Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 90 (9) S332–S347 (2025) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Dibutyltin(IV) formulations: Synthetic aspect, spectroscopic interpretation and computational calculation

SUCHITRA BUDANIA, ANKUR M KUMAR, POONAM CHAND and ASHA JAIN*

Department of Chemistry, University of Rajasthan, Jaipur-302004, Rajasthan, India

J. Serb. Chem. Soc. 90 (9) (2025) 1041–1054

TABLE S-I. ^{1}H NMR spectral data of dibutyltin(IV) complexes of sterically demanding substituted pyrazolones ($L_{(n)}H$) and mandelic acid (AH) in (δ) ppm

Complex formula	RCO:C(OH)N(C_6H_5)N:CCH_3 ($L_{(n)}H$)				$C_6H_5CH(OH)COOH$ (AH)				Bu_2Sn
	OH	Ring C_6H_5	Ring CH_3	Terminal R (CH_3/ CH_2CH_3/C_6H_5/ p-ClC_6H_4)	COOH	C_6H_5	OH	CH	
$Bu_2SnL_{(1)}A$ (1a)	-	7.17-7.85 (m,10H)	2.36 (s,3H)	2.39 (s,3H)	-	*	3.69 (s,1H)	5.11 (s,1H)	0.70-1.67 (18H)
$Bu_2SnL_{(2)}A$ (1b)	-	7.18-7.89 (m,10H)	2.43 (s,3H)	2.73 (q,2H), ** (3H)	-	*	3.73 (s,1H)	5.13 (s,1H)	0.70-1.68 (18H)
$Bu_2SnL_{(3)}A$ (1c)	-	7.19-7.89 (m,15H)	1.79 (s,3H)	*	-	*	3.64 (s,1H)	5.11 (s,1H)	0.66-1.67 (18H)
$Bu_2SnL_{(4)}A$ (1d)	-	7.19-7.89 (m,14H)	1.82 (s,3H)	*	-	*	3.69 (s,1H)	5.11 (s,1H)	0.70-1.68 (18H)

s(singlet); t(triplet); q(quartet); m(multiplet); *(merge with ring phenyl); **(merge with butyl region); R= -CH_3 ($L_{(1)}H$), -CH_2CH_3 ($L_{(2)}H$), -C_6H_5 ($L_{(3)}H$), p-ClC_6H_4- ($L_{(4)}H$)

* Corresponding author. E-mail: aashajain27@gmail.com

TABLE S-II. ^{13}C NMR spectral data of dibutyltin(IV) complexes of sterically demanding substituted pyrazolones ($L_{(n)}H$) and mandelic acid (AH) in (δ) ppm

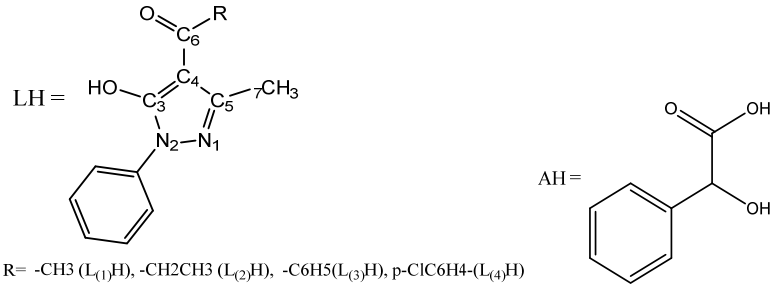
Complex formula.	$RCO:\overset{\frown}{C(OH)N(C_6H_5)N:}CCH_3$ **($L_{(n)}H$)**							$C_6H_5CH(OH)COOH$ **(AH)**			**Bu_2Sn**
	Ring C_6H_5	Terminal R= CH_3/ CH_2CH_3/ C_6H_5/ p-ClC_6H_4	C_3	C_4	C_5	C_6	C_7	COOH	C_6H_5	CH	
$Bu_2SnL_{(1)}A$ (1a)	120.93 - 148.92	27.99	162.01	104.76	138.48	193.15	17.52	179.60	*	73.51	13.42-28.73[ss]
$Bu_2SnL_{(2)}A$ (1b)	120.98 - 148.41	32.85 9.05	162.04	103.97	138.34	196.67	17.35	179.53	*	73.48	13.45-29.76
$Bu_2SnL_{(3)}A$ (1c)	120.92 - 149.35	*	162.60	104.61	139.47	192.42	16.44	179.77	*	73.56	13.40-32.38[ss]
$Bu_2SnL_{(4)}A$ (1d)	120.94 – 148.97	*	162.60	104.65	138.00	190.43	16.65	174.17	*	72.92	13.40-32.38[ss]

*merge with ring phenyl; [ss]splitted signals

TABLE S-III. Mass fragmentation pattern of dibutyltin(IV) complexes **1a-1d**

Fragments	Complex			
	$Bu_2SnL_{(1)}A$ (1a)	$Bu_2SnL_{(2)}A$ (1b)	$Bu_2SnL_{(3)}A$ (1c)	$Bu_2SnL_{(4)}A$ (1d)
$[M]^+$ (%intensity)	599.2868 (L.I.)	613.327 (n.o.)	661.327 (n.o.)	695.7827 (n.o.)
$[M-A]^+$ (%intensity)	449.2868 (100)	463.6000 (16.66)	511.9000 (6.66)	545.6388 (72.72)
$[F1]^+$ (%intensity)		381.7000 (15.55)		
$[F1-F2-CH_3]^+$ (%intensity)	335.0910 (4.61)	340.6000 (33.33)		
$[F1-F2-C_4H_9]^+$ (%intensity)			301.6000 (11.11)	
$[F1-F2-C_4H_9-CH_3]^+$ (%intensity)	279.1437 (37.39)	279.4000 (15.55)	279.4000 (100)	279.3088 (100)
$[F1-F2-2C_4H_9]^+$ (%intensity)	233.1190 (39.13)	231.4000 (30.00)		233.2572 (63.63)
$[SnO_2]^+$ (%intensity)	150.9696 (17.39)	149.2000	149.2000 (6.66)	151.0590 (18.18)
$[C_6H_5CO]^+/[C_6H_5N_2]^+$ (%intensity)		102.1000 (100)	102.1000 (17.77)	

$[M]^+ = [Bu_2SnL_{(n)}A]^+$; A = $C_8H_8O_3$; L.I. = Low Intensity; n.o. = not observed; F1 = M-A-C_6H_5; F2 = $CH_3/CH_2CH_3/C_6H_5/C_6H_4Cl$



R= -CH3 ($L_{(1)}H$), -CH2CH3 ($L_{(2)}H$), -C6H5($L_{(3)}H$), p-ClC6H4-($L_{(4)}H$)

Table S-IV. ^{1}H NMR spectral data of sterically demanding substituted pyrazolones ($L_{(n)}H$) and mandelic acid (AH) in (δ) ppm

Ligand formula	$RCO:C(OH)N(C_6H_5)N:CCH_3$ **($L_{(n)}H$)**				**$C_6H_5CH(OH)COOH$ (AH)**			
	OH	Ring C_6H_5	Ring CH_3	Terminal R (CH_3/ CH_2CH_3/ C_6H_5/ p-ClC_6H_4)	COOH	C_6H_5	OH	CH
AH*					11.81(s)	7.19-7.70(m)	3.50(s)	5.01(s)
$L_{(1)}H$**	11.51(bs)	7.17-7.83 (m)	2.51 (s)	2.45 (s)				
$L_{(2)}H$**	10.67 (bs)	7.23-7.86 (m)	2.39 (s)	2.73(q), 1.21(t)				
$L_{(3)}H$**	12.77 (bs)	7.25-7.93 (m)	2.08 (s)	*				
$L_{(4)}H$**	11.37(bs)	7.26-8.00 (m)	2.14 (s)	*				

*ref. 3;**ref28

Table S-V.[13]C NMR spectral data of sterically demanding substituted pyrazolones ($L_{(n)}H$) and mandelic acid (AH) in (δ) ppm

Ligand formula	$RCO:\overline{C(OH)N(C_6H_5)N:CCH_3}$ **($L_{(n)}H$)**							**$C_6H_5CH(OH)COOH$ (AH)**		
	Ring C_6H_5	Terminal R= CH_3/ CH_2CH_3/ C_6H_5/ p-ClC_6H_4	C_3	C_4	C_5	C_6	C_7	COOH	C_6H_5	CH
AH*								173.33	125.96-136.12	75.12
$L_{(1)}H$**	120.4 - 147.0	26.2	160.4	104.1	137.1	196.2	15.4			
$L_{(2)}H$**	120.40- 147.32	32.29 7.94	160.10	103.27	137.06	197.97	15.48			
$L_{(3)}H$**	120.75 - 147.98	126.69 - 131.90	161.42	103.58	137.56	192.05	15.84			
$L_{(4)}H$**	120.8 – 147.6	126.8 – 138.0	161.1	103.5	138.1	190.9	15.8			

*ref. 3;**ref28

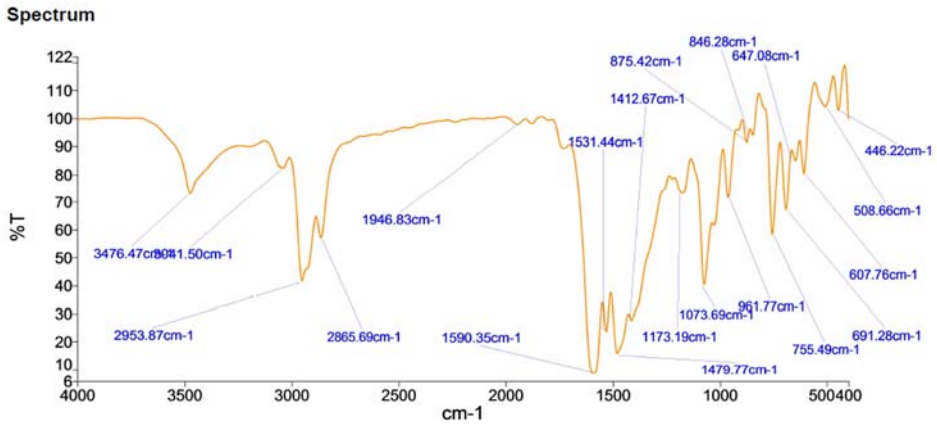


Fig S-1. IR Spectrum - Complex $Bu_2SnL_{(1)}A$(**1a**).

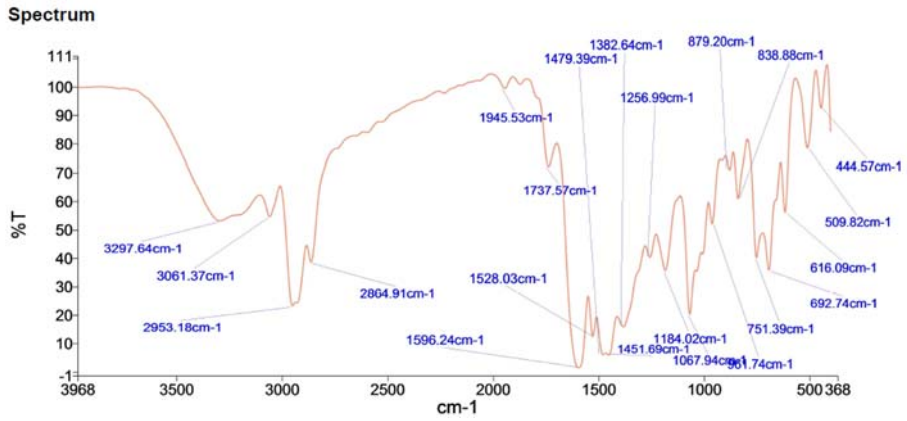


Fig S-2. IR Spectrum - Complex $Bu_2SnL_{(2)}A$ (**1b**).

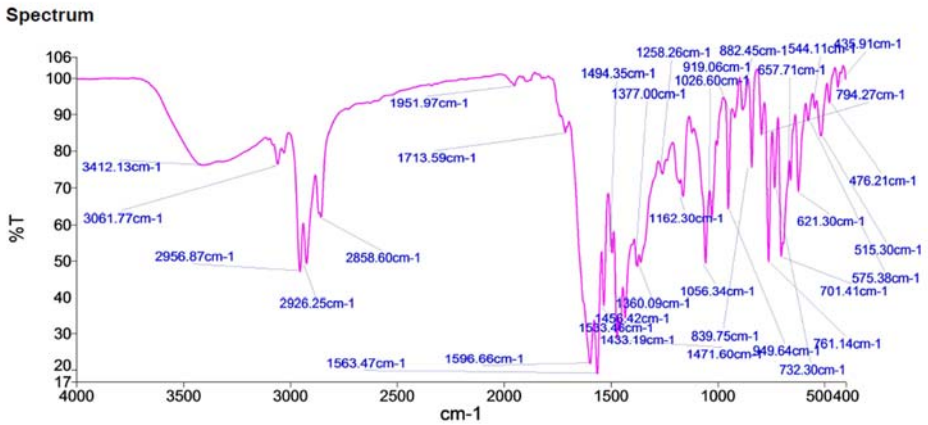


Fig S-3. **IR Spectrum** - Complex $Bu_2SnL_{(3)}A$ (**1c**).

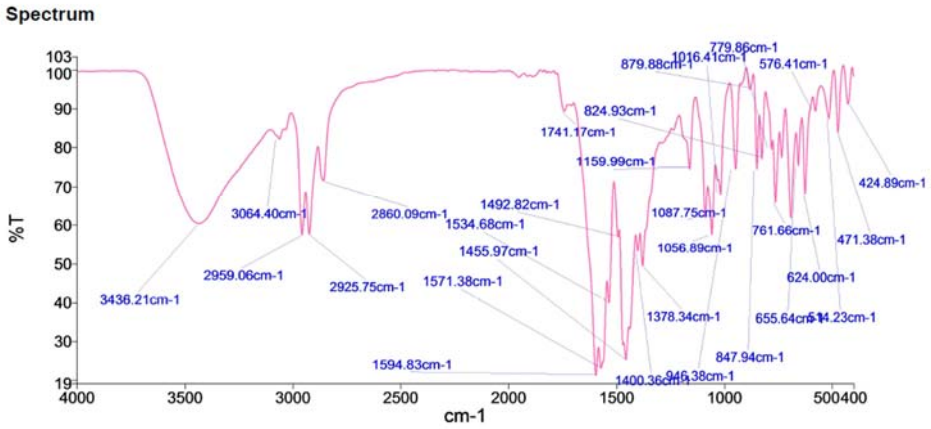


Fig S-4. **IR Spectrum** -Complex $Bu_2SnL_{(4)}A$ (**1d**).

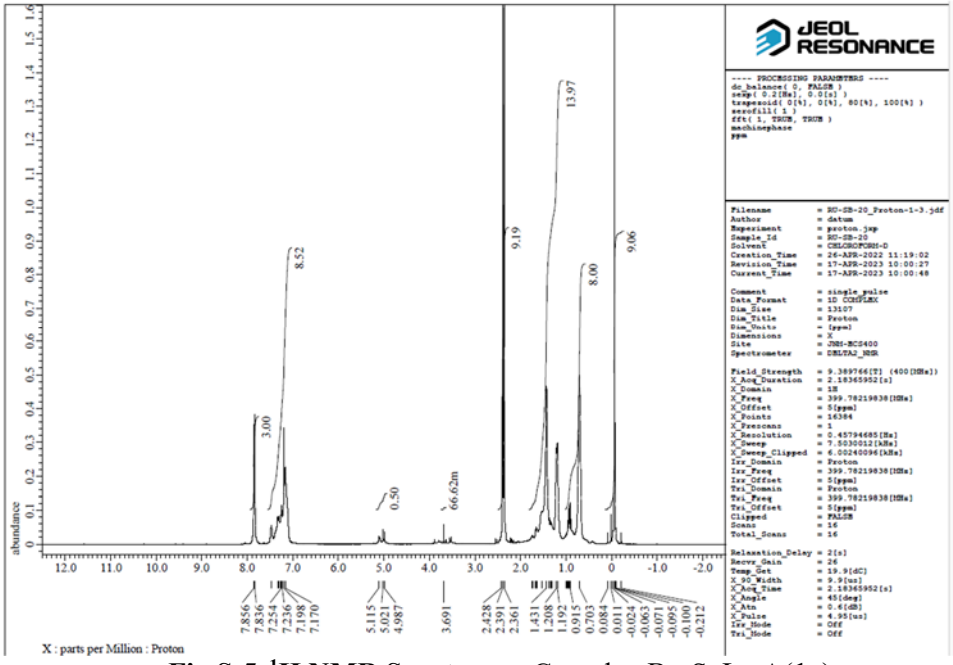


Fig S-5. ^{1}H NMR Spectrum - Complex $Bu_2SnL_{(1)}A$(**1a**).

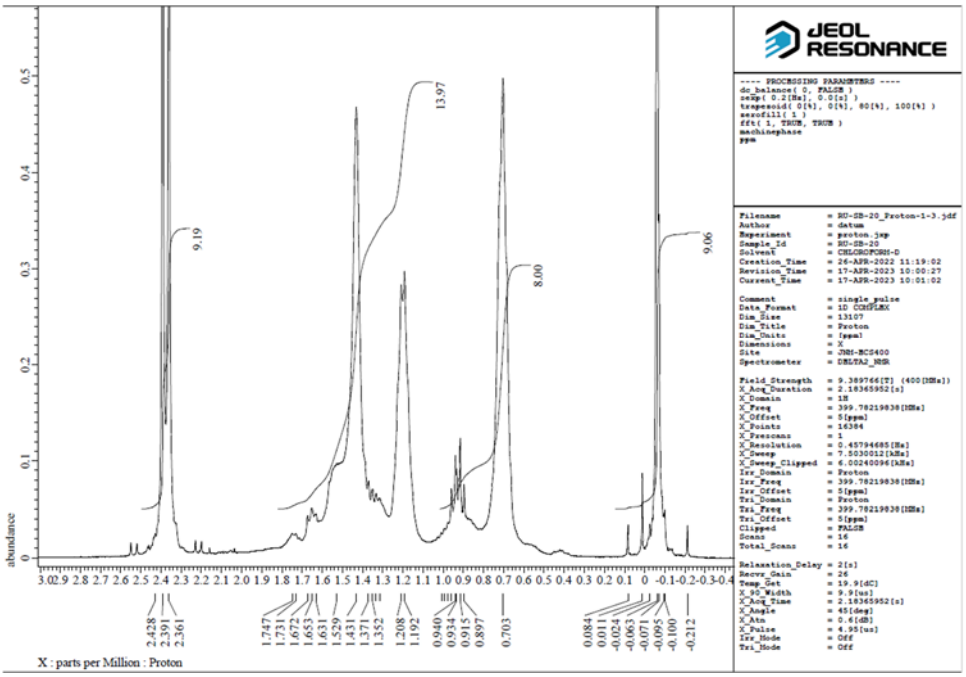


Fig S-6. ^{1}H NMR Spectrum - Complex $Bu_2SnL_{(1)}A$(**1a**) Expanded.

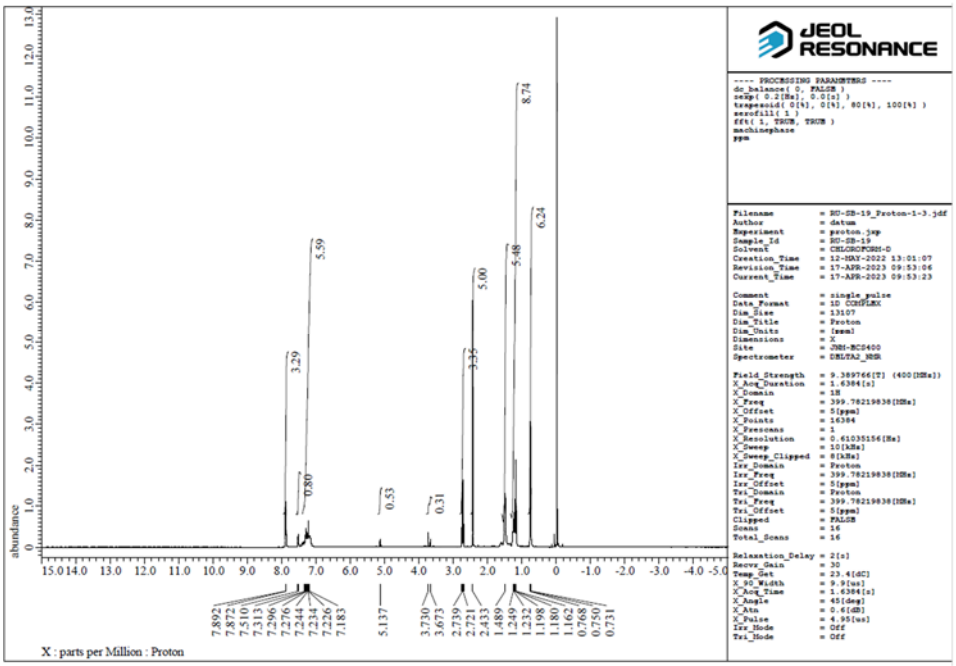


Fig S-7. ^{1}**H NMR Spectrum** - Complex $Bu_2SnL_{(2)}A$ (**1b**).

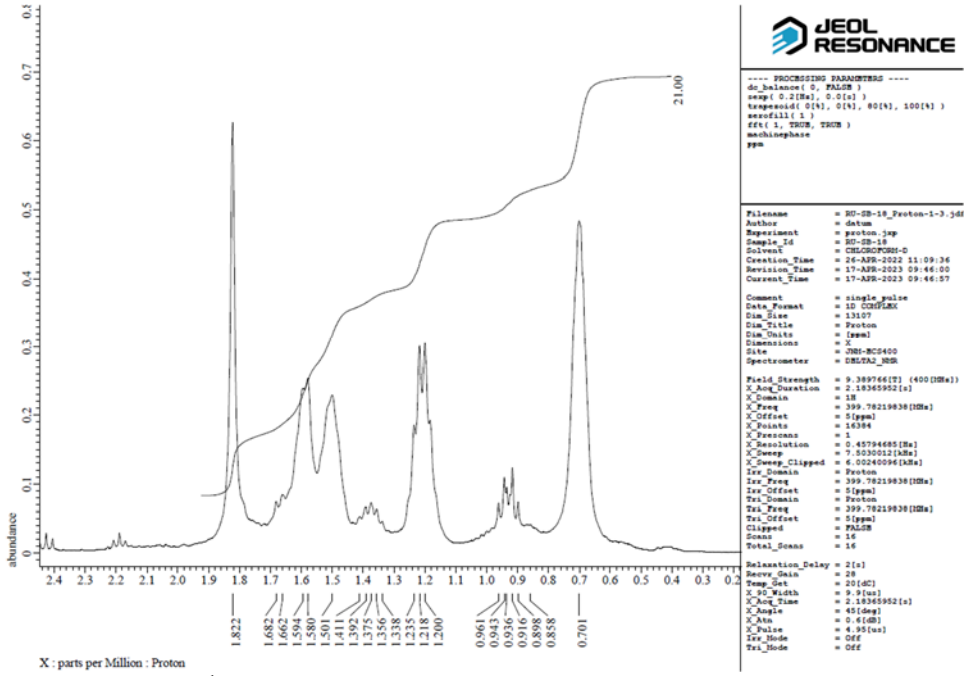


Fig S-8. ^{1}H NMR Spectrum - Complex $Bu_2SnL_{(2)}A$ (**1b**) Expanded.

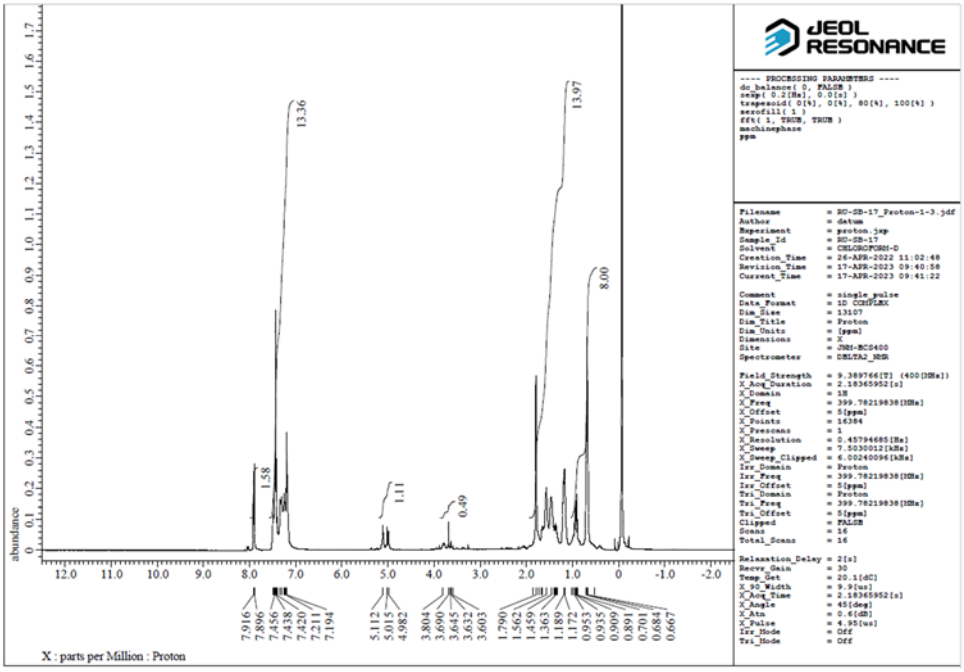


Fig S-9. ^{1}H NMR Spectrum - Complex $Bu_2SnL_{(3)}A$ (**1c**).

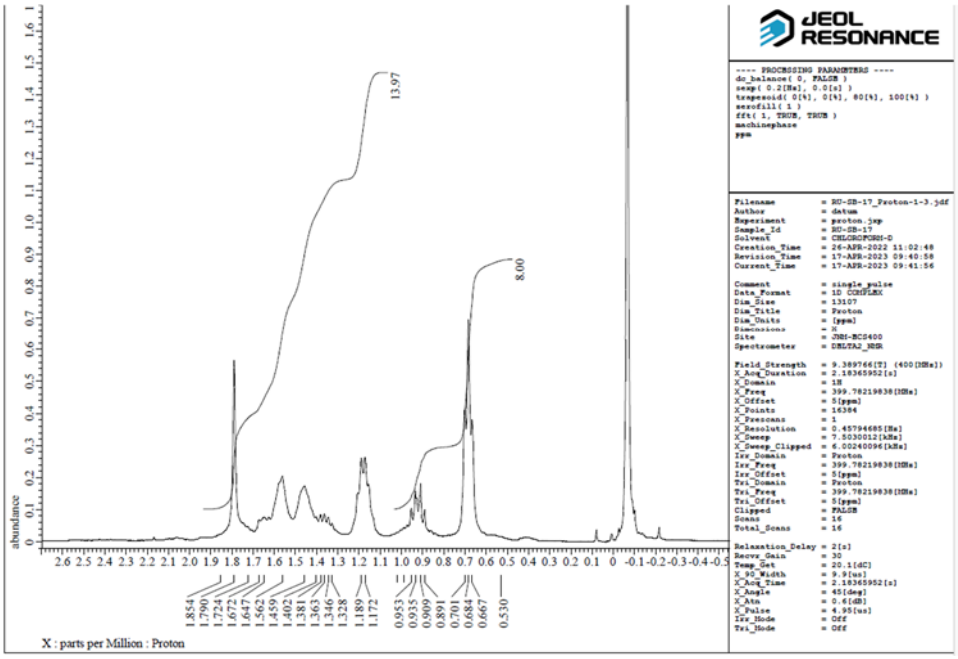


Fig S-10. **^{1}H NMR Spectrum** - Complex $Bu_2SnL_{(3)}A$ (**1c**)Expanded.

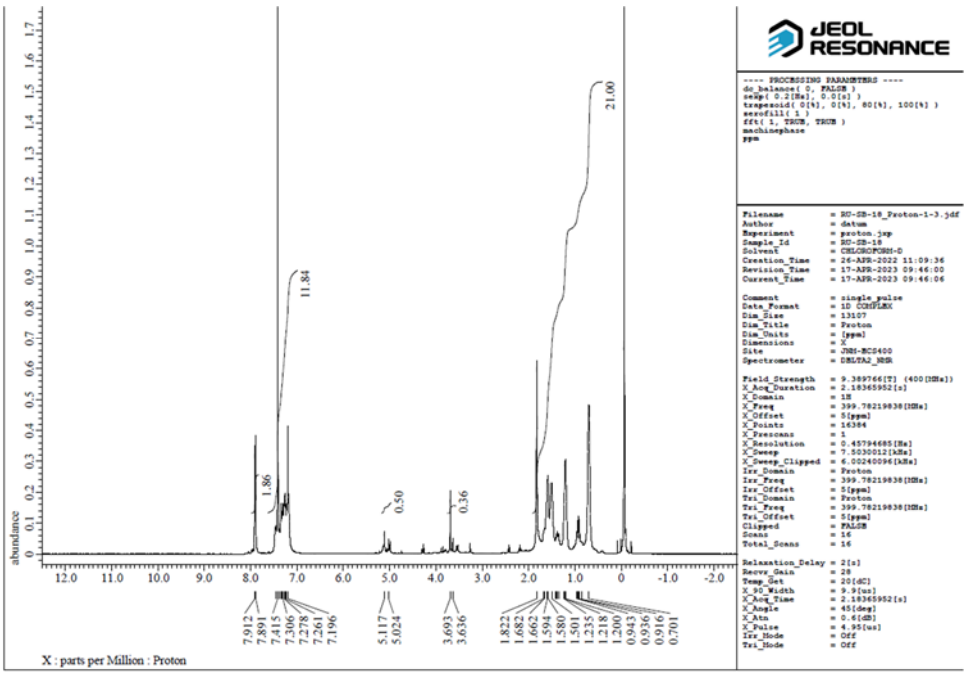


Fig S-11. **^{1}H NMR Spectrum** -Complex $Bu_2SnL_{(4)}A$ (**1d**).

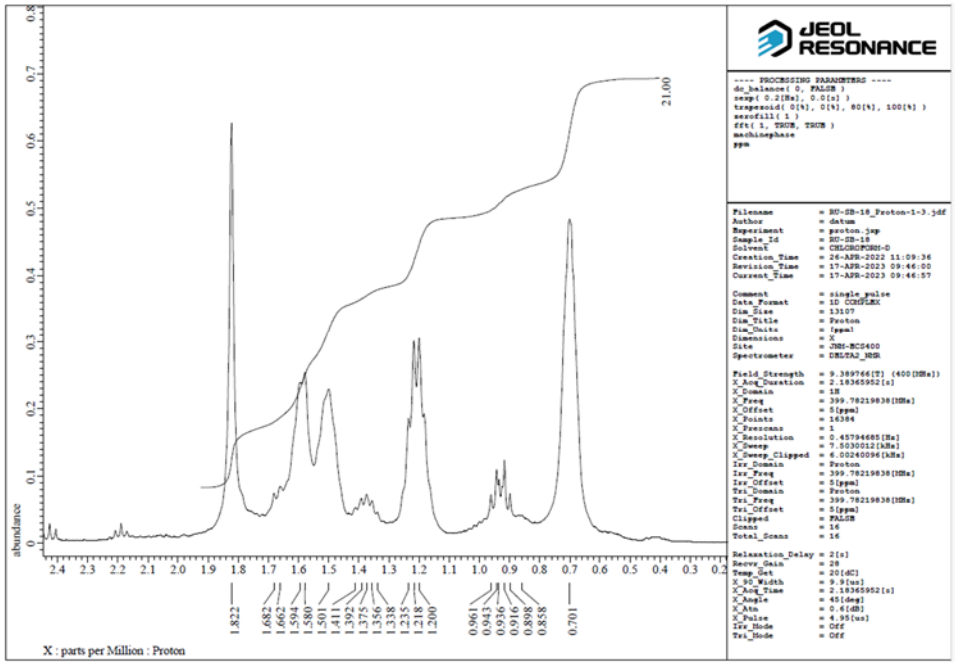


Fig S-12. **^{1}H NMR Spectrum** -Complex $Bu_2SnL_{(4)}A$ (**1d**) Expanded.

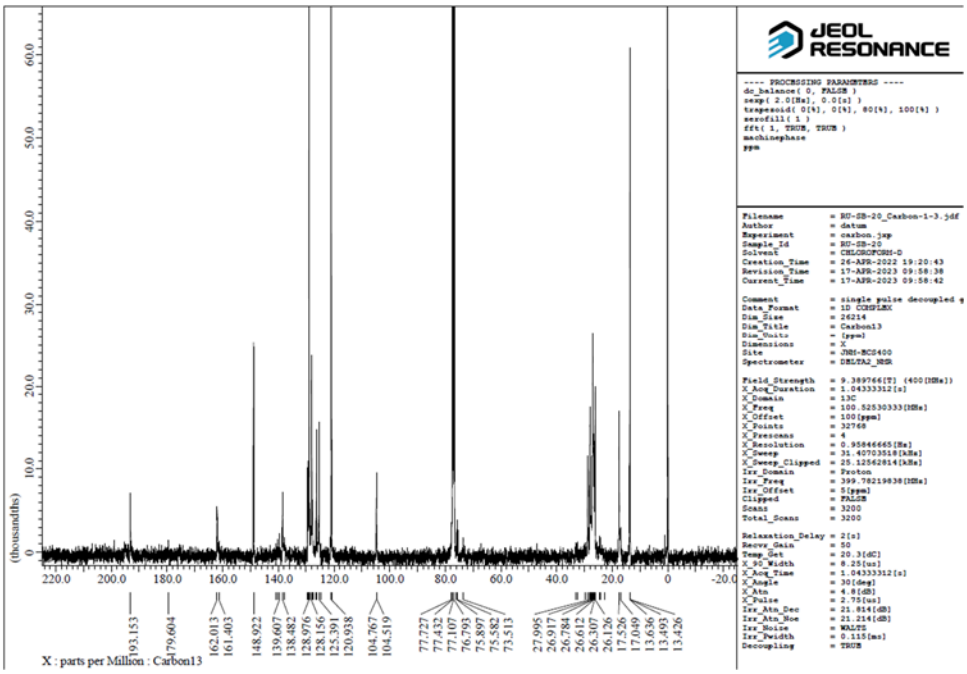


Fig S-13. **^{13}C NMR Spectrum** - Complex $Bu_2SnL_{(1)}A$(**1a**).

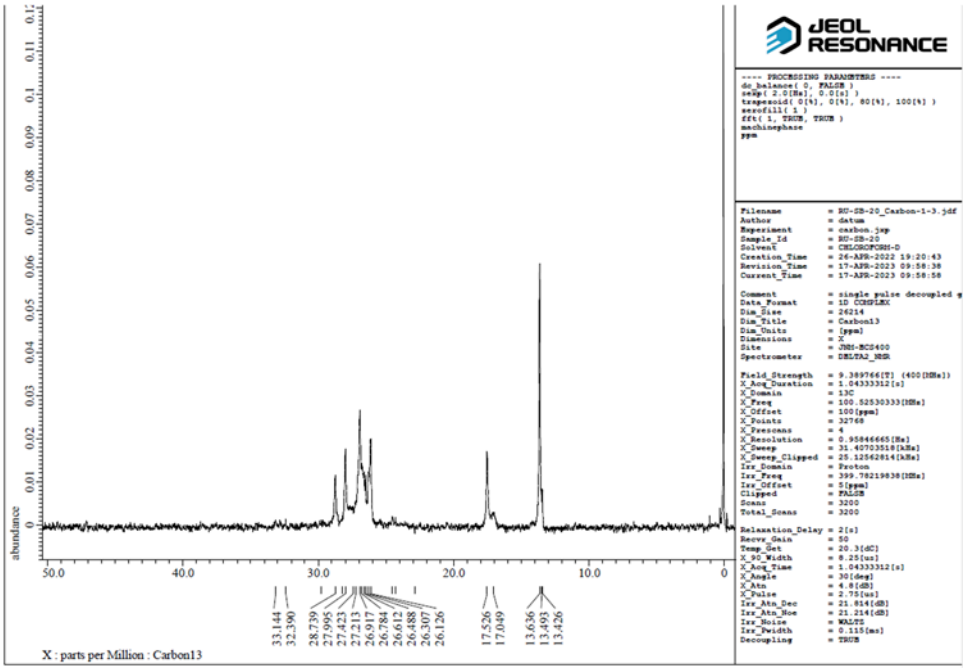


Fig S-14. 13C NMR Spectrum - Complex Bu2SnL(1)A(1a) Expanded.

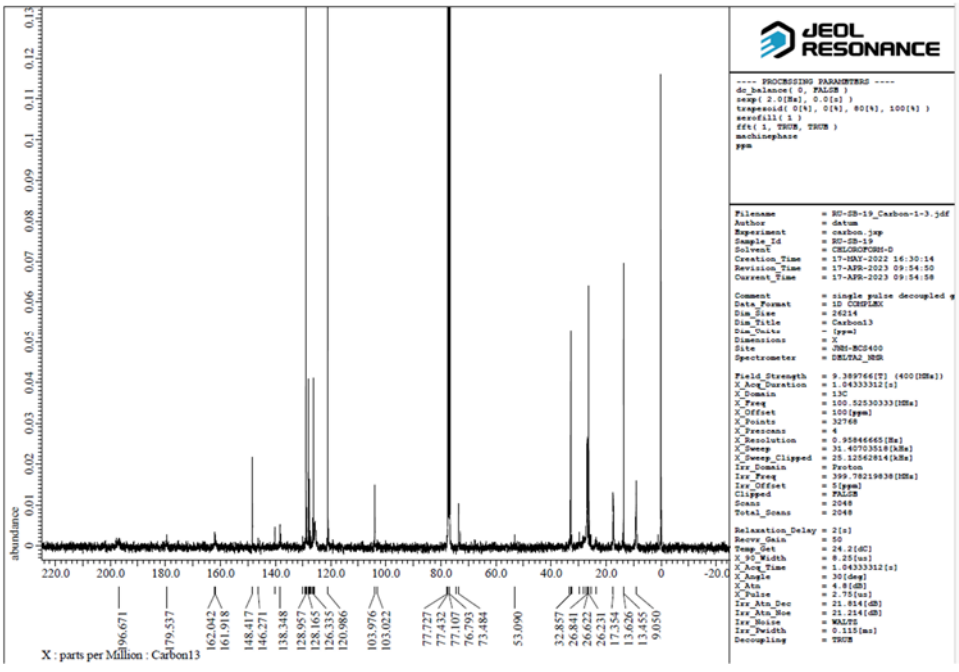


Fig S15. **^{13}C NMR Spectrum** - Complex $Bu_2SnL_{(1)}A$(**1a**) Expanded.

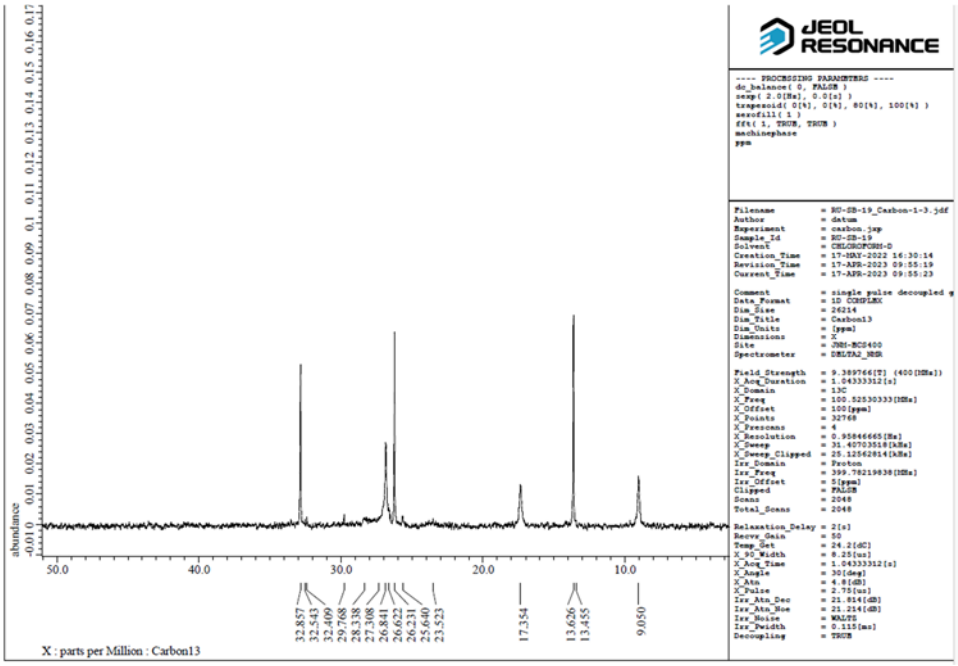


Fig S-16. **^{13}C NMR Spectrum** - Complex $Bu_2SnL_{(2)}A$ (**1b**) Expanded.

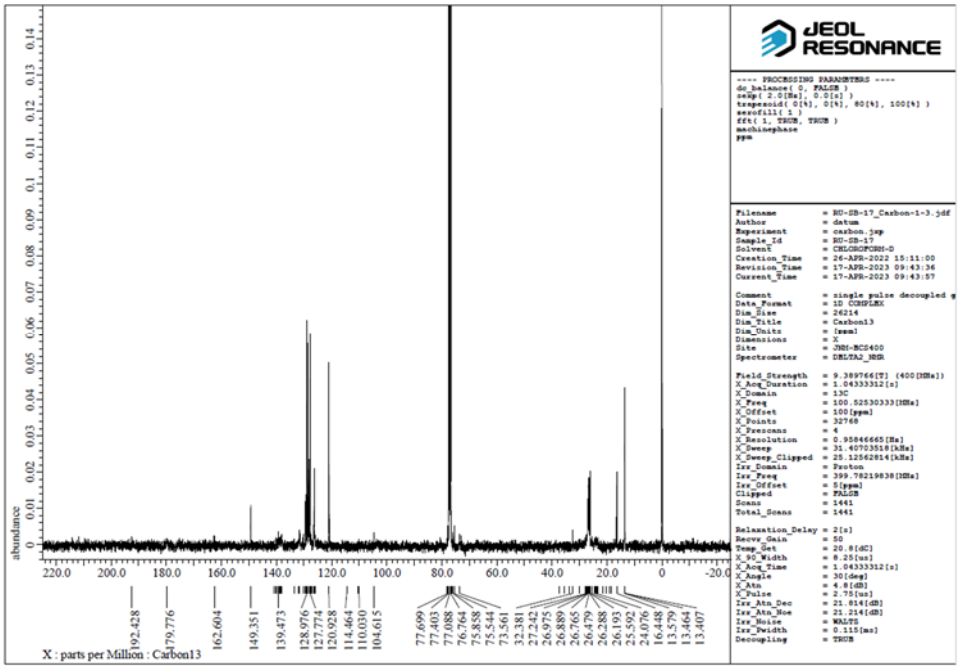


Fig S-17. ^{13}C NMR Spectrum - Complex $Bu_2SnL_{(3)}A$ (**1c**).

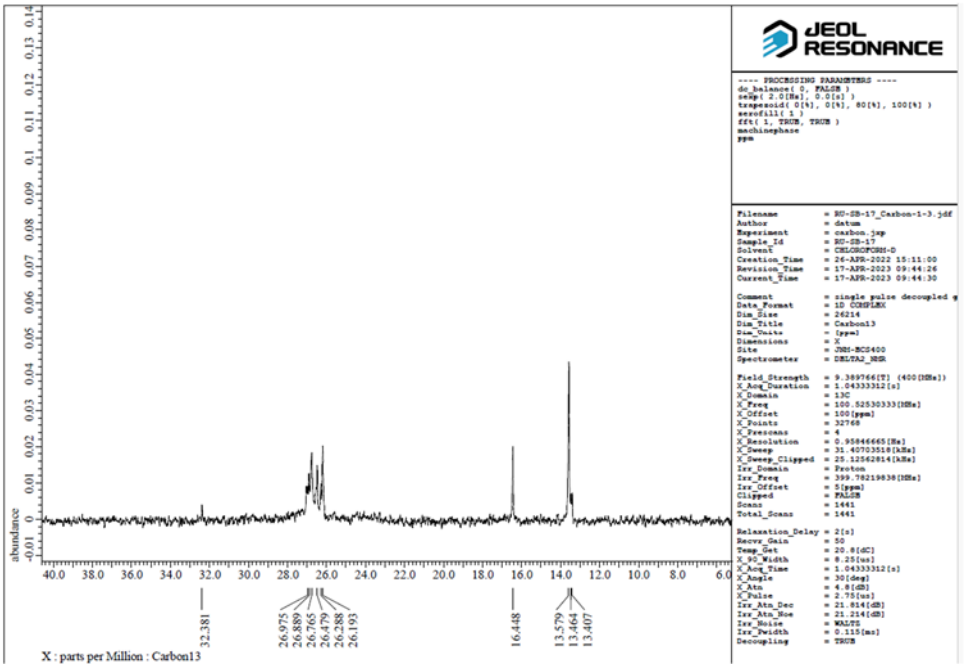


Fig S-18. **^{13}C NMR Spectrum** - Complex $Bu_2SnL_{(3)}A$ (**1c**).

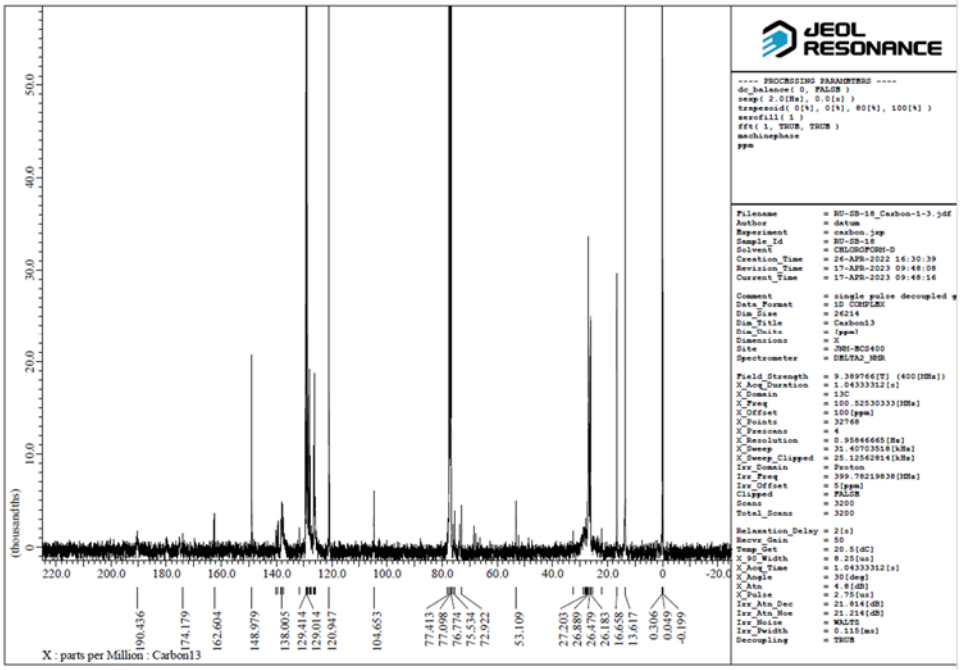


Fig S-19. **^{13}C NMR Spectrum** -Complex $Bu_2SnL_{(4)}A$ (**1d**).

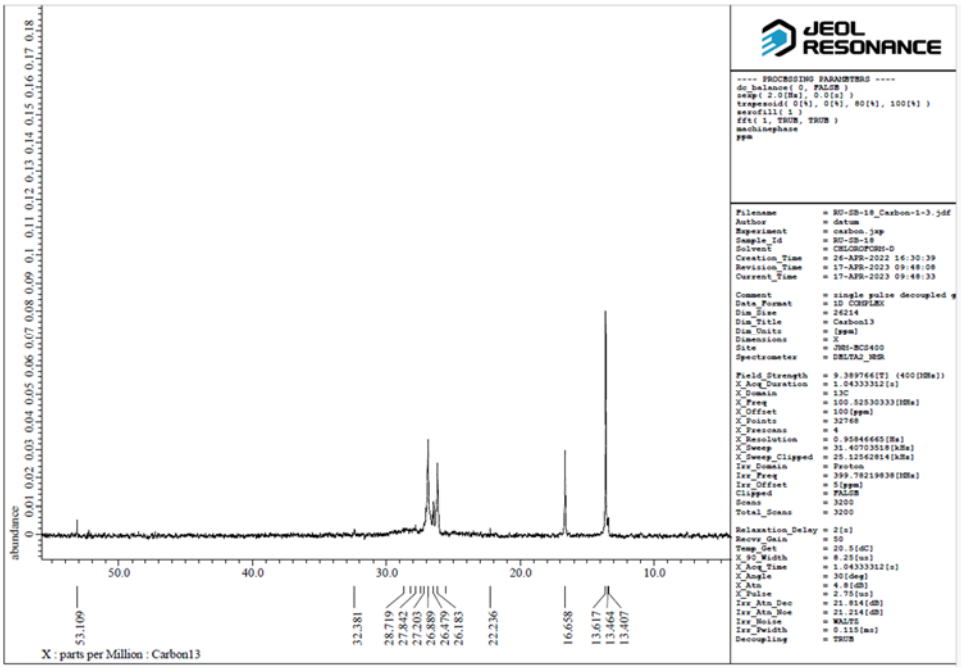


Fig S-20. ^{13}C NMR Spectrum -Complex $Bu_2SnL_{(4)}A$ **(1d)**Expanded.

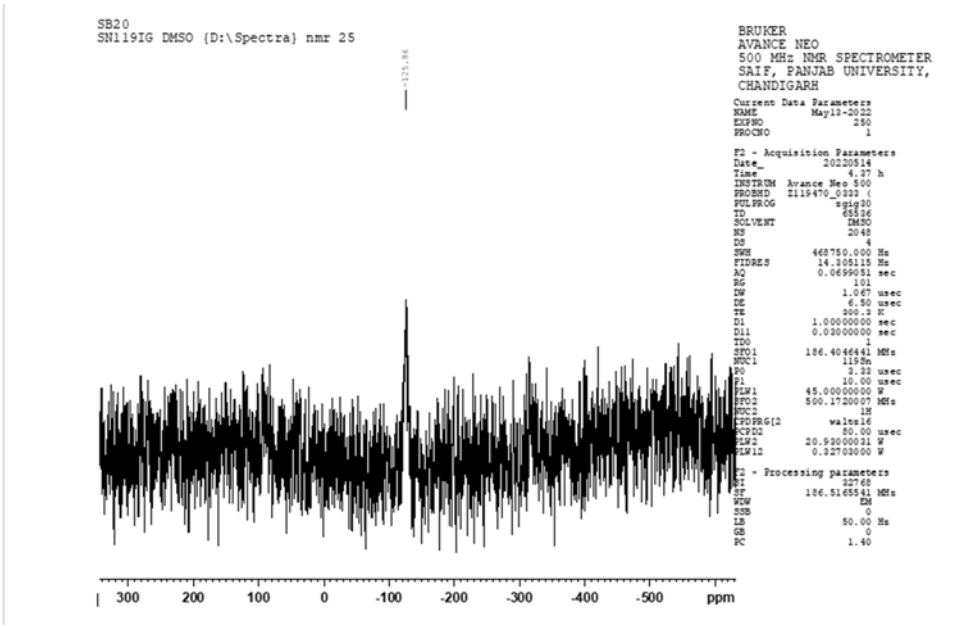


Fig S-21. ^{119}Sn NMR Spectrum - Complex $Bu_2SnL_{(1)}A$(1a).

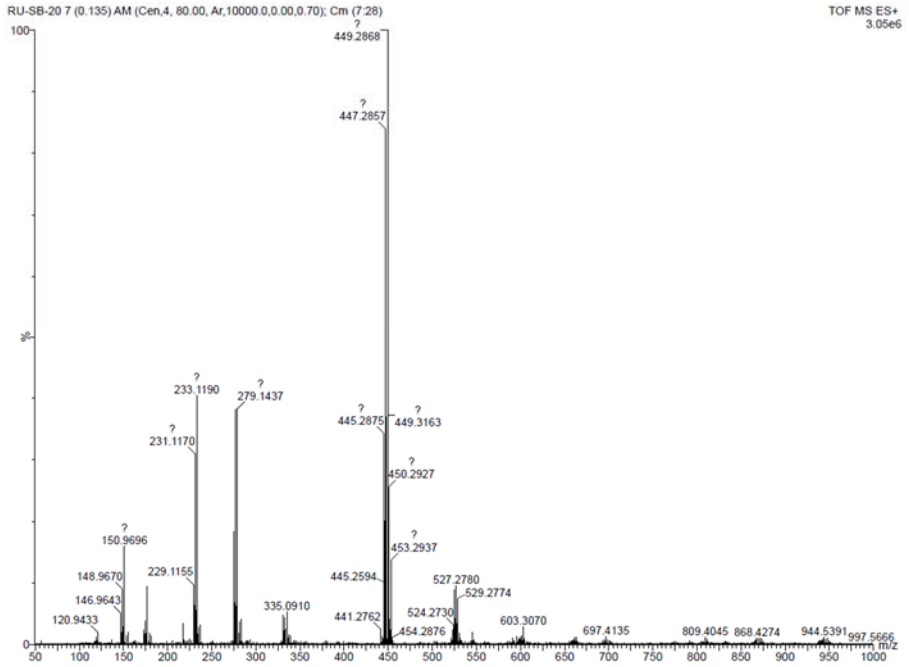


Fig S-22. **Mass Spectrum** - Complex $Bu_2SnL_{(1)}A$(**1a**).

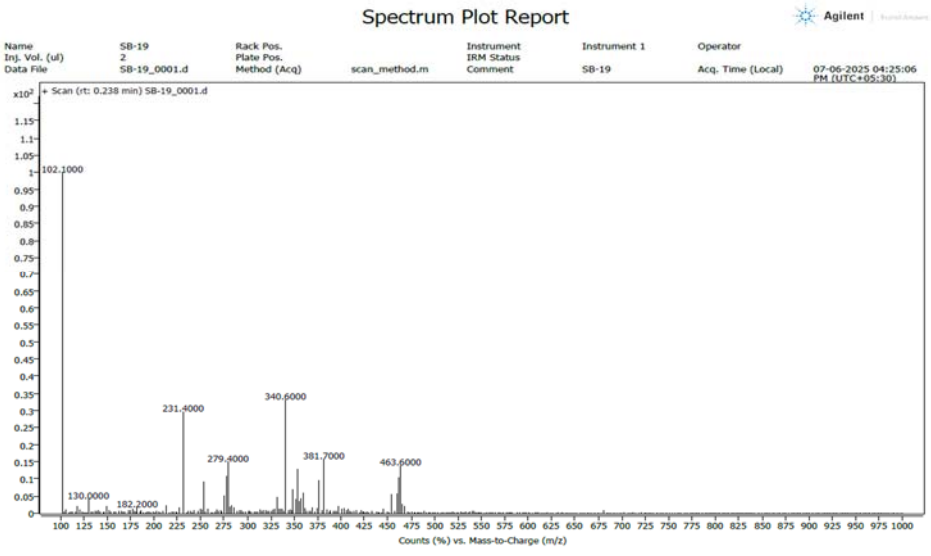


Fig S-23. Mass Spectrum - Complex $Bu_2SnL_{(2)}A$(1b).

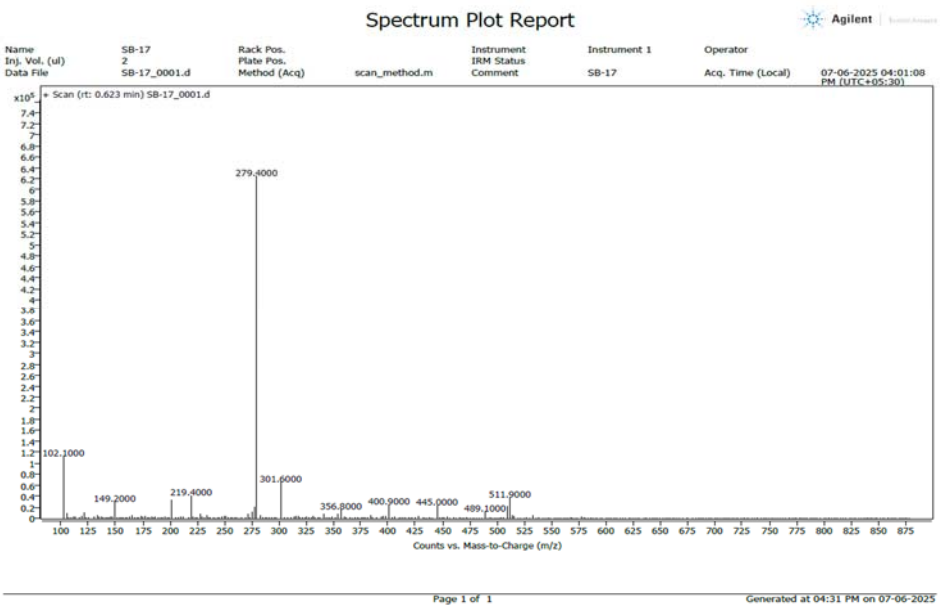


Fig S-24. Mass Spectrum - Complex $Bu_2SnL_{(3)}A$(1c).

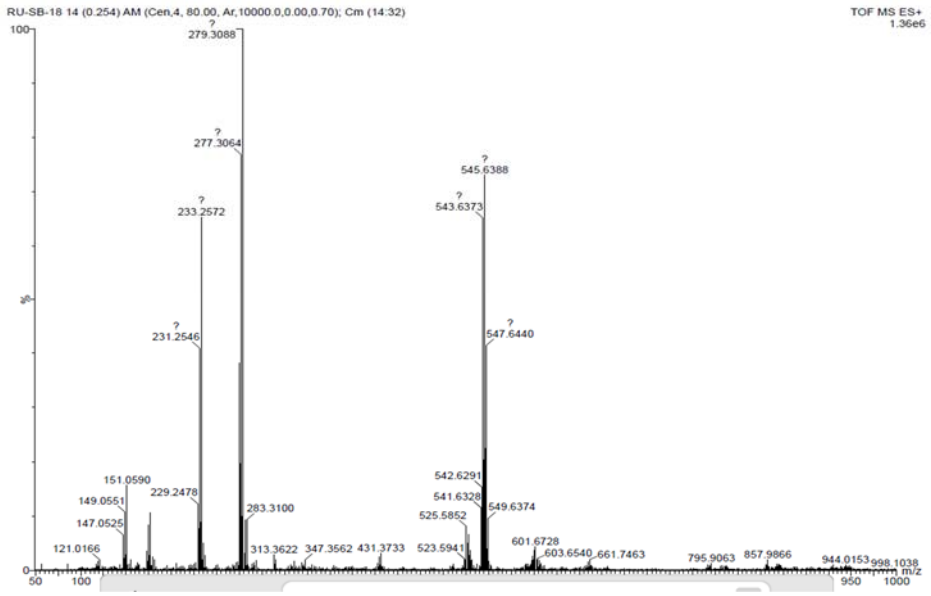


Fig S-25. Mass Spectrum -Complex $Bu_2SnL_{(4)}A$ (1d).