Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 76 (9) S1–S5 (2011) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Synthesis and antimicrobial activities of novel *N*-substituted 8-(1-alkyl/alkylsulphonyl/alkoxycarbonyl-benzimidazol-2--ylmethoxy)-5-chloroquinolines

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J. Serb. Chem. Soc. 76 (9) (2011) 1199–1206

SPECTRAL CHARACTERIZATION OF THE SYNTHESIZED COMPOUNDS

*[(5-Chloroquinolin-8-yl)oxy]acetic acid (**2**)*. Yield: 80 %; m. p. 222–225 °C. IR (KBr, cm^{-1}): 2799 (O–H stretching), 3068 (C–H stretching of aromatic ring), 1279 and 1257 (C–O–C stretching), 1107 (C–Cl stretching). ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 4.95 (2H, *s*, $-OCH_2$), 7.13 (1H, *d*, aromatic, J = 8.0 Hz), 7.67 (1H, *d*, J = 8.8 Hz, aromatic), 7.71–7.74 (1H, *m*, aromatic), 8.50 (1H, *d*, J = = 8.0 Hz, aromatic), 8.96–8.97 (1H, *m*, aromatic), 13.08 (1H, *bs*, –COOH). ^{13}C--NMR (100 MHz, DMSO-d_6, δ / ppm): 66.2 ($O–CH_2$), 110.92, 122.33, 124.02, 127.09, 127.50, 133.31, 140.64, 150.70, 153.57 (aromatic), 170.69 (–COOH). MS (*m*/*z*): 238.1 (M^+).

*8-[(1*H*-Benzimidazol-2-yl)methoxy]-5-chloroquinoline (**3**)*. Yield: 81 %; M. p. 214–217 °C. IR (KBr, cm^{-1}): 3340 (N–H stretching), 3048 (C–H stretching of aromatic ring), 1273 and 1257 (C–O–C stretching), 1101 (C–Cl stretching). ^{1}H--NMR (400 MHz, DMSO-d_6, δ / ppm): 5.65 (2H, *s*, $-OCH_2$), 7.22–7.25 (3H, *m*, aromatic), 7.54 (1H, *d*, J = 8.4 Hz, aromatic), 7.59–7.63 (3H, *m*, aromatic), 8.56 (1H, *d*, J = 8.6 Hz and J = 1.6 Hz, aromatic), 8.92 (1H, *bs*, aromatic), 12.8 (1H, *bs*, N–H). ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 65.05 ($O–CH_2$), 110.38, 115.09, 121.82, 122.25, 122.50, 126.30, 126.41, 132.41, 140.20, 149.30, 149.36, 152.93 (aromatic). MS (*m*/*z*): 310.1 (M^+).

*5-Chloro-8-[(1-methyl-1*H*-benzimidazol-2-yl)methoxy]quinoline (**4a**)*. M. p. 215–220 °C. IR (KBr, cm^{-1}): 3049 (C–H stretching of aromatic ring), 1254 and 1241 (C–O–C stretching), 1092 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 3.98 (3H, *s*, $-NCH_3$), 5.75 (2H, *s*, $-OCH_2$), 7.27–7.31 (3H, *m*, aromatic), 7.43–7.49 (2H, *m*, aromatic), 7.54–7.56 (1H, *m*, aromatic), 7.78–7.79

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(1H, *m*, aromatic), 8.52 (1H, *d*, *J* = 8.3 Hz, aromatic), 8.99 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 29.46 (CH_3 of N–methyl), 63.76 (O–CH_2), 108.77, 110.04, 118.81, 121.27, 121.65, 122.29, 122.37, 125.45, 126.09, 132.00, 135.40, 139.89, 141.08, 148.00, 148.99, 151.79 (aromatic). MS (*m*/*z*): 324.1 (M^+).

