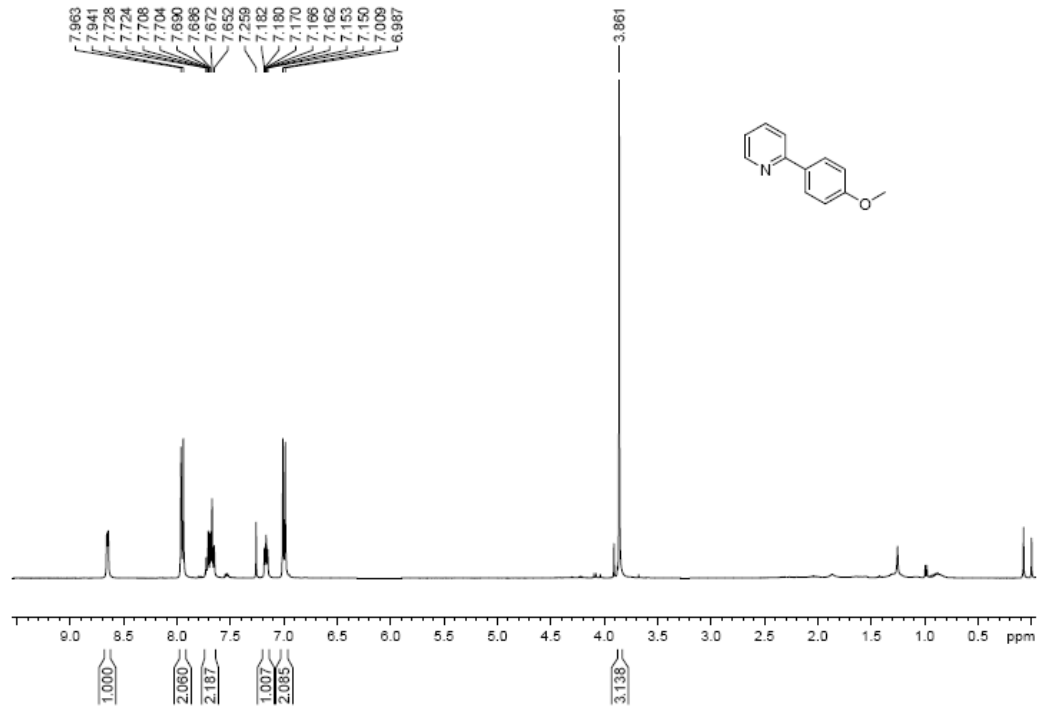
The NMR spectra.



