Supplementary Material for:

Mechanistic elucidation of monoalkyltin(IV)-catalyzed esterification

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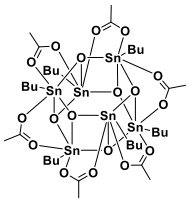
Materials and Methods

General

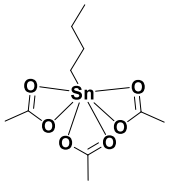
Dichloromethane was distilled from CaH_2, *n*-pentane from sodium/benzophenone and toluene from sodium under argon atmosphere. Ethanol was degassed, by bubbling nitrogen through for >30 min, and dried over 3Å molecular sieves. All other chemicals were obtained from Merck and were used without further purification. All air-sensitive materials were manipulated using standard Schlenk techniques or by the use of an argon-filled glovebox (MBraun Unilab). The NMR solvent $CDCl_3$ was dried over molecular sieves and degassed via three cycles of freeze-pump-thaw. Acetic acid-d_4 and Ethanol-d_6 were used without further purification. ^{1}H (500 or 400 MHz) and ^{13}C (125 or 100 Mhz) spectra were recorded on a Bruker DRX 500 MHz or a Bruker AVANCE 400 MHz spectrometer. ^{119}Sn NMR spectra were recorded on a Bruker DRX 500 MHz at 186 MHz and measured in the range of 100 to -700 ppm. ^{1}H and ^{13}C spectra were referenced against residual solvent signal, while ^{119}Sn spectra were externally calibrated against an 5% (v/v) solution of $SnMe_4$ in acetone. 2D ^{1}H DOSY spectra were recorded on a Bruker DRX 300 MHz spectrometer. FD-MS spectra were collected on an AccuTOF GC v 4g, JMS-T100GCV Mass spectrometer (JEOL, Japan) equipped with a Carbotec emitter or a LiFDi probe (FD) equipped with an FD Emitter, Linden CMS GmbH. A typical current rate of 51.2 mA/min over 1.2 min and a flashing current 40 mA on every spectra of 30 ms was used. ATR-FTIR spectra were recorded on a Bruker Alpha-P. GC analysis for heptylbenzoate and benzoic acid was performed on a Thermo Scientific Trace GC Ultra equipped with a Restek Stabilwax-DA column (30 m x 0.25 mm x 0.25 µm). Temperature program: initial temperature 50 °C, heat to 200 °C with 20 °C min^{-1}, hold for 10 min, heat to 250°C with 50 °C min^{-1}, hold for 3 minutes. Inlet temperature 250 °C, split ratio of 30, 1.0 mL min^{-1} helium flow, FID temperature 250 °C. Esterification reactions were performed in a Radley Discoveries 12 plus reaction station allowing a maximum of 12 simultaneous reactions under a nitrogen atmosphere.

Synthesis

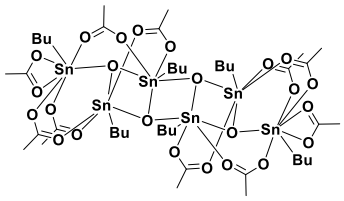
[*n*-BuSn(O)OAc]$_6$, *n*-BuSnOAc$_3$ and (*n*-BuSnOEt$_3$)$_4$ where synthesized according to literature procedures.[1–3]



1. [*n*-BuSn(O)OAc]$_6$: ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.09 (s, 3H, OOCC$\underline{H}_3$), 1.67 (m, 2H, C$\underline{H}_2$CH$_3$), 1.36 (m, 2H, C$\underline{H}_2$CH$_2$), 1.24 (m, 2H, SnC$\underline{H}_2$), 0.91 (t, *J* = 7.4 Hz, 3H, CH$_2$C$\underline{H}_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 179.88 (CH$_3$$\underline{C}$OO), 27.24 ($^3J$ ^{13}C - $^{119/117}$Sn = 57.5 Hz, $\underline{C}$H$_2$CH$_3$), 26.93 (^1J ^{13}C - ^{119}Sn = 1185.0 Hz, ^1J ^{13}C - ^{117}Sn = 1131.3 Hz, Sn$\underline{C}$H$_2$CH$_2$), 26.73 (^2J ^{13}C - $^{119/117}$Sn = 191.3 Hz, $\underline{C}$H$_2$CH$_2$), 24.48 (OOC$\underline{C}$H$_3$), 13.72 (CH$_2$$\underline{C}H_3$). ^{119}Sn{H} NMR (186 MHz, $CDCl_3$): δ -484.91. IR-ATR (cm^{-1}): 1595, 1593, 1448, 1421, 608. FD-MS (*m/z, pos*): Calculated for [$C_{31}H_{75}O_{18}Sn_6$] 1446.9101; found 1446.8201 [M-C_4H_9]$^+$



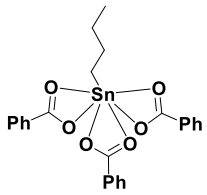
3. *n*-BuSnOAc$_3$: ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.15 (s, 9H, OOCC$\underline{H}_3$), 1.77 (m, 2H, C$\underline{H}_2$CH$_3$), 1.66 (m, 2H, SnC$\underline{H}_2$), 1.39 (s, 2H, C$\underline{H}_2$CH$_2$), 0.90 (t, *J* = 7.4 Hz, 3H, CH$_2$C$\underline{H}_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 184.16 (CH$_3$$\underline{C}$OO), 29.19 ($^3J$ ^{13}C - $^{119/117}$Sn = 61.3 Hz, $\underline{C}$H$_2$CH$_3$), 26.53 (^1J ^{13}C - ^{119}Sn = 1001.3 Hz, ^1J ^{13}C - ^{117}Sn = 957.5 Hz, Sn$\underline{C}$H$_2$CH$_2$), 25.64 (^2J ^{13}C - $^{119/117}$Sn = 166.3 Hz, $\underline{C}$H$_2$CH$_2$), 18.93 (OOC$\underline{C}$H$_3$), 13.67 (CH$_2$$\underline{C}H_3$). ^{119}Sn{H} NMR (186 MHz, $CDCl_3$): δ -531.51. IR-ATR (cm^{-1}): 1565, 1542, 1428, 1395, 1349, 699, 627.



[*n*-BuSn(O)(OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$

Efforts to synthesize [(*n*-BuSn(O)OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$ via a literature procedure[4] did not result in the isolation of [(*n*-BuSn(O)OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$ but rather [*n*-BuSn(O)OAc]$_6$. Instead, freeze drying of a solution of [*n*-BuSn(O)OAc]$_6$ (100 mg, 0.066 mmol) in 1 mL acetic acid gave [(*n*-BuSn(O)OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$ (113 mg, quantitative).

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.17 – 1.92 (m, 30H, OOCC$\underline{H}_3$), 1.81 – 1.15 (m, 34H , C$\underline{H}_2$), 0.96 – 0.79 (m, 18H, CH_3). ^{119}Sn{H} NMR (186 MHz, $CDCl_3$): δ -521.72, -554.17, -640.64. These ^{119}Sn NMR signals do not correspond to the -486, -522, -533 and -549 ppm reported in literature.[4] However, the signals at -486 and -533 ppm should not be assigned to [(*n*-BuSn(O)OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$ but rather to [*n*-BuSn(O)OAc]$_6$ and *n*-$BuSnOAc_3$, which are decomposition products. Due to this decomposition a pure ^{13}C NMR spectrum could not be recorded. In the ^{119}Sn{H} NMR spectrum obtained after the ^{13}C NMR measurement, additional peaks corresponding to decomposition products [*n*-BuSn(O)OAc]$_6$ (-484.84 ppm) and *n*-$BuSnOAc_3$ (-532.16 ppm) were observed.



4. *n*-BuSnOBz$_3$:

Under a nitrogen atmosphere AgOBz (6.48 g, 28.3 mmol) was suspended in 20 mL anhydrous DCM. Subsequently *n*-$BuSnCl_3$ (1.2 mL, 7.1 mmol) was slowly added and the reaction mixture was brought to reflux for 24 h. Filtration over celite and evaporation of the solvent resulted in a white solid material which was recrystallized from toluene/pentane to afford *n*-$BuSnOBz_3$ (3.15 g, 82% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 7.5 Hz, 6H, Ar$\underline{H}$), 7.61 (t, *J* = 7.4 Hz, 3H, Ar$\underline{H}$), 7.45 (t, *J* = 7.4 Hz, 6H, Ar$\underline{H}$), 2.04 (m, 2H, C$\underline{H}_2$), 1.83 (m, 2H, C$\underline{H}_2$), 1.45 (sext, *J* = 7.4 Hz, 2H, C$\underline{H}_2$), 0.90 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$).
^{13}C NMR (100 MHz, $CDCl_3$): δ 178.50 ($C_6H_5\underline{C}OO$), 134.02 ($\underline{C}_6H_5$), 131.26 ($\underline{C}_6H_5$), 128.37 ($\underline{C}_6H_5$), 127.58 ($\underline{C}_6H_5$)

29.58 (<u>C</u>H_2), 26.47 (<u>C</u>H_2), 25.56 (<u>C</u>H_2), 13.48 (<u>C</u>H_3). ^{119}Sn-^{13}C couplings were not well resolved. ^{119}Sn{H} NMR (186 MHz, $CDCl_3$): δ -535.56. IR-ATR (cm^{-1}): 1596, 1539, 1509, 1450, 1397, 1162, 1068, 1021, 827, 717, 681. FD-MS (*m/z, pos*): Calculated for [$C_{18}H_{19}O_4Sn_1$] 419.0309; found 419.0349 [M-OBz]$^+$; Calculated for [$C_{21}H_{15}O_6Sn_1$] 482.9895; found 482.9856 [M-C_4H_9]$^+$.

Single crystals suitable for XRD analysis were obtained via the slow vapor diffusion of *n*-hexane in a toluene solution. $C_{25}H_{24}O_6Sn$, Fw = 539.17, colorless block, 0.565×0.299×0.116 mm, orthorhombic, Pbca (No: 61)), a = 11.9618(3), b = 16.8603(4), c = 23.0411(6) Å, V = 4646.9(2) Å3, Z = 8, Dx = 1.541 g/cm3, m = 1.138 mm-1. 54938 Reflections were measured up to a resolution of (sin q/l)max = 0.63 Å-1. 4751 Reflections were unique (Rint = 0.0813), of which 3599 were observed [I>2s(I)]. 290 Parameters were refined without any restraints. R1/wR2 [I > 2s(I)]: 0.0277/0.0497. R1/wR2 [all refl.]: 0.0478/ 0.0553. S = 1.049. Residual electron density between -0.362 and 0.517 e/Å3. CCDC 2049109 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

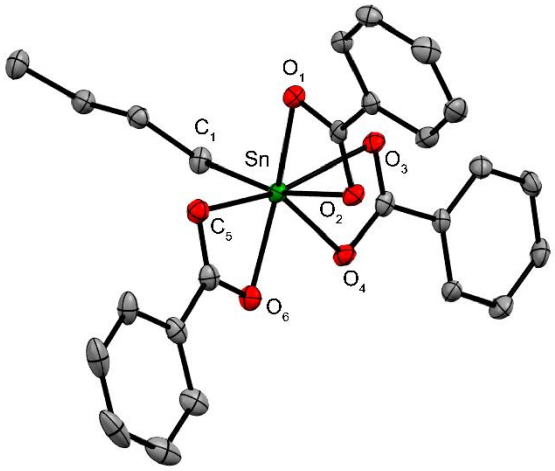
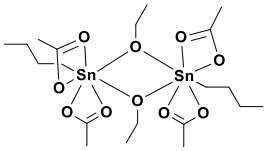


Fig. S1 ORTEP view of solid state structure of *n*-$BuSnOBz_3$. Ellipsoids are given at 50% probability level. H atoms are omitted for clarity. Selected bond distances (Å): Sn-O_1 = 2.373(2) , Sn-O_2 = 2.133(2) , Sn-O_3 = 2.242(2) , Sn-O_4 = 2.135(2) , Sn-O_5 = 2.328(2) , Sn-O_6 = 2.156(2) , Sn-C_1 = 2.118(3). Selected angles (°): C_1-Sn-O_1 = 93.94(8), C_1-Sn-O_5 = 96.39(8). Colors correspond to tin (green), oxygen (red) and carbon (gray).



5A. (*n*-BuSnOAc$_2$OEt)$_2$

Under a nitrogen atmosphere *n*-BuSnOAc$_3$ (345 mg, 0.987 mmol) and (*n*-BuSnOEt$_3$)$_4$ (42 mg, 0.122 mmol) were both dissolved in 2.5 mL anhydrous DCM. Afterwards the *n*-BuSnOEt$_3$ solution was transferred via a syringe and slowly added to the *n*-BuSnOAc$_3$ solution. After stirring for 1h the solvent was removed in *vacuo*, providing a yellowish oil (512 mg, quant.). Since the complex slowly decomposes at room temperature the ^{13}C NMR spectrum was recorded at 233 K.

^{1}H NMR (500 MHz, $CDCl_3$): δ 3.99 (br s, 4H, $CH_3C\underline{H}_2O$), 2.10 (s, 12H, $C\underline{H}_3COO$), 1.61 (m, 8H, $C\underline{H}_2C\underline{H}_2$), 1.34 (sext, *J* = 6.9 Hz, 4H, $C\underline{H}_2$), 1.18 (t, *J* = 6.8 Hz, 6H, $OCH_2C\underline{H}_3$), 0.89 (t, *J* = 7.3 Hz, 6H, $OC\underline{H}_2C\underline{H}_3$). ^{13}C NMR 233 K (125 MHz, $CDCl_3$): δ 182.61 ($CH_3\underline{C}OO$), 61.37 ($O\underline{C}H_2CH_3$), 27.74 ($\underline{C}H_2$), 27.06 ($\underline{C}H_2$), 26.27 ($\underline{C}H_2$), 20.06 ($\underline{C}H_3COO$), 18.44 ($\underline{C}H_3CH_2O$), 14.03 ($\underline{C}H_3CH_2CH_2$). ^{119}Sn-^{13}C couplings were not well resolved. ^{119}Sn{H} NMR (186 MHz, $CDCl_3$): δ -543.73. IR-ATR (cm^{-1}): 1560, 1411, 1048, 1021, 877, 662, 613, 546. LIFDI-FD-MS (*m/z, pos*): Calculated for [$C_{16}H_{31}O_{10}Sn_2$] 620.9963; found 620.9983 [M-C_4H_9]$^+$.

Catalysis

Procedure for esterification of benzoic acid and heptanol

In a carousel reaction station under a nitrogen atmosphere benzoic acid (610.6 mg, 5 mmol) was suspended in heptanol (7.14 mL, 50 mmol). Subsequently, the catalyst (1 mol%) and pentadecane (0.41 mL, 1.5 mmol) as internal standard were added. After 6h (at 150 °C) the conversion and yield were determined with GC analysis via the integration of the peak area of benzoic acid and heptylbenzoate.

Procedure for determination of the catalyst order

In a carousel reaction station under a nitrogen atmosphere benzoic acid (600 mg, 4.9 mmol) was suspended in heptanol (7 mL, 49 mmol). Subsequently, *n*-BuSnOOH (0.5, 1, 2 or 3 mol%), o-xylene (2 mL) and pentadecane (0.40 mL, 1.45 mmol) as internal standard were added. After 15, 30, 45 and 60 min (at 150 °C) samples were taken for GC analysis. The rate (M*s) was determined via a tangent line of the heptyl benzoate concentrations.

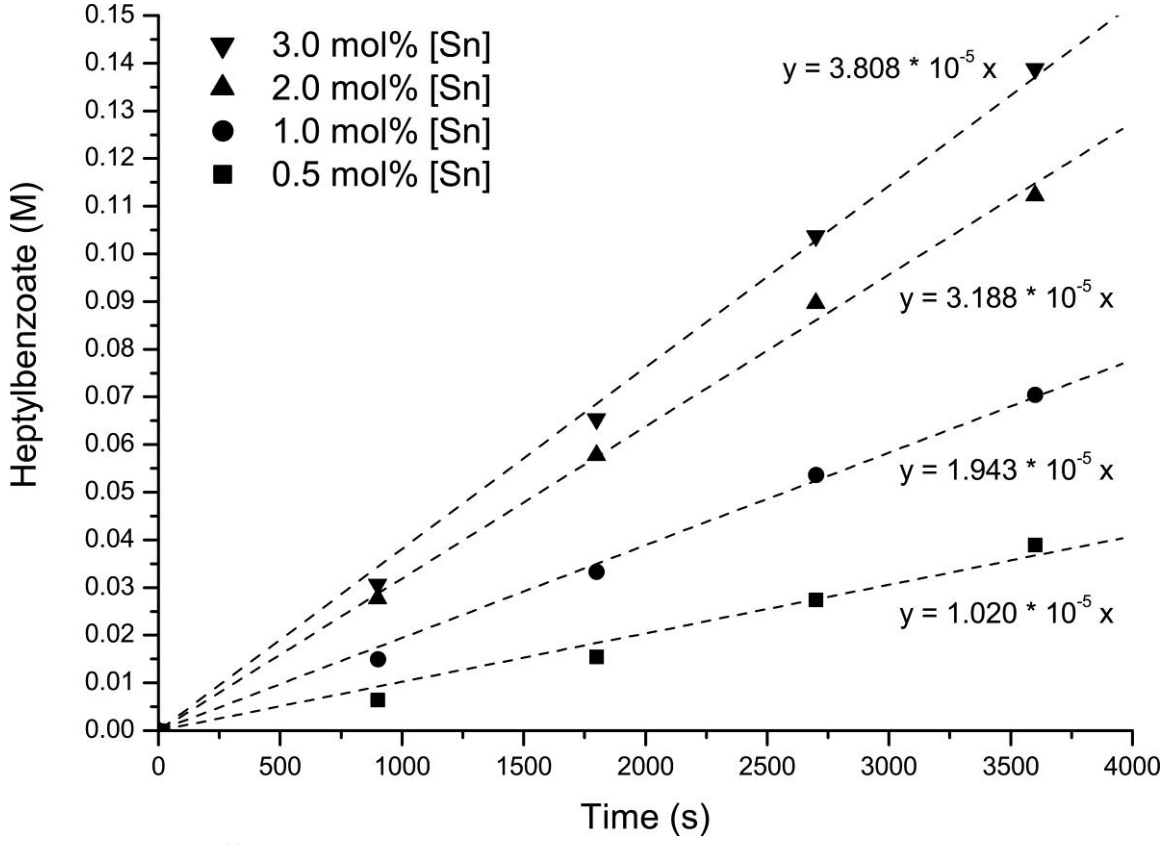


Fig. S2 Initial rate at different catalyst loadings

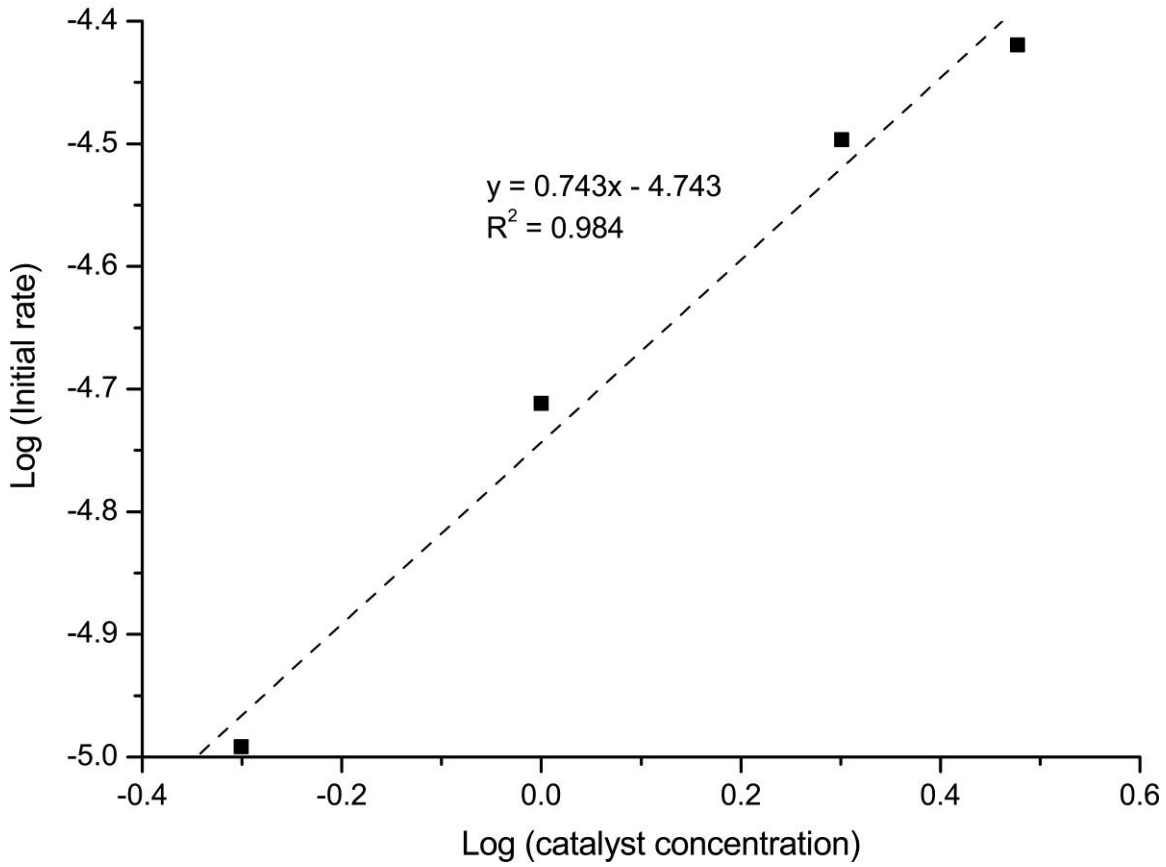


Fig. S3 Order in catalyst (*n*-BuSnOOH)

Procedure for esterification of acetic acid and ethanol

Activated molecular sieves (3Å, 2.0 g) and 1.2 mmol of tin catalyst (0.4 M) were loaded in a Schlenk reaction tube and placed under a nitrogen atmosphere. Anhydrous EtOH (1.5 mL) and acetic acid (1.5 mL) were added and the reaction mixture was heated to 90 °C in an oil bath. Aliquots (0.5 mL) for NMR analysis were taken after 5, 30 and 60 min and ^{119}Sn NMR spectra were directly measured at 90 °C (in a pre-heated NMR machine) and at 25 °C (sample cooled outside NMR machine). The conversion was monitored by ^{1}H NMR spectroscopy from the relative intensities of the methylene protons of EtOH at 3.68 ppm and ethylacetate at 4.09 ppm.

Computational details

Density functional theory calculations were performed using the TURBOMOLE software package, version 7.3.1,[5] coupled to the PQS Baker optimizer[6] via the BOpt package.[7-9] All structure optimizations were performed at the BP86[10-12]/def2-TZVP[13,14] level of theory on an m5 grid using Grimme's version 3 dispersion corrections (disp3)[15], with the corresponding effective core potential (def2-ECP) for Sn. This functional/basis set combination was found to be a good trade-off between accuracy in the geometric parameters of $Sn(OAc)_4$ compared to the known crystal structure[16], and computational costs (Table S1). All minima were characterized by no imaginary frequency in the Hessian matrix, while transition states had a single imaginary frequency. Energies were further refined using the M06-2x functional,[17,18] implemented via the XCFun library,[19] in combination with the def2-QZVPP basis set for Sn (with ECP) and def2-TZVP for all other elements, a very fine grid (7) and disp3 dispersion corrections. The M06-2x functional is optimized for main group elements is used for Sn-containing complexes.[20]

Functional	*Deviation in average Sn-O bond length*	*Absolute deviation in O-Sn-O angles*
BP86 / disp3	0.01839325	1.132
BP86	0.02534825	1.211
B3LYP / disp3	-0.0017655	1.225
M06-L / disp3	-0.03221675	0.7425
M06-2x / disp3	-0.01011175	0.9652

Table S1. Comparison of average geometric parameters of $Sn(OAc)_4$ versus published crystal structure, using different functionals, with or without disp3. All calculations were performed with the def2-TZVP basis set and grid size m5

Isotropic NMR shielding constants were calculated using the Gauge Including Atomic Orbital (GIAO) method[21] as implemented in TURBOMOLE, using the B3LYP functional[22-25] (with grid size 5) in combination with the TZVPPall basis set for Sn and def2-TZVP for all other elements. For comparison to experiment, relative chemical shifts were calculated by referencing to $Sn(CH_3)_4$. The calculated relative chemical shifts were compared to the experimentally obtained chemical shifts for three known compounds, measured at 25 °C in $CDCl_3$: *n*-$BuSn(OAc)_3$, $[n\text{-BuSn(O)OAc}]_6$ and $[(n\text{-BuSn(O)OAc})_2 n\text{-BuSn(OAc)}_3]_2$. Linear regression was

performed to fit the calculated chemical shifts to the experimental values. The B3LYP/TZVPPall combination gave a good fit (R^2 = 0.9933). Using the thus obtained fit parameters, other calculated chemical shifts were compared to the experimental shifts of unknown compounds.

