Supplementary material

Synthesis, spectroscopy, and density functional theory of organotin and organosilicon complexes of bioactive ligand containing nitrogen, sulfur donor atoms as antimicrobial agents: in-vitro and in-silico studies

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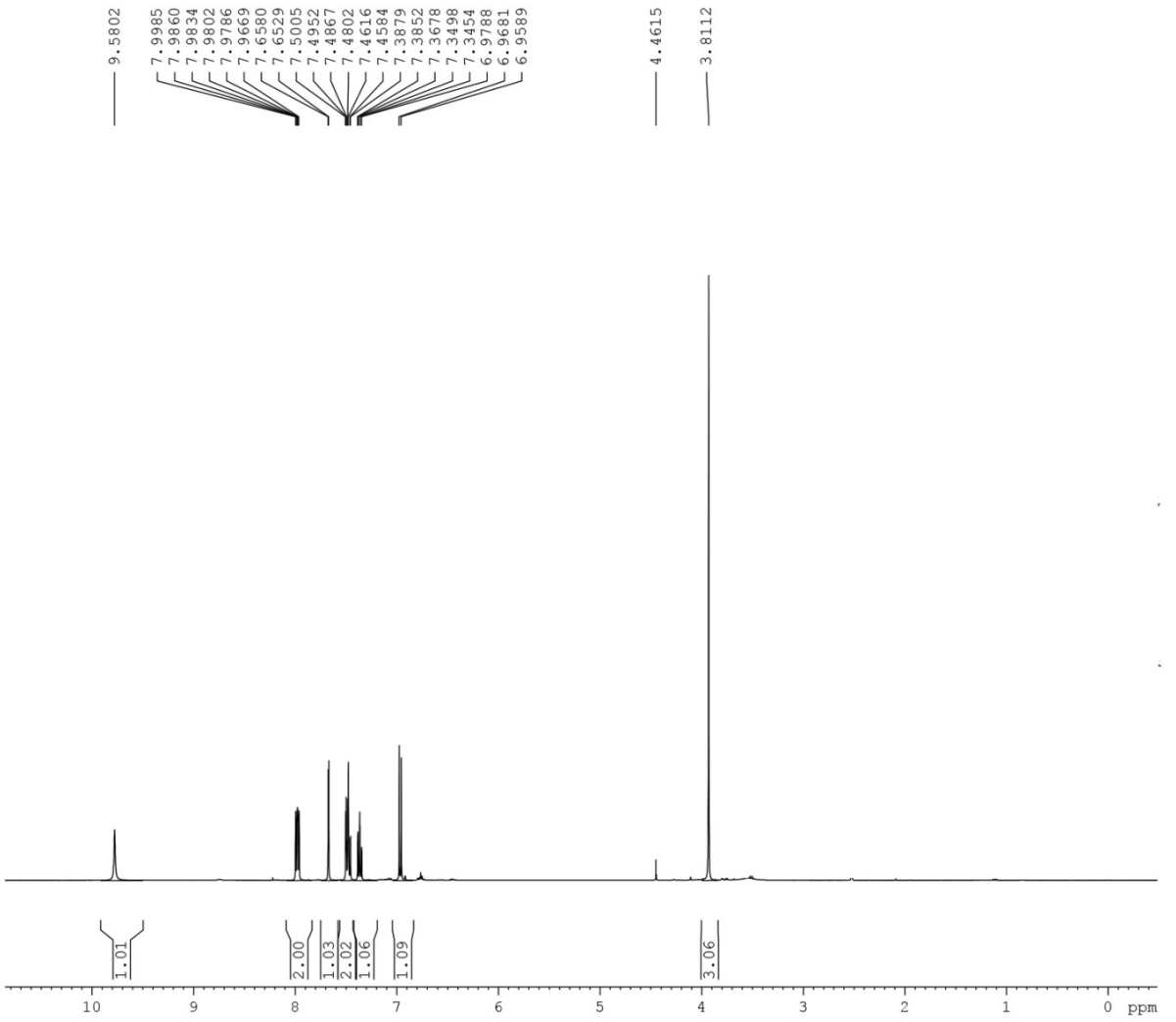

Fig. S1. [1]HNMR spectrum of compound LH.