*5-Chloro-8-[(1-ethyl-1*H*-benzimidazol-2-yl)methoxy]quinoline (**4b**)*. M. p. 225–228 °C. IR (KBr, cm^{-1}): 3049 (C–H stretching of aromatic ring), 1255 and 1242 (C–O–C stretching), 1095 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.40 (3H, *t*, *J* = 6.8 Hz, –CH_3), 4.51 (2H, *q*, *J* = 6.8 Hz, –NCH_2), 5.76 (2H, *s*, –OCH_2), 7.27–7.36 (3H, *m*, aromatic), 7.48–7.54 (3H, *m*, aromatic), 7.80–7.81 (1H, *m*, aromatic), 8.53 (1H, *d*, *J* = 8.2 Hz, aromatic), 8.98 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 15.19 (CH_3 of *N*-ethyl), 39.36 (N–CH_2), 64.64 (O–CH_2), 109.74, 110.93, 120.17, 122.32, 122.37, 123.26, 123.40, 126.50, 127.14, 133.06, 135.24, 140.82, 142.38, 148.49, 149.81, 152.71 (aromatic). MS (*m*/*z*): 338.1 (M^+).

*5-Chloro-8-[(1-propyl-1*H*-benzimidazol-2-yl)methoxy] quinoline (**4c**)*. M. p. 178–180 °C. IR (KBr, cm^{-1}): 3049 (C–H stretching of aromatic ring), 1254 and 1241 (C–O–C stretching), 1093 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 0.92 (3H, *t*, *J* = 7.2 Hz, –CH_3), 1.81–1.86 (2H, *m*, –CH_2 of *N*-propyl), 4.41 (2H, *t*, *J* = 7.3 Hz, –NCH_2), 5.76 (2H, *s*, –OCH_2), 7.27–7.30 (3H, *m*, aromatic), 7.47–7.56 (3H, *m*, aromatic), 7.80–7.81 (1H, *m*, aromatic), 8.53 (1H, *d*, *J* = 8.3 Hz, aromatic)**,** 8.98 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / / ppm): 11.30 (CH_3 of *N*-propyl), 23.22 (CH_2 of *N*-propyl), 46.03 (N–CH_2), 64.83 (O–CH_2), 110.03, 111.10, 120.12, 122.29, 122.37, 123.20, 123.44, 126.50, 127.13, 133.05, 135.63, 140.88, 142.29, 148.76, 149.79, 152.75 (aromatic). MS (m/z): 352.1 (M^+).

*8-[(1-Butyl-1*H*-benzimidazol-2-yl)methoxy]-5-chloroquinoline (**4d**)*. M. p. 174–178 °C. IR (KBr, cm^{-1}): 3050 (C–H stretching of aromatic ring), 1254 and 1241 (C–O–C stretching), 1093 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 0.81 (3H, *t*, *J* = 6.7 Hz, –CH_3 of *N*-butyl), 1.32–1.41 (2H, *m*, –CH_2 of *N*-butyl), 1.71–1.79 (2H, *m*, –CH_2 of *N*-butyl), 4.42 (2H, *t*, *J* = 6.7 Hz, –NCH_2), 5.75 (2H, *s*, –OCH_2), 7.27–7.34 (3H, *m*, aromatic), 7.49–7.54 (3H, *m*, aromatic), 7.78–7.79 (1H, *m*, aromatic), 8.52 (1H, *d*, *J* = 7.7 Hz, aromatic), 8.98 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.70 (CH_3 of *N*-butyl), 20.22 (CH_2 of *N*-butyl), 32.07 (CH_2 of *N*-butyl), 44.48 (N–CH_2), 64.73 (O–CH_2), 109.97, 110.96, 120.12, 122.28, 122.38, 123.20, 123.41, 126.51, 127.13, 133.06, 135.62, 140.86, 142.29, 148.66, 149.77, 152.70 (aromatic). MS (*m*/*z*): 366.2 (M^+).

