



SUPPLEMENTARY MATERIAL TO
**Synthesis of quinoline-attached furan-2(3H)-ones having
anti-inflammatory and antibacterial properties with reduced
gastro-intestinal toxicity and lipid peroxidation**

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

The splitting pattern abbreviations for the NMR signals are as follows: *s*, singlet; *d*, doublet; *dd*, double doublet; *t*, triplet; *q*, quartet; *m*, multiplet.

3-[(2-Chloroquinolin-3-yl)methylene]-5-phenyl furan-2(3H)-one (3a). Yield: 52 %; *R*_f 0.72; m.p. 136 °C; Anal. Calcd. for C₂₀H₁₂ClNO₂: C, 71.97; H, 3.62; N, 4.20 %. Found: C, 71.93; H, 3.61; N, 4.21 %; IR (KBr, cm⁻¹): 1740 (lactone C=O), 1560 (ArC=C), 1070 (ArC–N), 864 (ArC–H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 6.84 (1H, *s*, βH), 7.22–7.28 (5H, *m*, H-2,3,4,5,6, phenyl ring), 7.43 (2H, *m*, H-5,7, quinoline ring), 7.68 (1H, *t*, *J* = 7.3 Hz, H-6, quinoline ring), 7.92 (1H, *m*, H-8, quinoline ring), 8.28 (1H, *s*, H-4, quinoline ring), 8.38 (1H, *s*, olefinic H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 98.86, 125.67, 126.89, 127.60, 127.91, 128.06, 128.10, 128.60, 128.84, 129.04, 129.18, 131.22, 131.85, 138.00, 147.44, 150.44, 158.98, 168.07; MS (*m/z*): 334 (M⁺), 336 (M+2).

3-[(2,6-Dichloroquinolin-3-yl)methylene]-5-phenyl furan-2(3H)-one (3b). Yield: 56 %; *R*_f 0.74; m.p. 184 °C; Anal. Calcd. for C₂₀H₁₁Cl₂NO₂: C, 65.24 %; H, 3.01; N, 3.80 %. Found: C, 65.12; H, 3.02; N, 3.81 %; IR (KBr, cm⁻¹): 1740 (lactone C=O), 1562 (ArC=C), 1068 (ArC–N), 822 (ArC–H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 6.60 (1H, *s*, βH), 7.26–7.34 (5H, *m*, H-2,3,4,5,6, phenyl ring), 7.62 (1H, *d*, *J* = 1.9 Hz, H-5, quinoline ring), 7.68 (1H, *dd*, *J* = 8.6, 1.9 Hz, H-7, quinoline ring), 7.80 (1H, *d*, *J* = 8.5 Hz, H-8, quinoline ring), 7.94 (1H, *s*, H-4, quinoline ring), 8.24 (1H, *s*, olefinic H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 99.04, 124.91, 125.18, 126.73, 127.81, 128.91, 129.11, 130.72, 131.95,

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132.13, 132.64, 133.96, 138.12, 147.67, 150.61, 158.93, 168.13; MS (m/z): 368 (M^+), 370 ($M+2$).

3-[(2-Chloro-6-methoxyquinolin-3-yl)methylene]-5-phenyl furan-2(3H)-one (3c). Yield: 64 %; R_f : 0.82; m.p. 154 °C; Anal. Calcd. for $C_{21}H_{14}ClNO_3$: C, 69.33 %; H, 3.88%; N, 3.85%. Found: C, 69.58%; H, 3.87%; N, 3.86%; IR (KBr, cm^{-1}): 1740 (lactone C=O), 1562 (ArC=C), 1066 (ArC-N), 816 (ArC-H); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 3.86 (3H, s, OCH₃), 6.62 (1H, s, β H), 7.20–7.26 (5H, m, H-2,3,4,5,6, phenyl ring), 7.54 (1H, d, J = 1.8 Hz, H-5, quinoline ring), 7.60 (1H, dd, J = 8.0, 1.8 Hz, H-7, quinoline ring), 7.72 (1H, d, J = 8.0 Hz, H-8, quinoline ring), 7.92 (1H, s, H-4, quinoline ring), 8.02 (1H, s, olefinic H); ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 55.56, 98.93, 112.11, 123.73, 124.85, 125.19, 126.45, 128.87, 129.23, 129.46, 130.61, 132.17, 132.52, 138.04, 146.44, 150.31, 158.28, 167.95; MS (m/z): 364 (M^+), 366 ($M+2$).

