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SUPPLEMENTARY MATERIAL TO

An investigation of nucleophilic substitution reactions of 2,3-dichloro-1,4-naphthoquinone with various nucleophilic reagents

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

2-Chloro-3-((4-(diethylamino)phenyl)amino)naphthalene-1,4-dione ***(3)***. Compound **3** was synthesized in the reaction of **1** (0.5 g, 2.20 mmol) with **2** (0.36 g, 2.20 mmol) according to general procedure 1.

Yield: 67.53 % (0.52 g); blue solid; m.p.: 159–160 °C (Lit. 159 °C[1]); Anal. Calcd. for $C_{20}H_{19}ClN_2O_2$ (*FW*: 354.113): C, 67.70; H, 5.40; N, 7.89 %. Found: C, 67.65; H, 5.32; N, 7.81 %; R_f ($CHCl_3$): 0.34; IR (KBr, cm^{-1}): 3304 (N–H), 2965–2926 (CH aliphatic), 1672–1638 (C=O), 1524–1506 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.98 (3H, *t*, *J* = 7.32 Hz, CH_3), 3.24–3.36 (2H, *m*, NCH_2), 6.53–6.92 (4H, *m*, CH arom), 7.56–8.09 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 11.5 (CH_3), 43.4 (NCH_2), 111.4, 133.9, 124.4, 140.8, 125.2, 125.8, 125.9, 128.8, 131.5, 131.9, 145.2, (C arom, CH arom), 179.7, 176.2 (C=O); MS (*m*/*z* (relative abundance, %)): 381 (100) $[M+H]^+$.

2-((4-(Diethylamino)phenyl)amino)-3-(ethylthio)naphthalene-1,4-dione ***(5a)***. Compound **5a** was synthesized in the reaction of **3** (0.1 g, 0.28 mmol) with **4a** (0.017 g, 0.27 mmol) according to general procedure 2.

Yield: 93.45 % (0.1 g); gray oil; R_f (CH_2Cl_2): 0.25; Anal. Calcd. for $C_{22}H_{24}N_2O_2S$ (*FW*: 380.50): C, 69.44; H, 6.36; N, 7.36; S, 8.43 %. Found: C, 69.64; H, 6.48; N, 7.12; S, 8.74 %; IR (KBr, cm^{-1}): 3330 (N–H), 3018 (C–H arom), 2975–2929 (C–H aliphatic), 1664–1631 (C=O), 1593–1549 (C=C); ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 0.98 (3H, *t*, *J* =7.5 Hz, CH_3), 1.08 (6H, *t*, *J* =7.5 Hz, $NCH_2C\mathbf{H}_3$), 2.53–2.57 (2H, *m*, SCH_2), 3.26–3.30 (4H, *m*, NCH_2), 7.77 (1H, *s*, NH), 6.55 (2H, *d*, *J* = 7.3 Hz, CH arom), 6.86 (2H, *d*, *J* = 7.3 Hz, CH

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arom), 7.95–8.07 (4H, *m*, CH naphtho); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 11.5 (CH_3), 13.3 (**C**H_2CH_3), 28.6 (SCH_2), 43.4 (NCH_2),110.3, 112.5, 123.8, 125.4, 125.6, 125.8, 125.9, 129.7, 131.2, 132.8, 133.4, 144.7, 145.4, (CH arom, C arom), 179.6, 179.7 (C=O); MS (*m*/*z* (relative abundance, %)): 381 (100) $[M+H]^+$.

*2-(4-((Diethylamino)phenyl)amino)-3-((4-methyl-2-oxo-2*H*-chromen-7-yl)-thio)naphthalene-1,4-dione (**5b**)*. Compound **5b** was synthesized in the reaction of **3** (0.1 g, 0.28 mmol) with **4b** (0.05 g, 0.26 mmol) according to general procedure 2.

Yield: 64.28 % (0.09 g); blue oil; R_f ($CHCl_3$): 0.45; Anal. Calcd. for $C_{30}H_{26}N_2O_4S$ (*FW*: 510.60): C, 70.57; H, 5.13; N, 5.49; S, 6.28 %. Found: C, 70.33; H, 4.89; N, 5.26; S, 6.03 %; IR (KBr, cm^{-1}): 3253 (N–H), 3053 (C–H arom), 2962, 2923, 2852 (C–H aliphatic), 1734 (C=O lactone), 1666 (C=O quinone), 1597, 1537 (C=C),; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 1.07 (6H, *t*, *J* = 5.0 Hz, NCH_2C**H**$_3$), 1.48 (3H, *s*, CH_3), 6.01 (1H, *s*, CH vin), 3.24–3.26 (4H, *m*, NCH_2), 6.26–8.13 (11H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / / ppm) 11.4, 17.5 (CH_3), 43.5 (NCH_2), 123.0, 123.2, 124.4, 125.3, 125.9, 126.4, 127.4, 129.2, 131.6, 131.8, 132.8, 134.2, 140.8, 144.7, 145.2, 151.0, 152.5 (CH arom, C arom), 159.6 (C=O coumarin) 179.2, 179.8 (C=O); MS (*m*/*z* (relative abundance, %)): 511 (100) $[M+H]^+$.