*5-Chloro-8-[(1-pentyl-1*H*-benzimidazol-2-yl)methoxy]quinoline (**4e**)*. M. p. 147–150 °C. IR (KBr, cm^{-1}): 3054 (C–H stretching of aromatic ring), 1254 and 1240 (C–O–C stretching), 1093 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 0.73 (3H, *t*, *J* = 7.2 Hz, –CH_3 of *N*-pentyl), 1.13–1.22 (2H, *m*, –CH_2 of

N-pentyl), 1.27–1.34 (2H, *m*, –CH_2 of *N*-pentyl), 1.72–1.80 (2H, *m*, –CH_2 of *N*--pentyl), 4.42 (2H, *t*, *J* =7.7 Hz, –NCH_2), 5.76 (2H, *s*, –OCH_2), 7.28–7.32 (2H, *m*, aromatic), 7.33–7.37 (1H, *m*, aromatic), 7.47–7.56 (3H, *m*, aromatic), 7.78––7.81 (1H, *m*, aromatic), 8.52 (1H, *dd*, *J* = 8.6 Hz and 1.6 Hz, aromatic), 8.98 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.77 (CH_3 of *N*--pentyl), 22.32 (CH_2 of *N*-pentyl), 29.01 (CH_2 of *N*-pentyl), 29.71 (CH_2 of *N*--pentyl), 44.68 (N–CH_2), 64.73 (O–CH_2), 109.99, 110.93, 120.11, 122.28, 122.36, 123.20, 123.37, 126.50, 127.12, 133.05, 135.59, 140.84, 142.29, 148.68, 149.74, 152.70 (aromatic). MS (*m*/*z*): 380.2 (M^+).

*8-[(1-Benzyl-1*H*-benzimidazol-2-yl)methoxy]-5-chloroquinoline (**4f**)*. M. p. 208–210 °C. IR (KBr, cm^{-1}): 3061 (C–H stretching of aromatic ring), 1252 and 1239 (C–O–C stretching), 1093 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 5.68 (2H, *s*, –NCH_2), 5.70 (2H, *s*, –OCH_2), 6.92–6.93 (2H, *m*, aromatic), 7.0–7.1 (3H, *m*, aromatic), 7.23–7.38 (3H, *m*, aromatic), 7.36–7.38 (1H, *m*, aromatic), 7.44–7.51 (2H, *m*, aromatic), 7.82 (1H, *d*, *J* = 7.7 Hz, aromatic), 8.47 (1H, *d*, *J* = 8.3 Hz, aromatic), 8.88 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 47.61 (N–CH_2), 64.91 (O–CH_2), 110.21, 110.90, 120.18, 122.31, 122.56, 123.48, 123.58, 126.30, 126.33, 127.07, 127.46, 128.50, 132.91, 135.73, 136.04, 140.83, 142.29, 149.12, 149.73, 152.61 (aromatic). MS (*m*/*z*): 400.2 (M^+).

*8-{[1-(4-Bromobenzyl)-1*H*-benzimidazol-2-yl]methoxy}-5-chloroquinoline (**4g**)*. M. p. 244–248 °C. IR (KBr, cm^{-1}): 3060 (C–H stretching of aromatic ring), 1254 and 1241 (C–O–C stretching), 1091 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 5.68 (2H, *s*, –NCH_2), 5.71 (2H, *s*, –OCH_2), 6.78 (2H, *d*, *J* = 8.3 Hz, aromatic), 7.09 (2H, *d*, *J* = 8.3 Hz, aromatic), 7.25–7.31 (3H, *m*, aromatic), 7.35 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.47 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.55–7.58 (1H, *m*, aromatic), 7.80 (1H, *d*, *J* = 7.7 Hz, aromatic), 8.50 (1H, *d*, *J* = 8.5 Hz, aromatic), 8.84 (1H, *bs*, aromatic). MS (*m*/*z*): 480.1 (M^+).

*5-Chloro-8-{[1-(methylsulphonyl)-1*H*-benzimidazol-2-yl]methoxy}quinoline (**4h**)*. M. p. 183–186 °C. IR (KBr, cm^{-1}): 3055 (C–H stretching of aromatic ring), 1249 and 1237 (C–O–C stretching), 1165 (S=O stretching), 1096 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 3.81 (3H, *s*, –SO_2CH_3), 5.70 (2H, *s*, –OCH_2), 7.21 (1H, *d*, *J* = 8.4 Hz aromatic), 7.40–7.48 (2H, *m*, aromatic), 7.52––7.56 (1H, *m*, aromatic), 7.60 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.82 (1H, *d*, *J* = 7.2 Hz, aromatic), 7.97 (1H, *d*, *J* = 8.3 Hz, aromatic), 8.56 (1H, *dd*, *J* = 8.5 Hz and 1.5 Hz, aromatic), 8.82 (1H, *dd*, *J* = 8.3 Hz and 1.56 Hz, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 38.00 (SO_2–CH_3), 59.84 (O–CH_2), 104.23, 108.52, 116.25, 117.80, 118.71, 120.26, 121.40, 121.76, 122.53, 128.46, 128.76, 135.73, 136.52, 143.24, 144.73, 147.93 (aromatic). MS (*m*/*z*): 388.1 (M^+).

