Supporting Information

Palladium-Catalyzed Synthesis of Aldehydes from Aryl Halides and tert-Butyl Isocyanide using Formate salts as a Hydride Donor

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General information:

All reactants and reagents were purchased from commercial suppliers. All anhydrous solvents used in the reactions were dried and freshly distilled. TLC was performed on silica HSGF254 plates. Melting points were determined with a digital melting-point apparatus. $^1$H and $^{13}$C NMR spectra were obtained at 400/101 or 600/125 MHz, respectively. NMR spectra were run in a solution of deuterated chloroform (CDCl$_3$) or DMSO-$d_6$ and were reported in parts per million (ppm). LRMS analyses were carried out on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry.

Typical experimental procedure for reductive formylation reaction of aryl halides:

Into a 15 mL sealed tube was added aryl halides (0.7 mmol), tert-butyl isocyanide (0.84 mmol, 95 μL), Pd(OAc)$_2$ (0.032 mmol, 7 mg), dppe (0.063 mmol, 25 mg), HCO$_2$Na (1.4 mmol, 95 mg) and anhydrous DMSO (3.0 mL). The mixture was stirred at 120 °C under nitrogen. After completion of the reaction indicated by TLC, the mixture was extracted with Et$_2$O (3×10 mL). The combined organic layer was dried over Na$_2$SO$_4$, and the filtrate was then concentrated under vacuum. The residue was purified by column chromatography on silica gel using petroleum ether (30—60 °C)/Et$_2$O as eluent to provide the pure desired product.

4-Methylbenzaldehyde (2a):\(^1\)

![4-Methylbenzaldehyde (2a)](image)

Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 95% (80 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 9.96 (s, 1H), 7.77 (d, J = 8.0 Hz, 2H), 7.32 (d, J = 7.9 Hz, 2H), 2.43 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 192.1, 145.6, 134.2, 129.9, 129.8, 22.0. LRMS (ESI): m/z calcd for C$_8$H$_7$O [M + H]$^+$, 121.1; found, 121.0.

2-Methylbenzaldehyde (2b):\(^1\)

![2-Methylbenzaldehyde (2b)](image)

Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 65% (55 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 9.98 (s, 1H), 7.67 (d, J = 7.1 Hz, 2H), 7.45–7.38 (m, 2H), 2.43 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 192.6, 139.0, 136.5, 135.4, 130.1, 128.9, 127.3, 21.3. LRMS (ESI): m/z calcd for C$_8$H$_7$O [M + H]$^+$, 121.1; found, 121.0.

3,5-Dimethylbenzaldehyde (2c):\(^2\)

![3,5-Dimethylbenzaldehyde (2c)](image)

Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 84% (79 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 9.84 (s, 1H), 7.38 (s, 2H), 7.15 (s, 1H), 2.28 (s, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 192.8, 138.8, 136.6, 136.2, 127.6, 21.1. LRMS (ESI): m/z calcd for C$_8$H$_7$O [M + H]$^+$, 135.1; found, 134.9.
4-tert-Butylbenzaldehyde (2d): Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 90% (102 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.97 (s, 1H), 7.81 (d, $J$ = 8.4 Hz, 2H), 7.54 (d, $J$ = 8.3 Hz, 2H), 1.34 (s, 9H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 192.1, 158.5, 134.2, 129.8, 126.1, 35.4, 31.1. LRMS (ESI): $m/z$ calcd for C$_{11}$H$_{14}$O [M + H]$^+$, 163.1; found, 163.0.

4-Methoxybenzaldehyde (2e): Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 66% (63 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.78 (s, 1H), 7.74 (d, $J$ = 8.6 Hz, 2H), 6.90 (d, $J$ = 8.4 Hz, 2H), 3.78 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 190.8, 164.6, 132.0, 129.9, 114.3, 55.6. LRMS (ESI): $m/z$ calcd for C$_8$H$_8$O$_2$ [M + H]$^+$, 137.0; found, 136.9.

