Supporting Information

New efficient synthesis of benzofuro[2,3-b]pyrroles utilizing reactive nitrilium trapping approach by acid-promoted cascade addition/cyclization sequence

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General Information

Chemicals were purchased from Aldrich and Alfa Aesar Chemical Companies and used without further purification. Dried and distilled solvents were used. All reactions involving moisture sensitive reactants were performed using oven dried glassware. Chemicals were purchased from Aldrich and Alfa Aesar Chemical Companies and used without further purification. NMR spectra were recorded in CDCl$_3$ on a Jeol JNM ECP 400 and 600 NMR instrument. $^1$H NMR chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard (CDCl$_3$ at 7.26 ppm). Standard abbreviations were used to denote signal multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. $^{13}$C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard (CDCl$_3$ at 77.16 ppm). HRMS were obtained by EI on a double-focusing mass analyzer, ESI (positive ion mode) on TOF mass analyzer. All melting points were determined using open capillaries on an Electrothermal-9100 (Japan) instrument and are uncorrected.

Experimental procedure

General procedure

To a 25 ml oven dried R. B. flask successively added of 2-hydroxybenzaldehydes 1a (1 mmol), benzoylecyanitrile (2a), tert-butyl isocyanide (3a), p-TSA.H$_2$O (0.04 mmol) and 2.0 mL ethanol. The resulting mixture was stirred at 80 ºC for 4-6 h. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to ambient temperature and directly subjected to flash column chromatography on silica gel (60–120 mesh) using petroleum ether/ethylacetate = 80:20 as an eluant to afford the pure product 4a in good yield.
Characterization Data of the compounds

1-(tert-Butyl)-7-methoxy-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4a)

Yield: 91% (314 mg); Yellow solid; Mp: 94-96 °C; 
¹H NMR (600 MHz, CDCl₃) δ 7.98 – 7.93 (m, 2H), 7.47 – 7.42 (m, 2H), 7.38 – 7.33 (m, 1H), 7.13 (dd, J = 7.9, 1.4 Hz, 1H), 6.97 (t, J = 8.0 Hz, 1H), 6.88 (dd, J = 8.1, 1.4 Hz, 1H), 3.93 (s, 3H), 1.30 (s, 9H); ¹³C NMR (150 MHz, CDCl₃) δ 153.3, 151.3, 147.4, 142.4, 129.0, 128.9, 128.7, 124.6, 122.2, 120.5, 116.9, 115.6, 110.0, 104.3, 100.0, 93.8, 56.2, 54.1, 30.1; FT-IR (thin film): ν (cm⁻¹) 3060, 2965, 2921, 2223, 1597, 1561, 1490, 1468, 1438, 1365, 1275, 1250, 1221, 1097, 1090, 1010, 934, 911, 762, 732.; HRMS (ESI, m/z): calcd for C₂₂H₂₀N₂O₂ (M+H⁺) 344.1525, found 344.1529.

1-(tert-Butyl)-2-(4-fluorophenyl)-7-methoxy-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4b)

Yield: 84% (304.4 mg); Yellow solid; Mp: 102-104 °C; 
¹H NMR (600 MHz, CDCl₃) δ 7.95 – 7.91 (m, 2H), 7.16 – 7.13 (m, 2H), 7.10 (dd, J = 7.9, 1.4 Hz, 1H), 6.97 (t, J = 8.0 Hz, 1H), 6.87 (dd, J = 8.1, 1.3 Hz, 1H), 3.93 (s, 3H), 1.28 (s, 9H); ¹³C NMR (150 MHz, CDCl₃) 163.7, 162.1, 152.5, 151.3, 147.4, 142.4, 126.6, 126.6, 125.1, 125.1, 122.1, 120.6, 116.8, 116.3, 116.1, 115.6, 110.1, 104.4, 100.0, 93.5, 56.2, 54.1, 30.1; FT-IR (thin film): ν (cm⁻¹) 3071, 2967, 2932, 2223,
1596, 1567, 1503, 1468, 1438, 1394, 1365, 1277, 1232, 1159, 1088, 1010, 935, 834, 810, 732;
HRMS (ESI, m/z): calcd for C$_{22}$H$_{19}$FN$_2$O$_2$ (M+H$^+$) 362.1431, found: 362.1434.

1-(*tert*-Butyl)-2-(3-chlorophenyl)-7-methoxy-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4c)

Yield: 86% (326 mg); Yellow solid; Mp: 96-98 ºC; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.89 – 7.82 (m, 2H), 7.40 – 7.34 (m, 1H), 7.32 – 7.28 (m, 1H), 7.10 (dd, $J = 7.9, 1.4$ Hz, 1H), 6.97 (t, $J = 8.0$ Hz, 1H), 6.87 (dd, $J = 8.1, 1.4$ Hz, 1H), 3.93 (s, 3H), 1.31 (s, 9H);

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 152.1, 151.0, 147.3, 142.3, 135.1, 130.3, 128.6, 124.2, 122.4, 122.1, 120.6, 116.5, 115.2, 110.0, 103.5, 95.0, 56.1, 53.9, 30.2; HRMS (ESI, m/z): calcd for C$_{22}$H$_{19}$ClN$_2$O$_2$ (M+H$^+$) 378.1135, found: 378.1139.

1-(*tert*-Butyl)-7-ethoxy-2-(m-tolyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4d)

Yield: 82% (305.7 mg); Brown solid; Mp: 108-110 ºC; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.79 – 7.74 (m, 2H), 7.37 – 7.32 (m, 1H), 7.17 (d, $J = 7.9$ Hz, 1H), 7.11 (dd, $J = 7.9, 1.4$ Hz, 1H), 6.95 (t, $J = 8.0$ Hz, 1H), 6.86 (dd, $J = 8.1, 1.4$ Hz, 1H), 4.16 (q, $J = 7.0$ Hz, 2H), 2.42 (s, 3H), 1.48 (t, $J = 7.0$ Hz, 3H), 1.30 (s, 9H);

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 153.3, 151.5, 146.5, 142.4, 138.7,
129.7, 128.9, 128.7, 125.1, 122.1, 121.8, 120.5, 116.8, 115.7, 110.9, 103.9, 93.6, 64.8, 53.9, 30.2, 21.6, 15.0; HRMS (ESI, m/z): calcd for C_{24}H_{24}N_{2}O_{2} (M+H^+) 372.1838, found: 372.1841.

1-(tert-Butyl)-7-ethoxy-2-(4-fluorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4e)

![4e](image)

Yield: 71% (267.4 mg); Yellow solid; Mp: 100-102 °C; $^1$H NMR (600 MHz, CDCl$_3$) δ 7.96 – 7.90 (m, 2H), 7.15 – 7.12 (m, 2H), 7.08 (dd, $J = 7.9$, 1.4 Hz, 1H), 6.94 (t, $J = 8.0$ Hz, 1H), 6.85 (dd, $J = 8.1$, 1.4 Hz, 1H), 4.15 (q, $J = 7.0$ Hz, 2H), 1.47 (t, $J = 7.0$ Hz, 3H), 1.29 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 163.6, 162.0, 152.2, 151.7, 146.4, 142.4, 126.5, 125.6, 125.2, 122.0, 120.5, 116.7, 116.2, 115.6, 110.9, 103.6, 93.5, 64.8, 53.8, 30.2, 14.9; HRMS (ESI, m/z): calcd for C$_{23}$H$_{21}$FN$_{2}$O$_{2}$ (M+H$^+$) 376.1587, found: 376.1589.

1-(tert-Butyl)-2-(3-chlorophenyl)-7-ethoxy-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4f)

![4f](image)

Yield: 74% (290.5 mg); Yellow solid; Mp: 111-113°C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.90 – 7.81 (m, 2H), 7.40 – 7.35 (m, 1H), 7.32 – 7.28 (m, 1H), 7.09 – 7.04 (m, 1H), 6.95 (t, $J = 8.0$ Hz, 1H), 6.86 (dd, $J = 8.0$, 1.0 Hz, 1H), 4.20 – 4.14 (q, 2H), 1.49 (t, 3H), 1.32 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 152.5, 150.8, 146.4, 142.4, 135.1, 130.4, 128.6, 124.2, 122.4, 122.1, 120.6,
116.5, 115.3, 110.8, 102.9, 95.1, 64.9, 53.8, 30.3, 15.0; HRMS (ESI, m/z): calcd for C_{23}H_{21}ClN_{2}O_{2} (M+H\textsuperscript{+}) 392.1292, found: 392.1295.

**1-(tert-Butyl)-7-ethoxy-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4g)**

Yield: 80% (285.2 mg); Brown solid; Mp: 90-92 °C; \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.98 – 7.93 (m, 2H), 7.47 – 7.42 (m, 2H), 7.38 – 7.32 (m, 1H), 7.10 (dd, \(J = 7.9, 1.4\) Hz, 1H), 6.95 (t, \(J = 8.0\) Hz, 1H), 6.85 (dd, \(J = 8.1, 1.4\) Hz, 1H), 4.16 (q, 2H), 1.48 (t, 3H), 1.31 (s); \(^{13}\)C NMR (100 MHz, CDCl\textsubscript{3}) \(\delta\) 153.0, 151.7, 146.5, 142.4, 129.0, 128.8, 124.5, 122.1, 120.5, 116.8, 115.7, 110.8, 103.5, 93.8, 64.8, 53.8, 30.2, 15.0; HRMS (ESI, m/z): calcd for C_{23}H_{22}N_{2}O_{2} (M+H\textsuperscript{+}) 358.1681, found: 358.1684.

**1-(tert-Butyl)-5-chloro-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4h)**

Yield: 86% (299.8 mg); Brown solid; Mp: 106-108 °C; \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta\) 7.99 – 7.95 (m, 2H), 7.64 (d, \(J = 2.5\) Hz, 1H), 7.53 – 7.45 (m, 3H), 7.24 (dd, \(J = 8.7, 2.5\) Hz, 1H), 6.95 (d, \(J = 8.7\) Hz, 1H), 1.18 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\textsubscript{3}) \(\delta\) 157.1, 152.9, 146.1, 130.3, 129.9, 129.3, 128.7, 127.8, 125.6, 125.4, 120.4, 118.3, 114.8, 114.3, 114.0, 93.4, 57.3, 29.4; HRMS (ESI, m/z): calcd for C_{21}H_{17}ClN_{2}O (M+H\textsuperscript{+}) 348.1029, found: 348.1032.
1-(tert-Butyl)-5-chloro-2-(4-fluorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4i)

Yield: 78% (287 mg); Yellow solid; Mp: 98-100 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.97 – 7.92 (m, 2H), 7.60 (d, $J$ = 2.6 Hz, 1H), 7.22 (dd, $J$ = 8.7, 2.6 Hz, 1H), 7.20 – 7.15 (m, 2H), 6.94 (d, $J$ = 8.7 Hz, 1H), 1.18 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 164.9, 162.4, 156.0, 152.9, 146.4, 129.9, 128.7, 127.6, 127.5, 125.6, 124.2, 120.3, 118.3, 116.3, 116.4, 114.7, 113.3, 93.1, 57.1, 29.4.; HRMS (ESI, m/z): calcd for C$_{21}$H$_{16}$ClFN$_2$O (M+H$^+$) 366.0935, found: 366.0937.

1-(tert-Butyl)-5-chloro-2-(m-tolyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4j)

Yield: 79% (386.4 mg); Brown solid; Mp: 110-112 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.80 – 7.73 (m, 2H), 7.63 (d, $J$ = 2.5 Hz, 1H), 7.38 (t, $J$ = 7.7 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.23 (dd, $J$ = 8.7, 2.5 Hz, 1H), 6.95 (d, $J$ = 8.7 Hz, 1H), 2.43 (s, 3H), 1.18 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 157.3, 152.9, 146.1, 139.0, 131.2, 129.8, 129.1, 127.7, 125.9, 125.5, 122.6, 120.3, 118.4, 114.8, 113.7, 93.2, 57.2, 29.4, 21.6; HRMS (ESI, m/z): calcd for C$_{22}$H$_{19}$ClN$_2$O (M+H$^+$) 362.1186, found: 362.1189.

1-(tert-Butyl)-5-chloro-2-(3-chlorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4k)
Yield: 82% (314.2 mg); Yellow solid; Mp: 120-121 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.91 (dt, $J = 7.1$, 1.9 Hz, 1H), 7.85 (d, $J = 1.7$ Hz, 1H), 7.59 (d, $J = 2.5$ Hz, 1H), 7.44 – 7.39 (m, 2H), 7.25 – 7.21 (m, 1H), 6.94 (d, $J = 8.7$ Hz, 1H), 1.19 (s, 9H).; $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 154.9, 152.8, 147.1, 135.3, 130.6, 130.2, 130.0, 129.4, 128.8, 125.7, 125.1, 123.4, 120.3, 118.1, 114.3, 113.0, 94.5, 57.1, 29.5; HRMS (ESI, $m/z$): calcd for C$_{21}$H$_{16}$Cl$_2$N$_2$O (M+H$^+$) 382.0640, found: 382.0644.

1-\((\text{tert-Butyl})\)-2-phenyl-1\(H\)-benzofuro[2,3-b]pyrrole-3-carbonitrile (4l)

Yield: 90% (283 mg); Yellow solid; Mp: 88-90 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.99 – 7.95 (m, 2H), 7.67 (dd, $J = 7.7$, 1.6 Hz, 1H), 7.50 – 7.47 (m, 2H), 7.45 – 7.41 (m, 1H), 7.31 – 7.27 (m, 1H), 7.06 – 7.01 (m, 2H), 1.18 (s, 9H).; $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 156.6, 154.1, 146.2, 130.0, 129.9, 129.7, 129.4, 129.2, 128.7, 128.1, 125.3, 120.8, 118.9, 116.9, 115.3, 114.4, 93.7, 56.8, 29.4; HRMS (ESI, $m/z$): calcd for C$_{21}$H$_{18}$N$_2$O (M+H$^+$) 314.1419, found: 314.1422.

1-\((\text{tert-Butyl})\)-2-(4-fluorophenyl)-1\(H\)-benzofuro[2,3-b]pyrrole-3-carbonitrile (4m)
Yield: 79% (263 mg); Yellow solid; Mp: 94-96 °C; $^1$H NMR (600 MHz, CDCl$_3$) δ 8.00 – 7.94 (m, 2H), 7.65 (dd, $J = 7.7$, 1.6 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.20 – 7.16 (m, 2H), 7.05 – 7.01 (m, 2H), 1.18 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 162.7, 155.7, 154.1, 146.3, 130.0, 129.4, 127.5, 127.4, 120.9, 118.9, 116.8, 116.5, 116.4, 115.2, 93.5, 56.8, 29.4; HRMS (ESI, m/z): calcd for C$_{21}$H$_{17}$FN$_2$O (M+H$^+$) 332.1325, found: 332.1328.

1-(tert-Butyl)-2-(3-chlorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4n)

Yield: 88% (307 mg); Yellow solid; Mp: 109-111 °C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.91 (dt, $J = 7.3$, 1.7 Hz, 1H), 7.86 (t, $J = 1.7$ Hz, 1H), 7.63 (dd, $J = 7.7$, 1.6 Hz, 1H), 7.42-7.38 (m, 2H), 7.32 – 7.26 (m, 1H), 7.06 – 7.00 (m, 2H), 1.19 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 154.5, 154.0, 147.0, 135.3, 130.5, 130.1, 129.9, 129.6, 129.5, 125.0, 123.3, 121.0, 118.8, 116.7, 114.8, 113.9, 94.8, 56.8, 29.5; HRMS (ESI, m/z): calcd for C$_{21}$H$_{17}$ClN$_2$O (M+H$^+$) 348.1029, found: 348.1032.

1-(tert-Butyl)-2-(m-tolyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4o)
Yield: 91% (299 mg); Yellow solid; Mp: 91-93 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.83 – 7.75 (m, 2H), 7.67 (dd, \(J = 7.7, 1.6\) Hz, 1H), 7.37 (t, \(J = 7.7\) Hz, 1H), 7.31 – 7.27 (m, 1H), 7.26 – 7.22 (m, 1H), 7.08 – 6.99 (m, 2H), 2.43 (s, 3H), 1.18 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 156.9, 154.1, 145.9, 138.9, 130.9, 129.4, 129.1, 128.0, 125.8, 122.6, 118.9, 116.9, 115.3, 114.7, 93.5, 56.9, 29.4, 21.6; HRMS (ESI, \(m/z\)): calcd for C\(_{22}\)H\(_{20}\)N\(_2\)O (M+H\(^+\)) 328.1576, found: 328.1579.

5-bromo-1-(tert-Butyl)-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4p)

Yield: 76% (298.8 mg); Brown solid; Mp: 104-106 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.83 (dd, \(J = 8.4, 1.2\) Hz, 2H), 7.57 – 7.53 (m, \(J = 10.7, 5.1\) Hz, 2H), 7.45 – 7.41 (m, \(J = 7.5\) Hz, 2H), 7.35 (dd, \(J = 8.7, 2.6\) Hz, 1H), 6.93 (d, \(J = 8.7\) Hz, 1H), 1.26 (s, 9H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 157.1, 153.4, 146.2, 132.8, 131.7, 130.3, 127.8, 125.4, 120.8, 120.2, 118.9, 114.7, 113.5, 112.8, 93.5, 57.2, 29.4; HRMS (ESI, \(m/z\)): calcd for C\(_{21}\)H\(_{17}\)BrN\(_2\)O (M+H\(^+\)) 392.0524, found: 392.0528.

5-bromo-1-(tert-Butyl)-2-(p-tolyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4q)
Yield: 68% (277 mg); Brown solid; Mp: 119-121 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.84 (d, \(J = 8.2\) Hz, 2H), 7.75 (d, \(J = 2.4\) Hz, 1H), 7.33 (dd, \(J = 8.7, 2.4\) Hz, 1H), 7.27 (d, \(J = 8.3\) Hz, 2H), 6.87 (d, \(J = 8.7\) Hz, 1H), 2.40 (s, 3H), 1.17 (s, 9H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 157.2, 153.4, 146.2, 140.6, 132.5, 131.6, 129.9, 127.9, 125.3, 120.6, 119.0, 115.0, 112.6, 92.5, 56.8, 29.4, 21.6; HRMS (ESI, \(m/z\)): calcd for C\(_{22}\)H\(_{19}\)BrN\(_2\)O (M+H\(^+\)) 406.0681, found: 406.0685.

**5-bromo-1-(tert-Butyl)-2-(4-fluorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4r)**

Yield: 70% (287.3 mg); Brown solid; Mp: 130-132 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.99 – 7.94 (m, 2H), 7.76 (d, \(J = 2.4\) Hz, 1H), 7.38 (dd, \(J = 8.7, 2.4\) Hz, 1H), 7.19 (t, \(J = 8.7\) Hz, 2H), 6.90 (d, \(J = 8.7\) Hz, 1H), 1.18 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 165.0, 162.4, 156.2, 153.5, 146.1, 132.9, 131.6, 127.6, 127.6, 124.2, 120.9, 118.8, 116.8, 116.7, 116.4, 114.7, 113.8, 112.8, 93.3, 57.3, 29.4; HRMS (ESI, \(m/z\)): calcd for C\(_{21}\)H\(_{16}\)BrFN\(_2\)O (M+H\(^+\)) 410.0430, found: 410.0434.

**5-bromo-1-(tert-Butyl)-2-(3-chlorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4s)**
Yield: 72% (308 mg); Brown solid; Mp: 138-140 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.88 (dt, \(J = 7.1, 1.9\) Hz, 1H), 7.83 (td, \(J = 1.8, 0.7\) Hz, 1H), 7.71 (d, \(J = 2.4\) Hz, 1H), 7.43 – 7.38 (m, 2H), 7.35 (dd, \(J = 8.7, 2.4\) Hz, 1H), 6.89 (d, \(J = 8.7\) Hz, 1H), 1.19 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 154.6, 153.3, 147.4, 135.3, 132.7, 131.7, 130.6, 130.0, 129.4, 125.0, 123.2, 120.5, 118.7, 114.4, 112.7, 112.2, 94.4, 56.9, 29.4; HRMS (ESI, \(m/z\)): calcd for C\(_{21}\)H\(_{16}\)BrClN\(_2\)O (M+H\(^+\)) 426.0135, found: 426.0139.

