Supporting Information

DDQ: the chlorinating reagent and oxidant for the ligand-directed ortho-chlorination of 2-arylpypyridines

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Table 1. Optimization of the Reaction Conditions[^a]

<table>
<thead>
<tr>
<th>Entry</th>
<th>Palladium Source (mol%)</th>
<th>T (°C)</th>
<th>Solvent</th>
<th>Yield (%)[^b]</th>
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</table>

[^a]: Reaction conditions: 1a (0.3 mmol), palladium catalyst, and DDQ (3 equiv) in 2 mL of solvent under a nitrogen atmosphere at 120 °C for 3 h.[^b]: Isolated yield.[^c]: DDQ (2 equiv).[^d]: For 5 h.[^e]: Under air. 1-Chlorobenzoquinone (A1) (3 equiv) was used as the chlorinating reagent. 2-Chlorobenzoquinone (A1) (3 equiv) was used as the chlorinating reagent.

Experimental Section

General details

1H NMR and 13C NMR spectra were recorded on a Bruker DPX-400 spectrometer with CDCl₃ as the solvent and TMS as an internal standard. Melting points were measured by using a WC-1 microscopic apparatus. GC analysis was performed on Agilent 4890D gas chromatograph. Mass spectra were measured on an LC-MSD-Trap-XCT instrument. High resolution mass spectra were measured on a UHPLC Q-TOF HR-MS. The single crystal X-ray diffraction study was measured on a Xcalibur, Eos, Gemini diffractometer. Dichloromethane, ethyl acetate and hexane were used for column chromatography without further purification, and other solvents were purified according to the standard methods. The chemicals were obtained from commercial sources and used as-received unless otherwise noted.

General procedure for the palladium-catalyzed chlorination of 2-arylpypyridines

General procedure for the synthesis of 2j: to a solution of 2-(4-methoxyphenyl)-5-methylpyridine (0.3 mmol) in DMF (2 mL), DDQ (0.9 mmol) and PdCl₂ (5 mol%) were added. The resulting mixture was heated at 120 °C for 3 h. After the reaction was complete, the mixture was added into
H₂O (25 mL) and extracted with ethyl acetate (10 mL) three times. The combined organic layer was dried over anhydrous Na₂SO₄ and filtered. After removal of the solvent in vacuo, the residue was purified by column chromatography (petroleum/ethyl acetate=10:1) to afford the pure product. The yield of the isolated product was 99%.

2-(2,6-Dichlorophenyl)pyridine (2a)[1]
Light yellow liquid; ¹H NMR (400 MHz, CDCl₃): δ 7.26–7.30 (m, 1H), 7.32–7.35 (m, 2H), 7.39–7.42 (m, 2H), 7.81 (td, J = 7.70 Hz, 1.80 Hz, 1H), 8.74–8.77 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 122.9, 125.0, 128.1, 129.8, 134.6, 136.4, 138.4, 149.6, 155.5; HRMS-ESI (m/z) calcd for C₁₁H₈Cl₂N (M+H⁺): 224.0034, found: 224.0034.

2-[(2-Benzyloxy-6-chloro)phenyl]pyridine (2b)
Light yellow liquid; ¹H NMR (400 MHz, CDCl₃): δ 5.02 (s, 2H), 6.92 (d, J = 8.32 Hz, 1H), 7.09–7.17 (m, 3H), 7.21–7.29 (m, 5H), 7.35 (d, J = 7.76 Hz, 1H), 7.74 (td, J = 7.68 Hz, 1.40 Hz, 1H), 8.75 (d, J = 4.48 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 69.6, 110.6, 121.3, 121.4, 124.7, 125.6, 126.7, 127.4, 128.8, 129.0, 133.1, 135.0, 135.7, 148.4, 153.9, 156.3; HRMS-ESI (m/z) calcd for C₁₈H₁₅ClNO (M+H⁺): 296.0842, found: 296.0841.

