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SUPPLEMENTARY MATERIAL TO

Diorganotin(IV) complexes with hydroxamic acids derivatives of some histone deacetylases inhibitors

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SPECTRAL AND ANALYTICAL DATA OF LIGAND PRECURSORS AND COMPLEXES

*N-hydroxy-4-phenylbutanamide (**HL**$_1$):* Yield 434 mg (34.3%). Colorless crystals. IR (ATR): 3174w (ν(N-H)), 2979m, 2946m (ν$(CH_2)_{as}$), 2602m, 2496m, 1647m (ν(C=O)), 1474s (δ$(CH_2)_{sc}$), 1383m, 1364w, 1172m, 1035s, 851w, 807m, 757m (γ(C-H), 700m (Φ(C=C)), cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.25 (*dd,* 2H, J_3 = 7.5, 7.0, H-7 and H-9), 7.18 (*d,* 1H, J_3 = 7.0, H-8), 7.13 (*d,* 2H, J_3 = 7.5, H-6 and H-10), 2.60 (*t,* 2H, J_3 = 7.3, H-4), 2.10 (*bt,* 2H, J_3 = 7.0, H-2), 1.93 (*tt,* 2H, J_3 = 7.3, 7.0, H-3). ^{13}C NMR (100.6 MHz, $CDCl_3$, δ): 170.73 (C=O), 140.44 (C-5), 127.87 (C-6 and C-10 or C-7 and C-9), 127.85 (C-6 and C-10 or C-7 and C-9), 125.50 (C-8), 34.33 (C-4), 31.49 (C-2), 26.13 (C-3). ^{1}H NMR (400 MHz, DMSO-d_6, δ): 10.39 (*bs,* 1H, N-H), 8.77 (*bs,* 1H, O-H), 7.28 (*m*, 2H, H-6 and H-10), 7.18 (*m*, 3H, H-7, H-8 and H-9), 2.55 (*t,* 2H, J_3 = 7.1, H-4), 1.98 (*t*, 2H, J_3 = 7.4, H-2), 1.80 (*tt*, J_3 = 7.4, 7.1, 2H, H-3).^{13}C NMR (100.6 MHz, DMSO-d_6, δ): 169.12 (C=O), 141.90 (C-5), 128.54 (C-6 and C-10), 126.03 (C-7, C-8 and C-9), 34.85 (C-4), 32.02 (C-2), 27.25 (C-3).

*N-hydroxy-2-propylpentanamide (**HL**$_2$):* Yield 508 mg (45.7%). Colorless crystals. IR (ATR): 3176w (ν(N-H)), 3026w, 2957m (ν$(CH_3)_{as}$), 2930m (ν$(CH_2)_{as}$), 2873m (ν$(CH_2)_s$), 1627s (ν(C=O)), 1536m (ν(C-N) + ν$(CNH)_{bend}$), 1464s (δ$(CH_2)_{sc}$), 1381m, 1273w, 1113w, 1041m, 990w, 949m, 891w, 756m, cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.98 (*m*, 1H, H-2), 1.60 (*m*, 2H, H-3A), 1.40 (*m*, 2H, H-3B), 1.28 (*m*, 4H, H-4), 0.88 (*t,* J_3 = 7.2, 6H, H-5).^{13}C NMR (100.6 MHz, $CDCl_3$, δ): 174.47 (C=O), 44.15 (C-2), 34.83 (C-3), 20.80 (C-4), 14.15 (C-5). ^{1}H NMR (400 MHz, DMSO-d_6, δ): 10.36 (*s,* 1H, N-H), 8.68 (*s,* 1H, O-H), 1.96 (*m,* 1H, H-2), 1.43 (*m,* 2H, H-3A), 1.20 (*m,* 6H, H-3B and H-4), 0.83 (*t,* 6H, J_3 = 7.2, H-5). ^{13}C NMR (100.6 MHz, DMSO-d_6, δ): 171.39 (C=O), 41.89 (C-2), 34.45 (C-3), 19.97 (C-4), 13.78 (C-5).

