Supporting Information

Ligand-free Pd/C-catalyzed Suzuki-Miyaura Coupling Reaction for the Synthesis of Heterobiaryl Derivatives

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Experimental Section

General. All reactions were carried out under an argon atmosphere, unless otherwise noted. Aryl bromides were purchased from Tokyo Chemical Industry Co., Ltd., Aldrich Chemical Co., Inc. or Wako Pure Chemical Industries, Ltd. Aryl boronic acid esters were purchased from Aldrich Chemical Co., Inc. or Tokyo Chemical Industry Co., Ltd. Pd/C was gifted by N. E. Chemcat Co. Bases and solvents were purchased from Nacalai Tesque, Inc. or Wako Pure Chemical Industries, Ltd. All these materials were used without further purification.

$^1$H and $^{13}$C NMR spectra were recorded on a JEOL JNM EX-400 or JEOL JNM AL-400 spectrometer (400 MHz for $^1$H NMR and 100 MHz for $^{13}$C NMR). All NMR samples were prepared as CDCl$_3$ solutions. Chemical shifts ($\delta$) are expressed in ppm and are internally referenced (0.00 ppm for TMS-CDCl$_3$ for $^1$H NMR and 77.0 ppm for $^{13}$C NMR). EI Mass spectra were taken on a JEOL JMS-SX102A instrument. Elemental analyses were performed by YANACO MT-5 instrument. Flash column chromatography was performed using silica gel 60N [spherical neutral (63-210 $\mu$m)] from Kanto Chemical Co., Inc.

General Procedure of Suzuki-Miyaura Cross-Coupling Reaction

Method A: (eq 1; Table 1, entries 1-8; Table 2, entries 1-5, 7, 9 and 11):

To a test tube with a stir bar were added aryl bromide (250 $\mu$mol), arylboronic acid (375 $\mu$mol), Na$_3$PO$_4$·12H$_2$O (333 mg, 875 $\mu$mol), 10% Pd/C (9.3 mg, 8.75 $\mu$mol), H$_2$O (0.5 mL), and i-PrOH (0.5 mL) and the system was sealed with a septum. The air inside was replaced with argon (balloon) by three vacuum/argon cycles and the mixture was stirred at 80 °C. After a certain period, the mixture was diluted with H$_2$O (25 mL) and EtOAc (or Et$_2$O) (25 mL), and passed through a membrane filter (Millipore, Millex®–LH, 0.45 $\mu$m). The filtrate was separated into two layers and the aqueous layer was extracted with EtOAc (or Et$_2$O) (2 × 25 mL). The combined organic layers were washed with brine (25 mL), dried over Na$_2$SO$_4$ (or MgSO$_4$), and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel to give the corresponding biaryl.
Method B (Table 2, entries 6,8,10 and 12):
To a test tube with a stir bar were added aryl bromide (250 µmol), arylboronic acid (375 µmol), Na$_3$PO$_4$·12H$_2$O (333 mg, 875 µmol), 10% Pd/C (9.3 mg, 8.75 µmol), i-PrOH (1.0 mL) and the system was sealed with a septum. The air inside was replaced with argon (balloon) by three vacuum/argon cycles and the mixture was stirred at 80 °C. After a certain period, the mixture was diluted with H$_2$O (25 mL) and Et$_2$O (25 mL), and passed through a membrane filter (Millipore, Millex®–LH, 0.45 µm). The filtrate was separated into two layers and the aqueous layer was extracted with Et$_2$O (2 × 25 mL). The combined organic layers were washed with brine (25 mL), dried over MgSO$_4$, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel to give the corresponding biaryl.