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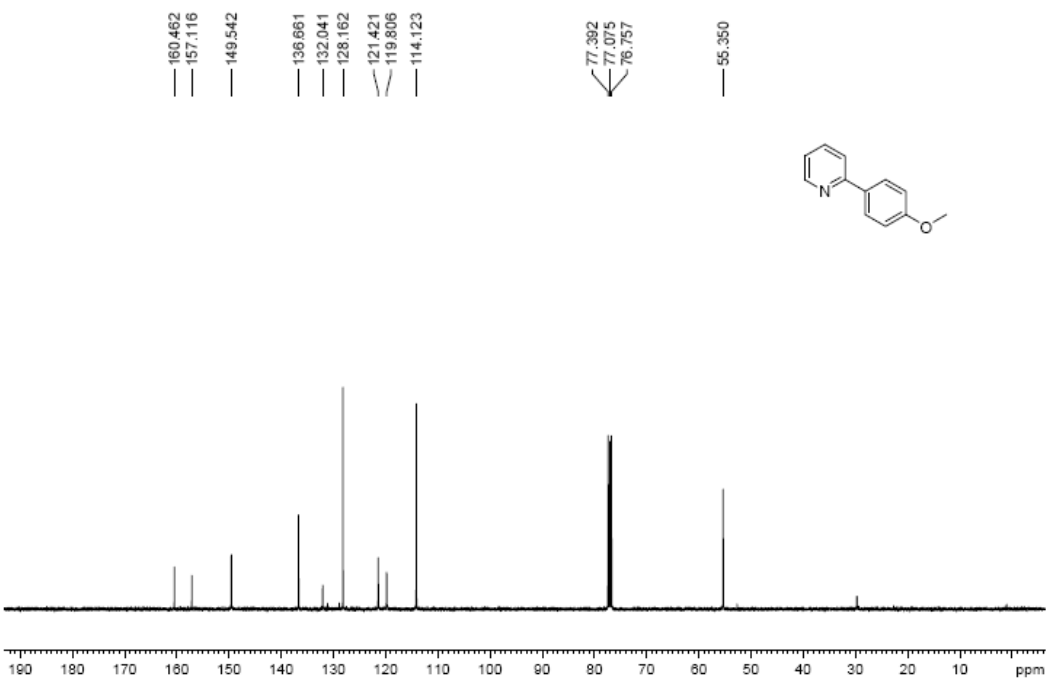
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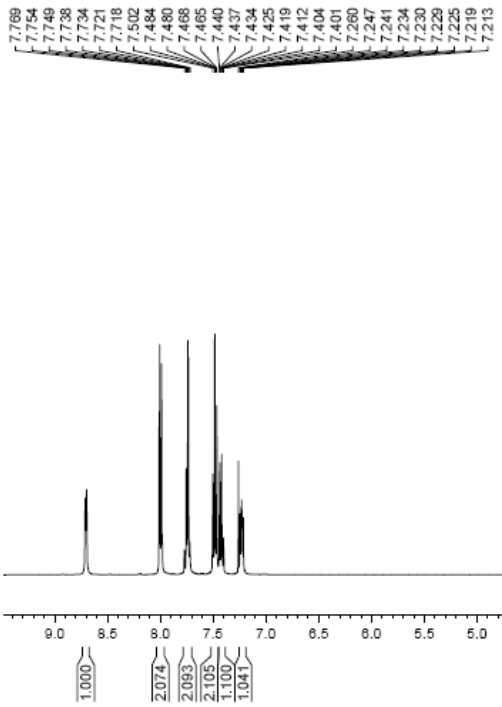
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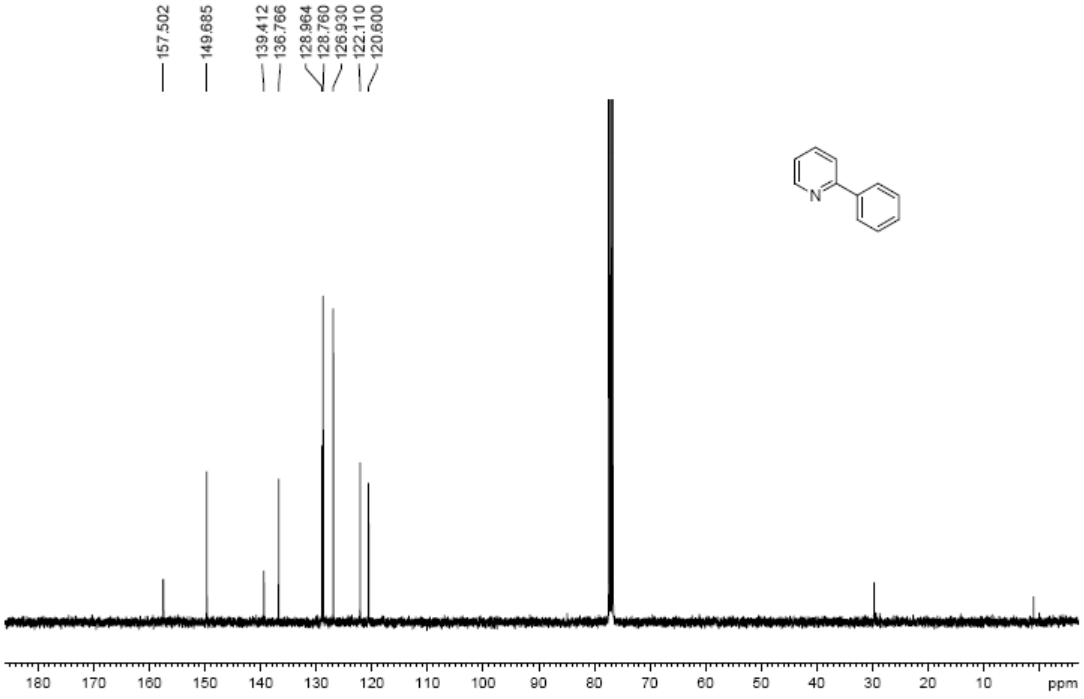
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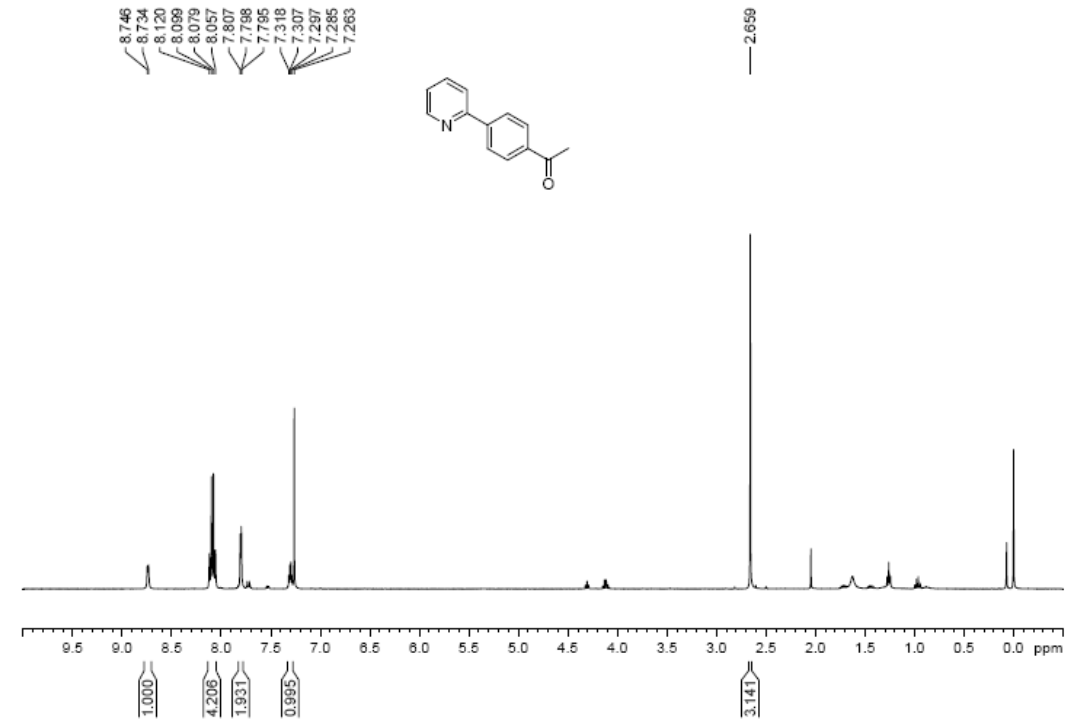
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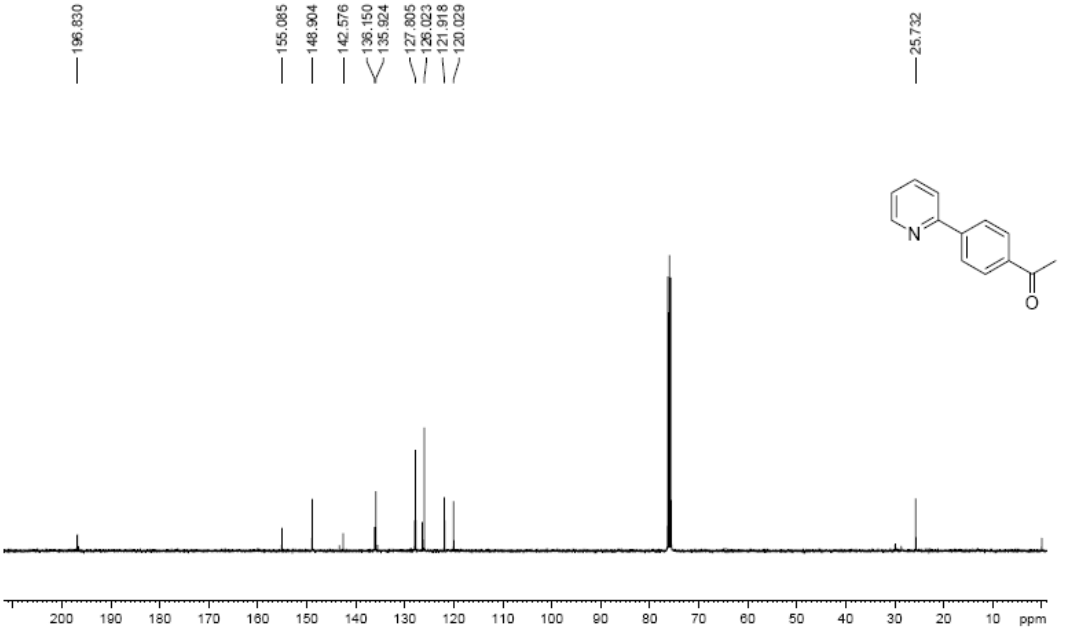
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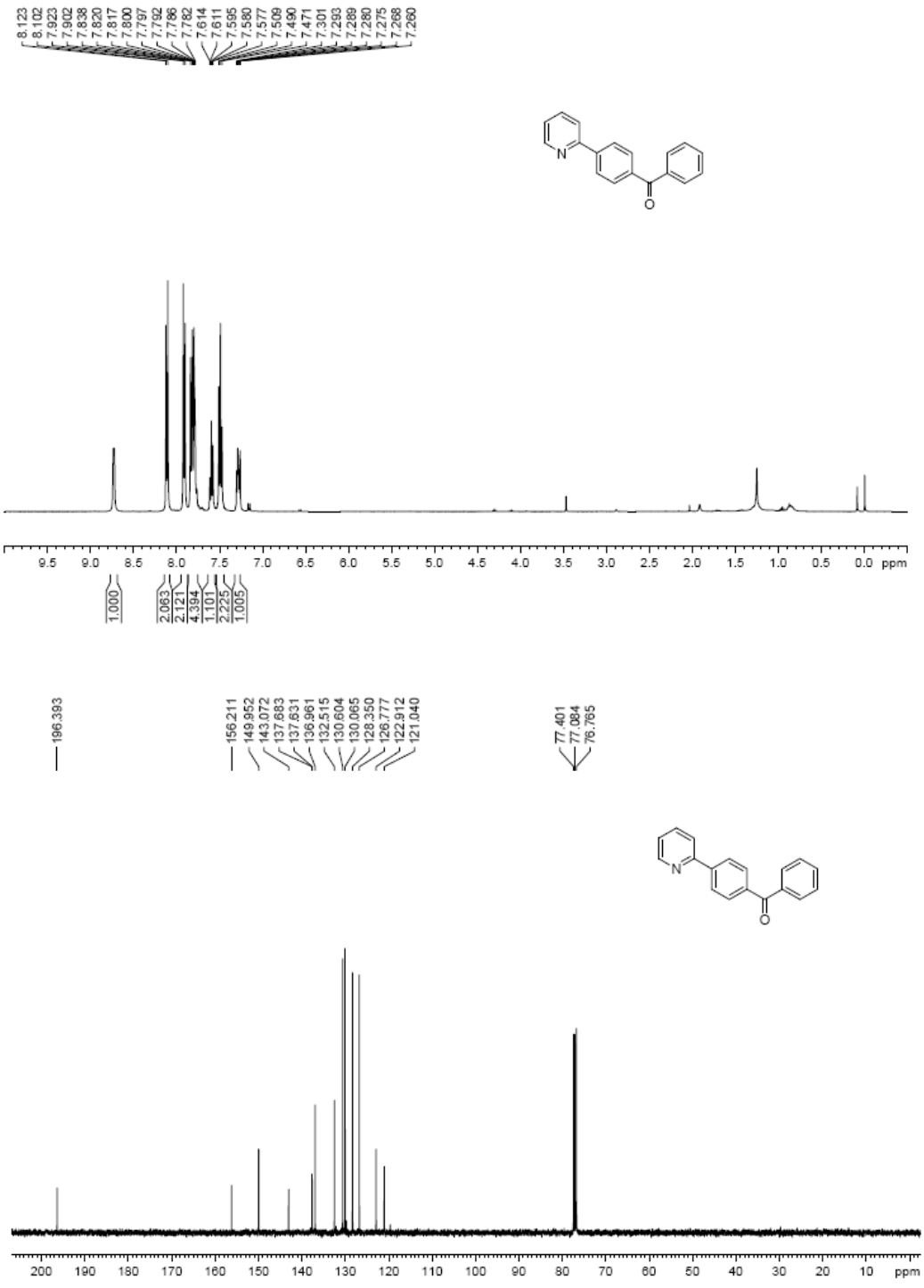
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O
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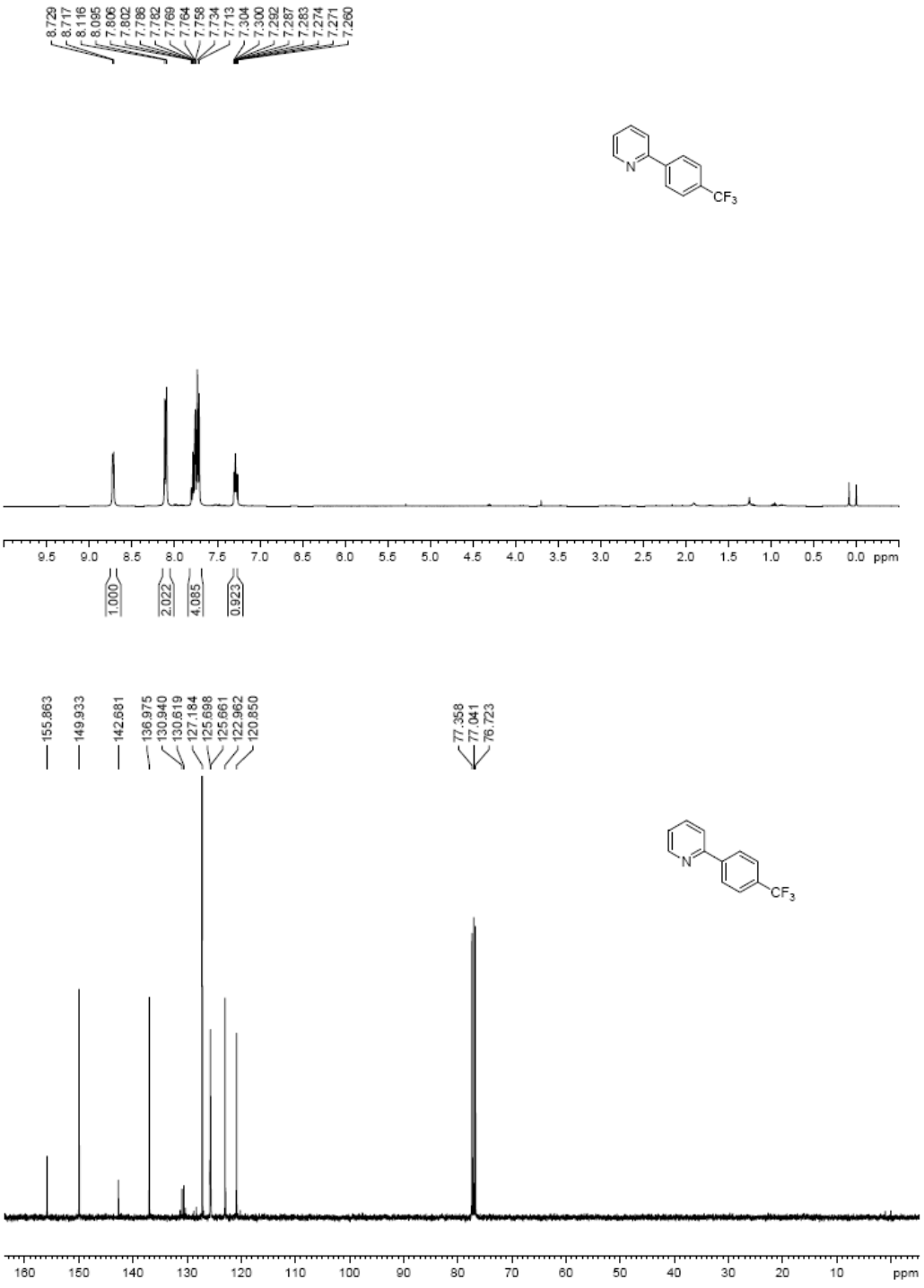
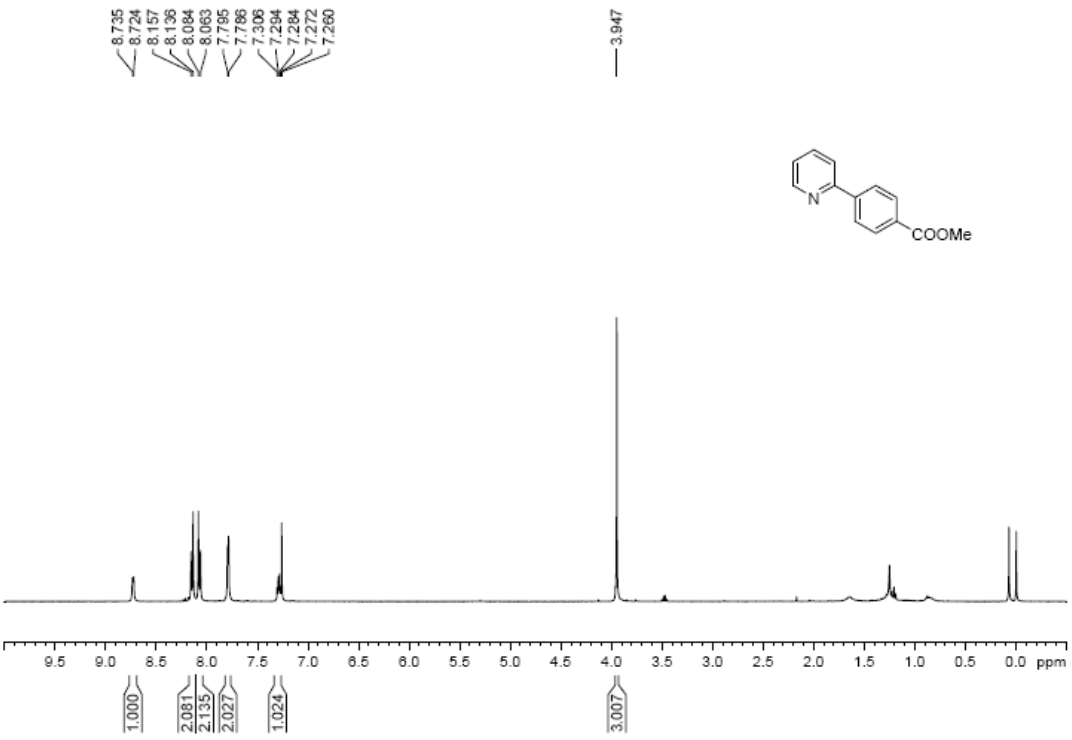
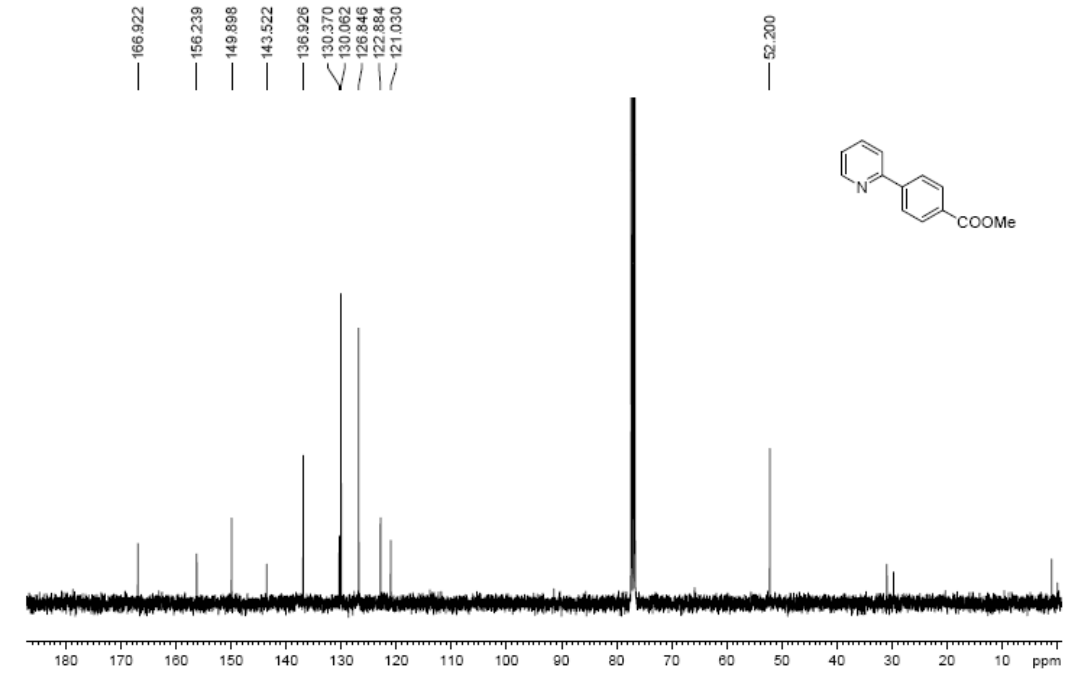
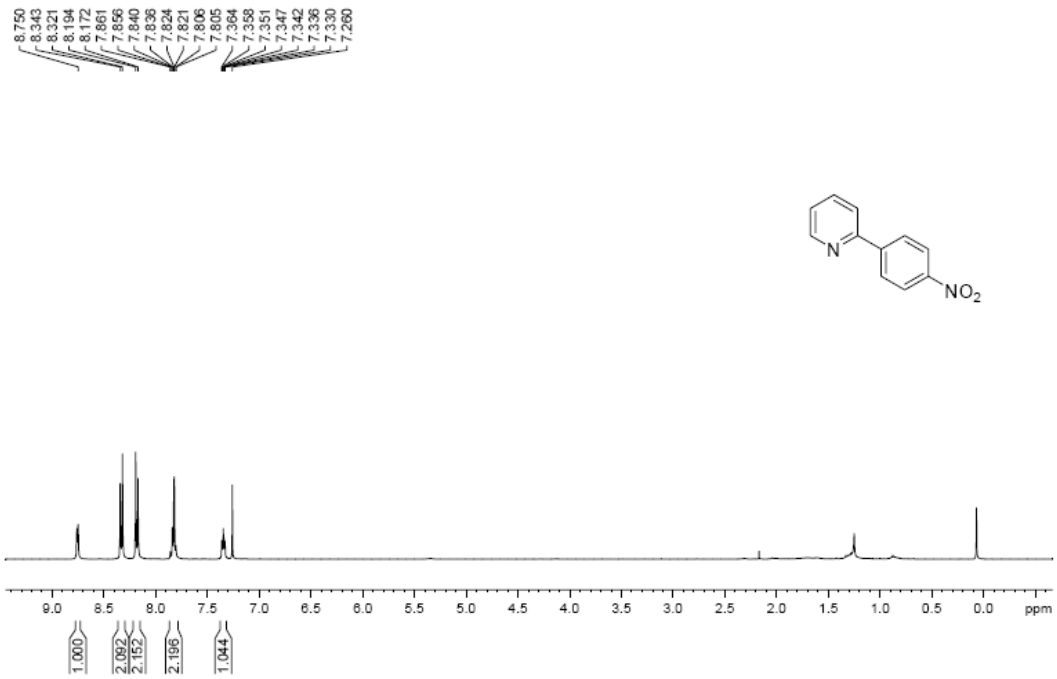
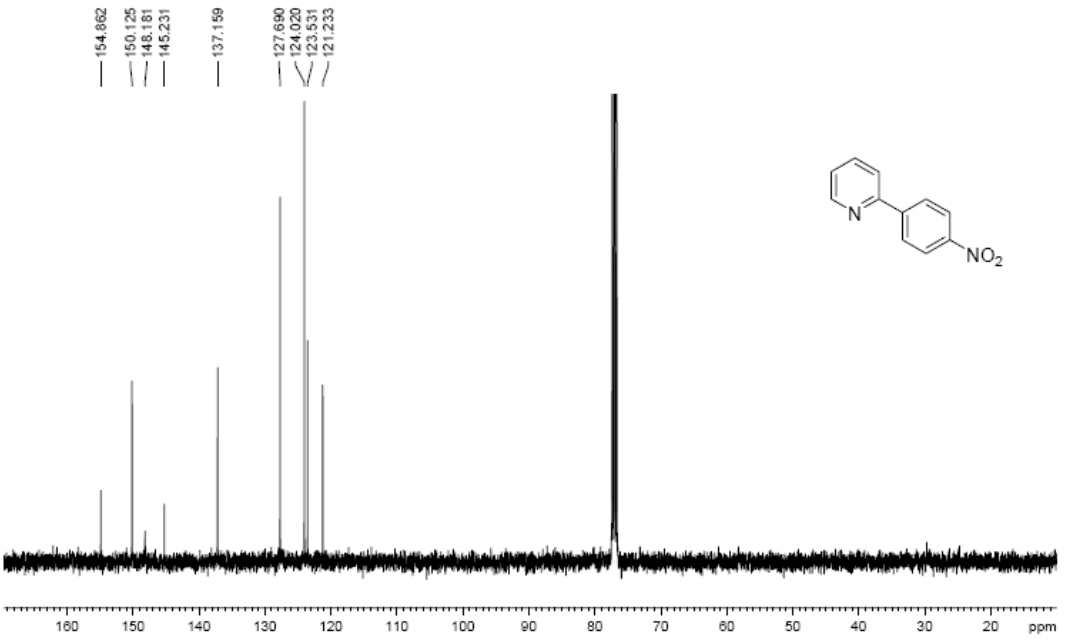
121.040
77.401
77.084
76.765
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