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*[$Ph_2Sn(L_1)_2$] (**1**)*: Yield 164 mg (94.8%). Colorless solid. IR (ATR): 3141w (ν(N-H)), 2929w (ν$(CH_2)_{as}$), 1596m (ν(C=O)), 1519m (ν(C-N) + ν$(CNH)_{bend}$), 1496m, 1454m (δ$(CH_2)_{sc}$), 1430m, 1363w, 1299w, 1152w, 1087w, 1071m, 992m, 952m, 731m (γ(C-H), 700s (Φ(C=C)), 540m (ν(Sn-O)), cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.75 (*dd,* 4H , J_3 = 6.60, J_4 = 2.90, H-2' and H-6'), 7.345 (*dd,* 4H, J_3 = 7.00, 6.60, H-3' and H-5'), 7.335 (*dd,* 2H, J_3 = 7.00, J_4 = 2.90, H-4'), 7.22 (*dd,* 4H, J_3 = 7.60, 7.20, H-7 and H-9), 7.15 (*dd*, 2H, J_3 = 7.60, J_4 = 1.70, H-8), 7.07 (*ddd*, 4H, J_3 = 7.20, J_4 = 1.70, –1.00, H-6 and H-10), 2.53 (*td,* 4H, J_3 = 7.70, J_4 = –1.00, H-4), 2.28 (*t,* 4H, J_3 = 7.00, H-2), 1.89 (*tt,* 4H, J_3 = 7.70, 7.00. H-3). ^{13}C NMR (100.6 MHz, $CDCl_3$, δ): 167.32 (C=O), 145.79 (C-1'), 141.10 (C-5), 134.86 (C-2' and C-6'), 129.86 (C-4'), 128.70 (C-3' and C-5'), 128.61 (C-6 and C-10), 128.59 (C-7 and C-9), 126.21 (C-8), 34.79 (C-4), 30.73 (C-2), 26.95 (C-3). ^{119}Sn NMR (149.2 MHz, $CDCl_3$, δ): –402.41 (*s,* Sn). Combustion analysis for $C_{15}H_{18}N_2O_4Sn$: Calculated. C 61.05 H 5.45, N 4.42; found C 60.93 H 5.57, N 4.45.

*[$Ph_2Sn(L_2)_2$] (**2**)*: Yield 98 mg (89 %). Colorless solid. IR (ATR): 3176w (ν(N-H)), 3048w, 2956s (ν$(CH_3)_{as}$), 2930m (ν$(CH_2)_{as}$), 2871m (ν$(CH_2)_s$), 1589s (ν(C=O)), 1525m (ν(C-N) + ν$(CNH)_{bend}$), 1464m (δ$(CH_2)_{sc}$), 1429m, 1380m, 1277w, 1120m, 1073m, 1045m, 995m, 953m, 899w, 728m (γ(C-H), 697s (Φ(C=C)), 540m (ν(Sn-O)), cm^{-1}. ^{1}H NMR (400 MHz, $CHCl_3$, δ): 7.59 (*m,* 4H, H-2' or H-3'), 7.30 (*m,* 2H, H-4'), 7.27 (*m,* 4H, H-2' or H-3'), 1.96 (*m,* 2H, H-2), 1.54 (*m,* 4H, H-3A), 1.28 (*m,* 8H, H-3B and H-4A), 1.07 (*m,* 4H, H-4B), 0.76 (*m*, 12H, CH_{3A} and CH_{3B}). ^{13}C NMR (100.6 MHz, $CDCl_3$, δ): 169.52 (C=O), 148.29 (C-1'), 135.56 (C-2' or C-3'), 128.38 (C-4'), 127.94 (C-2' or C-3'), 43.35 (C-2), 34.35 (C-3), 20.49 (C-4), 14.10 (C-5). ^{119}Sn NMR (149.2 MHz, $CDCl_3$, δ): –349.95 (*s,* Sn). Combustion analysis for $C_{28}H_{42}N_2O_4Sn$: Calculated. C 57.06, H 7.18, N 4.75; found C 57.45, H 7.32, N 4.70.

IR SPECTRA OF LIGAND PRECURSORS AND COMPLEXES

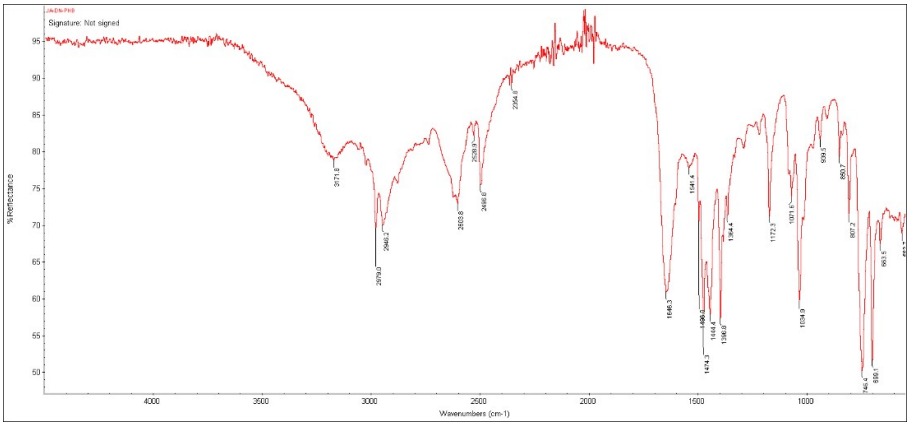

Fig. S-1. FTIR spectrum of *N*-hydroxy-4-phenylbutanamide (**HL$_1$**)

