One-pot synthesis of 2,3-diarylbenzofurans via sequential iodocyclization and Pd-catalyzed Suzuki coupling reactions of 2-alkynylanisoles with boronic acids in water

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Supporting Information

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Experimental section

Chemicals were either purchased or purified by standard techniques without special instructions. ^1H NMR and ^{13}C NMR spectra were measured on 500 MHz Bruker spectrometer, using CDCl_3 as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. Thin layer chromatography was performed using commercially prepared 60-mesh silica gel plates, and visualization was effected with short wavelength UV light (254 nm). All melting points are uncorrected. All reagents were used directly as obtained commercially unless otherwise noted. Column chromatography was performed using EM Silica gel 60 (300-400 mesh). Known compounds are identified by comparison with authentic samples.

Typical procedure for the sequential iodocyclization and Pd-catalyzed Suzuki coupling reaction of 2-alkynylanisoles with boronic acids in water: 2-phenylethynylanisole (0.5 mmol), iodine (0.5 mmol) were added in a Schlenk tube and stirred for 8 h at room temperature, then boronic acid (1 mmol), $\text{K}_3\text{PO}_4 \cdot 3\text{H}_2\text{O}$ (0.5 mmol), $\text{Pd}(\text{PPh}_3)_4$ (10 mol%), H_2O (2 mL) were added and stirred for another 24 h at 80 °C. After cooling to room temperature and extracted twice with EtOAc, the combined organic phase was washed with brine, dried over MgSO_4 , filtered, and evaporated under reduced pressure. The crude product was purified by flash chromatography over silica gel with petroleum ether to afford the desired product 2,3-diphenylbenzofuran (**3aa**) in 84 % yield.

(B) Analytical data for the products 3aa-3ig

2,3-diphenylbenzofuran 3aa. The product was obtained as a white solid in 84 % yield. m.p. 123-124 °C (lit.^{S1} 123-124 °C). ^1H NMR (CDCl_3 , 500 MHz) δ 7.65-7.67 (m, 2H), 7.55-7.56 (d, J = 5 Hz, 1H), 7.45-7.51 (m, 5H), 7.38-7.42 (m, 1H), 7.28-7.34 (m, 4H), 7.22-7.25 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 154.0, 150.5, 132.9, 130.7, 130.3, 129.8, 129.0, 128.4, 128.4, 127.6, 127.0, 124.7, 122.9, 120.0, 117.5, 111.1.

2-phenyl-3-(4-trifluoromethylphenyl)benzofuran 3ab. The product was obtained as a white solid in 74 % yield. m.p. 112-114 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.71-7.73 (d, J = 10 Hz, 2H), 7.57-7.64 (m, 5H), 7.48-7.49 (d, J = 5 Hz, 1H), 7.33-7.38 (m, 4H), 7.27-7.28 (d, J = 5 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 154.1, 151.3, 136.9, 130.2, 130.1, 129.8, 129.6, 128.9, 128.6, 127.3, 125.9 (q, $J_{\text{C-F}}$ = 3.62 Hz), 125.0, 124.2 (q, $J_{\text{C-F}}$ = 270.4 Hz), 123.3, 119.7, 116.1, 111.3; HRMS (ESI): Calcd 339.0991 for $\text{C}_{20}\text{H}_{14}\text{OF}^+$, Found: 339.0972 ($\text{M}+\text{H}$) $^+$.

2-phenyl-3-(4-fluorophenyl)benzofuran 3ac. The product was obtained as a white solid in 79 % yield. m.p. 112-114 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.63-7.64 (m, 2H), 7.55-7.56 (m, 1H), 7.45-7.48 (m, 3H), 7.30-7.35 (m, 4H), 7.23-7.25 (m, 1H), 7.15-7.18 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 162.4 (d, $J_{\text{C-F}}$ = 250 Hz), 154.0, 150.7, 131.4 (d, $J_{\text{C-F}}$ = 8.0 Hz), 130.5, 130.2, 128.8 (d, $J_{\text{C-F}}$ = 3.5 Hz), 128.5, 128.4, 127.0, 124.8, 123.0, 119.8, 116.5, 116.1 (d, $J_{\text{C-F}}$ = 22.5 Hz), 111.2; HRMS (ESI): Calcd 289.1023 for $\text{C}_{20}\text{H}_{14}\text{OF}^+$, Found: 289.1018 ($\text{M}+\text{H}$) $^+$.

2-phenyl-3-(4-chlorophenyl)benzofuran 3ad.^{S2} The product was obtained as a white solid in 80 % yield. m.p. 97-99 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.63-7.64 (m, 2H), 7.55-7.56 (m, 1H), 7.44-7.47 (m, 5H), 7.30-7.35 (m, 4H), 7.23-7.25 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 154.0,

150.8, 133.6, 131.4, 131.1, 130.4, 129.9, 129.3, 128.6, 128.5, 127.1, 124.9, 123.1, 119.8, 116.3, 111.2; HRMS (ESI): Calcd 305.0728 for $C_{20}H_{14}OCl^+$, Found: 305.0740 ($M+H$)⁺.

2-phenyl-3-(4-methylphenyl)benzofuran 3ae.^{S3} The product was obtained as a white solid in 90 % yield. m.p. 87-89 °C. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.66-7.68 (m, 2H), 7.53-7.55 (d, J = 10 Hz, 1H), 7.48-7.50 (d, J = 10 Hz, 1H), 7.38-7.40 (d, J = 10 Hz, 2H), 7.26-7.33 (m, 6H), 7.21-7.22 (m, 1H), 2.43 (s, 3H); ¹³C NMR (125 MHz, $CDCl_3$) δ 154.0, 150.4, 137.4, 130.8, 130.4, 129.8, 129.7, 129.6, 128.4, 128.3, 127.0, 124.6, 122.8, 120.1, 117.5, 111.1, 21.4; HRMS (ESI): Calcd 285.1274 for $C_{21}H_{17}O^+$, Found: 285.1291 ($M+H$)⁺.

2-phenyl-3-(4-ethylphenyl)benzofuran 3af. The product was obtained as colorless viscous oil in 86 % yield. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.67-7.68 (m, 2H), 7.49-7.54 (dd, J = 10 Hz, 2H), 7.40-7.42 (d, J = 10 Hz, 2H), 7.26-7.31 (m, 6H), 7.20-7.23 (m, 1H), 2.70-2.74 (q, J = 5 Hz, 2H), 1.29-1.32 (t, J = 10 Hz, 3H); ¹³C NMR (125 MHz, $CDCl_3$) δ 154.1, 150.4, 143.7, 130.9, 130.5, 130.0, 129.7, 128.5, 128.4, 128.3, 127.1, 124.7, 122.9, 120.0, 117.6, 111.1, 28.7, 15.4; HRMS (ESI): Calcd 321.1250 for $C_{22}H_{18}NaO^+$, Found: 321.1269 ($M+Na$)⁺.

2-phenyl-3-(4-biphenyl)benzofuran 3ag. The product was obtained as a white solid in 55 % yield. m.p. 135-137 °C. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.67-7.72 (m, 6H), 7.55-7.59 (m, 4H), 7.46-7.49 (m, 2H), 7.25-7.37 (m, 6H); ¹³C NMR (125 MHz, $CDCl_3$) δ 154.1, 150.7, 140.7, 140.3, 131.9, 130.7, 130.2, 130.1, 128.9, 128.5, 128.4, 127.6, 127.5, 127.2, 127.1, 124.8, 123.0, 120.1, 117.1, 111.2; HRMS (ESI): Calcd 347.1430 for $C_{26}H_{19}O^+$, Found: 347.1440 ($M+H$)⁺.

2-phenyl-3-(3,5-difluorophenyl)benzofuran 3ah. The product was obtained as a white solid in 38 % yield. m.p. 90-92 °C. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.65-7.67 (m, 2H), 7.56-7.57 (d, J = 5 Hz, 1H), 7.49-7.51 (d, J = 10 Hz, 1H), 7.34-7.37 (m, 4H), 7.26-7.29 (m, 1H), 7.02-7.04 (m, 2H), 6.83-6.88 (m, 1H); ¹³C NMR (125 MHz, $CDCl_3$) δ 163.5 (d, J_{C-F} = 247.4 Hz), 163.4 (d, J_{C-F} = 247.4 Hz), 154.0, 151.4, 136.3 (t, J_{C-F} = 10.1 Hz), 129.9, 129.4, 128.9, 128.7, 127.3, 125.1, 123.3, 119.6, 115.4, 112.7 (d, J_{C-F} = 25.3 Hz), 112.6 (d, J_{C-F} = 13.3 Hz), 111.4, 103.2 (t, J_{C-F} = 25.1 Hz); HRMS (ESI): Calcd 307.0929 for $C_{20}H_{13}OF_2^+$, Found: 307.0933 ($M+H$)⁺.

2-phenyl-3-(3,5-dimethylphenyl)benzofuran 3ai. The product was obtained as colorless viscous oil in 74 % yield. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.68-7.69 (d, J = 5 Hz, 2H), 7.52-7.54 (d, J = 10 Hz, 1H), 7.47-7.49 (d, J = 10 Hz, 1H), 7.27-7.32 (m, 4H), 7.20-7.23 (m, 1H), 7.11 (s, 2H), 7.04 (s, 1H), 2.34 (s, 6H); ¹³C NMR (125 MHz, $CDCl_3$) δ 154.0, 150.3, 138.5, 132.7, 130.9, 130.5, 129.4, 128.4, 128.2, 127.5, 126.9, 124.6, 122.8, 120.2, 117.8, 111.0, 21.4; HRMS (ESI): Calcd 321.1250 for $C_{22}H_{18}NaO^+$, Found: 321.1273 ($M+Na$)⁺.

2-phenyl-3-(2-fluorophenyl)benzofuran 3aj. The product was obtained as a white solid in 41 % yield. m.p. 73-75 °C. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.64-7.65 (m, 2H), 7.56-7.58 (m, 1H), 7.39-7.48 (m, 3H), 7.30-7.35 (m, 4H), 7.21-7.24 (m, 3H); ¹³C NMR (125 MHz, $CDCl_3$) δ 160.6 (d, J_{C-F} = 247.1 Hz), 154.2, 151.8, 132.4 (d, J_{C-F} = 3.75 Hz), 130.9, 130.3, 130.0 (d, J_{C-F} = 7.5 Hz), 128.8, 128.7, 126.8, 124.9, 124.8 (d, J_{C-F} = 3.75 Hz), 123.2, 120.8 (d, J_{C-F} = 16.25 Hz), 120.4, 116.5 (d, J_{C-F} = 21.25 Hz), 111.4, 111.3; HRMS (ESI): Calcd 289.1023 for $C_{20}H_{14}OF^+$, Found: 289.1020 ($M+H$)⁺.

2-phenyl-3-(2-chlorophenyl)benzofuran 3ak. The product was obtained as a white solid in 55 % yield. m.p. 80-82 °C. ¹H NMR ($CDCl_3$, 500 MHz) δ 7.56-7.59 (m, 4H), 7.39-7.42 (m, 2H), 7.28-7.37 (m, 6H), 7.21-7.24 (m, 1H); ¹³C NMR (125 MHz, $CDCl_3$) δ 153.8, 151.2, 134.7, 132.4, 132.1, 130.6, 130.2, 130.1, 129.5, 128.5, 128.4, 127.3, 126.3, 124.7, 122.9, 120.3, 115.0, 111.1; HRMS (ESI): Calcd 305.0728 for $C_{20}H_{14}OCl^+$, Found: 305.0728 ($M+H$)⁺.

2-phenyl-3-(2-methylphenyl)benzofuran 3al.^{S4} The product was obtained as colorless viscous oil in 66 % yield. ¹H NMR (CDCl₃, 500 MHz) δ 7.56-7.57 (m, 3H), 7.34-7.37 (m, 2H), 7.26-7.32 (m, 6H), 7.20-7.23 (m, 2H), 2.11 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 153.8, 150.2, 137.5, 132.2, 131.0, 130.6, 130.5, 128.5, 128.2, 128.1, 126.4, 125.9, 124.9, 124.6, 122.8, 120.2, 110.0, 101.3, 19.9.

2-phenyl-3-(3-methylphenyl)benzofuran 3am. The product was obtained as colorless viscous oil in 84 % yield. ¹H NMR (CDCl₃, 500 MHz) δ 7.66-7.68 (m, 2H), 7.53-7.55 (d, *J* = 10 Hz, 1H), 7.48-7.49 (m, 1H), 7.27-7.36 (m, 7H), 7.20-7.24 (m, 2H), 2.39 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 154.0, 150.4, 138.6, 132.8, 130.7, 130.4, 130.3, 128.9, 128.4, 128.3, 128.2, 127.0, 126.9, 124.6, 122.9, 120.1, 117.6, 111.1, 21.5; HRMS (ESI): Calcd 285.1274 for C₂₁H₁₇O⁺, Found: 285.1331 (M+H)⁺.

2,3-diphenyl-5-methylbenzofuran 3ba. The product was obtained as a white solid in 87 % yield. m.p. 115-117 °C (lit.^{S5} 114-115 °C). ¹H NMR (CDCl₃, 500 MHz) δ 7.63-7.65 (m, 2H), 7.40-7.50 (m, 6H), 7.27-7.30 (m, 4H), 7.13-7.14 (d, *J* = 8.5 Hz, 1H), 2.42 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 152.5, 150.6, 133.1, 132.4, 130.8, 130.4, 129.8, 129.0, 128.4, 128.2, 127.6, 127.0, 126.0, 119.8, 117.3, 110.6, 21.4; HRMS (ESI): Calcd 285.1274 for C₂₁H₁₇O⁺, Found: 285.1292 (M+H)⁺.

2-phenyl-3-(4-fluorophenyl)-5-methylbenzofuran 3bc. The product was obtained as a white solid in 81 % yield. m.p. 134-135 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.61-7.62 (m, 2H), 7.42-7.47 (m, 3H), 7.28-7.33 (m, 3H), 7.13-7.22 (m, 4H), 2.42 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 162.3 (d, *J*_{C-F} = 245.4 Hz), 152.4, 150.8, 132.6, 131.4 (d, *J*_{C-F} = 8.0 Hz), 130.6, 130.2, 128.9 (d, *J*_{C-F} = 3.38 Hz), 128.5, 128.4, 126.9, 126.1, 119.5, 116.3, 116.0 (d, *J*_{C-F} = 21.25 Hz), 110.7, 21.4; HRMS (ESI): Calcd 303.1180 for C₂₁H₁₆FO⁺, Found: 303.1204 (M+H)⁺.

2-phenyl-3-(4-ethylphenyl)-5-methylbenzofuran 3bf. The product was obtained as colorless viscous oil in 90 % yield. ¹H NMR (CDCl₃, 500 MHz) δ 7.65-7.67 (m, 2H), 7.40-7.43 (m, 3H), 7.27-7.31 (m, 6H), 7.12-7.14 (m, 1H), 2.72-2.77 (q, *J* = 10 Hz, 2H), 2.42 (s, 3H), 1.31-1.34 (t, *J* = 10 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 152.4, 151.1, 143.5, 132.3, 131.0, 130.5, 130.1, 129.7, 128.4, 128.3, 128.1, 126.9, 125.9, 119.9, 116.8, 110.6, 28.7, 21.3, 15.4; HRMS (ESI): Calcd 313.1587 for C₂₃H₂₁O⁺, Found: 313.1604 (M+H)⁺.

2-(4-methylphenyl)-3-phenylbenzofuran 3ca. The product was obtained as a white solid in 85 % yield. m.p. 98-99 °C (lit.^{S6} 96-97 °C). ¹H NMR (CDCl₃, 500 MHz) δ 7.46-7.55 (m, 8H), 7.30-7.31 (m, 3H), 7.12-7.13 (m, 2H), 2.35 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 153.9, 150.8, 138.3, 133.0, 130.3, 129.7, 129.1, 128.9, 127.8, 127.5, 126.9, 124.4, 122.8, 119.8, 116.8, 111.0, 21.3; HRMS (ESI): Calcd 285.1274 for C₂₁H₁₇O⁺, Found: 285.1281 (M+H)⁺.

2-(4-methylphenyl)-3-(4-fluorophenyl)benzofuran 3cc.^{S7} The product was obtained as a white solid in 80 % yield. m.p. 97-98 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.50-7.53 (m, 3H), 7.43-7.46 (m, 3H), 7.29-7.32 (m, 1H), 7.20-7.23 (m, 1H), 7.11-7.16 (m, 4H), 2.33 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 162.0 (d, *J*_{C-F} = 245 Hz), 153.9, 151.0, 138.6, 131.4 (d, *J*_{C-F} = 8.75 Hz), 130.3, 129.3, 129.0 (d, *J*_{C-F} = 3.38 Hz), 127.7, 127.0, 124.6, 123.0, 119.7, 116.0 (d, *J*_{C-F} = 21.38 Hz), 115.8, 111.1, 21.4; HRMS (ESI): Calcd 303.1180 for C₂₁H₁₆FO⁺, Found: 303.1194 (M+H)⁺.

2-(4-methylphenyl)-3-(4-ethylphenyl)benzofuran 3cf. The product was obtained as colorless viscous oil in 87 % yield. ¹H NMR (CDCl₃, 500 MHz) δ 7.49-7.57 (m, 4H), 7.40-7.42 (m, 2H), 7.28-7.32 (m, 3H), 7.20-7.23 (m, 1H), 7.12-7.13 (d, *J* = 5 Hz, 2H), 2.71-2.76 (q, *J* = 10 Hz, 2H),

2.34 (s, 3H), 1.30-1.33 (t, $J = 10$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 153.9, 150.7, 143.5, 138.3, 130.5, 130.1, 129.7, 129.1, 128.4, 128.0, 127.0, 124.4, 122.8, 120.0, 116.8, 110.0, 28.7, 21.3, 15.4; HRMS (ESI): Calcd 313.1587 for $\text{C}_{23}\text{H}_{21}\text{O}^+$, Found: 313.1602 ($\text{M}+\text{H}$) $^+$.

2-(4-methylphenyl)-3-phenyl-5-methylbenzofuran 3da. The product was obtained as a white solid in 88 % yield. m.p. 112-113 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.55 (d, $J = 8$ Hz, 2H), 7.46-7.52 (m, 4H), 7.39-7.44 (m, 2H), 7.28 (s, 1H), 7.11-7.14 (m, 3H), 2.43 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 152.4, 151.0, 138.3, 133.3, 132.4, 130.4, 129.9, 129.2, 128.9, 128.0, 127.5, 126.9, 125.7, 119.7, 116.7, 110.6, 21.4, 21.4; HRMS (ESI): Calcd 299.1430 for $\text{C}_{22}\text{H}_{19}\text{O}^+$, Found: 299.1444 ($\text{M}+\text{H}$) $^+$.

2-(4-methylphenyl)-3-(4-fluorophenyl)-5-methylbenzofuran 3dc. The product was obtained as a white solid in 80 % yield. m.p. 116-118 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.59 (d, $J = 8$ Hz, 2H), 7.49-7.55 (m, 3H), 7.30 (s, 1H), 7.20-7.26 (m, 5H), 2.51 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 162.3 (d, $J_{\text{C-F}} = 245$ Hz), 152.3, 151.1, 138.4, 132.5, 131.4 (d, $J_{\text{C-F}} = 8.0$ Hz), 130.3, 129.2, 129.1 (d, $J_{\text{C-F}} = 3.38$ Hz), 127.8, 126.9, 125.8, 119.4, 116.0 (d, $J_{\text{C-F}} = 21.25$ Hz), 115.6, 110.6, 21.4, 21.3; HRMS (ESI): Calcd 317.1336 for $\text{C}_{22}\text{H}_{18}\text{FO}^+$, Found: 317.1355 ($\text{M}+\text{H}$) $^+$.

2-(4-methylphenyl)-3-(4-ethylphenyl)-5-methylbenzofuran 3df. The product was obtained as a white solid in 89 % yield. m.p. 88-90 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.58 (d, $J = 8.0$ Hz, 2H), 7.43 (d, $J = 7.5$ Hz, 3H), 7.31 (d, $J = 8.5$ Hz, 3H), 7.13 (d, $J = 8.0$ Hz, 3H), 2.78 (q, $J = 7.5$ Hz, 2H), 2.43 (s, 3H), 2.36 (s, 3H), 1.35 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 152.4, 150.8, 143.5, 138.1, 132.3, 130.6, 130.4, 129.7, 129.1, 128.4, 128.2, 126.9, 125.7, 119.8, 116.7, 110.5, 28.7, 21.4, 21.4, 15.4; HRMS (ESI): Calcd 327.1743 for $\text{C}_{24}\text{H}_{23}\text{O}^+$, Found: 327.1749 ($\text{M}+\text{H}$) $^+$.

2-(4-fluorophenyl)-3-phenyl-5-methylbenzofuran 3ea. The product was obtained as a white solid in 80 % yield. m.p. 128-130 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.58-7.61 (m, 2H), 7.46-7.47 (m, 4H), 7.39-7.40 (m, 2H), 7.25 (s, 1H), 7.12-7.13 (m, 1H), 6.96-7.00 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 162.3 (d, $J_{\text{C-F}} = 247.5$ Hz), 152.4, 149.8, 132.8, 132.5, 130.3, 129.8, 129.0, 128.8 (d, $J_{\text{C-F}} = 8.75$ Hz), 127.7, 127.5 (d, $J_{\text{C-F}} = 3.38$ Hz), 126.0, 119.8, 115.5 (d, $J_{\text{C-F}} = 21.63$ Hz), 117.1, 110.6, 21.4; HRMS (ESI): Calcd 303.1180 for $\text{C}_{21}\text{H}_{16}\text{FO}^+$, Found: 303.1201 ($\text{M}+\text{H}$) $^+$.

2,3-di(4-fluorophenyl)-5-methylbenzofuran 3ec. The product was obtained as a white solid in 69 % yield. m.p. 139-140 °C. ^1H NMR (CDCl_3 , 500 MHz) δ 7.57-7.60 (m, 2H), 7.40-7.43 (m, 3H), 7.21 (s, 1H), 7.13-7.18 (m, 3H), 6.99-7.02 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 162.7 (d, $J_{\text{C-F}} = 247.6$ Hz), 162.7 (d, $J_{\text{C-F}} = 245.8$ Hz), 152.3, 149.9, 132.7, 131.4 (d, $J_{\text{C-F}} = 7.9$ Hz), 130.2, 128.8, 128.7, 126.8 (d, $J_{\text{C-F}} = 3.3$ Hz), 126.7 (d, $J_{\text{C-F}} = 8.1$ Hz), 126.1, 119.5, 116.1 (d, $J_{\text{C-F}} = 21.4$ Hz), 115.6 (d, $J_{\text{C-F}} = 21.8$ Hz), 110.7, 21.4; HRMS (ESI): Calcd 321.1085 for $\text{C}_{21}\text{H}_{15}\text{F}_2\text{O}^+$, Found: 321.1086 ($\text{M}+\text{H}$) $^+$.

2-(4-fluorophenyl)-3-(4-ethylphenyl)-5-methylbenzofuran 3ef. The product was obtained as colorless viscous oil in 82 % yield. ^1H NMR (CDCl_3 , 500 MHz) δ 7.61-7.64 (m, 2H), 7.37-7.41 (m, 3H), 7.26-7.30 (m, 3H), 7.11-7.13 (m, 1H), 6.97-7.01 (m, 2H), 2.71-2.76 (q, $J = 10$ Hz, 2H), 2.41 (s, 3H), 1.30-1.33 (t, $J = 5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 162.6 (d, $J_{\text{C-F}} = 247.4$), 153.9, 149.5, 143.8, 130.3, 129.8, 129.6, 128.9 (d, $J_{\text{C-F}} = 8.1$ Hz), 128.5, 127.1 (d, $J_{\text{C-F}} = 3.3$ Hz),

124.7, 122.9, 120.2, 117.3, 115.5 (d, J_{C-F} = 21.6 Hz), 111.0, 28.7, 15.4; HRMS (ESI): Calcd 331.1493 for $C_{23}H_{20}FO^+$, Found: 331.1497 (M+H)⁺.

2,3-diphenyl-5-chlorobenzofuran 3fa. The product was obtained as a white solid in 75 % yield. m.p. 111-113 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.62-7.64 (m, 2H), 7.43-7.47 (m, 7H), 7.25-7.31 (m, 4H); ¹³C NMR (125 MHz, CDCl₃) δ 152.4, 152.0, 132.2, 131.7, 130.2, 129.7, 129.1, 128.7, 128.6, 128.5, 127.9, 127.1, 124.8, 119.7, 117.1, 111.2; HRMS (ESI): Calcd 305.0728 for $C_{20}H_{14}OCl^+$, Found: 305.0738 (M+H)⁺.