Method C (Table 3, entries 1-6):
To a test tube with a stir bar were added aryl bromide (500 µmol), arylboronic acid (750 µmol), Na$_3$PO$_4$·12H$_2$O (285 mg, 750 µmol), 10% Pd/C (8.0 mg, 7.50 µmol), i-PrOH (2.0 mL) and the system was sealed with a septum. The air inside was replaced with argon (balloon) by three vacuum/argon cycles and the mixture was stirred at 80 °C. After a certain period, the mixture was diluted with H$_2$O (50 mL) and EtOAc (50 mL), and passed through a membrane filter (Millipore, Millex®–LH, 0.45 µm). The filtrate was separated into two layers and the aqueous layer was extracted with EtOAc (2 × 50 mL). The combined organic layers were washed with brine (50 mL), dried over Na$_2$SO$_4$, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel to give the corresponding biaryl.

4-(4’-Nitrophenyl)dibenzofuran
Yellow solid; mp 174–176 °C, $^1$H NMR δ 8.34 (d, $J$ = 8.8 Hz, 2H), 8.06 (d, $J$ = 8.8 Hz, 2H), 8.00 (d, $J$ = 7.6 Hz, 1H), 7.99 (d, $J$ = 7.6 Hz, 1H), 7.60 (d, $J$ = 8.2 Hz, 1H), 7.59 (d, $J$ = 8.2 Hz, 1H), 7.49 (t, $J$ = 8.2 Hz, 1H), 7.45 (t, $J$ = 8.2 Hz, 1H), 7.38 (t, $J$ = 7.6 Hz, 1H); $^{13}$C NMR δ 156.1, 153.1, 147.0, 142.9, 129.4, 127.7, 126.7, 125.4, 123.8, 123.4, 123.3, 123.2, 121.3, 120.8, 111.8; MS (EI) m/z 289 (M$^+$, 100%); HRMS (EI) Calcd for C$_{18}$H$_{11}$NO$_3$ (M$^+$) 289.0739. Found 289.0744. Anal. Calcd for C$_{18}$H$_{11}$NO$_3$·1/3 H$_2$O: C, 73.21; H, 3.98; N, 4.74. Found: C, 73.25; H, 4.04; N, 4.63.

2-(4’-Nitrophenyl)benzofuran$^1$
Yellow solid; $^1$H NMR δ 8.30 (d, $J$ = 8.8 Hz, 2H), 7.99 (d, $J$ = 8.8 Hz, 2H), 7.64 (d, $J$ =
8.0 Hz, 1H), 7.55 (d, \( J = 8.0 \) Hz, 1H), 7.37 (t, \( J = 8.0 \) Hz, 1H), 7.30–7.23 (m, 2H); \(^{13}\)C NMR \( \delta \) 155.4, 153.2, 147.3, 136.3, 128.6, 125.8, 125.2, 124.3, 123.5, 121.6, 111.5, 105.1; MS (EI) \( m/z \) 239 (M\(^+\), 100%); HRMS (EI) Calcd for C\(_{14}\)H\(_9\)NO\(_3\) (M\(^+\)) 239.0583. Found 239.0588.

2-(4'-Nitrophenyl)benzothiophene

Yellow solid; \(^1\)H NMR \( \delta \) 8.27 (d, \( J = 8.8 \) Hz, 2H), 7.87–7.84 (m, 4H), 7.70 (s, 1H), 7.42–7.38 (m, 2H); \(^{13}\)C NMR \( \delta \) 147.2, 141.2, 140.6, 140.3, 140.2, 126.8, 125.6, 125.1, 124.4, 124.3, 122.4, 122.4; MS (EI) \( m/z \) 255 (M\(^+\), 100%); HRMS (EI) Calcd for C\(_{14}\)H\(_9\)NO\(_2\)S (M\(^+\)) 255.0354. Found 255.0360.