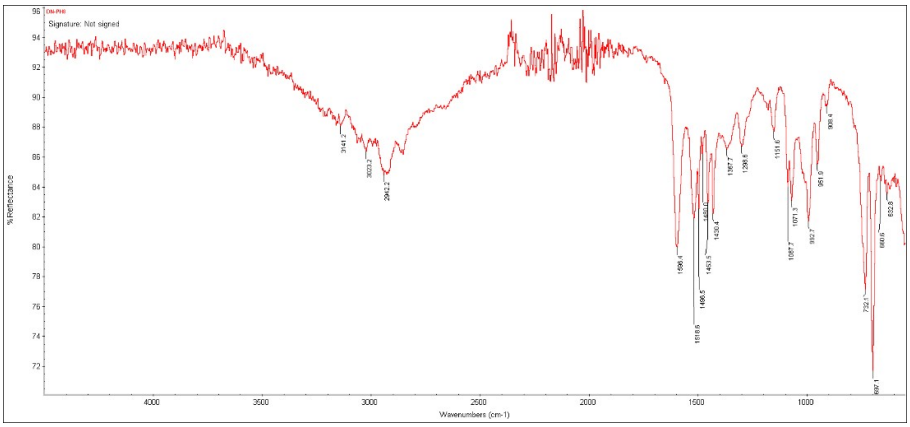

Fig. S-2. FTIR spectrum of [$Ph_2Sn(L_1)_2$] (**1**)

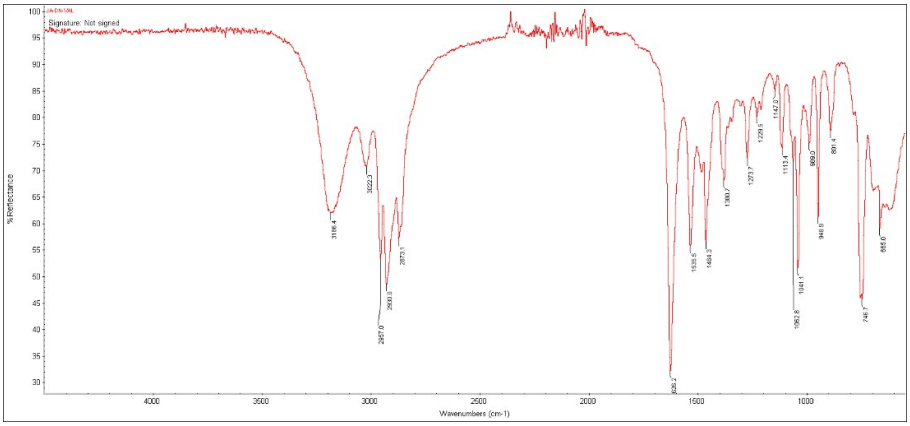

Fig. S-3. FTIR spectrum of *N*-hydroxy-2-propylpentanamide (**HL_2**)

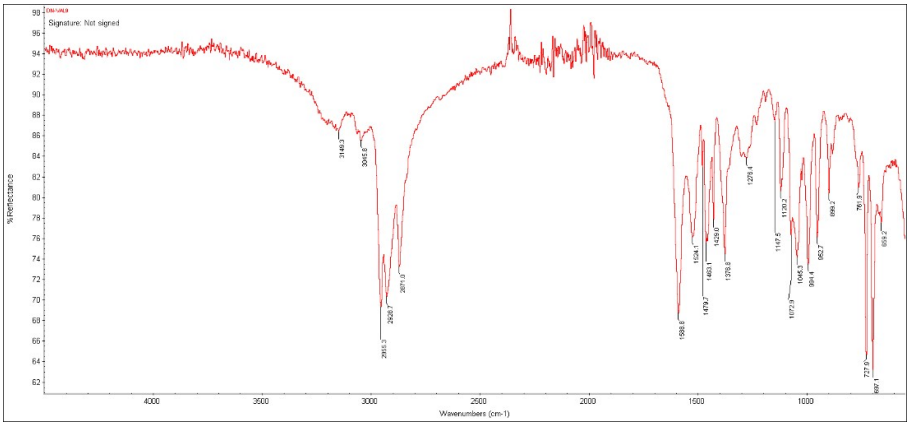

Fig. S-4. FTIR spectrum of $[Ph_2Sn(L_2)_2]$ (**2**)

NMR SPECTRA OF LIGAND PRECURSORS AND COMPLEXES

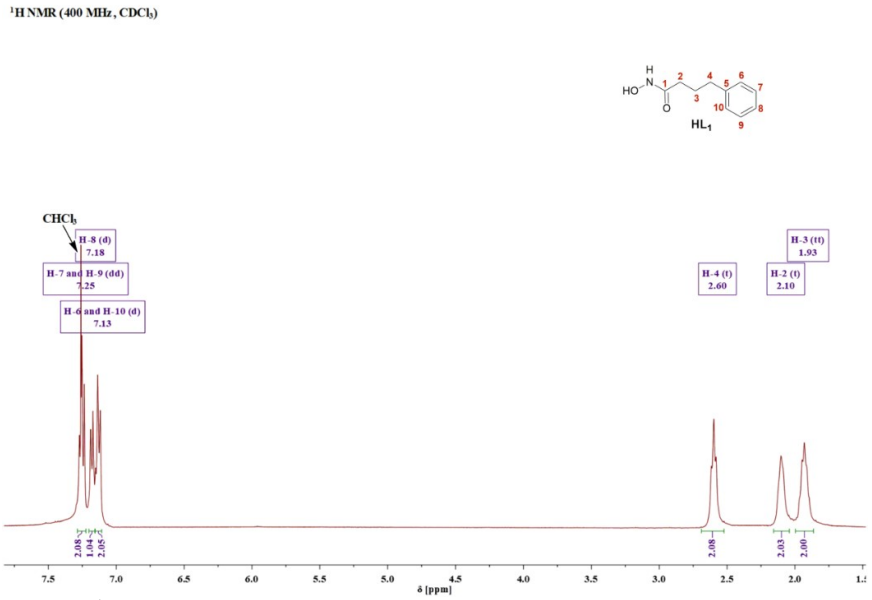

Fig. S-5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-hydroxy-4-phenylbutanamide (**HL$_1$**)

