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SUPPLEMENTARY MATERIAL TO

Syntheses and antimicrobial activities of 1-(3-benzyl-4-oxo-3,4--dihydroquinazolin-2-yl)-4-(substituted) thiosemicarbazide derivatives

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*3-Benzyl-2-thioxo-2,3-dihydro-1*H*-quinazolin-4-one* (***4***). Yield: 85 %; m.p.: 230–231 °C; Anal. Calcd for $C_{15}H_{12}N_2OS$: C, 67.14; H, 4.51; N, 10.44 %. Found: C, 67.19; H, 4.49; N, 10.46 %; IR (KBr, cm^{-1}): 3200 (NH), 1680 (C=O), 1208 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 4.65 (2H, *s*, CH_2), 7.01–7.03 (3H, *m*, Ar-H), 7.13 (2H, *d*, J = 7.5 Hz, Ar-H), 7.85–7.91 (4H, *m*, Ar-H), 8.15 (1H, *brs*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.75, 120.11, 121.79, 125.69, 126.25, 126.88, 127.23, 127.95, 132.89, 140.75, 145.89, 160.25, 162.89; MS (*m*/*z*): 268 (M^+).

*3-Benzyl-2-(methylsulphanyl)-3*H*-quinazolin-4-one* (***5***). Yield: 78 %; m.p.: 150–152 °C; Anal. Calcd for $C_{16}H_{14}N_2OS$: C, 68.06; H, 5.00; N, 9.92 %. Found: C, 68.03; H, 5.01; N, 9.96 %; IR (KBr, cm^{-1}): 1681 (C=O), 1616 (C=C); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.02 (3H, *s*, SCH_3), 4.35 (2H, *s*, CH_2), 7.00–7.02 (3H, *m*, Ar-H), 7.14 (2H, *d*, J = 7.5 Hz, Ar-H), 7.95–7.99 (4H, *m*, Ar-H); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 9.85, 39.89, 120.22, 121.65, 125.73, 126.55, 126.87, 127.42, 127.85, 132.65, 140.75, 145.89, 160.35, 162.75; MS (*m*/*z*): 282 (M^+).

*3-Benzyl-2-hydrazino-3*H*-quinazolin-4-one* (***6***). Yield: 81 %; m.p.: 242–245 °C; Anal. Calcd. for $C_{15}H_{14}N_4O$: C, 67.65; H, 5.30; N, 21.04 %. Found: C, 67.69; H, 5.32; N, 21.09 %; IR (KBr, cm^{-1}): 3383, 3295 ($NHNH_2$), 1677 (C=O); ^{1}H-NMR (300 MHz. $CDCl_3$, δ / ppm): 4.45 (2H, *s*, CH_2), 4.65 (2H, *s*, NH_2), 7.01–7.03 (3H, *m*, Ar-H), 7.14 (2H, *d*, J = 7.5 Hz, Ar-H), 8.01–8.03 (4H, *m*, Ar-H), 9.89 (1H, *s*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.89, 120.35,

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121.77, 125.65, 126.55, 126.88, 127.23, 127.95, 132.89, 140.85, 145.91, 160.25, 162.93; MS (*m*/*z*): 266 (M^+).

*1-[3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl]-4-[cyclohexyl]hydrazinecarbothioamide (**AS1**)*.[1] Yield: 76 %; m.p.: 215–218 °C; Anal. Calcd. for $C_{22}H_{25}N_5OS$: C, 64.84; H, 6.18; N, 17.18. Found: C, 64.81; H, 6.20; N, 17.22 %; IR (KBr, cm^{-1}): 3247 (NH), 3265 (NH), 3212 (NH), 1616 (C=O), 1600 (C=N), 1220 (C=S); ^{1}H-NMR (300 Hz, $CDCl_3$, δ / ppm): 1.42–1.69 (6H, *m*, CH_2), 1.78 (2H, *s*, CH_2), 1.82 (2H, *s*, CH_2), 2.99 (1H, *s*, CH), 4.72 (2H, *s*, CH_2), 7.11–7.62 (2H, *m*, Ar-H), 7.83–7.98 (1H, *m*, Ar-H), 8.04 (2H, *d*, J = 7.5 Hz, Ar-H), 8.10–8.14 (1H, *m*, Ar-H), 8.17 (2H, *d*, J = 8.0 Hz, Ar-H), 8.19–8.21 (1H, *m*, Ar-H), 8.85 (1H, *s*, NH), 8.96 (1H, *s*, NH), 11.15 (1H, *s*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 22.14, 25.89, 32.33, 39.89, 52.75, 120.56, 123.35, 123.68, 125.28, 127.78, 127.85, 128.61, 130.81, 131.86, 138.75, 158.69, 162.45, 183.74; MS (*m*/*z*): 407 (M^+).

N-*Benzyl-2-(3-benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)hydrazinecarbothioamide (**AS2**)*.[2] Yield: 72 %; m.p.: 231–233 °C; Anal. Calcd. for $C_{23}H_{21}N_5OS$: C, 66.41; H, 5.07; N, 16.83 %. Found: C, 66.38; H, 4.99; N, 16.85 %; IR (KBr, cm^{-1}): 3281 (NH), 3261 (NH), 3233 (NH), 1690 (C=O), 1620 (C=N), 1215 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 1.31 (2H, *s*, CH_2), 4.31 (2H, *s*, CH_2), 6.32–6.43 (2H, *m*, Ar-H), 6.83–6.91 (2H, *m*, Ar-H), 7.07 (2H, *d*, J = 8.0 Hz, Ar-H), 7.17 (2H, *d*, J = 7.5 Hz, Ar-H), 7.94 (2H, *d*, J = 8.0 Hz, Ar-H), 7.98–8.03 (1H, *m*, Ar-H), 8.10 (2H, *d*, J = 8.0 Hz, Ar-H), 8.31–8.38 (1H, *m*, Ar-H), 8.36 (1H, *s*, NH), 8.91 (1H, *s*, NH), 9.51 (1H, *s*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.87, 49.68, 120.71, 123.48, 123.68, 125.28, 125.68, 126.74, 127.22, 127.78, 127.85, 128.61, 130.81, 131.86, 138.75, 140.35, 158.69, 162.35, 183.58; MS (*m*/*z*): 415 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*phenylhydrazinecarbothioamide (**AS3**)*.[1] Yield: 72 %; m.p.: 150–153 °C; Anal. Calcd. for $C_{22}H_{19}N_5OS$: C, 65.81; H, 4.77; N, 17.44 %. Found: C, 65.78; H, 4.69; N, 17.39 %; IR (KBr, cm^{-1}): 3389 (NH), 3360 (NH), 3280 (NH), 1675 (C=O), 1600 (C=N), 1168 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 4.19 (2H, *s*, CH_2), 7.14–7.31 (2H, *m*, Ar-H), 7.51–7.74 (2H, *m*, Ar-H), 7.88 (2H, *d*, J = 8.0 Hz, Ar-H), 8.02 (2H, *d*, J = 7.5 Hz, Ar-H), 8.10 (2H, *d*, J = 8.0 Hz, Ar-H), 8.20–8.32 (1H, *m*, Ar-H), 8.38 (2H, *d*, J = 8.0 Hz, Ar-H), 8.45–8.49 (1H, *m*, Ar-H), 8.95 (1H, *s*, NH), 9.03 (1H, *s*, NH), 10.18 (1H, *s*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.77, 120.68, 123.55, 123.74 125.18, 125.36, 126.74, 127.22, 127.78, 127.85, 128.61, 130.81, 131.86, 138.75, 140.35, 158.69, 162.75, 183.75; MS (*m*/*z*): 401 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*(2-methylphenyl)hydrazinecarbothioate (**AS4**)*. Yield: 78 %; m.p.: 190–193 °C; Anal. Calcd. for $C_{23}H_{21}N_5OS$: C, 66.48; H, 5.09; N, 16.85 %. Found: C, 67.01; H, 5.20; N, 16.83