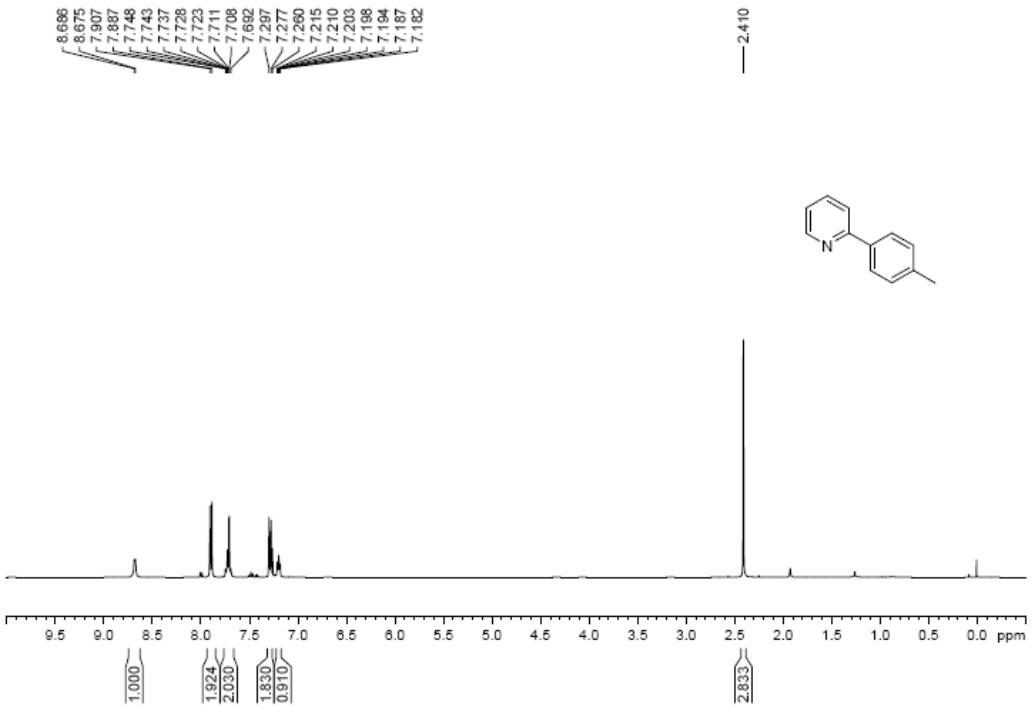

8.729
8.717
8.116
8.095
7.806
7.802
7.786
7.782
7.769
7.764
7.758
7.734
7.713
7.304
7.300
7.292
7.287
7.283
7.274
7.271
7.260
N
CF3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.022
4.085
0.923
155.863
149.933
142.681
136.975
130.940
130.619
127.184
125.698
125.661
122.962
120.850
77.358
77.041
76.723
N
CF3
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

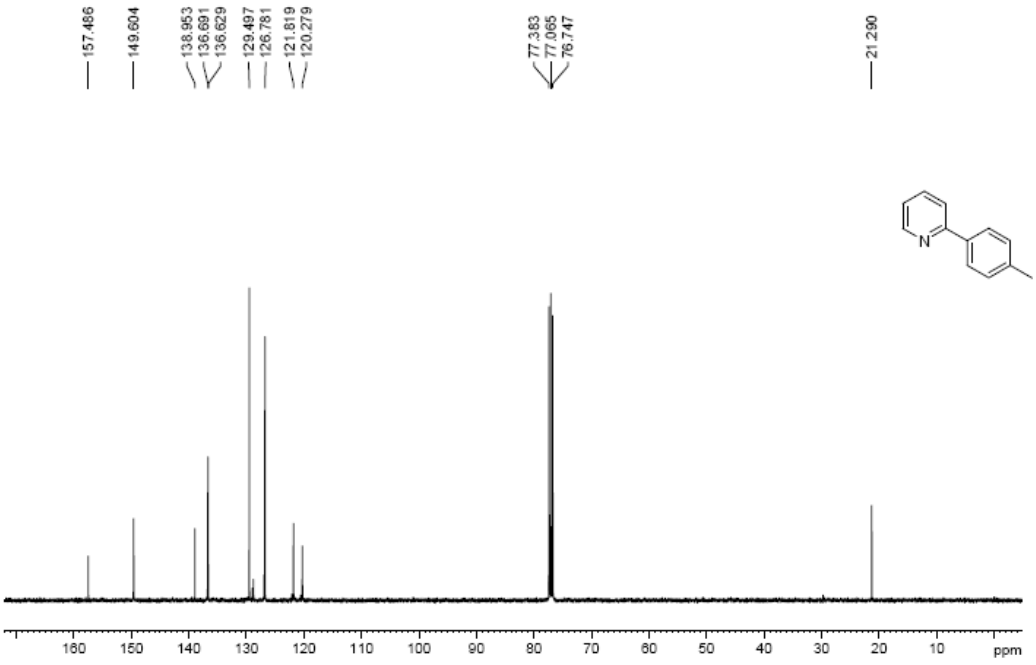

8.735
8.724
8.157
8.136
8.084
8.063
7.795
7.786
7.306
7.294
7.284
7.272
7.260
3.947
N
COOMe
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.081
2.135
2.027
1.024
3.007