3-[(2-Chloro-6-methylquinolin-3-yl)methylene]-5-phenyl furan-2(3H)-one (3d). Yield: 64 %; R_f : 0.80; m.p. 176 °C; Anal. Calcd. for $C_{21}H_{14}ClNO_2$: C, 72.52 %; H, 4.06%; N, 4.03%. Found: C, 72.53%; H, 4.07%; N, 4.01%; IR (KBr, cm^{-1}): 1740 (lactone C=O), 1558 (ArC=C), 1062 (ArC-N), 810 (ArC-H); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.15 (3H, s, CH₃), 6.88 (1H, s, β H), 7.18–7.25 (5H, m, H-2,3,4,5,6, phenyl ring), 7.49 (1H, d, J = 1.6 Hz, H-5, quinoline ring), 7.56 (1H, dd, J = 7.8, 1.6 Hz, H-7, quinoline ring), 7.84 (1H, d, J = 7.8 Hz, H-8, quinoline ring), 8.26 (1H, s, H-4, quinoline ring), 8.34 (1H, s, olefinic H). ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 21.06, 100.16, 124.96, 125.10, 125.27, 128.15, 128.90, 129.29, 129.52, 131.48, 131.83, 132.39, 134.12, 136.75, 137.84, 145.95, 150.21, 158.09, 167.83; MS (m/z): 348 (M^+), 350 ($M+2$).

3-[(2-Chloroquinolin-3-yl)methylene]-5-(4-methylphenyl) furan-2(3H)-one (3e). Yield: 34 %; R_f : 0.89; m.p. 204 °C; Anal. Calcd. for $C_{21}H_{14}ClNO_2$: C, 72.52 %; H, 4.06%; N, 4.03%. Found: C, 72.33%; H, 4.05%; N, 4.03%; IR (KBr, cm^{-1}): 1742 (lactone C=O), 1562 (ArC=C), 1066 (ArC-N), 812 (ArC-H); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.18 (3H, s, CH₃), 6.84 (1H, s, β H), 7.20 (2H, d, J = 8.3 Hz, H-3,5, phenyl ring), 7.39 (2H, d, J = 8.2 Hz, H-2,6, phenyl ring), 7.46 (2H, m, H-5,7, quinoline ring), 7.70 (2H, m, H-6,8, quinoline ring), 8.18 (1H, s, H-4, quinoline ring), 8.38 (1H, s, olefinic H). ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 21.14, 100.21, 124.13, 125.44, 127.68, 128.04, 128.83, 128.96, 128.99, 129.14, 129.48, 129.54, 131.39, 131.74, 137.77, 147.04, 150.38, 158.49, 167.84; MS (m/z): 348 (M^+), 350 ($M+2$).

3-[(2,6-Dichloroquinolin-3-yl)methylene]-5-(4-methylphenyl) furan-2(3H)-one (3f). Yield: 32 %; R_f : 0.9; m.p. 264 °C; Anal. Calcd. for $C_{21}H_{13}Cl_2NO_2$: C, 65.99 %; H, 3.43%; N, 3.66%. Found: C, 65.88%; H, 3.42%; N, 3.64%; IR (KBr, cm^{-1}): 1744 (lactone C=O), 1562 (ArC=C), 1064 (ArC-N), 822 (ArC-H); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.22 (3H, s, CH₃), 6.77 (1H, s, β H), 7.25 (2H, d, J = 8.0 Hz, H-3,5, phenyl ring), 7.49 (2H, d, J = 8.0 Hz, H-2,6, phenyl ring),

7.58 (1H, *d*, *J* = 2.1 Hz, H-5, quinoline ring), 7.64 (1H, *dd*, *J* = 8.6, 2.1 Hz, H-7, quinoline ring), 7.84 (1H, *d*, *J* = 8.6 Hz, H-8, quinoline ring), 8.02 (1H, *s*, H-4, quinoline ring), 8.34 (1H, *s*, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.18, 100.31, 124.54, 125.32, 126.16, 128.13, 128.96, 129.18, 129.56, 131.34, 132.06, 132.19, 132.73, 133.00, 137.84, 146.98, 150.42, 158.61, 167.93; MS (*m/z*): 382 (M⁺), 384 (M+2).

3-[(2-Chloro-6-methoxyquinolin-3-yl)methylene]-5-(4-methylphenyl) furan-2(3H)-one (3g). Yield: 48 %; *R*_f: 0.82; m.p. 242 °C; Anal. Calcd. for C₂₂H₁₆ClNO₃: C, 69.94; H, 4.27; N, 3.71 %. Found: C, 70.12; H, 4.28; N, 3.72 %; IR (KBr, cm⁻¹): 1796 (lactone C=C), 1557 (ArC=C), 1060 (ArC-N), 817 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.16 (3H, *s*, CH₃), 3.87 (3H, *s*, OCH₃), 6.85 (1H, *s*, βH), 7.21 (2H, *d*, *J* = 8.2 Hz, H-3,5, phenyl ring), 7.38 (2H, *d*, *J* = 8.1 Hz, H-2,6, phenyl ring), 7.32 (1H, *d*, *J* = 1.8 Hz, H-5, quinoline ring), 7.68 (1H, *s*, H-4, quinoline ring), 7.81 (1H, *d*, *J* = 8.1 Hz, H-7, quinoline ring), 8.26 (1H, *s*, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.16, 55.62, 100.24, 111.65, 123.78, 124.61, 126.08, 126.49, 128.90, 129.12, 129.64, 130.72, 132.18, 132.48, 138.11, 146.53, 150.18, 158.45, 167.74; MS (*m/z*): 378 (M⁺), 380 (M+2).

3-[(2-Chloro-6-methylquinolin-3-yl)methylene]-5-(4-methylphenyl) furan-2(3H)-one (3h). Yield: 48 %; *R*_f: 0.81; m.p. 190 °C; Anal. Calcd. for C₂₂H₁₆ClNO₂: C, 73.03; H, 4.46; N, 3.87 %. Found: C, 72.95; H, 4.45; N, 3.85 %; IR (KBr, cm⁻¹): 1795 (lactone C=O), 1558 (ArC=C), 1062 (ArC-N), 820 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.24 and 2.26 (6H, *s*, 2×CH₃), 6.63 (1H, *s*, βH), 7.28 (2H, *d*, *J* = 8 Hz, H-3,5, phenyl ring), 7.42 (2H, *d*, *J* = 8.1 Hz, H-2,6, phenyl ring), 7.53 (1H, *d*, *J* = 1.6 Hz, H-5, quinoline ring), 7.59 (1H, *dd*, *J* = 8.4, 1.6 Hz, H-7, quinoline ring), 7.74 (1H, *d*, *J* = 8.4 Hz, H-8, quinoline ring), 7.88 (1H, *s*, H-4, quinoline ring), 8.27 (1H, *s*, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.11, 21.29, 100.08, 124.32, 125.33, 125.74, 128.24, 129.06, 129.14, 129.62, 131.57, 131.90, 132.58, 134.18, 136.94, 137.78, 146.11, 150.05, 158.14, 167.90; MS (*m/z*): 362 (M⁺), 364 (M+2).

3-[(2-Chloroquinolin-3-yl)methylene]-5-(2,4-dimethylphenyl) furan-2(3H)-one (3i). Yield: 36 %; *R*_f: 0.92; m.p. 138 °C; Anal. Calcd. for C₂₂H₁₆ClNO₂: C, 73.03; H, 4.46; N, 3.87 %. Found: C, 73.18; H, 4.45; N, 3.86 %; IR (KBr, cm⁻¹): 1741 (lactone C=O), 1560 (ArC=C), 1064 (ArC-N), 824 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.18 and 2.22 (6H, *s*, 2 x CH₃), 6.61 (1H, *s*, βH), 7.11–7.18 (3H, *m*, H-3,5,6, phenyl ring), 7.42–7.76 (5H, *m*, H-4,5,6,7,8, quinoline ring), 8.25 (1H, *s*, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.42, 22.19, 102.20, 124.43, 126.90, 127.19, 127.89, 128.00, 128.29, 128.57, 128.67, 129.13, 131.78, 132.64, 137.01, 137.95, 141.24, 147.34, 150.44, 159.55, 167.94; MS (*m/z*): 362 (M⁺), 364 (M+2).

