Electronic Supplementary Information

One-pot microwave-assisted synthesis of organotin Schiff bases: An optical and electrochemical study towards their effect in organic solar cells

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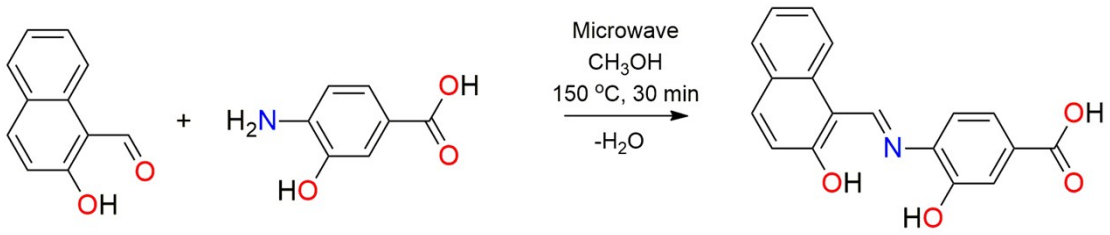
*2.7.5 (E)-3-hydroxy-4-(((2-hydroxynaphthalen-1-yl)methylene)amino)benzoic acid (**2a**)*



2a

An homogeneous mixture of 2-hydroxy-1-napthaldehyde 0.1 g (0.58 mmol), 2-aminophenol 0.0633 g (0.58 mmol) in methanol (5 mL) was irradiated using microwaves at 150°C for 30 min. The reaction progress was monitored by thin layer chromatography every 60 s. After cooling to room temperature, the excess of solvent was eliminated, and the product was filtered and washed with hexane. It was obtained as a yellow solid in 95% yield (0.27 g, 0.54 mmol); ^{1}H NMR (400.13 MHz, DMSO-d_6) δ (ppm): 6.80 (d, H3, ^{3}J = 8.0 Hz, 1H), 7.26-7.33 (t-d, H7, ^{3}J = 7.28 Hz, 1H), 7.47-7.51 (t-d, H8, ^{3}J = 7.48 Hz, 1H), 7.51-7.54 (d-d, H14, 1H), 7.57 (d-d, H13, ^{3}J = 8.0 Hz 1H), 7.67 (d-d, H16, ^{3}J = 9.0 Hz 1H), 7.82 (d, H6, ^{3}J = 8.0 Hz, 1H), 8.05 (d, H4, ^{3}J = 8.0 Hz, 1H), 8.40 (d, H9, ^{3}J = 8.3 Hz, 1H),

9.52 (S, 1H, N-H); 10.81 (S, 2H, OH) 15.48 (S, 1H, COOH); ^{13}C NMR (75.45 MHz, DMSO-d_6) δ (ppm): 108.25 -8-C1), 116.43 (C3), 116.97 (C9), 120.02 (C16), 121.25 (C14) 123.54 (C7), 125.31 (C15), 126.06 (C5), 128.17 (C8), 128.37 (C13), 129.14 (C6), 133.87 (C17), 138.91 (C10), 147.05 (C4), 149.11 (C11), 166.92 (C12), 179.02 (C2); 192.90 (COOH).

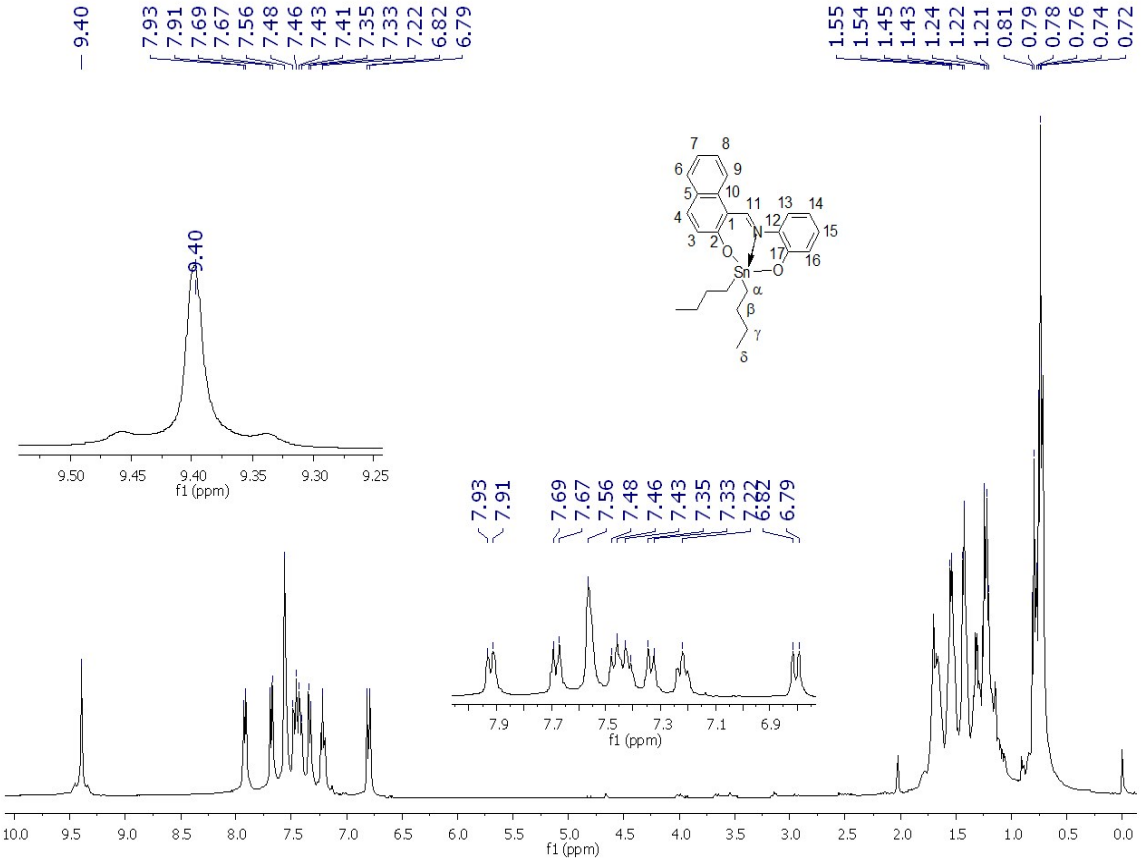


Fig. S1. ^{1}H NMR ($CDCl_3$) spectra of organotin compound **1**.

