



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: 0.69 g (75 %); mp 151–153 °C; IR (KBr, cm⁻¹): 2200, 1666; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 8.49 (1H, *d*, *J* = 1.80 Hz, Ar-H), 7.85 (1H, *dd*, *J* = 2.44 Hz & 8.24 Hz, Ar-H), 7.70–7.71 (1H, *m*, Ar-H), 7.53–7.57 (7H, *m*, Ar-H), 7.35–7.38 (3H, *m*, Ar-H), 3.51 (3H, *s*, N–CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 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; ESI-HRMS: [M+H]⁺ (*m/z*): 337.1327.

1-(3-Methyl-4-oxo-2-phenyl-3,4-dihydroquinazolin-6-yl)-2-phenylethane-1,2-dione (6): Yield: 70 mg (80 %); m.p.: 161–163 °C; IR (KBr, cm⁻¹): 1774, 1709, 1677; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 8.84 (1H, *d*, *J* = 1.18 Hz, Ar-H), 8.40 (1H, *dd*, *J* = 1.98 Hz & *J* = 8.5 Hz, Ar-H), 8.01 (2H, *dd*, *J* = 1.06 Hz & *J* = 8.24 Hz, Ar-H), 7.85 (1H, *d*, *J* = 8.54 Hz, Ar-H), 7.66–7.68 (1H, *m*, Ar-H), 7.52–7.60 (7H, *m*, Ar-H), 3.51 (3H, *s*, N–CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 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; HRMS: [M+H]⁺ (*m/z*): 369.1235.

3-Methyl-2-phenyl-6-(3-phenylquinoxalin-2-yl)quinazolin-4(3H)-one (8). White powder; m.p.: 219–220 °C; IR (KBr, cm⁻¹): 3062, 1674; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 8.61 (1H, *s*, Ar-H), 8.19–8.21 (2H, *m*, Ar-H), 7.79–7.84 (3H, *m*, Ar-H), 7.54–7.65 (8H, *m*, Ar-H), 7.34–7.39 (3H, *m*, Ar-H), 3.49 (3H, *s*,

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N-CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 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; ESI-HRMS: [M+H]⁺ (m/z): calcd. for C₂₉H₂₁N₄O: 441.1715. Found: 441.1706.

3-Methyl-2-phenyl-6-(3-phenylpyrazin-2-yl)quinazolin-4(3H)-one (10). White powder, m.p.: 180–181 °C; IR (KBr, cm⁻¹): 3057, 2924, 1680; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 8.66 (2H, s, Ar-H), 8.50 (1H, d, J = 2.3 Hz, Ar-H), 7.78 (1H, dd, J = 2.26 Hz & J = 8.30 Hz, Ar-H), 7.45–7.64 (8H, m, Ar-H), 7.31–7.34 (3H, m, Ar-H), 3.48 (3H, s, N-CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 162.2, 156.9, 152.9, 151.4, 147.3, 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; ESI-HRMS: [M+H]⁺ (m/z): calcd. for C₁₅H₁₉N₄O: 391.1558. Found: 391.1548.

6-(6-Bromo-3-phenylquinoxalin-2-yl)-3-methyl-2-phenylquinazolin-4(3H)-one (12a or 12a'). White powder; m.p.: 240–242 °C; IR (KBr) 3060, 1682 cm⁻¹; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 9.18 (1H, d, J = 2.5 Hz, Ar-H), 8.71 (1H, d, J = 2.5 Hz, Ar-H), 8.67 (1H, d, J = 1.9 Hz, Ar-H), 7.84 (1H, dd, J = 2.07 Hz & J = 8.5 Hz, Ar-H), 7.56–7.67 (9H, m, Ar-H), 7.39–7.30 (3H, m, Ar-H), 3.51 (3H, s, N-CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 162.3, 157.5, 153.7, 152.7, 147.7, 141.9, 140.0, 138.4, 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, 12.1, 120.5, 34.4; ESI-HRMS: [M+H]⁺ (m/z): calcd. for C₂₉H₂₀N₄OBr: 519.0820. Found: 519.0822.

6-(6-Chloro-3-phenylquinoxalin-2-yl)-3-methyl-2-phenylquinazolin-4(3H)-one (12b or 12b'). White powder; m.p.: 215–217 °C; IR (KBr, cm⁻¹): 3060, 2923, 1682; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 8.58 (1H, d, J = 8.4 Hz, Ar-H), 8.20 (1H, d, J = 2.29 Hz, Ar-H), 8.14 (1H, d, J = 9.1 Hz, Ar-H), 7.82 (1H, dd, J = 2.1 Hz & J = 9.0 Hz, Ar-H), 7.73 (1H, dd, J = 2.28 Hz & J = 8.85 Hz, Ar-H), 7.64–7.65 (1H, m, Ar-H), 7.53–7.59 (7H, m, Ar-H), 7.35–7.40 (3H, m, Ar-H), 3.50 (3H, s, N-CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 162.2, 157.0, 153.7, 152.7, 147.5, 141.7, 140.2, 138.3, 137.2, 135.3, 135.4, 133.8, 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; ESI-HRMS: [M+H]⁺ (m/z): calcd. for C₂₉H₂₀N₄OCl: 475.1325. Found: 475.1332.