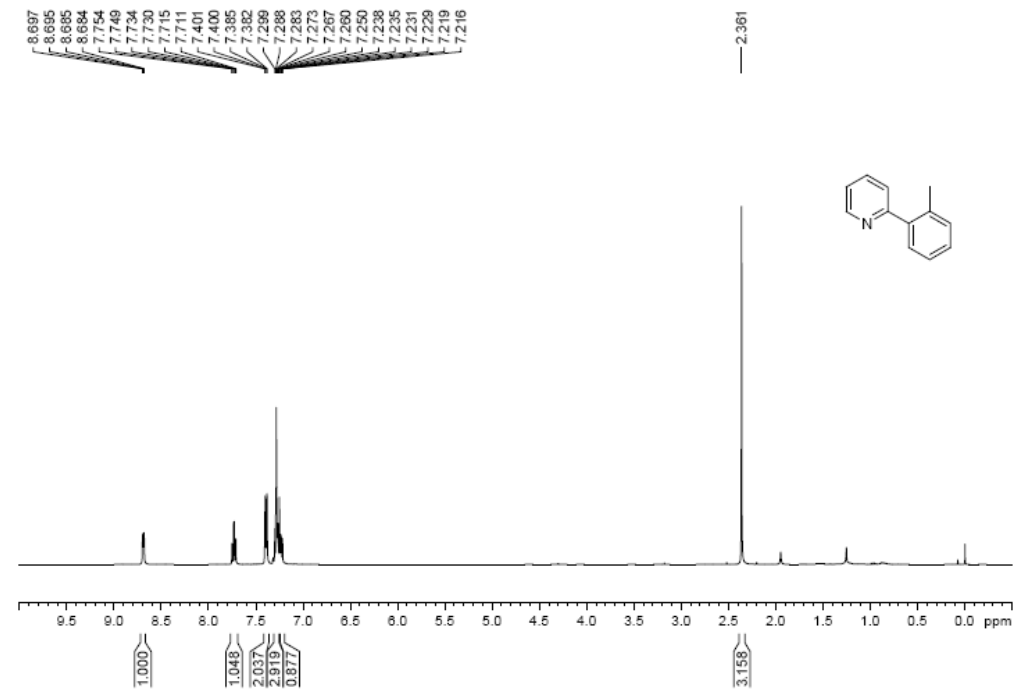

166.922
156.239
149.898
143.522
136.926
130.370
130.062
126.846
122.884
121.030
52.200
N
COOMe
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

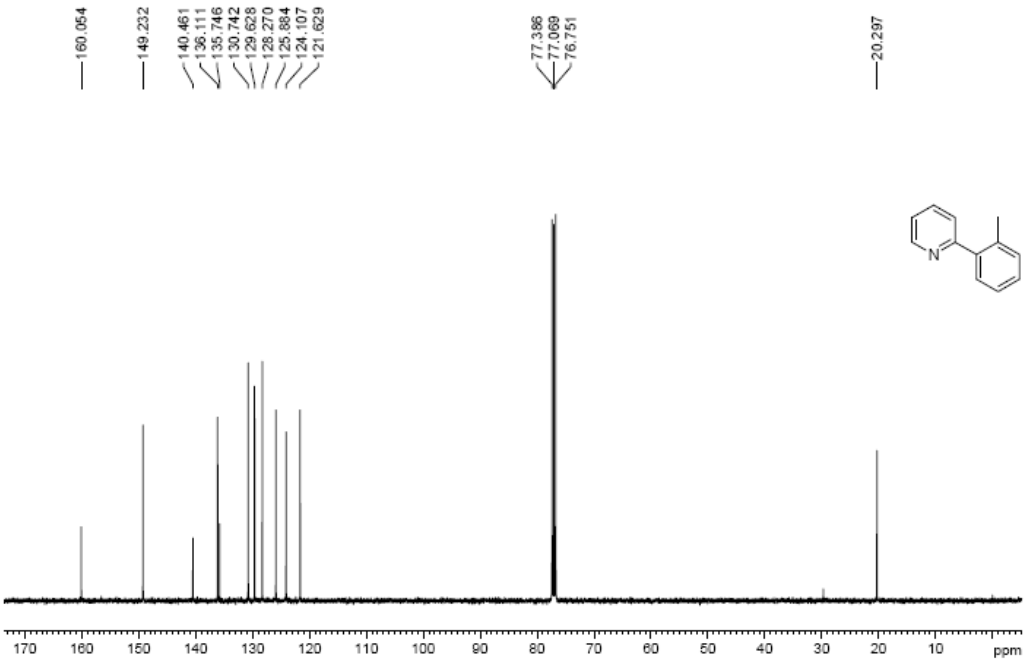

8.750
8.343
8.321
8.194
8.172
7.861
7.856
7.840
7.836
7.824
7.821
7.806
7.805
7.364
7.358
7.351
7.347
7.342
7.336
7.330
7.260
N
NO2
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.092
2.152
2.196
1.044

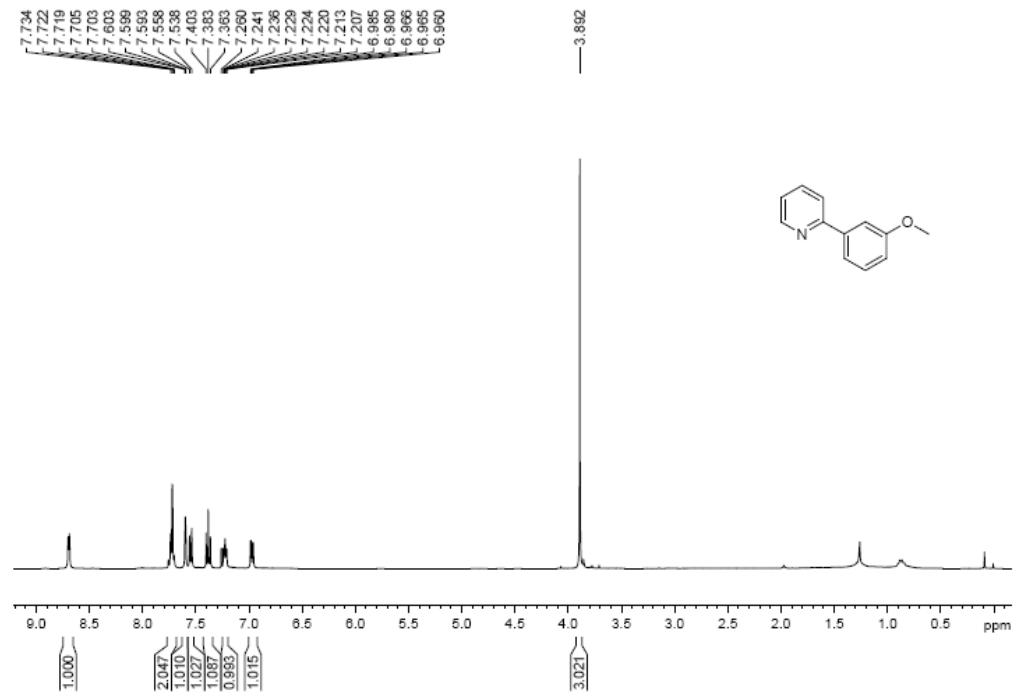

154.862
150.125
148.161
145.231
137.159
127.690
124.020
123.531
121.233
N
NO2
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

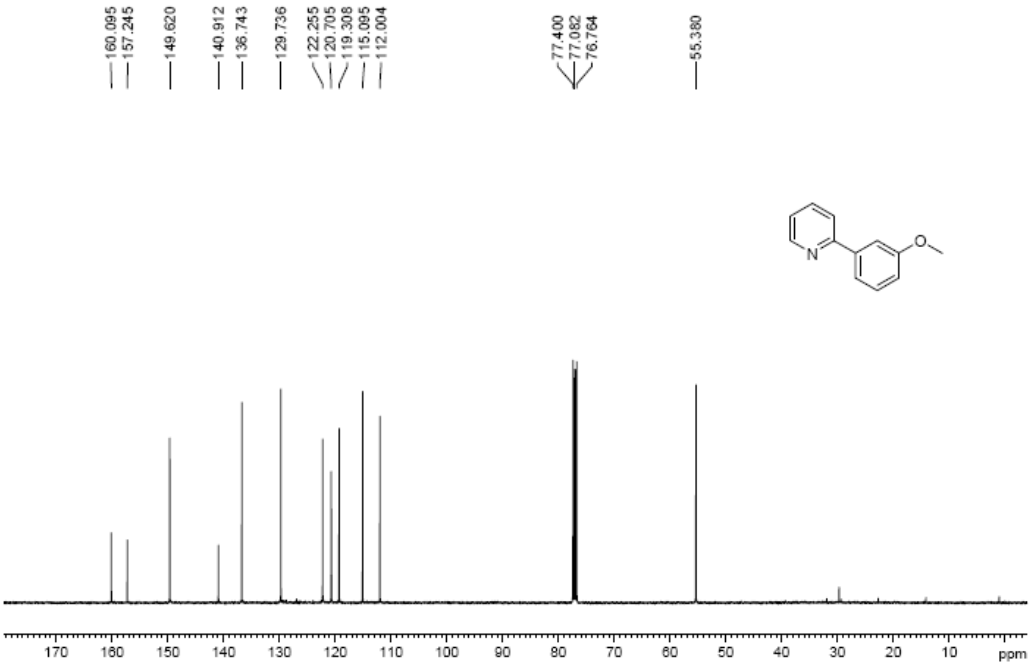

8.686
8.675
7.907
7.887
7.748
7.743
7.737
7.728
7.723
7.711
7.708
7.692
7.297
7.277
7.260
7.215
7.210
7.203
7.198
7.194
7.187
7.182
2.410
N
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.924
2.030
1.830
0.910
2.833

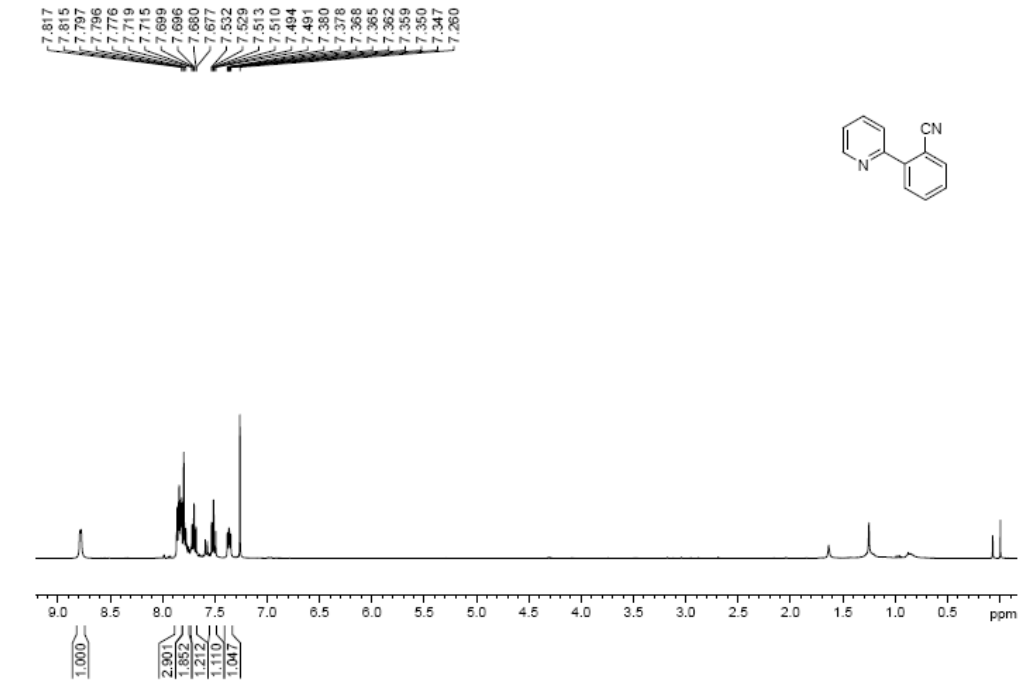

157.486
149.604
138.953
136.691
136.629
129.497
126.781
121.819
120.279
77.383
77.065
76.747
21.290
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.697
8.695
8.685
8.684
7.754
7.749
7.734
7.730
7.715
7.711
7.401
7.400
7.385
7.382
7.299
7.288
7.283
7.273
7.267
7.260
7.250
7.238
7.235
7.231
7.229
7.219
7.216
2.361
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 ppm
1.000
1.048
2.037
2.919
0.877
3.158