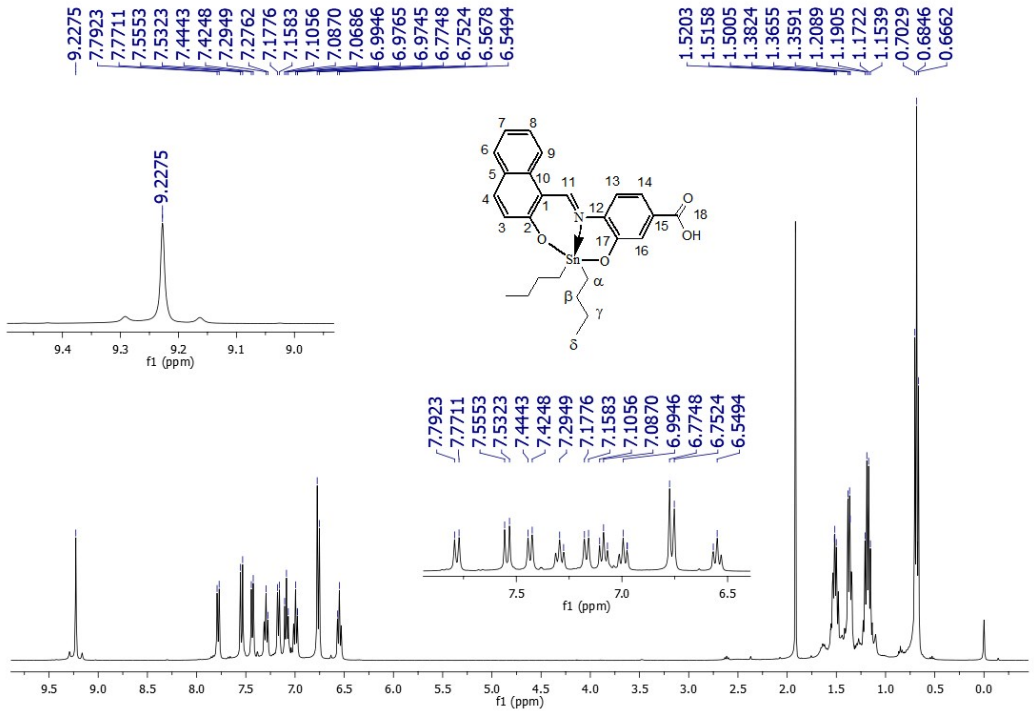


Fig. S2. ^{1}H NMR ($CDCl_3$) spectrum of organotin compound **2.**

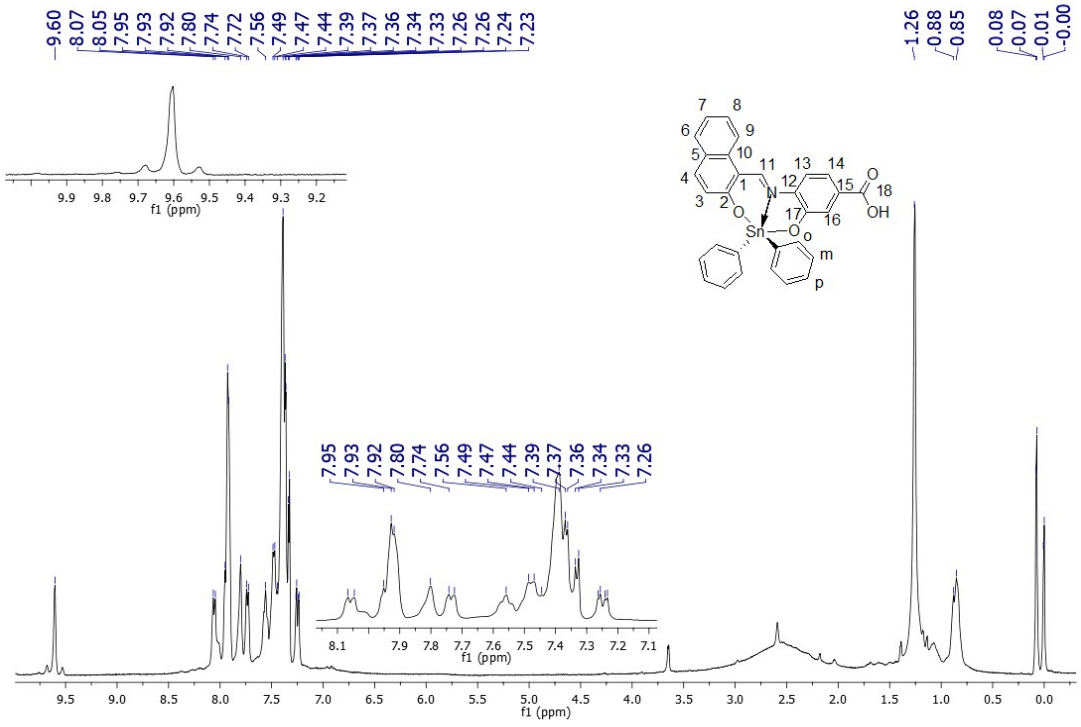


Fig. S3. ^{1}H NMR ($CDCl_3$) spectrum of organotin compound **3.**

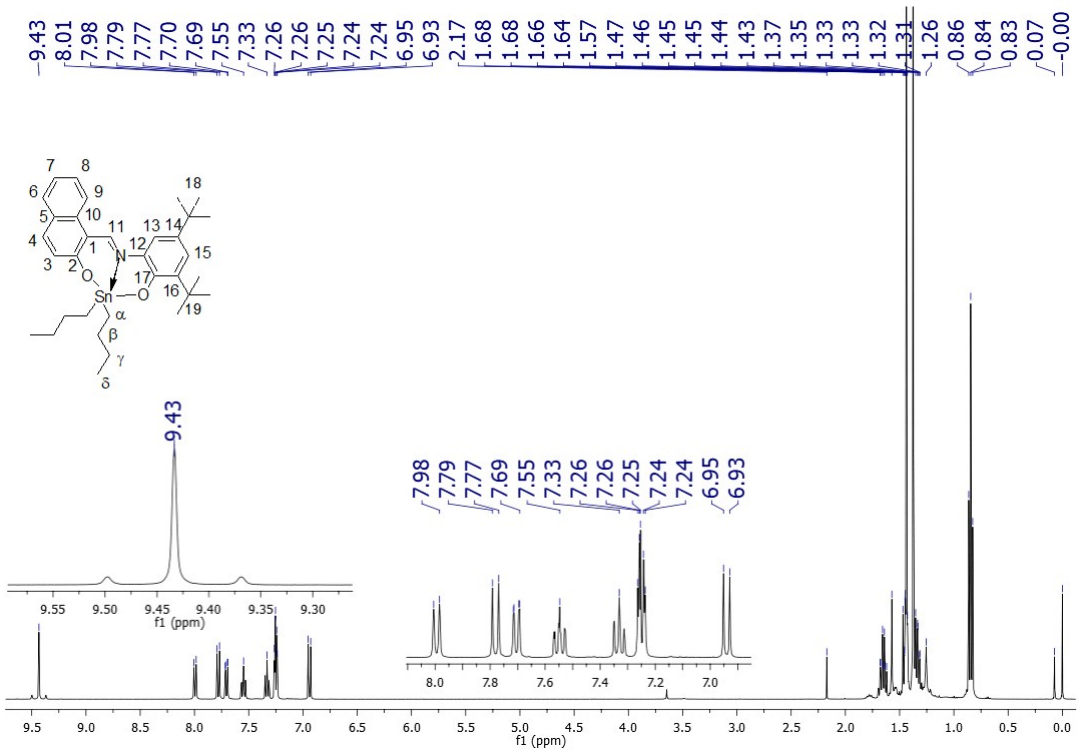


Fig. S4. ^{1}H NMR ($CDCl_3$) spectrum of organotin compound **4**.