3-Methoxybenzaldehyde (2f): Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 61% (58 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.97 (s, 1H), 7.47–7.42 (m, 2H), 7.39 (s, 1H), 7.18 (d, $J$ = 6.6 Hz, 1H), 3.86 (s, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 192.3, 160.2, 137.9, 130.1, 123.6, 123.6, 112.1, 55.6. LRMS (ESI): $m/z$ calcd for C$_8$H$_8$O$_2$ [M + H]$^+$, 137.0; found, 137.0.

3,4,5-Trimethoxybenzaldehyde (2g): Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 80% (93 mg). M.p 68- 70 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.88 (s, 1H), 7.14 (s, 2H), 3.94 (s, 9H). $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 191.2, 153.7, 143.6, 131.8, 106.8, 61.1, 56.4. LRMS (ESI): $m/z$ calcd for C$_{10}$H$_{12}$O$_4$ [M + H]$^+$, 167.1; found, 167.1.

4-Fluorobenzaldehyde (2h): Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 85% (74 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.98 (s, 1H), 7.95–7.89 (m, 2H), 7.22 (t, $J$ = 8.6 Hz, 2H). $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 190.6 (s), 166.6 (d, $J$ = 256.7 Hz), 133.1 (d, $J$ = 2.7 Hz), 132.3 (d, $J$ = 9.7 Hz), 116.4 (d, $J$ = 22.3 Hz). LRMS (ESI):
3,5-Difluorobenzaldehyde (2i):\(^6\)

![3,5-Difluorobenzaldehyde](image)

Prepared from corresponding aryl iodide for 6 h. Colorless oil. Yield: 55% (55 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.96 (s, 1H), 7.45–7.38 (dd, \(J = 6.9, 1.9\) Hz, 2H), 7.10 (tt, \(J = 8.4, 2.4\) Hz, 1H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 189.5 (t, \(J = 2.5\) Hz), 163.5 (dd, \(J = 252.5, 11.5\) Hz), 133.5 (s), 112.3 (m), 109.9 (t, \(J = 25.5\) Hz). LRMS (ESI): m/z calcd for C\(_7\)H\(_5\)FO [M + H]\(^+\), 125.0; found, 124.9.

4-Chlorobenzaldehyde (2j):\(^5\)

![4-Chlorobenzaldehyde](image)

prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 70% (69 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.98 (s, 1H), 7.82 (d, \(J = 8.5\) Hz, 2H), 7.51 (d, \(J = 8.4\) Hz, 2H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 191.0, 141.1, 134.8, 131.0, 129.6. LRMS (ESI): m/z calcd for C\(_7\)H\(_5\)ClO [M + H]\(^+\), 141.0; found, 141.0.

4-(Trifluoromethyl)benzaldehyde (2k):\(^3\)

![4-(Trifluoromethyl)benzaldehyde](image)

Prepared from corresponding aryl iodide for 3 h. Colorless oil. Yield: 73% (89 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.11 (s, 1H), 8.02 (d, \(J = 7.9\) Hz, 2H), 7.99 (d, \(J = 8.4\) Hz, 2H). \(^13\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 191.1 (s), 138.7 (d, \(J = 1.0\) Hz), 135.6 (q, \(J = 32.7\) Hz), 129.9 (s), 126.1 (q, \(J = 3.8\) Hz), 123.5 (q, \(J = 272.9\) Hz). LRMS (ESI): m/z calcd for C\(_8\)H\(_5\)F\(_3\)O [M + H]\(^+\), 175.0; found, 175.0.

4-Acetylbenzaldehyde (2l):\(^4\)

![4-Acetylbenzaldehyde](image)

Prepared from corresponding aryl iodide for 24 h. Colorless oil. Yield: 64% (66 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.12 (s, 1H), 8.11 (d, \(J = 8.1\) Hz, 2H), 7.99 (d, \(J = 8.4\) Hz, 2H). \(^13\)C NMR (151 MHz, CDCl\(_3\)) \(\delta\) 197.6, 191.8, 141.3, 139.2, 130.0, 129.0, 27.1. LRMS (ESI): m/z calcd for C\(_9\)H\(_8\)O\(_2\) [M + H]\(^+\), 149.1; found, 149.0.