2-[(2-Butoxy-6-chloro)phenyl]pyridine (2c)
Light yellow liquid; ¹H NMR (400 MHz, CDCl₃): δ 0.78 (t, J = 7.40 Hz, 3H), 1.15–1.25 (m, 2H), 1.48–1.55 (m, 2H), 3.87 (t, J = 6.36 Hz, 2H), 6.84 (d, J = 8.32 Hz, 1H), 7.04 (d, J = 8.00 Hz, 1H), 7.19–7.30 (m, 3H), 7.70 (td, J = 7.72 Hz, 1.48 Hz, 1H), 8.69 (d, J = 4.44 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 12.6, 17.9, 29.9, 67.6, 109.8, 120.6, 121.1, 124.6, 128.6, 128.7, 132.9, 134.8, 148.2, 154.0, 156.8; HRMS-ESI (m/z): calcd for C₁₅H₁₇ClNO (M+H⁺): 262.0999, found: 262.0998.

2-[(2-Chloro-5-methoxy)phenyl]pyridine (2d)
Light yellow liquid; ¹H NMR (400 MHz, CDCl₃): δ 3.80 (s, 3H), 6.87 (dd, J = 8.72 Hz, 2.88 Hz, 1H), 7.12 (d, J = 2.92 Hz, 1H), 7.24–7.27 (m, 1H), 7.34 (d, J = 8.80 Hz, 1H), 7.63 (d, J = 7.80 Hz, 1H), 7.73 (t, J = 7.60 Hz, 1H), 8.69 (d, J = 4.48 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 54.5, 115.0, 115.1, 121.4, 122.3, 123.8, 129.8, 134.8, 138.8, 148.4, 155.7, 157.3; HRMS-ESI (m/z) calcd for C₁₂H₁₁ClN (M+H⁺): 220.0529, found: 220.0523.

2-[(2-Chloro-5-methoxy)-5-methyl]pyridine (2e)
Light yellow liquid; ¹H NMR (400 MHz, CDCl₃): δ 2.39 (s, 3H), 3.82 (s, 3H), 6.87 (dd, J = 8.72 Hz, 2.76 Hz, 1H), 7.13 (d, J = 2.76 Hz, 1H), 7.34 (d, J = 8.80 Hz, 1H), 7.56 (s, 2H), 8.54 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 17.2, 54.6, 114.8, 115.0, 122.5, 123.3, 129.8, 131.1, 135.4, 138.8, 148.9, 153.0, 157.4; HRMS-ESI (m/z) calcd for C₁₃H₁₃ClN (M+H⁺): 234.0686, found: 234.0681.

2-[(2-Chloro-5-methyl)phenyl]pyridine (2f)
Light yellow liquid; ¹H NMR (400 MHz, CDCl₃): δ 2.34 (s, 3H), 7.11 (dd, J = 8.12 Hz, 1.56 Hz, 1H), 7.22–7.26 (m, 1H), 7.32 (d, J = 8.12 Hz, 1H), 7.40 (d, J = 1.24 Hz, 1H), 7.62 (d, J = 7.84 Hz, 1H), 7.71 (td, J = 7.76 Hz, 1.56 Hz, 1H), 8.69 (d, J = 4.56 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 19.8, 121.3, 123.9, 128.0, 128.8, 129.3, 131.1, 134.7, 135.9, 137.7, 148.5, 155.9; HRMS-ESI (m/z) calcd for C₁₂H₁₁ClN (M+H⁺): 204.0580, found: 204.0575.
2-[(2-Chloro-5-methyl)phenyl]-5-methylpyridine (2g)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 2.34 (s, 3H), 2.36 (s, 3H), 7.09 (d, $J = 7.40$ Hz, 1H), 7.31 (d, $J = 8.16$ Hz, 1H), 7.39 (s, 1H), 7.53 (s, 2H), 8.52 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 17.2, 19.8, 123.3, 128.0, 128.8, 129.1, 130.8, 131.0, 135.3, 135.8, 137.7, 148.9, 153.1; HRMS-ESI (m/z) calcd for C$_{13}$H$_{13}$ClN (M+H$^+$): 218.0737, found: 218.0741.

2-[(2-Chloro-5-isobutoxy)phenyl]pyridine (2h)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.00 (d, $J = 6.72$ Hz, 6H), 2.00–2.13 (m, 1H), 3.74 (d, $J = 6.44$ Hz, 2H), 6.88 (dd, $J = 8.76$ Hz, 1H), 7.14 (d, $J = 2.84$ Hz, 1H), 7.26 (t, $J = 7.28$ Hz, 1H), 7.32–7.36 (m, 1H), 7.63–7.66 (m, 1H), 7.71–7.76 (m, 1H), 8.67–8.71 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 18.2, 18.3, 27.3, 73.8, 115.4, 115.9, 121.4, 123.9, 129.8, 134.8, 135.7, 138.8, 148.5, 155.9, 157.1; HRMS-ESI (m/z) calcd for C$_{15}$H$_{17}$ClNO (M+H$^+$): 262.0999, found: 262.0996.

