

Supporting Information

Cu-Catalyzed Intermolecular [3+3] Annulation involving Oxidative Activation of Unreactive C(sp³)-H Bond: Access to Pyrimidine Derivatives from Amidines and Ketones

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Contents

A. General Methods.....	S2
B. General Procedure for the Preparation of 3	S3
C. Analytical Data	S4
D. NMR Spectra	S22

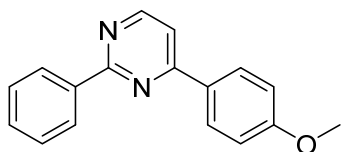
A. General Methods

Melting points were measured using a melting point instrument and are uncorrected. ^1H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC–MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100–400 mesh silica gel plates (GF₂₅₄). Unless otherwise noted, purchased chemicals were used without further purification.

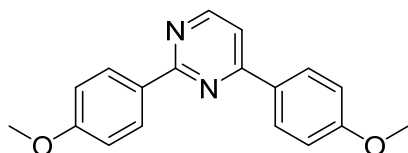
B. General Procedure for the Preparation of 3

A mixture of amidines (0.20 mmol), ketones (0.30 mmol), CuCl_2 (5 mol %), TEMPO (0.22 mmol, 1.1 equiv), Cs_2CO_3 (0.40 mmol, 2 equiv) was stirred in 1,2-DCB (1.0 mL) at 120 °C under an O_2 (1 atm) atmosphere for 24 h. After completion of the reaction (monitored by TLC), water (10 mL) was added to the reaction mixture, and the resulting mixture was extracted with ethyl acetate. The combined organic layers were then dried over MgSO_4 , filtered, and then concentrated in vacuum. The residue was purified by flash chromatography on silica gel to give the desired product (using the mixture of petroleum ether and ethyl acetate as eluents).

C. Analytical Data of 3

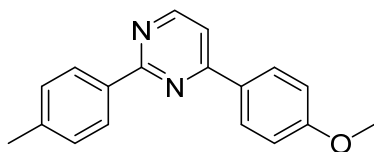


4-(4-Methoxyphenyl)-2-phenylpyrimidine (3aa).^[1] White solid: 84% yield (44 mg); mp 88–90 °C; IR (KBr) 3066, 2923, 2848, 1558, 1418, 1251, 1174, 1026, 823, 756, 693 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.72 (d, J = 4.0 Hz, 1H), 8.57 (d, J = 8.0 Hz, 2H), 8.16 (d, J = 8.0 Hz, 2H), 7.50–7.49 (m, 3H), 7.46 (d, J = 4.0 Hz, 1H), 6.99 (d, J = 8.0 Hz, 2H), 3.84 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 164.4, 163.4, 162.1, 157.2, 138.1, 130.6, 129.4, 128.8, 128.5, 128.3, 114.3, 113.7, 55.4 ppm; MS (EI, 70 eV) m/z 262.27, 247.25, 231.26, 219.24, 191.22, 159.21, 132.19, 117.17, 103.18; HRMS (ESI) calcd C₁₇H₁₅N₂O [M + H]⁺ m/z 263.1179, found m/z 263.1181.

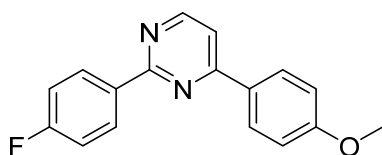


2,4-Bis(4-methoxyphenyl)pyrimidine (3ba). White solid: 85% yield (50 mg); mp 142–144 °C; IR (KBr) 3024, 2921, 2851, 1593, 1510, 1417, 1305, 1245, 1172, 1023, 821 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.72 (d, J = 8.0 Hz, 1H), 8.55 (d, J = 8.0 Hz, 2H), 8.20 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 8.0 Hz, 1H), 7.04 (d, J = 8.0 Hz, 4H), 3.90 (s, 3H), 3.89 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 164.2, 163.2, 162.0, 161.8, 157.4, 130.8, 129.9, 129.5, 128.7, 114.3, 113.8, 113.0, 55.4, 55.4 ppm; MS (EI, 70 eV) m/z 292.32, 277.29, 262.28, 249.27, 159.22, 132.19, 117.16; HRMS (ESI) calcd C₁₈H₁₇N₂O₂ [M + H]⁺ m/z 293.1285, found m/z

293.1290.

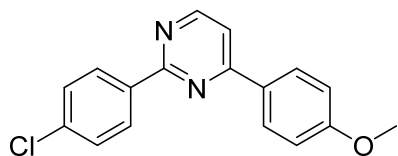


4-(4-Methoxyphenyl)-2-(p-tolyl)pyrimidine (3ca). White solid: 82% yield (45 mg); mp 93–95 °C; IR (KBr) 3059, 2924, 2853, 1560, 1511, 1421, 1253, 1175, 1114, 1029, 824 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.74 (d, $J = 4.0$ Hz, 1H), 8.45 (d, $J = 8.0$ Hz, 2H), 8.19 (d, $J = 8.0$ Hz, 2H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.01 (d, $J = 8.0$ Hz, 2H), 3.88 (s, 3H), 2.43 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.5, 163.3, 162.1, 157.4, 140.8, 135.3, 129.5, 129.3, 128.8, 128.2, 114.3, 113.4, 55.4, 21.5 ppm; MS (EI, 70 eV) m/z 276.30, 245.28, 233.26, 191.23, 159.20, 138.18, 132.18, 117.15; HRMS (ESI) calcd $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 277.1335, found m/z 277.1335.

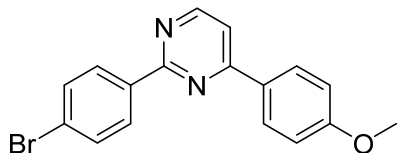


2-(4-Fluorophenyl)-4-(4-methoxyphenyl)pyrimidine (3da). White solid: 73% yield (41 mg); mp 118–120 °C; IR (KBr) 3068, 2921, 2851, 1647, 1562, 1510, 1413, 1251, 1176, 1027, 951, 823, 747 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.72 (d, $J = 4.0$ Hz, 1H), 8.58–8.55 (m, 2H), 8.17 (d, $J = 8.0$ Hz, 2H), 7.48 (d, $J = 8.0$ Hz, 1H), 7.19–7.15 (m, 2H), 7.02 (d, $J = 8.0$ Hz, 2H), 3.87 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.7 (d, $J = 250$ Hz), 163.5, 162.2, 157.5, 134.2 (d, $J = 3.0$ Hz), 130.4 (d, $J = 8.0$ Hz), 129.3, 128.7, 115.5, 115.3, 114.3, 113.5, 55.4 ppm; MS (EI, 70 eV) m/z 280.29, 265.23, 237.24, 159.21, 132.17, 121.15, 117.18; HRMS (ESI)

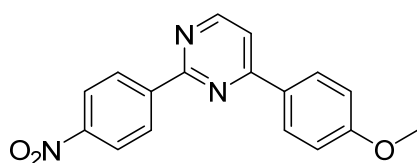
calcd C₁₇H₁₄FN₂O [M + H]⁺ *m/z* 281.1085, found *m/z* 281.1084.



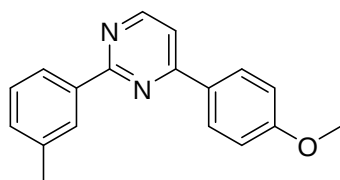
2-(4-Chlorophenyl)-4-(4-methoxyphenyl)pyrimidine (3ea). Yellow solid: 77% yield (46 mg); mp 119–121 °C; IR (KBr) 3061, 2923, 2852, 1663, 1564, 1512, 1457, 1377, 1258, 1172, 1102, 1029, 957, 822, 739 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.74 (d, *J* = 8.0 Hz, 1H), 8.51 (d, *J* = 8.0 Hz, 2H), 8.17 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 3.89 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 163.5, 163.4, 162.2, 157.5, 136.8, 136.5, 129.6, 129.2, 128.8, 128.7, 114.3, 113.8, 55.5 ppm; MS (EI, 70 eV) *m/z* 296.25, 281.21, 265.22, 253.21, 218.23, 159.21, 148.18, 132.16, 117.16; HRMS (ESI) calcd C₁₇H₁₄ClN₂O [M + H]⁺ *m/z* 297.0789, found *m/z* 297.0789.



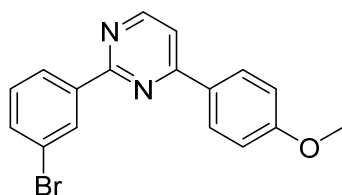
2-(4-Bromophenyl)-4-(4-methoxyphenyl)pyrimidine (3fa). Yellow solid: 76% yield (52 mg); mp 146–148 °C; IR (KBr) 3095, 2921, 2853, 1564, 1512, 1459, 1374, 1254, 1175, 1112, 1025, 957, 825, 743 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.72 (d, *J* = 4.0 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 2H), 8.16 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 4.0 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 3.87 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 163.5, 163.5, 162.2, 157.5, 136.9, 131.7, 129.9, 129.1, 128.8, 125.4, 114.3, 113.9, 55.5 ppm; MS (EI, 70 eV) *m/z* 340.20, 325.19, 297.18, 261.25, 218.22, 207.20, 183.10, 171.15, 159.22, 132.19, 117.16, 102.15, 89.16; HRMS (ESI) calcd C₁₇H₁₄BrN₂O [M + H]⁺ *m/z* 341.0284, found *m/z* 341.0288.



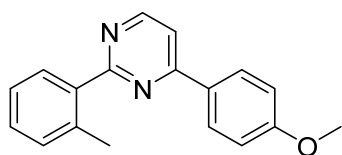
4-(4-Methoxyphenyl)-2-(4-nitrophenyl)pyrimidine (3ga). Yellow solid: 66% yield (41 mg); mp 153–155 °C; IR (KBr) 3109, 2918, 2851, 1566, 1515, 1444, 1345, 1250, 1181, 1105, 1025, 949, 864, 817, 749 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.78 (d, J = 8.0 Hz, 1H), 8.71 (d, J = 8.0 Hz, 2H), 8.31 (d, J = 8.0 Hz, 2H), 8.17 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 8.0 Hz, 1H), 7.04 (d, J = 8.0 Hz, 2H), 3.90 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 163.7, 162.4, 162.3, 157.7, 149.2, 143.8, 129.1, 128.8, 128.7, 123.6, 114.6, 114.4, 55.5 ppm; MS (EI, 70 eV) m/z 307.25, 277.24, 261.25, 218.22, 192.18, 159.19, 132.16, 117.14, 102.13, 89.13; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{13}\text{N}_3\text{NaO}_3$ $[\text{M} + \text{Na}]^+$ m/z 330.0849, found m/z 330.0857.



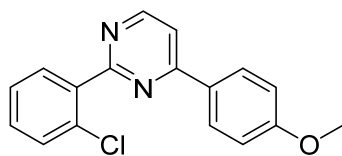
4-(4-Methoxyphenyl)-2-(m-tolyl)pyrimidine (3ha). White solid: 77% yield (43 mg); mp 93–95 °C; IR (KBr) 3067, 2924, 2853, 1562, 1513, 1420, 1252, 1175, 1028, 823, 699 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.75 (d, J = 4.0 Hz, 1H), 8.37 (s, 2H), 8.19 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 4.0 Hz, 1H), 7.42–7.38 (m, 1H), 7.31 (d, J = 4.0 Hz, 1H), 7.02 (d, J = 8.0 Hz, 2H), 3.88 (s, 3H), 2.47 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.6, 163.4, 162.1, 157.5, 138.1, 138.0, 131.4, 129.5, 128.8, 128.8, 128.5, 125.5, 114.3, 113.6, 55.4, 21.6 ppm; MS (EI, 70 eV) m/z 276.28, 245.26, 207.17, 191.19, 159.18, 138.19, 132.18, 117.15, 89.14; HRMS (ESI) calcd $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 277.1335, found m/z 277.1334.



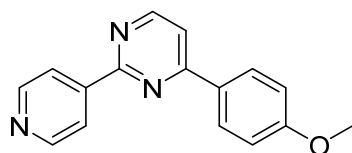
2-(3-Bromophenyl)-4-(4-methoxyphenyl)pyrimidine (3ia). Yellow solid: 67% yield (46 mg); mp 113–115 °C; IR (KBr) 3075, 2923, 2853, 1554, 1511, 1412, 1296, 1251, 1174, 1025, 823, 774 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.71 (d, J = 8.0 Hz, 2H), 8.48 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 4.0 Hz, 1H), 7.48 (d, J = 8.0 Hz, 1H), 7.37–7.33 (m, 1H), 7.02–6.99 (m, 2H), 3.86 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 163.5, 163.0, 162.2, 157.5, 140.1, 133.5, 131.3, 130.0, 129.0, 128.8, 126.8, 122.8, 114.3, 114.1, 55.4 ppm; MS (EI, 70 eV) m/z 340.21, 325.15, 299.17, 261.25, 218.21, 181.06, 159.19, 132.15, 117.15, 102.13, 89.14; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{14}\text{BrN}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 341.0284, found m/z 341.0285.



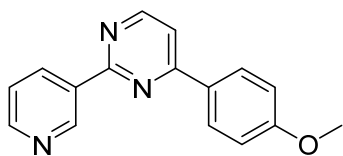
4-(4-Methoxyphenyl)-2-(o-tolyl)pyrimidine (3ja). Colorless oil: 69% yield (38 mg); IR (KBr) 3018, 2925, 2850, 1561, 1510, 1423, 1377, 1252, 1175, 1031, 826, 758 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.79 (d, J = 4.0 Hz, 1H), 8.14 (d, J = 8.0 Hz, 2H), 7.93 (d, J = 4.0 Hz, 1H), 7.52 (d, J = 4.0 Hz, 1H), 7.35–7.30 (m, 3H), 7.00 (d, J = 8.0 Hz, 2H), 3.86 (s, 3H), 2.64 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 167.5, 163.1, 162.1, 157.3, 138.5, 137.4, 131.3, 130.6, 129.3, 128.8, 125.9, 114.3, 113.0, 55.4, 21.4 ppm; MS (EI, 70 eV) m/z 276.28, 245.26, 207.17, 191.19, 159.18, 138.19, 132.18, 117.15, 89.14; HRMS (ESI) calcd $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 277.1335, found m/z 277.1332.



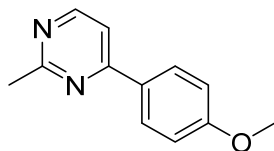
2-(2-Chlorophenyl)-4-(4-methoxyphenyl)pyrimidine (3ka). Colorless oil: 66% yield (39 mg); IR (KBr) 3069, 2922, 2851, 1566, 1511, 1419, 1296, 1251, 1175, 1120, 1029, 826, 755 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.82 (d, $J = 4.0$ Hz, 1H), 8.16 (d, $J = 8.0$ Hz, 2H), 7.87–7.85 (m, 1H), 7.58 (d, $J = 4.0$ Hz, 1H), 7.53–7.51 (m, 1H), 7.39–7.37 (m, 2H), 7.01 (d, $J = 8.0$ Hz, 2H), 3.86 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 165.3, 163.5, 162.2, 157.3, 138.0, 132.9, 131.9, 130.7, 130.3, 129.1, 129.0, 126.8, 114.4, 113.8, 55.4 ppm; MS (EI, 70 eV) m/z 296.21, 281.19, 261.25, 246.23, 218.20, 189.12, 159.19, 148.18, 132.13, 117.14, 102.11, 89.10; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{14}\text{ClN}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 297.0789, found m/z 297.0791.



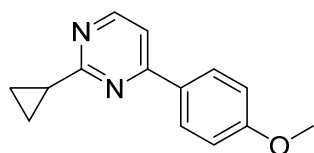
4-(4-Methoxyphenyl)-2-(pyridin-4-yl)pyrimidine (3la). White solid: 61% yield (32 mg); mp 128–130 $^{\circ}\text{C}$; IR (KBr) 3073, 2922, 2851, 1577, 1550, 1510, 1417, 1292, 1252, 1177, 1119, 1024, 826, 783, 648 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.79–8.78 (m, 3H), 8.40 (d, $J = 4.0$ Hz, 2H), 8.20–8.17 (m, 2H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.04 (d, $J = 8.0$ Hz, 2H), 3.89 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 163.7, 162.4, 162.4, 157.7, 150.3, 145.4, 128.8, 128.7, 122.1, 115.0, 114.4, 55.5 ppm; MS (EI, 70 eV) m/z 263.24, 248.21, 220.22, 192.18, 159.19, 132.05, 117.14, 104.13, 89.12; HRMS (ESI) calcd $\text{C}_{16}\text{H}_{14}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ m/z 264.1131, found m/z 264.1130.



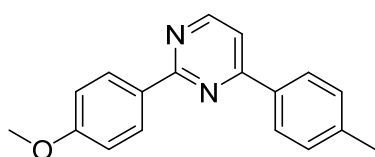
4-(4-Methoxyphenyl)-2-(pyridin-3-yl)pyrimidine (3ma). White solid: 44% yield (23 mg); mp 58–60 °C; IR (KBr) 3063, 2924, 2852, 1581, 1513, 1411, 1294, 1253, 1180, 1118, 1029, 827, 785, 707 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 9.75 (s, 1H), 8.81–8.71 (m, 3H), 8.18 (d, J = 8.0 Hz, 2H), 7.56 (d, J = 8.0 Hz, 1H), 7.45–7.42 (m, 1H), 7.04 (d, J = 8.0 Hz, 2H), 3.89 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 163.6, 162.6, 162.3, 157.7, 151.1, 149.9, 135.6, 133.6, 128.9, 128.8, 123.4, 114.4, 114.3, 55.5 ppm; MS (EI, 70 eV) m/z 263.28, 248.23, 220.23, 193.20, 159.18, 132.05, 115.61, 104.12, 89.13; HRMS (ESI) calcd $\text{C}_{16}\text{H}_{14}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ m/z 264.1131, found m/z 264.1128.



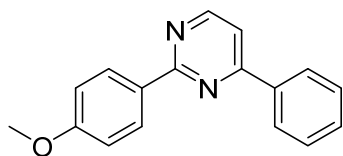
4-(4-Methoxyphenyl)-2-methylpyrimidine (3na). White solid: 65% yield (26 mg); mp 110–112 °C; IR (KBr) 3064, 2922, 2850, 1577, 1511, 1431, 1305, 1256, 1177, 1106, 1025, 822, 774 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.59 (d, J = 8.0 Hz, 1H), 8.05 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 4.0 Hz, 1H), 7.00 (d, J = 8.0 Hz, 2H), 3.87 (s, 3H), 2.77 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 168.2, 163.6, 162.0, 157.1, 129.3, 128.7, 114.3, 113.1, 55.4, 26.3 ppm; MS (EI, 70 eV) m/z 200.26, 185.21, 159.20, 132.14, 117.15, 89.14; HRMS (ESI) calcd $\text{C}_{12}\text{H}_{13}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 201.1022, found m/z 201.1028.



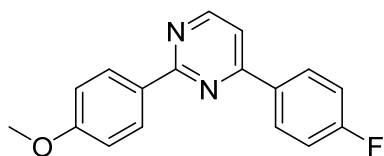
2-Cyclopropyl-4-(4-methoxyphenyl)pyrimidine (30a). Colorless oil: 69% yield (31 mg); IR (KBr) 3006, 2927, 2845, 1568, 1511, 1441, 1360, 1301, 1253, 1178, 1114, 1031, 918, 822 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.50 (d, $J = 8.0$ Hz, 1H), 8.04 (d, $J = 8.0$ Hz, 2H), 7.34 (d, $J = 4.0$ Hz, 1H), 6.97 (d, $J = 8.0$ Hz, 2H), 3.85 (s, 3H), 2.32–2.26 (m, 1H), 1.21–1.20 (m, 2H), 1.07–1.06 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 171.9, 163.0, 161.9, 156.9, 129.4, 128.6, 114.2, 112.6, 55.4, 18.3, 10.6 ppm; MS (EI, 70 eV) m/z 225.25, 210.22, 200.23, 182.21, 155.18, 133.16, 118.15, 89.14; HRMS (ESI) calcd $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 227.1179, found m/z 227.1177.



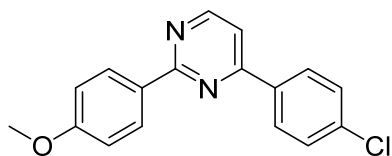
2-(4-Methoxyphenyl)-4-(p-tolyl)pyrimidine (3bb). White solid: 84% yield (46 mg); mp 117–119 $^{\circ}\text{C}$; IR (KBr) 3025, 2922, 2854, 1557, 1405, 1303, 1248, 1171, 1029, 806 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.73 (d, $J = 8.0$ Hz, 1H), 8.53 (d, $J = 8.0$ Hz, 2H), 8.09 (d, $J = 8.0$ Hz, 2H), 7.47 (d, $J = 8.0$ Hz, 1H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.01 (d, $J = 8.0$ Hz, 2H), 3.87 (s, 3H), 2.42 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.3, 163.7, 161.9, 157.6, 141.3, 134.3, 130.7, 130.0, 129.6, 127.1, 113.9, 113.5, 55.4, 21.5 ppm; MS (EI, 70 eV) m/z 276.33, 261.27, 233.27, 138.14, 115.18; HRMS (ESI) calcd $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 277.1335, found m/z 277.1335.



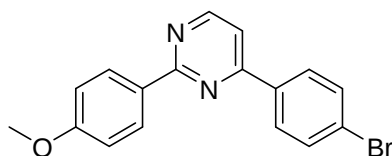
2-(4-Methoxyphenyl)-4-phenylpyrimidine (3bc).^[1] White solid: 86% yield (45 mg); mp 83–85 °C; IR (KBr) 3015, 2921, 2849, 1555, 1417, 1385, 1300, 1249, 1169, 1028, 834, 768, 691 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.75 (d, J = 8.0 Hz, 1H), 8.53 (d, J = 8.0 Hz, 2H), 8.19 (J = 8.0 Hz, 2H), 7.51–7.48 (m, 4H), 7.01 (d, J = 8.0 Hz, 2H), 3.86 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 164.4, 163.7, 161.9, 157.7, 137.1, 130.9, 130.6, 130.0, 128.9, 127.2, 113.9, 113.8, 55.4 ppm; MS (EI, 70 eV) m/z 262.31, 247.24, 219.25, 133.17, 102.14; HRMS (ESI) calcd C₁₇H₁₅N₂O [M + H]⁺ m/z 263.1179, found m/z 263.1178.



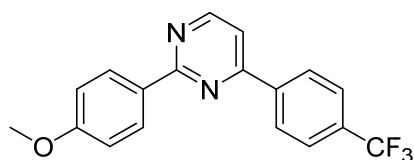
4-(4-Fluorophenyl)-2-(4-methoxyphenyl)pyrimidine (3bd). White solid: 91% yield (51 mg); mp 108–110 °C; IR (KBr) 3021, 2921, 2850, 1554, 1407, 1301, 1243, 1160, 1025, 820 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.72 (d, J = 8.0 Hz, 1H), 8.50 (d, J = 8.0 Hz, 2H), 8.19–8.16 (m, 2H), 7.42 (d, J = 8.0 Hz, 1H), 7.19–7.15 (m, 2H), 7.00 (d, J = 8.0 Hz, 2H), 3.86 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 164.9 (d, J = 249 Hz), 164.3, 162.6, 162.0, 157.8, 133.2 (d, J = 3.0 Hz), 130.5, 129.2, 129.2, 115.9 (d, J = 32 Hz), 113.9, 113.4, 55.4 ppm; MS (EI, 70 eV) m/z 280.30, 265.22, 237.24, 140.16, 133.14, 120.13, 103.14; HRMS (ESI) calcd C₁₇H₁₄FN₂O [M + H]⁺ m/z 281.1085, found m/z 281.1088.



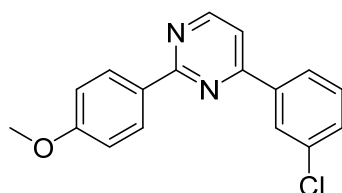
4-(4-Chlorophenyl)-2-(4-methoxyphenyl)pyrimidine (3be). Pale yellow solid: 88% yield (52 mg); mp 127–129 °C; IR (KBr) 3020, 2921, 2853, 1659, 1555, 1413, 1303, 1249, 1169, 1027, 814, 732 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.74 (d, J = 8.0 Hz, 1H), 8.50 (d, J = 8.0 Hz, 2H), 8.11 (d, J = 8.0 Hz, 2H), 7.47–7.42 (m, 3H), 7.01 (d, J = 8.0 Hz, 2H), 3.87 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.4, 162.5, 162.0, 157.9, 137.1, 135.5, 130.4, 130.0, 129.1, 128.4, 113.9, 113.5, 55.4 ppm; MS (EI, 70 eV) m/z 296.26, 281.23, 253.24, 218.24, 185.21, 148.20, 133.18, 103.17; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{14}\text{ClN}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 297.0789, found m/z 297.0795.



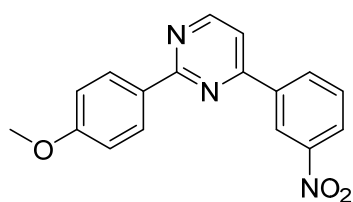
4-(4-Bromophenyl)-2-(4-methoxyphenyl)pyrimidine (3bf). Yellow solid: 86% yield (58 mg); mp 150–152 °C; IR (KBr) 3051, 2921, 2851, 1651, 1554, 1414, 1371, 1303, 1249, 1172, 1107, 1027, 815, 728, 654 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.74 (d, J = 8.0 Hz, 1H), 8.50 (d, J = 8.0 Hz, 2H), 8.04 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 8.0 Hz, 1H), 7.01 (d, J = 8.0 Hz, 2H), 3.87 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.4, 162.6, 162.0, 157.9, 136.0, 132.1, 130.3, 130.0, 128.7, 125.5, 113.9, 113.4, 55.4 ppm; MS (EI, 70 eV) m/z 340.22, 325.20, 299.19, 261.28, 218.27, 180.09, 170.19, 133.18, 101.17; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{14}\text{BrN}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 341.0284, found m/z 341.0285.



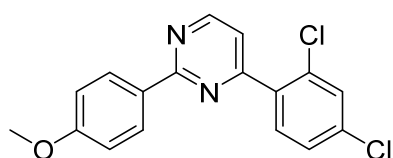
2-(4-Methoxyphenyl)-4-(4-(trifluoromethyl)phenyl)pyrimidine (3bg)^[2] White solid: 90% yield (59 mg); mp 145–147 °C; IR (KBr) 3060, 2923, 2851, 1601, 1554, 1459, 1376, 1324, 1253, 1128, 1027, 828, 706, 650 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.76 (d, J = 4.0 Hz, 1H), 8.50 (d, J = 8.0 Hz, 2H), 8.25 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 4.0 Hz, 1H), 7.01 (d, J = 8.0 Hz, 2H), 3.86 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 164.5, 162.2, 162.1, 158.1, 140.5, 132.43 (dd, J = 32.0 Hz), 130.2, 130.0, 127.5, 125.8 (dd, J = 4.0 Hz), 124.0 (d, J = 270.0 Hz), 114.0, 113.9, 55.4 ppm; MS (EI, 70 eV) m/z 330.30, 315.22, 287.27, 185.20, 170.17, 165.28, 133.12, 103.14; HRMS (ESI) calcd C₁₈H₁₄F₃N₂O [M + H]⁺ m/z 331.1053, found m/z 331.1054.



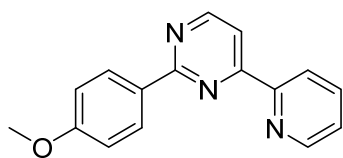
4-(3-Chlorophenyl)-2-(4-methoxyphenyl)pyrimidine (3bh). Pale yellow solid: 83% yield (49 mg); mp 68–70 °C; IR (KBr) 3020, 2921, 2849, 1552, 1414, 1302, 1249, 1169, 1028, 834, 785, 677 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.76 (d, J = 8.0 Hz, 1H), 8.51 (d, J = 8.0 Hz, 2H), 8.19 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.47–7.40 (m, 3H), 7.01 (d, J = 8.0 Hz, 2H), 3.87 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 164.5, 162.3, 162.0, 158.0, 138.9, 135.1, 130.8, 130.3, 130.1, 130.0, 127.3, 125.2, 113.9, 113.8, 55.4 ppm; MS (EI, 70 eV) m/z 296.30, 281.25, 253.25, 218.26, 133.18, 103.17; HRMS (ESI) calcd C₁₇H₁₄ClN₂O [M + H]⁺ m/z 297.0789, found m/z 297.0794.



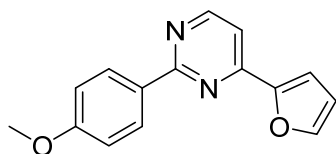
2-(4-Methoxyphenyl)-4-(3-nitrophenyl)pyrimidine (3bi). Yellow solid: 81% yield (50 mg); mp 165–167 °C; IR (KBr) 3089, 2917, 2849, 1562, 1511, 1408, 1338, 1241, 1077, 1015, 890, 797, 731, 645 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 9.03 (s, 1H), 8.87 (d, $J = 8.0$ Hz, 1H), 8.55–8.52 (m, 3H), 8.37 (d, $J = 8.0$ Hz, 1H), 7.74–7.70 (m, 1H), 7.58 (d, $J = 8.0$ Hz, 1H), 7.04 (d, $J = 8.0$ Hz, 2H), 3.91 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.7, 162.2, 161.2, 158.4, 148.9, 138.9, 132.8, 130.0, 129.9, 129.9, 125.3, 122.1, 114.0, 113.8, 55.4 ppm; MS (EI, 70 eV) m/z 307.30, 292.29, 261.30, 246.25, 218.26, 207.22, 191.24, 164.21, 133.19, 101.17; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{13}\text{N}_3\text{NaO}_3$ $[\text{M} + \text{Na}]^+$ m/z 330.0849, found m/z 330.0856.



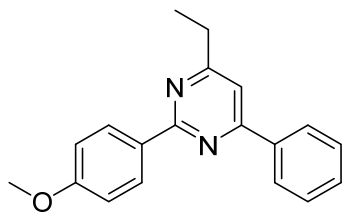
4-(2,4-Dichlorophenyl)-2-(4-methoxyphenyl)pyrimidine (3bj). Yellow solid: 92% yield (61 mg); mp 124–126 °C; IR (KBr) 3026, 2916, 2847, 1646, 1551, 1418, 1302, 1244, 1163, 1098, 1033, 800 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.79 (d, $J = 8.0$ Hz, 1H), 8.46 (d, $J = 8.0$ Hz, 2H), 7.54 (d, $J = 8.0$ Hz, 1H), 7.52–7.50 (m, 2H), 7.40 (d, $J = 8.0$ Hz, 1H), 6.99 (d, $J = 8.0$ Hz, 2H), 3.87 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.6, 162.7, 162.0, 157.1, 136.1, 135.7, 133.2, 132.6, 130.3, 130.2, 130.0, 127.6, 118.5, 113.9, 55.4 ppm; MS (EI, 70 eV) m/z 330.23, 315.20, 295.24, 252.21, 216.23, 170.11, 133.19, 103.16; HRMS (ESI) calcd $\text{C}_{17}\text{H}_{13}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 331.0399, found m/z 331.0401.



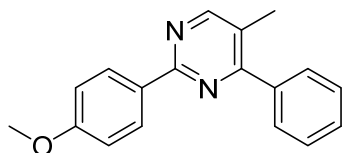
2-(4-Methoxyphenyl)-4-(pyridin-2-yl)pyrimidine (3bk). White solid: 83% yield (44 mg); mp 110–112 °C; IR (KBr) 3066, 2923, 2853, 1552, 1387, 1304, 1247, 1169, 1028, 841, 782 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.85 (d, $J = 8.0$ Hz, 1H), 8.70 (d, $J = 8.0$ Hz, 1H), 8.64 (d, $J = 8.0$ Hz, 1H), 8.53 (d, $J = 8.0$ Hz, 2H), 8.15 (d, $J = 8.0$ Hz, 1H), 7.86–7.82 (m, 1H), 7.38–7.35 (m, 1H), 7.01 (d, $J = 8.0$ Hz, 2H), 3.86 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.1, 162.7, 161.9, 158.3, 154.4, 149.4, 137.0, 130.5, 129.9, 125.3, 121.7, 114.3, 113.9, 55.4 ppm; MS (EI, 70 eV) m/z 263.30, 236.26, 220.24, 185.21, 133.20, 103.17; HRMS (ESI) calcd $\text{C}_{16}\text{H}_{13}\text{N}_3\text{NaO}$ $[\text{M} + \text{Na}]^+$ m/z 286.0951, found m/z 286.0955.



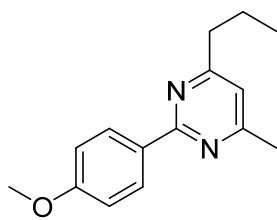
4-(Furan-2-yl)-2-(4-methoxyphenyl)pyrimidine (3bl). White solid: 76% yield (38 mg); mp 65–67 °C; IR (KBr) 3116, 2926, 2851, 1596, 1554, 1477, 1402, 1306, 1249, 1168, 1020, 828, 748, 682 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.73 (d, $J = 8.0$ Hz, 1H), 8.46 (d, $J = 8.0$ Hz, 2H), 7.59 (s, 1H), 7.39 (d, $J = 8.0$ Hz, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 6.58 (s, 1H), 3.87 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.3, 161.9, 157.7, 155.4, 152.3, 144.9, 130.4, 129.9, 113.8, 112.5, 112.2, 111.7, 55.4 ppm; MS (EI, 70 eV) m/z 252.27, 237.21, 223.25, 209.21, 180.22, 126.19, 103.17, 92.14; HRMS (ESI) calcd $\text{C}_{15}\text{H}_{13}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}]^+$ m/z 253.0972, found m/z 253.0975.



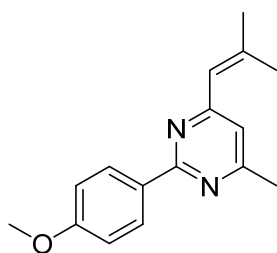
4-Ethyl-2-(4-methoxyphenyl)-6-phenylpyrimidine (bm). Colorless oil: 77% yield (45 mg); IR (KBr) 3066, 2926, 2853, 1578, 1528, 1454, 1375, 1304, 1248, 1170, 1030, 844, 768, 689 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.57 (d, $J = 8.0$ Hz, 2H), 8.18 (d, $J = 8.0$ Hz, 2H), 7.50–7.49 (m, 3H), 7.37 (s, 1H), 7.00 (d, $J = 8.0$ Hz, 2H), 3.86 (s, 3H), 2.88 (q, $J = 6.0$ Hz, 2H), 1.40 (t, q, $J = 6.0$ Hz, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 172.4, 164.0, 163.7, 161.7, 137.7, 131.1, 130.5, 130.0, 128.8, 127.2, 113.8, 112.1, 55.4, 31.3, 12.9 ppm; MS (EI, 70 eV) m/z 290.37, 274.28, 246.29, 145.24, 134.17, 102.14; HRMS (ESI) calcd $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 291.1492, found m/z 291.1496.



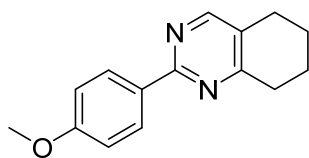
2-(4-Methoxyphenyl)-5-methyl-4-phenylpyrimidine (3bn). White solid: 79% yield (44 mg); mp 98–100 $^{\circ}\text{C}$; IR (KBr) 3194, 2923, 2851, 1572, 1419, 1303, 1246, 1098, 1024, 929, 846, 772, 694 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.58 (s, 1H), 8.45 (d, $J = 8.0$ Hz, 2H), 7.70 (d, $J = 8.0$ Hz, 2H), 7.50–7.42 (m, 3H), 6.97 (d, $J = 8.0$ Hz, 2H), 3.83 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 164.7, 162.3, 161.6, 159.1, 138.6, 130.6, 129.6, 129.2, 129.1, 128.3, 124.8, 113.8, 55.4, 17.0 ppm; MS (EI, 70 eV) m/z 275.30, 260.24, 232.25, 206.24, 133.13, 115.15, 103.13; HRMS (ESI) calcd $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 277.1335, found m/z 277.1336.



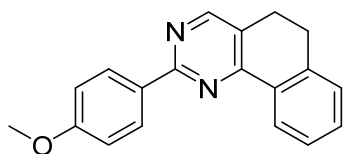
2-(4-Methoxyphenyl)-4-methyl-6-propylpyrimidine (3bo). Colorless oil: 80% yield (39 mg); IR (KBr) 3068, 2929, 2859, 1590, 1530, 1453, 1376, 1249, 1171, 1030, 957, 844, 792 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.40 (d, $J = 8.0$ Hz, 2H), 6.97 (d, $J = 8.0$ Hz, 2H), 6.84 (s, 1H), 3.87 (s, 3H), 2.72 (t, $J = 6.0$ Hz, 2H), 2.52 (s, 3H), 1.84–1.78 (m, 2H), 1.00 (t, $J = 6.0$ Hz, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 170.3, 166.5, 163.8, 161.5, 131.0, 129.8, 116.7, 113.7, 55.3, 39.8, 24.2, 22.0, 13.9 ppm; MS (EI, 70 eV) m/z 242.32, 227.27, 214.27, 184.27, 172.24, 134.20, 107.19; HRMS (ESI) calcd $\text{C}_{15}\text{H}_{19}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 243.1492, found m/z 243.1488.



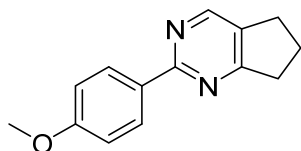
2-(4-Methoxyphenyl)-4-methyl-6-(2-methylprop-1-en-1-yl)pyrimidine (3bp). Colorless oil: 71% yield (36 mg); IR (KBr) 3069, 2922, 2853, 1651, 1578, 1522, 1451, 1374, 1305, 1168, 1032, 847, 792 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.41 (d, $J = 8.0$ Hz, 2H), 6.98 (d, $J = 8.0$ Hz, 2H), 6.76 (s, 1H), 6.22 (s, 1H), 3.86 (s, 3H), 2.51 (s, 3H), 2.33 (s, 3H), 2.00 (s, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 166.7, 163.8, 163.5, 161.5, 146.3, 131.2, 129.8, 123.5, 117.0, 113.7, 55.3, 28.1, 24.3, 20.7 ppm; MS (EI, 70 eV) m/z 253.31, 239.28, 224.23, 196.22, 183.22, 134.15, 120.12, 106.15; HRMS (ESI) calcd $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 255.1492, found m/z 255.1493.



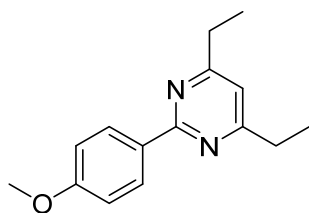
2-(4-Methoxyphenyl)-5,6,7,8-tetrahydroquinazoline (3bq). White solid: 88% yield (42 mg); mp 95–97 °C; IR (KBr) 3051, 2925, 2852, 1649, 1541, 1421, 1314, 1252, 1163, 1027, 953, 833, 773 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.38 (s, 1H), 8.34 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.0 Hz, 2H), 3.84 (s, 3H), 2.89 (t, J = 6.0 Hz, 2H), 2.71 (t, J = 6.0 Hz, 2H), 1.91–1.89 (m, 2H), 1.87–1.82 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 165.9, 161.8, 161.3, 157.0, 130.8, 129.4, 127.0, 113.8, 55.3, 32.1, 25.5, 22.4, 22.3 ppm; MS (EI, 70 eV) m/z 240.30, 225.25, 212.28, 186.24, 171.22, 155.20, 133.17, 120.19, 103.15; HRMS (ESI) calcd $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 241.1335, found m/z 241.1335.



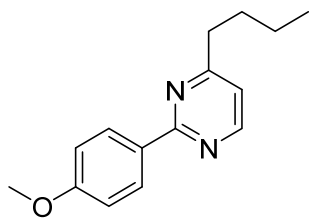
2-(4-Methoxyphenyl)-5,6-dihydrobenzo[h]quinazoline (3br). Yellow solid: 89% yield (51 mg); mp 124–126 °C; IR (KBr) 3065, 3008, 2928, 2844, 1585, 1419, 1295, 1250, 1167, 1104, 1031, 906, 847, 770, 732 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.51–8.48 (m, 4H), 7.39–7.37 (m, 2H), 7.23–7.21 (m, 1H), 7.01–6.98 (m, 2H), 3.85 (s, 3H), 2.97–2.93 (m, 2H), 2.90–2.86 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 163.0, 161.6, 159.1, 155.8, 139.3, 132.9, 131.0, 130.9, 129.6, 128.1, 127.3, 125.7, 125.2, 113.8, 55.4, 27.7, 24.3 ppm; MS (EI, 70 eV) m/z 288.36, 273.28, 260.27, 245.27, 229.23, 217.25, 186.23, 172.15, 144.19, 128.20, 102.13; HRMS (ESI) calcd $\text{C}_{19}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 289.1335, found m/z 289.1334.



2-(4-Methoxyphenyl)-6,7-dihydro-5H-cyclopenta[d]pyrimidine (3bs). White solid: 88% yield (40 mg); mp 99–101 °C; IR (KBr) 3079, 2918, 2843, 1590, 1538, 1461, 1422, 1381, 1309, 1244, 1175, 1107, 1028, 949, 897, 835, 786, 734 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.52 (s, 1H), 8.36 (d, $J = 8.0$ Hz, 2H), 6.97 (d, $J = 8.0$ Hz, 2H), 3.85 (s, 3H), 3.02 (d, $J = 7.5$ Hz, 2H), 2.94 (d, $J = 7.5$ Hz, 2H), 2.18–2.11 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 175.2, 163.0, 161.4, 152.0, 131.6, 130.8, 129.6, 113.8, 55.3, 34.2, 28.1, 22.7 ppm; MS (EI, 70 eV) m/z 226.27, 198.22, 183.19, 155.17, 133.09, 103.12; HRMS (ESI) calcd $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 227.1179, found m/z 227.1177.



4,6-Diethyl-2-(4-methoxyphenyl)pyrimidine (3bt). Colorless oil: 32% yield (15 mg); IR (KBr) 3118, 2922, 2853, 1649, 1540, 1461, 1379, 1250, 1172, 1032, 1024, 949, 847, 799 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.43 (d, $J = 8.0$ Hz, 2H), 6.97 (d, $J = 8.0$ Hz, 2H), 6.85 (s, 1H), 3.86 (s, 3H), 2.79 (t, $J = 6.0$ Hz, 4H), 2.79 (q, $J = 6.0$ Hz, 4H), 1.34 (t, $J = 6.0$ Hz, 6H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 171.50, 163.7, 161.5, 131.2, 129.8, 114.7, 113.7, 55.3, 31.0, 12.8 ppm; MS (EI, 70 eV) m/z 241.30, 226.26, 198.22, 185.19, 134.15, 103.12; HRMS (ESI) calcd $\text{C}_{15}\text{H}_{19}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 243.1492, found m/z 243.1492.

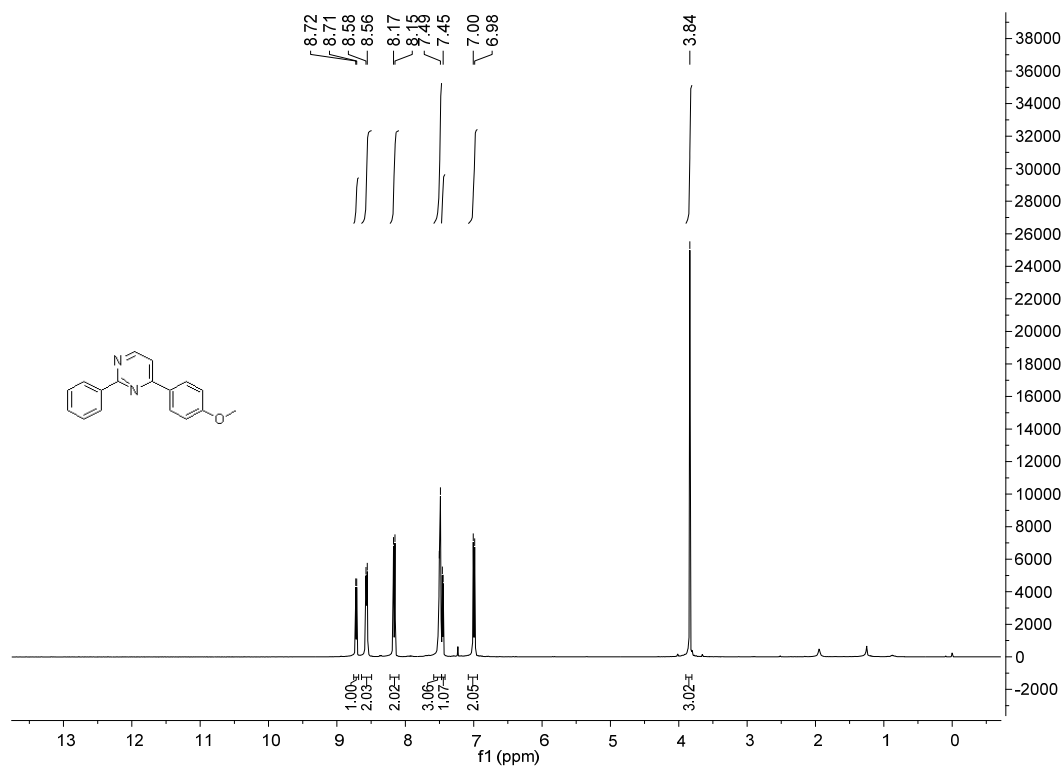


4-Butyl-2-(4-methoxyphenyl)pyrimidine (3bu). Colorless oil: 48% yield (23 mg); IR (KBr) 3077, 2925, 2856, 1556, 1513, 1451, 1387, 1250, 1169, 1030, 836, 753 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.59 (d, $J = 8.0$ Hz, 1H), 8.41 (d, $J = 8.0$ Hz, 2H), 7.00–6.94 (m, 3H), 3.86 (s, 3H), 2.78 (t, $J = 6.0$ Hz, 2H), 1.81–1.74 (m, 2H), 1.47–1.38 (m, 2H), 0.96 (q, $J = 6.0$ Hz, 3H) ppm; ^{13}C NMR (100 MHz, CDCl_3) δ 170.9, 164.0, 161.7, 156.7, 130.7, 129.8, 117.2, 113.8, 55.3, 37.7, 30.8, 22.4, 13.9 ppm; MS (EI, 70 eV) m/z 242.29, 227.26, 200.21, 170.19, 134.14, 103.14; HRMS (ESI) calcd $\text{C}_{15}\text{H}_{19}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ m/z 243.1492, found m/z 243.1493.

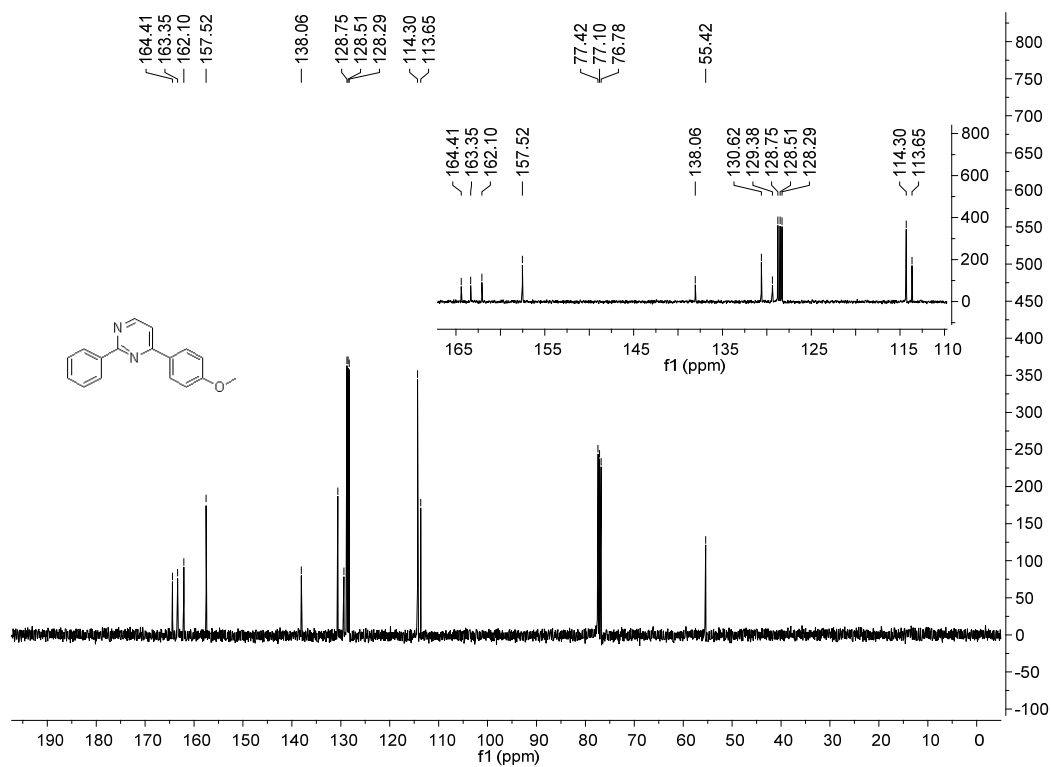
References:

- [1] W. Guo, C. Li, J. Liao, F. Ji, D. Liu, W. Wu, H. Jiang, *J. Org. Chem.* **2016**, *81*, 5538-5546.
- [2] J.-M. Begouin, M. Rivard, C. Gosmini, *Chem. Commun.* **2010**, *46*, 5972-5974.

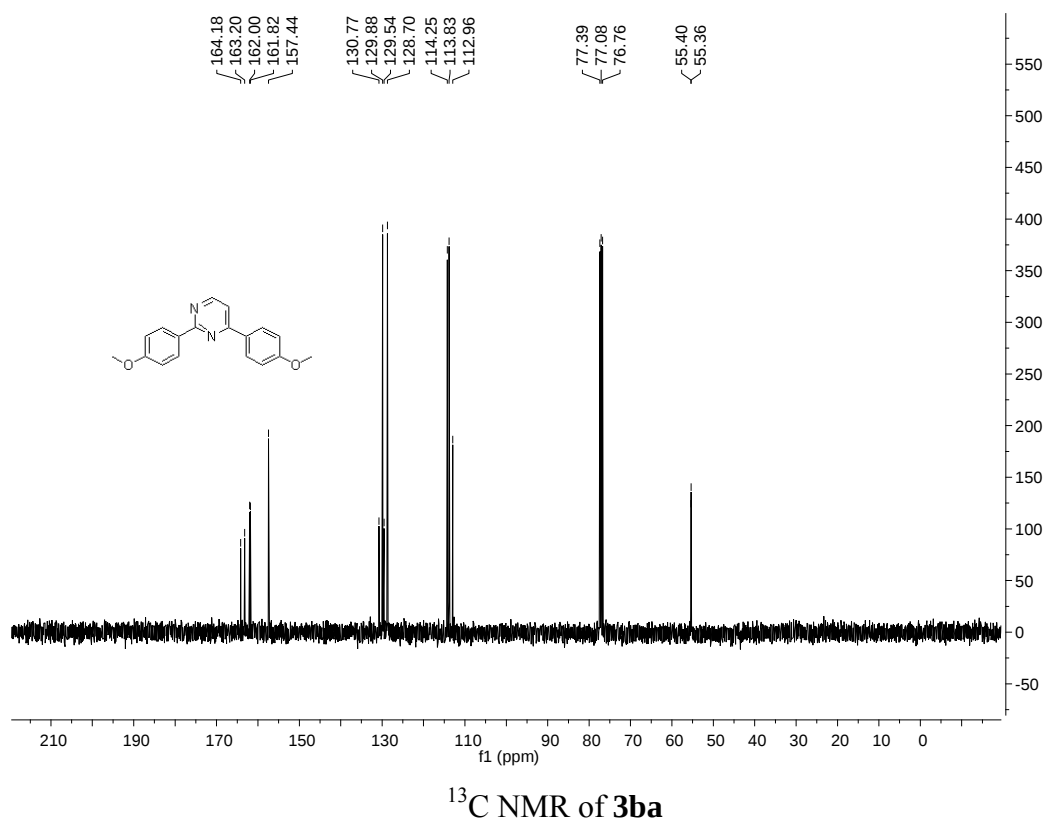
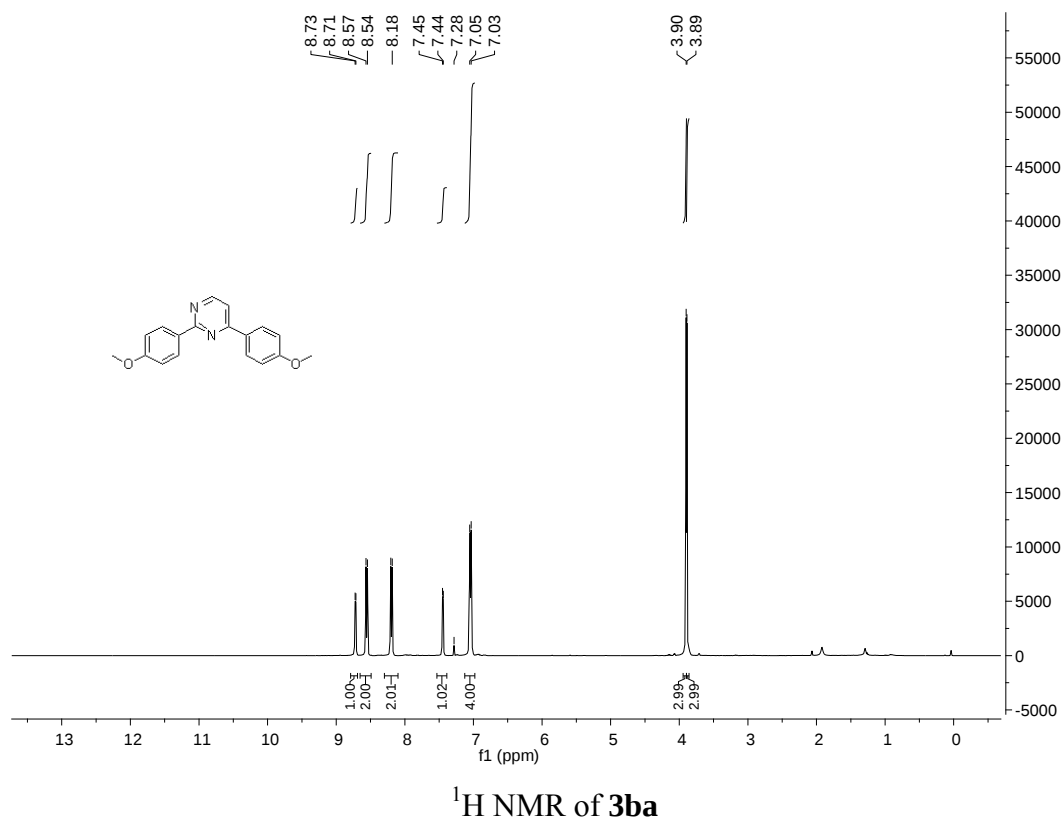
D. NMR Spectra

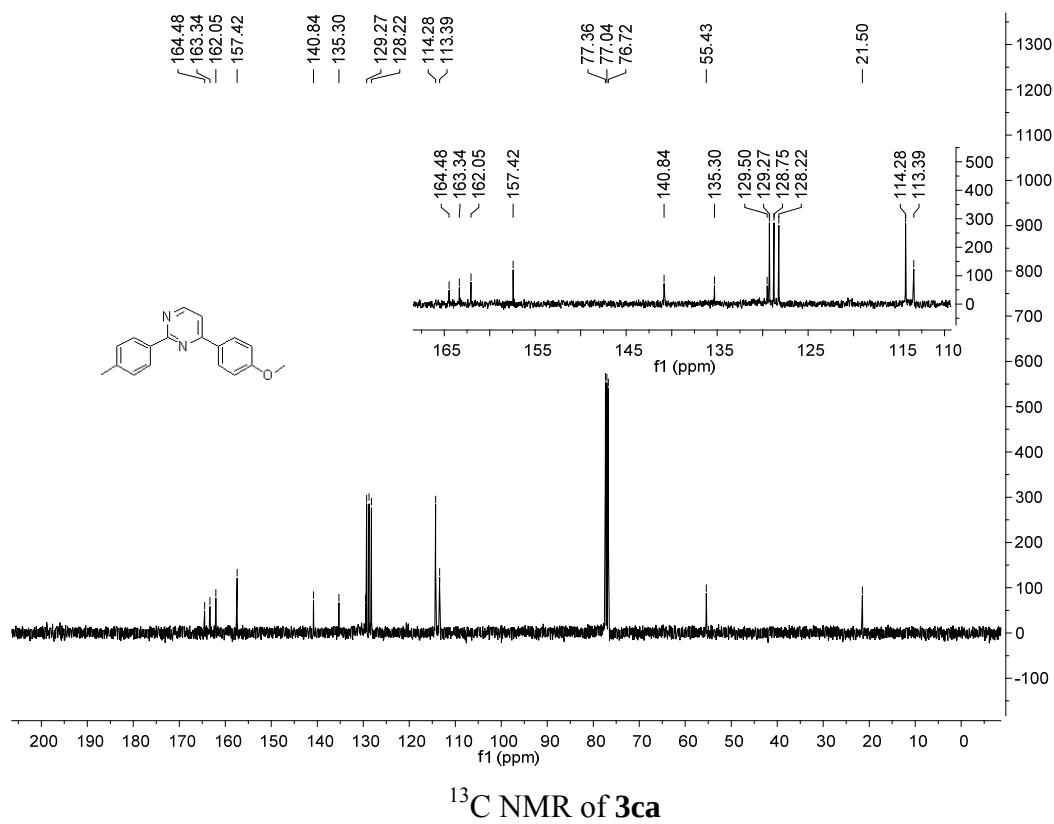
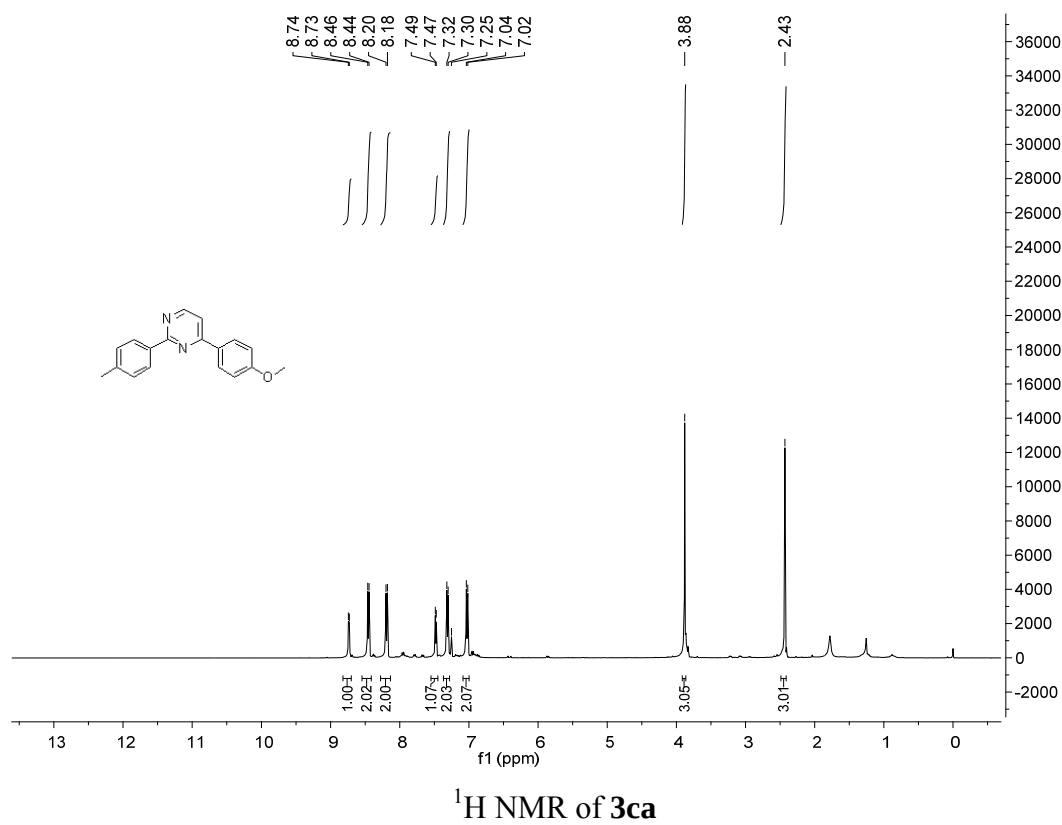


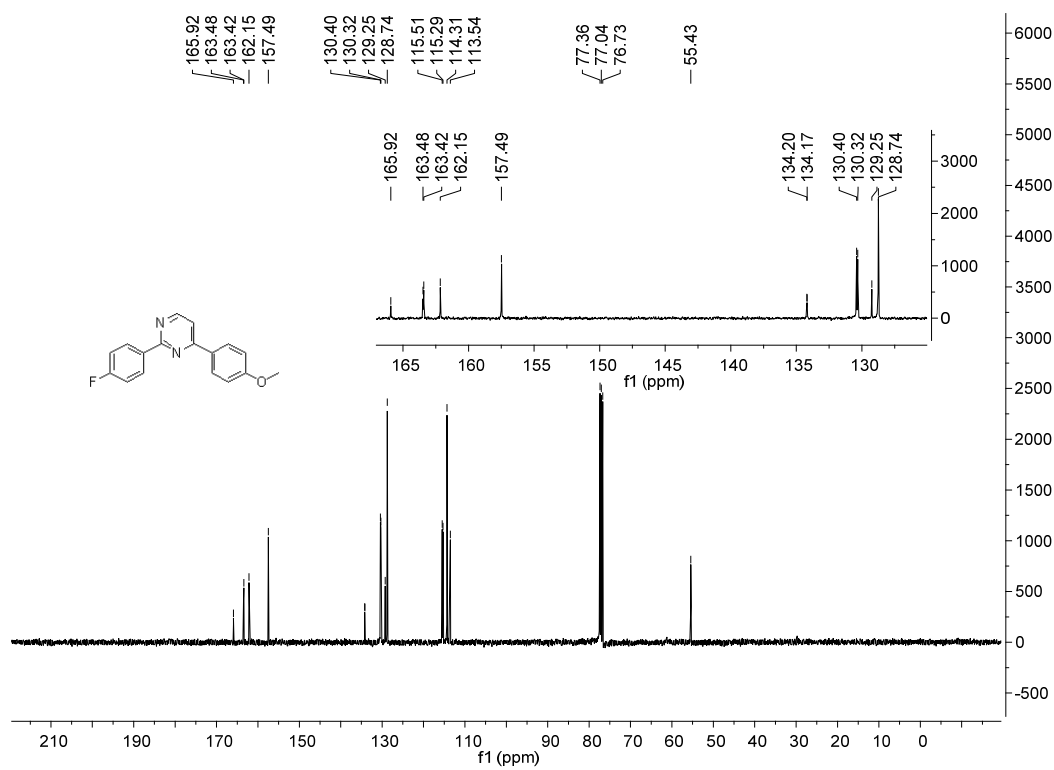
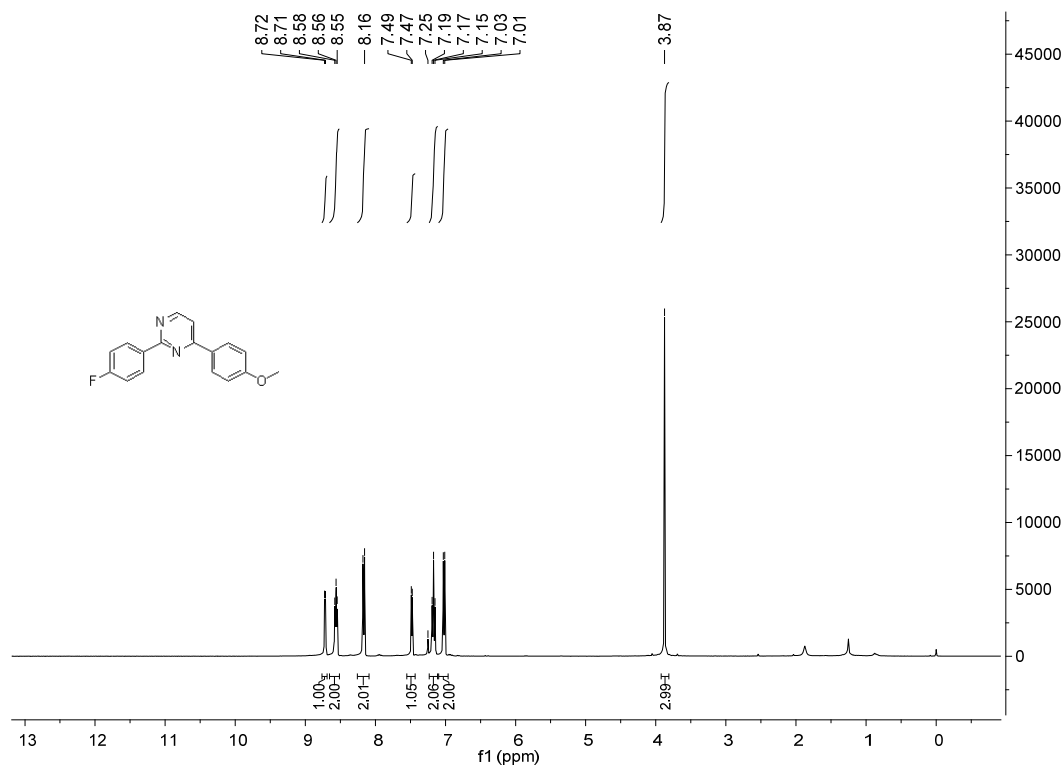
¹H NMR of **3aa**

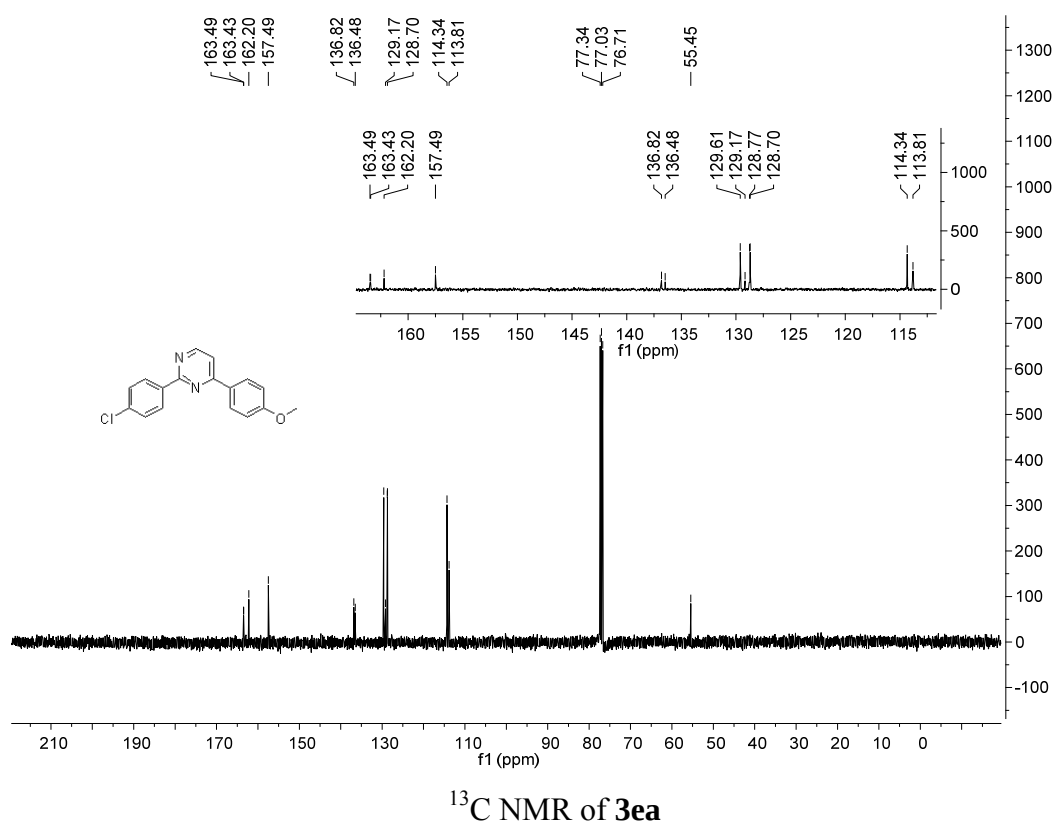
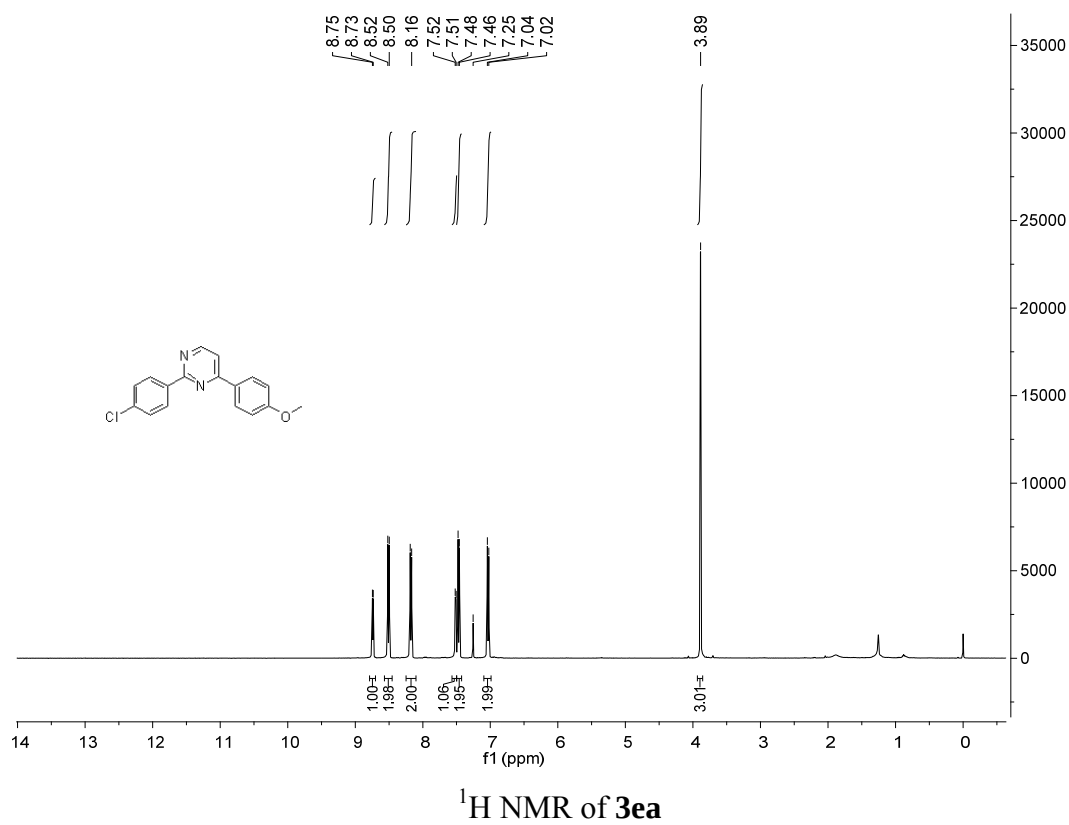


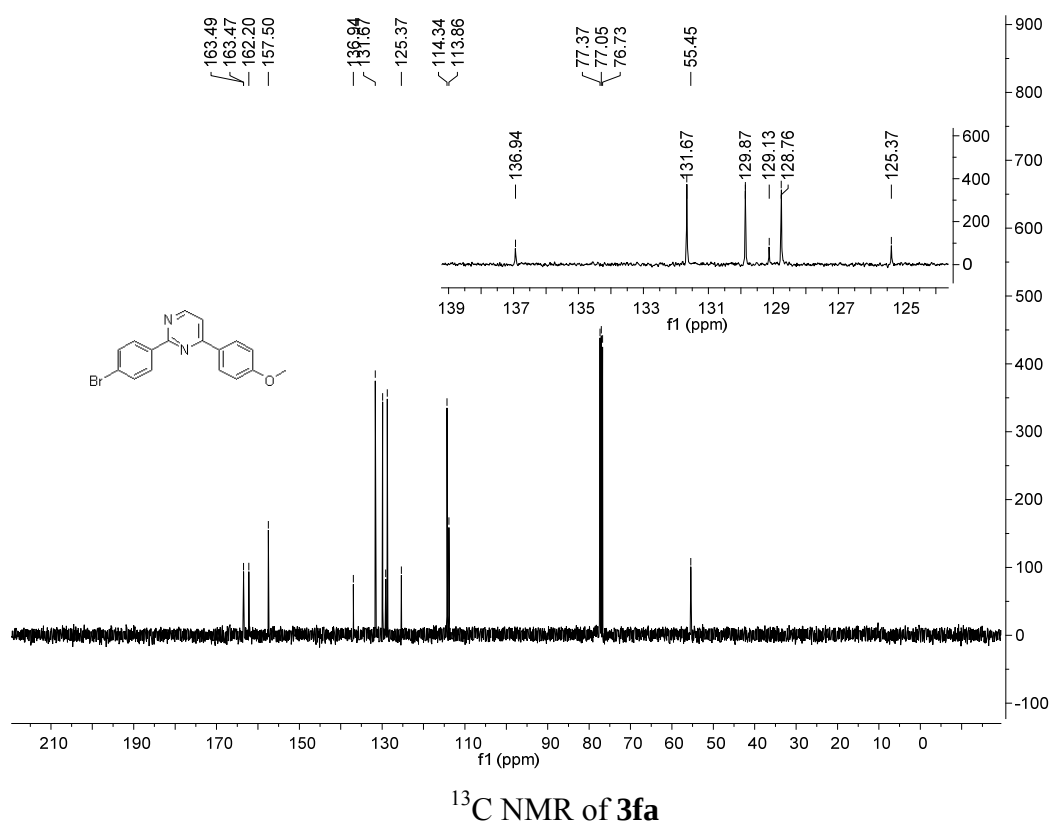
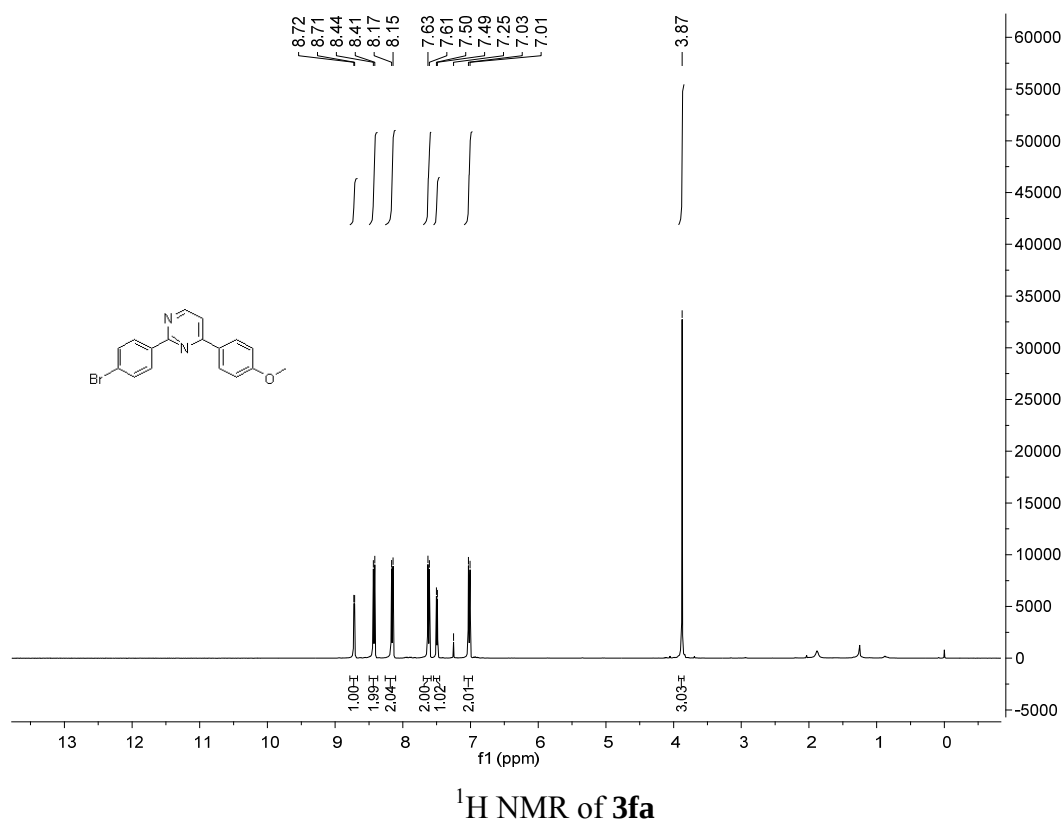
¹³C NMR of **3aa**

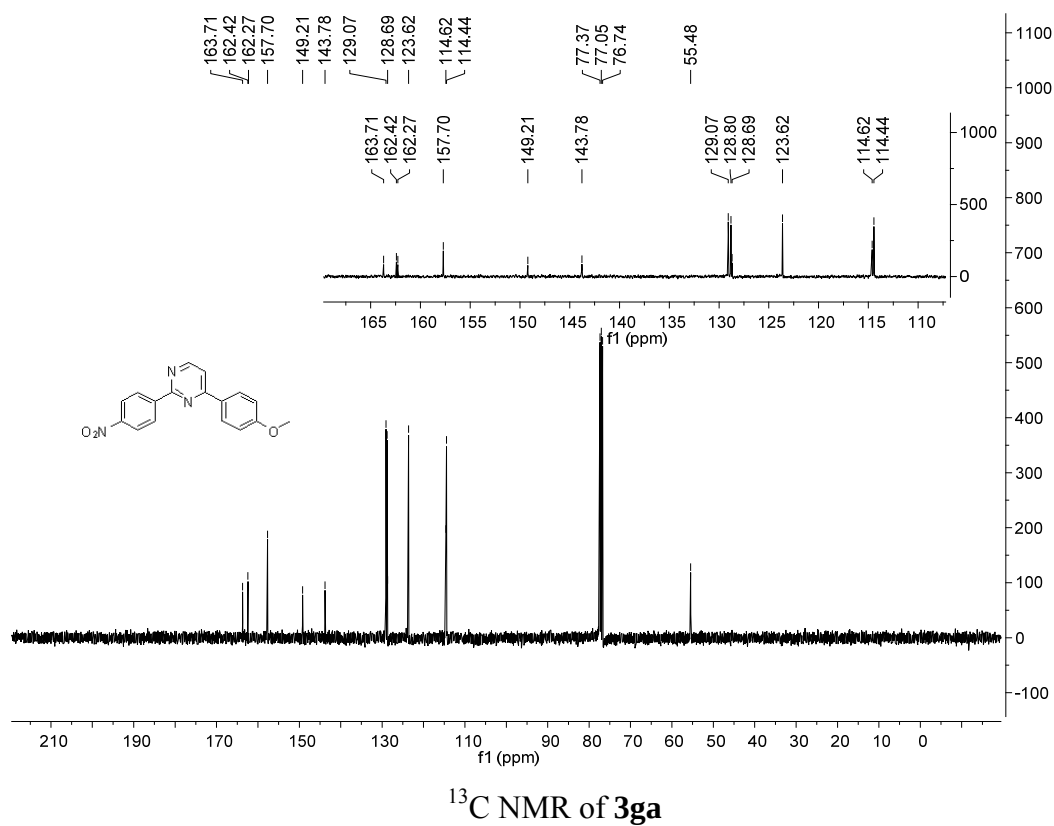
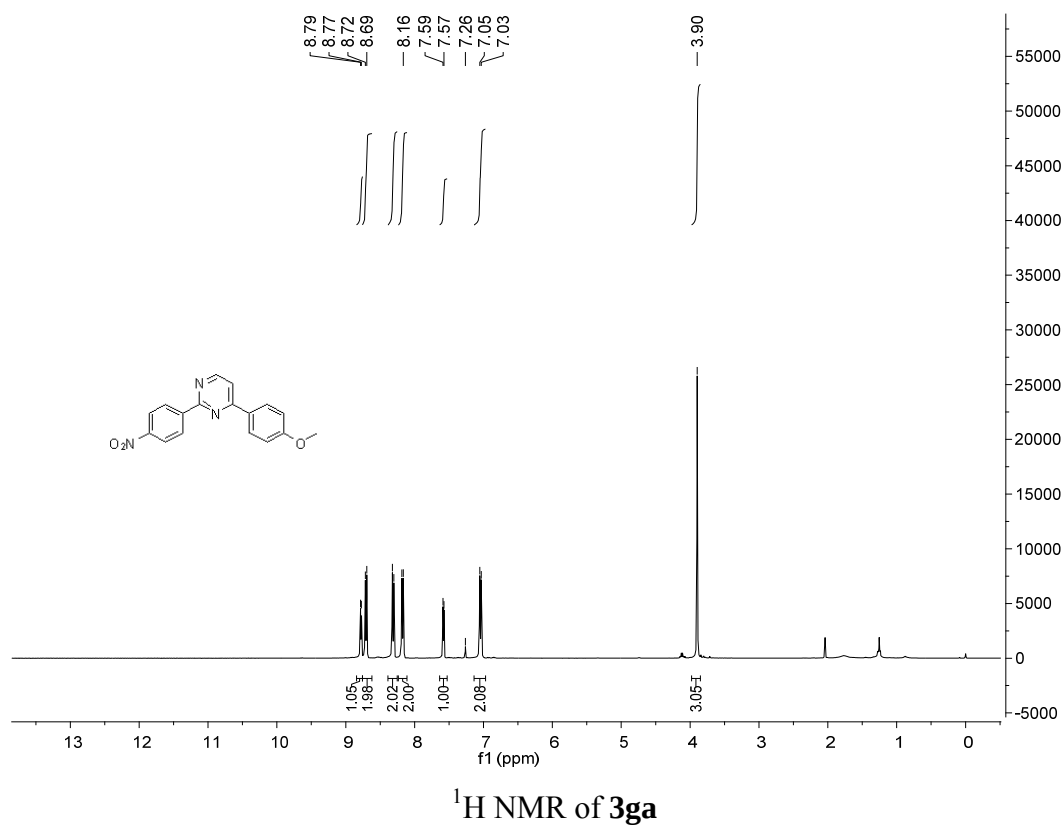


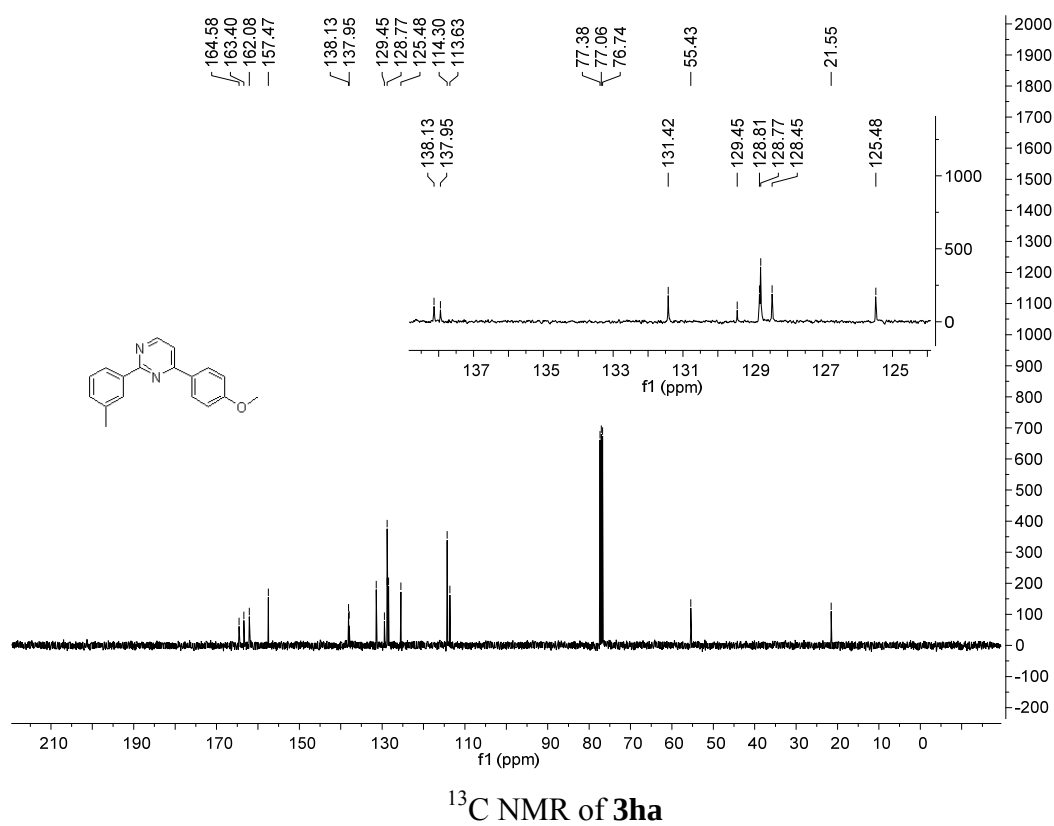
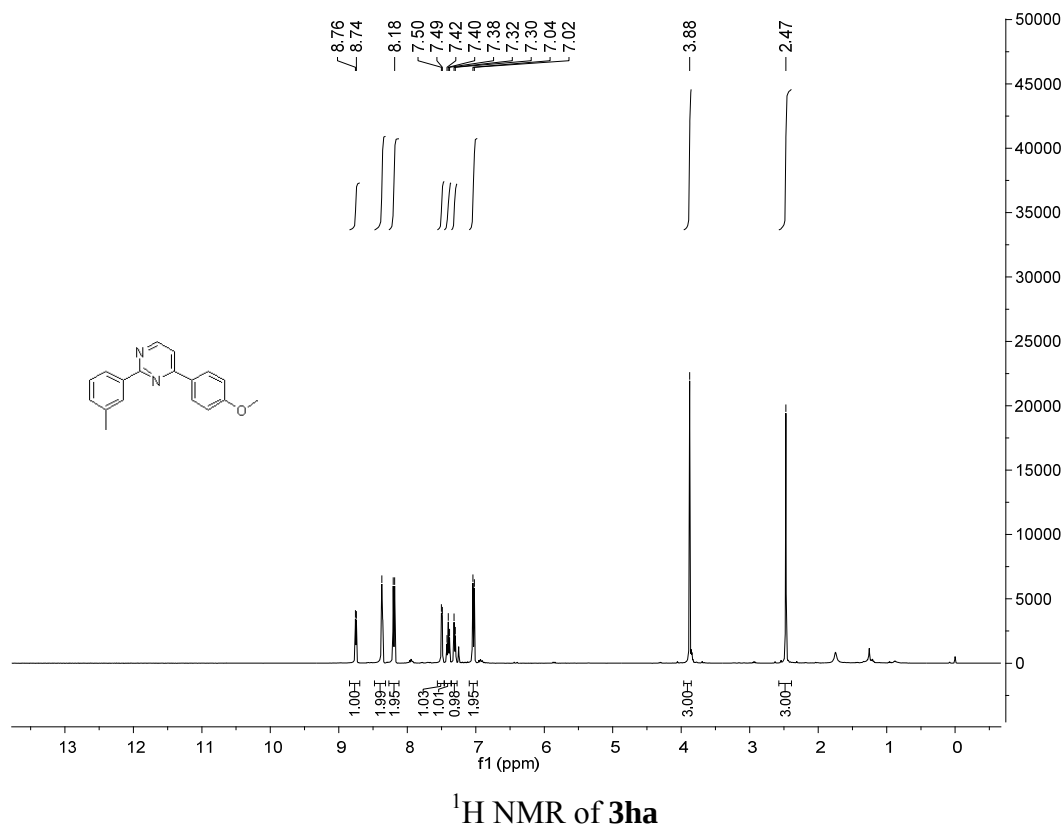


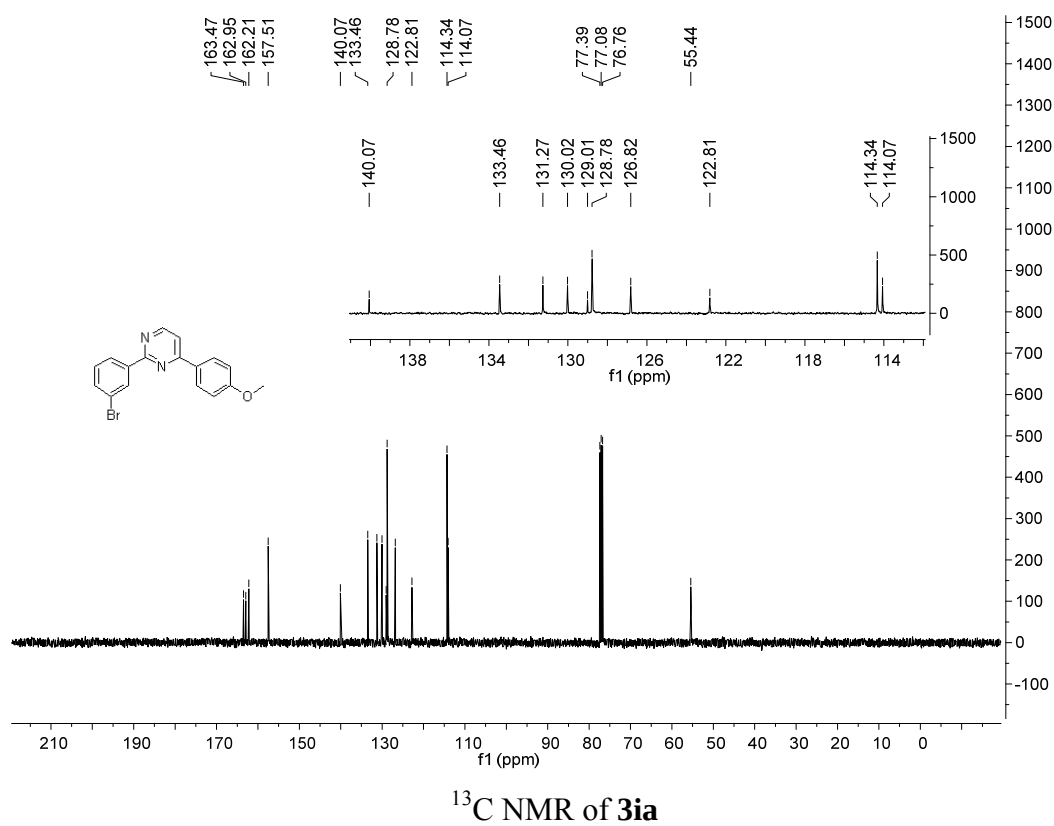
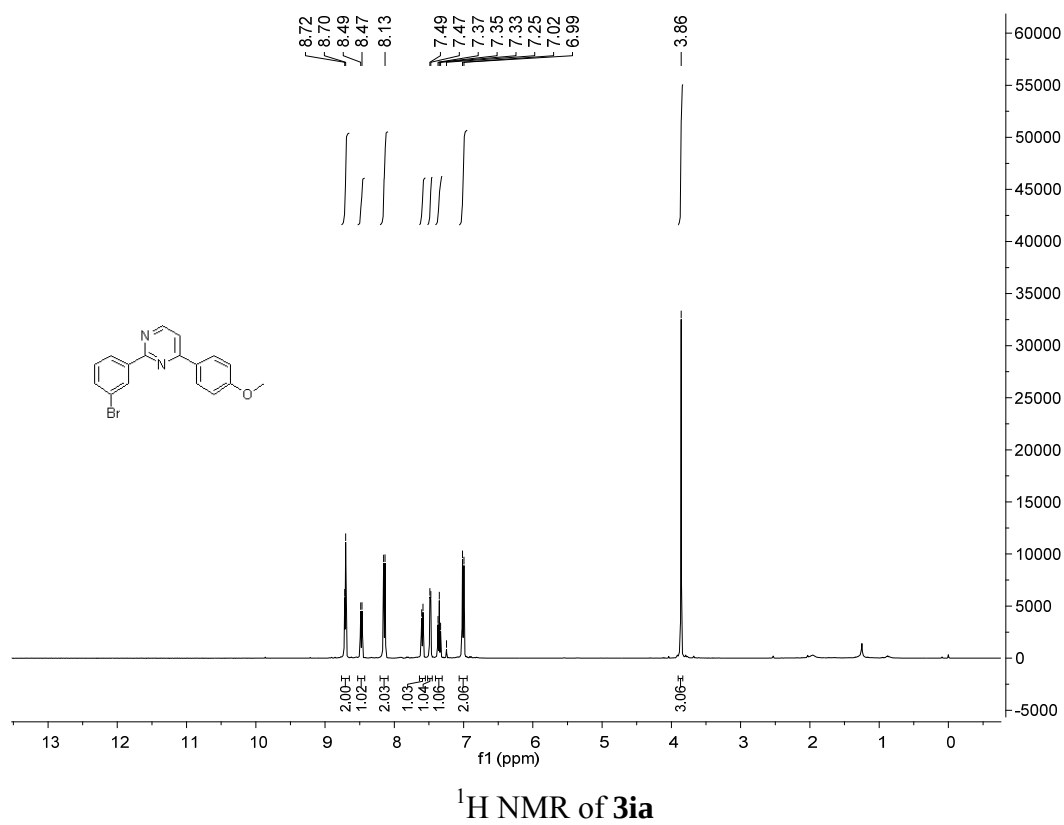


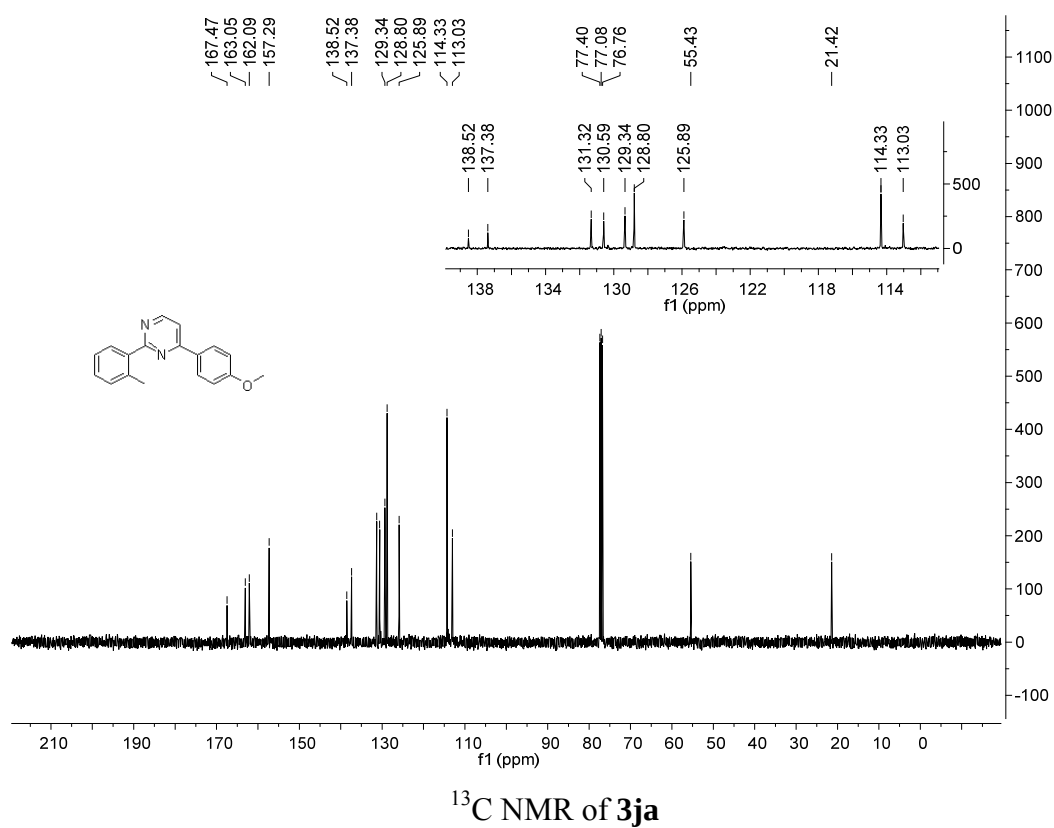
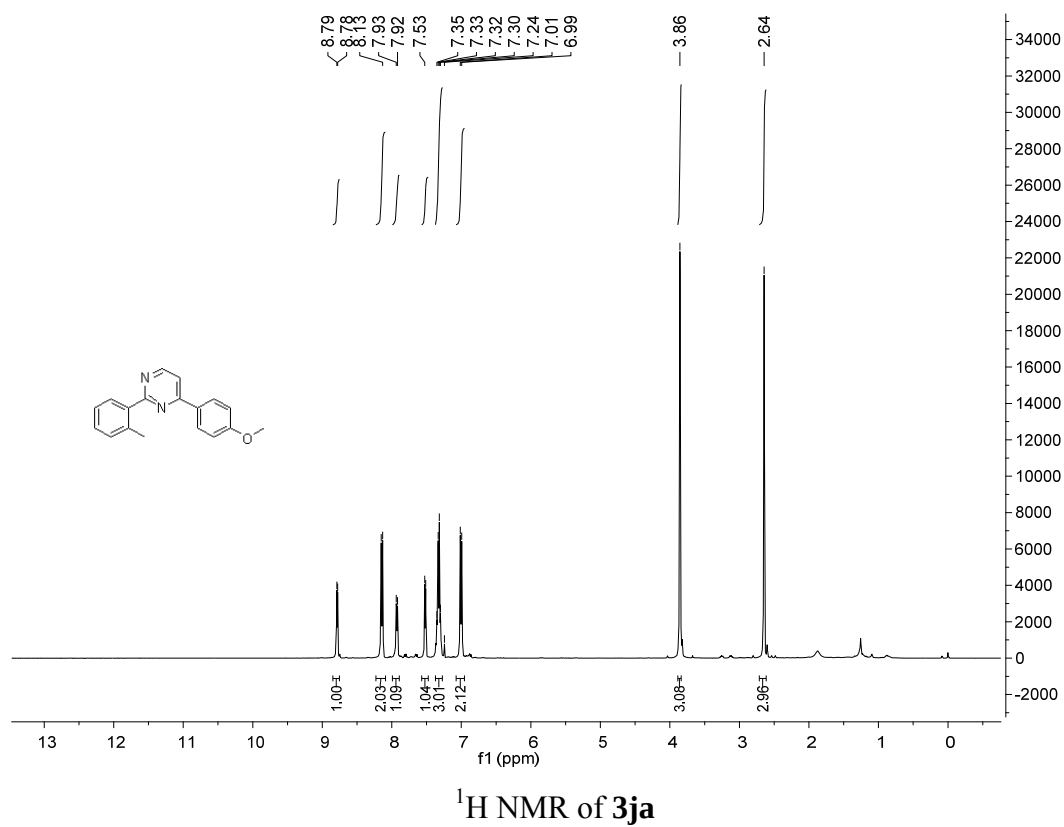


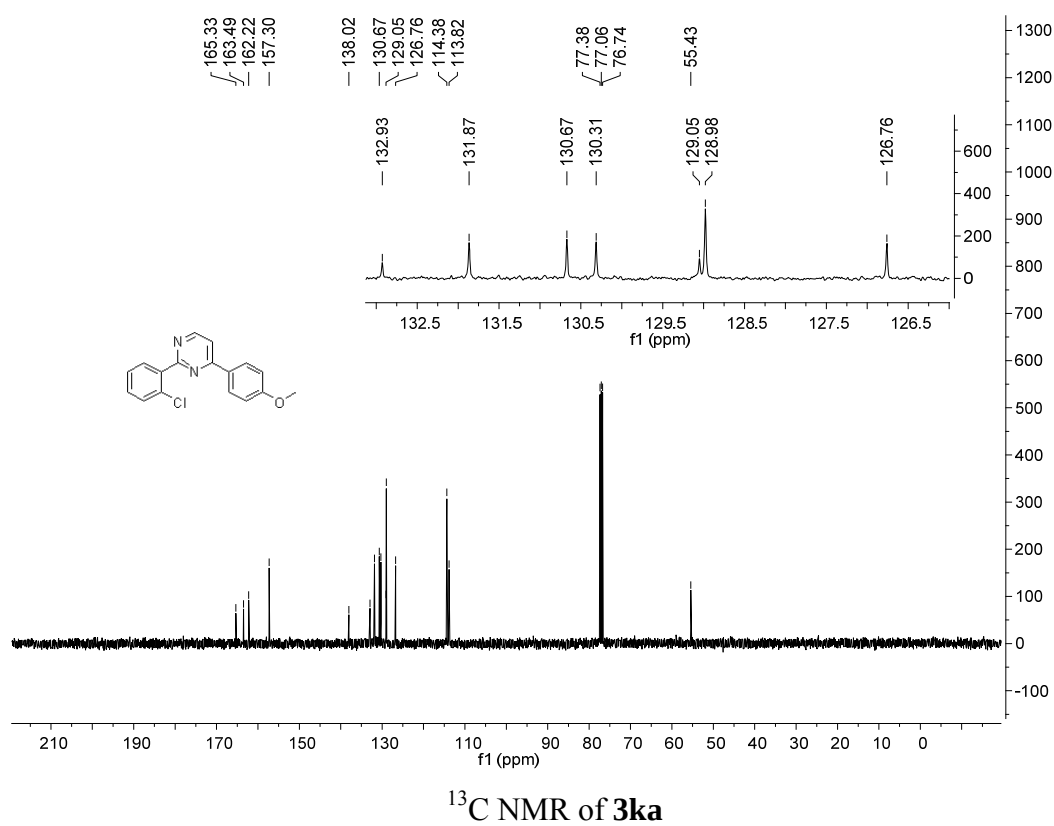
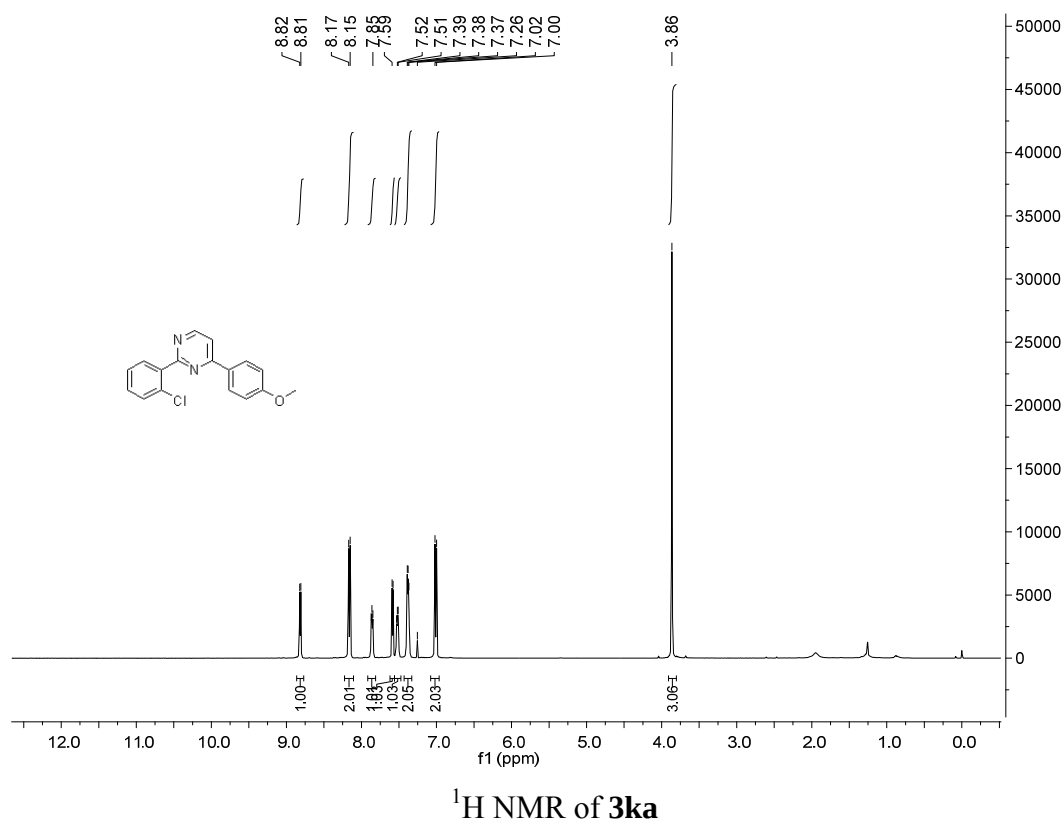


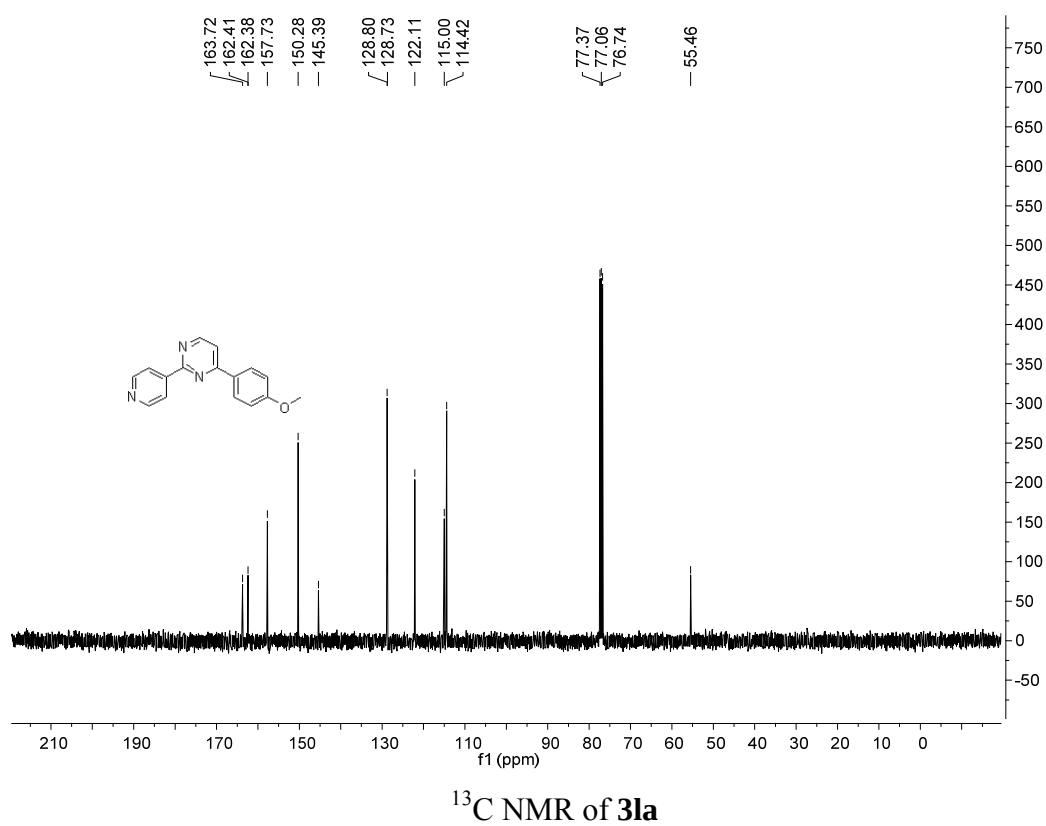
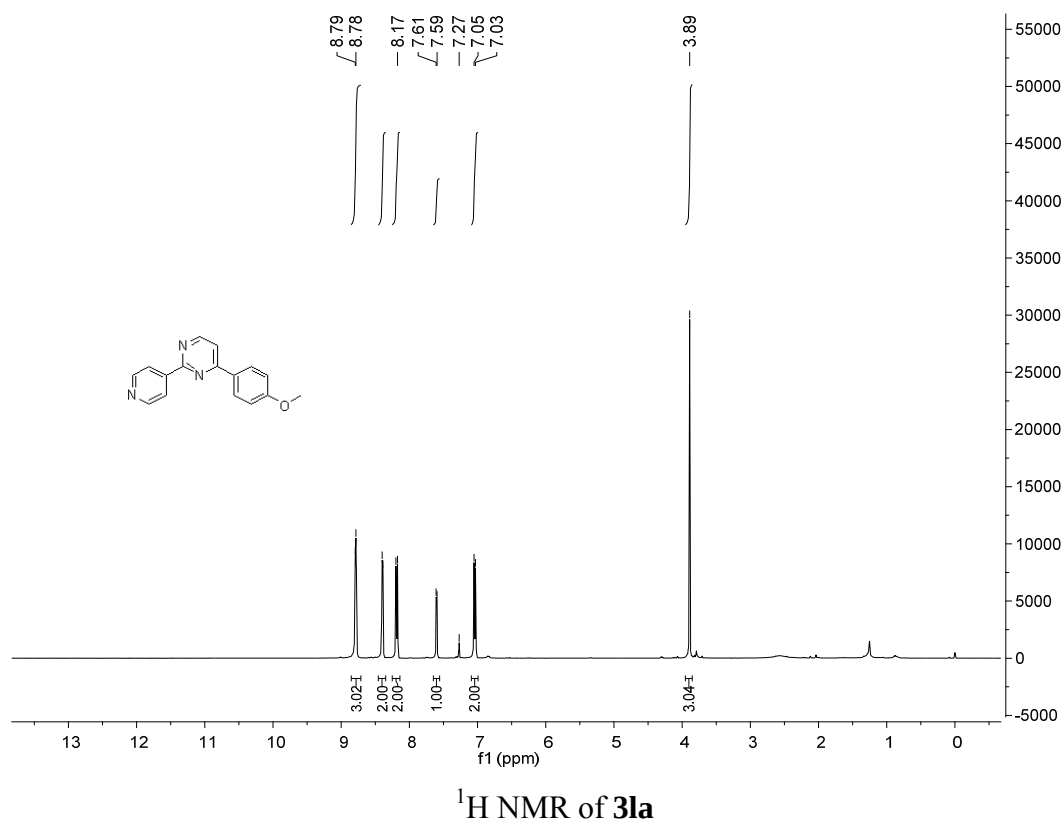


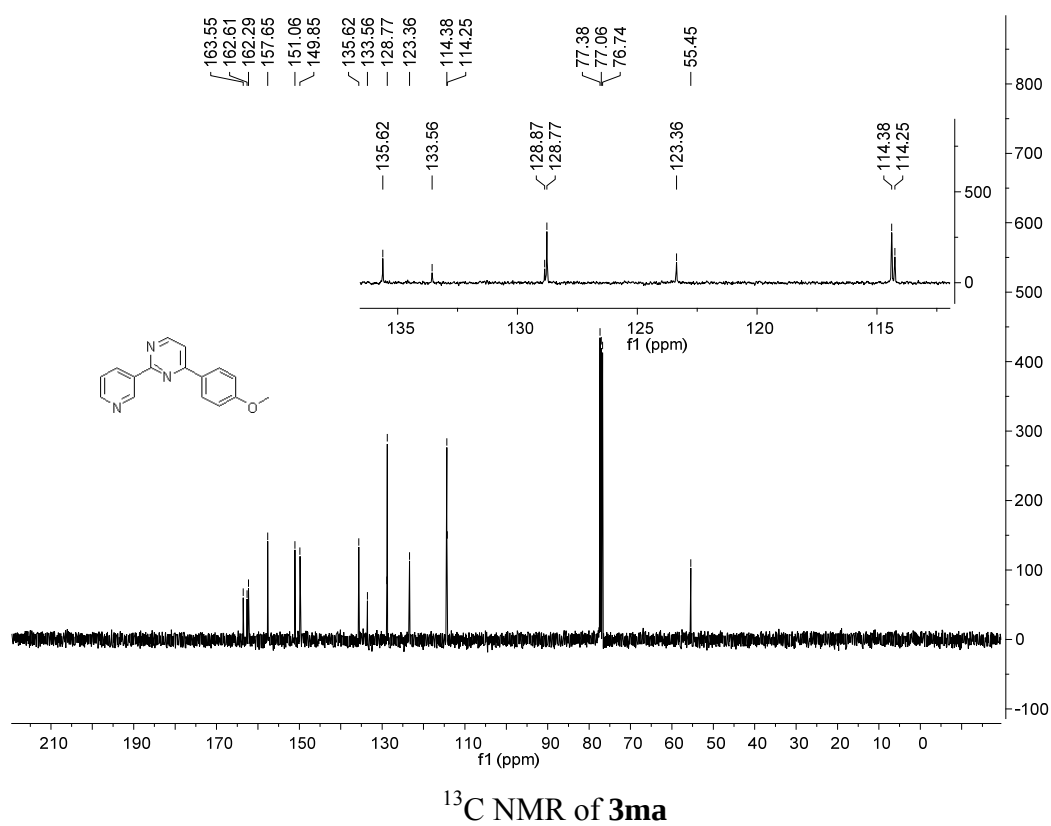
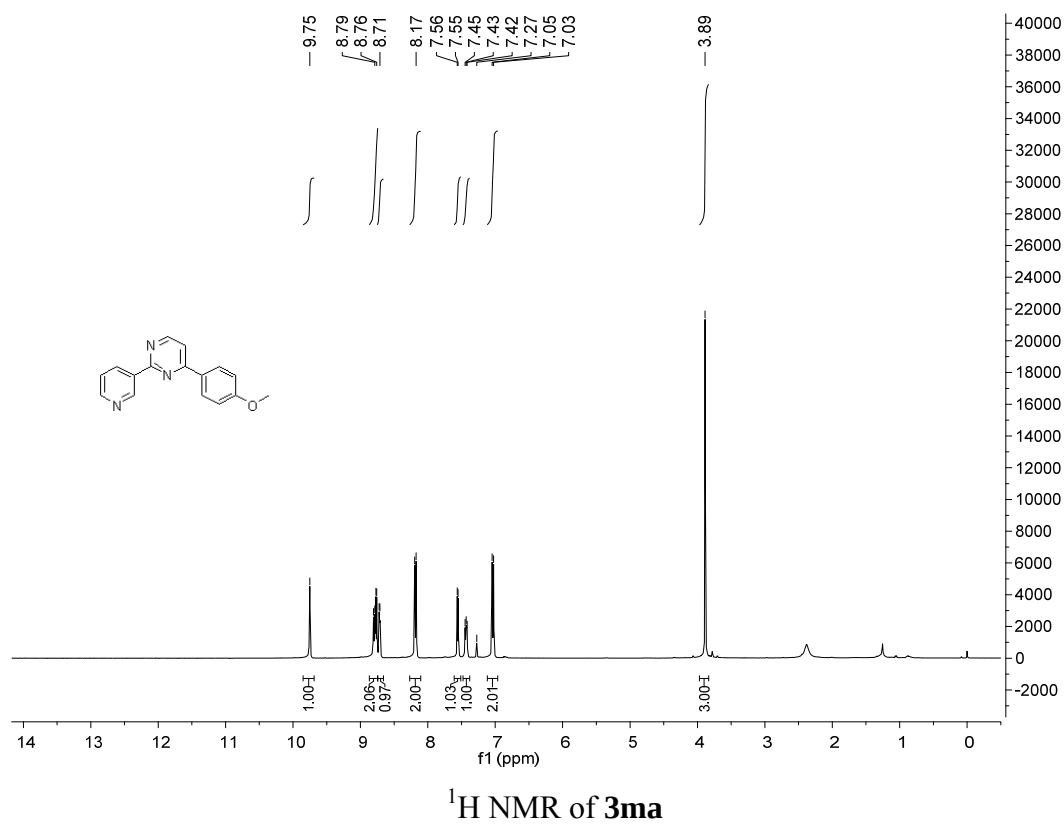


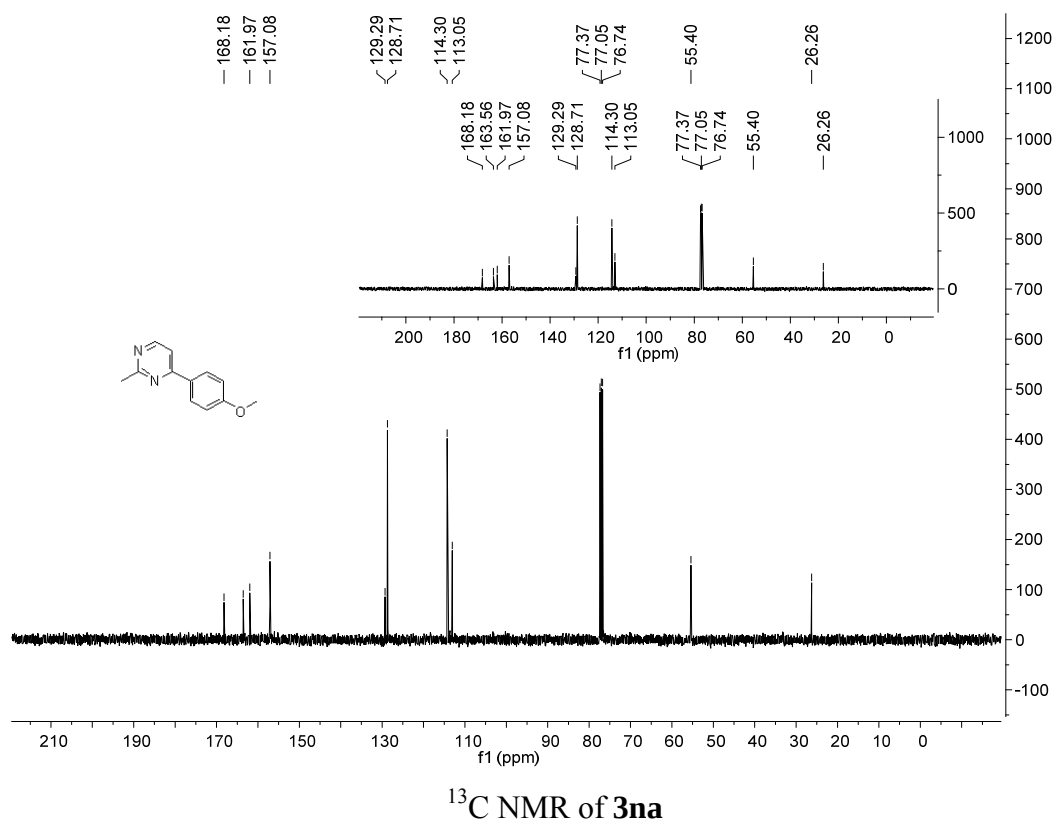
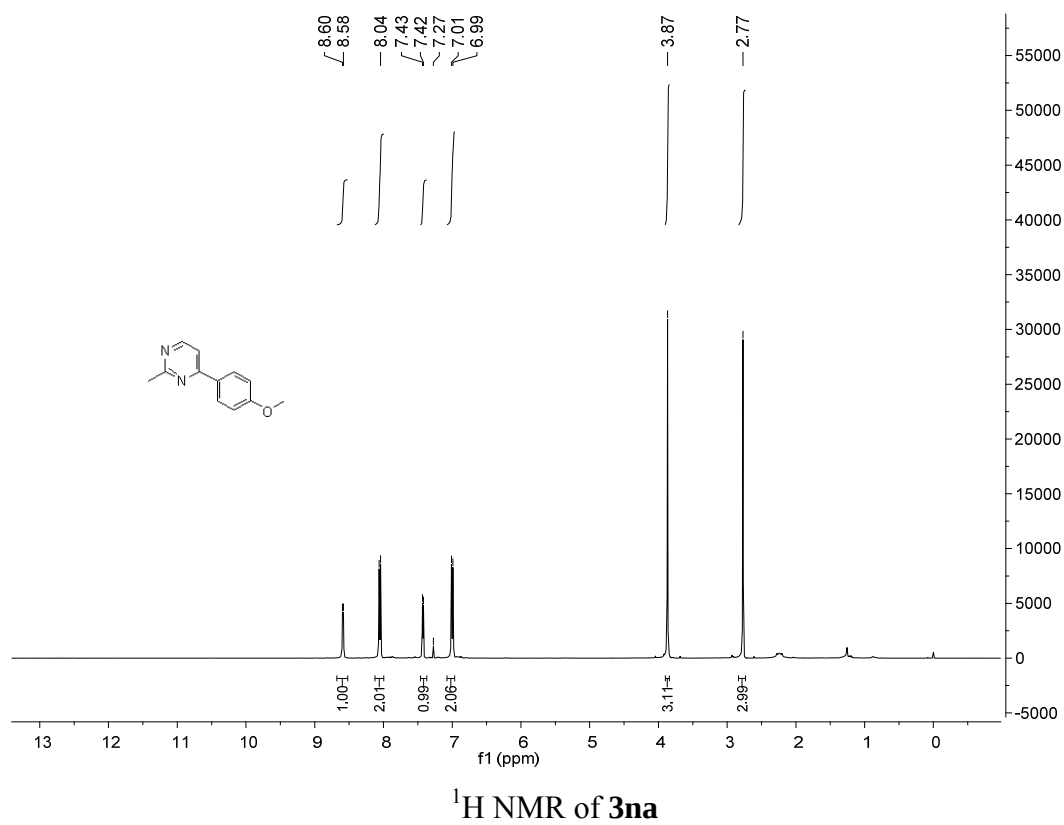


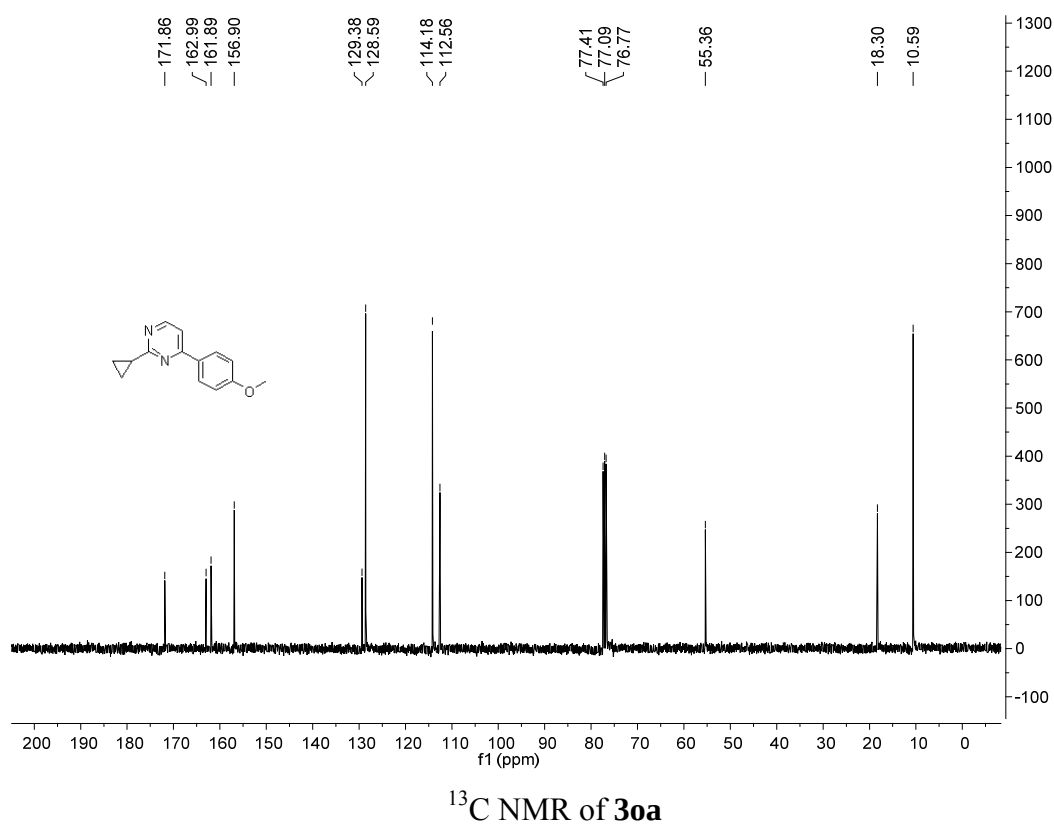
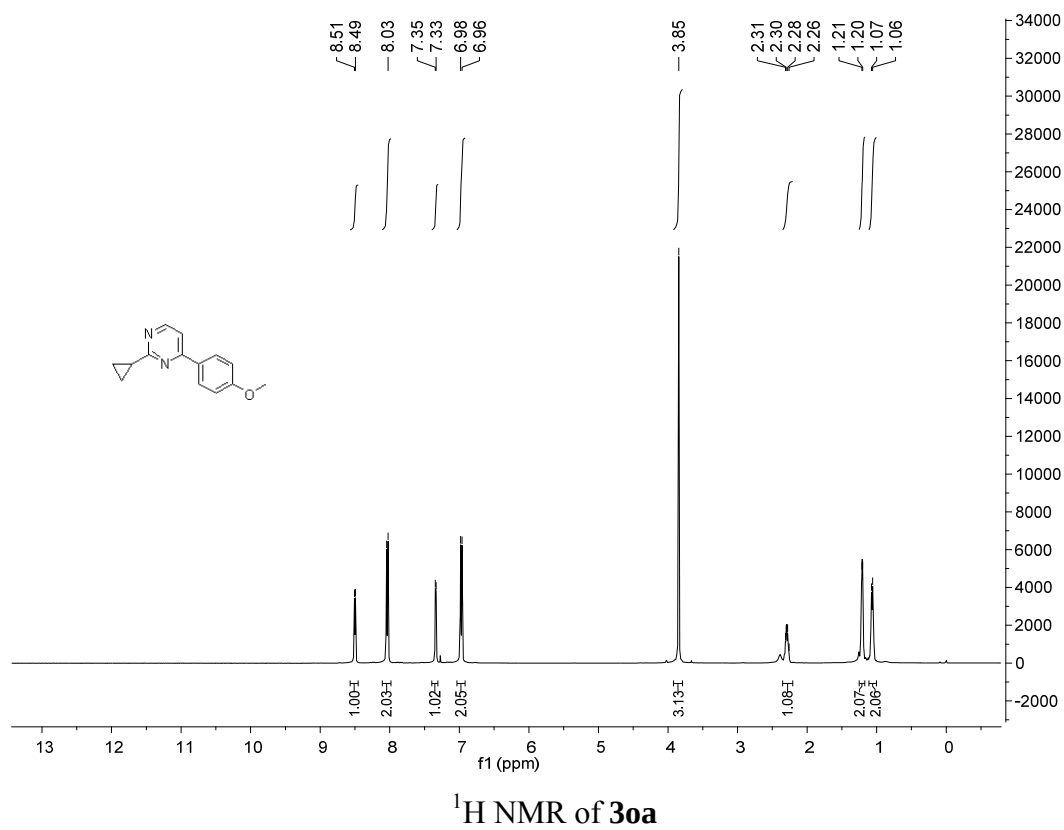


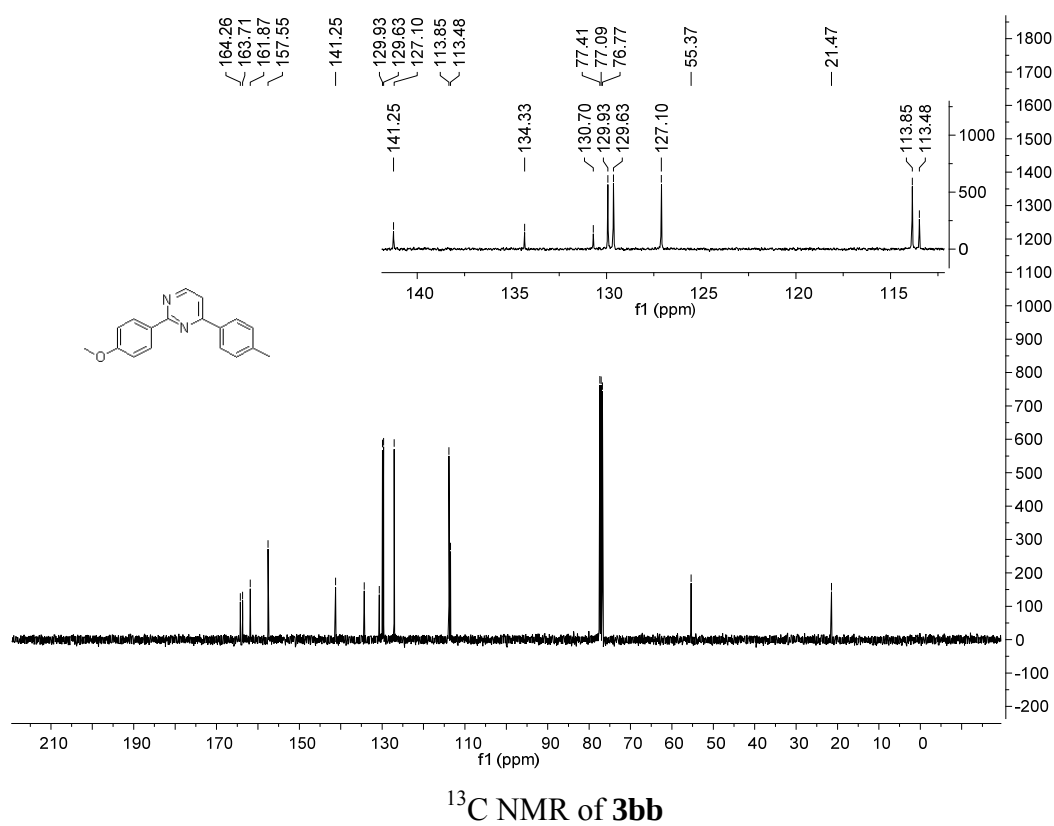
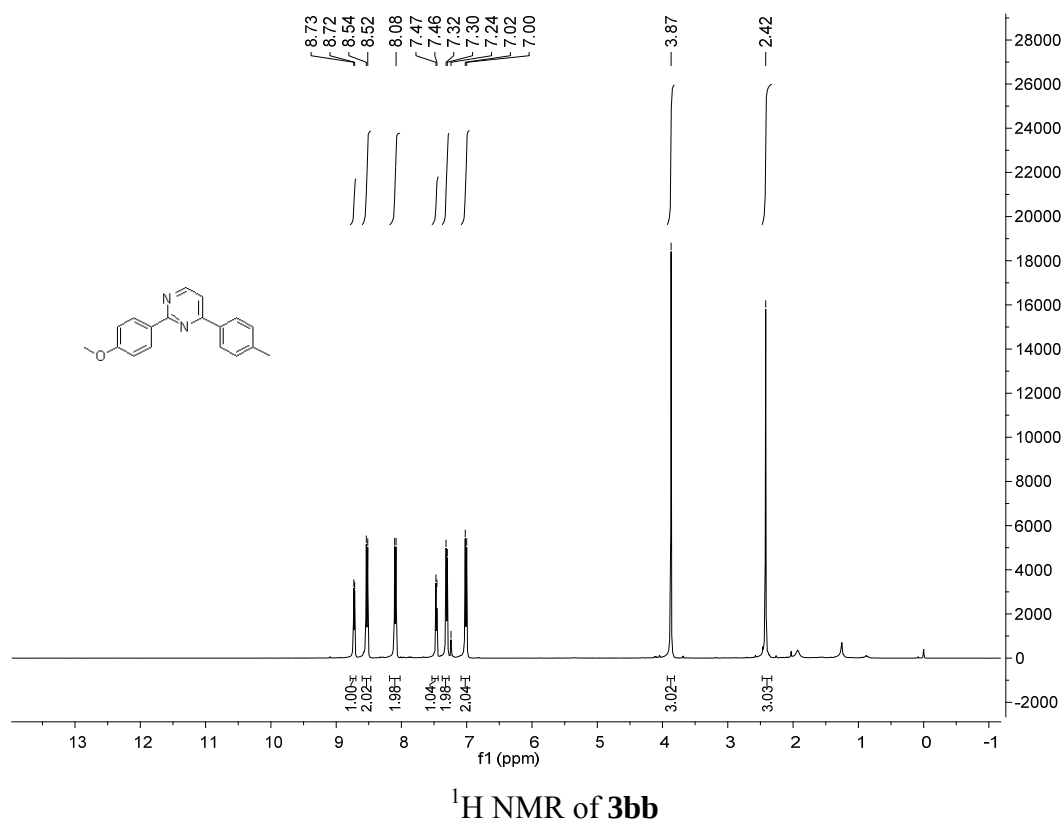


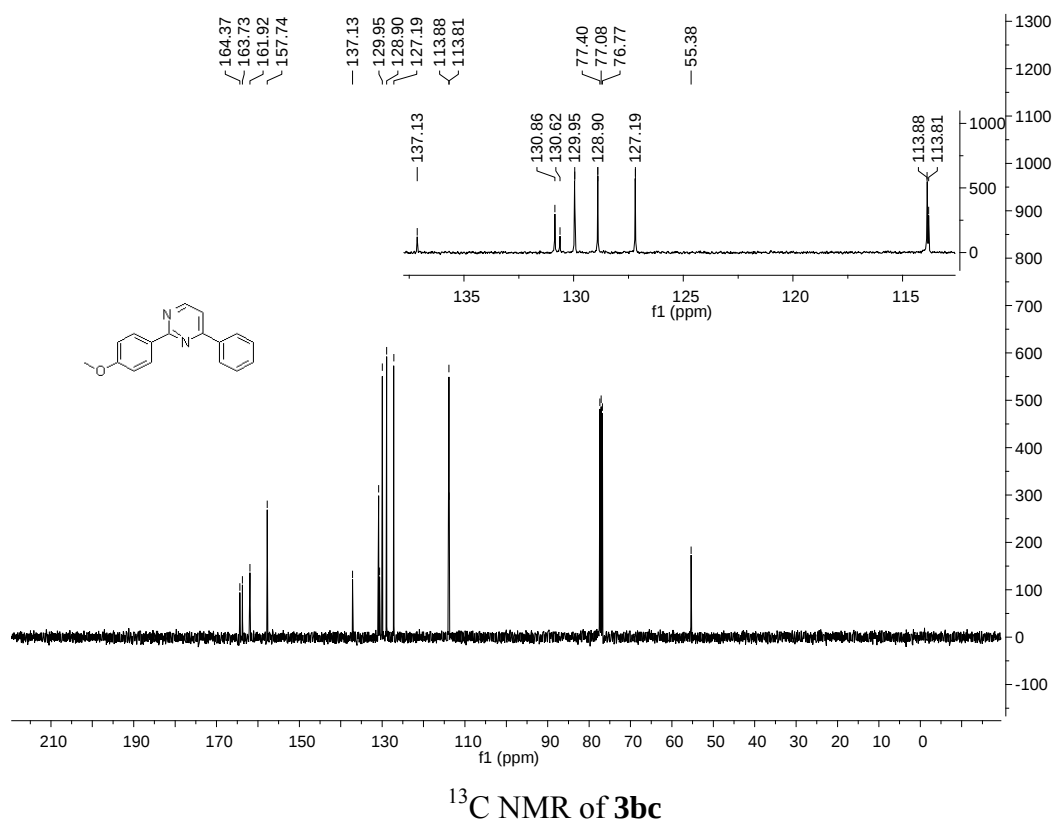
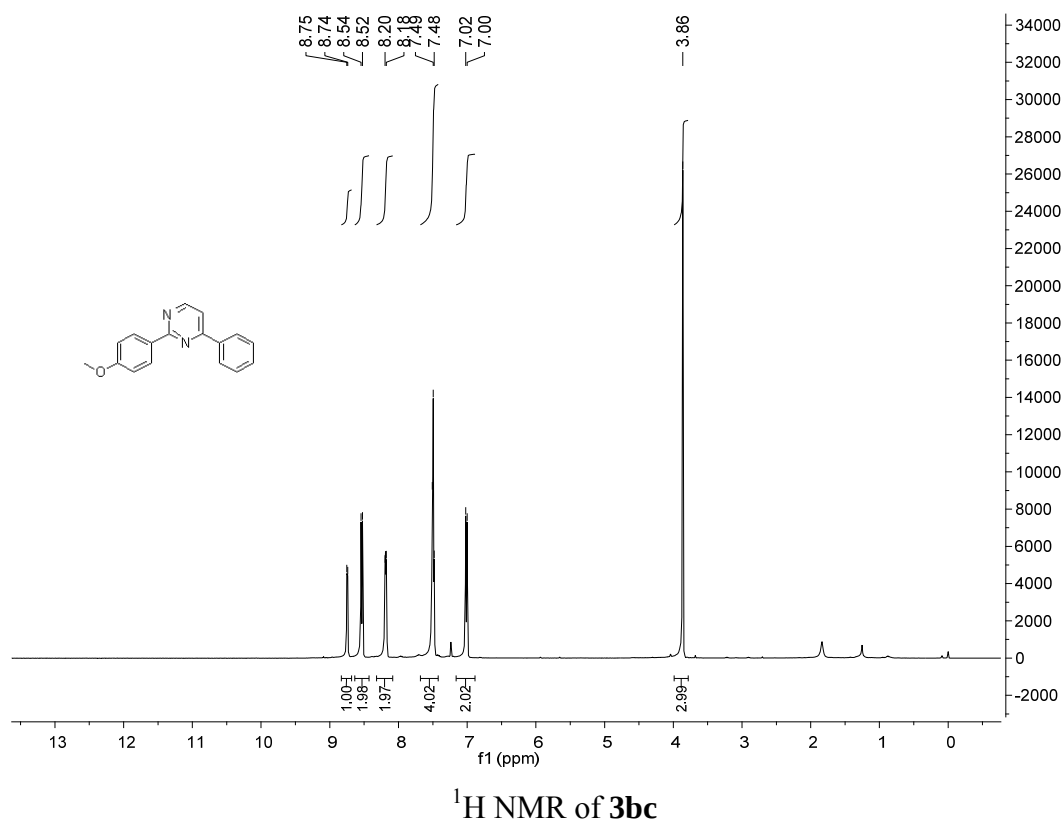


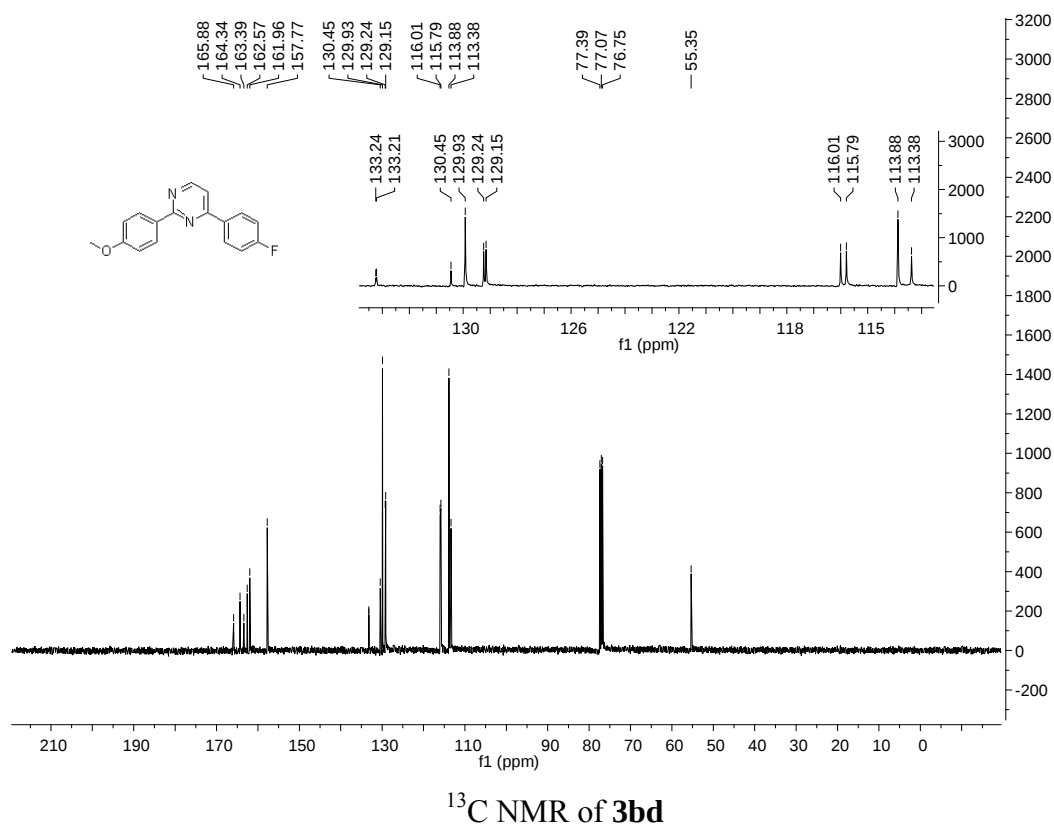
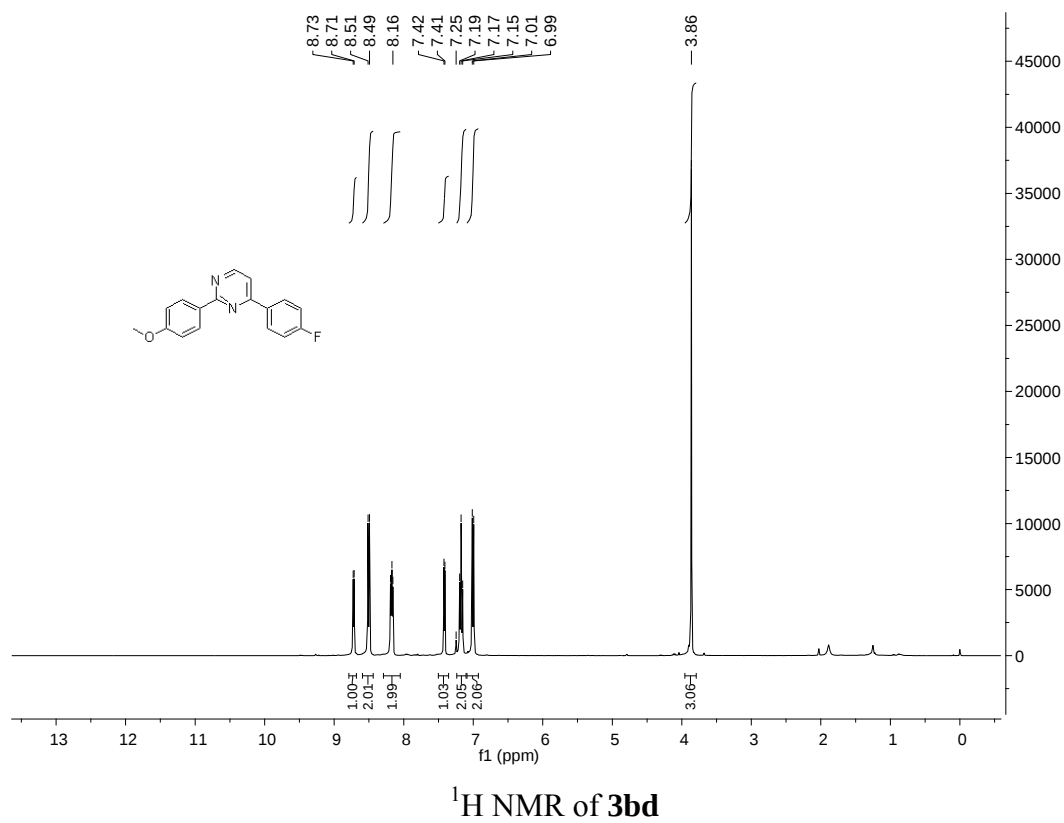


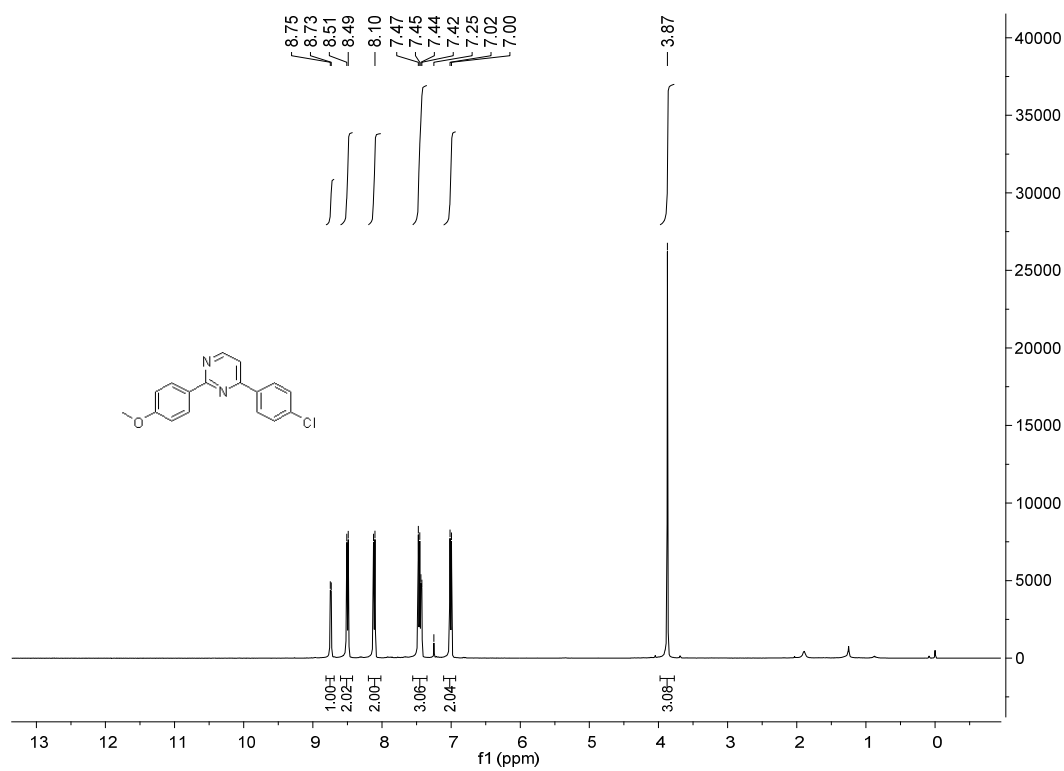




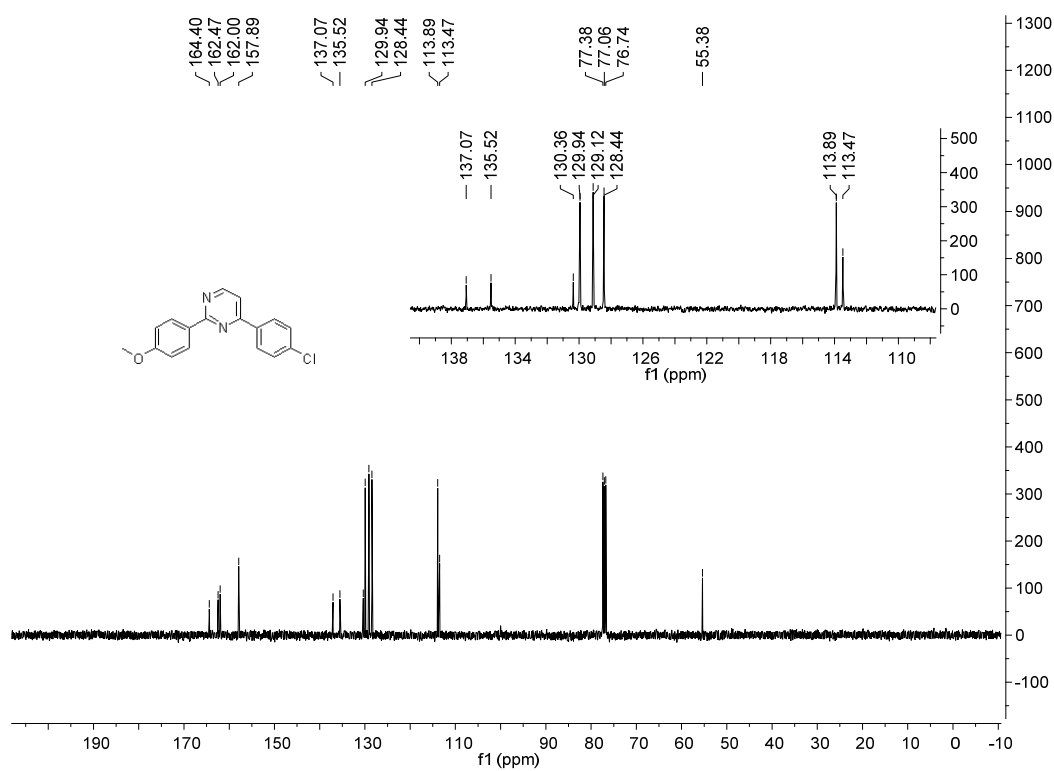








¹H NMR of 3be



¹³C NMR of 3be