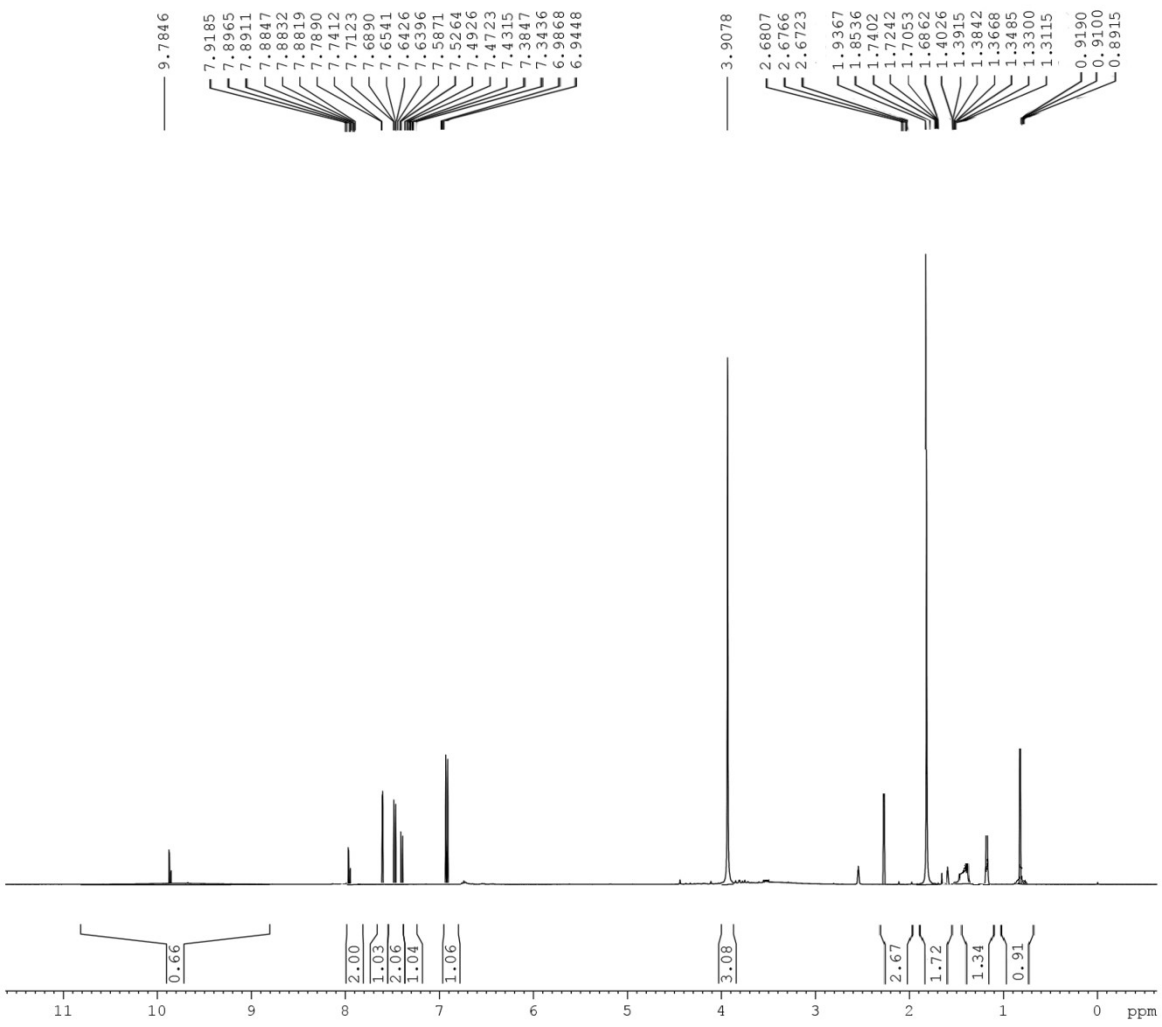

Fig. S2. ^{1}H-NMR spectrum of Compound 1.

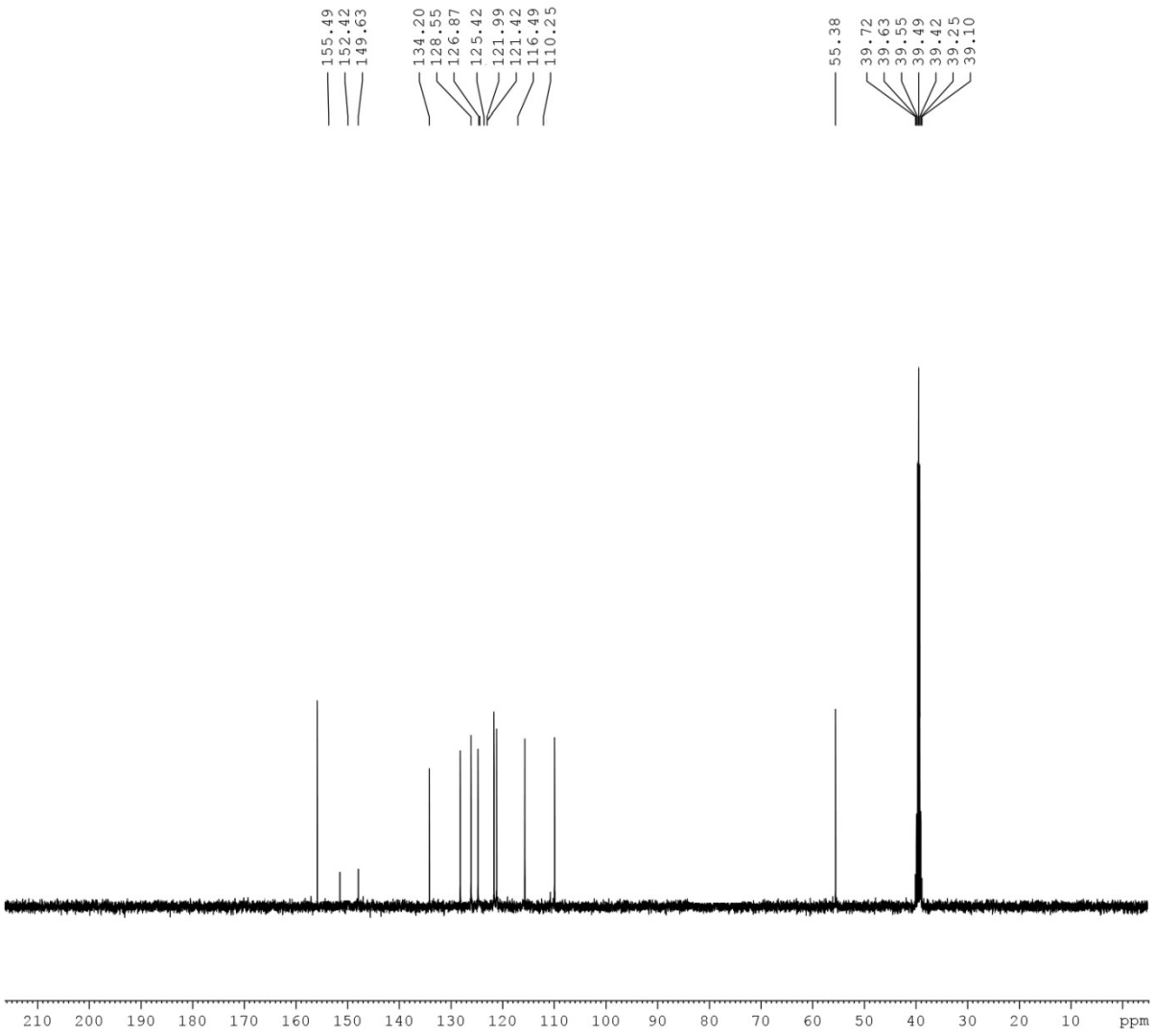

Fig. S3. ^{13}CNMR spectrum of compound LH.