2-[(2,6-Dichloro-4-methoxy)phenyl]pyridine (2i)
Yellow solid, mp 76–78 °C; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 3.84 (s, 3H), 6.96 (s, 2H), 7.30–7.34 (m, 2H), 7.79 (td, $J = 7.72$ Hz, 1.56 Hz, 1H), 8.74 (d, $J = 3.48$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 55.6, 113.9, 122.6, 125.4, 130.8, 134.8, 136.1, 149.3, 155.2, 159.5; HRMS-ESI (m/z) calcd for C$_{12}$H$_{10}$Cl$_2$NO (M+H$^+$): 254.0139, found: 254.0139.

2-[(2,6-Dichloro-4-methoxy)phenyl]-5-methylpyridine (2j)
White solid, mp 106–108 °C; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 2.41 (s, 3H), 3.83 (s, 3H), 6.95 (s, 2H), 7.21 (d, $J = 7.68$ Hz, 1H), 7.57–7.61 (m, 1H), 8.56 (dd, $J = 1.48$ Hz, 0.68 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 18.2, 55.6, 113.9, 124.8, 130.8, 134.8, 136.1, 149.4, 152.4, 159.4; HRMS-ESI (m/z) calcd for C$_{13}$H$_{12}$Cl$_2$NO (M+H$^+$): 268.0296, found: 268.0302.

2-[(2,6-Dichloro-4-tert-butyl)phenyl]pyridine (2k)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.33 (s, 9H), 7.30–7.33 (m, 2H), 7.40 (s, 2H), 7.80 (td, $J = 7.68$ Hz, 1.12 Hz, 1H), 8.74 (d, $J = 4.68$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 30.8, 34.8, 122.6, 124.9, 125.2, 133.9, 135.2, 136.1, 149.4, 153.7, 155.4; HRMS-ESI (m/z) calcd for C$_{15}$H$_{16}$Cl$_2$N (M+H$^+$): 280.0660, found: 280.0669.

2-[(2,6-Dichloro-4-tert-butyl)phenyl]-5-methylpyridine (2l)
Light yellow solid, mp 128–130 °C; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.33 (s, 9H), 2.41 (s, 3H), 7.23 (d, $J = 7.88$ Hz, 1H), 7.39 (s, 2H), 7.61 (dd, $J = 7.92$ Hz, 1.56 Hz, 1H), 8.57 (d, $J = 0.68$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 30.8, 34.8, 122.6, 124.9, 125.2, 133.9, 135.2, 136.1, 149.4, 153.7, 155.4; HRMS-ESI (m/z) calcd for C$_{16}$H$_{18}$Cl$_2$N (M+H$^+$): 294.0816, found: 294.0818.

2-[(2-Chloro-5-methyl)phenyl]-5-methylpyridine (2m)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 2.36 (s, 3H), 7.23 (s, 2H), 7.31–7.35 (m, 2H), 7.80 (td, $J = 7.68$ Hz, 1.60 Hz, 1H), 8.75 (d, $J = 4.40$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 20.7, 122.7, 125.1, 128.6, 134.0, 135.4, 136.2, 140.3, 149.5, 155.5; HRMS-ESI (m/z) calcd for C$_{12}$H$_{10}$Cl$_2$N (M+H$^+$): 238.0190, found: 238.0198.
2-[(2,6-Dichloro-4-methyl)phenyl]-5-methylpyridine (2n)
White solid, mp 81–83 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 2.36 (s, 3H), 2.41 (s, 3H), 7.22–7.24 (m, 3H), 7.61 (d, \(J = 7.72\) Hz, 1H), 8.58 (s, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 18.2, 20.6, 124.4, 128.5, 132.2, 134.1, 135.2, 136.7, 140.1, 149.8, 152.5; HRMS-ESI (m/z) calecd for C\(_{13}\)H\(_{12}\)Cl\(_2\)N (M+H\(^+\)): 252.0347, found: 252.0355.