160.054
149.232
140.461
136.111
135.746
130.742
129.628
128.270
125.884
124.107
121.629
77.386
77.069
76.751
20.297
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.734
7.722
7.719
7.705
7.703
7.603
7.599
7.593
7.558
7.538
7.403
7.383
7.363
7.260
7.241
7.236
7.229
7.224
7.220
7.213
7.207
6.985
6.980
6.966
6.965
6.960
3.892
N
O
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
ppm
1.000
2.047
1.010
1.027
1.087
0.993
1.015
3.021


160.095
157.245
149.620
140.912
136.743
129.736
122.255
120.705
119.308
115.095
112.004
77.400
77.082
76.764
55.380
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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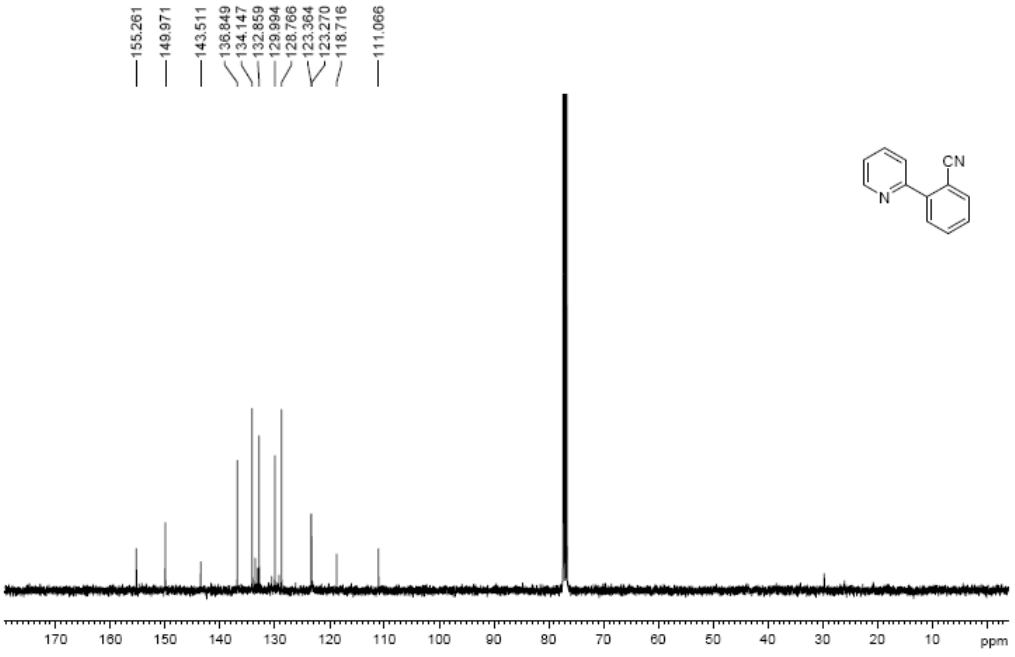
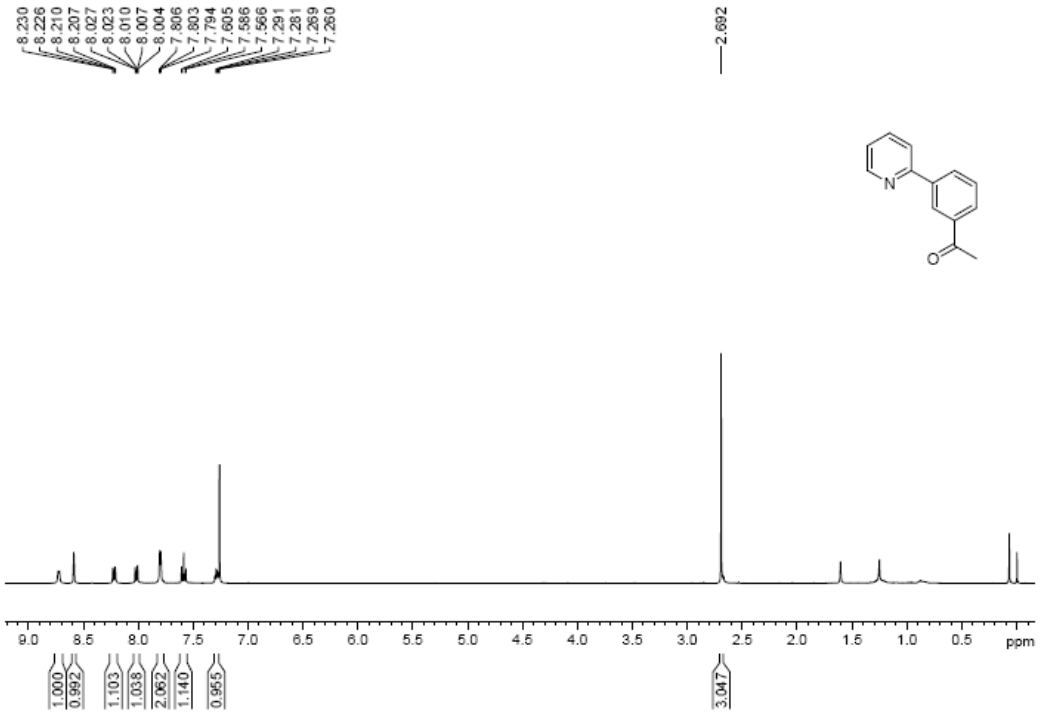
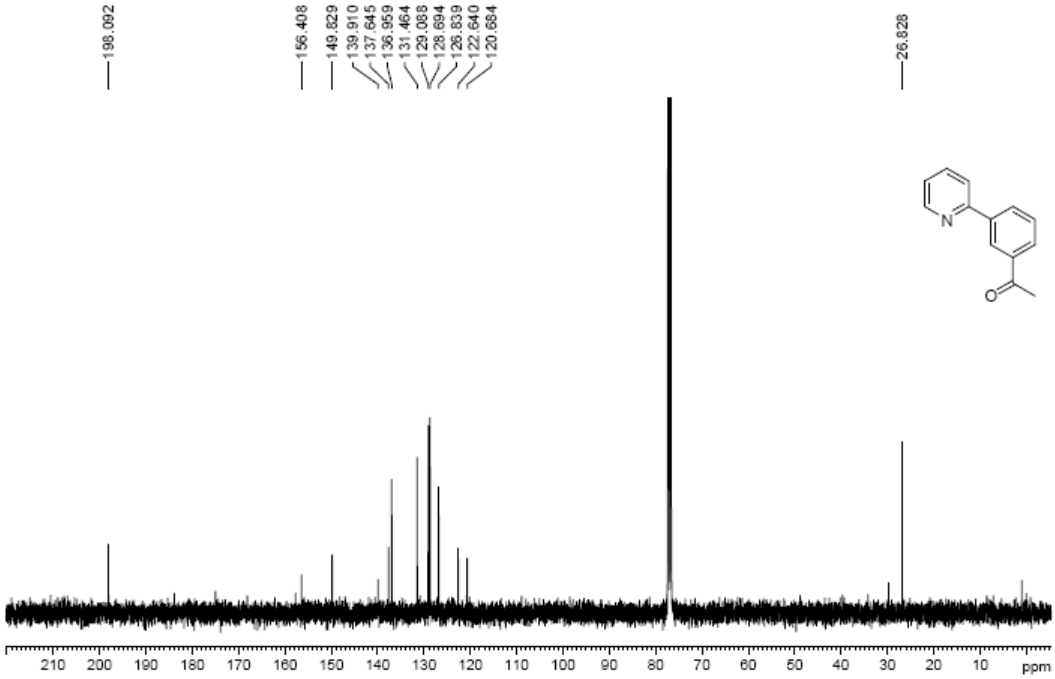
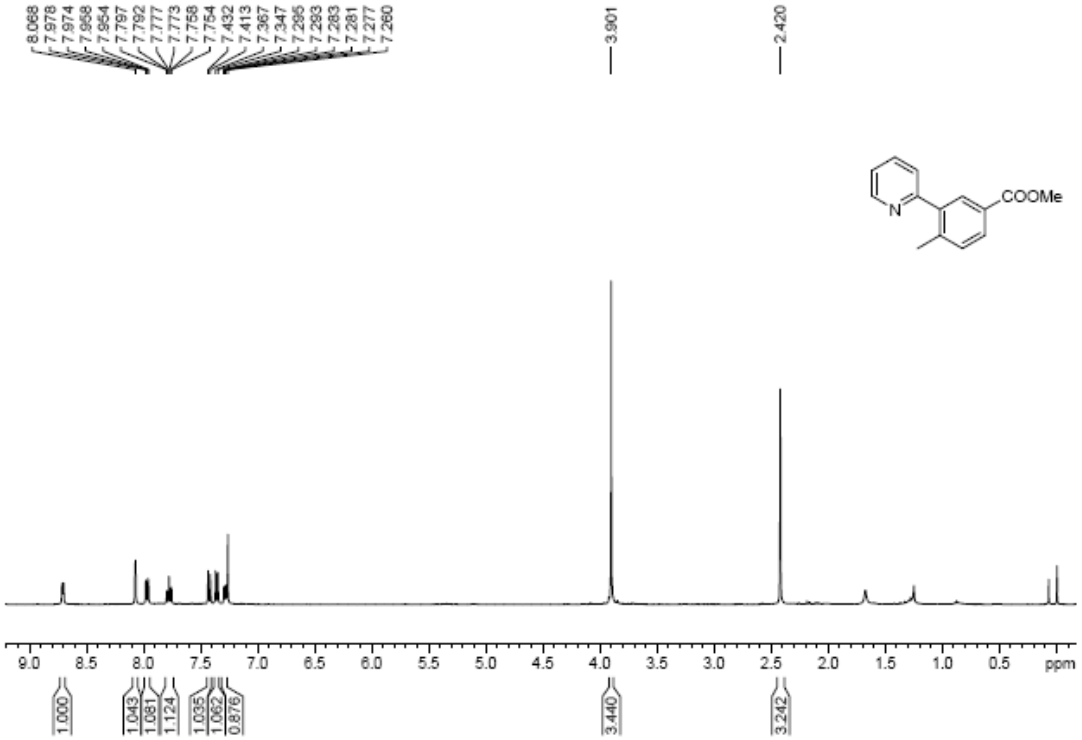
7.815
7.797
7.796
7.776
7.719
7.715
7.699
7.696
7.680
7.677
7.532
7.529
7.513
7.510
7.494
7.491
7.380
7.378
7.368
7.365
7.362
7.359
7.350
7.347
7.260
CN
N
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.000
2.901
1.852
1.212
1.110
1.047


155.261
149.971
143.511
136.849
134.147
132.859
129.994
128.766
123.364
123.270
118.716
111.066
CN
N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.230
8.226
8.210
8.207
8.027
8.023
8.010
8.007
8.004
7.806
7.803
7.794
7.605
7.586
7.566
7.291
7.281
7.269
7.260
2.692
N
O
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
ppm
1.000
0.992
1.103
1.038
2.062
1.140
0.955
3.047