3-Methyl-6-(5-nitro-3-phenylquinoxalin-2-yl)-2-phenylquinazolin-4(3H)-one (12c or 12c'). Yellow powder; m.p.: 247–249 °C; IR (KBr, cm⁻¹): 3056, 2923, 1673; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 8.46 (1H, d, J = 2 Hz, Ar-H), 8.41 (1H, dd, J = 1.06 Hz & J = 8.5 Hz, Ar-H), 8.20 (1H, dd, J = 1.22 Hz & J = 7.6 Hz, Ar-H), 8.10 (1H, dd, J = 2.13 Hz & J = 8.5 Hz, Ar-H), 7.83–7.86 (1H, m, Ar-H), 7.73 (1H, d, J = 8.39 Hz, Ar-H), 7.54–7.61 (7H, m, Ar-H), 7.39–7.46 (3H, m, Ar-H), 3.47 (3H, s, N-CH₃); ¹³C-NMR (75 MHz, CDCl₃, δ / ppm): 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; ESI-HRMS: $[M+H]^+$ (m/z): calcd. for $C_{29}H_{20}N_5O_3$: 486.1566. Found: 486.1552.

3-Methyl-6-(6-nitro-3-phenylquinoxalin-2-yl)-2-phenylquinazolin-4(3H)-one (12d or 12d'). Yellow powder; m.p.: 252–254 °C; IR (KBr, cm^{-1}): 3056, 2923, 1673; 1H -NMR (300 MHz, $CDCl_3$, δ / ppm): 9.10 (1H, *d*, $J = 2.3$ Hz, Ar-H), 8.61 (1H, *d*, $J = 1.2$ Hz, Ar-H), 8.56 (1H, *dd*, $J = 2.44$ Hz & $J = 9.15$ Hz, Ar-H), 8.31–8.32 (1H, *m*, Ar-H), 7.88 (1H, *dd*, $J = 2.13$ Hz & $J = 8.7$ Hz, Ar-H), 7.54–7.60 (1H, *m*, Ar-H), 7.54–7.55 (7H, *m*, Ar-H), 7.37–7.41 (3H, *m*, Ar-H), 3.51 (3H, *s*, N-CH₃); ^{13}C NMR (75 MHz, $CDCl_3$, δ / ppm): 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; ESI-HRMS: $[M+H]^+$ (m/z): calcd. for $C_{29}H_{20}N_5O_3$: 486.1566. Found: 486.1552.

3-Methyl-2-phenyl-6-(2-phenylpyrido[2,3-b]pyrazin-3-yl)quinazolin-4(3H)-one (12e or 12e'). White powder; m.p.: 238–240 °C; IR (KBr, cm^{-1}): 3060, 2922, 1672; 1H -NMR (300 MHz, $CDCl_3$, δ / ppm): 9.21 (1H, *d*, $J = 2.3$ Hz, Ar-H), 8.71 (1H, *d*, $J = 7.13$ Hz, Ar-H), 8.56–8.69 (3H, *m*, Ar-H), 7.55–7.67 (8H, *m*, Ar-H), 7.33–7.41 (3H, *m*, Ar-H) 3.51 (3H, *s*, N-CH₃); ^{13}C -NMR (125 MHz, $CDCl_3$, δ / ppm): 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; ESI-HRMS: $[M+H]^+$ (m/z): calcd. for $C_{28}H_{20}N_5O$: 442.1667. Found: 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, m.p.: 148–149 °C; IR (KBr, cm^{-1}): 3060, 2924, 1682; 1H -NMR (300 MHz, $CDCl_3$, δ / ppm): 8.58 (1H, *d*, $J = 1.91$ Hz, Ar-H), 8.38 (1H, *d*, $J = 2.1$ Hz, Ar-H), 8.05 (1H, *d*, Ar-H), 7.81–7.89 (2H, *m*, Ar-H), 7.53–7.67 (7H, *m*, Ar-H), 7.33–7.41 (3H, *m*, Ar-H), 3.50 (3H, *s*, N-CH₃); ^{13}C -NMR (75 MHz, $CDCl_3$, δ / ppm): 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; ESI-HRMS: $[M+H]^+$ (m/z): calcd. for $C_{28}H_{19}N_5OBr$: 520.0772. Found: 520.0795.