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Supplementary material

SUPPLEMENTARY MATERIAL TO

Synthesis and spectroscopic characterization of mononuclear/binuclear organotin(IV) complexes with 1*H*-1,2,4-triazole-3-thiol: Comparative studies of their antibacterial/antifungal potencies

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TABLE S-I. Physical data for the organotin(IV) complexes **1**–**8**

Compd.	Mol. formula	MW g mol^{-1}	M.p. °C	Yield %	Calcd. (found), %			
					C	H	N	S
HL	$C_2H_3N_3S$	101	232–34	–	23.73 (23.27)	2.96 (2.99)	41.53 (41.97)	31.64 (31.56)
1	$C_4H_8ClN_3SSn$	284.5	208–11	41.8	16.87 (16.76)	2.81 (2.71)	14.76 (14.68)	11.24 (11.39)
2	$C_{10}H_{20}ClN_3SSn$	368.5	219–22	91.2	32.56 (32.51)	5.42 (5.41)	11.39 (11.49)	8.68 (8.62)
3	$C_{14}H_{29}N_3SSn$	390	122–25	60	43.96 (42.93)	7.43 (7.27)	10.76 (10.63)	8.20 (8.39)
4	$C_{20}H_{17}N_3SSn$	450	197–99	93.2	53.33 (53.39)	3.77 (3.49)	9.33 (9.28)	7.11(7.20)
5	$C_7H_{13}Cl_2N_3S_3Sn_2$	544	202–04	58	15.44 (15.40)	2.38 (2.55)	7.72 (7.75)	17.64 (17.54)
6	$C_{19}H_{37}Cl_2N_3S_3Sn_2$	712	214–15	68.3	31.97 (31.86)	5.19 (5.23)	5.89 (5.73)	13.48 (13.66)
7	$C_{27}H_{55}N_3S_3Sn_2$	755	115–18	–	42.91 (42.75)	7.28 (7.21)	5.56 (5.51)	12.71 (12.70)
8	$C_{39}H_{31}N_3S_3Sn_2$	875	183–185	79.3	53.48 (53.22)	3.54 (3.46)	4.80 (4.42)	10.97 (10.80)

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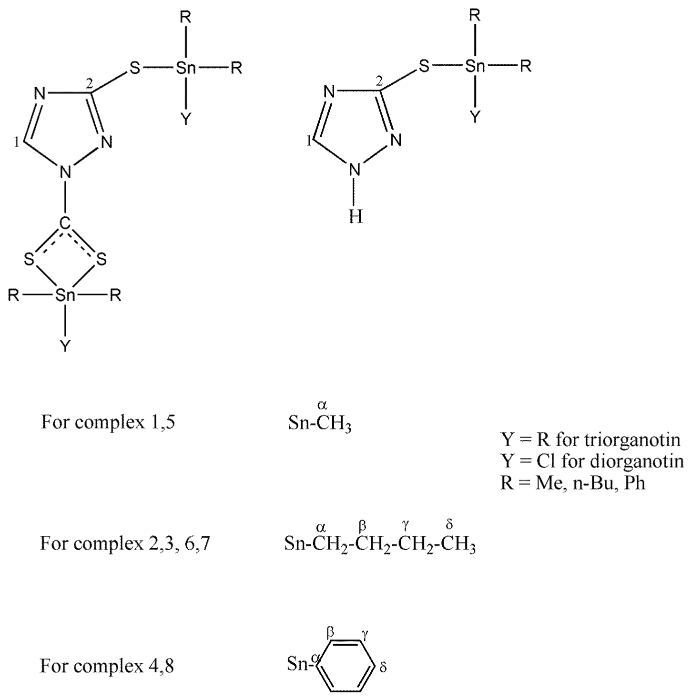
TABLE S-II. Infrared absorption bands (cm^{-1}) of organotin(IV) complexes **1–8**

Compd.	ν(S–H)	ν(N–H)	ν(C–N)	$ν(CS_2)_{asym}$	$ν(CS_2)_{sym}$	ν(Sn–C)	ν(Sn–S)	ν(Sn–Cl)
HL	2560	3148	–	–	–	–	–	–
1	–	3148	–	–	–	560	470	335
2	–	3149	–	–	–	535	447	328
3	–	3145	–	–	–	545	441	–
4	–	3143	–	–	–	265	437	–
5	–	–	1505	1048	973	563	471	336
6	–	–	1490	1044	976	539	449	320
7	–	–	1475	1051	972	556	445	–
8	–		1456	1034	963	263	438	–



Scheme S-1. Numbering scheme for NMR data.