*2-((4-(Diethylamino)phenyl)amino)-3-(propylthio)naphthalene-1,4-dione (**5c**)*. Compound **5c** was synthesized in the reaction of **3** (0.1 g, 0.282 mmol) with **4c** (0.02 g, 0.26 mmol) according to general procedure 2.

Yield: 62.72% (0.06 g); gray oil; R_f ($CHCl_3$): 0.40; Anal. Calcd. for $C_{23}H_{26}N_2O_2S$ (*FW*: 394.53): C, 70.02; H, 6.64; N, 7.10; S, 8.13 %. Found: C, 69.89; H, 6.31; N, 7.05; S, 8.21 %; IR (KBr, cm^{-1}): 3311 (N–H), 3071 (C–H arom), 2966, 2929, 2870 (C–H aliphatic), 1663 (C=O), 1591, 1562 (C=C); ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 0.74 (3H, *t*, *J* = 7.5 Hz, CH_3), 1.08 (6H, *t*, *J* = 7.5 Hz, NCH_2C**H**$_3$), 1.30–1.35 (2H, *m*, SCH_2C**H**$_2$), 2.50 (2H, *t*, *J* = 7.5 Hz, SCH_2), 3.25–3.29 (4H, *m*, NCH_2), 6.54 (1H, *bs*, NH), 6.57–6.87 (4H, *m*, CH arom), 7.94–8.06 (4H, *m*, CH naphtho); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm): 12.3, 13.0 (CH_3), 35.1 (CH_2), 40.15 (SCH_2), 43.5 (NCH_2), 112.8, 121.2, 123.2, 123.8, 125.4, 125.5, 125.6, 126.0, 129.7, 132.8, 133.3, 144.7, 145.3, (CH arom, C arom), 179.5, 179.7 (C=O); MS (*m*/*z* (relative abundance, %)): 395 (100) $[M+H]^+$.

*2-(Butylthio)-3-((4-(diethylamino)phenyl)amino)naphthalene-1,4-dione (**5d**)*. Compound **5d** was synthesized in the reaction of **3** (0.1 g, 0.28 mmol) with **4d** (0.025 g, 0.27 mmol) according to general procedure 2.

Yield: 69.52 % (0.08 g); gray oil; R_f ($CHCl_3$): 0.52; Anal. Calcd. for $C_{24}H_{28}N_2O_2S$ (*FW*: 408.56): C, 70.55; H, 6.91; N, 6.86; S, 7.85 %. Found: C, 70.32; H, 6.78; N, 6.61; S, 7.52 %; IR (KBr, cm^{-1}): 3307 (N–H), 3065 (C–H

arom), 2965, 2928, 2870 (C–H aliphatic), 1662, 1610 (C=O), 1591, 1544 (C=C),; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.78 (3H, *t*, *J* = 7.5 Hz, CH_3), 1.10 (6H, *t*, *J* = 15.0 Hz $NCH_2C\mathbf{H}_3$), 1.14–1.18 (2H, *m*, $C\mathbf{H}_2CH_3$), 1.24–1.29 (2H, *m*, $SCH_2C\mathbf{H}_2$), 2.50 (2H, *t*, *J* = 7.5 Hz, SCH_2), 3.25–3.29 (4H, *m*, NCH_2), 7.77 (1H, *bs*, NH), 6.52–6.87 (4H, *m*, CH arom), 7.94–8.06 (4H, *m*, CH naphtho); ^{13}C--NMR (125.66 MHz, $CDCl_3$, δ / ppm): 11.5, 12.6 (CH_3), 30.4, 32.8 (CH_2), 37.8 (SCH_2), 43.4 (NCH_2), 110.3, 112.9, 123.8, 125.5, 125.6, 125.9, 129.7, 131.2, 132.8, 133.3, 145.2, 144.7 (CH arom, C arom), 179.5, 179.7 (C=O); MS (*m*/*z* (relative abundance, %)): 409 (100). $[M+H]^+$.

*2-((4-(Diethylamino)phenyl)amino)-3-(octylthio)naphthalene-1,4-dione (**5e**)*. Compound **5e** was synthesized in the reaction of **3** (0.1 g, 0.28 mmol) with **4e** (0.041 g, 0.28 mmol) according to general procedure 2.

Yield: 83.20 % (0.109 g); blue oil; R_f ($CHCl_3$:ethyl acetate 3:1): 0.85; Anal. Calcd. for $C_{28}H_{36}N_2O_2S$ (*FW*: 464.66): C, 72.38; H, 7.81; N, 6.03; S, 6.90 %. Found: C, 72.19; H, 7.61; N, 5.81; S, 6.68 %; IR (KBr, cm^{-1}): 3318 (N–H), 3071 (C–H arom), 2964, 2926, 2853 (CH aliphatic), 1663, 1633 (C=O), 1592, 1548 (C=C),; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.77 (3H, *t*, *J* = 5.0 Hz, $CH_2C\mathbf{H}_3$), 1.08–1.11 (6H, *m*, $NCH_2C\mathbf{H}_3$), 1.14–1.18 (10H, *m*, $((CH_2)_5)$), 1.26––1.31 (2H, *m*, $SCH_2C\mathbf{H}_2$), 2.50 (2H, *t*, *J* = 7.5 Hz, SCH_2), 3.26–3.31 (4H, *m*, NCH_2), 7.77 (H, *s*, NH), 6.53 (2H, *d*, *J* = 5.0 Hz, CH arom), 6.87 (2H, *d*, *J* = 5.0 Hz, CH arom), 8.02 (2H, *dd*, *J* = 5.0 and 6.3 Hz, CH naphtho) 7.59 (2H, *t*, *J* = 7.5 Hz, CH naphtho); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 11.5 (CH_3), 13.0 (CH_3) thio, 30.7, 28.6, 28.4, 28.1, 28.0, 27.7 (CH_2), 33.1 (SCH_2), 43.5 (NCH_2), 110.3, 113.0, 123.8, 125.4, 125.7, 125.9, 129.7, 131.2, 132.8, 133.4, 144.7, 145.2 (CH arom, C arom), 179.6, 179.8 (C=O); MS (*m*/*z* (relative abundance, %)): 465 (100) $[M+H]^+$.

*3-Ethoxy-3-(((piperidin-2-yl)methyl)amino)naphthalene-1,4-dione (**7**)*. Compound **7** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **6** (0.25 g, 2.19 mmol) according to general procedure 2.

Yield: 34.73 % (0.33 g); blue oil; R_f ($CHCl_3$): 0.31; Anal. Calcd. for $C_{18}H_{22}N_2O_{43}$ (*FW*: 414.38): C, 68.77; H, 7.05; N, 8.91 %. Found: C, 68.52; H, 6.88; N, 8.58 %; IR (KBr, cm^{-1}): 3385 (N–H), 3010 (C–H arom), 2926, 2850 (C–H aliphatic), 1703, 1613 (C=O), 1594, 1505 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.76–0.82 (3H, *m*, CH_3), 1.17–1.26 (6H, *m*, CH_2 piper.), 1.50 (2H, *bs*, NH), 2.20–2.25 (4H, *m*, NCH_2), 2.78–2.81 (H, *m*, NCH), 4.57–4.60 (2H, *m*, OCH_2), 7.69–8.71 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / / ppm) 20.7 (CH_3), 28.3, 28.6, 28.9 (CH_2), 30.9, 35.2 (NCH_2), 52.3 (OCH_2), 124.6, 124.7, 127.3, 128.9, 130.1, 131.5, 131.7, 136.2 (CH arom, C arom), 174.7, 178.8 (C=O); MS (*m*/*z* (relative abundance, %)): 314 (100) $[M+H]^+$.

*2-(2-(((3-Chloro-1,4-dioxonaphthalen-2-yl)amino)methyl)piperidin-1-yl)-3--(((piperidin-2-yl)methyl)amino)naphthalene-1,4-dione (**8**)*. Compound **8** was

synthesized in the reaction of **1** (0.5g, 2.20 mmol) with **6** (0.25 g, 2.19 mmol) according to general procedure 1.

Yield: 50.79 % (0.64 g); brown solid; m.p.: 155–156 °C; R_f (CH_2Cl_2:petroleum ether 2:1, 40–60 °C): 0.41; Anal. Calcd. for $C_{32}H_{33}ClN_4O_4$ (*FW*: 573.08): C, 67.07; H, 5.80; N, 9.78 %. Found: C, 66.85; H, 5.56; N, 9.63 %; IR (KBr, cm^{-1}): 3400 (N–H), 3048 (C–H arom), 2938–2855 (C–H aliphatic), 1633––1614 (C=O), 1593 (C=C),; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 1.37–1.90 (12H, *m*, CH_2 piper.), 3.49 (4H, *t*, *J* = 7.3 Hz, NCH_2), 4.18 (4H, *t*, *J* = 7.3 Hz, NCH_2), 2.60–3.10 (2H, *m*, NCH), 7.77 (3H, m, NH), 7.45–8.06 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 28.6, 24.2, 22.5 (CH_2), 52.68, 52.74 (NCH_2), 108.9, 122.7, 125.2, 129.9, 130.9, 130.1, 131.8, 144.7, 157.5 (CH aromatic, C aromatic), 176.9 (C=O); MS (*m*/*z* (relative abundance, %)): 595 (100) $[M+Na]^+$).

*2-Ethoxy-3-(2-methyl-1*H*-indol-1-yl)naphthalene-1,4-dione (**10**)*. Compound **10** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **9** (0.288 g, 2.19 mmol) according to general procedure 3.

Yield: 9.66 % (0.14 g); blue oil; R_f ($CHCl_3$): 0.72; Anal. Calcd. for $C_{20}H_{15}NO_3$ (*FW*: 317.34): C, 75.70; H, 4.74; N, 4.41 %. Found: C, 75.51; H, 4.85; N, 4.12 5; IR (KBr, cm^{-1}): 3018 (C–H arom), 2926, 2854 (C–H aliphatic), 1717, 1664 (C=O), 1596, 1459 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 2.27 (3H, *s*, CH_3), 4.10 (3H, *s*, OCH_3), 7.01–8.18 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 12.8 (CH_3), 61.0 (OCH_3), 104.8, 126.1, 126.2, 126.3, 125.7, 129.8, 130.6, 131.1, 132.7, 132.9, 133.6, 134.3, 140.8 141.8, 146.5 (CH aromatic, C aromatic), 177.3 180.9 (C=O); MS (*m*/*z* (relative abundance, %)): 318 (100) $[M+H]^+$.

*2-((2-(2-(2-Aminoethoxy)ethoxy)ethyl)amino)-3-chloronaphthalene-1,4-dione (**12**)*. Compound **12** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **11** (0.652 g, 4.39 mmol) according to general procedure 1.

Yield: 3.22 % (0.048 g); brown oil; R_f (CH_3OH): 0.93; Anal. Calcd. for $C_{16}H_{19}ClN_2O_4$ (*FW*: 338.79): C, 56.72; H, 5.65; N, 8.27 %. Found: C, 56.63; H, 5.77; N, 8.36 %; IR (KBr, cm^{-1}): 3334 (N–H), 3012 (C–H arom), 2872 (C–H aliphatic), 1678, 1644 (C=O), 1574, 1515 (C=C),; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.97–4.04 (8H, *m*, OCH_2), 3.60–3.70 (4H, *m*, NCH_2), 7.47–7.99 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 43.4 (NCH_2), 68.9 (OCH_2), 69.4 (OCH_2**C**H_2NH), 76.2 (**C**$H_2CH_2NH_2$), 125.7, 131.4, 133.8 (CH aromatic, C aromatic), 179.3, 181.3 (C=O); MS (*m*/*z* (relative abundance, %)): 339 (100) $[M+H]^+$.

*2,2'-[1,2-Ethanediylbis(oxy-2,1-ethanediylimino)]bis(3-chloronaphthalene--1,4-dione) (**13**)*. Compound **13** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **11** (0.652 g, 4.39 mmol) according to general procedure 1.

Yield: 64.49% (0.75 g); red solid; m.p.: 150–152 °C (Lit 150–152 °C[2]); R_f ($CHCl_3$:ethyl acetate 1:1): 0.48; Anal. Calcd. for $C_{26}H_{22}ClN_2O_6$ (*FW*: 528.09) C, 58.99; H, 4.19; N, 5.29 %. Found: C, 58.78; H, 4.27; N, 5.16 %; IR (KBr, cm^{-1}): 3053 (C–H arom), 2900–2863 (C–H aliphatic), 1679–1636 (C=O), 1579–1513 (C=C), 3334 (N–H); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.72 (4H, *t*, *J* = 6.8 Hz, NCH_2), 4.0–4.04 (8H, *m*, OCH_2), 7.60–7.98 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 43.41 (NCH_2), 68.9, 69.4 (OCH_2), 125.7, 128.6, 131.5, 131.4, 133.8, 143.1, (CH arom, C arom), 179.3, 175.7 (C=O); MS (*m*/*z* (relative abundance, %)): 529 (38) $[M+H]^+$.

*2,2′-[1,2-Ethanediylbis(oxy-2,1-ethanediylimino)]bis[3-(buthylthio)naphthalene-1,4-dione] (**14d**)*. Compound **14d** was synthesized in the reaction of **13** (0.25 g, 0.47 mmol) with **4d** (0.061 g, 0.67 mmol) according to general procedure 2.

Yield: 57.76 % (0.17 g); red oil; R_f ($CHCl_3$): 0.35; Anal. Calcd. for $C_{34}H_{40}N_2O_6S_2$ (*FW*: 636.82): C, 64.13; H, 6.33; N, 4.40; S, 10.07 %. Found: C, 64.22; H, 6.46; N, 4.72; S, 10.25 %; IR (KBr, cm^{-1}): 3066 (C–H arom), 2956, 2927, 2870 (C–H aliphatic), 1674, 1629 (C=O), 1592, 1550 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.80 (6H, *t*, *J* = 7.5 Hz, CH_3), 1.29–1.34 (4H, *m*, CH_2), 1.45–1.51 (4H, *m*, $SCH_2C\mathbf{H}_2$), 2.72 (4H, *t*, *J* = 7.5 Hz, SCH_2), 3.69 (2H, *t*, *J* = 7.5 Hz, NCH_2), 4.08 (8H, *t*, *J* = 7.5 Hz, OCH_2), 7.47–8.02 (8H, *m*, C–H arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 12.6 ($CH_2\mathbf{C}H_3$), 21.0 ($\mathbf{C}H_2CH_3$), 30.9 (CH_2S), 33.7 ($\mathbf{C}H_2CH_2$–S), 44.4 ($NHCH_2$), 69.0 (O–$\mathbf{C}H_2CH_2NH$), 69.5 (OCH_2), 125.5, 125.7, 130.9, 132.7, 133.4 (CH arom, C arom), 179.1, 180.3 (C=O); MS (*m*/*z* (relative abundance, %)): 659 (100) $[M+Na]^+$.

*2,2′-[1,2-Ethanediylbis(oxy-2,1-ethanediylimino)]bis[3-(buthylthio)naphthalene-1,4-dione] (**14e**)*. Compound **14e** was synthesized in the reaction of **13** (0.3 g, 0.56 mmol) with **4e** (0.082 g, 0.56 mmol) according to general procedure 2.

Yield: 58.80 % (0.25 g); red oil; R_f ($CHCl_3$:ethyl acetate 2:3): 0.82; Anal. Calcd. for $C_{42}H_{56}N_2O_6S_2$ (*FW*: 749.03): C, 67.35; H, 7.54; N, 3.74; S, 8.56 %. Found: C, 66.98; H, 7.76; N, 3.45; S, 8.23 %; IR (KBr, cm^{-1}): 3066 (C–H arom), 2956, 2927, 2870 (C–H aliphatic), 1674, 1629 (C=O), 1592, 1550 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.80 (6H, *t*, *J* = 7.3 Hz, CH_3), 1.15–1.19 (12H, *m*, CH_2), 1.46–1.51 (12H, *m*, CH_2), 2.72 (4H, *t*, *J* = 7.3 Hz, SCH_2), 3.69 (4H, *t*, *J* = 6.8 Hz, NCH_2), 4.08 (8H, *t*, *J* = 6.8 Hz, OCH_2), 7.46–8.02 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 13.0 (CH_3), 34.0, 30.7, 28.9, 28.6, 28.1, 28.1 (CH_2), 38.2 (SCH_2), 44.4 ($NHCH_2$), 69.0 (O–$\mathbf{C}H_2CH_2NH$), 69.5 (OCH_2), 125.3, 125.5, 130.9, 132.7, 133.4 (CH arom, C arom), 179.0, 180.3 (C=O); MS (*m*/*z* (relative abundance, %)): 749 (100) $[M+H]^+$.

*2-Chloro-3-(4-methylpiperazin-1-yl)naphthalene-1,4-dione (**16**)*. Compound **16** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **15** (0.22 g, 2.19 mmol) according to general procedure 1.

Yield: 65 % (0.33 g); brown solid; m.p.: 105–106 °C (Lit. for **16**·HCl: 220––225 °C[3]); R_f (ethyl acetate): 0.73; Anal. Calcd. for $C_{15}H_{15}ClN_2O_2$ (*FW*: 290.74): C, 61.97; H, 5.20; N, 9.64 %. Found: C, 61.73; H, 5.11; N, 9.56 %; IR (KBr, cm^{-1}): 3072 (C–H arom), 2929, 2855 (C–H aliphatic), 1682, 1614 (C=O), 1592, 1562 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 1.18 (3H, *s*, NCH_3), 2.89–3.02 (8H, *m*, NCH_2), 7.99–8.88 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 28.6 (NCH_3), 44.7, 44.02 (NCH_2), 125.6, 125.9, 127.7, 127.9, 128.5, 128.8, 140.4 (CH arom, C arom), 175.4, 177.5 (C=O); MS (*m*/*z* (relative abundance, %)): 291 (100) $[M+H]^+$.

*2-(Butylthio)-3-(4-methylpiperazin-1-yl)naphthalene-1,4-dione (**17d**)*. Compound **17d** was synthesized in the reaction of **16** (0.50 g, 1.72 mmol) with **4d** (0.15 g, 1.66 mmol) according to general procedure 2.

Yield: 18.15 % (0.071 g); violet oil; R_f (ethyl acetate): 0.73; Anal. Calcd. for $C_{19}H_{24}N_2O_2S$ (*FW*: 344.47): C, 66.25; H, 7.02; N, 8.13; S, 9.31 %. Found: C, 65.96; H, 7.20; N, 7.82; S, 9.21 %; IR (KBr, cm^{-1}): 3005 (C–H arom), 2928, 2793 (C–H aliphatic), 1667, 1640 (C=O), 1591, 1563 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.84 (3H, *t*, J = 7.3 Hz, CH_3), 1.21–1.24 (4H, *m*, NCH_2), 1.32–1.36 (4H, *m*, NCH_2), 2.96 (2H, *t*, J = 7.3 Hz, SCH_2), 7.63–7.97 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 17.39 (CH_3), 27.52–29.84 (CH_2), 39.39 (SCH_2), 43.53 (NCH_3), 49.61 (NCH_2), 122.16, 127.25, 128.24, 128.9, 129.40, 146.51 (CH arom, C arom), 176.5, 177.5 (C=O); MS (*m*/*z* (relative abundance, %)): 345 (100) $[M+H]^+$.

*2-(4-Methylpiperazin-1-yl)-3-(*p*-tolylthio)naphthalene-1,4-dione (**17f**)*. Compound **17f** was synthesized in the reaction of **16** (0.50 g, 1.72 mmol) with **4f** (0.15 g, 0.39 mmol) according to general procedure 2.

Yield: 18.15 % (0.071 g); brown solid; m.p.: 278–279 °C, R_f ($CHCl_3$:ethyl acetate 2:1): 0.73; Anal. Calcd. for $C_{22}H_{22}N_2O_2S$ (*FW*: 378.49): C, 69.81; H, 5.86; N, 7.40; S, 8.47 %. Found: C, 69.29; H, 5.03; N, 7.26; S, 7.36 %; IR (KBr, cm^{-1}): 3000 (C–H arom), 2927, 2855 (C–H aliphatic), 1718, 1654 (C=O), 1593, 1491 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 1.40–1.45 (3H, *m*, CH_3), 1.18–2.26 (8H, *m*, NCH_2), 7.04–8.01 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 27.91 (C arom-CH_3), 42.8 (CH_3), 52.9, 53.21 (NCH_2), (C arom-S), 125.78, 126.17, 127.78, 128.24, 128.7, 128.76, 129.1, 129.8, 130.6, 131.2, 132.5, 133.3, 136.8 (CH arom, C arom), 175.3, 176.5 (C=O); MS (*m*/*z* (relative abundance, %)): 379 (100) $[M+H]^+$.

*2-Chloro-3-(3-((dimethylamino)methyl)-1*H*-indol-1-yl)naphthalene-1,4-dione (**19**)*. Compound **19** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **18** (0.38 g, 2.23 mmol) according to general procedure 1.

Yield: 54.82% (0.44 g); red solid; m.p.: 67–68 °C. R_f ($CHCl_3$:petroleum ether 1:1, 40–60 °C): 0.35; Anal. Calcd. for $C_{21}H_{17}N_2O_2$ (*FW*: 364.82): C, 69.14; H, 4.70; N, 8.77 %. Found: C, 68.84; H, 4.62; N, 8.49 %; IR (KBr, cm^{-1}):

3020 (C–H arom), 2961, 2926 (C–H aliphatic), 1676, 1643 (C=O), 1593, 1519 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.17 (6H, *s*, NCH_3), 3.37 (2H, *s*, NCH_2), 7.18 (1H, *s*, CH vin), 7.52–8.07 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 44.6 (NCH_3), 47.05 (NCH_2), 120.4, 126.7, 127.8, 129.3, 129.9 131.6, 131.9, 133.1, 133.9, 134.1, 134.4, 135.1, 135.6, 151.1 (CH arom, C arom), 178.1, 182.4 (C=O); MS (*m*/*z* (relative abundance, %)): 366 (100) $[M+H]^+$.

*2-(Butylthio)-3-(3-((dimethylamino)methyl)-1*H*-indol-1-yl)naphthalene-1,4--dione (**20d**)*. Compound **20d** was synthesized in the reaction of **19** (0.050 g, 0.13 mmol) with **4d** (0.012 g, 0.013 mmol) according to general procedure 2.

Yield: 52.24 % (0.03 g); red solid; m.p.: 134–135 °C; R_f ($CHCl_3$): 0.43; Anal. Calcd. for $C_{25}H_{26}N_2O_2S$ (*FW*: 418.55): C, 71.74; H, 6.26; N, 6.69; S, 7.66 %. Found: C,71.58; H, 6.13; N, 6.48; S, 7.46 %; IR (KBr, cm^{-1}): 3015 (C–H arom), 2961, 2926, 2871 (C–H aliphatic), 1655, 1592 (C=O), 1459, 1377 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.89 (3H, *t*, *J* = 7.2 Hz, CH_3), 1.18–1.55 (4H, *m*, CH_2), 2.70 (2H, *t*, *J* = 7.2 Hz, SCH_2), 3.37 (6H, *s*, NCH_3), 3.40 (2H, *s*, NCH_2), 7.19 (H, *s*, CH vin), 7.51–8.08 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 12.4 (CH_3), 22.2 ($\mathbf{C}H_2CH_3$), 30.9 ($SCH_2\mathbf{C}H_2$), 31.5 (SCH_2), 32.8 (NCH_3), 36.1 (NCH_2), 125.3, 125.5, 125.7, 125.8, 125.9, 128.7, 129.6, 130.9, 131.3, 131.7, 132.8, 133.5, 133.9, 143.8 (CH arom, C arom), 179.4, 180.5 (C=O); MS (*m*/*z* (relative abundance, %): 441 (12) $[M+H]^+$.

*2-Chloro-3-((2-(hydroxymethyl)phenyl)amino)naphthalene-1,4-dione (**22**)*. Compound **22** was synthesized in the reaction of **1** (0.50 g, 2.20 mmol) with **21** (0.27 g, 2.19 mmol) according to general procedure 1.

Yield: 58 % (0.4 g); red oil; R_f ($CHCl_3$): 0.32; Anal. Calcd. for $C_{17}H_{12}ClNO_3$ (*FW*: 313.74): C, 65.08; H, 3.86; N, 4.46 %. Found: C, 65.25; H, 4.08; N, 4.29 %; IR (KBr, cm^{-1}): 3010 (C–H arom), 3365 (N–H), 2910–2871 (C–H aliphatic), 1674–1606 (C=O), 1568–1505 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.81–3.87 (2H, *m*, OCH_2), 4.20 (1H, *m*, OH), 7.01 (1H, *s*, NH), 7.46–8.09 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 68.4 (CH_2O), 108.5, 110, 127, 127.1, 129.1, 132.1, 135.2, 138.5, 143.2, 167.3 (CH arom, C arom), 175.2, 180.8 (C=O); MS (*m*/*z* (relative abundance, %)): 314 (100) $[M+H]^+$.

*2-(2-((Hydroxymethyl)phenyl)amino)-3-(propylthio)naphthalene-1,4-dione (**23c**)*. Compound **23c** was synthesized in the reaction of **22** (0.1 g, 0.31 mmol) with **4c** (0.02 g, 0.026 mmol) according to general procedure 2.

Yield: 81.80 % (0.09 g); pink oil; R_f ($CHCl_3$:Ethyl acetate 3:1): 0.66; Anal. Calcd. for $C_{20}H_{19}NO_3S$ (*FW*: 353.43): C, 67.97; H, 5.42; N, 3.96; S, 9.07 %. Found: C, 67.74; H, 5.28; N, 3.84; S, 8.77 %; IR (KBr, cm^{-1}): 3439 (O–H), 3289 (N–H), 3010 (C–H arom), 2962, 2929, 2871 (C–H aliphatic), 1667, 1636 (C=O), 1585, 1548 (C=C); ^{1}H-NMR 500 MHz, $CDCl_3$, δ / ppm): 0.70 (3H, *t*, *J* = 7.3 Hz,

CH_3), 1.44 (1H, *bs*, OH), 1.12–1.28 (2H, *m*, CH_2), 2.50 (2H, *t*, *J* = 7.3 Hz, SCH_2), 4.73 (2H, *s*, OCH_2), 6.80 (1H, *s*, NH), 7.57–8.08 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 21.9 (CH_3), 28.6 (SCH_2**C**H_2), 34.5 (SCH_2), 63.0 (CH_2O), 121.8, 123.3, 125.6, 125.8, 126.5, 127.1, 127.8, 129.8, 130.5, 131.7, 132.5, 133.4, 137.4, 144.8 (CH arom, C arom), 179.4, 180.0 (C=O); MS (*m*/*z* (relative abundance, %)): 354 (100) $[M+H]^+$.

*2-(Butylthio)-3-((2-(hydroxymethyl)phenyl)amino)naphthalene-1,4-dione (**23d**)*. Compound **23d** was synthesized in the reaction of **22** (0.10 g, 0.31 mmol) with **4d** (0.020 g, 0.022 mmol) according to general procedure 2.

Yield: 81.80 % (0.09 g); pink oil; R_f ($CHCl_3$:ethyl acetate 3:1): 0.36; Anal. Calcd. for $C_{21}H_{21}NO_3S$ (*FW*: 367.46): C, 68.64; H, 5.76; N, 3.81, S, 8.73 %. Found: C, 68.52; H, 5.94; N, 3.97, S, 8.52 %; IR (KBr, cm^{-1}): 3293 (N–H), 3011 (C–H arom), 2958, 2929, 2872 (C–H aliphatic), 1667, 1636 (C=O), 1586, 1548 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.74 (3H, *t*, *J* = 7.3 Hz, CH_3), 1.44 (1H, *bs*, OH), 1.18–1.24 (4H, *m*, CH_2), 2.49 (2H, *t*, *J* = 7.3 Hz, SCH_2), 4.74 (2H, *s*, OCH_2), 6.85 (1H, *s*, NH), 7.57–8.08 (8H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 20.7 (CH_3), 28.6 (SCH_2CH_2**C**H_2), 30.6 (SCH_2**C**H_2), 32.2 (SCH_2), 63.0 (CH_2O), 117.7 121.8, 123.2, 125.6, 125.8, 127, 127.7, 128.7, 129.8, 130.5, 132.5, 133.3, 144.7 (CH arom, C arom), 179.4, 180.0 (C=O); MS (*m*/*z* (relative abundance, %)): 366 (100) $[M+H]^+$.

*2-Chloro-3-(*N*-(2-hydroxyethyl)-*N*-phenylamino)naphthalene-1,4-dione (**25**)*. Compound **25** was synthesized in the reaction of **1** (1 g, 4.404 mmol) with **24** (0.64 g, 4.40 mmol) according to general procedure 1.

Yield: 45.18% (0.65 g); violet oil; R_f ($CHCl_3$): 0.45; Anal. Calcd. for $C_{18}H_{14}ClNO_3$ (*FW*: 327.76): C, 65.96; H, 4.31; N, 4.27 %. Found: C, 65.68; H, 4.62; N, 4.44 %; IR (KBr, cm^{-1}): 3330 (OH), 3067 (C–H arom), 2940, 2880 (C–H aliphatic), 1731, 1674 (C=O), 1593, 1557 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 1.20 (1H, *s*, OH), 3.80 (2H, *t*, *J* = 6.8 Hz, NCH_2), 4.01(2H, *t*, *J* = 6.8 Hz, OCH_2), 7.25–8.14 (9H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / / ppm) 52.5 (NCH_2), 60.1 (CH_2O), 116.8, 126.6, 127.9, 128, 128.1, 128.3, 130.6, 132.7, 133, 133.1, 133.4, 144.8, 147.2 (CH arom, C arom), 177.0, 181.1 (C=O); MS (*m*/*z* (relative abundance, %)): 327 (100) $[M]^+$.

*2-Chloro-3-((2-(diethylamino)ethyl)amino)naphthalene-1,4-dione (**27**)*. Compound **27** was synthesized in the reaction of **1** (1 g, 4.40 mmol) with **26** (0.51 g, 4.38 mmol) according to general procedure 1.

Yield: 70% (0.95 g); yellow solid; m.p.: 86–87 °C (Lit. for **27**·HCl m.p.: 242 °C[4]); R_f ($CHCl_3$): 0.44; Anal. Calcd. for $C_{16}H_{19}ClN_2O_2$ (*FW*: 306.11): C, 62.64; H, 6.24; N, 9.13 %. Found: C, 62.82; H, 6.36; N, 9.23 %; IR (KBr, cm^{-1}): 3267 (N–H), 3002 (C–H arom), 2966, 2931, 2887 (C–H aliphatic), 1682, 1639 (C=O), 1594, 1576 (C=C),; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.81–0.84 (6H, *m*, CH_3), 3.75–3.79 (8H, *m*, $NHCH_2$), 7.53–8.09 (4H, *m*, CH arom); ^{13}C-

-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 10.9 (CH_3), 40.8 (NH–CH_2), 50.5 (N**C**H_2CH_3), 65.9 (NCH_2), 108.7, 158.4, 125.6, 131.2, 133.6 (CH arom, C arom), 183.6, 179.8 (C=O); MS (*m*/*z* (relative abundance, %)): 309 (100) $[M+H]^+$.

*2-(Butylthio)-3-((2-(diethylamino)ethyl)amino)naphthalene-1,4-dione (**28d**)*. Compound **28d** was synthesized in the reaction of **27** (0.1 g, 0.24 mmol) with **4d** (0.021 g, 0.058 mmol) according to general procedure 1.

Yield: 75 % (0.06 g); red oil; R_f (methanol): 0.56; Anal. Calcd. for $C_{20}H_{28}N_2O_2S$ (*FW*: 360.51): C, 66.63; H, 7.83; N, 7.77; S, 8.89 %. Found: C, 66.87; H, 7.92; N, 7.69; S, 8.76 %; IR (KBr, cm^{-1}): 3266 (N–H), 3096 (C–H arom), 2959, 2927, 2871 (C–H aliphatic), 1673, 1628 (C=O), 1592, 1557 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.80 (3H, *t*, *J* = 7.3 Hz, CH_3), 0.86 (6H, *t*, *J* = 7.3 Hz, CH_3), 1.00–1.29 (4H, *m*, CH_2), 1.30–1.37 (1H, *m*, NH), 2.64 (2H, *t*, *J* = 7.3 Hz, SCH_2), 2.72 (6H, *t*, NCH_2), 3.90 (1H, *bs*, NH), 7.64–8.07 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / ppm) 12.6, 13.1 (CH_3), 31.0, 21.6 (CH_2), 37.8 (SCH_2), 42.0 ($NHCH_2$), 45.4, 50.6 (NCH_2), 125.2, 125.5, 130.8, 132.9, 133 (CH arom, C arom), 179.2, 180.7 (C=O); MS (*m*/*z* (relative abundance, %)): 361 (100)) $[M+H]^+$.

*2-(2-((Diethylamino)ethyl)amino)-3-(octylthio)naphthalene-1,4-dione (**28e**)*. Compound **28e** was synthesized in the reaction of **27** (0.50 g, 1.62 mmol) with **4e** (0.23 g, 1.57 mmol) according to general procedure 1.

Yield: 65 % (0.44 g); red oil; R_f ($CHCl_3$): 0.87; Anal. Calcd. for $C_{24}H_{36}N_2O_2S$ (*FW*: 416.62): C, 69.19; H, 8.71; N, 6.72; S, 7.70 %. Found: C, 68.98; H, 9.02; N, 6.51; S, 7.54 %; IR (KBr, cm^{-1}): 3258 (N–H), 3065 (C–H arom), 2956, 2925, 2853 (C–H aliphatic), 1673, 1630 (C=O), 1592, 1552 (C=C); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 0.77–0.87 (9H, *m*, CH_3), 1.01–1.20 (12H, *m*, (CH_2), 2.61 (2H, *t*, *J* = 7.2 Hz, SCH_2), 2.72 (6H, *t*, *J* = 7.2 Hz, NCH_2), 3.90 (1H, *bs*, NH), 7.63–8.07 (4H, *m*, CH arom); ^{13}C-NMR (125.66 MHz, $CDCl_3$, δ / / ppm) 13.05, 13.07 (CH_3), 21.6, 28.2, 28.6, 28.9, 30.3, 30.7 (CH_2), 38.2 (SCH_2), 42.0 ($NHCH_2$), 45.4, 50.6, (N**C**H_2), 125.2, 125.5, 129.8, 130.8, 132.2, 132.9, 133.3, 137.1 (CH arom, C arom), 179.1, 180.6 (C=O); MS (*m*/*z* (relative abundance, %)): 417 (100) $[M+H]^+$.

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