

**Supporting Information**

**Preparation of 7-Alkylamino-2-methylquinoline-5,8-diones**

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**Experimental Section**

**6-Amino-7-bromo-2-methylquinoline-5,8-dione (4b).** mp 218-220 °C dec; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.26 (d, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 5.80 (bs, 2H), 2.77 (s, 3H); <sup>13</sup>C NMR (50 MHz, DMSO-d<sub>6</sub> + CDCl<sub>3</sub>) .175.4, 173.0, 160.8, 147.1, 143.8, 132.8, 126.2, 125.9, 99.7, 22.8; MS (EI) 268 (M<sup>+</sup>, 100), 266 (M<sup>+</sup>), 240, 238, 212, 210, 187, 159, 131, 120, 104, 92, 77, 68, 52, 39. Anal. Calcd for C<sub>10</sub>H<sub>7</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 44.97; H, 2.64; N, 10.49. Found: C, 45.26; H, 3.01; N, 10.15.

**7-Amino-6-bromo-2-methylquinoline-5,8-dione (5b).** mp 247 °C dec; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.37 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 5.80 (bs, 2H), 2.75 (s, 3H); <sup>13</sup>C NMR (50 MHz, DMSO-d<sub>6</sub> + CDCl<sub>3</sub>) .177.2, 173.0, 163.3, 146.8, 146.5, 133.3, 125.1, 123.4, 102.0, 47.7, 23.7; MS (EI) 268 (M<sup>+</sup>), 266 (M<sup>+</sup>), 187 (100), 159, 143, 131, 119, 104, 92, 77, 65, 52, 39. Anal. Calcd for C<sub>10</sub>H<sub>7</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 44.97; H, 2.64; N, 10.49. Found: C, 45.30; H, 2.79; N, 10.28.

**7-Bromo-6-n-butylamino-2-methylquinoline-5,8-dione (4c).** mp 127-128 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.18 (d, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 6.15 (bs, 1H), 3.87 (q, *J* = 6.7 Hz, 2H), 2.73 (s, 3H), 1.60-1.80 (m, 2H), 1.35-1.60 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .179.1, 174.4, 165.1, 147.1, 145.4, 134.4, 126.0, 124.0, 44.7, 32.4, 24.8, 19.4, 13.3; MS (EI) 324 (M<sup>+</sup>), 322 (M<sup>+</sup>, 100), 281, 279, 254, 252, 227, 225, 201, 187, 174, 158, 144, 129, 116, 104, 89, 77, 63, 52, 41. Anal. Calcd for C<sub>14</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 52.03; H, 4.68; N, 8.67. Found: C, 51.97; H, 4.92; N, 8.59.

MHz, CDCl<sub>3</sub>) . 8.32 (d, *J* = 7.8 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 6.17 (bs, 1H), 3.90 (q, *J* = 6.8 Hz, 2H), 2.72 (s, 3H), 1.60-1.71 (m, 2H), 1.38-1.58 (m, 2H), 0.98 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .178.5, 175.3, 163.3, 146.7, 134.9, 128.1, 127.3, 45.2, 32.8, 24.8, 19.7, 13.6; MS (EI) 324 (M<sup>+</sup>), 322 (M<sup>+</sup>, 100), 307, 305, 292, 253, 251, 197, 195, 172, 142, 116, 89, 63, 52, 39. Anal. Calcd for C<sub>14</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 52.03; H, 4.68; N, 8.67. Found: C, 52.21; H, 4.87; N, 8.28.

**6-Benzylamino-7-bromo-2-methylquinoline-5,8-dione (4d).** mp 141-142 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.20 (d, *J* = 8.2 Hz, 1H), 7.29-7.45 (m, 7H), 6.22 (bs, 1H), 5.08 (d, *J* = 8.2 Hz, 2H), 2.74 (s, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .179.5, 175.1, 165.7, 147.4, 145.7, 145.7, 137.5, 134.9, 129.0, 128.1, 127.6, 126.4, 124.5, 49.3, 25.3; MS (EI) 358 (M<sup>+</sup>), 356 (M<sup>+</sup>, 100), 278, 268, 266, 221, 155, 121, 107. Anal. Calcd for C<sub>17</sub>H<sub>13</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 57.16; H, 3.67; N, 7.84. Found: C, 57.22; H, 3.82; N, 7.98.

