



SUPPLEMENTARY MATERIAL TO

Synthesis, antimicrobial and antioxidative activity of some new isatin derivatives

GAVRILO M. ŠEKULARAC^{1#}, JASMINA B. NIKOLIĆ^{2#}, PREDRAG PETROVIĆ³,
BRANKO BUGARSKI³, BOBAN ĐUROVIĆ⁴ and SAŠA Ž. DRMANIĆ^{2**}

¹Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, Belgrade, Serbia, ²Department of Organic Chemistry, Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, ³Department of Chemical Engineering, Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia and ⁴Faculty of Technical Science, Kneza Miloša 7, 38220 Kosovska Mitrovica, Serbia

J. Serb. Chem. Soc. 79 (11) (2014) 1347–1355

I. CHARACTERIZATION OF THE SYNTHESIZED COMPOUNDS

1,3-Dihydro-3-[(5-mercapto-1,3,4-thiadiazol-2-yl)imino]-2H-indol-2-one (1). Yield: 74 %; m.p.: 183–185 °C; Anal. Calcd. for C₁₀H₆N₄OS₂: C, 45.8; H, 2.30; N, 21.4 %. Found: C, 46.0; H, 2.37; N 21.5 %. IR (KBr, cm⁻¹): 3418 (NH), 1743 (C=O), 1733 (C=N), 1616 (C=N); ¹H-NMR (250 MHz, DMSO-*d*₆, δ / ppm): 11.03 (1H, s, NH), 7.60–6.90 (4H, *m*, isatin-Ph), 3.4 (1H, s, SH); ¹³C-NMR (62.89 MHz, DMSO-*d*₆, δ / ppm): 184.0 (C–SH), 180.1 (N–C=N), 162.0 (C=N), 159.1 (C=O), 131.6 (isatin-Ph).

1,3-Dihydro-3-(2-benzothiazolylimino)-2H-indol-2-one (2). Yield: 78 %; m.p.: 164–166 °C; IR (KBr, cm⁻¹): 3315 (NH), 1715 (C=O), 1650 (C=N), 1575 (C=N); ¹H-NMR (250 MHz, DMSO-*d*₆, δ / ppm): 11.05 (1H, s, NH), 7.60–6.90 (4H, *m*, isatin-Ph), 7.3–8.2 (4H, *m*, benzothiazol); ¹³C-NMR (62.89 MHz, DMSO-*d*₆, δ / ppm): 166.3 (S–C=N), 159.1 (C=N), 152.6 (C=O), 127.9 (isatin-Ph), 136.5 (benzothiazole).

1,3-Dihydro-3-[(4-cyanophenyl)imino]-2H-indol-2-one (3). Yield: 73 %; m.p.: 257–259 °C; IR (KBr, cm⁻¹): 3446 (NH), 2228 (CN), 1742 (C=O), 1727 (C=N), 1611 (C=N); ¹H-NMR (250 MHz, DMSO-*d*₆, δ / ppm): 11.05 (1H, s, NH), 7.94–6.94 (4H, *m*, isatin-Ph), 7.68 (2H, *d*, *J* = 7.5 Hz, benzene); ¹³C-NMR (62.89 MHz, DMSO-*d*₆, δ / ppm): 163.1 (C=N), 153.2 (C=O), 132.4 (isatin-Ph), 128.2 (benzene), 119.2 (C–CN).

* Corresponding author. E-mail: drmana@tmf.bg.ac.rs

1,3-Dihydro-3-[(5-nitro-2-thiazolyl)imino]-2H-indol-2-one (4). Yield: 79 %; m.p.: 178–180 °C. IR (KBr, cm^{-1}): 3431 (NH), 1751 (C=O), 1741 (C=N), 1633 (C=N), 1367 (NO_2); $^1\text{H-NMR}$ (250 MHz, $\text{DMSO-}d_6$, δ / ppm): 11.04 (1H, s, NH), 8.80 (1H, s, CH=C), 7.59–6.87 (4H, m, isatin-Ph); $^{13}\text{C-NMR}$ (62.89 MHz, $\text{DMSO-}d_6$, δ / ppm): 184.6 (S–C=N), 173.7 (C=N), 158.3 (N–C=N), 150.7 (C=O), 147.5 (S–C– NO_2), 125.4 (isatin-Ph).