4-(4'-Acetylphenyl)dibenzofuran

Colorless solid; mp 109–111 °C, \(^1\)H NMR \( \delta \) 8.08 (d, \( J = 8.0 \) Hz, 2H), 7.98 (d, \( J = 8.0 \) Hz, 1H), 7.96 (d, \( J = 8.0 \) Hz, 1H), 7.94 (d, \( J = 8.0 \) Hz, 1H), 7.59 (d, \( J = 8.0 \) Hz, 1H), 7.58 (d, \( J = 8.0 \) Hz, 1H), 7.45 (t, \( J = 8.0 \) Hz, 1H), 7.40 (t, \( J = 8.0 \) Hz, 1H), 7.35 (t, \( J = 8.0 \) Hz, 1H); \(^{13}\)C NMR \( \delta \) 197.6, 156.1, 153.3, 141.1, 136.1, 128.8, 128.6, 127.4, 126.7, 125.1, 124.5, 123.9, 123.2, 122.9, 120.7, 120.5, 111.8, 26.6; MS (EI) \( m/z \) 286 (M\(^+\), 81%); HRMS (EI) Calcd for C\(_{20}\)H\(_{14}\)O\(_2\) (M\(^+\)) 286.0994. Found 286.0987. Anal. Calcd for C\(_{20}\)H\(_{14}\)O\(_2\): C, 83.90; H, 4.93. Found: C, 83.75; H, 5.08.

2-(4'-Acetylphenyl)benzofuran

Colorless solid; mp 177–179 °C, \(^1\)H NMR \( \delta \) 8.00 (d, \( J = 8.6 \) Hz, 2H), 7.90 (d, \( J = 8.6 \) Hz, 2H), 7.59 (d, \( J = 8.4 \) Hz, 1H), 7.52 (d, \( J = 8.4 \) Hz, 1H), 7.32 (t, \( J = 8.4 \) Hz, 1H), 7.22 (t, \( J = 8.4 \) Hz, 1H), 2.60 (s, 3H); \(^{13}\)C NMR \( \delta \) 197.2, 155.2, 154.5, 136.5, 134.5, 128.9, 125.1, 124.7, 123.2, 121.3, 111.3, 103.6, 26.6; MS (EI) \( m/z \) 236 (M\(^+\), 90%); HRMS (EI) Calcd for C\(_{16}\)H\(_{12}\)O\(_2\) (M\(^+\)) 236.0837. Found 236.0830. Anal. Calcd for C\(_{16}\)H\(_{12}\)O\(_2\)·1/7 H\(_2\)O: C, 80.46; H, 5.18. Found: C, 80.85; H, 5.26.

4-(4'-Methoxyphenyl)dibenzofuran

Collorless solid; mp 86–88 °C, \(^1\)H NMR \( \delta \) 7.97 (d, \( J = 8.0 \) Hz, 1H), 7.89–7.85 (m, 3H), 7.59 (d, \( J = 8.0 \) Hz, 2H), 7.56 (d, \( J = 8.0 \) Hz, 2H), 7.45 (t, \( J = 8.0 \) Hz, 1H), 7.39 (t, \( J = 8.0 \) Hz, 1H), 7.34 (t, \( J = 8.0 \) Hz, 1H), 7.07 (d, 2H); \(^{13}\)C NMR \( \delta \) 159.3, 156.1, 153.3, 129.9, 128.8, 127.1, 126.4, 125.5, 124.8, 124.3, 123.1, 122.7, 120.6, 119.0, 114.1, 111.8, 55.3; MS (EI) \( m/z \) 289 (M\(^+\), 100%); HRMS (EI) Calcd for C\(_{19}\)H\(_{14}\)O\(_2\) (M\(^+\)) 274.0994. Found 274.0998. Anal. Calcd for C\(_{19}\)H\(_{14}\)O\(_2\)·1/6.5 H\(_2\)O: C, 82.36; H, 5.20. Found: C, 82.36; H, 5.21.
4-(2′-Tolyl)dibenzofuran
Colorless oil; $^1$H NMR $\delta$ 7.97 (d, $J = 7.8$ Hz, 1H), 7.94 (d, $J = 7.8$ Hz, 1H) 7.50 (d, $J = 7.8$ Hz, 1H), 7.43–7.31 (m, 8H), 2.24 (s, 3H); $^{13}$C NMR $\delta$ 156.2, 153.6, 136.8, 136.4, 130.3, 130.2, 128.3, 128.1, 127.1, 126.3, 125.7, 124.3, 124.2, 122.7, 122.7, 120.7, 119.6, 111.8, 20.2; MS (EI) m/z 258 (M$^+$, 100%); HRMS (EI) Calcd for C$_{19}$H$_{14}$O (M$^+$) 258.1045. Found 258.1055. Anal. Calcd for C$_{19}$H$_{14}$O: C, 88.34; H, 5.46. Found: C, 88.10; H, 5.68.