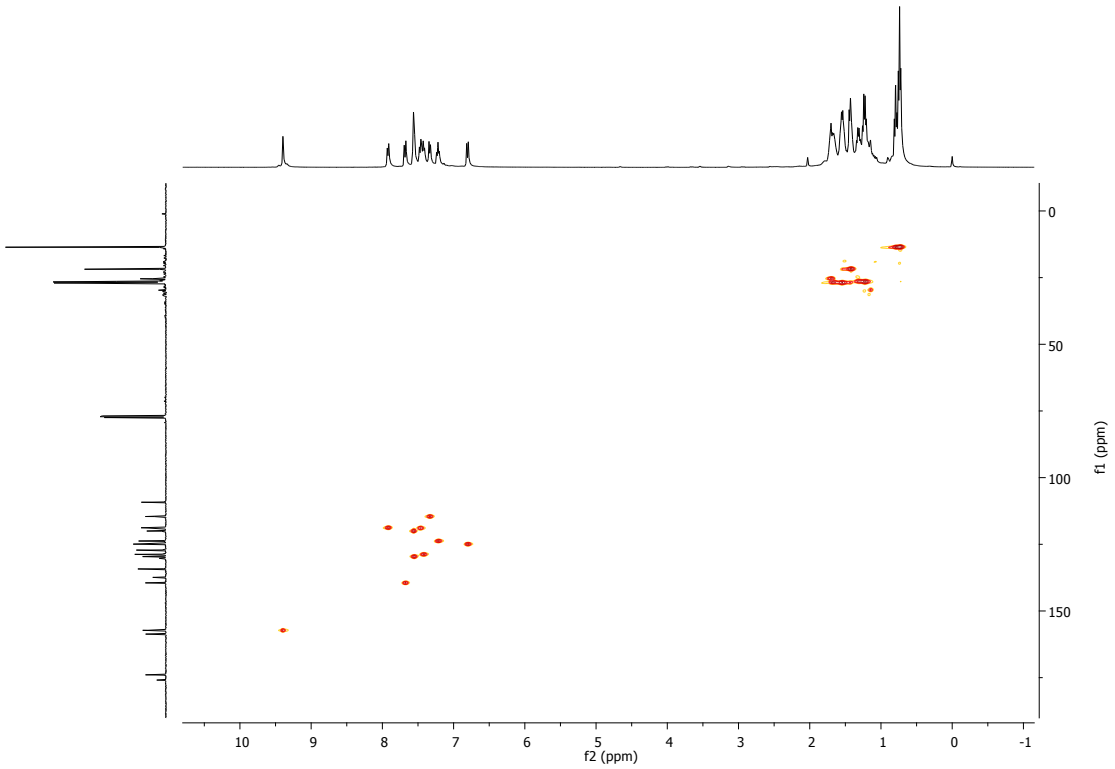


Fig. S5. HETCOR ($CDCl_3$) spectrum of organotin compound **1.**

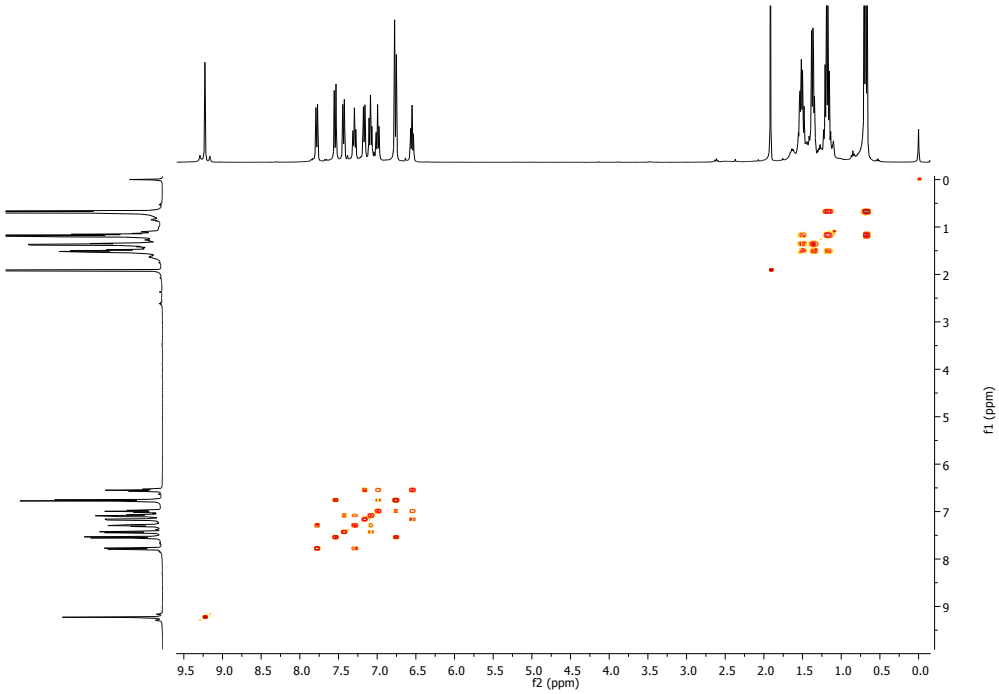


Fig. S6. HETCOR ($CDCl_3$) spectrum of organotin compound **2.**

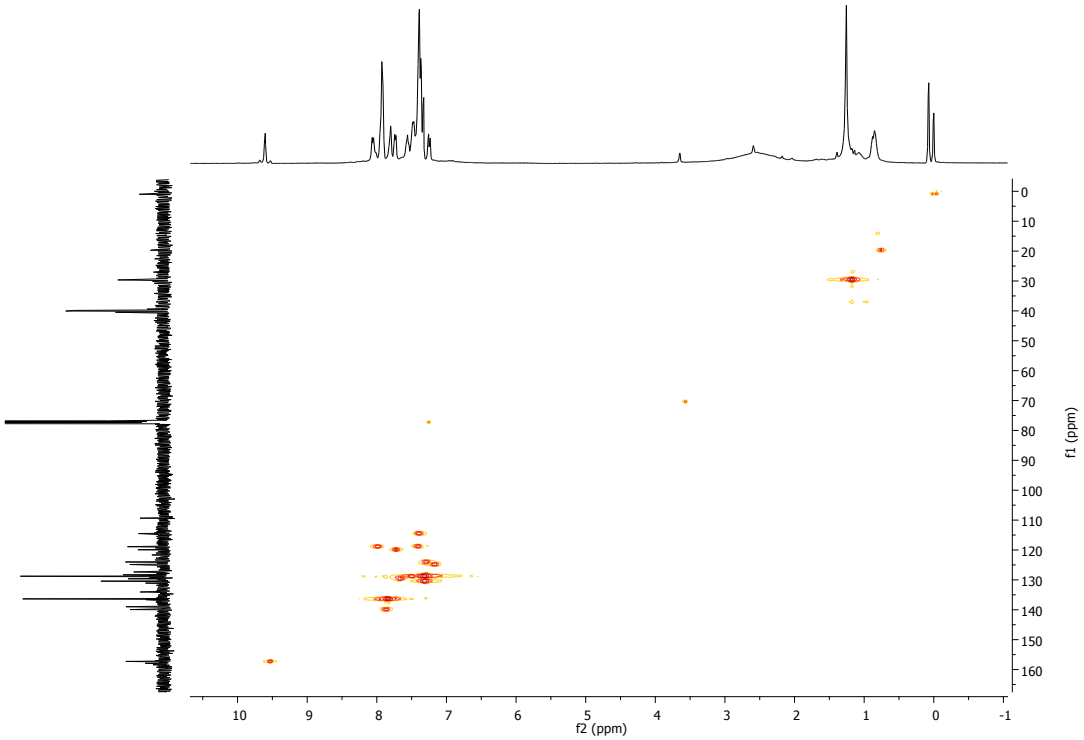


Fig. S7. HETCOR ($CDCl_3$) spectrum of organotin compound **3.**

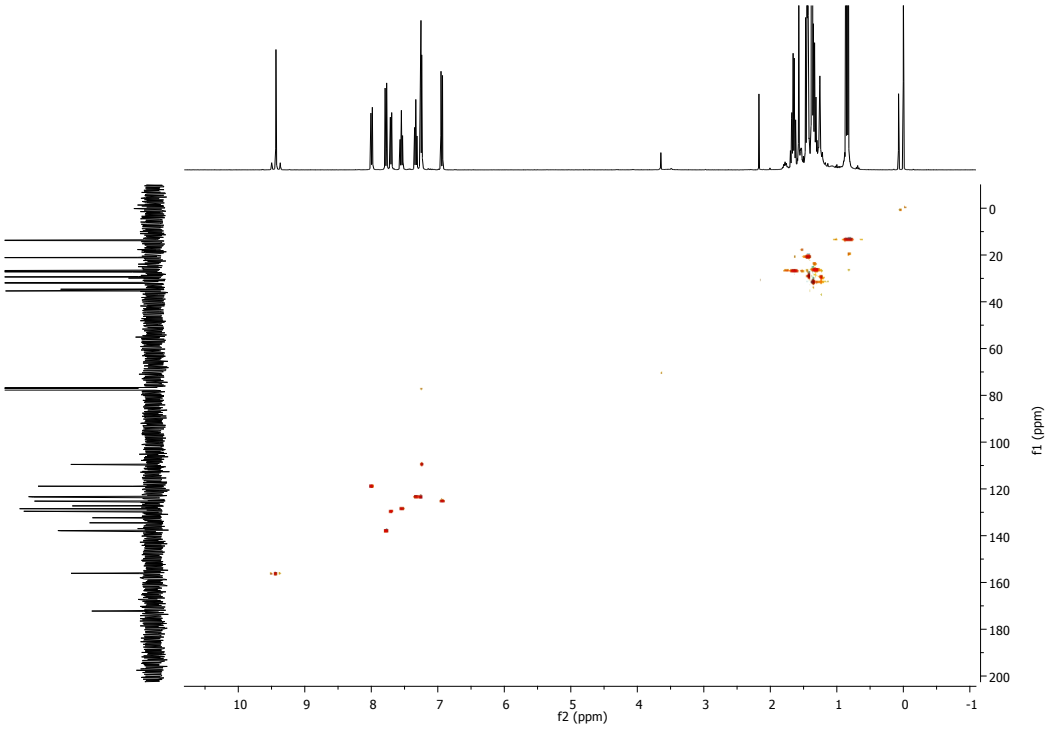


Fig. S8. HETCOR ($CDCl_3$) spectrum of organotin compound **4**

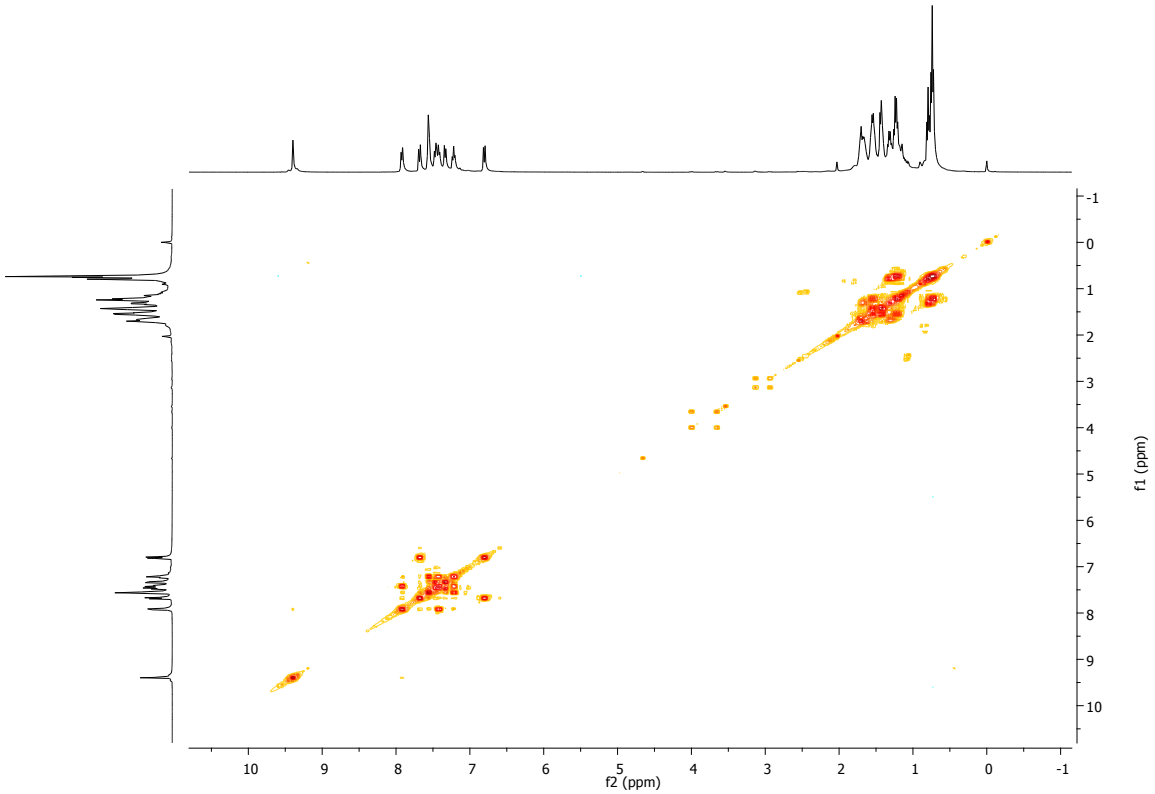


Fig. S9. COSY ($CDCl_3$) spectrum of organotin compound **1.**

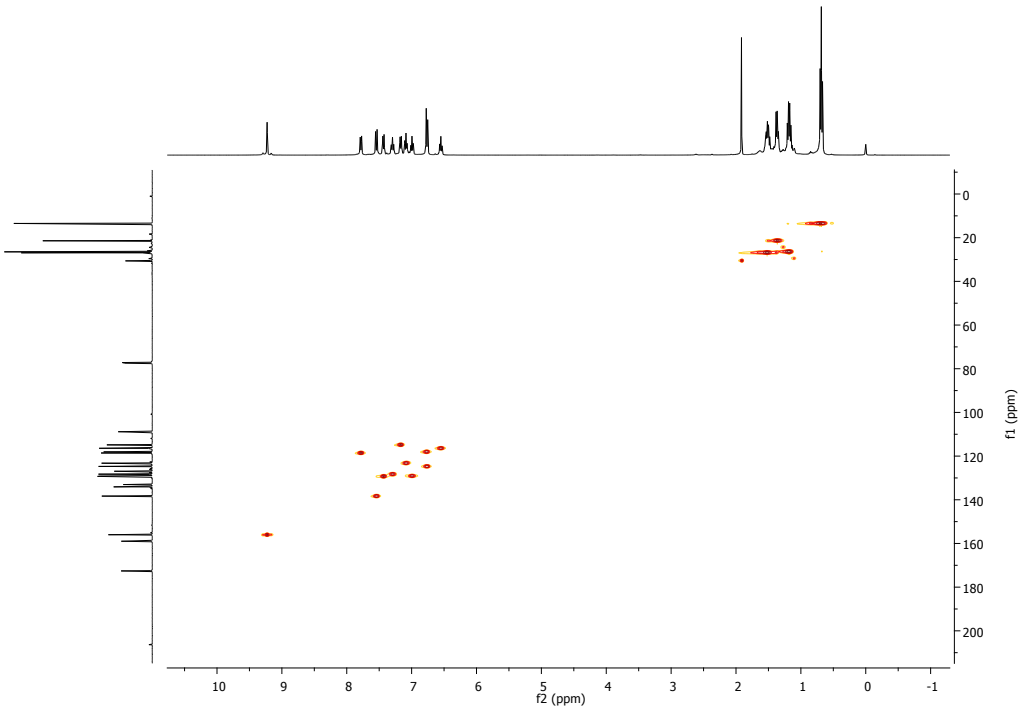


Fig. S10. COSY ($CDCl_3$) spectrum of organotin compound **2.**

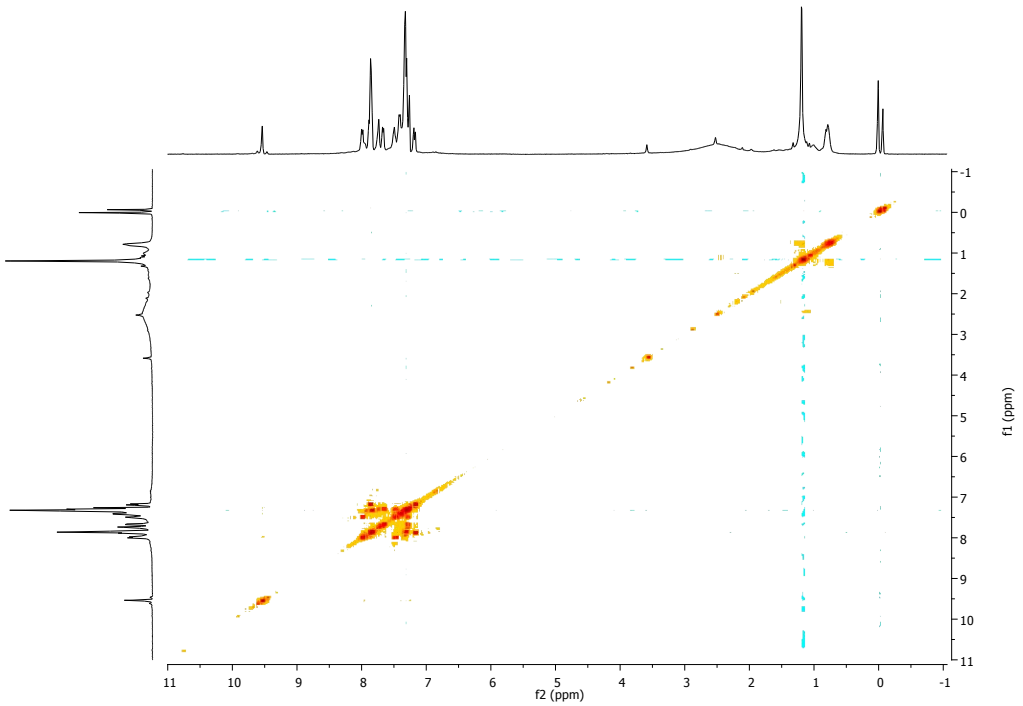


Fig. S11. COSY ($CDCl_3$) spectrum of organotin compound **3.**

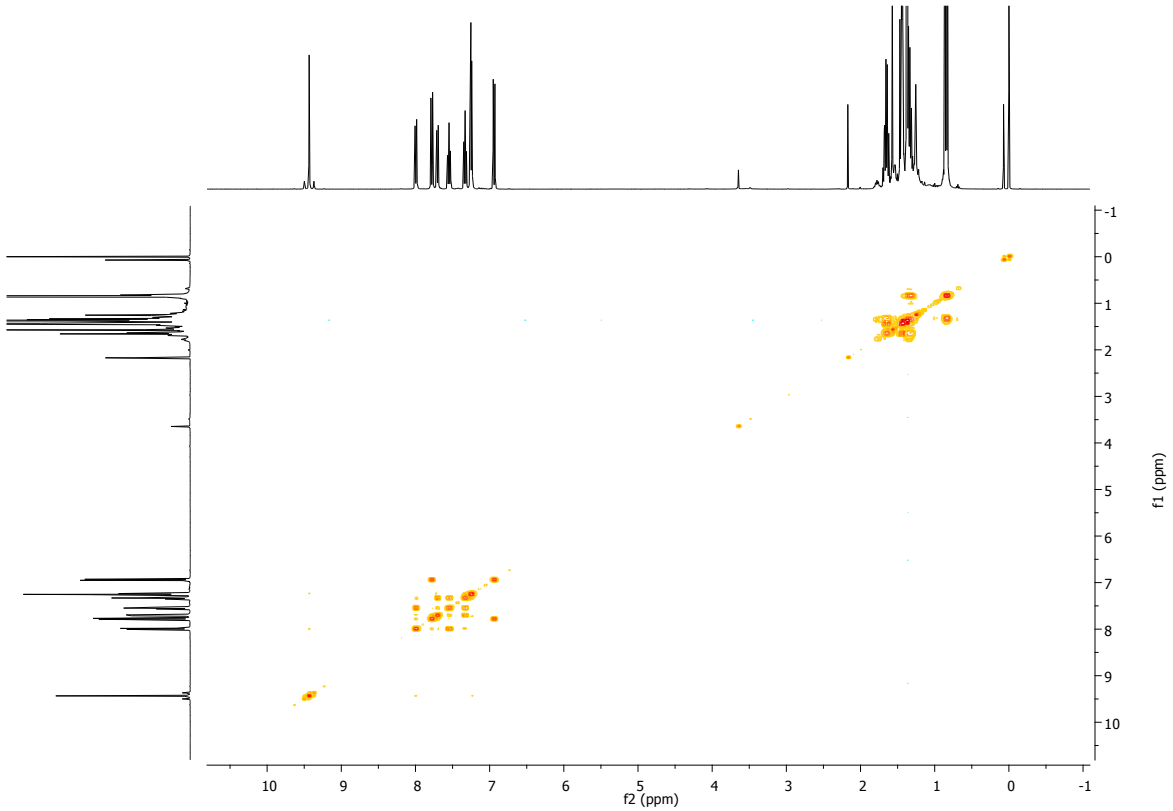


Fig. S12. COSY ($CDCl_3$) spectrum of organotin compound **4**.