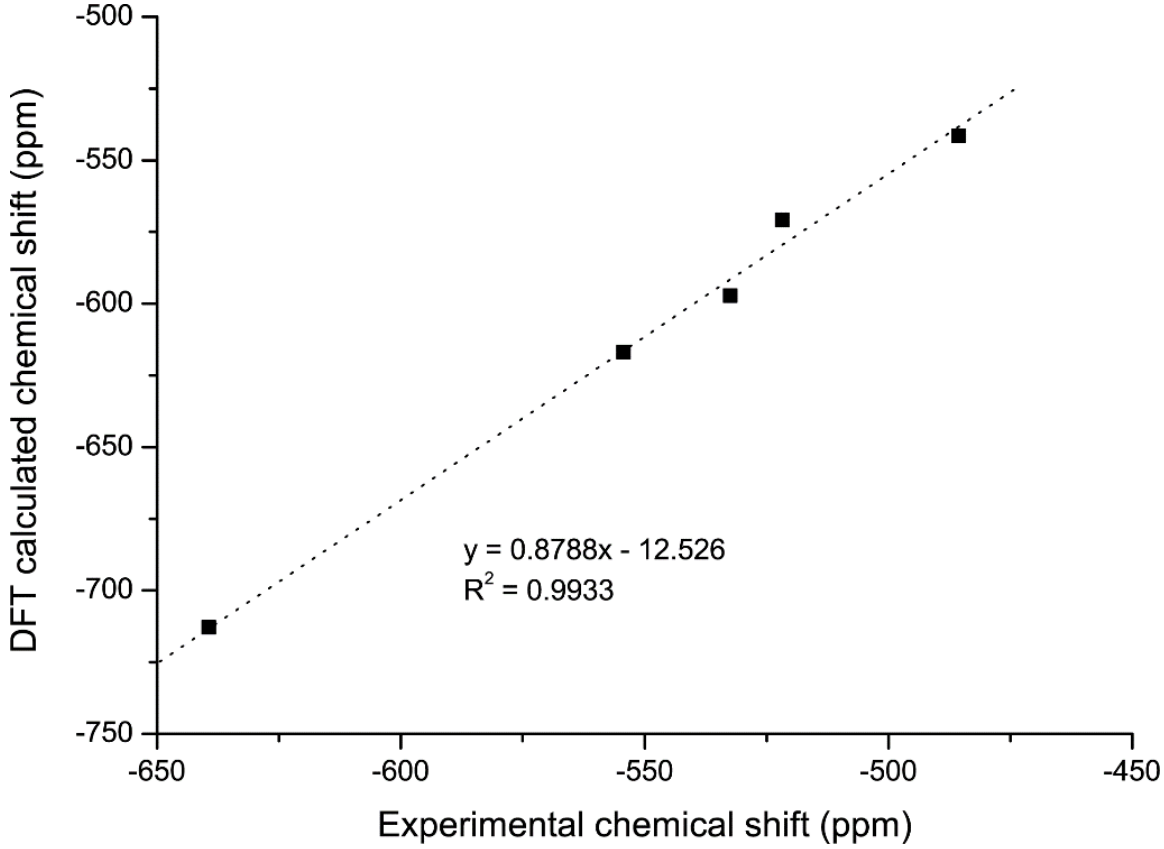


Fig. S4 Correlation between experimental and calculated ^{119}Sn chemical shifts for B3LYP/TZVPPall

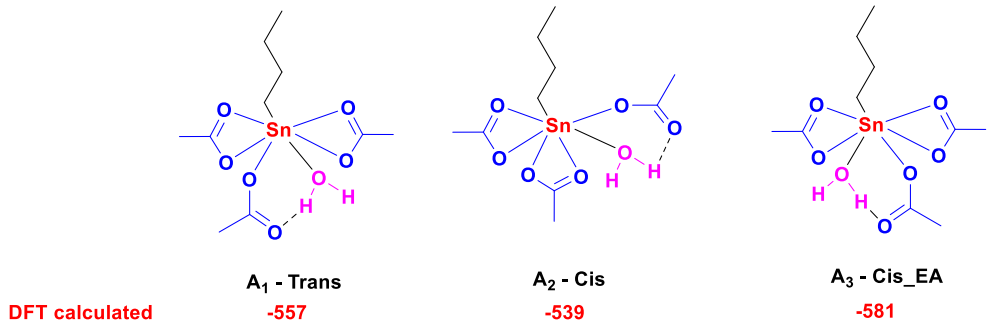


Fig. S5 DFT calculated ^{119}Sn NMR chemical shifts (in red, in ppm) of adducts of **3** with a single H_2O molecule

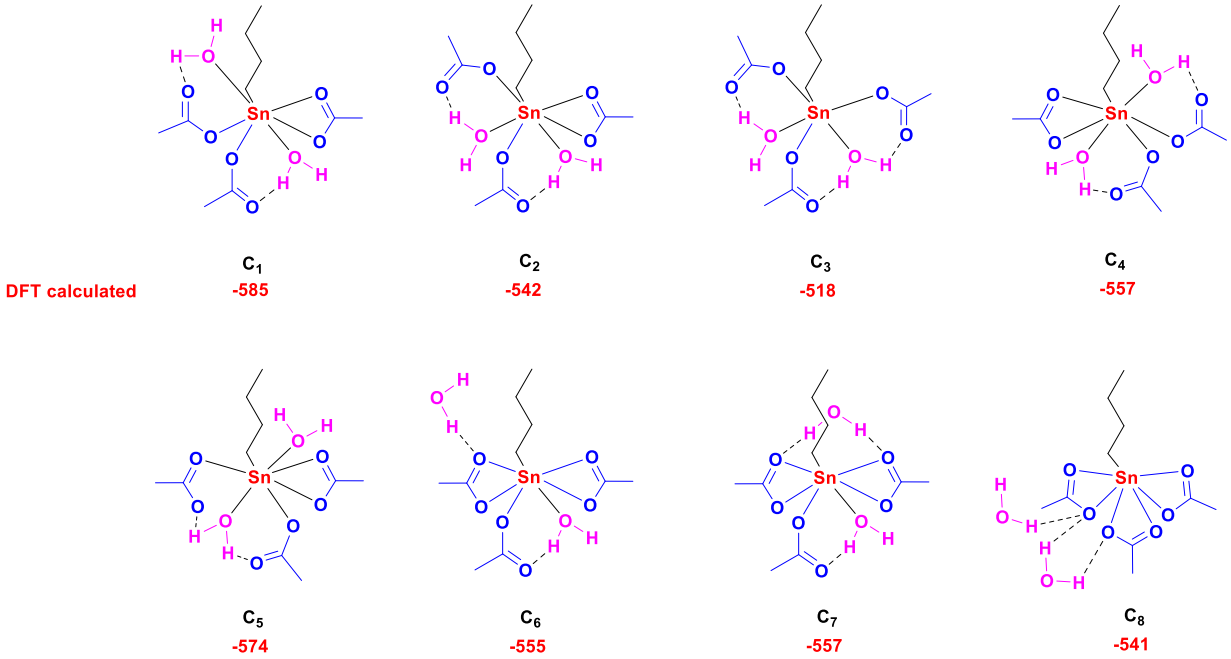
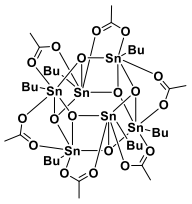


Fig. S6 DFT calculated ^{119}Sn NMR chemical shifts (red, in ppm) of adducts of **3** with two H_2O molecules

Spectra



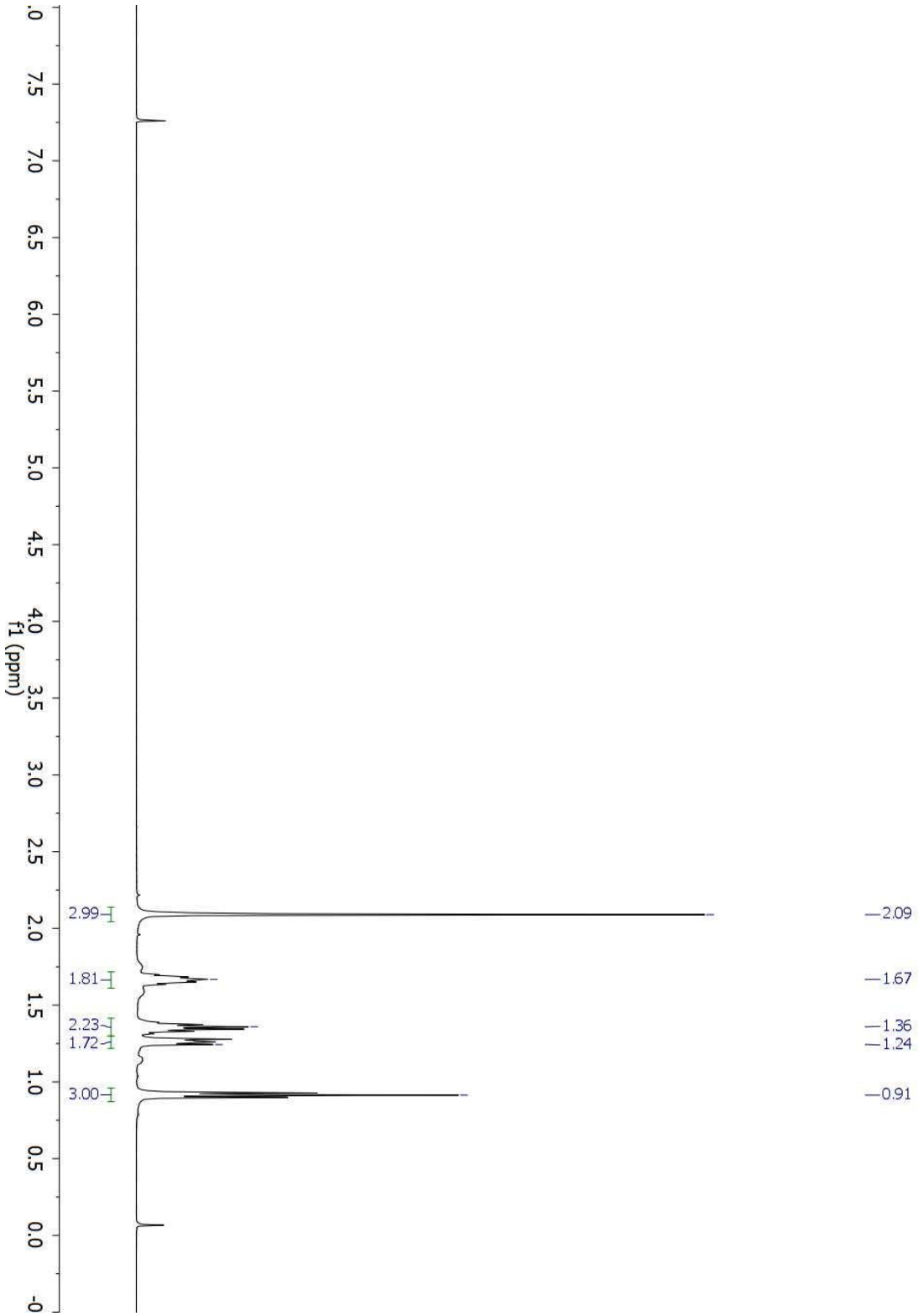


Fig. S7 ^{1}H NMR of **2** ([*n*-BuSn(O)OAc]$_6$), $CDCl_3$ at 298 K

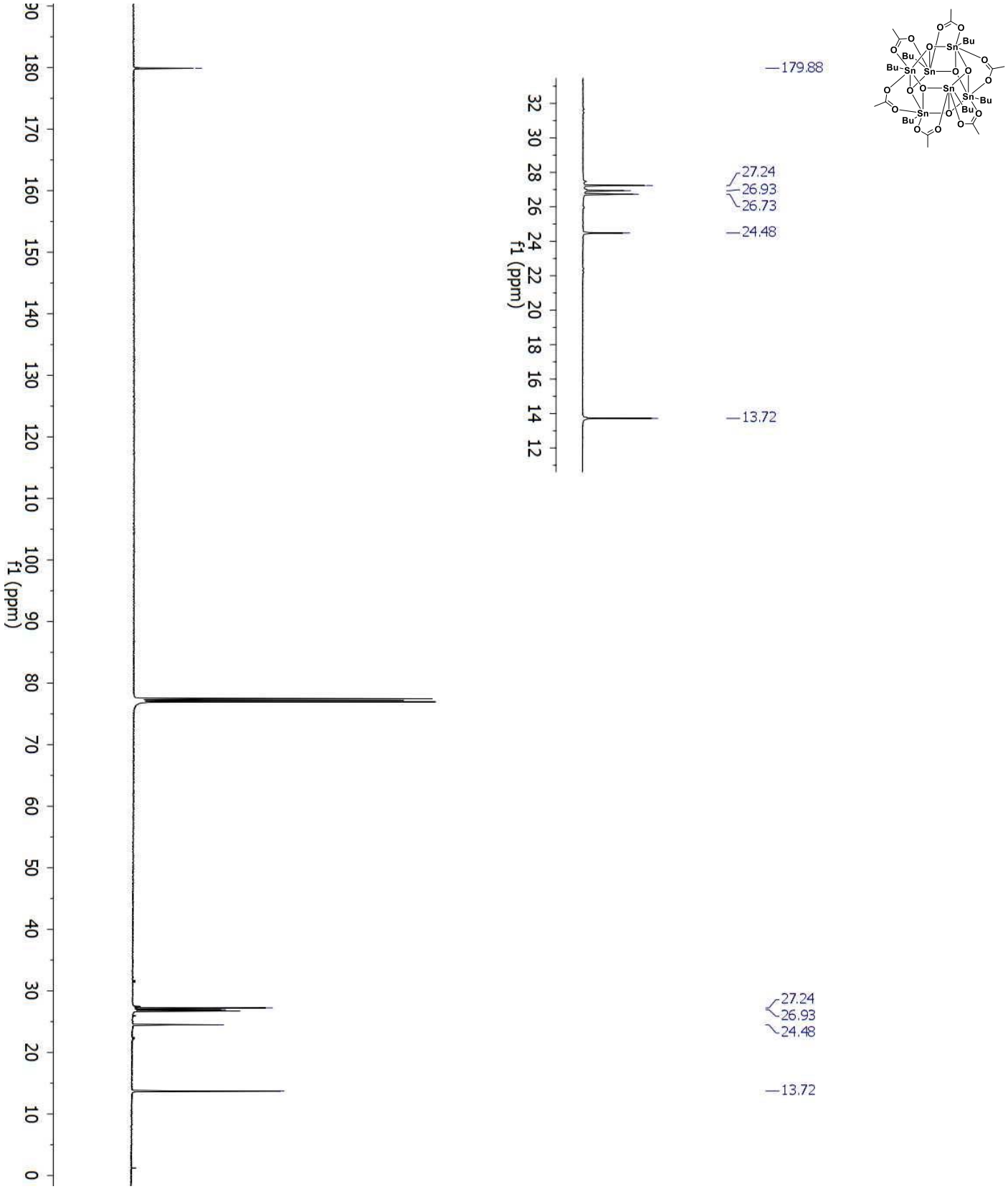


Fig. S8 ^{13}C NMR of **2**, $CDCl_3$ at 298 K

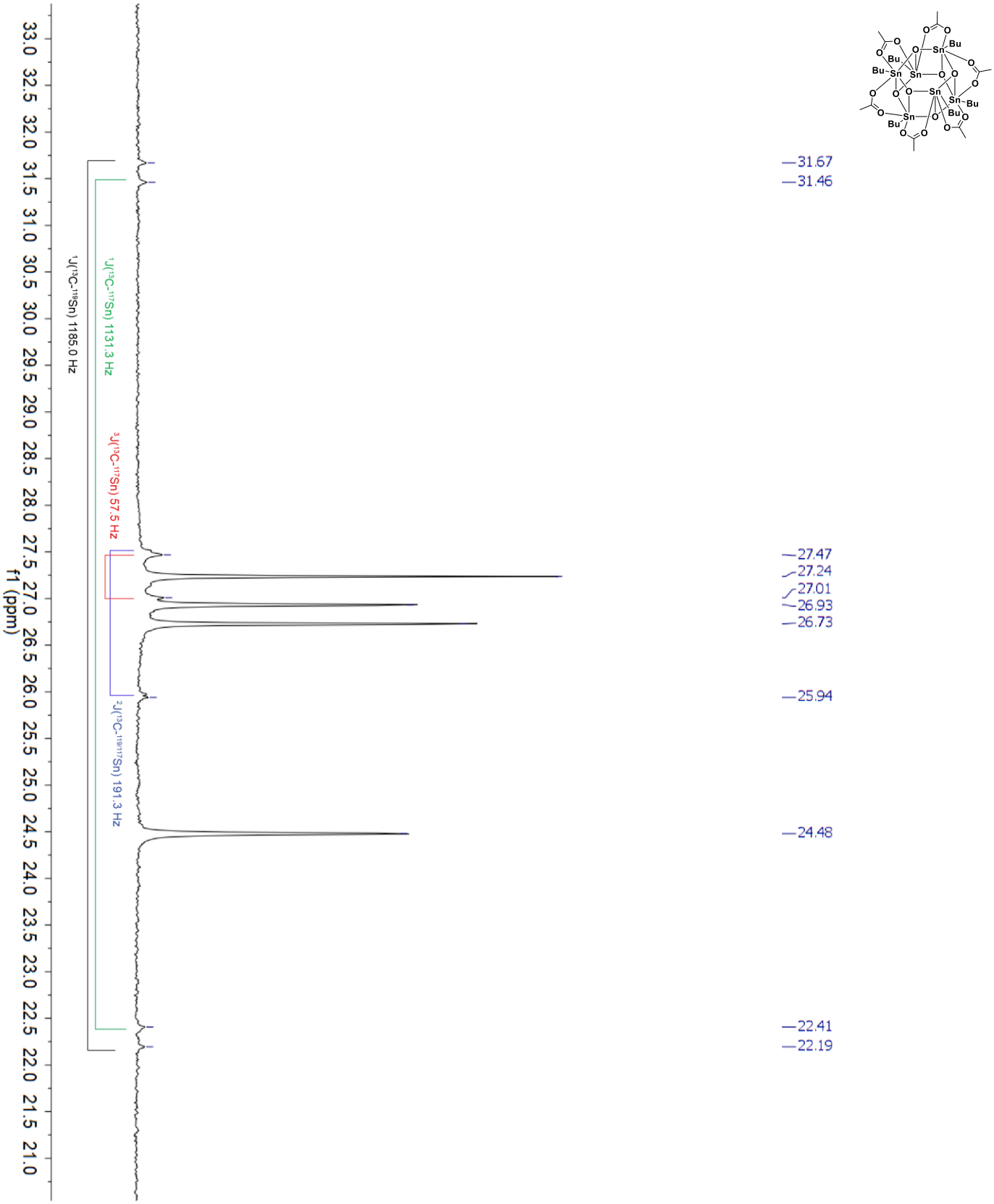


Fig. S9 *J*-coupling of ^{13}C – ^{119}Sn ^{13}C NMR of **2**, $CDCl_3$ at 298 K

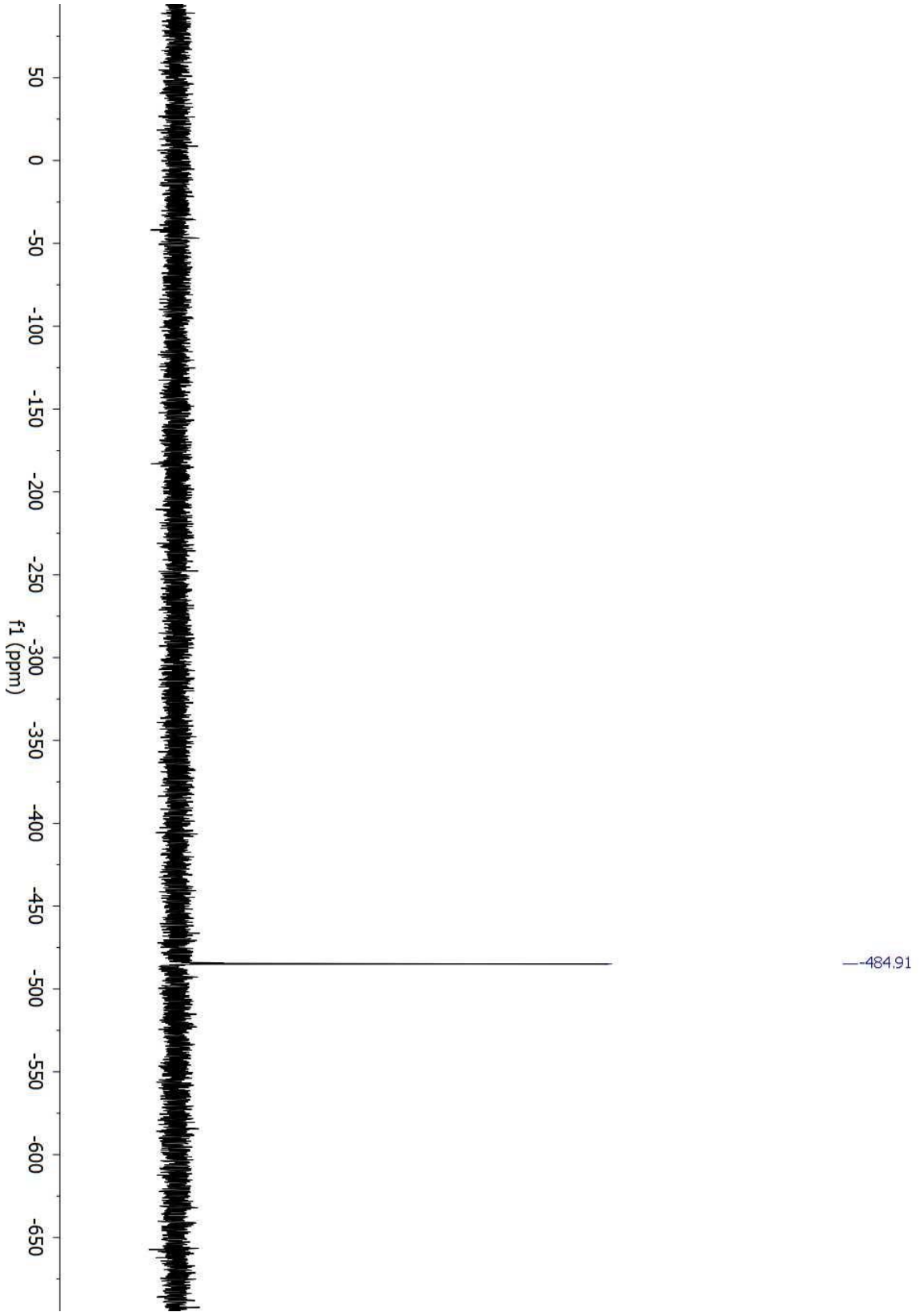


Fig. S10 $^{119}Sn\{H\}$ NMR of **2**, $CDCl_3$ at 298 K

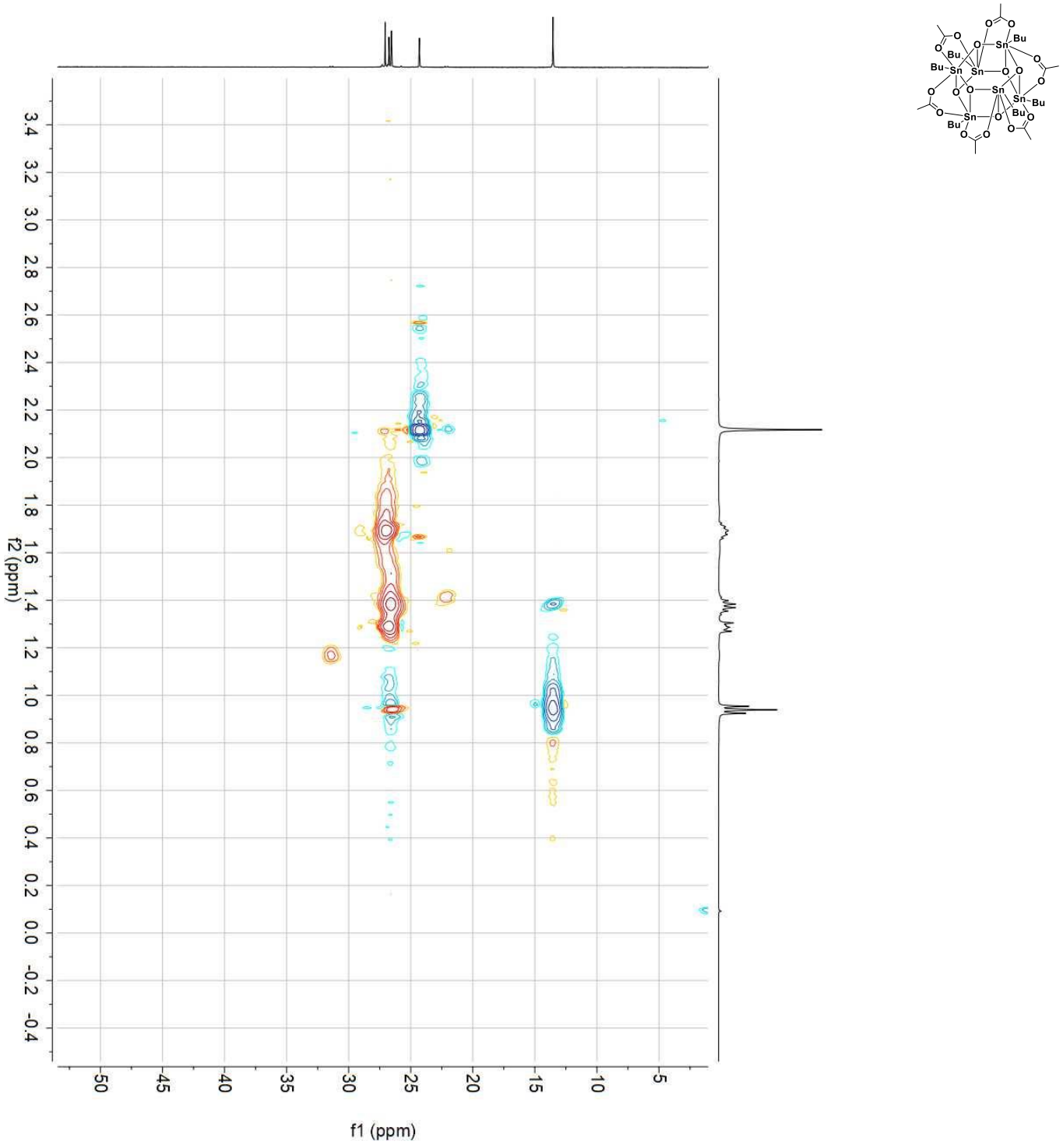


Fig. S11 ^{1}H-^{13}C HSQC NMR of **2**, $CDCl_3$ at 298 K

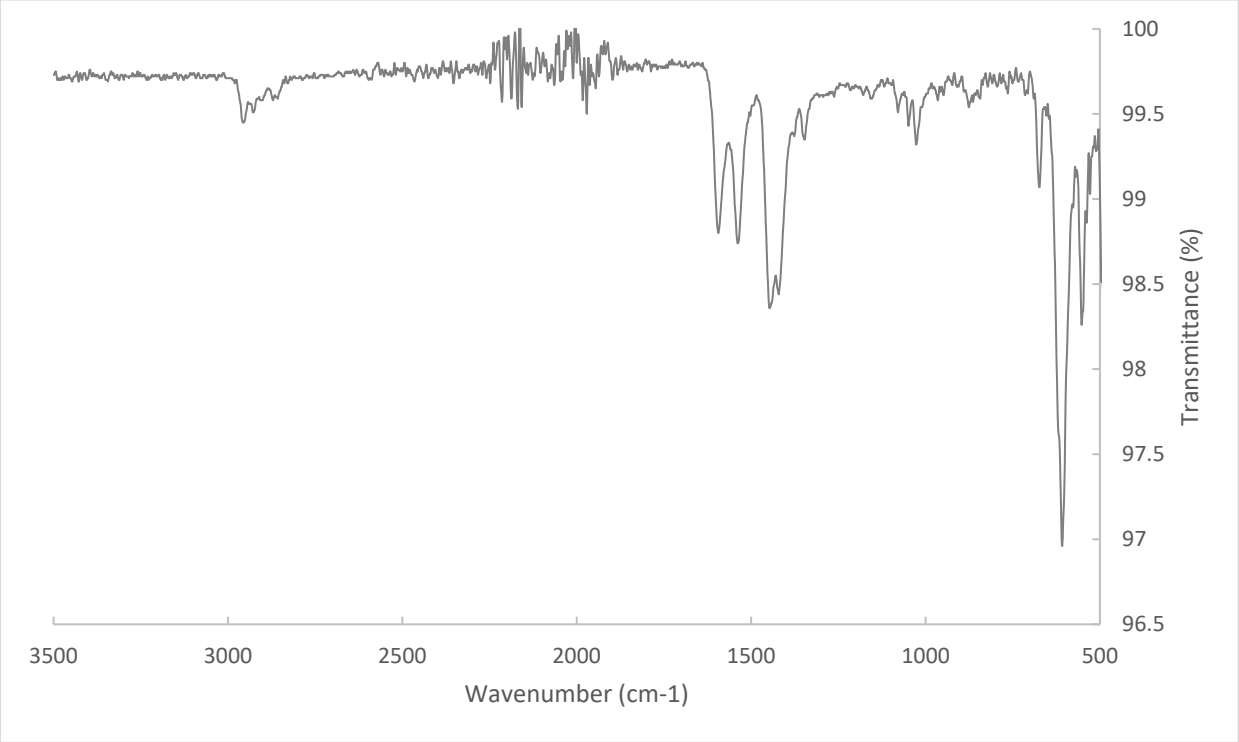
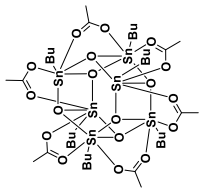


