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Synthesis, Characterization and Antifungal Assessment of Optically Active Bis-organotin Compounds Derived from (S)-BINOL Diesters

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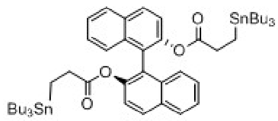
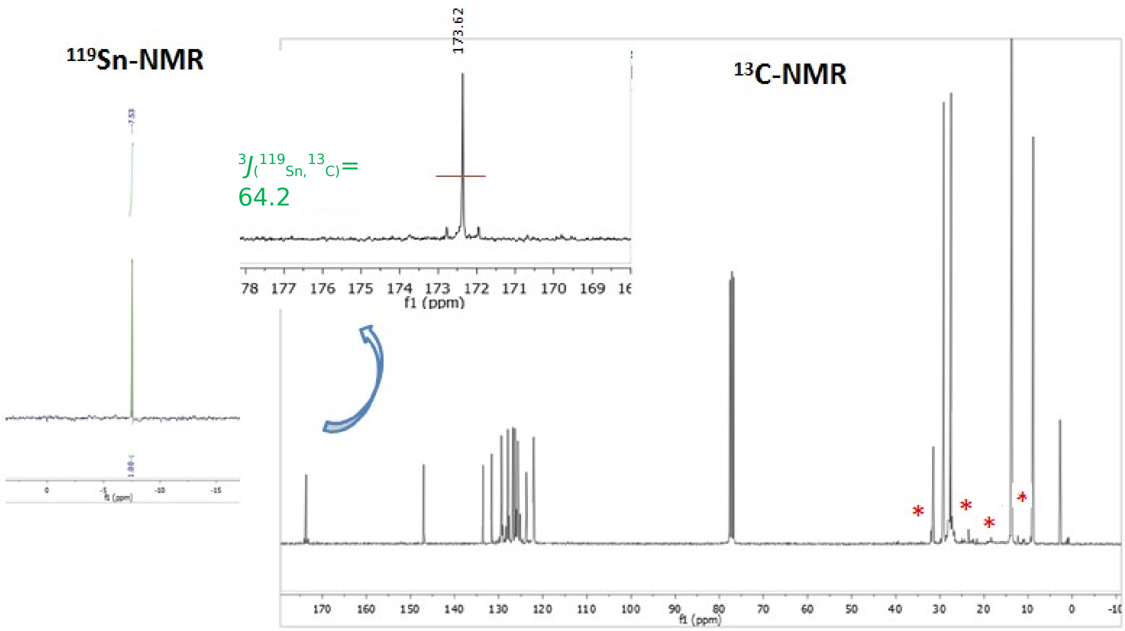
SUPPLEMENTARY MATERIAL

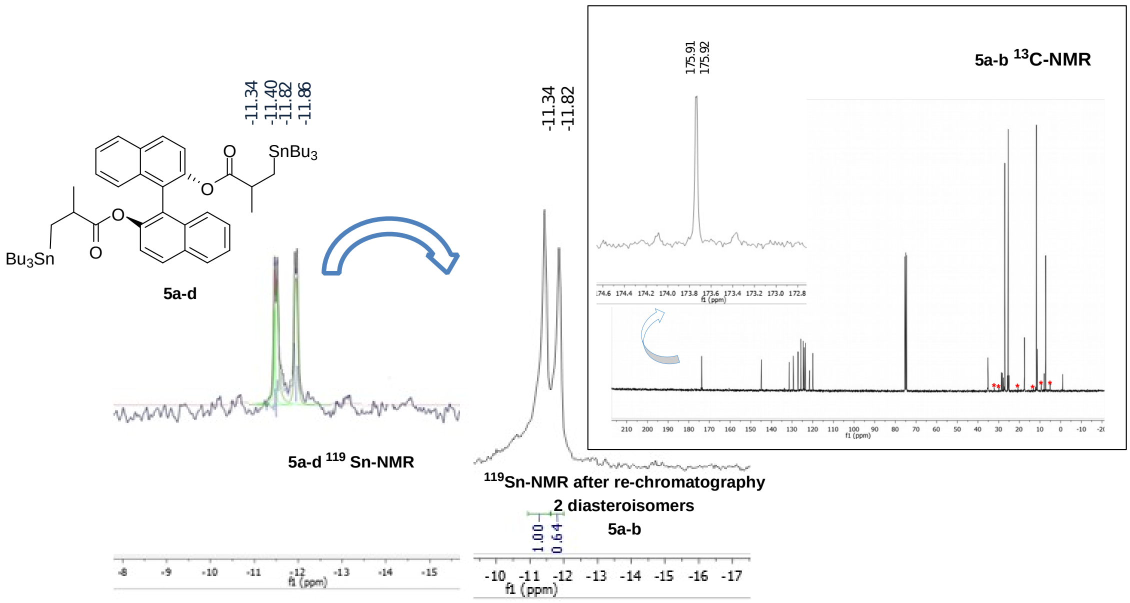


(S)-3



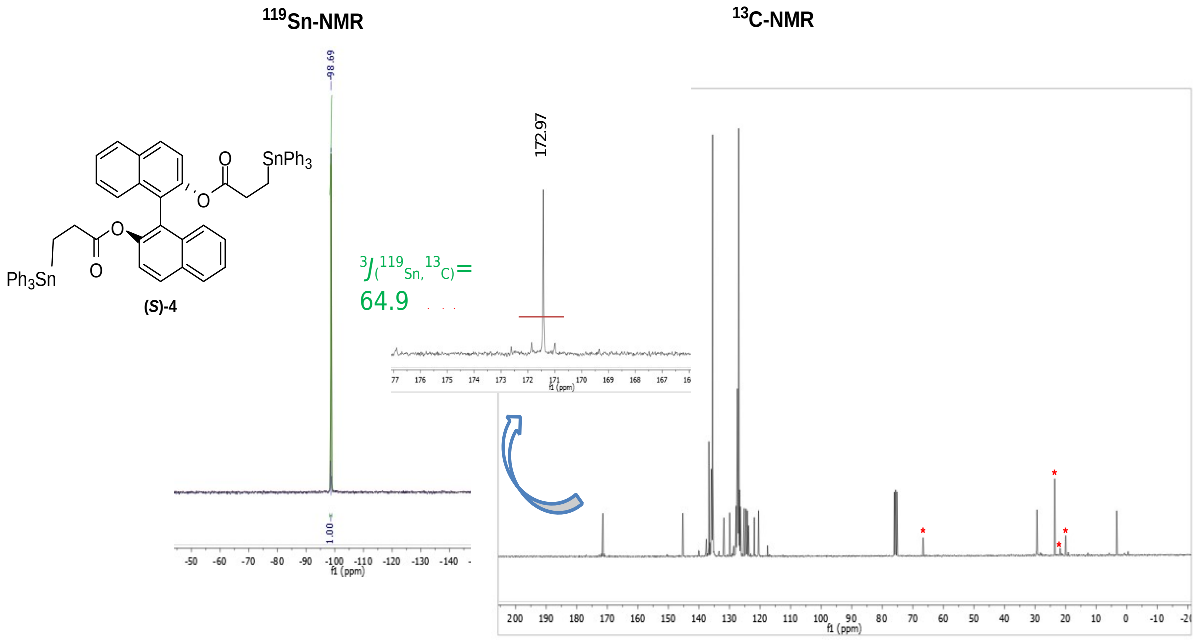
Note: Impurities coming from the solvent are present and marked with *

Fig. (SP1).



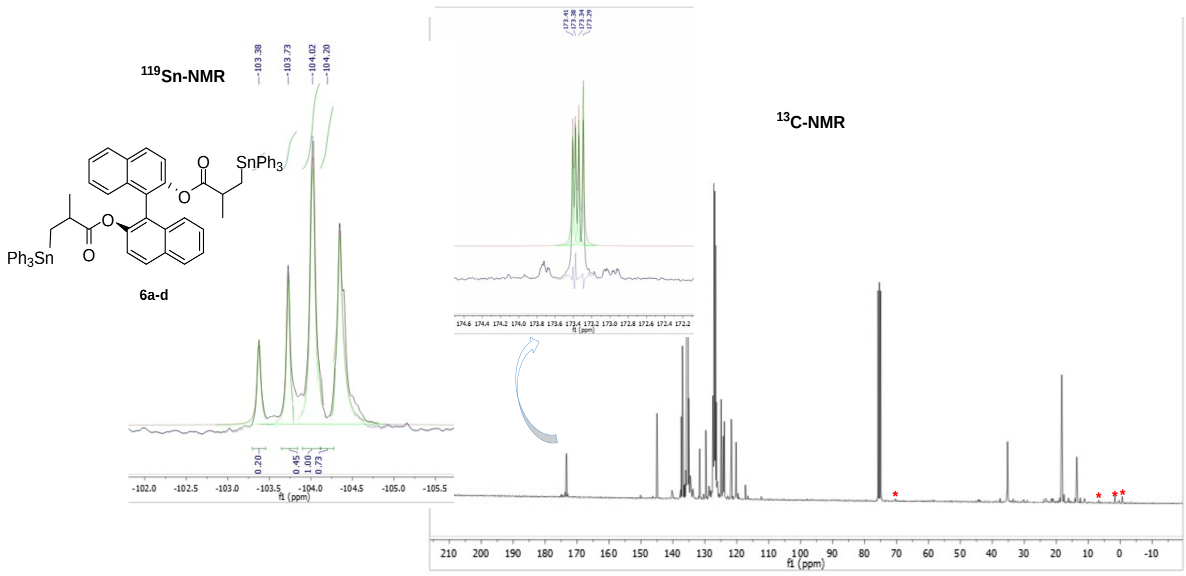
Note: Impurities coming from the solvent are present and marked with *. $^{3}J(^{119}Sn,^{13}C)$ can be observed for the C=O signal.

Fig. (SP2).



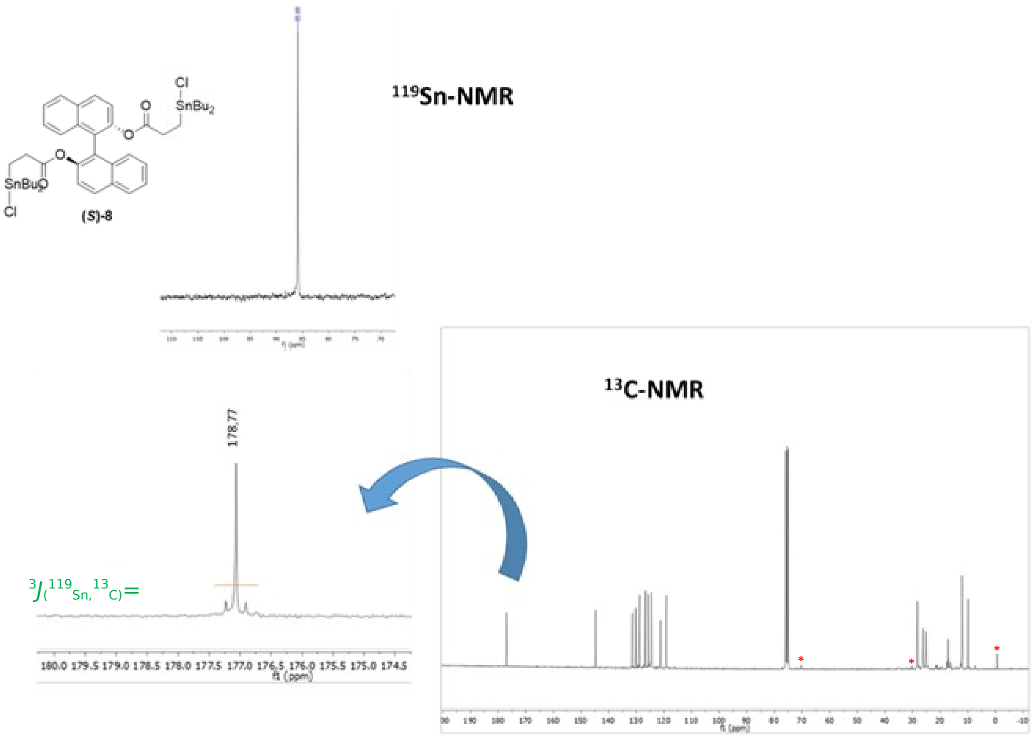
Note: Impurities coming from the solvent are present and marked with *.

Fig. (SP3).



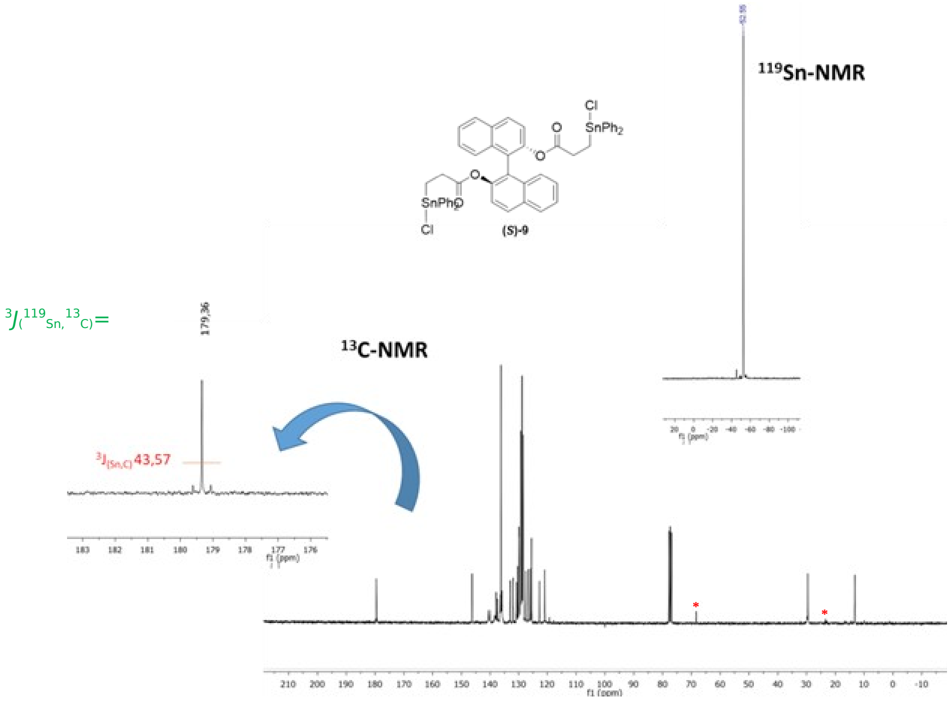
Note: Impurities coming from the solvent are present and marked with *. $^{3}J(^{119}Sn,^{13}C)$ can be observed for the C=O signal.

Fig. (SP4).



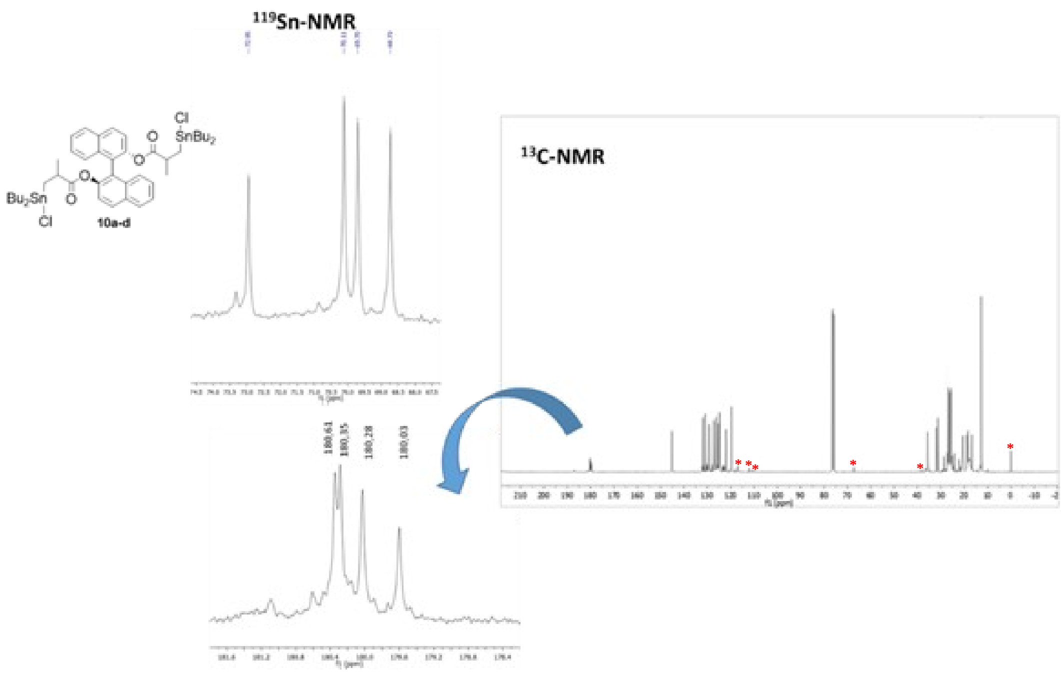
Note: Impurities coming from the solvent are present and marked with *.