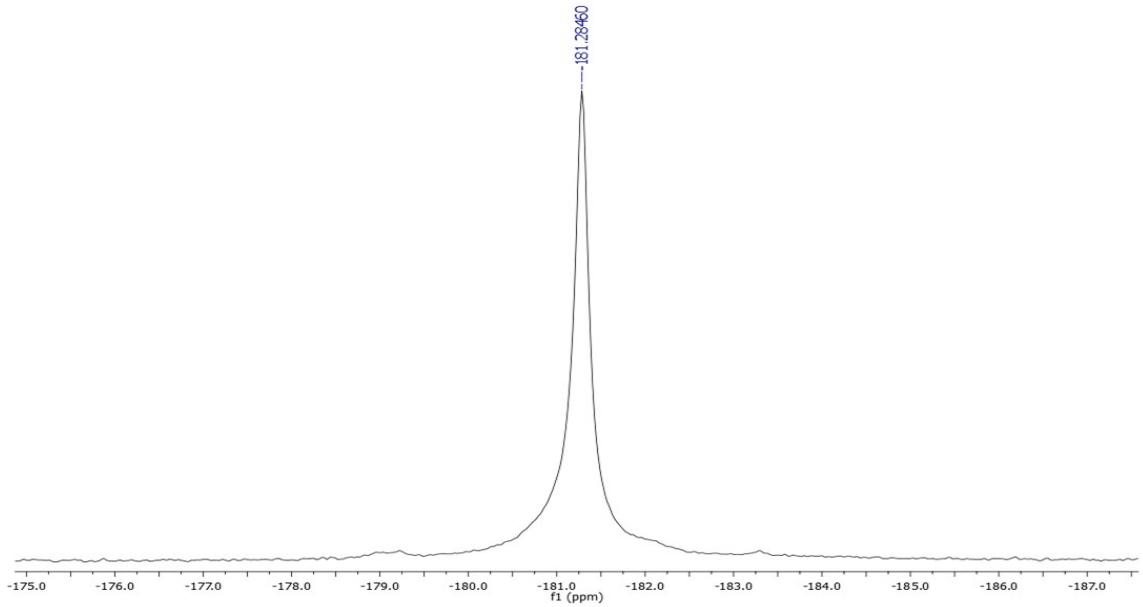


Fig. S13. ^{119}Sn NMR ($CDCl_3$) spectrum of organotin compound **1.**

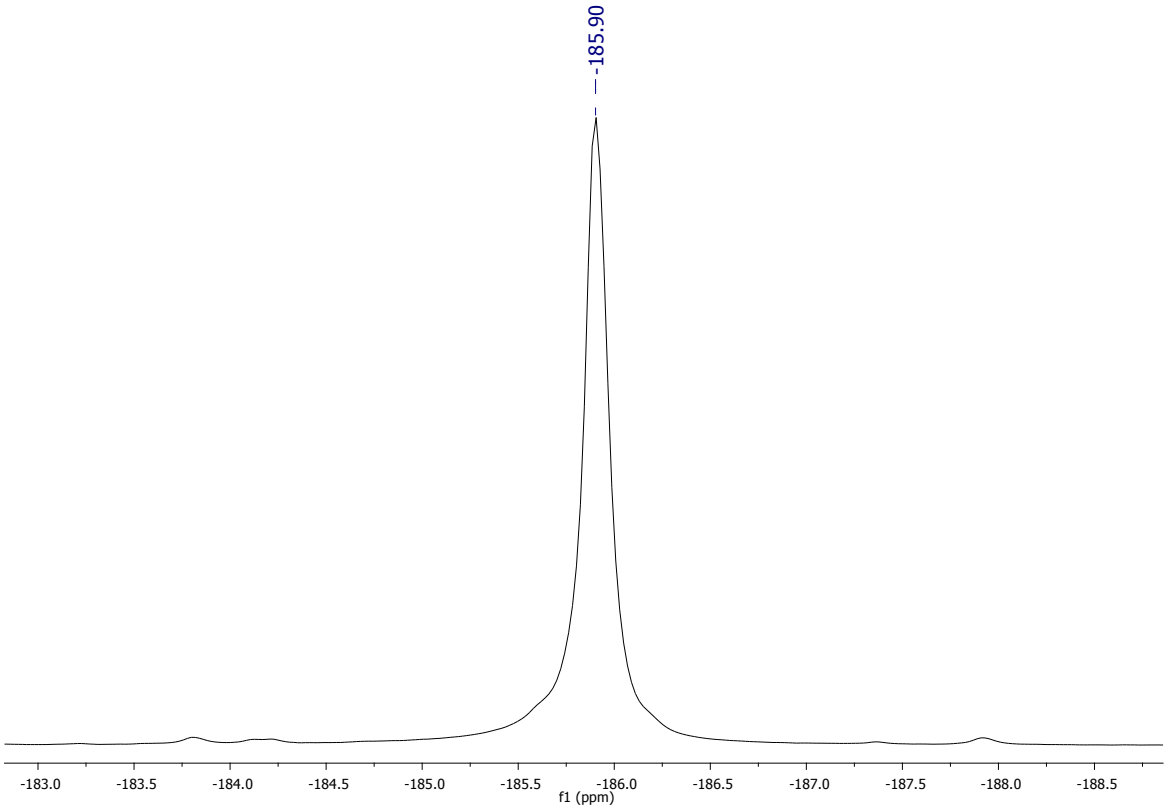


Fig. S14. ^{119}Sn NMR ($CDCl_3$) spectrum of compound **2.**

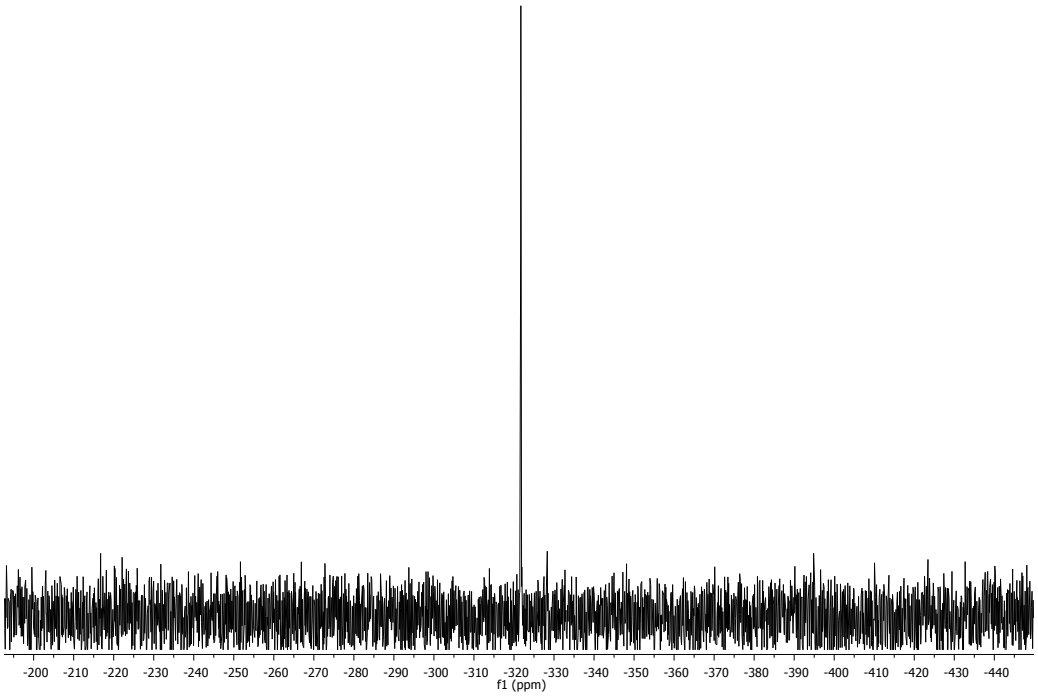


Fig. S15. ^{119}Sn NMR ($CDCl_3$) spectrum of organotin compound **3.**

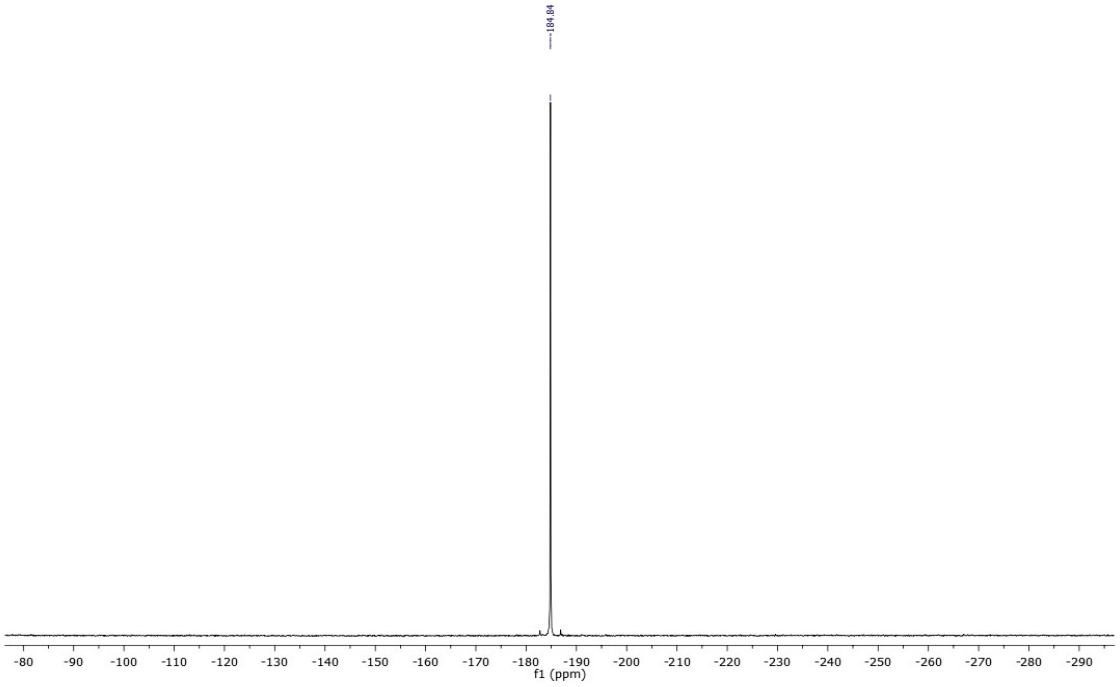


Fig. S16. ^{119}Sn NMR ($CDCl_3$) spectrum of organotin compound **4.**

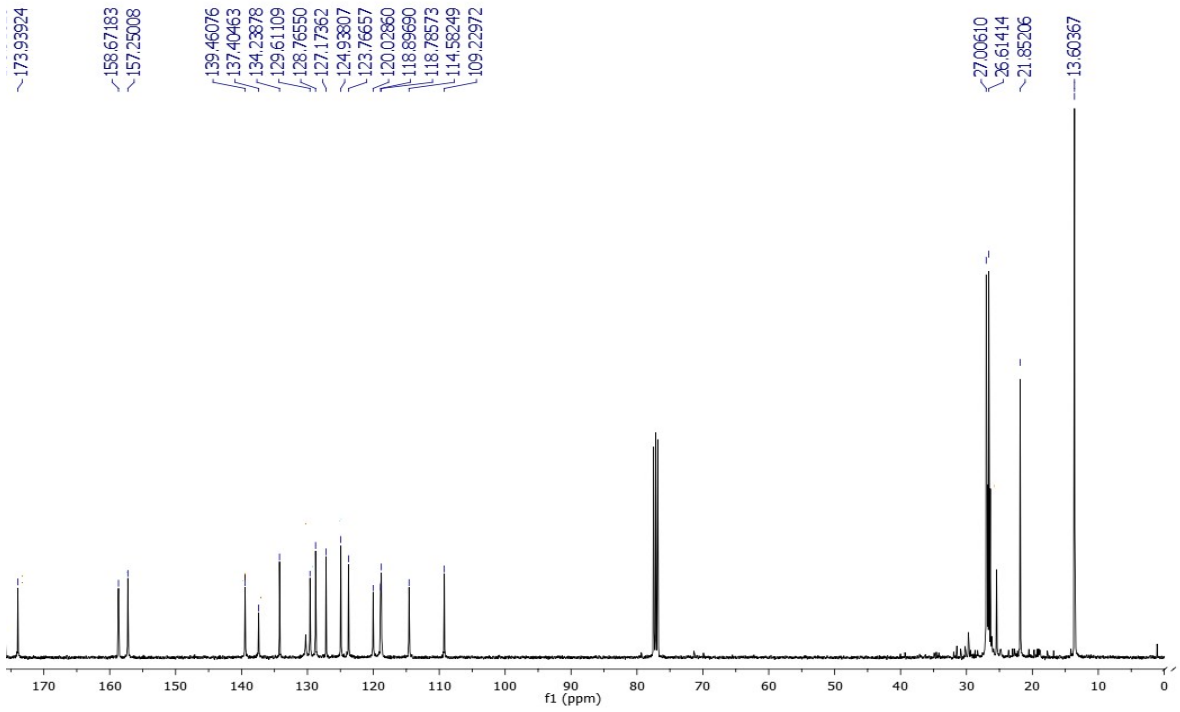