2-Phenylpyridine
Colorless oil; $^1$H NMR $\delta$ 8.65–8.64 (m, 1H), 7.99–7.96 (m, 2H), 7.63–7.57 (m, 2H), 7.44–7.33 (m, 3H), 7.22–7.08 (m, 1H); $^{13}$C NMR $\delta$ 157.1, 149.4, 139.1, 136.4, 128.7, 128.5, 126.6, 121.8, 120.2; MS (EI) m/z 155 (M$^+$, 100%); HRMS (EI) Calcd for C$_{11}$H$_9$N (M$^+$) 155.0735. Found 155.07447.

2-(4′-Tolyl)pyridine
Colorless oil; $^1$H NMR $\delta$ 8.66 (d, $J = 4.8$ Hz, 1H), 7.88 (d, $J = 8.0$ Hz, 2H), 7.68–7.67 (m, 2H), 7.26 (d, $J = 8.0$ Hz, 2H), 7.18–7.14 (m, 1H), 2.38 (s, 3H); $^{13}$C NMR $\delta$ 157.4, 149.5, 138.8, 136.6, 136.5, 129.4, 126.7, 121.7, 120.1, 21.2; MS (EI) m/z 169 (M$^+$, 100%); HRMS (EI) Calcd for C$_{12}$H$_{11}$N (M$^+$) 169.0892. Found 169.0897.

2-(4′-Chlorophenyl)pyridine
Colorless oil; $^1$H NMR $\delta$ 8.69 (d, $J = 4.8$ Hz, 1H), 7.94 (d, $J = 8.8$ Hz, 2H), 7.68–7.62 (m, 2H), 7.15–7.11 (m, 1H), 7.02 (d, $J = 8.8$ Hz, 2H), 3.82 (s, 3H); $^{13}$C NMR $\delta$ 160.4, 157.0, 149.4, 136.5, 131.9, 128.0, 121.3, 119.6, 114.0, 55.2; MS (EI) m/z 185 (M$^+$, 100%); HRMS (EI) Calcd for C$_{11}$H$_{11}$NO (M$^+$) 185.0841. Found 185.0838.

2-(4′-Methoxyphenyl)pyridine
Colorless solid; $^1$H NMR $\delta$ 8.63 (d, $J = 4.8$ Hz, 1H), 7.94 (d, $J = 8.8$ Hz, 2H), 7.68–7.62 (m, 2H), 7.15–7.11 (m, 1H), 7.02 (d, $J = 8.8$ Hz, 2H), 3.82 (s, 3H); $^{13}$C NMR $\delta$ 160.4, 157.0, 149.4, 136.5, 131.9, 128.0, 121.3, 119.6, 114.0, 55.2; MS (EI) m/z 185 (M$^+$, 100%); HRMS (EI) Calcd for C$_{11}$H$_{11}$NO (M$^+$) 185.0841. Found 185.0838.

2-(4′-Methylenedioxy)pyridine
Colorless oil; $^1$H NMR $\delta$ 8.63 (d, $J = 4.8$ Hz, 1H), 7.94 (d, $J = 8.8$ Hz, 2H), 7.68–7.62 (m, 2H), 7.15–7.11 (m, 1H), 7.02 (d, $J = 8.8$ Hz, 2H), 3.82 (s, 3H); $^{13}$C NMR $\delta$ 160.4, 157.0, 149.4, 136.5, 131.9, 128.0, 121.3, 119.6, 114.0, 55.2; MS (EI) m/z 185 (M$^+$, 100%); HRMS (EI) Calcd for C$_{11}$H$_{11}$NO (M$^+$) 185.0841. Found 185.0838.