Fig. (SP5).



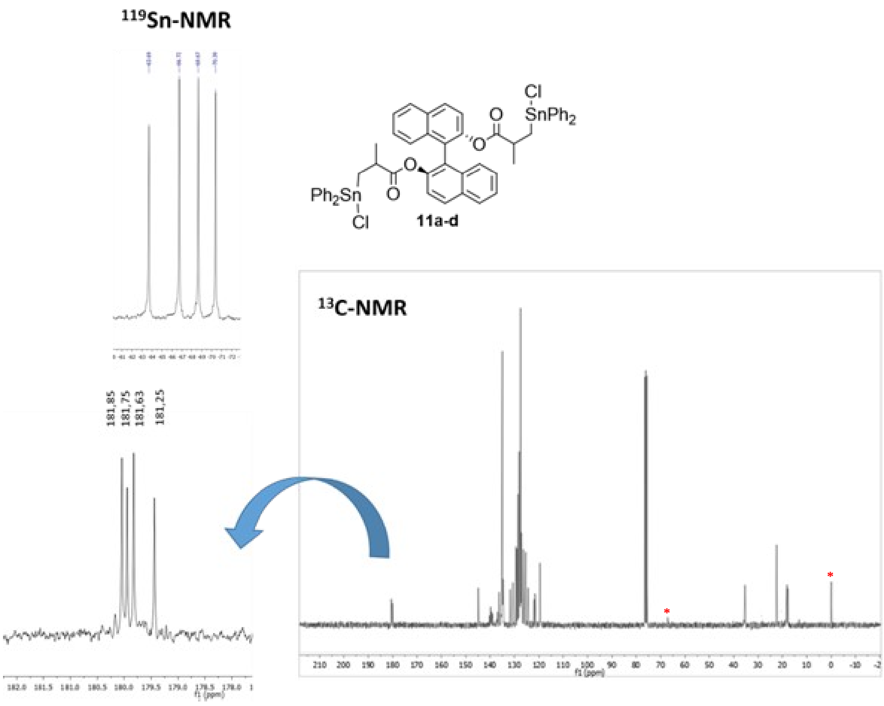
Note: Impurities coming from the solvent are present and marked with *.

Fig. (SP6).



Note: Impurities coming from the solvent are present and marked with *. $^3J(^{119}Sn,^{13}C)$ can be observed for the C=O signal.

Fig. (SP7).



Note: Impurities coming from the solvent are present and marked with *. $^3J(^{119}Sn,^{13}C)$ can be observed for the C=O signal.

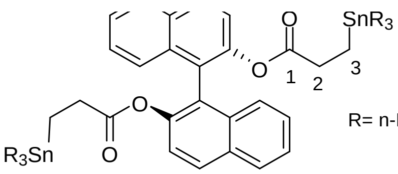
Fig. (SP8).

Table S1. ^{1}H-NMR data for compounds (*S*)-3 and (*S*)-4.

Cpd.	Chemical shift (δ, ppm)[a]
(*S*)-3	0.71-0.88 (30H, m, 6CH$_2$, 6CH$_3$), 0.86-1.00 (12H, m, 6CH$_2$), 1.11-1.31 (12H, m, 6CH$_2$), 1.40 (4H, t $^2J_{(H, Sn)}$= 60.6, Hz, $^3J_{(H,H)}$= 8.71, 2CH$_2$), 2.46 (4H, t, $^3J_{(H, Sn)}$= 11.8, Hz, $^3J_{(H,H)}$= 8.71, 2CH$_2$), 7.03-7.12 (4H, m, Ar-H), 7.15-7.37 (6H, m, Ar-H), 7.77-7.99 (2H, m, Ar-H).
(*S*)-4	1.41 (4H, t $^2J_{(H, Sn)}$= 61.8, Hz, $^3J_{(H,H)}$= 7.42, 2CH$_2$), 2.51 (4H, t, $^3J_{(H,H)}$= 7.42, 2CH$_2$), 7.23 (2H, $^3J_{(H,H)}$= 8.9 Hz, Ar-H), 7.36-7.45 (4H, m, Ar-H), 7,46-7.58 (20H, m, Ar-H), 7.62-7.65 (12H, m, Ar-H), 7.97-8.00 (4H, m, Ar-H).

[a] In CDCl$_3$; chemical shift, δ, in ppm relative to TMS; ^nJ couppling constant in Hz (in brackets); multiplicity (in brackets): s = singlet, d= doublet, t= triplet, m= multiplet.

Table S2. ^{13}C-NMR data for compounds (*S*)-3 and (*S*)-4.



R= n-Bu (**(*S*)-3**); Ph (**(*S*)-4**)

Cpd.	Chemical shift (δ, ppm)[a]			
	C$_1$ $^3J_{(Sn,C)}$	C$_2$ $^2J_{(Sn,C)}$	C$_3$ $^1J_{(Sn,C)}$	Other signals
(*S*)-3	173.62 (64.2)	31.17 (16.4)	2.72 (468.8)	8.83 (323.2), 13.80, 27.39(56.3), 29.14(19.5), 110.82, 117.76, 124.04, 124.20, 127.48, 128.41, 129.45, 131.43, 133.39, 151.74
(*S*)-4	171.42 (64.9)	29.34 (18.4)	5.02 (390.1)	122.03, 123.44, 125.35, 125.72, 126.13, 126.74, 128.54, 128.85, 128.97, 129.06, 131.48, 133.36, 137.06 (35.3), 137.48, 138.28 (504.5), 146.81

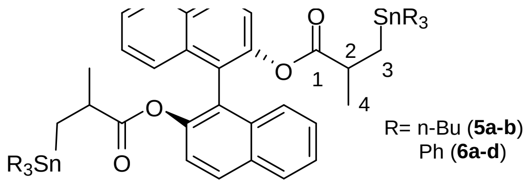
[a] In CDCl$_3$; chemical shift, δ, in ppm relative to TMS; $^nJ(^{119}Sn,^{13}C)$ coupling constant in Hz (in brackets).

Table S3. ^{1}H-NMR data for compounds 5a-b and 6a-d.

Cpd.	Chemical shifts (δ, ppm)[a]
5a-b	0.46 (8H, dd, $^3J_{(H,H)}$= 6.9 Hz, $^2J_{(H,H)}$= 2.3 Hz, 4CH$_2$), 0.60-0.67 (24H, m, 12CH$_2$), 0.81 (36H, t, $^3J_{(H,H)}$= 7.3 Hz, 12CH$_3$), 1.11-1.22 (36H, m, 4CH$_3$, 12CH$_2$), 1.23-1.33 (24H, m, 12CH$_2$), 2.23-2.42 (4H, m, 4CH), 7.21-4.23 (8H, m, Ar-H), 7.28-7.42 (8H, m, Ar-H), 7.77-7.93 (8H, m, Ar-H).
6a-d	0.42-0.60 (24H, m, 8CH$_3$), 0.84-1.08 (16H, m, 8CH$_2$), 2.39-2.66 (8H, m, 8CH), 6.92-7.12 (16H, m, Ar-H), 7.38-7.55 (64H, m, Ar-H), 7.59-7.70 (56H, m, Ar-H), 7.84-7.93 (32H, m, Ar-H)

[a] In CDCl$_3$; chemical shift, δ, in ppm relative to TMS; ^nJ coupling constant in Hz (in brackets); multiplicity (in brackets): s = singlett, d= doublet, t= triplet, m= multiplet.

Table S4. ^{13}C-NMR data for compounds 5a-b and 6a-d.



Cpd.	Chemical shifts (δ, ppm)[a]				
	C$_1$ $^3J_{(Sn,C)}$ [b]	C$_2$ $^2J_{(Sn,C)}$ [b]	C$_3$ $^1J_{(Sn,C)}$ [b]	C$_4$ $^3J_{(Sn,C)}$ [b]	Other signals
5a-b	175.91 175.92	37.30 (23.6) 37.33 (20.2)	9.39 (309.9) 9.41 (323.6)	19.73 (22.8)	12.27 (281.5), 13.84, 27.32 (55.5), 29.20 (17.0), 122.11, 123.81, 123.83, 125.70, 126.27, 126.76, 127.93,129.30, 129.34, 131.59, 131.61, 133.56,133.60, 147.02
6a-d	173.29 173.34 173.38 173.41	35.34 35.29 35.27 35.23	13.72 13.70 13.62 13.59	18.29	120.22, 120.25, 120.29, 120.31,121.72, 121.75, 123.90, 123.94, 124.25,124.26, 124.36, 124.90, 124.92, 126.13,126.18, 126.41, 126.39, 126.74, 126.94,126.99, 127.06, 127.11, 127.13, 129.68,129.71, 129.73, 131.54, 131.56, 131.61,131.62, 153.33, 135.71,136.98, 137.01, 137.03, 137.36,144.95, 144.09, 145.01

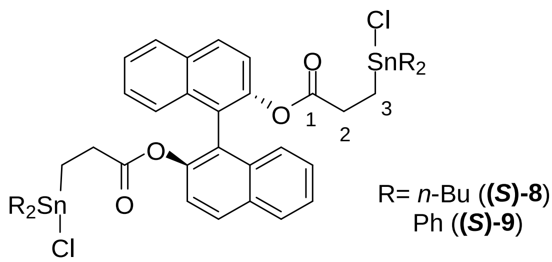
[a] In CDCl$_3$; chemical shift, δ, in ppm relative to TMS; $^nJ(^{119}Sn,^{13}C)$ coupling constant in Hz (in brackets); [b] Overlapping signals for **6a-d**.

Table S5. ^{1}H-NMR data for (*S*)-8 and (S)-9.

Cpd.	Chemical Shift (δ, ppm)[a]
(*S*)-8	0.77 (4H, dd, $^3J_{(H,H)}$= 7.3 Hz, 2 x CH$_2$), 0.83 (4H, dd, $^3J_{(H,H)}$= 7.3 Hz, 2 x CH$_2$), 1.06-1.39 (20H, m, 4 x CH$_3$, 4 x CH$_2$), 1.43-4.56 (8H, m, 4 x CH$_2$), 2.22-2.33 (4H, m, 2 x CH$_2$), 2.49-2.60 (4H, m, 2 x CH$_2$), 7.02-7.33 (6H, m, Ar-H), 7.43 (2H, dt, $^3J_{(H,H)}$= 8.2 Hz, $^4J_{(H,H)}$= 1.8 Hz, Ar-H), 7.89 (2H, d, $^3J_{(H,H)}$= 8.2 Hz, Ar-H), 7.43 (2H, d, $^3J_{(H,H)}$= 8.2 Hz, Ar-H),
(*S*)-9	1.26-1.30 (2H, m, CH$_2$), 1.30-1.40 (2H, m, CH$_2$), 2.16-2.28 (4H, m, 2 x CH$_2$), 6.83-7.07 (8H, m, Ar-H), 7.21-7.42 (20H, m, Ar-H), 7.82-7.89 (4H, m, Ar-H)

[a] In CDCl$_3$; chemical shift, δ, in ppm relative to TMS; ^nJ couppling constant in Hz (in brackets); multiplicity (in brackets): d= doublet, dd= double doublet, dt= double triplet, t= triplet, m= multiplet.

Table S6. ^{13}C-NMR data for (*S*)-8 and (S)-9.



Cpd.	Chemical Shift (δ, ppm)[a]			
	C$_1$ $^3J_{(Sn,C)}$	C$_2$ $^2J_{(Sn,C)}$	C$_3$ $^1J_{(Sn,C)}$	Other signs
(*S*)-8	178.77 (24.4)	29.96 (27.2)	11.59 (388.6)	13.81, 18.11 (647.0), 18.80, 26.88 (85.1), 27.86 (41.1), 120.83, 123.06, 126.24, 126.46, 127.40, 128.39, 130.48, 131.92, 133.06, 146.34

Cpd.	Chemical Shift (δ, ppm)[a]			
	C_1 $^3J_{(Sn,C)}$	C_2 $^2J_{(Sn,C)}$	C_3 $^1J_{(Sn,C)}$	Other signs
(*S*)-9	179.36 (43.6)	29.38 (32.8)	13.04 (513.0)	120.72, 122.57, 125.30, 125.64, 126.38, 127.31, 128.22, 128.58, 129.10, 129.17, 129.65, 130.14, 130.49, 131.66, 132.723, 136.11 (45.3), 146.13

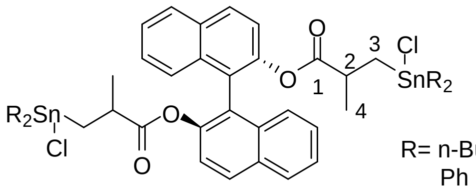
[a] In $CDCl_3$; chemical shift, δ, in ppm relative to TMS; $^nJ(^{119}Sn,^{13}C)$ coupling constant in Hz (in brackets);

Tabla S7. ^{1}H-NMR data for 10a-d and 11a-d.

Cpd.	Chemical Shift (δ, ppm)[a]
10a-d	0.18 (6H, d, $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.30 (6H, d $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.59 (6H, d $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.76-0.91 (22H, m, 2CH_3, 4 x 2CH_2), 1.04-1.84 (144H, m, 4 x 12CH_2, 4 x 4CH_3), 2.37-2.91 (8H,m, 4 x 2CH), 7.04-7.32 (24H, m, Ar-H), 7.40-7.45 (8H, m, Ar-H); 7.86-7.97 (16H, m, Ar-H)
11a-d	0.04 (6H, d, $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.19 (6H, d, $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.28 (6H, d, $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.44 (6H, d, $^3J_{(H,H)}$= 7.2 Hz, 2 x CH_3), 0.89-1.34 (16H, m, 4 x 2CH_2), 2.32-2.78 (8H, m, 4 x 2CH), 6.61-7.22 (112H, m, Ar-H), 7.78-7.88 (16H, m, Ar-H)

[a] In $CDCl_3$; chemical shift, δ in ppm relative to TMS; ^nJ coupling constant in Hz (in brackets); multiplicity (in brackets): d= doublet, t= triplet, m= multiplet.

Table S8. ^{13}C-NMR data for 10a-d and 11a-d.