198.092
156.408
149.829
139.910
137.645
136.959
131.464
129.088
128.694
126.839
122.640
120.684
26.828
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.068
7.978
7.974
7.968
7.954
7.797
7.792
7.777
7.773
7.758
7.754
7.432
7.413
7.367
7.347
7.295
7.293
7.283
7.281
7.277
7.260
3.901
2.420
COOMe
N
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
ppm
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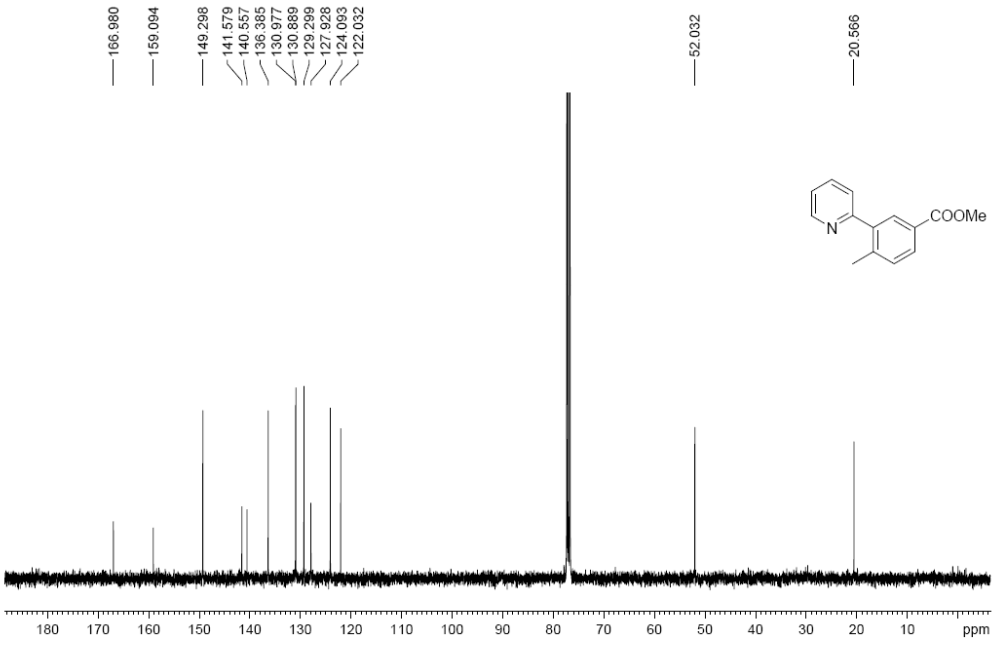
1.081
1.124
1.035
1.062
0.876
3.440
3.242


166.980
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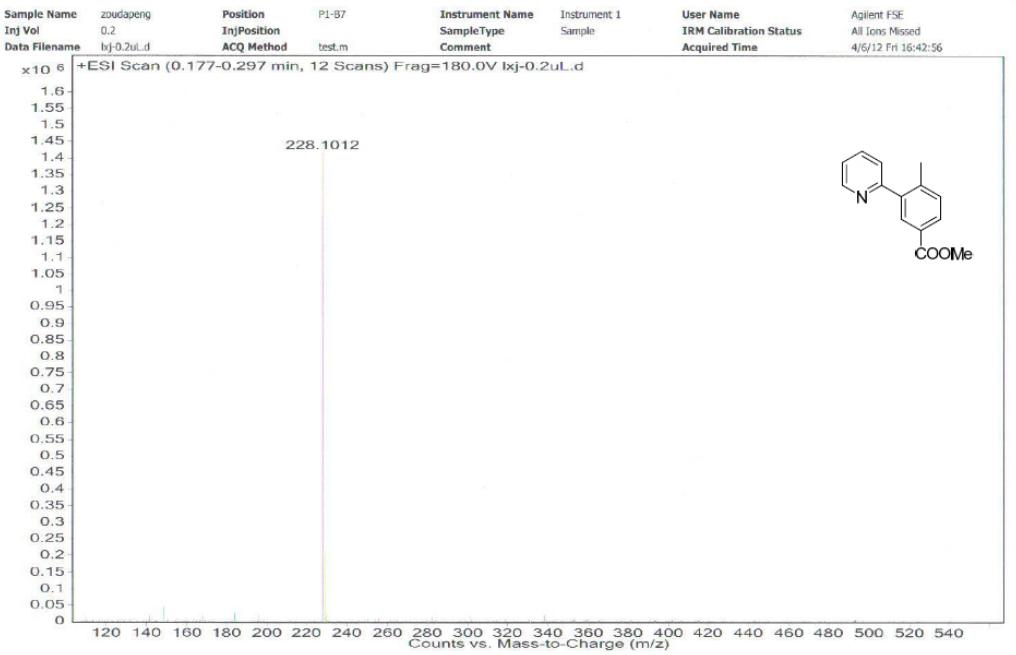
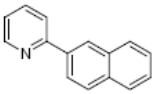
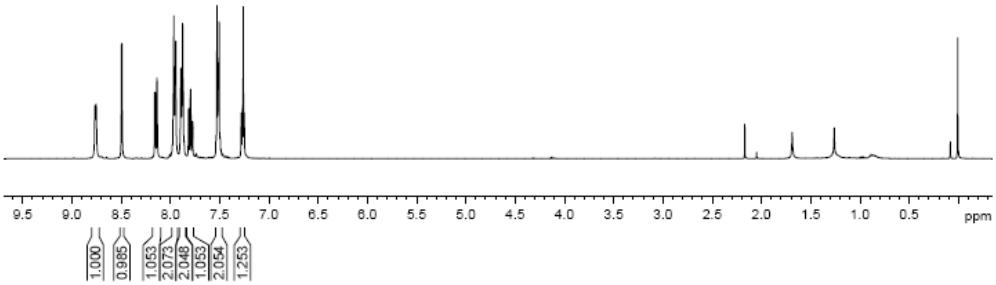
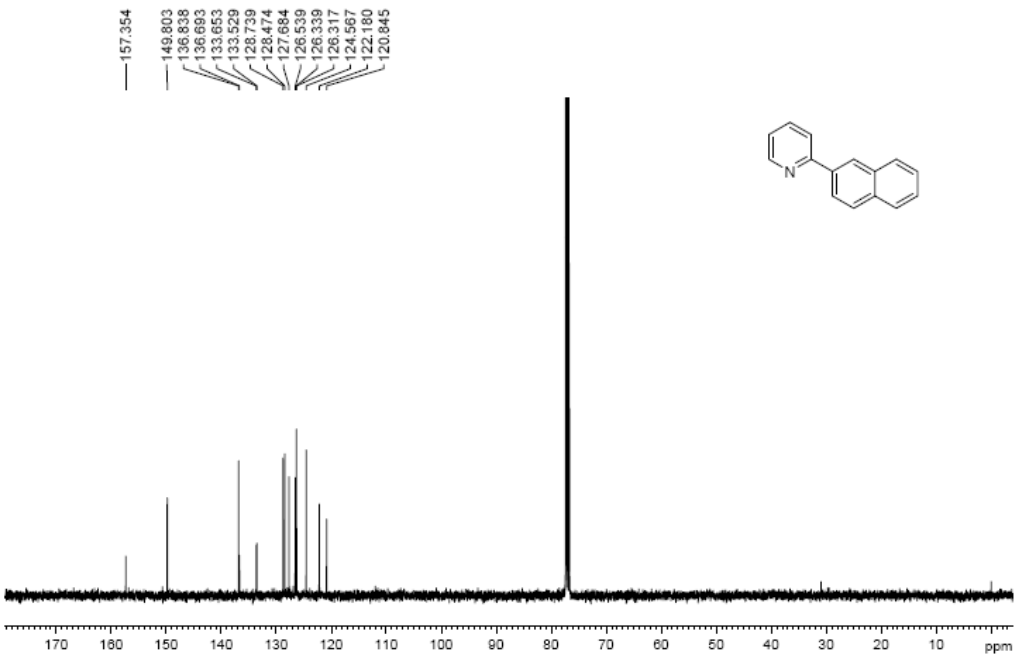
149.298
141.579
140.557
136.385
130.977
130.889
129.299
127.928
124.093
122.032
52.032
20.566
COOMe
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Sample Name zoudapeng
Position P1-B7
Instrument Name Instrument 1
User Name Agilent FSE
Inj Vol 0.2
InjPosition
SampleType Sample
IRM Calibration Status All Ions Missed
Data Filename lxj-0.2uL.d
ACQ Method test.m
Comment
Acquired Time 4/6/12 Fri 16:42:56
+ESI Scan (0.177-0.297 min, 12 Scans) Frag=180.0V lxj-0.2uL.d
x10 6
228.1012
COOMe
Counts vs. Mass-to-Charge (m/z)


7.965
7.959
7.954
7.946
7.893
7.876
7.869
7.816
7.811
7.797
7.793
7.777
7.773
7.537
7.535
7.527
7.519
7.513
7.504
7.496
7.494
7.282
7.279
7.270
7.267
7.260
7.251
7.249




ppm
1.000
0.985
1.053
2.073
2.048
1.053
2.054
1.253


157.354
149.803
136.838
136.693
133.653
133.529
128.739
128.474
127.684
126.539
126.339
126.317
124.567
122.180
120.845
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.842
7.827
7.823
7.808
7.804
7.624
7.621
7.606
7.603
7.582
7.562
7.544
7.532
7.528
7.515
7.511
7.503
7.497
7.491
7.482
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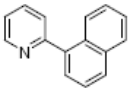
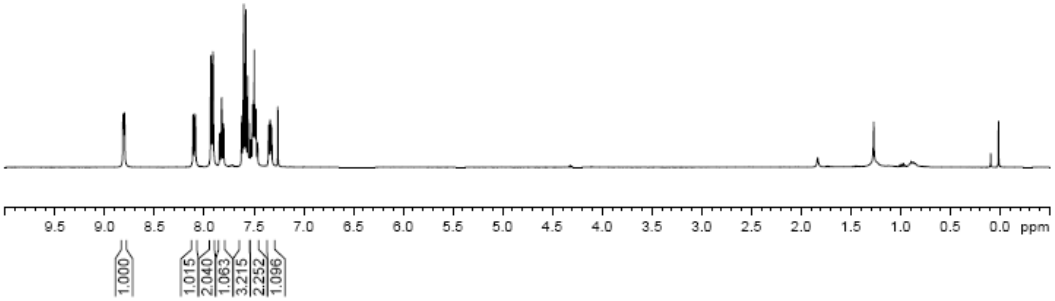
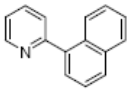
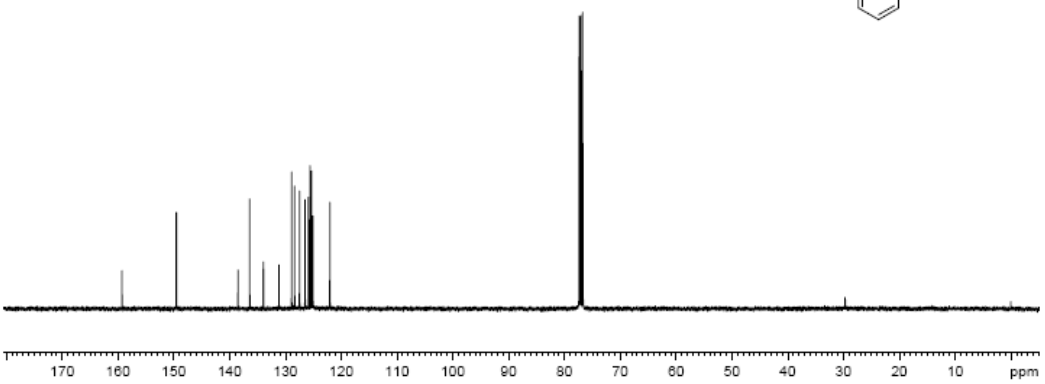
7.339
7.335
7.332
7.323
7.320
7.260

