

Supporting Information

One-pot Oxidative Decarboxylation–Friedel-Crafts Reaction of Acyclic α -Amino Acid Derivatives Activated by the Combination of Iodobenzene Diacetate/Iodine and Iron Dust

Renhua Fan,* Weixun Li and Bing Wang*

1-((2,5-dimethoxyphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2b): ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.25 (m, 5H), 6.79-6.78 (m, 2H), 6.73-6.72 (m, 2H), 3.73 (s, 3H), 3.65 (s, 3H), 2.68 (s, 4H); ^{13}C NMR δ 176.9, 153.2, 151.4, 137.6, 128.53, 128.50, 127.7, 127.2, 117.7, 113.0, 111.1, 56.2, 55.6, 53.7, 28.2; IR (neat cm^{-1}): ν = 2935, 1705, 1496, 1386, 1221, 1171; HRMS calcd for $\text{C}_{19}\text{H}_{19}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 348.1212, found: 348.1210.

1-((3,4-dimethoxyphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2c): ^1H NMR (400 MHz, CDCl_3) δ 7.30-7.23 (m, 5H), 6.97 (d, J = 1.8 Hz, 1H), 6.93 (dd, J = 8.2, 1.8 Hz, 1H), 6.81 (d, J = 8.2 Hz, 1H), 6.49 (s, 1H), 3.85 (s, 3H), 3.79 (s, 3H), 2.70 (s, 4H); ^{13}C NMR δ 176.9, 148.87, 148.83, 137.7, 130.2, 128.4, 128.1, 127.6, 121.8, 112.7, 110.8, 58.3, 56.0, 55.9, 28.2; IR (neat cm^{-1}): ν = 2937, 1774, 1705, 1592, 1516, 1464, 1358; HRMS calcd for $\text{C}_{19}\text{H}_{19}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 348.1212, found: 348.1210.

1-(benzo[d][1,3]dioxol-5-yl)(phenyl)methylpyrrolidine-2,5-dione (2d): ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.24 (m, 5H), 6.85 (d, J = 1.8 Hz, 1H), 6.78 (dd, J = 8.2, 1.8 Hz, 1H), 6.73 (d, J = 8.2 Hz, 1H), 6.45 (s, 1H), 5.92 (s, 2H), 2.69 (s, 4H); ^{13}C NMR δ 176.8, 147.8, 147.3, 137.6, 131.5,

128.4, 128.3, 127.8, 122.6, 109.6, 108.0, 101.3, 58.3, 28.2; IR (neat cm^{-1}): $\nu = 2900, 1774, 1705, 1444, 1489, 1362$; HRMS calcd for $\text{C}_{18}\text{H}_{15}\text{NNaO}_4$ ($[\text{M}+\text{Na}]^+$): 332.0899, found: 332.0894.

1-((4-methoxy-3,5-dimethylphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2e): ^1H NMR (400 MHz, CDCl_3) δ 7.30-7.26 (m, 5H), 6.96 (s, 2H), 6.44(s, 1H), 3.71 (s, 3H), 2.74 (s, 4H), 2.24 (s, 6H); ^{13}C NMR δ 176.8, 156.6, 137.8, 133.0, 130.8, 129.3, 128.5, 128.3, 127.7, 59.7, 58.1, 28.3, 16.3; IR (neat cm^{-1}): $\nu = 2924, 1708, 1540, 1456, 1378, 1171$; HRMS calcd for $\text{C}_{20}\text{H}_{21}\text{NNaO}_3$ ($[\text{M}+\text{Na}]^+$): 346.1419, found: 346.1414.

1-((5-tert-butyl-2-ethoxyphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2f): ^1H NMR (400 MHz, CDCl_3) δ 7.37-7.23 (m, 6H), 7.14 (d, $J = 2.3$ Hz, 1H), 6.77-6.75 (m, 2H), 4.02-3.94 (m, 2H), 2.67 (s, 4H), 1.32 (t, $J = 7.4$ Hz, 3H), 1.18 (s, 9H); ^{13}C NMR δ 176.8, 154.3, 142.4, 138.0, 128.5, 128.4, 127.6, 125.4, 125.3, 110.3, 63.7, 54.0, 34.1, 31.5, 31.4, 28.2, 15.0; IR (neat cm^{-1}): $\nu = 2961, 1708, 1503, 1477, 1360, 1250$; HRMS calcd for $\text{C}_{23}\text{H}_{27}\text{NNaO}_3$ ($[\text{M}+\text{Na}]^+$): 388.1889, found: 388.1904.

1-((2-ethoxyphenyl)(phenyl)methyl)pyrrolidine-2,5-dione **and**

1-((4-ethoxyphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2g): ^1H NMR (400 MHz, CDCl_3) δ 7.35-7.21 (m, 6.55H), 7.04, (d, $J = 7.3$ Hz, 0.45H), 6.86-6.82 (m, 2H), 6.73, (s, 0.45H), 6.5 (s, 0.55H), 4.05-3.95 (m, 2H), 2.71 (s, 2H), 2.76 (s, 2H), 1.41 (t, $J = 6.9$ Hz, 1.55H) 1.32 (t, $J = 6.9$ Hz, 1.45H) ; ^{13}C NMR δ 176.8, 158.6, 156.4, 137.9, 130.9, 130.3, 129.6, 129.0, 128.6, 128.5, 128.4, 128.3, 127.6, 126.0, 120.0, 114.3, 110.9, 63.6, 63.5, 58.0, 54.0, 28.3, 28.2, 14.9; IR (neat cm^{-1}): $\nu = 2979, 1705, 1610, 1512, 1492, 1359, 1045$; HRMS calcd for $\text{C}_{19}\text{H}_{19}\text{NNaO}_3$ ($[\text{M}+\text{Na}]^+$): 332.1263, found: 332.1258.

1-(mesityl(phenyl)methyl)pyrrolidine-2,5-dione (2i): ^1H NMR (400 MHz, CDCl_3) δ 7.28-7.24 (m, 3H), 7.04 (d, $J = 7.7$ Hz, 2H), 6.82 (s, 2H), 6.77 (s, 1H), 2.76 (s, 4H), 2.24 (s, 3H), 2.06 (s, 6H); ^{13}C NMR δ 176.7, 138.8, 138.1, 137.6, 130.4, 130.3, 128.6, 127.1, 126.7, 56.0, 28.2, 21.8, 20.9; IR

(neat cm^{-1}): $\nu = 2922, 1777, 1708, 1610, 1450, 1351, 1172$; HRMS calcd for $\text{C}_{20}\text{H}_{21}\text{NNaO}_2$ ($[\text{M}+\text{Na}]^+$): 330.1470, found: 330.1461.

1-((2,5-dimethylphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2j): ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.16 (m, 5H), 7.12 (s, 1H), 7.06 (d, $J = 7.8$ Hz, 1H), 7.02 (d, $J = 7.8$ Hz, 1H), 6.63 (s, 1H), 2.73 (s, 4H), 2.26 (s, 3H), 2.19 (s, 3H); ^{13}C NMR δ 177.0, 137.4, 135.7, 135.5, 133.2, 130.5, 129.8, 128.7, 128.5, 128.4, 127.6, 56.0, 28.2, 21.3, 19.3; IR (neat cm^{-1}): $\nu = 2923, 1775, 1705, 1497, 1381, 1358, 1175$; HRMS calcd for $\text{C}_{19}\text{H}_{19}\text{NNaO}_2$ ($[\text{M}+\text{Na}]^+$): 316.1314, found: 316.1313.

1-((3,4-dimethylphenyl)(phenyl)methyl)pyrrolidine-2,5-dione **and**

1-((2,3-dimethylphenyl)(phenyl)methyl)pyrrolidine-2,5-dione (2k): ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.27 (m, 5H), 7.07-7.06 (m, 3H), 6.70 (s, 0.2H), 6.49 (s, 0.8H), 2.71 (s, 0.8H), 2.70 (s, 3.2H), 2.28 (s, 0.6H), 2.24 (s, 2.4H), 2.22 (s, 2.4H), 2.12 (s, 0.6H); ^{13}C NMR δ 177.0, 176.9, 137.8, 137.0, 136.7, 136.3, 135.1, 134.8, 130.1, 129.7, 128.6, 128.5, 128.4, 127.7, 127.2, 126.4, 125.3, 58.3, 56.5, 28.3, 28.2, 20.9, 19.9, 19.5, 15.3; IR (neat cm^{-1}): $\nu = 2922, 1705, 1496, 1357, 1174$; HRMS calcd for $\text{C}_{19}\text{H}_{19}\text{NNaO}_2$ ($[\text{M}+\text{Na}]^+$): 316.1314, found: 316.1306.

1-(furan-2-yl(phenyl)methyl)pyrrolidine-2,5-dione (2m): ^1H NMR (400 MHz, CDCl_3) δ 7.54-7.34 (m, 6H), 6.45 (s, 1H), 6.34 (dd, $J = 3.2, 1.8$ Hz, 1H), 6.16 (d, $J = 3.2$ Hz, 1H), 2.72 (s, 4H); ^{13}C NMR δ 176.4, 150.4, 142.3, 136.2, 128.9, 128.7, 128.6, 110.6, 109.9, 52.8, 28.2; IR (neat cm^{-1}): $\nu = 2919, 1708, 1498, 1376, 1355, 1176$; HRMS calcd for $\text{C}_{15}\text{H}_{13}\text{NNaO}_3$ ($[\text{M}+\text{Na}]^+$): 278.0793, found: 278.0790.

1-(phenyl(thiophen-2-yl)methyl)pyrrolidine-2,5-dione (2n): ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.25 (m, 6H), 7.04 (d, $J = 3.6$ Hz, 1H), 6.97 (dd, $J = 5.0, 3.6$ Hz, 1H), 6.75 (s, 1H), 2.71 (s, 4H); ^{13}C NMR δ 176.3, 140.1, 137.6, 128.5, 128.3, 128.2, 126.6, 126.2, 54.0, 28.2; IR (neat cm^{-1}): ν

= 2925, 1706, 1386, 1363, 1175, 1120 cm^{-1} ; HRMS calcd for $\text{C}_{15}\text{H}_{13}\text{NNaO}_2\text{S}$ ($[\text{M}+\text{Na}]^+$): 294.0567,
found: 294.0555.