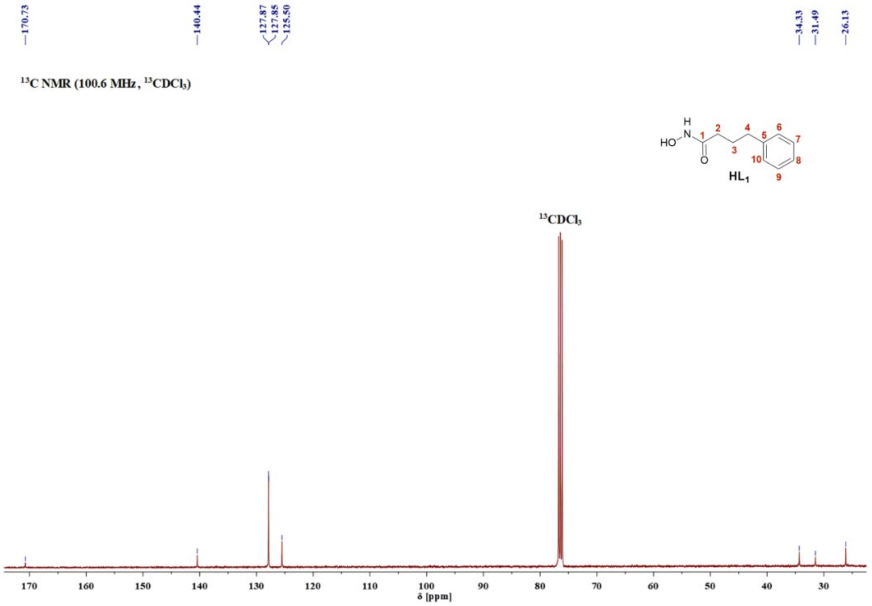

Fig. S-6. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of *N*-hydroxy-4-phenylbutanamide (**HL$_1$**)

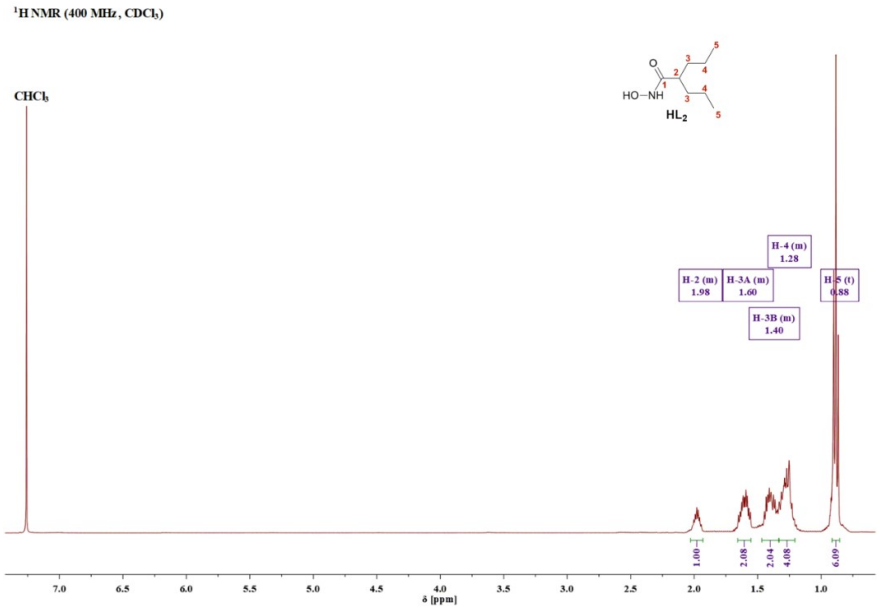

Fig. S-7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-hydroxy-2-propylpentanamide (**HL_2**)