*5-Chloro-8-{[1-(phenylsulphonyl)-1*H*-benzimidazol-2-yl] methoxy}quinoline (**4i**)*. M. p. 173–177 °C. IR (KBr, cm^{-1}): 3059 (C–H stretching of aromatic ring),

1248 and 1235 (C–O–C stretching), 1178 (S=O stretching), 1093 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 5.89 (2H, *s*, $–OCH_2$), 7.25 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.33–7.42 (4H, *m*, aromatic), 7.52–7.59 (3H, *m*, aromatic), 7.75 (1H, *d*, *J* = 7.5 Hz, aromatic), 7.95 (1H, *d*, *J* = 7.4 Hz, aromatic), 8.36 (2H, *dd*, *J* = 8.4 Hz and 2.8 Hz, aromatic), 8.55 (1H, *dd*, *J* = 8.5 Hz and 1.6 Hz, aromatic), 9.01 (1H, *dd*, *J* = 8.3 Hz and 1.7 Hz, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 64.93 ($O–CH_2$), 110.13, 113.39, 121.02, 122.44, 123.49, 124.94, 125.94, 126.46, 127.26, 128.12, 129.40, 132.87, 133.07, 134.64, 137.61, 140.81, 141.66, 148.26, 149.74, 153.08 (aromatic). MS (*m*/*z*): 450.2 (M^+).

*5-Chloro-8-{[1-(4-methylphenylsulphonyl)-1*H*-benzimidazol-2-yl]methoxy}-quinoline (**4j**)*. M. p. 181–184 °C. IR (KBr, cm^{-1}): 3057 (C–H stretching of aromatic ring), 1256 and 1240 (C–O–C stretching), 1175 (S=O stretching), 1092 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.33 (3H, *s*, $–CH_3$), 5.88 (2H, *s*, $–OCH_2$), 7.17 (2H, *d*, *J* = 8.4 Hz, aromatic), 7.25 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.33–7.44 (2H, *m*, aromatic), 7.54 (1H, *d*, *J* = 7.4 Hz, aromatic), 7.57–7.60 (1H, *m*, aromatic), 7.75 (1H, *d*, *J* = 7.5 Hz, aromatic), 7.95 (1H, *d*, *J* = 8.1 Hz, aromatic), 8.20 (2H, *d*, *J* = 8.4 Hz, aromatic), 8.57 (1H, *dd*, *J* = 8.5 Hz and 1.6 Hz, aromatic), 9.02 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 21.69 (CH_3), 64.95 ($O–CH_2$), 110.12, 113.40, 120.96, 122.43, 123.43, 124.84, 125.82, 126.46, 127.24, 128.11, 130.02, 132.89, 133.05, 134.66, 140.81, 141.69, 145.98, 148.25, 149.72, 153.13 (aromatic). MS (*m*/*z*): 464 (M^+).

*Methyl 2-{[(5-chloroquinolin-8-yl)oxy]methyl}-1*H*-benzimidazole-1-carboxylate (**4k**)*. M. p. 140–144 °C. IR (KBr, cm^{-1}): 3060 (C–H stretching of aromatic ring), 1758 (C=O stretching), 1255 and 1233 (C–O–C stretching), 1093 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 4.08 (3H, *s*, $–OCH_3$), 5.83 (2H, *s*, $–OCH_2$), 7.17 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.36–7.40 (2H, *m*, aromatic), 7.52–7.57 (2H, *m*, aromatic), 7.77 (1H, *d*, *J* = 7.4 Hz, aromatic), 7.95 (1H, *dd*, *J* = = 7.1 Hz and 1.6 Hz, aromatic), 8.55 (1H, *dd*, *J* = 8.5 Hz and 1.6 Hz, aromatic), 8.99 (1H, *bs*, aromatic). MS (*m*/*z*): 368.1 (M^+).