2-(2,6-Dichlorophenyl)-5-methylpyridine (2o)
Yellow solid, mp 90–93 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 2.42 (s, 3H), 7.23–7.29 (m, 2H), 7.38–7.41 (m, 2H), 7.63 (dd, \(J = 7.92\) Hz, 1.60 Hz, 1H), 8.59 (t, \(J = 0.56\) Hz, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 18.2, 124.2, 127.9, 129.5, 132.4, 134.6, 136.8, 138.1, 149.8, 152.4; HRMS-ESI (m/z) calecd for C\(_{12}\)H\(_{10}\)Cl\(_2\)N (M+H\(^+\)): 238.0190, found: 238.0194.

2-[(4-Bromo-2,6-dichloro)phenyl]pyridine (2p)
White solid, mp 88–90 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 7.29–7.37 (m, 2H), 7.59 (s, 2H), 7.81 (td, \(J = 7.76\) Hz, 1.72 Hz, 1H), 8.74–8.76 (m, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 122.0, 123.0, 124.8, 130.7, 135.2, 136.3, 137.3, 149.6, 154.4; HRMS-ESI (m/z) calecd for C\(_{11}\)H\(_{7}\)BrCl\(_2\)N (M+H\(^+\)): 301.9139, found: 301.9143.

2-[(4-Bromo-2,6-dichloro)phenyl]-5-methylpyridine (2q)
White solid, mp 100–103 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 2.42 (s, 3H), 7.21 (d, \(J = 7.88\) Hz, 1H), 7.57–7.64 (m, 3H), 8.58 (d, \(J = 0.52\) Hz, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 18.2, 121.8, 124.2, 130.7, 132.7, 135.4, 136.8, 137.3, 150.0, 151.5; HRMS-ESI (m/z) calecd for C\(_{12}\)H\(_{9}\)BrCl\(_2\)N (M+H\(^+\)): 315.9295, found: 315.9304.

2-[(2,6-Dichloro-4-fluoro)phenyl]pyridine (2r)
Light yellow liquid; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 7.19 (d, \(J = 8.20\) Hz, 2H), 7.30–7.38 (m, 2H), 7.82 (td, \(J = 7.72\) Hz, 1.40 Hz, 1H), 8.75 (d, \(J = 4.56\) Hz, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 115.7 (d, \(J = 24.3\) Hz), 122.9, 125.1, 134.7 (d, \(J = 4.1\) Hz), 135.2 (d, \(J = 11.5\) Hz), 136.3, 149.5, 154.5, 161.3 (d, \(J = 251.4\) Hz); HRMS-ESI (m/z) calecd for C\(_{11}\)H\(_{7}\)Cl\(_2\)FN (M+H\(^+\)): 241.9940, found: 241.9945.

2-[(2,6-Dichloro-4-fluoro)phenyl]-5-methylpyridine (2s)
White solid, mp 81–83 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 2.42 (s, 3H), 7.16–7.23 (m, 3H), 7.61–7.64 (m, 1H), 8.57–8.59 (m, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 18.2, 115.6 (d, \(J = 24.3\) Hz), 124.5, 132.6, 134.7 (d, \(J = 3.9\) Hz), 135.4 (d, \(J = 11.5\) Hz), 136.8, 150.0, 151.6, 161.2 (d, \(J = 251.2\) Hz); HRMS-ESI (m/z) calecd for C\(_{12}\)H\(_{9}\)Cl\(_2\)FN (M+H\(^+\)): 256.0096, found: 256.0096.

2-[(2,6-Dichloro-4-ethoxycarbonyl)phenyl]pyridine (2t)
Light yellow liquid; \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 1.43 (t, \(J = 7.16\) Hz, 3H), 4.42 (q, \(J = 7.16\) Hz, 2H), 7.33–7.40 (m, 2H), 7.84 (td, \(J = 7.72\) Hz, 1.72 Hz, 1H), 8.07 (s, 2H), 8.76–8.79 (m, 1H); \(^13\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 13.2, 60.9, 122.3, 123.8, 128.1, 131.2, 133.9, 135.6, 141.1, 148.8, 153.8, 163.2; HRMS-ESI (m/z) calecd for C\(_{14}\)H\(_{12}\)Cl\(_2\)NO\(_2\) (M+H\(^+\)): 296.0248, found: 296.0245.
2-[(2,6-Dichloro-4-ethoxycarbonyl)phenyl]-5-methylpyridine (2u)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.42 (t, $J = 7.12$ Hz, 3H), 2.43 (s, 3H), 4.41 (q, $J = 7.12$ Hz, 2H), 7.22–7.28 (m, 1H), 7.64 (d, $J = 7.72$ Hz, 1H), 8.06 (s, 2H), 8.60 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 14.1, 18.3, 61.8, 124.1, 129.0, 131.9, 132.9, 135.0, 136.9, 142.1, 150.1, 151.8, 164.1; HRMS-ESI (m/z) calcd for C$_{15}$H$_{14}$Cl$_2$NO$_2$ (M+H$^+$): 310.0402, found: 310.0407.