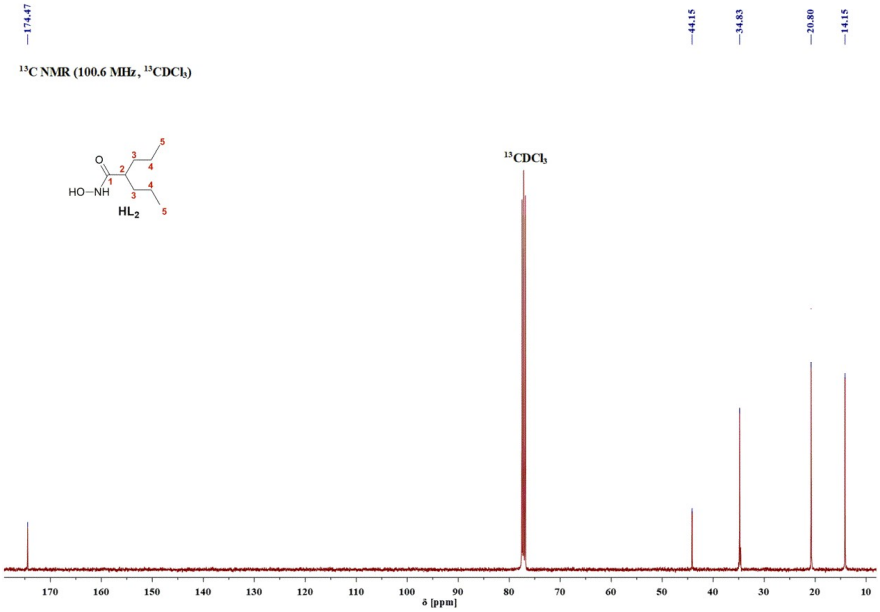

Fig. S-8. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of *N*-hydroxy-2-propylpentanamide (**HL_2**)

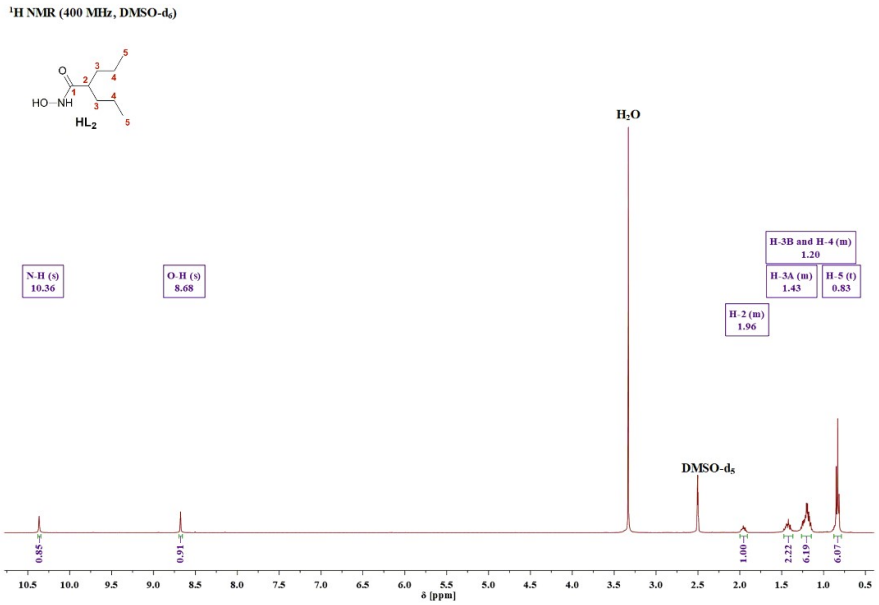

Fig. S-9. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of *N*-hydroxy-2-propylpentanamide (**HL$_2$**)

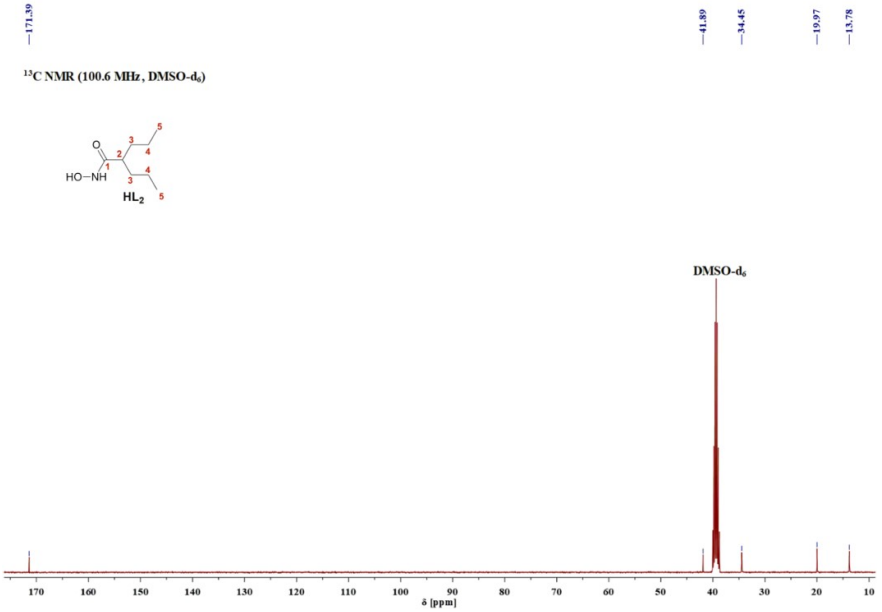

Fig. S-10. ^{13}C NMR spectrum (100.6 MHz, DMSO-d_6) of *N*-hydroxy-2-propylpentanamide (**HL$_2$**)