Fig. S12 IR-ATR spectrum of **2**



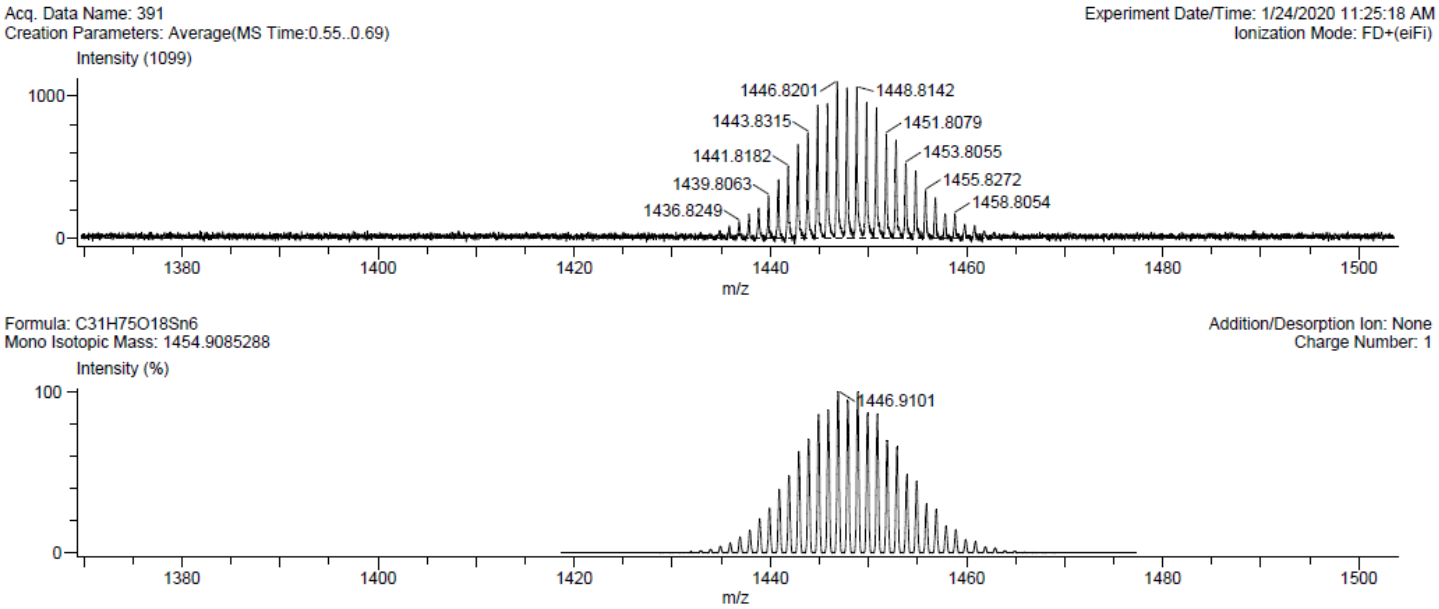


Fig. S13 FD-MS spectrum of **2**

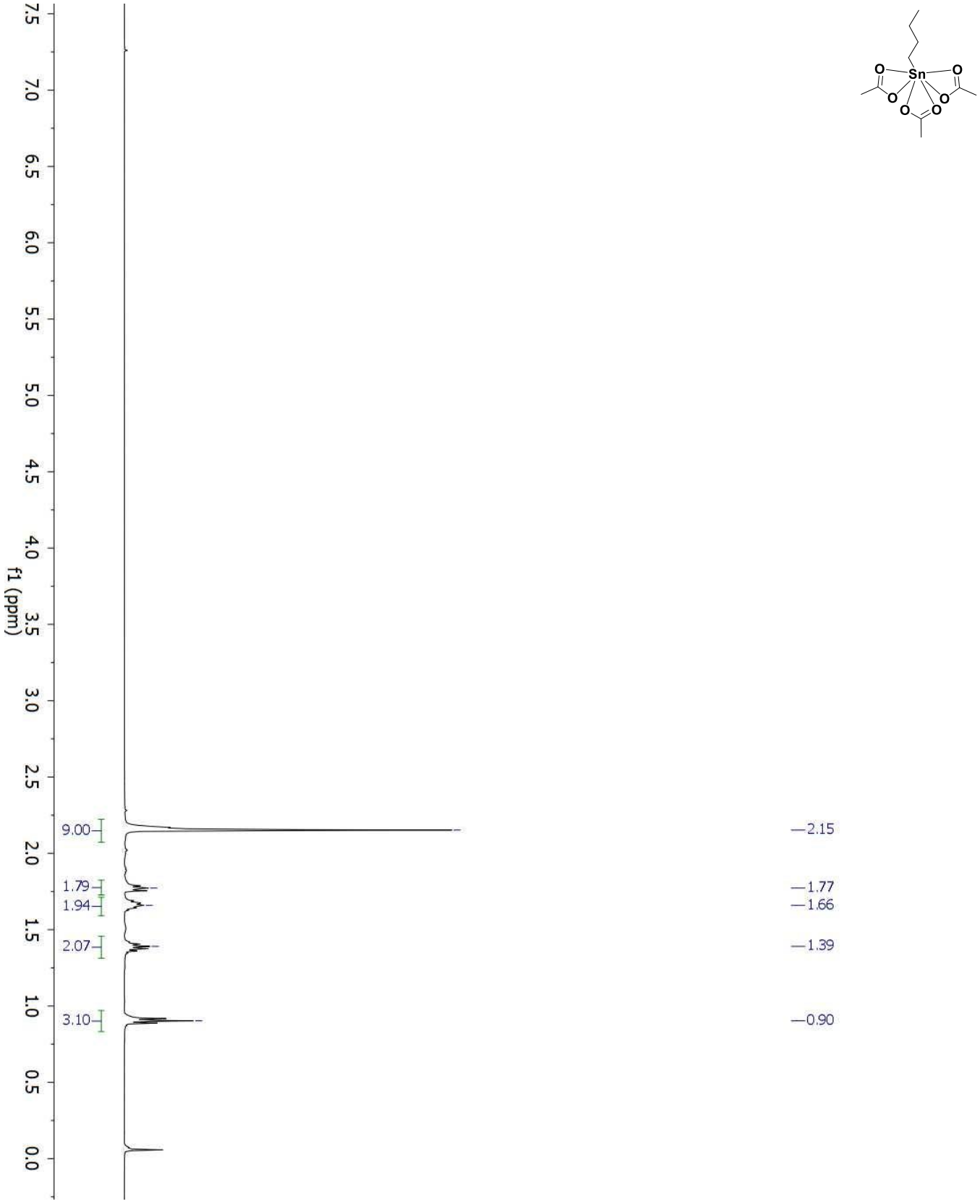


Fig. S14 ^{1}H NMR of **3** (*n*-BuSnOAc$_3$), $CDCl_3$ at 298 K

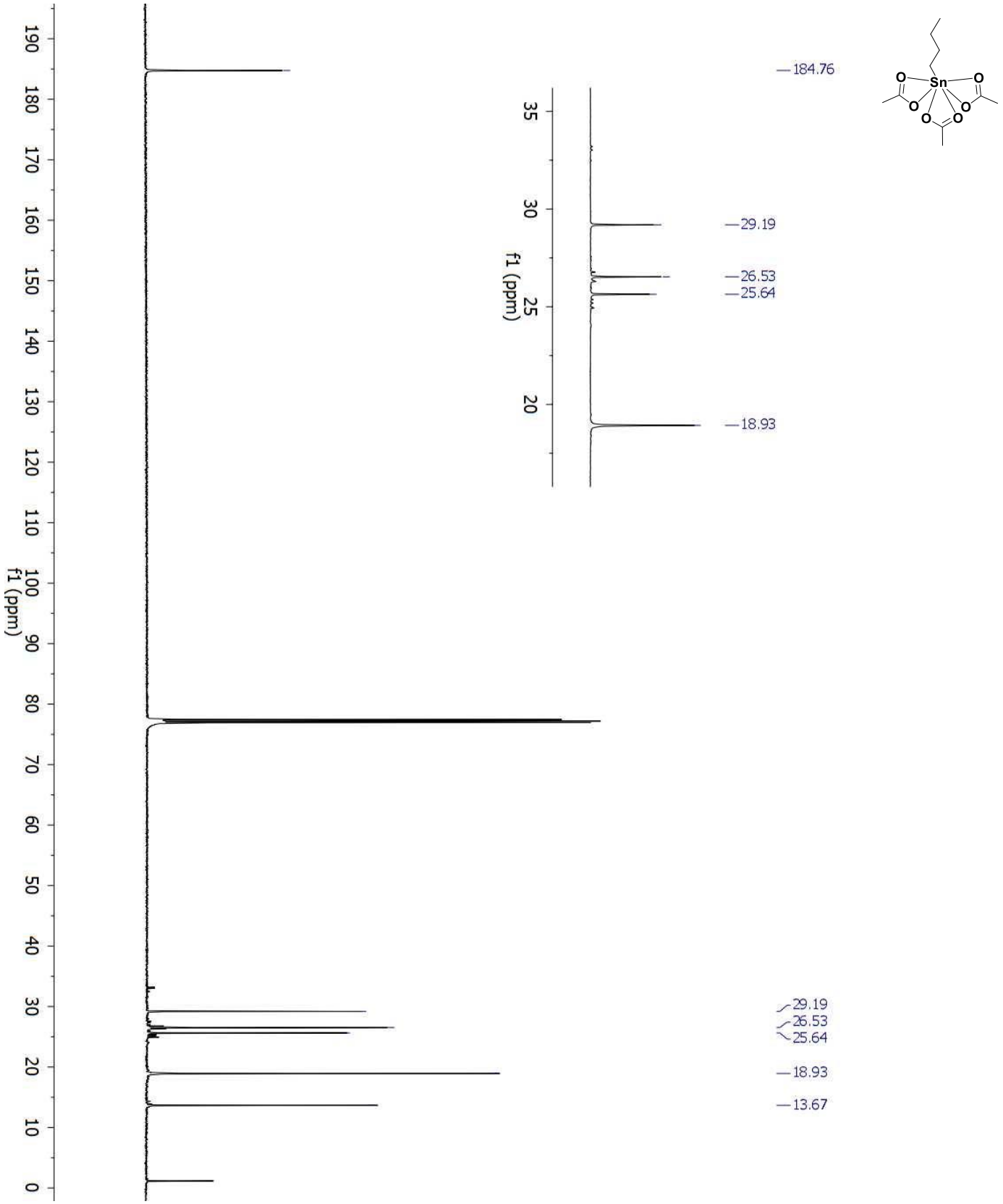


Fig. S15 ^{13}C NMR of **3**, $CDCl_3$ at 298 K

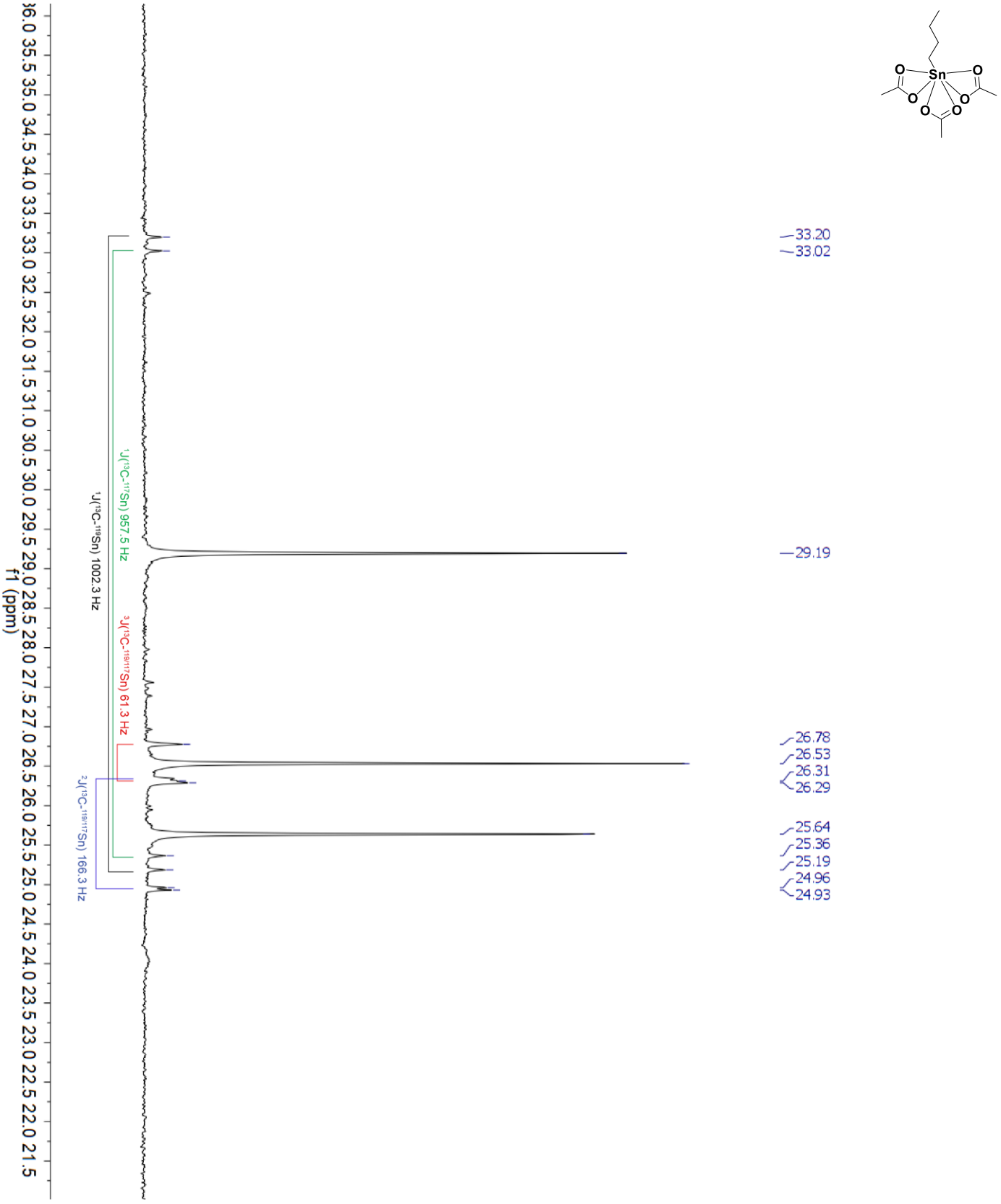


Fig. S16 *J*-coupling of ^{13}C – ^{119}Sn ^{13}C NMR of **3**, $CDCl_3$ at 298 K

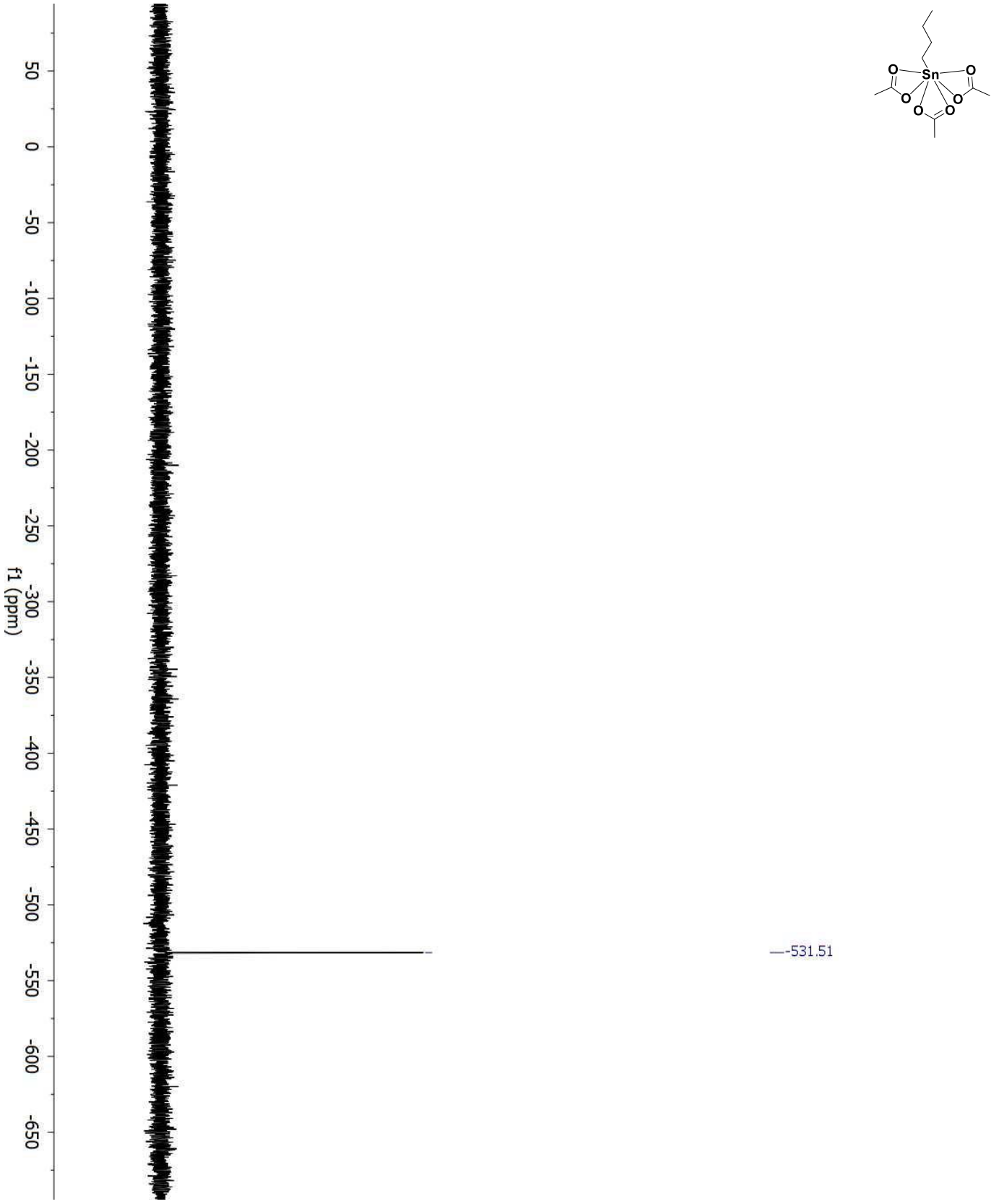


Fig. S17 ^{119}Sn{H} NMR of **3**, $CDCl_3$ at 298 K

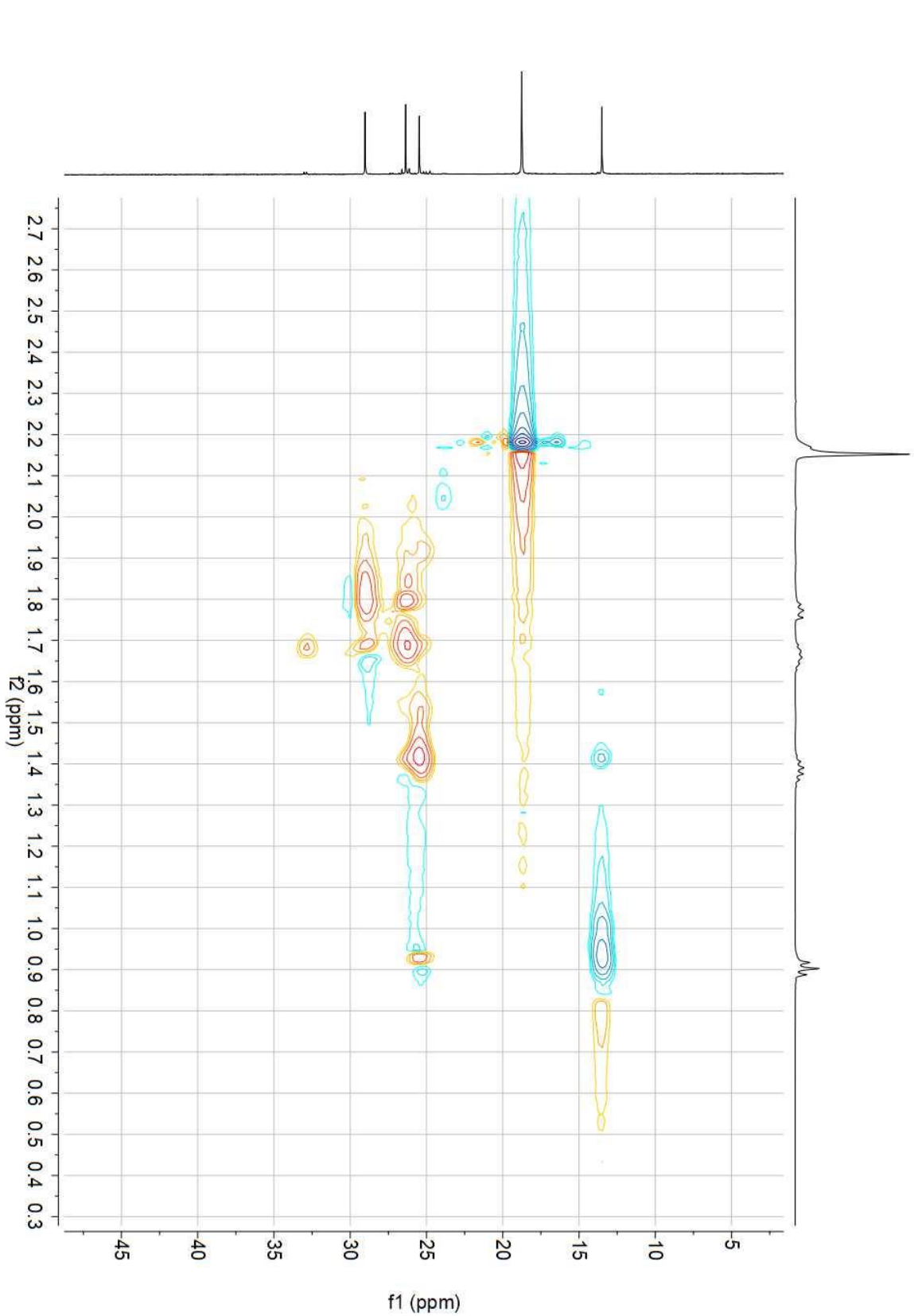


Fig. S18 ^{1}H-^{13}C HSQC NMR of **3**, $CDCl_3$ at 298 K

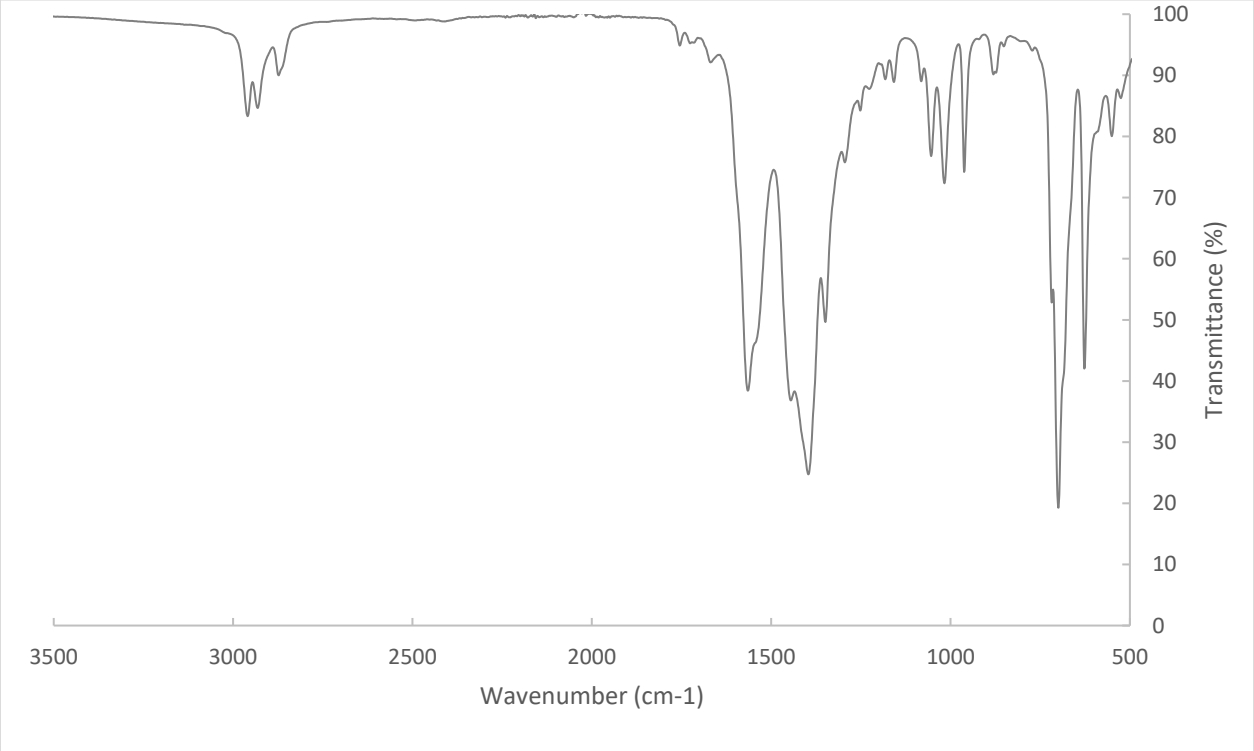


Fig. S19 IR-ATR spectrum of **3**

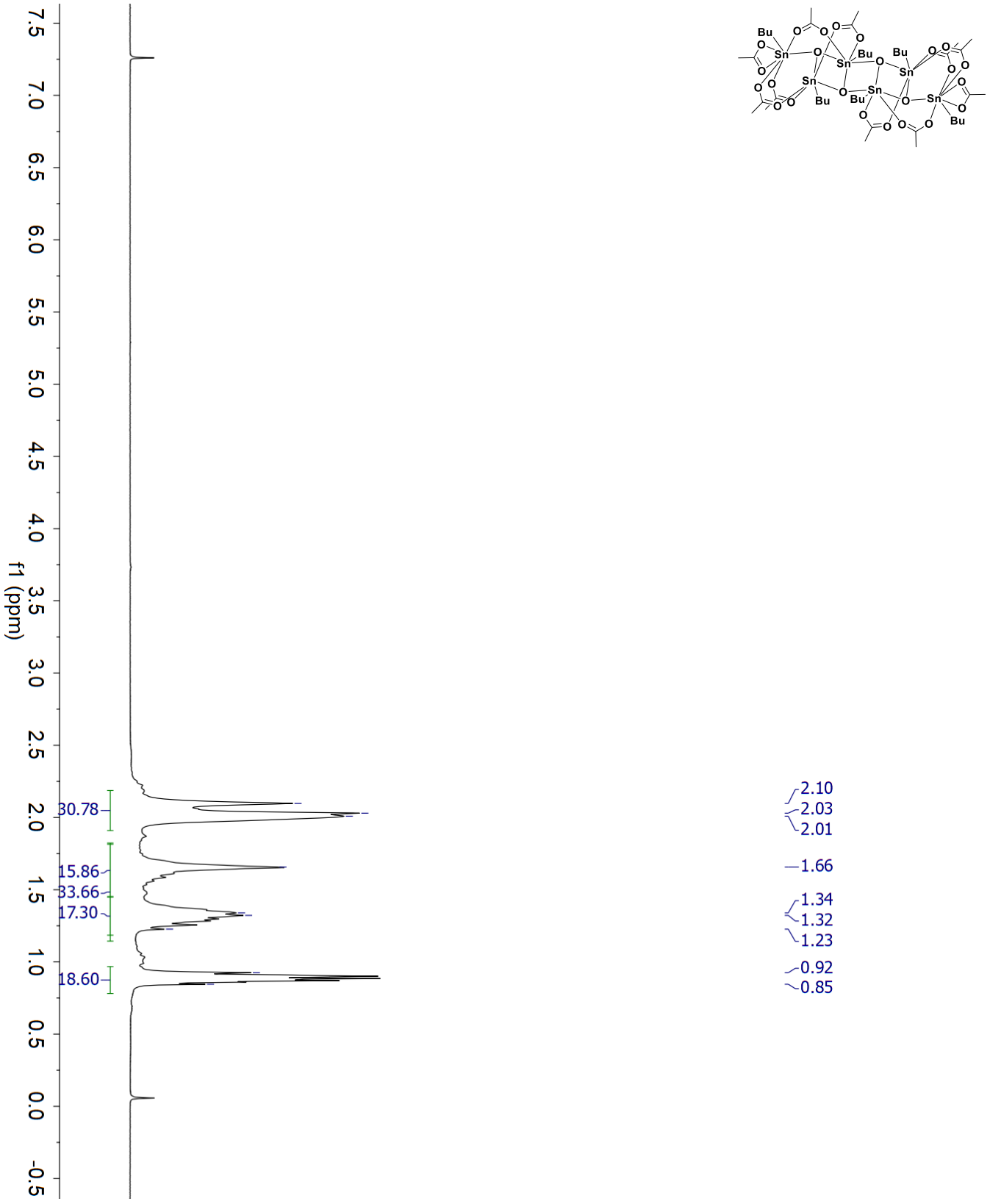


Fig. S20 ^{1}H NMR of [*n*-BuSn(O)(OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$, $CDCl_3$ at 298 K