2-(3′,4′-Methylenedioxy)pyridine
Colorless oil; $^1$H NMR $\delta$ 8.63 (d, $J = 4.8$ Hz, 1H), 7.68 (t, $J = 7.4$ Hz, 1H), 7.61 (d, $J = 7.4$ Hz, 1H), 7.52 (s, 1H), 7.48 (d, $J = 8.4$ Hz, 1H), 7.16 (dd, $J = 7.4$ Hz, 4.8 Hz, 1H), 6.89 (d, $J = 8.4$ Hz, 1H), 6.00 (s, 2H); $^{13}$C NMR $\delta$ 156.8, 149.4, 148.4, 148.2, 136.6, 133.8, 121.6, 120.8, 119.9, 108.3, 107.3, 101.2; MS (EI) m/z 199 (M$^+$, 100%); HRMS (EI) Calcd for C$_{12}$H$_9$NO$_2$ (M$^+$) 199.0633. Found 199.0640. Anal. Caled for C$_{12}$H$_9$NO$_2$·1/9 H$_2$O: C, 71.63; H, 4.62; N, 6.96. Found: C, 71.78; H, 4.59; N, 6.93.

2-(4′-Chlorophenyl)pyridine
Colorless oil; $^1$H NMR $\delta$ 8.69 (d, $J = 4.0$ Hz, 1H), 7.94 (d, $J = 8.6$ Hz, 2H), 7.75(t, $J =
7.6 Hz, 1H), 7.69 (d, $J = 7.6$ Hz, 1H), 7.45 (d, $J = 8.6$ Hz, 2H), 7.02 (dd, $J = 7.6$ Hz, 4.0 Hz, 1H); $^{13}$C NMR δ 156.9, 150.4, 138.5, 137.5, 135.8, 129.6, 128.8, 123.0, 121.0; MS (EI) $m/z$ 189 (M$^+$, 100%); HRMS (EI) Calcd for C$_{11}$H$_8$ClN (M$^+$) 189.0345. Found 189.0347.

3-(4'-Methoxyphenyl)pyridine

Colorless solid; $^1$H NMR δ 8.83 (s, 1H), 8.55 (d, $J = 4.7$ Hz, 1H), 7.82 (d, $J = 7.7$ Hz, 1H), 7.50 (d, $J = 8.6$ Hz, 2H), 7.32 (dd, $J = 4.7$ Hz, 7.7 Hz, 1H), 7.00 (d, $J = 8.6$ Hz, 2H), 3.84 (s, 3H); $^{13}$C NMR δ 159.7, 147.5, 147.4, 136.3, 133.9, 130.0, 128.1, 123.5, 114.5, 55.2; MS (EI) $m/z$ 185 (M$^+$, 100%); HRMS (EI) Calcd for C$_{12}$H$_{11}$NO (M$^+$) 185.0841. Found 185.0832.

4-(4'-Methoxyphenyl)pyridine

Colorless solid; $^1$H NMR δ 8.62 (d, $J = 5.8$ Hz, 2H), 7.57 (d, $J = 8.8$ Hz, 2H), 7.45 (d, $J = 5.8$ Hz, 2H), 6.98 (d, $J = 8.8$ Hz, 2H), 3.84 (s, 3H); $^{13}$C NMR δ 160.5, 149.7, 147.9, 130.1, 128.0, 121.0, 114.5, 55.3; MS (EI) $m/z$ 185 (M$^+$, 100%); HRMS (EI) Calcd for C$_{12}$H$_{11}$NO (M$^+$) 185.0841. Found 185.0831.