10-Chlorobenzo[h]quinoline (2v)$^{[1]}$
Light yellow solid, mp 64–66 °C; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.51–7.56 (m, 2H), 7.67 (d, $J = 8.80$ Hz, 1H), 7.81 (d, $J = 7.76$ Hz, 2H), 8.13–8.17 (m, 1H), 9.09–9.12 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 121.7, 126.6, 127.5, 127.6, 127.7, 128.2, 131.5, 132.3, 135.7, 136.3, 146.5, 147.6; HRMS-ESI (m/z) calcd for C$_{13}$H$_9$ClN (M+H$^+$): 214.0424, found: 214.0418.

2-[2-(3-Chlorothienyl)]pyridine (2w)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.00 (d, $J = 5.32$ Hz, 1H), 7.18–7.23 (m, 1H), 7.35 (d, $J = 5.32$ Hz, 1H), 7.75 (td, $J = 7.92$ Hz, 1.72 Hz, 1H), 8.23 (d, $J = 8.12$ Hz, 1H), 8.61 (d, $J = 4.64$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 120.5, 121.9, 122.2, 126.3, 129.8, 136.4, 136.8, 149.3, 150.8; HRMS-ESI (m/z) calcd for C$_9$H$_7$ClNS (M+H$^+$): 195.9988, found: 195.9996.

2-[2-(3-Chlorothienyl)]-5-methylpyridine (2x)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 2.36 (s, 3H), 6.99 (d, $J = 5.32$ Hz, 1H), 7.32 (d, $J = 5.32$ Hz, 1H), 7.56 (d, $J = 8.12$ Hz, 1H), 8.11 (d, $J = 8.20$ Hz, 1H), 8.44 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 18.3, 120.3, 121.5, 125.8, 129.9, 132.1, 137.0, 137.2, 148.3, 149.9; HRMS-ESI (m/z) calcd for C$_{10}$H$_9$ClNS (M+H$^+$): 210.0144, found: 210.0148.

([(5-Methoxy-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]pyridine (3a)
Light yellow liquid; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 1.18 (s, 12H), 2.29 (s, 3H), 3.81 (s, 3H), 6.85–6.88 (m, 1H), 7.28 (t, $J = 8.00$ Hz, 1H), 7.42–7.48 (m, 2H), 7.52–7.55 (m, 1H), 8.43 (s, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 17.1, 24.0, 54.3, 82.5, 110.7, 113.7, 118.1, 119.2, 128.6, 130.7, 136.3, 139.9, 149.0, 153.5, 159.0; HRMS-ESI (m/z) calcd for C$_9$H$_7$ClNS (M+H$^+$-Bpin): 200.1075, found: 200.1087.

Crystal data for compound 2j:
The molecular structure of the dichlorinated product (2j) was unambiguously determined by the single crystal X-ray diffraction study (Fig. 1). CCDC 917218 contains the supplementary crystallographic data for 2j. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/datarequest/cif. Crystal, data for compound 2j: C$_{13}$H$_{11}$Cl$_2$NO, $M = 268.13$, Triclinic, $a = 6.2427(4)$ Å, $\alpha = 74.492(6)^\circ$, $b = 8.5337(6)$ Å, $\beta = 77.526(6)^\circ$, $c = 12.7695(10)$ Å, $\gamma = 81.552(5)^\circ$, $V = 637.16(8)$ Å$^3$, T = 291.15 K, space group = P$\bar{1}$, $Z = 2$, Number of reflections = 4499, Independent reflections = 2279, [R(int) = 0.0212], Final R indices [I>2$\sigma$(I)] $R_1 = 0.0389$, wR$_2 = 0.1078$, R indices (all data) $R_1 = 0.0443$, wR$_2 = 0.1131$. 

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Figure 1. Molecular structure of 2j

References:
The reductive product of DDQ detected by GC-Mass: