

## Supporting Information

## A Convenient Method for Synthesis of Benzo[d]thiazoles in Water and Solvent Free Condition

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**2-Methylbenzo[d]thiazole (7):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3062 ( $\text{sp}^2$  C-H), 2924–2853 ( $\text{sp}^3$  C-H), 1702 (C=N), 1520–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83–7.81 (1H, d,  $J = 8.4$ ), 7.59–7.56 (1H, d,  $J = 7.8$ ), 7.24–7.21 (1H, t,  $J = 4.05$ ), 7.14–7.11 (1H, t,  $J = 4.05$ ), 2.58 (3H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  166.6, 153.2, 135.5, 125.7, 124.5, 122.2, 121.2; EI, MS  $m/z$  (%): 149.25 (100,  $\text{M}^+$ ).

**2-Ethylbenzo[d]thiazole (8):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3062 ( $\text{sp}^2$  C-H), 2924–2853 ( $\text{sp}^3$  C-H), 1702 (C=N), 1520–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (1H, d,  $J = 8.0$  Hz), 7.78 (1H, d,  $J = 8.0$  Hz), 7.40 (1H, t,  $J = 7.6$  Hz), 7.28 (1H, t,  $J = 7.6$  Hz), 3.10 (2H, q,  $J = 7.6$  Hz), 1.43 (3H, t,  $J = 7.6$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  167.8, 161.9, 154.2, 134.8, 129.1, 126.4, 126.2, 124.8, 124.8, 121.5, 114.3, 55.4; EI, MS  $m/z$  (%): 163.24 (100,  $\text{M}^+$ ).

**2-Pentylbenzo[d]thiazole (9):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3062 ( $\text{sp}^2$  C-H), 2924–2853 ( $\text{sp}^3$  C-H), 1702 (C=N), 1520–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (1H, d,  $J = 8.1$  Hz), 7.83–7.82 (1H, m), 7.45–7.42 (1H, m), 7.35–7.32 (1H, m), 3.10 (2H, t,  $J = 7.7$  Hz), 1.88 (2H, q,  $J = 7.7$  Hz), 1.45–1.34 (4H, m), 0.91 (3H, t,  $J = 7.3$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.4, 153.2, 135.1, 125.8, 124.5, 122.4, 121.4, 34.3, 31.3, 29.4, 22.3, 13.9; EI, MS  $m/z$  (%): 219.35 (100,  $\text{M}^+$ ).

**2-Heptylbenzo[d]thiazole (10):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3062 ( $\text{sp}^2$  C-H), 2924–2853 ( $\text{sp}^3$  C-H), 1702 (C=N), 1520–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97–7.95 (1H, d,  $J = 8.1$  Hz), 7.78–7.76 (1H, d,  $J = 7.8$  Hz), 7.40–7.37 (1H, t,  $J = 4.05$  Hz), 7.30–7.27 (1H, t,  $J = 4.05$ ), 3.09–3.04 (2H, t,  $J = 7.65$  Hz), 1.89–1.79 (2H, m), 1.42–1.26 (8H, m), 0.89–0.84 (3H, t,  $J = 6.75$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.2, 153.2, 135.1, 125.7, 124.5, 122.4, 121.4, 34.3, 31.6, 29.6, 29.1, 28.9, 22.6, 14.0; EI, MS  $m/z$  (%): 233.40 (100, M-15).

**2-Undecylbenzo[d]thiazole (11):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3063 ( $\text{sp}^2$  C-H), 2951–2851 ( $\text{sp}^3$  C-H), 1779–1703 (C=N), 1520–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00–7.97 (1H, d,  $J = 8.1$  Hz), 7.86–7.83 (1H, d,  $J = 8.1$  Hz), 7.48–7.43 (1H, t,  $J = 7.05$  Hz), 7.37–7.33 (1H, t,  $J = 6.9$  Hz), 3.15–3.10 (2H, t,  $J = 3.75$  Hz), 1.94–1.84 (2H, m), 1.45–1.27 (16H, m), 0.92–0.87 (3H, t,  $J = 6.75$  Hz);  $^{13}\text{C-NMR}$

(75 MHz,  $\text{CDCl}_3$ )  $\delta$  172.4, 153.2, 135.1, 125.8, 124.5, 122.5, 121.4, 34.3, 31.9, 29.7, 29.6, 29.4, 29.34, 29.31, 29.1, 22.7, 14.1; EI, MS  $m/z$  (%): 289.51 (100, M-15).

**2-(Methoxymethyl)benzo[d]thiazole (12):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3104–3065 ( $\text{sp}^2$  C-H), 2922 ( $\text{sp}^3$  C-H), 1700 (C=N), 1514–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00–7.97 (1H, d,  $J = 8.1$  Hz), 7.87–7.84 (1H, d,  $J = 7.8$  Hz), 7.46–7.42 (1H, t,  $J = 7.05$  Hz), 7.36–7.32 (1H, t,  $J = 7.05$  Hz), 4.83 (2H, s), 3.50 (3H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  170.0, 153.0, 134.9, 126.0, 125.0, 122.9, 121.7, 71.9, 59.2; EI, MS  $m/z$  (%): 165.21 (100,  $\text{M}^+$ ).

**2-Cyclohexylbenzo[d]thiazole (13):** mp 117–119 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3104–3065 ( $\text{sp}^2$  C-H), 2922 ( $\text{sp}^3$  C-H), 1700 (C=N), 1514–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (1H, d,  $J = 8.1$  Hz), 7.85–7.83 (1H, m), 7.45–7.42 (1H, m), 7.35–7.31 (1H, m), 3.10 (1H, tt,  $J = 3.3, 11.7$  Hz), 2.23–2.18 (2H, m), 1.91–1.86 (2H, m), 1.79–1.74 (1H, m), 1.68–1.60 (2H, m), 1.49–1.40 (2H, m), 1.36–1.27 (1H, m);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  177.6, 153.1, 134.5, 125.7, 124.4, 122.5, 121.5, 43.4, 33.4, 26.0, 25.7; EI, MS  $m/z$  (%): 21833 (100,  $\text{M}^+$ ).

**2-Phenylbenzo[d]thiazole (14):** mp 103–105 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3064 ( $\text{sp}^2$  C-H), 2924–2853 ( $\text{sp}^3$  C-H), 1650 (C=N), 1478–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41–7.38 (1H, m), 7.52–7.48 (4H, m), 7.92–7.90 (1H, d,  $J = 8.1$  Hz), 8.12–8.08 (3H, m);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  168.1, 154.1, 135.0, 133.6, 131.0, 129.0, 127.5, 126.3, 125.2, 123.2, 121.6; EI, MS  $m/z$  (%): 211.28 (100,  $\text{M}^+$ ).

**2-(4-Methoxyphenyl)benzo[d]thiazole (15):** Solid, mp 117–119 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3057 ( $\text{sp}^2$  C-H), 2993–2858 ( $\text{sp}^3$  C-H), 1604 (C=N), 1620–1432 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05–8.02 (3H, m), 7.87 (1H, d,  $J = 7.7$  Hz), 7.49–7.45 (1H, m), 7.37–7.34 (1H, m), 7.01–6.98 (2H, m), 3.88 (3H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  167.8, 161.9, 154.2, 134.8, 129.1, 126.4, 126.2, 124.8, 122.8, 121.5, 114.3, 55.4; EI, MS  $m/z$  (%): 242.31 (100,  $\text{M}^+$ ).

**2-Benzylbenzo[d]thiazole (16):** Liquid, IR (KBr,  $\text{cm}^{-1}$ ): 3104–3065 ( $\text{sp}^2$  C-H), 2922 ( $\text{sp}^3$  C-H), 1700 (C=N), 1514–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (1H, d,  $J = 8.4$  Hz), 7.79 (1H, d,  $J = 7.7$  Hz), 7.47–7.44 (1H, m), 7.39–7.28 (6H, m), 4.45 (2H, s);  $^{13}\text{C-NMR}$  (75 MHz,

$\text{CDCl}_3$ )  $\delta$  171.2, 153.2, 137.2, 135.6, 129.1, 128.8, 127.3, 125.9, 124.8, 122.7, 121.5, 40.6; EI, MS  $m/z$  (%): 225.31 (100,  $\text{M}^+$ ).

**2-Phenethylbenzo[d]thiazole (17):** mp 59–60 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3081–3025 ( $\text{sp}^2$  C-H), 2955–2852 ( $\text{sp}^3$  C-H), 1708–1690 (C=N), 1492–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.02 (1H, d), 7.85 (1H, d), 7.34 (7H, m), 3.45 (2H, m), 3.22 (2H, m);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  171.2, 153.2, 137.2, 135.6, 129.1, 128.8, 127.3, 125.9, 124.8, 122.7, 121.5, 40.6; EI, MS  $m/z$  (%): 239.34 (100,  $\text{M}^+$ ).

***N,N*-Dimethyl-4-(6-methylbenzo[d]thiazole-2-yl)aniline (18):** mp 189–191 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3078 ( $\text{sp}^2$  C-H), 2976–2935 ( $\text{sp}^3$  C-H), 1736–1707 (C=N), 1639–1459 (C=C), 1242–1175 (C-N), 915 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97–7.94 (2H, d,  $J=9.0$  Hz), 7.90–7.87 (2H, d,  $J=8.4$  Hz), 7.64 (1H, s), 7.28–7.25 (1H, d,  $J=8.7$  Hz), 6.77–6.74 (2H, d,  $J=9.0$  Hz), 3.06 (6H, s), 2.49 (3H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  167.8, 152.4, 152.0, 134.6, 134.2, 128.7, 127.5, 121.7, 121.5, 121.2, 111.7, 40.2, 21.5; EI, MS  $m/z$  (%): 268.38 (100,  $\text{M}^+$ ).

**6-Methyl-2-(4-nitrophenyl)benzo[d]thiazole (19):** mp 132–133 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3325–3231 ( $\text{sp}^2$  C-H), 3014–2911 ( $\text{sp}^3$  C-H), 1600–1475 (C=C), 1688 (C=N), 1517–1337 (N=O), 847 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35–8.32 (2H, d,  $J=8.7$  Hz), 8.25–8.22 (2H, d,  $J=8.7$  Hz), 8.02–7.99 (1H, d,  $J=8.4$  Hz), 7.74 (1H, s), 7.38–7.35 (1H, d,  $J=8.4$  Hz), 2.54 (3H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  163.7, 152.2, 148.8, 139.3, 136.6, 135.6, 128.6, 128.0, 124.2, 123.3, 121.5, 21.6; EI, MS  $m/z$  (%): 270.31 (100,  $\text{M}^+$ ).

**2-(3-Chlorophenyl)benzo[d]thiazole (16):** mp 97–99 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3060 ( $\text{sp}^2$  C-H), 2920–2840 ( $\text{sp}^3$  C-H), 1650 (C=N);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.23–7.36 (3H, m), 7.49 (1H, s), 7.52–7.50 (2H, m), 8.12 (1H, d,  $J=2.1$  Hz), 8.23 (1H, d,  $J=3.1$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  121.7, 121.8, 125.2, 125.6, 125.9, 127.4, 128.8, 130.7, 135.8, 136.7, 155.6, 168.3; EI, MS  $m/z$  (%): 245.72 (100,  $\text{M}^+$ ).

**4-(Benzo[d]thiazol-2-yl)benzotrile (17):** mp 167–169 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3050 ( $\text{sp}^2$  C-H), 2920–2850 ( $\text{sp}^3$  C-H), 1650 (C=N);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.51–7.53 (2H, m), 7.57 (2H, d,  $J=4.3$  Hz), 7.66 (2H, d,  $J=4.1$  Hz), 8.14 (1H, d,  $J=2.1$  Hz), 8.20 (1H, d,  $J=2.2$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  121.7, 121.8, 125.2, 125.6, 125.9, 127.4, 128.8, 130.7, 135.8, 136.7, 155.6, 168.3; EI, MS  $m/z$  (%): 236.29 (100,  $\text{M}^+$ ).

**2-(Thiophen-2-yl)benzo[d]thiazole (18):** mp 100–102 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3062 ( $\text{sp}^2$  C-H), 2924–2853 ( $\text{sp}^3$  C-H), 1702 (C=N), 1520–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06–8.04 (1H, d,  $J=8.1$  Hz), 7.88–7.85 (1H, d,  $J=8.1$  Hz), 7.67–7.66 (1H, d,  $J=3.6$  Hz), 7.53–7.47 (2H, m), 7.40–7.36 (1H, t,  $J=6.9$  Hz), 7.16–7.14 (1H, t,  $J=4.35$ );  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  161.4, 153.6, 137.3, 134.6, 129.3, 128.6, 128.0, 126.4, 125.2, 122.9, 121.4; EI, MS  $m/z$  (%): 217.35 (100,  $\text{M}^+$ ).

**2-(Thiophen-2-ylmethyl)benzo[d]thiazole (19):** mp 78–80 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3104–3065 ( $\text{sp}^2$  C-H), 2922 ( $\text{sp}^3$  C-H), 1700 (C=N), 1514–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04–8.02 (1H, d,  $J=7.8$  Hz), 7.83–7.81 (1H, d,  $J=7.5$  Hz), 7.50–7.45 (1H, t,  $J=7.05$  Hz), 7.39–7.34 (1H, t,  $J=7.05$  Hz), 7.27–7.26 (1H, d,  $J=5.1$  Hz), 7.07–7.06 (1H, d,  $J=2.4$  Hz), 7.02–7.00 (1H, t,  $J=4.2$  Hz), 4.66 (1H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  170.3, 153.2, 138.7, 135.6, 127.2, 127.0, 126.0, 125.3, 125.0, 122.9, 121.6, 34.6; EI, MS  $m/z$  (%): 231.34 (100,  $\text{M}^+$ ).

**2-(Furan-2-yl)benzo[d]thiazole (20):** mp 108–109 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3104–3065 ( $\text{sp}^2$  C-H), 2922 ( $\text{sp}^3$  C-H), 1700 (C=N), 1514–1434 (C=C), 780 (C-S);  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.13 (1H, s), 8.04 (1H, d,  $J=7.8$  Hz), 7.88 (1H, d,  $J=7.8$  Hz), 7.55 (1H, s), 7.49 (1H, dd,  $J=7.5$  Hz, 7.8 Hz), 7.38 (1H, dd,  $J=7.5$  Hz, 7.8 Hz), 6.99 (1H, s);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5, 154.1, 144.6, 143.0, 134.7, 126.7, 125.4, 123.2, 122.2, 121.9, 109.6; EI, MS  $m/z$  (%): 201.26 (100,  $\text{M}^+$ ).

