Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 78 (8) S91–S92 (2013) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Synthesis, spectroscopic characterization and pharmacological evaluation of oxazolone derivatives

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J. Serb. Chem. Soc. 78 (8) (2013) 1127–1134

ANALYTIC AND SPECTRAL DATA FOR THE SYNTHESIZED COMPOUNDS

4-[(Z)-(4-Chloro-3-nitrophenyl)methylidene]-2-phenyl-5(4H)-oxazolone (***2***). R_f: 0.67 (ethyl acetate: hexane, 2:8); Anal. Calcd. for $C_{16}H_9ClN_2O_4$: C, 58.46; H, 2.76; N, 8.52 %. Found: C, 58.41; H, 2.77; N, 8.50 %; IR (KBr, cm^{-1}): 1799, 1659, 1536, 1451, 1324, 1172, 868, 644; ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 7.13 (1H, *s*, 6-H), 7.52–7.68 (5H, *m*, Ar-H), 8.15–8.18 (2H, *m*, Ar-H), 8.80 (1H, *s*, Ar-H); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 166.70, 164.98, 146.80, 136.57, 135.84, 132.77, 132.03, 129.36, 129.16, 128.68, 127.88, 126.23, 125.60, 125.49; EI-MS (*m*/*z* (relative abundance, %)): 330 (M+2, 12.3), 328 (M^+, 37.5), 105 (100), 77 (71.6), 44 (93.1).

4-[(Z,2E)-3-(4-Methoxyphenyl)-2-propenylidene]-2-phenyl-5(4H)-oxazolone (***3***). R_f: 0.70 (ethyl acetate: hexane, 2:8); Anal. Calcd. for $C_{19}H_{15}NO_3$: C, 74.74; H, 4.95; N, 4.59 %. Found: C, 74.70; H, 4.97; N, 4.57 %; IR (KBr, cm^{-1}): 1781, 1652, 1593, 1328, 1256, 1161, 865; ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 3.84 (3H, *s*, OCH_3), 7.38 (1H, *d*, *J* = 14.5 Hz, C**H**–CH=CH), 7.42 (1H, *d*, *J* = 9.8 Hz, CH–CH=C**H**), 6.95 (1H, *dd*, *J* = 9.8, 14.5 Hz, CH–C**H**=CH), 7.45–7.58 (5H, *m*, Ar-H), 7.92–8.12 (4H, *m*, Ar-H); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 166.03, 162.37, 159.32, 135.13, 134.20, 132.51, 132.03, 129.45, 129.42, 129.36, 129.16, 128.71, 127.81, 114.57, 14.02; EI-MS (*m*/*z* (relative abundance, %)): 305 (M^+, 39.2), 277 (3.0), 105 (100), 77 (29.4), 44 (68.3).

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*4-[(Z)-(4-Chloro-3-nitrophenyl)methylidene]-2-methyl-5(4H)-oxazolone (**4**).* R_f: 0.77 (ethyl acetate:hexane, 2:8); Anal. Calcd. for $C_{11}H_7ClN_2O_4$: C, 49.55; H, 2.65; N, 10.51 %. Found: C, 49.57; H, 2.61; N, 10.53 %; IR (KBr, cm^{-1}): 3072, 1805, 1661, 1607, 1533, 1360, 1261, 1168, 890, 657, 629; ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.42 (3H, *s*, CH_3), 7.24 (1H, *s*, 6-H), 7.57–8.10 (2H, *m*, Ar-H), 8.70 (1H, *s*, Ar-H); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 168.38, 160.19, 146.88, 136.57, 132.77, 129.90, 128.61, 125.64, 125.41, 125.01, 11.12; EI-MS (*m*/*z* (relative abundance, %)): 268 (M^{+2}, 59.4), 266 (M^+, 29), 105 (3.9), 114 (64.5) 77 (35), 44 (100).

*4-[(Z)-(3,5-Dibromo-4-hydroxyphenyl)methylidene]-2-methyl-5(4H)-oxazolone (**5**).* R_f: 0.65 (ethyl acetate:hexane, 2:8); Anal. Calcd. for $C_{11}H_7Br_2NO_3$: C, 36.60; H, 1.95; N, 3.88 %. Found: C, 36.62; H, 1.94; N, 3.85 %; IR (KBr, cm^{-1}): 3071, 1760, 1670, 1580, 1479, 1302, 1139, 876, 646; ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.14 (3H, *s*, CH_3), 7.24 (1H, *s*, 6-H), 7.97 (2H, *s*, Ar-H), 9.88 (1H, *s*, OH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 168.38, 160.19, 151.51, 131.35, 129.02, 126.27, 125.52, 113.41, 14.03; EI-MS (*m*/*z* (relative abundance, %)): 364 (M+4, 10), 362 (M+2, 12), 360 (M^+, 39), 105 (100), 77 (12), 44 (91.8).

*4-[(Z)-(3,5-Dibromo-4-hydroxyphenyl)methylidene]-2-phenyl-5(4H)-oxazolone (**6**).* R_f: 0.72 (ethyl acetate:hexane, 2:8); Anal. Calcd. for $C_{16}H_9Br_2NO_3$: C, 45.42; H, 2.14; N, 3.31 %. Found: C, 45.40; H, 2.15; N, 3.32 %; IR (KBr, cm^{-1}): 3075, 1650, 1541, 1416, 1241, 652, 644; ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 7.26 (1H, *s*, 6-H), 7.97 (2H, *s*, Ar-H), 7.24–8.32 (5H, *m*, Ar-H) 9.88 (1H, *s*, OH); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 166.70, 164.91, 151.51, 134.96, 132.01, 131.31, 129.10, 127.88, 127.11, 126.27, 113.44; EI-MS (*m*/*z* (relative abundance, %)): 427 (M+4, 2) 425 (M+2, 3), 423 (M^+, 2.5), 105 (100), 77 (76.8), 44 (73.5).

*4-[(Z)-(2-Ethoxyphenyl)methylidene]-2-phenyl-5(4H)-oxazolone (**7**).* R_f: 0.72 (ethyl acetate: hexane, 2:8); Anal. Calcd. for $C_{18}H_{15}NO_3$: C, 73.71; H, 5.15; N, 4.78 %. Found: C, 73.70; H, 5.17; N, 4.77 %; IR (KBr, cm^{-1}): 1788, 1768, 1664, 1595, 1557, 1488, 1447, 1248, 1168, 1045; ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 1.50 (3H, *t*, J = 6.5 Hz, C**H**$_3$CH$_2$O), 4.15 (2H, *q*, J = 6.5 Hz, CH$_3$C**H**$_2$O), 6.88––7.08 (5H, *m*, Ar-H), 7.24 (1H, *s*, 6-H), 7.35–8.87 (4H, *m*, Ar-H); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 166.70, 164.98, 157.80, 132.03, 130.96, 129.92, 129.36, 129.16, 128.74, 127.88, 127.69, 122.04, 121.31, 117.24, 64.52, 13.83: EI-MS (*m*/*z* (relative abundance, %)): 293 (M^+, 38.1), 265 (3.7), 105 (100), 77 (77.2).