Fig. S17. ^{13}C NMR ($CDCl_3$) spectrum of compound **1**

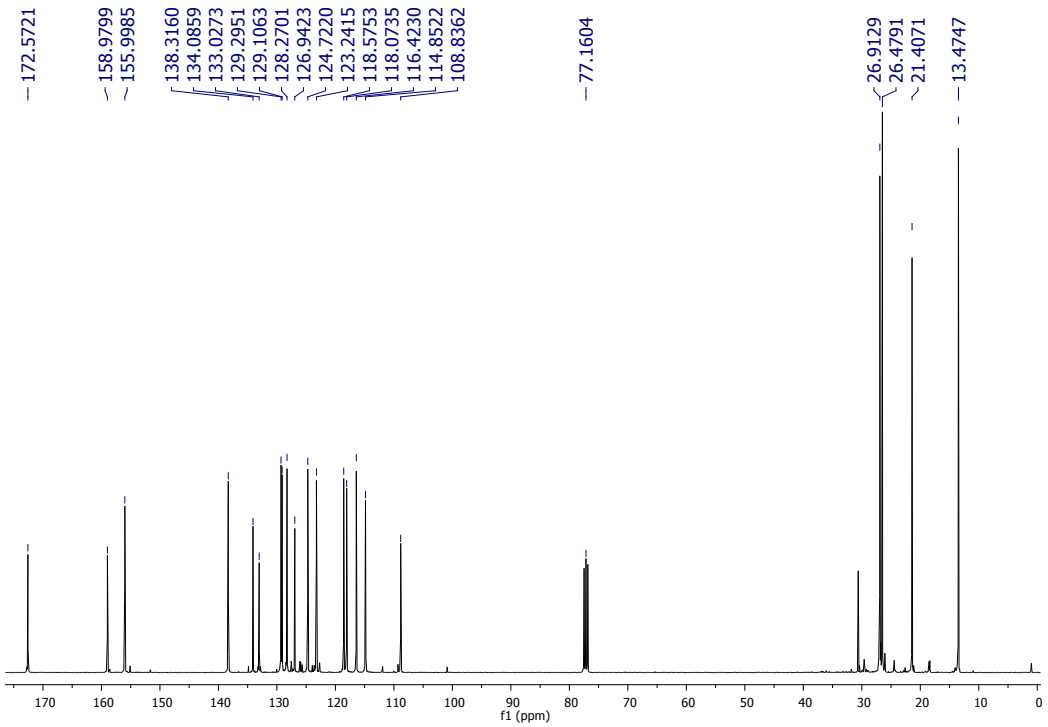


Fig. S18.^{13}CNMR spectrum of organotin compound **2.**

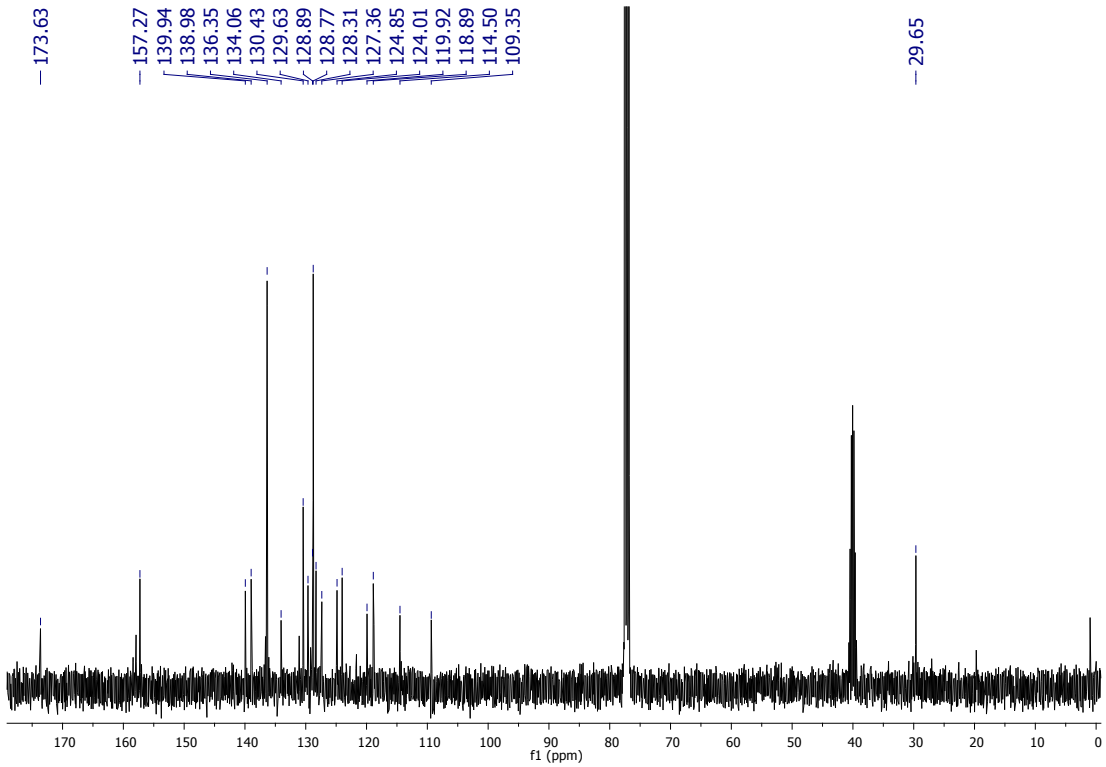


Fig. S19.^{13}C NMR ($CDCl_3$) spectrum of organotin compound **3.**

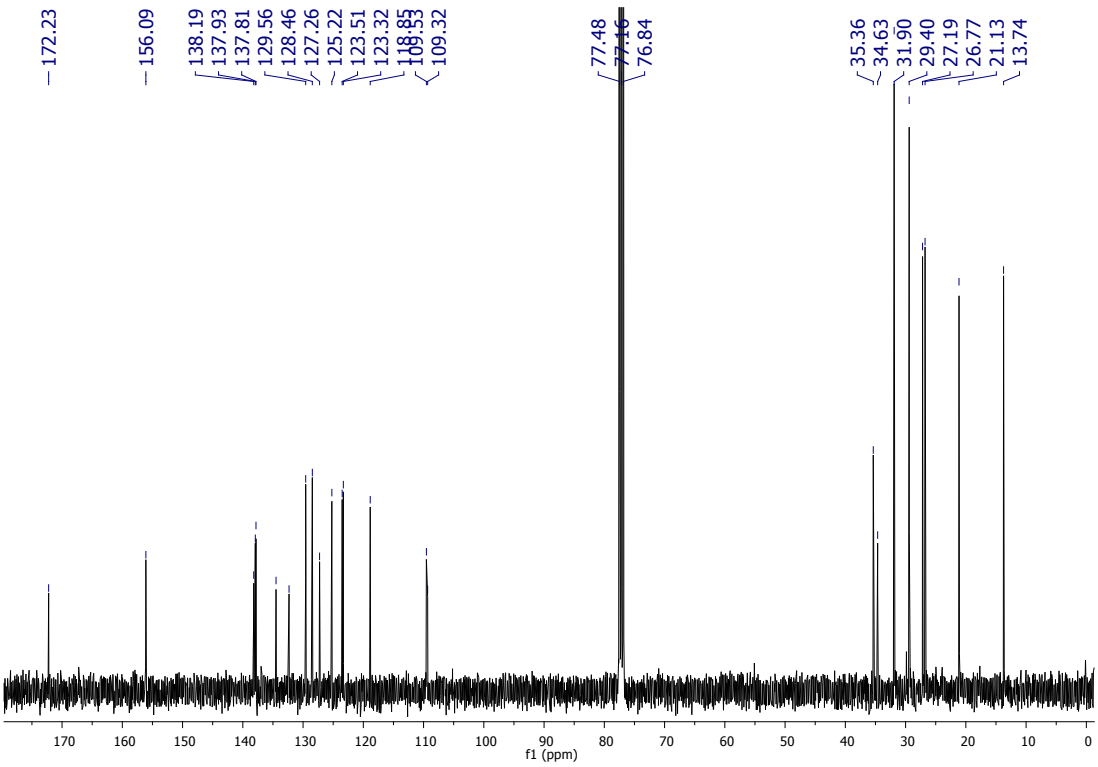


Fig. S20. ^{13}CNMR ($CDCl_3$) spectrum of organotin compound **4.**

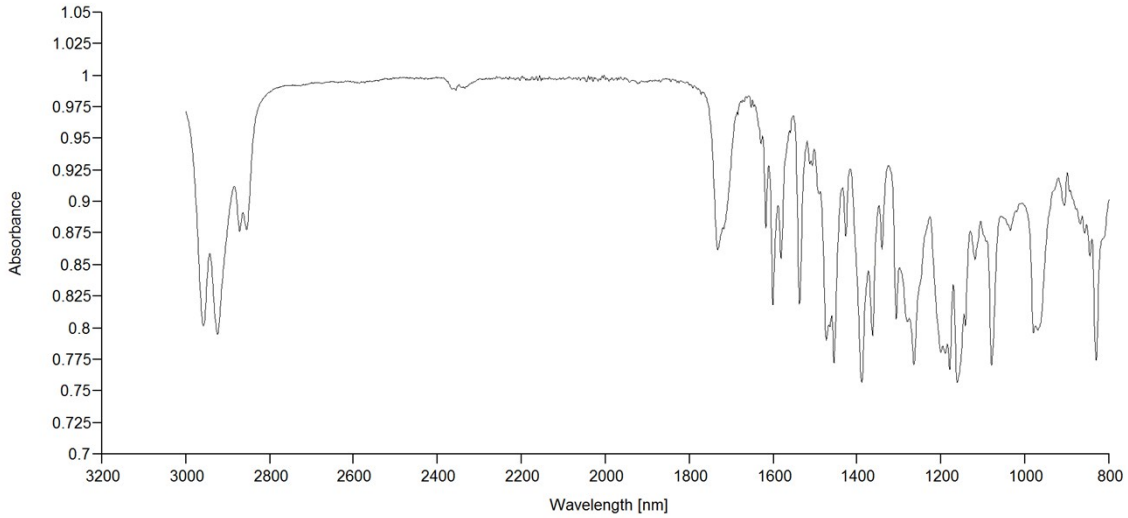


Fig. S21. Infrared spectrum of organotin compound **1**.

