SUPPORTING INFORMATION

First Cross-Coupling Reaction of Potassium Aryltrifluoroborates with Organic Chlorides in Aqueous Media Catalyzed by an Oxime-Derived Palladacycle

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General. Unless otherwise noted all commercials reagents and dry solvents were used without further purification. All reactions were carried out in absence of light and under argon atmosphere. Melting points were determined with a Reichert Thermovar hot plate apparatus and are uncorrected. IR spectra were recorded on a Nicolet 510 P-FT. ^{1}H-NMR (300 or 400 MHz) and ^{13}C-NMR (75 or 100 MHz) spectra were obtained on a Bruker AC-300 and Bruker AC-400, respectively, using $CDCl_3$ as solvent and TMS as internal standard, unless otherwise stated. Low-resolution electron impact (EI) mass spectra were obtained at 70 eV on a Shimadzu QP-5000. Analytical TLC was performed on Merck aluminum sheets with silica gel 60 F_{254}. Silica gel 60, (0.04-0.06 mm) was employed for flash chromatography. Microwave reactions were performed with a CEM Discover Synthesis Unit (CEM Corp., Matthews, NC) with a continuous focused microwave power delivery system in glass vessels (10 mL) sealed with a septum under magnetic stirring. The temperature of the reaction mixture inside the vessel was monitored using a calibrated infrared temperature control under the reaction vessel.

General procedure for aryl chlorides. A 2 M solution of K_2CO_3 (1 mL, 2 mmol) was added to an emulsion of aryl chloride (1 mmol), TBAB (see, Table 1), potassium aryltrifluoroborate (1.5 mmol) and commercially available complex **1** (0.01-1 mol% Pd, Table 1) in water (2 mL). The mixture was stirred and heated under reflux and the reaction was monitored by GC until completion. In the case of MW heating, a 10 mL pressure tube sealed with a septum was used and the mixture was stirred and heated in a microwave reactor (30 W, 1 bar, 100 ºC, 15-20 min and 40 psi of air stream cooling). Then, the crude reaction was cooled at room temperature and the product was extracted with diethyl ether (3 x 15 mL) and the combined organic layers were washed with water (3 x 15 mL) and dried over magnesium sulphate. The solvent was removed under vacuum and the products were purified by recrystallization or by flash chromatography.

General procedure for recycling experiments for the reaction of 4-chloroacetophenone with $PhBF_3K$. The reaction mixture described before was cooled at room temperature and extracted in the reaction flask with diethyl ether (6 x 5 mL) to afford the product. To the aqueous phase kept in the reaction flask was added again the reagents expect palladacycles **1** and the mixture was heated again until the reaction was finished.

General procedure for allyl and benzyl chlorides.: A 1M solution of KOH (2 mL, 2 mmol) was added to a solution of allyl or benzyl chloride (1 mmol), TBAB (322 mg, 1 mmol), potassium phenyltrifluoroborate (276 mg, 1.5 mmol) and catalyst **1** (0.29 mg, 0.1 mol% Pd) in acetone (3 mL) in a round-bottom flask. The mixture was stirred at rt or heated at 50 ºC and the reaction was monitored by GC until completion. In the case of MW heating, a 10 mL pressure tube sealed with a septum was used and the mixture was stirred and heated in a microwave reactor (30 W, 1 bar, 50 ºC, 15-20 min and 40 psi of air stream cooling). Then, the crude reaction was cooled at room temperature and the product was extracted with diethyl ether (3 x 15 mL) and the combined organic layers were washed with water (3 x 15 mL) and dried over magnesium sulphate. The solvent was removed under slight vacuum and the products were purified by flash chromatography.

General procedure for recycling experiments for the reaction of cinnamyl and benzyl chloride with $PhBF_3K$. The reaction mixture described before was cooled at room temperature and extracted in the reaction flask with diethyl ether (6 x 5 mL) to afford the product. To the aqueous phase kept in the reaction flask was added again the reagents expect palladacycles **1** and acetone (3 mL). Then the mixture was heated again until the reaction was finished.

Compounds **2aa**, **2ba**, **2cb**, **2cc**, **2da**, **2ea**, **2fa**, **3a**, **3b**, **3c**, **4a** and **4c** are commercially available. Compounds **2ga**, **2ha**, **4b** and **4b** have been previously reported.

4-Acetylbiphenyl (2aa): White solid; M.p. = 121-123 ºC; R_f = 0.55 (Hexane/Ethyl acetate 3:1); IR (KBr) ν = 1680, 1601 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 8.03-8.00 (m, 2H, ArH), 7.69-7.66 (m, 2H, ArH), 7.63-7.60 (m, 2H, ArH), 7.49-7.38 (m, 3H, ArH), 2.62 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 197.7 (CO), 145.7, 139.8, 135.8 (ArC), 129.0, 128.9, 128.3, 127.3, 127.2 (ArCH), 26.6 (CH_3); MS (m/z, %): 196 (M^+,45), 181 (M^+-15, 100), 153 (36), 152 (54), 151 (20), 76 (65).

4-Biphenylacetic acid (2ba): White solid; M.p. = 163-164 ºC; R_f = 0.51 (Hexane/Ethyl acetate 1:1); IR (KBr) ν = 1688 (C=O) cm^{-1}; H-NMR (Methanol-d_4, 300 MHz) δ_H (ppm) = 7.63-7.33 (m, 9H, ArH), 3.66 (s, 2H, CH_2); ^{13}C-NMR (Methanol-d_4, 75 MHz) δ_C (ppm) = 175.5 (CO_2H), 142.1, 141.1, 135.1 (ArC), 130.8, 129.8, 128.2, 128.0, 127.9 (ArCH), 41.5 (CH_2); MS (m/z, %): 213 (M^++1, 10), 212 (M^+, 19), 194 (M^+-18, 7), 169 (16), 168 (16), 167 (48), 166 (21), 165 (28), 164 (38), 163 (24), 141 (16), 139 (11), 128 (45), 126 (13), 115 (24), 91 (10), 82 (56), 76 (48), 65 (70).

2-Cyano-4'-methyl-1,1'-biphenyl (2cb): White solid; M.p. = 47-49 ºC; R_f = 0.50 (Hexane/Ethyl acetate 5:1); IR (KBr) ν = 2223 (C≡N) cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.74-7.72 (m, 1H, ArH), 7.63-7.58 (m, 1H, ArH), 7.49-7.37 (m, 4H, ArH), 7.29 (d, 2H, J = 8.05 Hz, ArH), 2.41 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 145.6 138.7, 135.3 (ArC), 133.8, 132.8, 130.0, 129.5, 128.7, 127.3 (ArCH), 119.0 (CN), 111.2 (ArC), 21.3 (CH_3); MS (m/z, %): 193 (M^+, 100), 165 (35), 82 (17).

2-Cyano-2'-methyl-1,1'-biphenyl (2cc): Colorless oil; R_f = 0.53 (Hexane/Ethyl acetate 5:1); H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.74 (d, 1H, J = 7.7 Hz, ArH), 7.64-7.60 (m, 1H, ArH), 7.46-7.42 (m, 1H, ArH), 7.38-7.26 (m, 4H, ArH), 7.20 (d, 1H, J = 7.7 Hz, ArH), 2.19 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 145.9, 138.1, 135.8 (ArC), 132.9, 132.5, 130.6, 130.5, 129.5, 128.8, 127.6, 126.0, 118.2 (ArCH), 112.9 (CN), 20.0 (CH_3); MS (m/z, %): 193 (M^+, 100), 165 (58), 152 (10).

4-Methoxybiphenyl (2da): White solid; M.p. = 88-89 ºC; R_f = 0.15 (Hexane); IR (KBr) ν = 3064, 3056, 3032, 3001, 1606, 1522, 1251, 1035 cm^{-1}; H-NMR ($CDCl_3$, 300

MHz) δ_H (ppm) = 7.55-7.28 (m, 7H, ArH), 6.96 (d, 2H, *J* = 9.1 Hz, ArH), 3.81 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 159.3 (ArC-O), 140.9, 133.9 (ArC), 128.8, 128.3, 126.8, 126.7, 114.3 (ArCH), 55.4 (CH_3); MS (m/z, %): 184 (M^+, 100), 169 (M^+-15, 44), 141 (37), 139 (10), 115 (30).

4-Biphenyl-4-amine (2ea): Brown solid; M.p. = 51 ºC; R_f = 0.31 (Hexane/Ethyl acetate 3:1); IR (KBr): ν = 3424, 3382, 3300, 3206, 1617 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.55-7.37 (m, 7H, ArH), 6.76 (d, 2H, *J* = 8.6 Hz, ArH), 3.71 (br. s., 2H, NH_2); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 145.9, 141.2, 131.6 (ArC), 128.7, 128.1, 126.4, 126.3, 115.4 (ArCH); MS (m/z, %): 169 (M^+, 100), 84(12).

3-Phenylpyridine (2fa): Brown oil; R_f = 0.32 (Hexane/Ethyl acetate 1:1); IR (film) ν = 1678, 1607, 1579 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 8.85 (s, 1H, ArH), 8.59 (d, 1H, *J* = 4.9 Hz, ArH), 7.87 (dd, 1H, *J* = 8.0 and 1.8 Hz, ArH), 7.59-7.33 (m, 6H, ArH); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 148.6, 148.3 (ArCH), 137.9, 136.7 (ArC), 134.5, 129.2, 128.2, 127.2, 123.6 (ArCH); MS (m/z, %): 155 (M^+, 100), 154 (M^+-1, 51), 127 (17), 77 (12), 64 (13), 51 (29).

4,5-Diphenyl-2-methyl-3(2*H*)-pyridazinone (**2ga**):[1] White solid; M.p. = 180 ºC; R_f = 0.50 (Hexane/Ethyl acetate 1:1); IR (KBr): ν = 1630 (C=O) cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.86 (s, 1H, ArH), 7.28-7.19 (m, 8H, ArH), 7.12-7.10 (m, 2H, ArH), 3.87 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 160.5 (CO), 140.8 (ArC), 138.1 (ArCH), 136.9, 135.2, 132.7 (ArC), 130.6, 129.2, 128.7, 128.6, 128.4, 128.0 (ArCH), 40.7 (CH_3); MS (m/z, %): 262 (M^+, 32), 261 (100), 191 (20), 189 (19).

2,4,6-Triphenylpyrimidine (2ha):[2] White solid; M.p. = 82 ºC; R_f = 0.14 (Hexane/Ethyl acetate 5:1); H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 8.74-8.72 (m, 2H, ArH), 8.30-8.27 (m, 4H, ArH), 8.00 (s, 1H, ArH), 7.56-7.53 (m, 9H, ArH); ^{13}C-NMR ($CDCl_3$, 75 MHz)

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[1] Maes, B. U. W.; R'Kyek, O.; Kosmrlj, J.; Lemière, G. L. F.; Esmans, E.; Rozenski, J.; Dommisse, R. A.; Haemers, A. *Tetrahedron* **2001**, *57*, 1323-1330.
[2] Schomaker, J. M.; Delia, T. J. *J. Org. Chem.* **2001**, *66*, 7125-7128.

δ_C (ppm) = 165.0, 164.6, 138.3, 137.7, 130.9, 130.8, 129.1, 128.6, 127.5, 127.4, 110.4; MS (m/z, %): 308 (M^+, 76), 205 (78), 204 (82), 102 (100), 77 (33), 76 (31).

(*E*)-1,3-Diphenylpropene (3a): Yellowish oil; R_f = 0.31 (Hexane); IR (film) ν = 3075, 3056, 2896, 1722, 1705, 1601 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.37-7.19 (m, 10H, ArH), 6.46 (d, 1H, *J* =15.9 Hz, CH), 6.40-6.30 (m, 1H, CH), 3.55 (d, 2H, *J* = 6.7 Hz, CH_2); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 140.3, 137.6 (ArC), 132.1, 129.3, 128.74, 126.68, 128.6, 127.2 126.3, 126.2 (ArCH and CH), 39.4 (CH_2); MS (m/z, %): 194 (M^+, 100), 193 (62), 179 (51), 178 (46), 116 (65), 115 (92), 103 (31), 91 (48), 77 (21) 65 (33).

Allylbenzene (3b): Colorless oil; R_f = 0.56 (hexane); IR (film) ν = 3082, 3025, 2977, 1642, 1603, 1495, 1072 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.30-7.16 (m,5H, ArH), 6.03-5.89 (m, 1H, CH), 5.10-5.03 (m, 2H, CH_2), 3.37 (d, 2H, *J* = 6.7 Hz, CH_2); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 140.1 (ArC), 137.6 (CH), 128.7, 128.5 (2 x ArCH), 126.2 (ArCH), 115.9 (=CH_2), 40.4 (CH_2); MS (m/z, %): 118 (M^+, 75), 117 (100), 115 (43), 91 (52), 65 (23), 58 (29) 51 (27).

2-Methyl-3-phenylpropene (3c): Colorless oil; : R_f = 0.35 (Hexane); IR (film) ν =3045, 2992, 2936, 1661, 1510, 1468 cm^{-1}; H-NMR ($CDCl_3$, 400 MHz) δ_H (ppm) = 7.28-7.16 (m, 5H, ArH), 4.80 (s, 1H, =CH*H*), 4.72 (s, 1H, =C*H*H), 3.30 (s, 2H, CH_2), 1.66 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 145.1(C), 139.8 (ArC), 129.0, 128.4, 128.3, 126.1 (ArCH), 112.0 (=CH_2), 44.7 (CH_2), 22.1 (CH_3); MS (m/z, %): 132 (M^+, 71), 117 (100), 115 (53), 91 (76).

2,3-Diphenylpropene (3d): Colorless solid; M.p. = 53 ºC; R_f = 0.45 (Hexane); IR (film) ν = 3056, 3025, 2911, 1624, 1602, 1492, 1440 cm^{-1}; H-NMR ($CDCl_3$, 400 MHz) δ_H (ppm) = 7.42 (dd, 2H, *J* = 8.6 and 1.5 Hz, ArH), 7.29-7.16 (m, 8H, ArH), 5.48 (s, 1H, =CH*H*), 5.01 (d, 1H, *J* = 1.1 Hz, =C*H*H), 3.83 (s, 2H, CH_2); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ_C (ppm) = 147.0 (C), 140.9, 139.6 (ArC), 129.1, 128.5, 128.4, 127.6, 126.3, 126.2 (ArCH), 114.7 (=CH_2), 41.7 (CH_2); MS (m/z, %): 195 (M^++1, 16), 194 (M^+, 100), 193 (M^+-1, 43), 178 (85), 116 (51), 103 (89).

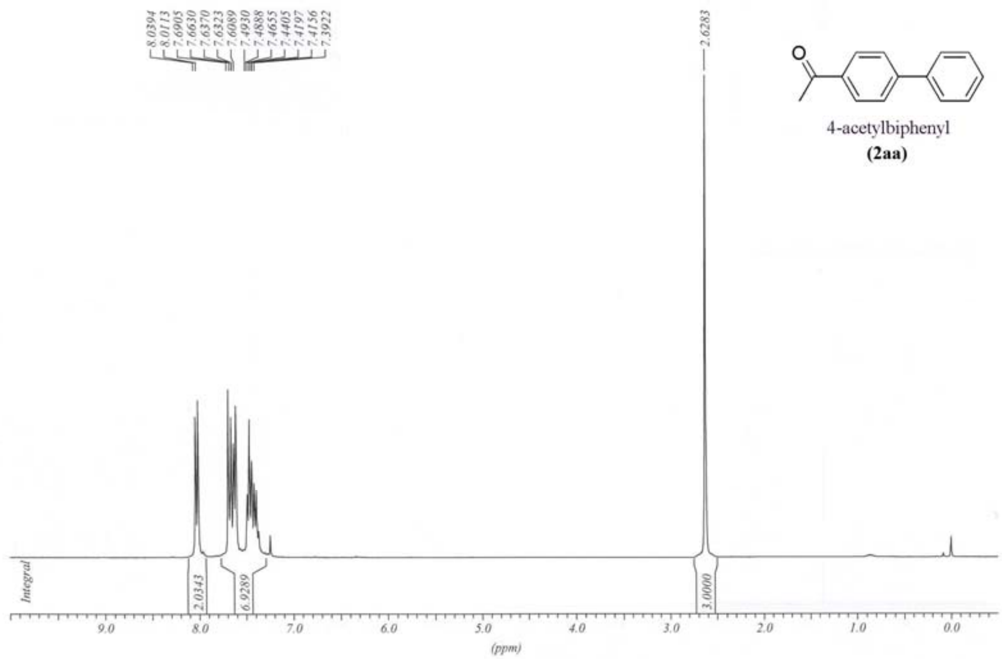
Diphenylmethane (4a): Colorless oil: $R_f = 0.51$ (Hexane); IR (film) ν = 3025, 1600, 1493, 1028 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.27-7.15 (m, 10H, ArH), 3.95 (s, 2H, CH_2); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 141.2 (2 x ArC), 129.1, 128.6 (4 x ArCH), 126.2 (2 x ArCH), 42.1 (CH_2); MS (m/z, %): 168 (M^+, 79), 167 (100), 153 (31), 115 (16), 91 (25).

3-Benzylanisole (4b):[3] Colorless oil; $R_f = 0.51$ (Hexane/Ethyl acetate 6:1); IR (film): ν = 1258, 1050 cm^{-1}; H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 7.27-7.13 (m, 6H, ArH), 6.77-6.70 (m, 3H, ArH), 3.91 (s, 2H, CH_2), 3.71 (s, 3H, CH_3); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 159.8, 142.8, 141.0 (ArC), 129.5, 128.9, 128.5, 126.2, 121.4, 114.9, 111.4 (ArCH), 55.1 (CH_3), 42.0 (CH_2); MS (m/z, %): 198 (M^+, 100), 183 (M^+-15, 20), 167 (49), 165 (47) 153 (18), 152 (19), 91 (23), 65 (16).

4-Chlorobenzylbenzene (4c): Colorless oil; $R_f = 0.48$ (Hexane); IR (film): ν = 3081, 3059, 3026, 2913, 1602, 1489, 1452, 1406, 1092, 1015 cm^{-1}; H-NMR ($CDCl_3$, 400 MHz) δ_H (ppm) = 7.27-7.15 (m, 5H, ArH), 7.13-7.11 (m, 2H, ArH), 7.06-7.04 (m, 2H, ArH), 3.88 (s, 2H, CH_2); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ_C (ppm) = 140.6, 139.7, 131.9 (ArC), 130.3, 128.9, 128.7, 127.3, 127.2, 126.4 (ArCH), 41.3 (CH_2); MS (m/z, %): 204 (M^++2, 13), 203 (M^++1, 7), 202 (M^+, 41), 167 (100), 165 (45), 152 (16), 91 (5).

5-Benzyl-2-chloropyridine (4d):[4] Colorless oil; $R_f = 0.38$ (Hexane/Ethyl acetate 9:1); H-NMR ($CDCl_3$, 300 MHz) δ_H (ppm) = 8.24 (d, 1H, *J* = 1.8 Hz, ArH), 7.39 (dd, 1H, *J* = 8.5 and 2.4 Hz, ArH), 7.31-7.12 (m, 6H, ArH), 3.92 (s, 2H, CH_2); ^{13}C-NMR ($CDCl_3$, 75 MHz) δ_C (ppm) = 149.7 (ArCH), 149.4 (ArC), 139.3 (ArCH), 139.2, 135.5 (ArC), 128.8, 126.7, 124.0 (ArCH), 38.2 (CH_2); MS (m/z, %): 205 (M^++2, 33), 203 (M^+, 100), 202 (M^+-1, 85), 168 (M^+-35, 57), 140 (15), 139 (30), 115 (22), 91 (28) 70 (66), 65 (34), 63 (43).

[3] Vanier, C.; Lorgé, F.; Wagner, A. ; Mioskowski, C. *Angew. Chem. Int. Ed.* **2000**, *39*, 1679.
[4] Lantzsch, R. *Eur. Pat. Appl.* **1993**, 10.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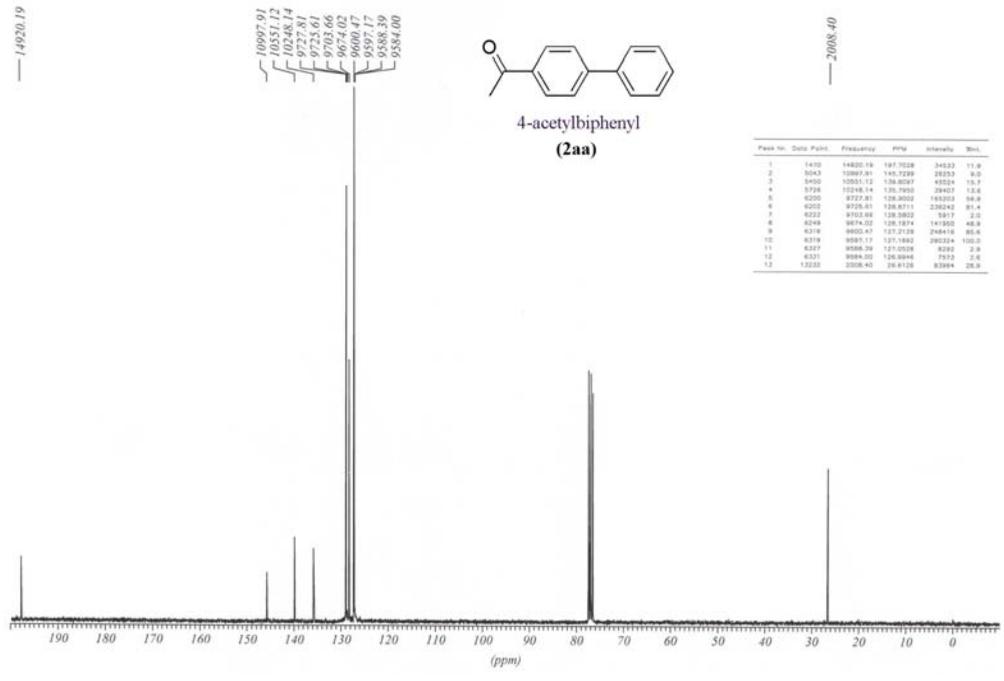
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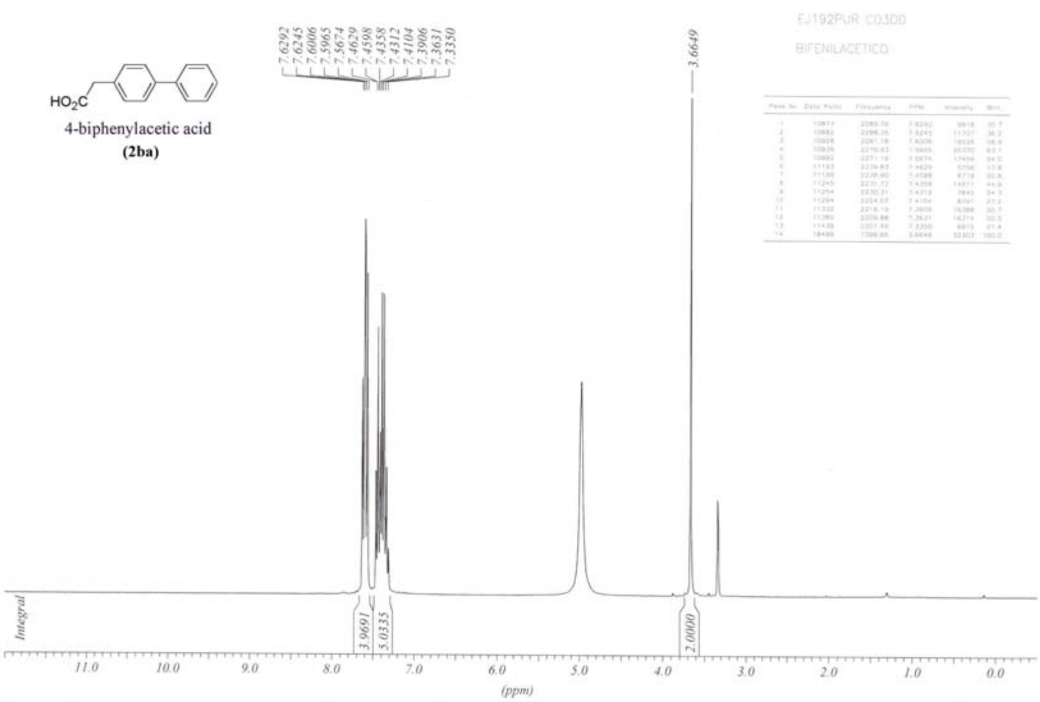
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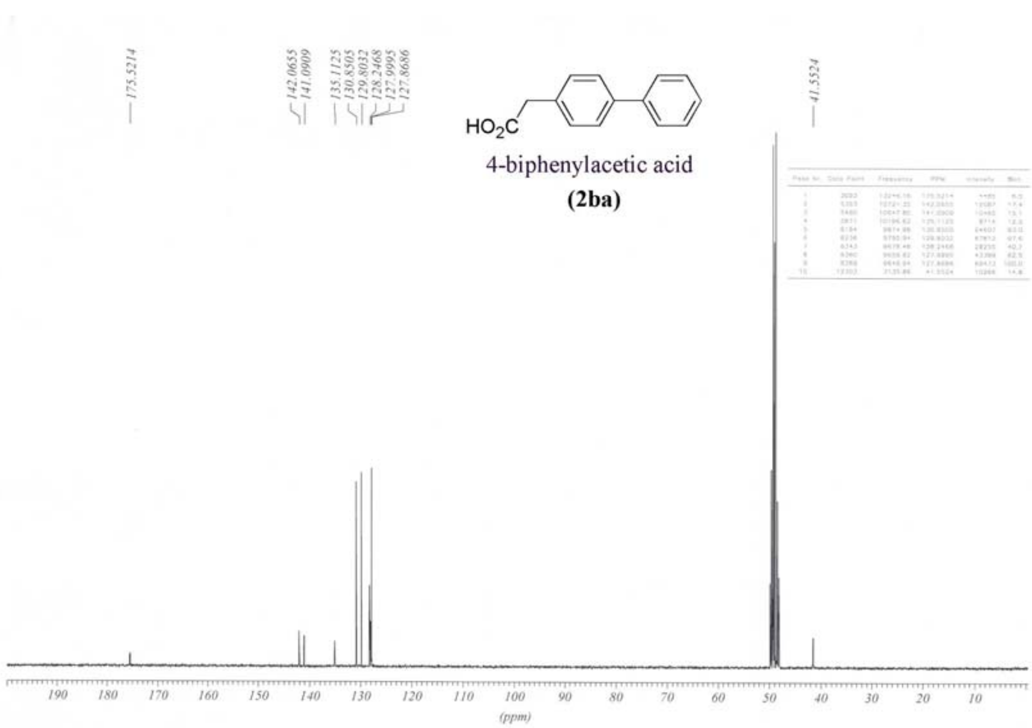
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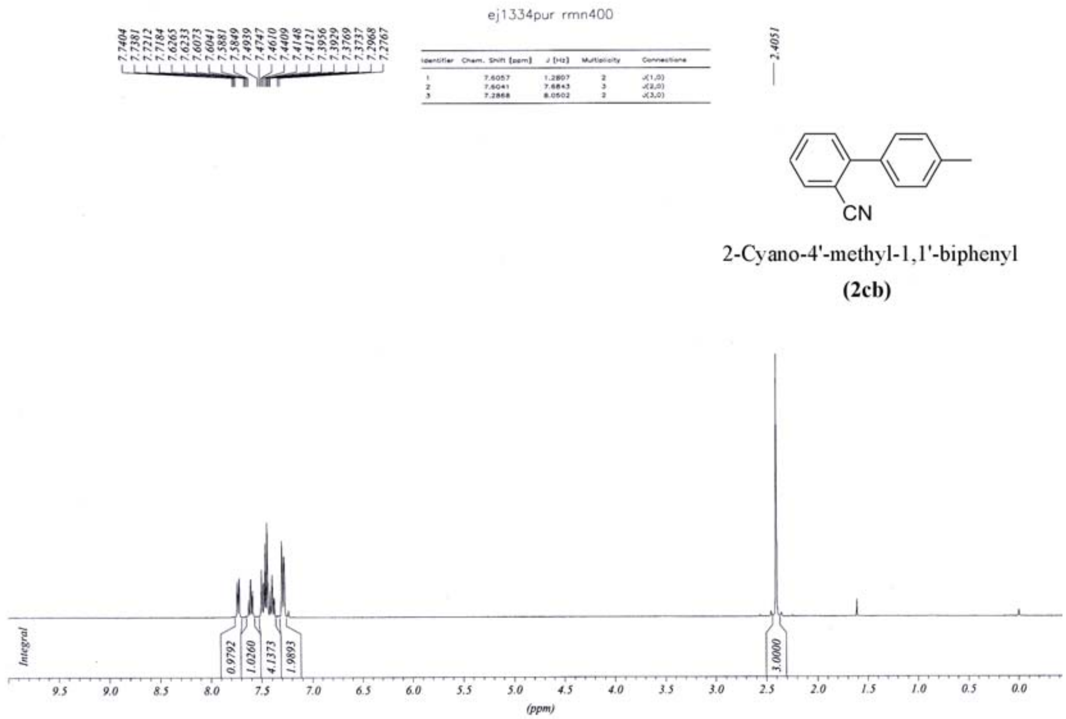

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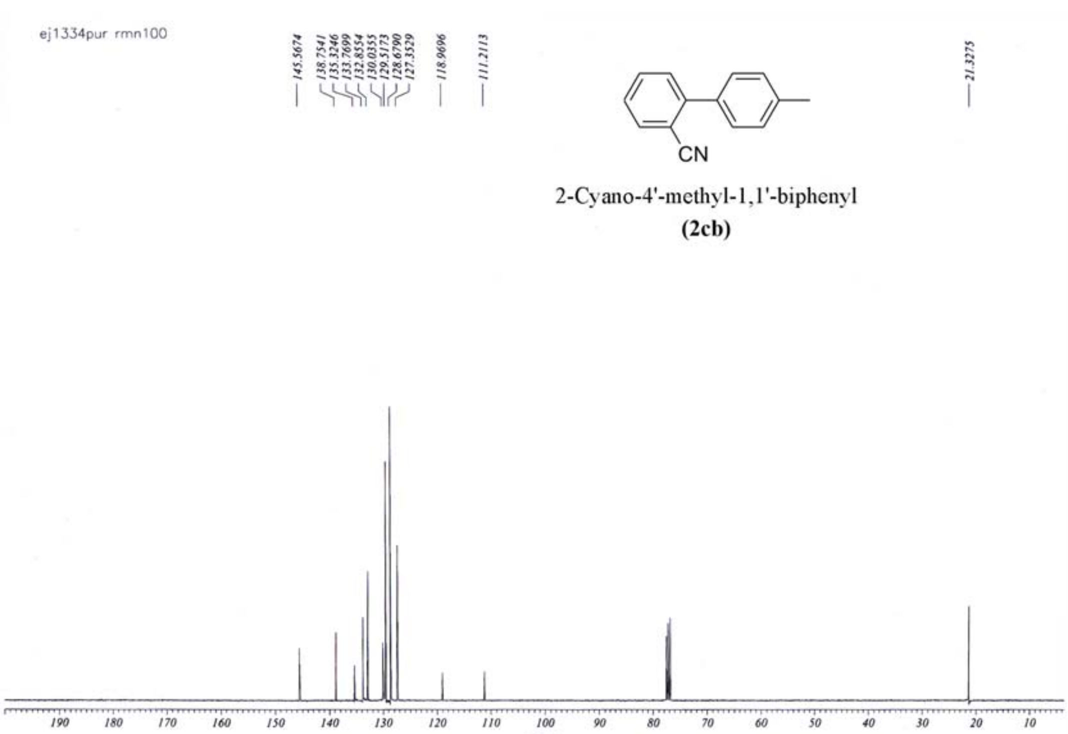
2-Cyano-4'-methyl-1,1'-biphenyl

(2cb)



2-Cyano-4'-methyl-1,1'-biphenyl

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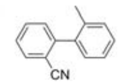

2-Cyano-2'-methyl-1,1'-biphenyl

(2cc)

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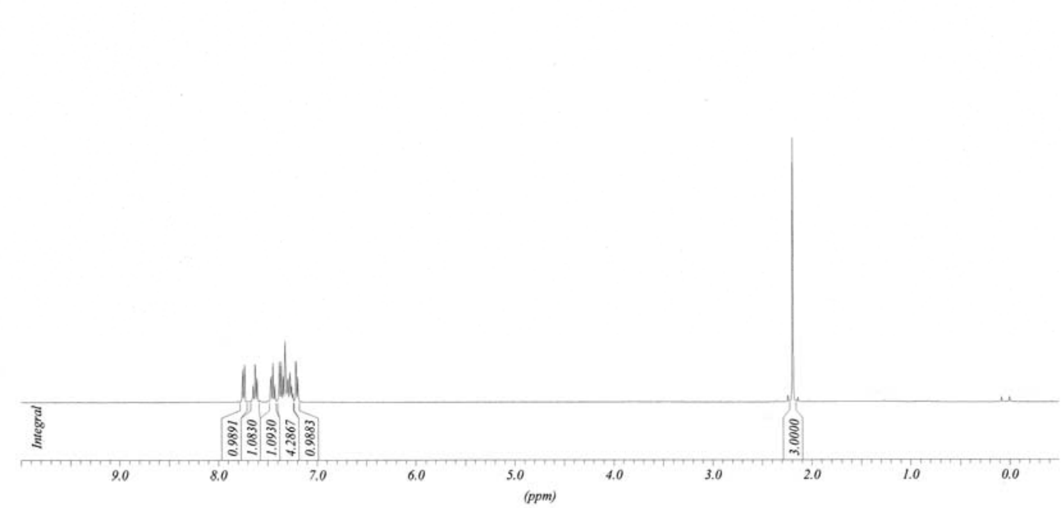
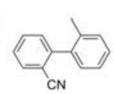
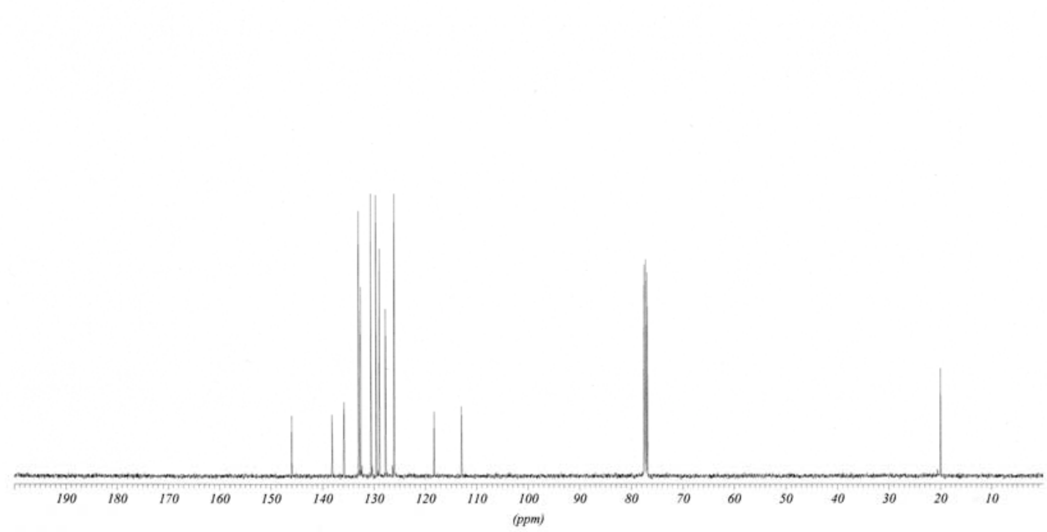
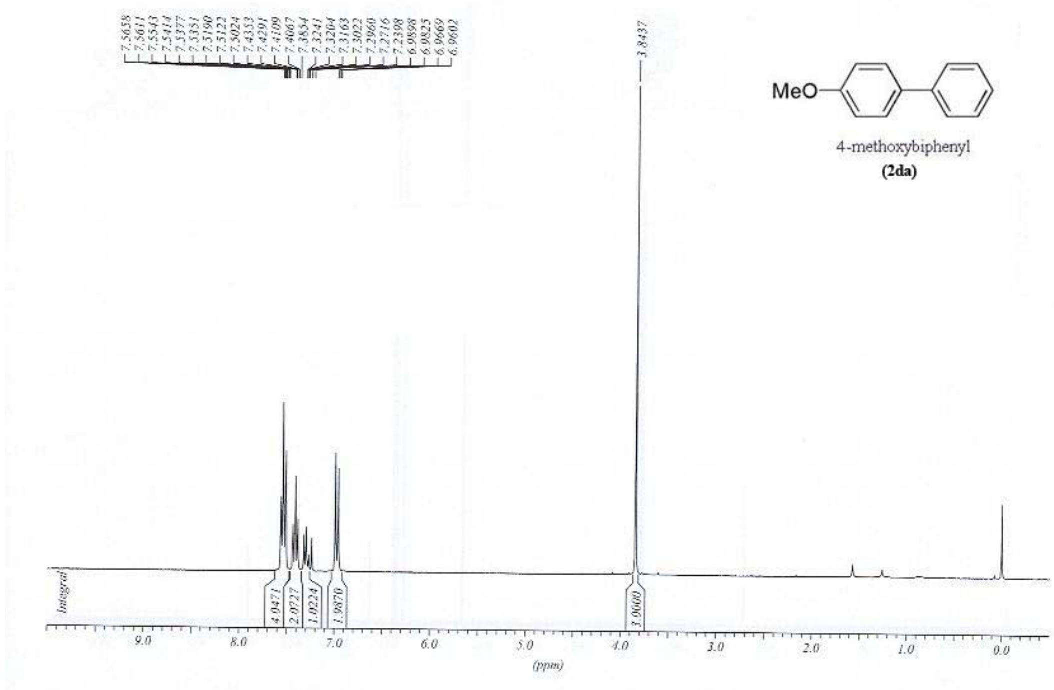




2-Cyano-2'-methyl-1,1'-biphenyl

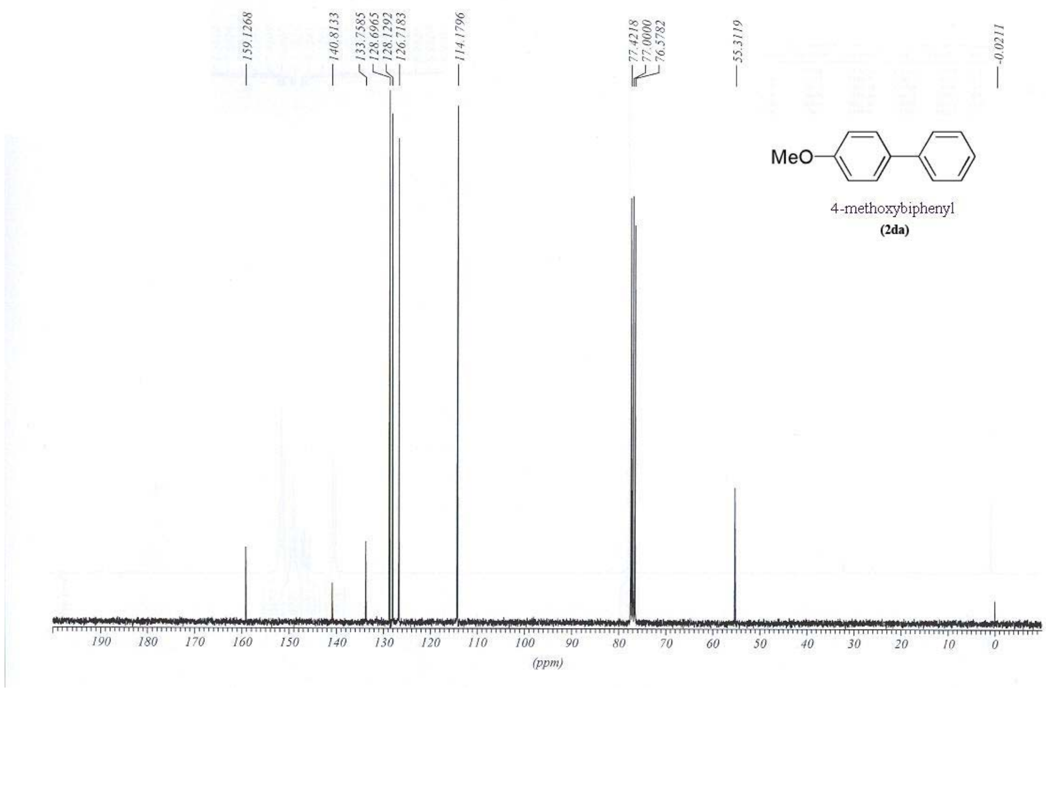
(2cc)





4-methoxybiphenyl

(2da)



4-methoxybiphenyl

(2da)

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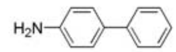

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(2ea)

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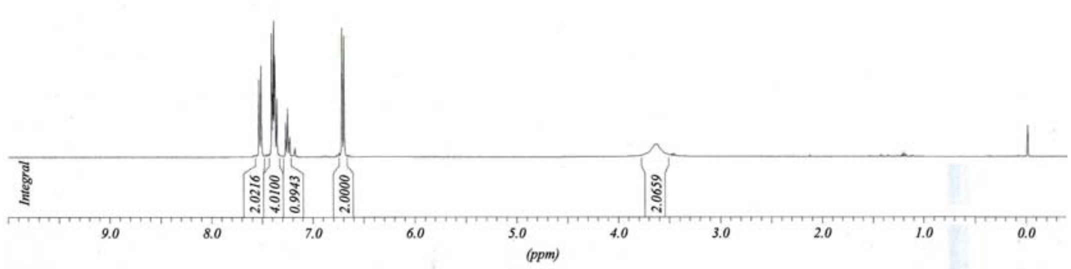
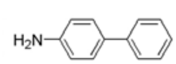
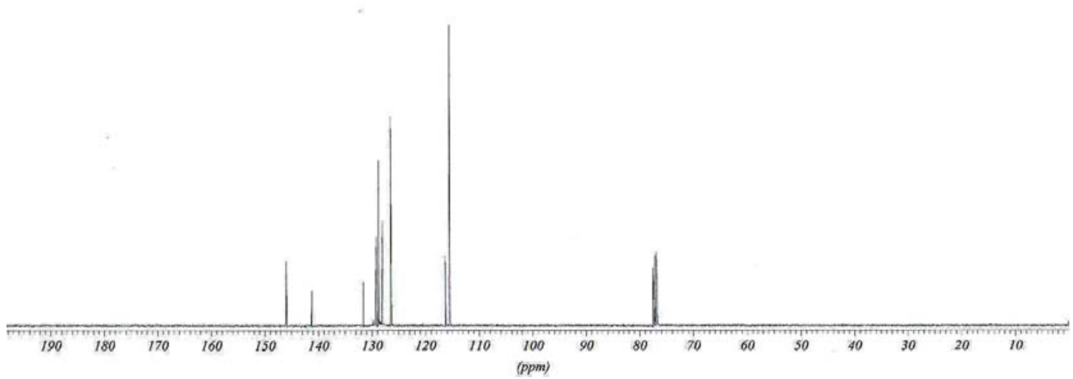
2	7.5095	1.0978	2	J(2,0)
3	6.7052	8.7820	2	J(3,0)

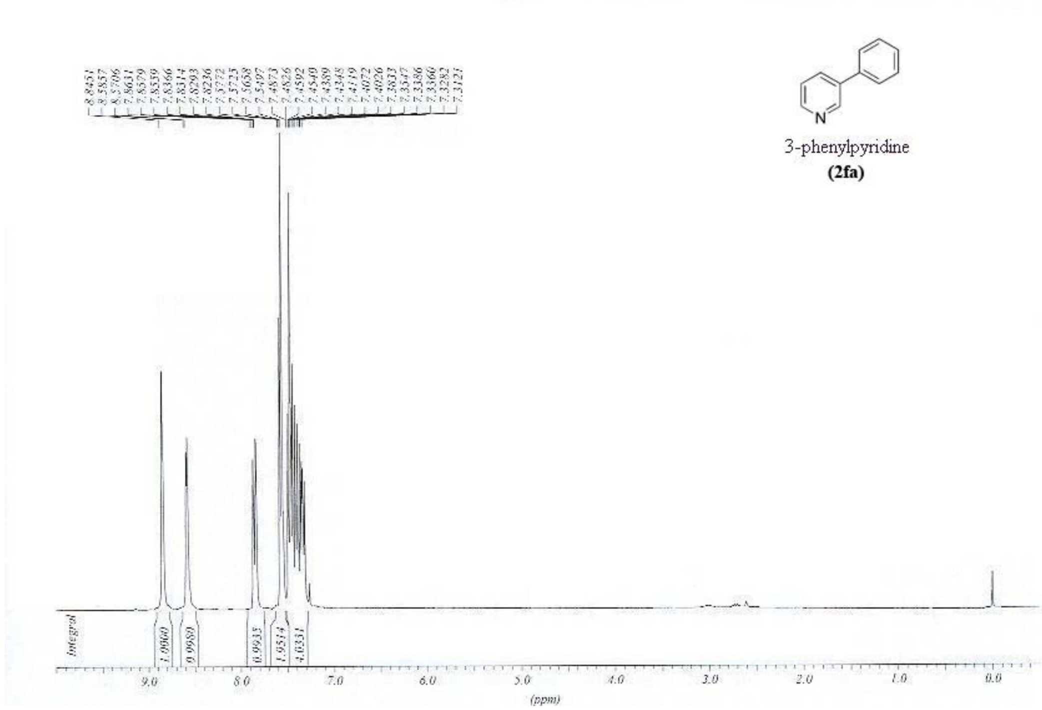


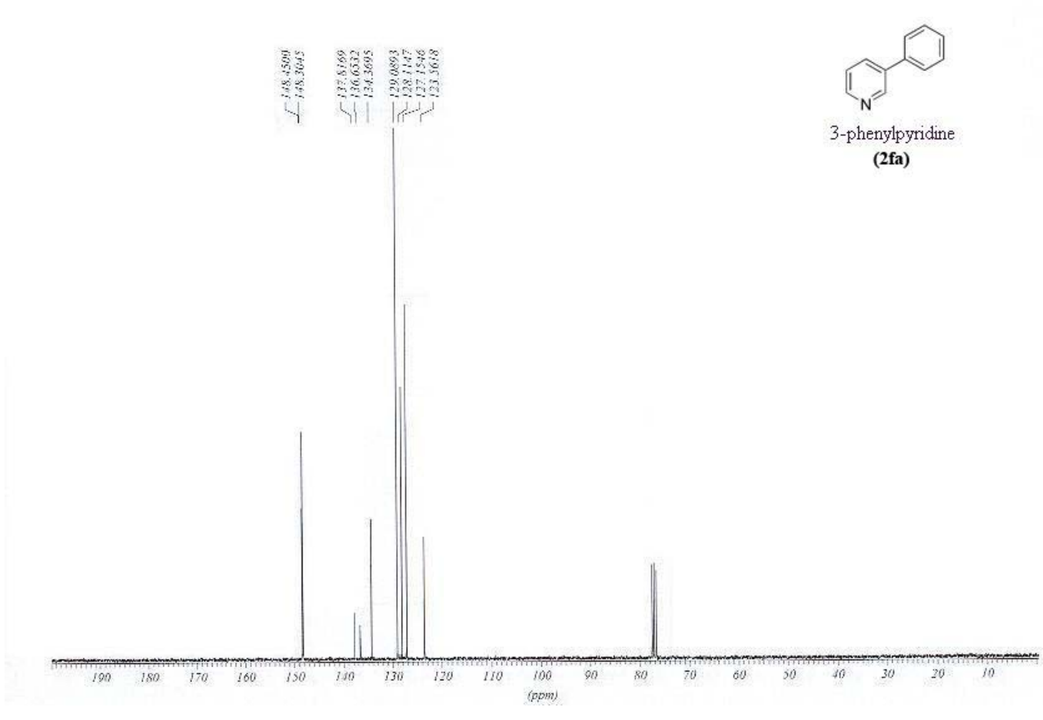
145.9180
141.1929
131.5445 128.7399 128.0388 126.4384 126.3317
115.4639

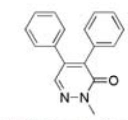


biphenyl-4-amine
(2ea)



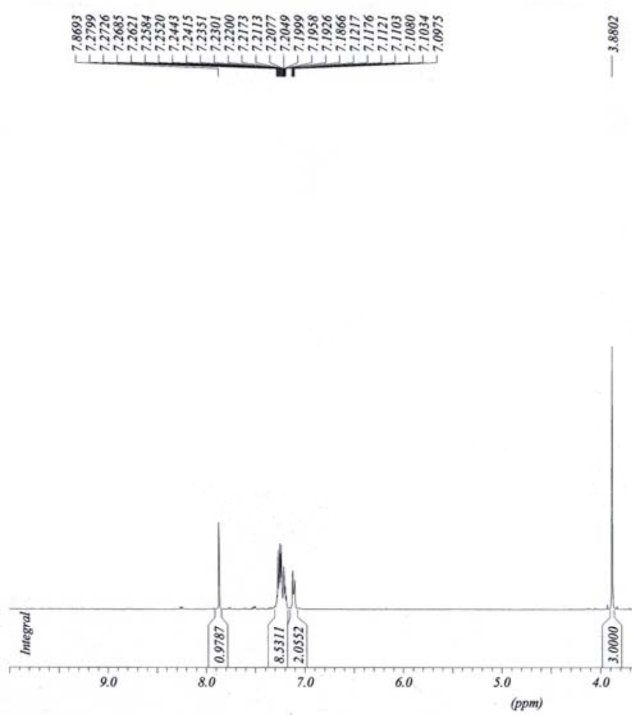

3-phenylpyridine
(2fa)
integral
(ppm)

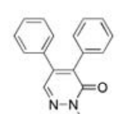

3-phenylpyridine
(2fa)
148.4509
148.3045
137.8169
136.6532
134.3695
129.0893
128.1147
127.1546
123.5618
(ppm)



2-methyl-4,5-diphenylpyridazin-3(*2H*)-one

(2ga)

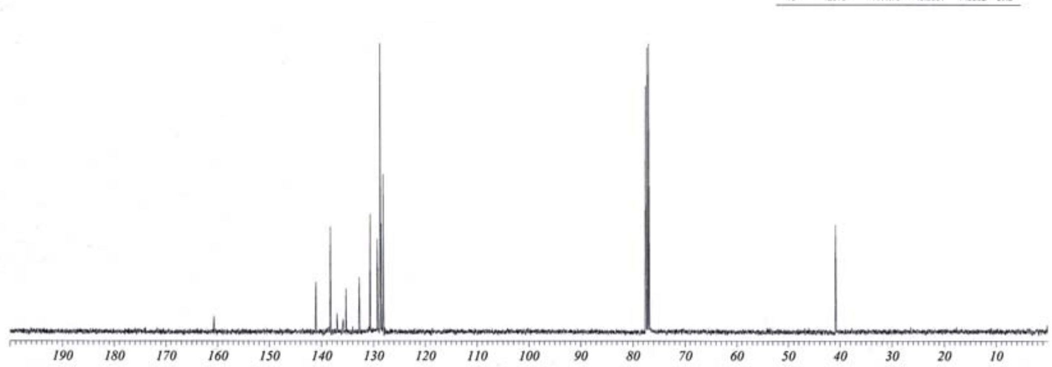


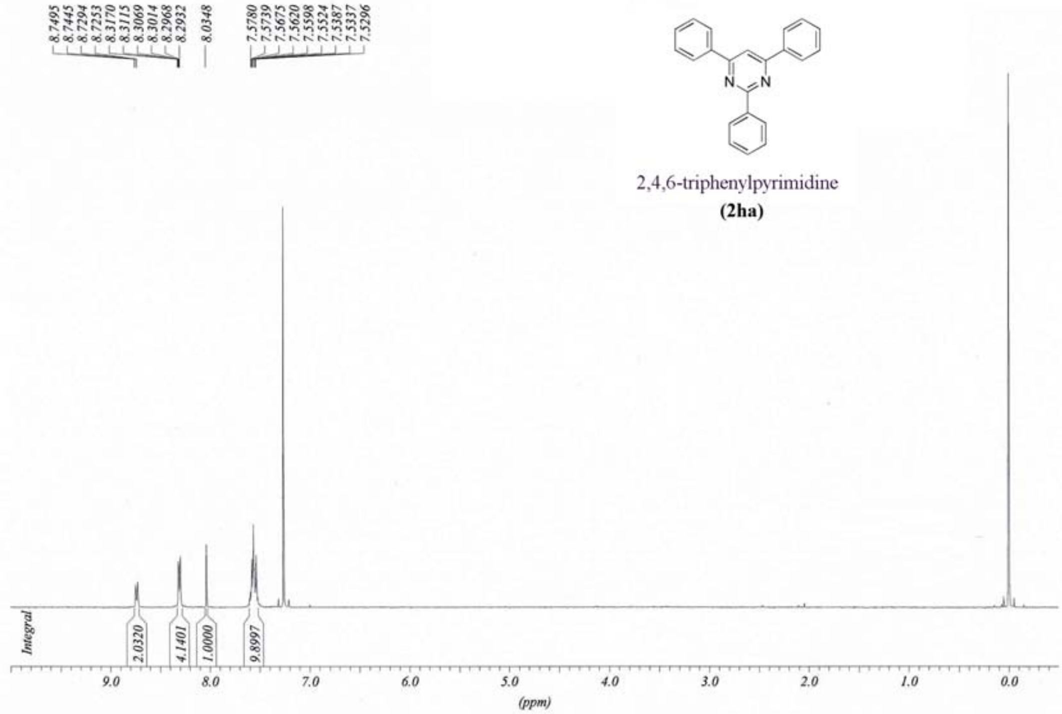


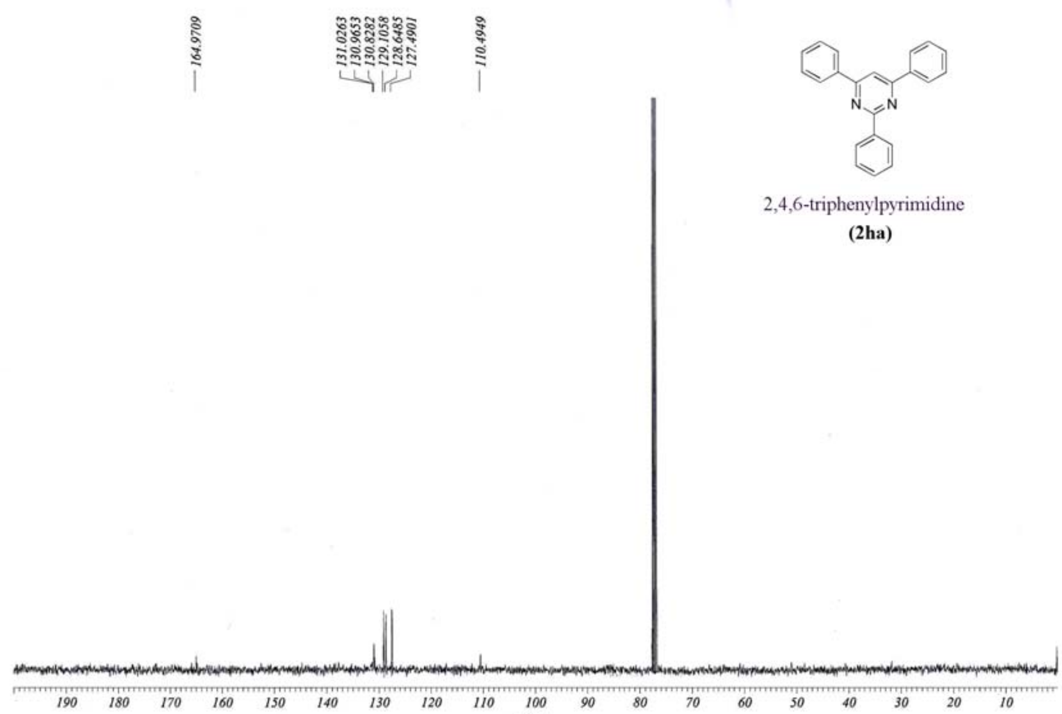
2-methyl-4,5-diphenylpyridazin-3(*2H*)-one

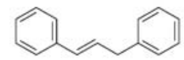
(2ga)

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	4222	16159.33	160.6116	21359	5.5
2	5511	14162.59	140.9643	67761	17.4
3	5686	13911.15	138.2664	143171	36.7
4	5772	13782.33	136.9860	24912	6.4
5	5852	13659.65	135.7666	17186	4.4
6	5886	13607.51	135.2484	58983	15.1
7	6053	13351.41	132.7029	74608	19.1
8	6162	13138.24	130.5843	160619	41.2
9	6284	12997.16	129.1820	126411	32.4
10	6315	12949.62	128.7095	159067	40.8
11	6318	12945.02	128.6637	389625	100.0
12	6333	12922.01	128.4351	147670	37.9
13	6354	12889.81	128.1150	25218	6.5
14	6358	12883.67	128.0540	213687	54.8
15	12078	4111.79	40.8681	145392	37.3



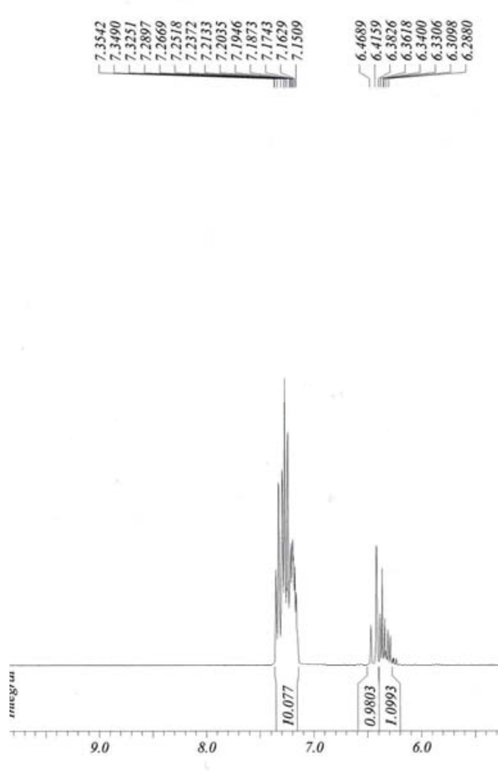

8.7495
8.7445
8.7294
8.7253
8.3170
8.3115
8.3069
8.3014
8.2968
8.2932
8.0348
7.5780
7.5739
7.5675
7.5620
7.5598
7.5524
7.5387
7.5337
7.5296
2,4,6-triphenylpyrimidine
(2ha)
Integral
2.0320
4.1401
1.0000
9.8997
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

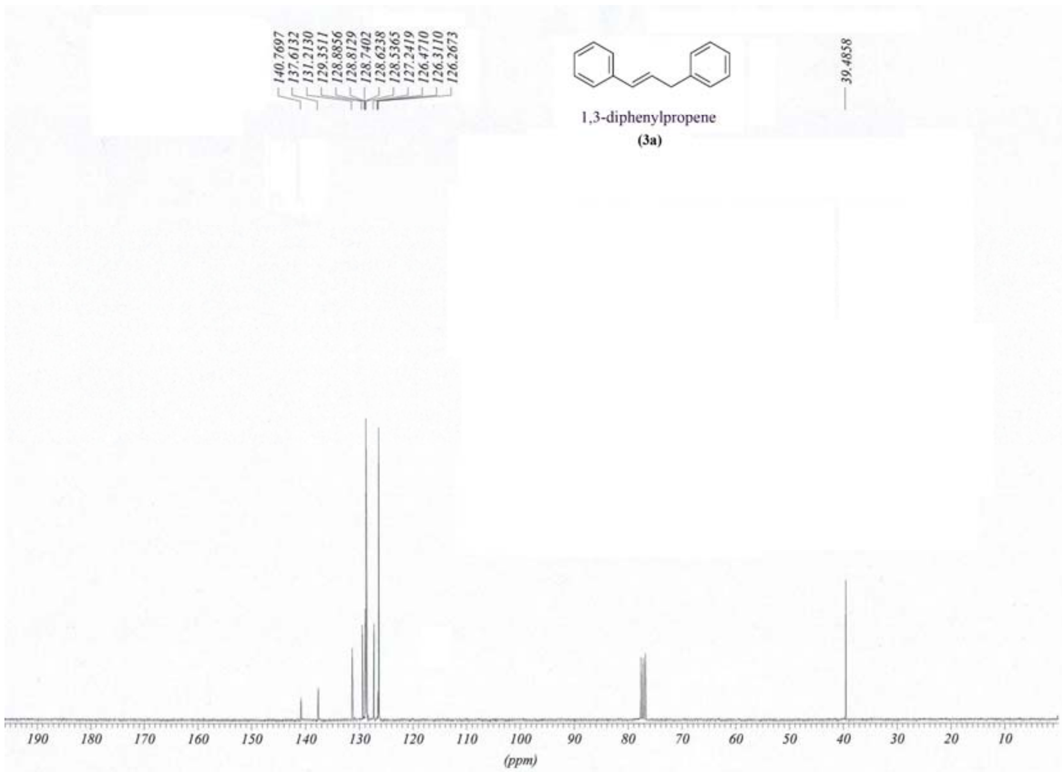

164.9709
131.0263
130.9653
130.8282
129.1058
128.6485
127.4901
110.4949
2,4,6-triphenylpyrimidine
(2ha)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

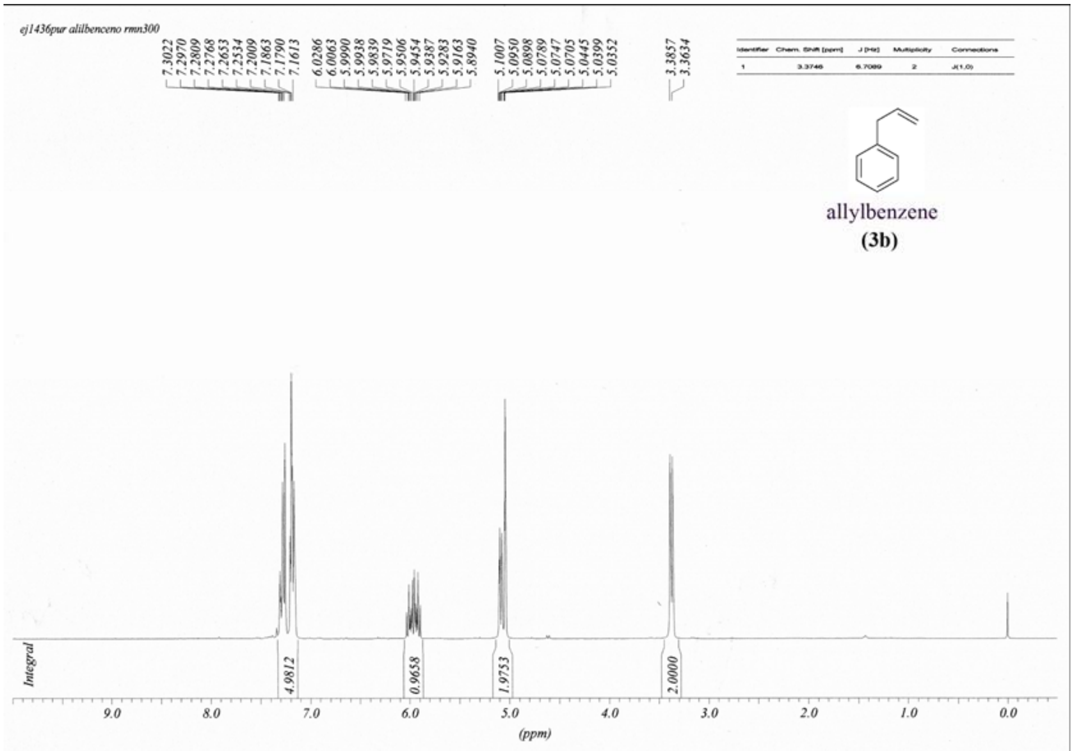


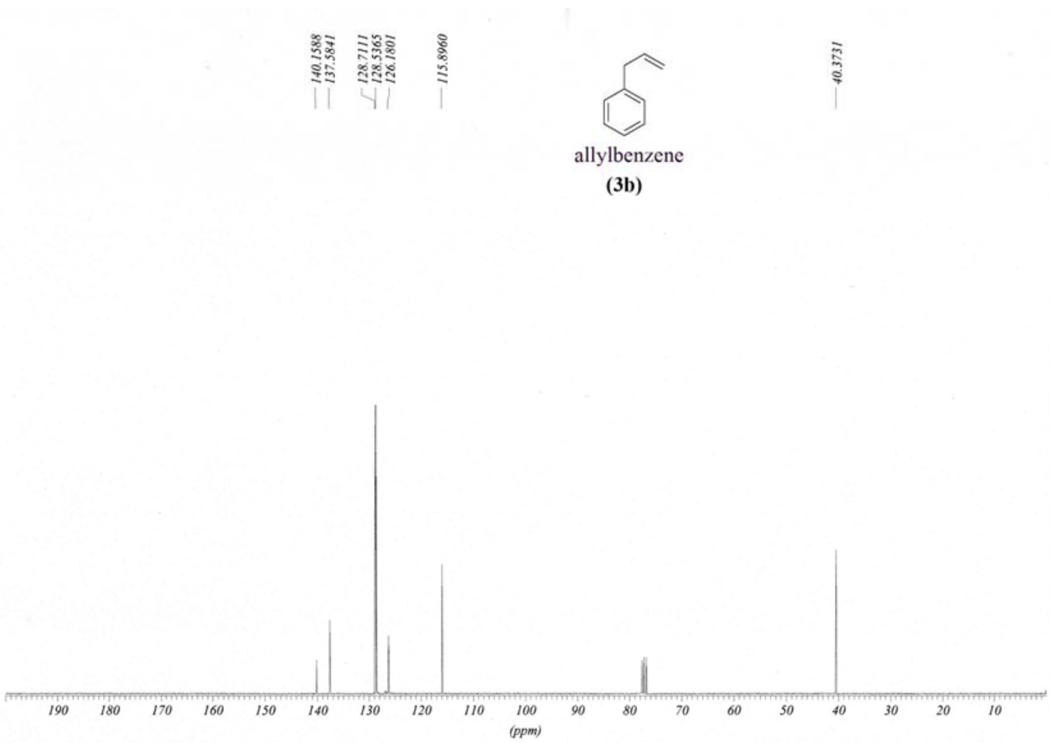
1,3-diphenylpropene
(3a)

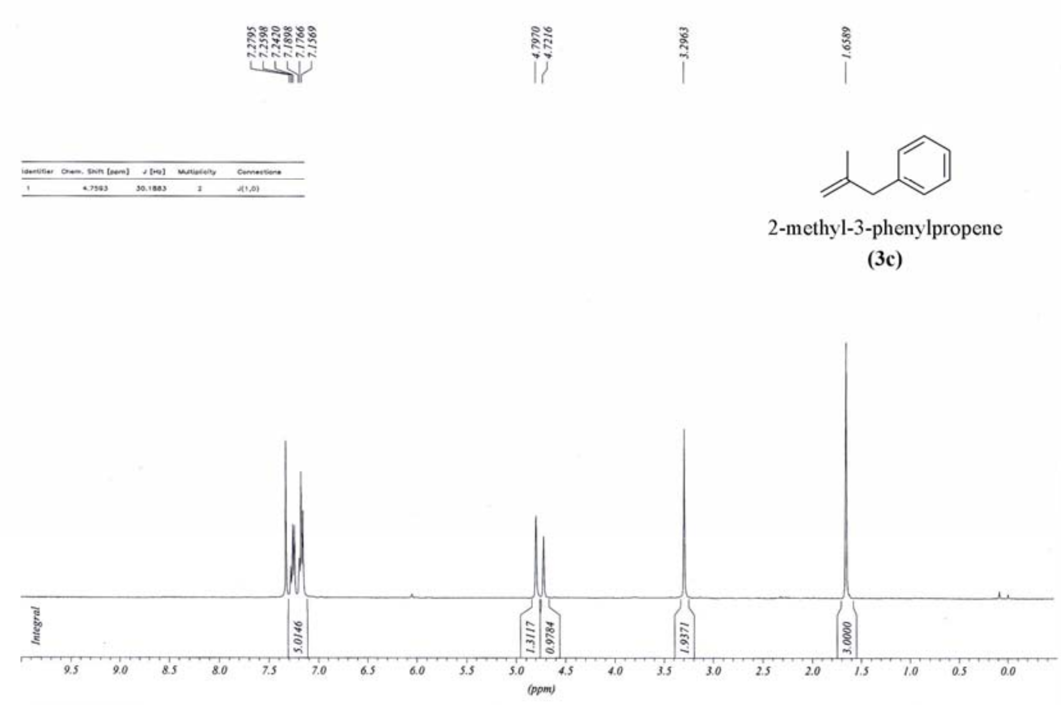
Identifier	Chem. Shift [ppm]	J [Hz]	Multiplicity	Connections
1	6.4424	15.9141	2	J(1,0)
2	3.5274	6.3968	2	J(2,0)



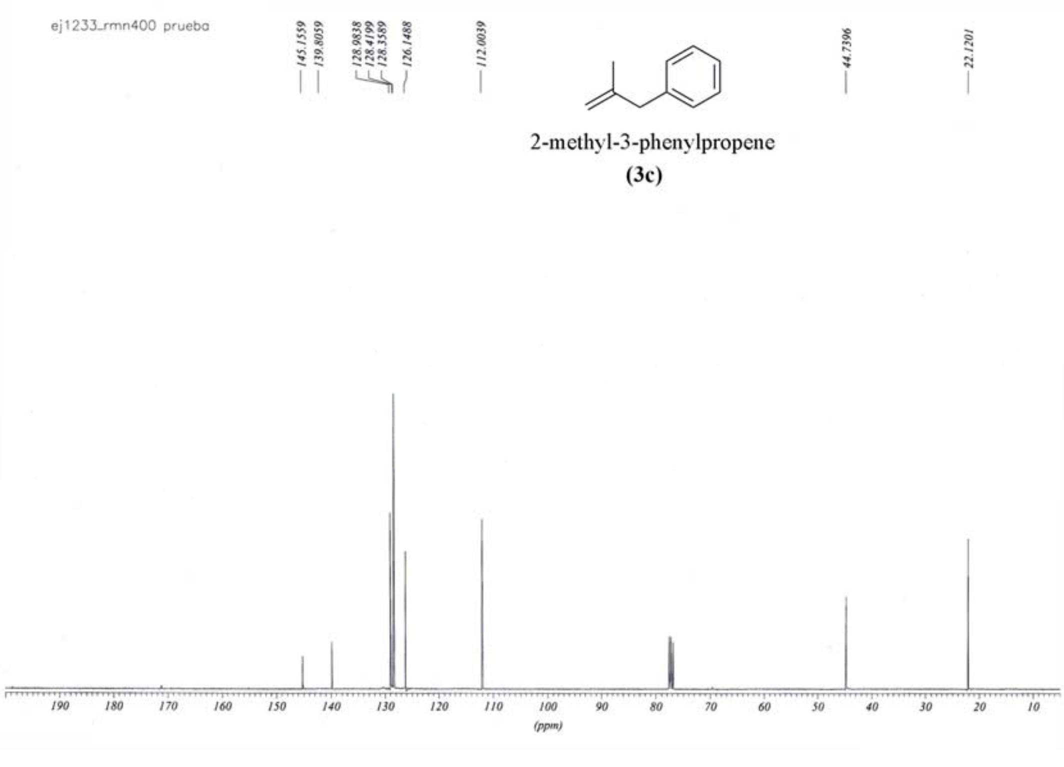


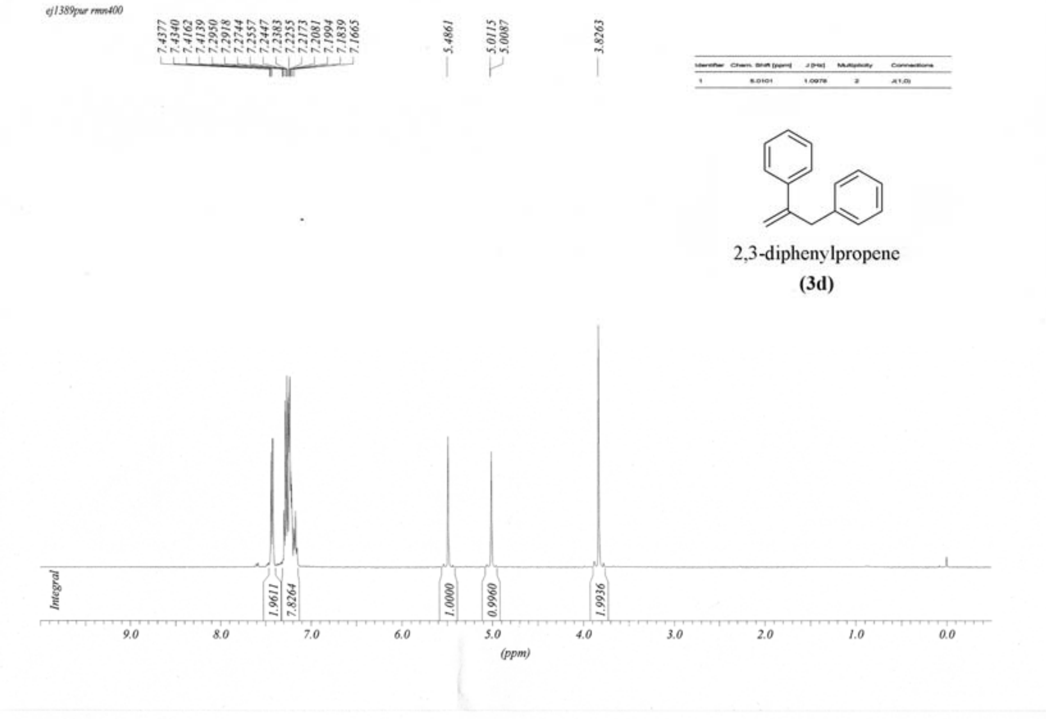

ej1436pur alilbenceno rmn300
allylbenzene
(3b)
Integral
4.9812
0.9658
1.9753
2.0000
(ppm)

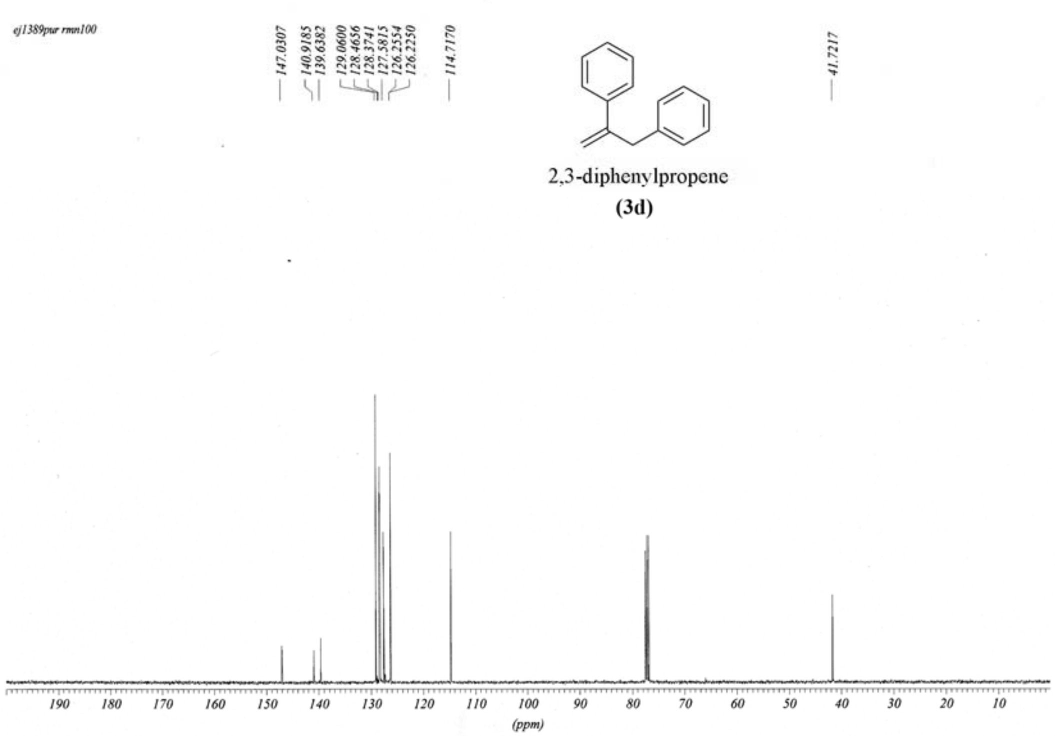

140.1588
137.5841
128.7111
128.5365
126.1801
115.8960
40.3731
allylbenzene
(3b)
(ppm)

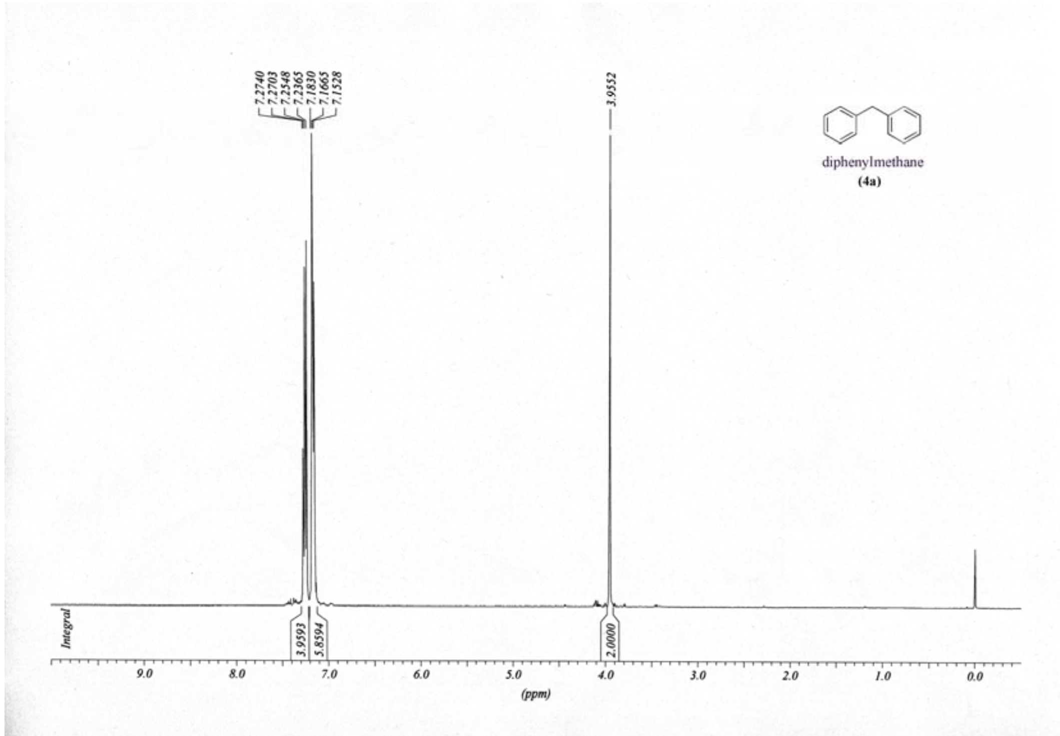


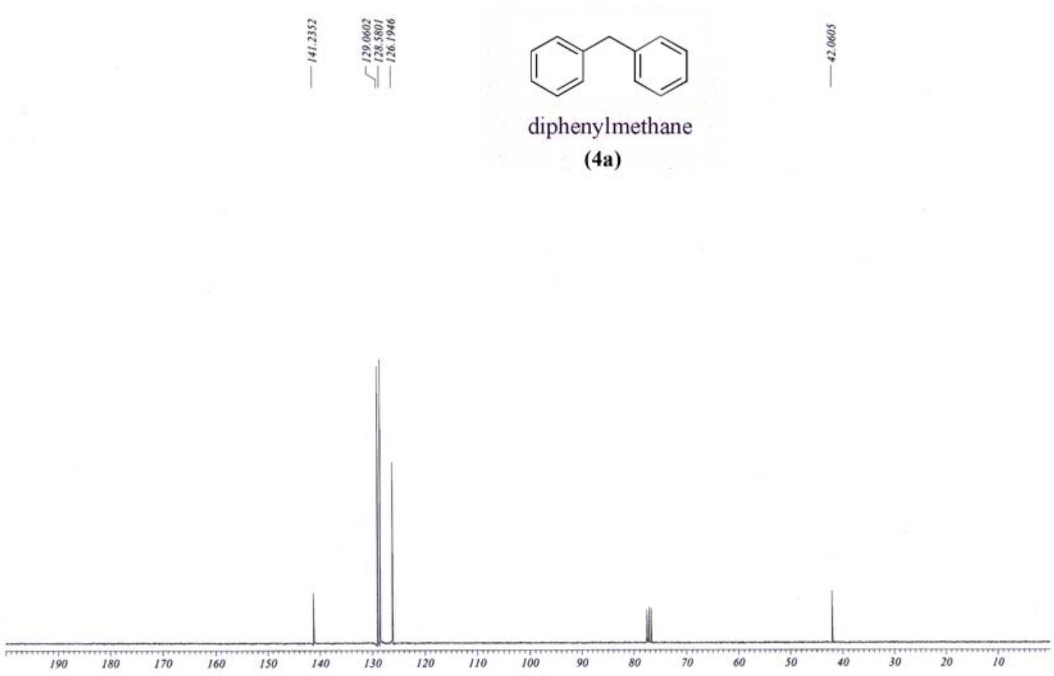
Identifier	Chem. Shift [ppm]	J [Hz]	Multiplicity	Connections
1	4.7593	30.1883	2	J(1,0)

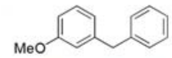



ej1389pur rmn400
7.4377
7.4340
7.4162
7.4139
7.2950
7.2918
7.2744
7.2557
7.2447
7.2383
7.2235
7.2173
7.2081
7.1994
7.1839
7.1665
5.4861
5.0115
5.0087
3.8263
2,3-diphenylpropene
(3d)
Integral
1.9611
7.8264
1.0000
0.9960
1.9936
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

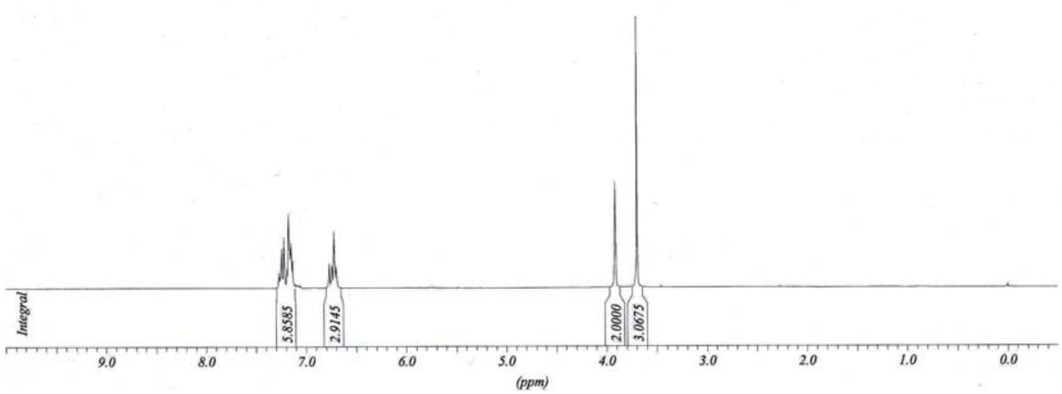

ej1389pur rmn100
147.0307
140.9185
139.6382
129.0600
128.4656
128.3741
127.5815
126.2554
126.2250
114.7170
41.7217
2,3-diphenylpropene
(3d)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

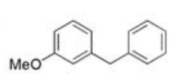

7.2740
7.2703
7.2548
7.2365
7.1830
7.1665
7.1528
3.9552
diphenylmethane
(4a)
Integral
3.9593
5.8594
2.0000
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


141.2352
129.0602
128.5801
126.1946
42.0605
diphenylmethane
(4a)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

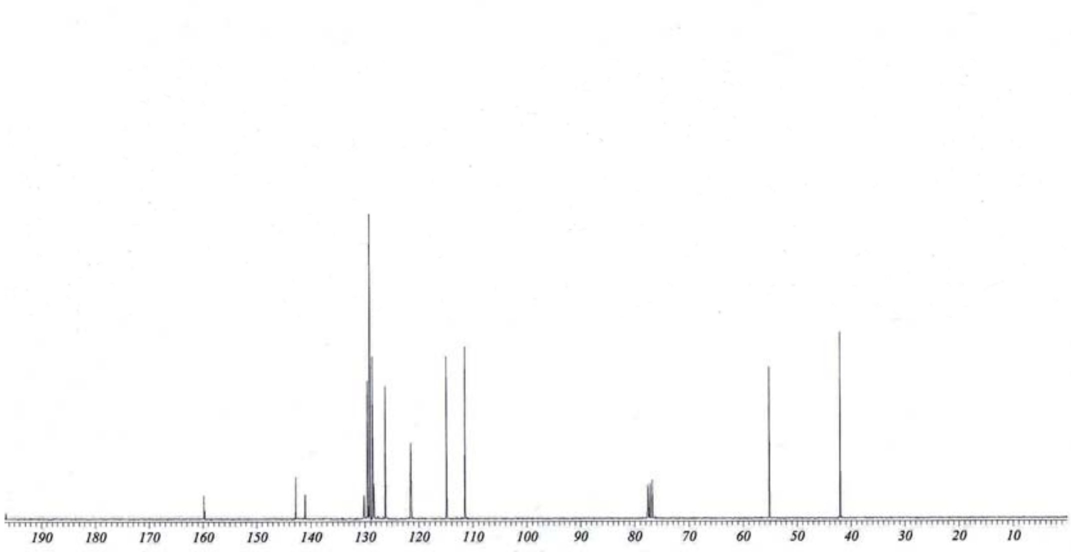


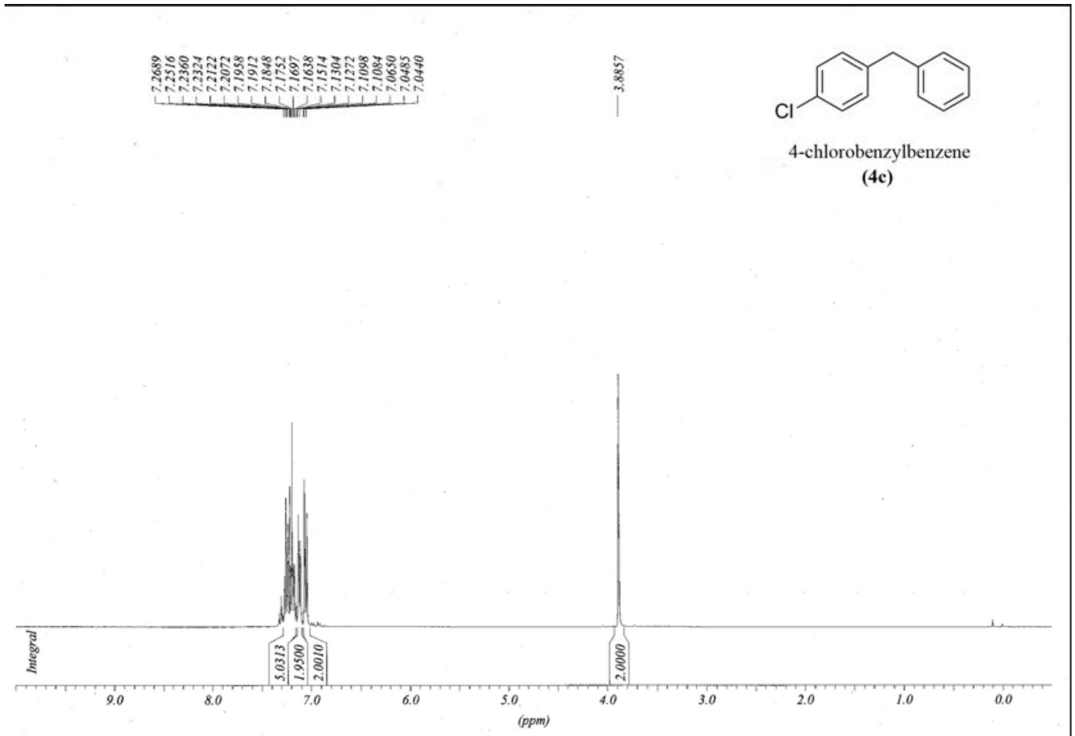
1-benzyl-3-methoxybenzene
(4b)



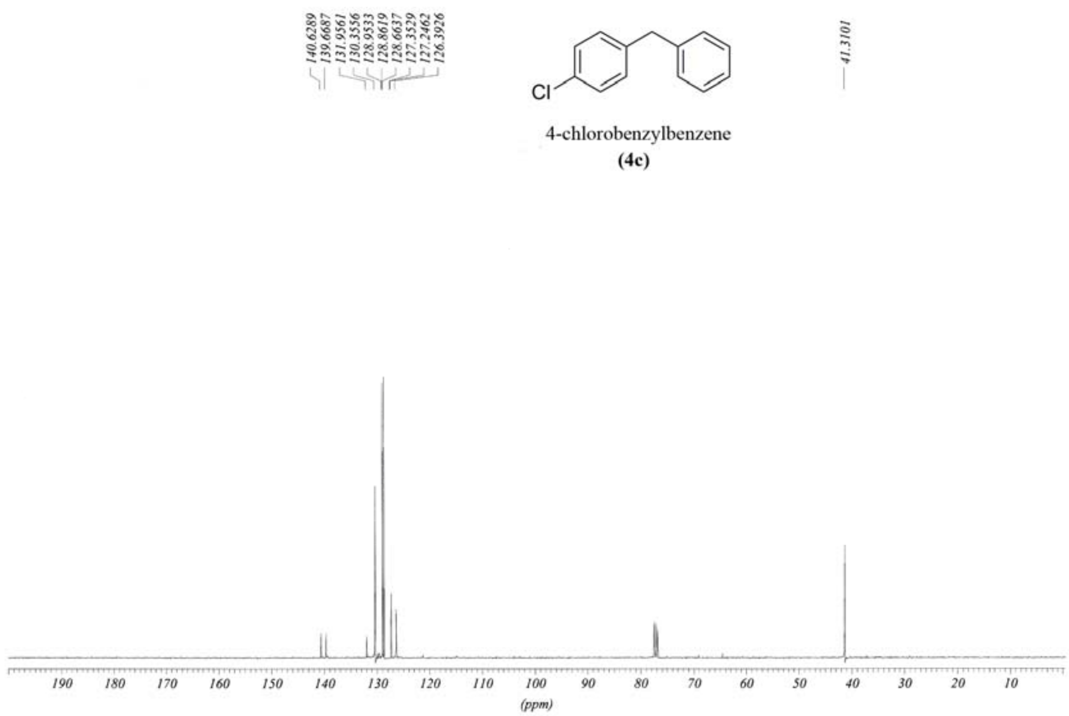


1-benzyl-3-methoxybenzene
(4b)

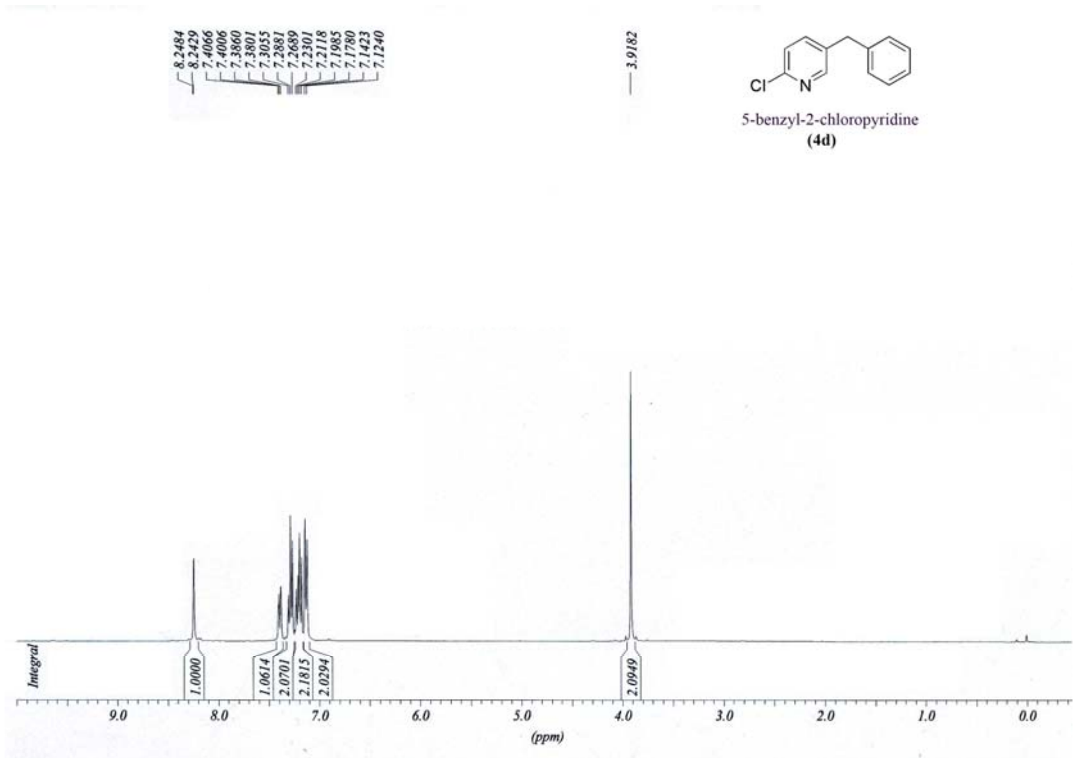




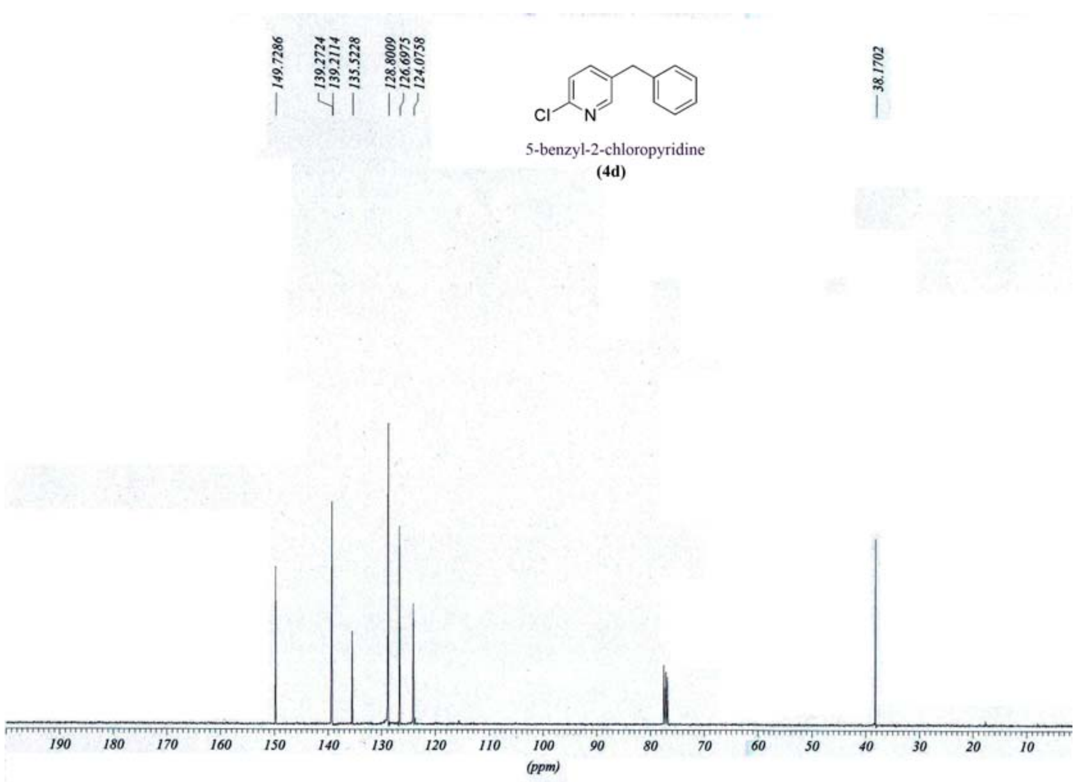
4-chlorobenzylbenzene
(4c)



4-chlorobenzylbenzene
(4c)



8.2484
8.2429
7.4066
7.4006
7.3860
7.3801
7.3055
7.2881
7.2689
7.2301
7.2118
7.1985
7.1780
7.1423
7.1240
3.9182
Cl
N
5-benzyl-2-chloropyridine
(4d)
Integral
1.0000
1.0614
2.0701
2.1815
2.0294
2.0949
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)



149.7286
139.2724
139.2114
135.5228
128.8009
126.6975
124.0758
38.1702
Cl
N
5-benzyl-2-chloropyridine
(4d)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)