3-[(2,6-Dichloroquinolin-3-yl)methylene]-5-(2,4-dimethylphenyl) furan-2(3H)-one (**3j**). Yield: 42 %; R_f : 0.87; m.p. 184 °C; Anal. Calcd. for $C_{22}H_{15}Cl_2NO_2$: C, 66.68; H, 3.82; N, 3.53 %. Found: C, 66.72; H, 3.80; N, 3.54 %; IR (KBr, cm^{-1}): 1742 (lactone C=O), 1562 (ArC=C), 1062 (ArC-N), 821 (ArC-H); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.28 and 2.32 (6H, s, 2 x CH_3), 6.60 (1H, s, βH), 7.06 (1H, d, $J = 1.5$ Hz, H-3, phenyl ring), 7.14 (1H, dd, $J = 7.2, 1.5$ Hz, H-5, phenyl ring), 7.32 (1H, d, $J = 7.2$ Hz, H-6, phenyl ring), 7.56 (1H, d, $J = 1.7$ Hz, H-5, quinoline ring), 7.62 (1H, dd, $J = 7.4, 1.7$ Hz, H-7, quinoline ring), 7.80 (1H, d, $J = 7.4$ Hz, H-8, quinoline ring), 8.10 (1H, s, H-4, quinoline ring), 8.28 (1H, s, olefinic H). ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 21.49, 22.21, 102.34, 124.56, 126.97, 127.25, 127.98, 128.21, 128.69, 130.81, 131.54, 131.85, 132.73, 133.65, 137.18, 138.11, 141.33, 147.62, 150.73, 159.87, 168.05; MS (m/z): 396 (M^+), 398 ($M+2$).

3-[(2-Chloro-6-methoxyquinolin-3-yl)methylene]-5-(2,4-dimethylphenyl) furan-2(3H)-one (**3k**). Yield: 36 %; R_f : 0.92; m.p. 200 °C; Anal. Calcd. for $C_{23}H_{18}ClNO_3$: C, 70.50; H, 4.63; N, 3.57 %. Found: C, 70.66; H, 4.62; N, 3.58 %; IR (KBr, cm^{-1}): 1756 (lactone C=O), 1612 (ArC=C), 1060 (ArC-N), 818 (ArC-H); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.28 and 2.34 (6H, s, $2 \times CH_3$), 3.98 (3H, s, OCH_3), 6.62 (1H, s, βH), 6.96 (1H, d, $J = 1.6$ Hz, H-3, phenyl ring), 7.11 (1H, dd, $J = 7.2, 1.6$ Hz, H-5, phenyl ring), 7.26 (1H, d, $J = 7.2$ Hz, H-6, phenyl ring), 7.34 (1H, d, $J = 1.8$ Hz, H-5, quinoline ring), 7.52 (1H, dd, $J = 7.7, 1.8$ Hz, H-7, quinoline ring), 7.64 (1H, d, $J = 7.6$ Hz, H-8, quinoline ring), 7.72 (1H, s, H-4, quinoline ring), 8.26 (1H, s, olefinic H). ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 21.45, 22.11, 103.04, 111.59, 124.16, 126.33, 127.02, 127.19, 129.56, 131.83, 131.92, 132.08, 133.14, 137.09, 137.67, 142.11, 146.43, 150.76, 158.93, 159.46, 167.71; MS (m/z): 392 (M^+), 394 ($M+2$).

3-[(2-Chloro-6-methylquinolin-3-yl)methylene]-5-(2,4-dimethylphenyl) furan-2(3H)-one (**3l**). Yield: 32 %; R_f : 0.91; m.p. 174 °C; Anal. Calcd. for $C_{23}H_{18}ClNO_2$: C, 73.50; H, 4.83; N, 3.73 %. Found: C, 73.53; H, 4.82; N, 3.72 %; IR (KBr, cm^{-1}): 1755 (lactone C=O), 1610 (ArC=C), 1068 (ArC-N), 824 (ArC-H); 1H -NMR: 2.20, 2.24 and 2.30 (9H, s, $3 \times CH_3$), 6.60 (1H, s, βH), 7.15–7.22 (3H, m, H-3,5,6, phenyl ring), 7.48 (1H, d, $J = 1.7$ Hz, H-5, quinoline ring), 7.56 (1H, dd, $J = 7.8, 1.7$ Hz, H-7, quinoline ring), 7.68 (1H, d, $J = 7.7$ Hz, H-8, quinoline ring), 7.78 (1H, s, H-4, quinoline ring), 8.28 (1H, s, olefinic H). ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 20.98, 21.31, 21.84, 101.63, 124.11, 124.38, 126.93, 128.12, 129.16, 130.92, 131.12, 131.65, 132.78, 132.94, 137.16, 137.91, 138.11, 141.69, 146.21, 150.39, 158.64, 167.84; MS (m/z): 376 (M^+), 378 ($M+2$).