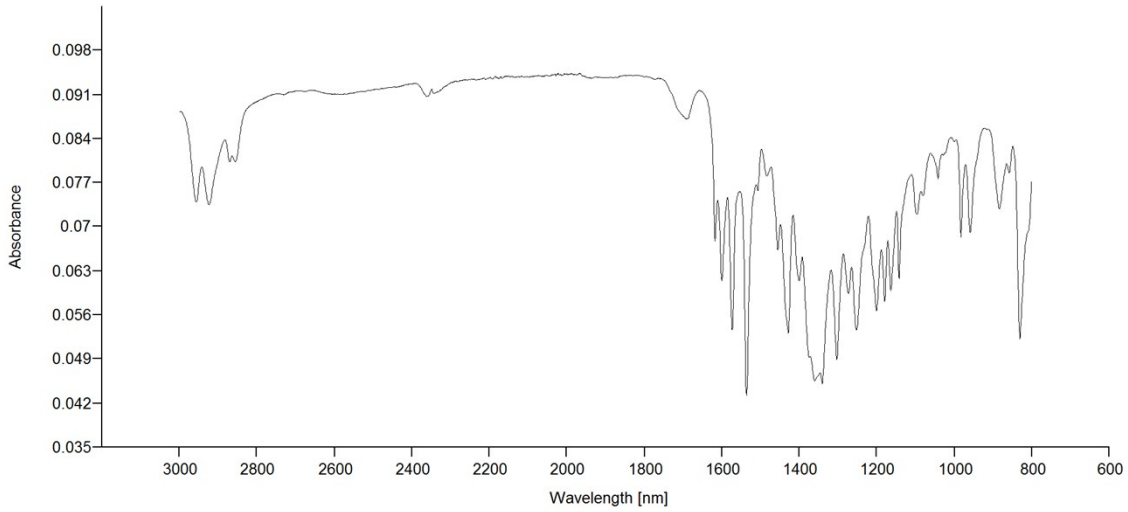


Fig. S22. Infrared spectrum of organotin compound **2.**

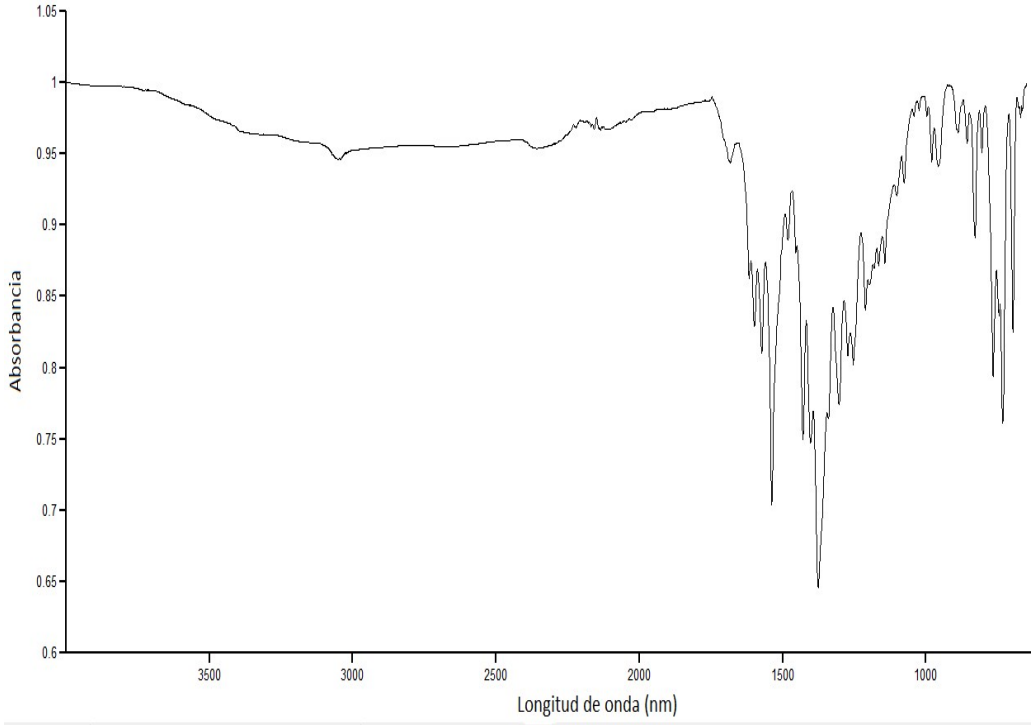


Fig. S23. Infrared spectrum of organotin compound **3.**

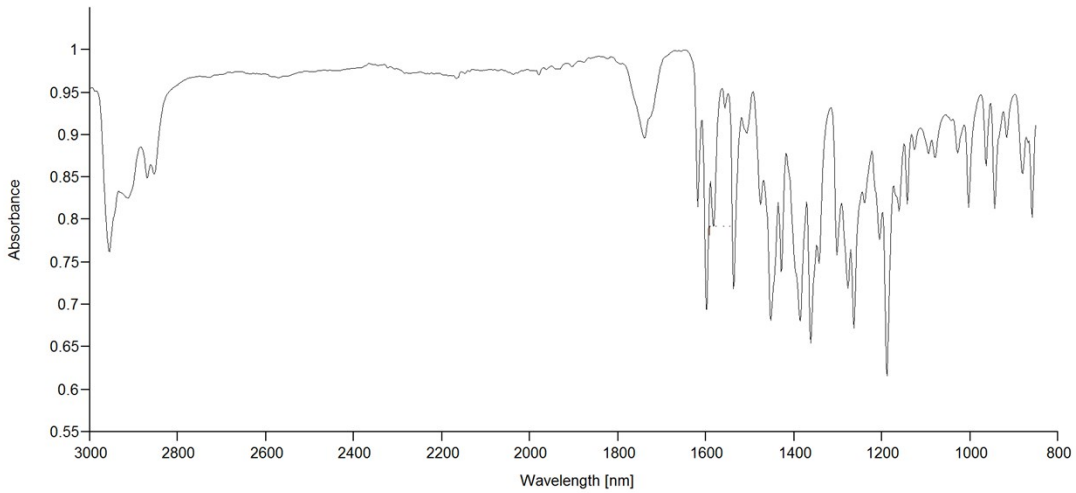


Fig. S24. Infrared spectrum of organotin compound **4.**

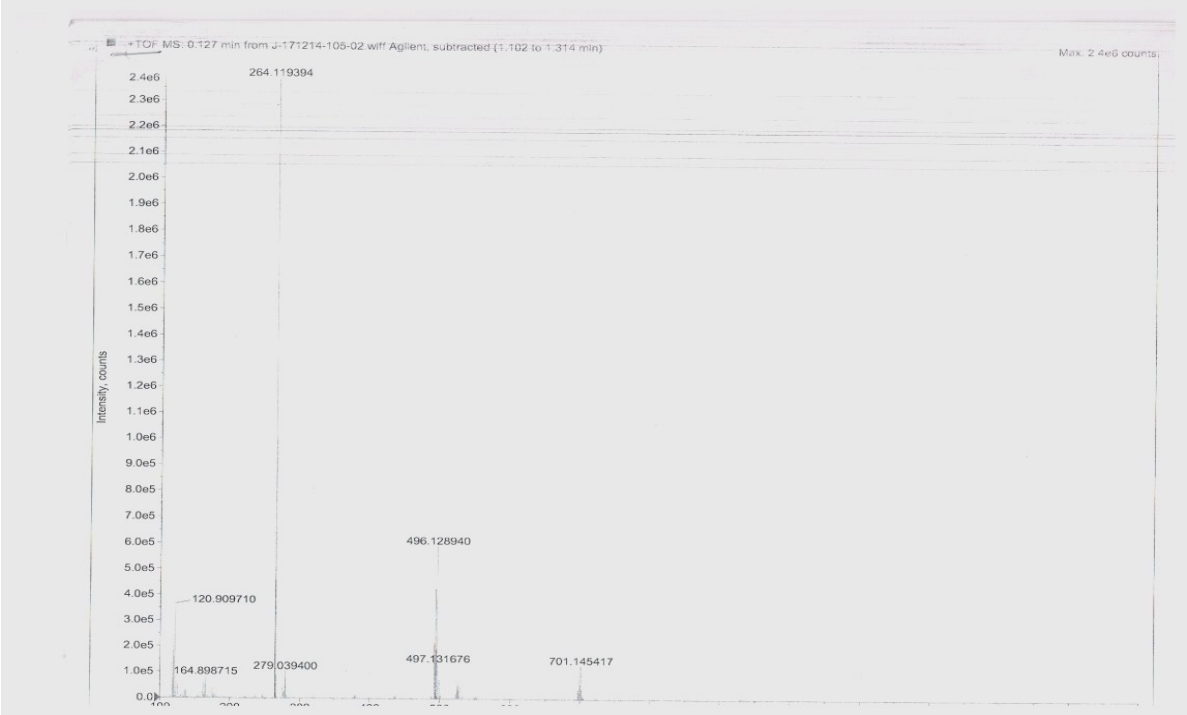


Fig. S25. Mass spectrum of organotin compound **1.**

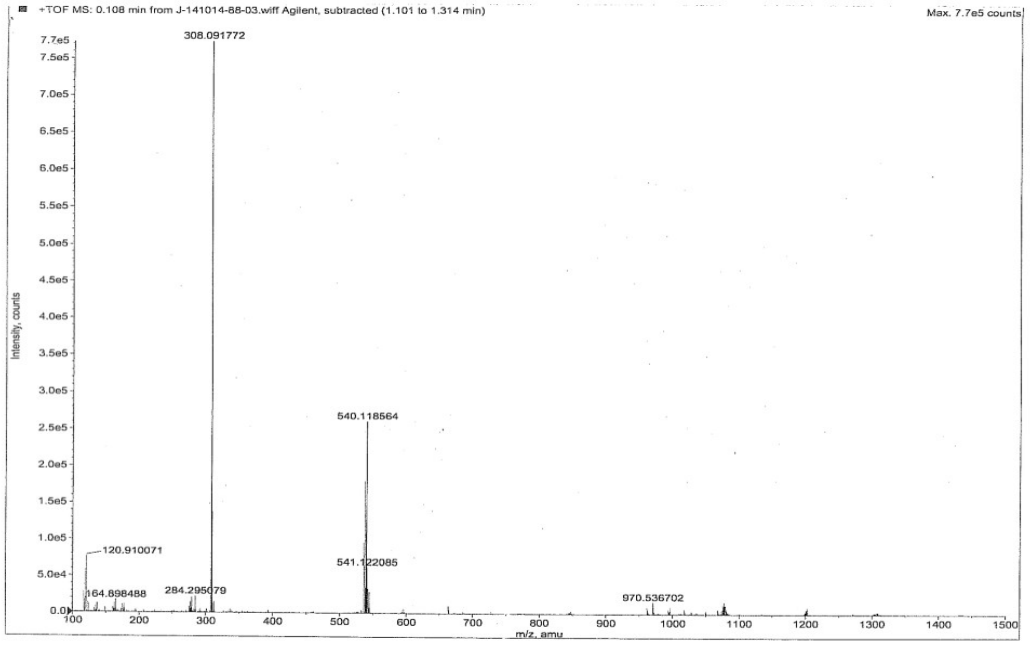


Fig. S26. Mass spectrum of organotin compound **2**.