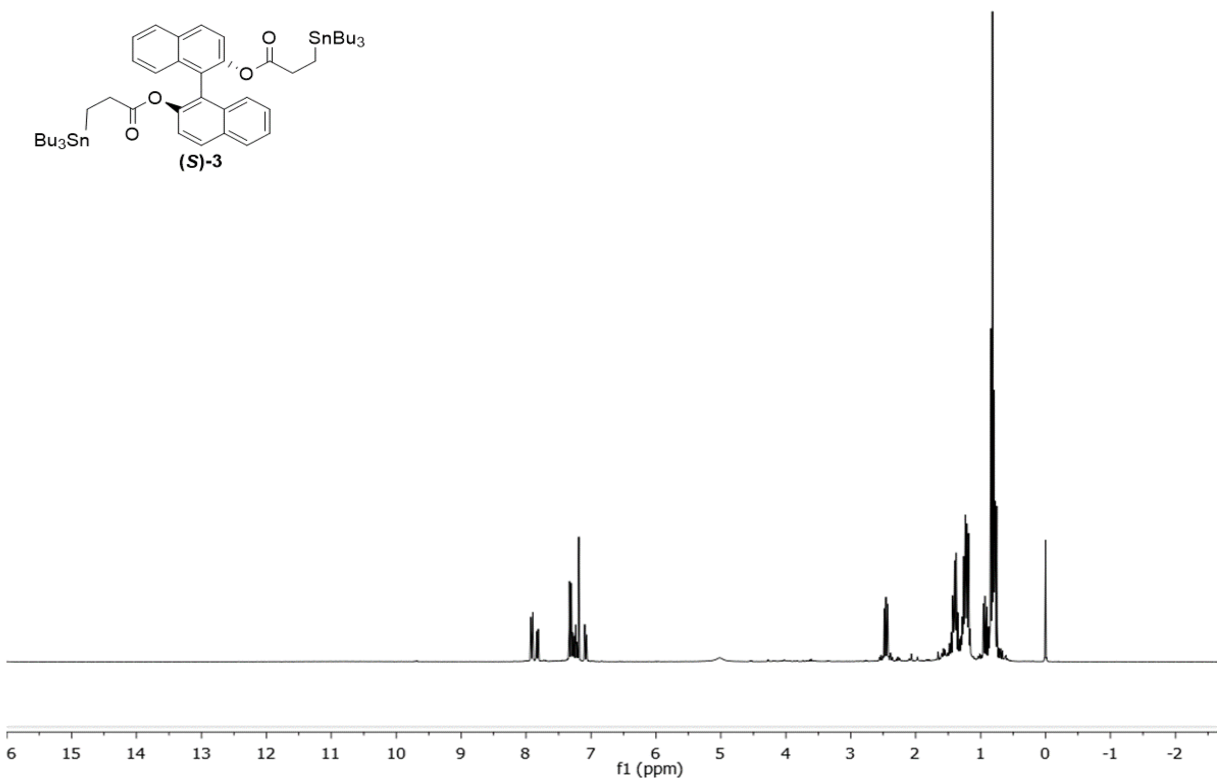
Cpd.	Chemical Shift (δ, ppm)[a]				
	C_1 $^3J_{(Sn,C)}$[b]	C_2 $^2J_{(Sn,C)}$[b]	C_3 $^1J_{(Sn,C)}$[b]	C_4 $^3J_{(Sn,C)}$[c]	Other signs
10a-d	180.03 180.28 180.35 180.61	35.55 35.62 35.66 35.74	20.55 20.56 20.73 20.85	18.33 18.63 18.90 19.00	12.68, 25.43, 25.57, 26.08, 26.28, 31.27, 31.87, 119.65, 121.97, 124.74, 125.32, 126.22, 127.20, 129.07, 130.71, 131.82, 145.12
11a-d	181.25 181.63 181.75 181.85	36.45 36.53 36.60 36.73	23.32 23.40	18.78 19.08 19.18 19.32	118.77, 118.93, 119.00, 120.74, 120.94, 121.28, 123.60, 123.71, 123.78, 123.83, 124.63, 124.73, 124.78, 125.60, 125.70, 126.81, 127.42, 127.85, 128.26, 128.75, 129.91, 129.99, 130.11, 130.99, 131.01, 131.08, 134.41, 144.20, 144.29, 144.31, 144.36

[a] In $CDCl_3$; chemical shift, δ, in ppm relative to TMS; [b] Overlapping signals for **11a-d**; [c] Not

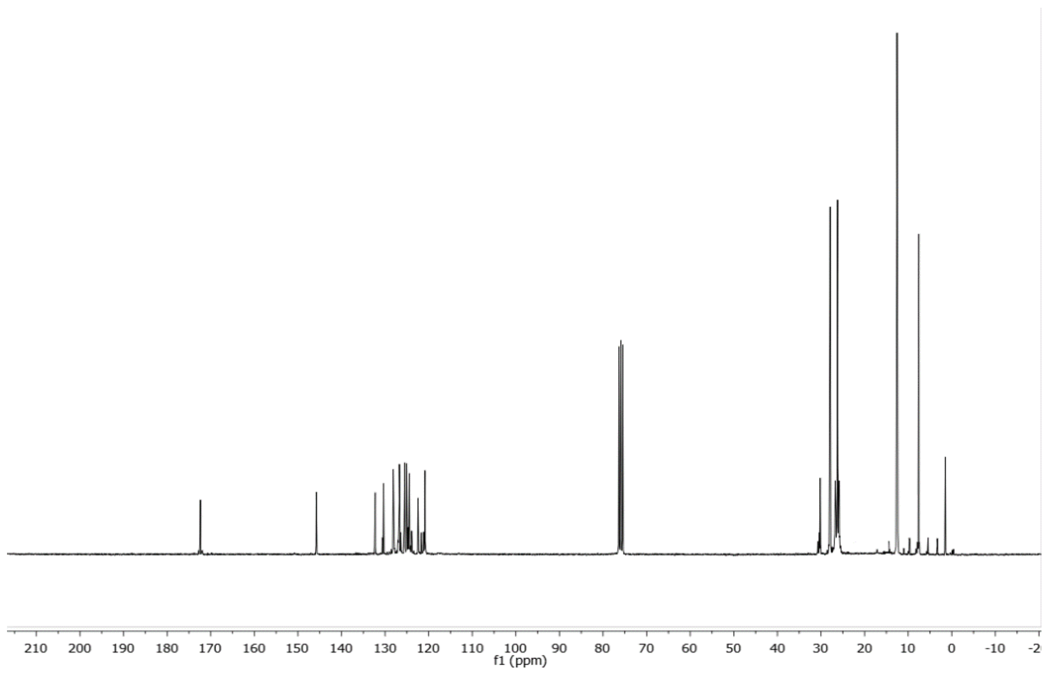
NMR-spectra of new products

(*S*)-1,1'-binaphthalene-2,2'-diyl-bis[3-(tri-*n*-buthylestannyl)propanoate] (*S*)-3

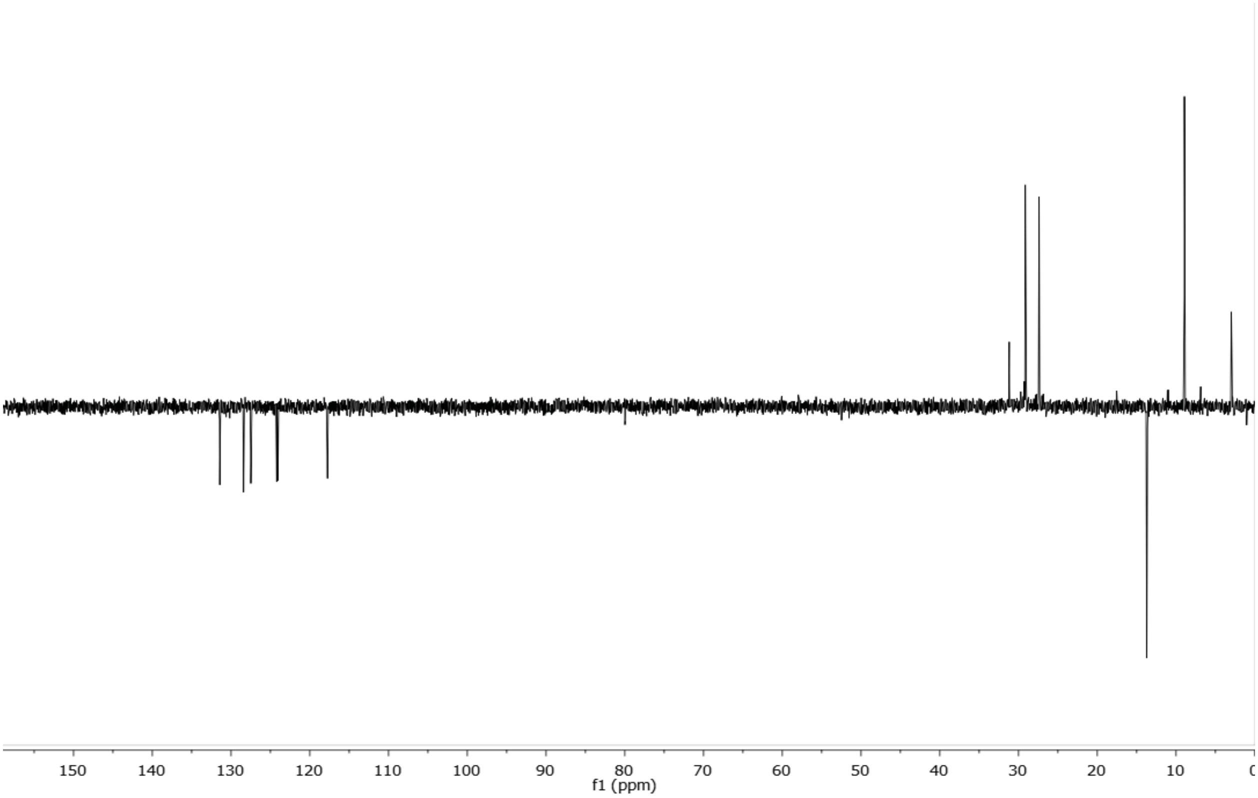
^{1}H-NMR (300MHz, $CDCl_3$)



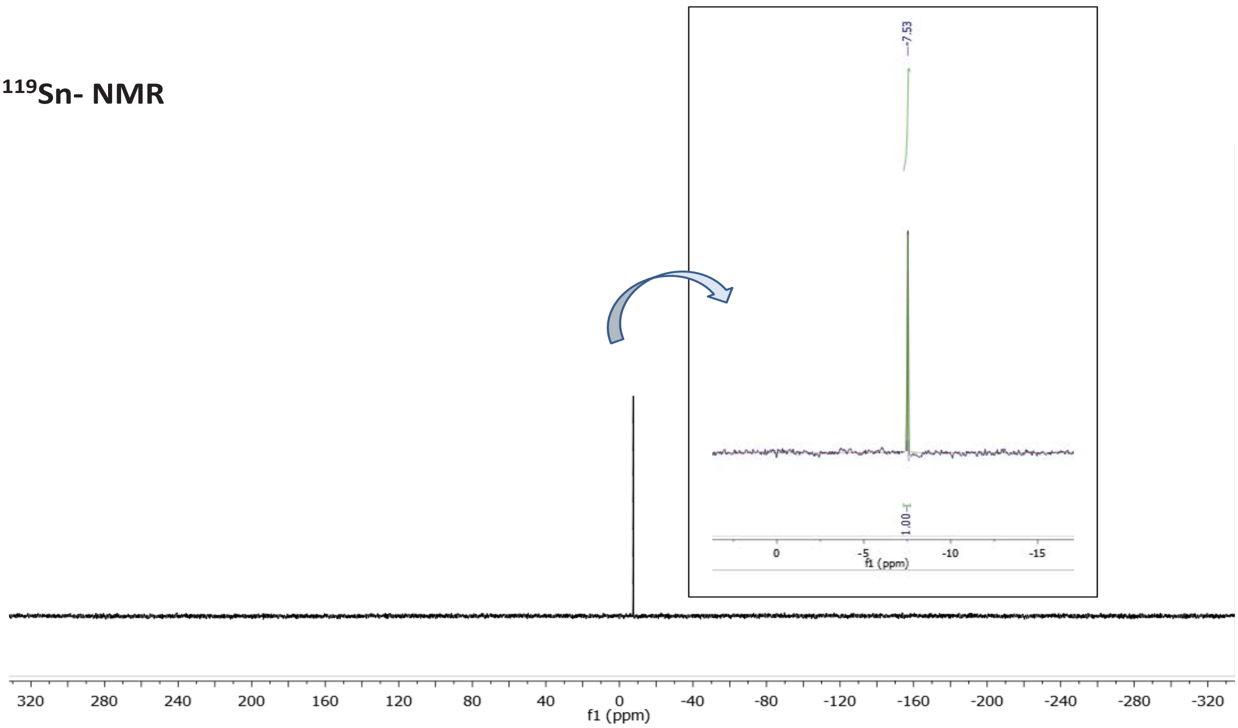
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

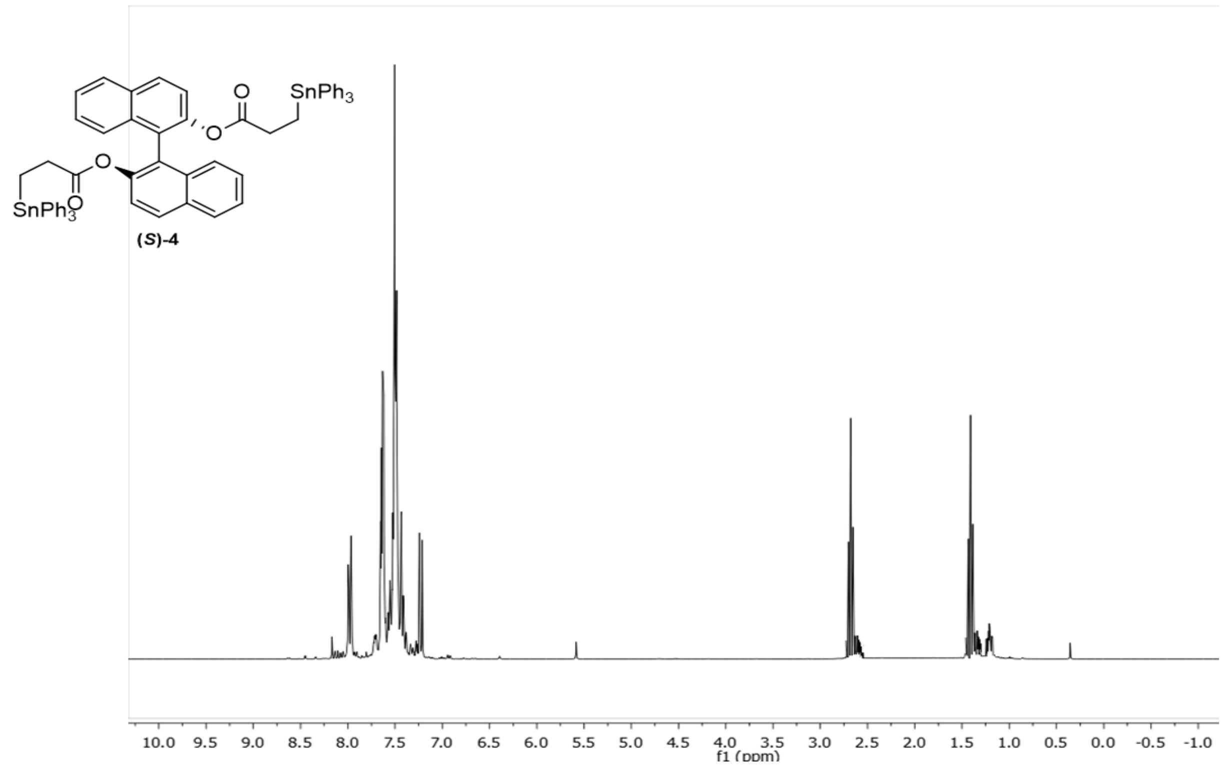


^{119}Sn- NMR

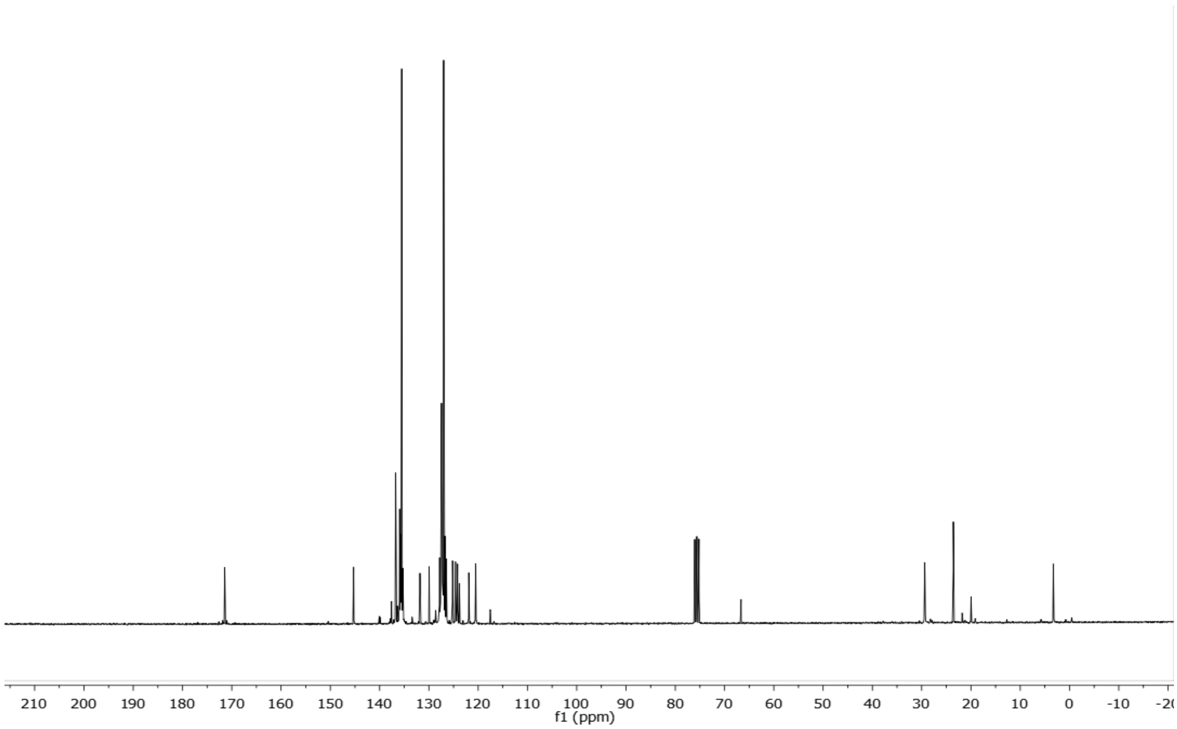


(*S*)-1,1'-binaphthalene-2,2'-diyl-bis[3-(triphenylestannyl)propanoate] (*S*)-4

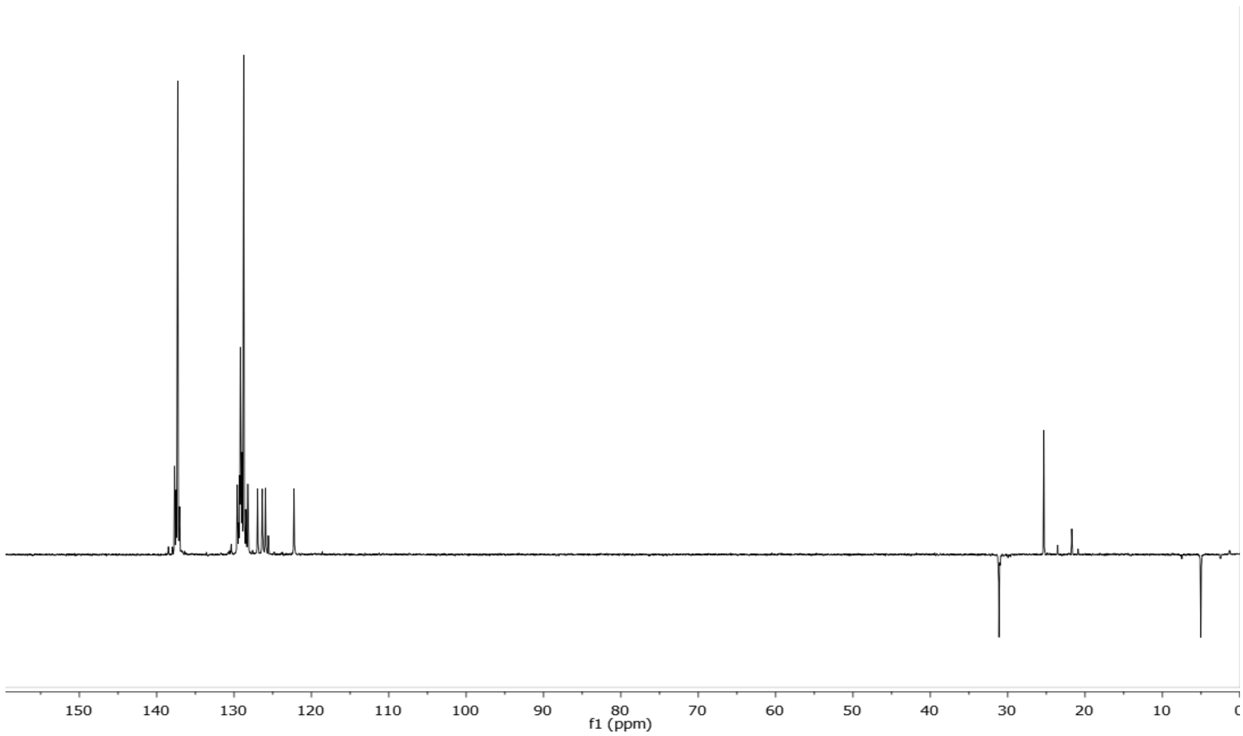
^{1}H- NMR (300MHz, $CDCl_3$)



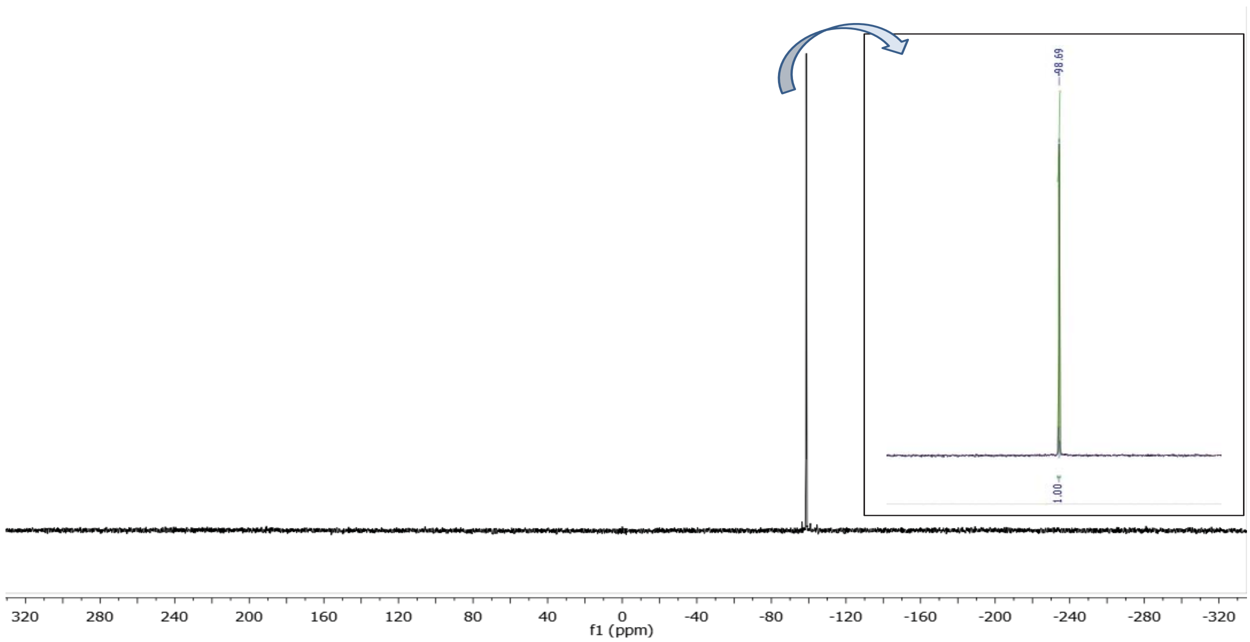
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

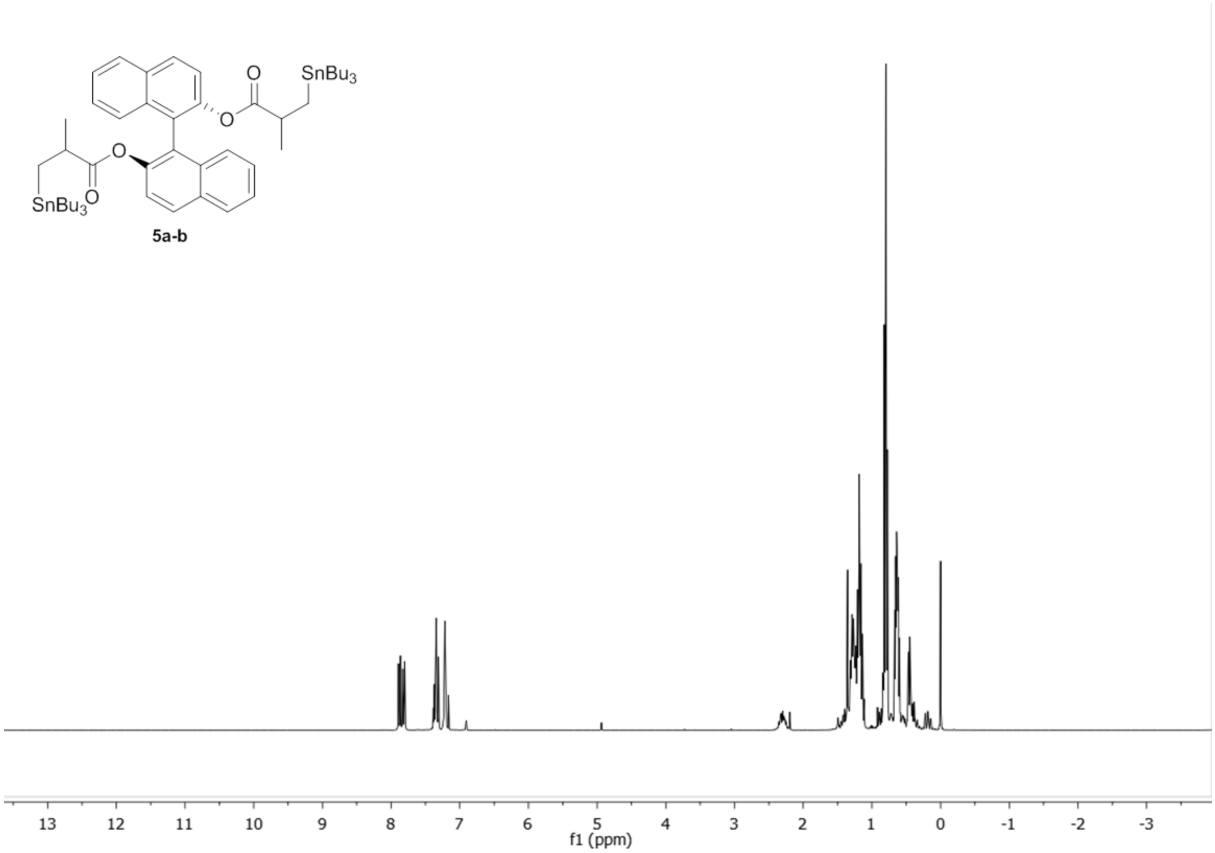


^{119}Sn- NMR

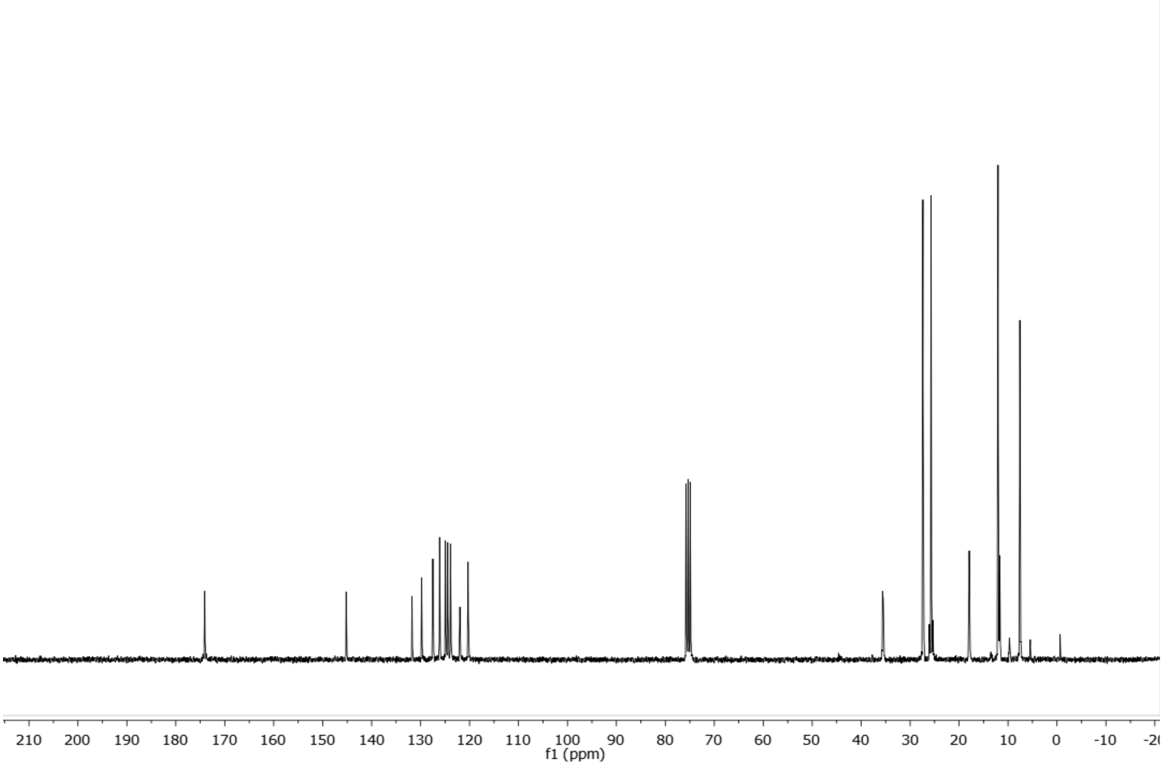


1,1'-binaphthalene-2,2'-diyl-bis[2-methyl-3-(tri-*n*-buthylestannyl)propanoate] 5a-b

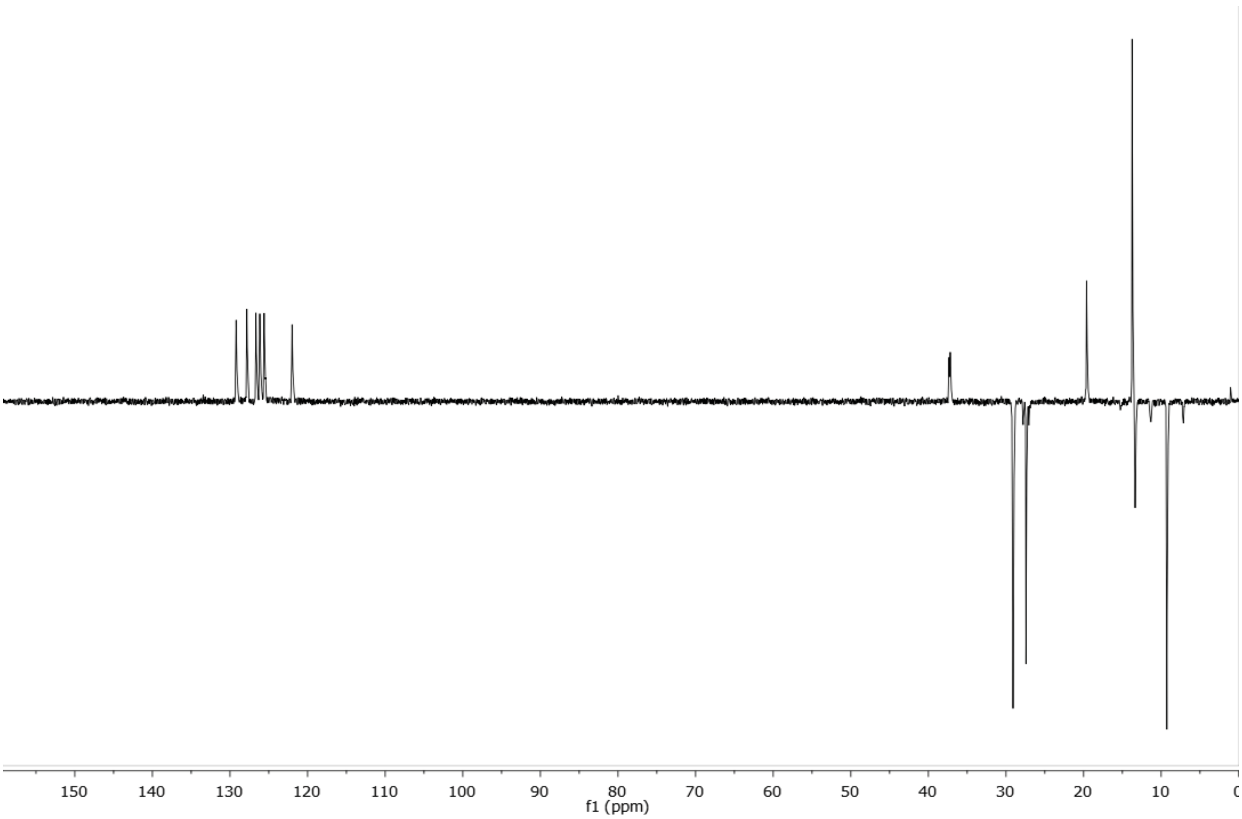
^{1}H- NMR (300MHz, $CDCl_3$)



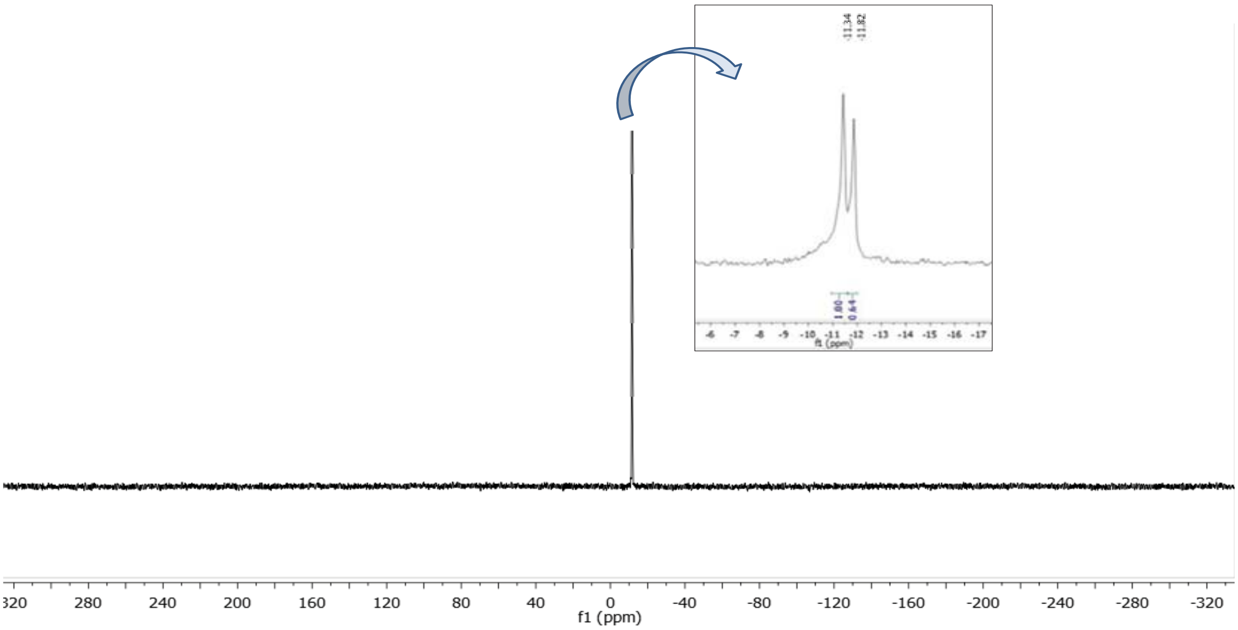
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

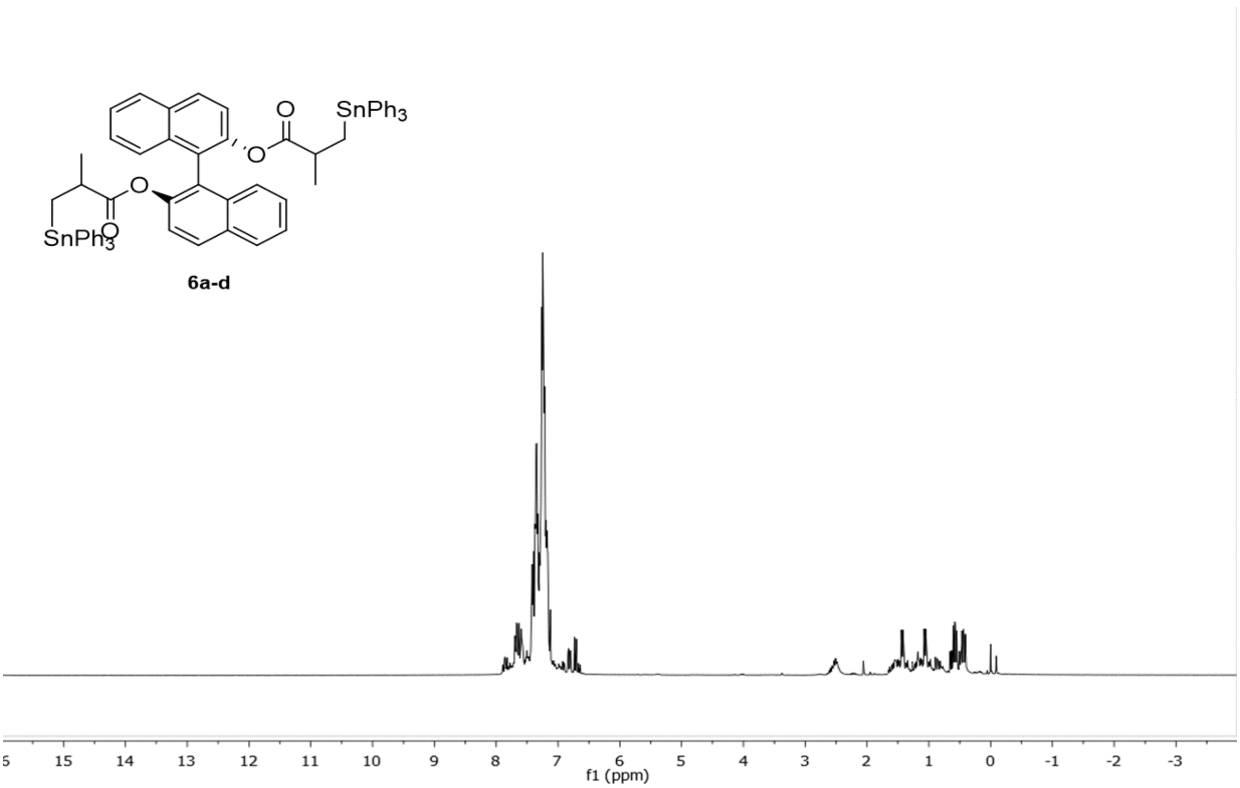


^{119}Sn- NMR

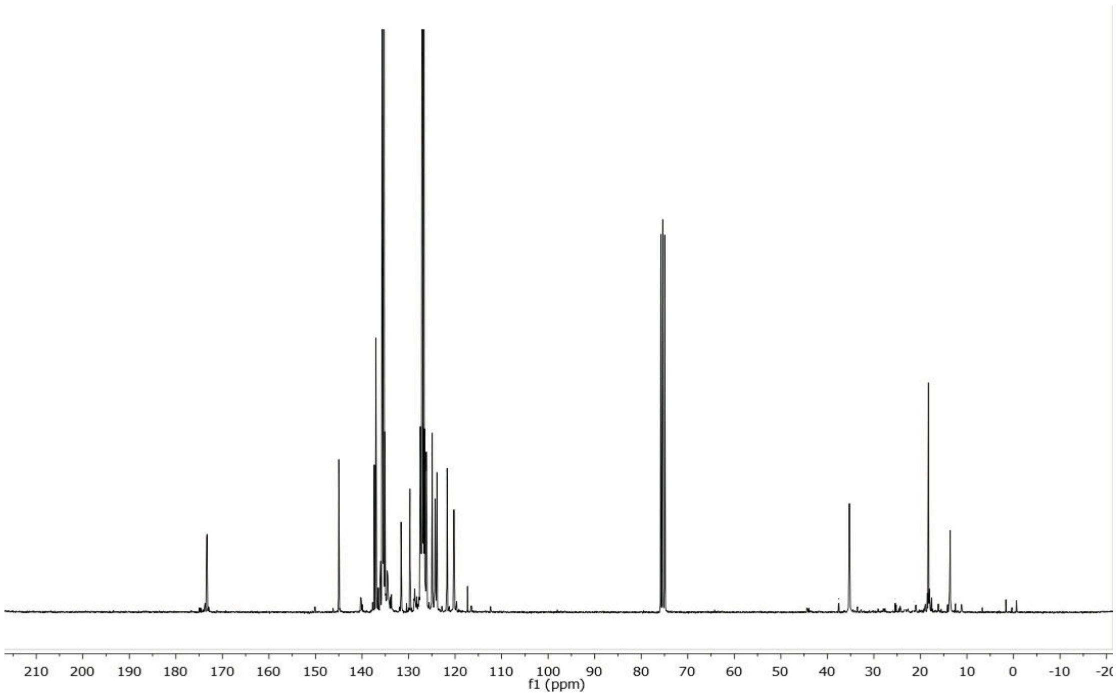


1,1'-binaphthalene-2,2'-diyl-bis[2-methyl-3-(triphenylestannyl)propanoate] 6a-d

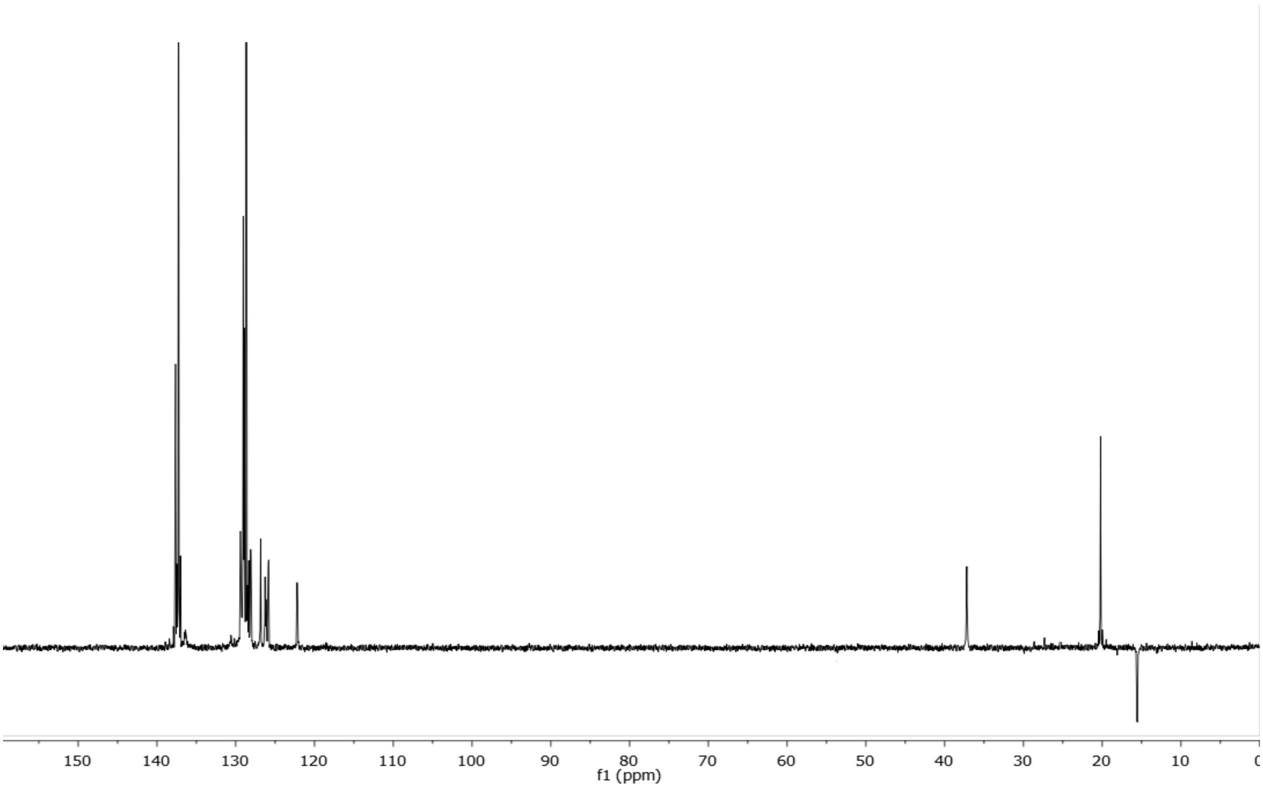
^{1}H- NMR (300MHz, $CDCl_3$)



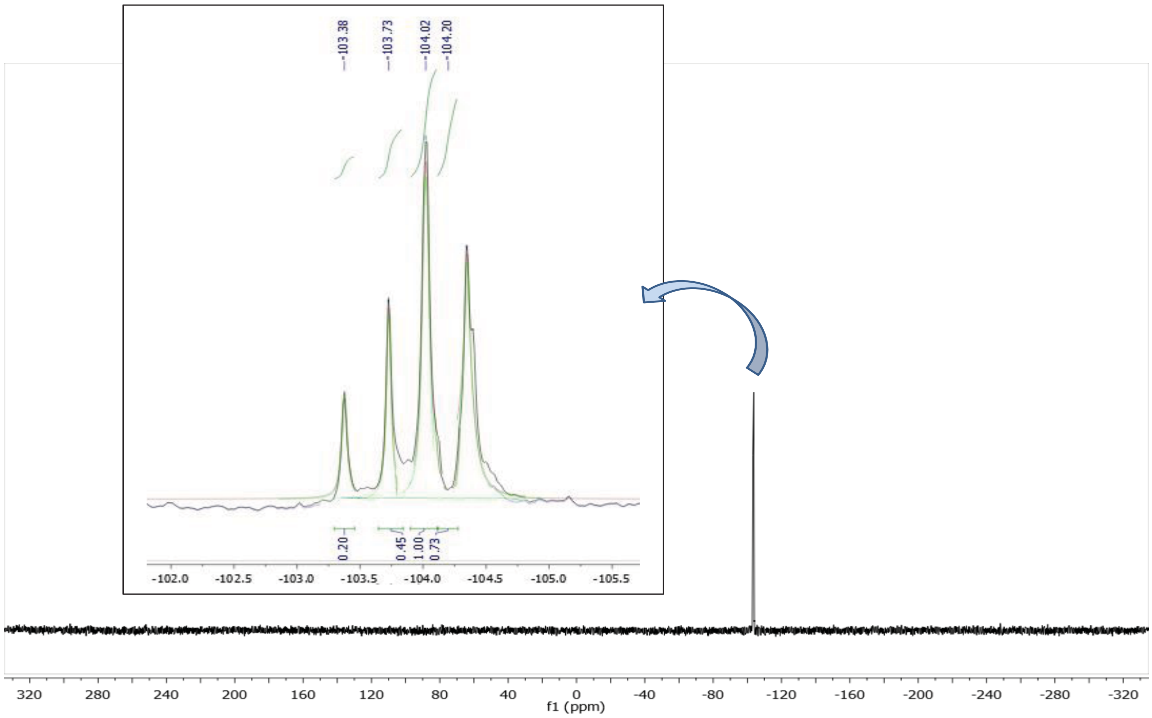
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

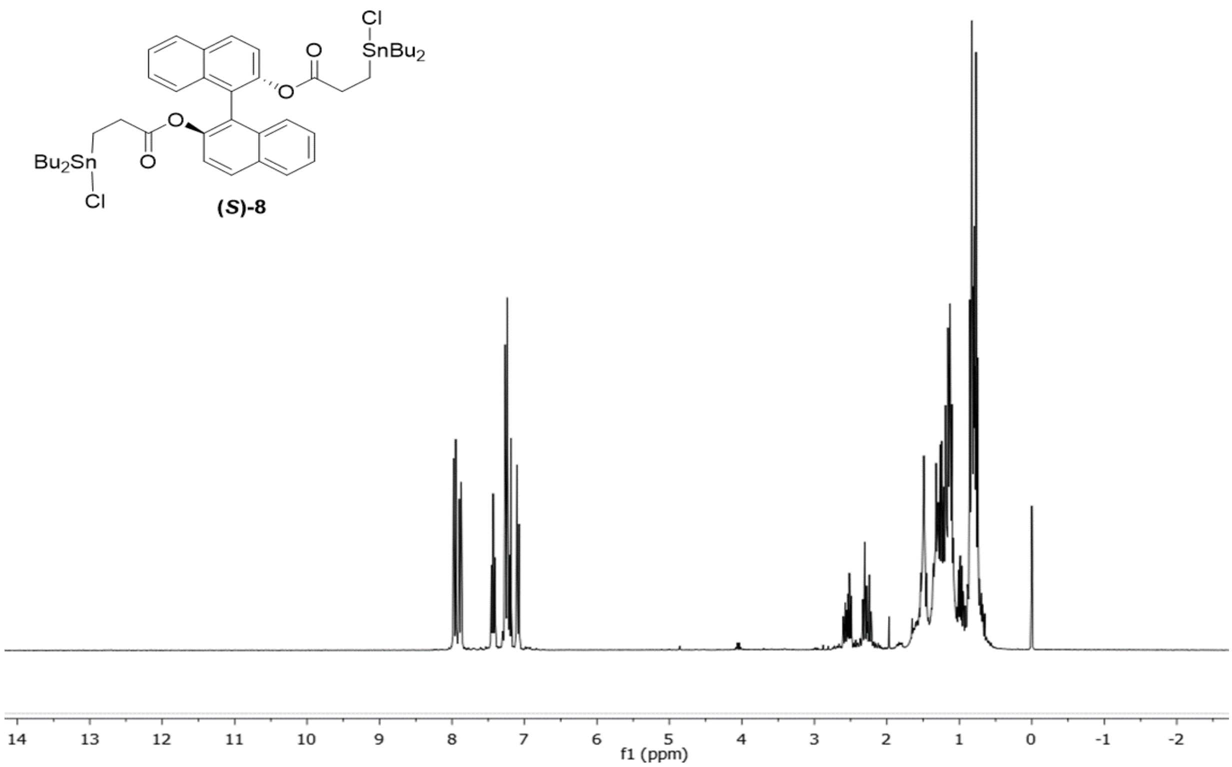


^{119}Sn- NMR

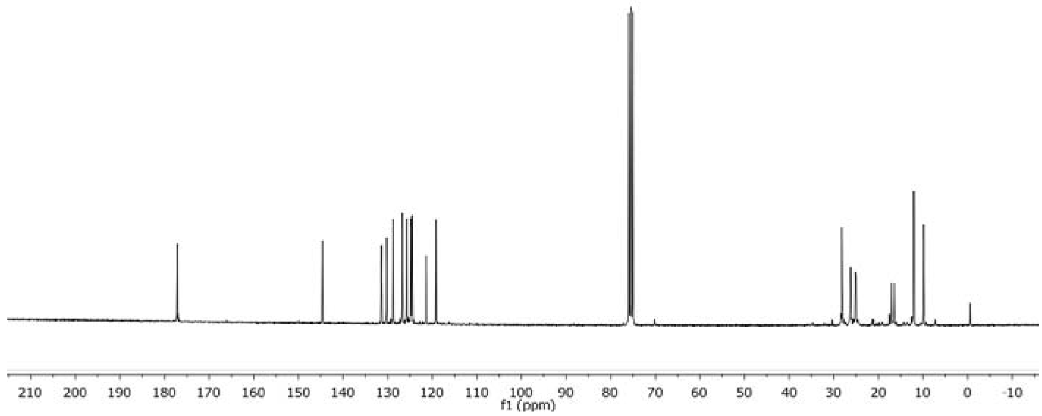


(*S*)-1,1'-binaphthalene-2,2'-diyl-bis[3-(chlorodi-*n*-buthylestannyl)propanoate] (*S*)-8

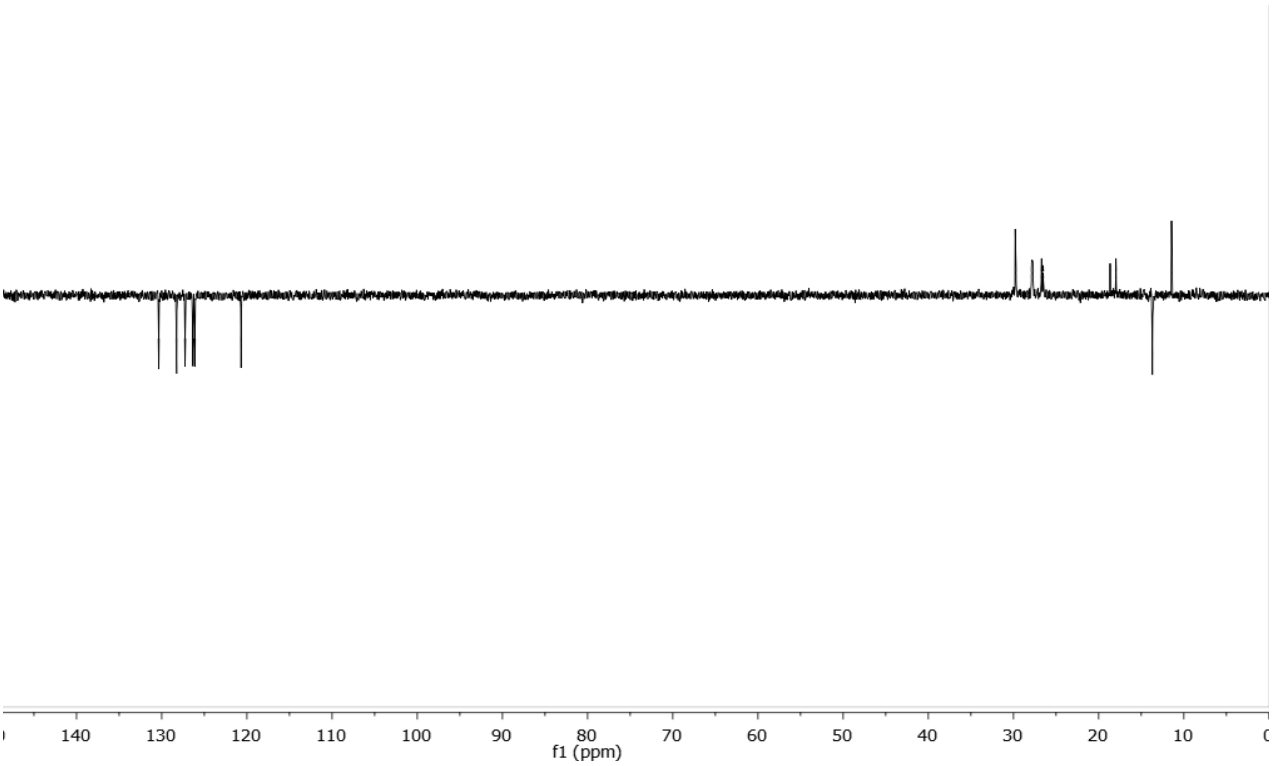
^{1}H- NMR (300MHz, $CDCl_3$)



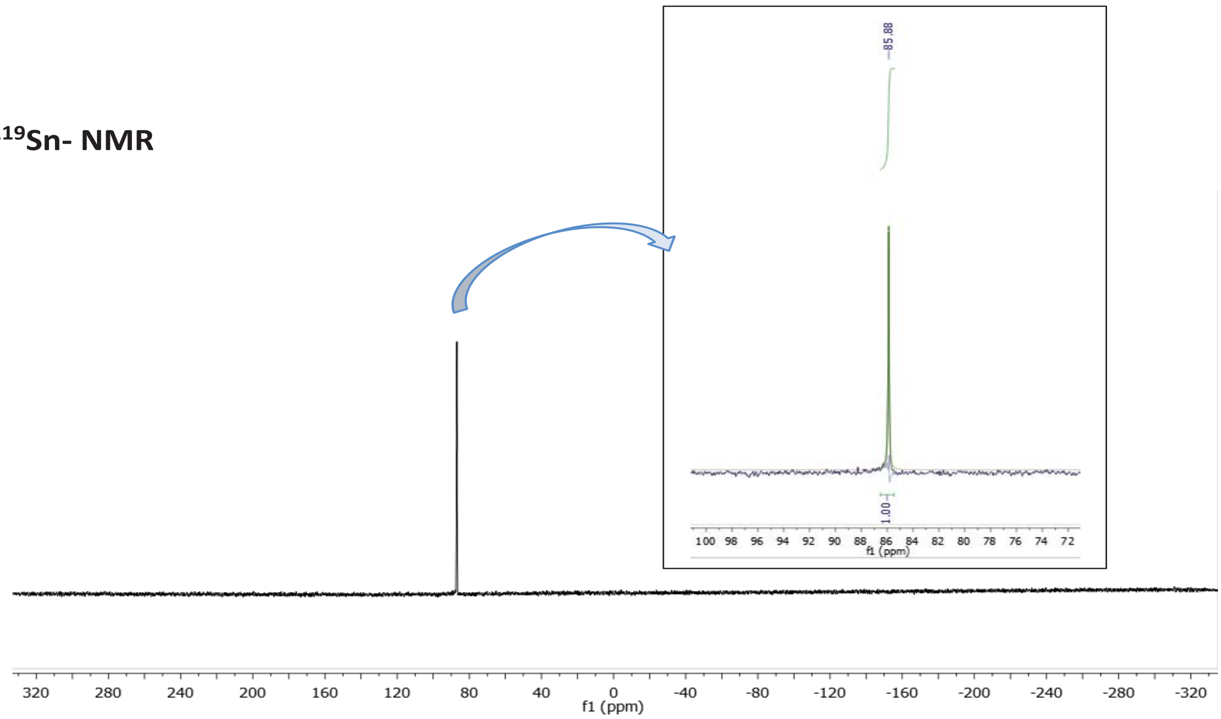
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

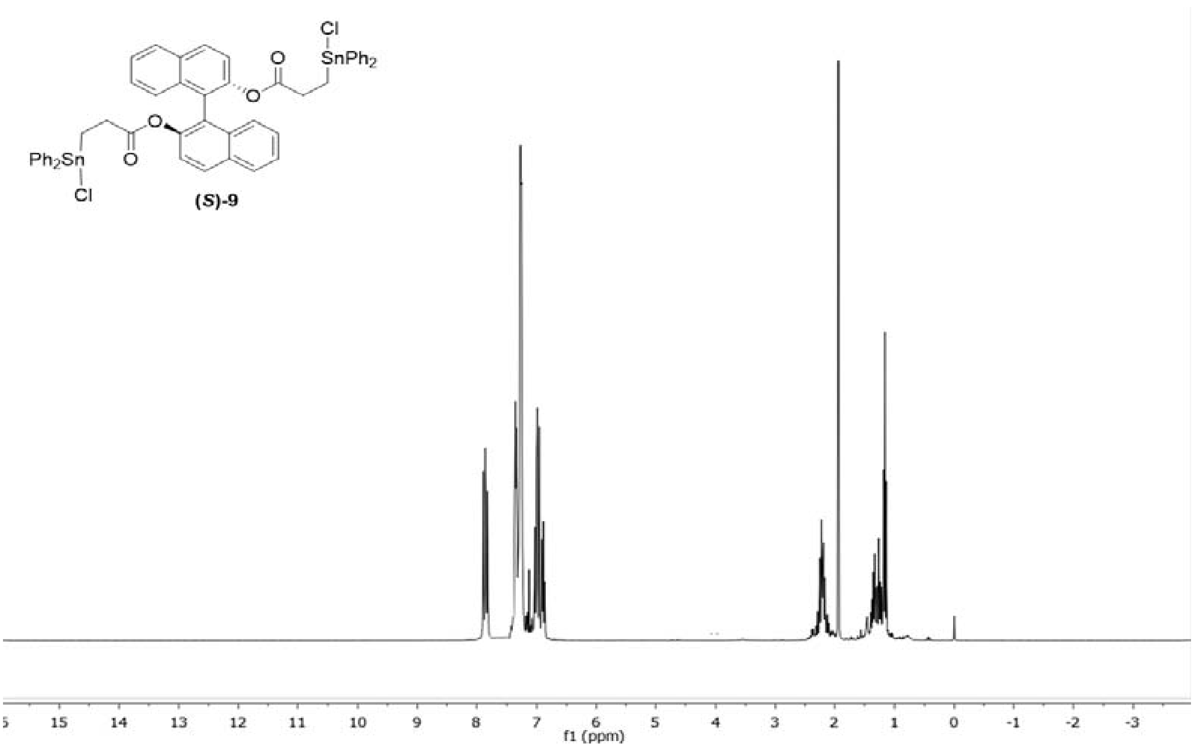


^{119}Sn- NMR

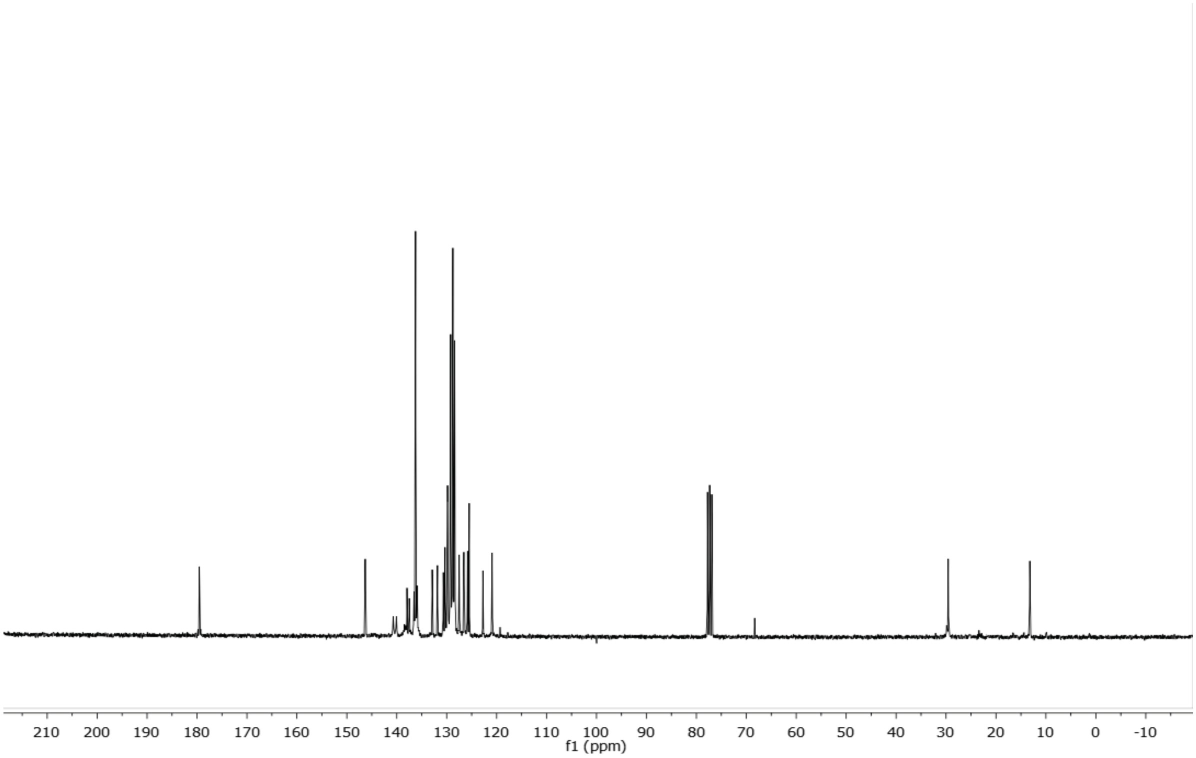


(*S*)-1,1'-binaphthalene-2,2'-diyl-bis[3-(chlorodiphenylestannyl)propanoate] (*S*)-9

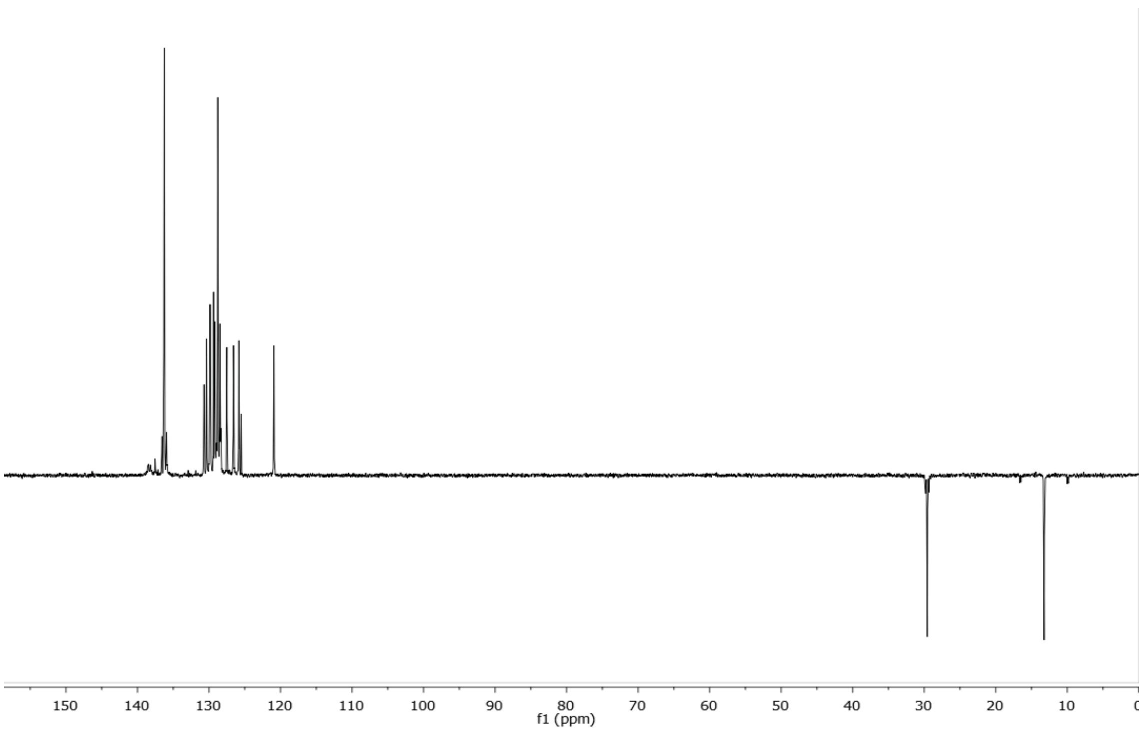
^{1}H- NMR (300MHz, $CDCl_3$)



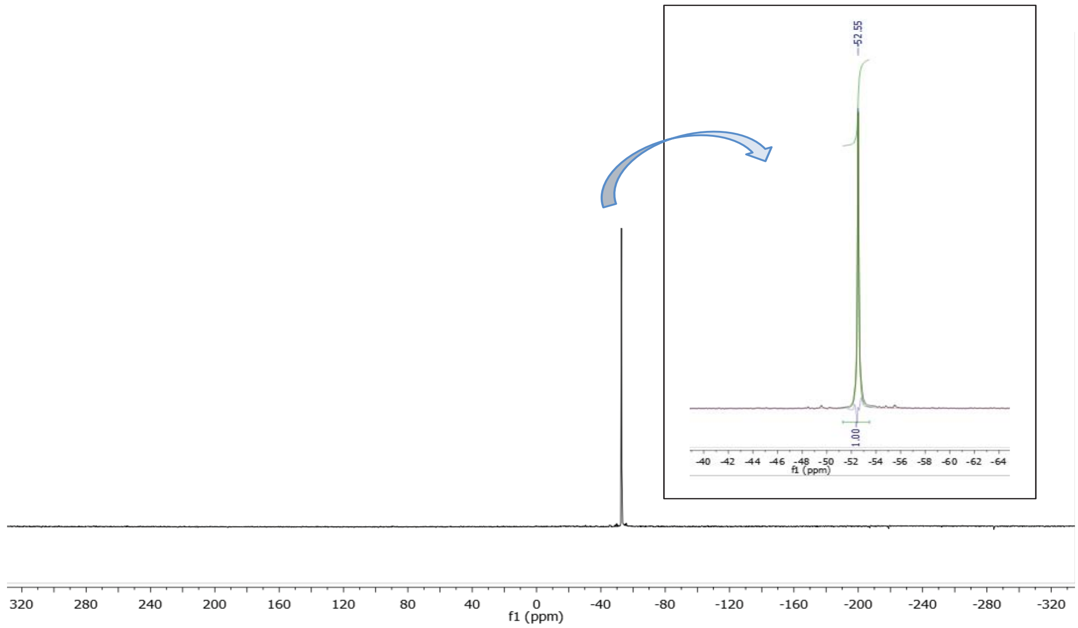
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

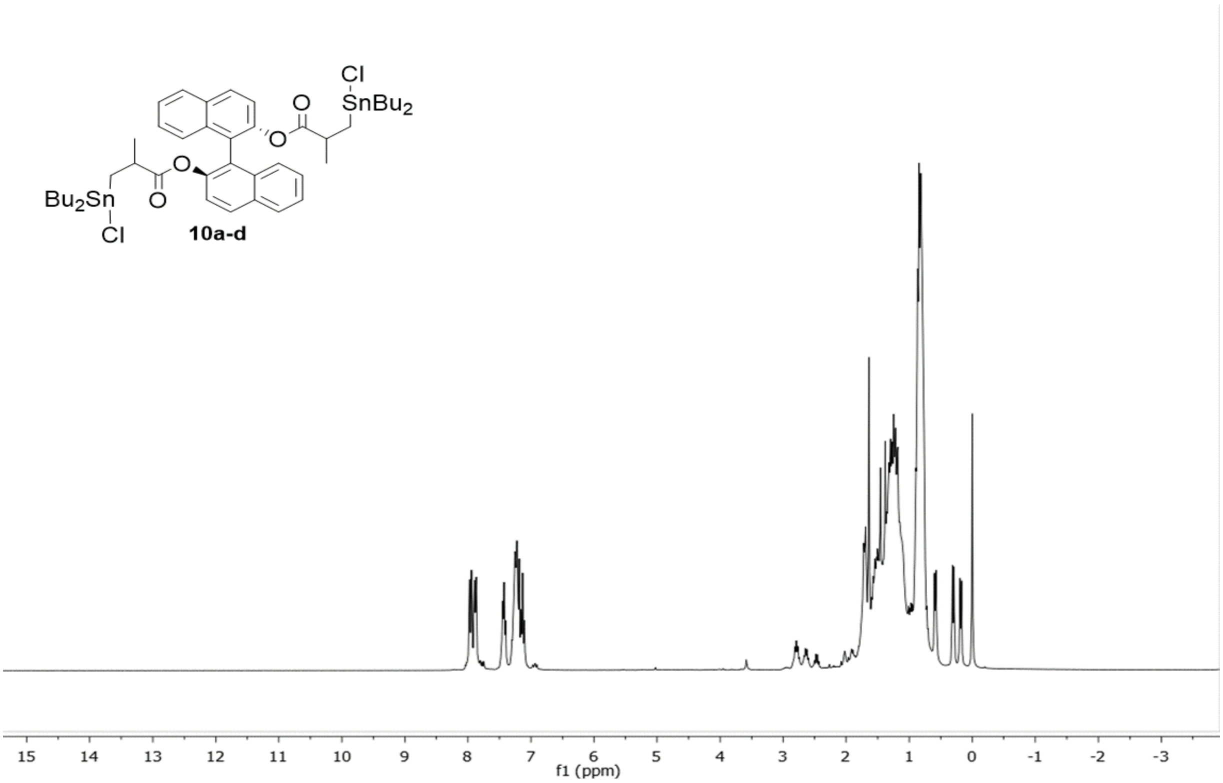


^{119}Sn- NMR

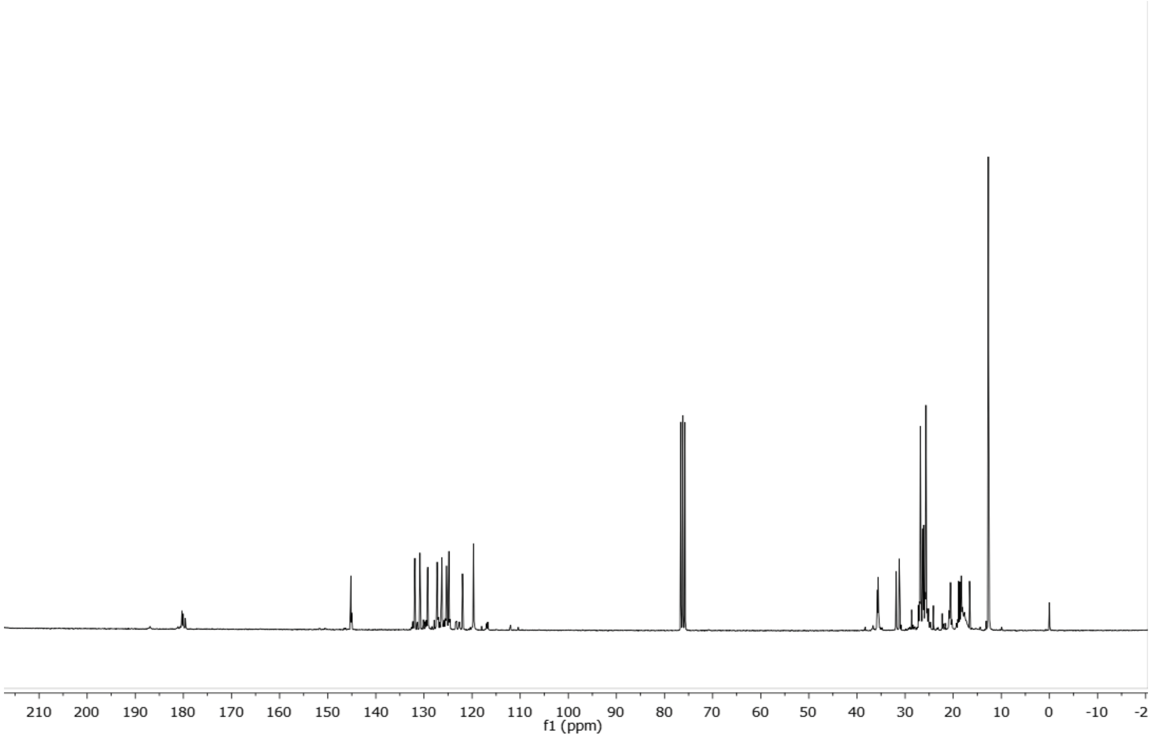


1,1'-binaphthalene-2,2'-diyl-bis[3-(chlorodi-*n*-buthylestannyl)-2-methyl propanoate] (10a-d)

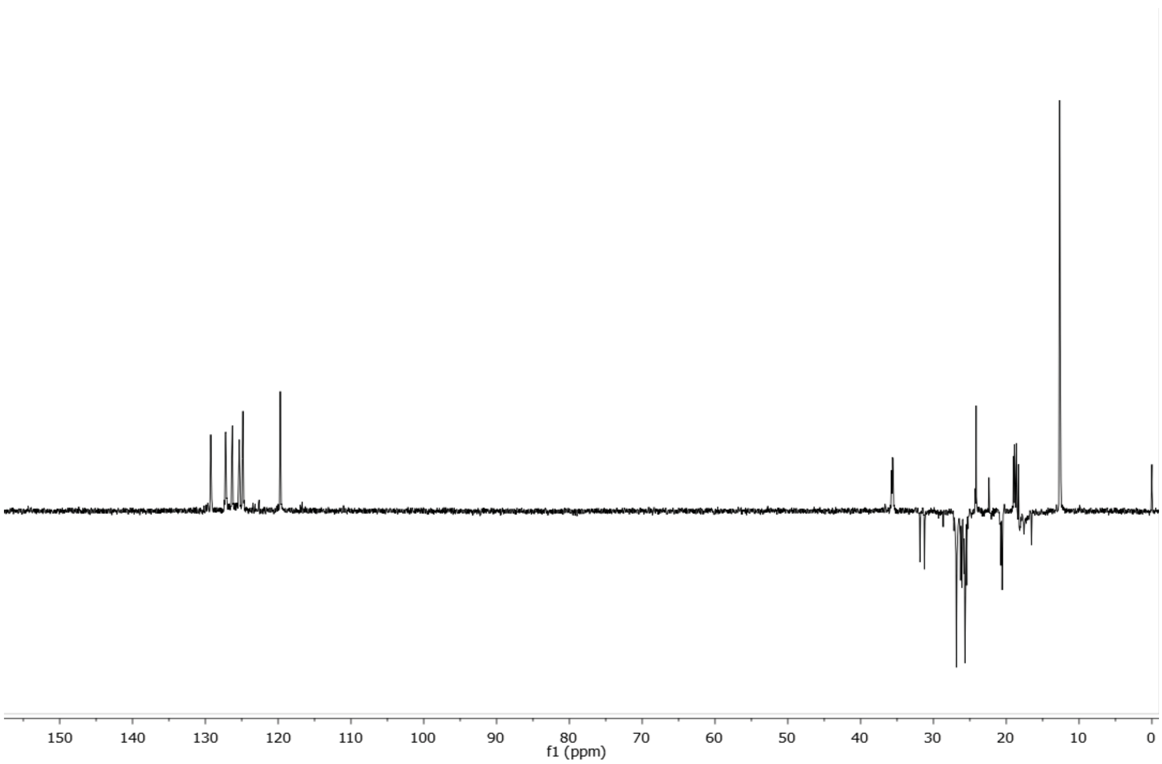
^{1}H- NMR (300MHz, $CDCl_3$)



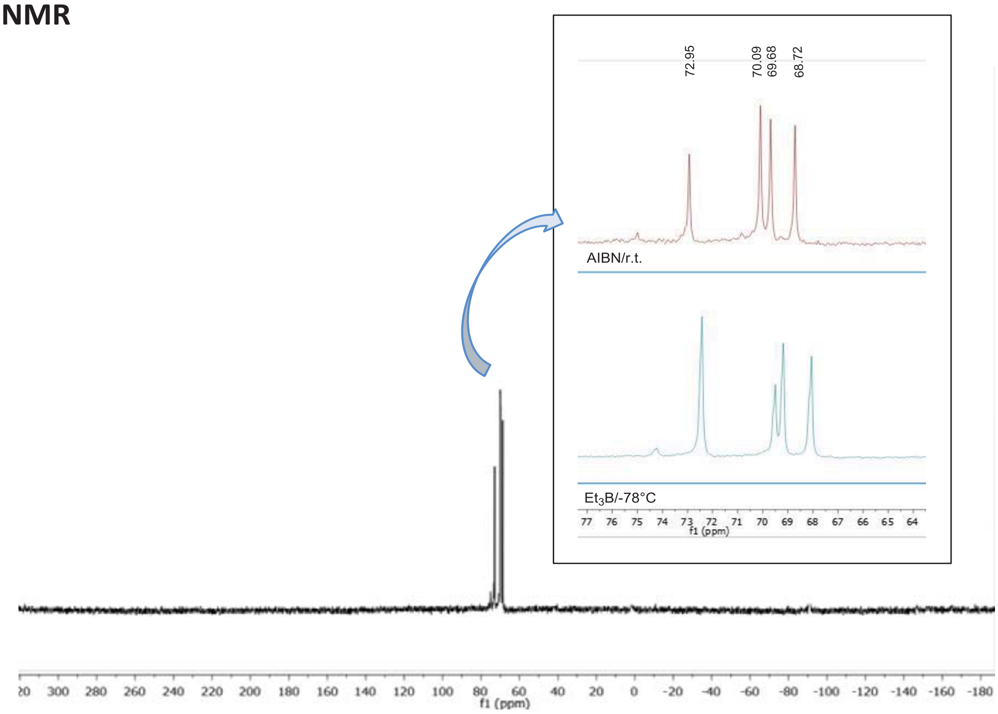
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR

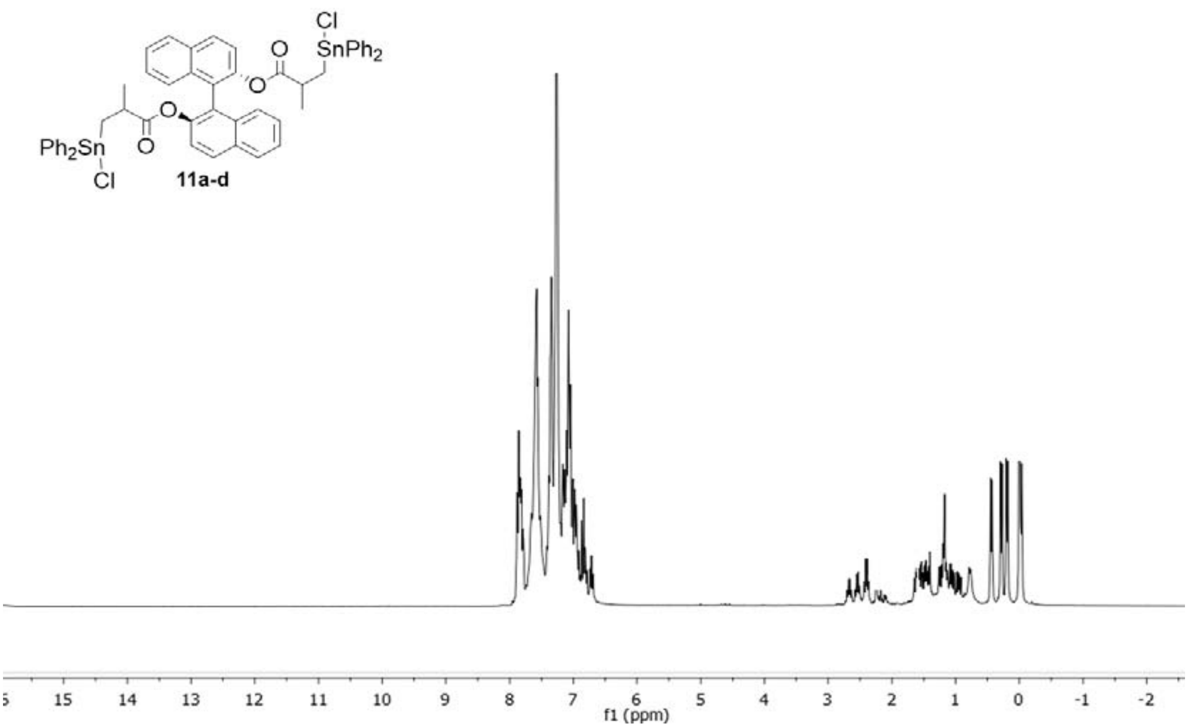


^{119}Sn- NMR

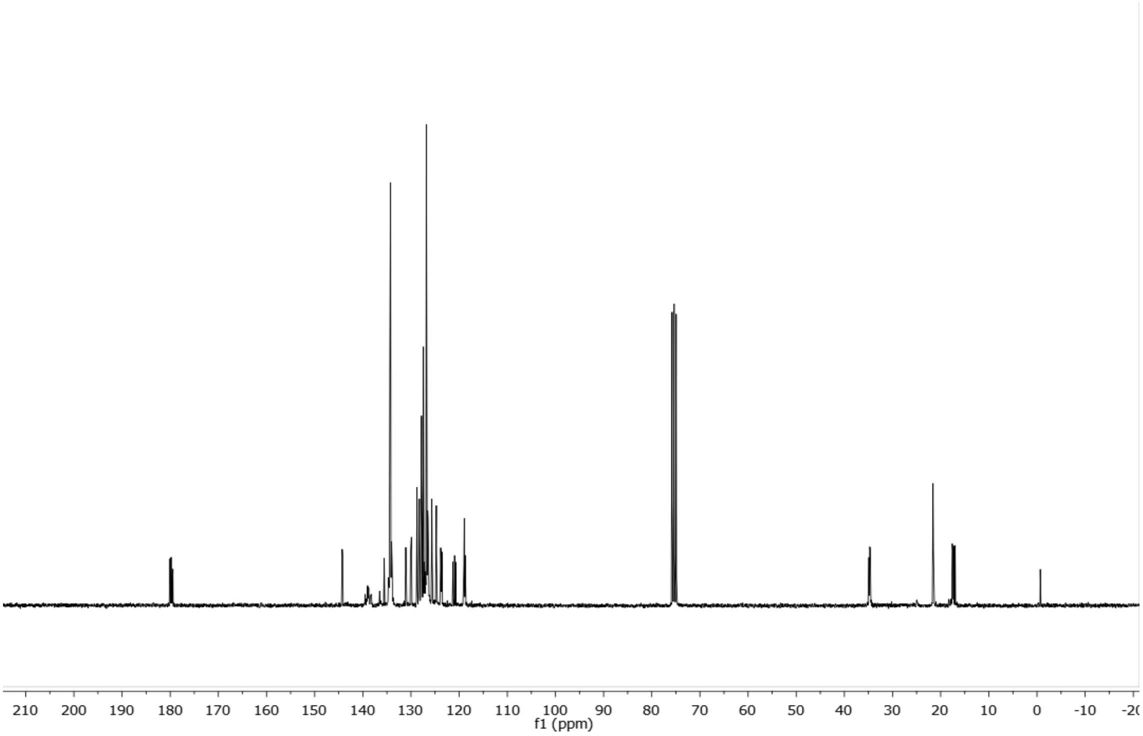


1,1'-binaphthalene-2,2'-diyl-bis[3-(chlorodiphenylestannyl)-2-methyl propanoate] (11a-d)

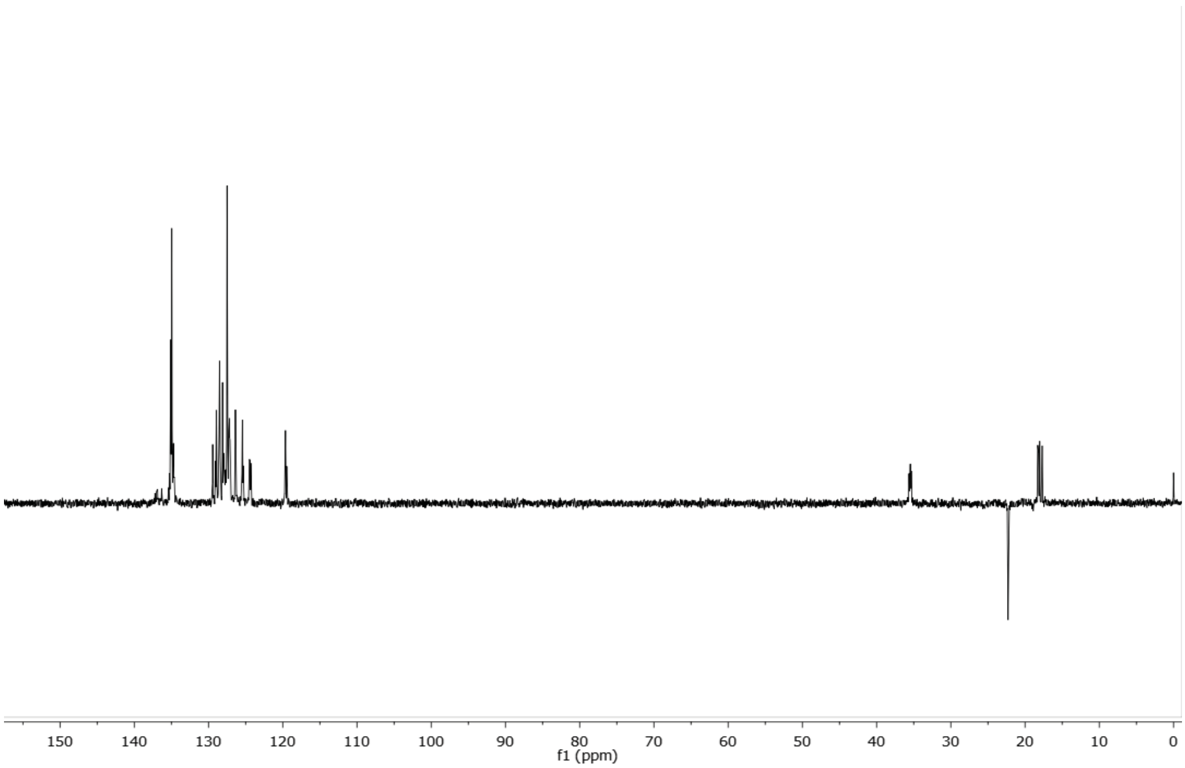
^{1}H- NMR (300MHz, $CDCl_3$)



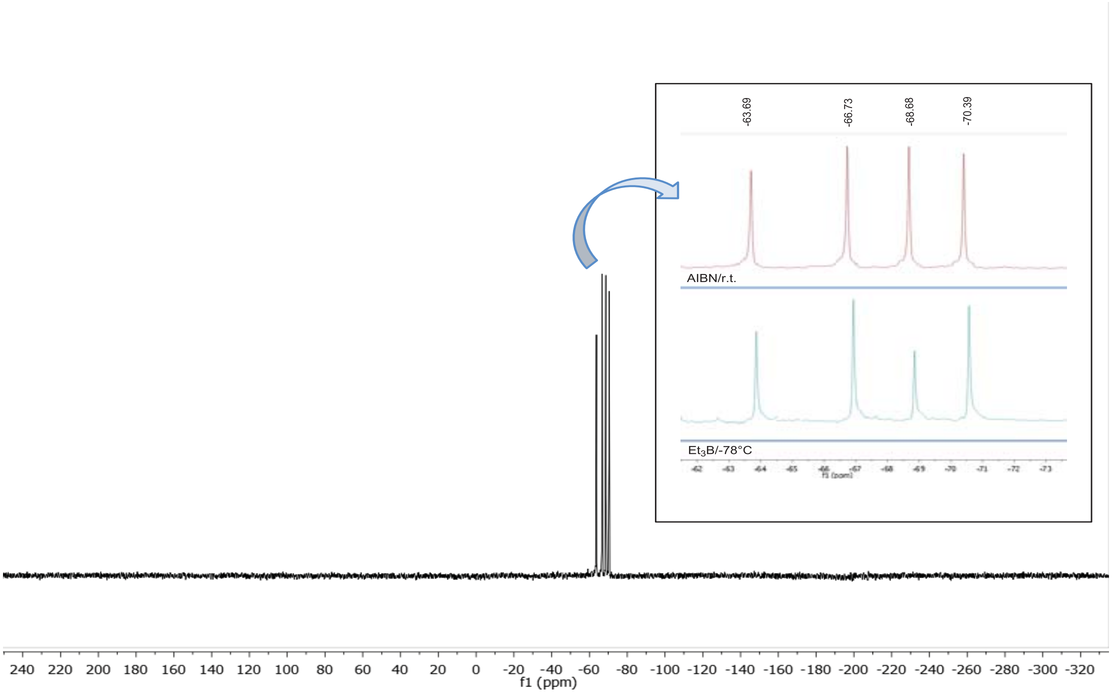
^{13}C- NMR (75MHz, $CDCl_3$)



DEPT- NMR



^{119}Sn- NMR



Crystallographic Information

Summary of Data CCDC 1589534

Compound Name:
Formula: C38 H26 O4
Unit Cell Parameters: a 10.3051(5) b 15.1494(7) c 17.4971(5) P212121

Table S1. Crystal data and structure refinement for **(*S*)-1e**

Identification code	arc364
Empirical formula	C38 H26 O4
Moiety formula	C38 H26 O4
Formula weight	546.59
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 10.3051(5) A alpha = 90 deg.

b = 15.1494(7) A beta = 90 deg.

c = 17.4971(5) A gamma = 90 deg.

Volume 2731.6(2) A^3

Z, Calculated density 4, 1.329 Mg/m^3

Absorption coefficient 0.085 mm^-1

F(000) 1144

Crystal size .15 x .1 x .06 mm

Theta range for data collection 2.29 to 27.00 deg.

Limiting indices -13<=h<=11, -19<=k<=11, -20<=l<=22

Reflections collected / unique 13044 / 3364 [R(int) = 0.0610]

Reflection observed [I>2sigma(I)] 2443

Completeness to theta = 27.00 99.9 %

Absorption correction None

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 3364 / 0 / 379

Goodness-of-fit on F^2 0.928

Final R indices [I>2sigma(I)] R1 = 0.0371, wR2 = 0.0639

R indices (all data) R1 = 0.0656, wR2 = 0.0701

Largest diff. peak and hole 0.177 and -0.203 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ***(S)*-1e**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	2876(1)	1600(1)	2634(1)	19(1)
O(2)	3348(2)	1537(1)	1366(1)	26(1)
O(3)	4919(2)	-718(1)	3272(1)	18(1)

O(4)	3955(2)	-298(1)	2162(1)	24(1)
C(1)	2552(2)	1545(2)	1871(1)	21(1)
C(2)	1136(2)	1517(2)	1776(1)	22(1)
C(3)	634(2)	1547(2)	1074(1)	22(1)
C(4)	-732(2)	1521(2)	840(1)	20(1)
C(5)	-1736(2)	1271(2)	1327(1)	24(1)
C(6)	-3010(2)	1256(2)	1072(1)	26(1)
C(7)	-3305(2)	1483(2)	327(1)	27(1)
C(8)	-2320(2)	1730(2)	-168(1)	26(1)
C(9)	-1050(2)	1745(2)	84(1)	23(1)
C(10)	4193(2)	1667(2)	2832(1)	17(1)
C(11)	4632(2)	1136(2)	3415(1)	16(1)
C(12)	3748(2)	504(2)	3807(1)	16(1)
C(13)	3880(2)	-391(2)	3706(1)	18(1)
C(14)	4911(3)	-543(2)	2494(1)	20(1)
C(15)	6182(2)	-692(2)	2151(1)	21(1)
C(16)	7284(2)	-772(2)	2545(1)	21(1)
C(17)	8590(2)	-855(2)	2222(1)	22(1)
C(18)	8815(2)	-1062(2)	1456(1)	25(1)
C(19)	10059(2)	-1073(2)	1168(1)	29(1)
C(20)	11106(2)	-870(2)	1631(1)	28(1)
C(21)	10900(2)	-678(2)	2396(1)	28(1)
C(22)	9657(2)	-687(2)	2689(1)	25(1)
C(23)	3086(2)	-1014(2)	4074(1)	19(1)
C(24)	2161(2)	-731(2)	4577(1)	18(1)
C(25)	1995(2)	184(2)	4729(1)	17(1)
C(26)	2771(2)	807(2)	4329(1)	16(1)

C(27)	2590(2)	1716(2)	4485(1)	19(1)
C(28)	1709(2)	1987(2)	5024(1)	21(1)
C(29)	966(2)	1366(2)	5432(1)	22(1)
C(30)	1104(2)	483(2)	5288(1)	20(1)
C(31)	5974(2)	1197(2)	3628(1)	17(1)
C(32)	6796(2)	1801(2)	3242(1)	18(1)
C(33)	6254(2)	2359(2)	2674(1)	21(1)
C(34)	4982(2)	2294(2)	2470(1)	19(1)
C(35)	8135(2)	1830(2)	3421(1)	22(1)
C(36)	8648(2)	1290(2)	3968(1)	23(1)
C(37)	7824(2)	711(2)	4371(1)	23(1)
C(38)	6527(2)	664(2)	4212(1)	19(1)

Table S3. Anisotropic displacement parameters (A^2 x 10^3) for ***(S)*-1e**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	19(1)	24(1)	15(1)	1(1)	-2(1)	1(1)
O(2)	25(1)	36(1)	17(1)	-2(1)	2(1)	1(1)
O(3)	17(1)	22(1)	16(1)	-1(1)	3(1)	3(1)
O(4)	20(1)	31(1)	22(1)	-3(1)	-3(1)	3(1)
C(1)	25(1)	19(2)	19(1)	2(1)	-2(1)	1(1)
C(2)	21(1)	23(2)	22(1)	-1(1)	2(1)	2(1)
C(3)	22(1)	23(2)	22(1)	0(1)	3(1)	1(1)

C(4)	19(1)	18(2)	21(1)	-3(1)	-1(1)	1(1)
C(5)	26(2)	24(2)	23(1)	-3(1)	1(1)	-1(1)
C(6)	23(2)	23(2)	33(1)	-4(1)	6(1)	-2(1)
C(7)	24(2)	21(2)	37(2)	-5(1)	-5(1)	3(1)
C(8)	28(2)	26(2)	24(1)	0(1)	-8(1)	2(1)
C(9)	24(1)	24(2)	22(1)	2(1)	0(1)	0(1)
C(10)	15(1)	18(2)	17(1)	-2(1)	-0(1)	-1(1)
C(11)	21(1)	14(1)	12(1)	-3(1)	1(1)	0(1)
C(12)	17(1)	17(2)	14(1)	-1(1)	-2(1)	0(1)
C(13)	17(1)	23(2)	15(1)	-3(1)	-1(1)	1(1)
C(14)	24(1)	18(2)	18(1)	-2(1)	0(1)	-5(1)
C(15)	21(1)	24(2)	19(1)	-2(1)	2(1)	0(1)
C(16)	21(1)	22(2)	20(1)	-0(1)	4(1)	-2(1)
C(17)	21(1)	21(2)	24(1)	-1(1)	-0(1)	2(1)
C(18)	19(1)	31(2)	25(1)	-3(1)	0(1)	0(1)
C(19)	25(2)	39(2)	23(1)	-2(1)	5(1)	0(2)
C(20)	19(1)	31(2)	33(1)	1(1)	6(1)	1(1)
C(21)	18(1)	35(2)	30(1)	-1(1)	-2(1)	3(1)
C(22)	21(1)	33(2)	21(1)	0(1)	0(1)	-1(1)
C(23)	19(1)	16(1)	21(1)	0(1)	-4(1)	-1(1)
C(24)	16(1)	22(2)	18(1)	4(1)	-2(1)	-4(1)
C(25)	15(1)	22(2)	14(1)	1(1)	-3(1)	1(1)
C(26)	18(1)	19(1)	13(1)	1(1)	-4(1)	-1(1)
C(27)	20(1)	19(2)	17(1)	0(1)	-2(1)	-3(1)
C(28)	21(1)	21(2)	21(1)	-3(1)	-3(1)	2(1)
C(29)	20(1)	30(2)	17(1)	-1(1)	2(1)	2(1)
C(30)	15(1)	27(2)	17(1)	2(1)	-0(1)	-0(1)

C(31)	22(1)	14(1)	15(1)	-5(1)	3(1)	0(1)
C(32)	18(1)	19(2)	16(1)	-4(1)	0(1)	0(1)
C(33)	26(2)	17(1)	20(1)	1(1)	4(1)	-4(1)
C(34)	20(1)	21(2)	17(1)	-1(1)	1(1)	2(1)
C(35)	21(1)	24(2)	20(1)	-4(1)	3(1)	-5(1)
C(36)	19(1)	25(2)	24(1)	-3(1)	-3(1)	-2(1)
C(37)	24(1)	21(2)	22(1)	0(1)	-6(1)	2(1)
C(38)	24(1)	16(2)	18(1)	-0(1)	1(1)	-0(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **(*S*)-1e**.

	x	y	z	U(eq)
H(9)	585	1479	2210	26
H(15)	1245	1590	670	27
H(23)	-1546	1108	1839	29
H(20)	-3685	1089	1412	32
H(11)	-4179	1469	155	33
H(18)	-2518	1890	-680	31
H(7)	-380	1908	-261	28
H(19)	6229	-737	1610	25
H(4)	7216	-774	3086	25
H(26)	8103	-1196	1131	30
H(12)	10199	-1221	647	35
H(3)	11960	-863	1426	33

H(24)	11613	-539	2718	33
H(17)	9527	-577	3218	30
H(13)	3192	-1626	3974	22
H(5)	1623	-1150	4828	22
H(1)	3084	2142	4214	23
H(21)	1600	2599	5122	25
H(10)	366	1561	5808	27
H(6)	599	67	5566	24
H(14)	6789	2786	2432	25
H(22)	4635	2670	2086	23
H(25)	8685	2231	3156	26
H(2)	9551	1304	4075	27
H(16)	8178	347	4761	27
H(8)	5991	272	4495	23