TABLE S-III. ^{1}H-NMR data (ppm) of the organotin(IV) complexes **1–8** in DMSO-d_6

Compd.	–CH	–NH	–SH	R
HL	8.21	11.48	13.357	–
1	8.24	11.45	–	1.03 (*s*)
2	8.24	11.48	–	1.62–1.58 (*m*, H*α*), 1.40–1.47 (*m*, H*β*), 1.32–1.23 (*m*, H*γ*), 0.87 (*t*, H*δ*), ^3J = 7.2 Hz
3	8.24	11.43	–	1.54–1.46 (*m*, H*α*), 1.44–1.39 (*m*, H*β*), 1.27–1.13 (*m*, H*γ*), 0.81 (t, H*δ*), ^3J = 7.0 Hz
4	8.23	11.30	–	7.97–7.72 (*m*), 7.52–7.36 (*m*)

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TABLE S-III. Continued

Compd.	–CH	–NH	–SH	R
5	8.20	–	–	1.46, *s*, ^2J [79/76], Hα
6	8.21	–	–	1.63–1.55 (*m*, Hα), 1.39–1.47 (*m*, Hβ), 1.31–1.25 (*m*, Hγ), 0.87 (*t*, ^3J = 7.2 Hz, Hδ)
7	8.23	–	–	1.52–1.48 (*m*, Hα), 1.44–1.40 (*m*, Hβ), 1.26–1.12 (*m*, Hγ), 0.80 (t, ^3J = 7.0 Hz, Hδ)
8	8.23	–	–	7.96–7.74 (*m*), 7.48–7.31 (*m*)

Table S-IV. ^{13}C-NMR data (ppm) of the organotin(IV) complexes **5–8**; Chemical shifts (δ) in ppm and $^nJ[^{119/117}Sn, ^{13}C]$ values in Hz are listed in square brackets

Compd.	1C	2C	–CSS	R
HL	140.44	165.57	–	–
5	140.78	153.36	191.36	10.6 (C-α, ^1J[570,545])
6	140.65	154.16	193.80	26.5 (C-α, ^1J[496/479]), 29.3 (C-β, ^2J[44]), 28.3 (C-γ, ^3J[112/109]), 14.7 (C-δ)
7	140.32	153.15	194.85	25.4 (C-α, ^1J[346/332]), 29.2 (C-β, ^2J[34]), 27.1 (C-γ, ^3J[68/62]), 13.5 (C-δ)
8	140.35	152.15	191.78	138.1 (C-α), 136.3 (C-β, ^2J[47.3/45]), 129.1 (C-γ, ^3J[61.5/59.2]), 129.5 (C-δ, ^4J [12.8])

TABLE S-V. (C–Sn–C) angles based on the NMR parameters of complexes **5–7**

Compd.	$^1J(^{119}Sn, ^{13}C)$ / Hz	$^2J(^{119}Sn, ^1H)$ / Hz	Angle, °	
			^1J	^2J
5	570	79	126.75	124
6	495	–	120.1	–
7	346	–	107.1	–

Table S-VI. Mass fragments, *m*/*z*, and relative abundance of the organotin(IV) complexes **1–8**; n.o. – not observed

Compd.	Mass fragmentation: *m*/*z* (intensity, %)
HL	101 (100) $[C_2H_3N_3S]^+$, 74 (87.4) $[CH_2N_2S]^+$, 60 (27.4) $[CH_2NS]^+$, 47 (10.8) $[NHS]^+$, 42 (70.5) $[CH_2N_2]^+$
1	285 (1.2) $[(CH_3)_2Sn(–SN_3C_2H_2)Cl]^+$, 270 (4.2) $[(CH_3)Sn(–SN_3C_2H_2)Cl]^+$, 255 (2.0) $[Sn(–SN_3C_2H_2)Cl]^+$, 155 (38.8) $[SnCl]^+$, 100 (100) $[(SN_3C_2H_2)]^+$, 250 (3.0) $[(CH_3)_2Sn(–SN_3C_2H_2)]^+$, 220 (5.0) $[Sn(–SN_3C_2H_2)]^+$, 120 (8.1) $[Sn]^+$, 185 (19.2) $[(CH_3)_2SnCl]^+$, 150 (2.2) $[(CH_3)_2Sn]^+$, 135 (6.1) $[CH_3–Sn]^+$
2	369 (11.1) $[(Bu)_2Sn(–SN_3C_2H_2)Cl]^+$, 334 (97.6) $[(Bu)_2Sn(–SN_3C_2H_2)]^+$, 312 (5.8) $[(Bu)Sn(–SN_3C_2H_2)Cl]^+$, 220 (68.0) $[Sn(–SN_3C_2H_2)]^+$, 100 (11.8) $[(SN_3C_2H_2)]^+$, 120 (9.5) $[Sn]^+$, 269 (20.9) $[Sn–Bu_2Cl]^+$, 212 (13) $[SnBu–Cl]^+$, 155 (16.2) $[SnCl]^+$, 57 (92.5) $[Bu]^+$
3	391 (0.5) $[(Bu)_3Sn(–SN_3C_2H_2)]^+$, 277 (12.3) $[(Bu)Sn(–SN_3C_2H_2)]^+$, 220 (35.6) $[Sn(–SN_3C_2H_2)]^+$, 100 (100) $[(SN_3C_2H_2)]^+$, 120 (8.0) $[Sn]^+$, 291 (15.6) $[(Bu)_3 Sn]^+$, 234 (20.9) $[(Bu)_2 Sn]^+$, 177 (21.68) $[Bu(Sn)]^+$