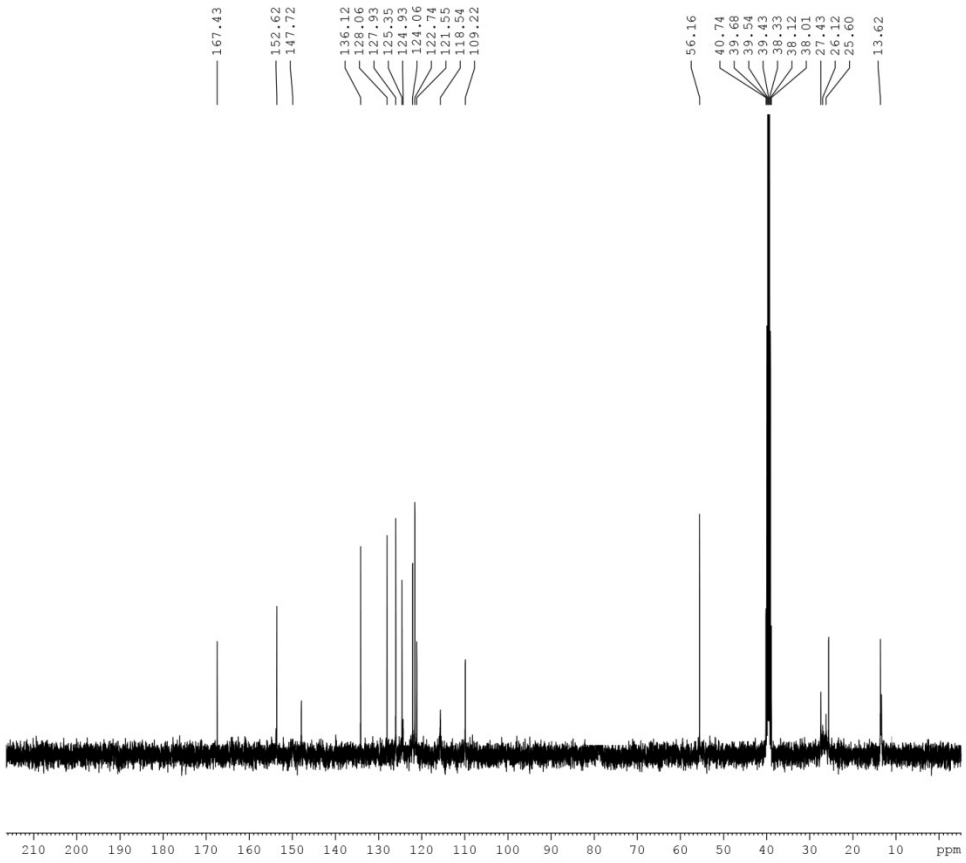

Fig. S4. ^{13}CNMR spectrum of Compound 1.

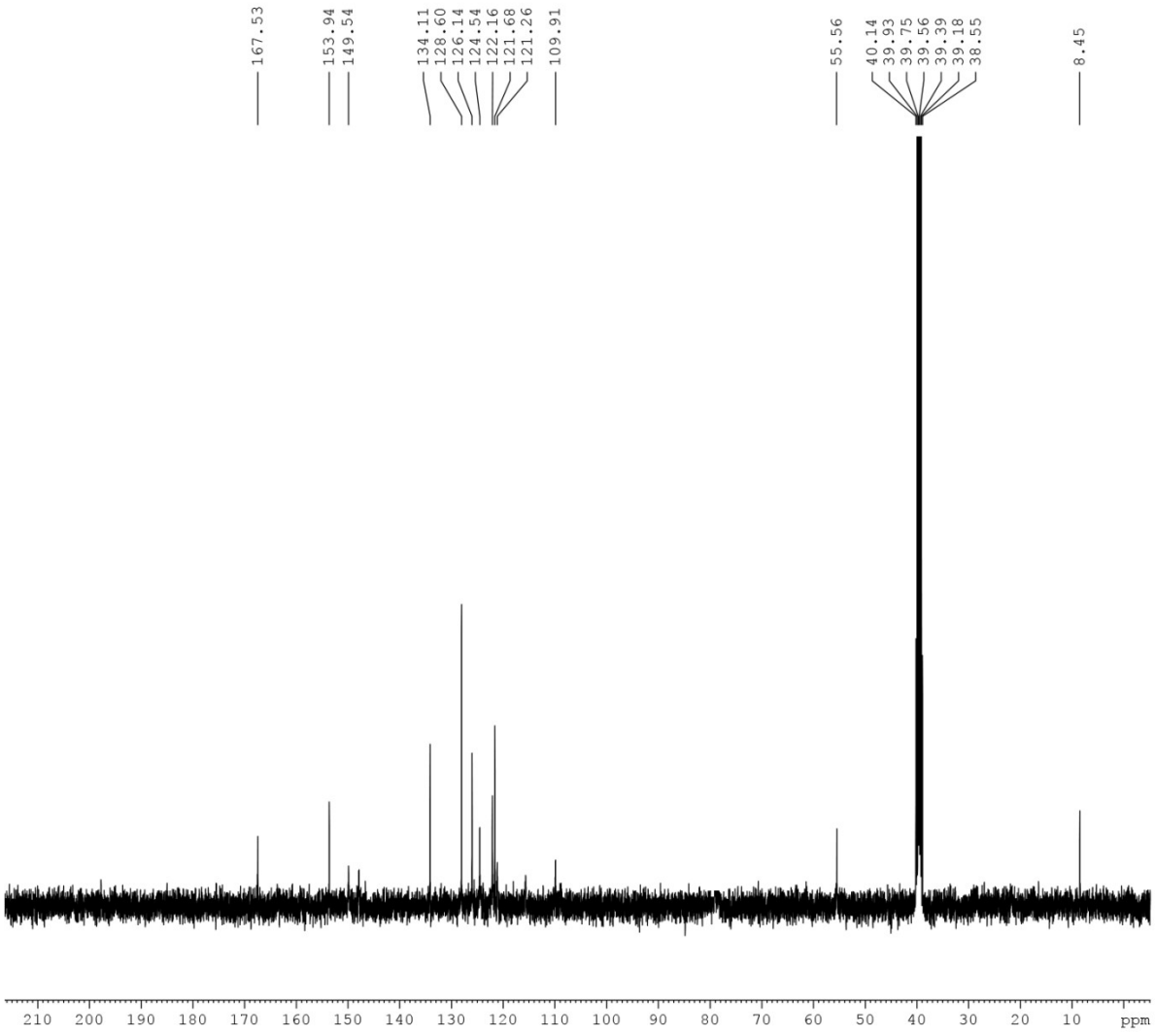

Fig. S5. ^{13}CNMR spectrum of Compound 3.

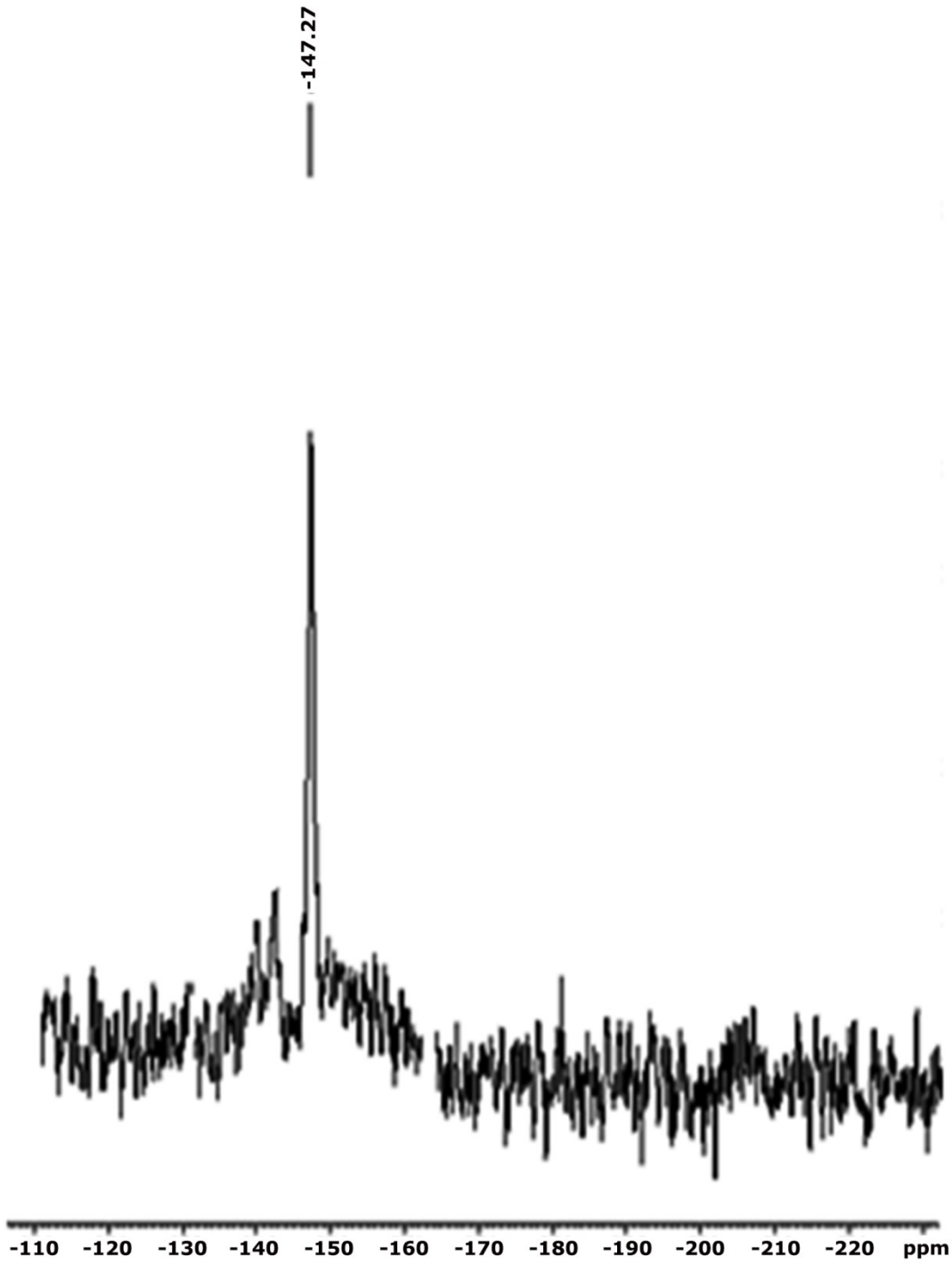

Fig. S6. ^{13}CNMR spectrum of compound 1.

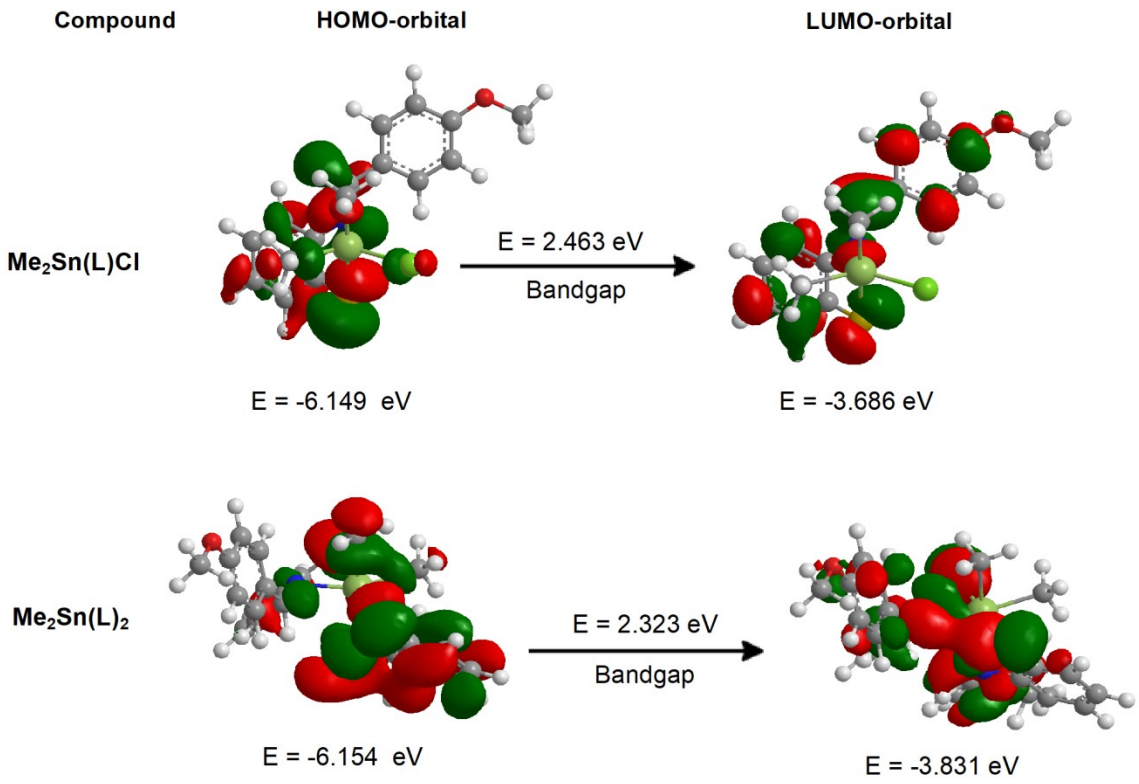

Fig. S7. HOMO-LUMO orbital energy of $Me_2Sn(L)Cl$ and $Me_2Sn(L)_2$ complexes.

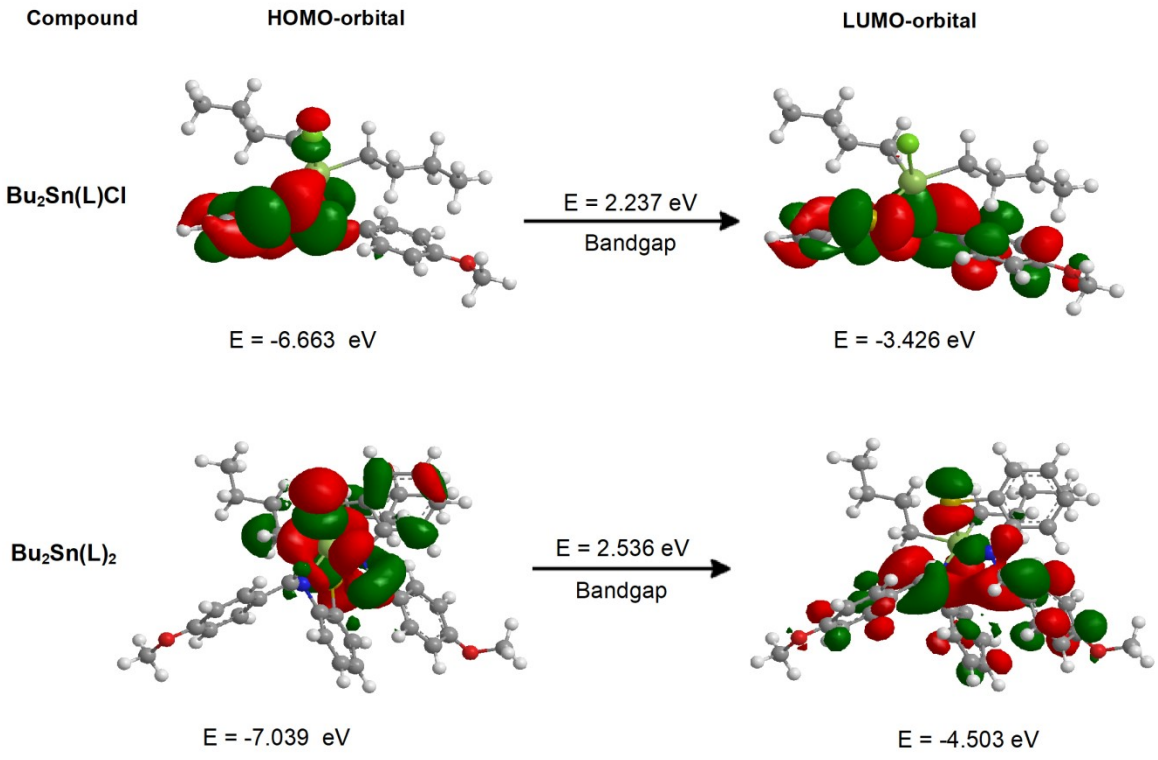

Fig. S8. HOMO-LUMO orbital energy of $Bu_2Sn(L)Cl$ and $Bu_2Sn(L)_2$ complexes..

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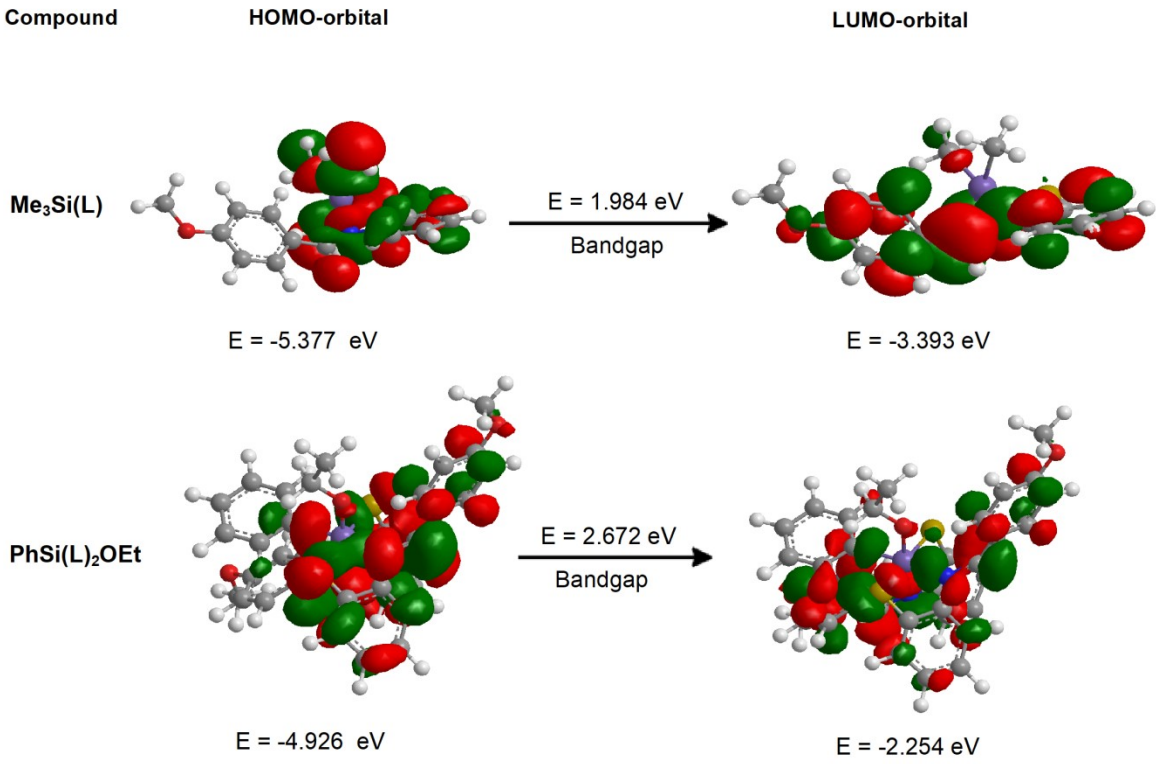

Fig. S9. HOMO-LUMO orbital energy of Me_3SiL and $PhSi(L)_2OEt$ complexes.

Table S1. The Mulliken atomic charge distribution calculated by DFT/b3lyp/LanL2DZ of 2-(4-methoxyphenyl)-2,3-dihydrobenzo[d]thiazole.

Atoms	Atomic Charges	Atoms	Atomic Charges	Atoms	Atomic Charges
2-(4-methoxyphenyl)-2,3-dihydrobenzo[d]thiazole (LH)					
C1	-0.377027	C11	-0.389594	H21	0.240289
C2	0.388747	C12	-0.384616	H22	0.070969
C3	-0.313680	C13	0.373760	H23	0.185948
C4	-0.284709	C14	-0.312966	H24	0.235227
C5	-0.232886	C15	-0.449352	H25	0.257816
C6	-0.229901	O16	-0.306562	H26	0.218792
N7	-0.026410	C17	-0.502166	H27	0.306404
S8	-0.000639	H18	0.215803	H28	0.236769
C9	-0.340779	H19	0.230725	H29	0.207511
C10	0.527442	H20	0.236300	H30	0.218783

Table S2. The Mulliken atomic charge distribution calculated by DFT/b3lyp/LanL2DZ of Chloro2-{(4-methoxybenzylidene)amino}benzenethiolate dimethyltin(IV) complex

Atoms	Atomic Charges	Atoms	Atomic Charges	Atoms	Atomic Charges
C1	-0.220974	C14	-0.771397	H27	0.254667
C2	-0.296970	C15	-0.390025	H28	0.269248
C3	-0.325579	O16	-0.280865	H29	0.191374
C4	0.566850	C17	-0.499291	H30	0.198699
C5	-0.457746	Sn18	1.000187	H 31	0.252765
C6	-0.253287	Cl19	-0.338001	H 32	0.198457
N7	-0.500072	C20	-0.956147	H33	0.225781
C8	-0.437270	C21	-0.815560	H 34	0.232950
S9	-0.058092	H22	0.230881	H35	0.259473
C10	0.632059	H23	0.225641	H36	0.204028
C11	-0.409149	H24	0.201432	H37	0.850791
C12	-0.442595	H25	0.250019	H38	0.386167
C13	0.355501	H26	0.230429	H39	0.235619

Table S3. The Mulliken atomic charge distribution calculated by DFT/b3lyp/LanL2DZ of Bis-[2-{(4-methoxybenzylidene)amino}benzenethiolate]dimethyltin(IV) complex.

Atoms	Atomic Charges	Atoms	Atomic Charges	Atoms	Atomic Charges
C1	-0.281112	C24	0.523088	H47	0.212805
C2	-0.243806	C25	-0.422910	H48	0.221767
C3	-1.905496	S26	-0.279592	H49	0.240216
C4	0.402921	N27	-0.442550	H50	1.157126
C5	-0.410464	C28	-0.445932	H51	0.288013
C6	-0.260645	C29	-0.053916	H52	0.252535
N7	-0.416760	C30	0.546697	H53	0.267491
C8	-0.412631	C31	-0.478641	H54	0.268081
S9	-0.005637	C32	-0.415195	H55	0.185405
C10	0.381958	C33	0.401304	H56	0.225533
C11	-0.457528	C34	-0.706699	H57	0.220839
C12	-0.404315	O35	-0.910452	H58	0.204345
C13	0.391413	C36	-0.300624	H59	0.248799
C14	-0.559299	C37	-0.506650	H60	0.231527
C15	-0.917188	H38	0.246322	H61	0.243132
O16	-0.300106	H39	0.241318	H62	0.219176
C17	-0.504850	H40	1.301250	H63	0.230493
Sn18	1.030009	H41	0.270187	H64	0.326132
C19	-0.634523	H42	0.271470	H65	0.238801
C20	-1.038559	H43	0.246388	H66	0.215357
C21	-0.222549	H44	0.221642	H67	0.222850
C22	-0.290280	H45	0.257703		
C23	-0.347385	H46	1.922207		