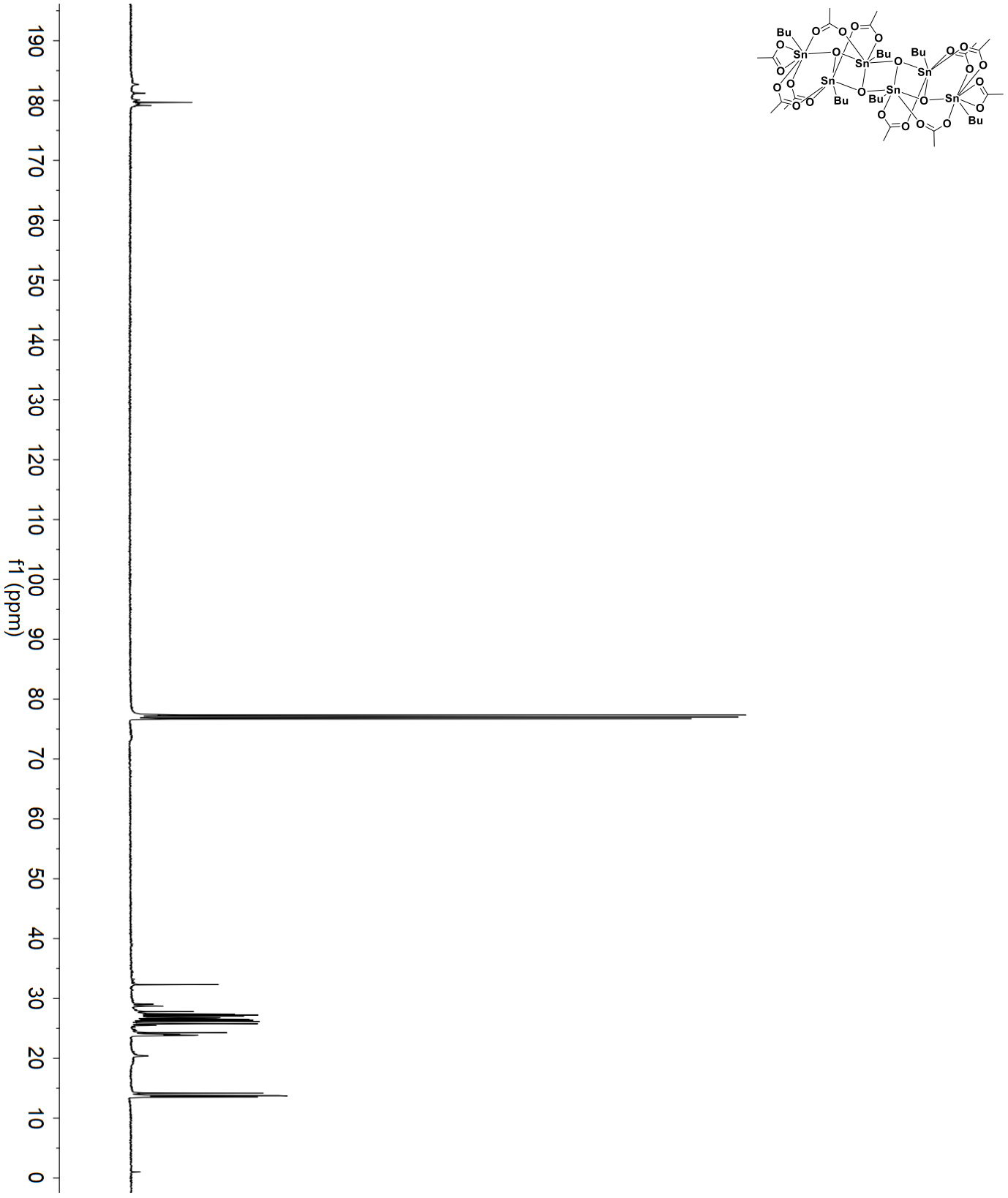


Fig. S21 ^{13}C NMR of [*n*-BuSn(O)(OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$, $CDCl_3$ at 298 K

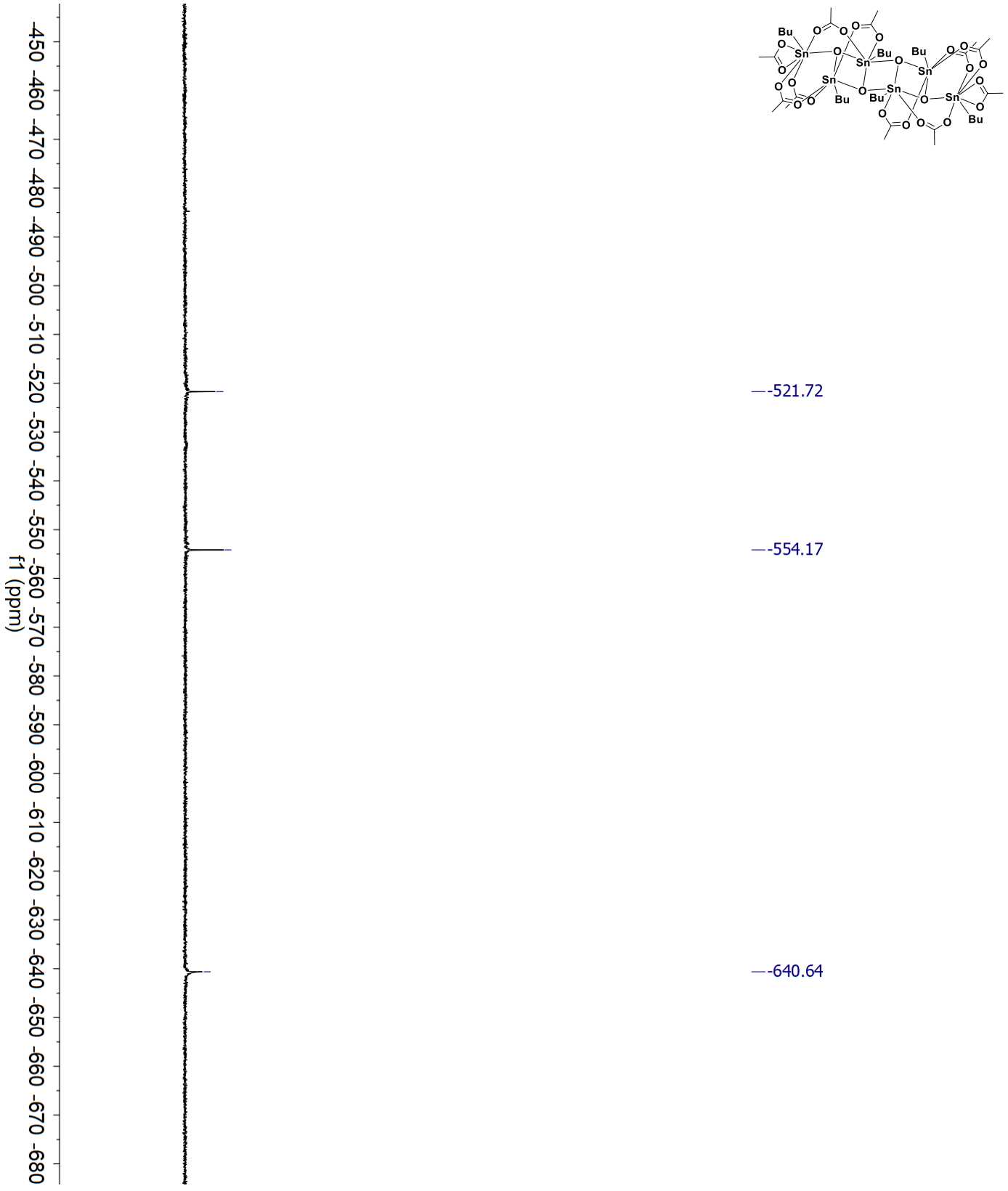


Fig. S22 ^{119}Sn NMR of [*n*-BuSn(O)(OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$, $CDCl_3$ at 298 K

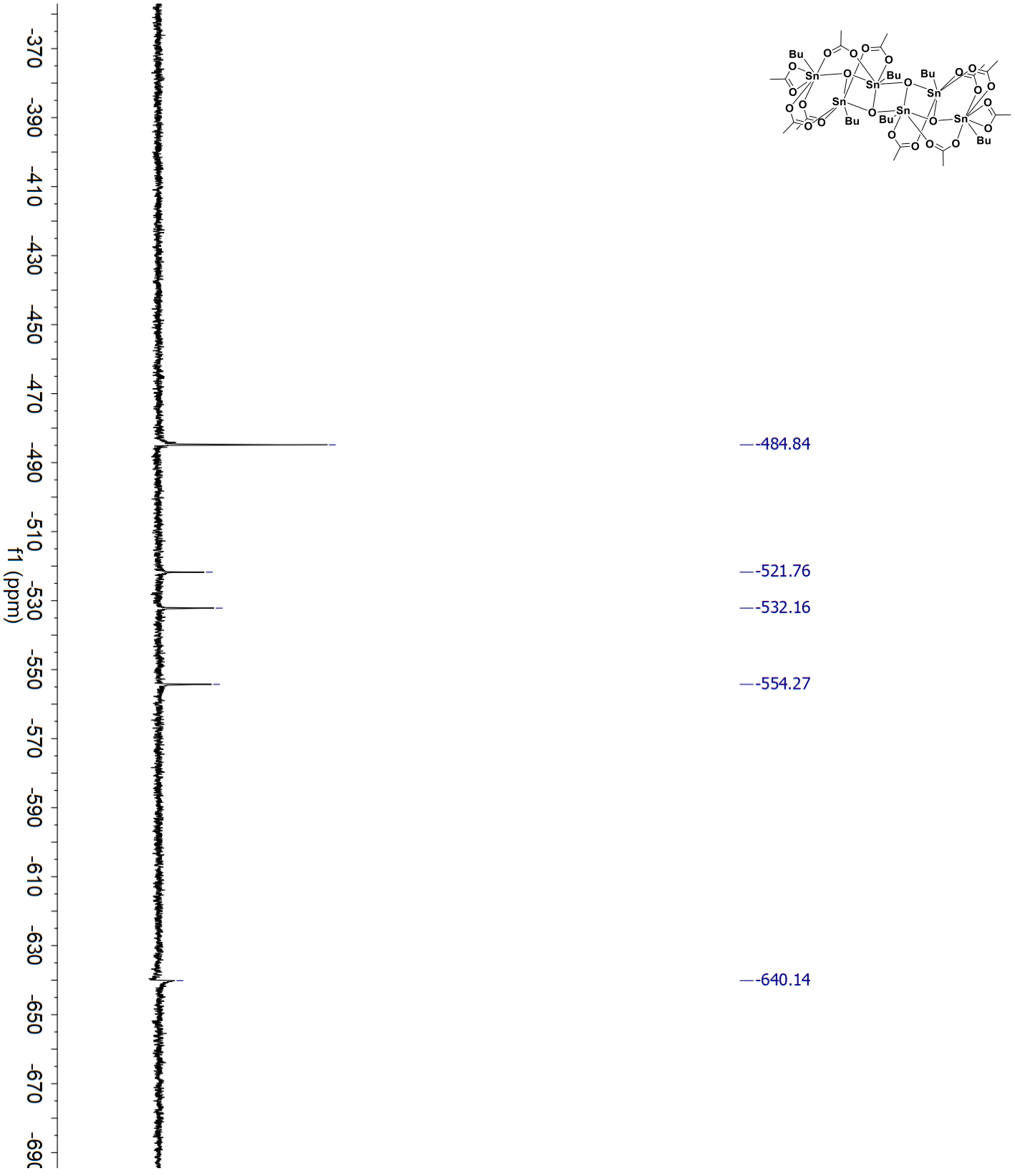


Fig. S23 ^{119}Sn NMR of [*n*-BuSn(O)(OAc)$_2$*n*-BuSn(OAc)$_3$]$_2$ after ^{13}C NMR, $CDCl_3$ at 298 K

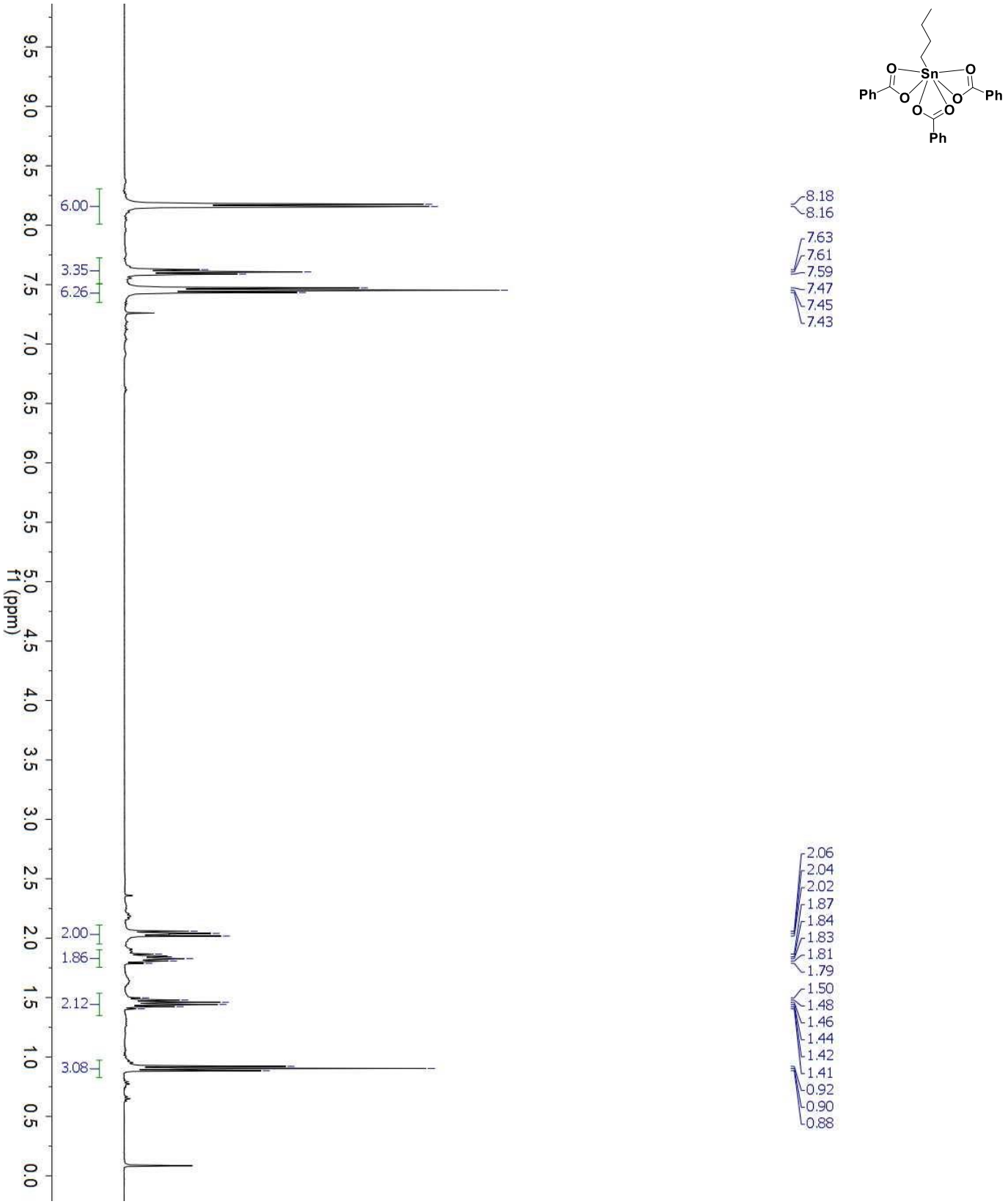


Fig. S24 ^{1}H NMR of **4** (*n*-BuSnOBz$_3$), $CDCl_3$ at 298 K

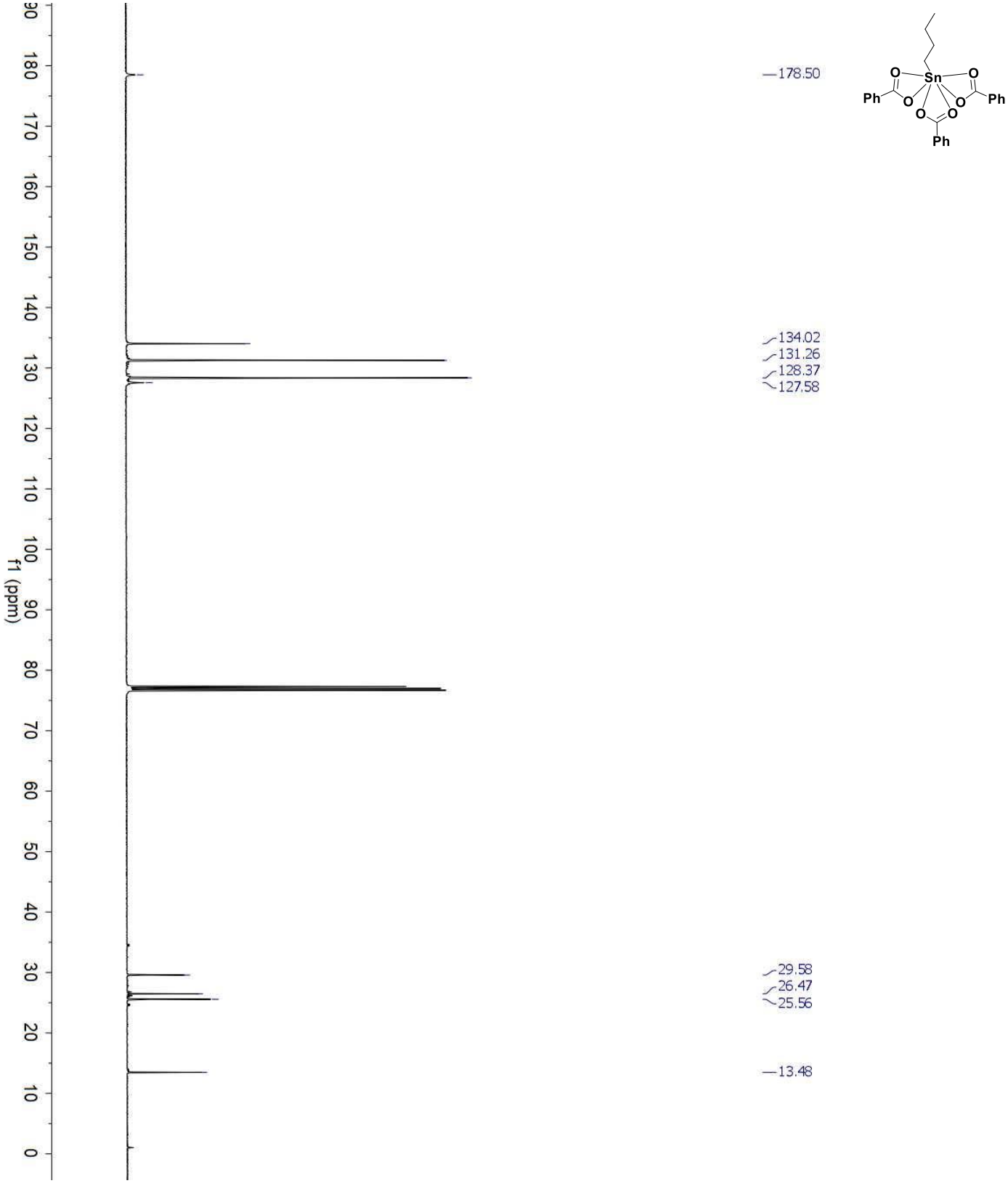


Fig. S25 ^{13}C NMR of **4**, $CDCl_3$ at 298 K

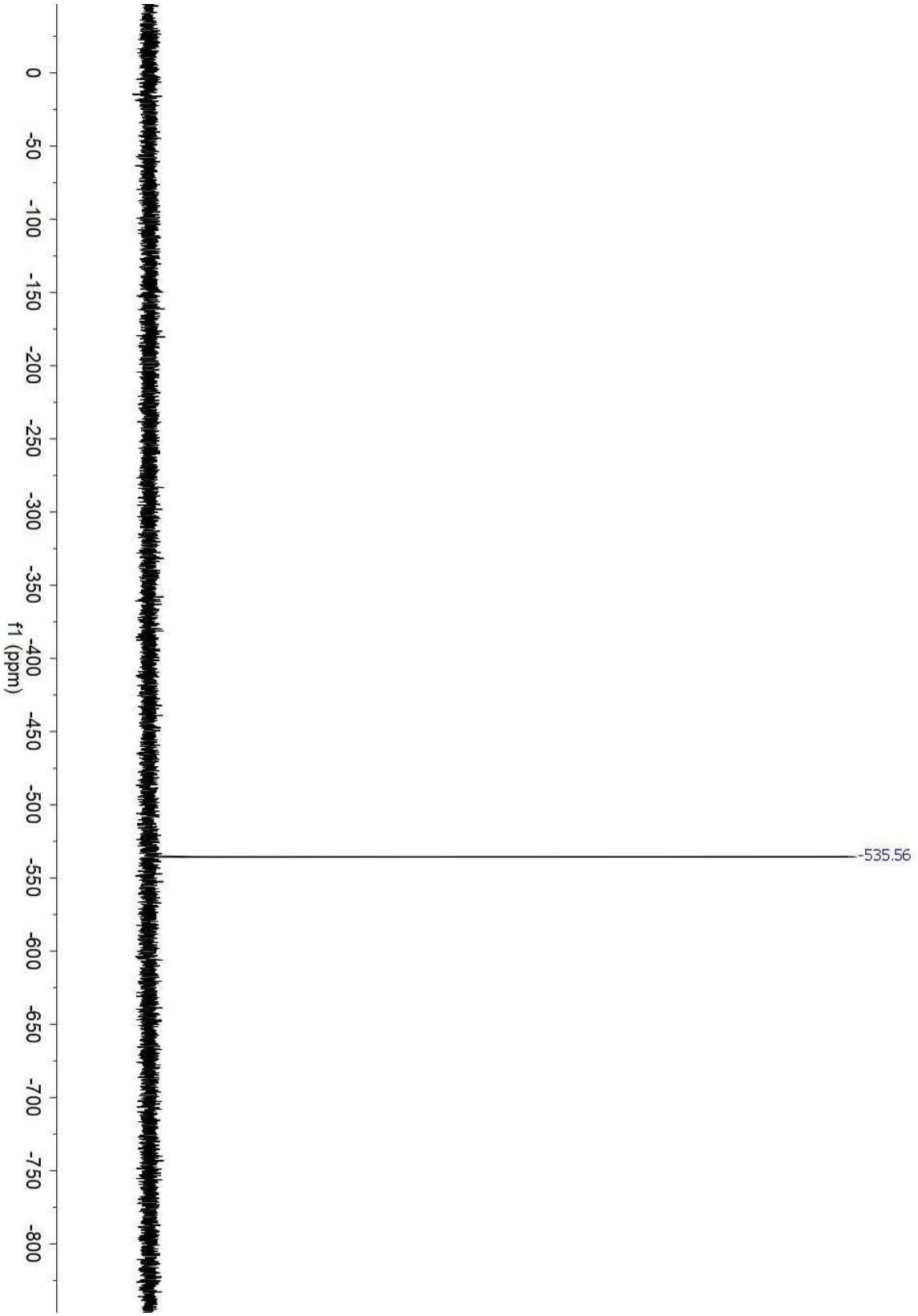


Fig. S26 $^{119}Sn\{H\}$ NMR of **4**, $CDCl_3$ at 298 K

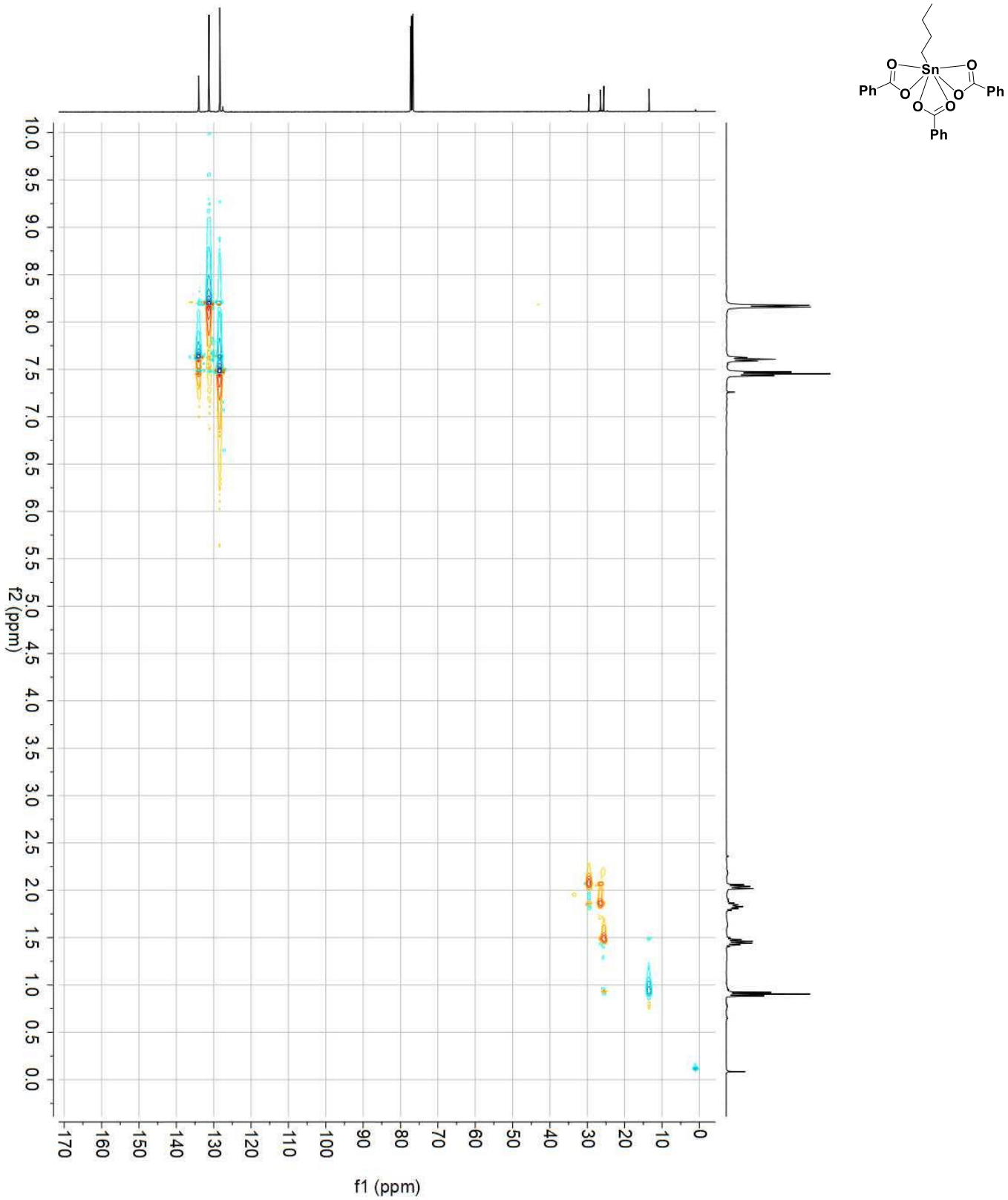


Fig. S27 ^{1}H-^{13}C HSQC NMR of **4**, $CDCl_3$ at 298 K

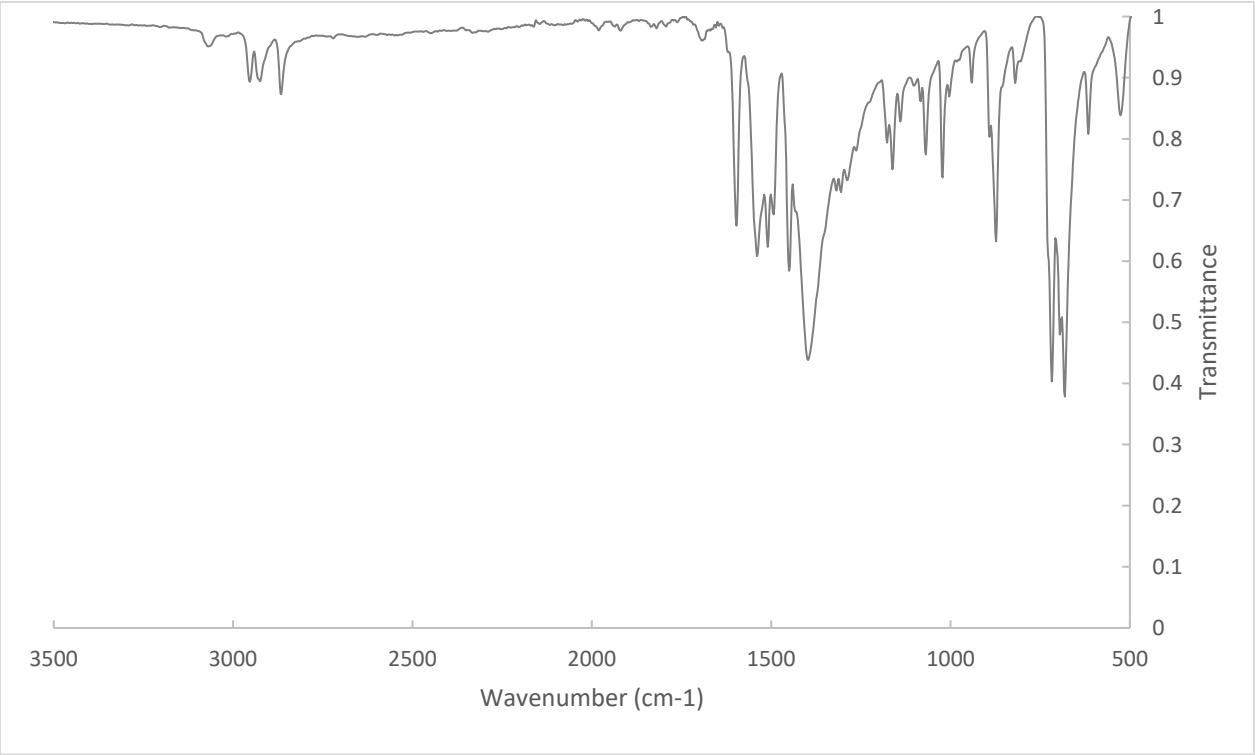
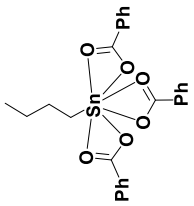
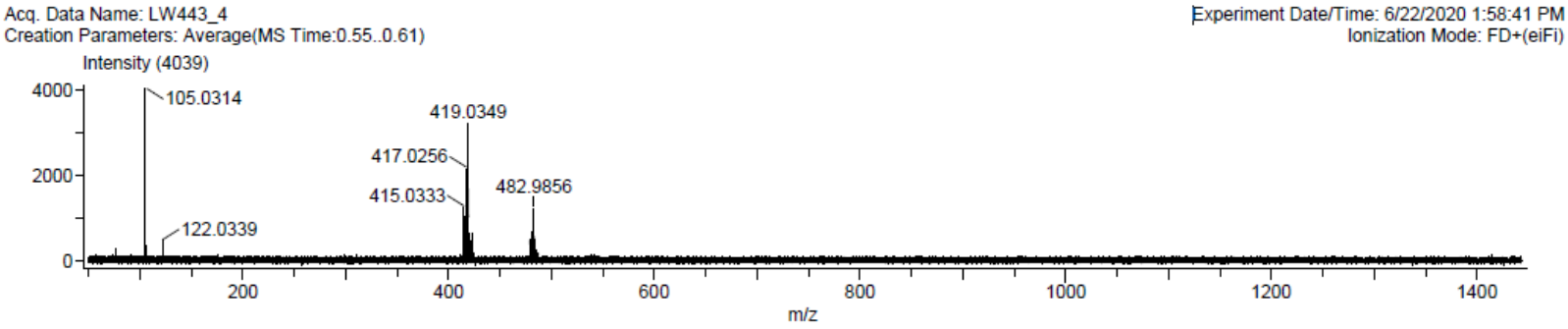
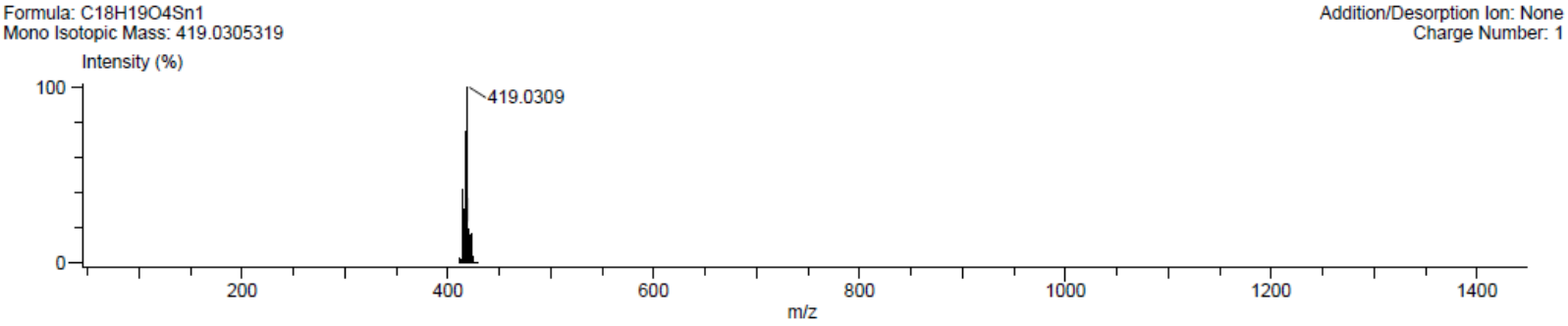


Fig. S28 IR-ATR spectrum of **4**







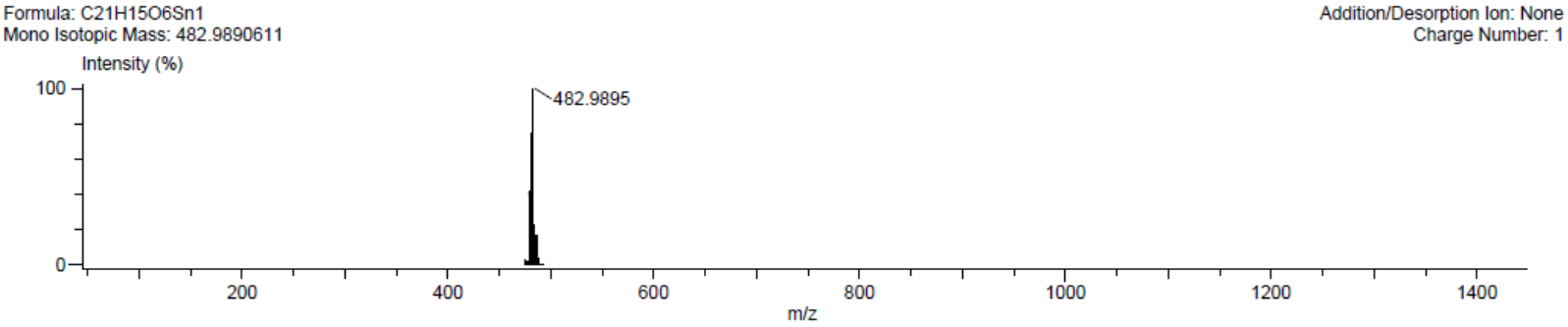
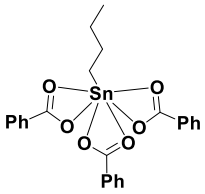