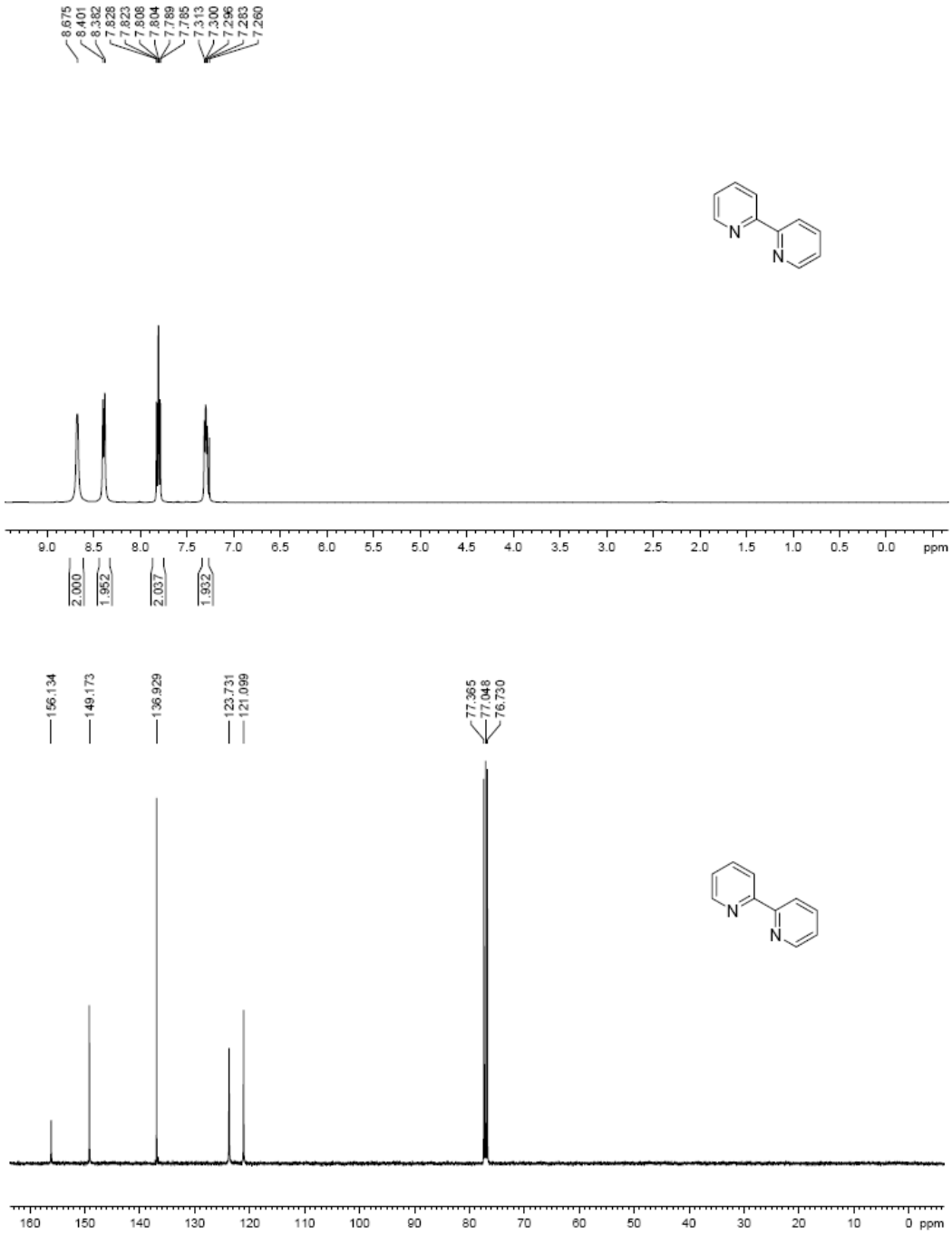



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.015
2.040
1.063
3.215
2.252
1.096

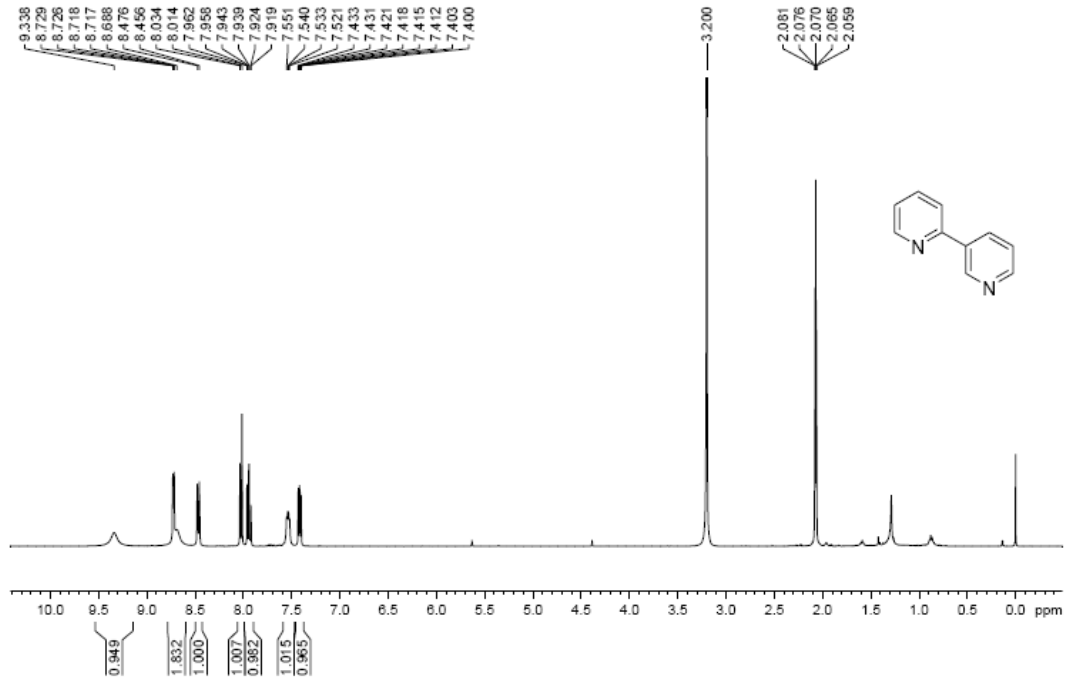

159.283
149.557
138.522
136.411
133.953
131.171
128.906
128.367
127.485
126.495
125.883
125.610
125.311
125.071
122.038
77.386
77.069
76.751

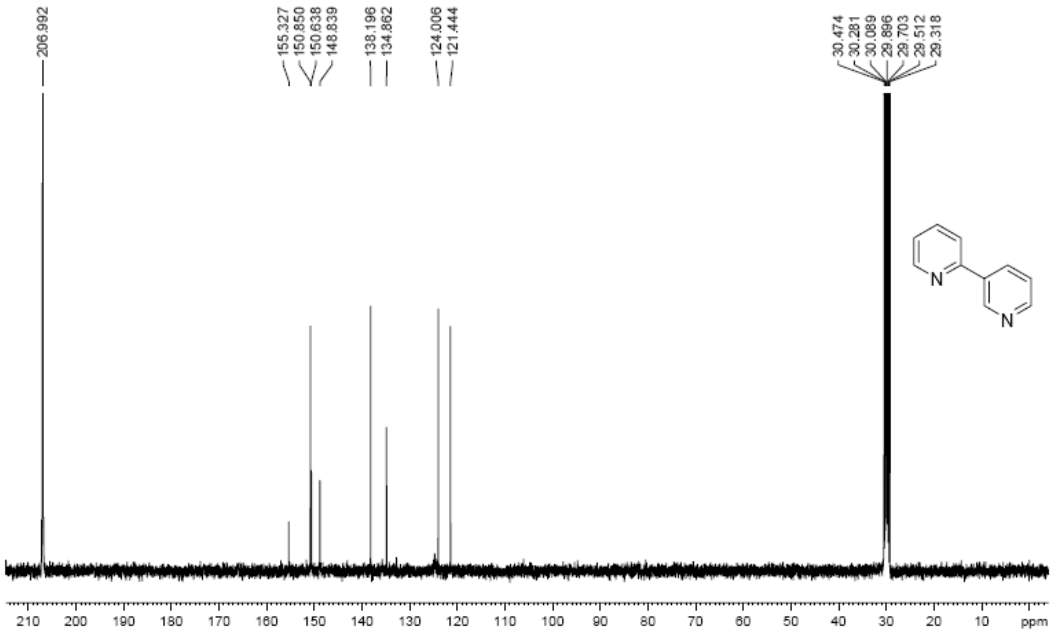


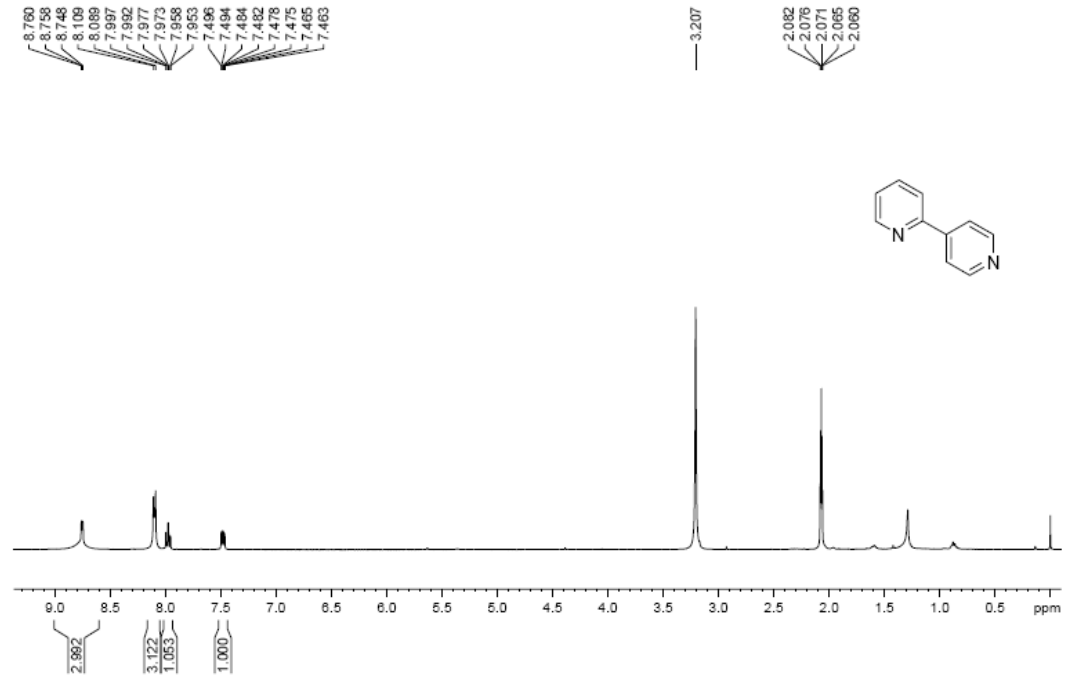

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

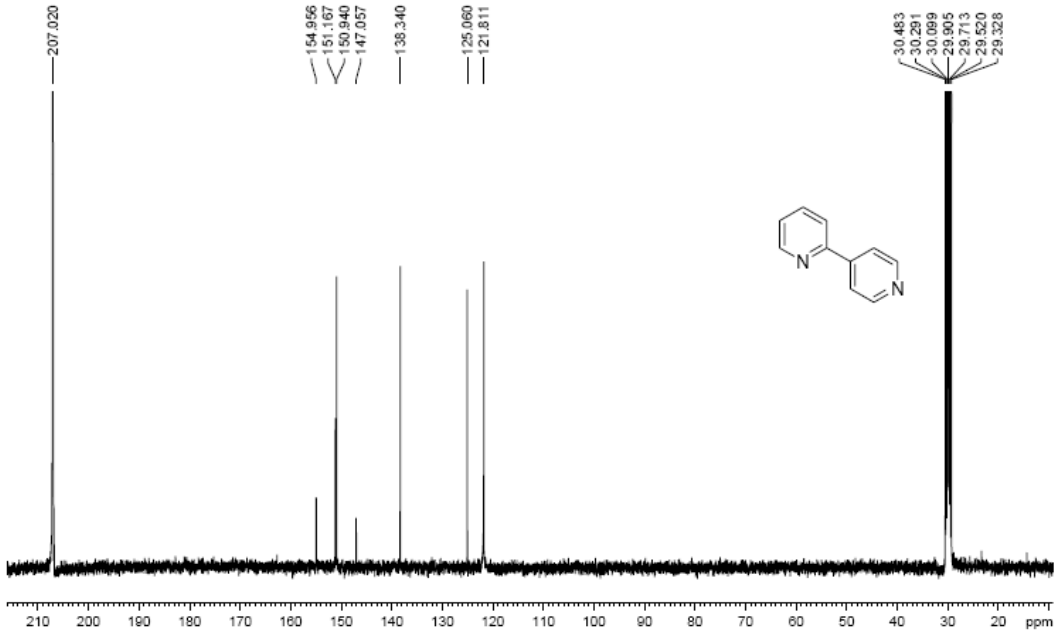

8.675
8.401
8.382
7.828
7.823
7.808
7.804
7.789
7.785
7.313
7.300
7.296
7.283
7.260
N
N
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.000
1.952
2.037
1.932
156.134
149.173
136.929
123.731
121.099
77.365
77.048
76.730
N
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

