Supporting Information for

Rhodium-Catalyzed Regioselective C-H Functionalization via Decarbonylation of Acid Chlorides and C-H Bond Activation under Phosphine-Free Conditions

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Experimental procedures and analytical data

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1. General Considerations

Unless otherwise noted, the starting materials were commercially available and the reactions were carried out under nitrogen atmosphere. Toluene and xylene were dried from Na/benzophenone and distilled prior to use. The inorganic bases were dried at 160 °C for 3 h, and 4A molecular sieves were activated at 500 °C for 2 h, and then cooled to ambient temperature before use. $[Rh(COD)Cl]_2$ was commercially purchased or prepared according to the reported method.[1] The commercially available acid chlorides were redistilled prior to use and chlorides **2b**-**h** and **2j** were synthesized by reacting their corresponding mother acids with thionyl chloride.[2] 2-Arylpyridines (**1b-g**)[3] and 1-(pyridin-2-yl)-1,2,3,4-tetrahydroquinoline (**1i**)[4] were prepared according to the literature methods. All the melting points were uncorrected. ^1H and $^{13}C\{^1H\}$ NMR spectra were obtained with a 400 MHz NMR spectrometer, and the chemical shift values were relative to $CDCl_3$. Products **3a**,[5] **3j**,[5] **3n**[5] and **3o**[6] are known compounds and they were identified by comparison of their NMR features with those reported data and further confirmed by HRMS analysis.

References

(1) Schenck, T. G.; Downes, J. M.; Milne, C. R. C.; Mackenzie, P. B.; Boucher, T. G.; Whelan, J.; Bosnich, B. *Inorg. Chem.* **1985**, *24*, 2334.

(2) Andersson, C. M.; Hallberg, A. *J. Org. Chem.* **1988**, *53*, 235.

(3) Chow, H.-F.; Wan, C.-W. *J. Org. Chem.* **2001,** *66,* 5042.

(4) Wagaw, S.; Buchwald, S. L. *J. Org. Chem.* **1996,** *61,* 7240.

(5) Oi, S.; Fukita, S.; Hirata, N.; Watanuki, N.; Miyano, S.; Inoue, Y. *Org. Lett.* **2001**, *3*, 2579.

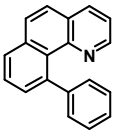
(6) Oi, S.; Fukita, S.; Inoue, Y. *Chem. Commun.* **1998**, 2439.

2. Experimental procedures

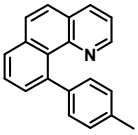
A typical procedure for arylation of benzo[h]quinoline (1a) and 2-substituted pyridines (1e-i)–phenylation of 1a using benzoyl chloride as the coupling partner: In a glovebox, to a 25-mL Schlenk tube were successively added the catalyst $[Rh(COD)Cl]_2$ (12 mg, 0.025 mmol), Na_2CO_3 (106 mg, 1 mmol), 4A molecular sieves (600 mg), benzo[*h*]quinoline **1a** (89 mg, 0.5 mmol), benzoyl chloride **2a** (105 mg, 0.75 mmol) and xylene (3 mL). The Schlenk tube was equipped with an air condenser and the mixture was stirred at 145 °C under nitrogen atmosphere for 16 h. After cooled to ambient temperature, the resulting mixture was filtered through a short pad of celite and rinsed with 10 mL toluene. The combined filtrate was evaporated all the volatiles under reduced pressure. The resultant residue was purified by flash silica gel column chromatography (eluent: petroleum ether (60-90 °C) / EtOAc = 30 : 1, v/v), affording the target product **3a** as a white solid (118.0 mg, 93%).

A typical procedure for diarylation of 2-substituted pyridines (1b-d)–diphenylation of 2-phenylpyridine (1b) using benzoyl chloride as the coupling partner: In a glovebox, to a 25-mL Schlenk tube were successively added the catalyst $[Rh(COD)Cl]_2$ (24.0 mg, 0.05 mmol), Na_2CO_3 (159 mg, 1.5 mmol), 4A molecular sieves (600 mg), 2-phenylpyridine **1b** (78.0 mg, 0.5 mmol), benzoyl chloride **2a** (281 mg, 2.0 mmol) and xylene (3 mL). The Schlenk tube was equipped with an air condenser and the mixture was stirred at 145 °C under nitrogen atmosphere for 16 h. After cooled to ambient temperature, the resulting mixture was filtered through a short pad of celite and rinsed with 10 mL toluene. The combined filtrate was evaporated all the volatiles under reduced pressure. The resultant residue was purified by flash silica gel column chromatography (eluent: petroleum ether (60-90 °C) / EtOAc / Et_3N = 100 : 5 : 1, v/v/v), affording the target product **3j** as a white solid (110.3 mg, 72%).

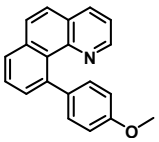
3. Analytical data



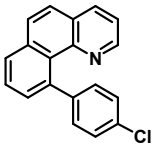
10-Phenyl-7,8-benzoquinoline (3a)[5]: White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (dd, J = 4.2, 1.8 Hz, 1H), 8.11 (dd, J = 8.0, 1.8 Hz, 1H), 7.97 (dd, J = 7.9, 1.2 Hz, 1H), 7.90 (d, J = 8.8 Hz, 1H), 7.76-7.71 (m, 2H), 7.63 (dd, J = 7.2, 1.3 Hz, 1H), 7.51-7.43 (m, 5H), 7.35 (dd, J = 8.0, 4.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 147.0, 146.5, 141.8, 135.3, 135.1, 131.6, 129.1, 128.8, 128.4, 128.0, 127.5, 127.3, 127.1, 126.0, 125.8, 121.1.



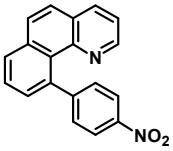
10-(4-Methylphenyl)-7,8-benzoquinoline (3b): Viscous yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (dd, J = 4.2, 1.7 Hz, 1H), 8.11 (dd, J = 8.0, 1.6 Hz, 1H), 7.98 (d, J = 7.8 Hz, 1H), 7.91 (d, J = 8.8 Hz, 1H), 7.78-7.72 (m, 2H), 7.67 (d, J = 7.2 Hz, 1H), 7.42-7.34 (m, 5H), 2.59 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 146.90, 146.86, 143.5, 141.8, 135.2, 135.1, 131.7, 129.1, 128.7, 128.3, 128.2, 127.8, 127.2, 127.1, 125.9, 121.1, 21.4. HRMS calcd. for $C_{20}H_{15}N$ $[M]^+$: 269.1204; found: 269.1193.



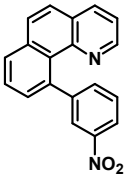
10-(4-Methoxylphenyl)-7,8-benzoquinoline (3c): White solid; m.p. 121-122 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (dd, J = 4.2, 1.7 Hz, 1H), 8.09 (dd, J = 8.0, 1.8 Hz Hz, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.86 (d, J = 8.8 Hz, 1H), 7.71-7.67 (m, 2H), 7.58 (dd, J = 7.2, 1.0 Hz, 1H), 7.36-7.32 (m, 3H), 6.99 (d, J = 8.6 Hz, 2H), 3.99 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.0, 147.0, 141.5, 139.0, 135.4, 135.2, 131.8, 129.9, 129.2, 128.4, 127.9, 127.3, 127.2, 126.0, 121.1, 112.9, 55.4. HRMS calcd. for $C_{20}H_{15}NO$ $[M]^+$: 285.1154; found: 285.1146.



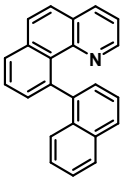
10-(4-Chlorophenyl)-7,8-benzoquinoline (3d): White solid; m.p. 82 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (dd, J = 4.2, 1.6 Hz, 1H), 8.11 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 7.8 Hz, 1H), 7.87 (d, J = 8.8 Hz, 1H), 7.73-7.68 (m, 2H), 7.52 (d, J = 7.2 Hz, 1H), 7.41-7.30 (m, 5H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 147.0, 146.7, 145.0, 140.5, 135.4, 135.1, 131.6, 131.4, 130.2, 129.0, 128.4, 127.6, 127.4, 127.2, 126.2, 121.3. HRMS calcd. for $C_{19}H_{12}ClN$ $[M]^+$: 289.0658; found: 289.0647.



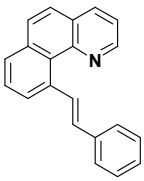
10-(4-Nitrophenyl)-7,8-benzoquinoline (3e): Pale yellow solid; m.p. 159 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (dd, J = 4.1, 1.5 Hz, 1H), 8.26 (d, J = 8.6 Hz, 2H), 8.11 (dd, J = 8.0, 1.5 Hz, 1H), 8.00 (d, J = 7.9 Hz, 1H), 7.89 (d, J = 8.8 Hz, 1H), 7.75-7.70 (m, 2H), 7.47-7.45 (m, 3H), 7.35 (dd, J = 8.0, 4.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 153.9, 146.9, 146.1, 139.2, 135.5, 134.9, 130.7, 129.5, 129.0, 128.6, 128.2, 127.4, 127.1, 126.4, 122.8, 121.5. HRMS calcd. for $C_{19}H_{12}N_2O_2$ $[M]^+$: 300.0899; found: 300.0895.



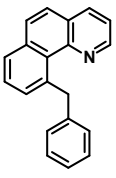
10-(3-Nitrophenyl)-7,8-benzoquinoline (3f): Pale yellow solid; m.p. 92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (dd, J = 4.2, 1.7 Hz, 1H), 8.25-8.23 (m, 2H), 8.13 (dd, J = 8.0, 1.7 Hz, 1H), 8.01 (dd, J = 7.9, 0.7 Hz, 1H), 7.90 (d, J = 8.8 Hz, 1H), 7.76-7.68 (m, 3H), 7.57-7.52 (m, 2H), 7.35 (dd, J = 8.0, 4.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 148.1, 147.8, 147.0, 146.3, 139.0, 135.6, 135.2, 131.3, 129.1, 128.8, 128.4, 128.1, 127.5, 127.3, 126.4, 124.1, 121.5, 120.9. HRMS calcd. for $C_{19}H_{12}N_2O_2$ $[M]^+$: 300.0899; found: 300.0902.



10-(1-Naphthyl)-7,8-benzoquinoline (3g): Yellow solid; m.p. 88-89 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.08 (m, 2H), 8.04-7.95 (m, 4H), 7.84-7.80 (m, 1H), 7.75-7.64 (m, 3H), 7.50-7.43 (m, 2H), 7.35 (d, J = 8.4 Hz, 1H), 7.17-7.14 (m, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 147.3, 146.5, 145.0, 139.6, 135.0, 134.7, 133.3, 133.1, 131.7, 130.4, 128.4, 128.3, 128.0, 127.3, 127.1, 126.5, 126.3, 126.1, 125.6, 125.2, 125.1, 124.7, 120.9. HRMS calcd. for $C_{23}H_{15}N$ $[M+H]^+$: 306.1283; found: 306.1279.

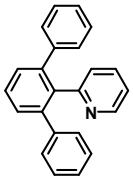


10-(β-Styryl)-7,8-benzoquinoline (3h): Brown viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (d, J = 16 Hz, 1H), 9.09 (dd, J = 4.2, 1.7 Hz, 1H), 8.16 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 7.4 Hz, 1H), 7.90-7.78 (m, 3H), 7.72-7.67 (m, 2H), 7.52-7.47 (m, 3H), 7.36 (m, 1H), 7.03 (d, J = 16 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 148.2, 147.9, 138.9, 138.6, 135.6, 135.0, 134.8, 128.9, 128.7, 128.6, 128.2, 128.1, 127.7, 127.6, 127.0, 126.8, 126.4, 125.8, 120.9. HRMS calcd. for $C_{21}H_{15}N$ $[M]^+$: 281.1204; found: 281.1210.

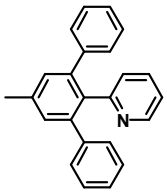


10-Benzyl-7,8-benzoquinoline (3i): White solid; m.p. 89-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (dd, J = 4.2, 1.9 Hz, 1H), 8.12 (dd, J = 8.0, 1.7 Hz, 1H), 7.86-7.82 (m, 2H), 7.67-7.61 (m, 2H), 7.55 (d, J = 7.3 Hz, 1H), 7.44 (dd, J = 8.0, 4.3 Hz, 1H), 7.29-7.20 (m, 4H), 7.14-7.11 (m, 1H), 5.40 (s, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ148.2, 147.1, 143.2, 140.6, 135.6, 135.4, 132.0, 129.7, 129.3, 128.9,

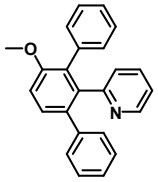
128.0, 127.6, 127.4, 125.7, 125.3, 120.9, 43.6. HRMS calcd. for $C_{20}H_{15}N$ $[M+H]^+$: 270.1283; found: 270.1284.



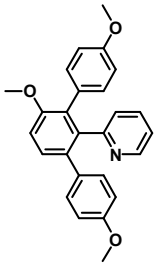
2-(2,6-Diphenyl)-phenylpyridine (3j)[5]: White solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 4.8 Hz, 1H), 7.55-7.53 (m, 1H), 7.50-7.48 (m, 2H), 7.32-7.31 (m, 1H), 7.19-7.13 (m, 10H), 6.94-6.90 (m, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.9, 148.5, 141.9, 141.6, 138.5, 135.0, 129.7, 129.5, 128.3, 127.7, 126.9, 126.4, 121.0.



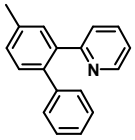
2-(2,6-Diphenyl-4-methyl)-phenylpyridine (3k): White solid; m.p. 134 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 4.6 Hz, 1H), 7.32-7.28 (m, 3H), 7.17-7.11 (m, 10H), 6.93-6.88 (m, 2H), 2.50 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.0, 148.4, 141.9, 141.8, 138.0, 135.8, 135.1, 130.3, 129.7, 127.7, 127.1, 126.3, 120.9, 21.4. HRMS calcd. for $C_{24}H_{19}N$ $[M]^+$: 321.1517; found: 321.1516.



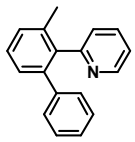
2-(2,6-Diphenyl-5-methoxyl)-phenylpyridine (3l): White solid; m.p. 173-174 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 4.3 Hz, 1H), 7.46 (d, J = 8.5 Hz, 1H), 7.27-7.23 (m, 1H), 7.14-7.11 (m, 11H), 6.86-6.83 (m, 2H), 3.83 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 158.8, 156.3, 148.3, 141.5, 140.5, 136.9, 134.8, 134.3, 131.0, 130.8, 130.4, 129.8, 127.7, 127.3, 126.7, 126.3, 126.0, 120.8, 111.0, 56.1. HRMS calcd. for $C_{24}H_{19}NO$ $[M]^+$: 337.1467; found: 337.1462.



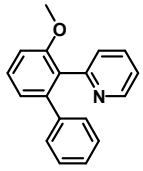
2-(2,6-Di(4-methoxylphenyl)-3-methoxyl)-phenylpyridine (3m): Yellow solid; m.p. 155 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 4.3 Hz, 1H), 7.41 (d, J = 8.5, 1H), 7.29-7.26 (m, 1H), 7.10 (d, J = 8.6 Hz, 1H), 7.04-7.00 (m, 4H), 6.88-6.83 (m, 2H), 6.72-6.68 (m, 4H), 3.82 (s, 3H), 3.73 (s, 6H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.1, 157.8, 156.2, 148.3, 140.6, 134.9, 134.0, 133.8, 132.0, 130.7, 130.3, 130.0, 129.1, 126.6, 120.7, 113.1, 112.8, 110.9, 56.0, 55.1, 55.0. HRMS calcd. for $C_{26}H_{23}NO_3$ $[M+H]^+$: 398.1756; found: 398.1770.



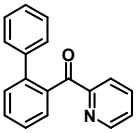
2-(5-Methyl-2-phenyl)-phenylpyridine (3n)[5]: Viscous yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, J = 4.7 Hz, 1H), 7.56 (s, 1H), 7.38-7.29 (m, 3H), 7.25-7.15 (m, 5H), 7.10 (dd, J = 6.8, 5.2 Hz, 1H), 6.88 (d, J = 7.9 Hz, 1H), 2.47 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.4, 149.4, 141.3, 139.2, 137.9, 137.5, 135.2, 131.1, 130.5, 129.8, 129.4, 128.1, 126.6, 125.6, 121.4, 21.2.



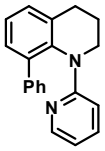
2-(6-Methyl -2-phenyl)-phenylpyridine (3o)[6]: Yellow viscous liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, J = 4.7 Hz, 1H), 7.46 (dt, J = 7.6, 1.6 Hz, 1H), 7.38 (t, J = 7.5 Hz, 1H), 7.32-7.29 (m, 2H), 7.15-7.08 (m, 6H), 6.90 (d, J = 7.8 Hz, 1H), 2.21 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.4, 148.7, 141.5, 141.1, 139.2, 136.6, 135.7, 129.5, 129.3, 128.0, 127.5, 126.1, 125.5, 121.2, 20.4.



2-(6-Phenyl-2-methoxyl)-phenylpyridine (3p): White solid; m.p. 86-87 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, J = 4.6 Hz, 1H), 7.49-7.42 (m, 2H), 7.15-7.07 (m, 7H), 7.04-7.01 (m, 2H), 3.80 (s, 3H).. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 157.3, 156.8, 148.8, 142.9, 141.1, 135.7, 129.7, 129.3, 129.0, 127.7, 126.5, 126.4, 122.6, 121.4, 110.2, 56.1. HRMS calcd. for $C_{18}H_{15}NO$ $[M]^+$: 261.1154; found: 261.1145.

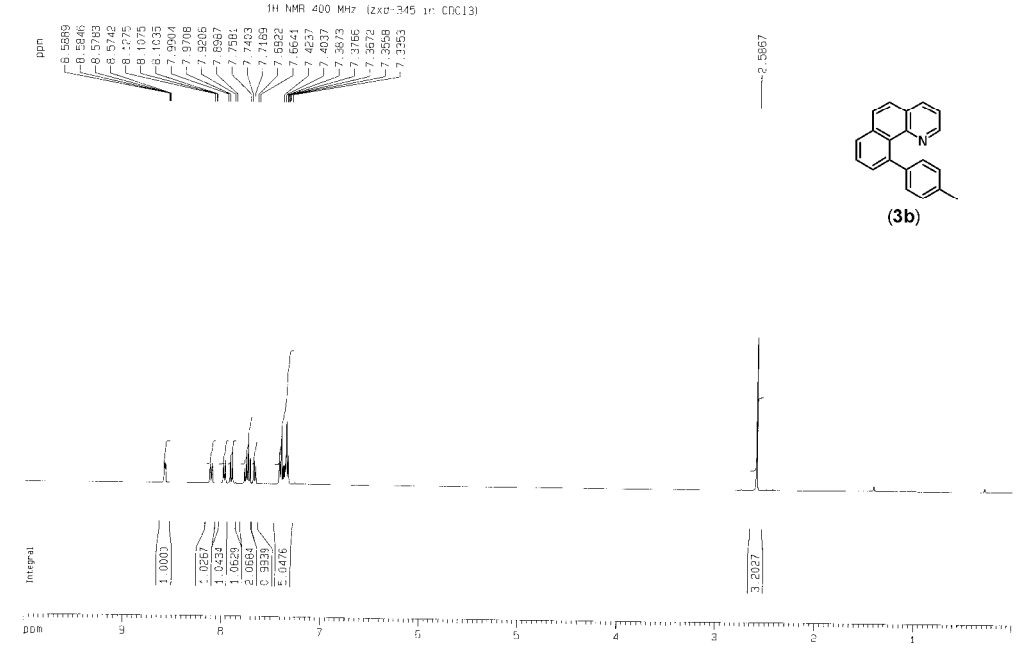


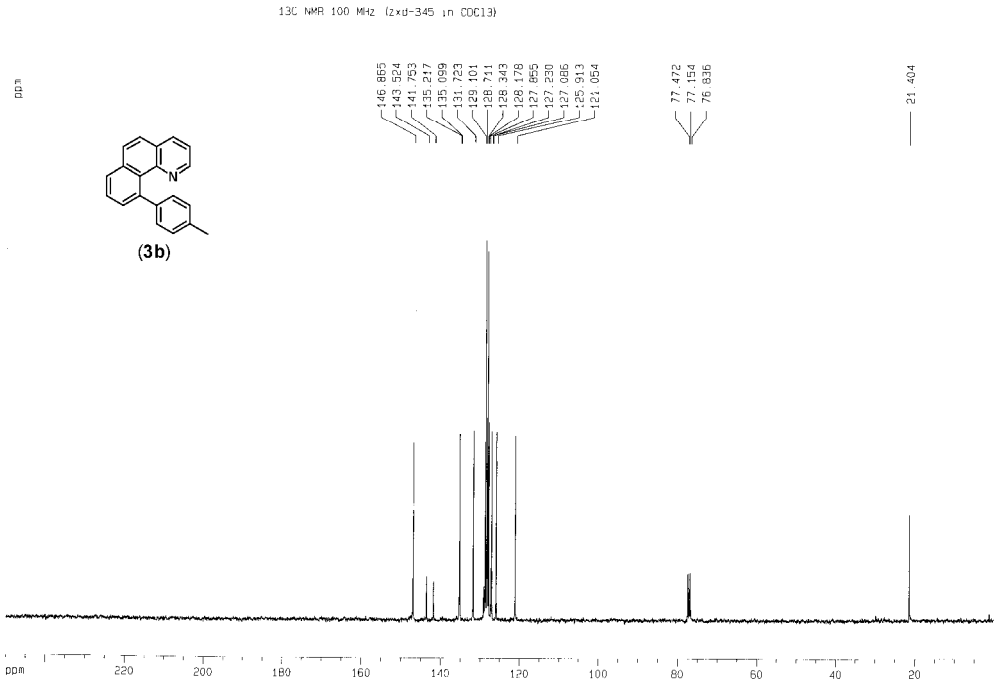
2-Biphenyl 2-pyridinyl methanone (3q): White solid; m.p. 110 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, J = 4.5 Hz, 1H), 7.81 (d, J = 7.8 Hz, 1H), 7.68-7.59 (m, 3H), 7.52-7.47 (m, 2H), 7.27-7.09 (m, 6H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 198.6, 154.7, 148.9, 142.0, 140.8, 138.5, 136.5, 131.0, 129.9, 129.5, 129.2, 128.2, 127.3, 127.2, 126.1, 123.8. HRMS calcd. for $C_{18}H_{13}NO$ $[M+K]^+$: 298.0634; found: 298.0642.

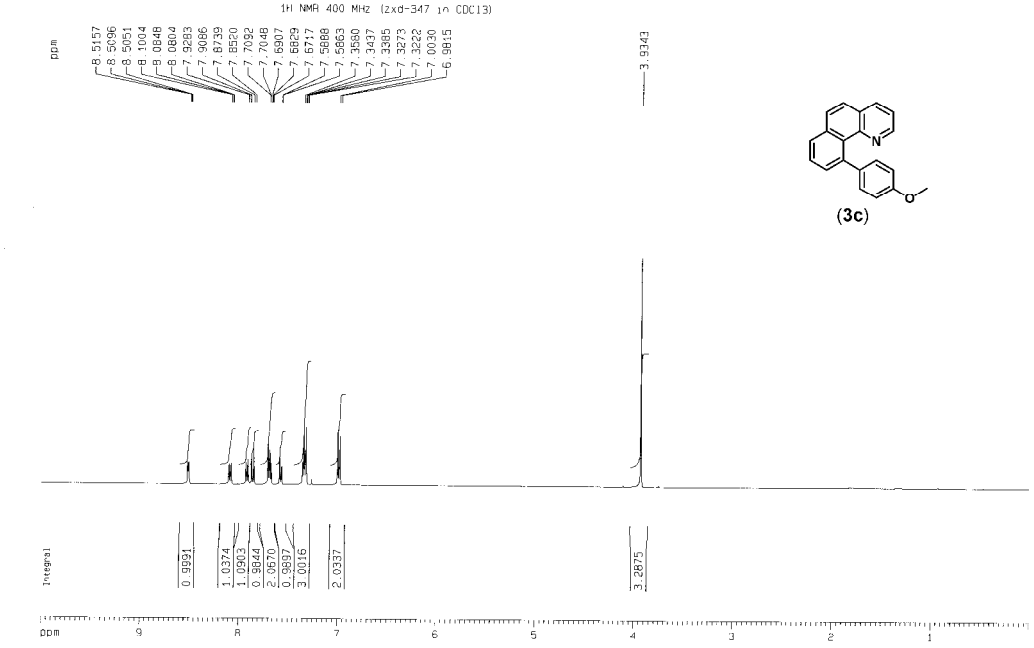


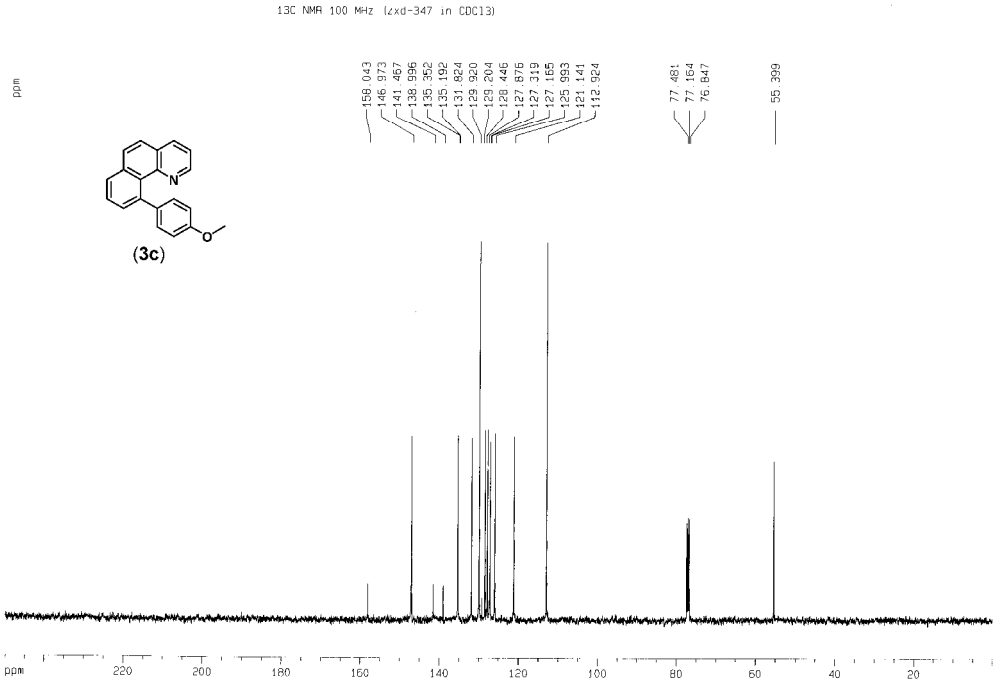
8-Phenyl-1-(2-pyridinyl)-1,2,3,4-tetrahydroquinoline (3r): Pale yellow solid; m.p. 103-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, J = 4.9, 1.5 Hz, 1H), 7.32-7.30 (m, 2H), 7.24-7.12 (m, 5H), 7.06-7.02 (m, 1H), 6.99-6.95 (m, 1H), 6.37 (dd, J = 7.0, 5.0 Hz, 1H), 6.24 (d, J = 8.5 Hz, 1H), 4.07 (t, J = 6.2 Hz, 2H), 2.78 (t, J = 6.6 Hz, 2H), 2.09-2.02 (m, 2H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 157.3, 147.3, 140.2, 138.8, 136.2, 135.9, 135.5, 129.0, 128.4, 128.0, 126.6, 124.4, 113.9, 111.1, 45.9, 27.6, 24.7. HRMS calcd. for $C_{20}H_{18}N_2$ $[M+H]^+$: 287.1548; found: 287.1552.

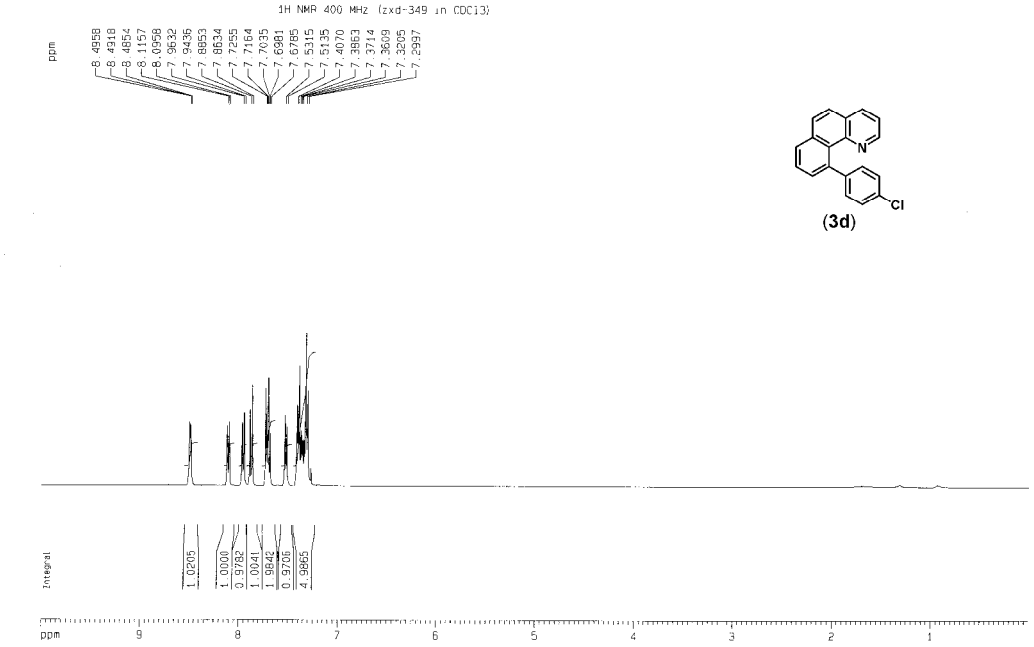
4. Copies of NMR spectra for new compounds

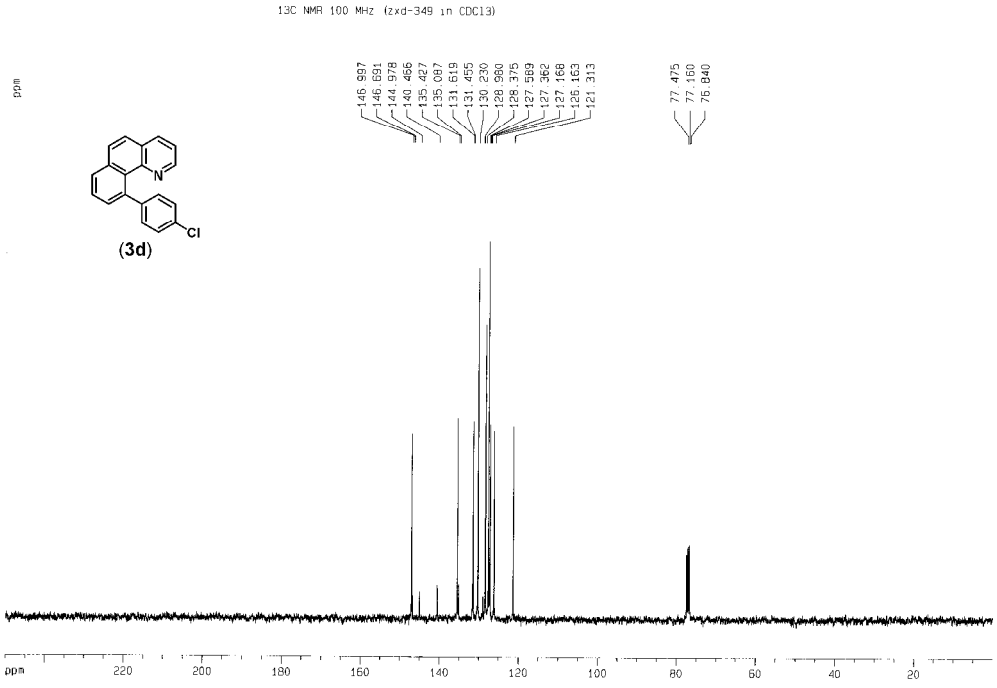


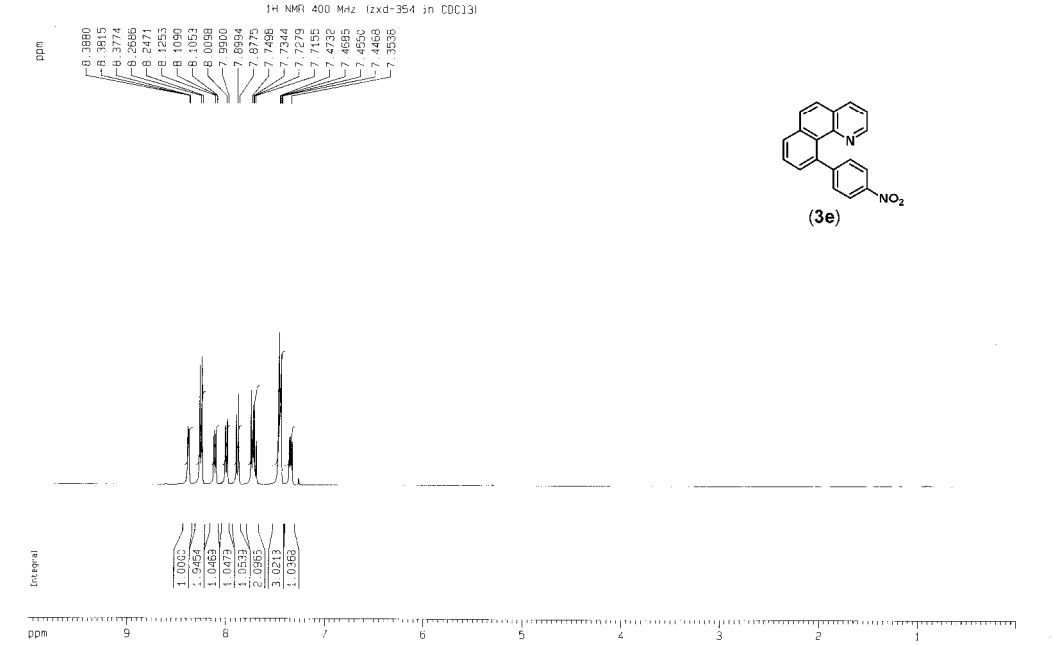


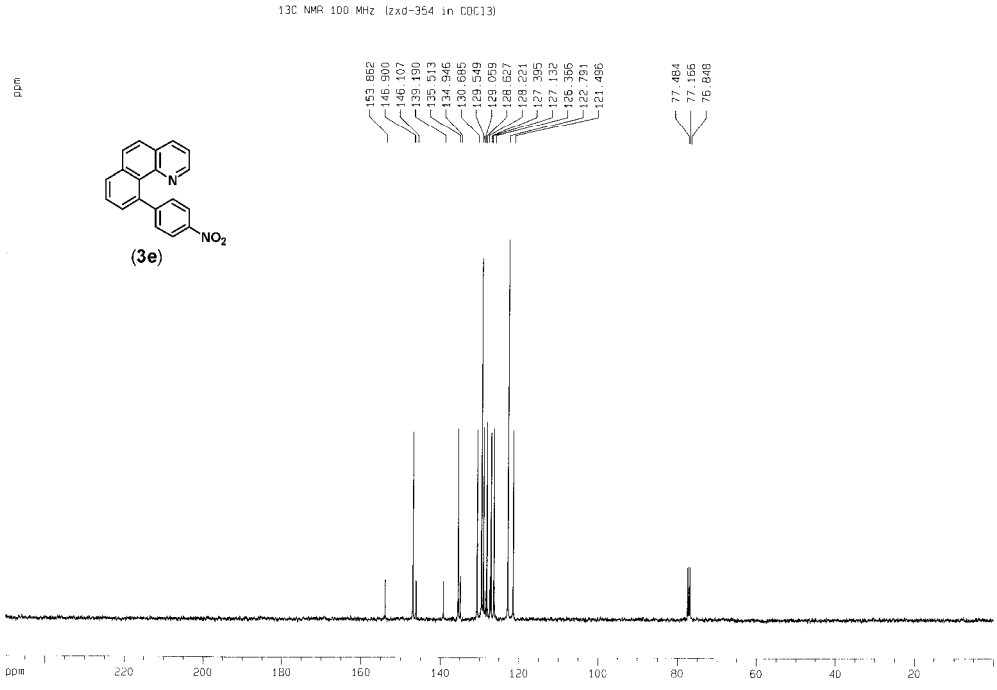

1H NMR 400 MHz (zxd-347 in CDCl3)
ppm
8.5157
8.5096
8.5051
8.1004
8.0848
8.0804
7.9283
7.9086
7.8739
7.8520
7.7092
7.7046
7.6907
7.6829
7.6717
7.5888
7.5863
7.3580
7.3437
7.3385
7.3273
7.3222
7.0030
6.9815
3.9343
(3c)
Integral
0.9991
1.0374
1.0903
0.9844
2.0670
0.9897
3.0016
2.0337
3.2875
ppm

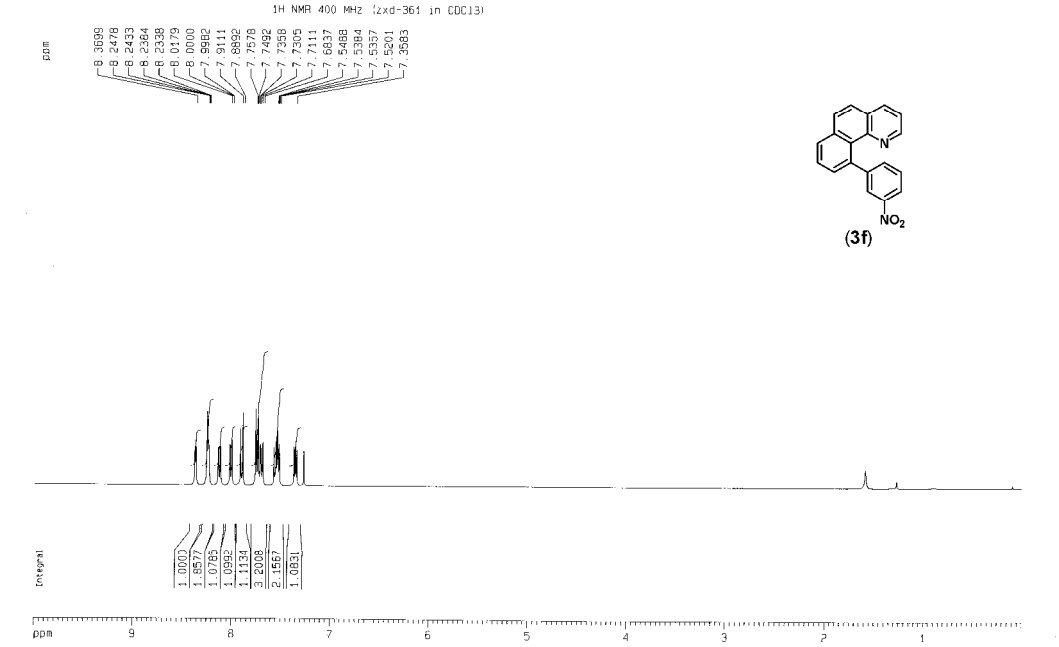

13C NMR 100 MHz (zxd-347 in CDCl3)
ppm
158.043
146.973
141.467
138.996
135.352
135.192
131.824
129.920
129.204
128.446
127.876
127.319
127.165
125.993
121.141
112.924
77.481
77.164
76.847
55.399
(3c)
ppm

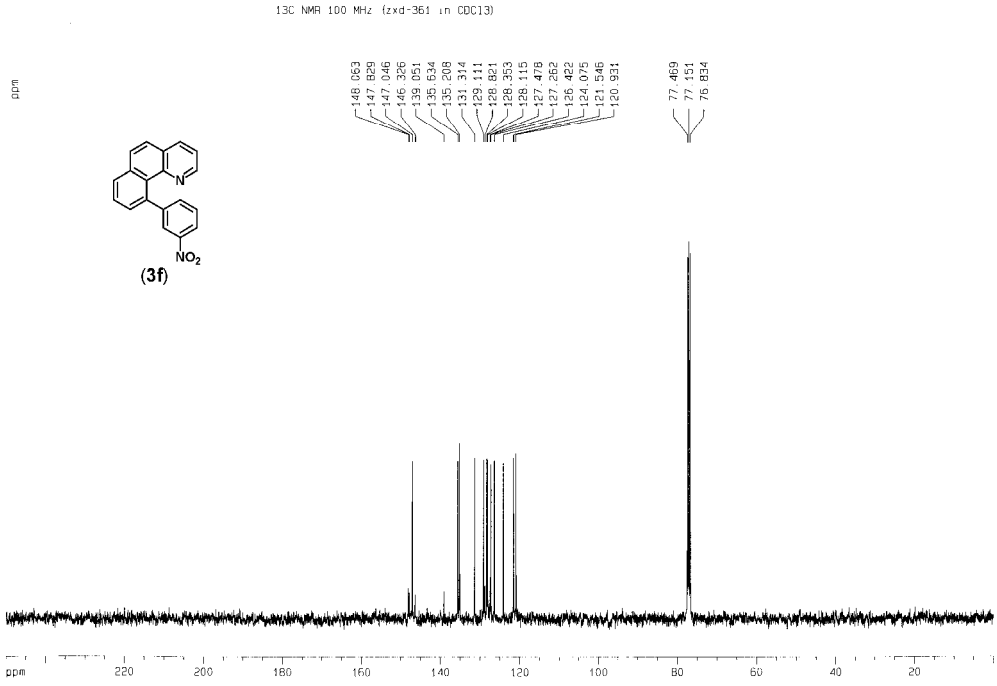

1H NMR 400 MHz (zxd-349 in CDCl3)
ppm
8.4958
8.4918
8.4654
8.1157
8.0958
7.9632
7.9436
7.8853
7.8634
7.7255
7.7164
7.7035
7.6981
7.6785
7.5315
7.5135
7.4070
7.3863
7.3714
7.3609
7.3205
7.2997
Cl
(3d)
Integral
1.0205
1.0000
0.9782
1.0041
1.9842
0.9706
4.9865
ppm
9
8
7
6
5
4
3
2
1

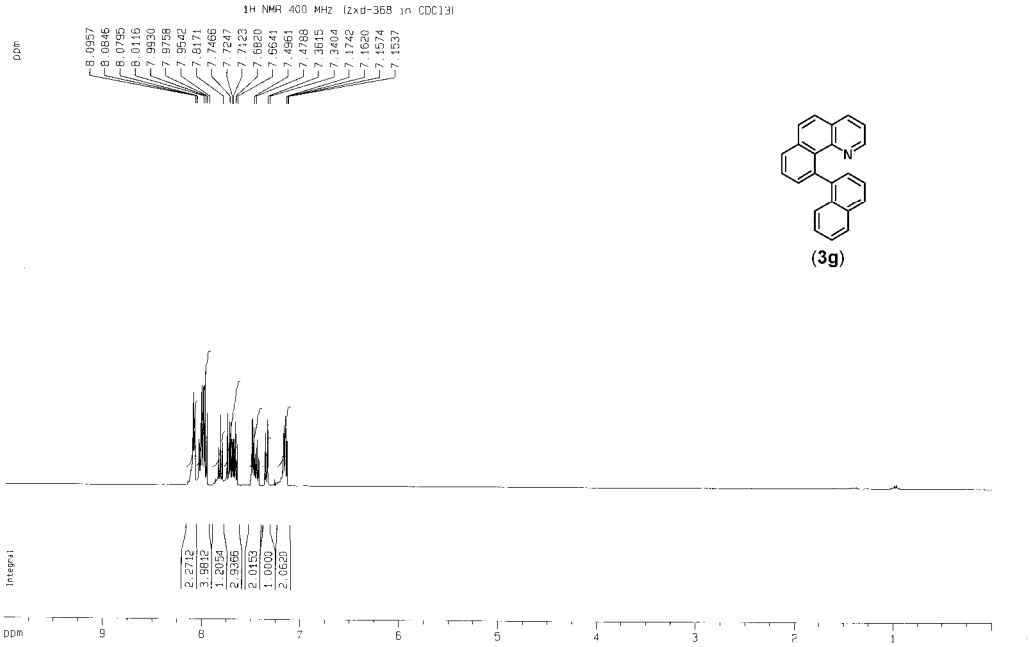

13C NMR 100 MHz (zxd-349 in CDCl3)
ppm
146.997
146.691
144.978
140.456
135.427
135.097
131.619
131.455
130.230
128.980
128.375
127.569
127.362
127.168
126.163
121.313
77.475
77.160
76.840
Cl
(3d)
ppm
220
200
180
160
140
120
100
80
60
40
20


1H NMR 400 MHz (zxd-354 in CDCl3)
ppm
8.3980
8.3815
8.3774
8.2686
8.2471
8.1253
8.1090
8.1053
8.0098
7.9900
7.8994
7.8775
7.7498
7.7344
7.7279
7.7155
7.4732
7.4685
7.4556
7.4468
7.3535
N
NO2
(3e)
Integral
1.0003
1.9454
1.0469
1.0479
1.0539
2.0965
3.0213
1.0368
ppm
9
8
7
6
5
4
3
2
1


13C NMR 100 MHz (zxd-354 in CDCl3)
ppm
153.862
146.900
146.107
139.190
135.513
134.946
130.685
129.549
129.059
128.627
128.221
127.395
127.132
126.366
122.791
121.496
77.484
77.165
76.848
N
NO2
(3e)
ppm
220
200
180
160
140
120
100
80
60
40
20

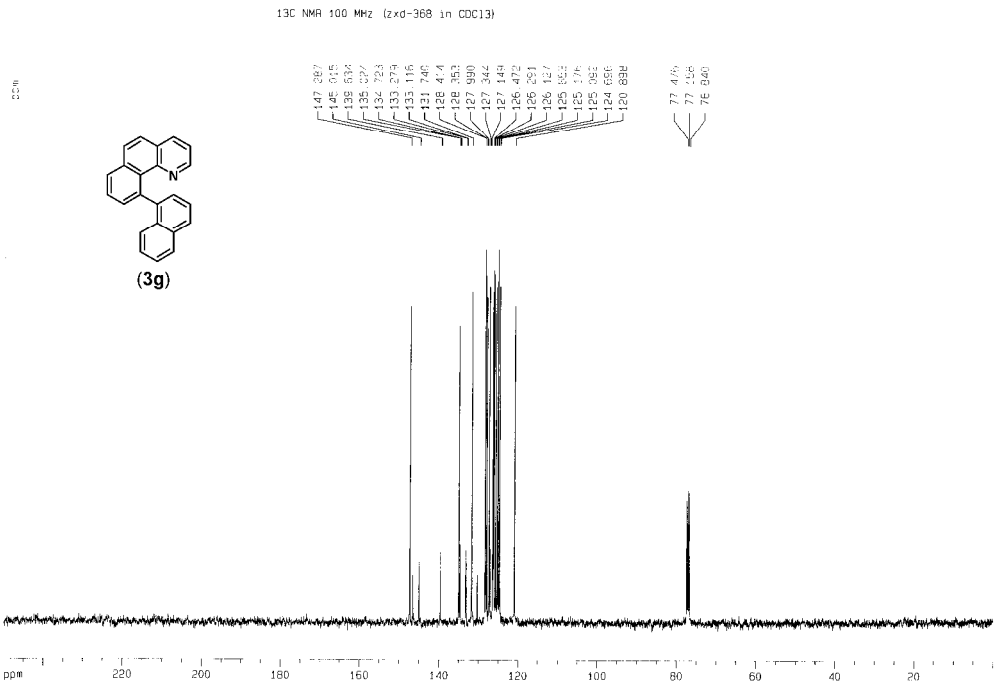

1H NMR 400 MHz (zxd-361 in CDCl3)
ppm
8.3699
8.2478
8.2433
8.2364
8.2338
8.0179
8.0000
7.9982
7.9111
7.8892
7.7578
7.7492
7.7356
7.7305
7.7111
7.6837
7.5488
7.5384
7.5357
7.5201
7.3583
N
NO2
(3f)
Integral
1.0000
1.8577
1.0785
1.0992
1.1134
3.2008
2.1567
1.0831
ppm
9
8
7
6
5
4
3
2
1


13C NMR 100 MHz (zxd-361 in CDCl3)
ppm
148.063
147.829
147.046
146.326
139.051
135.634
135.208
131.314
129.111
128.821
128.353
128.115
127.478
127.262
126.482
124.075
121.546
120.931
77.469
77.151
76.834
N
NO2
(3f)
ppm
220
200
180
160
140
120
100
80
60
40
20


1H NMR 400 MHz (zxd-368 in CDCl3)
ppm
8.0957
8.0846
8.0795
8.0116
7.9930
7.9758
7.9542
7.8171
7.7466
7.7247
7.7123
7.6820
7.6641
7.4961
7.4788
7.3615
7.3404
7.1742
7.1620
7.1574
7.1537
Integral
2.2712
3.9812
1.2054
2.9366
2.0153
1.0000
2.0628
ppm
9
8
7
6
5
4
3
2
1

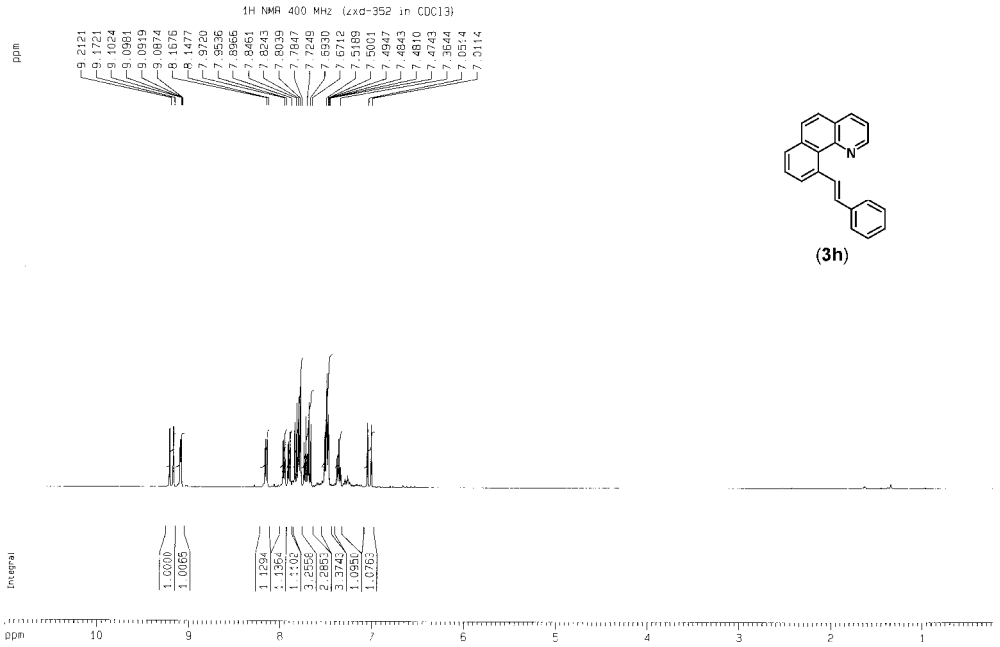
N

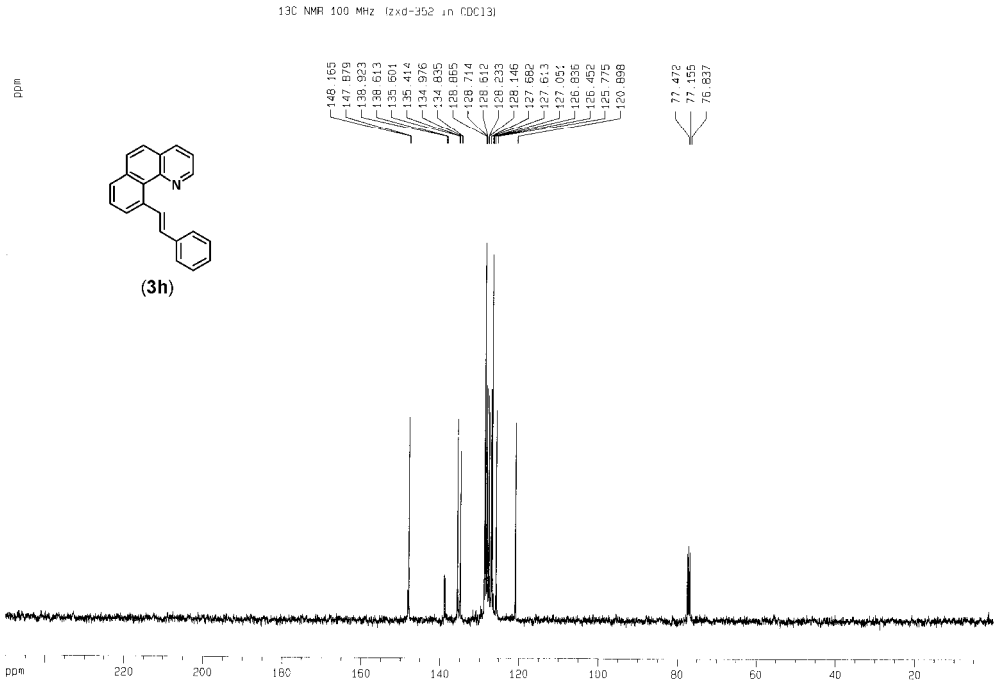
(3g)

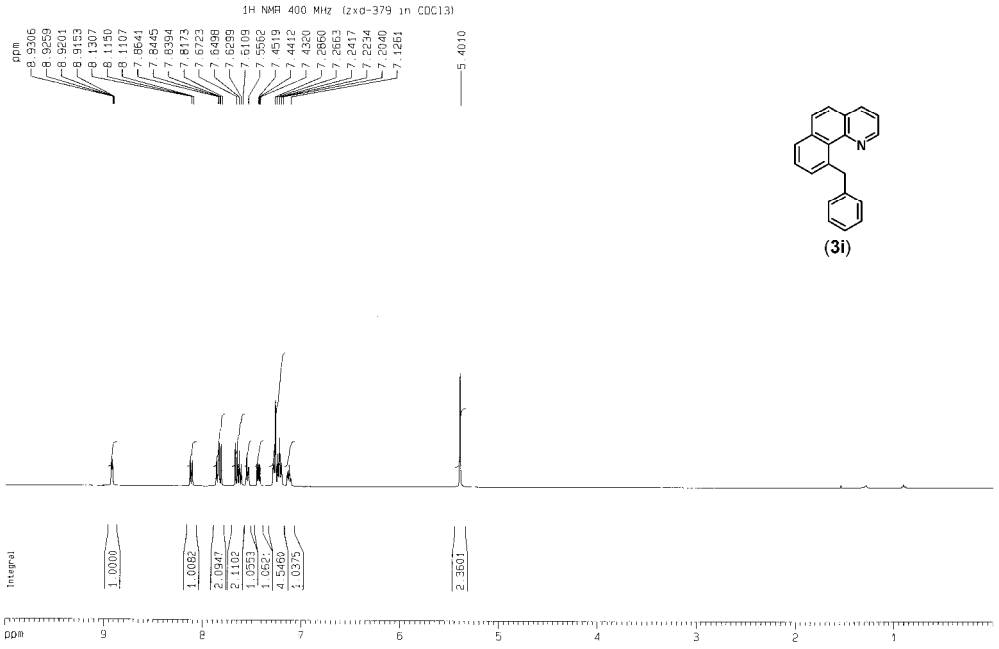

13C NMR 100 MHz (zxd-368 in CDCl3)
ppm
220
200
180
160
140
120
100
80
60
40
20

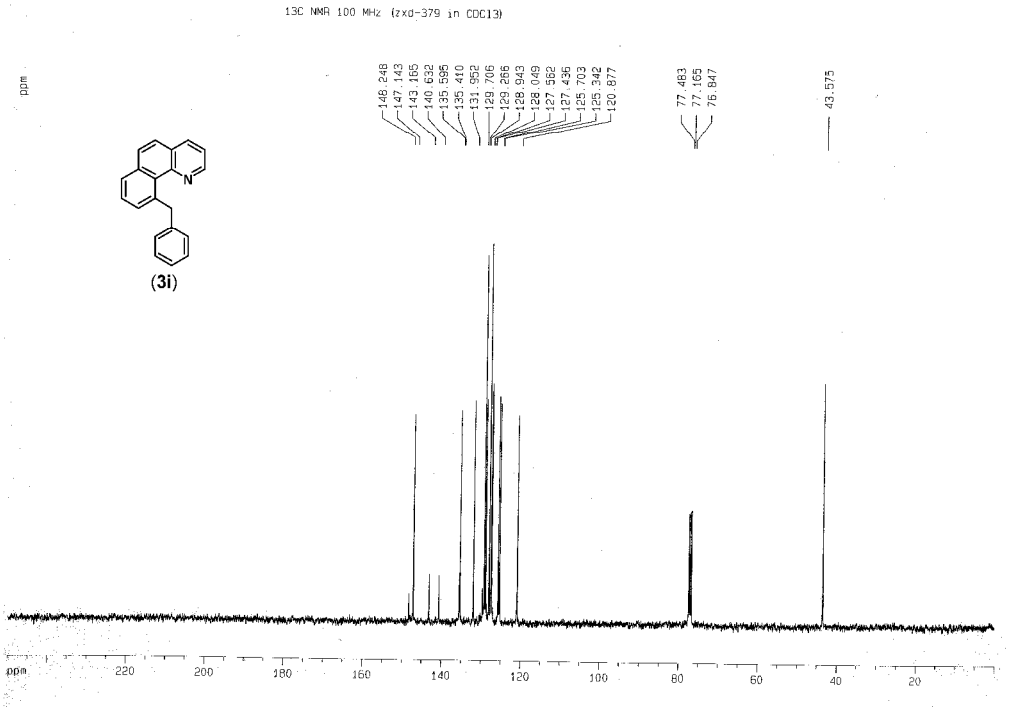
N

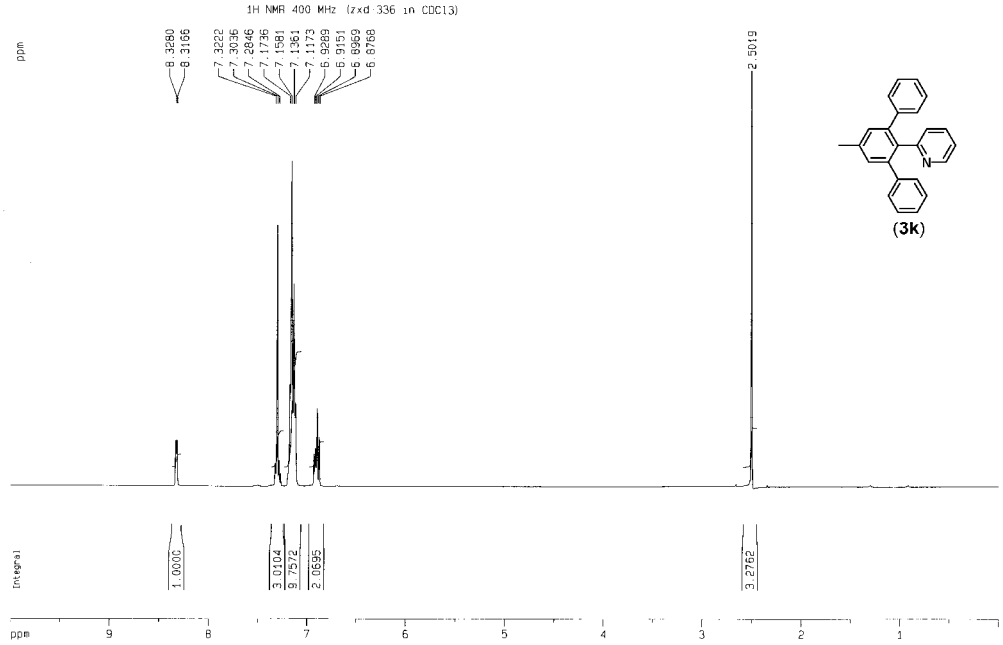
(3g)

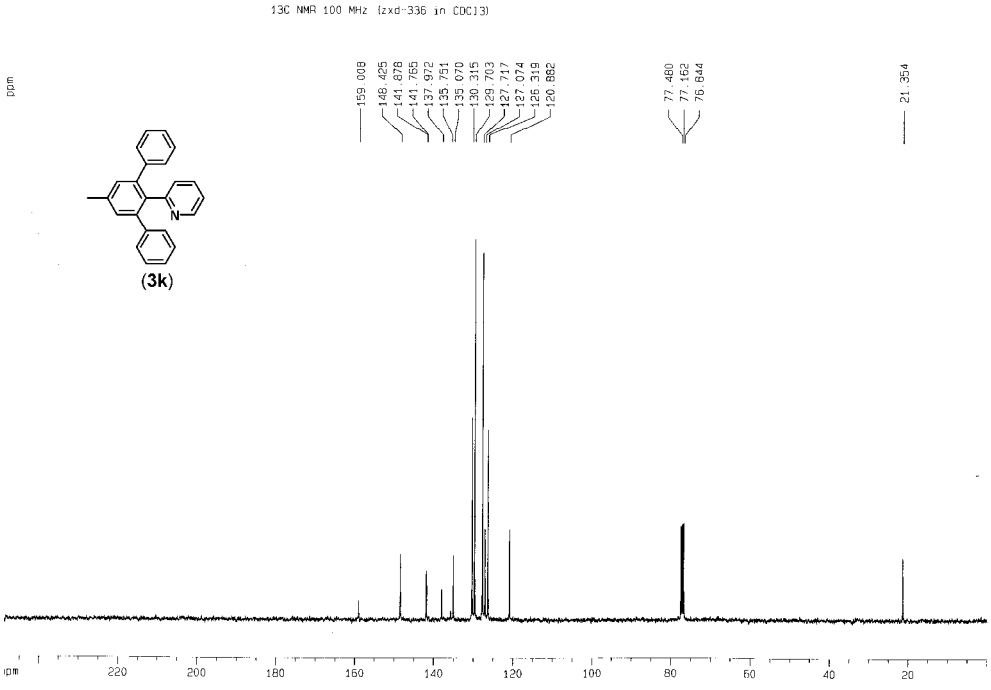

1H NMR 400 MHz (zxd-352 in CDCl3)
ppm
9.2121
9.1721
9.1024
9.0981
9.0919
9.0874
8.1676
8.1477
7.9720
7.9536
7.8966
7.8461
7.8243
7.8039
7.7847
7.7249
7.6930
7.6712
7.5189
7.5001
7.4947
7.4843
7.4810
7.4743
7.3644
7.0514
7.0114
(3h)
Integral
1.0000
1.0065
1.1294
1.1364
1.1102
3.2556
2.2853
3.3743
1.0945
1.0763
ppm
10
9
8
7
6
5
4
3
2
1

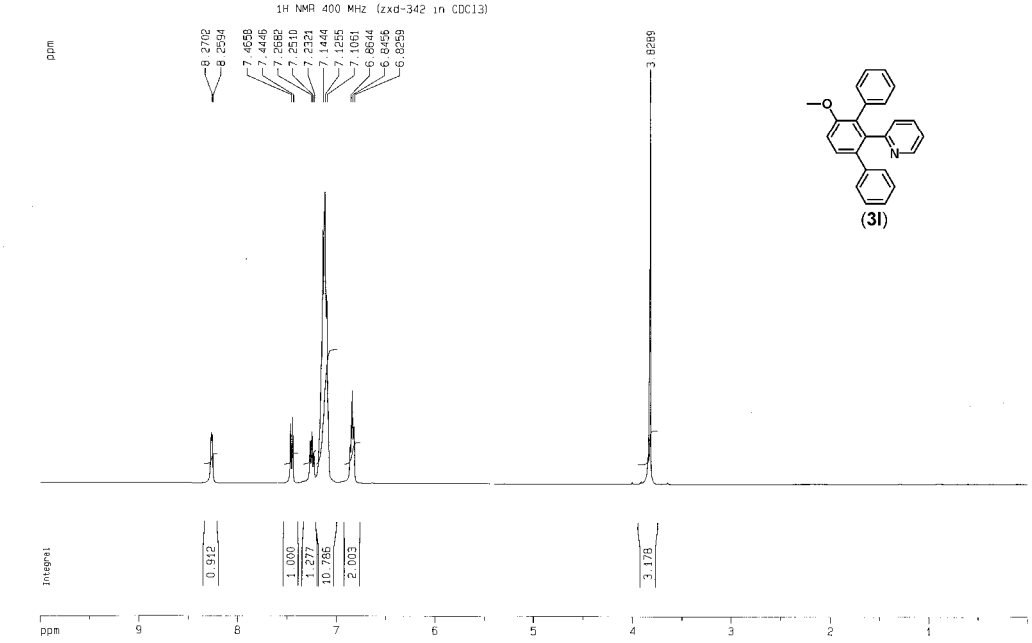

13C NMR 100 MHz (zxd-352 in CDCl3)
ppm
148.165
147.879
138.923
138.613
135.601
135.414
134.976
134.835
128.865
128.714
128.612
128.233
128.146
127.682
127.613
127.051
126.836
126.452
125.775
120.898
77.472
77.155
76.837
(3h)
ppm
220
200
180
160
140
120
100
80
60
40
20

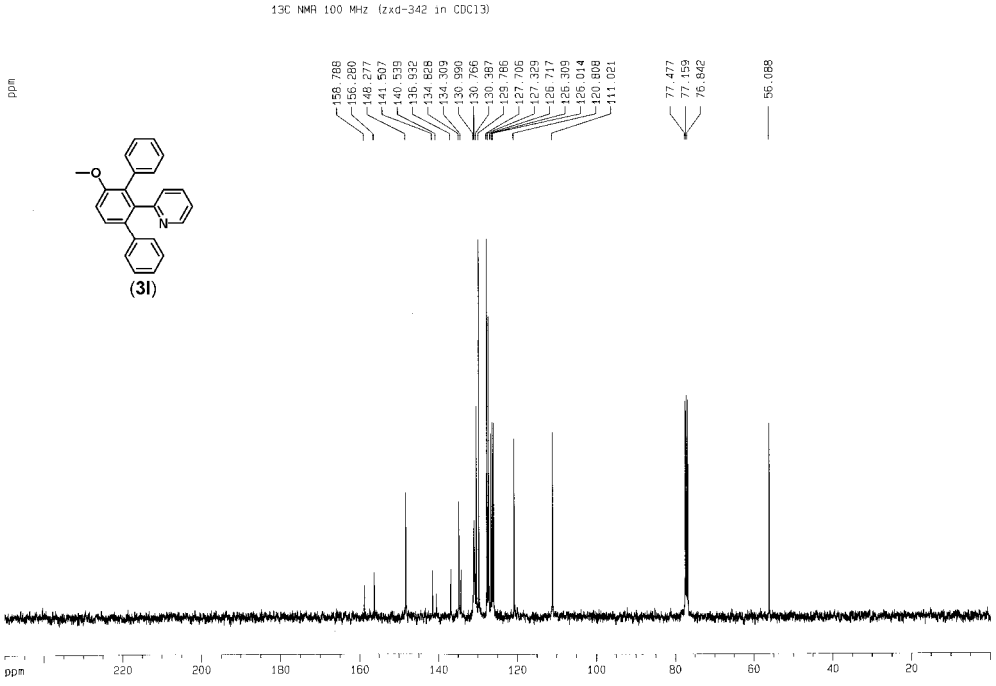

1H NMR 400 MHz (zxd-379 in CDCl3)
ppm
8.9306
8.9259
8.9201
8.9153
8.1307
8.1150
8.1107
7.8641
7.8445
7.8394
7.8173
7.6723
7.6498
7.6299
7.6109
7.5562
7.4519
7.4412
7.4320
7.2860
7.2663
7.2417
7.2234
7.2040
7.1261
5.4010
(3i)
Integral
1.0000
1.0082
2.0947
2.1102
1.0953
1.0621
4.5460
1.0375
2.3601
ppm

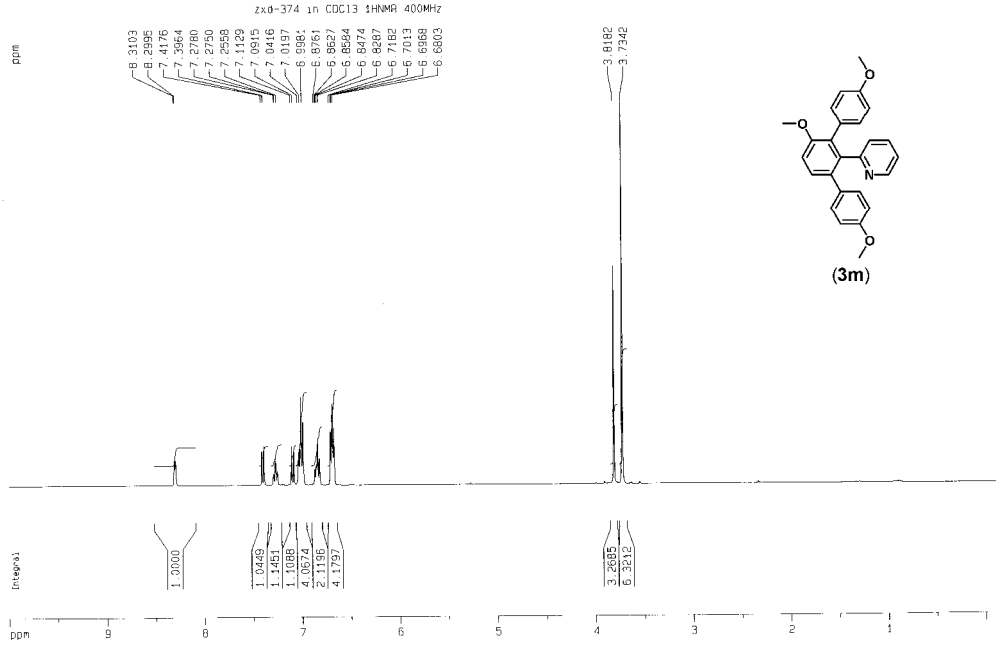

13C NMR 100 MHz (zxd-379 in CDCl3)
ppm
146.248
147.143
143.165
140.632
135.595
135.410
131.952
129.706
129.286
128.943
128.049
127.562
127.436
125.703
125.342
120.877
77.483
77.165
76.847
43.575
(3i)
ppm

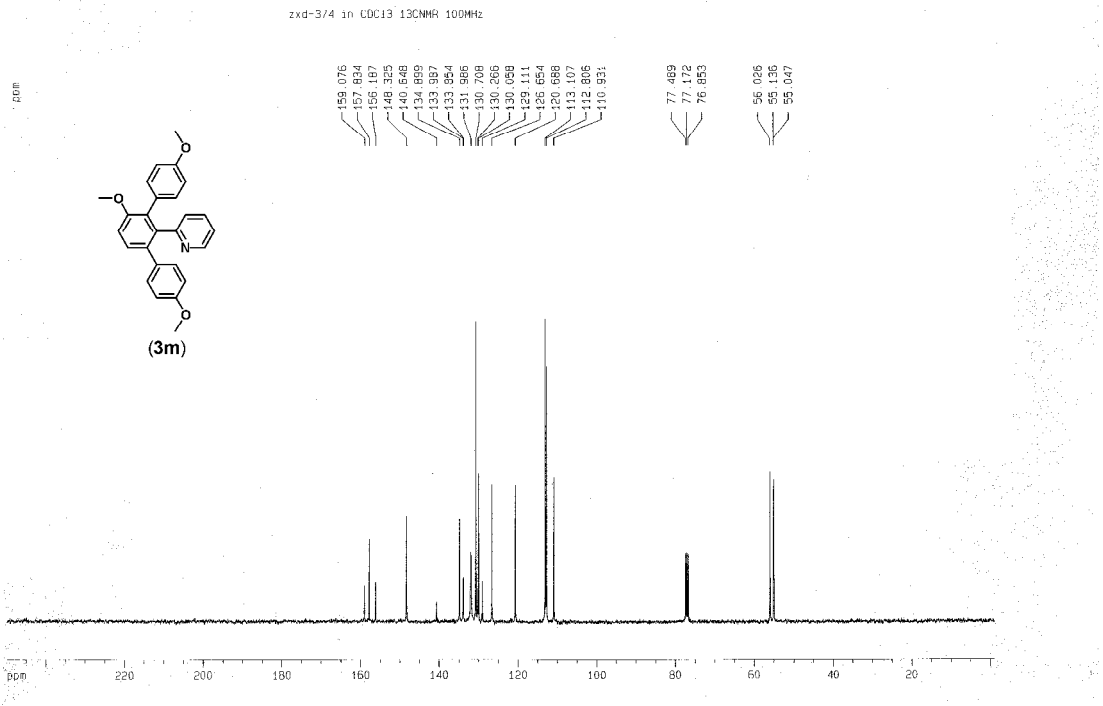

1H NMR 400 MHz (zxd-336 in CDCl3)
ppm
8.3280
8.3166
7.3222
7.3036
7.2846
7.1736
7.1581
7.1361
7.1173
6.9289
6.9151
6.8969
6.8768
2.5019
Integral
1.0000
3.0104
9.7572
2.0695
3.2762
ppm
9
8
7
6
5
4
3
2
1
(3k)

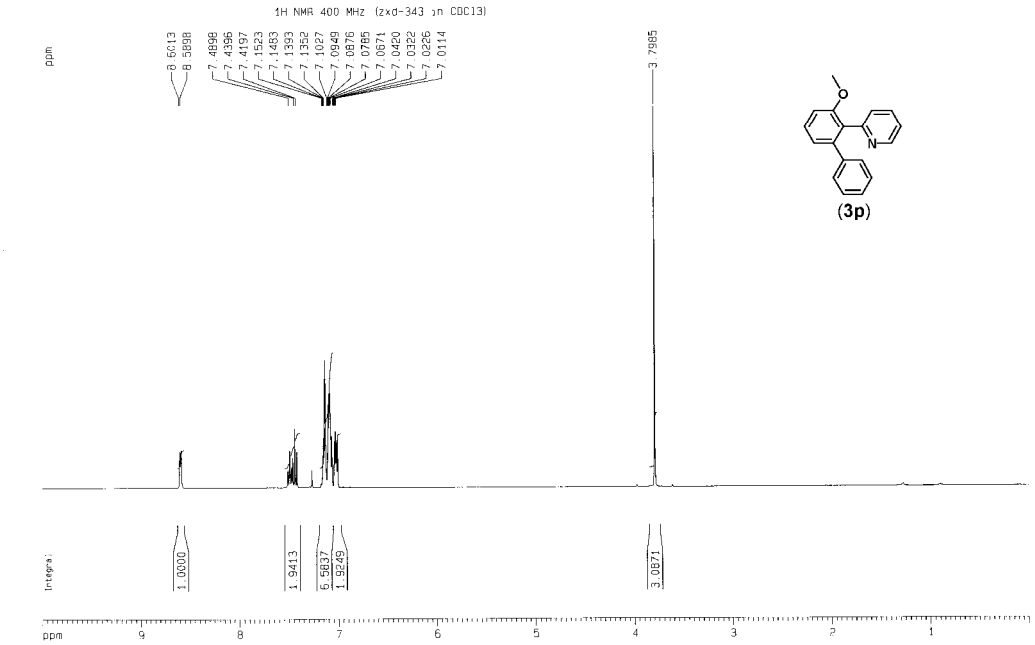

13C NMR 100 MHz (zxd-336 in CDCl3)
ppm
159.008
148.425
141.878
141.765
137.972
135.751
135.070
130.315
129.703
127.717
127.074
125.319
120.882
77.480
77.162
76.844
21.354
(3k)
ppm
220
200
180
160
140
120
100
80
60
40
20

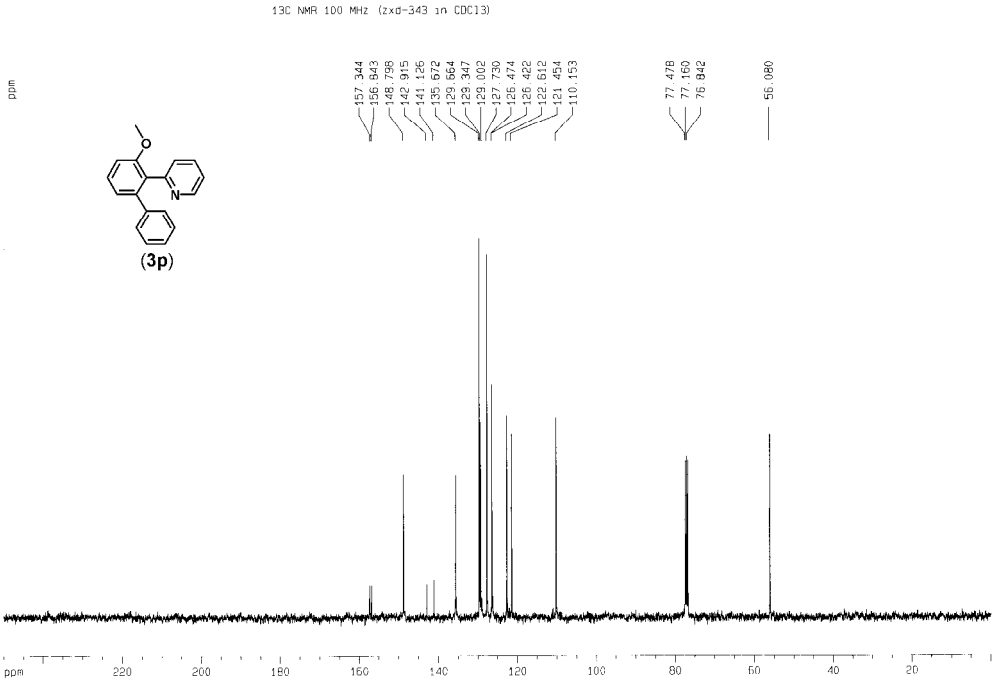

1H NMR 400 MHz (zxd-342 in CDCl3)
ppm
8.2702
8.2594
7.4658
7.4446
7.2682
7.2510
7.2321
7.1444
7.1256
7.1061
6.8644
6.8456
6.8259
3.8289
Integral
0.912
1.000
1.277
10.786
2.003
3.178
ppm
9
8
7
6
5
4
3
2
1
(3l)

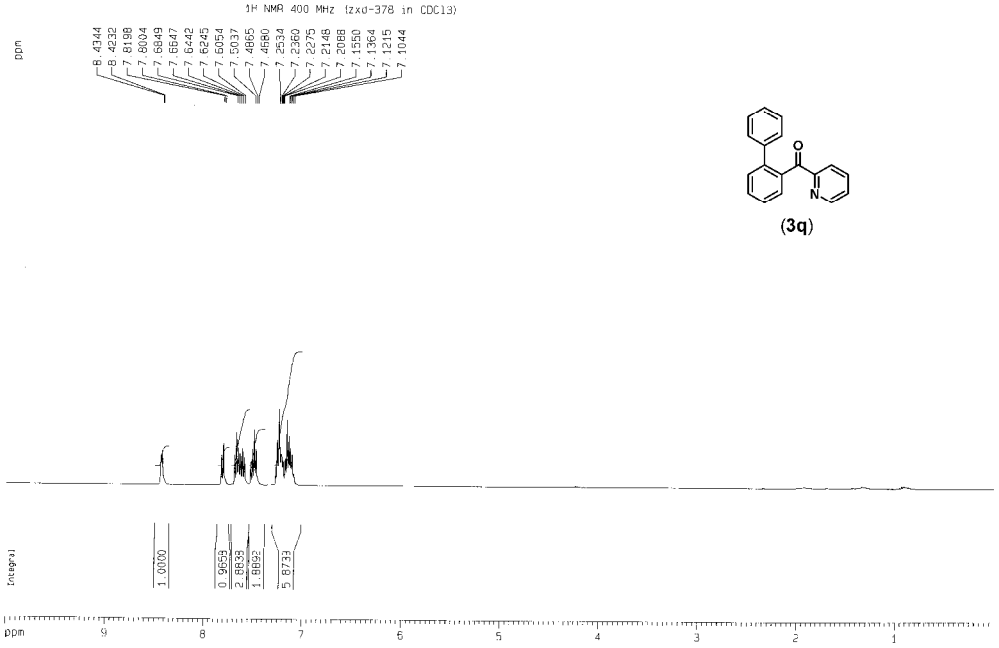

13C NMR 100 MHz (zxd-342 in CDCl3)
ppm
158.788
156.280
148.277
141.507
140.539
136.932
134.828
134.309
130.990
130.766
130.387
129.786
127.706
127.329
126.717
126.309
126.014
120.808
111.021
77.477
77.159
76.842
56.088
(3l)
ppm
220
200
180
160
140
120
100
80
60
40
20

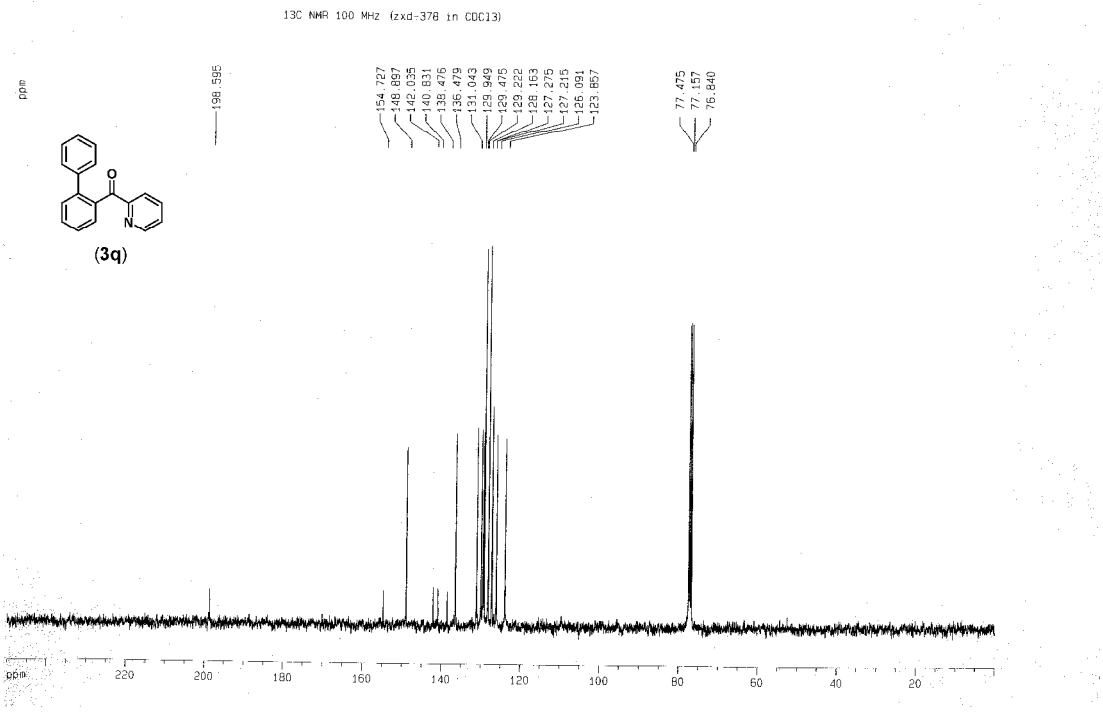

zxd-374 in CDCl3 1HNMR 400MHz
ppm
8.3103
8.2995
7.4176
7.3964
7.2780
7.2750
7.2558
7.1129
7.0915
7.0416
7.0197
6.9982
6.8761
6.8627
6.8584
6.8474
6.8287
6.7182
6.7013
6.6968
6.6803
3.8182
3.7942
Integral
1.0000
1.0449
1.1451
1.1088
4.0674
2.1196
4.1797
3.2685
6.3212
ppm
9
8
7
6
5
4
3
2
1
(3m)

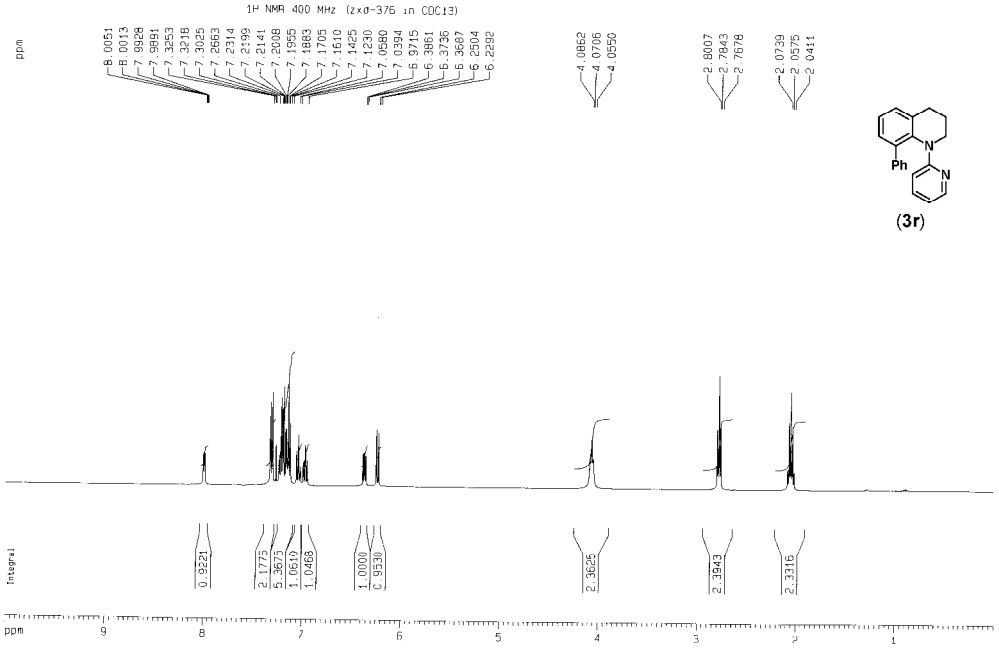

zxd-374 in CDCl3 13CNMR 100MHz
ppm
159.076
157.834
156.187
148.325
140.648
134.899
133.957
133.954
131.986
130.708
130.266
130.058
129.111
126.654
120.688
113.107
112.806
110.931
77.489
77.172
76.853
56.026
55.136
55.047
ppm
220
200
180
160
140
120
100
80
60
40
20
(3m)

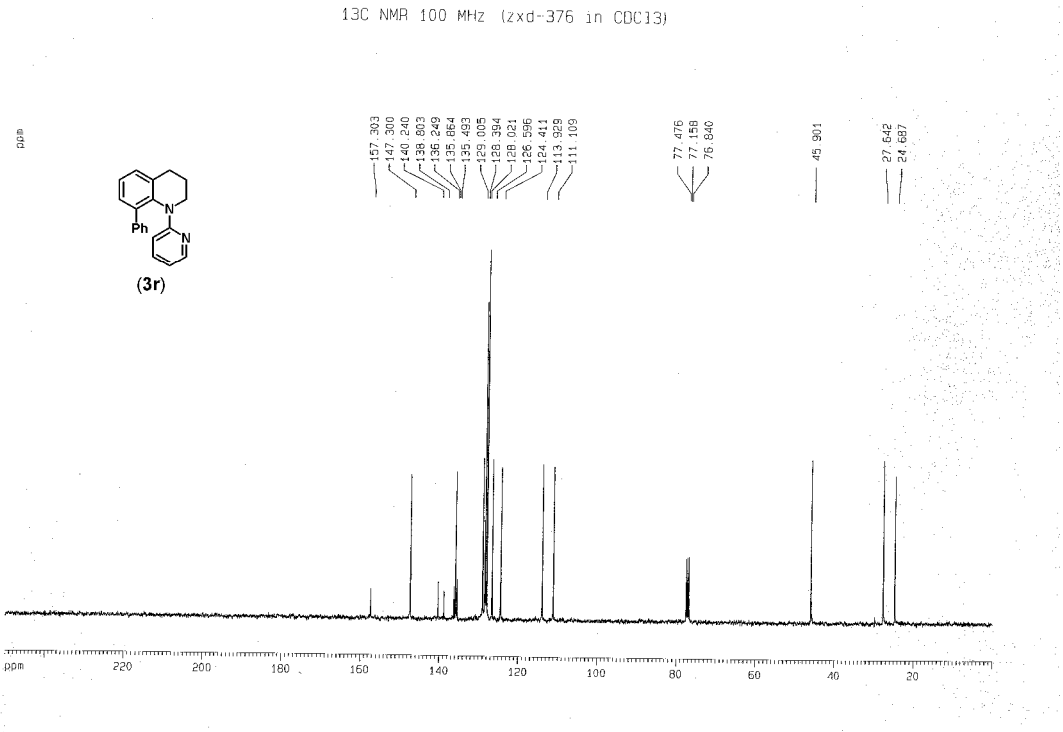

1H NMR 400 MHz (zxd-343 in CDCl3)
ppm
8.6613
8.5898
7.4898
7.4396
7.4197
7.1523
7.1483
7.1393
7.1352
7.1027
7.0949
7.0876
7.0785
7.0671
7.0420
7.0322
7.0226
7.0114
3.7985
Integral
1.0000
1.9413
6.5837
1.9249
3.0871
ppm
9
8
7
6
5
4
3
2
1
(3p)


13C NMR 100 MHz (zxd-343 in CDCl3)
ppm
157.344
156.843
148.796
142.915
141.126
135.672
129.864
129.347
129.002
127.730
126.474
126.422
122.612
121.454
110.153
77.478
77.160
76.842
56.080
ppm
220
200
180
160
140
120
100
80
60
40
20
(3p)


1H NMR 400 MHz (zxd-378 in CDCl3)
ppm
8.4344
8.4232
7.8198
7.8004
7.6849
7.6647
7.6442
7.6245
7.6054
7.5037
7.4865
7.4680
7.2534
7.2360
7.2275
7.2148
7.2088
7.1550
7.1364
7.1215
7.1044
O
N
(3q)
Integral
1.0000
0.9659
2.8638
1.8892
5.8733
ppm


13C NMR 100 MHz (zxd-378 in CDCl3)
ppm
198.595
154.727
148.897
142.035
140.831
138.476
136.479
131.043
129.949
129.475
129.222
128.163
127.275
127.215
126.091
123.857
77.475
77.157
76.840
O
N
(3q)
ppm


1H NMR 400 MHz (zxd-376 in CDCl3)
ppm
8.0051
8.0013
7.9928
7.9891
7.3253
7.3218
7.3025
7.2663
7.2314
7.2199
7.2141
7.2008
7.1955
7.1883
7.1705
7.1610
7.1425
7.1230
7.0980
7.0394
6.9715
6.3861
6.3736
6.3687
6.2504
6.2292
4.0862
4.0706
4.0550
2.8007
2.7843
2.7678
2.0739
2.0575
2.0411
Ph
N
N
(3r)
Integral
0.9221
2.1775
5.3675
1.0610
1.0468
1.0000
0.9530
2.3625
2.3943
2.3316
ppm
9
8
7
6
5
4
3
2
1


13C NMR 100 MHz (zxd-376 in CDCl3)
ppm
157.303
147.300
140.240
138.803
136.249
135.864
135.493
129.005
128.394
128.021
126.596
124.411
113.928
111.109
77.476
77.158
76.840
45.901
27.642
24.687
Ph
N
N
(3r)
ppm
220
200
180
160
140
120
100
80
60
40
20