**7-Benzylamino-6-bromo-2-methylquinoline-5,8-dione (5d).** mp 169-171 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.30 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.2 Hz, 1H), 7.35 (s, 5H), 6.35 (bs, 1H), 5.08 (d, *J* = 7.8 Hz, 2H), 2.71 (s, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .178.2, 175.3, 163.4, 146.5, 145.2, 137.5, 134.8, 128.8, 128.0, 127.8, 127.4, 127.0, 49.2, 24.7; MS (EI) 358 (M<sup>+</sup>), 356 (M<sup>+</sup>, 100), 277, 253, 91. Anal. Calcd for C<sub>17</sub>H<sub>13</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 57.16; H, 3.67; N, 7.84. Found: C, 57.09; H, 4.02; N, 7.77.

**7-Bromo-2-methyl-6-methylaziridinylquinoline-5,8-dione (4e).** mp 138-139 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.25 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 2.76 (s, 3H), 2.60-2.70 (m, 1H), 2.52-2.58 (m, 2H), 1.57 (d, *J* = 5.6 Hz, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .178.0, 175.4, 164.7, 153.9, 146.2, 134.5, 126.8, 125.1, 119.3, 37.9, 37.2, 24.8, 17.5; MS (EI) 308 (M<sup>+</sup>), 306 (M<sup>+</sup>), 267, 265, 227, 195, 186, 172, 158, 144, 130, 116, 102, 77, 64, 56, 41 (100). Anal. Calcd for C<sub>13</sub>H<sub>11</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 50.84; H, 3.61; N, 9.12. Found: C, 50.52; H, 3.92; N, 8.82.

MHz, CDCl<sub>3</sub>) . 8.32 (d, *J* = 7.8 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 1H), 2.75 (s, 3H), 2.62-2.78 (m, 1H), 2.52-2.60 (m, 2H), 1.57 (d, *J* = 5.6 Hz, 3H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .177.1, 176.1, 163.9, 154.9, 145.6, 134.6, 127.4, 125.9, 117.7, 38.1, 37.2, 24.7, 17.5; MS (EI) 308 (M<sup>+</sup>), 306 (M<sup>+</sup>), 281, 279, 253, 251, 227 (100), 225, 198, 186, 172, 144, 129, 115, 102, 64, 56, 44. Anal. Calcd for C<sub>13</sub>H<sub>11</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 50.84; H, 3.61; N, 9.12. Found: C, 50.62; H, 3.98; N, 8.98.

**7-Bromo-6-cyclohexylamino-2-methylquinoline-5,8-dione (4f).** mp 109-110 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.21 (d, *J* = 8.2 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 6.01 (bs, 1H), 4.42-4.65 (m, 1H), 2.75 (s, 3H), 2.05-2.12 (m, 2H), 1.61-1.95 (m, 3H), 1.20-1.60 (m, 5H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .179.6, 174.8, 165.5, 147.5, 144.9, 134.7, 126.1, 124.3, 52.5, 34.3, 25.1, 24.3; MS (EI) 350 (M<sup>+</sup>), 348 (M<sup>+</sup>), 307, 305 (100), 269, 267, 252, 197, 141, 113, 89, 77, 65, 53, 41. Anal. Calcd for C<sub>16</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 55.03; H, 4.91; N, 8.02. Found: C, 54.90; H, 5.00; N, 7.70.

**6-Bromo-7-cyclohexylamino-2-methylquinoline-5,8-dione (5f).** mp 159-160 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.34 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 6.09 (bs, 1H), 4.42-4.62 (m, 1H), 2.73 (s, 3H), 2.05-2.13 (m, 2H), 1.65-1.83 (m, 3H), 1.20-1.60 (m, 5H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .178.6, 175.3, 163.3, 146.1, 145.5, 134.9, 128.1, 124.3, 53.0, 34.4, 25.2, 24.8, 24.4; MS (EI) 350 (M<sup>+</sup>), 348 (M<sup>+</sup>), 307, 305, 269, 267, 251 (100), 225, 187, 169, 143, 92, 55, 41. Anal. Calcd for C<sub>16</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 55.03; H, 4.91; N, 8.02. Found: C, 54.66; H, 5.18; N, 8.04.