5-(4-Bromophenyl)3-[(2-chloroquinolin-3-yl)methylene] furan-2(3H)-one (**3m**). Yield: 30 %; R_f : 0.85; m.p. 216 °C; Anal. Calcd. for $C_{20}H_{11}BrClNO_2$: C, 58.21; H, 2.69; N, 3.39 %. Found: C, 58.38; H, 2.70; N, 3.38 %; IR (KBr, cm^{-1}): 1748

(lactone C=O), 1612 (ArC=C), 1062 (ArC-N), 826 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 6.71 (1H, s, βH), 7.36 (2H, d, J = 8.8 Hz, H-3,5, phenyl ring), 7.48 (2H, d, J = 8.7 Hz, H-2,6, phenyl ring), 7.58–7.68 (4H, m, H-5,6,7,8, quinoline ring), 8.08 (1H, s, H-4, quinoline ring), 8.16 (1H, s, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 99.34, 125.66, 126.55, 126.65, 126.88, 127.02, 127.95, 128.04, 128.66, 129.94, 131.95, 132.36, 138.02, 147.51, 150.37, 158.04, 167.66; MS (m/z): 413 (M⁺), 415 (M+2).

5-(4-Bromophenyl)-3-[(2,6-dichloroquinolin-3-yl)methylene] furan-2(3H)-one (3n). Yield: 32 %; R_f: 0.86; m.p. 156 °C; Anal. Calcd. for C₂₀H₁₀BrCl₂NO₂: C, 53.73; H, 2.25; N, 3.13 %. Found: C, 53.62; H, 2.23; N, 3.12 %; IR (KBr, cm⁻¹): 1750 (lactone C=O), 1580 (ArC=C), 1060 (ArC-N), 818 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 6.60 (1H, s, βH), 7.35–7.66 (7H, m, H-5,7,8 of quinoline ring merged with H-2,3,5,6 of phenyl ring), 8.04 (1H, s, H-4, quinoline ring), 8.21 (1H, s, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 100.12, 125.69, 126.43, 126.63, 127.09, 128.14, 128.26, 128.48, 130.06, 131.88, 132.29, 134.39, 138.14, 146.53, 150.84, 158.13, 167.74; MS (m/z): 447 (M⁺), 449 (M+2).

5-(4-Bromophenyl)-3-[(2-chloro-6-methoxyquinolin-3-yl)methylene] furan-2(3H)-one (3o). Yield: 38 %; R_f: 0.89; m.p. 264 °C; Anal. Calcd. for C₂₁H₁₃BrClNO₃: C, 56.98; H, 2.96; N, 3.16 %. Found: C, 56.83; H, 2.97; N, 3.17 %; IR (KBr, cm⁻¹): 1748 (lactone C=O), 1612 (ArC=C), 1064 (ArC-N), 812 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.78 (1H, s, OCH₃), 6.64 (1H, s, βH), 7.34–7.58 (7H, m, H-5,7,8 of quinoline ring merged with H-2,3,5,6 of phenyl ring), 7.94 (1H, s, H-4, quinoline ring), 8.08 (1H, s, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 55.68, 99.14, 111.36, 124.52, 124.89, 125.38, 126.48, 126.51, 127.14, 128.19, 131.75, 133.43, 136.31, 144.46, 149.35, 158.06, 160.08, 167.68; MS (m/z): 443 (M⁺), 445 (M+2).

5-(4-Bromophenyl)-3-[(2-chloro-6-methylquinolin-3-yl)methylene] furan-2(3H)-one (3p). Yield: 42 %; R_f: 0.83; m.p. 174 °C; Anal. Calcd. for C₂₁H₁₃BrClNO₂: C, 59.11 ; H, 3.07; N, 3.28 %. Found: C, 58.96; H, 3.08; N, 3.29 %; IR (KBr, cm⁻¹): 1748 (lactone C=O), 1602 (ArC=C), 1066 (ArC-N), 810 (ArC-H); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.20 (1H, s, CH₃), 6.60 (1H, s, βH), 7.34 (2H, d, J = 8.6 Hz, H-3,5, phenyl ring), 7.44 (2H, d, J = 8.6 Hz, H-2,6, phenyl ring), 7.50 (1H, d, J = 1.9 Hz, H-5, quinoline ring), 7.60 (1H, dd, J = 8.3, 1.9 Hz, H-7, quinoline ring), 7.78 (1H, d, J = 8.4 Hz, H-8, quinoline ring), 7.96 (1H, s, H-4, quinoline ring), 8.21 (1H, s, olefinic H). ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 20.93, 99.44, 125.18, 125.21, 126.32, 126.72, 127.19, 127.98, 128.27, 131.76, 131.84, 131.93, 136.53, 138.19, 146.12, 148.49, 158.19, 167.70; MS (m/z): 427 (M⁺), 429 (M+2).