Supplementary Data


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Table of Contents:

1. Synthesis of 1,4-Bis(2-aminophenyl)-2-phenylbutane-1,4-dione derivatives 6a-o ..................1
5. Biological testing ........................................................................................................................................14
6. 1H and 13C NMR Spectra of Synthesised Compounds ........................................................................15
7. CCDC Deposition Data ...........................................................................................................................49
1. Synthesis of 1,4-Bis(2-aminophenyl)-2-phenylbutane-1,4-dione derivatives 6a-m

1,4-Bis(2-aminophenyl)-2-(4-chlorophenyl)butane-1,4-dione (6a).

1-(2-Aminophenyl)-3-(4-chlorophenyl)prop-2-en-1-one (0.5 mmol, 0.129 g) and 2-oxindole (0.5 mmol, 0.067 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.091 g, 48 %); mp 65 °C. 1H NMR (400 MHz, DMSO-\textit{d}_6) δ 7.98 (dd, J = 8.5, 1.5 Hz, 1H), 7.85 – 7.35 (m, 4H), 7.26 – 7.15 (m, 4H), 7.10 (s, 2H), 6.51 (ddd, J = 9.7, 8.2, 6.9, 1.2 Hz, 2H), 5.33 (dd, J = 10.8, 3.3 Hz, 1H), 4.05 – 3.99 (m, 1H), 3.18 (dd, J = 17.7, 3.2 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 200.10, 199.31, 151.96, 151.01, 139.04, 134.17, 134.02, 131.58, 131.50, 131.25, 129.90, 128.71, 117.08, 116.90, 116.12, 116.09, 115.75, 114.41, 114.33, 46.64, 43.51. IR (ATR): ν max = 3479, 3352, 2362, 2355, 1918, 1641, 1581 cm–1. HRMS (ESI+, 47 V): m/z calcd for C_{22}H_{19}ClN_2O_2 [M + H]: 379.1208; found: 379.1204.

1,4-Bis(2-aminophenyl)-2-(4-bromophenyl)butane-1,4-dione (6b).

1-(2-Aminophenyl)-3-(4-bromophenyl)prop-2-en-1-one (0.5 mmol, 0.151 g) and 2-oxindole (0.5 mmol, 0.067 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.086 g, 41 %); mp 144 °C. 1H NMR (600 MHz, DMSO-\textit{d}_6) δ 7.97 (dd, J = 8.5, 1.5 Hz, 1H), 7.84 (dd, J = 8.3, 1.6 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.37 – 7.34 (m, 2H), 7.21 (dddd, J = 24.3, 8.4, 6.9, 1.5 Hz, 4H), 7.10 (s, 2H), 6.51 (ddd, J = 8.5, 6.2, 1.2 Hz, 2H), 6.51 (ddd, J = 15.3, 8.2, 6.9, 1.2 Hz, 2H), 5.32 (dd, J = 10.7, 3.3 Hz, 1H), 4.03 (dd, J = 17.7, 10.8 Hz, 1H), 3.18 (dd, J = 17.7, 3.3 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 200.03, 199.30, 151.97, 151.02, 139.49, 134.18, 134.04, 131.65, 131.59, 131.26, 130.29, 130.02, 117.08, 116.90, 116.10, 115.73, 114.41, 114.33, 46.70, 43.46. IR (ATR): ν max = 3478, 3349, 3053, 2913, 2794, 2363, 1942, 1901, 1795, 1640, 1577 cm–1. HRMS (ESI+, 47 V): m/z calcd for C_{22}H_{19}BrN_2O_2 [M + H]: 423.0703; found: 423.0697.

1,4-Bis(2-aminophenyl)-2-phenylbutane-1,4-dione (6c).

1-(2-Aminophenyl)-3-phenylprop-2-en-1-one (0.5 mmol, 0.112 g) and 2-oxindole (0.5 mmol, 0.067 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.058 g, 34 %); mp 160 °C. 1H NMR (600 MHz, DMSO-\textit{d}_6) δ 7.99 (dd, J = 8.4, 1.5 Hz, 1H), 7.85 (dd, J = 8.3, 1.5 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.30 (t, J = 7.7 Hz, 2H), 7.28 – 7.13 (m, 5H), 7.10 (s, 2H), 6.72 (ddd, J = 11.8, 8.4, 1.2 Hz, 2H), 6.51 (ddd, J = 18.1, 8.1, 6.9, 1.2 Hz, 2H), 5.30 (dd, J = 10.9, 3.2 Hz, 1H), 4.06 (dd, J = 17.7, 10.8 Hz, 1H), 3.16 (dd, J = 17.7, 3.2 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 200.40, 199.30, 151.97, 151.02, 140.06, 134.14, 133.89, 131.64, 131.26, 128.79, 128.03, 126.76, 117.03, 116.89, 116.18, 115.95, 114.41, 114.27, 47.42, 43.74. IR (ATR): ν max = 3475, 3349, 3053, 2913, 2794, 2363, 1942, 1901, 1795, 1640, 1577 cm–1. HRMS (ESI+, 47 V): m/z calcd for C_{22}H_{20}N_2O_2 [M + Na]: 367.1417; found: 367.1415.
1,4-Bis(2-aminophenyl)-2-(4-fluorophenyl)butane-1,4-dione (6d).

1-(2-Aminophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (0.5 mmol, 0.175 g) and 2-oxindole (0.5 mmol, 0.067 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.085 g, 41 %); mp 164 °C. 1H NMR (600 MHz, DMSO-d6) δ 7.90 (dd, J = 8.4, 1.5 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.22 (dddd, J = 23.4, 8.4, 6.9, 1.5 Hz, 4H), 7.12 (s, 2H), 6.73 (ddd, J = 8.4, 5.0, 1.2 Hz, 2H), 6.51 (ddd, J = 11.3, 8.1, 6.9, 1.2 Hz, 2H), 4.85 (td, J = 17.7, 3.3 Hz, 1H), 1H. 13C NMR (151 MHz, DMSO) δ 199.74, 199.12, 152.03, 151.04, 144.90, 134.22, 134.15, 131.25, 130.45, 129.93, 129.63, 129.31, 128.91, 127.79, 127.58, 127.37, 127.16, 126.93, 125.65, 125.63, 125.13, 123.33, 121.53, 117.12, 116.91, 116.06, 115.73, 114.41, 47.14, 44.70. IR (ATR): νmax = 3452, 3341, 3046, 2920, 2364, 1927, 1613, 1579 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H19F3N2O2 [M + H]: 413.1471; found: 413.1469.

1,4-Bis(2-aminophenyl)-2-(4-iodophenyl)butane-1,4-dione (6e).

1-(2-Aminophenyl)-3-(4-iodophenyl)prop-2-en-1-one (0.5 mmol, 0.146 g) and 2-oxindole (0.5 mmol, 0.020 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.085 g, 41 %); mp 164 °C. 1H NMR (600 MHz, DMSO-d6) δ 7.90 (dd, J = 8.4, 1.5 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.22 (dddd, J = 23.4, 8.4, 6.9, 1.5 Hz, 4H), 7.12 (s, 2H), 6.73 (ddd, J = 8.4, 5.0, 1.2 Hz, 2H), 6.51 (ddd, J = 11.3, 8.1, 6.9, 1.2 Hz, 2H), 4.85 (td, J = 17.7, 3.3 Hz, 1H), 1H. 13C NMR (151 MHz, DMSO) δ 199.74, 199.12, 152.03, 151.04, 144.90, 134.22, 134.15, 131.25, 130.45, 129.93, 129.63, 129.31, 128.91, 127.79, 127.58, 127.37, 127.16, 126.93, 125.65, 125.63, 125.13, 123.33, 121.53, 117.12, 116.91, 116.06, 115.73, 114.41, 47.14, 44.70. IR (ATR): νmax = 3452, 3341, 3046, 2920, 2364, 1927, 1613, 1579 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H19I2N2O2 [M + H]: 471.0564; found: 471.0562.

1,4-Bis(2-aminophenyl)-2-(4-(trifluoromethyl)phenyl)butane-1,4-dione (6f).

1-(2-Aminophenyl)-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (0.5 mmol, 0.146 g) and 2-oxindole (0.5 mmol, 0.020 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.085 g, 41 %); mp 164 °C. 1H NMR (600 MHz, DMSO-d6) δ 7.90 (dd, J = 8.4, 1.5 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.22 (dddd, J = 23.4, 8.4, 6.9, 1.5 Hz, 4H), 7.12 (s, 2H), 6.73 (ddd, J = 8.4, 5.0, 1.2 Hz, 2H), 6.51 (ddd, J = 11.3, 8.1, 6.9, 1.2 Hz, 2H), 4.85 (td, J = 17.7, 3.3 Hz, 1H), 1H. 13C NMR (151 MHz, DMSO) δ 199.74, 199.12, 152.03, 151.04, 144.90, 134.22, 134.15, 131.25, 130.45, 129.93, 129.63, 129.31, 128.91, 127.79, 127.58, 127.37, 127.16, 126.93, 125.65, 125.63, 125.13, 123.33, 121.53, 117.12, 116.91, 116.06, 115.73, 114.41, 47.14, 44.70. IR (ATR): νmax = 3452, 3341, 3046, 2920, 2364, 1927, 1613, 1579 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H19F3N2O2 [M + H]: 471.0564; found: 471.0562.
1,4-Bis(2-aminophenyl)-2-(thiophen-2-yl)butane-1,4-dione (6g).

1-(2-Aminophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (2 mmol, 0.459 g) and 2-oxindole (2 mmol, 0.264 g) were dissolved in DMSO (5 ml) at room temperature. Sodium hydroxide (2 mmol, 0.080 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.256 g, 37 %); mp 60 °C. 1H NMR (400 MHz, DMSO-d6) δ 8.07 (dd, J = 8.4, 1.5 Hz, 1H), 7.86 (dd, J = 5.1, 1.2 Hz, 1H), 7.26 – 7.20 (m, 2H), 7.17 (s, 2H), 7.13 – 7.03 (m, 3H), 6.94 (dd, J = 5.1, 3.5 Hz, 1H), 6.74 (dd, J = 8.4, 3.1, 1.2 Hz, 2H), 6.55 (dddd, J = 8.1, 4.0, 1.2 Hz, 2H), 5.62 (dd, J = 10.7, 3.3 Hz, 1H), 4.08 (dd, J = 17.7, 10.7 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 199.32, 199.00, 152.06, 151.04, 142.13, 134.25, 134.14, 131.61, 131.23, 127.00, 125.85, 125.10, 117.07, 116.91, 115.97, 115.46, 114.45, 114.34, 44.09, 42.16. IR (ATR): νmax = 3465, 3344, 2646, 2321, 2113, 1931, 1611, 1576 cm–1. HRMS (ESI+, 47 V): m/z calcd for C20H18N2O2S [M + Na]: 373.0981; found: 373.0983.

1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-chlorophenyl)butane-1,4-dione (6h).

1-(2-Aminophenyl)-3-(4-chlorophenyl)prop-2-en-1-one (0.5 mmol, 0.129 g) and 6-bromooxindole (0.5 mmol, 0.106 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 7 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.059 g, 26 %); mp 203 °C. 1H NMR (600 MHz, DMSO-d6) δ 7.94 (d, J = 8.8 Hz, 1H), 7.84 (dd, J = 8.3, 1.5 Hz, 1H), 7.44 – 7.27 (m, 6H), 7.25 – 7.21 (m, 1H), 7.10 (s, 2H), 6.97 (d, J = 2.0 Hz, 1H), 6.73 (dd, J = 8.4, 1.2 Hz, 1H), 6.64 (dd, J = 8.7, 2.0 Hz, 1H), 6.52 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 5.29 (dd, J = 10.8, 3.3 Hz, 1H), 4.02 (dd, J = 17.8, 10.8 Hz, 1H), 3.20 (dd, J = 17.7, 3.3 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 199.86, 199.26, 152.84, 151.03, 138.62, 134.23, 133.57, 131.64, 131.28, 129.91, 128.77, 127.86, 118.85, 117.10, 116.90, 116.03, 114.81, 114.41, 46.71, 43.47. IR (ATR): νmax = 3478, 3350, 2362, 1606, 1596, 1548 cm –1. HRMS (ESI+, 47 V): m/z calcd for C22H18BrClN2O2 [M + H]: 457.0313; found: 457.0314.

1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-bromophenyl)butane-1,4-dione (6i).

1-(2-Aminophenyl)-3-(4-bromophenyl)prop-2-en-1-one (0.5 mmol, 0.151 g) and 6-bromooxindole (0.5 mmol, 0.106 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 7 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale yellow solid (0.087 g, 35 %); mp 216 °C. 1H NMR (400 MHz, DMSO-d6) δ 7.93 (d, J = 8.8 Hz, 1H), 7.84 (dd, J = 8.3, 1.5 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.44 – 7.28 (m, 4H), 7.23 (d4dd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.10 (s, 2H), 6.97 (d, J = 2.0 Hz, 1H), 6.73 (dd, J = 8.4, 1.2 Hz, 1H), 6.64 (dd, J = 8.7, 2.0 Hz, 1H), 6.52 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 5.28 (dd, J = 10.8, 3.3 Hz, 1H), 4.06 – 3.97 (m, 1H), 3.20 (dd, J = 17.8, 3.2 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 199.79, 199.23, 152.84, 151.03, 139.05, 134.23, 133.56, 131.74, 131.28, 129.91, 128.77, 127.86, 118.85, 117.10, 116.90, 116.85, 116.11, 115.90, 114.80, 114.41, 46.79, 43.41, 40.15, 39.94, 39.73, 39.52, 39.31, 38.10, 38.89. IR (ATR): νmax =3608, 3475, 3349, 2360, 2356, 2035, 1606, 1549 cm–1. HRMS (ESI+, 47 V): m/z calcd for C22H18Br2ClN2O2 [M + H] 500.9808; found: 500.9807.
1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-phenylbutane-1,4-dione (6j).

1-(2-Aminophenyl)-3-phenylprop-2-en-1-one (0.5 mmol, 0.112 g) and 6-bromooxindole (0.5 mmol, 0.106 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 7 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure light brown solid (0.065 g, 31 %); mp 76 °C. 1H NMR (600 MHz, DMSO-<sup>d6</sup>) δ 7.95 (d, J = 8.8 Hz, 1H), 7.84 (dd, J = 8.3, 1.6 Hz, 1H), 7.51 – 7.24 (m, 6H), 7.26 – 7.19 (m, 2H), 7.11 (s, 2H), 6.96 (d, J = 2.0 Hz, 1H), 6.73 (dd, J = 8.4, 1.2 Hz, 1H), 6.64 (dd, J = 8.7, 2.1 Hz, 1H), 6.52 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 5.26 (dd, J = 10.9, 3.3 Hz, 1H), 4.05 (dd, J = 17.8, 10.8 Hz, 1H), 3.19 (dd, J = 17.7, 3.2 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 200.14, 199.46, 152.80, 151.01, 139.62, 134.18, 133.59, 131.27, 128.83, 128.02, 127.69, 126.88, 118.80, 117.05, 116.89, 116.11, 115.00, 114.41, 47.51, 43.68, 30.69. IR (ATR): ν max = 3479, 3348, 2363, 2034, 1963, 1605, 1595, 1549 cm –1. HRMS (ESI+, 47 V): m/z calcd for C<sub>22</sub>H<sub>19</sub>BrN<sub>2</sub>O<sub>2</sub> [M + H]: 423.0703; found: 423.0697.

1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-fluorophenyl)butane-1,4-dione (6k).

1-(2-Aminophenyl)-3-(4-fluorophenyl)prop-2-en-1-one (0.5 mmol, 0.121 g) and 6-bromooxindole (0.5 mmol, 0.106 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 7 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure light brown solid (0.089 g, 40 %); mp 170 °C. 1H NMR (600 MHz, DMSO-<sup>d6</sup>) δ 7.96 (d, J = 8.8 Hz, 1H), 7.84 (dd, J = 8.2, 1.5 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.37 (d, J = 34.9 Hz, 2H), 7.23 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.19 – 7.05 (m, 4H), 6.97 (d, J = 2.0 Hz, 1H), 6.73 (dd, J = 8.4, 1.2 Hz, 1H), 6.65 (dd, J = 8.7, 2.1 Hz, 1H), 6.52 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 5.29 (dd, J = 10.9, 3.3 Hz, 1H), 4.04 – 3.95 (m, 1H), 3.19 (dd, J = 17.7, 3.2 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 200.14, 199.38, 161.96, 160.35, 152.84, 151.02, 135.73, 135.71, 134.21, 133.59, 131.29, 129.96, 129.90, 127.78, 118.83, 117.08, 116.89, 116.06, 115.64, 115.00, 114.86, 114.41, 46.53, 43.66. IR (ATR): ν max = 3454, 3339, 3075, 2659, 1890, 1737, 1576, 1527 cm –1. HRMS (ESI+, 47 V): m/z calcd for C<sub>22</sub>H<sub>18</sub>BrFN<sub>2</sub>O<sub>2</sub> [M + H]: 441.0608; found: 441.0609.

1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-iodophenyl)butane-1,4-dione (6l).

1-(2-Aminophenyl)-3-(4-iodophenyl)prop-2-en-1-one (0.5 mmol, 0.175 g) and 6-bromooxindole (0.5 mmol, 0.106 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 7 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure yellow solid (0.097 g, 35 %); mp 212 °C. 1H NMR (600 MHz, DMSO-<sup>d6</sup>) δ 7.92 (d, J = 8.8 Hz, 1H), 7.84 (dd, J = 8.2, 1.5 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.37 (d, J = 34.9 Hz, 2H), 7.23 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.19 – 7.05 (m, 4H), 6.97 (d, J = 2.0 Hz, 1H), 6.73 (dd, J = 8.4, 1.2 Hz, 1H), 6.65 (dd, J = 8.7, 2.1 Hz, 1H), 6.52 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 5.29 (dd, J = 10.9, 3.3 Hz, 1H), 4.04 – 3.95 (m, 1H), 3.19 (dd, J = 17.7, 3.2 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 199.75, 199.24, 152.83, 151.02, 139.45, 135.76, 134.22, 133.55, 131.27, 130.42, 127.86, 118.84, 117.10, 116.90, 116.03, 114.80, 114.41, 93.01, 54.91, 46.95, 43.66. IR (ATR): ν max = 3467, 3337, 2920, 2854, 1945, 1737, 1572, 1545 cm –1. HRMS (ESI+, 47 V): m/z calcd for C<sub>22</sub>H<sub>18</sub>BrIN<sub>2</sub>O<sub>2</sub> [M + H]: 548.9669; found: 548.9668.
1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-(trifluoromethyl)phenyl)butane-1,4-dione (6m).

1-(2-Aminophenyl)-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (0.5 mmol, 0.146 g) and 6-bromooxindole (0.5 mmol, 0.106 g) were dissolved in DMSO (1 ml) at room temperature. Sodium hydroxide (0.5 mmol, 0.020 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 7 hrs. After completion of the reaction, water (100 ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 50 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure light brown solid (0.076 g, 31 %); mp 183 °C. 1H NMR (600 MHz, DMSO-d6) δ 7.96 (d, J = 8.8 Hz, 1H), 7.85 (dd, J = 8.2, 1.5 Hz, 1H), 7.69 (d, J = 8.2 Hz, 2H), 7.38 (s, 2H), 7.24 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H), 7.11 (s, 2H), 6.98 (d, J = 2.1 Hz, 1H), 6.74 (dd, J = 8.4, 1.2 Hz, 1H), 6.65 (dd, J = 8.7, 2.0 Hz, 1H), 6.52 (ddd, J = 9.2, 1.2 Hz, 1H), 6.40 (dd, J = 10.8, 3.3 Hz, 1H), 4.06 (dd, J = 17.8, 10.8 Hz, 1H), 3.26 (dd, J = 17.7, 3.3 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 199.51, 199.06, 152.88, 151.05, 144.46, 134.27, 133.54, 131.31, 128.91, 128.01, 127.90, 127.91, 127.48, 127.27, 126.91, 125.69, 125.67, 125.64, 125.11, 123.31, 118.89, 117.17, 116.91, 115.98, 114.79, 114.42, 47.22, 43.44. IR (ATR): ν max = 3478, 3347, 3054, 2917, 2362, 1603, 1532 cm –1. HRMS (ESI+, 47 V): m/z calcd for C23H18BrF3N2O2 [M + Na]: 513.0396; found: 513.0395.

1,4-Bis(2-aminophenyl)-2-(4-methoxyphenyl)butane-1,4-dione (6n).

1-(2-Aminophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (1 mmol, 0.253 g) and 2-oxindole (1 mmol, 0.133 g) were dissolved in DMSO (2 ml) at room temperature. Sodium hydroxide (1 mmol, 0.040 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (150ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 75 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale solid (0.147 g, 39 %); mp 66 °C. 1H NMR (400 MHz, DMSO-d6) δ 7.98 (dd, J = 8.4, 1.5 Hz, 1H), 7.84 (dd, J = 8.3, 1.5 Hz, 1H), 7.33 – 7.02 (m, 8H), 6.90 – 6.84 (m, 2H), 6.72 (dd, J = 8.6, 1.2 Hz, 2H), 6.51 (dddd, J = 13.5, 8.2, 7.0, 1.2 Hz, 2H), 5.24 (dd, J = 10.8, 3.2 Hz, 1H), 4.07 – 3.98 (m, 1H), 3.69 (s, 3H), 3.12 (dd, J = 17.7, 3.2 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 200.68, 199.69, 158.08, 151.87, 150.97, 134.10, 133.79, 131.80, 131.64, 131.23, 129.05, 117.00, 116.89, 116.23, 115.94, 114.40, 114.24, 114.21, 55.00, 46.51, 43.73. IR (ATR): ν max = 2834, 2160, 2040, 1979, 1736, 1637, 1610, 1577 cm–1.

1,4-Bis(2-aminophenyl)-2-(3,4,5-trimethoxyphenyl)butane-1,4-dione (6o).

1,4-bis(2-aminophenyl)-2-(3,4,5-trimethoxyphenyl)butane-1,4-dione (1 mmol, 0.313 g) and 2-oxindole (1 mmol, 0.133 g) were dissolved in DMSO (2 ml) at room temperature. Sodium hydroxide (1 mmol, 0.040 g) was added and the reaction mixture was stirred at room temperature in an open vessel for 5 hrs. After completion of the reaction, water (150ml) was added and the crude mixture acidified to pH 4-6, followed by extraction with DCM (3 x 75 ml), washing combined organic fractions with brine and drying over sodium sulfate. The crude product was purified by column chromatography (hexane/ethyl acetate) and concentrated in vacuo to yield an analytically pure pale solid (0.141 g, 32 %); mp 81 °C. 1H NMR (400 MHz, DMSO-d6) δ 8.06 (dd, J = 8.4, 1.5 Hz, 1H), 7.88 (dd, J = 8.3, 1.5 Hz, 1H), 7.30 – 6.97 (m, 6H), 6.82 – 6.62 (m, 4H), 6.53 (dddd, J = 8.2, 7.0, 3.2, 1.2 Hz, 2H), 5.23 (dd, J = 11.0, 3.0 Hz, 1H), 4.18 – 4.05 (m, 1H), 3.70 (d, J = 8.6 Hz, 6H), 3.60 (s, 3H), 3.15 (dd, J = 17.8, 3.0 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 200.38, 199.69, 152.99, 151.82, 150.97, 150.30, 136.30, 135.52, 134.10, 133.88, 131.71, 131.37, 116.99, 116.87, 116.20, 114.37, 114.30, 105.37, 59.88, 55.91, 55.79, 47.54, 43.82. IR (ATR): ν max = 2936, 2835, 2161, 1977, 1736, 1637, 1610, 1577 cm–1.


1,4-Bis(2-aminophenyl)-2-(4-chlorophenyl)butane-1,4-dione (0.13 mmol, 0.05 g) was dissolved in T3P® in 50% DMF (0.26 mmol, 0.083 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH2Cl2 (3 x 30 mL). The combined organic extracts were washed with brine, dried over Na2SO4 filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.031 g, 64 %); mp 201 °C. 1H NMR (600 MHz, DMSO-d6) δ 9.95 (s, 1H), 8.88 (s, 1H), 8.59 (dd, J = 8.6, 1.3 Hz, 1H), 8.08 (dd, J = 8.3, 1.3 Hz, 1H), 7.94 (dd, J = 8.0, 1.7 Hz, 1H), 7.84 – 7.82 (m, 1H), 7.73 – 7.70 (m, 1H), 7.61 (dd, J = 8.5, 1.0 Hz, 1H), 7.51 – 7.48 (m, 1H), 7.23 – 7.20 (m, 2H), 7.04 – 7.01 (m, 1H), 6.80 – 6.77 (m, 2H), 5.60 (s, 1H). 13C NMR (151 MHz, DMSO) δ 189.08, 172.01, 152.96, 147.74, 142.79, 142.03, 134.76, 133.63, 131.59, 130.50, 129.83, 129.40, 128.58, 128.35, 126.51, 123.05, 123.25, 122.35, 121.70, 120.47, 114.09, 60.41. IR (ATR): νmax = 3331, 3059, 2927, 2365, 1657, 1594 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H15ClN2O [M + H]: 371.0946; found: 371.0940.


1,4-Bis(2-aminophenyl)-2-(4-bromophenyl)butane-1,4-dione (0.57 mmol, 0.240 g) was dissolved in T3P® in 50% DMF (1.14 mmol, 0.363 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (200 mL) was added and the mixture was extracted with CH2Cl2 (3 x 60 mL). The combined organic extracts were washed with brine, dried over Na2SO4 filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure pale solid (0.132 g, 56 %); mp 281 °C. 1H NMR (600 MHz, DMSO-d6) δ 9.95 (s, 1H), 8.88 (s, 1H), 8.59 (dd, J = 8.7, 1.2 Hz, 1H), 8.08 (dd, J = 8.4, 1.3 Hz, 1H), 7.94 (dd, J = 8.0, 1.7 Hz, 1H), 7.83 (ddd, J = 8.2, 6.8, 1.3 Hz, 1H), 7.72 (ddd, J = 8.4, 6.9, 1.3 Hz, 1H), 7.61 (dd, J = 8.4, 1.1 Hz, 1H), 7.49 (ddd, J = 8.5, 7.0, 1.7 Hz, 1H), 7.40 – 7.31 (m, 2H), 7.03 (ddd, J = 8.0, 6.9, 1.1 Hz, 1H), 6.74 – 6.68 (m, 2H), 5.58 (s, 1H). 13C NMR (151 MHz, DMSO) δ 189.01, 152.97, 147.74, 142.79, 142.02, 135.21, 133.63, 131.26, 130.50, 129.83, 129.39, 128.92, 126.50, 123.03, 122.35, 120.27, 120.17, 120.11, 120.03, 114.04, 60.46. IR (ATR): νmax = 3254, 3179, 3078, 3017, 2321, 2115, 1657, 1595 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H15BrN2O [M + H]: 415.0441; found: 415.0443.


1,4-Bis(2-aminophenyl)-2-phenylbutane-1,4-dione (0.1 mmol, 0.03 4 g) was dissolved in T3P® in 50% DMF (1.14 mmol, 0.363 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (200 mL) was added and the mixture was extracted with CH2Cl2 (3 x 60 mL). The combined organic extracts were washed with brine, dried over Na2SO4 filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.016 g, 48 %); mp 115 °C. 1H NMR (600 MHz, DMSO-d6) δ 9.95 (s, 1H), 8.88 (s, 1H), 8.59 (dd, J = 8.7, 1.2 Hz, 1H), 8.08 (dd, J = 8.4, 1.3 Hz, 1H), 7.94 (dd, J = 8.0, 1.7 Hz, 1H), 7.83 (ddd, J = 8.2, 6.8, 1.3 Hz, 1H), 7.72 (ddd, J = 8.4, 6.9, 1.3 Hz, 1H), 7.61 (dd, J = 8.4, 1.1 Hz, 1H), 7.49 (ddd, J = 8.5, 7.0, 1.7 Hz, 1H), 7.40 – 7.31 (m, 2H), 7.03 (ddd, J = 8.0, 6.9, 1.1 Hz, 1H), 6.74 – 6.68 (m, 2H), 5.58 (s, 1H). 13C NMR (151 MHz, DMSO) δ 189.55, 153.16, 147.71, 142.77, 141.98, 135.79, 133.44, 130.51, 129.72, 129.38, 128.38, 126.92, 126.55, 126.42, 123.20, 122.34, 120.27, 120.16, 119.91, 114.24, 61.21. IR (ATR): νmax = 3298, 3207, 3025, 2922, 2321, 2115, 1657, 1595, 1522 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H16N2O [M + H]: 371.0946; found: 371.0940.

1,4-Bis(2-aminophenyl)-2-(4-fluorophenyl)butane-1,4-dione (0.1 mmol, 0.036 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.018 g, 51 %); mp 104 °C. 1H NMR (600 MHz, DMSO-d₆) δ 9.95 (s, 1H), 8.87 (s, 1H), 8.60 (dd, J = 8.6, 1.3 Hz, 1H), 8.07 (dd, J = 8.4, 1.3 Hz, 1H), 7.94 (dd, J = 8.0, 1.7 Hz, 1H), 7.83 (dd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.71 (dd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.61 (dd, J = 8.4, 1.1 Hz, 1H), 7.49 (dd, J = 8.5, 7.0, 1.7 Hz, 1H), 7.04 – 6.97 (m, 3H), 6.84 – 6.79 (m, 2H), 5.58 (d, J = 1.4 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 189.31, 161.80, 160.19, 152.93, 147.71, 142.78, 142.00, 133.54, 131.83, 131.81, 130.49, 129.78, 129.39, 128.71, 128.65, 126.47, 123.10, 122.35, 120.27, 120.14, 119.99, 115.26, 115.12, 114.28, 60.34, 29.59. IR (ATR): ν max = 3328, 3208, 3066, 2924, 1654, 1592, 1526 cm –1. HRMS (ESI +, 47 V): m/z calcd for C₂₃H₁₅F₁N₂O [M + H]: 355.1241; found: 355.1240.


1-(2-Aminophenyl)-4-(2-aminophenyl)-2-(4-(iodo)phenyl)butane-1,4-dione (0.1 mmol, 0.047 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.027 g, 58 %); mp 194 °C. 1H NMR (600 MHz, DMSO-d₆) δ 9.94 (s, 1H), 8.88 (s, 1H), 8.58 (dd, J = 8.5, 1.3 Hz, 1H), 8.07 (dd, J = 8.3, 1.3 Hz, 1H), 7.94 (dd, J = 8.0, 1.7 Hz, 1H), 7.84 – 7.81 (m, 1H), 7.73 – 7.70 (m, 1H), 7.60 (dd, J = 8.4, 1.1 Hz, 1H), 7.51 – 7.47 (m, 3H), 7.03 (dd, J = 8.0, 7.0, 1.1 Hz, 1H), 6.59 – 6.55 (m, 2H), 5.57 (s, 1H). 13C NMR (151 MHz, DMSO) δ 189.02, 153.00, 147.73, 142.79, 142.00, 137.09, 135.64, 133.63, 130.50, 129.81, 129.39, 128.98, 126.50, 123.02, 122.33, 120.27, 120.18, 120.02, 114.00, 93.03, 60.59. IR (ATR): ν max = 3255, 2918, 2850, 2321, 2113, 2098, 1923, 1661, 1594, 1521 cm⁻¹. HRMS (ESI+, 47 V): m/z calcd for C₂₃H₁₅IN₂O [M + H]: 463.0305; found: 463.0302.


1-(2-Aminophenyl)-4-(2-aminophenyl)-2-(4-(trifluoromethyl)phenyl)butane-1,4-dione (0.1 mmol, 0.041 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.024 g, 59 %); mp 222 °C. 1H NMR (600 MHz, DMSO-d₆) δ 9.98 (s, 1H), 8.92 (s, 1H), 8.58 (dd, J = 8.3, 1.4 Hz, 1H), 8.09 (dd, J = 8.4, 1.2 Hz, 1H), 7.98 (dd, J = 8.0, 1.7 Hz, 1H), 7.84 (dd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.72 (dd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.59 (dd, J = 8.4, 1.1 Hz, 1H), 7.54 – 7.48 (m, 3H), 7.04 (dd, J = 8.0, 6.9, 1.1 Hz, 1H), 6.99 (d, J = 8.1 Hz, 2H), 5.74 – 5.71 (m, 1H). 13C NMR (151 MHz, DMSO) δ 188.72, 152.96, 147.78, 142.17, 142.04, 133.77, 130.53, 129.89, 129.42, 127.65, 127.58, 126.57, 125.28, 125.25, 122.98, 122.35, 120.37, 120.26, 114.00, 70.70. IR (ATR): ν max = 3263, 3193, 3071, 3029, 2921, 2321, 2113, 1900, 1656, 1594, 1521 cm⁻¹. HRMS (ESI+, 47 V): m/z calcd for C₂₅H₁₅F₃N₂O [M + H]: 463.0302; found: 463.0305.


1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-(chloro)phenyl)butane-1,4-dione (0.1 mmol, 0.046 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄, filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.027 g, 60 %); mp 230 °C. ¹H NMR (600 MHz, DMSO-d₆) δ 10.00 (s, 1H), 8.90 (s, 1H), 8.58 (dd, J = 8.8, 1.2 Hz, 1H), 8.09 (dd, J = 8.4, 1.3 Hz, 1H), 7.89 (d, J = 1.8 Hz, 1H), 7.84 (dd, J = 8.4, 2.1 Hz, 2H), 7.73 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.25 – 7.22 (m, 2H), 7.19 (dd, J = 8.5, 1.8 Hz, 1H), 6.81 – 6.77 (m, 2H), 5.63 (s, 1H). ¹³C NMR (151 MHz, DMSO) δ 188.54, 152.93, 147.77, 141.65, 134.75, 132.64, 131.76, 130.00, 129.42, 128.57, 128.48, 127.05, 126.71, 122.96, 122.34, 122.24, 122.13, 120.26, 114.39, 59.75, 54.91. IR (ATR): ν max = 3061, 2322, 2109, 1896, 1656, 1583, 1515 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₃H₁₄BrClN₂O [M + H]: 449.0051; found: 449.0055.


1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-(bromo)phenyl)butane-1,4-dione (0.1 mmol, 0.050 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄, filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.034 g, 69 %); mp 221 °C. ¹H NMR (600 MHz, DMSO-d₆) δ 10.00 (s, 1H), 8.90 (s, 1H), 8.59 – 8.56 (m, 1H), 8.09 (dd, J = 8.4, 1.2 Hz, 1H), 7.89 (d, J = 1.9 Hz, 1H), 7.86 – 7.83 (m, 2H), 7.73 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.39 – 7.36 (m, 2H), 7.19 (dd, J = 8.5, 1.8 Hz, 1H), 6.73 – 6.70 (m, 2H), 5.61 (s, 1H). ¹³C NMR (151 MHz, DMSO) δ 188.48, 152.93, 147.77, 143.63, 132.64, 131.39, 130.00, 129.42, 128.90, 128.00, 127.06, 127.01, 122.97, 122.35, 122.25, 122.11, 120.30, 114.34, 60.27. IR (ATR): ν max = 3171, 3062, 2321, 1909, 1672, 1585, 1521 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₃H₁₄Br₂N₂O [M + H]: 492.9546; found: 492.9551.


1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-phenylbutane-1,4-dione (0.08 mmol, 0.034 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄, filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.022 g, 66 %); mp 261 °C. ¹H NMR (600 MHz, DMSO-d₆) δ 10.00 (s, 1H), 8.90 (s, 1H), 8.59 – 8.56 (m, 1H), 8.09 (dd, J = 8.4, 1.3 Hz, 1H), 7.89 (d, J = 1.9 Hz, 1H), 7.86 – 7.83 (m, 2H), 7.73 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.39 – 7.36 (m, 2H), 7.19 (dd, J = 8.5, 1.8 Hz, 1H), 6.73 – 6.70 (m, 2H), 5.61 (s, 1H). ¹³C NMR (151 MHz, DMSO) δ 189.02, 153.12, 147.74, 143.63, 132.64, 131.39, 130.00, 129.42, 128.90, 128.00, 127.06, 127.01, 122.97, 122.35, 122.25, 122.11, 120.30, 114.34, 60.27. IR (ATR): ν max = 3345, 3228, 3064, 2919, 2321, 1640, 1587, 1520 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₃H₁₄BrN₂O [M + H]: 415.0441; found: 415.0440.

1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-fluorophenyl)butane-1,4-dione (0.1 mmol, 0.044 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH2Cl2 (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na2SO4 filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.021 g, 49 %); mp 312 °C. 1H NMR (600 MHz, DMSO-d6) δ 10.00 (s, 1H), 8.89 (s, 1H), 8.58 (dd, J = 8.7, 1.4 Hz, 1H), 8.09 (dd, J = 8.4, 1.3 Hz, 1H), 7.90 (d, J = 1.9 Hz, 1H), 7.84 (dd, J = 8.4, 6.6 Hz, 2H), 7.74 – 7.71 (m, 1H), 7.19 (dd, J = 8.5, 1.8 Hz, 1H), 7.03 – 6.99 (m, 2H), 6.83 – 6.80 (m, 2H), 5.61 – 5.60 (m, 1H). 13C NMR (151 MHz, DMSO) δ 188.78, 161.88, 160.27, 152.90, 147.75, 143.62, 141.61, 132.63, 131.43, 129.95, 129.41, 128.72, 128.66, 126.95, 126.68, 122.90, 122.35, 122.20, 120.26, 115.40, 115.26, 114.58, 60.15. IR (ATR): νmax = 3336, 3209, 3068, 2920, 2322, 1894, 1648, 1586, 1502 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H14BrFN2O [M + H]: 433.0346; found: 433.0347.


1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-iodophenyl)butane-1,4-dione (0.1 mmol, 0.055 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH2Cl2 (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na2SO4 filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.036 g, 66 %); mp 229 °C. 1H NMR (600 MHz, DMSO-d6) δ 9.99 (s, 1H), 8.89 (s, 1H), 8.59 – 8.56 (m, 1H), 8.09 (dd, J = 8.4, 1.3 Hz, 1H), 7.89 (d, J = 1.9 Hz, 1H), 7.86 – 7.82 (m, 2H), 7.73 (ddd, J = 8.3, 6.8, 1.3 Hz, 1H), 7.55 – 7.51 (m, 2H), 7.19 (dd, J = 8.5, 1.9 Hz, 1H), 6.59 – 6.55 (m, 2H), 5.59 (s, 1H). 13C NMR (151 MHz, DMSO) δ 188.50, 152.98, 147.77, 143.64, 141.63, 137.22, 135.25, 132.64, 129.99, 129.42, 128.95, 127.06, 126.71, 122.96, 122.34, 122.25, 122.11, 120.26, 114.31, 93.27, 60.40, 54.91. IR (ATR): νmax = 3264, 3065, 2919, 2652, 2062, 1669, 1585, 1522 cm–1. HRMS (ESI+, 47 V): m/z calcd for C23H14BrIN2O [M + H]: 540.9407; found: 540.9406.


1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-(trifluoromethyl)phenyl)butane-1,4-dione (0.1 mmol, 0.049 g) was dissolved in T3P® in 50% DMF (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH2Cl2 (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na2SO4 filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.033 g, 68 %); mp 248 °C. 1H NMR (600 MHz, DMSO-d6) δ 10.02 (s, 1H), 8.93 (s, 1H), 8.57 (dd, J = 8.6, 1.3 Hz, 1H), 8.10 (dd, J = 8.5, 1.3 Hz, 1H), 7.90 (s, 1H), 7.88 (m, 1H), 7.74 (ddd, J = 8.3, 6.8, 1.4 Hz, 1H), 7.55 (d, J = 8.2 Hz, 2H), 7.21 (dd, J = 8.5, 1.8 Hz, 1H), 7.00 (d, J = 8.1 Hz, 2H), 5.76 – 5.74 (m, 1H). 13C NMR (151 MHz, DMSO) δ 188.20, 152.92, 147.82, 141.83, 140.27, 132.69, 130.08, 129.45, 127.82, 127.59, 127.40, 127.21, 126.78, 125.45, 125.42, 125.37, 124.94, 123.09, 122.36, 122.30, 120.32, 114.33, 60.50. IR (ATR): νmax = 3343, 3073, 2319, 1925, 1656, 1586, 1520 cm–1. HRMS (ESI+, 47 V): m/z calcd for C24H14BrF3N2O [M + H]: 540.9407; found: 540.9406.


1,4-Bis(2-aminophenyl)-2-(4-chlorophenyl)butane-1,4-dione (0.4 mmol, 0.152 g) and benzaldehyde (0.4 mmol, 0.042 g) was dissolved in T3P® in 50% EtOAc (1.2 mmol, 0.380 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.083 g, 46%); mp 132 °C. 1H NMR (400 MHz, DMSO-d₆) δ 10.00 (s, 1H), 8.56 (dd, J = 8.6, 1.3 Hz, 1H), 8.09 (dd, J = 8.0, 1.7 Hz, 1H), 7.88 – 7.84 (m, 1H), 7.81 – 7.77 (m, 1H), 7.65 – 7.58 (m, 3H), 7.57 – 7.51 (m, 4H), 7.14 – 7.11 (m, 2H), 7.09 – 7.05 (m, 1H), 6.61 – 6.58 (m, 2H), 5.57 (d, J = 1.3 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 189.23, 161.21, 146.72, 143.57, 143.32, 139.76, 134.82, 133.93, 131.41, 130.33, 130.25, 129.40, 129.23, 128.58, 128.29, 128.22, 128.75, 126.54, 122.88, 122.26, 120.28, 120.20, 120.16, 113.39, 58.42, 54.89. IR (ATR): νmax = 3332, 3058, 2923, 2321, 2110, 1894, 1653, 1586, 1519 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₉H₁₉ClN₂O [M + H]: 447.1259; found: 447.1256.


1,4-Bis(2-aminophenyl)-2-(4-fluorophenyl)butane-1,4-dione (0.2 mmol, 0.072 g) and benzaldehyde (0.2 mmol, 0.021 g) was dissolved in T3P® in 50% EtOAc (0.6 mmol, 0.190 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.058 g, 67%); mp 136 °C. 1H NMR (600 MHz, DMSO-d₆) δ 10.00 (s, 1H), 8.59 – 8.53 (m, 1H), 8.09 (dd, J = 8.3, 1.3 Hz, 1H), 8.03 (dd, J = 8.0, 1.7 Hz, 1H), 7.57 – 7.43 (m, 4H), 7.09 – 7.05 (m, 1H), 6.90 (t, J = 8.8 Hz, 2H), 6.60 (td, J = 5.7, 2.7 Hz, 2H), 5.57 (d, J = 1.7 Hz, 1H). 13C NMR (151 MHz, DMSO) δ 189.52, 161.66, 161.24, 160.05, 146.71, 143.55, 143.32, 139.83, 133.87, 131.86, 130.31, 130.27, 129.41, 129.25, 128.57, 128.21, 127.91, 127.85, 126.53, 126.28, 126.17, 126.12, 115.08, 113.57, 58.32, 30.95, 22.05, 13.96. IR (ATR): νmax = 3342, 3058, 2343, 2107, 1653, 1605, 1520 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₉H₁₉F₁N₂O [M + H]: 431.1554; found: 431.1552.


1,4-Bis(2-aminophenyl)-2-(thiophen-2-yl)butane-1,4-dione (0.2 mmol, 0.072 g) and benzaldehyde (0.2 mmol, 0.021 g) was dissolved in T3P® in 50% EtOAc (0.6 mmol, 0.190 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.015 g, 18%); mp 262 °C. 1H NMR (400 MHz, DMSO-d₆) δ 10.09 (s, 1H), 8.61 – 8.57 (m, 1H), 8.09 (dd, J = 8.3, 1.3 Hz, 1H), 8.03 (dd, J = 8.0, 1.7 Hz, 1H), 7.86 (dd, J = 8.2, 6.7, 1.3 Hz, 1H), 7.72 (dd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.64 – 7.60 (m, 2H), 7.59 (d, J = 8.3 Hz, 1H), 7.57 – 7.43 (m, 4H), 7.09 – 7.05 (m, 1H), 6.90 (t, J = 8.8 Hz, 2H), 6.60 (td, J = 5.7, 2.7 Hz, 2H), 5.57 (d, J = 1.7 Hz, 1H). 13C NMR (101 MHz, DMSO) δ 188.38, 160.50, 161.66, 161.24, 160.05, 146.71, 143.55, 143.32, 139.83, 133.87, 131.86, 130.31, 130.27, 129.41, 129.25, 128.57, 128.21, 127.91, 127.85, 126.53, 126.28, 126.17, 126.12, 115.08, 113.57, 58.32, 30.95, 22.05, 13.96. IR (ATR): νmax = 3342, 3058, 2343, 2107, 1653, 1605, 1520 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₇H₁₈N₂OS [M + H]: 431.1554; found: 431.1552.

1,4-Bis(2-aminophenyl)-2-(4-methoxyphenyl)butane-1,4-dione (0.3 mmol, 0.112 g) and benzaldehyde (0.3 mmol, 0.032 g) was dissolved in T3P® in 50% EtOAc (0.9 mmol, 0.285 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.060 g, 45 %); mp 118 °C. ¹H NMR (400 MHz, DMSO-d₆) δ 9.96 (s, 1H), 8.58 – 8.54 (m, 1H), 8.08 (dd, J = 8.4, 1.3 Hz, 1H), 8.03 – 8.00 (m, 1H), 7.87 – 7.82 (m, 1H), 7.73 – 7.69 (m, 1H), 7.63 – 7.58 (m, 3H), 7.55 – 7.48 (m, 4H), 7.07 – 7.04 (m, 1H), 6.64 – 6.61 (m, 2H), 6.53 – 6.47 (m, 2H), 5.56 (d, J = 1.2 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (101 MHz, DMSO) δ 190.03, 161.34, 157.91, 146.66, 143.49, 143.34, 139.99, 133.68, 130.24, 130.18, 129.39, 129.23, 128.49, 128.16, 127.53, 127.00, 126.43, 123.13, 122.23, 120.29, 120.19, 120.04, 113.80, 113.76, 58.35, 54.90. IR (ATR): νmax = 2834, 2161, 2045, 1978, 1637, 1610, 1578 cm⁻¹.


1,4-Bis(2-aminophenyl)-2-(3,4,5-trimethoxyphenyl)butane-1,4-dione (0.3 mmol, 0.130 g) and benzaldehyde (0.3 mmol, 0.032 g) was dissolved in T3P® in 50% EtOAc (0.9 mmol, 0.285 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.090 g, 60 %); mp 147 °C. ¹H NMR (400 MHz, DMSO-d₆) δ 10.02 (s, 1H), 8.60 – 8.51 (m, 1H), 8.08 (dd, J = 8.4, 1.3 Hz, 1H), 8.00 (dd, J = 8.0, 1.7 Hz, 1H), 7.85 (ddd, J = 8.3, 6.8, 1.2 Hz, 1H), 7.77 – 7.70 (m, 1H), 7.68 – 7.49 (m, 8H), 7.09 – 7.05 (m, 1H), 5.79 (s, 1H), 5.58 (d, J = 1.2 Hz, 1H), 3.50 (s, 3H), 3.37 (s, 6H). ¹³C NMR (101 MHz, DMSO) δ 189.62, 161.34, 157.91, 144.66, 143.20, 139.99, 136.24, 130.22, 130.10, 129.41, 128.47, 128.19, 126.48, 123.32, 122.30, 120.19, 120.08, 119.93, 113.72, 103.53, 59.85, 58.98, 55.57. IR (ATR): νmax = 2835, 2161, 2050, 1735, 1637, 1609, 1579 cm⁻¹.
4. Synthesis of 6,6-Dimethyl-7-phenyl-5,6,7,13-tetrahydro-8H-benzo[6,7]azepino[3,2-c]quinolin-8-one derivatives 12a-b

6,6-Dimethyl-7-(4-(trifluoromethyl)phenyl)-5,6,7,13-tetrahydro-8H-benzo[6,7]azepino[3,2-c]quinolin-8-one (12a).

1-(2-Aminophenyl)-4-(2-aminophenyl)-2-(4-(trifluoromethyl)phenyl)butane-1,4-dione (0.1 mmol, 0.041 g) and acetone (1 drop) was dissolved in T3P® in 50% EtOAc (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.032 g, 74%); mp 141 °C. ¹H NMR (600 MHz, DMSO-d₆) δ 8.74 (s, 1H), 7.88 (dd, J = 8.1, 1.7 Hz, 1H), 7.51 (d, J = 8.2 Hz, 2H), 7.35 (dd, J = 7.9, 1.4 Hz, 1H), 7.31 (dd, J = 8.5, 6.8, 1.7 Hz, 1H), 7.23 (dd, J = 8.3, 1.2 Hz, 1H), 7.15 (d, J = 8.2 Hz, 2H), 7.05 (dd, J = 8.2, 7.2, 1.4 Hz, 1H), 6.87 (ddd, J = 7.9, 6.8, 1.1 Hz, 1H), 6.65 (ddd, J = 8.0, 1.2 Hz, 1H), 6.58 (td, J = 7.5, 1.2 Hz, 1H), 6.28 (s, 1H), 4.94 (d, J = 1.7 Hz, 1H) 1.53 (s, 3H), 1.21 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 186.64, 144.24, 144.14, 141.33, 132.51, 132.15, 130.05, 129.50, 127.36, 124.83, 124.81, 122.66, 121.10, 118.92, 118.14, 116.23, 115.83, 115.72, 113.27, 58.03, 28.60, 27.84. IR (ATR): νmax = 3344, 3054, 2981, 1922, 1613, 1602, 1517 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₆H₂₁F₃N₂O [M + H]: 435.1679; found: 435.1675.

11-Bromo-6,6-dimethyl-7-(4-(trifluoromethyl)phenyl)-5,6,7,13-tetrahydro-8H-benzo[6,7]azepino[3,2-c]quinolin-8-one (12b).

1-(2-Amino-4-bromophenyl)-4-(2-aminophenyl)-2-(4-(trifluoromethyl)phenyl)butane-1,4-dione (0.1 mmol, 0.049 g) and acetone (1 drop) was dissolved in T3P® in 50% EtOAc (0.3 mmol, 0.095 g) and the reaction mixture was stirred at 80 °C for 24 h. Water (100 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic extracts were washed with brine, dried over Na₂SO₄ filtered, and the solvent removed under reduced pressure. The crude product was purified by column chromatography (hexane/ethyl acetate) to give an analytically pure solid (0.033 g, 64%); mp 248 °C. ¹H NMR (600 MHz, DMSO-d₆) δ 8.84 (s, 1H), 7.79 (d, J = 8.6 Hz, 1H), 7.50 (d, J = 1.9 Hz, 1H), 7.33 (dd, J = 8.0, 1.4 Hz, 1H), 7.14 (d, J = 8.1 Hz, 2H), 7.07 – 7.01 (m, 2H), 6.65 (ddd, J = 8.1, 1.2 Hz, 1H), 6.58 (td, J = 7.5, 1.2 Hz, 1H), 6.30 (s, 1H), 4.97 – 4.94 (m, 1H), 1.51 (s, 3H), 1.19 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 186.18, 144.24, 144.14, 141.33, 132.51, 132.15, 130.05, 129.50, 127.36, 124.83, 124.81, 122.66, 121.10, 118.92, 118.14, 116.23, 115.83, 115.72, 113.27, 58.03, 28.60, 27.84. IR (ATR): νmax = 3376, 3267, 2972, 2321, 2113, 1517 cm⁻¹. HRMS (ESI⁺, 47 V): m/z calcd for C₂₆H₂₁BrF₃N₂O [M + Na]: 535.0603; found: 535.0605.
5. General Information and Biology

General Information:

$^1$H and $^{13}$C NMR spectra were obtained in the specified solvents on a Bruker Avance III 400 Prodigy and a Bruker Avance III 600 Cryo spectrometer. Chemical shifts ($\delta$) are in parts per million (ppm) internally referenced relative to the solvent nuclei. Multiplicities are assigned as singlet (s), doublet (d), doublet of doublet (dd), doublet of doublet of doublet (ddd), doublet of triplet (dt), triplet (t), quartet (q), pentet (p), hextet (h), septet (sept), multiplet (m) where appropriate, and the observed coupling constants ($J$) are described in Hertz (Hz). Melting points were measured using an Optimelt melting point apparatus and are uncorrected. High-resolution ESI$^+$ mass spectra (HRMS) were recorded using a Thermo LTQ Orbitrap XL instrument with electrospray ionisation at the UNSW Bioanalytical Mass Spectrometry Facility. Infrared spectral data were recorded on Agilent Cary 630 FTIR spectrometer fitted with a diamond attenuated total reflectance (ATR) sample interface. Commercially available reagents were purchased from Sigma Aldrich and Alfa Aesar and used without further purification.

Biology Experimental:

*AlamarBlue® Cell Viability Assay*

MCF-7 breast cancer adenocarcinoma cells (MCF-7) at a density of $3 \times 10^3$ cells/well were seeded in triplicates on the surface of a 96-well plate and incubated at 37 °C in 5% CO$_2$ for 24 h. The test samples were made to a stock solution (20 mM concentration) with sterile DMSO. The samples were then diluted to 100 μM, 50 μM, 25 μM, 10 μM, 5 μM and 1 μM concentrations in Dulbecco’s Modified Eagle Media (DMEM). DMEM culture medium was removed from each well and replaced with 200 μL of the test samples accordingly to the concentrations. Culture medium and cells with culture medium were employed as negative and positive controls, respectively. The well plate was incubated at 37 °C in 5% CO$_2$ for 72 h. After incubation, the test sample solutions were carefully removed and replaced with 200 μL DMEM culture medium with the addition of alamarBlue® reagent (10% v/v). The fluorescence was measured using excitation wavelength of 570 nm and emission wavelength of 585 nm by a fluorescence microplate reader after 4 h incubation. All procedures were performed under sterile conditions.
6. $^1\text{H}$ and $^{13}\text{C}$ NMR Spectra of Synthesised Compounds
7. CCDC Deposition Data

Compound 6i

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

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Click on the hyperlinks for more details of the test.

![Graph of Compound 6i]
### Compound 7b

**Bond precision:** $\text{C-C} = 0.0030 \ \text{Å}$  
**Wavelength:** $0.71073$

**Cell:**  
- $a=11.6284(10)$  
- $b=12.7024(11)$  
- $c=12.0155(10)$  
- $\alpha=90$  
- $\beta=107.180(2)$  
- $\gamma=90$

**Temperature:** 150 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Volume</strong></td>
<td>1695.6(3)</td>
</tr>
<tr>
<td><strong>Space group</strong></td>
<td>P $2_1/c$</td>
</tr>
<tr>
<td><strong>Hall group</strong></td>
<td>$-P \ 2ybc$</td>
</tr>
<tr>
<td><strong>Moity formula</strong></td>
<td>C$<em>{23}$ H$</em>{15}$ Br N$_2$ O</td>
</tr>
<tr>
<td><strong>Sum formula</strong></td>
<td>C$<em>{23}$ H$</em>{15}$ Br N$_2$ O</td>
</tr>
<tr>
<td><strong>Mr</strong></td>
<td>415.27</td>
</tr>
<tr>
<td><strong>$D_x, g \ cm^{-3}$</strong></td>
<td>1.627</td>
</tr>
<tr>
<td><strong>$Z$</strong></td>
<td>4</td>
</tr>
<tr>
<td><strong>$\mu (\text{mm}^{-1})$</strong></td>
<td>2.441</td>
</tr>
<tr>
<td><strong>$F_{000}$</strong></td>
<td>840.0</td>
</tr>
<tr>
<td><strong>$F_{000}'$</strong></td>
<td>839.15</td>
</tr>
<tr>
<td><strong>$h,k,l_{\text{max}}$</strong></td>
<td>15,16,15</td>
</tr>
<tr>
<td><strong>$N_{\text{ref}}$</strong></td>
<td>3929</td>
</tr>
<tr>
<td><strong>$T_{\text{min}}, T_{\text{max}}$</strong></td>
<td>0.725, 0.803</td>
</tr>
<tr>
<td><strong>$T_{\text{min}}'$</strong></td>
<td>0.600</td>
</tr>
<tr>
<td><strong>Correction method</strong></td>
<td># Reported T Limits</td>
</tr>
<tr>
<td><strong>AbsCorr</strong></td>
<td>MULTI-SCAN</td>
</tr>
</tbody>
</table>

**Data completeness** = 0.996  
**Theta(max)** = 27.582  
**R(reflections)** = 0.0373 (3119)  
**wr2(reflections)** = 0.0950 (3912)

**$S$** = 1.017  
**Npar** = 244
### Compound 12b

**Bond precision:** $\text{C-C} = 0.0051 \text{ Å}$  \hspace{1cm} **Wavelength**=0.71073

**Cell:** 
- $a = 17.7029(13)$
- $b = 17.0250(14)$
- $c = 16.7413(15)$
- $\alpha = 90^\circ$
- $\beta = 90.744(3)^\circ$
- $\gamma = 90^\circ$

**Temperature:** 100 K

**Volume:** Calculated 5045.3(7)  \hspace{1cm} **Reported** 5045.3(7)

**Space group:** $P 21/c$  \hspace{1cm} **Hall group:** $-P 2ybc$

**Hall group:** $P 1 21/c 1$  \hspace{1cm} **Moiety formula:** $\text{C}_26 \text{H}_20 \text{Br} \text{F}_3 \text{N}_2 \text{O}$, $\text{C}_2 \text{H}_6 \text{O}$

**Sum formula:** $\text{C}_{28} \text{H}_{26} \text{Br} \text{F}_3 \text{N}_2 \text{O}_2$  \hspace{1cm} **C}_{56} \text{H}_{52} \text{Br}_2 \text{F}_6 \text{N}_4 \text{O}_4$

**Mr:** 559.41  \hspace{1cm} **Dx,g cm$^{-3}$:** 1.473

**Dx,g cm$^{-3}$:** 1.473  \hspace{1cm} **Z:** 8

**Mu (mm$^{-1}$):** 1.680  \hspace{1cm} **F000:** 2288.0

**F000:** 2288.0  \hspace{1cm} **F000’:** 2286.83

**h,k,lmax:** 21,20,19  \hspace{1cm} **Nref:** 8880

**Nref:** 8691  \hspace{1cm} **Tmin, Tmax:** 0.671,0.860

**Tmin, Tmax:** 0.505  \hspace{1cm} **AbsCorr = MULTI-SCAN**

**Correction method:** # Reported T Limits: Tmin=0.464 Tmax=0.746

**Data completeness:** 0.979  \hspace{1cm} **Theta(max):** 24.998

**R(reflections):** 0.0569( 7010)  \hspace{1cm} **wr2(reflections):** 0.1545( 8691)

**S = 1.168**  \hspace{1cm} **Npar = 676**