2-(4-methylphenyl)-3-phenyl-5-chlorobenzofuran 3ga. The product was obtained as a white solid in 80 % yield. m.p. 148-150 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.51 (d, J = 8.5 Hz, 2H), 7.42-7.46 (m, 7H), 7.25-7.26 (m, 1H), 7.11 (d, J = 8.0 Hz, 2H), 2.34 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 152.3, 152.2, 138.9, 132.3, 131.8, 129.7, 129.2, 129.1, 128.6, 128.1, 127.8, 127.4, 127.0, 124.6, 119.5, 112.0, 21.4; HRMS (ESI): Calcd 319.0884 for $C_{21}H_{16}ClO^+$, Found: 319.0879 (M+H)⁺.

2-(4-fluorophenyl)-3-phenyl-5-chlorobenzofuran 3ha. The product was obtained as a white solid in 60 % yield. m.p. 126-128 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.60-7.63 (m, 2H), 7.41-7.50 (m, 7H), 7.27-7.29 (m, 1H), 6.99-7.03 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 162.9 (d, J_{C-F} = 245.3 Hz), 152.3, 151.1, 132.0, 131.6, 129.6, 129.2, 129.0 (d, J_{C-F} = 8.1 Hz), 128.8, 128.1, 126.4 (d, J_{C-F} = 3.3 Hz), 124.9, 119.7, 116.9, 115.7 (d, J_{C-F} = 21.6 Hz), 112.1; HRMS (ESI): Calcd 323.0633 for $C_{20}H_{13}ClFO^+$, Found: 323.0648 (M+H)⁺.

2-(4-biphenyl)-3-phenylbenzofuran 3ia. The product was obtained as a white solid in 90 % yield. m.p. 139-141 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.72-7.74 (m, 2H), 7.53-7.60 (m, 7H), 7.48-7.50 (m, 3H), 7.41-7.44 (m, 3H), 7.32-7.35 (m, 2H), 7.23-7.25 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 154.1, 150.3, 141.0, 140.4, 132.9, 130.4, 129.9, 129.6, 129.1, 128.9, 127.7, 127.6, 127.4, 127.1, 127.0, 124.8, 123.0, 120.1, 117.7, 111.1; HRMS (ESI): Calcd 347.1430 for $C_{26}H_{19}O^+$, Found: 347.1437 (M+H)⁺.

2,3-di(4-biphenyl)benzofuran 3ig. The product was obtained as a white solid in 60 % yield. m.p. 153-155 °C. ¹H NMR (CDCl₃, 500 MHz) δ 7.79 (d, J = 10 Hz, 2H), 7.69-7.74 (m, 4H), 7.56-7.63 (m, 8H), 7.47-7.50 (m, 2H), 7.42-7.45 (m, 2H), 7.33-7.38 (m, 3H), 7.27-7.28 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 154.1, 150.4, 141.0, 140.7, 140.4, 131.9, 130.3, 130.2, 129.6, 128.9, 128.8, 128.1, 127.7, 127.6, 127.5, 127.4, 127.1, 127.1, 127.0, 124.8, 123.0, 120.1, 117.3, 111.2; HRMS (ESI): Calcd 423.1743 for $C_{32}H_{23}O^+$, Found: 423.1753 (M+H)⁺.

