

## Supplementary Materials

# Design, Synthesis, and Bioactivity of Novel Quinazolinone Scaffolds Containing Pyrazole Carbamide Derivatives as Anti-fungal Agents

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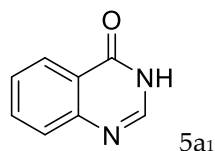
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### Instruments and Chemicals

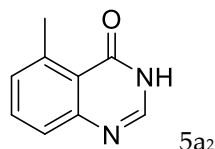
<sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded in CDCl<sub>3</sub> or DMSO-*d*<sub>6</sub> using 600 and 150 MHz spectrophotometers (Bruker BioSpin GmbH, Rheinstetten, Germany), respectively. All solvents were distilled and dried using standard methods before use.

### General procedure for the preparation of quinazolin-4-ones (5a<sub>1</sub>-a<sub>32</sub>)

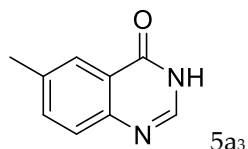
Anthranilic acid or its substituted derivatives (10 mmol) were mixed with formamidine acetate (20 mmol) in ethylene glycol monomethyl ether and the reaction mixture was subsequently stirred at 95–130°C. The mixture was then poured into cold water, thereby precipitating a large amount of solid. The crude product was subsequently obtained by filtration and was dissolved in a hot 10% NaOH solution, heated for 5–6 minutes with charcoal, and filtered, and the clear solution was subsequently neutralized (pH=7) using 1N HCl. The precipitated crystals were filtered out, washed with cooled water, and dried to obtain the quinazolin-4-ones.



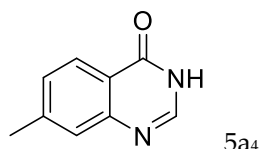
quinazolin-4(3*H*)-one, white solid, yield 86%, 217.5–218.3°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.24 (s, 1H), 8.12 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.09 (s, 1H), 7.81 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.68–7.63 (m, 1H), 7.52 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.73, 148.77, 145.39, 134.32, 127.24, 126.75, 125.84, 122.64. HRMS (ESI): calculated for C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 147.05529, found: 147.05556.



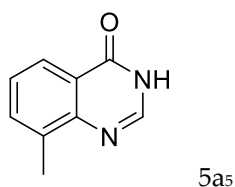
5-methylquinazolin-4(3*H*)-one, white solid, yield 86%, 223.5–224.9 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.01 (s, 1H), 7.99 (s, 1H), 7.60 (dd, *J* = 7.7 Hz, 1H), 7.49–7.43 (m, 1H), 7.23 (dt, *J* = 7.4, 1.1 Hz, 1H), 2.76 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 161.67, 150.32, 145.14, 140.03, 133.29, 128.96, 125.34, 22.55. HRMS (ESI): calculated for C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 161.07094, found: 161.07095.



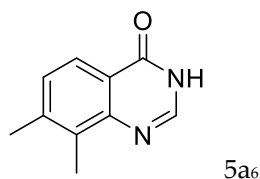
6-methylquinazolin-4(3H)-one, white solid, yield 85%, 259.8-259.9°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.15 (s, 1H), 8.02 (s, 1H), 7.91 (d, *J* = 2.0 Hz, 1H), 7.62 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 2.43 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.73, 146.79, 144.58, 136.51, 135.65, 127.14, 125.24, 122.40, 20.85. HRMS (ESI): calculated for C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 161.07094, found: 161.07095.



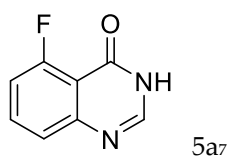
7-methylquinazolin-4(3H)-one, white solid, yield 81%, 243.1-244.5°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.14 (s, 1H), 8.05 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.46 (s, 1H), 7.33 (dd, *J* = 8.0, 1.6 Hz, 1H), 2.44 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.63, 148.90, 145.43, 144.81, 128.15, 126.88, 125.70, 120.24, 21.32. HRMS (ESI): calculated for C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 161.07094, found: 161.07095.



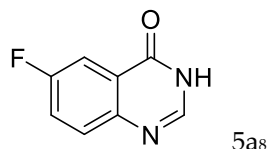
8-methylquinazolin-4(3H)-one, white solid, yield 82%, 255.8-256.9°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.22 (s, 1H), 8.10 (s, 1H), 7.95 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 2.51 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 161.16, 147.30, 144.45, 135.47, 134.82, 126.33, 123.59, 122.63, 17.36. HRMS (ESI): calculated for C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 161.07094, found: 161.07095.