4-Formylbenzonitrile (2m):\(^1\)

![4-Formylbenzonitrile](image)
Prepared from corresponding aryl iodide for 6 h. Colorless oil. Yield: 49% (45 mg). \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\) 10.03 (s, 1H), 7.94 (d, \(J = 8.3\) Hz, 2H), 7.79 (d, \(J = 8.2\) Hz, 2H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 190.8, 138.8, 133.0, 129.9, 117.8, 117.6. LRMS (ESI): m/z calcd for C\(_9\)H\(_9\)NO [M + H]\(^+\), 164.1; found, 164.0.

**Biphenyl-4-carbaldehyde (2n):**

![Biphenyl-4-carbaldehyde](image)

Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 77% (98 mg). Mp. 55–56 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.00 (s, 1H), 7.89 (d, \(J = 8.1\) Hz, 2H), 7.69 (d, \(J = 8.2\) Hz, 2H), 7.58 (d, \(J = 7.6\) Hz, 2H), 7.44 (t, \(J = 7.5\) Hz, 2H), 7.38 (t, \(J = 7.1\) Hz, 1H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 191.9, 147.0, 139.6, 135.1, 130.2, 129.0, 128.5, 127.6, 127.3. LRMS (ESI): m/z calcd for C\(_{13}\)H\(_7\)O [M + H]\(^+\), 183.1; found, 183.0.

**4-(dimethylamino)benzaldehyde (2o):**

![4-(dimethylamino)benzaldehyde](image)

Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 90% (94 mg). M.p 69–71 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.73 (s, 1H), 7.73 (d, \(J = 7.7\) Hz, 2H), 6.69 (d, \(J = 7.5\) Hz, 2H), 3.08 (s, 6H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 190.4, 154.4, 132.1, 125.3, 111.1, 40.2. LRMS (ESI): m/z calcd for C\(_9\)H\(_{11}\)NO [M + H]\(^+\), 150.1; found, 150.1.

**4-Hydroxymethylbenzaldehyde (2p):**

![4-Hydroxymethylbenzaldehyde](image)

Prepared from corresponding aryl iodide for 6 h. Colorless oil. Yield: 94% (90 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.90 (s, 1H), 7.79 (d, \(J = 7.9\) Hz, 2H), 7.47 (d, \(J = 7.9\) Hz, 2H), 4.73 (s, 2H), 3.69 (brs, 1H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 192.52, 148.27, 135.32, 130.00, 126.92, 64.16. LRMS (ESI): m/z calcd for C\(_8\)H\(_6\)O\(_2\) [M + H]\(^+\), 137.1; found, 137.1.

**N-(4-formylphenyl)acetamide (2q):**

![N-(4-formylphenyl)acetamide](image)

Prepared from corresponding aryl iodide for 6 h. Yellow solid. Yield: 82% (94 mg). M.p 155–157 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.91 (s, 1H), 8.07 (s, 1H), 7.83 (d, \(J = 8.5\) Hz, 2H), 7.72 (d, \(J = 8.4\) Hz, 2H), 2.23 (s, 3H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 191.3, 169.1, 143.8, 132.3, 131.3, 119.4, 24.9. LRMS (ESI): m/z calcd for C\(_9\)H\(_8\)NO\(_2\) [M + H]\(^+\), 164.1; found, 164.0.
Ethyl-4-formylbenzoate (2r):[^1]

Prepared from corresponding aryl iodide for 6 h. Colorless liquid. Yield: 91% (113 mg). ^1H NMR (400 MHz, CDCl₃) δ 10.09 (s, 1H), 8.19 (d, J = 8.4 Hz, 2H), 7.94 (d, J = 8.6 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H). ^13C NMR (101 MHz, CDCl₃) δ 191.8, 165.6, 139.1, 135.5, 130.2, 129.6, 61.7, 14.3.

LRMS (ESI): m/z calcd for C₁₀H₁₀O₂ [M + H]^+, 179.1; found, 179.0.