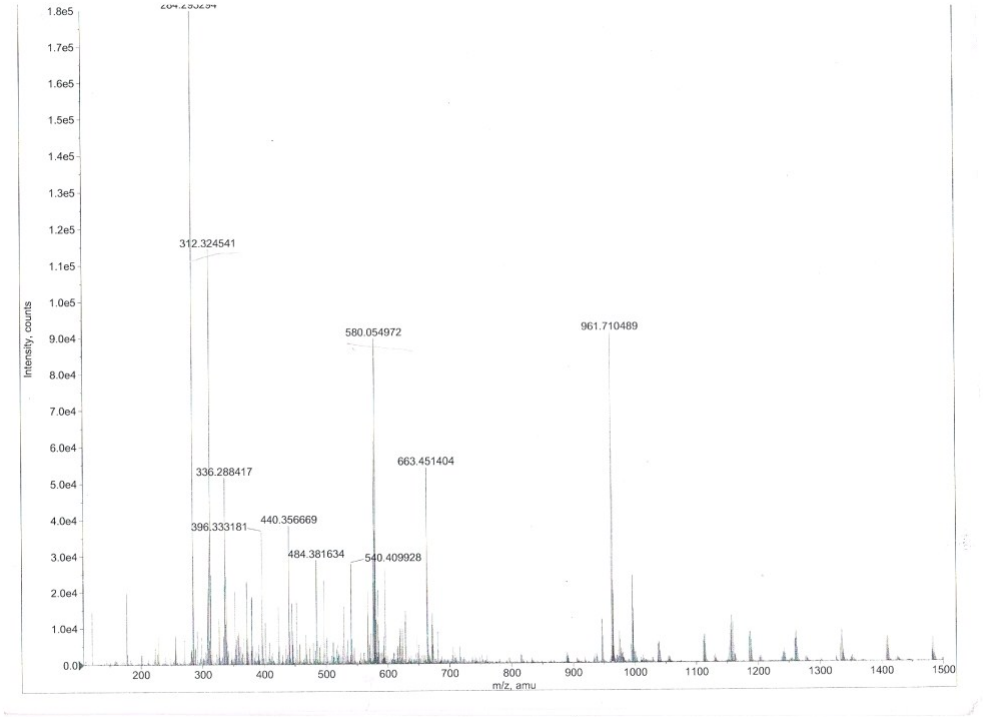


Fig. S27. Mass spectrum of organotin compound **3.**

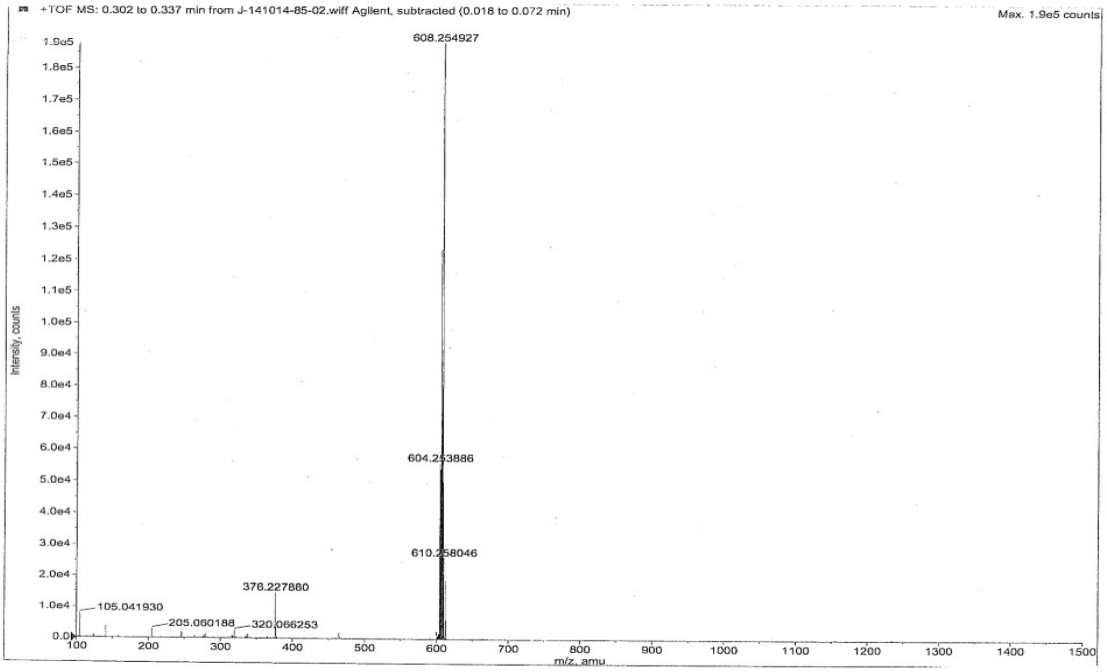


Fig. S28. Mass spectrum of organotin compound **4**.

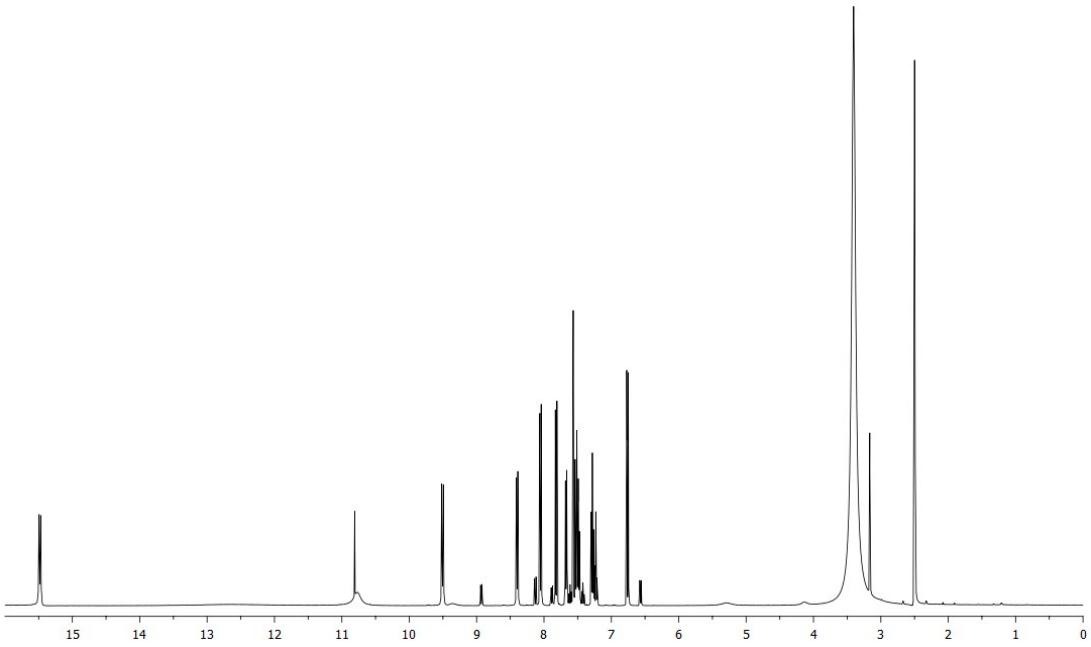


Fig. S29. ^{1}H NMR (DMSO-d_6) spectrum of ligand **2a**

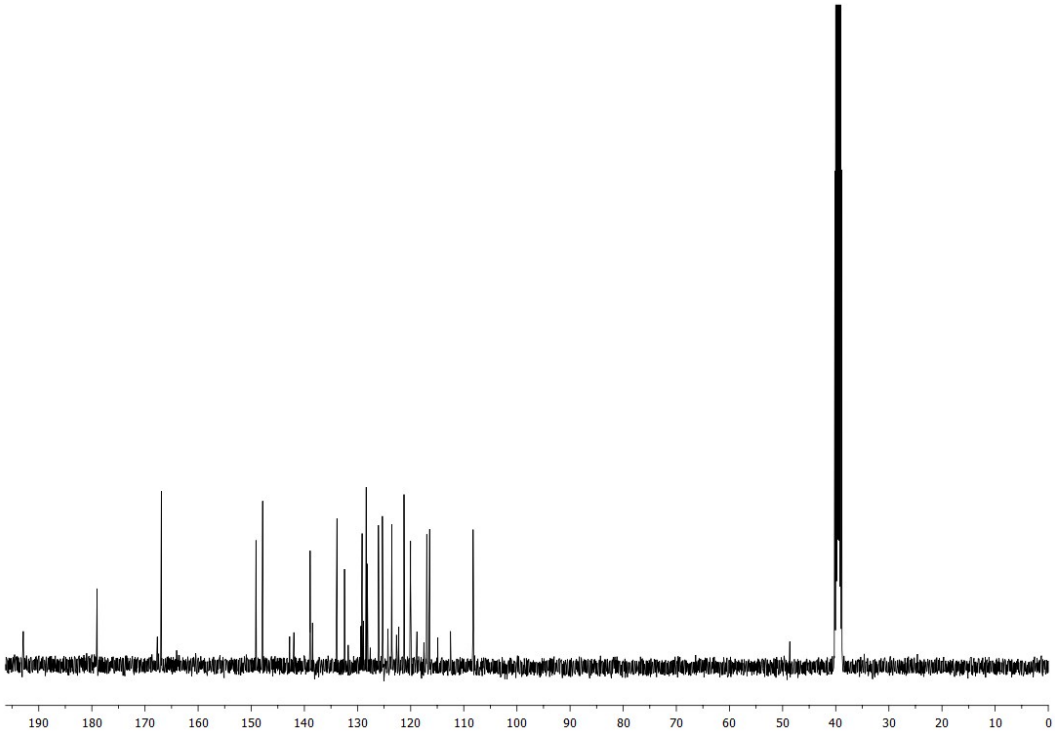


Fig. S30. ^{13}C NMR (DMSO-d_6) spectrum of ligand **2a**

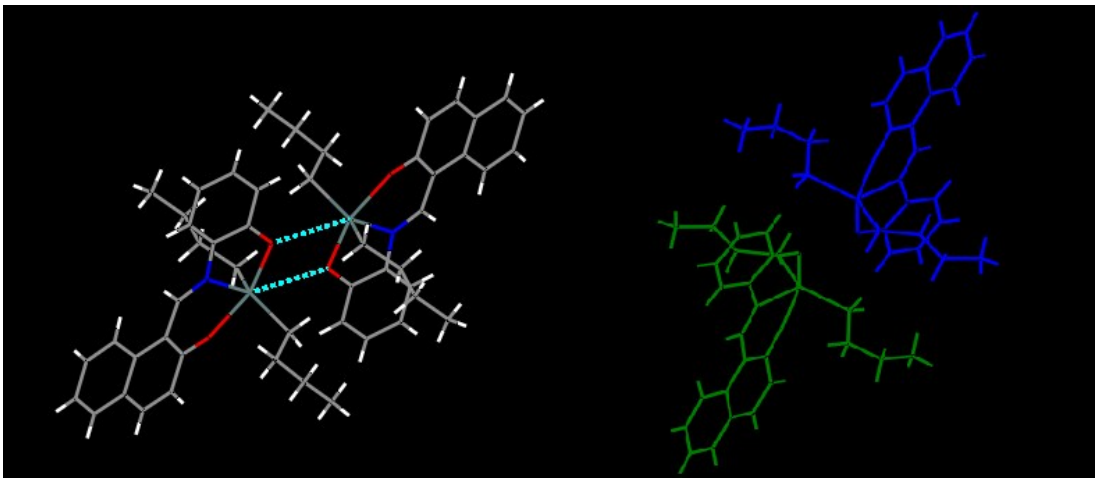


Fig. 31. Intermolecular interaction of organotin compound **1**.