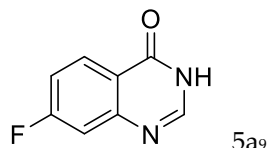
7,8-dimethylquinazolin-4(3H)-one, White solid, yield 83%, 261.0-262.8°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.10 (s, 1H), 8.06 (d, *J* = 2.5 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 2.44 (s, 3H), 2.36 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 161.19, 146.97, 144.18, 142.93, 133.43, 128.45, 122.74, 120.54, 20.56, 13.01. HRMS (ESI): calculated for C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 175.08659, found: 175.08668.



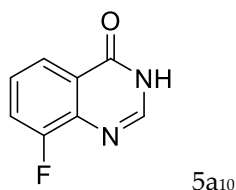
5-fluoroquinazolin-4(3H)-one, white solid, yield 77%, 291.7-292.6°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.27 (s, 1H), 8.07 (s, 1H), 7.76 (td, *J* = 8.2, 5.5 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.24 (dd, *J* = 11.1, 8.2, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.41 (d, *J* = 263.0 Hz), 158.02, 150.95, 146.41, 134.90 (d, *J* = 10.3 Hz), 123.31, 113.11 (d, *J* = 20.0 Hz), 112.12 (d, *J* = 6.0 Hz). HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>FN<sub>2</sub>O [M+H]<sup>+</sup>: 165.04587, found: 165.04592.



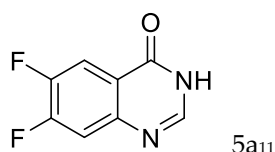
6-fluoroquinazolin-4(3*H*)-one, white solid, yield 78%, 253.4-258.6°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.36 (s, 1H), 8.07 (s, 1H), 7.76 (dd, *J* = 8.6, 3.0 Hz, 1H), 7.73 (dd, *J* = 8.9, 5.0 Hz, 1H), 7.67 (td, *J* = 8.6, 3.0 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.11 (ds, *J* = 245.6 Hz), 160.25, 145.69, 144.90, 130.16 (d, *J* = 8.4 Hz), 123.92 (d, *J* = 8.5 Hz), 122.85 (d, *J* = 24.2 Hz), 110.53 (d, *J* = 23.5 Hz). HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>FN<sub>2</sub>O [M+H]<sup>+</sup>: 165.04587, found: 165.04592.



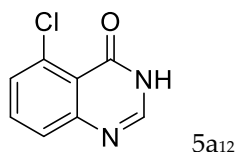
7-fluoroquinazolin-4(3*H*)-one, white solid, yield 81%, 246.2-247.2°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.34 (s, 1H), 8.17 (dd, *J* = 8.8, 6.3 Hz, 1H), 8.13 (s, 1H), 7.44 (dd, *J* = 10.2, 2.6 Hz, 1H), 7.38 (td, *J* = 8.8, 2.6 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 165.57 (d, *J* = 250.6 Hz), 160.05, 150.96 (d, *J* = 12.5 Hz), 146.86, 129.00 (d, *J* = 11.1 Hz), 119.65, 115.31 (d, *J* = 23.6 Hz), 112.34 (d, *J* = 21.5 Hz). HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>FN<sub>2</sub>O [M+H]<sup>+</sup>: 165.04587, found: 165.04592.



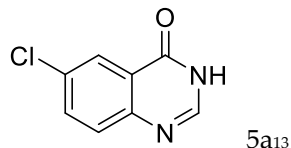
8-fluoroquinazolin-4(3*H*)-one, white solid, yield 75%, 274.5-274.6°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.45 (s, 1H), 8.14 (s, 1H), 7.94 – 7.90 (m, 1H), 7.67 (ddd, *J* = 10.7, 8.0, 1.3 Hz, 1H), 7.50 (td, *J* = 8.0, 4.8 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.85 (d, *J* = 3.5 Hz), 156.48 (d, *J* = 253.4 Hz), 146.03, 137.96 (d, *J* = 11.3 Hz), 127.01 (d, *J* = 7.7 Hz), 124.67, 121.60 (d, *J* = 3.7 Hz), 119.77 (d, *J* = 18.6 Hz). HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>FN<sub>2</sub>O [M+H]<sup>+</sup>: 165.04587, found: 165.04592.