*Ethyl 2-{[(5-chloroquinolin-8-yl)oxy]methyl}-1*H*-benzimidazole-1-carboxylate (**4l**)*. M. p. 134–138 °C. IR (KBr, cm^{-1}): 3063 (C–H stretching of aromatic ring), 1758 (C=O stretching), 1259 and 1230 (C–O–C stretching), 1090 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.43 (3H, *t*, *J* = 7.1 Hz, $–CH_3$), 4.53 (2H, *q*, *J* = 7.1 Hz, $–COOCH_2$), 5.82 (2H, *s*, $–OCH_2$), 7.17 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.34–7.41 (2H, *m*, aromatic), 7.52–7.58 (2H, *m*, aromatic), 7.77 (1H, *d*, *J* = 8.2 Hz, aromatic), 7.97 (1H, *d*, *J* = 8.5 Hz, aromatic), 8.56 (1H, *d*, *J* = = 8.4 Hz, aromatic), 9.0 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 14.10 ($–CH_3$), 64.54 ($COO–CH_2$), 66.26 ($O–CH_2$), 110.08, 114.92, 120.54, 122.40, 123.25, 124.67, 125.48, 126.29, 127.13, 132.88, 133.01, 140.70, 142.08, 149.81, 150.02, 150.08, 153.38 (aromatic). MS (*m*/*z*): 382.2 (M^+).

*Benzyl 2-{[(5-chloroquinolin-8-yl)oxy]methyl}-1*H*-benzimidazole-1-carboxylate (**4m**)*. M. p. 167–170 °C. IR (KBr, cm^{-1}): 3060 (C–H stretching of aromatic ring), 1759 (C=O stretching), 1254 and 1238 (C–O–C stretching), 1098 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 5.36 (2H, *m*, $–COOCH_2$), 5.66 (2H, *s*, $–OCH_2$), 6.94 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.17–7.31 (7H, *m*, aromatic), 7.38 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.47–7.50 (1H, *m*, aromatic), 7.67–7.70 (1H, *m*, aromatic), 7.89–7.91 (1H, *m*, aromatic), 8.47 (1H, *d*, *J* = 8.4 Hz, aromatic), 8.92 (1H, *bs*, aromatic). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 66.24 ($O–CH_2$), 70.14 ($COO–CH_2$), 109.94, 114.98, 120.61, 122.37, 123.19, 124.74, 125.65, 126.27, 127.13, 128.73, 128.86, 129.03, 132.91, 133.10, 133.74, 140.77, 142.12, 149.72, 149.84, 149.88, 153.35 (aromatic). MS (*m*/*z*): 466.2 (M^+).

*2,2,2-Trichloroethyl 2-{[(5-chloroquinolin-8-yl)oxy]methyl}-1*H*-benzimidazole-1-carboxylate (**4n**)*. M. p. 121–125 °C. IR (KBr, cm^{-1}): 3064 (C–H stretching of aromatic ring), 1759 (C=O stretching), 1253 and 1230 (C–O–C stretching), 1099 (C–Cl stretching). ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 5.10 (2H, *s*, $–COOCH_2$), 5.66 (2H, *s*, $–OCH_2$), 7.16 (1H, *d*, *J* = 8.4 Hz, aromatic), 7.37–7.45 (2H, *m*, aromatic), 7.51–7.56 (2H, *m*, aromatic), 7.79 (1H, *dd*, *J* = 7.2 Hz and 2.0 Hz, aromatic), 8.10 (1H, *dd*, *J* = 7.0 Hz and 1.3 Hz, aromatic), 8.54 (1H, *dd*, *J* = = 8.5 Hz and 1.6 Hz, aromatic), 8.97 (1H, *bs*, aromatic). MS (*m*/*z*): 486.1 (M^+).