5-(4'-Methoxyphenyl)pyrimidine

Colorless solid; $^1$H NMR δ 9.16 (s, 1H), 8.92 (s, 2H), 7.52 (d, $J = 8.4$ Hz, 2H), 7.04 (d, $J = 8.4$ Hz, 2H), 3.87 (s, 3H); $^{13}$C NMR δ 160.4, 156.7, 154.3, 133.8, 128.0, 126.4, 114.8, 55.3; MS (EI) $m/z$ 186 (M$^+$, 100%); HRMS (EI) Calcd for C$_{11}$H$_{10}$N$_2$O (M$^+$) 186.0793. Found 186.0798.

2-(3'-Quinolyl)benzofuran

Collorless solid; mp 134–136 °C, $^1$H NMR δ 9.31 (s, 1H), 8.50 (s, 1H), 8.10 (d, $J = 8.2$ Hz, 1H), 7.84 (d, $J = 8.2$ Hz, 1H), 7.68 (t, $J = 8.2$ Hz, 1H), 7.60 (d, $J = 7.8$ Hz, 1H), 7.55–7.51 (m, 2H), 7.31 (t, $J = 7.8$ Hz, 1H), 7.24 (t, $J = 7.8$ Hz, 1H), 7.17 (s, 1H); $^{13}$C NMR δ 155.1, 153.1, 147.6, 147.5, 130.7, 129.7, 129.3, 128.8, 128.1, 127.7, 127.3, 125.0, 123.6, 123.3, 121.2, 111.2, 102.9; MS (EI) $m/z$ 245 (M$^+$, 100%); HRMS (EI) Calcd for C$_{17}$H$_{11}$NO (M$^+$) 245.0841. Found 245.0835. Anal. Calcd for C$_{17}$H$_{11}$NO: C, 83.25; H, 4.52; N, 5.71. Found: C, 82.97; H, 4.77; N, 5.62.

4-(3'-Quinolyl)dibenzofuran

Collorless solid; mp 145–147 °C, $^1$H NMR δ 9.46 (s, 1H), 8.59 (s, 1H), 8.18 (d, $J = 8.8$ Hz, 1H), 7.93 (t, $J = 6.4$ Hz, 2H), 7.88 (d, $J = 8.0$ Hz, 1H), 7.23 (t, $J = 7.4$ Hz, 1H), 7.66
(d, J = 8.0 Hz, 1H), 7.58–7.54 (m, 2H), 7.50–7.40 (m, 2H), 7.34 (t, J = 7.8 Hz, 1H); $^{13}$C NMR δ 156.0, 153.3, 150.6, 147.3, 135.0, 129.5, 129.2, 129.1, 128.0, 127.8, 127.3, 126.8, 126.5, 125.0, 123.8, 123.3, 122.8, 122.2, 120.6, 120.4, 111.7; MS (EI) m/z 295 (M⁺, 100%); HRMS (EI) Calcd for C$_{21}$H$_{13}$NO (M⁺) 295.0997. Found 295.0986. Anal. Calcd for C$_{21}$H$_{13}$NO·1/11 H$_2$O: C, 84.93; H, 4.47; N, 4.72. Found: C, 84.98; H, 4.60; N, 4.71.

3-(2'-Thienyl)quinoline
Collorless solid; ¹H NMR δ 9.17 (s, 1H), 8.21 (s, 1H), 8.07 (d, J = 8.2 Hz, 1H), 7.77 (d, J = 8.2 Hz, 1H), 7.65 (t, J = 8.2 Hz, 1H), 7.51 (t, J = 8.2 Hz, 1H), 7.45 (d, J = 3.6 Hz, 1H), 7.35 (d, J = 5.2 Hz, 1H), 7.12 (dd, J = 5.2 Hz, 3.6 Hz, 1H); $^{13}$C NMR δ 148.6, 147.3, 140.8, 131.4, 129.3, 129.3, 128.4, 127.9, 127.8, 127.6, 127.3, 126.1, 124.4; MS (EI) m/z 211 (M⁺, 100%); HRMS (EI) Calcd for C$_{13}$H$_{9}$NS (M⁺) 211.0456. Found 211.0461.