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TABLE S-VI. Continued

Compd.	Mass fragmentation: *m*/*z* (intensity, %)
4	451 (3.9) $[(Ph)_3Sn(–SN_3C_2H_2)]^+$, 100 (100) $[(SN_3C_2H_2)]^+$, 374 (36.8) $[(Ph)_2Sn(–SN_3C_2H_2)]^+$, 297 (3.5) $[(Ph)Sn(–SN_3C_2H_2)]^+$, 220 (4.2) $[C_2H_3N_3SSn]^+$, 100 (9.5) $[C_2H_3N_3S]^+$, 351 (48.3) $[(Ph)_3Sn]^+$, 274 (2.6) $[(Ph)_2Sn]^+$, 197 (45.6) $[Ph–Sn]^+$, 77 (20.9) $[Ph]^+$, 51 (16.3) $[C_4H_3]^+$, 120 (12.7) $[Sn]^+$
5	545 (<0.5) $[(CH_3)_2ClSn(–S–CS)–NC_2HN_2S(–Sn(CH_3)_2Cl]$, 469 (1.2) $[(CH_3)_2ClSn(–NC_2HN_2S)(–Sn(CH_3)_2Cl]^+$, 285 (4.1) $[(CH_3)_2Sn(–SN_3C_2H_2)Cl]^+$, 185 (6.5) $[(CH_3)_2SnCl]^+$, 100 (100) $[(SN_3C_2H_2)]^+$, 76 (7.1) $[S–CS]^+$, 196 (2.4) $[Sn–(S–CS)]^+$, 143 (2.8) $[CS–NC_2HN_2S]^+$
6	713 (n.o) $[(Bu)_2ClSn(–S–CS)–NC_2HN_2S(–Sn(Bu)_2Cl]$, 637 (<0.5) $[(Bu)_2ClSn(–NC_2HN_2S)(–Sn(Bu)_2Cl]^+$, 369 (4.6) $[(Bu)_2Sn(–SN_3C_2H_2)Cl]^+$, 269 (100) $[(Bu)_2SnCl]^+$, 100 (16) $[(SN_3C_2H_2)]^+$, 76 (7.1) $[S–CS]^+$, 196 (6.4) $[Sn–(S–CS)]^+$
7	757 (n.o.) $[(Bu)_3Sn(–S–CS)–NC_2HN_2S(–Sn(Bu)_3)]^+$, 681 (2.4) $[(Bu)_3Sn–NC_2HN_2S(–Sn(Bu)_3)]^+$, 291 (2.1) $[(Bu)_3\ Sn]^+$, 196 (6.4) $[Sn–(S–CS)]^+$, 76 (10.3) $[S–CS]^+$, 120 (2.0) $[Sn]^+$, 57 (3.3) $[Bu]^+$
8	877 (n.o.) $[(Ph)_3Sn(–S–CS)–NC_2HN_2S(–Sn(Ph)_3)]^+$, 801 (<0.5) $[(Ph)_3Sn–NC_2HN_2S(–Sn(Ph)_3)]^+$, 350 (4.8) $[Ph_2SnC_6H_4]^+$, 723 (1.1) $[(Ph)Sn(–S–CS)–NC_2HN_2S(–Sn(Ph)_3)]^+$, 196 (16.9) $[Sn–C_6H_4]^+$, 154 (83.1) $[Ph–Ph]^+$, 76 (12.3) $[S–CS]^+$, 451 (1.9) $[(Ph)_3Sn(–SN_3C_2H_2)]^+$

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