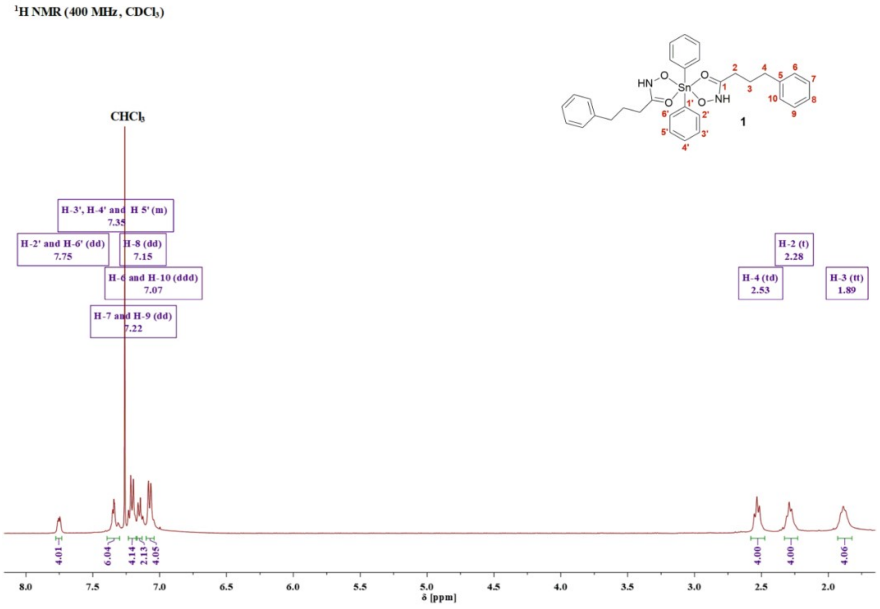

Fig. S-11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of $[Ph_2Sn(L_1)_2]$ (**1**)

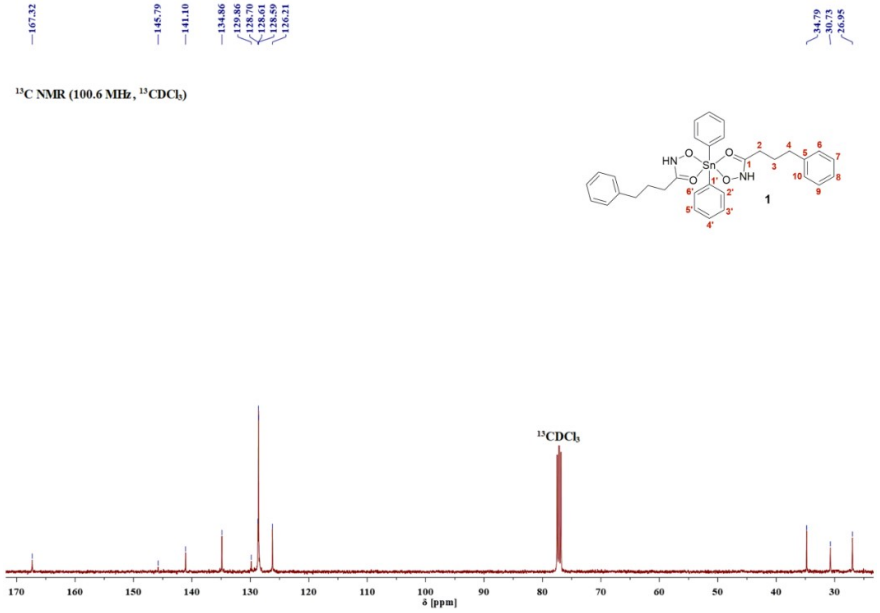

Fig. S-12. ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$) of $[Ph_2Sn(L_1)_2]$ (**1**)

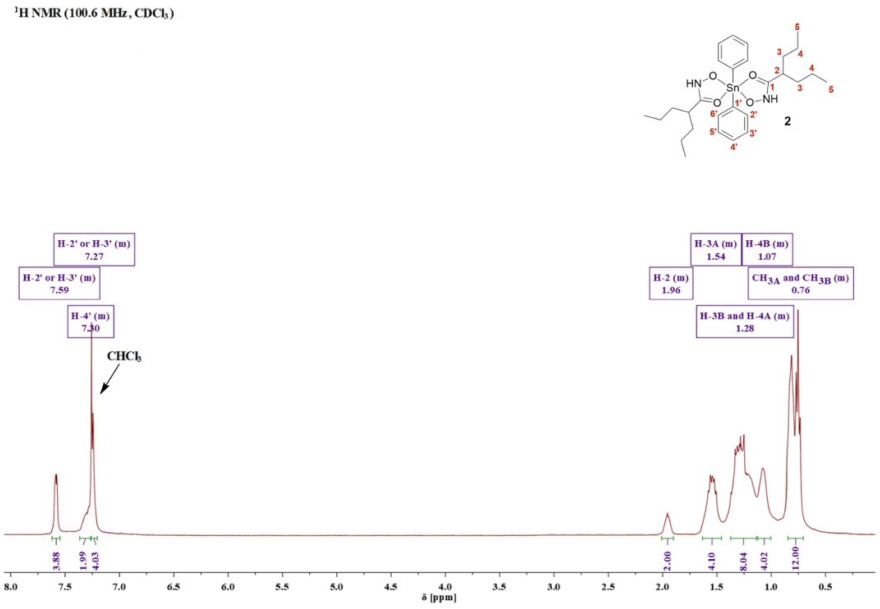

Fig. S-13. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of $[Ph_2Sn(L_2)_2]$ (**2**)