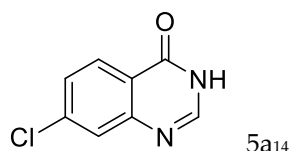
6,7-difluoroquinazolin-4(3*H*)-one, white solid, yield 83%, 259.3-260.9°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.47 (s, 1H), 8.13 (s, 1H), 8.00 (dd, *J* = 10.4, 8.7 Hz, 1H), 7.72 (dd, *J* = 11.4, 7.3 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.50, 153.75 (dd, *J* = 253.7, 13.6 Hz), 148.54 (dd, *J* = 249.1, 13.6 Hz), 146.82 (d, *J* = 11.1 Hz), 146.36, 119.93 (d, *J* = 6.1 Hz), 115.27 (d, *J* = 17.4 Hz), 113.39 (d, *J* = 18.7 Hz). HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>F<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 183.03645, found: 183.03604.



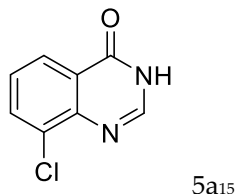
5-chloroquinazolin-4(3*H*)-one, white solid, yield 68%, 207.7-209.0°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.29 (s, 1H), 8.07 (s, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 7.60 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.52 (dd, *J* = 7.8, 1.2 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.00, 151.31, 146.28, 134.24, 132.42, 129.25, 126.89, 119.63. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup>: 181.01632, found: 181.01650.



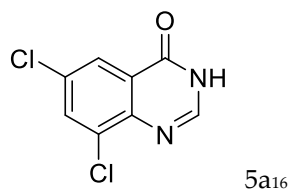
6-chloroquinazolin-4(3*H*)-one, white solid, yield 71%, 269.8-271.1°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.42 (s, 1H), 8.10 (s, 1H), 8.01 (d, *J* = 2.5 Hz, 1H), 7.80 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.86, 147.53, 145.94, 134.50, 131.13, 129.57, 124.89, 123.92. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup>: 181.01632, found: 181.01650.



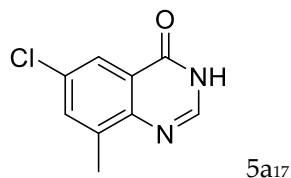
7-chloroquinazolin-4(3*H*)-one, white solid, yield 69%, 251.0-253.0°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.36 (s, 1H), 8.11 (s, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.64 (d, *J* = 2.1 Hz, 1H), 7.48 (dd, *J* = 8.5, 2.1 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.24, 149.87, 146.92, 138.98, 127.97, 127.04, 126.40, 121.47. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup>: 181.01632, found: 181.01650.



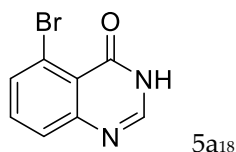
8-chloroquinazolin-4(3*H*)-one, white solid, yield 71%, 305.5-307.2°C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.50 (s, 1H), 8.21 (s, 1H), 8.07 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.95 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.24, 146.38, 145.23, 134.46, 130.82, 127.10, 125.03, 124.36. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup>: 181.01632, found: 181.01650.



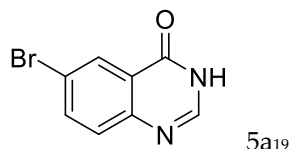
6,8-dichloroquinazolin-4(3*H*)-one, white solid, yield 68%, >310 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.68 (s, 1H), 8.24 (s, 1H), 8.12 (s, 1H), 8.02 (s, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.32, 146.81, 144.27, 134.04, 132.38, 130.72, 125.05, 124.18. HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>Cl<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 214.97734, found: 214.97717.



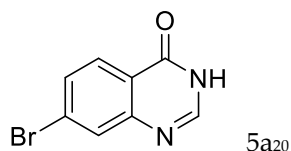
**6-chloro-8-methylquinazolin-4(3H)-one**, white solid, yield 59%, >310 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.42 (s, 1H), 8.13 (s, 1H), 7.88 (d, *J* = 2.5 Hz, 1H), 7.73 (d, *J* = 2.5 Hz, 1H), 2.51 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.16, 146.16, 144.99, 138.58, 134.47, 130.54, 123.79, 122.40, 17.08. HRMS (ESI): calculated for C<sub>9</sub>H<sub>7</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup>: 195.03197, found: 195.03183.