2-(5'-Pyrimidyl)benzofuran
Collorless solid; ¹H NMR δ 9.15 (s, 1H), 9.10 (s, 1H), 7.57 (d, J = 7.8 Hz, 2H), 7.51 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.8 Hz, 1H), 7.24 (t, J = 7.8 Hz, 1H); $^{13}$C NMR δ 157.6, 155.0, 152.4, 149.4, 128.0, 125.4, 124.6, 123.4, 121.2, 111.2, 103.9; MS (EI) m/z 196 (M⁺, 100%); HRMS (EI) Calcd for C$_{12}$H$_{8}$N$_{2}$O (M⁺) 196.0637. Found 196.0642.

2-[2'-(5'-Methyl)thienyl]benzofuran
Collorless solid; mp 85–87 °C, ¹H NMR δ 7.48 (d, J = 7.0 Hz, 1H), 7.45 (d, J = 7.0 Hz, 1H), 7.25 (d, J = 4.0 Hz, 1H), 7.23–7.18 (m, 2H), 6.73 (s, 1H), 6.72 (d, J = 4.0 Hz, 1H), 2.48 (s, 3H); $^{13}$C NMR δ 154.4, 151.5, 140.8, 130.9, 129.2, 126.1, 124.6, 123.9, 123.0, 120.5, 110.9, 100.2, 15.3; MS (EI) m/z 214 (M⁺, 100%); HRMS (EI) Calcd for C$_{13}$H$_{10}$OS (M⁺) 214.0452. Found 214.0444. Anal. Calcd for C$_{13}$H$_{10}$OS: C, 72.87; H, 4.70. Found: C, 72.92; H, 4.81.

2-(5'-Indoyl)benzofuran
Collorless solid; mp 156–158 °C, ¹H NMR δ 8.18 (s, 1H), 8.05 (brs, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.54 (d, J = 7.2 Hz, 1H), 7.52 (d, J = 7.2 Hz, 1H), 7.35 (d, J = 8.8 Hz, 1H), 7.26–7.18 (m, 3H), 7.15 (t, J = 7.2 Hz, 1H), 6.93 (s, 1H), 6.60–6.59 (m, 1H); $^{13}$C NMR δ 157.6, 154.7, 135.9, 129.7, 128.1, 125.1, 123.5, 122.7, 122.6, 120.4, 119.7, 117.6, 111.4, 110.9, 103.3, 99.4; MS (EI) m/z 233 (M⁺, 100%); HRMS (EI) Calcd for C$_{16}$H$_{11}$NO (M⁺) 233.0841. Found 233.0835. Anal. Calcd for C$_{16}$H$_{11}$NO·1/3 H$_2$O: C,
80.32; H, 4.91; N, 5.85. Found: C, 80.46; H, 4.90, N, 5.82.
References
4-(4'-Nitrophenyl)dibenzofuran

Supplementary Material (ESI) for Chemical Communications
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2-\((4'\text{-Acetylphenyl})\text{benzofuran}\)
4-(4'-Acetylphenyl)dibenzofuran
4-(4'-Methoxyphenyl)dibenzofuran
4-(2'-Tolyl)dibenzofuran

[Chemical structure image]

Supplementary Material (ESI) for Chemical Communications
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2-(3',4'-Methylenedioxy)pyridine

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\begin{align*}
\text{H} & \quad \text{O} \\
\text{N} & \quad \text{O}
\end{align*}
\]
2-(3'-Quinolyl)benzofuran
4-(3'-Quinolyl)dibenzofuran
2-[2''-(5''-Methyl)thienyl]benzofuran

Supplementary Material (ESI) for Chemical Communications
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2-(5'-Indoyl)benzofuran

Supplementary Material (ESI) for Chemical Communications
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