%; IR (KBr, cm^{-1}): 3323 (NH), 3305 (NH), 3274 (NH), 1604 (C=O), 1610 (C=N), 1243 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.42 (3H, *s*, CH_3), 4.71 (2H, *s*, CH_2), 6.80 (1H, *brs*, NH), 6.71–6.78 (2H, *m*, Ar-H), 7.01–7.08 (1H, *m*, Ar-H), 7.25 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.48 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.66 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.83–7.92 (1H, *m*, ArH), 7.99 (2H, *d*, *J* = 7.5 Hz, Ar-H), 8.32–8.41 (1H, *m*, Ar-H), 8.86 (1H, *brs*, NH), 10.50 (1H, *brs*, NH); ^{13}C--NMR (75 MHz, $CDCl_3$, δ / ppm): 12.58, 39.85, 120.68, 123.55, 123.74 125.18, 125.36, 126.74, 127.22, 127.78, 127.85, 128.61, 130.81, 131.86, 138.75, 138.85, 140.35, 158.69, 162.75, 181.75; MS (*m*/*z*): 415 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*(4-methylphenyl)hydrazinecarbothioate (**AS5**)*.[3] Yield: 74 %; m.p.: 260–263 °C; Anal. Calcd. for $C_{23}H_{21}N_5OS$: C, 66.48; H, 5.09; N, 16.85 %. Found: C, 66.50; H, 5.12; N, 16.87 %; IR (KBr, cm^{-1}): 3340 (NH), 3288 (NH), 3259 (NH), 1612 (C=O), 1174 (C=N), 1255 (C=S); ^{1}H-NMR ($CDCl_3$, δ / ppm): 2.56 (3H, *s*, CH_3), 4.78 (2H, *s*, CH_2), 6.85 (1H, *brs*, NH), 7.09–7.13 (2H, *m*, Ar-H), 7.25–7.36 (1H, *m*, Ar-H), 7.55 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.81 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.87 (2H, *d*, *J* = = 7.5 Hz, Ar-H), 7.92–7.96 (1H, *m*, Ar-H), 8.00 (2H, *d*, *J* = 8.0 Hz, Ar-H), 8.06––8.09 (1H, *m*, Ar-H), 8.94 (1H, *brs*, NH), 10.62 (1H, *brs*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 12.98, 39.85, 120.52, 123.71, 123.84, 125.42, 125.87, 126.74, 127.22, 127.78, 127.85, 128.61, 130.81, 131.86, 138.75, 140.45, 158.69, 162.59, 183.61; MS (*m*/*z*): 415 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*3-methoxyphenylhydrazinecarbothioate (**AS6**)*.[1] Yield: 70 %; m.p.: 205–208 °C; Anal. Calcd. for $C_{23}H_{21}N_5O_2S$: C, 64.02; H, 4.91; N, 16.23 %. Found: C, 64.01; H, 4.88; N, 16.32 %; IR (KBr, cm^{-1}): 3353 (NH), 3321 (NH), 3274 (NH), 1640 (C=O), 1621 (C=N), 1286 (OCH_3), 1243 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.31 (3H, *s*, OCH_3), 5.23 (2H, *s*, CH_2), 6.83 (1H, *brs*, NH), 7.13–7.17 (1H, *m*, Ar-H), 7.21–7.25 (2H, *m*, Ar-H), 7.34 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.45 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.54 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.59–7.62 (1H, *m*, Ar-H), 7.68 (2H, *d*, *J* = 7.5 Hz, Ar-H), 8.06–8.09 (1H, *m*, Ar-H), 8.53 (1H, *brs*, NH), 10.31 (1H, *brs*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.89, 53.85, 108.75, 109.87, 117.85, 120.48, 123.51, 123.25, 125.42, 127.53, 127.85, 128.61, 129.57, 129.99, 130.81, 131.86, 137.57, 138.75, 158.69, 162.42, 179.53; MS (*m*/*z*): 431 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*4-methoxyphenylhydrazinecarbothioate (**AS7**)*. Yield: 79 %; m.p.: 210–212 °C; Anal. Calcd. for $C_{23}H_{21}N_5O_2S$: C, 64.02; H, 4.91; N, 16.23 %. Found: C, 64.05; H, 4.92; N, 16.26 %; IR (KBr, cm^{-1}): 3310 (NH), 3300 (NH), 3260 (NH), 1682 (C=O), 1608 (C=N), 1290 (OCH_3), 1212 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 3.92 (3H, *s*, OCH_3), 4.15 (2H, *s*, CH_2), 6.52 (1H, *brs*, NH), 6.52–6.56 (1H, *m*, Ar-H), 6.91–6.94 (2H, *m*, Ar-H), 7.24 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.33 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.42 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.82–7.88 (1H, *m*, Ar-H), 8.13 (2H, *d*, *J* =

= 7.5 Hz, Ar-H), 8.21–8.26 (1H, *m*, ArH), 8.81 (1H, *brs*, NH), 10.63 (1H, *brs*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.75, 53.75, 120.61, 123.85, 123.98, 125.42, 125.87, 126.74, 127.22, 127.78, 127.85, 128.35, 128.61, 130.81, 131.86, 138.75, 140.45, 156.79, 162.59, 181.61; MS (*m*/*z*): 431 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*(4-chlorophenyl)hydrazinecarbothioate (**AS8**)*. Yield: 83 %; m.p.: 188–190 °C; Anal. Calcd. for $C_{22}H_{18}ClN_5OS$: C, 60.47; H, 4.12; N, 16.01 %. Found: C, 60.45; H, 4.13; N, 16.06 %; IR (KBr, cm^{-1}): 3321 (NH), 3310 (NH), 3221 (NH), 1690 (C=O), 1620 (C=N), 1210 (C=S); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 4.36 (2H, *s*, CH_2), 6.52–6.57 (2H, *m*, Ar-H), 6.92–6.95 (1H, *m*, Ar-H), 7.07 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.14 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.65 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.81–7.84 (1H, *m*, Ar-H), 7.91 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.93–7.97 (1H, *m*, Ar-H), 9.21 (1H, *brs*, NH), 10.51 (1H, *brs*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 39.75, 120.45, 123.77, 123.89, 125.23, 125.87, 126.81, 127.09, 127.58, 128.34, 127.99, 128.61, 130.81, 131.86, 138.75, 140.45, 156.79, 162.59, 181.61; MS (*m*/*z*): 435 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*(4-nitrophenyl)hydrazinecarbothioate (**AS9**)*. Yield: 72 %; m.p.: 251–253 °C; Anal. calcd. for $C_{22}H_{18}N_6O_3S$: C, 59.02; H, 4.02; N, 18.83 %. Found: C, 59.06; H, 4.00; N, 18.85 %; IR (KBr, cm^{-1}): 3342 (NH), 3313 (NH), 3262 (NH), 1691 (C=O), 1615 (C=N), 1222 (C=S); ^{1}H-NMR (300 MHz. $CDCl_3$, δ / ppm): 4.22 (2H, *s*, CH_2), 6.61–6.65 (2H, *m*, Ar-H), 6.72–6.78 (1H, *m*, ArH), 7.07 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.15 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.44 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.78–7.80 (1H, *m*, Ar-H), 7.91 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.93–7.95 (1H, *m*, A-rH), 8.62 (1H, *brs*, NH), 8.81 (1H, *brs*, NH), 10.51 (1H, *brs*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$ δ ppm): 39.83, 120.39, 123.47, 123.84, 125.42, 125.87, 126.74, 127.22, 127.78, 127.85, 128.35, 128.61, 130.81, 131.66, 138.75, 139.45, 158.69, 161.79, 181.61; MS (*m*/*z*): 446 (M^+).

2-(3-Benzyl-4-oxo-3,4-dihydroquinazolin-2-yl)-N-*(pyridin-2-yl)hydrazinecarbothioate (**AS10**)*. Yield: 79 %; m.p.: 171–172 °C; Anal. Calcd. for $C_{21}H_{18}N_6OS$: C, 62.53; H, 4.45; N, 21.03 %. Found: C, 62.56; H, 4.46; N, 21.05 %; IR (KBr, cm^{-1}): 3350 (NH), 3323 (NH), 3242 (NH), 1691 (C=O), 1615 (C=N), 1210 (C=S); ^{1}H-NMR ($CDCl_3$, δ / ppm): 4.12 (2H, *s*, CH_2), 6.50–6.53 (1H, *m*, Ar-H), 6.51–6.53 (2H, *m*, ArH), 7.25 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.17 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.13 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.35–7.39 (1H, *m*, Ar-H), 7.44 (2H, *d*, *J* = 7.5 Hz, Ar-H), 7.64–7.66 (1H, *m*, Ar-H), 8.35 (1H, *s*, NH), 8.82 (1H, *s*, NH), 9.50 (1H, *s*, NH); ^{13}C-NMR (75 MHz, $CDCl_3$ δ / ppm): 39.83, 108.75, 112.89, 120.48, 123.51, 123.25, 125.42, 127.53, 127.85, 128.35, 128.61, 130.81, 131.86, 137.89, 138.75, 147.75, 157.85, 158.69, 161.78, 181.25; MS (*m*/*z*): 402 (M^+).

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