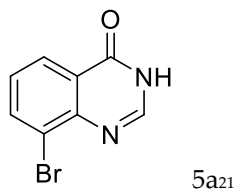
**5-bromoquinazolin-4(3H)-one**, white solid, yield 68%, 243.6-243.7 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.31 (s, 1H), 8.08 (s, 1H), 7.72 (dd, *J* = 6.9, 2.1 Hz, 1H), 7.66 -7.58 (m, 2H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.01, 151.12, 145.96, 134.44, 132.91, 127.51, 120.49, 119.91. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup>: 224.96580, found: 224.96560.



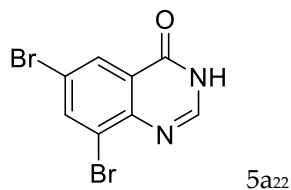
**6-bromoquinazolin-4(3H)-one**, white solid, yield 41%, 270.6-271.9 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.42 (s, 1H), 8.16 (d, *J* = 2.4 Hz, 1H), 8.12 (s, 1H), 7.93 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.75, 147.74, 146.10, 137.24, 129.66, 128.02, 127.93, 124.26, 119.30. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup>: 224.96580, found: 224.96560.



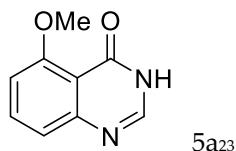
**7-bromoquinazolin-4(3H)-one**, white solid, yield 57%, 270.6-271.9 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.38 (s, 1H), 8.11 (s, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 2.0 Hz, 1H), 7.65 (dd, *J* = 8.5, 2.0 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.42, 149.94, 146.92, 129.88, 129.50, 128.04, 127.99, 121.78. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup>: 224.96580, found: 224.96560.



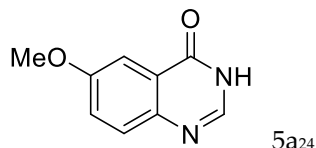
**8-bromoquinazolin-4(3H)-one**, white solid, yield 63%, >310 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.50 (s, 1H), 8.21 (s, 1H), 8.12 (td, *J* = 7.5, 1.4 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.25, 146.46, 146.24, 137.78, 127.61, 125.73, 124.27, 121.84. HRMS (ESI): calculated for C<sub>8</sub>H<sub>5</sub>BrN<sub>2</sub>O [M+H]<sup>+</sup>: 224.96580, found: 224.96560.



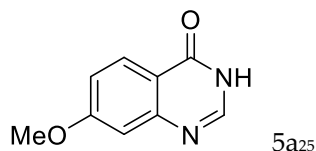
6,8-dibromoquinazolin-4(3H)-one, white solid, yield 48%, >310 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.67 (s, 1H), 8.35 (s, 1H), 8.24 (s, 1H), 8.18 (s, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.33, 147.02, 145.60, 139.65, 127.95, 125.26, 123.44, 119.11. HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>Br<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 302.87632, found: 302.87534.



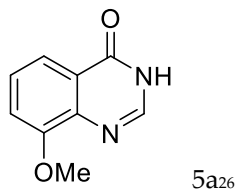
5-methoxyquinazolin-4(3H)-one, white solid, yield 72%, 210.5 - 211.2 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 11.91 (s, 1H), 7.95 (s, 1H), 7.66 (t-like, *J* = 8.2 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 3.84 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.77, 159.04, 151.35, 145.83, 134.75, 119.12, 112.34, 108.46, 56.06. HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>Br<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 302.87632, found: 302.87534.



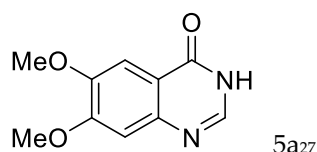
6-methoxyquinazolin-4(3H)-one, white solid, yield 70%, 246.6-247.9 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.18 (s, 1H), 7.98 (s, 1H), 7.62 (d, *J* = 8.9 Hz, 1H), 7.50 (d, *J* = 3.0 Hz, 1H), 7.41 (dd, *J* = 8.9, 3.0 Hz, 1H), 3.87 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.52, 157.74, 143.21, 143.10, 128.94, 123.75, 123.45, 105.82, 55.61. HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>Br<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 302.87632, found: 302.87534.



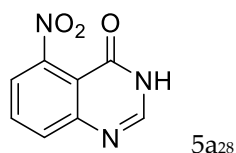
7-methoxyquinazolin-4(3H)-one, white solid, yield 67%, 263.8-263.9 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.09 (s, 1H), 8.05 (s, 1H), 8.01 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.11 – 7.06 (m, 2H), 3.88 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 163.92, 160.29, 151.02, 146.00, 127.46, 116.19, 116.03, 108.40, 55.69. HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>Br<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 302.87632, found: 302.87534.



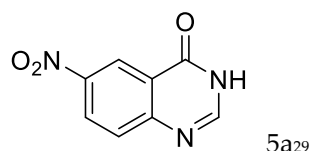
8-methoxyquinazolin-4(3H)-one, white solid, yield 89%, 296.6 - 297.9 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.25 (s, 1H), 8.02 (s, 1H), 7.66 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.44 (dd, *J* = 8.0 Hz, 1H), 7.36 (dd, *J* = 8.0, 1.3 Hz, 1H), 3.89 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.61, 154.54, 143.94, 139.27, 127.03, 123.68, 116.78, 114.93, 55.96. HRMS (ESI): calculated for C<sub>8</sub>H<sub>4</sub>Br<sub>2</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 302.87632, found: 302.87534.



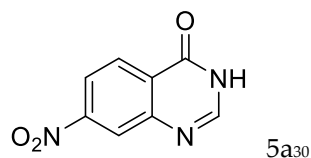
7,8-dimethoxyquinazolin-4(3H)-one, white solid, yield 80%, 264.3-268.3 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.07 (s, 1H), 7.98 (s, 1H), 7.43 (s, 1H), 7.12 (s, 1H), 3.89 (s, 3H), 3.86 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.15, 154.52, 148.62, 144.92, 143.90, 115.64, 108.05, 104.96, 55.99, 55.75. HRMS(ESI): calculated for C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 207.07642, found: 207.07626.



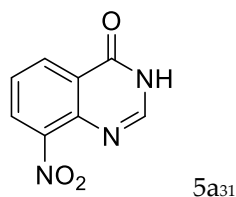
5-nitroquinazolin-4(3H)-one, red brown solid, yield 39%, 253.2-255.1 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.74 (s, 1H), 8.23 (s, 1H), 7.98-7.93 (m, 1H), 7.88 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.81 (dd, *J* = 7.6, 1.2 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 157.43, 149.70, 148.18, 147.22, 134.66, 130.06, 120.50, 113.06. HRMS(ESI): calculated for C<sub>8</sub>H<sub>5</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 192.04037, found: 192.04003.



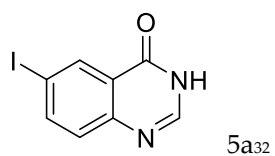
6-nitroquinazolin-4(3H)-one, light yellow solid, yield 42%, 283.6-284.2 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.73 (s, 1H), 8.75 (d, *J* = 2.7 Hz, 1H), 8.51 (dd, *J* = 8.9, 2.7 Hz, 1H), 8.28 (s, 1H), 7.82 (d, *J* = 8.9 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 160.11, 153.00, 148.91, 145.02, 129.15, 128.32, 122.73, 121.96. HRMS(ESI): calculated for C<sub>8</sub>H<sub>5</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 192.04037, found: 192.04003.



7-nitroquinazolin-4(3H)-one, red brown solid, yield 71%, 266.9-267.3 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.66 (s, 1H), 8.35 (d, *J* = 2.3 Hz, 1H), 8.32 (d, *J* = 8.7 Hz, 1H), 8.25 (s, 1H), 8.22 (dd, *J* = 8.7, 2.3 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.83, 151.04, 149.14, 147.73, 128.20, 126.98, 122.21, 120.35. HRMS(ESI): calculated for C<sub>8</sub>H<sub>5</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 192.04037, found: 192.04003.



8-nitroquinazolin-4(3H)-one, red brown solid, yield 49%, 216.9-217.3 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.70 (s, 1H), 8.34 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.27 (dd, *J* = 7.8, 1.5 Hz, 1H), 8.24 (s, 1H), 7.65 (t-like, *J* = 8.0 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.33, 148.16, 146.66, 140.47, 129.56, 127.74, 126.42, 124.04. HRMS(ESI): calculated for C<sub>8</sub>H<sub>5</sub>N<sub>3</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 192.04037, found: 192.04003.



6-iodoquinazolin-4(3H)-one, white solid, yield 88%, 271.7-273.2 °C. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 12.40 (s, 1H), 8.37 (d, *J* = 2.1 Hz, 1H), 8.12 (s, 1H), 8.08 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.45 (d, *J* = 8.5 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ 159.53, 148.03, 146.15, 142.74, 134.19, 129.45, 124.46, 91.86. HRMS(ESI): calculated for C<sub>8</sub>H<sub>5</sub>IN<sub>2</sub>O [M+H]<sup>+</sup>: 272.95193, found: 272.95200.