



SUPPLEMENTARY MATERIAL TO
**Lanthanum triflate-triggered synthesis of
tetrahydroquinazolinone derivatives of *N*-allylquinolone
and their biological assessment**

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ANALYTICAL AND SPECTROSCOPIC CHARACTERIZATION DATA
OF **5a–p** AND **6a–h**

4-(1-Allyl-2-oxo-1,2-dihydroquinolin-3-yl)-4,6,7,8-tetrahydroquinazolinone-2,5(1H,3H)-dione (5a). White powder; Yield: 87 %; m.p.: 192–194 °C; Anal. Calcd. for C₂₀H₁₉N₃O₃ (FW: 349.38): C, 68.75; H, 5.48; N, 12.03 %. Found: C, 68.52; H, 5.84; N, 12.30 %; IR (KBr, cm⁻¹): 3435, 3352 (N–H str.), 1711, 1639, 1593 (C=O str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.97–2.54 (6H, *m*, 3CH₂), 4.90–5.05 (2H, *d*, *J*_{trans} = 17.2 Hz, *J*_{cis} = 10.8 Hz, N–CH₂–CH=CH₂), 5.18 (2H, *d*, *J* = 4.8 Hz, N–CH₂–CH), 5.94 (1H, *m*, CH=CH₂), 5.36 (1H, *s*, quinazolinone H₄), 7.08–7.60 (5H, *m*, Ar–H), 7.80 (1H, *s*, NH), 9.52 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.28 (CH₂), 26.54 (CH₂), 36.80 (CH₂–CO), 44.39 (allylic N–CH₂–CH=CH₂), 49.31 (quinazolinone C₄), 105.51, 115.30, 117.23, 120.20, 122.54, 129.66, 130.92, 132.26, 133.02, 135.28, 138.67, 152.04 (12C, Ar-C and allylic C=C), 156.69 (C=O), 160.72 (C=O), 193.67 (C=O); MS (*m/z*): 350.2 [M+1]⁺.

4-(1-Allyl-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-4,6,7,8-tetrahydroquinazolinone-2,5(1H,3H)-dione (5b). White powder; Yield: 85 %; m.p.: 282–284 °C; Anal. Calcd. for C₂₂H₂₃N₃O₃ (FW: 377.44): C, 70.01; H, 6.14; N, 11.13 %. Found: C, 70.32; H, 6.53; N 10.84 %; IR (KBr, cm⁻¹): 3431, 3346 (N–H str.), 1708, 1634, 1604 (C=O str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 0.98 (3H, *s*, CH₃), 1.03 (3H, *s*, CH₃), 2.07–2.46 (4H, *m*, 2CH₂) 4.98–5.09 (2H, *d*, *J*_{trans} = 17.2 Hz, *J*_{cis} = 10.8 Hz, N–CH₂–CH=CH₂), 5.21 (2H, *d*, *J* = 4.8 Hz, N–CH₂–CH), 5.97 (1H, *m*, CH=CH₂), 5.41 (1H, *s*, quinazolinone H₄), 7.11–7.68 (5H, *m*, Ar-H), 9.01 (1H, *s*, NH), 10.43 (1H, *s*, NH); ¹³C-NMR (100 MHz,

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DMSO- d_6 , δ / ppm): 20.28 (CH₃), 20.84 (CH₃), 32.79 (C(CH₃)₂), 39.12 (CH₂), 48.87 (CH₂-CO), 49.94 (allylic N-CH₂-CH=CH₂), 50.14 (quinazolinone C₄), 105.52, 115.76, 118.12, 121.03, 122.87, 130.35, 131.73, 132.91, 133.54, 136.37, 139.24, 152.98 (12C, Ar-C and allylic C=C), 156.60 (C=O), 161.73 (C=O), 193.66 (C=O); MS (m/z): 378.3 [M+1]⁺.

4-(1-Allyl-2-oxo-1,2-dihydroquinolin-3-yl)-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (5c). White powder; Yield: 85 %; m.p.: 197–199 °C; Anal. Calcd. for C₂₀H₁₉N₃O₂S (FW: 365.45): C, 65.73; H, 5.24; N, 11.50 %. Found: C, 66.05; H, 5.01; N, 11.23 %; IR (KBr, cm⁻¹): 3392, 3240 (N-H str.), 1650, 1606 (C=O str.), 1183 (C=S str.); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.99–2.64 (6H, *m*, 3CH₂), 4.90–5.05 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.18 (2H, *d*, $J = 4.8$ Hz, N-CH₂-CH), 5.96 (1H, *m*, CH=CH₂), 5.40 (1H, *s*, quinazolinone H₄), 7.16–7.82 (5H, *m*, Ar-H), 8.97 (1H, *s*, NH), 10.61 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO- d_6 , δ / ppm): 21.24 (CH₂), 26.43 (CH₂), 36.73 (CH₂-CO), 44.32 (allylic N-CH₂-CH=CH₂), 48.56 (quinazolinone C₄), 105.08, 115.12, 117.09, 120.18, 122.47, 129.24, 130.74, 132.10, 133.14, 135.23, 138.45, 153.07 (12C, Ar-C and allylic C=C), 157.87 (C=O), 175.83 (C=S), 194.19 (C=O); MS (m/z): 366.2 [M+1]⁺.

4-(1-Allyl-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (5d). White powder; Yield: 78 %; m.p.: 285–287 °C; Anal. Calcd. for C₂₂H₂₃N₃O₂S (FW: 393.50): C, 67.15; H, 5.89; N, 10.68 %. Found: C, 66.89; H, 6.23; N, 10.94 %; IR (KBr, cm⁻¹): 3390, 3227 (N-H str.), 1656, 1634 (C=O str.), 1174 (C=S str.); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.06 (3H, *s*, CH₃), 1.09 (3H, *s*, CH₃), 2.29–2.56 (4H, *m*, 2CH₂) 4.92–5.01 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.26 (2H, *d*, $J = 4.8$ Hz, N-CH₂-CH), 5.87–5.94 (1H, *m*, CH=CH₂), 5.38 (1H, *s*, quinazolinone H₄), 7.02–7.63 (5H, *m*, Ar-H), 8.87 (1H, *s*, NH), 9.92 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO- d_6 , δ / ppm): 26.29 (CH₃), 28.87 (CH₃), 33.44 (C(CH₃)₂), 39.35 (CH₂), 49.94 (CH₂-CO), 50.02 (allylic N-CH₂-CH=CH₂), 51.29 (quinazolinone C₄), 105.08, 115.71, 118.06, 120.97, 122.78, 130.27, 131.65, 132.88, 133.51, 136.32, 139.19, 152.86 (12C, Ar-C and allylic C=C), 156.76 (C=O), 180.34 (C=S), 194.50 (C=O); MS (m/z): 394.4 [M+1]⁺.

4-(1-Allyl-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione (5e). White powder; Yield: 82 %; m.p.: 210–212 °C; Anal. Calcd. for C₂₁H₂₁N₃O₃ (FW: 363.41): C, 69.41; H, 5.82; N, 11.56 %. Found: C, 69.30; H, 5.45; N, 11.39 %; IR (KBr, cm⁻¹): 3437, 3348 (N-H str.), 1701, 1611, 1598 (C=O str.); ¹H-NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.96–2.51 (6H, *m*, 3CH₂), 2.42 (3H, *s*, CH₃), 4.97–5.08 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.21 (2H, *d*, $J = 4.8$ Hz, N-CH₂-CH), 5.97 (1H, *m*, CH=CH₂), 5.38 (1H, *s*, quinazolinone H₄), 7.06–7.57 (4H, *m*, Ar-H), 7.82 (1H, *s*, NH), 9.53 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO- d_6 , δ / ppm): 20.69

(CH₃), 21.23 (CH₂), 26.52 (CH₂), 36.78 (CH₂-CO), 44.36 (allylic N-CH₂-CH=CH₂), 49.33 (quinazolinone C₄), 105.23, 115.17, 117.19, 120.14, 122.49, 129.61, 130.87, 132.11, 132.92, 135.03, 138.39, 151.98 (12C, Ar-C and allylic C=C), 156.23 (C=O), 161.54 (C=O), 193.55 (C=O); MS (*m/z*): 364.1 [M+1]⁺.

4-(1-Allyl-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-4,6,7,8-tetrahydroquinazolin-2,5(1H,3H)-dione (5f). White powder; Yield: 79 %; m.p.: 308–310 °C; Anal. Calcd. for C₂₃H₂₅N₃O₃ (FW: 391.46): C, 70.57; H, 6.44; N, 10.73 %. Found: C, 70.71; H, 6.69; N, 10.40 %; IR (KBr, cm⁻¹): 3440, 3359 (N-H str.), 1680, 1626, 1604 (C=O str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 0.98 (3H, *s*, CH₃), 1.02 (3H, *s*, CH₃), 2.07–2.46 (4H, *m*, 2CH₂), 2.28 (3H, *s*, CH₃), 4.97–5.05 (2H, *d*, *J*_{trans} = 17.2 Hz, *J*_{cis} = 10.8 Hz, N-CH₂-CH=CH₂), 5.13 (2H, *d*, *J* = 4.8 Hz, N-CH₂-CH), 5.92 (1H, *m*, CH=CH₂), 5.38 (1H, *s*, quinazolinone H₄), 7.06–7.43 (4H, *m*, Ar-H), 8.87 (1H, *s*, NH), 10.14 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 20.31 (CH₃), 21.12 (CH₃), 22.70 (CH₃) 32.81 (C(CH₃)₂), 39.24 (CH₂), 49.03 (CH₂-CO), 49.86 (allylic N-CH₂-CH=CH₂), 50.21 (quinazolinone C₄), 105.67, 115.88, 118.17, 121.28, 122.93, 130.42, 131.80, 132.96, 133.67, 136.41, 139.26, 153.01 (12C, Ar-C and allylic C=C), 156.66 (C=O), 161.85 (C=O), 193.74 (C=O); MS (*m/z*): 392.6 [M+1]⁺.

4-(1-Allyl-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (5g). Pale yellow powder; Yield: 82 %; m.p.: 211–213 °C; Anal. Calcd. for C₂₁H₂₁N₃O₂S (FW: 379.48): C, 66.47; H, 5.58; N, 11.07 %. Found: C, 66.48; H, 5.27; N, 11.03 %; IR (KBr, cm⁻¹): 3391, 3230 (N-H str.), 1652, 1611 (C=O str.), 1179 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.86–2.44 (6H, *m*, 3CH₂), 3.28 (3H, *s*, CH₃) 4.93–5.04, (2H, *d*, *J*_{trans} = 17.2 Hz, *J*_{cis} = 10.8 Hz, N-CH₂-CH=CH₂), 5.19 (2H, *d*, *J* = 4.8 Hz, N-CH₂-CH), 5.95 (1H, *m*, CH=CH₂), 5.37 (1H, *s*, quinazolinone H₄), 7.12–7.78 (4H, *m*, Ar-H), 8.91 (1H, *s*, NH), 10.83 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.11 (CH₃), 21.35 (CH₂), 26.41 (CH₂), 36.75 (CH₂-CO), 44.38 (allylic N-CH₂-CH=CH₂), 48.47 (quinazolinone C₄), 105.19, 115.21, 117.14, 120.24, 122.54, 129.32, 130.79, 132.13, 133.16, 135.39, 138.67, 153.16 (12C, Ar-C and allylic C=C), 156.94 (C=O), 176.34 (C=S), 194.21 (C=O); MS (*m/z*): 380.5 [M+1]⁺.

4-(1-Allyl-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (5h). White powder; Yield: 79 %; m.p.: 291–293 °C; Anal. Calcd. for C₂₃H₂₅N₃O₂S (FW: 407.53): C, 67.79; H, 6.18; N, 10.31 %. Found: C, 68.06; H, 6.24; N, 10.67 %; IR (KBr, cm⁻¹): 3394, 3217 (N-H str.), 1657, 1639 (C=O str.), 1173 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 0.98 (3H, *s*, CH₃), 1.02 (3H, *s*, CH₃), 2.35 (3H, *s*, CH₃), 2.07–2.51 (4H, *m*, 2CH₂), 4.82–4.98 (2H, *d*, *J*_{trans} = 17.2 Hz, *J*_{cis} = 10.8 Hz, N-CH₂-CH=CH₂), 5.13 (2H, *d*, *J* = 4.8 Hz, N-CH₂-CH), 5.88 (1H, *m*, CH=CH₂), 5.35 (1H, *s*, quinazolinone H₄), 7.19–7.60 (4H, *m*, Ar-H), 9.06 (1H,

s, NH), 10.50 (1H, s, NH); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ / ppm): 20.51 (CH₃), 27.83 (CH₃), 29.16 (CH₃), 32.77 (C(CH₃)₂), 39.11 (CH₂), 49.07 (CH₂-CO), 50.13 (allylic N-CH₂-CH=CH₂), 50.90 (quinazolinone C₄), 105.57, 115.18, 117.02, 121.12, 122.97, 129.19, 131.37, 132.95, 133.77, 136.81, 140.26, 153.93 (12C, Ar-C and allylic C=C), 157.83 (C=O), 175.22 (C=S), 193.90 (C=O); MS (m/z): 408.3 [M+1]⁺.

4-(1-Allyl-6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione (**5i**). Pale yellow powder; Yield: 84 %; m.p.: 217–219 °C; Anal. Calcd. for C₂₁H₂₁N₃O₄ (FW: 379.41): C, 66.48; H, 5.58; N, 11.08 %. Found: C, 66.20; H, 5.59; N, 11.30 %; IR (KBr, cm⁻¹): 3402, 3265 (N-H str.), 1695, 1632, 1630 (C=O str.); ^1H -NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.94–2.53 (6H, m, 3CH₂), 3.72 (3H, s, OCH₃), 4.96–5.11 (2H, d, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.33 (2H, d, $J = 4.8$ Hz, N-CH₂-CH), 6.02 (1H, m, CH=CH₂), 5.63 (1H, s, quinazolinone H₄), 7.08–7.68 (4H, m, Ar-H), 8.18 (1H, s, NH), 10.29 (1H, s, NH); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ / ppm): 21.28 (CH₂), 26.61 (CH₂), 37.17 (CH₂-CO), 44.32 (allylic N-CH₂-CH=CH₂), 48.26 (quinazolinone C₄), 55.62 (OCH₃), 106.18, 116.82, 117.96, 120.55, 123.01, 130.13, 131.26, 132.43, 133.12, 135.27, 138.46, 152.05 (12C, Ar-C and allylic C=C), 157.06 (C=O), 162.28 (C=O), 194.13 (C=O); MS (m/z): 380.5 [M+1]⁺.

4-(1-Allyl-6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione (**5j**). Pale yellow powder; Yield: 82 %; m.p.: 295–297 °C; Anal. Calcd. for C₂₃H₂₅N₃O₄ (FW: 407.46): C, 67.80; H, 6.18; N, 10.31 %. Found: C, 67.45; H, 6.34; N, 10.22 %; IR (KBr, cm⁻¹): 3442, 3356 (N-H str.), 1671, 1626, 1602 (C=O str.); ^1H -NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.02 (3H, s, CH₃), 1.04 (3H, s, CH₃), 2.05–2.42 (4H, m, 2CH₂), 3.86 (3H, s, OCH₃), 4.99–5.08 (2H, d, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.15 (2H, d, $J = 4.8$ Hz, N-CH₂-CH), 5.96 (1H, m, CH=CH₂), 5.43 (1H, s, quinazolinone H₄), 7.07–7.41 (4H, m, Ar-H), 8.92 (1H, s, NH), 10.10 (1H, s, NH); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ / ppm): 20.26 (CH₃), 21.09 (CH₃), 32.94 (C(CH₃)₂), 39.27 (CH₂), 49.12 (CH₂-CO), 49.86 (allylic N-CH₂-CH=CH₂), 50.21 (quinazolinone C₄), 55.86 (OCH₃), 105.71, 116.01, 118.25, 121.32, 122.97, 130.46, 131.84, 132.99, 133.70, 136.44, 139.29, 153.10 (12C, Ar-C and allylic C=C), 156.82 (C=O), 161.93 (C=O), 193.81 (C=O); MS (m/z): 408.7 [M+1]⁺.

4-(1-Allyl-6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**5k**). Pale yellow powder; Yield: 87 %; m.p.: 225–227 °C; Anal. Calcd. for C₂₁H₂₁N₃O₃S (FW: 395.47): C, 63.78; H, 5.35; N, 10.63 %. Found: C, 63.91; H, 5.28; N, 10.38 %; IR (KBr, cm⁻¹): 3401, 3241 (N-H str.), 1651, 1609 (C=O str.), 1186 (C=S str.); ^1H -NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.89–2.48 (6H, m, 3CH₂), 3.89 (3H, s, OCH₃), 4.96–5.07, (2H, d,

$J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.26 (2H, *d*, $J = 4.8$ Hz, N-CH₂-CH), 5.97 (1H, *m*, CH=CH₂), 5.38 (1H, *s*, quinazolinone H₄), 7.07–7.64 (4H, *m*, Ar-H), 9.01 (1H, *s*, NH), 10.91 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.39 (CH₂), 26.47 (CH₂), 36.82 (CH₂-CO), 44.45 (allylic N-CH₂-CH=CH₂), 48.53 (quinazolinone C₄), 55.58 (OCH₃), 104.98, 115.17, 117.21, 120.22, 122.48, 129.29, 130.81, 132.09, 133.13, 135.32, 138.64, 153.22 (12C, Ar-C and allylic C=C), 155.92 (C=O), 175.21 (C=S), 194.39 (C=O); MS (*m/z*): 396.1 [M+1]⁺.

4-(1-Allyl-6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**5l**). Pale yellow powder; Yield: 82 %; m.p.: 296–298 °C; Anal. Calcd. for C₂₃H₂₅N₃O₃S (FW: 423.53): C, 65.23; H 5.95; N, 9.92 %. Found: C, 64.95; H 5.87; N, 9.56 %; IR (KBr, cm⁻¹): 3395, 3220 (N-H str.), 1656, 1634 (C=O str.), 1174 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.01 (3H, *s*, CH₃), 1.04 (3H, *s*, CH₃), 2.08–2.49 (4H, *m*, 2CH₂), 3.85 (3H, *s*, OCH₃), 4.96–5.02 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.24 (2H, *d*, $J = 4.8$ Hz, N-CH₂-CH), 6.02 (1H, *m*, CH=CH₂), 5.76 (1H, *s*, quinazolinone H₄), 7.16–7.59 (4H, *m*, Ar-H), 8.42 (1H, *s*, NH), 10.69 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 27.62 (CH₃), 28.96 (CH₃), 32.82 (C(CH₃)₂), 40.38 (CH₂), 50.17 (CH₂-CO), 51.25 (allylic N-CH₂-CH=CH₂), 51.97 (quinazolinone C₄), 55.14 (OCH₃), 106.26, 115.89, 117.36, 121.18, 123.16, 129.41, 131.42, 133.02, 133.94, 137.13, 140.45, 154.15 (12C, Ar-C and allylic C=C), 159.24 (C=O), 177.10 (C=S), 195.72 (C=O); MS (*m/z*): 424.2 [M+1]⁺.

4-(1-Allyl-6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione (**5m**). White powder; Yield: 86 %; m.p.: 230–232 °C; Anal. Calcd. for C₂₀H₁₈ClN₃O₃ (FW: 383.83): C, 62.58; H 4.73; N, 10.95 %. Found: C, 62.43; H 5.12; N, 11.03 %; IR (KBr, cm⁻¹): 3440, 3357 (N-H str.), 1703, 1642, 1603 (C=O str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.98–2.59 (6H, *m*, 3CH₂), 4.98–5.14 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N-CH₂-CH=CH₂), 5.47 (2H, *d*, $J = 4.8$ Hz, N-CH₂-CH), 5.82 (1H, *m*, CH=CH₂), 5.66 (1H, *s*, quinazolinone H₄), 7.05–7.60 (4H, *m*, Ar-H), 7.98 (1H, *s*, NH), 10.11 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.27 (CH₂), 26.38 (CH₂), 36.82 (CH₂-CO), 44.41 (allylic N-CH₂-CH=CH₂), 48.15 (quinazolinone C₄), 105.53, 115.18, 117.20, 120.41, 123.23, 129.98, 131.12, 132.36, 133.09, 135.12, 138.19, 152.01. (12C, Ar-C and allylic C=C), 156.96 (C=O), 161.83 (C=O), 194.02 (C=O); MS (*m/z*): 384.9 [M+1]⁺.

4-(1-Allyl-6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-4,6,7,8-tetrahydroquinazoline-2,5(1H,3H)-dione (**5n**). Pale yellow powder; Yield: 84 %; m.p.: 286–288 °C; Anal. Calcd. for C₂₂H₂₂ClN₃O₃ (FW: 411.88): C, 64.15; H 5.38; N, 10.20 %. Found: C, 64.41; H 5.43; N, 9.85 %; IR (KBr, cm⁻¹): 3445, 3364 (N-H str.), 1660, 1620, 1600 (C=O str.); ¹H-NMR (400 MHz, DMSO-*d*₆,

δ / ppm): 0.99 (3H, *s*, CH₃), 1.02 (3H, *s*, CH₃), 2.02–2.37 (4H, *m*, 2CH₂), 4.95–5.01 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N–CH₂–CH=CH₂), 5.10 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.92 (1H, *m*, CH=CH₂), 5.41 (1H, *s*, quinazolinone H₄), 7.02–7.38 (4H, *m*, Ar–H), 8.89 (1H, *s*, NH), 10.03 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 27.56 (CH₃), 29.11 (CH₃), 32.45 (C(CH₃)₂), 39.51 (CH₂), 49.22 (CH₂–CO), 49.93 (allylic N–CH₂–CH=CH₂), 50.76 (quinazolinone C₄), 106.04, 116.98, 118.79, 121.55, 123.11, 130.88, 131.99, 133.07, 133.87, 136.91, 139.36, 153.26 (12C, Ar-C and allylic C=C), 157.12 (C=O), 162.05 (C=O), 194.13 (C=O); MS (*m/z*): 412.7 [M+1]⁺.

4-(1-Allyl-6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**5o**). Yellowish-orange powder; Yield: 81 %; m.p.: 234–236 °C; Anal. Calcd. for C₂₀H₁₈ClN₃O₂S (FW: 399.89): C, 60.07; H 4.54; N, 10.51 %. Found: C, 59.90; H 4.45; N, 10.57 %; IR (KBr, cm⁻¹): 3396, 3236 (N–H str.), 1647, 1601 (C=O str.), 1184 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.85–2.37 (6H, *m*, 3CH₂), 4.92–5.01, (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH=CH₂), 5.20 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N–CH₂–CH), 5.93 (1H, *m*, CH=CH₂), 5.30 (1H, *s*, quinazolinone H₄), 7.11–7.64 (4H, *m*, Ar–H), 8.71 (1H, *s*, NH), 10.75 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.31 (CH₂), 26.44 (CH₂), 36.76 (CH₂–CO), 44.41 (allylic N–CH₂–CH=CH₂), 48.49 (quinazolinone C₄), 104.71, 114.98, 117.03, 120.08, 122.28, 129.15, 130.67, 131.97, 133.01, 135.19, 138.43, 153.11 (12C, Ar-C and allylic C=C), 155.42 (C=O), 175.12 (C=S), 194.27 (C=O); MS (*m/z*): 400.8 [M+1]⁺.

4-(1-Allyl-6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**5p**). Pale yellow powder; Yield: 76 %; m.p.: 302–304 °C; Anal. Calcd. for C₂₂H₂₂ClN₃O₂S (FW: 427.95): C, 61.74; H 5.18; N, 9.82 %. Found: C, 61.55; H 5.50; N, 9.53 %; IR (KBr, cm⁻¹): 3398, 3229 (N–H str.), 1662, 1645 (C=O str.), 1175 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 0.98 (3H, *s*, CH₃), 1.01 (3H, *s*, CH₃), 2.04–2.39 (4H, *m*, 2CH₂), 4.89–4.96 (2H, *d*, $J_{\text{trans}} = 17.2$ Hz, $J_{\text{cis}} = 10.8$ Hz, N–CH₂–CH=CH₂), 5.15 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.87 (1H, *m*, CH=CH₂), 5.54 (1H, *s*, quinazolinone H₄), 7.02–7.47 (4H, *m*, Ar–H), 7.92 (1H, *s*, NH), 9.87 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 26.26 (CH₃), 27.01 (CH₃), 32.07 (C(CH₃)₂), 41.19 (CH₂), 49.03 (CH₂–CO), 50.86 (allylic N–CH₂–CH=CH₂), 52.04 (quinazolinone C₄), 105.12, 115.16, 116.45, 121.36, 122.73, 129.17, 131.10, 132.59, 133.47, 136.87, 139.55, 153.37 (12C, Ar-C and allylic C=C), 158.65 (C=O), 176.32 (C=S), 193.33 (C=O); MS (*m/z*): 429.1 [M+1]⁺.

4-(1-Allyl-2-oxo-1,2-dihydroquinolin-3-yl)-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6a**). White powder; Yield: 74 %; m.p.: 248–250 °C; Anal. Calcd. for C₂₆H₂₃N₃O₂S (FW: 441.54): C, 70.72; H 5.25; N, 9.52 %. Found: C, 70.88; H 5.63; N, 9.39 %; IR (KBr, cm⁻¹): 3464 (N–H str.), 1670, 1653 (C=O str.), 1182 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ /

/ ppm): 1.76–2.32 (6H, *m*, 3CH₂), 4.82–4.98 (2H, *d*, $J_{\text{trans}} = 17.6$ Hz, $J_{\text{cis}} = 10.4$ Hz, N–CH₂–CH=CH₂), 5.11 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.82 (1H, *m*, CH=CH₂), 5.29 (1H, *s*, quinazolinone H₄), 7.12–7.81 (10H, *m*, Ar–H), 9.76 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.38 (CH₂), 26.51 (CH₂), 36.49 (CH₂–CO), 45.13 (allylic N–CH₂–CH=CH₂), 49.25 (quinazolinone C₄), 105.41, 115.03, 116.75, 120.18, 122.47, 127.91, 128.34, 129.16, 130.20, 131.12, 132.26, 133.46, 133.85, 135.87, 138.67, 154.31 (16C, Ar-C and allylic C=C), 161.25 (C=O), 165.18 (C=S), 194.46 (C=O); MS (*m/z*): 442.3 [M+1]⁺.

4-(1-Allyl-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6b**). Pale yellow powder; Yield: 83 %; m.p.: 234–236 °C; Anal. Calcd. for C₂₈H₂₇N₃O₂S (FW: 469.60): C, 71.61; H 5.80; N, 8.95 %. Found: C, 71.38; H 5.41; N, 9.19 %; IR (KBr, cm⁻¹): 3471, (N–H str.), 1653, 1630 (C=O str.), 1176 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.09 (3H, *s*, CH₃), 1.11 (3H, *s*, CH₃), 2.26–2.72 (4H, *m*, 2CH₂), 4.96–5.01 (2H, *d*, $J_{\text{trans}} = 17.6$ Hz, $J_{\text{cis}} = 10.4$ Hz, N–CH₂–CH=CH₂), 5.17 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.94 (1H, *m*, CH=CH₂), 5.44 (1H, *s*, quinazolinone H₄), 7.25–7.73 (10H, *m*, Ar–H), 10.84 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 28.03 (CH₃), 28.80 (CH₃), 32.60 (C(CH₃)₂), 37.58 (CH₂), 41.27 (CH₂–CO), 44.69 (allylic N–CH₂–CH=CH₂), 50.42 (quinazolinone C₄), 105.64, 115.50, 117.18, 119.92, 121.27, 122.82, 126.62, 128.64, 129.60, 131.24, 131.75, 132.80, 133.92, 137.02, 138.49, 154.56 (16C, Ar-C and allylic C=C), 160.00 (C=O), 166.78 (C=S), 194.62 (C=O); MS (*m/z*): 470.4 [M+1]⁺.

4-(1-Allyl-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6c**). White powder; Yield: 74 %; m.p.: 262–264 °C; Anal. Calcd. for C₂₇H₂₅N₃O₂S (FW: 455.57): C, 71.18; H 5.53; N, 9.22 %. Found: C, 70.79; H 5.32; N, 9.25 %; IR (KBr, cm⁻¹): 3470 (N–H str.), 1651, 1622 (C=O str.), 1184 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.81–2.42 (6H, *m*, 3CH₂), 2.70 (3H, *s*, CH₃), 4.86–5.01 (2H, *d*, $J_{\text{trans}} = 17.6$ Hz, $J_{\text{cis}} = 10.4$ Hz, N–CH₂–CH=CH₂), 5.16 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.88 (1H, *m*, CH=CH₂), 5.34 (1H, *s*, quinazolinone H₄), 7.21–8.01 (9H, *m*, Ar–H), 10.03 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 20.86 (CH₃), 21.94 (CH₂), 27.12 (CH₂), 36.54 (CH₂–CO), 45.44 (allylic N–CH₂–CH=CH₂), 49.77 (quinazolinone C₄), 105.22, 115.11, 116.81, 120.22, 122.53, 128.02, 128.67, 129.29, 130.31, 131.14, 132.34, 133.48, 133.89, 136.10, 138.83, 154.51 (16C, Ar-C and allylic C=C), 162.82 (C=O), 166.17 (C=S), 194.69 (C=O); MS (*m/z*): 456.3 [M+1]⁺.

4-(1-Allyl-6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6d**). White powder; Yield: 77 %; m.p.: 251–253 °C; Anal. Calcd. for C₂₉H₂₉N₃O₂S (FW: 483.62): C, 72.02; H 6.04; N, 8.69 %. Found: C, 72.13; H 6.21, N, 8.42 %; IR (KBr, cm⁻¹): 3459, (N–H str.), 1654, 1633 (C=O str.), 1180 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆,

δ / ppm): 0.86 (3H, *s*, CH₃), 0.95 (3H, *s*, CH₃), 1.87–2.32 (4H, *m*, 2CH₂), 2.29 (3H, *s*, CH₃), 4.85–5.04 (2H, *d*, $J_{\text{trans}} = 17.6$ Hz, $J_{\text{cis}} = 10.4$ Hz, N–CH₂–CH=CH₂), 5.19 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.91 (1H, *m*, CH=CH₂), 5.37 (1H, *s*, quinazolinone H₄), 7.06–7.72 (9H, *m*, Ar–H), 9.98 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 20.47 (CH₃), 27.85 (CH₃), 29.73 (CH₃), 32.48 (C(CH₃)₂), 39.59 (CH₂), 49.91 (CH₂–CO), 50.28 (allylic N–CH₂–CH=CH₂), 51.40 (quinazolinone C₄), 105.37, 115.44, 117.21, 117.67, 121.41, 123.37, 126.78, 127.22, 129.38, 130.55, 131.62, 133.31, 134.54, 137.23, 140.46, 154.33 (16C, Ar-C and allylic C=C), 158.14 (C=O), 166.52 (C=S), 194.43 (C=O); MS (*m/z*): 484.7 [M+1]⁺.

4-(1-Allyl-6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6e**). Pale yellow powder; Yield: 79 %; m.p.: 276–278 °C; Anal. Calcd. for C₂₇H₂₅N₃O₃S (FW: 471.57): C, 68.77; H 5.34; N, 8.91 %. Found: C, 68.84; H 5.46; N, 8.67 %; IR (KBr, cm⁻¹): 3435 (N–H str.), 1653, 1624 (C=O str.), 1178 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.88–2.27 (6H, *m*, 3CH₂), 3.81 (3H, *s*, OCH₃), 4.94–4.99 (2H, *d*, $J_{\text{trans}} = 17.6$ Hz, $J_{\text{cis}} = 10.4$ Hz, N–CH₂–CH=CH₂), 5.15 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 5.93 (1H, *m*, CH=CH₂), 5.40 (1H, *s*, quinazolinone H₄), 7.17–7.75 (9H, *m*, Ar–H), 9.34 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 21.21 (CH₂), 28.33 (CH₂), 37.42 (CH₂–CO), 45.88 (allylic N–CH₂–CH=CH₂), 49.59 (quinazolinone C₄), 56.02 (OCH₃), 105.66, 109.16, 110.13, 116.59, 119.95, 120.33, 122.82, 127.64, 128.81, 129.45, 131.99, 133.39, 137.08, 140.85, 153.80, 154.72, (16C, Ar-C and allylic C=C), 160.96 (C=O), 178.21 (C=S), 195.04 (C=O); MS (*m/z*): 472.3 [M+1]⁺.

4-(1-Allyl-6-methoxy-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6f**). Pale yellow powder; Yield: 85 %; m.p.: 289–291 °C; Anal. Calcd. for C₂₉H₂₉N₃O₃S (FW: 499.62): C, 69.71; H 5.85; N, 8.41 %. Found: C, 69.37; H 5.66; N, 8.65 %; IR (KBr, cm⁻¹): 3473, (N–H str.), 1657, 1631 (C=O str.), 1185 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.04 (3H, *s*, CH₃), 1.06 (3H, *s*, CH₃), 2.08–2.48 (4H, *m*, 2CH₂), 3.89 (3H, *s*, OCH₃), 5.01–5.12 (2H, *d*, $J_{\text{trans}} = 17.6$ Hz, $J_{\text{cis}} = 10.4$ Hz, N–CH₂–CH=CH₂), 5.22 (2H, *d*, $J = 4.8$ Hz, N–CH₂–CH), 6.05 (1H, *m*, CH=CH₂), 5.46 (1H, *s*, quinazolinone H₄), 7.14–8.02 (9H, *m*, Ar–H), 10.06 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 27.82 (CH₃), 29.75 (CH₃), 32.69 (C(CH₃)₂), 40.15 (CH₂), 50.13 (CH₂–CO), 50.29 (allylic N–CH₂–CH=CH₂), 51.24 (quinazolinone C₄), 55.19 (OCH₃), 105.45, 115.37, 117.38, 118.01, 121.63, 123.51, 126.90, 127.47, 129.50, 130.47, 131.85, 133.49, 134.77, 137.39, 140.62, 154.60 (16C, Ar-C and allylic C=C), 158.48 (C=O), 166.75 (C=S), 194.71 (C=O); MS (*m/z*): 500.4 [M+1]⁺.

4-(1-Allyl-6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6g**). Pale yellow powder; Yield: 73

%; m.p.: 285–287 °C; Anal. Calcd. for C₂₆H₂₂ClN₃O₂S (FW: 475.99): C, 65.61; H 4.66, N; 8.83 %. Found: C, 65.84; H 4.58; N, 8.44 %; IR (KBr, cm⁻¹): 3467 (N–H str.), 1673, 1648 (C=O str.), 1178 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 2.06–2.79 (6H, *m*, 3CH₂), 4.95–5.00 (2H, *d*, *J*_{trans} = 17.6 Hz, *J*_{cis} = 10.4 Hz, N–CH₂–CH=CH₂), 5.18 (2H, *d*, *J* = 4.8 Hz, N–CH₂–CH), 5.94 (1H, *m*, CH=CH₂), 5.40 (1H, *s*, quinazolinone H₄), 7.17–8.01 (9H, *m*, Ar–H), 10.89 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 20.78 (CH₂), 28.23 (CH₂), 37.13 (CH₂–CO), 44.86 (allylic N–CH₂–CH=CH₂), 50.63 (quinazolinone C₄), 106.23, 115.32, 117.25, 117.51, 121.42, 122.58, 126.82, 128.64, 129.57, 130.67, 132.60, 132.71, 133.13, 135.06, 137.21, 157.03 (16C, Ar–C and allylic C=C), 159.87 (C=O), 166.72 (C=S), 194.85 (C=O); MS (*m/z*): 476.6 [M+1]⁺.

4-(1-Allyl-6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-7,7-dimethyl-1-phenyl-2-thioxo-2,3,4,6,7,8-hexahydroquinazolin-5(1H)-one (**6h**). Yellowish-orange powder; Yield: 73 %; m.p.: 301–303 °C; Anal. Calcd. for C₂₈H₂₆ClN₃O₂S (FW: 504.04): C, 66.72; H 5.20; N, 8.34 %. Found: C, 66.63; H 5.04; N, 8.63 %; IR (KBr, cm⁻¹): 3452, (N–H str.), 1670, 1644 (C=O str.), 1182 (C=S str.); ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 1.01 (3H, *s*, CH₃), 1.04 (3H, *s*, CH₃), 2.01–2.43 (4H, *m*, 2CH₂), 4.98–5.06 (2H, *d*, *J*_{trans} = 17.6 Hz, *J*_{cis} = 10.4 Hz, N–CH₂–CH=CH₂), 5.19 (2H, *d*, *J* = 4.8 Hz, N–CH₂–CH), 5.97 (1H, *m*, CH=CH₂), 5.41 (1H, *s*, quinazolinone H₄), 7.08–7.76 (9H, *m*, Ar–H), 9.87 (1H, *s*, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 26.89 (CH₃), 29.46 (CH₃), 32.39 (C(CH₃)₂), 40.01 (CH₂), 49.98 (CH₂–CO), 50.09 (allylic N–CH₂–CH=CH₂), 51.19 (quinazolinone C₄), 105.37, 115.22, 117.26, 117.89, 121.47, 123.32, 126.78, 127.34, 129.41, 130.38, 131.81, 133.32, 134.52, 137.23, 140.49, 154.71 (16C, Ar–C and allylic C=C), 160.12 (C=O), 166.81 (C=S), 195.08 (C=O); MS (*m/z*): 505.2 [M+1]⁺.