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SUPPLEMENTARY MATERIAL TO

Reactions of tin and triorganotin(IV) isopropoxides with thymol derivative: synthesis, characterization and *in vitro* antimicrobial screening

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TABLE S-I. Amount of 2-propanol in the azeotropic mixture formed during the preparation of the complexes

Complex	Calculated, g	Found, g
2	0.598	0.538
3	0.598	0.538
4	0.300	0.270
5	0.300	0.272
6	0.299	0.269

PHYSICAL, ANALYTICAL AND SPECTRAL DATA OF THE LIGAND AND COMPLEXES

*H_2hbgl (**1**)*. Yield: 5.9 g, 80 %; Colour: yellow; m.p.: 70 °C; Anal. Calcd. for $C_{13}H_{19}NO_3$: C, 65.74; H, 8.00; N 6.04 %. Found: C, 65.84; H, 8.10; N, 5.80 %; IR (KBr/CsI, cm^{-1}): 3390 (–OH stretching of phenolic group), 3056 (–CH stretching of aromatic ring), 2956, 2856 (asymmetric and symmetric stretching of $–CH_3$ or $–CH_2$), 1582 (asymmetric stretching of carboxylate group), 1413 (symmetric stretching of carboxylate group); ^{1}H-NMR (300 MHz, DMSO, δ / ppm): 6.50 (1H, *d*, *J* = 7.8 Hz, Ar-H), 6.90 (1H, *d*, *J* = 8 Hz, Ar-H); 8.38 (1H, *s*, phenolic –OH), 7.15 (1H, *br*, –NH), 2.13 (3H, *s*, $–CH_3$), 1.81 (2H, *s*, Ar–C$\mathbf{H}_2$–), 3.10 (2H, *s*, $–CH_2$–), 1.12 (6H, *d*, *J* = 6.9 Hz, -CH(C$\mathbf{H}_3$)$_2$); ESI-MS (*m/z* (relative abundance (%)): $[C_{13}H_{19}NO_3]^+$ 237.9 (48), $[C_{11}H_{15}O]^+$ 163.1 (30).

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[Sn(OPr^i)$_2$(hbgl)] ***(2)***. Yield: 1.42 g, 67 %; Colour: yellowish brown; m.p.: 155 °C; Anal. Calcd for $C_{19}H_{31}NO_5Sn$: C, 48.28; H, 6.56; N, 3.09; Sn, 25.13 %. Found: C, 48.34; H, 6.59; N, 2.99; Sn, 25.19 %; IR (KBr/CsI, cm^{-1}): 3100 (N–H stretching of amine), 2963, 2868 (asymmetric and symmetric stretching of –CH_3 or –CH_2 groups), 1613 (asymmetric stretching of carboxylate group), 1412 (symmetric stretching of carboxylate group), $\Delta\nu$: 201, 500 (Sn–O stretching); ^{1}H-NMR (300 MHz, DMSO, δ / ppm): 7.13 (1H, *d*, *J* = 7.8 Hz, Ar-H), 6.77 (1H, *d*, *J* = 7.8 Hz, Ar-H), 6.58 (1H, *d*, –NH), 2.30 (3H, *s*, –CH_3), 1.15 (3H, *d*, *J* = 2.7 Hz, –CH(C**H**$_3$)$_2$), 1.76 (3H, *d*, *J* = 2.7 Hz, -CH(C**H**$_3$)$_2$); molar conductance (10^{-3} M DMSO, µS cm^{-1}): 21.

[Sn(OPr^i)$_2$(Hhbgl)$_2$] ***(3)***. Yield: 2.057 g, 64 %; Colour: brown; m.p.: 160 °C; Anal. Calcd. for $C_{32}H_{50}N_2O_8Sn$: C, 54.12; H, 7.04; N, 4.07; Sn, 16.73 %. Found: C, 54.22; H, 7.14; N, 4.01; Sn 16.79 %; IR (KBr/CsI, cm^{-1}): 3394 (–OH stretching of phenolic group), 3200–3000 (–NH/–CH stretching of amine and aromatic ring), 2961, 2871 (asymmetric and symmetric stretching of –CH_3 or –CH_2 group), 1588 (asymmetric stretching of carboxylate group), 1415 (symmetric stretching of carboxylate group), $\Delta\nu$:173, 503 (Sn–O stretching); ^{1}H-NMR (300 MHz, MeOD, δ / ppm): 6.45–6.96 (4H, *m*, Ar-H), 8.06 (1H, *s*, phenolic –OH), 8.54 (1H, *s*, phenolic –OH), 2.20 (6H, *s*, CH_3); molar conductance (10^{-3} M DMSO, µS cm^{-1}): 25.