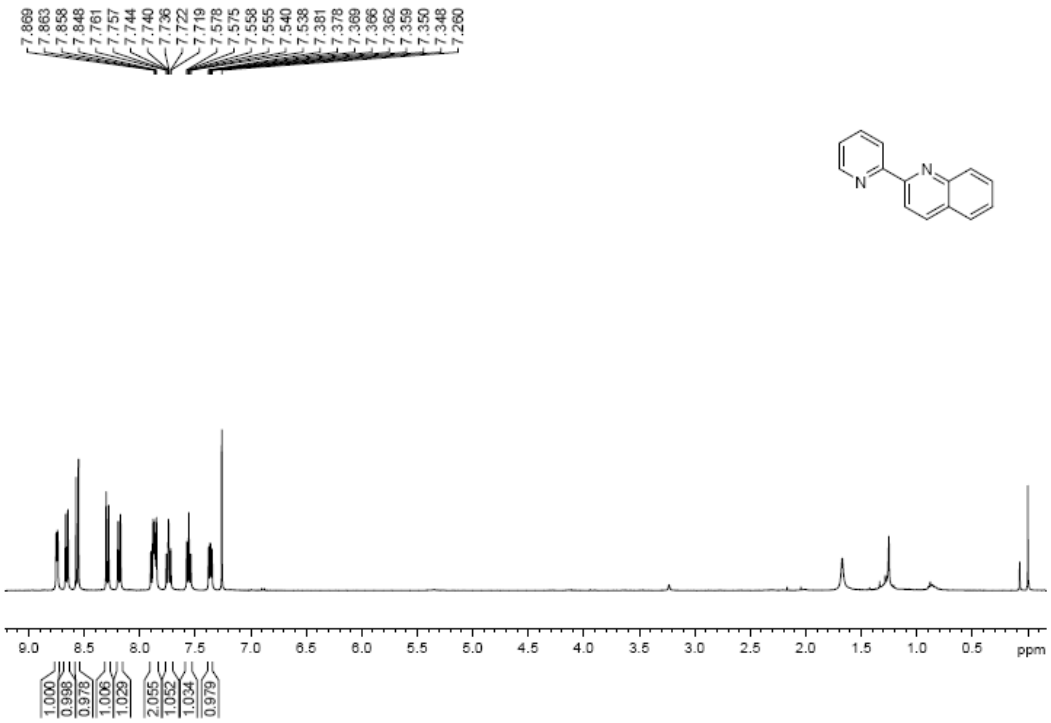
5

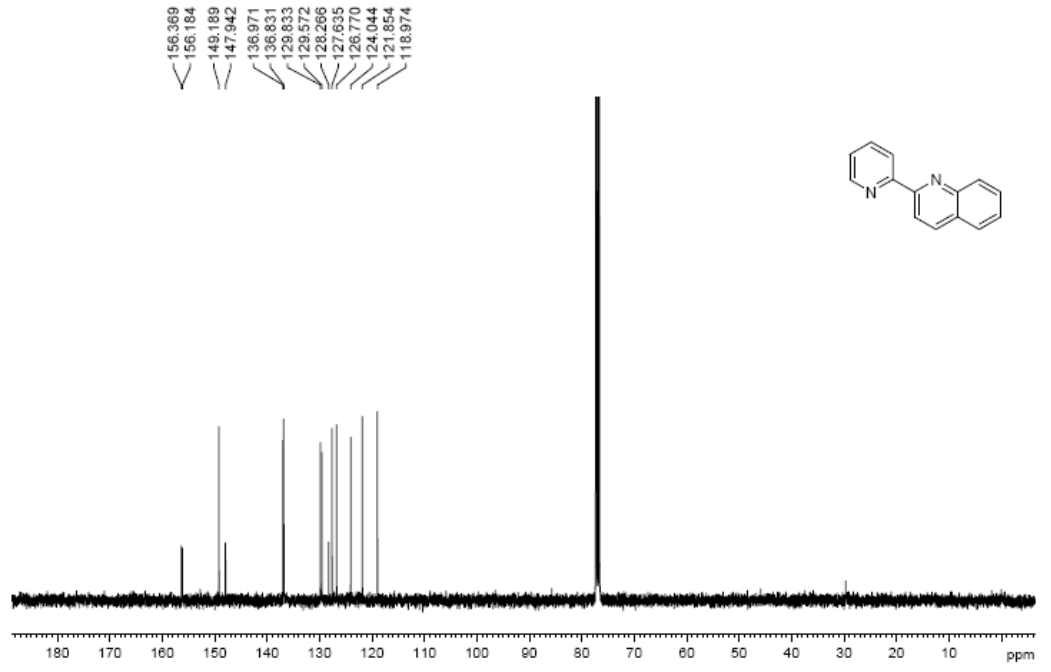

9.338
8.729
8.726
8.718
8.717
8.688
8.476
8.456
8.034
8.014
7.962
7.958
7.943
7.939
7.924
7.919
7.551
7.540
7.533
7.521
7.433
7.431
7.421
7.418
7.415
7.412
7.403
7.400
3.200
2.081
2.076
2.070
2.065
2.059
N
N
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.949
1.832
1.000
1.007
0.982
1.015
0.965

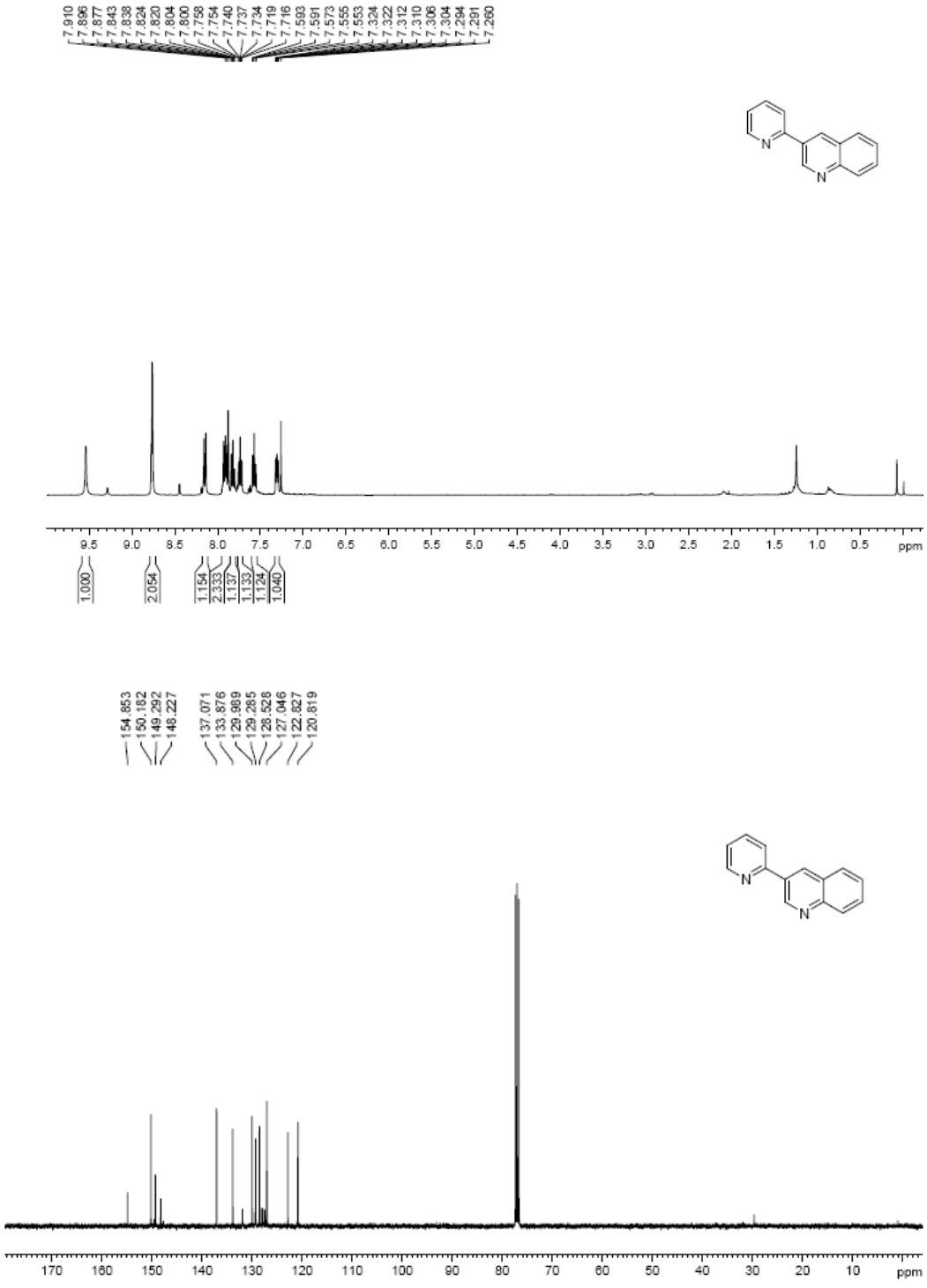

206.992
155.327
150.850
150.638
148.839
138.196
134.862
124.006
121.444
30.474
30.281
30.089
29.896
29.703
29.512
29.318
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.760
8.758
8.748
8.109
8.089
7.997
7.992
7.977
7.973
7.958
7.953
7.496
7.494
7.484
7.482
7.478
7.475
7.465
7.463
3.207
2.082
2.076
2.071
2.065
2.060
N
N
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
ppm
2.992
3.122
1.053
1.000


207.020
154.956
151.167
150.940
147.057
138.340
125.060
121.811
30.483
30.291
30.099
29.905
29.713
29.520
29.328
N
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.869
7.863
7.858
7.848
7.761
7.757
7.744
7.740
7.736
7.722
7.719
7.578
7.575
7.558
7.555
7.540
7.538
7.381
7.378
7.369
7.366
7.362
7.359
7.350
7.348
7.260
N
N
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 ppm
1.000
0.998
0.978
1.006
1.029
2.055
1.052
1.034
0.979


156.369
156.184
149.189
147.942
136.971
136.831
129.833
129.572
128.266
127.635
126.770
124.044
121.854
118.974
N
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.910
7.896
7.877
7.843
7.838
7.824
7.820
7.804
7.800
7.758
7.754
7.740
7.737
7.734
7.719
7.716
7.593
7.591
7.573
7.555
7.553
7.324
7.322
7.312
7.310
7.306
7.304
7.294
7.291
7.260
N
N
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 ppm
1.000
2.054
1.154
2.333
1.137
1.133
1.124
1.040
154.853
150.162
149.292
148.227
137.071
133.876
129.989
129.285
128.528
127.046
122.827
120.819
N
N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm