Electronic Supplementary Information for

Organotin Schiff bases as Halofluorochromic dyes: Green synthesis, chemio-photophysical characterization, DFT, and their fluorescent bioimaging *in vitro*

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Table S1. Reaction time and yields by two synthetic routes of **1**-**8**.

Comp.	Conventional heating		Microwave irradiation		Reaction time improve
	Time (h)	Yield (%)	Time (min)	Yield (%)	
1	24	78	3	83	480
2	24	63	6	86	240
3	24	60	3	97	480
4	24	59	6	89	240
5	24	72	3	91	480
6	24	63	6	88	240
7	24	57	3	90	480
8	24	62	6	87	240

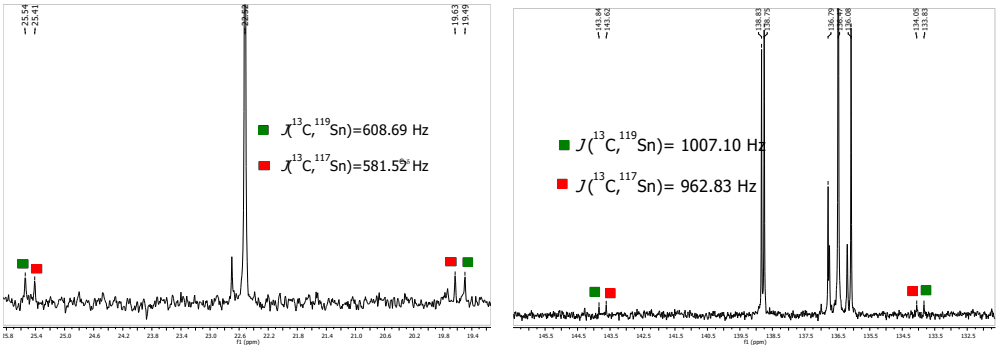


Figure S1. ^{13}C NMR Spectrum of compound **7** (left) and **6** (right) with zoom on an aliphatic and aromatic zone, respectively.

Table S2. Crystal data for compound **1**

Empirical formula	$C_{21}H_{26}N_2O_5Sn$
Formula weight	505.13
Temperature, K	293(2)
Wavelength	0.71073
Crystal system	Monoclinic
Space group	*P*2(1)/*c*
a, Å	9.67160 (10)
b, Å	16.2257 (3)
c, Å	14.4268 (15)
α	90.00 °
β	100.982(2)°
γ	90.00°
V, Å^3	2132.42 (5)
Z	4
$\rho_{calc,mg.cm^{-3}}$	1.573
μ, mm^{-1}	1.232
2θ range for data collection	2.924 – 27.466°
Index ranges	-18 ≤ *h* ≤ 18,
No. of reflns collected	43394
No. of indep reflns	3977
[R_{int}]	0.0311
Goodness of fit	1.054
*R*1, w*R*2 (I>2σ(I))	0.0317/0.0765
*R*1, w*R*2 (all data)	0.0429/0.0843

Table S3. Emission data of compounds **1-8** at different pH values.

Comp.	pH 5	pH 6	pH 7	pH 8	Effect below pH 7
1	519	517	538	524	Hypochromic
2	525	541	517	542	Hypochromic
3	513	515	530	529	Hypochromic
4	491	490	492	492	Hyperchromic
6	550	554	560	571	Hyperchromic
7	519	517	538	528	Hypochromic
8	524	553	525	541	Hypochromic

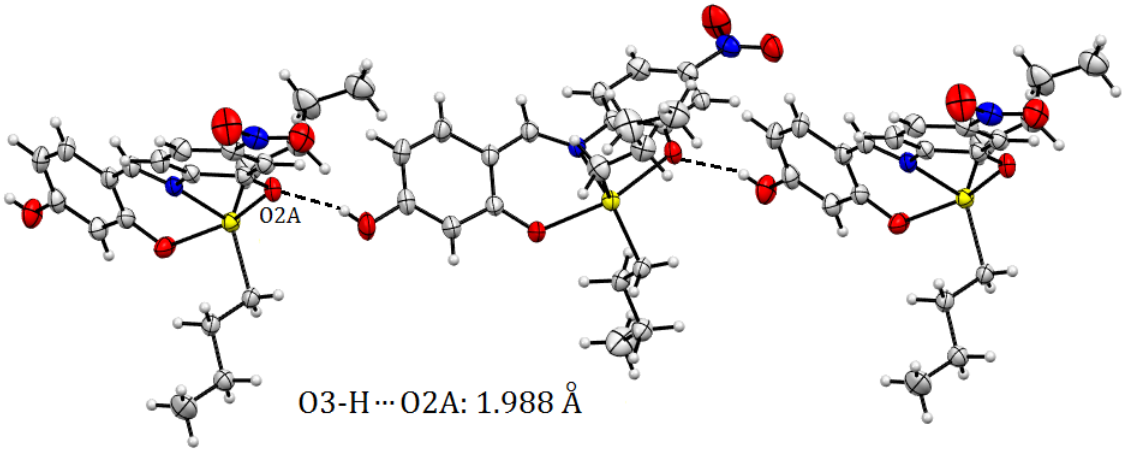


Figure S2. Intermolecular interaction of compound **1**

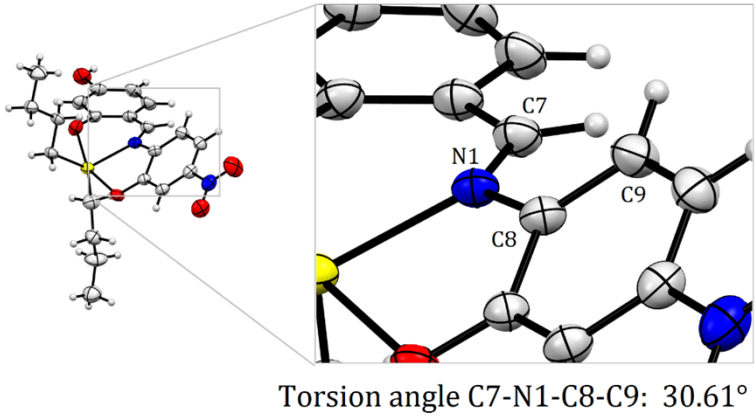


Figure S3. Torsion angle of compound **1.**

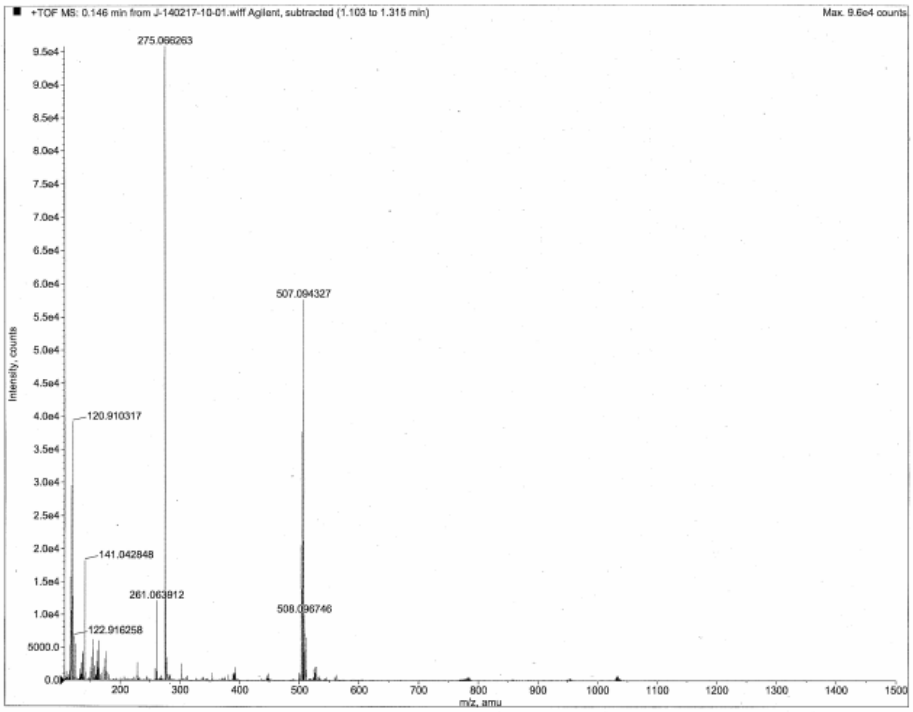


Figure S4. Mass spectrum of compound **1**

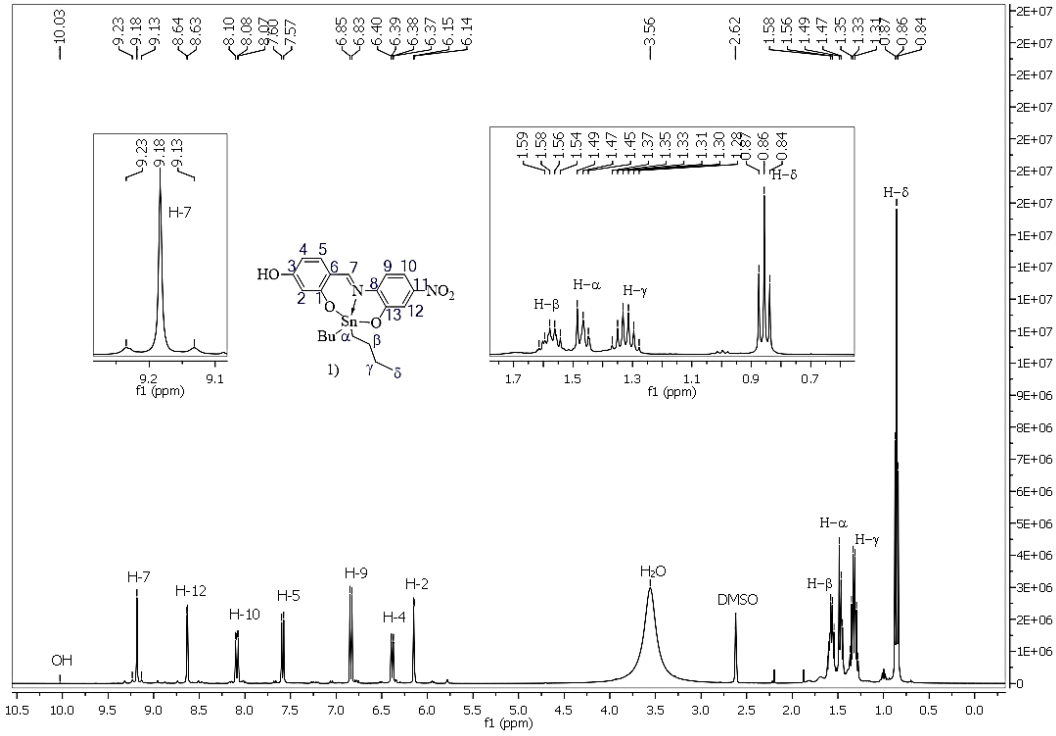


Figure S5. ^{1}H NMR (DMSO-d_6) spectrum of compound **1**.

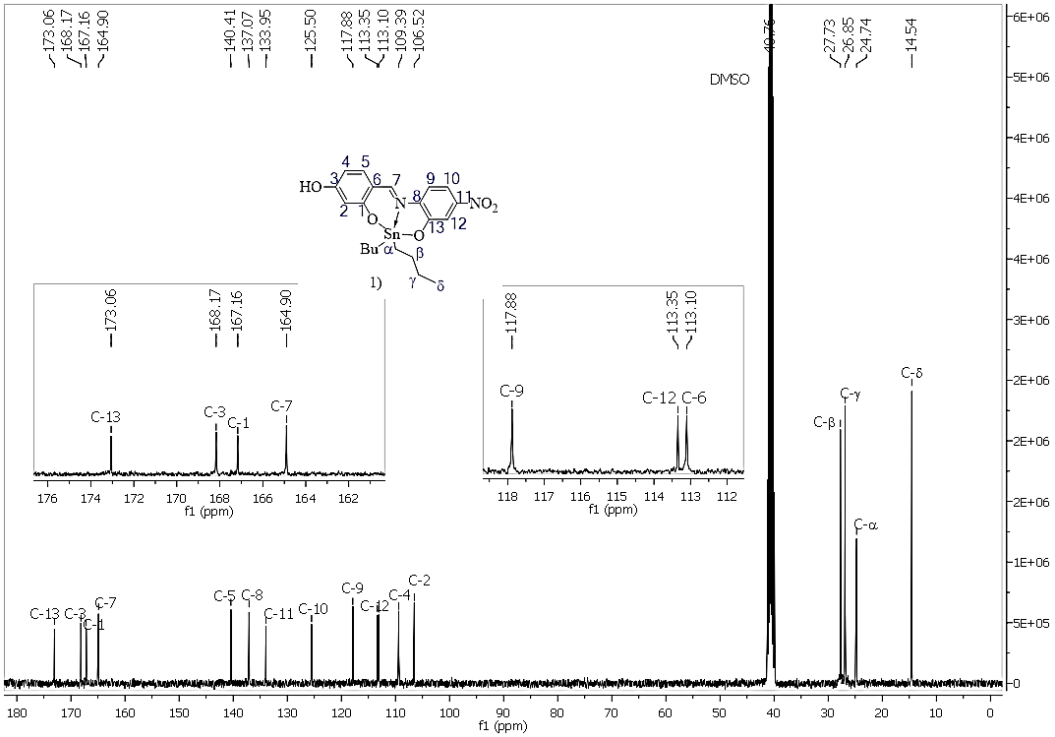


Figure S6. ^{13}C NMR (DMSO-d_6) spectrum of compound **1**.

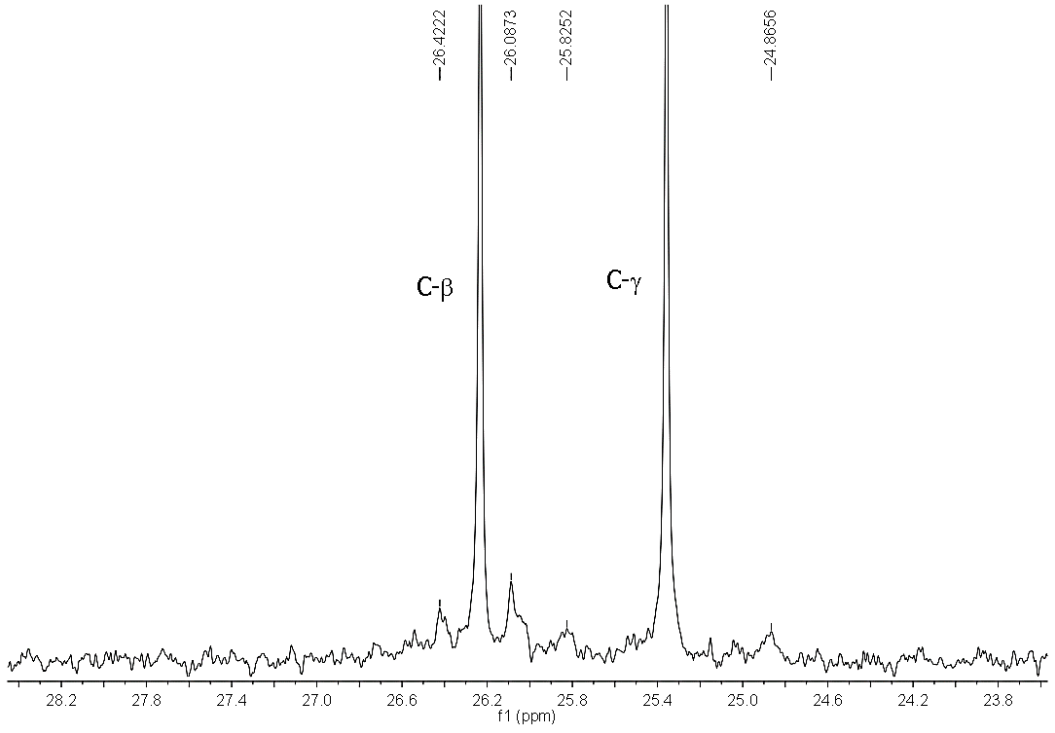


Figure S7. ^{13}C NMR extension spectrum corresponding aliphatic region of compound **1**.

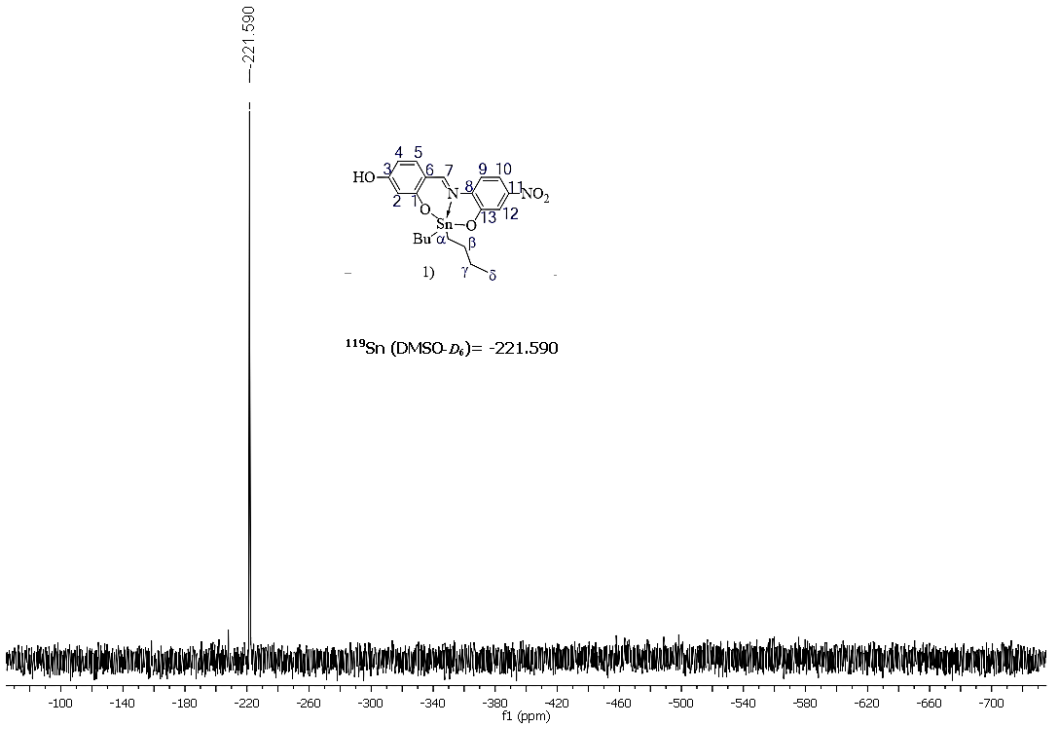


Figure S8. ^{119}Sn NMR (DMSO-d_6) spectrum of compound **1**.

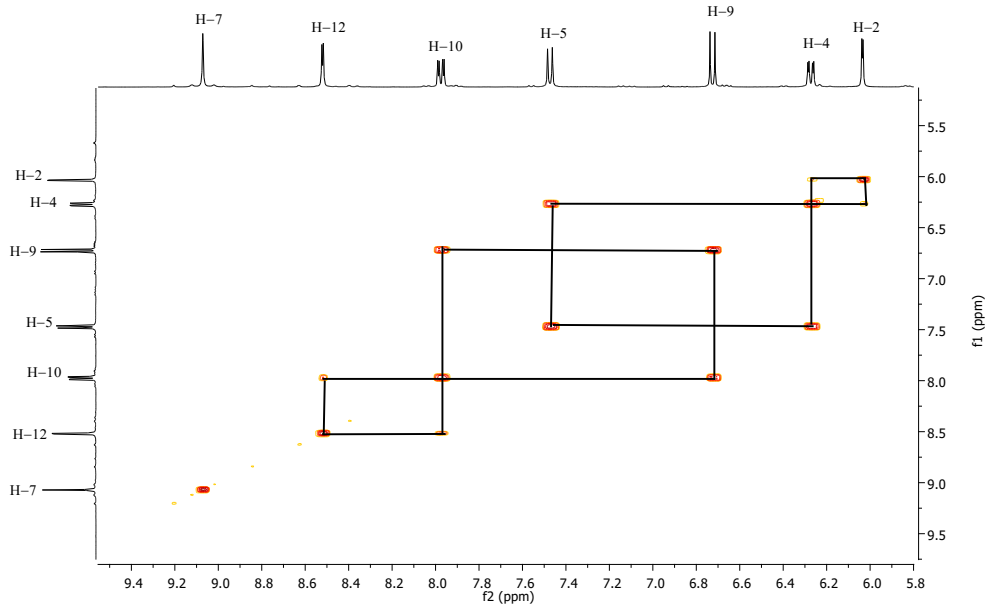


Figure S9. COSY correlation (δ_H/δ_H) spectrum corresponding aromatic region of compound **1.**

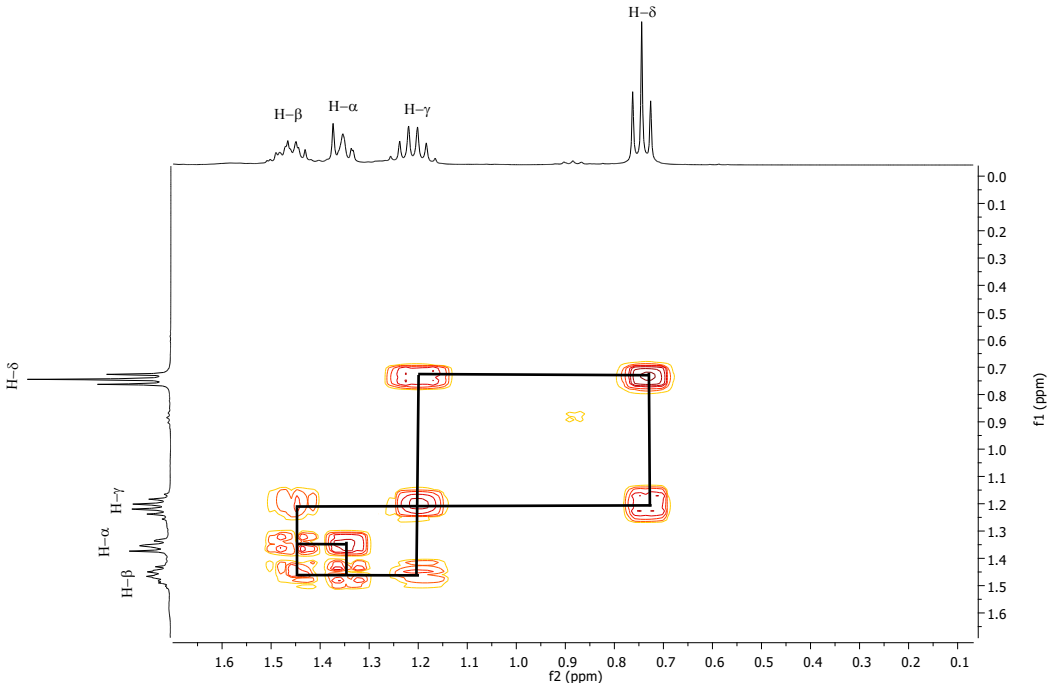


Figure S10. COSY correlation (δ_H/δ_H) spectrum corresponding aliphatic region of compound **1**.

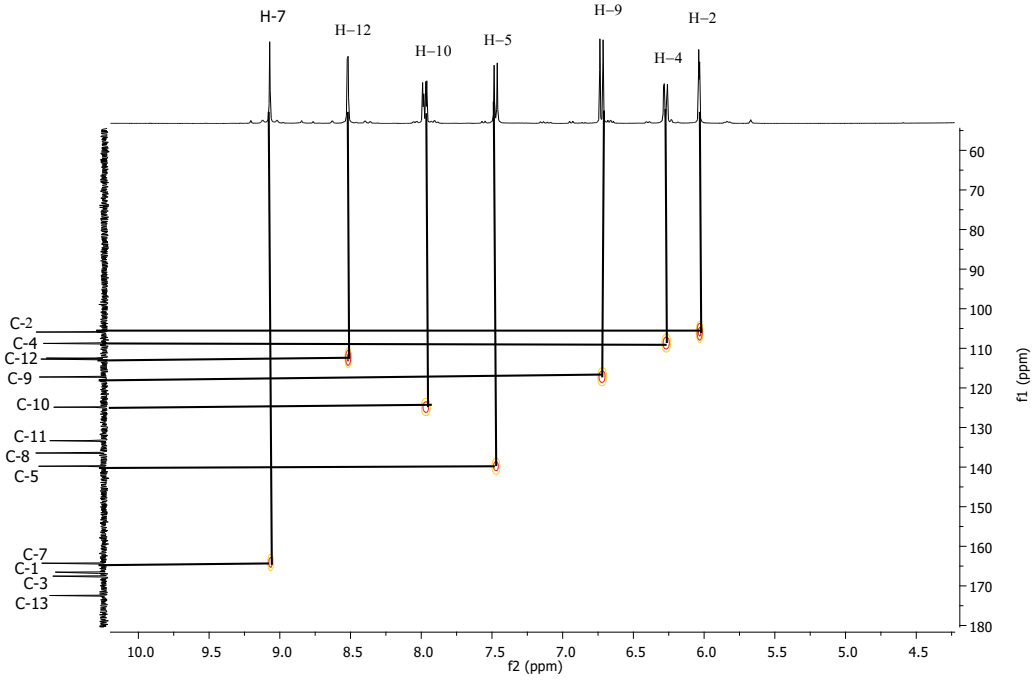


Figure S11. HSQC correlation (δH/δC) spectrum corresponding aromatic region of compound **1**.

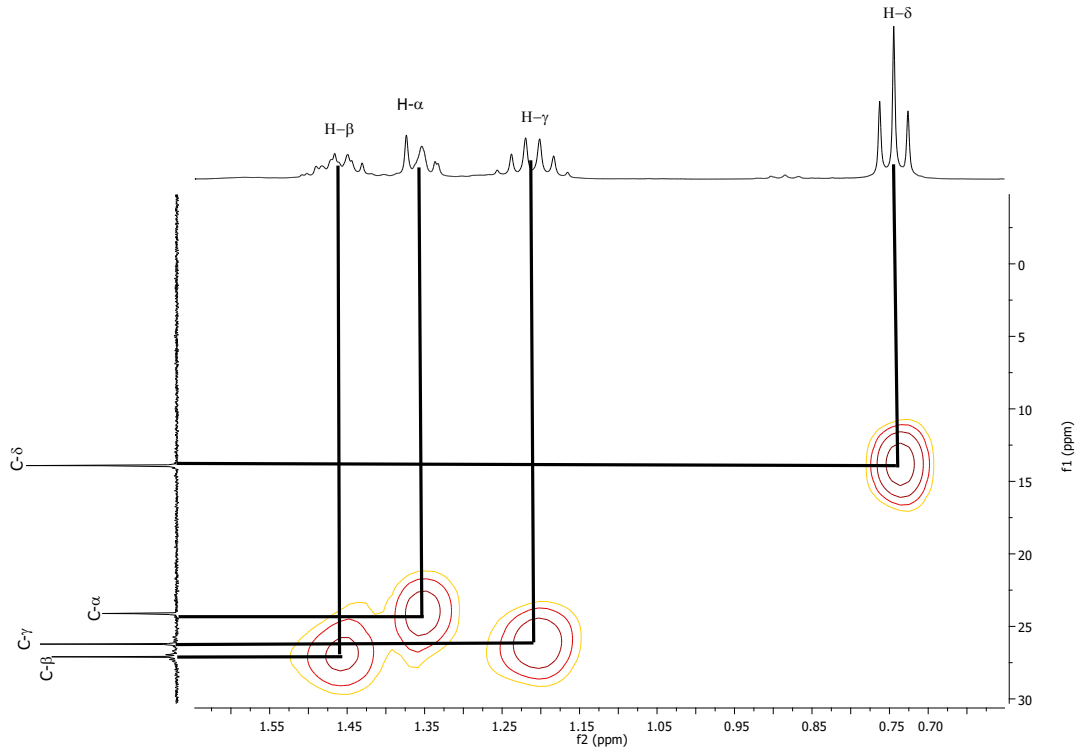


Figure S12. HSQC correlation (δH/δC) spectrum corresponding aliphatic region of compound **1**.

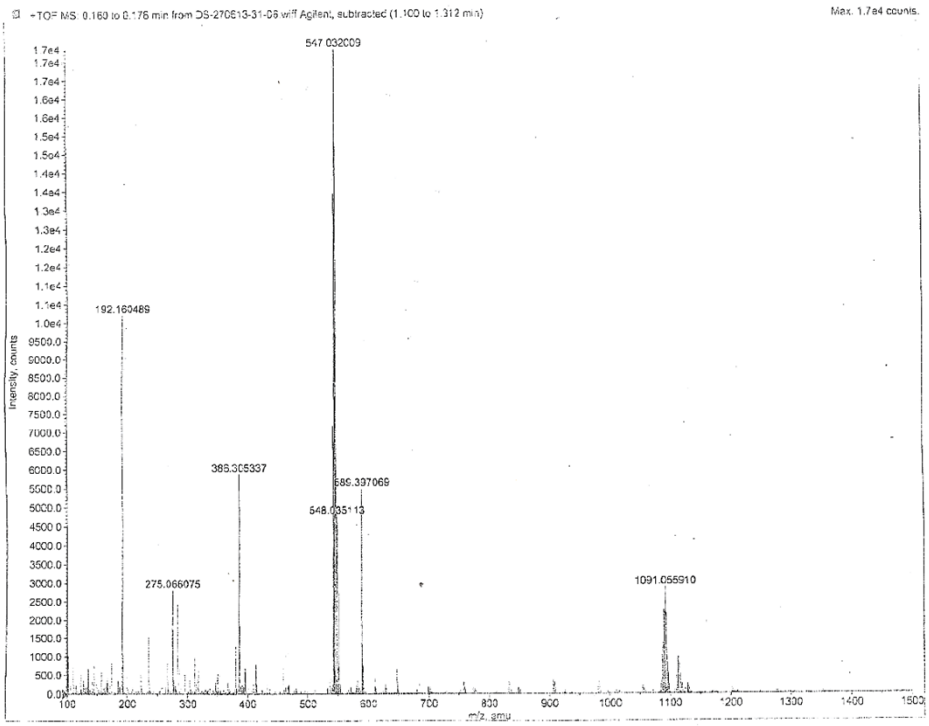


Figure S13. Mass spectrum of compound **2.**

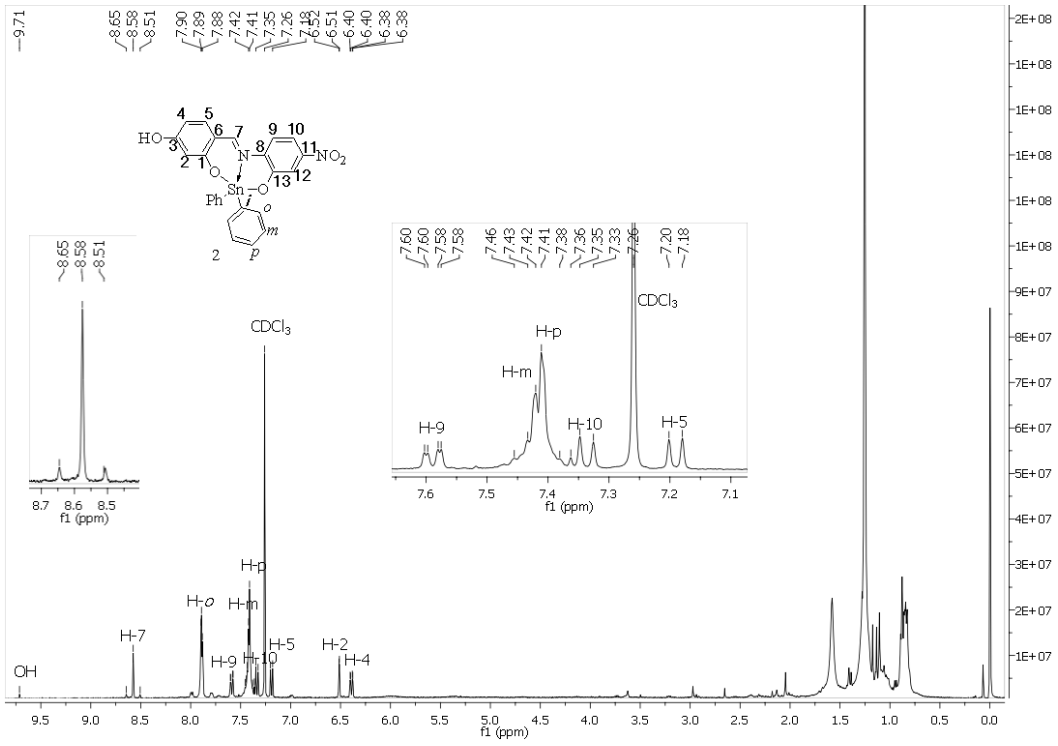


Figure S14. ^{1}H NMR ($CDCl_3$) spectrum of compound **2**.

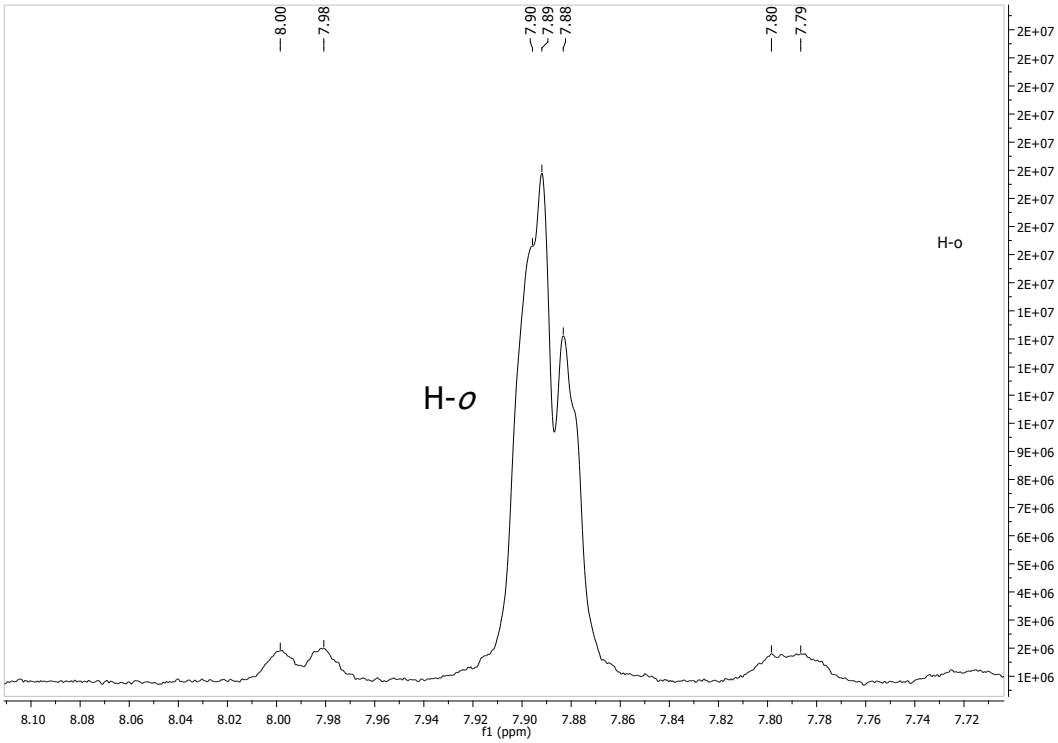


Figure S15. ^{1}H NMR for H-*o* spectrum of compound **2**.

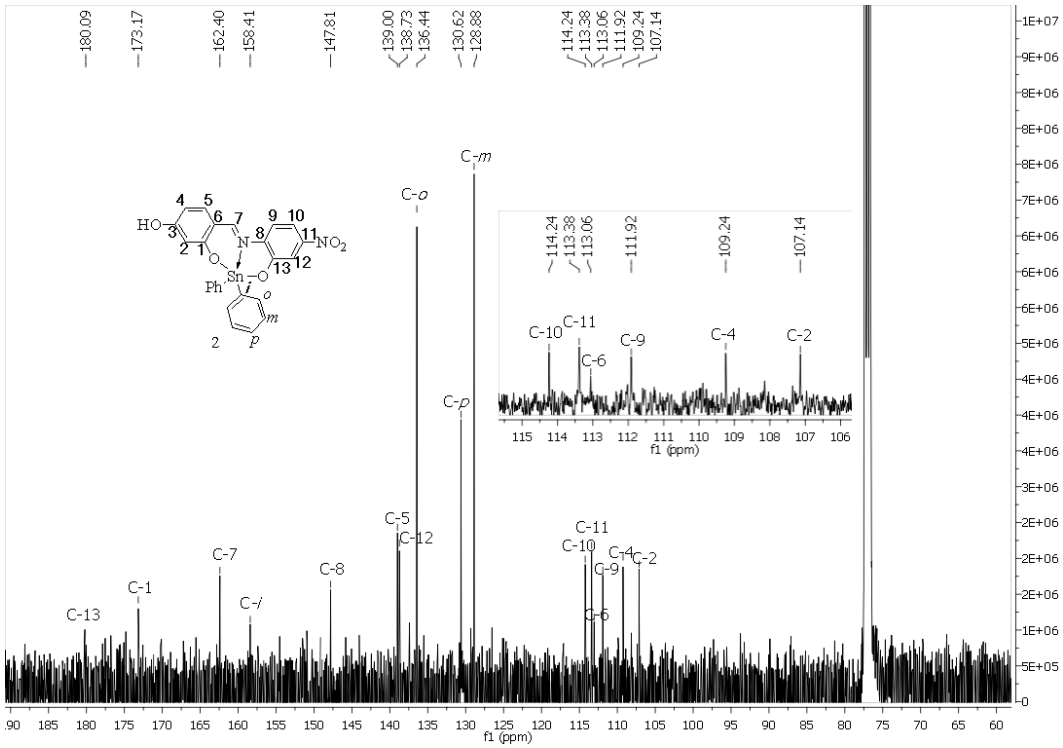


Figure S16 ^{13}C NMR ($CDCl_3$) spectrum of compound **2**.

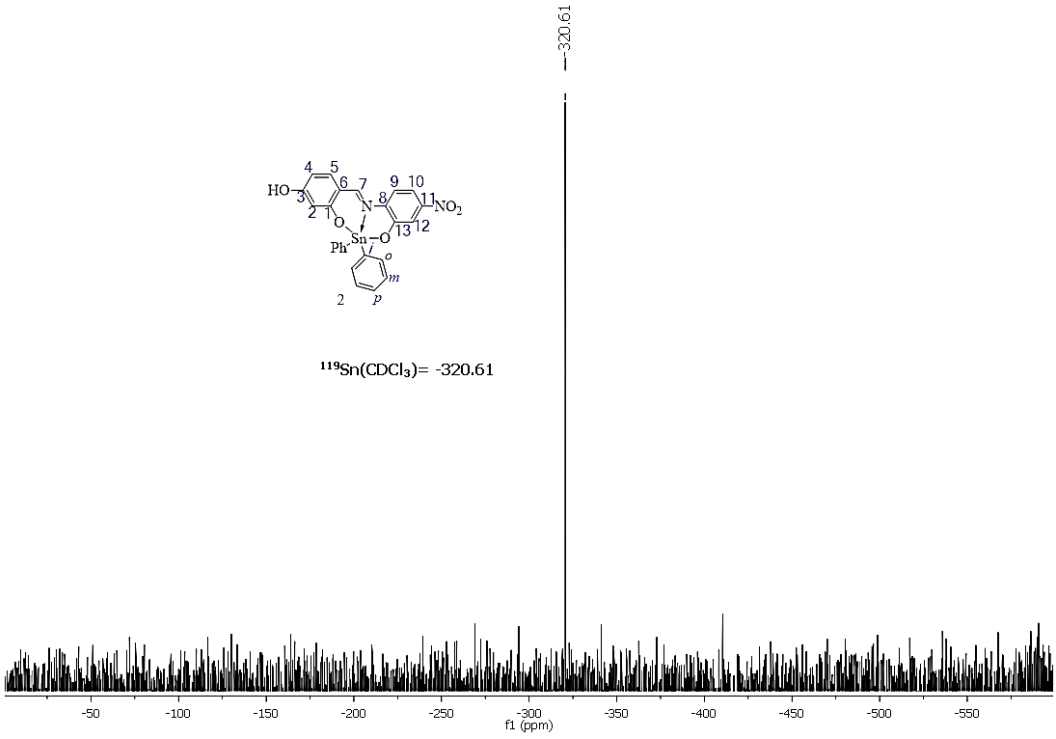


Figure S17. ^{119}Sn NMR ($CDCl_3$) spectrum of compound **2**.

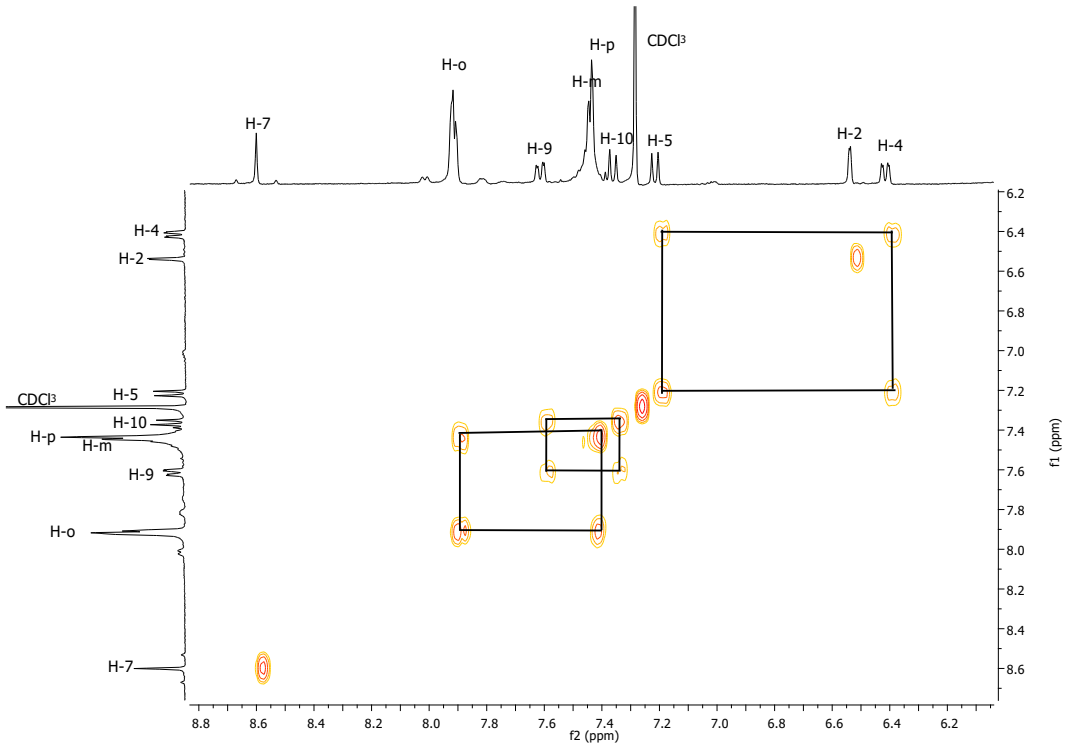


Figure S18. COSY correlation (δ_H/δ_H) spectrum corresponding of compound **2**.

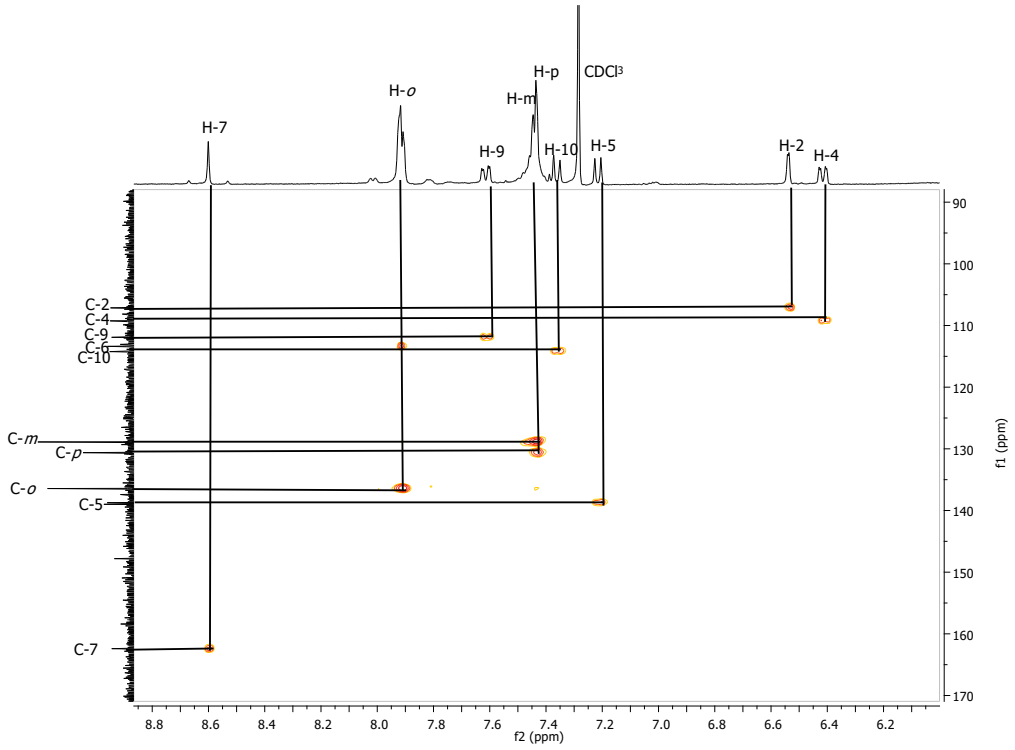


Figure S19. HSQC correlation (δH/δC) spectrum corresponding of compound **2.**

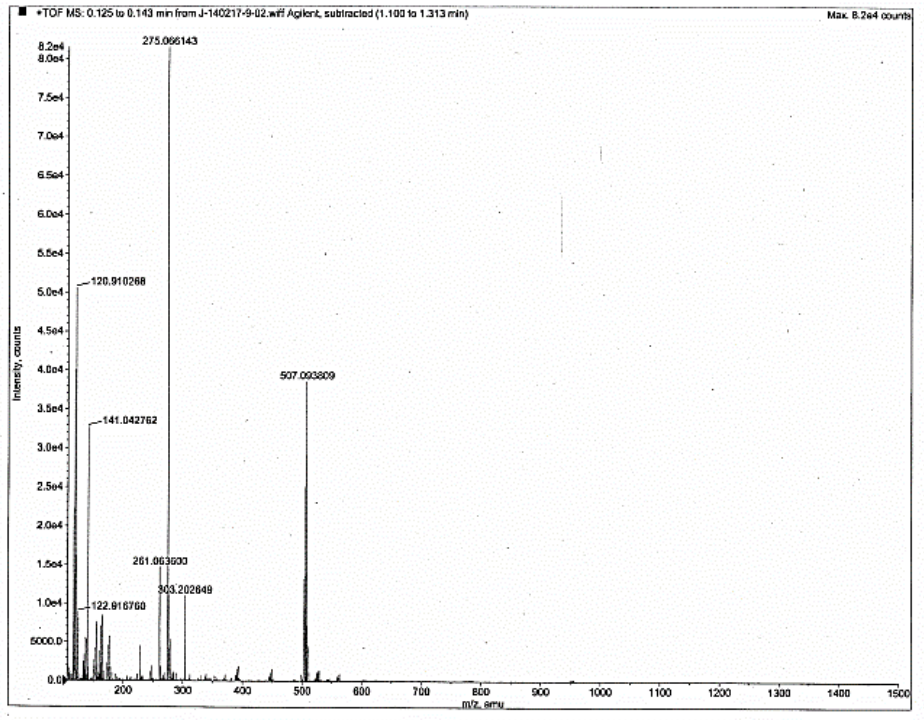


Figure S20. Mass spectrum of compound **3.**

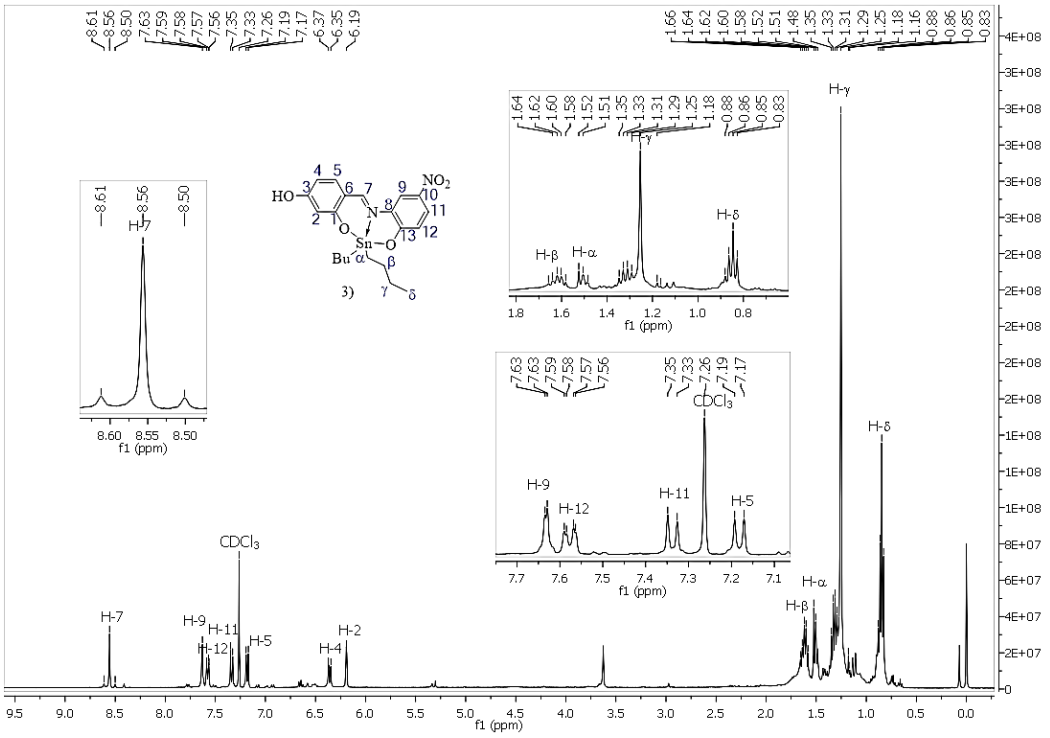


Figure S21. ^{1}H NMR ($CDCl_3$) spectrum of compound **3**.

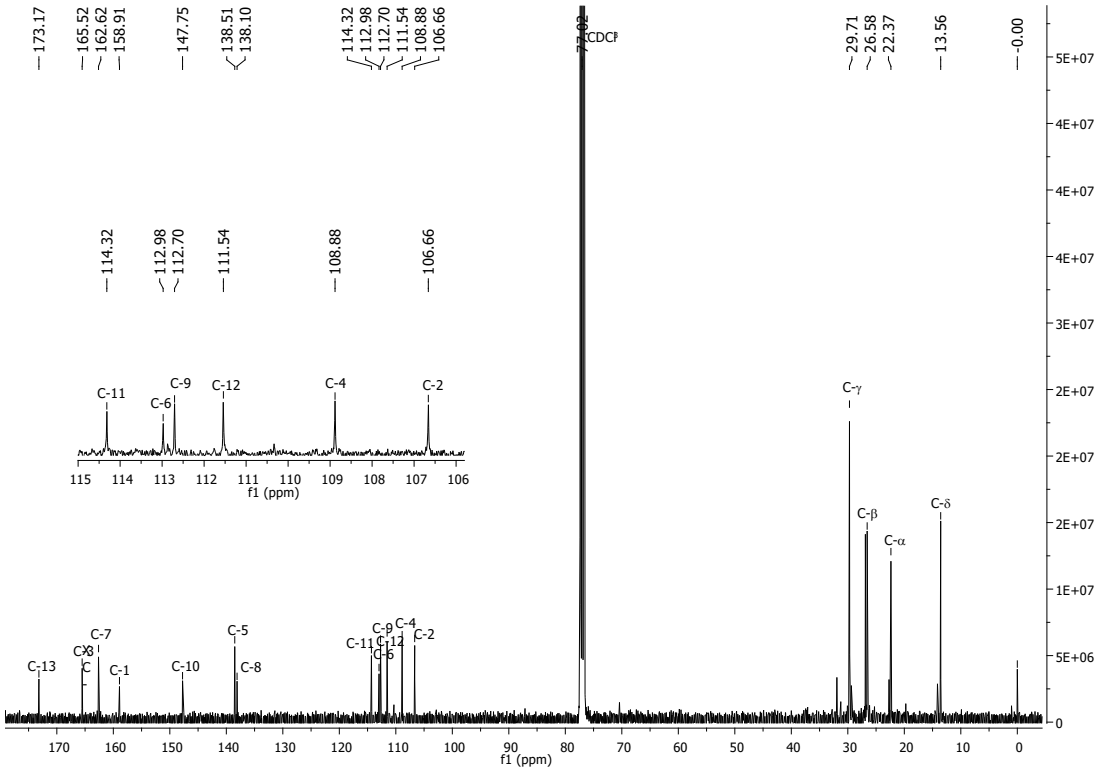


Figure S22. ^{13}C NMR ($CDCl_3$) spectrum of compound **3**.

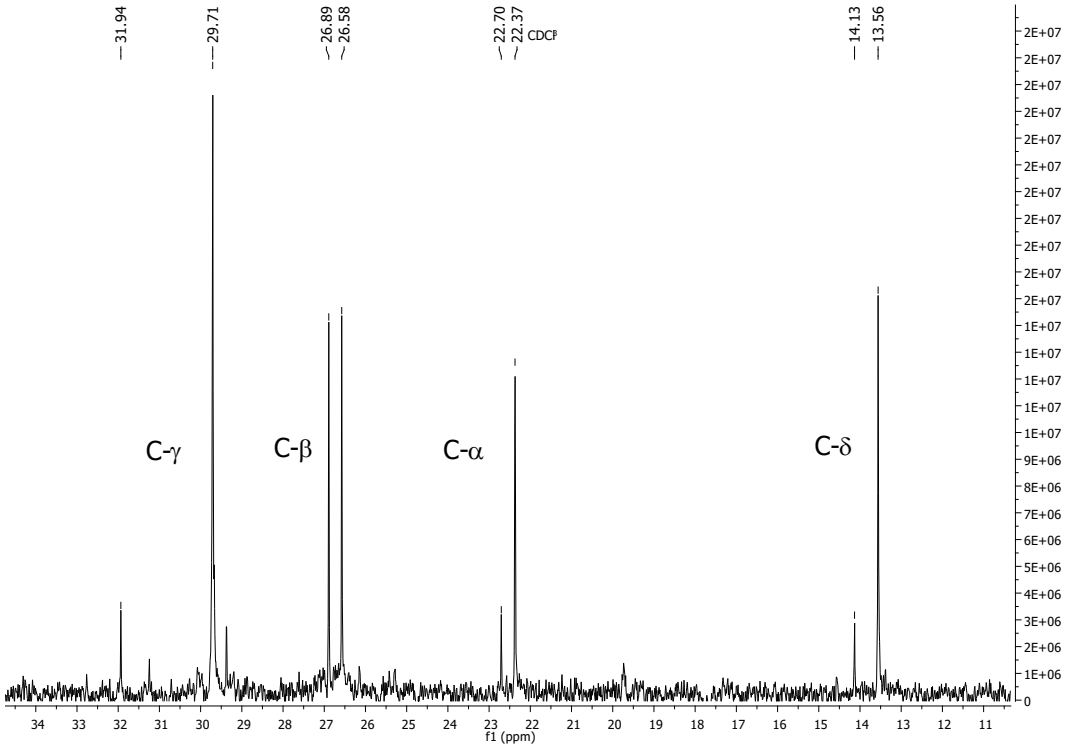


Figure S23. ^{13}C NMR ($CDCl_3$) expansion spectrum of compound **3**.

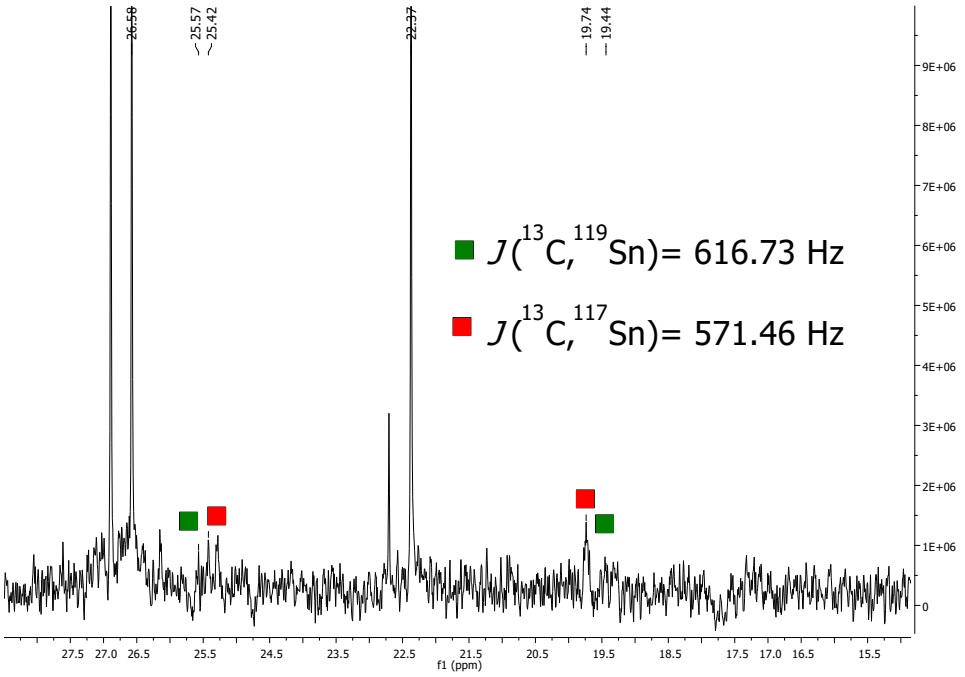


Figure S24. Coupling constant $J(^{13}C,^{119/117}Sn)$ of compound **3.**

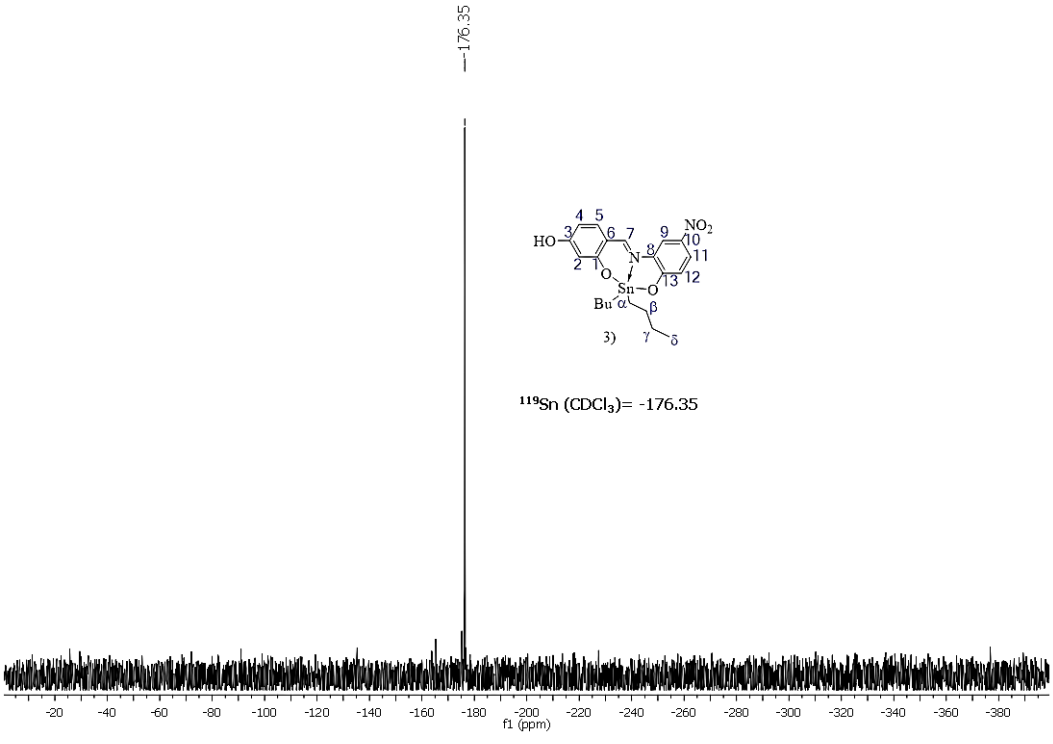


Figure S25. ^{119}Sn NMR ($CDCl_3$) spectrum of compound **3**.

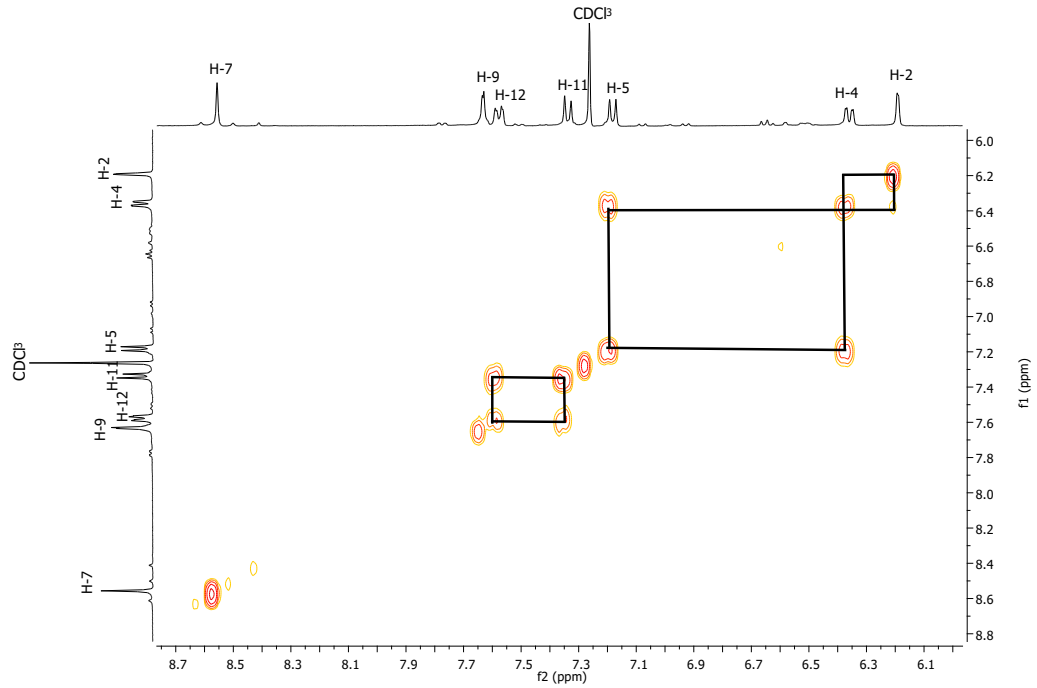


Figure S26. COSY correlation (δ_H/δ_H) spectrum corresponding aromatic region of compound **3.**

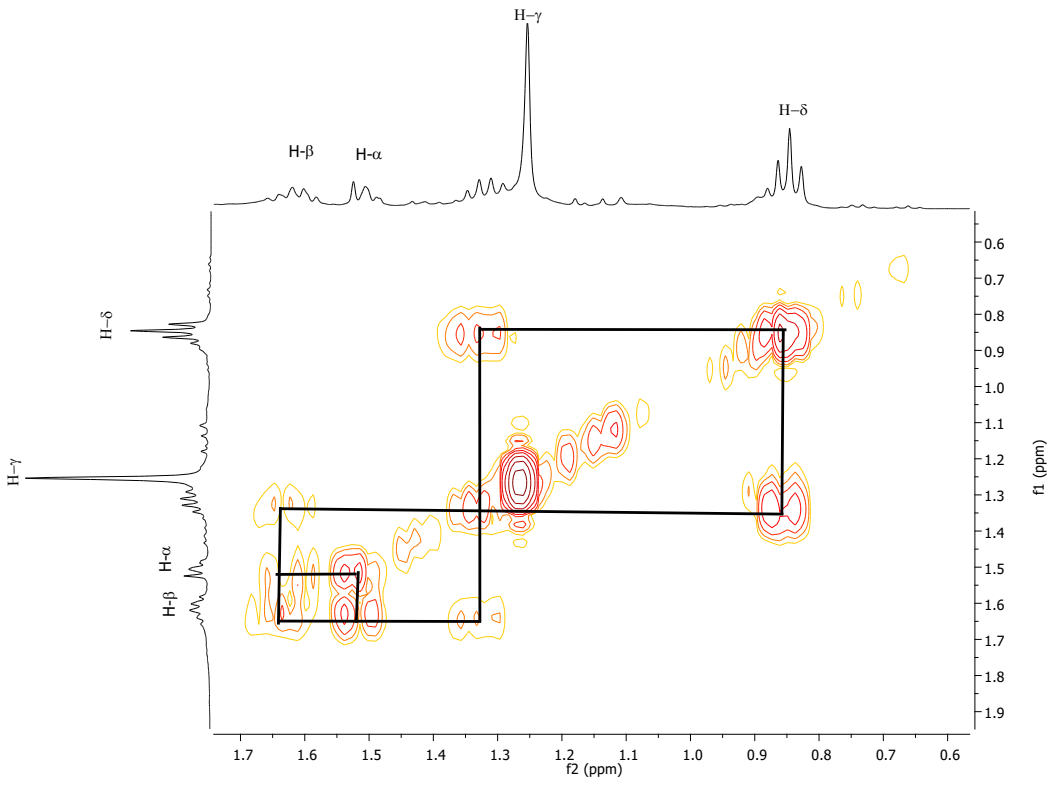


Figure S27. COSY correlation (δ_H/δ_H) spectrum aliphatic region of compound **3**.

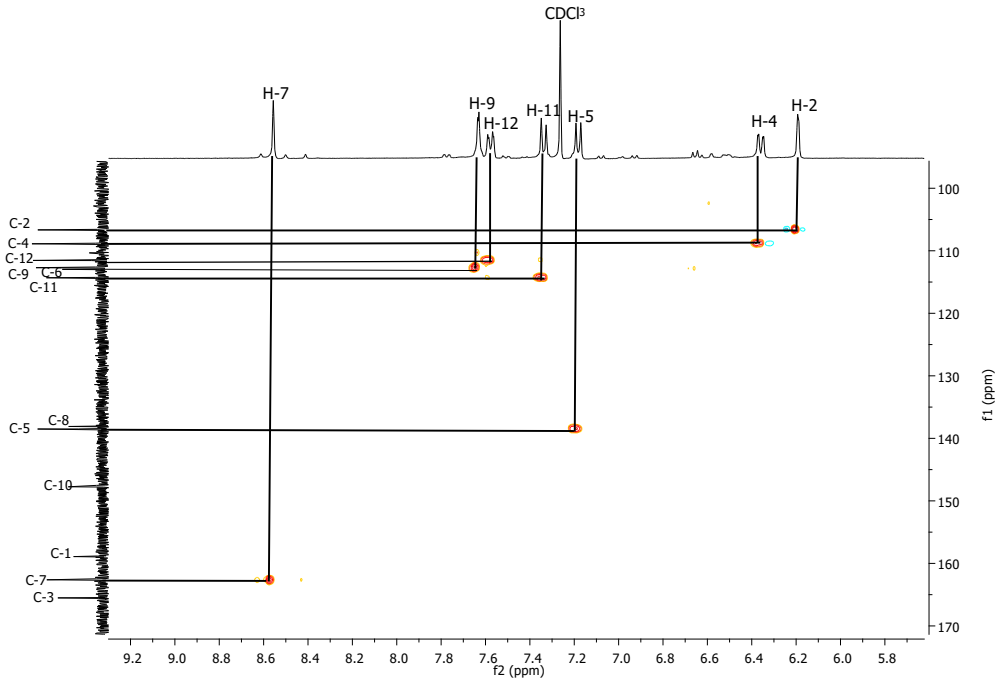


Figure S28. HSQC correlation (δH/δC) spectrum corresponding aromatic region of compound **3**.

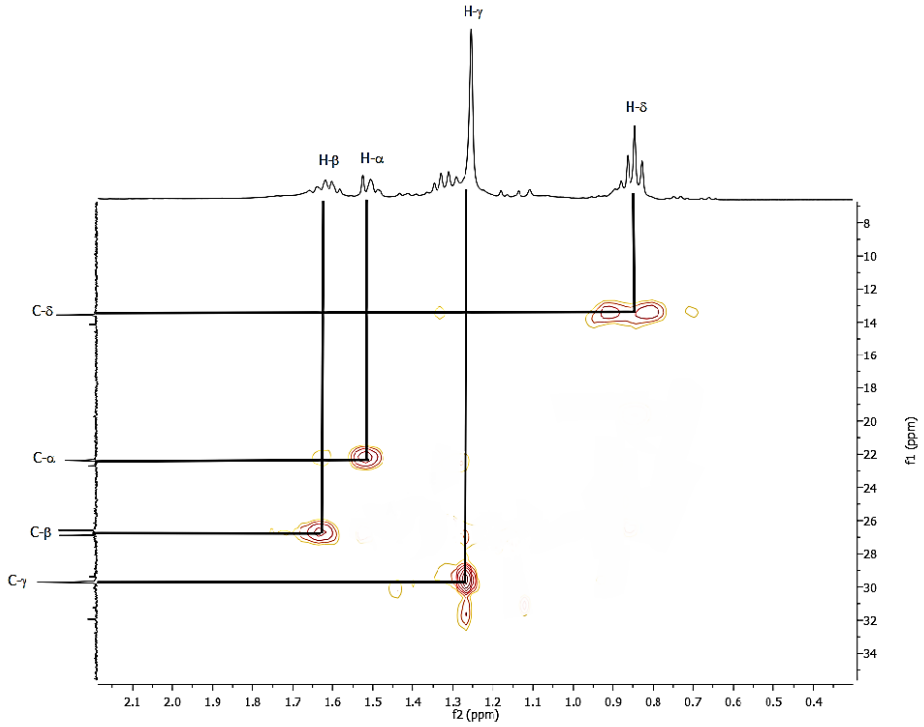


Figure S29. HSQC correlation (δH/δC) spectrum corresponding aliphatic region of compound **3**.

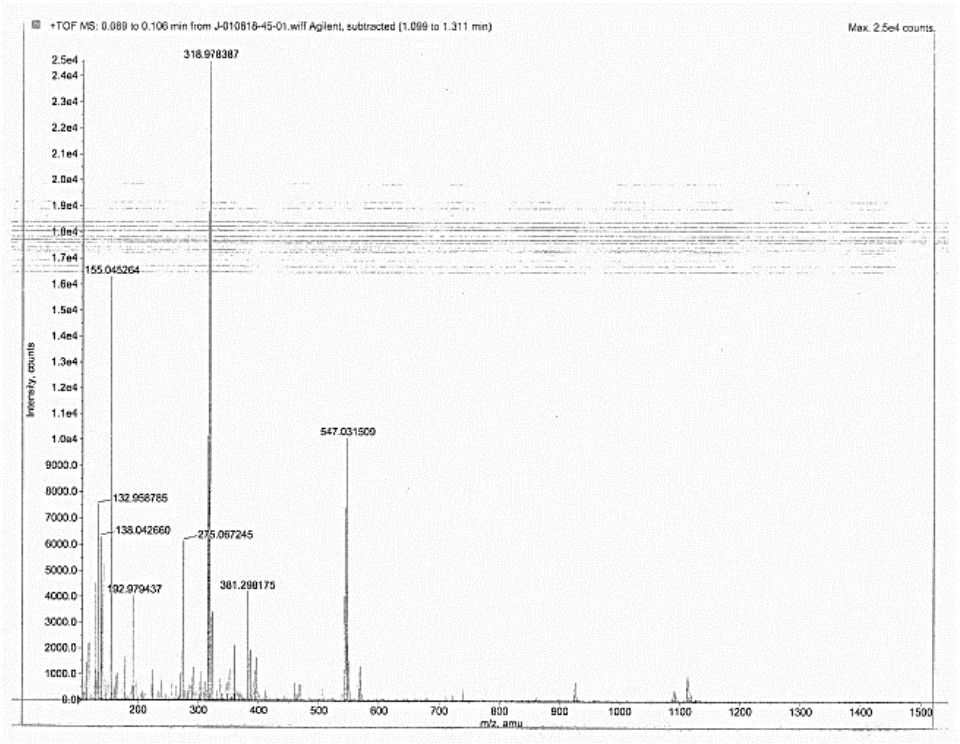


Figure S30. Mass spectrum of compound **4.**

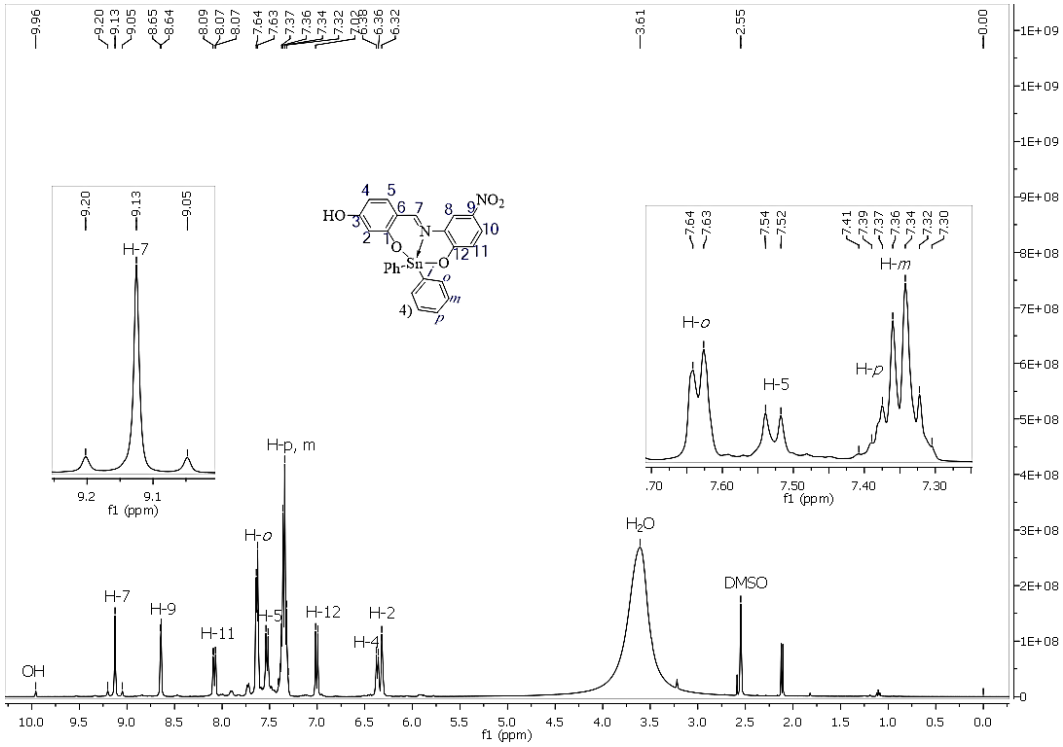


Figure S31. ^{1}H NMR (DMSO-d_6) spectrum of compound **4**.

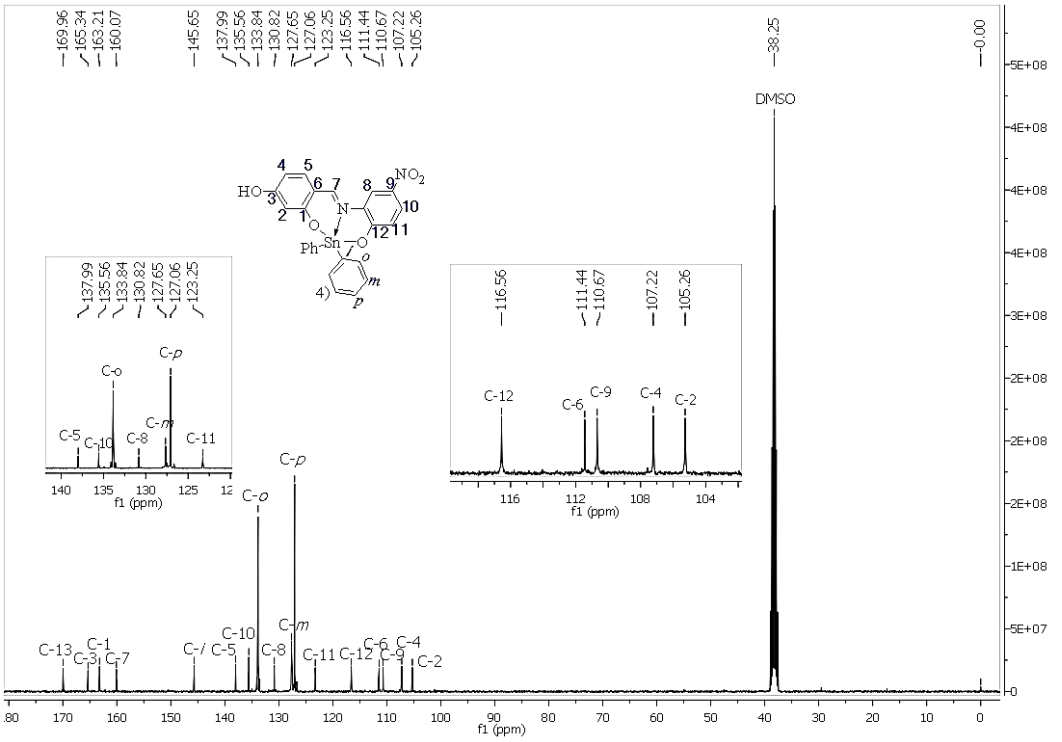


Figure S32. ^{13}C NMR (DMSO-d_6) spectrum of compound **4**.

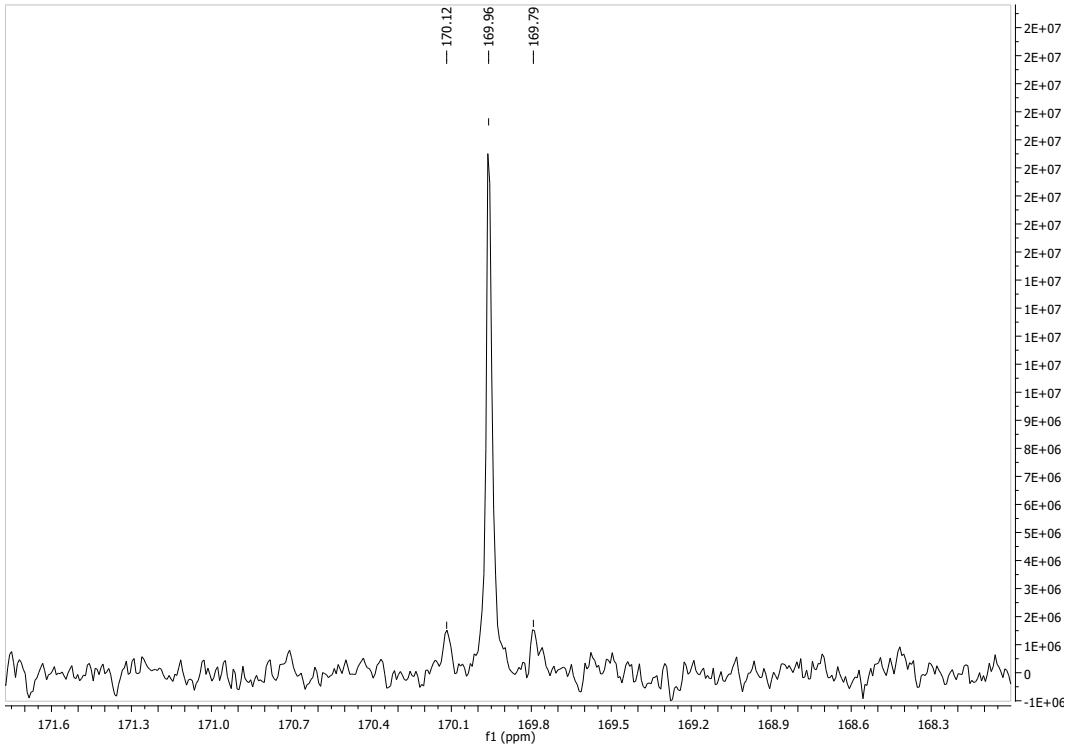


Figure S33. ^{13}C NMR expansion spectrum of compound **4**.

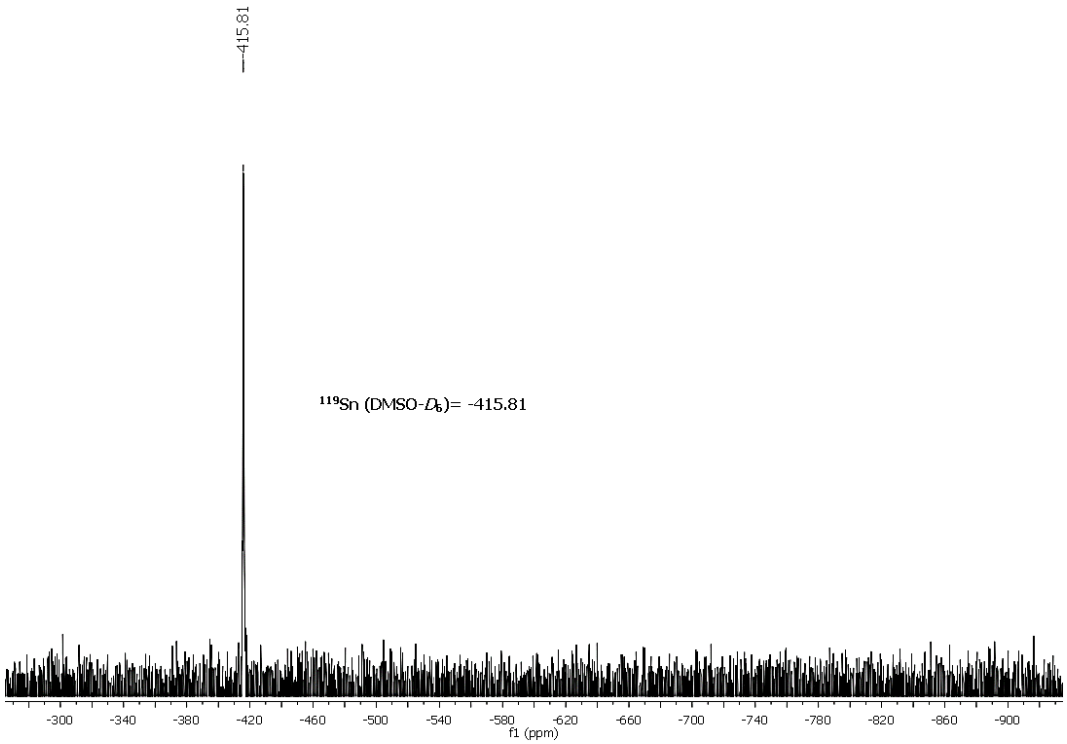


Figure S34. ^{119}Sn NMR (DMSO-d_6) spectrum of compound **4**.

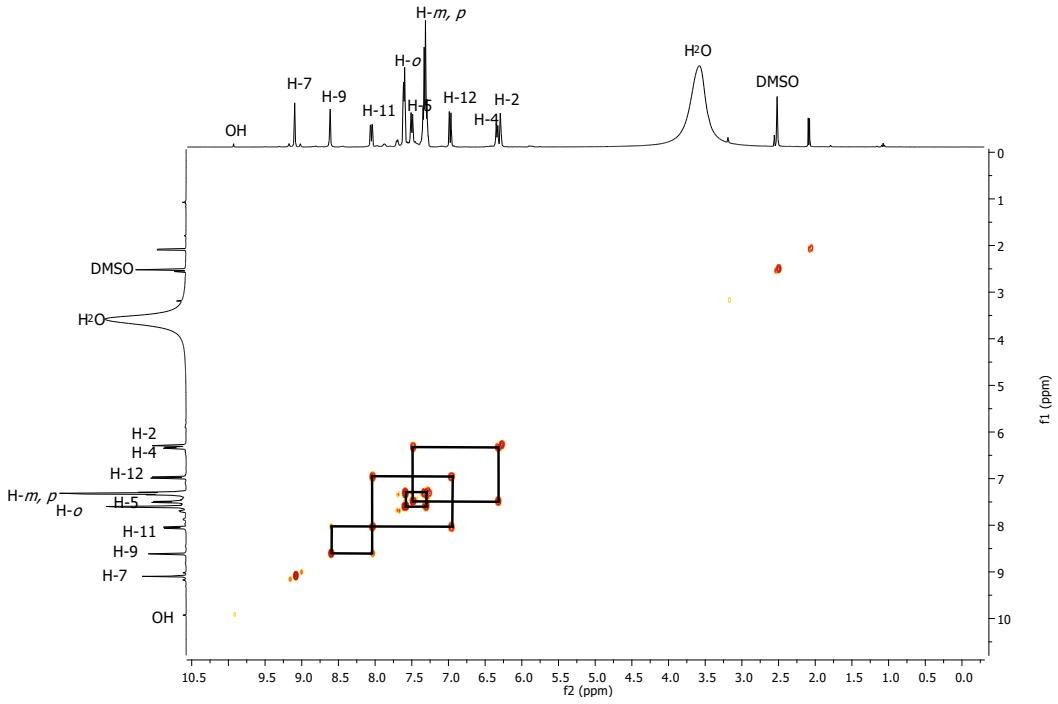


Figure S35. COSY correlation (δ_H/δ_H) spectrum corresponding of compound **4**.

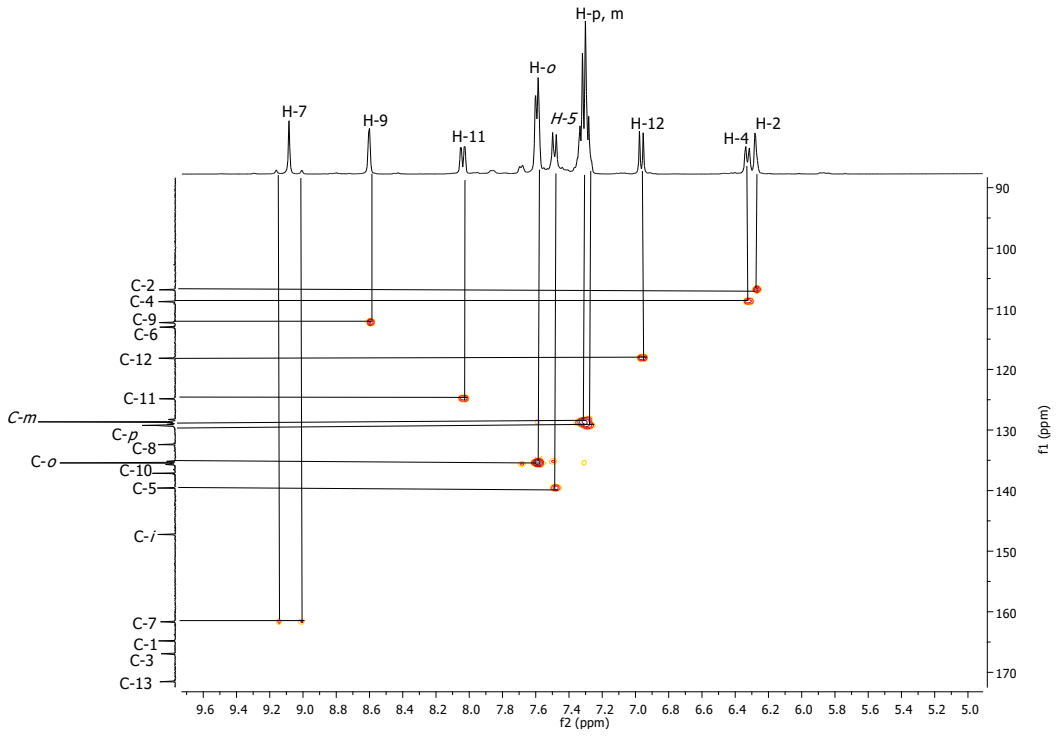


Figure S36. HSQC correlation (δH/δC) spectrum corresponding of compound **4**.

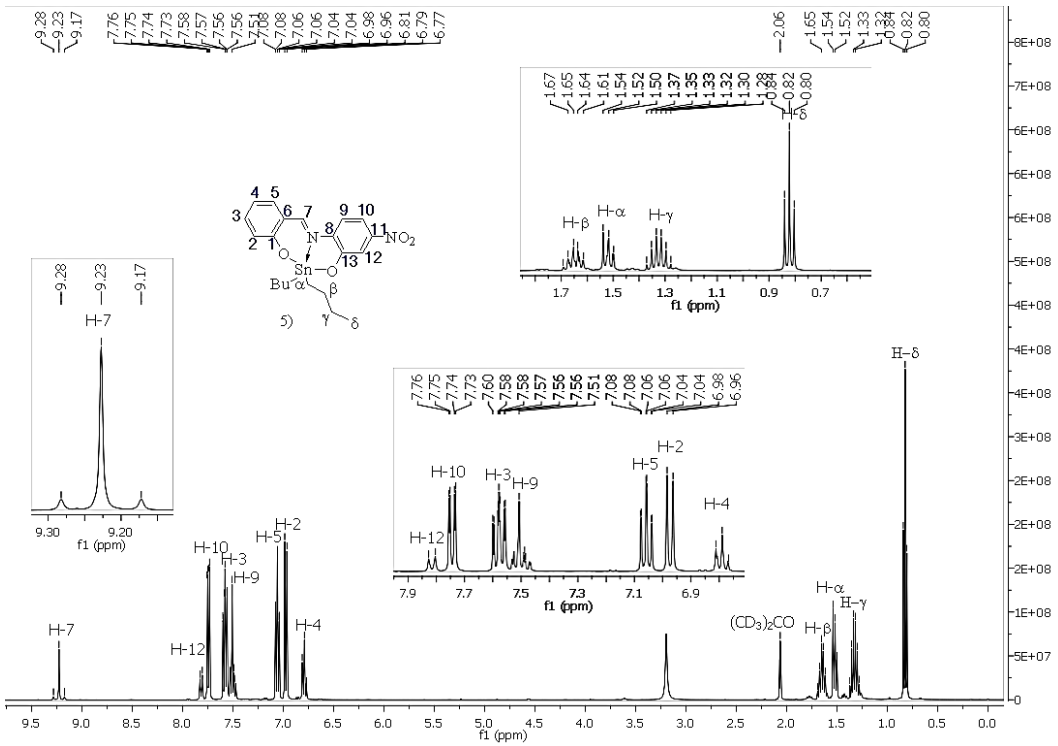


Figure S37. ^{1}H NMR ($(CD_3)_2CO$) spectrum of compound **5**.

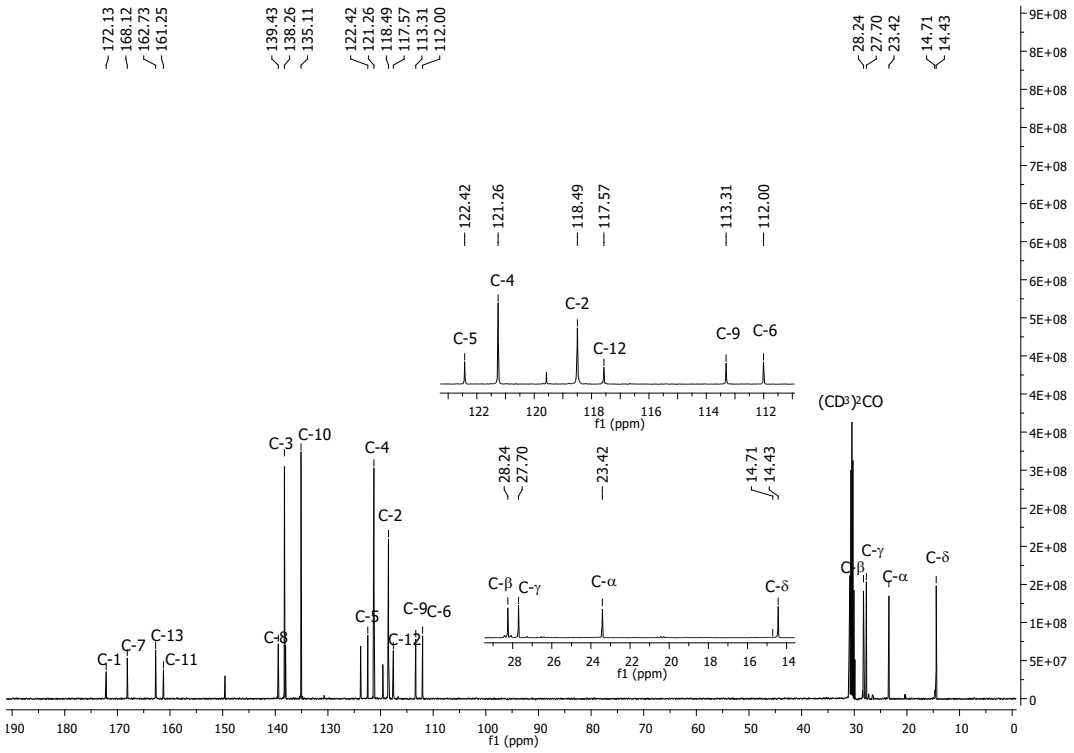


Figure S38. ^{13}C NMR ($(CD_3)_2CO$) spectrum of compound **5**.

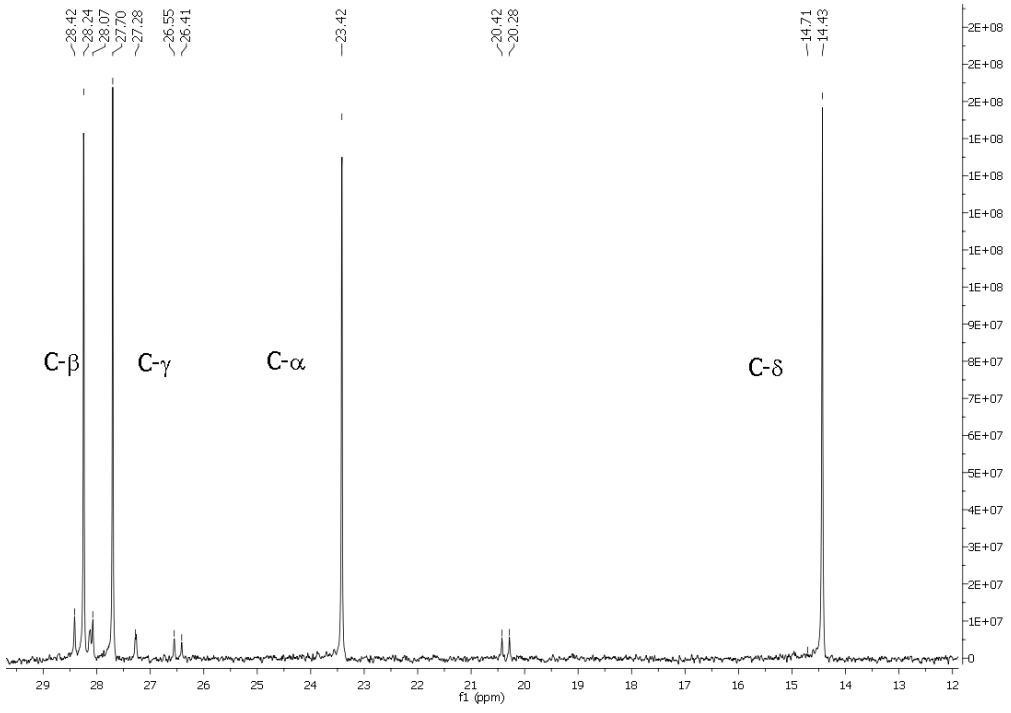


Figure S39. ^{13}C NMR expansion spectrum of compound **5**.

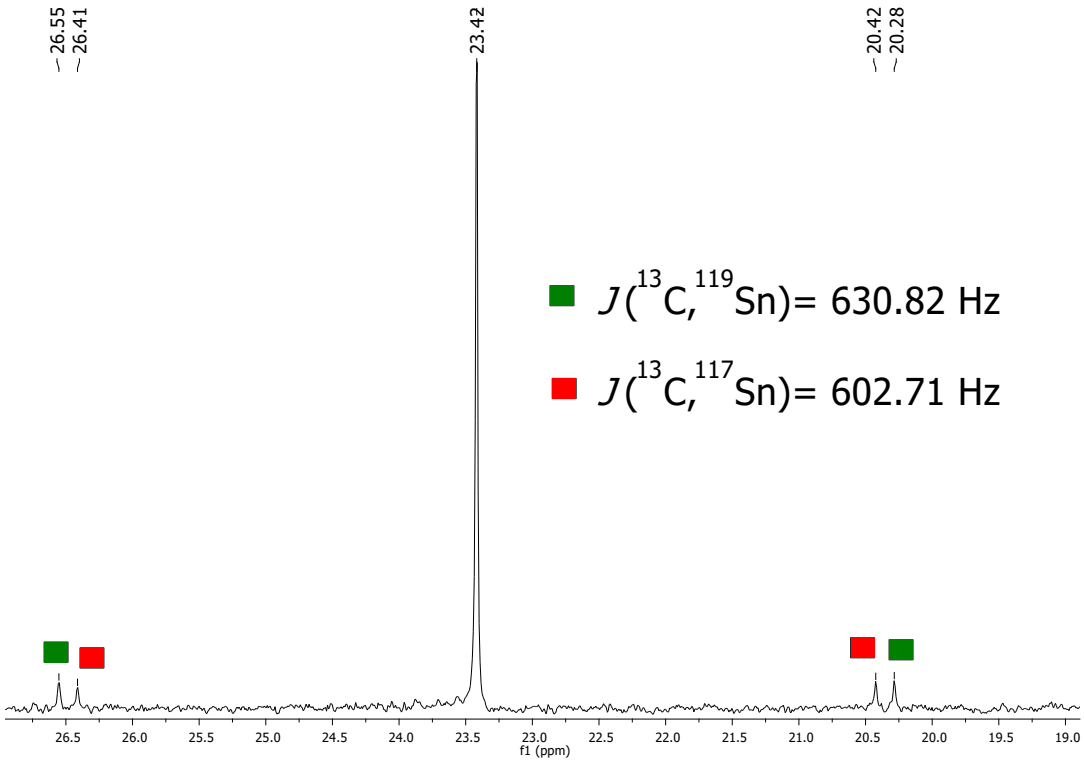


Figure S40. Coupling constant $J(^{13}C,^{119/117}Sn)$ of compound **5.**

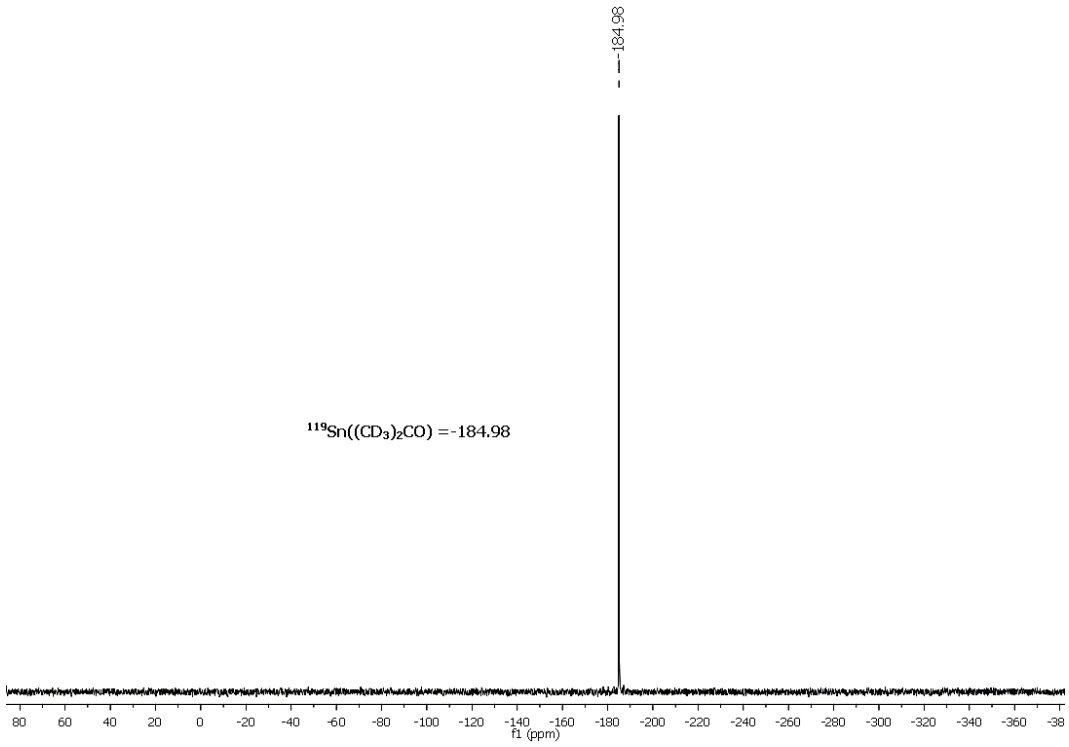


Figure S41. ^{119}Sn NMR ($(CD_3)_2CO$) spectrum of compound **5**.

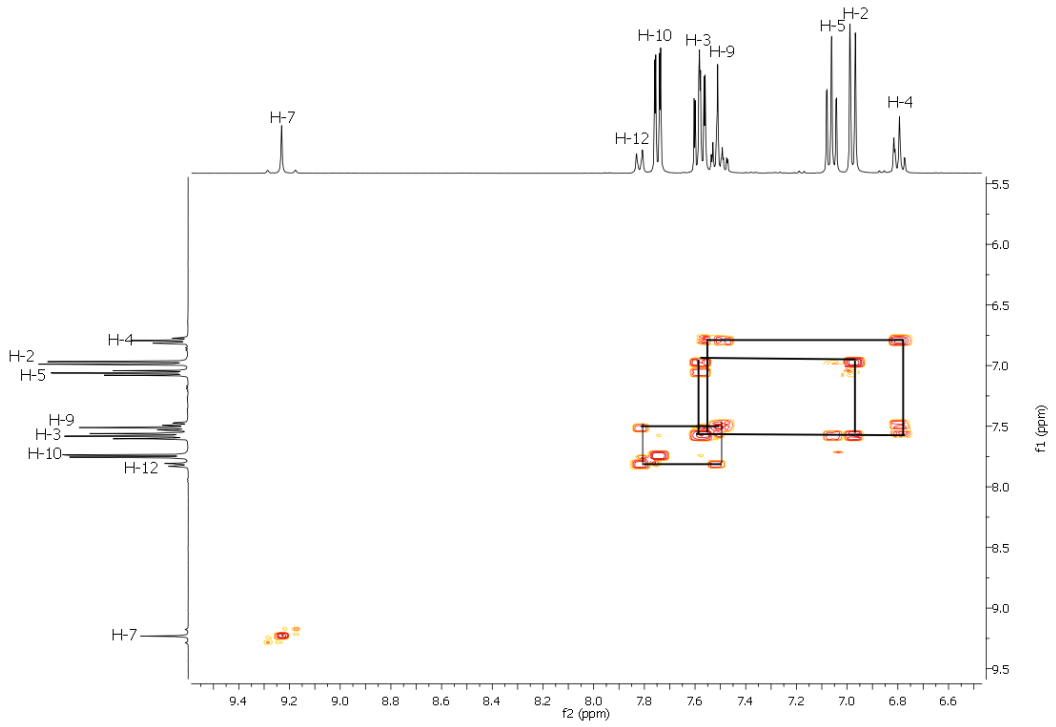


Figure S42. COSY correlation (δ_H/δ_H) spectrum corresponding aromatic region of compound **5.**

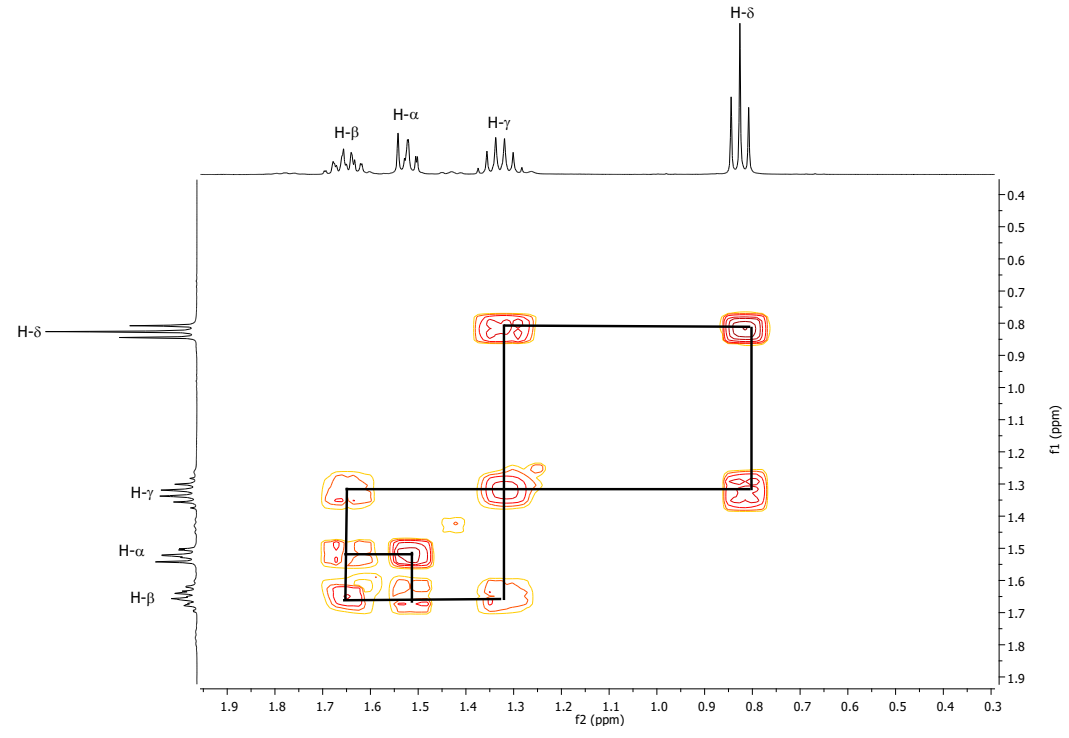


Figure S43. COSY correlation (δ_H/δ_H) spectrum corresponding aliphatic region of **5**.

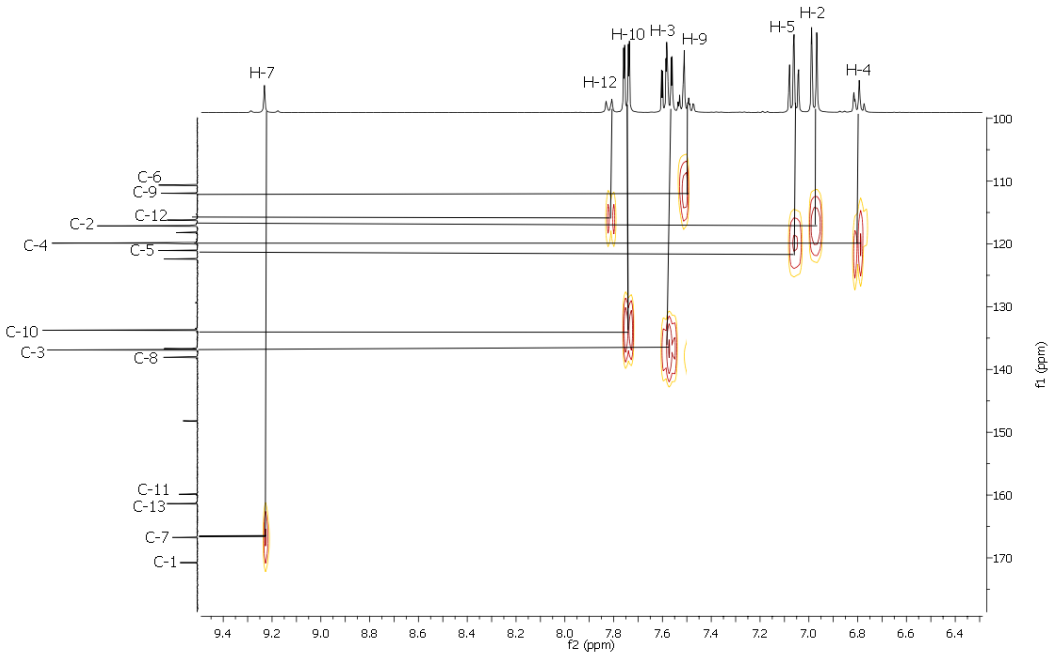


Figure S44. HSQC correlation (δH/δC) spectrum corresponding aromatic region of compound **5**.

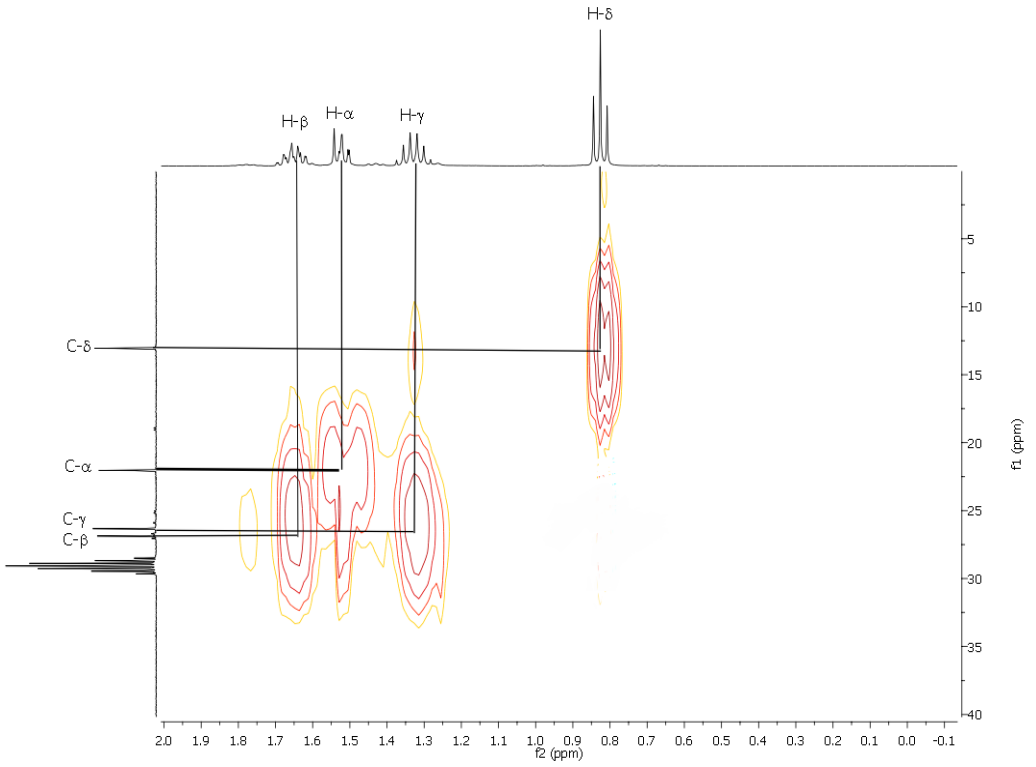


Figure S45. HSQC correlation (δH/δC) spectrum corresponding aliphatic region of compound **5**.

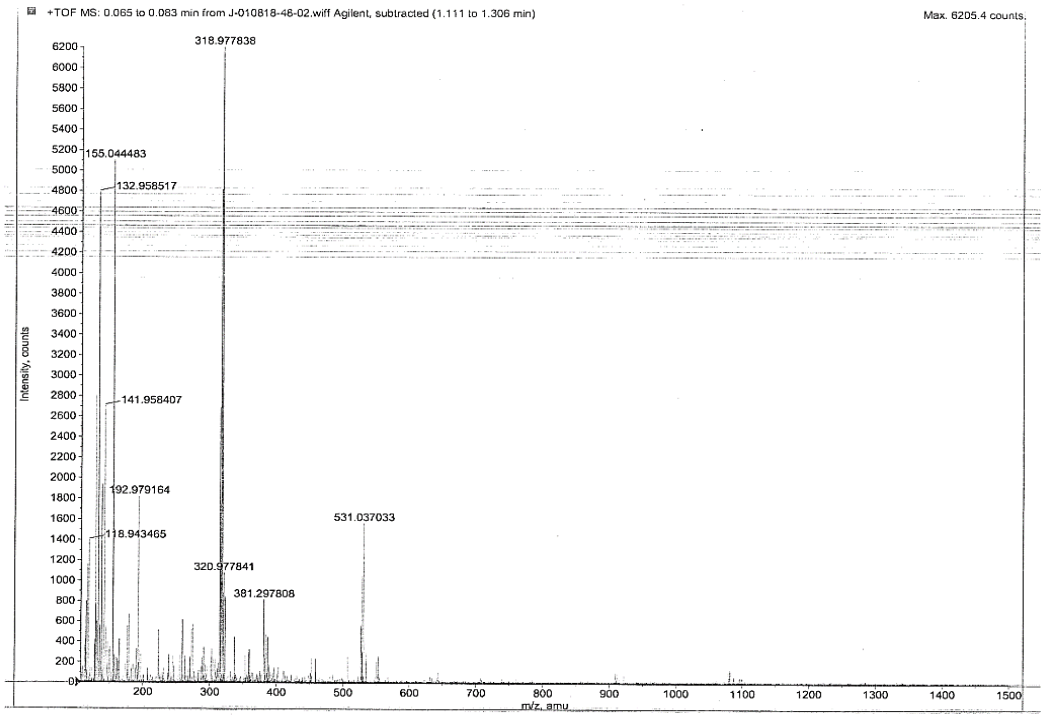


Figure S46. Mass spectrum of compound **6.**

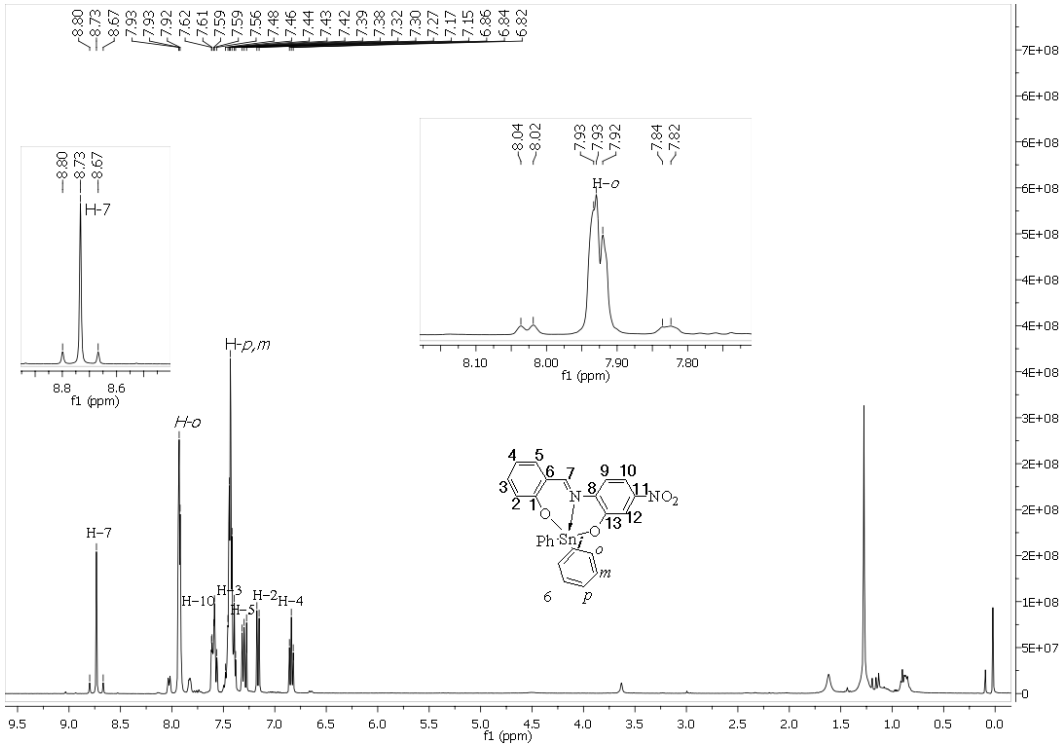


Figure S47. ^{1}H NMR ($CDCl_3$) spectrum of compound **6**.

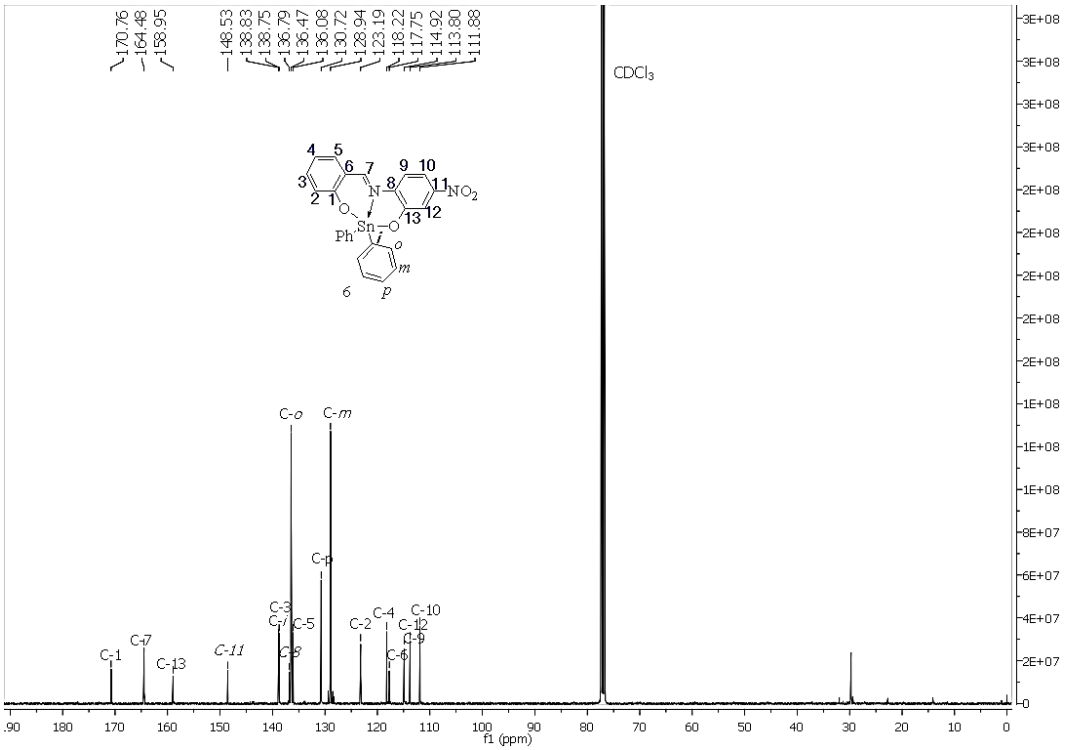


Figure S48. ^{13}C NMR ($CDCl_3$) spectrum of compound **6**.

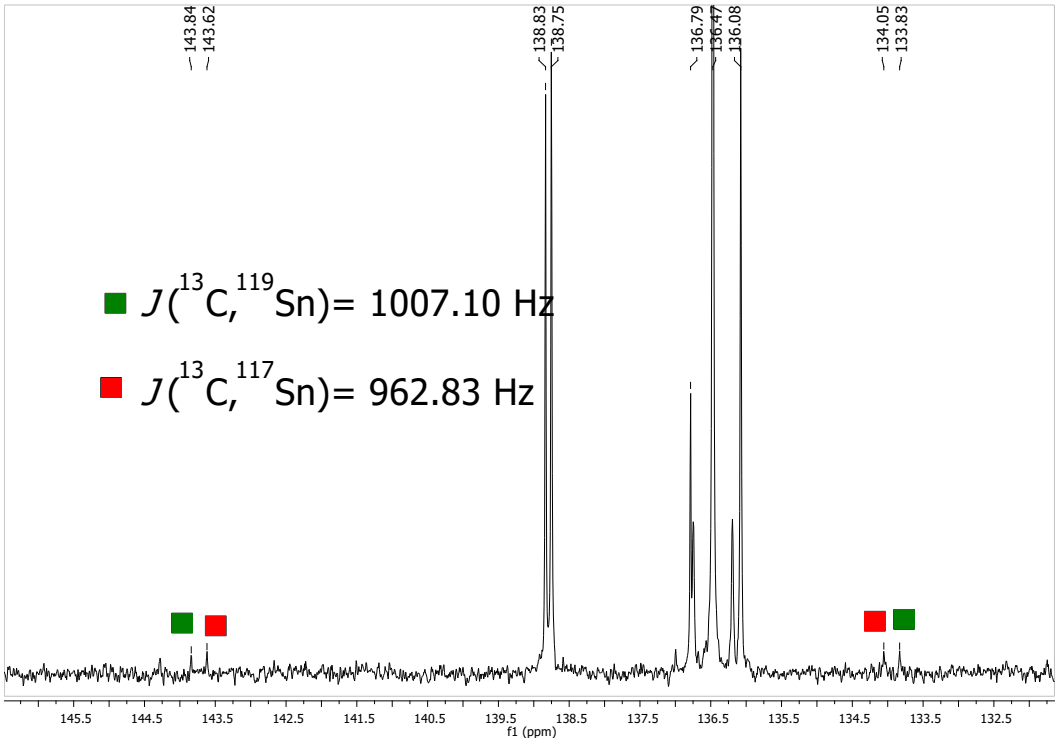


Figure S49. Coupling constant $J(^{13}C,^{119/117}Sn)$ of compound **6.**

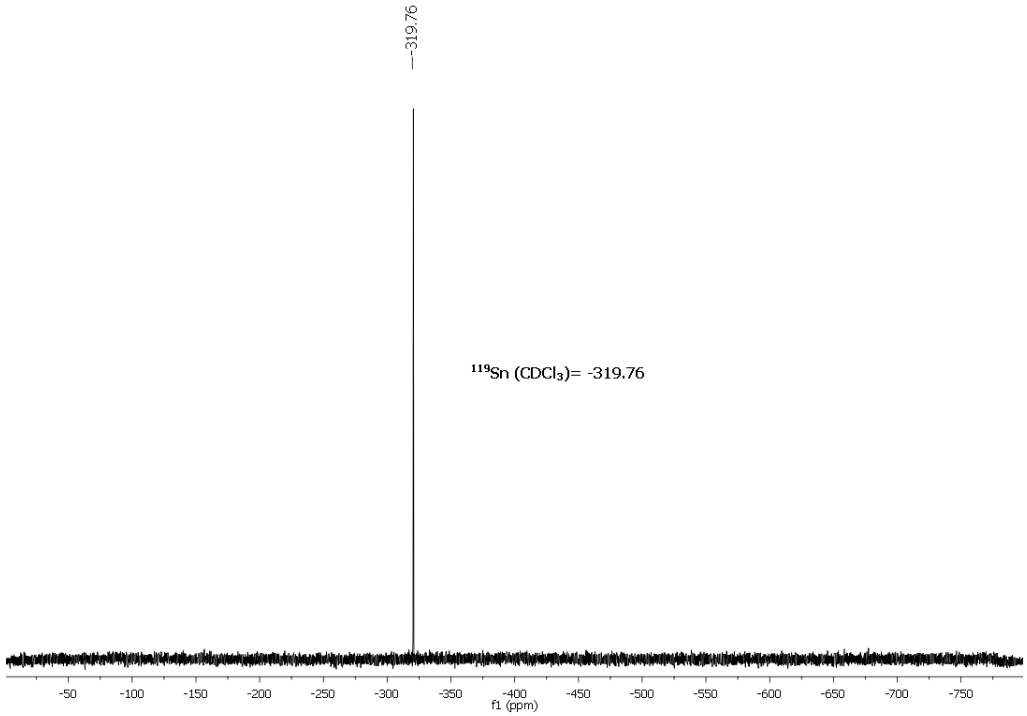


Figure S50. ^{119}Sn NMR ($CDCl_3$) spectrum of compound **6**.

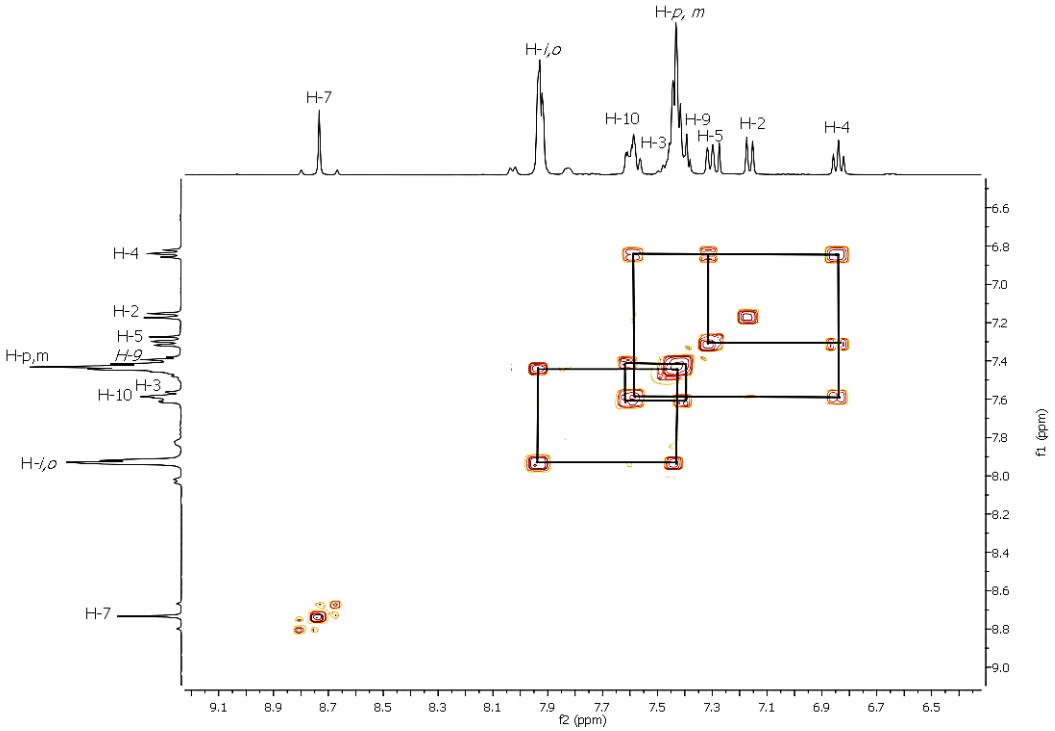


Figure S51. COSY correlation (δ_H/δ_H) spectrum corresponding of compound **6**.

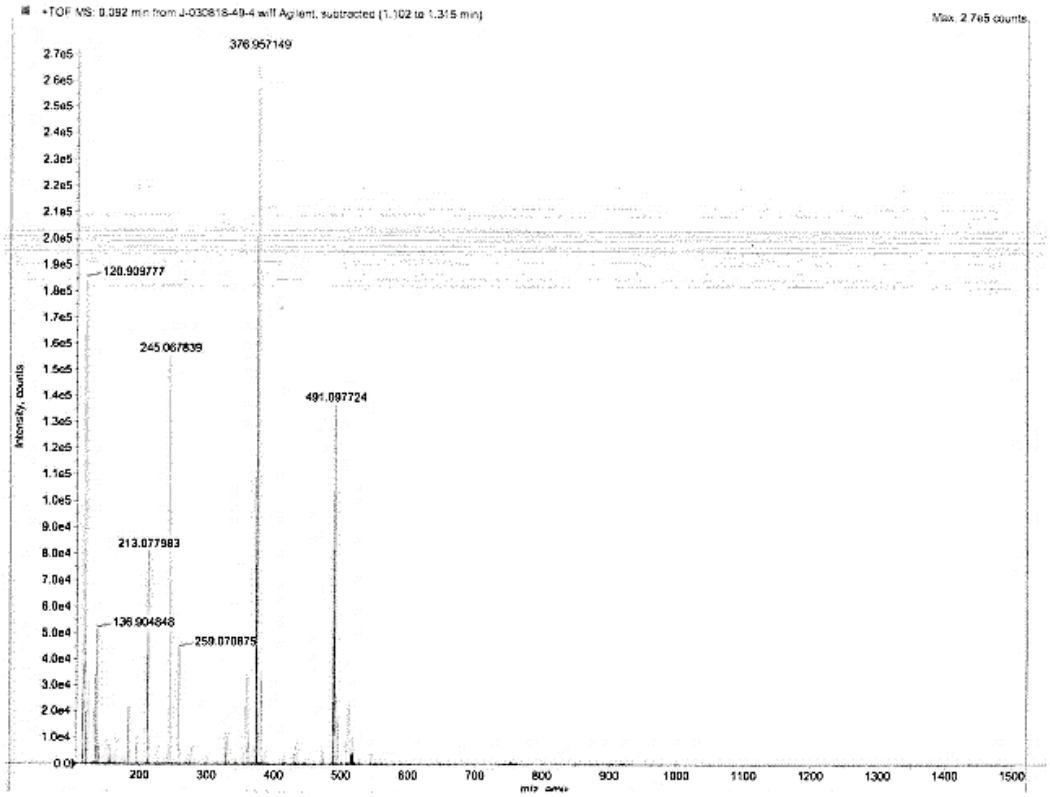


Figure S52. Mass spectrum of compound **7.**

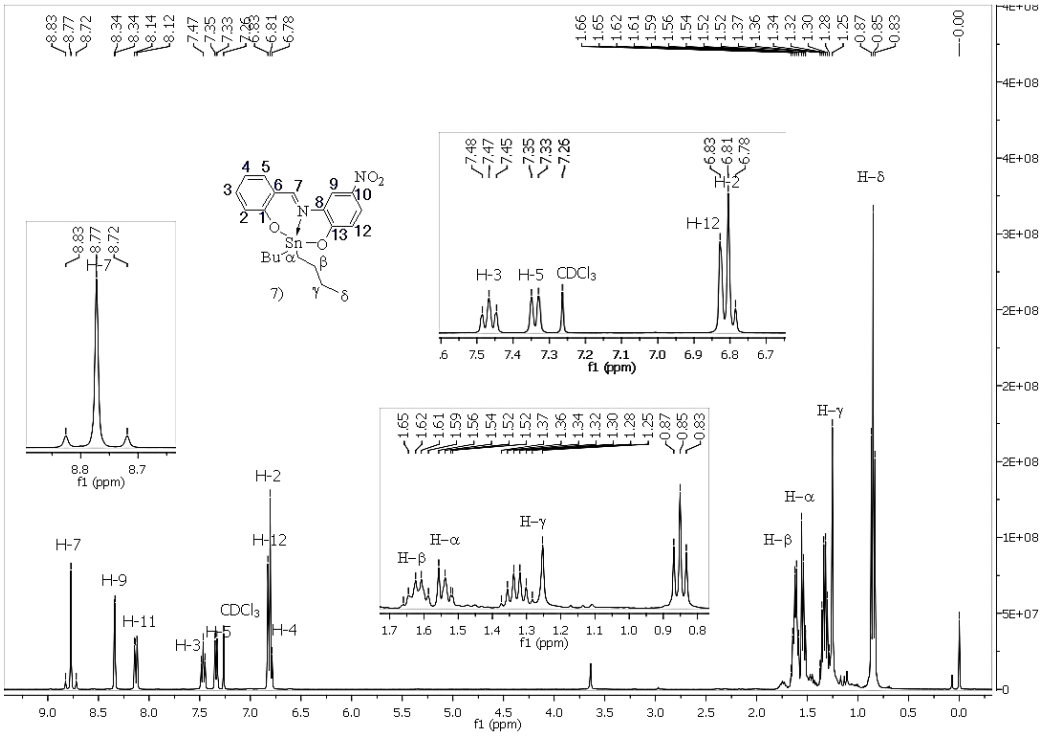


Figure S53. ^{1}H NMR ($CDCl_3$) spectrum of compound **7**.

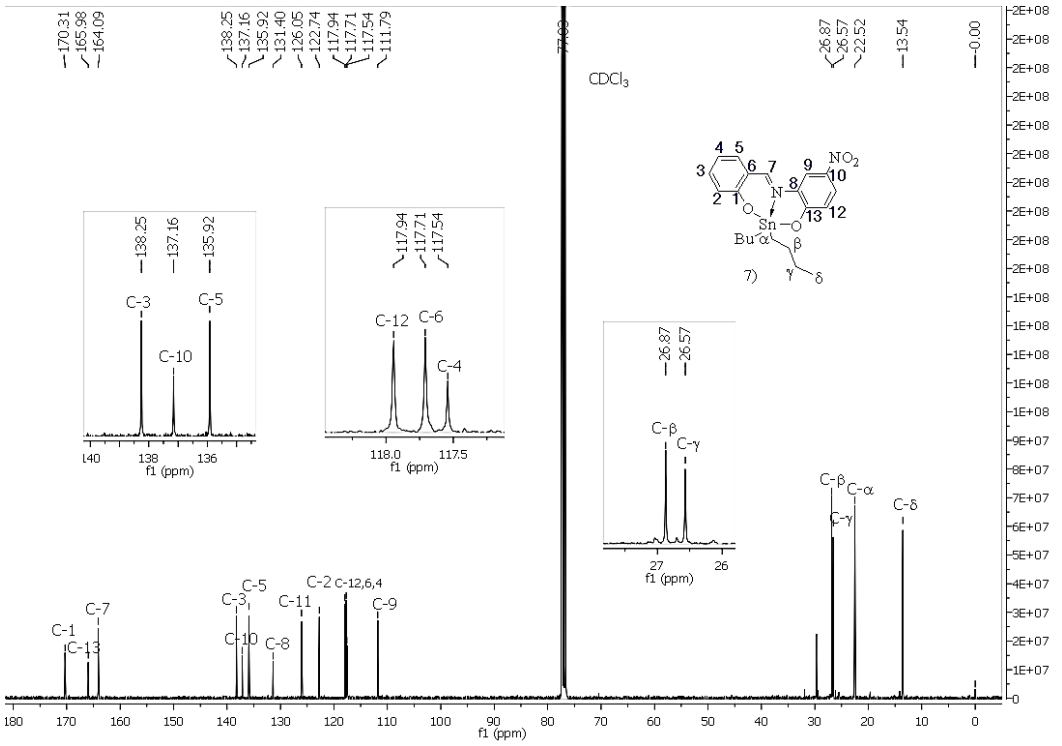


Figure S54. ^{13}C NMR ($CDCl_3$) spectrum of compound **7**.

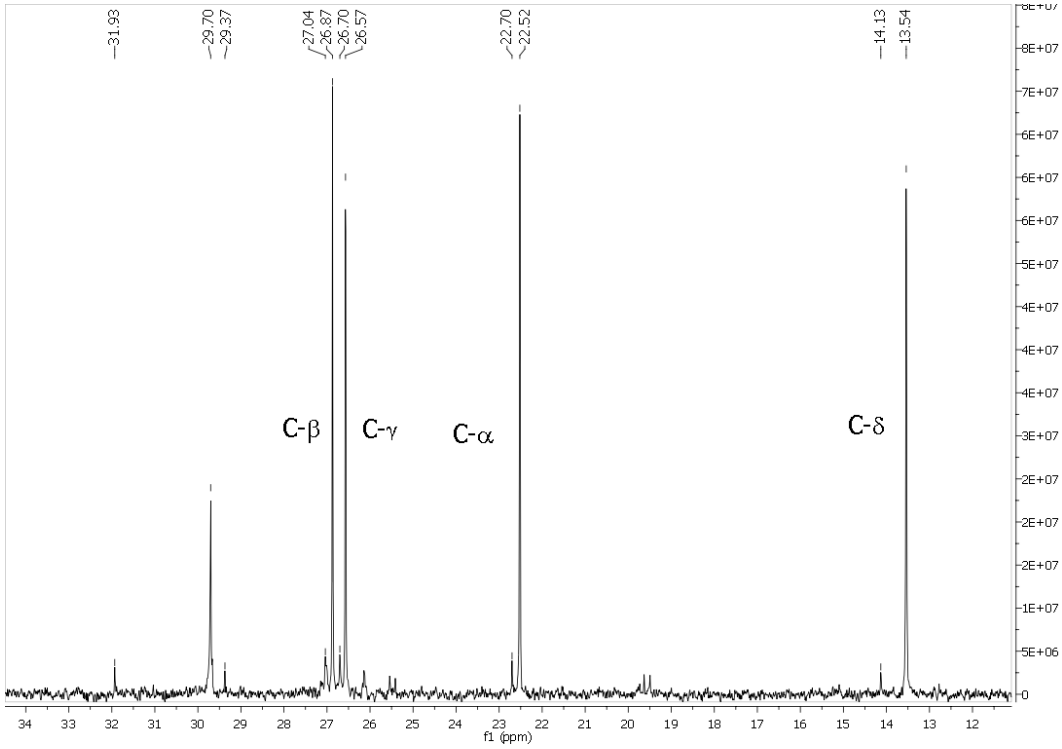


Figure S55. ^{13}C NMR expansion spectrum of compound **7**.

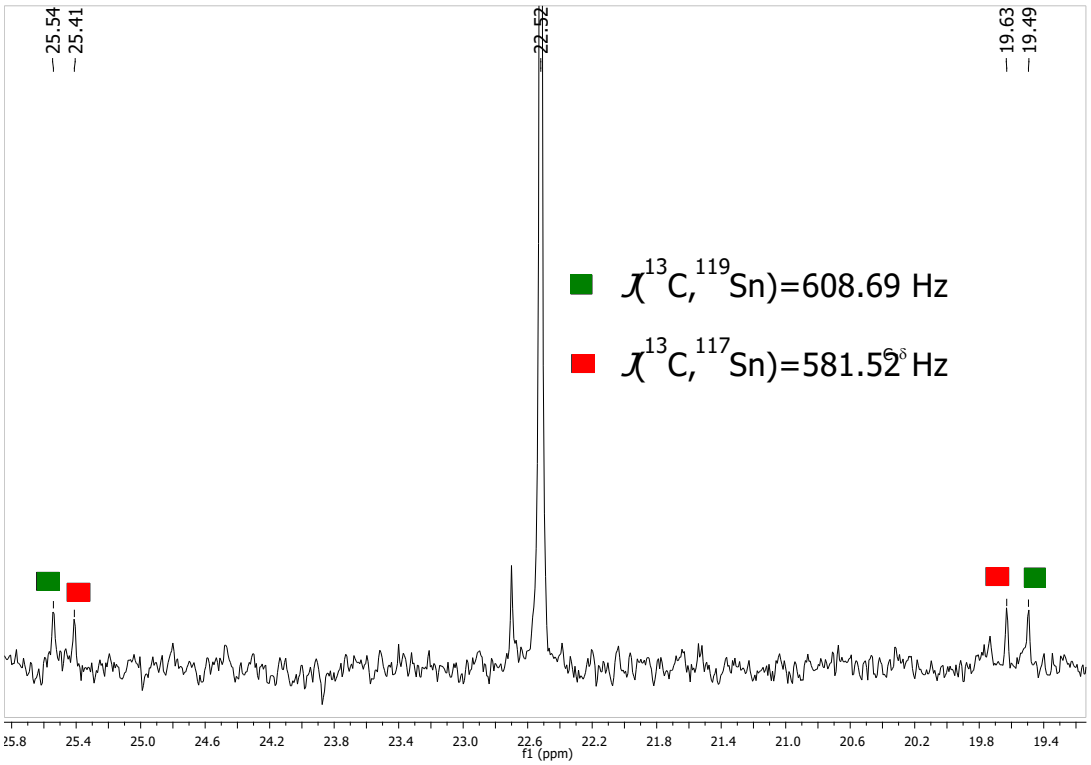


Figure S56. Coupling constant $J(^{13}C,^{119/117}Sn)$ of compound **7.**

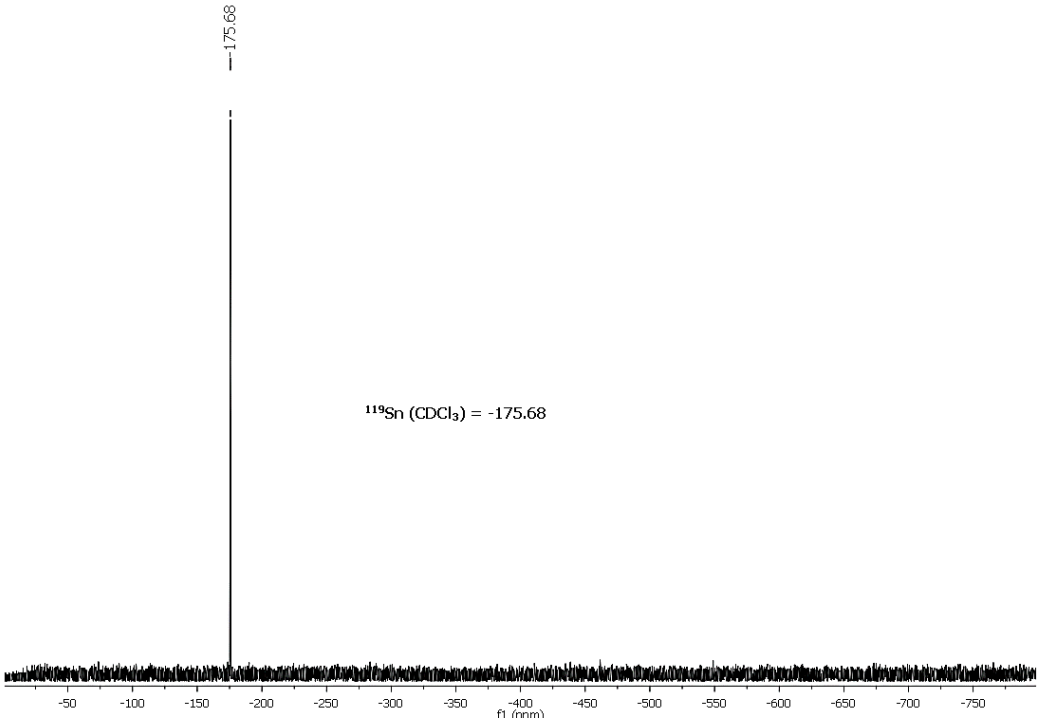


Figure S57. ^{119}Sn NMR ($CDCl_3$) spectrum of compound **7**.

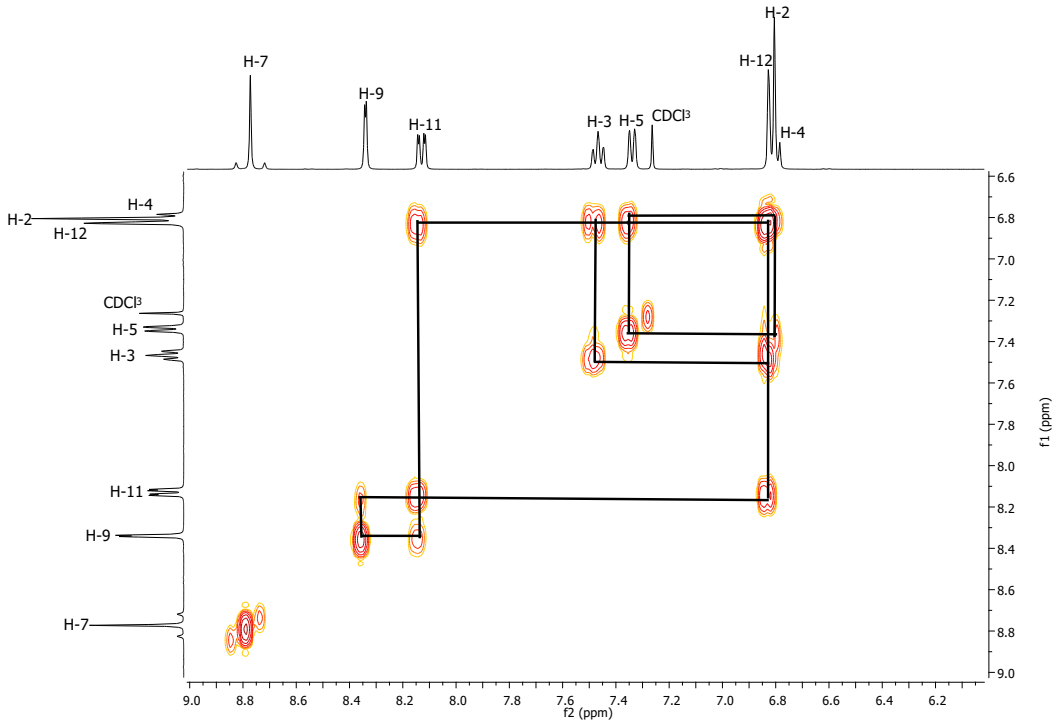


Figure S58. COSY correlation (δ_H/δ_H) spectrum corresponding aromatic region of compound **7.**

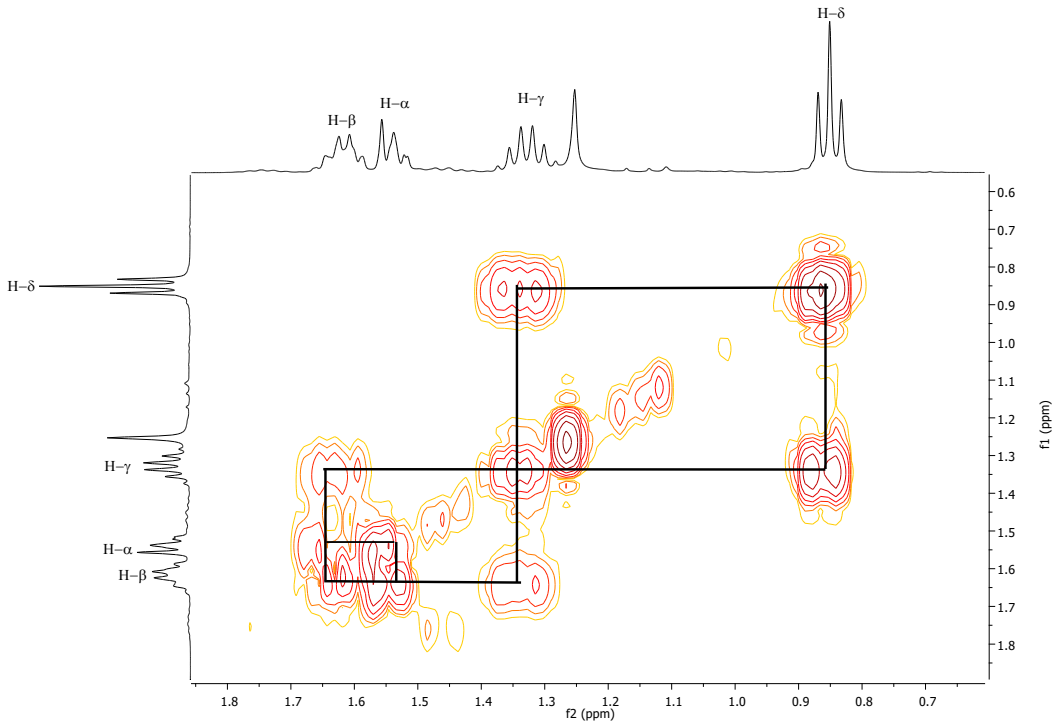


Figure S59. COSY correlation (δ_H/δ_H) spectrum corresponding aliphatic region of compound **7**.

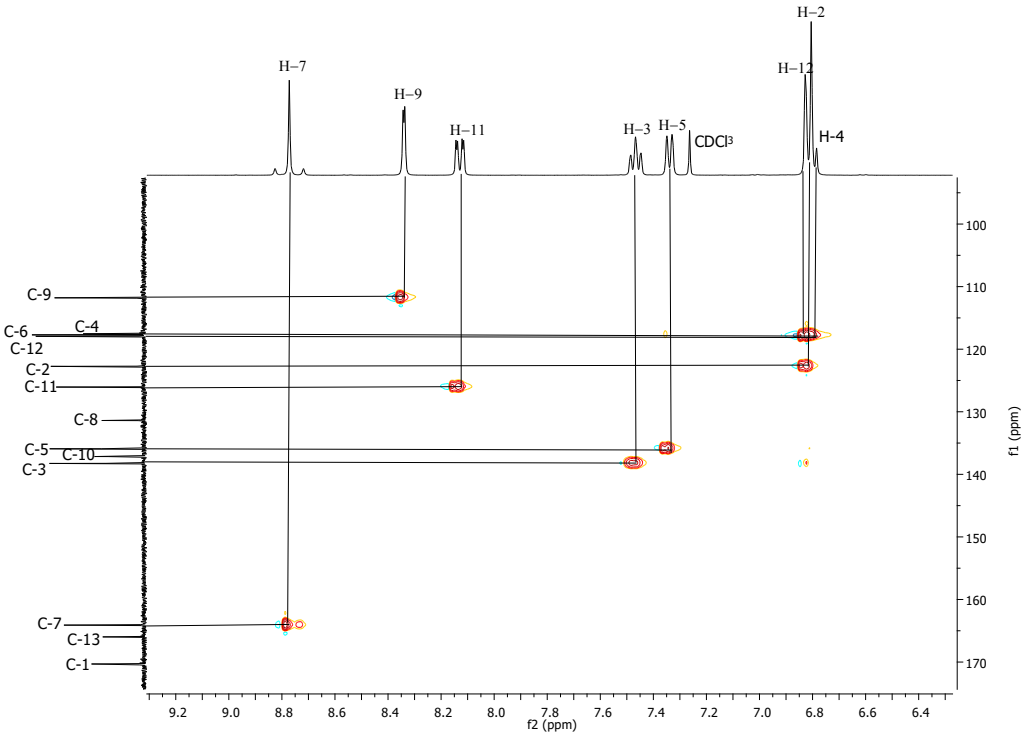


Figure S60. HSQC correlation (δH/δC) spectrum corresponding aromatic region of compound **7**.

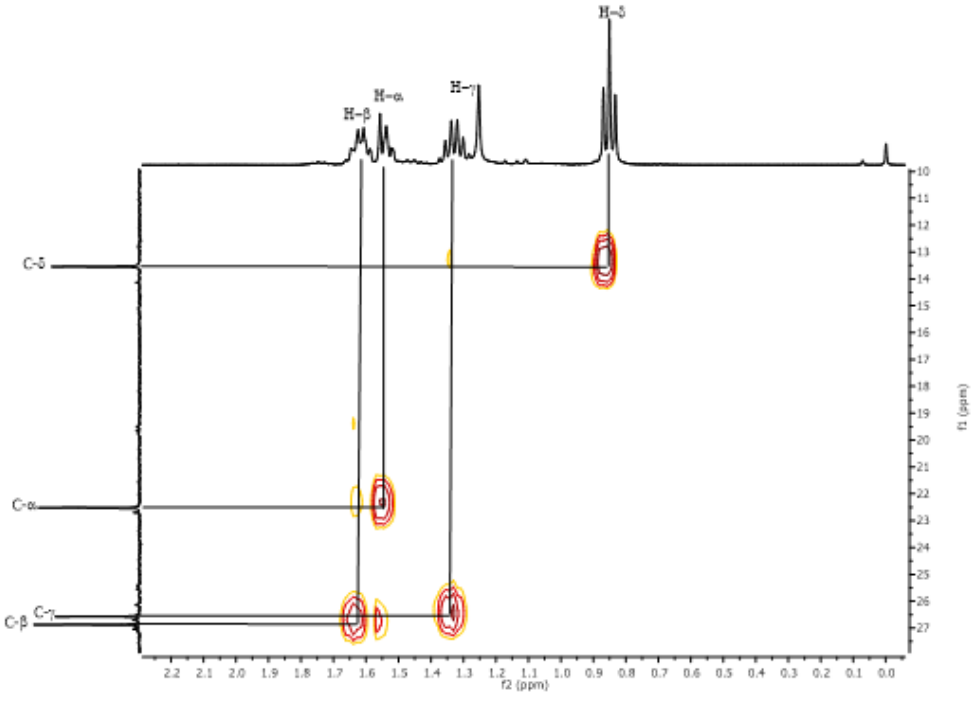


Figure S61. HSQC correlation (δH/δC) spectrum corresponding aliphatic region of compound **7**.

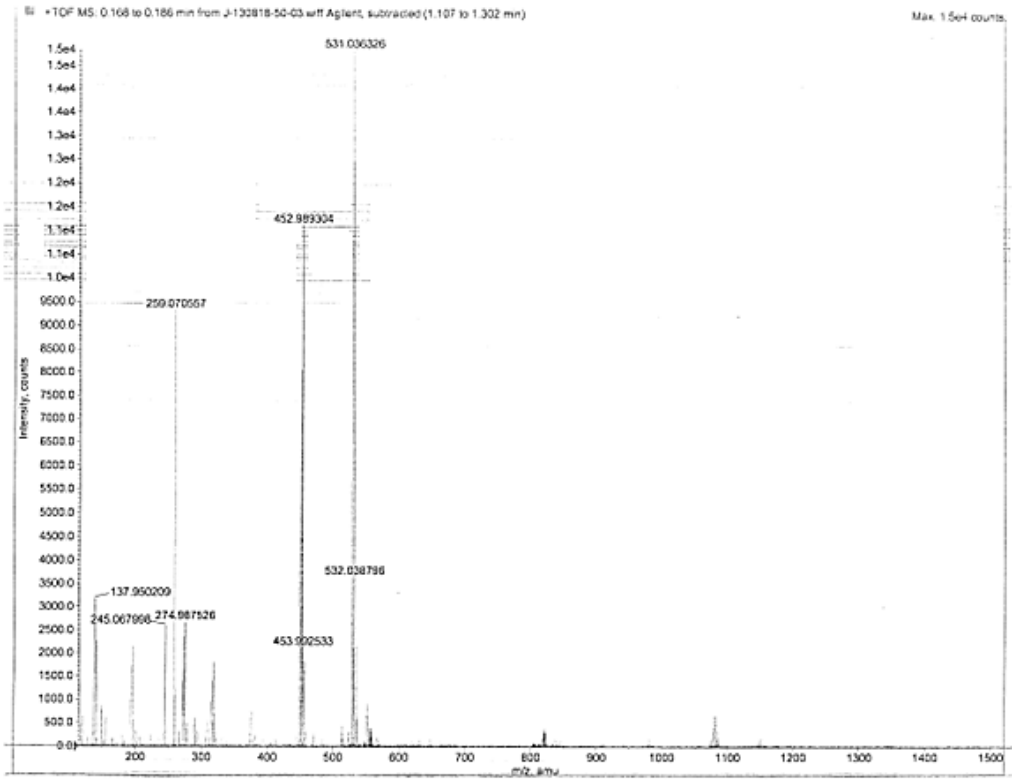


Figure S62. Mass spectrum of compound **8.**

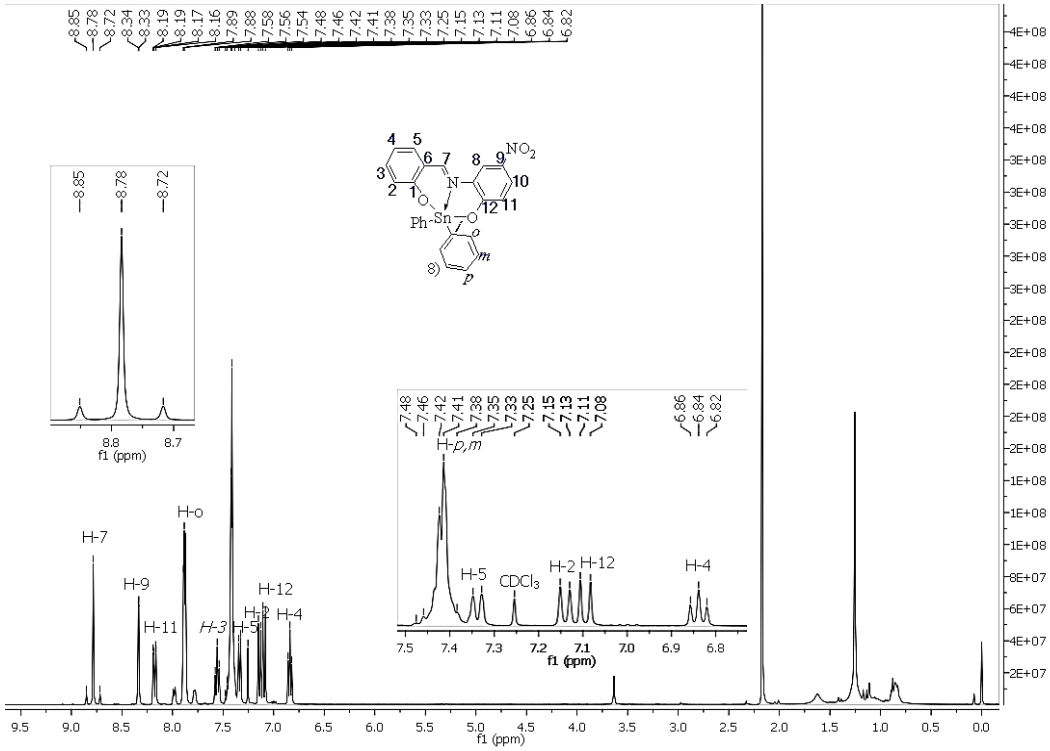


Figure S63. ^{1}H NMR ($CDCl_3$) spectrum of compound **8**.

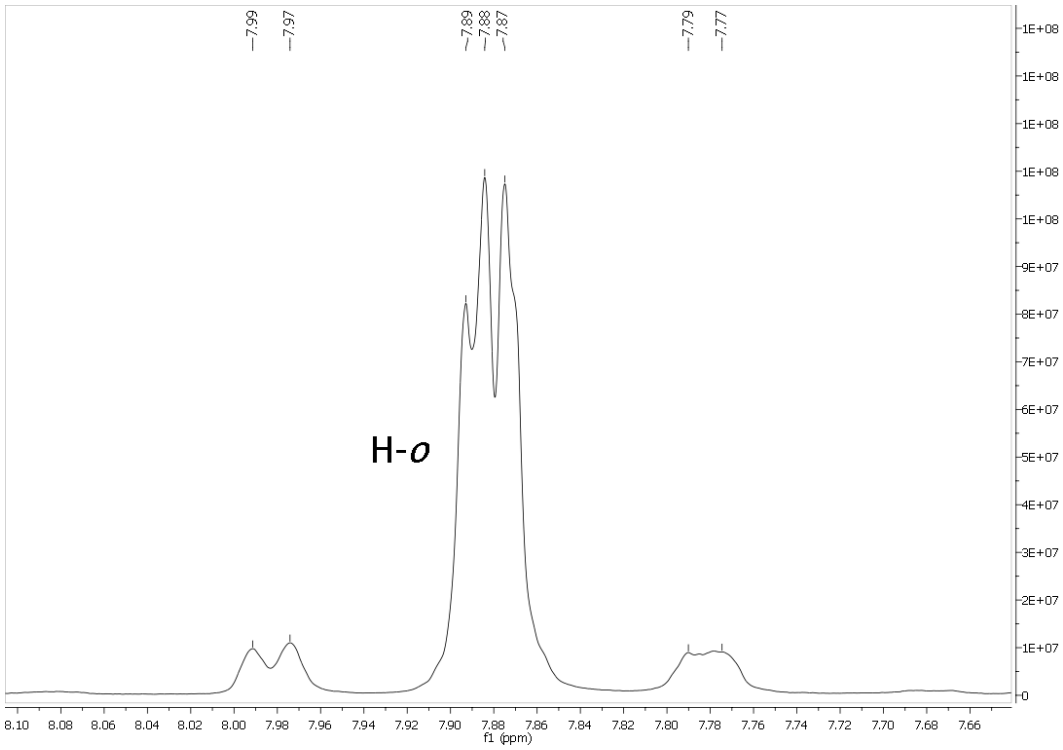


Figure S64. ^{1}H NMR H-*o* spectrum of compound **8**.

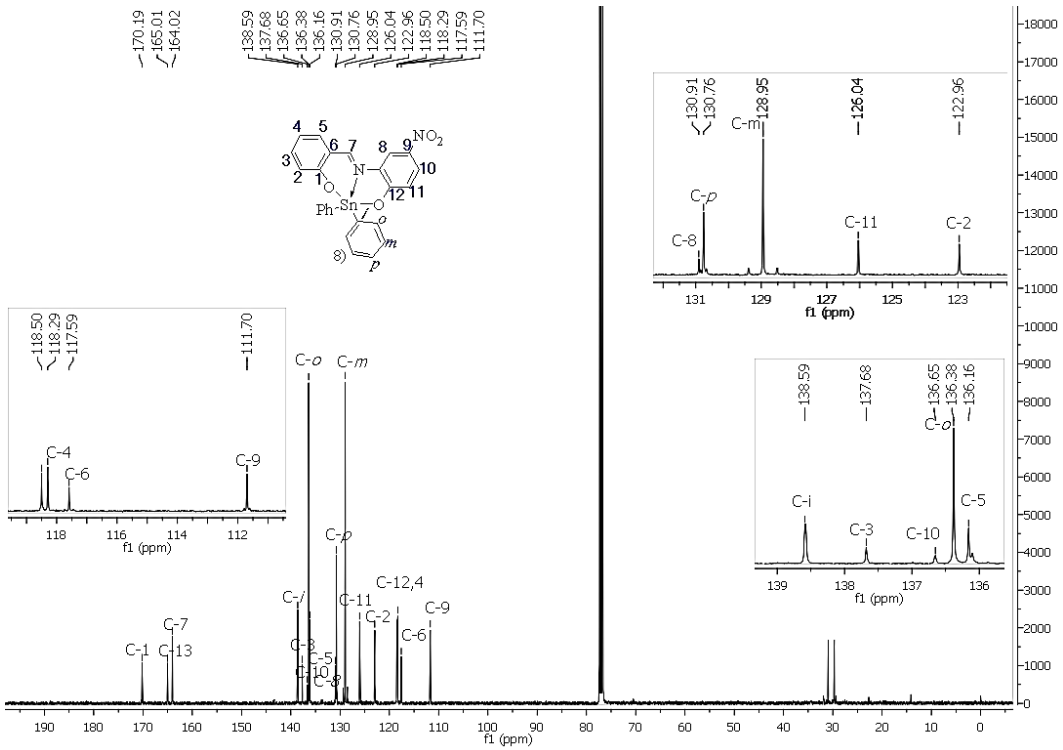


Figure S65. ^{13}C NMR ($CDCl_3$) spectrum of compound **8**.

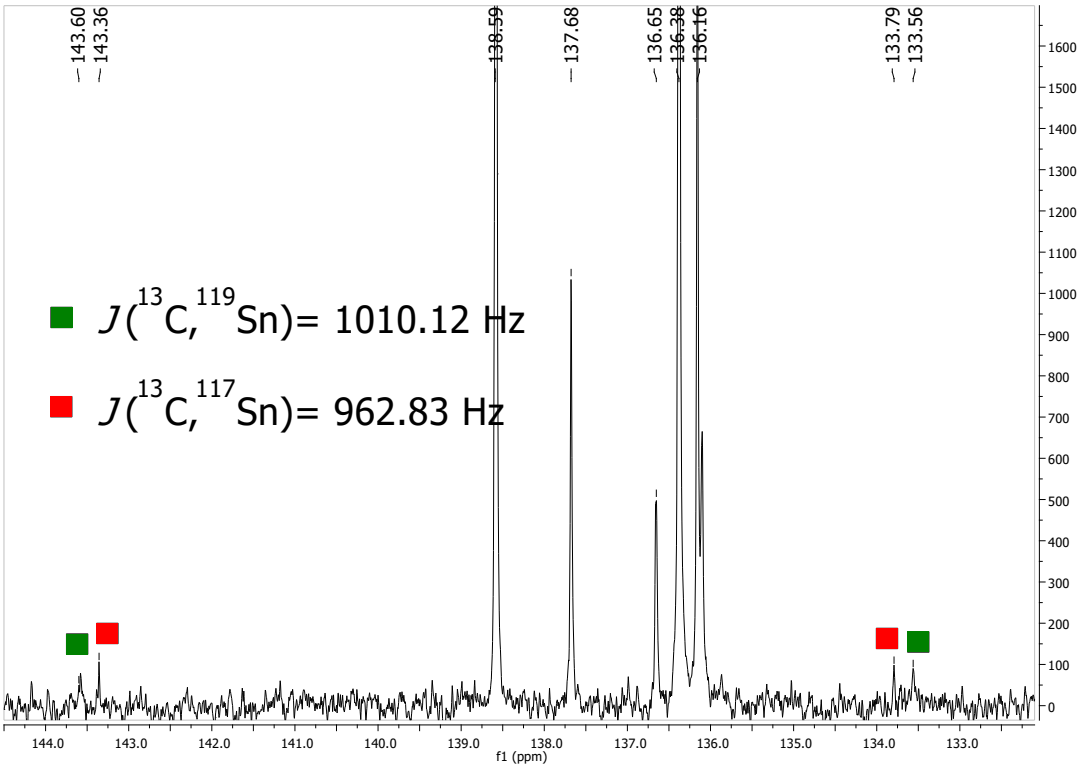


Figure S66. Coupling constant $J(^{13}C,^{119/117}Sn)$ of compound **8**

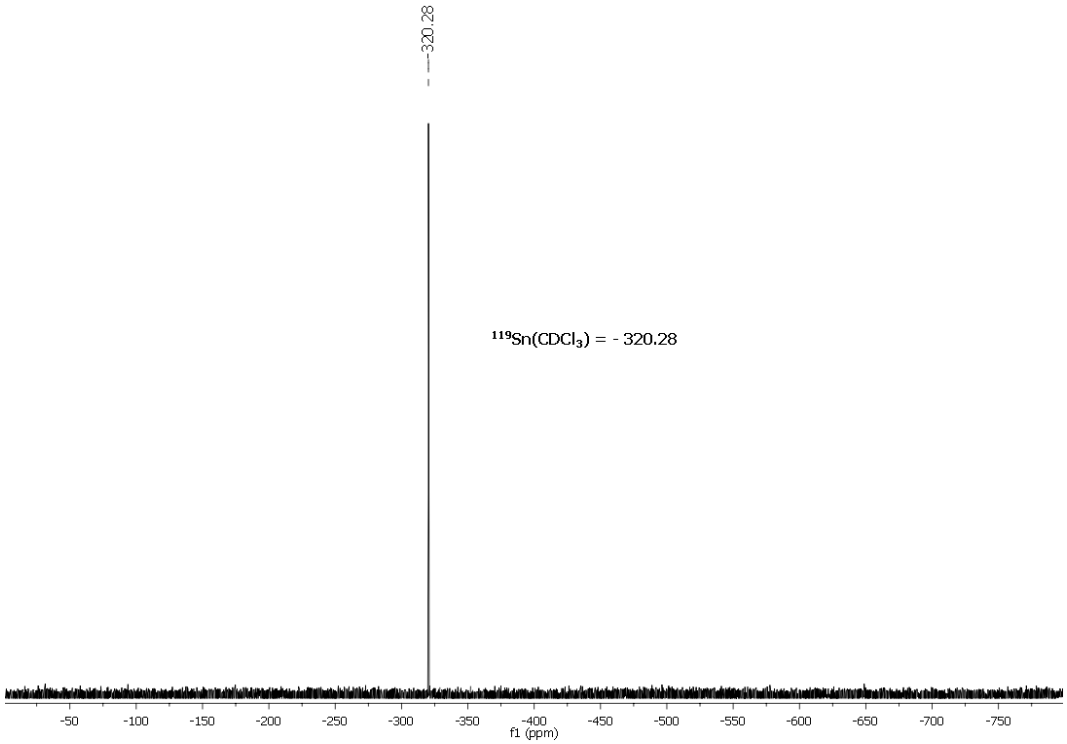


Figure S67. ^{119}Sn NMR ($CDCl_3$) spectrum of compound **8**.

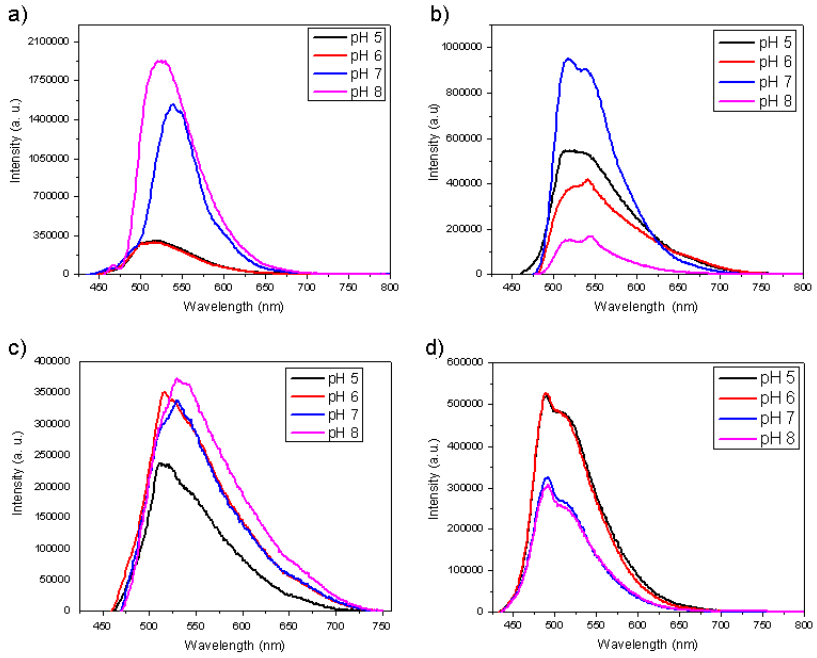


Figure S68. Emission spectra of halochromism for compound **1** a), **2** b), **3** c), and **4** d).

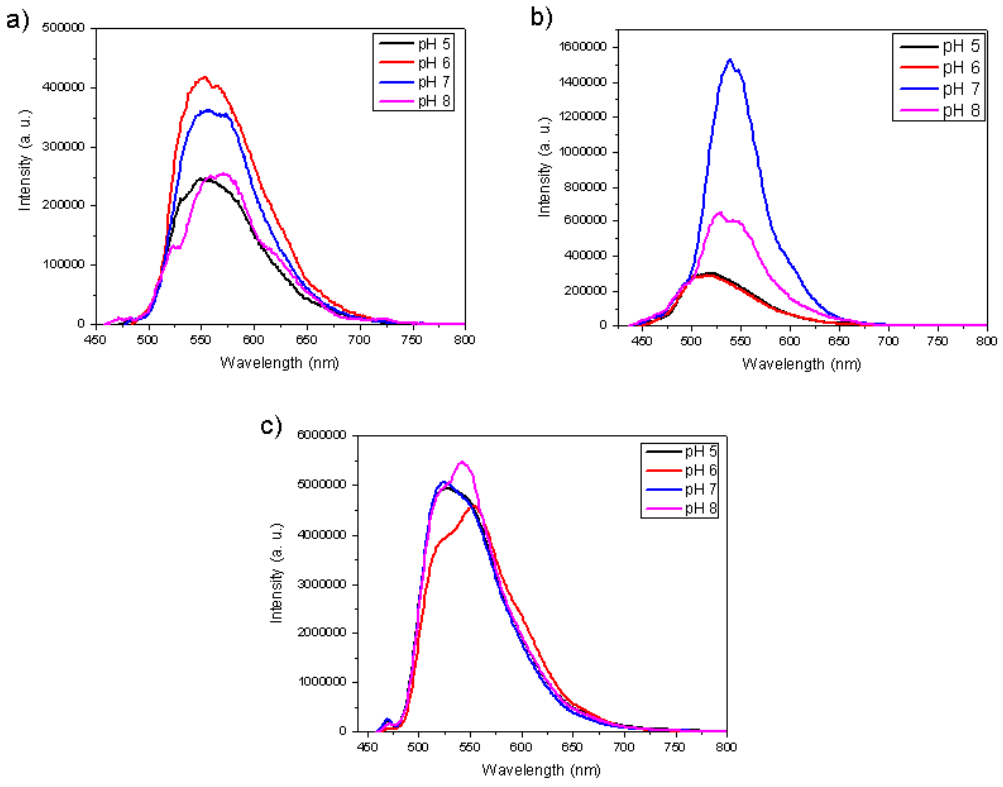


Figure S69. Emission spectra of halochromism for compounds **6** a), **7** b) and **8** c)**.**

Table S4. Structural parameters obtained through X-ray diffraction structure ($\mathbf{1_c}$) and theoretically calculated ($\mathbf{1A^0_{Theo}}$) to compound **1**. Where α and γ are bond angles in º, and *d* is the bond lengths in Å.

System	$\mathbf{1}_c$	$\mathbf{1A}^0$ Theo
d(O3-H)	0.708	0.962
d(N-Sn)	2.174	2.237
d(Sn-O1)	2.118	2.138
d(Sn-O2)	2.182	2.122
d(Sn-C18)	2.119	2.161
d(Sn-C14)	2.105	2.157
d(C7-N1)	1.320	1.297
d(C8-N1)	1.415	1.409
d(C1-O1)	1.311	1.312
α(O1-Sn1-O2)	154.93º	156.68
α(C18-Sn1-N1)	116.90º	117.79
α(C14-Sn1-N1)	105.10º	111.59
α(C14-Sn1-C18)	137.95º	130.60
α(C18-Sn1-O1)	91.00º	94.69
α(C18-Sn1-O2)	94.27º	94.27
α(C14-Sn1-O1)	93.59º	93.13
α(C14-Sn1-O2)	93.71º	97.25
α(O1-Sn1-N1)	81.22º	81.63
α(O2-Sn1-N1)	74.54º	75.14
γ(C7-N1-C8-C9)	30.61°	21.07

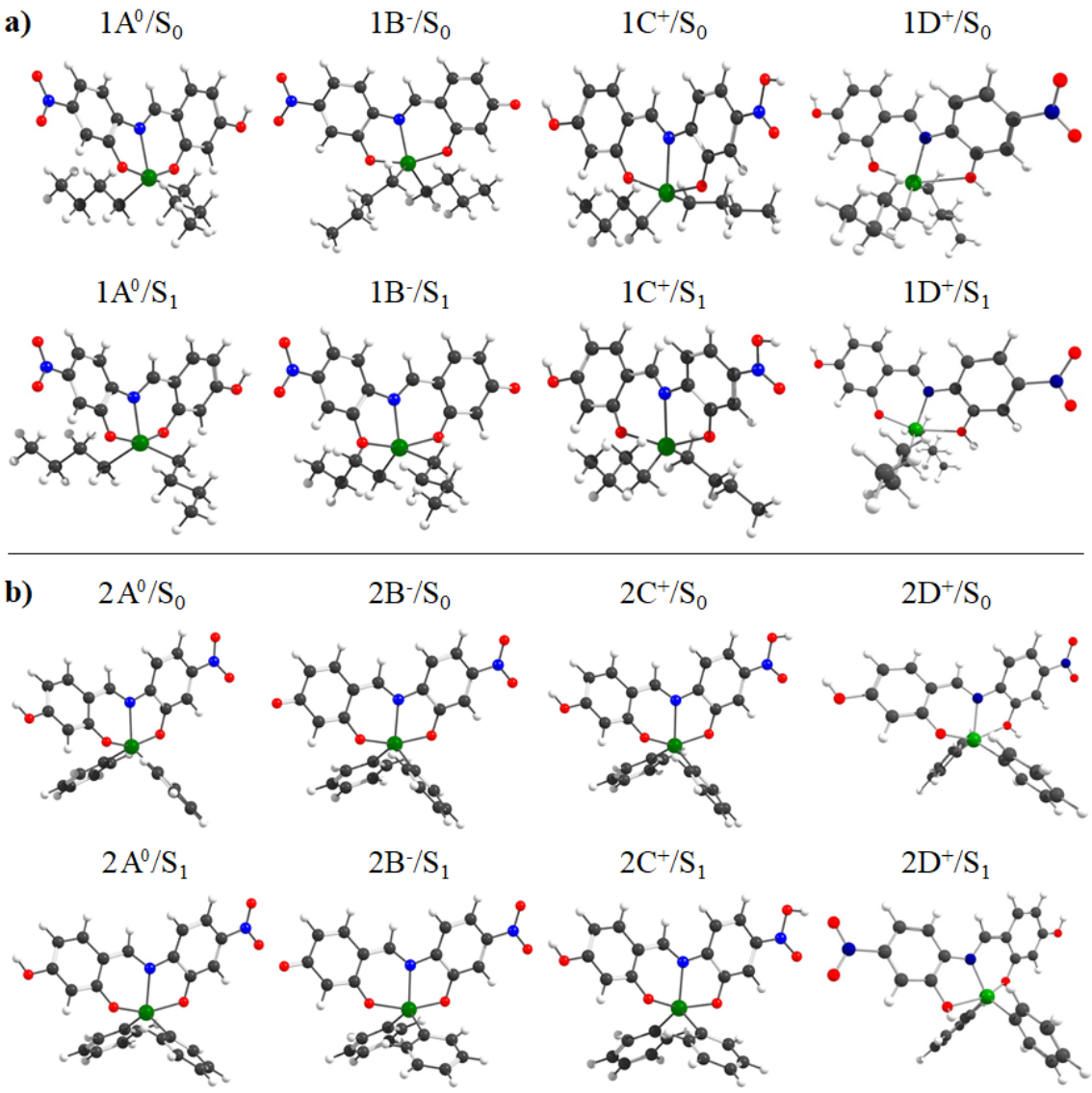


Figure. S70. Optimized structures of **1** and **2** in the ground (S_0) and the first-singlet excited (S_1) state: neutral (**A**^{0}), basic (**B**$^{-}$) and acid (**C**$^{+}$ and **D**$^{+}$) media. Atoms are denoted with red (oxygen), blue (nitrogen), gray (carbon), light gray (hydrogen), and green (tin) spheres.

Table S5. Torsion angle $\gamma(C_7\text{-}N_1\text{-}C_8\text{-}C_9)$ and bond lengths $d(Sn\text{-}O_2)$ (in Å).

System	A^0/S_0	A^0/S_1	B^-/S_0	B^-/S_1	C^+/S_0	C^+/S_1	D^+/S_0	D^+/S_1
1 $\gamma(C_7\text{-}N_1\text{-}C_8\text{-}C_9)$	30.61°	26.04°	0.25°	10.18°	-0.70°	34.24°	31.6°	17.9°
2 $\gamma(C_7\text{-}N_1\text{-}C_8\text{-}C_9)$	21.87°	29.78°	11.65°	30.17°	18.87°	9.93°	30.8°	16.0°
1 $d(Sn\text{-}O_2)$	2.121	2.098	2.147	2.063	2.134	2.126	2.653	2.434
2 $d(Sn\text{-}O_2)$	2.115	2.274	2.126	2.066	2.135	2.087	2.611	2.480

Table S6. Singlet→Singlet absorption data in compounds **1** and **2** in the neutral ($\mathbf{A^0}$), basic ($\mathbf{B^-}$), and acid ($\mathbf{C^+}$ and $\mathbf{D^+}$) media considering the solvent effect (Aqueous Solutions, Ɛ=58.5, and refraction=1.33). Where λ_a is the theoretical absorption wavelength (nm), *f* is the oscillator strength, H (HOMO), L (LUMO) and A is the assignment of transitions.

	CAM-B3LYP				B3LYP			
Systems	$^*\lambda_a$	***f***	**Active MOs**	**A**	λ_a	***f***	**Active MOs**	**A**
$\mathbf{1A^0}$	398 (474)*	0.562	H→L	n→π*	527	0.342	H→L	n→π*
	292 (338)*	0.417	H-2→L	π→π*	383	0.464	H-2→L	π→π*
$\mathbf{1B^-}$	427	0.899	H→L	n→π*	566	0.591	H→L	n→π*
	334	0.324	H-2→L	π→π*	370	0.464	H→L+1	n→π*
	307	0.139	H→L+1	n→π*	333	0.155	H-1→L+1	π→π*
$\mathbf{1C^+}$	562	0.417	H→L	n→π*	689	0.193	H→L	n→π*
	445	0.400	H-1→L	π→π*	506	0.617	H-2→L	π→π*
	378	0.783	H-2→L	π→π*	404	0.466	H→L+1	π→π*
$\mathbf{1D^+}$	344	0.675	H→L	n→π*	469	0.294	H→L	n→π*
	305	0.336	H-1→L	π→π*	406	0.336	H-1→L	π→π*
	286	0.145	H-2→L	π→π*	339	0.122	H-2→L	π→π*
$\mathbf{2A^0}$	388 (466)*	0.584	H→L	n→π*	495	0.384	H→L	n→π*
	291 (338)*	0.265	H-2→L	π→π*	368	0.460	H-3→L	π→π*
$\mathbf{2B^-}$	419	0.897	H→L	n→π*	567	0.593	H→L	n→π*
	332	0.348	H-2→L	π→π*	364	0.515	H-2→L	π→π*
	304	0.120	H→L+1	n→π*	334	0.100	H→L+1	n→π*
$\mathbf{2C^+}$	549	0.383	H→L	n→π*	649	0.187	H→L	n→π*
	440	0.474	H-1→L	π→π*	542	0.575	H-1→L	π→π*
	383	0.672	H-2→L	π→π*	320	0.401	H-1→L+1	π→π*
$\mathbf{2D^+}$	341	0.692	H→L	n→π*	447	0.333	H→L	n→π*
	306	0.364	H-1→L	π→π*	399	0.353	H-1→L	π→π*
	285	0.104	H-2→L	π→π*	334	0.131	H→L+1	π→π*

*Experimental absorption wavelength.

Table S7. Singlet→Singlet emission data in compounds **1** and **2** in the neutral (**A⁰**), basic (**B⁻**), and acid (**C⁺** and **D⁺**) media considering the solvent effect (Aqueous Solutions, ε=58.5, and refraction=1.33). Where λ_e is the theoretical emission wavelength (nm), *f* is the oscillator strength, A is the assignment of transitions, $k_{rd,}$ and τ_{rad} are the rate of radiative transfer (s^{-1}) and radiative transfer lifetime (s), respectively.

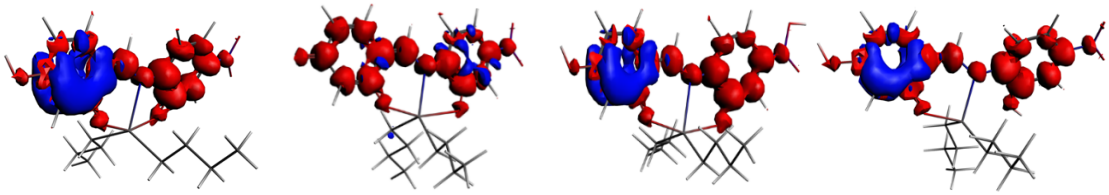
	CAM-B3LYP					B3LYP				
Systems	$^{*}\lambda_e$	***f***	$k_{rad}\,10^8$	$\tau_{rad}\,10^{-9}$	**A**	λ_e	***f***	$k_{rad}\,10^8$	$\tau_{rad}\,10^{-9}$	**A**
1A⁰	447	0.454	2.77	3.60	*π→π	576	0.285	6.85	1.46	*π→π
1B⁻	449	0.661	5.56	1.80	*π→π	778	0.362	1.01	9.85	*π→π
1C⁺	564	0.058	0.22	45.4	*π→π	753	0.068	0.20	48.9	*π→π
1D⁺	417	0.239	2.33	4.28	*π→π	656	0.059	0.53	18.9	*π→π
2A⁰	440	0.414	3.58	2.79	*π→π	566	0.258	1.33	7.33	*π→π
2B⁻	439	0.017	0.01	101.4	*π→π	500	0.013	0.08	117.9	*π→π
2C⁺	549	0.354	2.24	4.64	*π→π	495	0.018	0.01	96.6	*π→π
2D⁺	470	0.581	4.17	2.40	*π→π	444	0.189	1.37	7.29	*π→π

*Experimental emission wavelength is 547 and 532 to **1** and **2**, respectively.

Table S8. Morokuma-Ziegler EDA for all systems in the neutral (**A⁰**), basic (**B⁻**), and acid (**C⁺** and **D⁺**) media. All values are in kcal mol^{-1}.

Molecule	ΔE_{Int}	ΔE_{Pauli}	ΔE_{Disp}	ΔE_{Elec}	ΔE_{Orb}
1A⁰	-8901.7	25537.1	-75.60 (0.2%)	-6450.1 (15.8%)	-34363.3 (84.0%)
1B⁻	-8856.1	25174.1	-74.1 (0.2%)	-6360.0 (15.7%)	-33956.1 (84.1%)
1C⁺	-8846.8	32246.8	-75.8 (0.2%)	-6490.2 (15.8%)	-34527.6 (84.0%)
1D⁺	-8853.2	32264.9	-76.5 (0.2%)	-6496.8 (15.8%)	-34544.8 (84.0%)
2A⁰	-9034.0	35744.0	-82.6 (0.2%)	-7206.0 (16.1%)	-37489.4 (83.7%)
2B⁻	-8994.4	35329.4	-82.2 (0.2%)	-7135.3 (16.1%)	-37106.3 (83.7%)
2C⁺	-8980.2	36039.6	-83.4 (0.2%)	-7267.9 (16.1%)	-37668.4 (83.7%)
2D⁺	-8986.4	36082.4	-84.4 (0.2%)	-7276.7 (16.1%)	-37707.7 (83.7%)

Table S9. Contours of the NOCV deformation density (**ρ**) and the contribution of the interaction to the total orbital interaction (***k***) are presented in kcal mol^{-1} for all systems in the neutral (**A^0**), basic (**B$^-$**) and acid (**C$^+$** and **D$^+$**) media.

Systems	**1A^0**	**1B$^-$**	**1C$^+$**	**1D$^+$**
k_1	-720.9	-729.2	-696.0	-699.0
ρ				
Systems	**1A^0**	**1B$^-$**	**1C$^+$**	**2D$^+$**
k_1	-746.2	-778.5	-737.8	-711.3
ρ