[Ph$_3$Sn(Hhbgl)] ***(4)***. Yield: 1.764 g, 67 %; Colour: brown; m.p.: >300 °C; Anal. Calcd. for $C_{31}H_{33}NO_3Sn$: C, 63.41; H, 5.80; N, 2.39; Sn, 20.23 %. Found: C, 63.46; H, 5.84; N, 2.34; Sn, 20.28 %; IR (KBr/CsI, cm^{-1}): 3426 (–OH stretching of phenolic group), 3056 (–CH stretching of aromatic ring), 2958, 2868 (asymmetric and symmetric stretching of –CH_3 or –CH_2 groups), 1604 (asymmetric stretching of carboxylate group), 1417 (symmetric stretching of carboxylate group), $\Delta\nu$: 187, 558 (Sn–O stretching), 279, 207 (asymmetric and symmetric stretching of Sn–C); ^{1}H-NMR (300 MHz, DMSO, δ / ppm): 7.22––7.58 (17H, *m*, Ar-H and Sn–C_6H_5), 7.76 (1H, *br*, phenolic –OH), 7.33 (1 H, *br*, –NH), 2.13 (3H, *s*, –CH_3), 1.08 (3H, *d*, *J* = 5.1 Hz, –CH(C**H**$_3$)$_2$), 1.05 (3H, *d*, *J* = = 5.1 Hz, -CH(C**H**$_3$)$_2$); molar conductance (10^{-3} M DMSO, µS cm^{-1}): 17.

[Bu$_3$Sn(Hhbgl)] ***(5)***. Yield: 1.644 g, 69 %; Colour: brown; m.p.: >300 °C; Anal. Calcd. for $C_{25}H_{45}NO_3Sn$: C, 57.06; H, 8.56; N, 2.67; Sn, 22.58 %. Found: C, 57.15; H, 8.61; N, 2.61; Sn, 22.62 %; IR (KBr/CsI, cm^{-1}): 3500–3000 (–OH stretching of phenolic group), 2962, 2863 (asymmetric and symmetric stretching of –CH_3 or –CH_2 groups), 1591 (asymmetric stretching of carboxylate group), 1406 (symmetric stretching of carboxylate group), $\Delta\nu$: 185, 501 (Sn–O stretching), 528, 469 (asymmetric and symmetric stretching of Sn–C); ^{1}H-NMR (300 MHz, DMSO, δ / ppm): 7.12 (1H, *d*, *J* = 7.8 Hz, Ar-H), 6.77 (1H, *d*, *J* = 7.5 Hz, Ar-H), 8.00 (1H, *s*, phenolic –OH), 6.88 (1H, *s*, –NH), 2.30 (3H, *s*, CH_3), 0.78

and 0.90–1.21 (27 H, *t*, *m*, Sn–C_4H_9); molar conductance (10^{-3} M DMSO, µS cm^{-1}): 18.

*[Me_3Sn(Hhbgl)] (**6**)*. Yield: 1.304 g, 72 %; Colour: cream; m.p.: >300 °C; Anal. Calcd for $C_{16}H_{27}NO_3Sn$: C, 47.99; H, 6.75; N, 3.50; Sn, 29.67 %. Found: C, 47.91; H, 6.71; N, 3.46; Sn, 29.70 %; IR (KBr/CsI, cm^{-1}): 3404 (–OH stretching of phenolic group), 2959, 2863 (asymmetric and symmetric stretching of $–CH_3$ or $–CH_2$ groups), 1626 (asymmetric stretching of carboxylate group), 1410 (symmetric stretching of carboxylate group), $\Delta\nu$: 216, 555 (Sn–O stretching); ^{1}H-NMR (300 MHz, DMSO, δ / ppm): 6.89 (1H, *d*, *J* = 6 Hz, Ar-H), 6.48 (1H, *d*, *J* = 6.09 Hz, Ar-H), 7.80 (1H, *s*, phenolic –OH), 4.90 (1H, *br*, –NH), 0.99 (3H, *d*, *J* = 5.13 Hz, –CH(C**H**$_3$)$_2$), 1.07 (3H, *d*, *J* = 4.44 Hz, –CH(C**H**$_3$)$_2$), 0.42 (9H, *s*, Sn–CH_3, ^2J $^{117/119}$Sn- ^{1}H = 68.0 Hz); molar conductance (10^{-3} M DMSO, µS cm^{-1}): 32.