

## Supplementary Material To

### PEG mediated synthesis of 6-pyrazinyl- / fused pyrazinylquinazolin-4(3H)-ones using Castro-Stephen coupling, oxidation and cyclocondensation reactions

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#### ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

*3-Methyl-2-phenyl-6-(phenylethynyl)quinazolin-4(3H)-one (5)*: Yield (0.69g, 75%), mp 151-153 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 8.49 (d, *J* = 1.80 Hz, 1H, Ar-H), 7-85 (dd, *J* = 2.44 Hz, 8.24 Hz, 1H, Ar-H), 7.70-7.71 (m, 1H, Ar-H), 7.53-7.57 (m, 7H, Ar-H), 7.35-7.38 (m, 3H, Ar-H), 3.51 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>) δ 161.9, 156.5, 146.7, 136.8, 135.1, 131.6, 130.1, 129.9, 128.8, 128.5, 128.3, 127.9, 127.6, 122.7, 122.0, 120.4, 90.9, 88.4, 34.3; IR (KBr) 2200, 1666 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> *m/z* 337.1327.

*1-(3-Methyl-4-oxo-2-phenyl-3,4-dihydroquinazolin-6-yl)-2-phenylethane-1,2-dione (6)*: Yield (70mg, 80%); mp 161-163 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 8.84 (d, 1H, *J* = 1.18 Hz, Ar-H), 8.40 (dd, *J* = 1.98 Hz, 8.5Hz, 1H, Ar-H), 8.01 (dd, *J* = 1.06 Hz, 8.24 Hz, 2H, Ar-H), 7.85(d, 1H, *J* = 8.54 Hz, Ar-H), 7.66-7.68 (m, 1H, Ar-H), 7.52-7.60 (m, 7H, Ar-H), 3.51 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>) δ 193.6, 192.7, 161.8, 158.9, 151.3, 134.9, 134.6, 132.6, 130.8, 130.5, 129.8, 128.9, 128.8, 128.5, 127.8, 120.2, 34.4; IR (KBr) 1774, 1709, 1677cm<sup>-1</sup>; HRMS: [M+H]<sup>+</sup> *m/z* 369.1235.

*3-Methyl-2-phenyl-6-(3-phenylquinoxalin-2-yl)quinazolin-4(3H)-one (8)*: White powder, mp 219-220 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 8.61 (s, 1H, Ar-H), 8.19-8.21 (m, 2H, Ar-H), 7.79-7.84 (m, 3H, Ar-H), 7.54 - 7.65 (m, 8H, Ar-H), 7.34 -7.39 (m, 3H, Ar-H), 3.49 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>) δ 162.3, 156.9, 153.3, 151.2, 147.3, 141.2, 138.7, 137.8, 135.5, 130.2, 130.1, 129.8, 129.2, 129.1, 128.8, 128.5, 128.1, 127.3, 120.3, 34.3; IR (KBr)

33 3062, 1674 cm<sup>-1</sup>. ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>29</sub>H<sub>21</sub>N<sub>4</sub>O: *m/z* 441.1715; found at *m/z*  
34 441.1706.

35 *3-Methyl-2-phenyl-6-(3-phenylpyrazin-2-yl)quinazolin-4(3H)-one (10)*: White powder, mp  
36 180-181 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 8.66 (s, 2H, Ar-H), 8.50 (d, *J* = 2.3 Hz, 1H, Ar-  
37 H), 7.78 (dd, *J* = 2.26 Hz, 8.30 Hz, 1H, Ar-H), 7.45-7.64 (m, 8H, Ar-H), 7.31-7.34 (m, 3H,  
38 Ar-H), 3.48 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>) δ 162.2, 156.9, 152.9, 151.4, 147.3,  
39 142.5, 142.2, 138.1, 137.4, 135.3, 130.2, 129.6, 128.9, 128.5, 128.2, 127.9, 127.3, 120.5, 34.3;  
40 IR (KBr) 3057, 2924, 1680 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>15</sub>H<sub>19</sub>N<sub>4</sub>O: *m/z*  
41 391.1558; found at *m/z* 391.1548.

42 *6-(6-Bromo-3-phenylquinoxalin-2-yl)-3-methyl-2-phenylquinazolin-4(3H)-one (12a or*  
43 *12a')*: White powder, mp 240-242 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 9.18 (d, *J* = 2.5 Hz, 1H,  
44 Ar-H), 8.71 (d, *J* = 2.5 Hz, 1H, Ar-H), 8.67 (d, *J* = 1.9 Hz, 1H, Ar-H), 7.84 (dd, *J* = 2.07 Hz,  
45 8.5 Hz, 1H, Ar-H), 7.56 - 7.67 (m, 9H, Ar-H), 7.39 - 7.30 (m, 3H, Ar-H), 3.51 (s, 3H, N-  
46 CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>) δ 162.3, 157.5, 153.7, 152.7, 147.7, 141.9, 140.0, 138.4,  
47 137.3, 135.5, 135.2, 133.9, 131.5, 130.5, 130.3, 129.8, 129.3, 128.9, 128.6, 127.9, 127.5,  
48 12.1, 120.5, 34.4; IR (KBr) 3060, 1682 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for  
49 C<sub>29</sub>H<sub>20</sub>N<sub>4</sub>OBr: *m/z* 519.0820; found at *m/z* 519.0822.

50 *6-(6-Chloro-3-phenylquinoxalin-2-yl)-3-methyl-2-phenylquinazolin-4(3H)-one (12b or 12b')*:  
51 White powder, mp 215-217 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 8.58 (d, *J* = 8.4 Hz, 1H, Ar-H),  
52 8.20 (d, *J* = 2.29 Hz, 1H, Ar-H), 8.14 (d, *J* = 9.1 Hz, 1H, Ar-H), 7.82 (dd, *J* = 2.1 Hz, 9.0  
53 Hz, 1H, Ar-H), 7.73 (dd, *J* = 2.28 Hz, 8.85 Hz, 1H, Ar-H), 7.64-7.65 (m, 1H, Ar-H), 7.53 -  
54 7.59 (m, 7H, Ar-H), 7.35 - 7.40 (m, 3H, Ar-H), 3.50 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz,  
55 CDCl<sub>3</sub>) δ 162.2, 157.0, 153.7, 152.7, 147.5, 141.7, 140.2, 138.3, 137.2, 135.3, 135.4, 133.8,  
56 131.5, 130.5, 130.2, 129.8, 129.7, 129.3, 128.9, 128.6, 127.9, 127.4, 124.0, 120.4, 34.4;  
57 IR(KBr) 3060, 2923, 1682 Cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>29</sub>H<sub>20</sub>N<sub>4</sub>OCl: *m/z*  
58 475.1325; found at *m/z* 475.1332.

59 *3-Methyl-6-(5-nitro-3-phenylquinoxalin-2-yl)-2-phenylquinazolin-4(3H)-one (12c or 12c')*:  
60 Yellow powder, mp 247-249 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>) δ 8.46 (d, *J* = 2 Hz, 1H, Ar-H),  
61 8.41 (dd, *J* = 1.06 Hz, 8.5 Hz, 1H, Ar-H), 8.20 (dd, *J* = 1.22 Hz, 7.6 Hz, 1H, Ar-H), 8.10 (dd,  
62 *J* = 2.13 Hz, 8.5 Hz, 1H, Ar-H), 7.83-7.86 (m, 1H, Ar-H), 7.73 (d, *J* = 8.39 Hz, 1H, Ar-H),  
63 7.54-7.61 (m, 7H, Ar-H), 7.39-7.46 (m, 3H, Ar-H), 3.47 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz,

CDCl<sub>3</sub>)  $\delta$  162.1, 157.3, 154.9, 153.5, 148.1, 147.1, 140.9, 137.9, 136.2, 135.7, 135.7, 135.2, 133.8, 133.2, 130.3, 129.9, 129.7, 129.1, 128.9, 128.7, 128.4, 128.0, 127.8, 124.6, 120.2, 34.5; IR(KBr) 3056, 2923, 1673 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>29</sub>H<sub>20</sub>N<sub>5</sub>O<sub>3</sub>:  $m/z$  486.1566; found at  $m/z$  486.1552.

*3-Methyl-6-(6-nitro-3-phenylquinoxalin-2-yl)-2-phenylquinazolin-4(3H)-one (12d or 12d')*: Yellow powder, mp 252-254 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)  $\delta$  9.10 (d,  $J$  = 2.3 Hz, 1H, Ar-H), 8.61 (d,  $J$  = 1.2 Hz, 1H, Ar-H), 8.56 (dd,  $J$  = 2.44 Hz, 9.15 Hz, 1H, Ar-H), 8.31-8.32 (m, 1 H, Ar-H), 7.88 (dd,  $J$  = 2.13 Hz, 8.7 Hz, 1H, Ar-H), 7.54-7.60 (m, 1H, Ar-H), 7.54-7.55 (m, 7 H, Ar-H), 7.37-7.41 (m, 3H, Ar-H), 3.51 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)  $\delta$  162.2, 157.4, 156.2, 154.2, 148.1, 143.6, 140.1, 137.7, 136.6, 135.1, 130.8, 130.3, 130.1, 129.8, 128.9, 128.7, 128.1, 128.0, 127.6, 125.6, 123.6, 120.5, 34.4; IR (KBr) 3056, 2923, 1673 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>29</sub>H<sub>20</sub>N<sub>5</sub>O<sub>3</sub>:  $m/z$  486.1566; found at  $m/z$  486.1552.

*3-Methyl-2-phenyl-6-(2-phenylpyrido[2,3-b]pyrazin-3-yl)quinazolin-4(3H)-one (12e or 12e')*: White powder, mp 238-240 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)  $\delta$  9.21 (d,  $J$  = 2.3 Hz, 1H, Ar-H), 8.71 (d,  $J$  = 7.13 Hz, 1H, Ar-H), 8.56-8.69 (m, 3H, Ar-H), 7.55-7.67 (m, 8H, Ar-H), 7.33-7.41 (m, 3H, Ar-H), 3.51 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)  $\delta$  162.2, 157.1, 156.1, 154.3, 153.1, 149.7, 147.7, 138.1, 137.7, 137.1, 136.2, 135.1, 130.2, 129.6, 128.8, 128.6, 128.4, 127.3, 127.2, 125.3, 120.4, 34.3; IR (KBr) 3060, 2922, 1672 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>28</sub>H<sub>20</sub>N<sub>5</sub>O:  $m/z$  442.1667; found at  $m/z$  442.1650.

*6-(7-Bromo-2-phenylpyrido[2,3-b]pyrazin-3-yl)-3-methyl-2-phenylquinazolin-4(3H)-one (12f or 12f')*: White powder, mp 148-149 °C. <sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)  $\delta$  8.58 (d,  $J$  = 1.91 Hz, 1H, Ar-H), 8.38 (d,  $J$  = 2.1 Hz, 1H, Ar-H), 8.05 (d, 1H, Ar-H), 7.81-7.89 (m, 2H, Ar-H), 7.53-7.67 (m, 7H, Ar-H), 7.33-7.41 (m, 3H, Ar-H), 3.50 (s, 3H, N-CH<sub>3</sub>); <sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)  $\delta$  162.1, 157.3, 156.3, 155.4, 154.0, 148.1, 147.8, 139.4, 137.4, 136.7, 136.4, 135.3, 135.0, 130.3, 130.1, 130.1, 129.0, 12.7, 128.4, 128.0, 127.4, 121.1, 120.5, 34.4; IR (KBr) 3060, 2924, 1682 cm<sup>-1</sup>; ESI-HRMS: [M+H]<sup>+</sup> calculated for C<sub>28</sub>H<sub>19</sub>N<sub>5</sub>OBr:  $m/z$  520.0772; found at  $m/z$  520.0795.