Supporting Information

An Efficient Three Component Synthesis of Pyrrole Derivatives Catalyzed by Iodobenzene and Oxone[®]

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GENERAL INFORMATION

All chemicals were commercially available and used without further purification. All previously reported products were identified by comparison of their NMR spectra, melting points with literature data. Melting point was determined on a Buchi B-545 melting point apparatus. ¹H NMR spectra were recorded on 300 MHz spectrometer in CDCl₃. Column chromatography was performed on silica gel (SiO₂: 60-120 mesh).

General Experimental Procedure for Synthesis of Pyrrole derivatives

To a previously stirred mixture of iodobenzene (0.2 mmol) and Oxone[®] (1.0 mmol) in ethanol (10 mL) for 15 min at room temperature, amine (1 mmol), nitrostyrene (1.1 mmol), 1,3-dicarbonyl compound (1 mmol) and 4 Å molecular sieves (0.100 g) were added. The resultant reaction mixture was stirred at reflux temperature. After the completion of the reaction

(monitored by TLC), the reaction mixture was diluted with water (20 mL) and extracted with ethyl acetate (3 X 30 mL). The combined organic layer was washed with brine and dried over anhydrous sodium sulphate. The solvent was evaporated and crude residue was purified by column chromatography to obtain the pure product.

Characterization data of compounds

1-(2-methyl-1,4-diphenyl-1*H*-pyrrol-3-yl)ethanone (Table 2, entry 1):^[1] White solid; Mp 104-106 °C [Lit. Mp 105-107 °C]; IR (neat): 3059, 3029, 1651, 1503, 1402, 1223 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 2.10 (s, 3H), 2.42 (s, 3H), 6.67 (s, 1H), 7.31-7.43 (m, 7H), 7.45-7.50 (m, 3H).

1-[4-(4-chlorophenyl)-2-methyl-1-phenyl-1*H*-pyrrol-3-yl]ethanone (Table 2, entry 2):^[2] Yellow solid; Mp 98-100 °C [Lit. Mp 99-101 °C]; IR (neat): 3057, 3006, 1651, 1501, 1404, 1222 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 2.09 (s, 3H), 2.43 (s, 3H), 6.65 (s, 1H), 7.30-7.39 (m, 6H), 7.46-7.54 (m, 3H).

Ethyl 2-methyl-1,4-diphenyl-1*H*-pyrrole-3-carboxylate (Table 2, entry 3):^[2] Red sticky liquid; IR (neat): 3055, 2979, 1694, 1504, 1223 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.13 (t, 3H), 2.45 (s, 3H), 4.17 (q, 2H), 6.70 (s, 1H), 7.25-7.35 (m, 5H), 7.39-7.48 (m, 5H).

Ethyl 2-methyl-4-(4-methylphenyl)-1-phenyl-1*H*-pyrrole-3-carboxylate (Table 2, entry 4):^[2] Yellow oil; IR (neat): 3035, 2980, 1693, 1517, 1221 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.14 (t, 3H), 2.30 (s, 3H), 2.46 (s, 3H), 4.18 (q, 2H), 6.68 (s, 1H), 7.15-7.20 (m, 2H), 7.31-7.44 (m, 7H).

1-(1-Benzyl-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (Table 2, entry 5):^[2] White solid; Mp 50-53 °C [Lit. Mp 51-54 °C]; IR (neat): 3020, 2932, 1647, 1529, 1456, 1355, 1215 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 2.08 (s, 3H), 2.40 (s, 3H), 5.03 (s, 2H), 6.55 (s, 1H), 7.10 (d, *J* = 7.0 Hz, 2H), 7.28-7.60 (m, 8H).

1-[1-benzyl-4-(4-fluorophenyl)-2-methyl-1*H*-pyrrol-3-yl]ethanone (Table 2, entry 6):^[3]

Yellow oil; IR (neat): 3038, 2927, 1649, 1525, 1434, 1221 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): 2.04 (s, 3H), 2.43 (s, 3H), 5.02 (s, 2H), 6.57 (s, 1H), 7.08 (m, 4H), 7.22–7.30 (m, 6H).

Ethyl 1-benzyl-2-methyl-4-phenyl-1*H*-pyrrole-3-carboxylate (Table 2, entry 7):^[3]

Sticky solid; IR (neat): 3043, 2926, 1689, 1540, 1415, 1280 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): 1.13 (t, 3H); 2.47 (s, 3H); 4.15 (q, 2H); 5.06 (s, 2H); 6.49 (s, 1H); 7.10 (d, 2H); 7.15–7.33 (s, 2H).

1-(2-methyl-1-phenethyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (Table 2, entry 8):^[4]

White solid, Mp 84–86 °C [Lit. Mp 85–87 °C]; IR (neat): 3056, 2939, 1638, 1502, 1226 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): 2.00 (s, 3H), 2.38 (s, 3H), 3.01 (t, 2H), 4.05 (q, 2H), 6.38 (s, 1H), 7.09 (d, 2H), 7.23–7.38 (m, 8H).

Ethyl 2-methyl-4-phenyl-1-(2-phenylethyl)-1*H*-pyrrole-3-carboxylate (Table 2, entry 9):

Brown sticky liquid; IR (neat): 3060, 2927, 1690, 1524, 1417, 1281 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.11 (t, 3H), 2.41 (s, 3H), 3.00 (t, 2H), 4.05 (t, 2H), 4.13 (q, 2H), 6.44 (s, 1H), 7.09 (d, 2H), 7.23–7.34 (m, 8H); ¹³C NMR (CDCl₃, 100 MHz): δ 165.9, 137.7, 135.9, 130.1, 129.3, 128.7, 128.7, 127.4, 126.9, 126.0, 119.5, 59.3, 48.3, 37.6, 14.0, 11.2; Elem. Anal. Found: C, 79.06; H, 6.87; N, 4.07; Calcd. for C₂₂H₂₃N₁O₂: C, 79.25; H, 6.95, N, 4.20.

1-[1-(4-methoxyphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl]ethanone (Table 2, entry 10):^[11]

Yellow solid; Mp 89–91 °C [Lit. Mp 90–91 °C]; IR (neat): 3010, 2933, 1645, 1512, 1252 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 2.08 (s, 3H), 2.37 (s, 3H), 3.86 (s, 3H), 6.62 (s, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 7.24 (d, *J* = 8.9 Hz, 2H), 7.30–7.35 (m, 1H), 7.36–7.38 (m, 4H).

1-[1-(4-Bromophenyl)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrol-3-yl]-ethanone (Table 2,

entry 11):^[11] Red solid, Mp 116–118 °C [Lit. Mp 119–121 °C]; IR (neat): 3009, 2928, 1646, 1402,

1242 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 2.07 (s, 3H), 2.42 (s, 3H), 3.81 (s, 3H), 6.64 (s, 1H), 6.94 (d, *J* = 8.5 Hz, 2H), 7.22-7.33 (m, 4H), 7.58 (d, *J* = 8.5 Hz, 2H).

Ethyl 1-(4-bromophenyl)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (Table 2, entry 12): Yellow solid; Mp 118-120 °C ; IR (neat): 3105, 2924, 1681, 1523, 1489, 1240 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.17 (t, 3H), 2.44 (s, 3H), 3.83 (s, 3H), 4.19 (q, 2H), 6.64 (s, 1H), 6.88-6.90 (d, *J* = 8 Hz, 2H), 7.19-7.21 (d, *J* = 8 Hz, 2H), 7.33-7.35 (d, *J* = 8 Hz, 2H), 7.61-7.63 (d, *J* = 8 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz): δ 165.7, 158.4, 138.0, 136.2, 132.5, 130.3, 127.8, 127.7, 126.6, 121.8, 120.3, 113.1, 113.0, 59.5, 55.3, 14.2, 12.7; Elem. Anal. Found: C, 60.72; H, 4.79; N, 3.29; Calcd. for C₂₁H₂₀BrN₁O₃: C, 60.88; H, 4.87, N, 3.38.

1-[1,4-bis(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl]ethanone (Table 2, entry 13): Red solid; Mp 166-168 °C; IR (neat): 3076, 3049, 1651, 1512, 1494, 1222 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 2.08 (t, 3H), 2.39 (s, 3H), 6.63 (s, 1H), 7.26-7.37 (m, 6H), 7.46-7.48 (d, *J* = 8.8 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz): δ 197.2, 162.3, 161.1, 135.4, 134.2, 132.9, 130.4, 128.5, 127.4, 125.3, 122.7, 120.5, 116.5, 115.2, 31.2, 12.9; Elem. Anal. Found: C, 66.18; H, 4.26; N, 3.97; Calcd. for C₁₉H₁₅Cl₂N₁O₁: C, 66.29; H, 4.39, N, 4.07.

Ethyl 1-(4-chlorophenyl)-2-methyl-4-phenyl-1*H*-pyrrole-3-carboxylate (Table 2, entry 14):^[5] White solid; Mp 98-100 °C [Lit. Mp 99-100 °C]; IR (neat): 3017, 2984, 1693, 1526, 1499, 1227 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.13 (t, 3H), 2.44 (s, 3H), 4.18 (q, 2H), 6.67 (s, 1H), 7.26-7.35 (m, 5H), 7.39-7.41 (d, *J* = 8 Hz, 2H), 7.45-7.47 (d, *J* = 8 Hz, 2H).

1-[4-(4-Chlorophenyl)-1-cyclohexyl-2-methyl-1*H*-pyrrol-3-yl]-ethanone (Table 2, entry 15):^[1] White solid; Mp 99-101 °C [Lit. Mp 98-100 °C]; IR (neat) 2930, 2855, 1646, 1506, 1415 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.21-1.26 (m, 2H), 1.39-1.48 (m, 2H), 1.57-1.65 (m, 2H),

1.78 (d, $J = 13$ Hz, 2H), 1.92 (d, $J = 13$ Hz, 2H), 2.00 (s, 3H), 2.46 (s, 3H), 3.91 (t, 1H), 6.56 (s, 1H), 7.26 (d, $J = 8.7$ Hz, 2H), 7.32 (d, $J = 8.7$ Hz, 2H).

Ethyl 2-methyl-4-phenyl-1-(2-phenylethyl)-1*H*-pyrrole-3-carboxylate (Table 2, entry 9):

Ethyl 1-(4-bromophenyl)-4-(4-methoxyphenyl)-2-methyl-1*H*-pyrrole-3-carboxylate (Table 2, entry 12):

1-[1,4-bis(4-chlorophenyl)-2-methyl-1*H*-pyrrol-3-yl]ethanone (Table 2, entry 13):

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