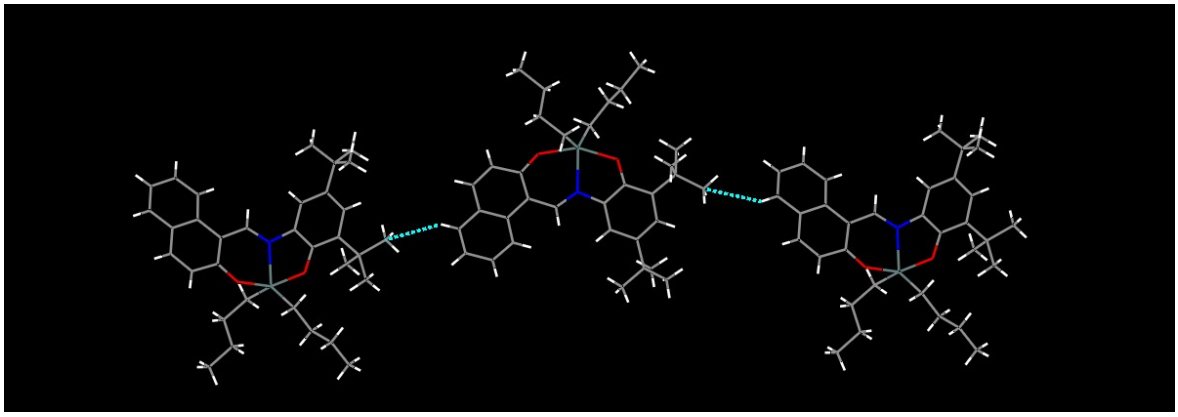


Fig. 32. Intermolecular interactions of organotin compound **4.**

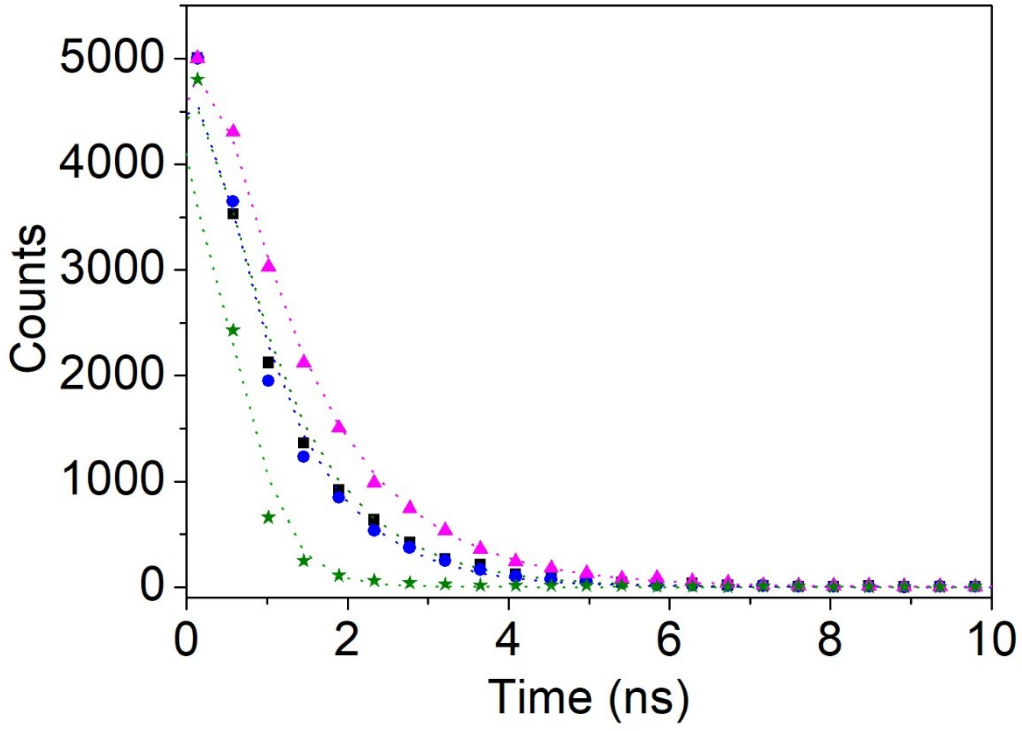


Figure S33. TSPC data for **1-4** in $CHCl_3$ by exciting at 455 nm. Dotted lines: fitted curves. Symbols: experimental decays; squares=**1**, circles=**2**, triangles=**3**, stars=**4**.

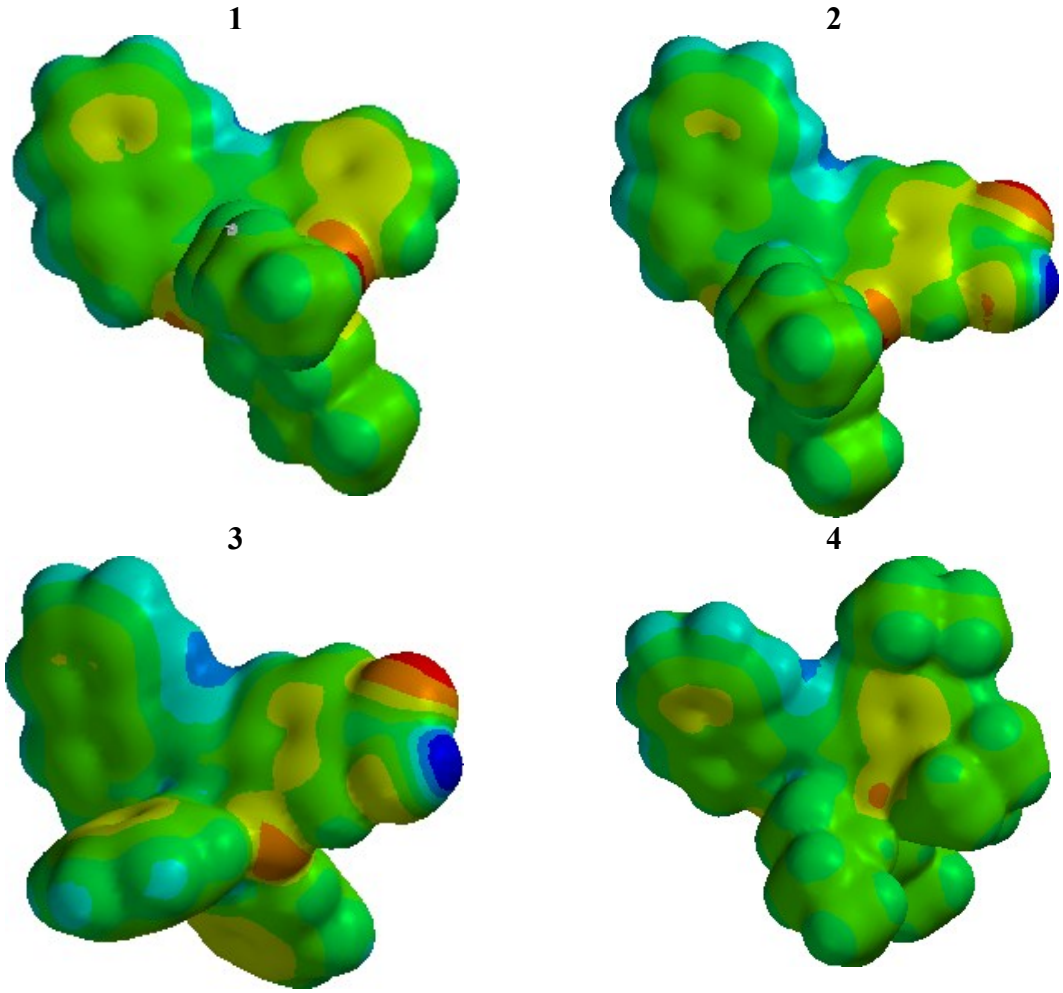


Figure S34. Electrostatic potential map for Sn-complexes.

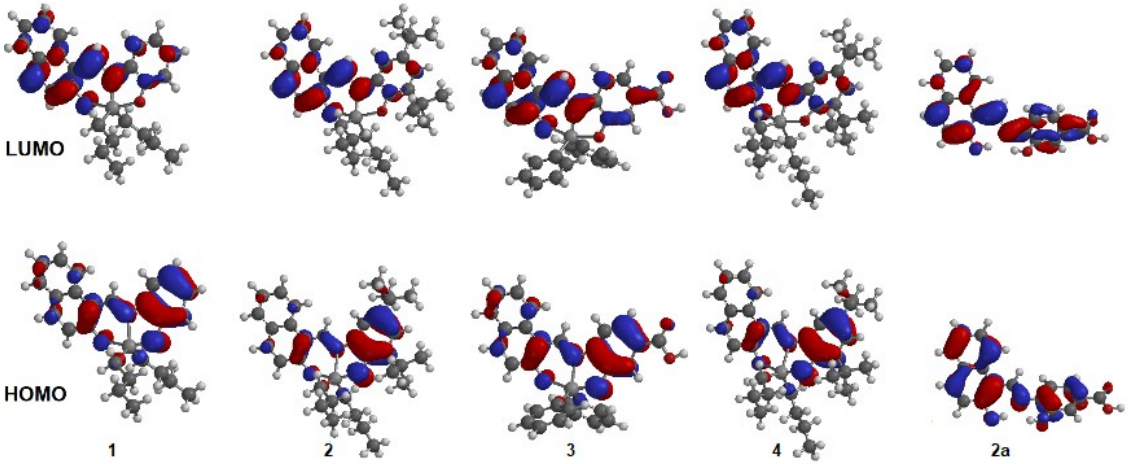


Figure S35. HOMO and LUMO frontier molecular orbitals for the whole series studied in this work.

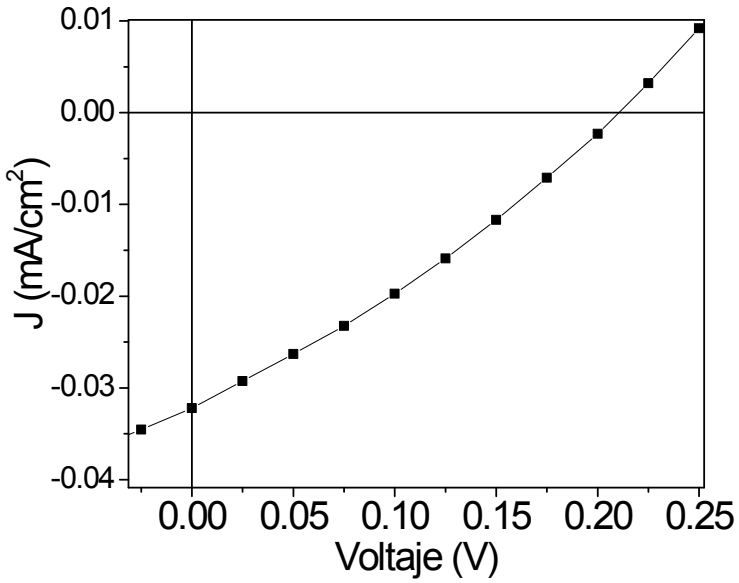
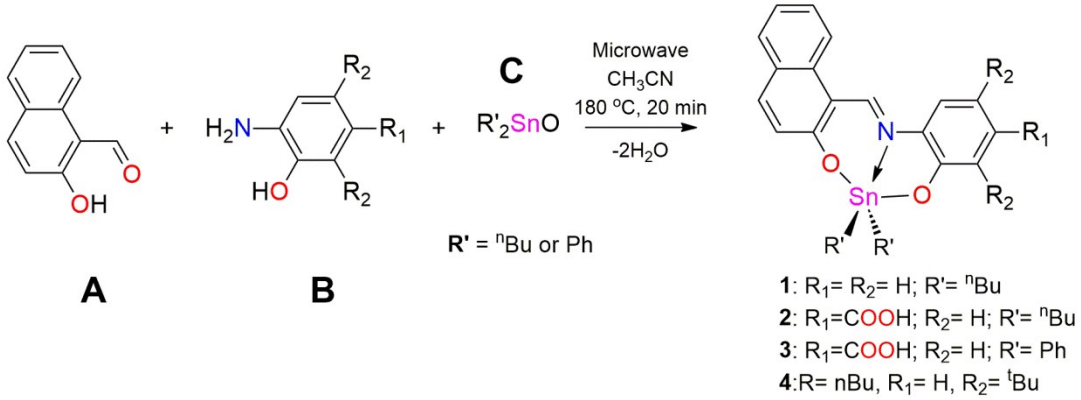


Figure S36. a) J-V curve of a solar cell in configuration: ITO/PEDOT/P3HT+**2**/TiO_2/FM

Calculation of ecological parameters of the organotin compounds synthesis

a) Experimental atomic economy



The calculation of the experimental atomic economy was performed first calculating the atom economy of the synthesis, and then multiplied by the percent yield. Enviromental (E) factor was calculated using the experimental yield for each reaction.

Table S1. Experimental atomic economy calculations.

	Precursor [g/Mol]				**Product** [g/Mol]	**Theoretical atomic Economy** (%)	**Experimental atomic Economy** (%)
Compound	A	B	C	D	F		
1		109.05	248.94		495.12	100	95
2	172.05	153.04	248.94		539.11	100	75
3		153.04	288.92		495.27	86	64
4		221.18	248.94		607.25	100	91

Table S2. Experimental environmental (E) factor.

Compound	**Waste** [%]	**Product** [%]	**Environmental (E)Factor**
1	5	95	0.05
2	25	75	0.33
3	36	64	0.56
4	9	91	0.09