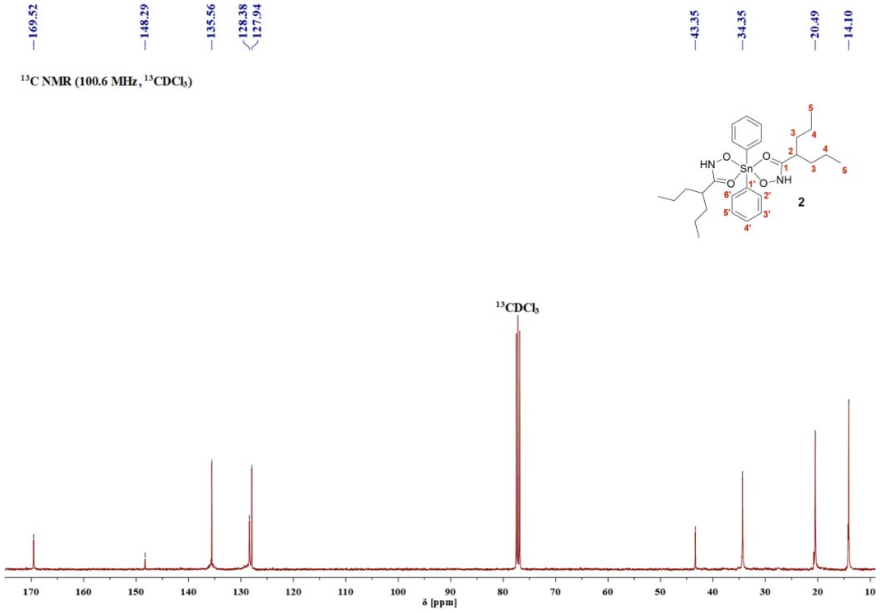

Fig. S-14. ^{13}C NMR spectrum (100.6 MHz, $^{13}CDCl_3$) of $[Ph_2Sn(L_2)_2]$ (**2**)

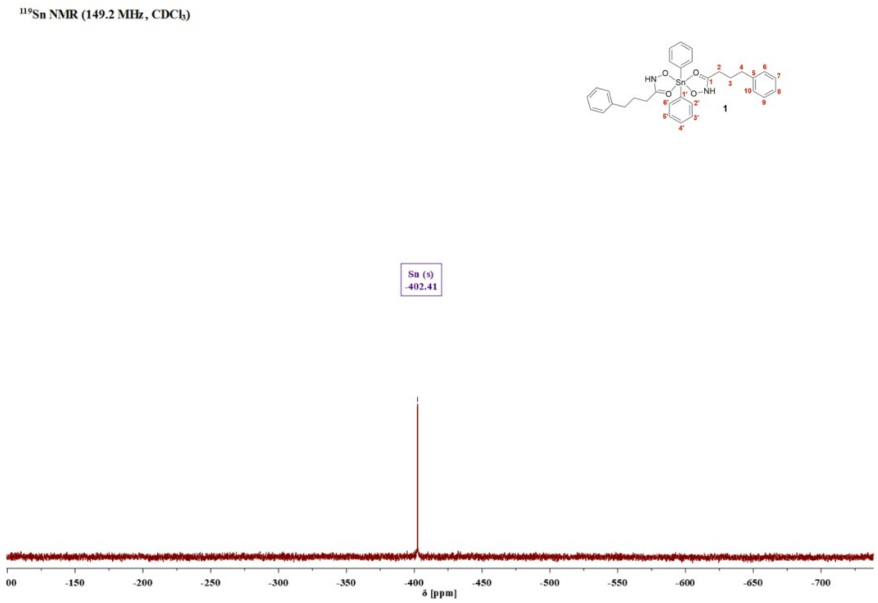

Fig. S-15. ^{119}Sn NMR spectrum (149.2 MHz, $CDCl_3$) of $[Ph_2Sn(L_1)_2]$ (**1**)

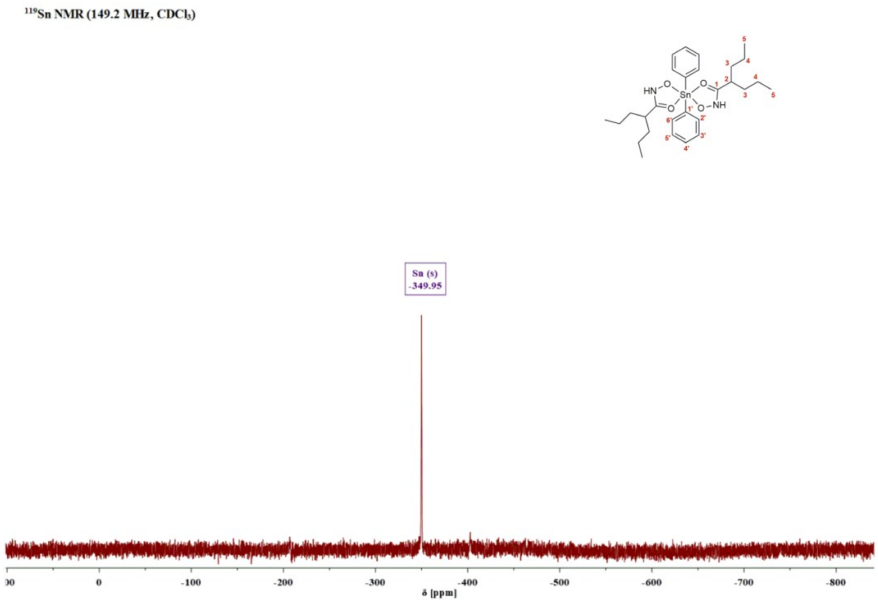

Fig. S-16. ^{119}Sn NMR spectrum (149.2 MHz, $CDCl_3$) of $[Ph_2Sn(L_2)_2]$ (**2**)

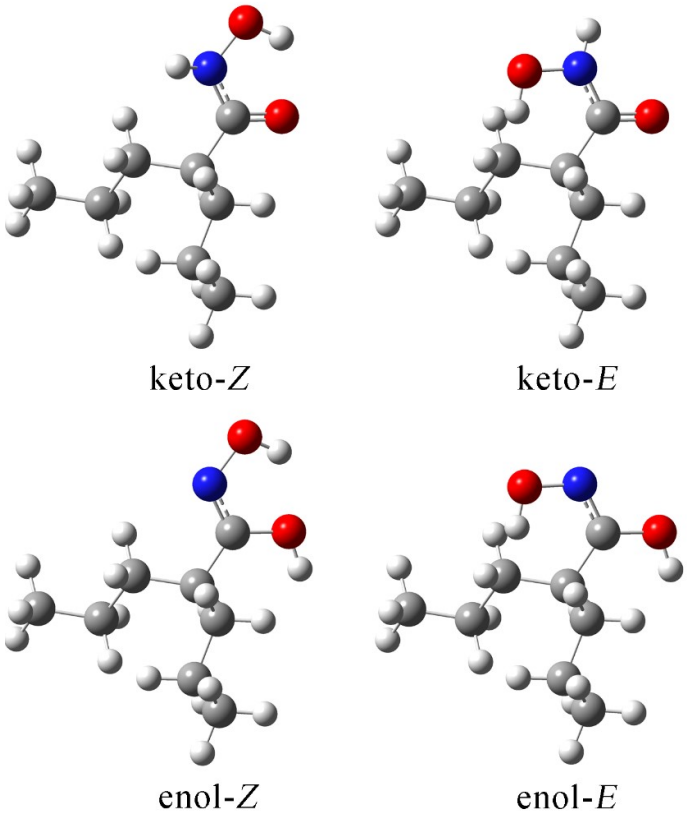

Fig. S-17. Optimized isomers (B3LYP-D3BJ/6-311++G(d,p) level of theory) of **HL_2**

Table S-I. Experimental and theoretical (at B3LYP-D3BJ/6-311++G(d,p) level of theory) of **HL_2**

^{1}H chemical shifts [ppm]			^{13}C chemical shifts [ppm]		
H atom	Experimental	Theoretical	C atom	Experimental	Theoretical
C5-H	0.88	0.88	C5	14.2	15.8
C4-H	1.28	1.28	C4	20.8	27.2
C3-H	1.40	1.30	C3	34.8	38.5
C2-H	1.98	2.06	C2	44.1	49.6
O-H	8.68	6.98	C1	174.5	171.5
N-H	10.36	7.66			
R		0.978	R		0.994
MAE [ppm]		0.04	MAE [ppm]		4.0

Table S-II. Experimental and theoretical (at B3LYP-D3BJ/6-311++G(d,p) level of theory) of complex **2**.

^{1}H chemical shifts [ppm]			^{13}C chemical shifts [ppm]		
H atom	Experimental	Theoretical	C atom	Experimental	Theoretical
C5-H	0.76	0.58	C5	14.1	16.5
C4-HA	1.07	0.78	C4	20.5	22.0
C4-HB	1.28	0.89	C3	34.4	38.1
C3-HA	1.28	0.95	C2	43.4	48.0
C3-HB	1.54	1.29	C2’	127.9	133.7
C2-H	1.96	1.53	C6’	127.9	125.0
C2’-H	7.27	7.22	C4’	128.3	128.7
C6’-H	7.27	7.22	C3’	135.6	130.0
C4’-H	7.30	7.28	C5’	135.6	130.0
C3’-H	7.59	7.54	C1’	148.3	147.7
C5’-H	7.59	8.08	C1	169.5	169.6
R		0.992	R		0.991
MAE [ppm]		0.22	MAE [ppm]		3.0