**7-Bromo-6-cyclopentylamino-2-methylquinoline-5,8-dione (4g).** mp 122-123 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.22 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 6.07 (bs, 1H), 4.80-5.10 (m, 1H), 2.76 (s, 3H), 2.05-2.20 (m, 2H), 1.56-1.83 (m, 6H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .178.9, 174.4, 165.2, 147.0, 144.7, 134.5, 126.0, 123.8, 55.4, 34.8, 24.9, 23.4; MS (EI) 336 (M<sup>+</sup>), 334 (M<sup>+</sup>), 307, 305 (100), 281, 253, 227, 207, 187, 144, 117, 89. Anal. Calcd for C<sub>15</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 53.75; H, 4.51; N, 8.36. Found: C, 54.11; H, 4.74; N, 8.76.

MHz, CDCl<sub>3</sub>) . 8.22 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 6.15 (bs, 1H), 4.82-5.10 (m, 1H), 2.73 (s, 3H), 2.05-2.21 (m, 2H), 1.57-1.83 (m, 6H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .177.9, 174.7, 162.8, 145.6, 144.8, 134.5, 127.8, 126.8, 55.6, 34.8, 24.4, 23.5; MS (EI) 336 (M<sup>+</sup>), 334 (M<sup>+</sup>), 307, 305, 281, 255 (100), 237, 225, 198, 187, 169, 143, 116, 92, 77, 41. Anal. Calcd for C<sub>15</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 53.75; H, 4.51; N, 8.36. Found: C, 53.74; H, 4.69; N, 8.55.

**7-Bromo-6-*t*-butylamino-2-methylquinoline-5,8-dione (4h).** mp 136-137 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.22 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 5.85 (bs, 1H), 2.75 (s, 3H), 1.55 (s, 9H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) .179.3, 174.6, 165.1, 148.8, 146.9, 134.8, 126.3, 125.4, 110.6, 56.2, 31.0, 25.1; MS (EI) 324 (M<sup>+</sup>), 322 (M<sup>+</sup>), 309, 307, 268 (100), 266, 240, 238, 212, 210, 187, 159, 131, 104, 57, 41. Anal. Calcd for C<sub>14</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 52.03; H, 4.68; N, 8.67. Found: C, 51.92; H, 4.88; N, 8.57.

**6-Bromo-7-*t*-butylamino-2-methylquinoline-5,8-dione (5h).** mp 115-116 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) . 8.30 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 5.88 (bs, 1H), 2.74 (s, 3H), 1.57 (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) .178.2, 175.0, 163.4, 149.7, 146.1, 134.5, 127.7, 126.3, 108.8, 56.4, 31.0, 24.9; MS (EI) 324 (M<sup>+</sup>), 322 (M<sup>+</sup>), 309, 307, 291, 268, 266, 187 (100), 169, 143, 104, 57, 41. Anal. Calcd for C<sub>14</sub>H<sub>15</sub>BrN<sub>2</sub>O<sub>2</sub>: C, 52.03; H, 4.68; N, 8.67. Found: C, 52.40; H, 4.78; N, 8.98.

**2-Methyl-6-piperidinylquinoline-5,8-dione (6a).** mp 115-116 °C; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.18 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 6.17 (s, 1H), 3.54 (bs, 4H), 2.74 (s, 3H), 1.74 (bs, 6H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) . 182.5, 181.9, 164.4, 152.7, 147.5, 134.6, 127.0, 126.0, 110.2, 50.2, 25.6, 25.0, 24.0; MS (EI) 256 (M<sup>+</sup>, 100), 227, 213, 201, 188, 172, 161, 144, 117, 84, 41. Anal. Calcd for C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>: C, 70.29; H, 6.29; N, 10.93. Found: C, 70.20; H, 6.43; N, 11.15.

(d,  $J = 8.0$  Hz, 1H), 7.44 (d,  $J = 8.0$  Hz, 1H), 6.15 (s, 1H), 5.22 (bs, 2H), 2.77 (s, 3H);  $^{13}\text{C}$  NMR (50 MHz, DMSO-d<sub>6</sub>) .180.0, 178.9, 162.2, 148.0, 146.4, 132.2, 124.0, 123.5, 101.5, 22.9; MS (EI) 188 (M<sup>+</sup>, 100), 160, 132, 120, 104, 93, 77, 68, 52, 39. Anal. Calcd for C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>: C, 63.82; H, 4.28; N, 14.89. Found: C, 63.51; H, 4.48; N, 15.26.

**7-n-Butylamino-2-methylquinoline-5,8-dione (7c).** mp 139-140 °C;  $^1\text{H}$  NMR (200 MHz, CDCl<sub>3</sub>) .8.31 (d,  $J = 8.0$  Hz, 1H), 7.50 (d,  $J = 8.0$  Hz, 1H), 6.06 (bs, 1H), 5.75 (s, 1H), 3.22 (q,  $J = 6.7$  Hz, 2H), 2.73 (s, 3H), 1.60-1.80 (m, 2H), 1.38-1.58 (m, 2H), 0.98 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (50 MHz, CDCl<sub>3</sub>) .181.7, 180.4, 162.7, 148.1, 146.1, 133.3, 128.6, 128.1, 99.8, 42.4, 30.1, 24.8, 20.1, 13.6; MS (EI) 244 (M<sup>+</sup>), 215, 201, 189, 174, 161, 146, 117, 92, 65, 41. Anal. Calcd for C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>: C, 68.83; H, 6.60; N, 11.47. Found: C, 69.16; H, 6.98; N, 11.62.

**6-n-Butylamino-2-methylquinoline-5,8-dione (6c).** mp 142-144 °C;  $^1\text{H}$  NMR (200 MHz, CDCl<sub>3</sub>) .8.23 (d,  $J = 8.2$  Hz, 1H), 7.42 (d,  $J = 8.0$  Hz, 1H), 5.93 (bs, 1H), 5.90 (s, 1H), 3.16-3.26 (m, 2H), 2.76 (s, 3H), 1.62-1.98 (m, 2H), 1.42-1.54 (m, 2H), 0.98 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (50 MHz, CDCl<sub>3</sub>) .181.5, 181.4, 165.4, 148.9, 147.4, 134.2, 125.9, 125.0, 101.4, 77.6, 77.0, 76.4, 42.3, 30.1, 25.3, 20.1, 13.5; MS (EI) 244 (M<sup>+</sup>), 227, 215, 201 (100), 174, 161, 145, 117, 101, 92, 44, 32. Anal. Calcd for C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>: C, 68.83; H, 6.60; N, 11.47. Found: C, 68.88; H, 6.92; N, 11.63.

**7-Cyclohexylamino-2-methylquinoline-5,8-dione (7f).** mp 208-209 °C;  $^1\text{H}$  NMR (200 MHz, CDCl<sub>3</sub>) .8.30 (d,  $J = 8.0$  Hz, 1H), 7.50 (d,  $J = 8.0$  Hz, 1H), 5.97 (bd,  $J = 7.8$  Hz, 1H), 5.78 (s, 1H), 3.20-3.40 (m, 1H), 2.73 (s, 3H), 1.95-2.15 (m, 2H), 1.60-1.85 (m, 3H), 1.22-1.44 (m, 5H);  $^{13}\text{C}$  NMR (50 MHz, CDCl<sub>3</sub>) .181.7, 180.5, 162.7, 146.9, 146.2, 134.3, 128.6, 128.0, 99.9, 51.4, 31.8, 25.4, 24.8, 24.5; MS (EI) 270 (M<sup>+</sup>), 253, 227 (100), 189, 161, 117, 92, 55, 41. HRMS (EI) m/z 270.1374, calcd for C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub> 270.1368.

$\text{CDCl}_3$ ) . 8.23 (d,  $J = 8.0$  Hz, 1H), 7.42 (d,  $J = 7.8$  Hz, 1H), 5.93 (s, 1H), 5.85 (bd,  $J = 7.4$  Hz, 1H), 3.20-3.40 (m, 1H), 1.95-2.15 (m, 2H), 1.60-1.90 (m, 3H), 1.20-1.55 (m, 5H);  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) .181.6, 181.3, 165.3, 148.8, 146.1, 134.1, 125.7, 125.0, 101.5, 51.2, 31.7, 25.3, 24.4; MS (EI) 270 ( $M^+$ , 100), 251, 227, 189, 161, 117, 92, 55, 41. Anal. Calcd for  $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_2$ : C, 71.09; H, 6.71; N, 10.36. Found: C, 71.26; H, 6.91; N, 10.61..

**7-Cyclopentylamino-2-methyl-quinoline-5,8-dione (7g).** mp 178-179 °C;  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) . 8.31 (d,  $J = 8.2$  Hz, 1H), 7.50 (d,  $J = 8.0$  Hz, 1H), 5.99 (bs, 1H), 5.78(s, 1H), 3.75-3.95 (m, 1H), 2.74 (s, 3H), 1.95-2.13 (m, 2H), 1.60-1.85 (m, 6H);  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) .181.6, 180.5, 162.7, 147.6, 146.2, 134.3, 128.6, 128.0, 100.5, 54.0, 32.6, 24.8, 24.0; MS (EI) 256 ( $M^+$ , 100), 227, 213, 189, 161, 117, 92, 41. Anal. Calcd for  $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_2$ : C, 70.29; H, 6.29; N, 10.93. Found: C, 70.41; H, 6.62; N, 10.95.

**6-Cyclopentylamino-2-methyl-quinoline-5,8-dione (6g).** mp 161-163 °C;  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) . 8.22 (d,  $J = 8.2$  Hz, 1H), 7.41 (d,  $J = 8.0$  Hz, 1H), 5.92(s, 1H), 5.87 (bd,  $J = 6.2$  Hz, 1H), 3.72-3.90 (m, 1H), 2.76 (s, 3H), 1.95-2.13 (m, 2H), 1.60-1.85 (m, 6H);  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) .181.5, 181.2, 165.4, 148.8, 146.8, 134.2, 125.8, 125.0, 102.0, 53.8, 32.6, 25.3, 23.9. MS (EI) 256 ( $M^+$ ), 227 (100), 213, 189, 161, 117, 89, 65, 41; Anal. Calcd for  $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_2$ : C, 70.29; H, 6.29; N, 10.93. Found: C, 70.11; H, 6.57; N, 10.93.

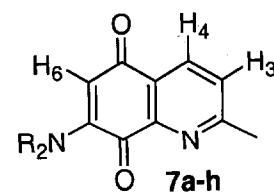
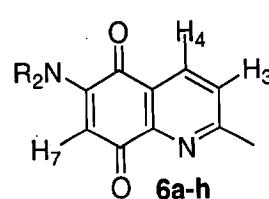
**7-t-Butylamino-2-methylquinoline-5,8-dione (7h).** mp 142-144 °C;  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) . 8.30 (d,  $J = 8.2$  Hz, 1H), 7.50 (d,  $J = 8.0$  Hz, 1H), 6.08 (bs, 1H), 5.99 (s, 1H), 2.73 (s, 3H), 1.47 (s, 9H);  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) .181.4, 180.8, 162.7, 146.0, 134.2, 128.3, 128.0, 101.8, 51.8, 28.2, 24.8; MS (EI) 244 ( $M^+$ ), 229, 221, 188, 161 (100), 132, 107, 93, 57, 41. HRMS (EI) m/z 244.1214, calcd for  $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_2$  244.1212.

8.23 (d,  $J = 8.0$  Hz, 1H), 7.42 (d,  $J = 8.2$  Hz, 1H), 6.13 (s, 1H), 5.97 (bs, 1H), 2.76 (s, 3H), 1.46 (s, 9H);  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) . 181.9, 181.1, 165.3, 148.5, 145.1, 134.3, 125.8, 125.0, 103.2, 51.7, 28.1, 25.3; MS (EI) 244 ( $\text{M}^+$ ), 229 (100), 189, 160, 132, 92, 57, 32. HRMS (EI) m/z 244.1212, calcd for  $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_2$  244.1212.

**6-Methoxy-2-methylquinoline-5,8-dione (6i).** **6i** was prepared by the same method as for **7i** by 37% yield, mp 204-206 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) . 8.32 (d,  $J = 8.0$  Hz, 1H), 7.56 (d,  $J = 8.0$  Hz, 1H), 6.34 (s, 3H), 3.97 (s, 3H), 2.78 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) . 182.9, 179.1, 165.0, 159.6, 146.7, 134.4, 126.9, 125.4, 109.9, 56.3, 24.9; MS (EI) 203 ( $\text{M}^+$ , 100), 188, 175, 145, 117, 104, 77, 69, 53, 39. Anal. Calcd for  $\text{C}_{11}\text{H}_9\text{NO}_3$ : C, 65.02; H, 4.46; N, 6.89. Found: C, 65.32; H, 4.55; N, 7.10.

**Table S1.** The Chemical Shifts of  $\text{H}_4$  and  $\text{H}_3$  of **4a-h** and **5a-h**.

$\text{R}_2\text{N}$	<b>4a-h</b>	$\text{H}_3$	$\text{H}_4$	<b>5a-h</b>	$\text{H}_3$	$\text{H}_4$
piperidinyl	<b>4a</b>	7.37	8.12	<b>5a</b>	7.45	8.20
amino	<b>4b</b>	7.46	8.26	<b>5b</b>	7.51	8.37
<i>n</i> -butylamino	<b>4c</b>	7.44	8.19	<b>5c</b>	7.48	8.30
2-methylaziridinyl	<b>4e</b>	7.46	8.20	<b>5e</b>	7.50	8.26
c-hexylamino	<b>4f</b>	7.38	8.17	<b>5f</b>	7.45	8.29
c-pentylamino	<b>4g</b>	7.42	8.22	<b>5g</b>	7.49	8.34
<i>t</i> -butylamino	<b>4h</b>	7.40	8.19	<b>5h</b>	7.45	8.27

**Table S2.** The Chemical Shifts of H<sub>3</sub>, H<sub>4</sub> and H<sub>7</sub> or H<sub>6</sub> of **6a-h** and **7a-h**.

R <sub>2</sub> N	<b>6a-h</b>	H <sub>3</sub>	H <sub>4</sub>	H <sub>7</sub>	<b>7a-h</b>	H <sub>3</sub>	H <sub>4</sub>	H <sub>6</sub>
piperidinyl	<b>6a</b>	7.42	8.18	6.16	<b>7a</b>	7.47	8.24	6.01
amino	<b>6b</b>	7.44	8.26	6.15	<b>7b</b>	7.50	8.28	6.03
<i>n</i> -butylamino	<b>6c</b>	7.42	8.23	5.90	<b>7c</b>	7.49	8.31	5.75
2-methylaziridinyl	<b>6e</b>	7.46	8.28	5.95	<b>7e</b>	7.52	8.29	5.79
<i>c</i> -hexylamino	<b>6f</b>	7.37	8.19	5.88	<b>7f</b>	7.46	8.26	5.74
<i>c</i> -pentylamino	<b>6g</b>	7.36	8.18	5.87	<b>7g</b>	7.43	8.23	5.70
<i>t</i> -butylamino	<b>6h</b>	7.37	8.18	6.09	<b>7h</b>	7.50	8.30	5.99

**6,7-dipiperidinyl-2-methylquinoline-5,8-dione (8a).** **3** (812 mg, 2.45 mmol) was dissolved in neat piperidine (15 mL) in a two-neck flask (200 mL). The mixture was heated from rt to reflux and retained in refluxing for 10 min. The mixture was concentrated *in vacuo* and extracted with EtOAc. The organic layer was dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated *in vacuo*. The residue was purified by flash column chromatography (20% EtOAc/hexane) to give **8a** (457 mg, 1.35 mmol, 55%, a dark-violet solid), **7a** (108 mg, 0.42 mmol, 17%, a yellow solid), and **6a** (104 mg, 0.41 mmol, 16%, a yellow solid). **8a**: mp 185 °C dec; <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) . 8.14 (d, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 3.31 (s, 8H), 2.70 (s, 3H), 1.67 (s, 12H); <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) . 181.1, 180.6, 161.7, 145.5, 142.7, 139.9, 132.2, 124.9, 124.5, 50.5, 50.3, 25.0, 23.3, 22.73, 22.70; MS (EI) 339 (M<sup>+</sup>), 332, 296, 282 (100), 272, 255, 240, 227, 215, 190, 84, 88, 41. HRMS (EI) m/z 339.1967, calcd for C<sub>20</sub>H<sub>25</sub>N<sub>3</sub>O<sub>2</sub> 339.1947.