1,3-Dihydro-3-[(5-methyl-2-pyridyl)imino]-2H-indol-2-one (5). Yield: 72 %; m.p.: 204–206 °C; Anal. calcd. for $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}$: C, 71.0; H, 4.6; N, 17.7 %. Found: C, 71.3; H, 4.4; N, 17.5 %; IR (KBr, cm^{-1}): 3447 (NH), 3193 (C=N aromatic), 1753 (C=O), 1733 (C=N), 1626 (C=N); $^1\text{H-NMR}$ (250 MHz, $\text{DMSO-}d_6$, δ / ppm): 11.07 (1H, s, NH), 7.96–7.23 (4H, m, isatin-Ph), 8.33–6.88 (3H, m, pyridine), 2.33 (3H, s, CH_3); $^{13}\text{C-NMR}$ (62.89 MHz, $\text{DMSO-}d_6$, δ / ppm): 163.6 (C=N), 152 (C=O), 130.6 (isatin-Ph), 138.3 (pyridine), 19.5 (CH_3).

1,3-Dihydro-3-[(4-nitrophenyl)imino]-2H-indol-2-one (6). Yield: 79 %; m.p.: 149–151 °C; IR (KBr, cm^{-1}): 3446 (NH), 1742 (C=O), 1727 (C=N), 1611 (C=N), 1367 (NO_2); $^1\text{H-NMR}$ (250 MHz, $\text{DMSO-}d_6$, δ / ppm): 11.02 (1H, s, NH), 7.90–7.83 (4H, m, isatin-Ph), 6.87 (2H, d, $J = 7.5$ Hz, benzene); $^{13}\text{C-NMR}$ (62.89 MHz, $\text{DMSO-}d_6$, δ / ppm): 164.7 (C=N), 155 (C=O), 131.0 (isatin-Ph), 162.3 (C–N), 147.5 (C– NO_2), 141.5 (benzene).

II. ANTIOXIDATIVE ACTIVITY

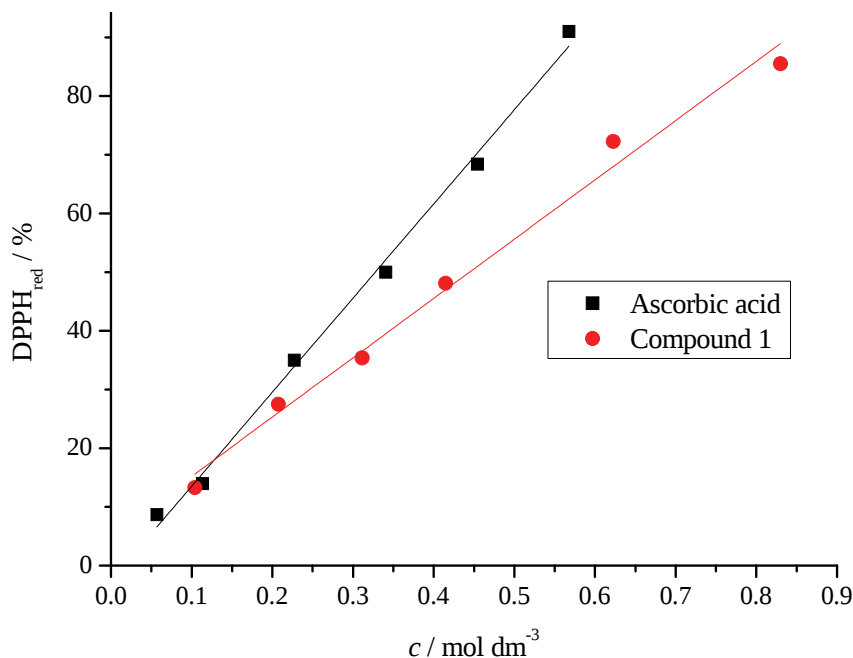


Fig. S-1. DPPH Scavenging activity of compound **1** compared to ascorbic acid.