

Supporting Information
for
Palladium-Catalyzed Intermolecular Coupling of Aryl Halides and Amides

Jingjun Yin and Stephen L. Buchwald*

General Considerations All reactions were carried out under an argon atmosphere in flame-dried glassware. Elemental analyses were performed by Atlantic Microlabs Inc, Norcross, GA. Anhydrous 1,4-dioxane was purchased from Aldrich Chemical Co. and was used without further purification. THF was distilled under argon from sodium benzophenone ketyl. All aryl halides, p-nitrophenyl triflate, amides, carbamates, and sulfonamides were purchased from commercial sources and were used without further purification. Palladium acetate and tris(dibenzylideneacetone) dipalladium(0) were purchased from Strem Chemical company. Xantphos¹ and 4-tert-butylphenyl triflate^{2,3} were prepared according to the literature procedures. Cesium carbonate was purchased from Chemtall Chemical Company; the bulk of this material was stored under nitrogen in a Vacuum Atmospheres glovebox. Small portions (ca. 10 g) were removed from the glovebox in glass vials, stored in the air in desiccators filled with anhydrous calcium sulfate, and weighed in the air. IR spectra reported in this paper were obtained by placing neat samples directly on the DiComp probe of an ASI REACTIR in situ IR instrument or were recorded on a Perkin Elmer 1600 series FT-IR spectrometer. Yields in Tables 1 and 2 refer to isolated yields (average of two runs) of compounds estimated to be $\geq 95\%$ pure as determined by ¹H NMR, and GC analysis or combustion analysis. The procedures described in this section are representative, thus the yields may differ from those given in Tables 1 and 2.

General Procedure for Pd-Catalyzed Couplings of Aryl Halides/Triflates and Amides/Carbamates/Sulfonamides

A flame-dried resealable Schlenk tube was charged with Pd(OAc)₂ (2.2 mg, 0.01 mmol, 1 mol %), Xantphos (8.7 mg, 0.015 mmol, 1.5 mol %), the solid reactant(s) (1.0 mmol of the aryl halide/triflate and 1.2 mmol of the amide/carbamate/sulfonamide), and Cs₂CO₃ (456 mg, 1.4 mmol). The Schlenk tube was capped with a rubber septum, evacuated and backfilled with argon; this evacuation/backfill sequence was repeated one additional time. The liquid reactant(s) and 1,4-dioxane (1 mL) were added through the septum. The septum was replaced with a teflon screwcap. The Schlenk tube was sealed, and the mixture was stirred at the indicated temperature (45-110 °C) for the indicated time in Tables 1 and 2 (6-44 h) until the starting aryl halide or triflate had been completely consumed as judged by GC analysis. The reaction mixture was then cooled to room temperature, diluted with dichloromethane (10 mL), filtered, and concentrated in vacuo. The crude material was purified by flash chromatography on silica gel.

Workup Method B (for Table 1, entry 7 only) Following the completion of the reaction, the reaction mixture was cooled to room temperature and then diluted with ethyl acetate (8 mL) and 1 N HCl (6 mL). The aqueous layer was washed with ethyl acetate (8 mL). The combined organic layers were extracted with 1 N NaOH (4 x 8 mL) and were discarded. The product went into the aqueous layer in this case. The combined aqueous layers were acidified with 1 N HCl (50 mL) and extracted with ethyl acetate (50 mL). This ethyl acetate layer was dried over MgSO₄ and concentrated to give the pure product.

N-(4-Cyanophenyl)benzamide (Table 1, entry 1)⁴ The general procedure using THF as solvent, 1.1 equivalents of benzamide and 1.5 equivalents of Cs₂CO₃ gave 208 mg (94%) of the title compound as a white solid: mp 166-167 °C (lit. mp 167±2 °C),⁴ ¹H NMR (300 MHz, CDCl₃) δ 8.22 (br s, 1 H), 7.89-7.88 (m, 1 H), 7.87-7.85 (m, 1 H), 7.82 (t, J = 2.2 Hz, 1 H), 7.79 (t, J = 2.2 Hz, 1 H), 7.65 (t, J = 2.1 Hz, 1 H), 7.62 (t, J = 2.2 Hz, 1 H), 7.60-7.56 (m, 1 H), 7.52-7.46 (m, 2 H); ¹³C NMR (75 MHz, CDCl₃) δ 166.2, 142.3, 134.3, 133.5, 132.7,

129.1, 127.4, 120.2, 119.1, 107.5; IR (NaCl, cm^{-1}) 3349, 2226, 1660, 1590, 1520, 1504, 1408.

N-(4-Cyanophenyl)benzamide (Table 1, entry 2)⁴ The general procedure using THF as solvent gave 214 mg (96%) of the title compound as a white solid.

N-(4-Cyanophenyl)-N-methylacetamide (Table 1, entry 3)⁵ The general procedure using THF as solvent and 1.5 equivalents of Cs_2CO_3 gave 168 mg (97%) of the title compound as a white solid: mp 142-144 °C (lit. mp 142 °C);⁵ ^1H NMR (300 MHz, CDCl_3) δ 7.73 (dd, J = 6.7, 2.1 Hz, 2 H), 7.34 (dd, J = 6.7, 2.1 Hz, 2 H), 3.32 (s, 3 H), 1.99 (br s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 169.7, 148.1, 133.5, 127.5, 118.0, 110.9, 37.3, 22.7; IR (NaCl, cm^{-1}) 2228, 1657, 1601, 1508, 1381, 1355.

N-(4-Cyanophenyl)-N-phenylacetamide (Table 1, entry 4)⁶ The general procedure gave 225 mg (95%) of the title compound as a white solid: mp 94-95 °C (lit. mp 96-97 °C);⁶ ^1H NMR (300 MHz, CDCl_3) δ 7.59 (dt, J = 6.9, 1.2 Hz, 2 H), 7.50-7.35 (m, 5 H), 7.27-7.24 (m, 2 H), 2.07 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.5, 146.6, 132.8, 130.2, 128.7, 126.1, 118.6, 109.2, 24.6; IR (NaCl, cm^{-1}) 2227, 1683, 1603, 1504, 1493, 1369, 1325, 1298.

N-(4-Cyanophenyl)-N-phenylacetamide (Table 1, entry 5)⁶ The general procedure gave 176 mg (75%) of the title compound as a white solid.

Benzyl N-(4-formylphenyl)carbamate (Table 1, entry 6)⁷ The general procedure using THF as solvent gave 252 mg (99%) of the title compound as a white solid: mp 132-133 °C (lit. mp 129-131.5 °C);⁷ ^1H NMR (300 MHz, CDCl_3) δ 9.91 (s, 1 H), 7.85 (dt, J = 9.0, 2.0 Hz, 2 H), 7.57 (dt, J = 8.8, 2.0 Hz), 2 H), 7.44-7.35 (m, 5 H), 7.00 (br s, 1 H), 5.24 (s, 2 H); ^{13}C NMR (75 MHz, CDCl_3) δ 153.1, 144.0, 135.7, 131.7, 131.5, 128.8, 128.7, 128.5, 118.2, 67.6; IR (neat, cm^{-1}) 3323, 1745, 1683, 1668, 1590, 1536, 1324, 1224, 1170, 1046.

N-(4-Formylphenyl)-p-toluenesulfonamide (Table 1, entry 7)⁸ The general procedure using $\text{Pd}_2(\text{dba})_3$ (2.3 mg, 0.0025 mmol, 1 mol % Pd per mmol halide) on a 0.5 mmol scale and using **Workup Method B** gave 125 mg (91%) of the title compound as a white solid: mp 186-187 °C (lit. mp 188-188.5 °C);⁸ ^1H NMR (300 MHz, acetone- d_6) δ 9.87

(s, 1 H), 9.57 (br s, 1 H), 7.82-7.77 (m, 4 H), 7.44-7.34 (m, 4 H), 2.35 (s, 3 H); ^{13}C NMR (75 MHz, acetone- d_6) δ 191.3, 144.9, 144.4, 137.6, 133.1, 131.7, 130.5, 127.9, 119.4, 21.5; IR (neat, cm^{-1}) 3231, 1683, 1598, 1586, 1339, 1220, 1154..

N-(2-Carbomethoxyphenyl)-N-methylacetamide (Table 1, entry 8)⁹ The general procedure gave 202 mg (98%) of the title compound as a pale yellow solid: mp 37-39 °C (lit. mp 39-40 °C);⁹ ^1H NMR (300 MHz, CDCl_3) δ 8.10 (dd, J = 6.6, 1.8 Hz, 2 H), 7.28 (dd, J = 6.6, 1.8 Hz, 2 H), 3.94 (s, 3 H), 3.30 (s, 3 H), 1.94 (br s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.0, 166.0, 148.4, 131.0, 129.2, 126.8, 52.1, 37.2, 22.7; IR (neat, cm^{-1}) 1722, 1664, 1602, 1509, 1274.

N-(4-Carbomethoxyphenyl)-N-methyl-p-toluenesulfonamide (Table 1, entry 9)¹⁰ The general procedure gave 277 mg (87%) of the title compound as a white solid, mp 103-105 °C (lit. mp 100-102 °C).¹⁰ This material contained ca. 4% N, N-dimethyl-p-toluenesulfonamide as judged by ^1H NMR, GC, and GC-MS analysis. Data for the title compound: ^1H NMR (300 MHz, CDCl_3) δ 7.98-7.94 (m, 2 H), 7.39 (d, J = 8.2 Hz, 2 H), 7.24-7.18 (m, 4 H), 3.91 (s, 3 H), 3.18 (s, 3 H), 2.40 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 166.4, 145.7, 144.0, 133.1, 130.3, 129.6, 128.4, 127.8, 125.6, 52.4, 37.8, 21.8; IR (neat, cm^{-1}) 1718, 1598, 1459, 1440, 1343, 1278, 1162.

N-(2-Carbomethoxyphenyl)benzamide (Table 1, entry 10)⁹ The general procedure using $\text{Pd}_2(\text{dba})_3$ (4.6 mg, 0.005 mmol, 1 mol % Pd) gave 237 mg (93%) of the title compound as a white solid: mp 97-98 °C (lit. mp 93-95 °C);⁹ ^1H NMR (300 MHz, CDCl_3) δ 12.06 (br s, 1 H), 8.95 (dd, J = 8.6, 0.8 Hz, 1 H), 8.12-8.05 (m, 3 H), 7.66-7.51 (m, 4 H), 7.14 (td, J = 7.6, 1.2 Hz, 1 H), 3.99 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 168.8, 165.4, 141.7, 134.7, 131.9, 130.9, 128.7, 127.3, 122.5, 120.2, 114.9, 52.5; IR (neat, cm^{-1}) 3269, 1695, 1671, 1590, 1536.

N-(2'-Carbomethoxyphenyl)-2-azetidinone (Table 1, entry 11) The general procedure using $\text{Pd}_2(\text{dba})_3$ (4.6 mg, 0.005 mmol, 1 mol % Pd per mmol halide) gave 163 mg (80%) of the title compound as a pale yellow oil: ^1H NMR (300 MHz, CDCl_3) δ 7.75-7.72

(m, 1 H), 7.50-7.48 (m, 2 H), 7.21 (ddd, $J = 7.7, 5.9, 2.8$ Hz, 1 H), 3.92 (s, 3 H), 3.76 (t, $J = 4.7$ Hz, 2 H), 3.13 (t, $J = 4.7$ Hz, 2 H); ^{13}C NMR (75 MHz, CDCl_3) δ 167.3, 165.5, 136.0, 132.3, 130.5, 124.8, 123.7, 121.2, 52.6, 40.7, 36.6; IR (neat, cm^{-1}) 1749, 1722, 1602, 1579, 1494, 1451, 1366, 1293, 1254. Anal. Calcd. for $\text{C}_{11}\text{H}_{11}\text{NO}_3$: C, 64.38; H, 5.40. Found: C, 64.40; H, 5.49.

N-(3-Carbomethoxyphenyl)benzamide (Table 1, entry 12)¹¹ The general procedure using $\text{Pd}_2(\text{dba})_3$ (4.6 mg, 0.005 mmol, 1 mol % Pd) gave 240 mg (94%) of the title compound as a white solid: mp 134-135 °C (lit. mp 130-131 °C);¹¹ ^1H NMR (300 MHz, CDCl_3) δ 8.16 (t, $J = 1.9$ Hz, 1 H), 8.07 (ddd, $J = 8.0, 2.2, 1.1$ Hz, 1 H), 8.02 (br s, 1 H), 7.91-7.88 (m, 2 H), 7.83 (dt, $J = 8.0, 1.3$ Hz, 1 H), 7.61-7.44 (m, 4 H), 3.93 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 166.8, 166.2, 138.3, 134.6, 132.1, 130.8, 129.2, 128.8, 127.3, 125.6, 125.0, 121.4, 52.5; IR (neat, cm^{-1}) 3285, 1725, 1652, 1594, 1529, 1432, 1293, 1231.

Ethyl N-(3-carbomethoxyphenyl)-N-ethylcarbamate (Table 1, entry 13) The general procedure using $\text{Pd}_2(\text{dba})_3$ (9.2 mg, 0.01 mmol, 2 mol % Pd) gave 165 mg (66%) of the title compound as a pale yellow oil: ^1H NMR (300 MHz, CDCl_3) δ 7.89-7.84 (m, 2 H), 7.42-7.37 (m, 2 H), 4.12 (q, $J = 7.1$ Hz, 2 H), 3.87 (s, 3 H), 3.71 (q, $J = 7.1$ Hz, 2 H), 1.18 (t, $J = 7.1$ Hz, 3 H), 1.12 (t, $J = 7.1$ Hz, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 166.4, 155.1, 142.1, 131.8, 131.0, 128.9, 128.1, 127.4, 61.7, 52.3, 45.2, 14.7, 13.9; IR (neat, cm^{-1}) 1725, 1702, 1606, 1586, 1447, 1270, 1239. Anal. Calcd. for $\text{C}_{13}\text{H}_{17}\text{NO}_4$: C, 62.14; H, 6.82. Found: C, 62.31; H, 6.84.

N-(2-Methyl-6-nitrophenyl)acetamide (Table 1, entry 14)¹² The general procedure using $\text{Pd}_2(\text{dba})_3$ (4.6 mg, 0.005 mmol, 1 mol % Pd) gave 181 mg (93%) of the title compound as a white solid: mp 157-158 °C (lit. mp 155-157 °C);¹² ^1H NMR (300 MHz, CDCl_3) δ 8.33 (br s, 1 H), 7.84 (d, $J = 8.2$ Hz, 1 H), 7.53 (d, $J = 7.7$ Hz, 1 H), 7.29 (t, $J = 7.8$ Hz, 1 H), 2.34 (s, 3 H), 2.25 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3) δ 168.4, 145.0, 138.4, 136.2, 129.7, 126.5, 122.9, 24.0, 19.3; IR (neat, cm^{-1}) 3304, 1664, 1286, 1517, 1359, 1266.

N-(4-Nitrophenyl)-N-methylbenzamide (Table 1, entry 15)¹³ The general procedure gave 181 mg (71%) of the title compound as a pale yellow solid: mp 107-108 °C (lit. mp 109 °C);¹³ ¹H NMR (300 MHz, CDCl₃) δ 8.13-8.08 (m, 2 H), 7.37-7.31 (m, 3 H), 7.26-7.16 (m, 4 H), 3.57 (s, 3 H); ¹³C NMR (75 MHz, CDCl₃) δ 170.4, 150.5, 144.8, 134.9, 130.4, 128.6, 128.2, 126.5, 124.4, 38.1; IR (neat, cm⁻¹) 1644, 1606, 1586, 1521, 1494, 1332, 1100.

N-(4-*t*-Butylphenyl)benzamide (Table 2, entry 1)¹⁴ The general procedure using Pd₂(dba)₃ (9.2 mg, 0.01 mmol, 4 mol % Pd per mmol halide) and 2 mL dioxane per mmol halide on a 0.5 mmol scale gave 118 mg (93%) of the title compound as a white solid: mp 140-142 °C (lit. mp 143-144 °C);¹⁴ ¹H NMR (300 MHz, CDCl₃) δ 7.89-7.86 (m, 2 H), 7.78 (br s, 1 H), 7.59-7.47 (m, 5 H), 7.41 (dt, J = 6.6, 2.2 Hz, 2 H), 1.34 (s, 9 H); ¹³C NMR (75 MHz, CDCl₃) δ 166.0, 147.5, 135.4, 135.0, 131.7, 128.6, 127.2, 125.8, 120.4, 34.6, 31.6; IR (neat, cm⁻¹) 3308, 2961, 1652, 1590, 1521, 1494, 1405, 1320, 1297, 1266.

N-(4-*t*-Butylphenyl)benzamide (Table 2, entry 2)¹⁴ The general procedure using Pd₂(dba)₃ (5.8 mg, 0.00625 mmol, 2.5 mol % Pd per mmol halide) and 2 mL dioxane per mmol halide on a 0.5 mmol scale gave 115 mg (91%) of the title compound as a white solid.

N-(4-*t*-Butylphenyl)benzamide (Table 2, entry 3)¹⁴ The general procedure using Pd₂(dba)₃ (5.8 mg, 0.00625 mmol, 2.5 mol % Pd per mmol halide) and 2 mL dioxane per mmol halide on a 0.5 mmol scale gave 120 mg (94%) of the title compound as a pale yellow solid.

N-(4'-*t*-Butylphenyl)-4-methoxybenzamide (Table 2, entry 4) The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 2 mol % Pd per mmol halide) and 2 mL dioxane per mmol halide on a 0.5 mmol scale gave 121 mg (85%) of the title compound as a white solid: mp 165-166 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.85 (d, J = 8.2 Hz, 2 H), 7.71 (br s, 1 H), 7.55 (d, J = 8.5 Hz, 2 H), 7.39 (d, J = 8.5 Hz, 2 H), 6.98 (d, J = 8.2 Hz, 2 H), 3.89 (s, 3 H), 1.34 (s, 9 H); ¹³C NMR (75 MHz, CDCl₃) δ 165.5, 162.3, 147.2, 125.6, 129.1, 127.3, 125.8, 120.2, 113.9, 55.6, 34.6, 31.6; IR (neat, cm⁻¹) 3308, 2953, 1648, 1598, 1532, 1509, 1332, 1251. Anal. Calcd. for C₁₈H₂₁NO₂: C, 76.29; H, 7.47. Found: C, 76.05; H, 7.56.

N-(4-*t*-Butylphenyl)acetamide (Table 2, entry 5)¹⁵ The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 2 mol % Pd per mmol halide) and 2 mL dioxane per mmol halide on a 0.5 mmol scale gave 85 mg (89%) of the title compound as a white solid: mp 165-166 °C (lit. mp 171.5-173 °C);¹⁵ ¹H NMR (300 MHz, CDCl₃) δ 7.42 (d, J = 8.8 Hz, 2 H), 7.34 (d, J = 8.5 Hz, 2 H), 7.20 (br s, 1 H), 2.18 (s, 3 H), 1.32 (s, 9 H); ¹³C NMR (75 MHz, CDCl₃) δ 168.8, 147.2, 135.4, 125.8, 120.1, 34.6, 31.6, 24.6; IR (neat, cm⁻¹) 3289, 3254, 3188, 3123, 3061, 2961, 1668, 1606, 1548, 1513, 1324, 1266.

N-(4-*t*-Butylphenyl)-N-methylformamide (Table 2, entry 6)¹⁶ The general procedure gave 163 mg (85%) of the title compound as a pale yellow solid: mp 49-50 °C (lit. mp 51 °C);¹⁶ ¹H NMR (300 MHz, CDCl₃) δ 8.46 (s, 1 H), 7.43 (dt, J = 8.5, 2.0 Hz, 2 H), 7.11 (dt, J = 8.5, 2.0 Hz, 2 H), 3.32 (s, 3 H), 1.35 (s, 9 H); ¹³C NMR (75 MHz, CDCl₃) δ 162.1, 149.3, 139.4, 126.4, 122.0, 34.5, 32.1, 31.4; IR (neat, cm⁻¹) 2961, 2872, 1679, 1606, 1509, 1336, 1270.

N-(4-*t*-Butylphenyl)-2-pyrrolidinone (Table 2, entry 7) The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 2 mol % Pd per mmol halide) on a 0.5 mmol scale gave 99 mg (91%) of the title compound as a white solid: mp 67-69 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.55-7.50 (m, 2 H), 7.42-7.37 (m, 2 H), 3.87 (t, J = 7.0 Hz, 2 H), 2.62 (t, J = 8.0 Hz, 2 H), 2.17 (pent, J = 7.6 Hz, 2 H), 1.33 (s, 9 H); ¹³C NMR (75 MHz, CDCl₃) δ 174.0, 147.3, 136.7, 125.6, 119.7, 48.9, 34.4, 32.8, 31.4, 18.2; IR (neat, cm⁻¹) 2961, 1695, 1602, 1393, 1305, 1224. Anal. Calcd. for C₁₄H₁₉NO: C, 77.38; H, 8.81. Found: C, 77.53; H, 8.81.

N-(3-Methoxyphenyl)-N-methylformamide (Table 2, entry 8)¹⁷ The general procedure gave 162 mg (98%) of the title compound as a colorless oil: ¹H NMR (300 MHz, CDCl₃) δ 8.48 (s, 1 H), 7.30 (t, J = 8.0 Hz, 1 H), 6.82-6.73 (m, 2 H), 6.69 (t, J = 2.3 Hz, 1 H), 3.82 (s, 3 H), 3.30 (s, 3 H); ¹³C NMR (75 MHz, CDCl₃) δ 162.3, 160.5, 143.4, 130.4, 114.5, 111.4, 108.6, 55.6, 32.2; IR (neat, cm⁻¹) 1671, 1590, 1494, 1459, 1336, 1274, 1224.

N-Phenyl-2-azetidinone (Table 2, entry 9)¹⁸ The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 1 mol % Pd per mmol halide) gave 140 mg (95%) of the title

compound as a white solid: mp 77-78.5 °C (lit. mp 75-76 °C);¹⁸ ¹H NMR (300 MHz, CDCl₃) δ 7.40-7.31 (m, 4 H), 7.13-7.07 (m, 1 H), 3.65 (t, J = 4.4 Hz, 2 H), 3.13 (t, J = 4.4 Hz, 2 H); ¹³C NMR (75 MHz, CDCl₃) δ 164.4, 138.5, 129.1, 123.8, 116.1, 38.1, 36.2; IR (neat, cm⁻¹) 1737, 1598, 1502, 1463, 1382.

N-Phenyl-2-pyrrolidinone (Table 2, entry 10)¹⁸ The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 1 mol % Pd per mmol halide) gave 158 mg (98%) of the title compound as a white solid: mp 65-66 °C (lit. mp 66-67°C);¹⁸ ¹H NMR (300 MHz, CDCl₃) δ 7.61-7.57 (m, 2 H), 7.8-7.31 (m, 2 H), 7.15-7.09 (m, 1 H), 3.81 (t, J = 7.0 Hz, 2 H), 2.57 (t, J = 8.0 Hz, 2 H), 2.16-2.06 (m, 2 H); ¹³C NMR (75 MHz, CDCl₃) δ 174.1, 139.3, 128.7, 124.3, 119.8, 48.8, 32.8, 18.1; IR (neat, cm⁻¹) 1679, 1594, 1490, 1397, 1305, 1227.

N-Phenyl-δ-valerolactam (Table 2, entry 11)¹⁸ The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 1 mol % Pd per mmol halide) gave 158 mg (90%) of the title compound as a white solid: mp 100-101 °C (lit. mp 94-95 °C);¹⁸ ¹H NMR (300 MHz, CDCl₃) δ 7.38-7.32 (m, 2 H), 7.24-7.18 (m, 3 H), 3.60-3.56 (m, 2 H), 2.54-2.49 (m, 2 H), 1.92-1.86 (m, 4 H); ¹³C NMR (75 MHz, CDCl₃) δ 169.6, 143.1, 128.8, 126.4, 125.9, 51.5, 32.7, 23.4, 21.3; IR (neat, cm⁻¹) 1640, 1594, 1490, 1428, 1347, 1328, 1305.

N-Phenyl-ε-caprolactam (Table 2, entry 12)¹⁸ The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 1 mol % Pd per mmol halide) gave 172 mg (91%) of the title compound as a pale yellow solid: mp 72-73 °C (lit. mp 69-70.5 °C);¹⁸ ¹H NMR (300 MHz, CDCl₃) δ 7.37-7.31 (m, 2 H), 7.22-7.16 (m, 3 H), 3.73-3.71 (m, 2 H), 2.68-2.66 (m, 2 H), 1.79 (br s, 6 H); ¹³C NMR (75 MHz, CDCl₃) δ 175.2, 144.3, 128.8, 126.1, 126.0, 52.9, 37.6, 29.7, 28.8, 23.5; IR (neat, cm⁻¹) 2941, 1652, 1590, 1490, 1467, 1409, 1336, 1216.

N-(4'-Chlorophenyl)-2-azetidinone (Table 2, entry 13)¹⁹ The general procedure using Pd₂(dba)₃ (4.6 mg, 0.005 mmol, 1 mol % Pd per mmol halide) gave 171 mg (94%) of the title compound as a white solid: mp 132-133 °C (lit. mp 131-132.5 °C);¹⁹ ¹H NMR (300 MHz, CDCl₃) δ 7.30 (s, 4 H), 3.63 (t, J = 4.4 Hz, 2 H), 3.14 (t, J = 4.4 Hz, 2 H); ¹³C NMR (75

MHz, CDCl₃) δ 164.4, 137.0, 129.2, 128.7, 117.4, 38.3, 36.5; IR (neat, cm⁻¹) 1733, 1598, 1494, 1378.

References

1. Kranenburg, M.; van der Burgt, Y. E. M.; Kamer, P. C. J.; van Leeuwen, P. W. N. M. *Organometallics* **1995**, 14, 3081-3089.
2. Echavarren, A. M.; Stille, J. K. *J. Am. Chem. Soc.* **1987**, 109, 5478-5486.
3. Larhed, M.; Andersson, C.-M.; Hallberg, A. *Tetrahedron* **1994**, 50, 285-304.
4. Vuihorgne, M.; LePotier, I.; Auzeil, N.; Bacqué, E.; Paris, J. M.; Fleury, M. B. *Tetrahedron* **1994**, 50, 6307-6332.
5. Kakimoto, S.; Tone, I. *J. Med. Chem.* **1965**, 8, 867-868.
6. Dharmasena, P. M.; Oliveira-Campos, A.-M. F.; Raposo, M. M. M.; Shannon, P. V. R. *J. Chem. Res. miniprint* **1994**, 8, 1601-1611.
7. Witek, S.; Bielawski, J.; Bielawski, A. *J. Prakt. Chem.* **1979**, 321, 804-812.
8. Burmistrow, S. I.; Mysyk, D. D. *Ukr. Khim. Zh. (Russ. Ed.)* **1964**, 30, 1321-1324.
9. Williams, A.; Salvadori, G. *J. Chem. Soc., Perkin Trans. 2* **1972**, 883-889.
10. Papaioannou, D.; Athanassopoulos, C.; Magafa, V.; Karamanos, N.; Stavropoulos, G.; Napoli, A.; Sindona, G.; Aksnes, D. W.; Francis, G. W. *Acta. Chem. Scand.* **1994**, 48, 324-333.
11. Williams, A.; Douglas, K. T. *J. Chem. Soc., Perkin Trans. 2* **1972**, 2112-2115.
12. Newman, M. S.; Kannan, R. *J. Org. Chem.* **1976**, 41, 3356-3359.
13. Broxton, T. J.; Deady, L. W. *J. Org. Chem.* **1974**, 39, 2767-2769.
14. Acheson, R. M.; Harvey, W. C. *J. Chem. Soc., Perkin Trans. 1* **1976**, 465-470.
15. Brunce, N. J. *Can. J. Chem.* **1977**, 55, 383-392.
16. Dallacker, F.; Eschelbach, F.-E. *Liebigs Ann. Chem.* **1965**, 689, 171-178.
17. Yoder, C. H.; Sandberg, J. A.; Moore, W. S. *J. Am. Chem. Soc.* **1974**, 96, 2260-2262.
18. Shakespeare, W. C. *Tetrahedron Lett.* **1999**, 40, 2035-2038.
19. Manhas, M. S.; Jeng, S. J. *J. Org. Chem.* **1967**, 32, 1246-1248.