1-cyclohexyl-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4t)

Yield: 61% (207.6 mg); Yellow solid; Mp: 113-115 °C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.96 – 7.91 (m, 2H), 7.57 (dd, \(J = 7.7, 1.6\) Hz, 1H), 7.49 – 7.44 (m, 2H), 7.41 – 7.36 (m, 1H), 7.30 – 7.25 (m, 1H), 7.07 – 6.99 (m, 2H), 3.32 – 3.05 (m, 1H), 1.99 – 1.88 (m, 2H), 1.75 – 1.69 (m, 2H), 1.63 – 1.57 (m, 1H), 1.30 – 1.13 (m, 5H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 154.2, 153.5, 148.9, 129.8, 129.6, 129.4, 128.3, 124.8, 121.1, 118.0, 116.6, 115.3, 105.4, 94.1, 55.8, 33.6, 25.4, 24.7; HRMS (ESI, \(m/z\)): calcd for C\(_{23}\)H\(_{20}\)N\(_2\)O (M+H\(^+\)) 340.1576, found: 340.1579.

5-chloro-1-cyclohexyl-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4u)
Yield: 58% (217.4 mg); Yellow solid; Mp: 120-122 °C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.93 – 7.86 (m, 2H), 7.49 – 7.48 (m, 1H), 7.46 – 7.42 (m, 2H), 7.40 – 7.37 (m, 1H), 7.16 (dd, $J$ = 8.7, 2.5 Hz, 1H), 6.91 (d, $J$ = 8.7 Hz, 1H), 3.26 – 3.15 (m, 1H), 1.98 – 1.90 (m, 2H), 1.75 – 1.70 (m, 2 Hz), 1.62 – 1.56 (m, 1H), 1.30 – 1.16 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 153.9, 152.1, 149.7, 129.4, 129.1, 128.4, 128.1, 128.0, 126.8, 125.6, 124.7, 119.1, 115.0, 102.9, 93.6, 55.4, 33.6, 25.4, 24.7; HRMS (ESI, $m/z$): calcd for C$_{23}$H$_{19}$ClN$_2$O (M+H$^+$) 374.1186, found: 374.1189.
$^1$H NMR and $^{13}$C NMR of compound (4b)
$^1$H NMR and $^{13}$C NMR of compound (4c)
$^1$H NMR and $^{13}$C NMR of compound (4d)
$^1$H NMR and $^{13}$C NMR of compound (4e)
${}^{1}H$ NMR and ${}^{13}C$ NMR of compound (4f)
$^1$H NMR and $^{13}$C NMR of compound (4g)
$^1$H NMR and $^{13}$C NMR of compound (4h)
$^{1}$H NMR and $^{13}$C NMR of compound (4i)
$^1$H NMR and $^{13}$C NMR of compound (4j)
$^1$H NMR and $^{13}$C NMR of compound (4k)
$^1$H NMR and $^{13}$C NMR of compound (4l)
$^1$H NMR and $^{13}$C NMR of compound (4m)
$^1$H NMR and $^{13}$C NMR of compound (4n)
$^1$H NMR and $^{13}$C NMR of compound (4o)
$^1$H NMR and $^{13}$C NMR of compound (4p)
$^1$H NMR and $^{13}$C NMR of compound (4q)
$^1$H NMR and $^{13}$C NMR of compound (4r)
$^1$H NMR and $^{13}$C NMR of compound (4s)
$^1$H NMR and $^{13}$C NMR of compound (4t)
$^1$H NMR and $^{13}$C NMR of compound (4u)
$^1$H NMR and $^{13}$C NMR of compound (5)