2,3-Dihydrobenzo[b][1,4]dioxine-6-carbaldehyde (2s):[^3]

Prepared from corresponding aryl iodide for 3 h. White solid. Yield: 73% (84 mg). M.p 51–53 °C. ^1H NMR (400 MHz, CDCl₃) δ 9.80 (s, 1H), 7.38 (d, J = 5.9 Hz, 2H), 6.96 (d, J = 8.7 Hz, 1H), 4.32 (d, J = 3.9 Hz, 2H), 4.28 (d, J = 4.4 Hz, 2H). ^13C NMR (101 MHz, CDCl₃) δ 190.8, 149.3, 143.9, 130.6, 124.2, 118.3, 117.8, 64.7, 64.0. LRMS (ESI): m/z calcd for C₁₃H₁₀O₂ [M + H]^+, 165.1; found, 165.0.

1-Naphthaldehyde (2t):[^1]

Prepared from corresponding aryl iodide for 3 h. Yellow oil. Yield: 80% (87 mg). ^1H NMR (400 MHz, CDCl₃) δ 10.36 (s, 1H), 9.24 (d, J = 8.6 Hz, 1H), 8.05 (d, J = 8.2 Hz, 1H), 7.93 (d, J = 6.9 Hz, 1H), 7.88 (d, J = 8.1 Hz, 1H), 7.66 (t, J = 7.7 Hz, 1H), 7.57 (q, J = 7.1 Hz, 2H). ^13C NMR (101 MHz, CDCl₃) δ 193.7, 136.8, 135.4, 133.8, 131.4, 130.6, 129.4, 128.6, 127.0, 124.9. LRMS (ESI): m/z calcd for C₁₃H₉O [M + H]^+, 157.1; found, 157.0.

Thiophene-2-carbaldehyde (2u):[^1]

Prepared from corresponding aryl iodide for 8 h. Yellow oil. Yield: 38% (30 mg). ^1H NMR (400 MHz, CDCl₃) δ 9.95 (s, 1H), 7.80–7.77 (m, 2H), 7.22 (t, J = 4.3 Hz, 1H). ^13C NMR (101 MHz, CDCl₃) δ 183.1, 144.0, 136.5, 135.2, 128.4. LRMS (ESI): m/z calcd for C₇H₈OS [M + H]^+, 113.0; found, 113.0.

Pyridine-3-carbaldehyde (2v):[^1]

Prepared from corresponding aryl iodide for 3 h. Yellow oil. Yield: 69% (52 mg) ^1H NMR (400 MHz, CDCl₃) δ 10.14 (s, 1H), 9.11 (s, 1H), 8.87 (d, J = 4.6 Hz, 1H), 8.20 (dt, J = 7.9, 1.9 Hz, 1H), 7.52 (dd, J = 7.7, 5.0
Hz, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 190.8, 154.7, 152.0, 135.9, 131.4, 124.2. LRMS (ESI): $m/z$ calcd for C$_{10}$H$_6$NO [M + H]$^+$, 158.1; found, 158.0.

Benzo[b]thiophene-3-carbaldehyde (2w):$^3$

![Image of Benzo[b]thiophene-3-carbaldehyde](image)

Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 57% (65 mg). M.p 49–50 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 10.13 (s, 1H), 8.68 (d, $J$ = 7.7 Hz, 1H), 8.31 (s, 1H), 7.88 (d, $J$ = 7.9 Hz, 1H), 7.48 (dt, $J$ = 22.8, 7.3 Hz, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 185.5, 143.4, 140.5, 136.5, 135.2, 126.2, 124.9, 122.5. LRMS (ESI): $m/z$ calcd for C$_{10}$H$_6$OS [M + H]$^+$, 163.0; found, 162.9.

1-Methyl-1H-indole-5-carbaldehyde (2x):$^6$

![Image of 1-Methyl-1H-indole-5-carbaldehyde](image)

Prepared from corresponding aryl iodide for 6 h. White solid. Yield: 36% (40 mg). M.p 79–81 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 10.03 (s, 1H), 8.15 (s, 1H), 7.80 (d, $J$ = 8.6 Hz, 1H), 7.40 (d, $J$ = 8.6 Hz, 1H), 7.15 (d, $J$ = 3.1 Hz, 1H), 6.65 (d, $J$ = 3.0 Hz, 1H), 3.84 (s, 3H). $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 192.7, 140.1, 130.9, 129.4, 128.3, 126.6, 122.0, 109.9, 103.4, 33.3. LRMS (ESI): $m/z$ calcd for C$_{10}$H$_6$NO [M + H]$^+$, 160.1; found, 159.9.

Isoquinoline-6-carbaldehyde (2y):$^6$

![Image of Isoquinoline-6-carbaldehyde](image)

Prepared from corresponding aryl iodide for 3 h. Yellow solid. Yield: 87% (96 mg). M.p 73–75 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 10.37 (s, 1H), 9.31 (s, 1H), 8.96 (d, $J$ = 6.0 Hz, 1H), 8.69 (d, $J$ = 6.0 Hz, 1H), 8.20 (t, $J$ = 8.2 Hz, 2H), 7.75 (dd, $J$ = 8.0, 7.3 Hz, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 192.7, 153.0, 146.4, 140.0, 134.9, 133.4, 130.7, 128.8, 126.7, 117.9. LRMS (ESI): $m/z$ calcd for C$_{10}$H$_6$NO [M + H]$^+$, 158.1; found, 158.0.

Quinoline-2-carbaldehyde (2z):$^6$

![Image of Quinoline-2-carbaldehyde](image)

Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 68% (75 mg). M.p 69–71 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 10.23 (s, 1H), 8.31 (d, $J$ = 8.4 Hz, 1H), 8.25 (d, $J$ = 8.5 Hz, 1H), 8.03 (d, $J$ = 8.4 Hz, 1H), 7.90 (d, $J$ = 8.2 Hz, 1H), 7.83 (dd, $J$ = 8.3, 7.1 Hz, 1H), 7.69 (t, $J$ = 7.5 Hz, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 193.9, 152.7, 148.0, 137.5, 130.6, 130.5, 130.2, 129.3, 128.0, 117.5. LRMS (ESI): $m/z$ calcd for C$_{10}$H$_6$NO [M + H]$^+$, 158.1; found, 158.0.

Quinoline-3-carbaldehyde (2aa):$^6$

![Image of Quinoline-3-carbaldehyde](image)
Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 76% (84 mg). M.p 70–72 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 10.22 (s, 1H), 9.34 (s, 1H), 8.60 (s, 1H), 8.16 (d, J = 8.5 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.86 (dd, J = 8.4, 7.0 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 190.8, 150.6, 149.2, 140.3, 132.8, 129.8, 129.5, 128.6, 128.0, 127.1. LRMS (ESI): m/z calcd for C$_{18}$H$_{18}$NO [M + H]$^+$, 158.1; found, 158.0.

2-Methylquinoline-6-carbaldehyde (2bb):$^{13}$

Prepared from corresponding aryl bromide for 30 h. White solid. Yield: 87% (104 mg). M.p 73–75 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 10.10 (s, 1H), 8.23 (s, 1H), 8.12 (m, 2H), 8.04 (d, J = 8.7 Hz, 1H), 7.34 (d, J = 8.4 Hz, 1H), 2.74 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 191.5, 162.4, 150.6, 137.4, 133.7, 133.4, 129.9, 126.9, 125.9, 123.2, 25.72. LRMS (ESI): m/z calcd for C$_{15}$H$_{19}$NO [M + H]$^+$, 172.1; found, 172.0.

Anthracene-9-carbaldehyde (2cc):$^{14}$

Prepared from corresponding aryl bromide for 30 h. Yellow solid. Yield: 56% (81 mg). M.p 113–114 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 11.36 (s, 1H), 8.85 (d, J = 9.0 Hz, 2H), 8.47 (s, 1H), 7.90 (d, J = 8.4 Hz, 2H), 7.58 (t, J = 7.8 Hz, 2H), 7.45 (t, J = 7.5 Hz, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 192.9, 135.2, 132.0, 130.9, 129.3, 129.0, 125.6, 124.5, 123.5. LRMS (ESI): m/z calcd for C$_{17}$H$_{16}$NO [M + H]$^+$, 207.1; found, 206.9.

4-(1H-pyrrol-1-yl)benzaldehyde (2dd):$^{15}$

Prepared from corresponding aryl iodide for 6 h. Brown solid. Yield: 92% (110 mg). M.p 92–94 °C. $^1$H NMR (CDCl$_3$, 400 MHz) δ 9.98 (s, 1H), 7.94 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.19 (s, 2H), 6.41 (s, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 190.9, 145.0, 133.3, 131.5, 119.7, 119.1, 112.0. LRMS (ESI): m/z calcd for C$_{17}$H$_{14}$NO [M + H]$^+$, 172.1; found, 172.1.

3-Iodobenzaldehyde (2ee):$^{16}$

Prepared from 1,3-diodobenzene for 12 h. Yellow solid. Yield: 45% (73 mg). M.p 58–59 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 9.92 (s, 1H), 8.21 (s, 1H), 7.96 (d, J = 7.8 Hz, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.33 – 7.18 (m, 1H), 7.35 – 7.26 (m, 1H). $^{13}$C NMR (151 MHz, CDCl$_3$) δ 190.8, 143.3, 138.6, 138.1, 130.8, 129.0, 94.8.
LRMS (ESI): m/z calcd for CrH5IO [M + H]+, 232.9; found, 233.0.

Spectra data for NMR of aldehydes

$^1$H NMR spectrum of compound 2a

$^{13}$C NMR spectrum of compound 2a
$^1$H NMR spectrum of compound 2b

$^{13}$C NMR spectrum of compound 2b
$^1$H NMR spectrum of compound 2c

$^{13}$C NMR spectrum of compound 2c
$^1$H NMR spectrum of compound 2d

$^{13}$C NMR spectrum of compound 2d
$^1$H NMR spectrum of compound 2e

$^{13}$C NMR spectrum of compound 2e
$^1$H NMR spectrum of compound 2f

$^{13}$C NMR spectrum of compound 2f
$^1$H NMR spectrum of compound 2g

$^{13}$C NMR spectrum of compound 2g
$^1$H NMR spectrum of compound 2h

$^{13}$C NMR spectrum of compound 2h
$^1$H NMR spectrum of compound 2i

$^{13}$C NMR spectrum of compound 2i
$^1$H NMR spectrum of compound 2j

$^{13}$C NMR spectrum of compound 2j
$^1$H NMR spectrum of compound 2k

$^{13}$C NMR spectrum of compound 2k
$^1$H NMR spectrum of compound 2l

$^{13}$C NMR spectrum of compound 2l
$^1$H NMR spectrum of compound 2m

$^{13}$C NMR spectrum of compound 2m
$^1$H NMR spectrum of compound 2n

$^{13}$C NMR spectrum of compound 2n
$^1$H NMR spectrum of compound 2p

$^{13}$C NMR spectrum of compound 2p
\(^1\)H NMR spectrum of compound 2q

\[^{13}\text{C} \] NMR spectrum of compound 2q
$^1$H NMR spectrum of compound 2r

$^{13}$C NMR spectrum of compound 2r
\(^1\)H NMR spectrum of compound 2s

\[^{13}\]C NMR spectrum of compound 2s
$^1$H NMR spectrum of compound 2t

$^{13}$C NMR spectrum of compound 2t
$^1$H NMR spectrum of compound 2u

$^{13}$C NMR spectrum of compound 2u
$^1$H NMR spectrum of compound 2v

$^{13}$C NMR spectrum of compound 2v
$^1$H NMR spectrum of compound 2w

$^{13}$C NMR spectrum of compound 2w
\(^1\)H NMR spectrum of compound 2x

\(^{13}\)C NMR spectrum of compound 2x
$^1$H NMR spectrum of compound 2y

$^{13}$C NMR spectrum of compound 2y
$^1$H NMR spectrum of compound 2z

13C NMR spectrum of compound 2z
$^1$H NMR spectrum of compound 2aa

$^{13}$C NMR spectrum of compound 2aa
$^1$H NMR spectrum of compound 2bb

$^{13}$C NMR spectrum of compound 2bb
1H NMR spectrum of compound 2cc

13C NMR spectrum of compound 2cc
\(^1\)H NMR spectrum of compound 2dd

\(^{13}\)C NMR spectrum of compound 2dd
\textsuperscript{1}H NMR spectrum of compound \textit{2ee}

\textsuperscript{13}C NMR spectrum of compound \textit{2ee}