Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 84 (10) S319 (2019) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

In vitro anticancer evaluation of novel triphenyltin(IV) compounds with some *N*-acetyl-*S*-naphthoquinonylcysteine derivatives

NEBOJŠA Đ. PANTELIĆ[1,2], MARTINA LERBS[1], KATHARINA WOLF[1], LUDGER A. WESSJOHANN[1] and GORAN N. KALUĐEROVIĆ[1,3]*

[1]*Department of Bioorganic Chemistry, Leibniz-Institute of Plant Biochemistry, Weinberg 3, D 06120 Halle (Saale), Germany,* [2]*Department of Chemistry and Biochemistry, Faculty of Agriculture, University of Belgrade, Nemanjina 6, Belgrade-Zemun, Serbia and* [3]*Department of Engineering and Natural Sciences, University of Applied Sciences Merseburg, Eberhard-Leibnitz-Strasse 2, 06217 Merseburg, Germany*

J. Serb. Chem. Soc. 84 (10) (2019) 1119–1127

N-{2-[(3,4-Dihydro-3,4-dioxo-1-naphtyl)thio]-1-{[(triphenylstannyl)oxy]carbonyl}ethyl}--acetamide **(1)**: Yield 85.7 mg (80.7 %). Anal. Calcd. for $C_{33}H_{27}NO_5SSn$: C, 59.30; H, 4.07; N, 2.10; S, 4.80 %. Found: C, 59.60; H, 4.10; N, 2.13; S, 4.67 %. IR (ATR): 1699 (*s*) (ν C=O), 1640 (*s*) (ν_a COO^-), 1372 (*s*) (ν_s COO^-), 450 (*s*) (ν Sn–O), cm^{-1}. ^{1}H-NMR (400.13 MHz, DMSO, *δ*): 8.12 (*d*, *J* = 8.1 Hz, 1H, NH), 8.01 (*d*, *J* = 7.8 Hz, 2H, $C^{10}H$, $C^{11}H$), 7.81 (*m*, 9H, *o*- and *p*-protons in $SnPh_3$), 7.68 (*m*, 2H, C^8H, C^9H), 7.42 (*m*, 6H, *m*-protons in $SnPh_3$), 6.41 (*s*, 1H, C^6H), 4.50 (*m*, 1H, C^2H), 3.30 (*d*, *J* = 13.0 Hz, 2H, C^3H), 1.80 (*s*, 3H, $C^{15}H$) ppm. ^{13}C--NMR (100.6 MHz, DMSO, *δ*): 178.64 (C4), 175.64 (C5), 175.10 (C8), 169.29 (C14), 157.19 (C7), 142.63 (C1'), 136.18 (C2', C4', C6'), 134.93 (C10), 133.05 (C9), 131.12 (C12), 130.44 (C13), 128.89 (C6), 128.24 (C3', C5'), 124.86 (C11), 119.89 (C8), 53.57 (C2), 33.69 (C3), 22.40 (C15) ppm. ^{119}Sn{1H} NMR (149.2 MHz, $CDCl_3$, *δ*): –83.3 ppm. ESI-HRMS (*m*/*z*): calculated for $[C_{33}H_{28}NO_5SSn]^+$ 670.0705, observed 670.0702 $[M+H]^+$.

N-{2-[(1,4-Dihydro-1,4-dioxo-2-naphtyl)thio]-1-{[(triphenylstannyl)oxy]carbonyl}ethyl}--acetamide **(2)**: Yield: 88.2 mg (84.1 %). Anal. Calcd. for $C_{33}H_{27}NO_5SSn$: C, 59.30; H, 4.07; N, 2.10; S, 4.80 %. Found: C, 59.17; H, 3.96; N, 2.17; S, 4.82 %. IR (ATR): 1700 (*s*) (ν C=O), 1645 (*s*) (ν_a COO^-), 1368 (*s*) (ν_s COO^-), 450 (*s*) (ν Sn–O), cm^{-1}. ^{1}H-NMR (400.13 MHz, DMSO, *δ*): 8.11 (*d*, *J* = 8.3 Hz, 1H, NH), 7.98–8.03 (*m*, 4H, C^8H, C^9H, $C^{10}H$, $C^{11}H$), 7.82–7.85 (*m*, 9H, *o*- and *p*-protons in $SnPh_3$), 7.42 (*q*, J_1 = 14.0 Hz, J_2 = 6.9 Hz, 6H, *m*-protons in $SnPh_3$), 6.73 (*s*, 1H, C^5H), 4.46 (*dd*, J_1 = 8.9 Hz, J_2 = 7.5 Hz, 1H, C^2H), 3.25 (*d*, *J* = 13.6 Hz, 2H, C^3H), 1.80 (*s*, 3H, $C^{15}H$) ppm. ^{13}C-NMR (100.6 MHz, DMSO, *δ*): 181.72 (C4), 180.84 (C7), 172.25 (C1), 169.24 (C14), 153.84 (C6), 142.67 (C1'), 136.19 (C2', C4', C6'), 134.72 (C10), 133.64 (C9), 131.61 (C12), 131.38 (C13), 128.89 (C5), 128.23 (C'3, C'5), 126.31 (C8), 126.02 (C11), 54.87 (C2), 32.63 (C3), 22.38 (C15) ppm. ^{119}Sn{1H} NMR (149.2 MHz, $CDCl_3$, *δ*): –84.5 ppm. ESI-HRMS (*m*/*z*): calculated for $[C_{33}H_{28}NO_5SSn]^+$ 670.0705, observed 670.0709 $[M+H]^+$.

* Corresponding author. E-mail: goran.kaluderovic@hs-merseburg.de