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¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(4-(trifluoromethyl)phenyl)benzofuran (**3ab**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(4-(trifluoromethyl)phenyl)benzofuran (**3ab**)

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(4-fluorophenyl)benzofuran (**3ac**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(4-fluorophenyl)benzofuran (**3ac**)

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(4-chlorophenyl)benzofuran (**3ad**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(4-chlorophenyl)benzofuran (**3ad**)

c1ccc(cc1)-c2cc(ccc2)-c3cc4ccccc4o3-c5ccccc5

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(3,5-difluorophenyl)benzofuran (**3ah**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(3,5-difluorophenyl)benzofuran (**3ah**)

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(3,5-dimethylphenyl)benzofuran (**3ai**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(3,5-dimethylphenyl)benzofuran (**3ai**)

c1ccc(cc1)-c2c3ccccc3c(c2)c4ccccc4F

S16

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(2-methylphenyl)benzofuran(**3al**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(2-methylphenyl)benzofuran (**3al**)

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(3-methylphenyl)benzofuran (**3am**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(3-methylphenyl)benzofuran (**3am**)

¹H NMR (CDCl₃, 500 MHz) of 2,3-diphenyl-5-methylbenzofuran (**3ba**)

¹³C NMR (CDCl₃, 125 MHz) of 2,3-diphenyl-5-methylbenzofuran (**3ba**)

¹H NMR (CDCl₃, 500 MHz) of 2-phenyl-3-(4-ethylphenyl)-5-methylbenzofuran (**3bf**)

¹³C NMR (CDCl₃, 125 MHz) of 2-phenyl-3-(4-ethylphenyl)-5-methylbenzofuran (**3bf**)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-methylphenyl)-3-(4-fluorophenyl)benzofuran (**3cc**)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-methylphenyl)-3-(4-fluorophenyl)benzofuran (**3cc**)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-methylphenyl)-3-(4-ethyl)benzofuran (**3cf**)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-methylphenyl)-3-(4-ethyl)benzofuran (**3cf**)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-methylphenyl)-3-phenyl-5-methylbenzofuran (**3da**)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-methylphenyl)-3-phenyl-5-methylbenzofuran (**3da**)

Chemical structure: Cc1ccc(cc1)-c2oc3cc(C)ccc3c2-c4ccc(F)cc4

¹³C NMR peaks (ppm): 163.264, 161.302, 152.318, 151.085, 138.426, 132.463, 131.492, 131.429, 130.306, 129.199, 129.124, 129.097, 127.823, 126.877, 125.813, 119.405, 116.072, 115.902, 115.611, 110.625, 21.372, 21.337.

¹³C NMR (CDCl₃, 125 MHz) of
2-(4-methylphenyl)-3-(4-fluorophenyl)-5-methylbenzofuran (**3dc**)

¹H NMR (CDCl₃, 500 MHz) of
2-(4-methylphenyl)-3-(4-ethylphenyl)-5-methylbenzofuran (**3df**)

¹³C NMR (CDCl₃, 125 MHz) of
2-(4-methylphenyl)-3-(4-ethylphenyl)-5-methylbenzofuran (**3df**)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-fluorophenyl)-3-phenyl-5-methylbenzofuran (**3ea**)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-fluorophenyl)-3-phenyl-5-methylbenzofuran (**3ea**)

¹H NMR (CDCl₃, 500 MHz) of 2,3-di(4-fluorophenyl)-5-methylbenzofuran (**3ec**)

¹³C NMR (CDCl₃, 125 MHz) of 2,3-di(4-fluorophenyl)-5-methylbenzofuran(**3ec**)

¹H NMR (CDCl₃, 500 MHz) of
2-(4-fluorophenyl)-3-(4-ethylphenyl)-5-methylbenzofuran (**3ef**)

¹³C NMR (CDCl₃, 125 MHz) of
2-(4-fluorophenyl)-3-(4-ethylphenyl)-5-methylbenzofuran (**3ef**)

¹H NMR (CDCl₃, 125 MHz) of 2,3-diphenyl-5-chlorobenzofuran (**3fa**)

¹³C NMR (CDCl₃, 500 MHz) of 2,3-diphenyl-5-chlorobenzofuran (**3fa**)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-methylphenyl)-3-phenyl-5-chlorobenzofuran (**3ga**)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-methylphenyl)-3-phenyl-5-chlorobenzofuran(**3ga**)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-fluorophenyl)-3-phenyl-5-chlorobenzofuran (3ha)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-fluorophenyl)-3-phenyl-5-chlorobenzofuran (3ha)

¹H NMR (CDCl₃, 500 MHz) of 2-(4-biphenyl)-3-phenylbenzofuran (**3ia**)

¹³C NMR (CDCl₃, 125 MHz) of 2-(4-biphenyl)-3-phenylbenzofuran (**3ia**)