Fig. S29 FD-MS spectrum of **4**



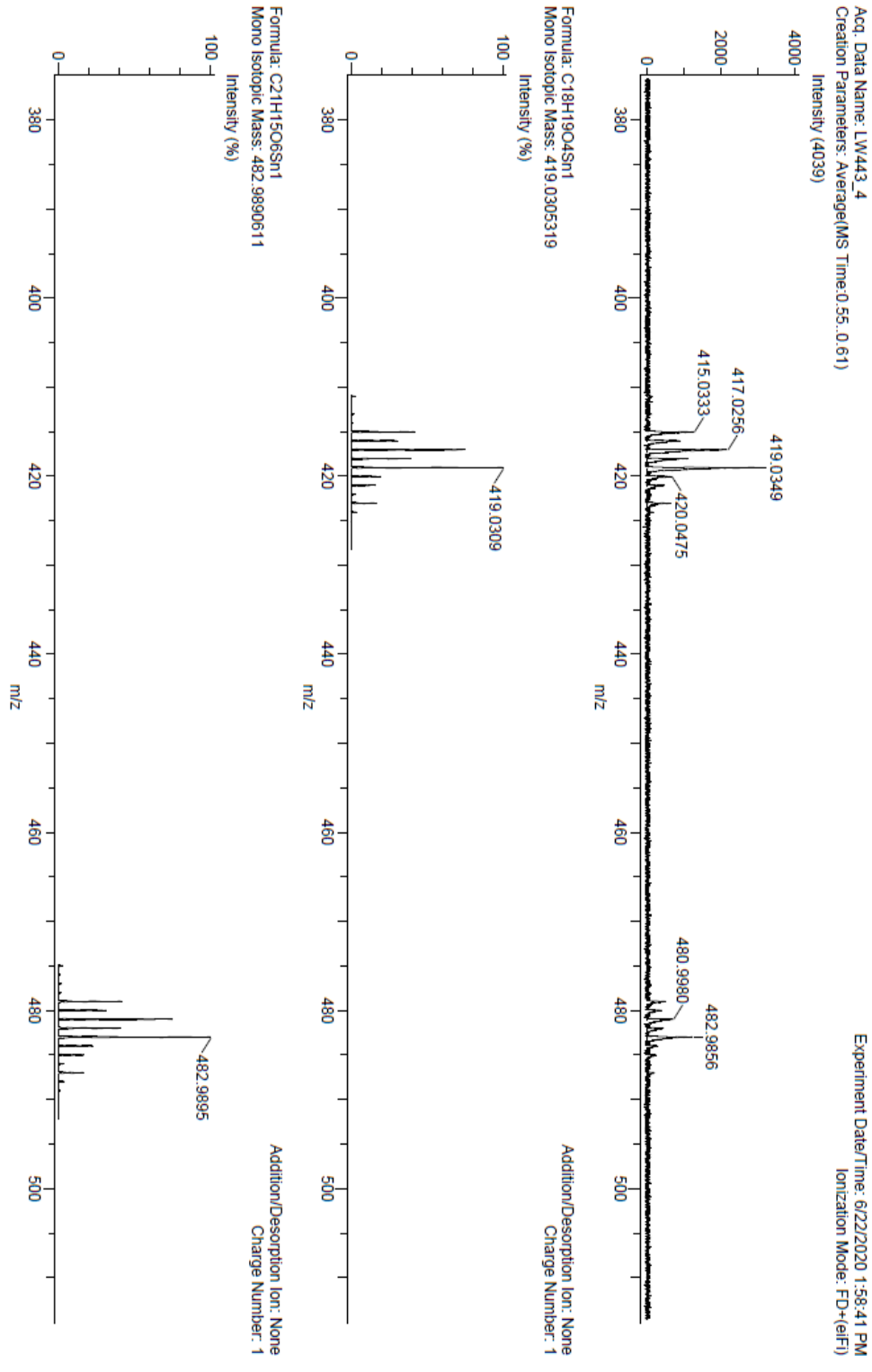


Fig. S30 FD-MS spectrum of **4**

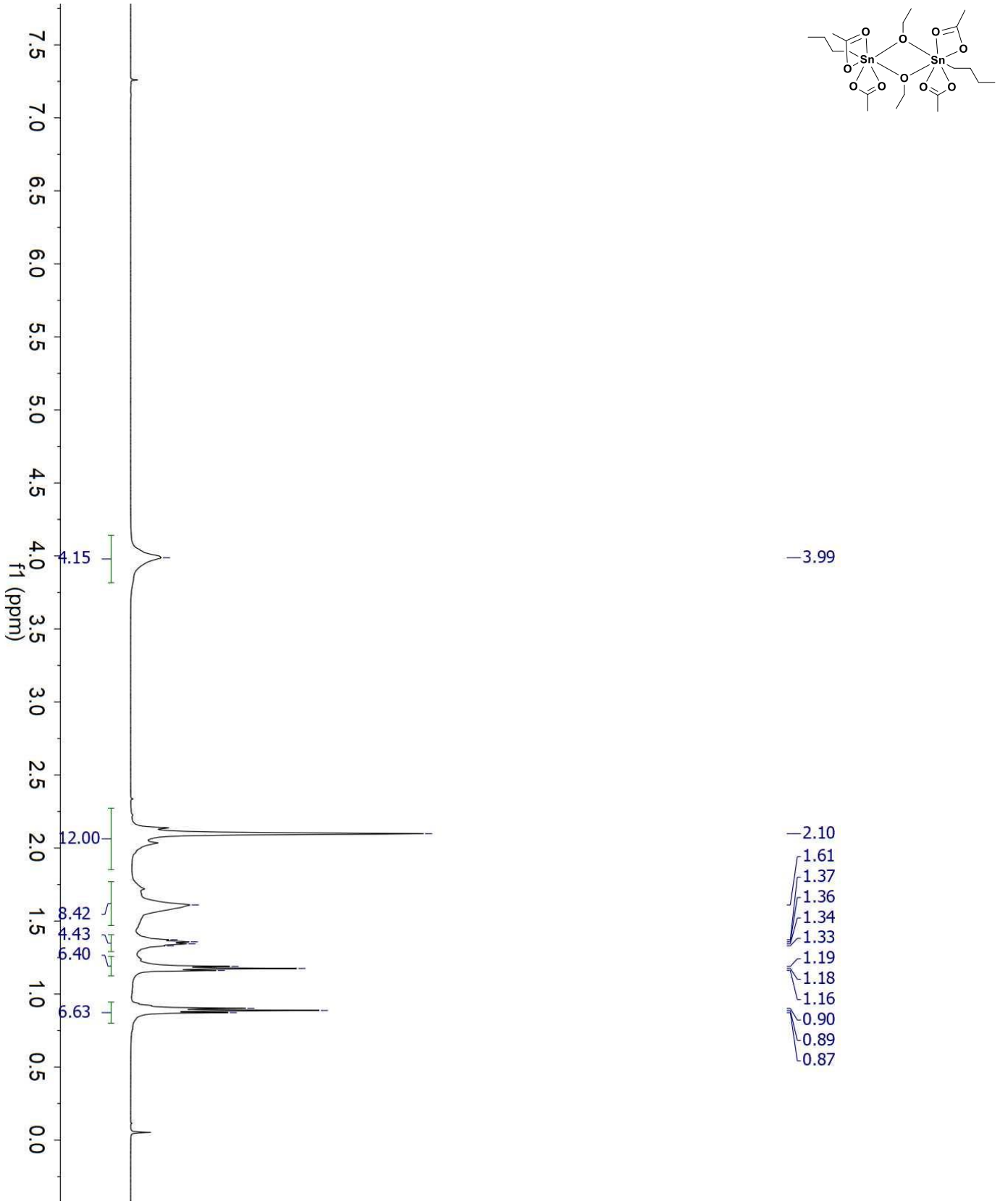


Fig. S31 ^{1}HNMR of **5A** (*n*-BuSnOAc$_2$EtO)$_2$ at 298 K, $CDCl_3$ at 298 K

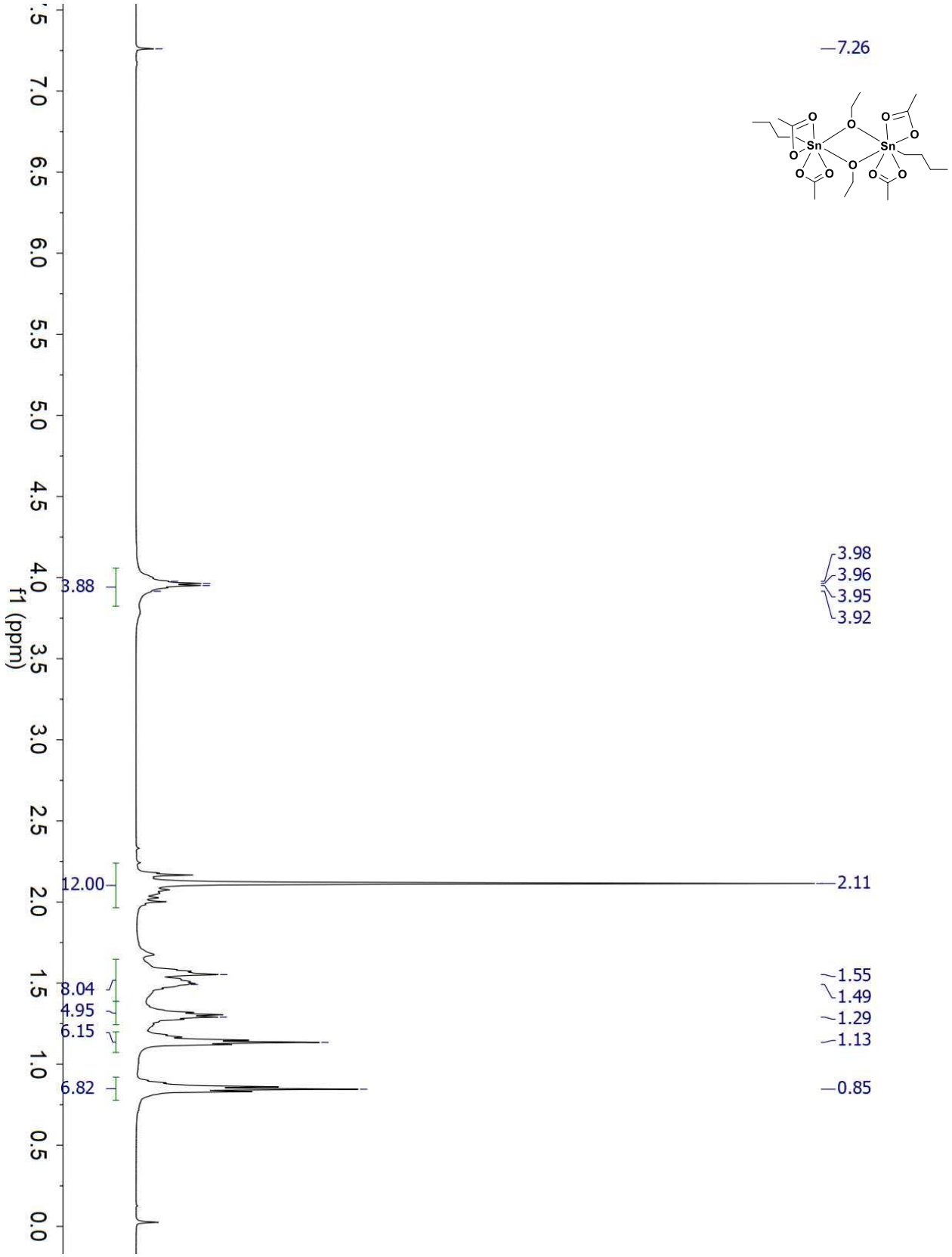


Fig. S32 ^{1}HNMR of **5A** at 233 K, $CDCl_3$

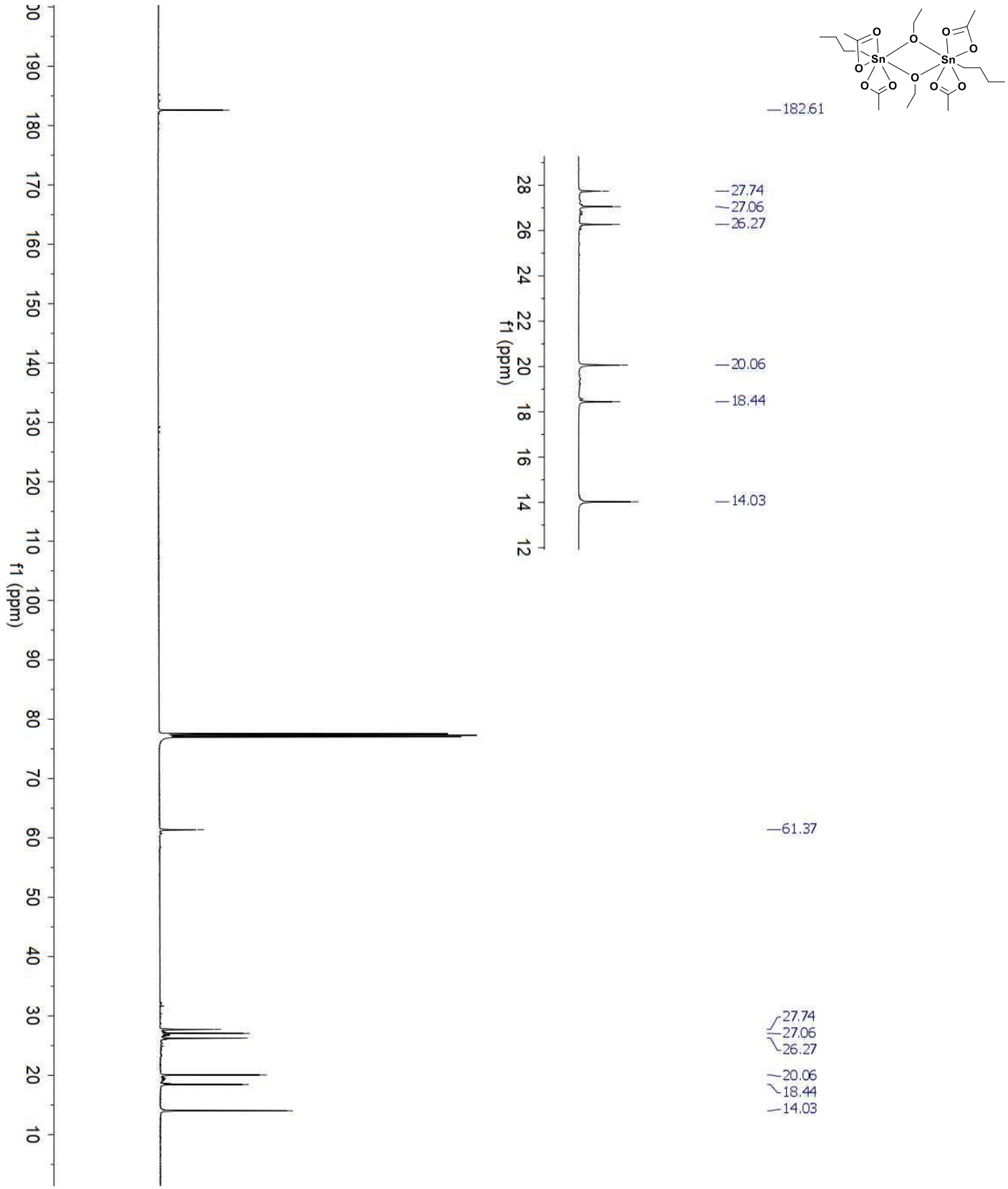


Fig. S33 ^{13}C NMR of **5A** at 233 K, $CDCl_3$

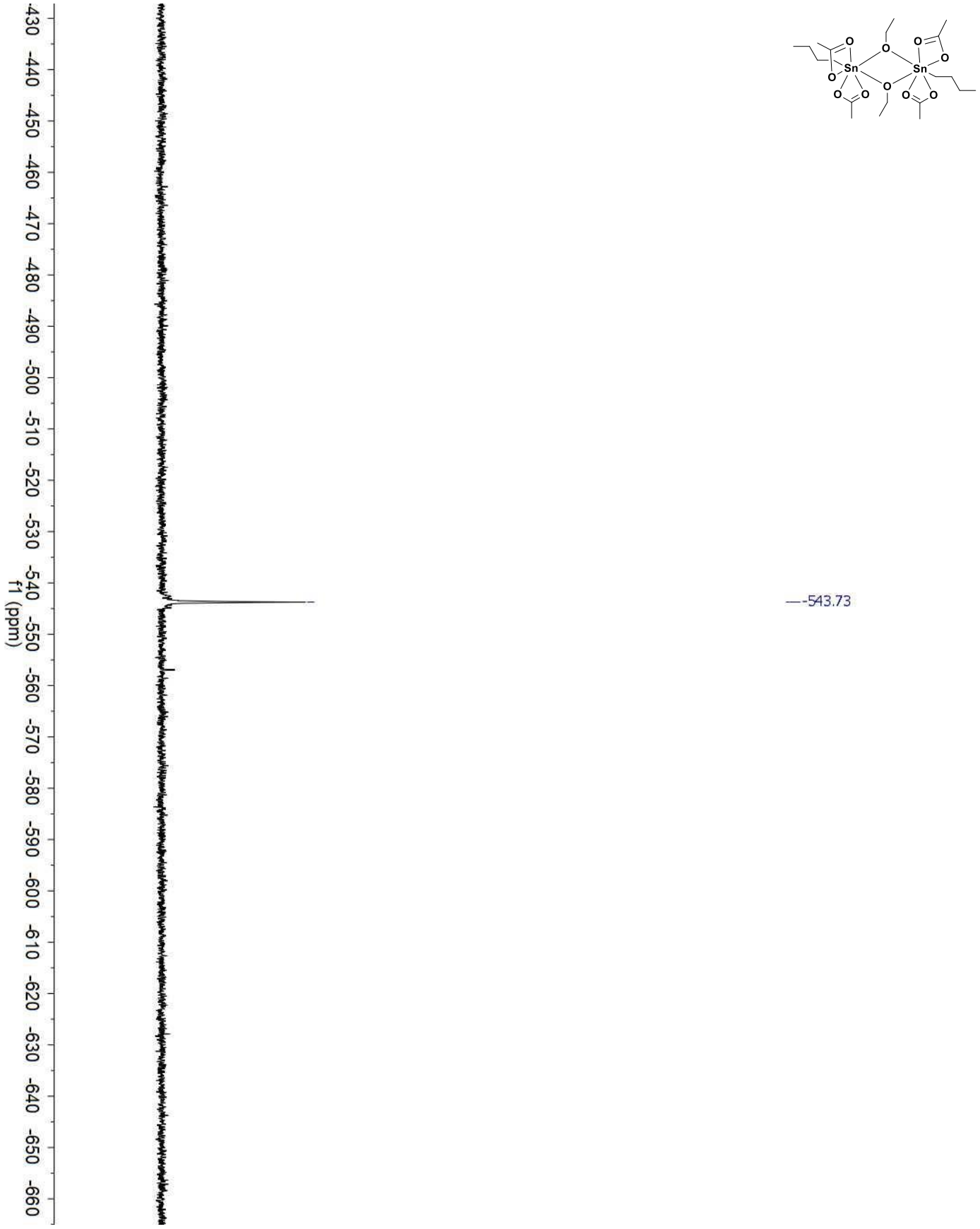


Fig. S34 $^{119}Sn\{H\}$ NMR of **5A**, $CDCl_3$ at 298 K

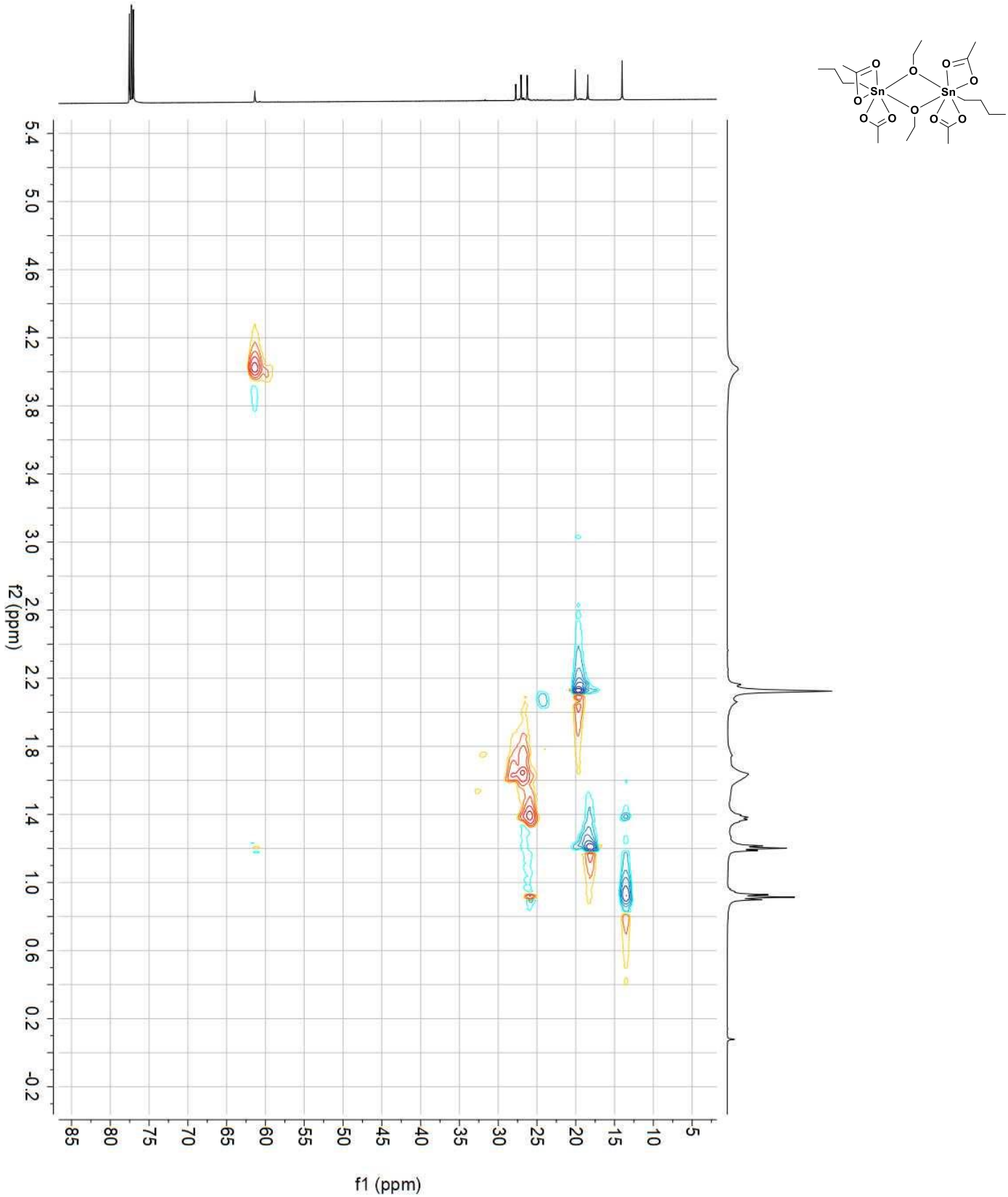


Fig. S35 ^{1}H-^{13}C HSQC NMR of **5A**, $CDCl_3$ at 298 K

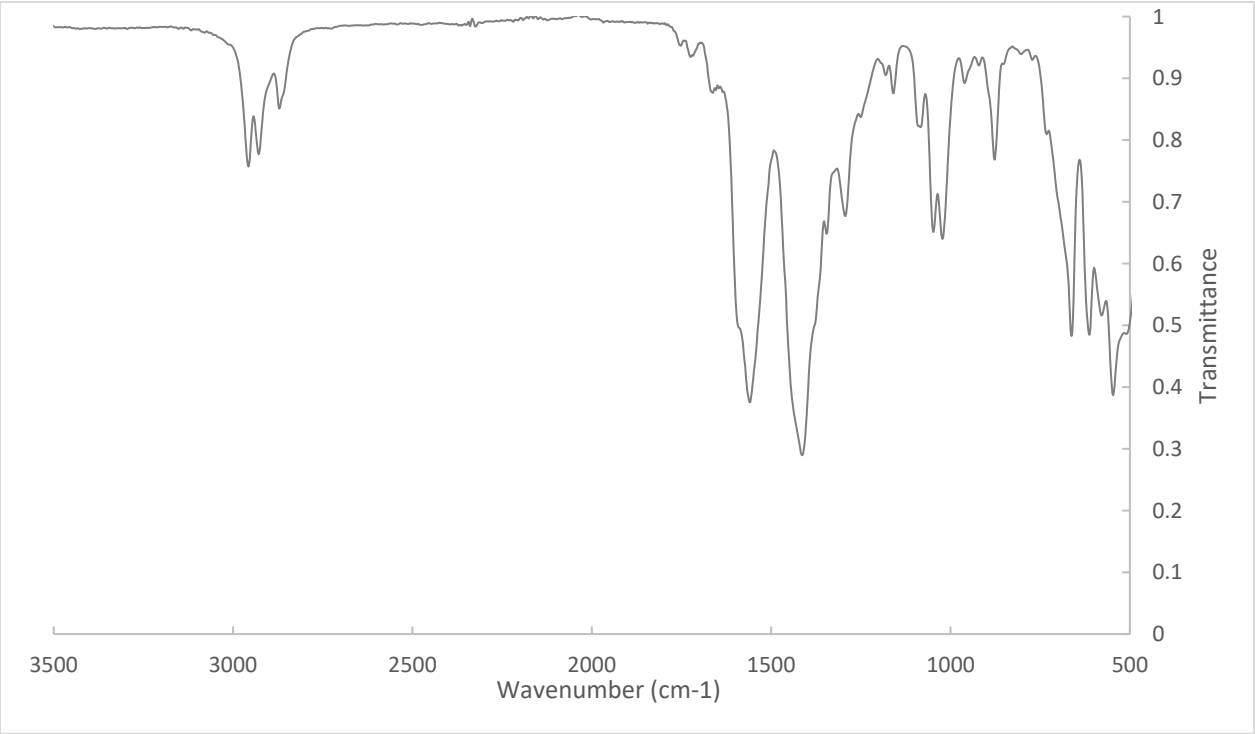
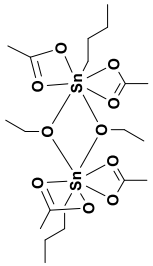
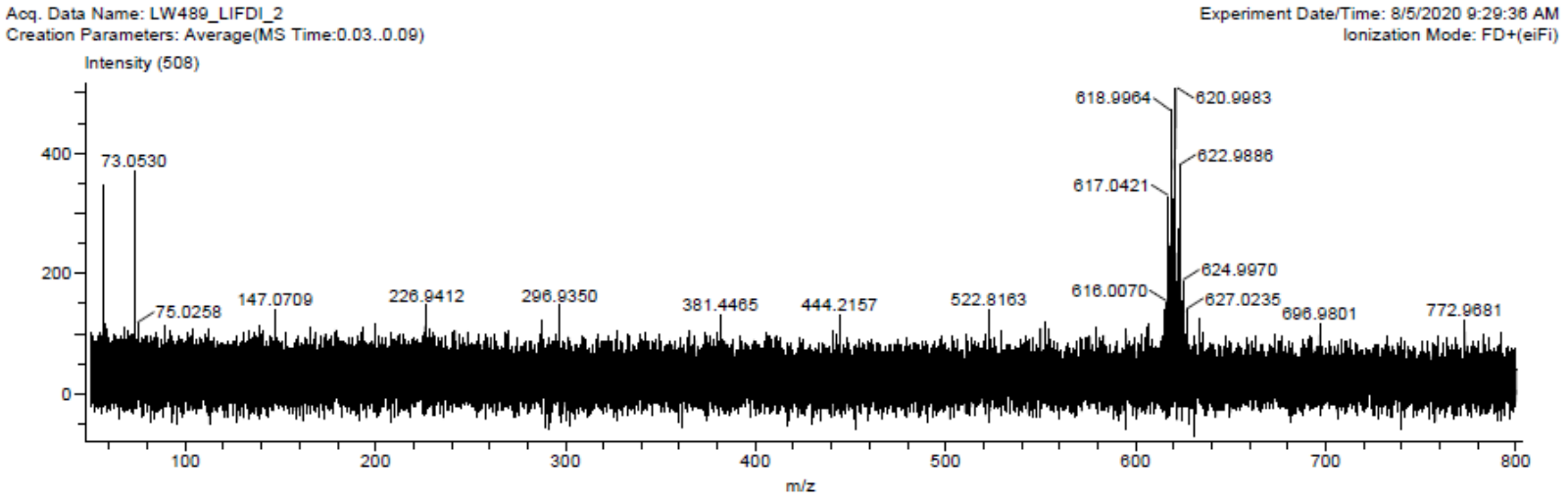


Fig. S36 IR-ATR spectrum of **5A**





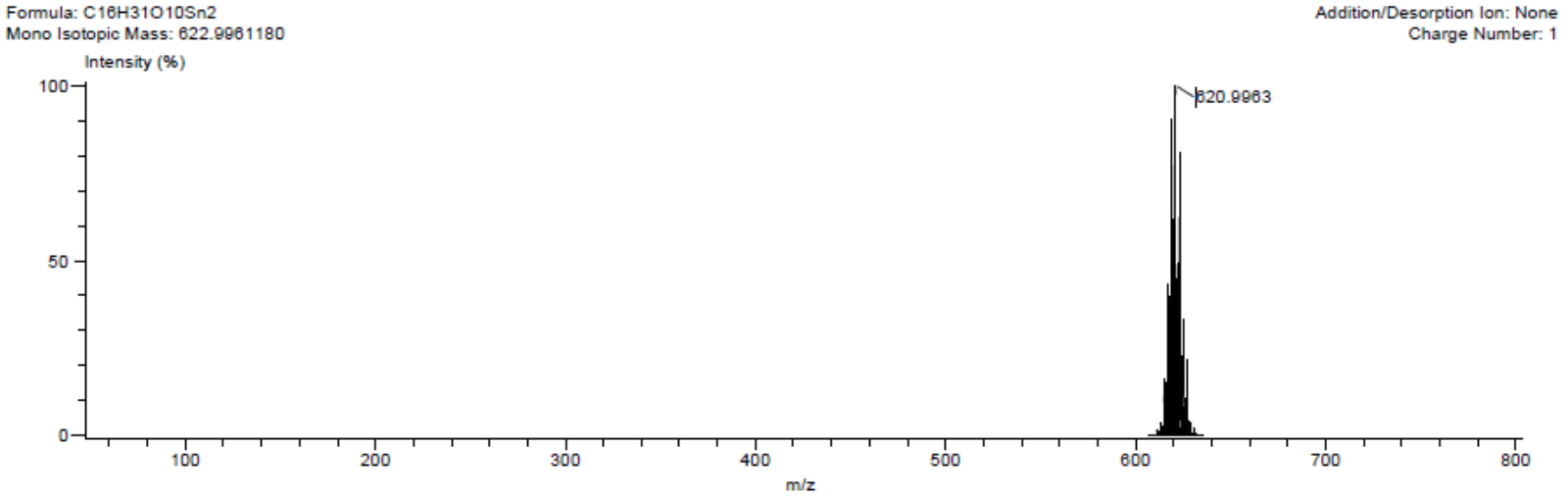
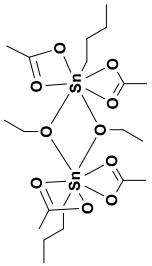
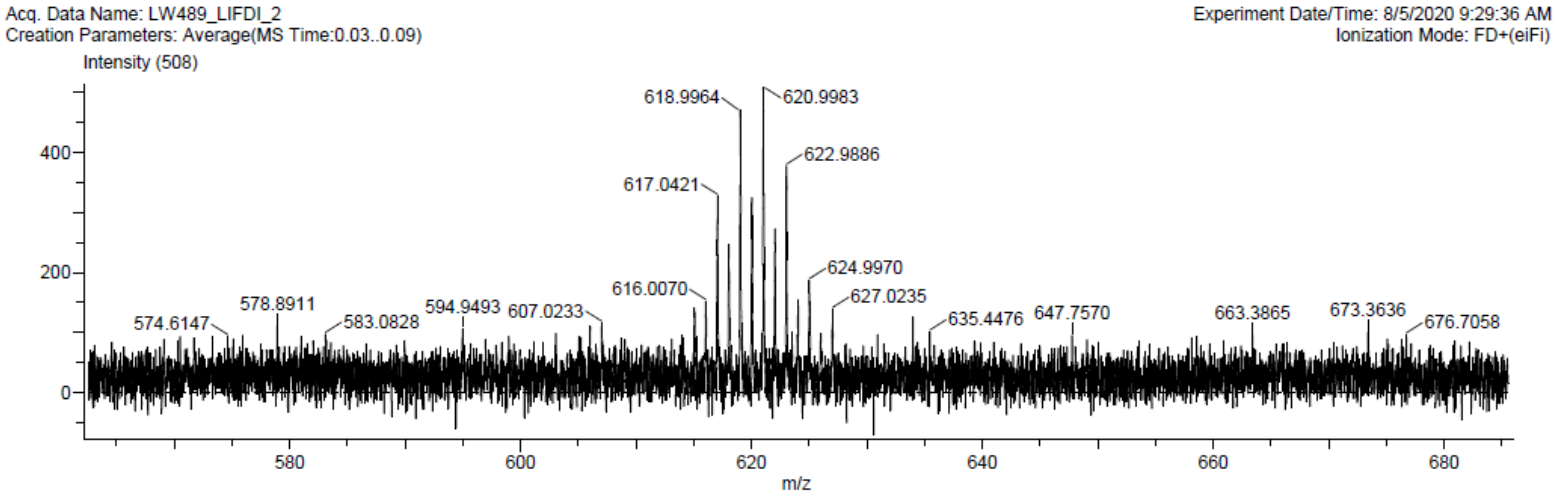


Fig. S37 LIFDI FD-MS spectrum of **5A**





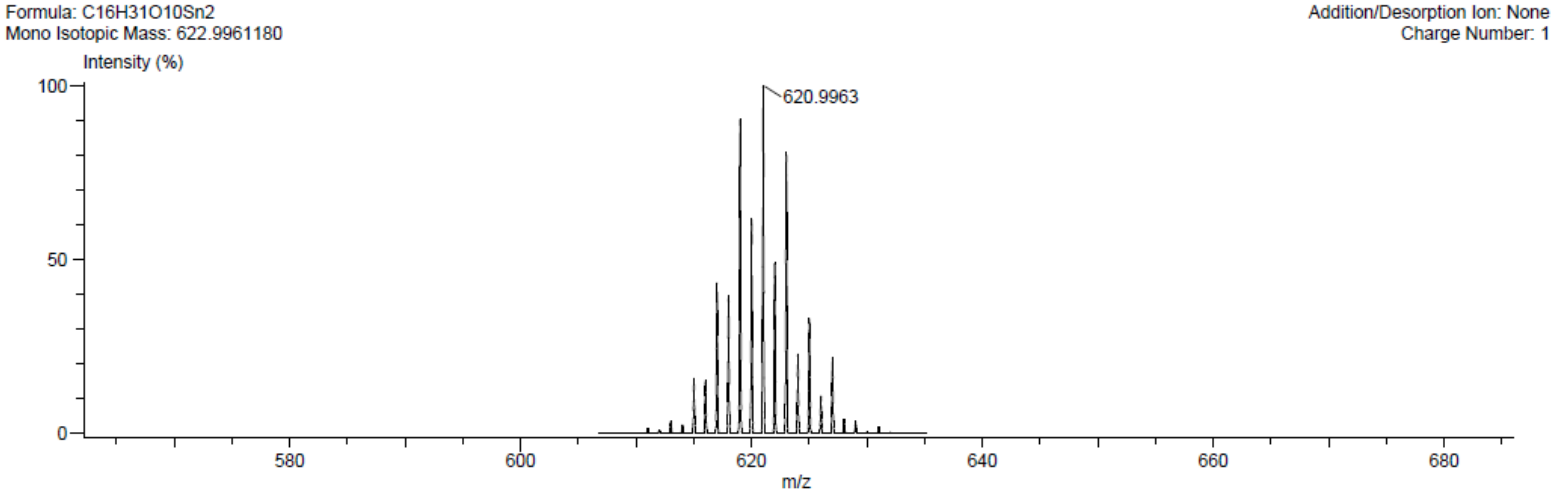


Fig. S38 LIFDI FD-MS spectrum of **5A**

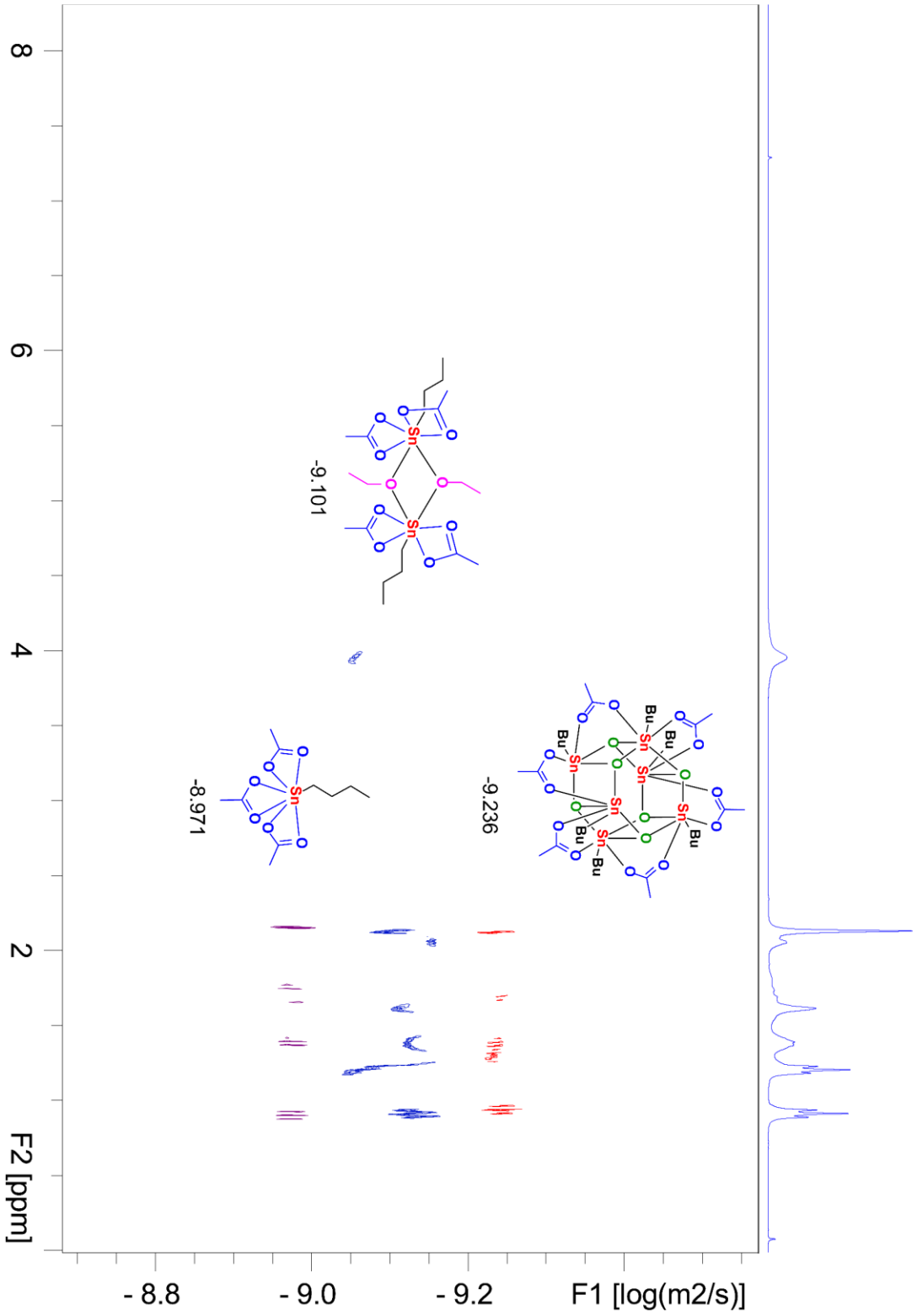


Fig. S39 2D ^{1}H DOSY spectrum of monomer **3** (purple trace), dimer **5A** (blue trace, with ^{1}H NMR on horizontal axis) and cluster **2** (red trace) in $CDCl_3$ at 298K

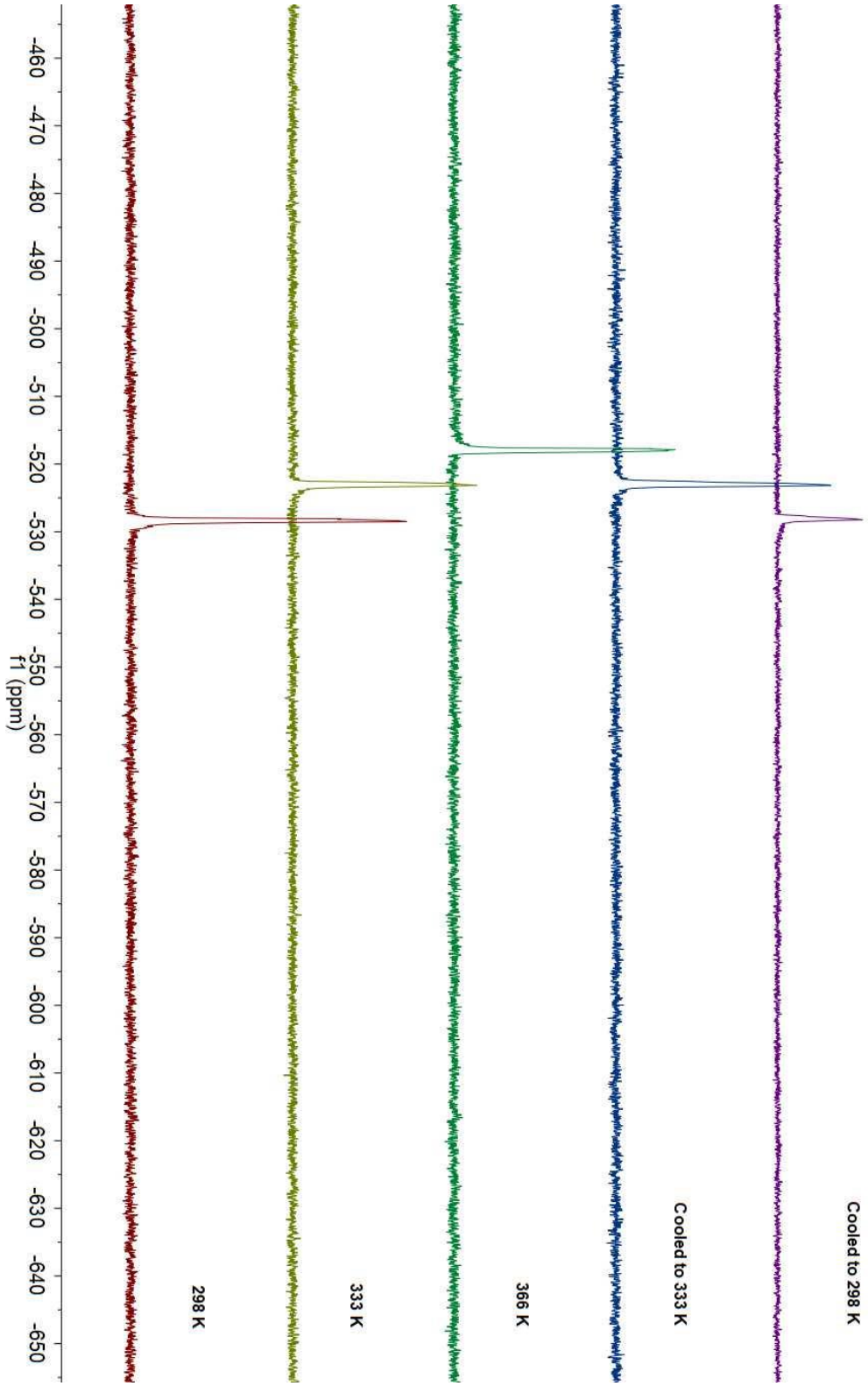


Fig. S40 VT ^{119}Sn{H} NMR of **3** (0.4 M in Sn), Acetic acid-d_4 at 298 K

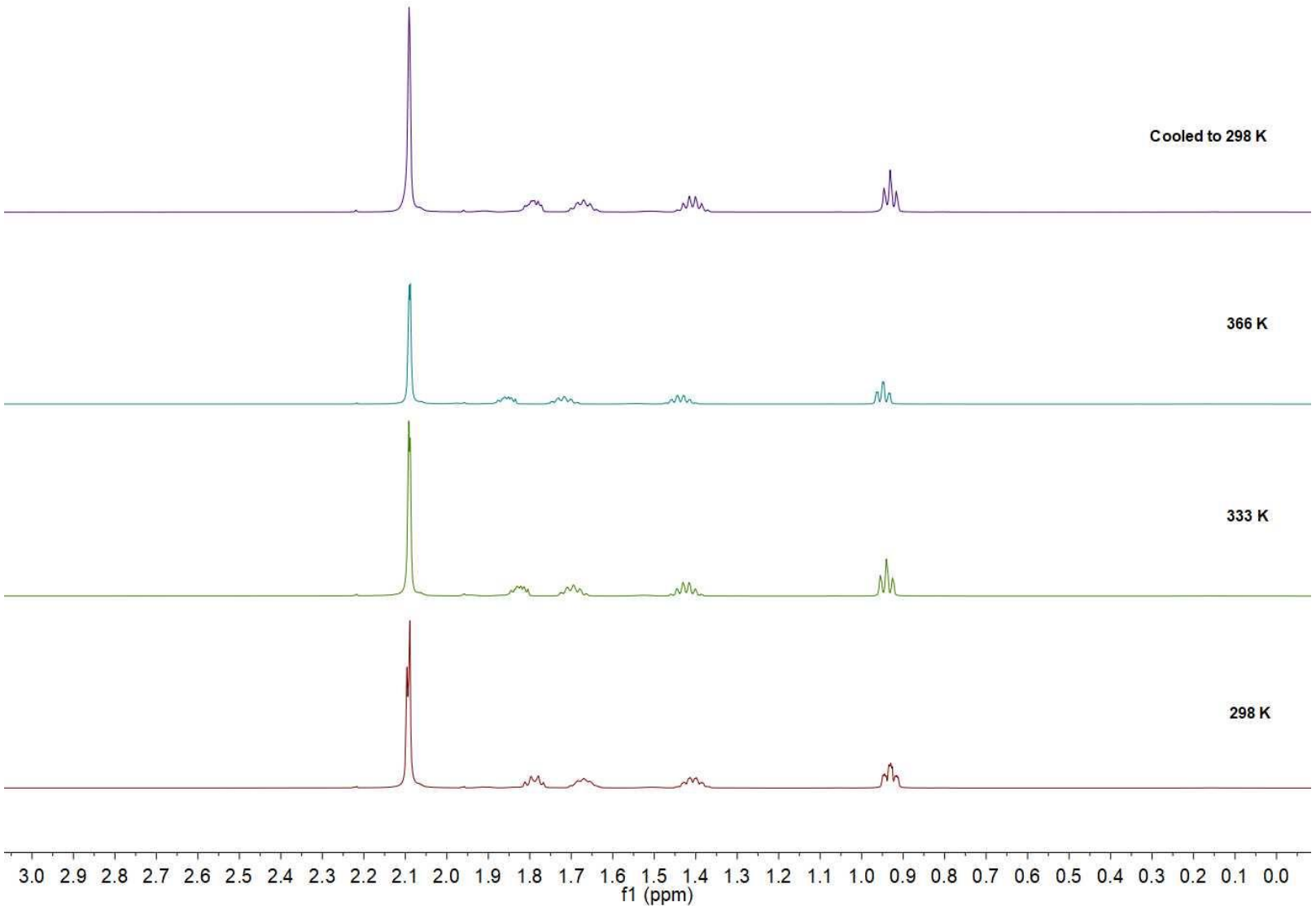


Fig. S41 VT ^{1}H NMR of **3** (0.4 M in Sn), Acetic acid-d_4

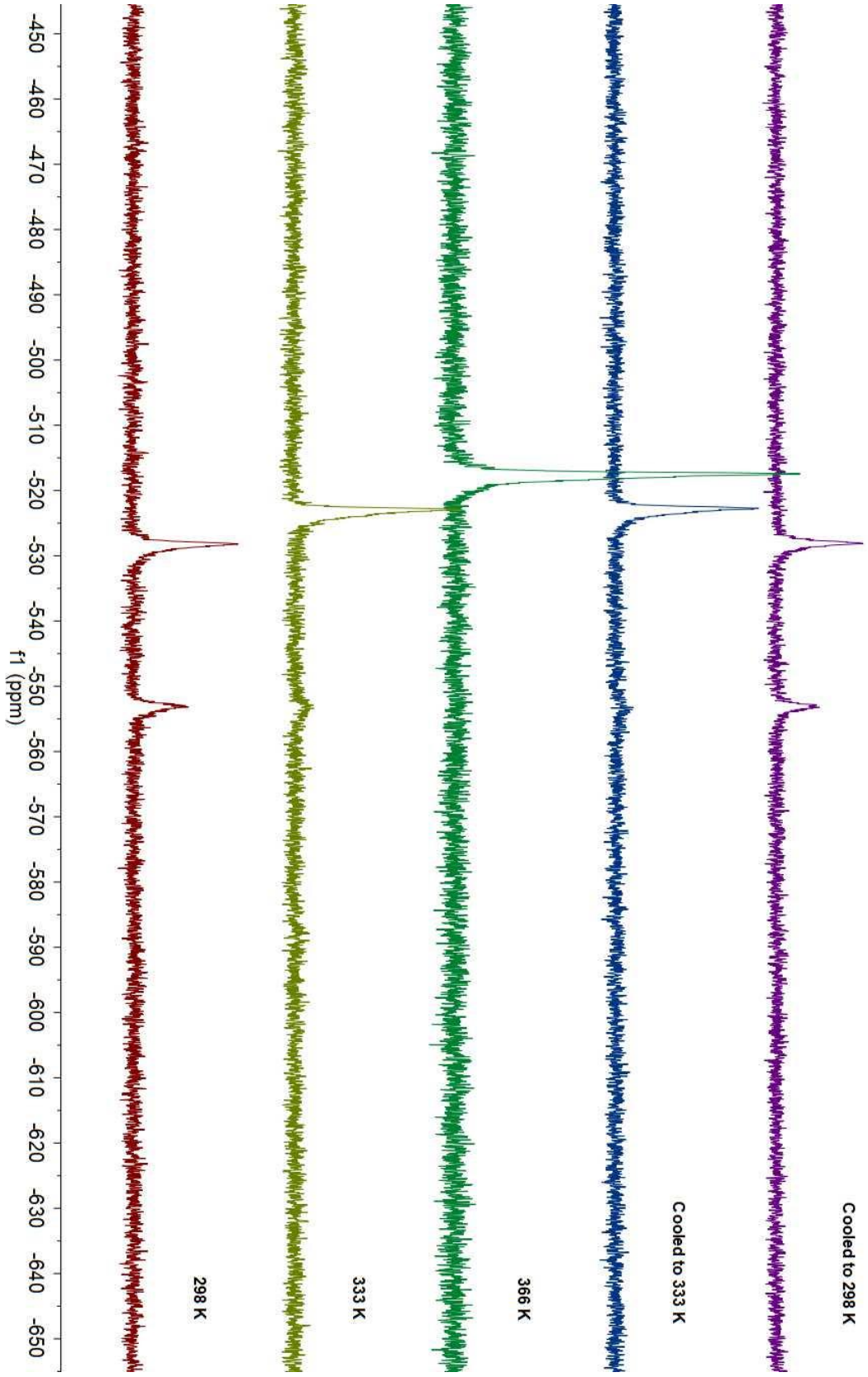


Fig. S42 VT ^{119}Sn{H} NMR of **2** (0.4 M in Sn), Acetic acid-d_4

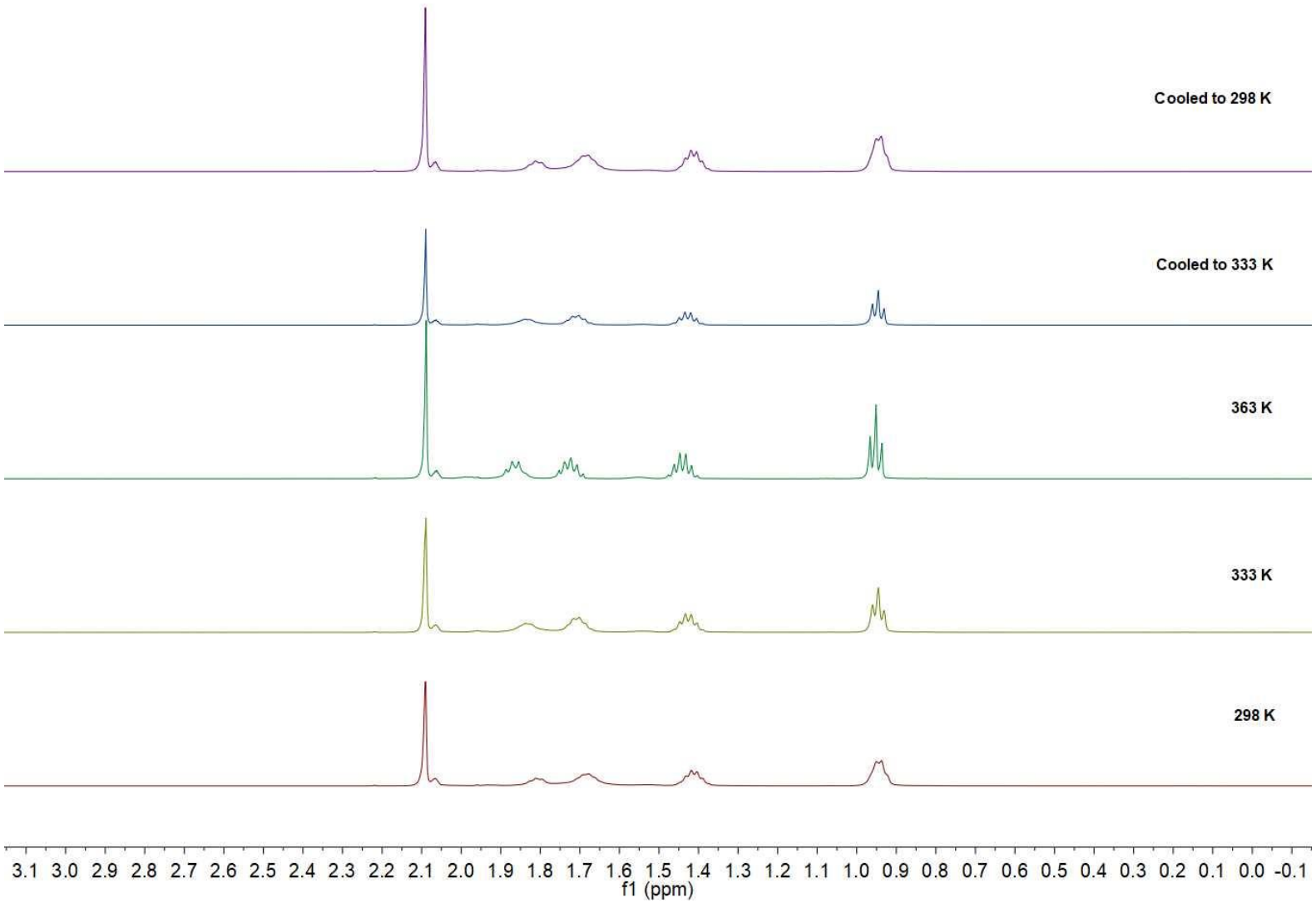


Fig. S43 VT ^{1}H NMR of **2** (0.4 M in Sn), Acetic acid-d_4

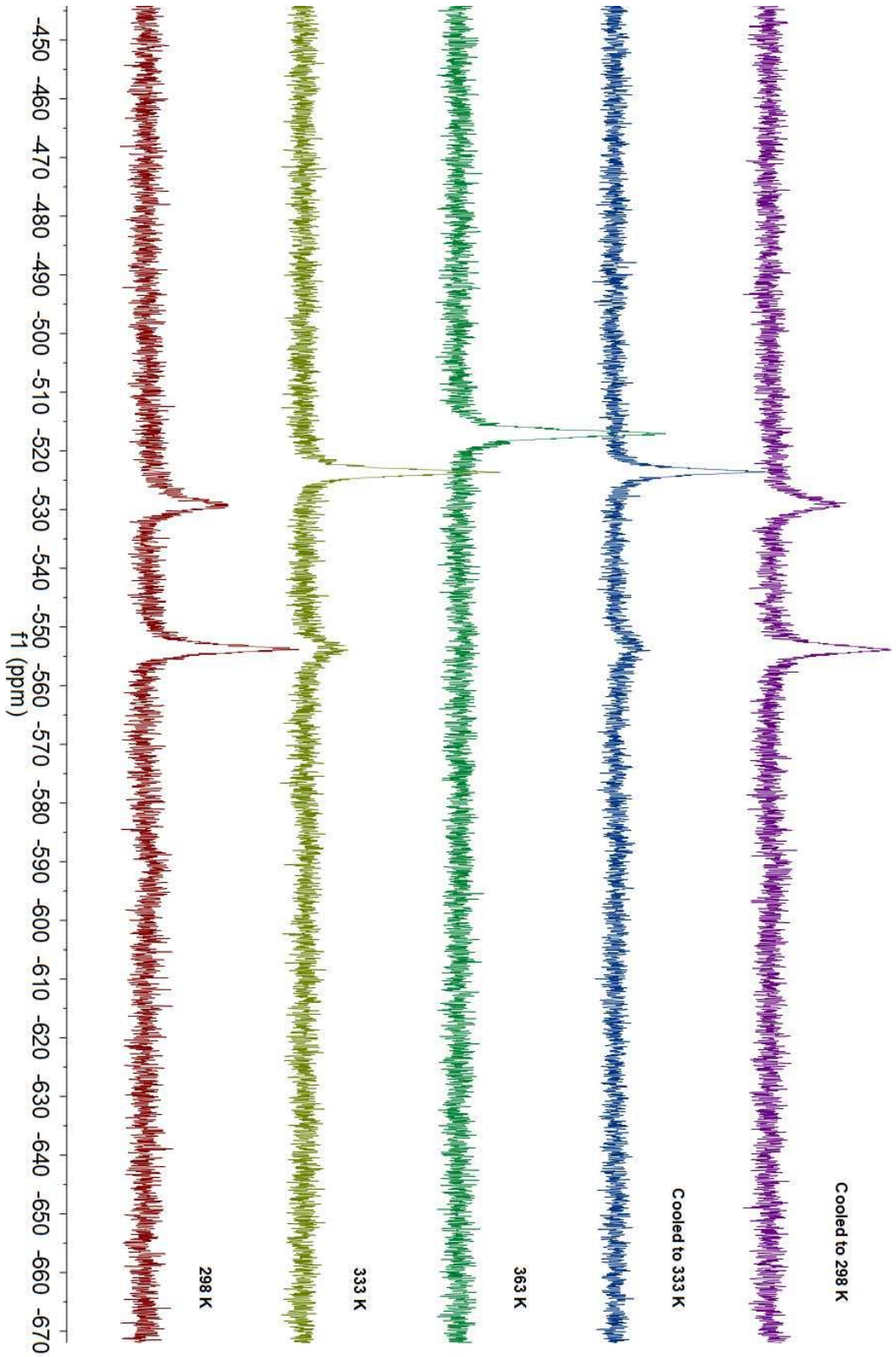


Fig. S44 VT ^{119}Sn{H} NMR of **1** (0.4 M in Sn), Acetic acid-d_4

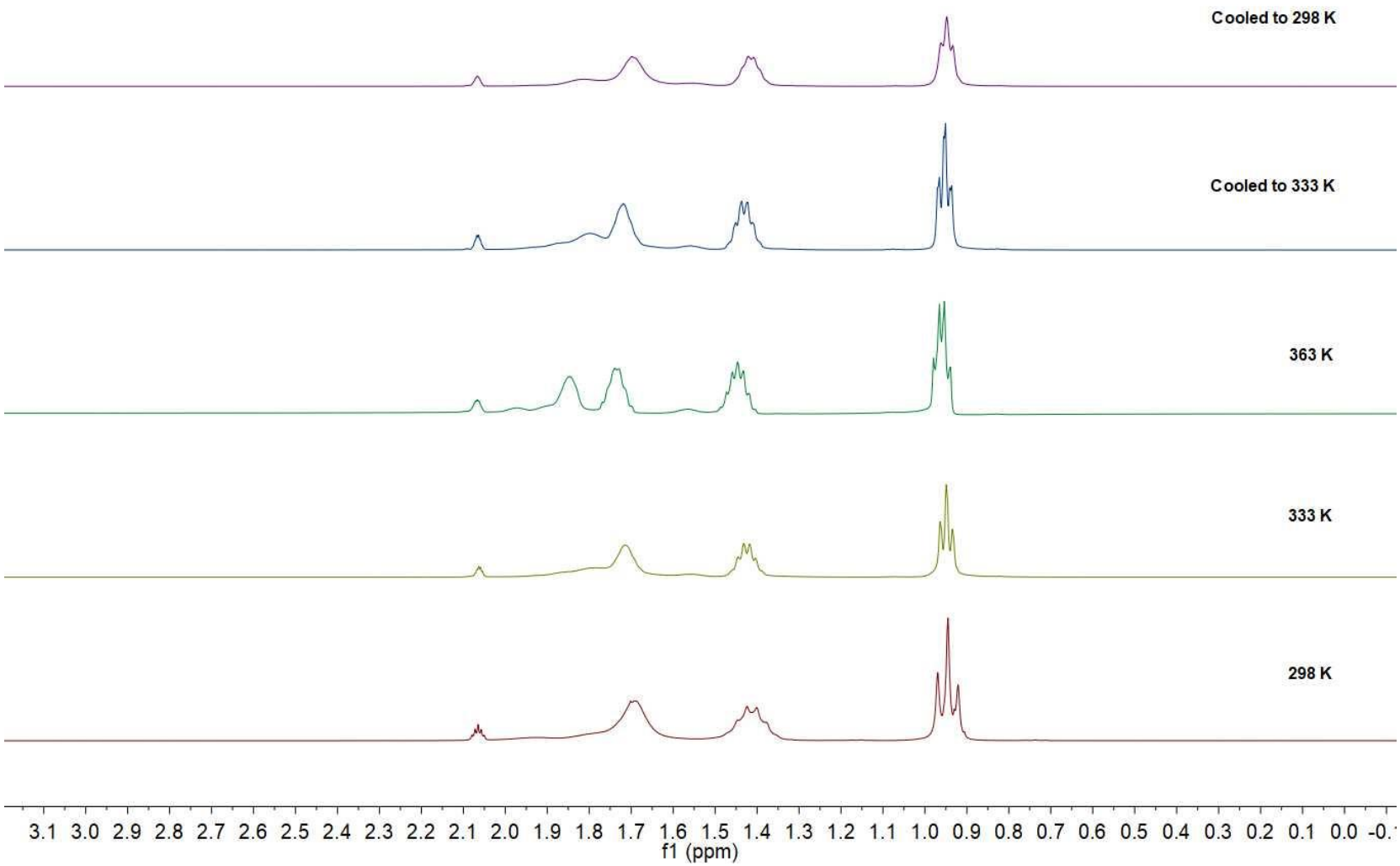


Fig. S45 VT ^{1}H NMR of **1** (0.4 M in Sn), Acetic acid-d_4

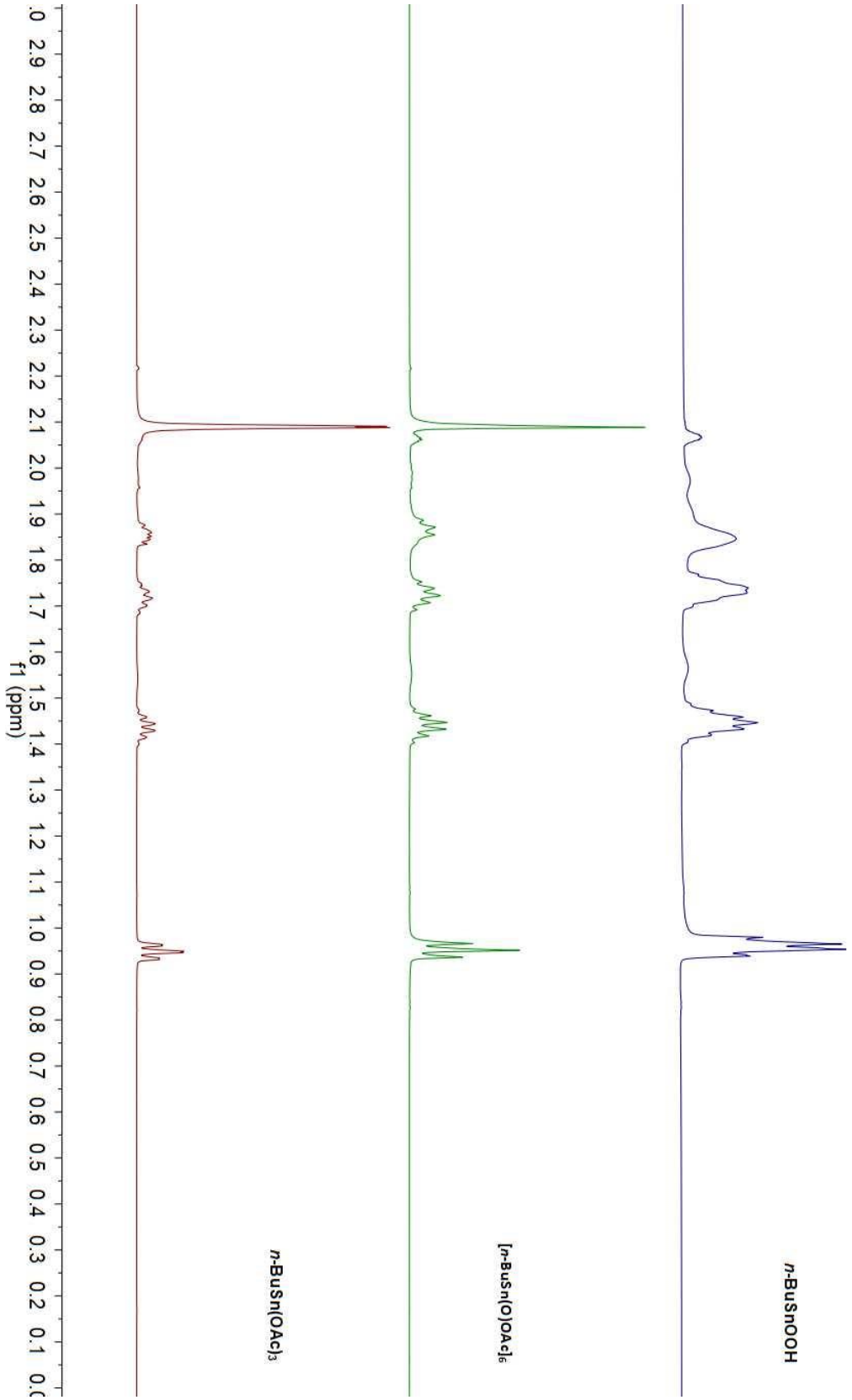


Fig. S46 ^{1}H NMR of [*n*-BuSn(O)OAc]$_6$, *n*-BuSnOAc$_3$ and BuSnOOH (0.4 M in Sn) at 363 K, Acetic acid-d$_4$

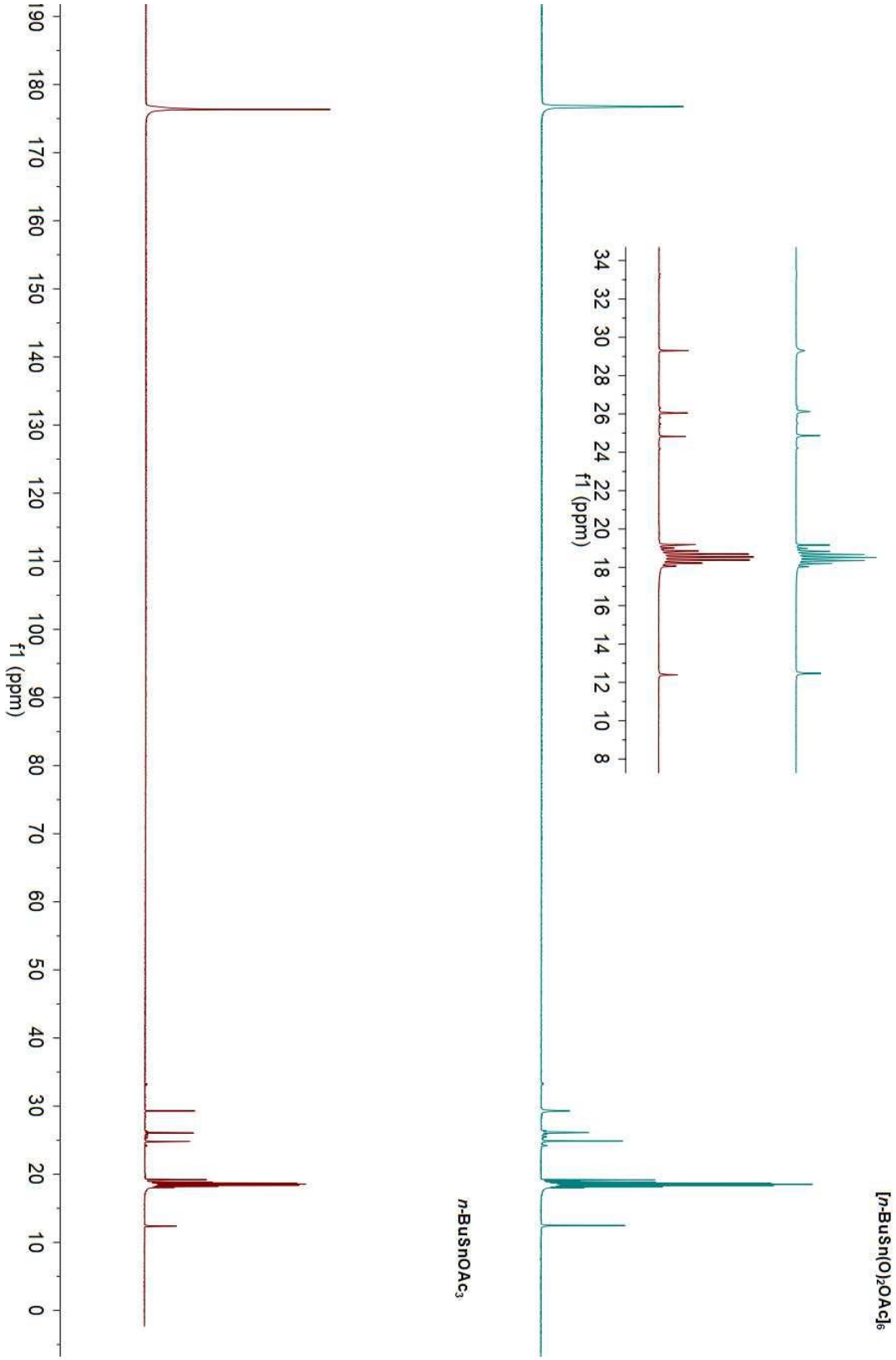


Fig. S47 ^{13}C NMR of [*n*-BuSn(O)OAc]$_6$ and *n*-BuSnOAc$_3$ (0.4 M in Sn) at 366 K, Acetic acid-d$_4$ at 298 K

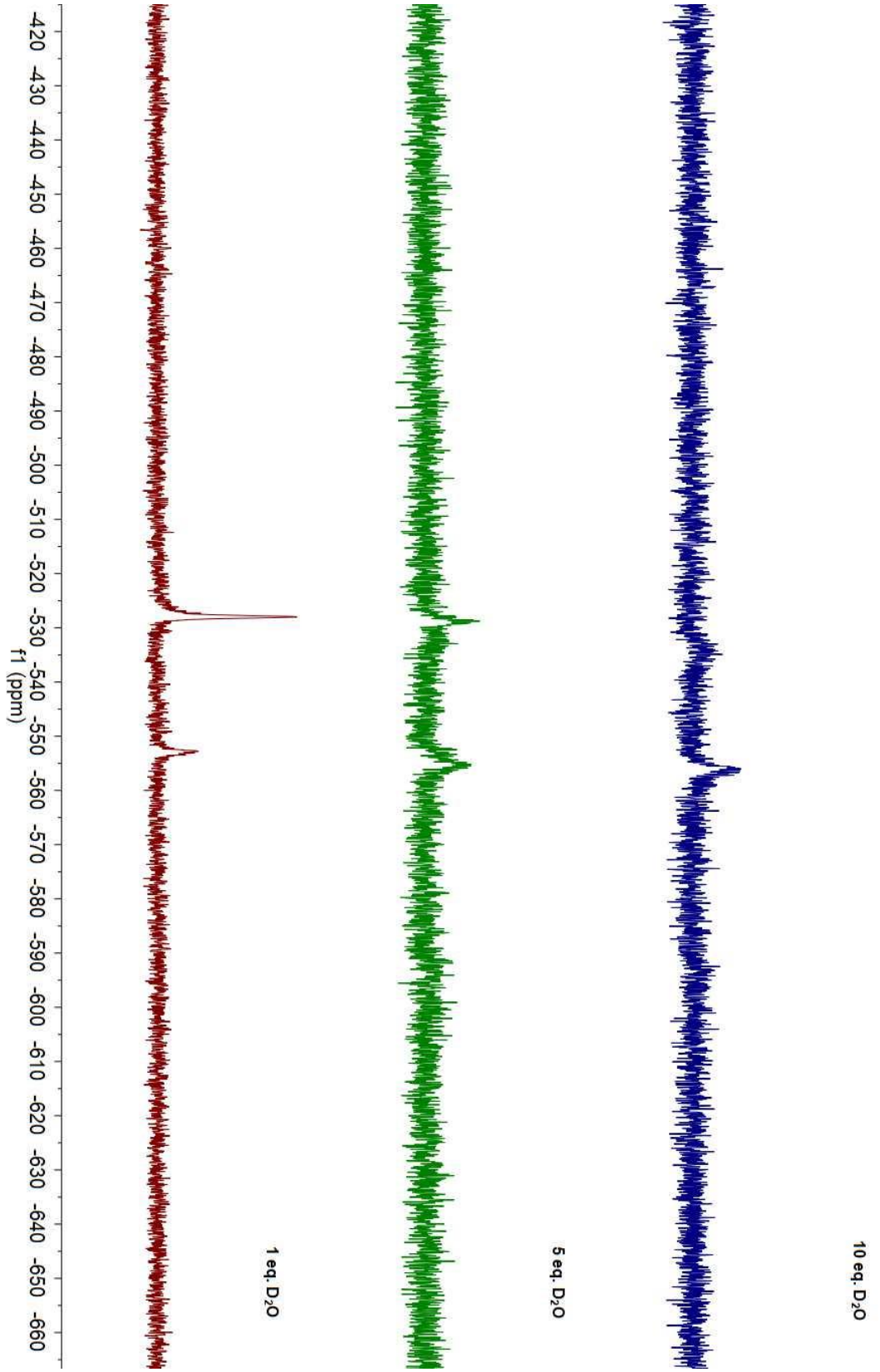


Fig. S48 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) with 1, 5 and 10 equivalents D_2O at 298K , Acetic acid (measured unlocked)

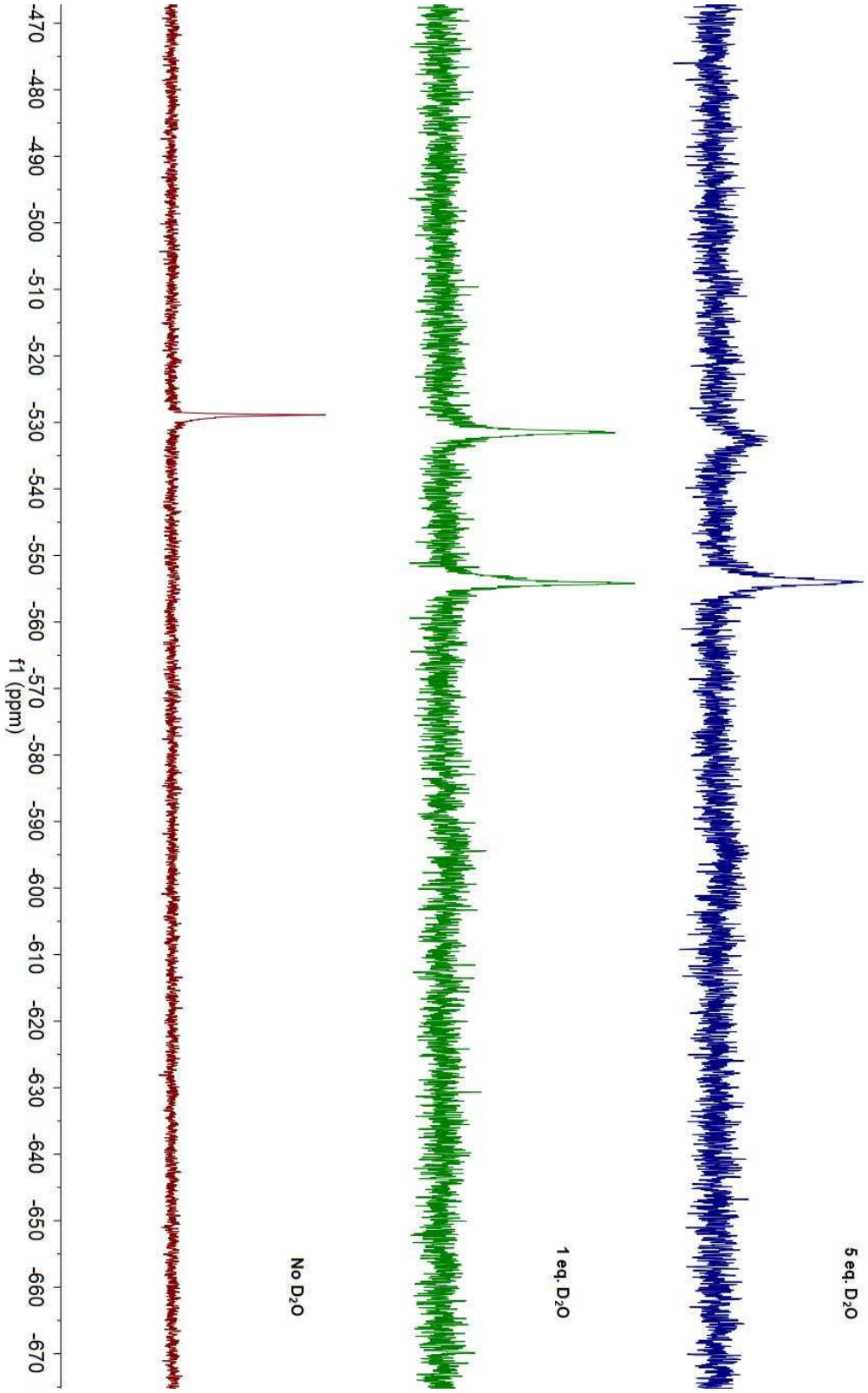


Fig. S49 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) with no, 1 and 5 equivalents D_2O at 298K , Acetic acid/EtOH 1:1 (measured unlocked)

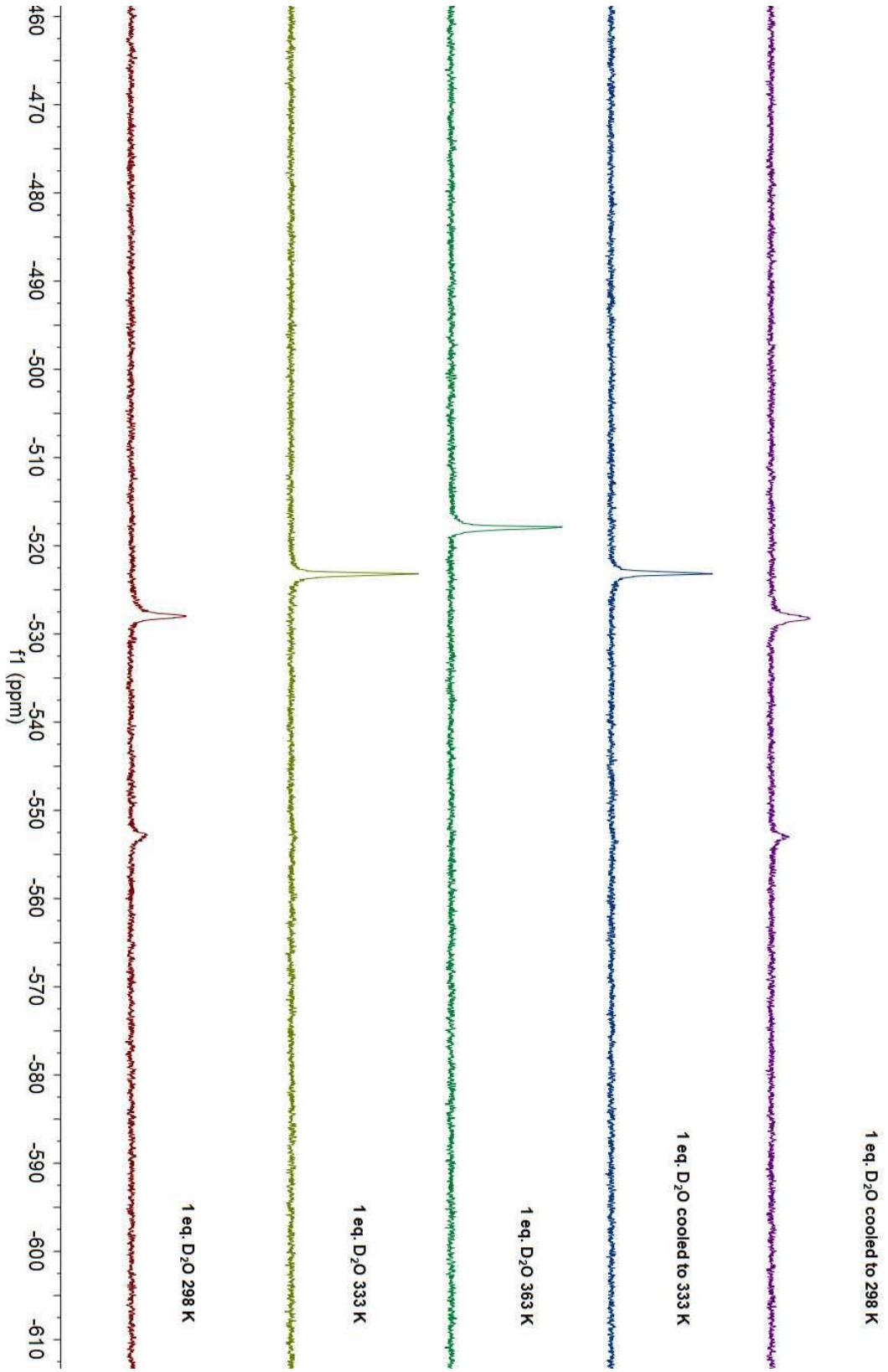


Fig. S50 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) with 1 equivalent D_2O at 298K, 333K and 363K, in acetic acid (measured unlocked).

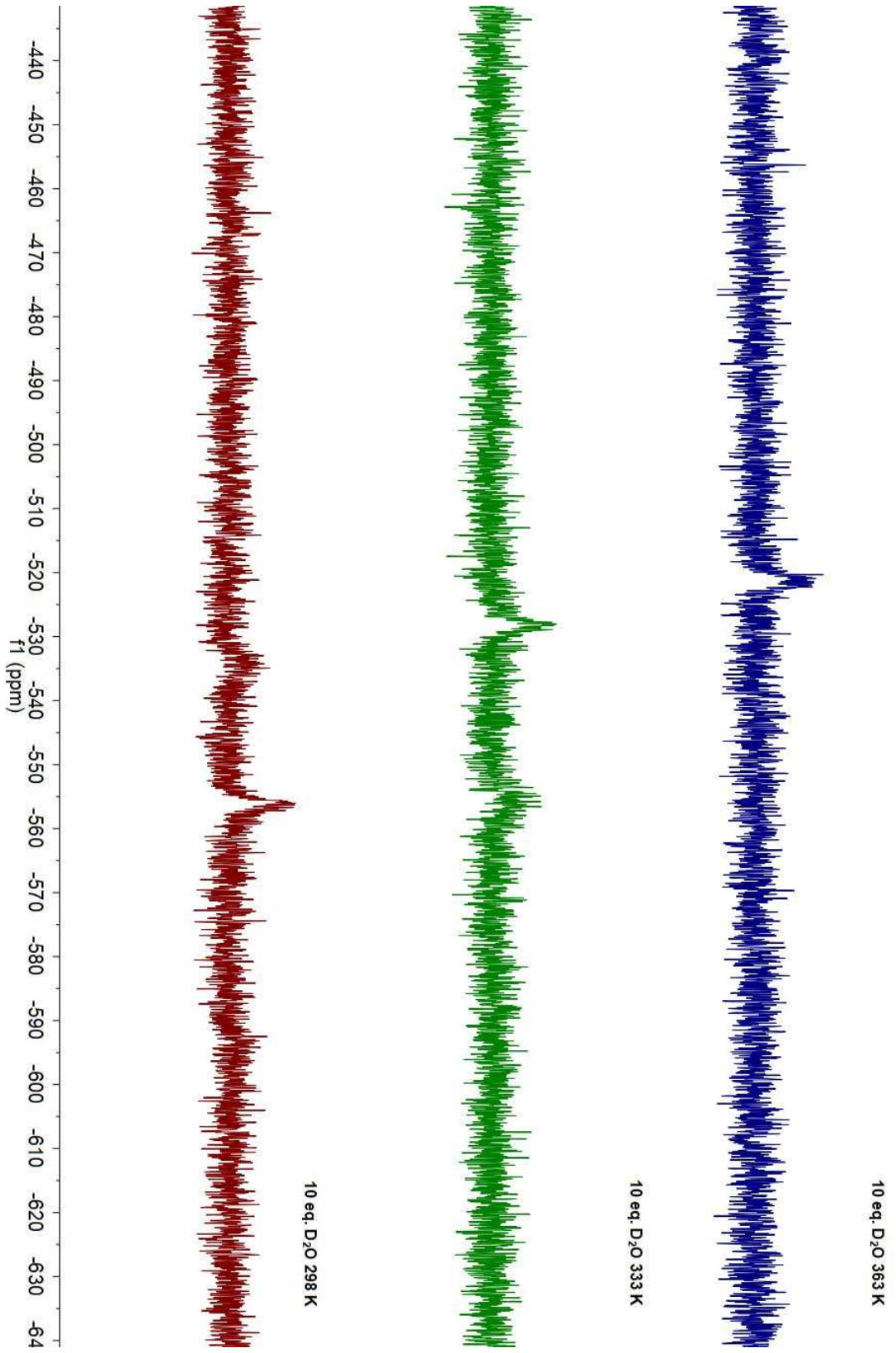


Fig. S51 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) with 10 equivalents D_2O at 298K, 333K and 363K, Acetic acid (measured unlocked).

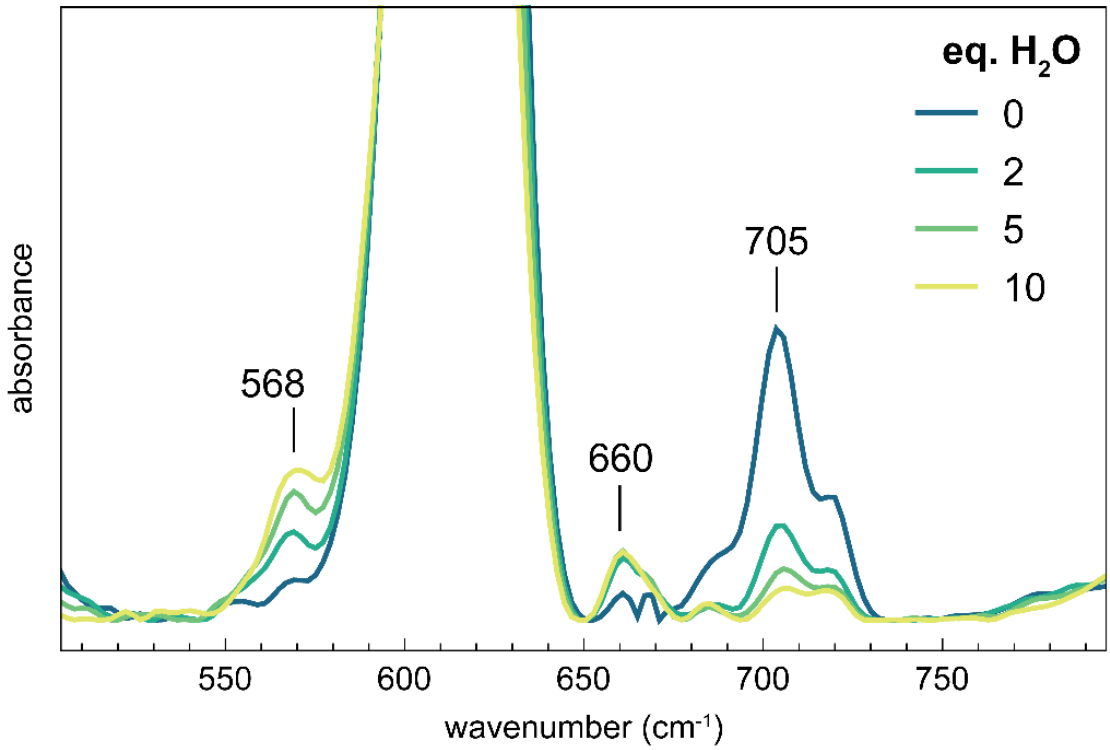


Fig. S52 IR-ATR spectrum of **3** with 0, 2, 5 and 10 equivalents of H_2O.

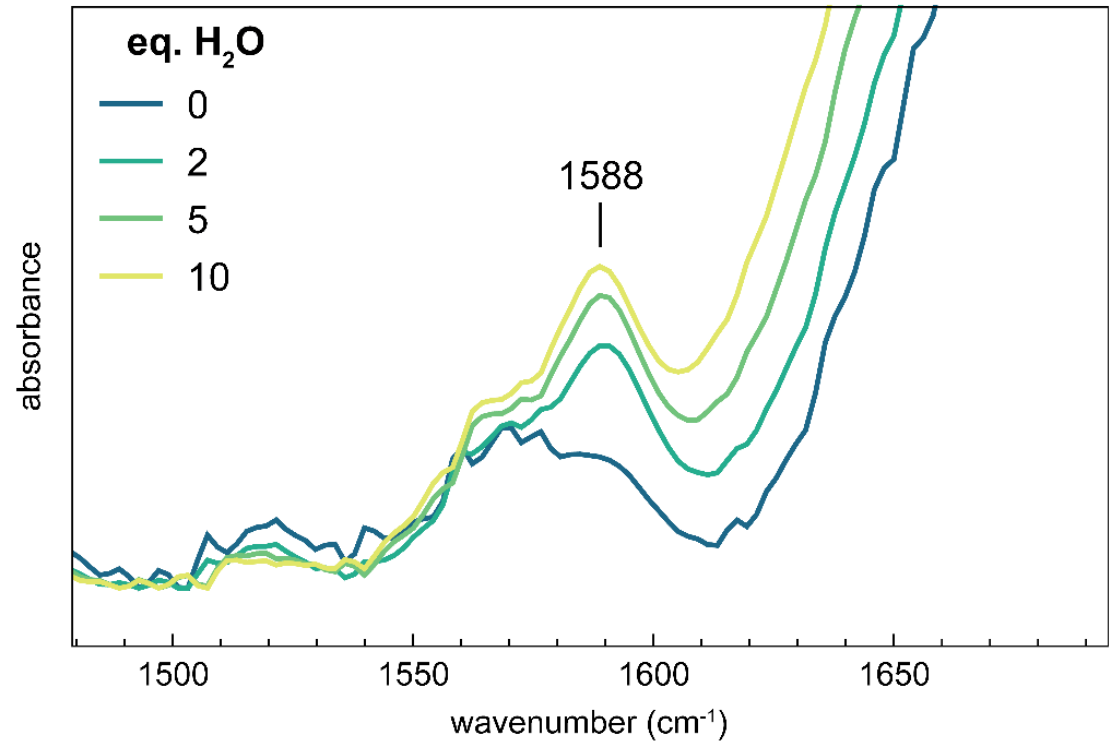


Fig. S53 IR-ATR spectrum of **3** with 0, 2, 5 and 10 equivalents of H_2O.

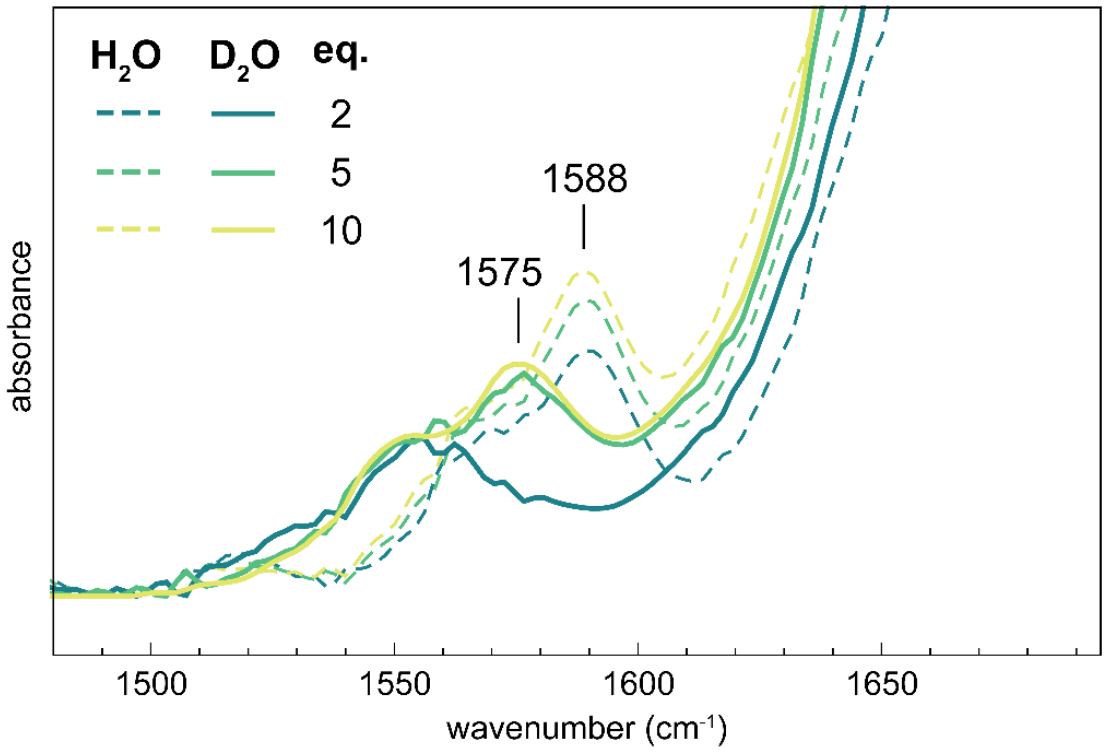


Fig. S54 IR-ATR spectrum of **3** with 0, 2, 5 and 10 equivalents of H_2O or D_2O

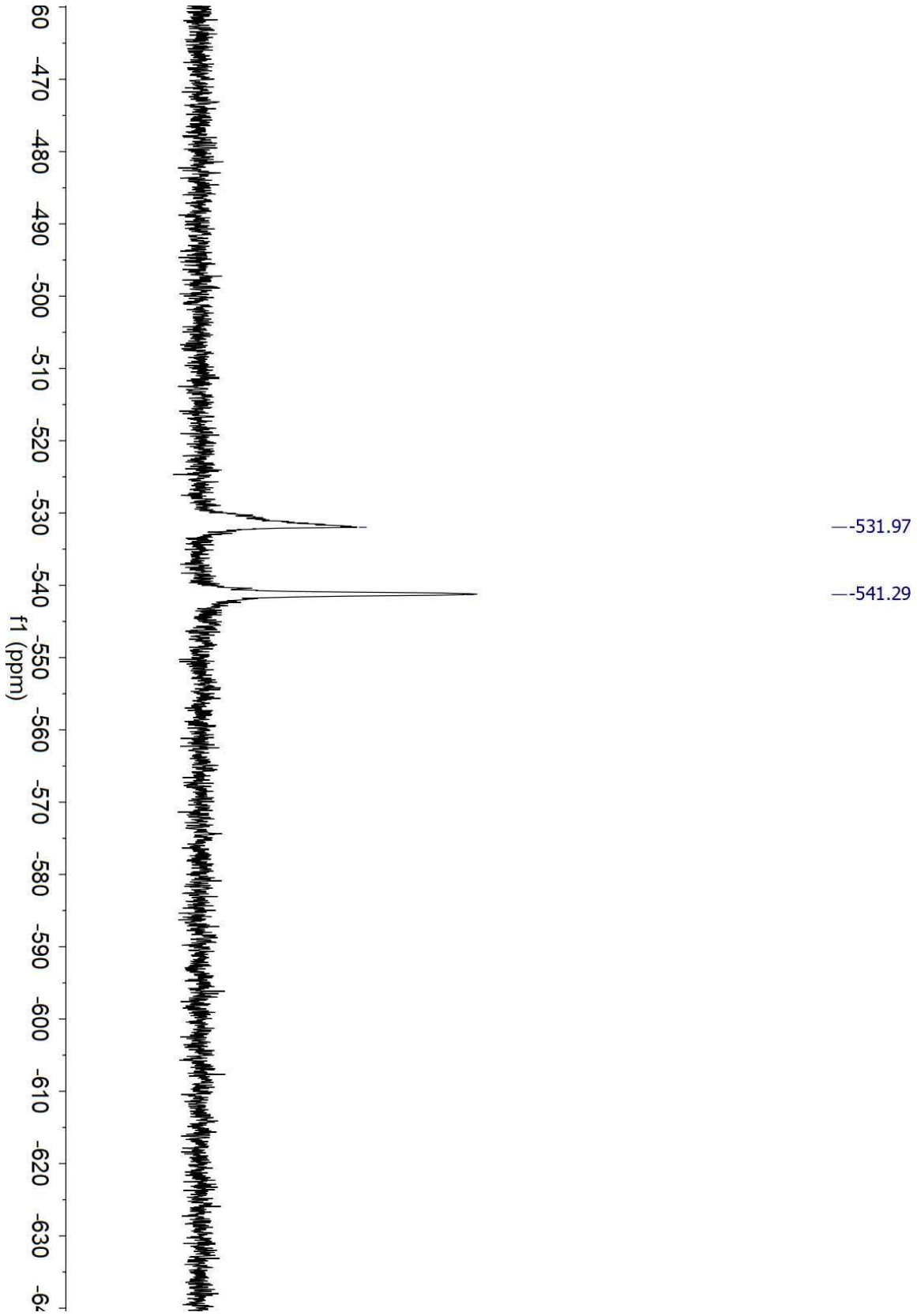


Fig. S55 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) in EtOH at 298 K (measured unlocked).

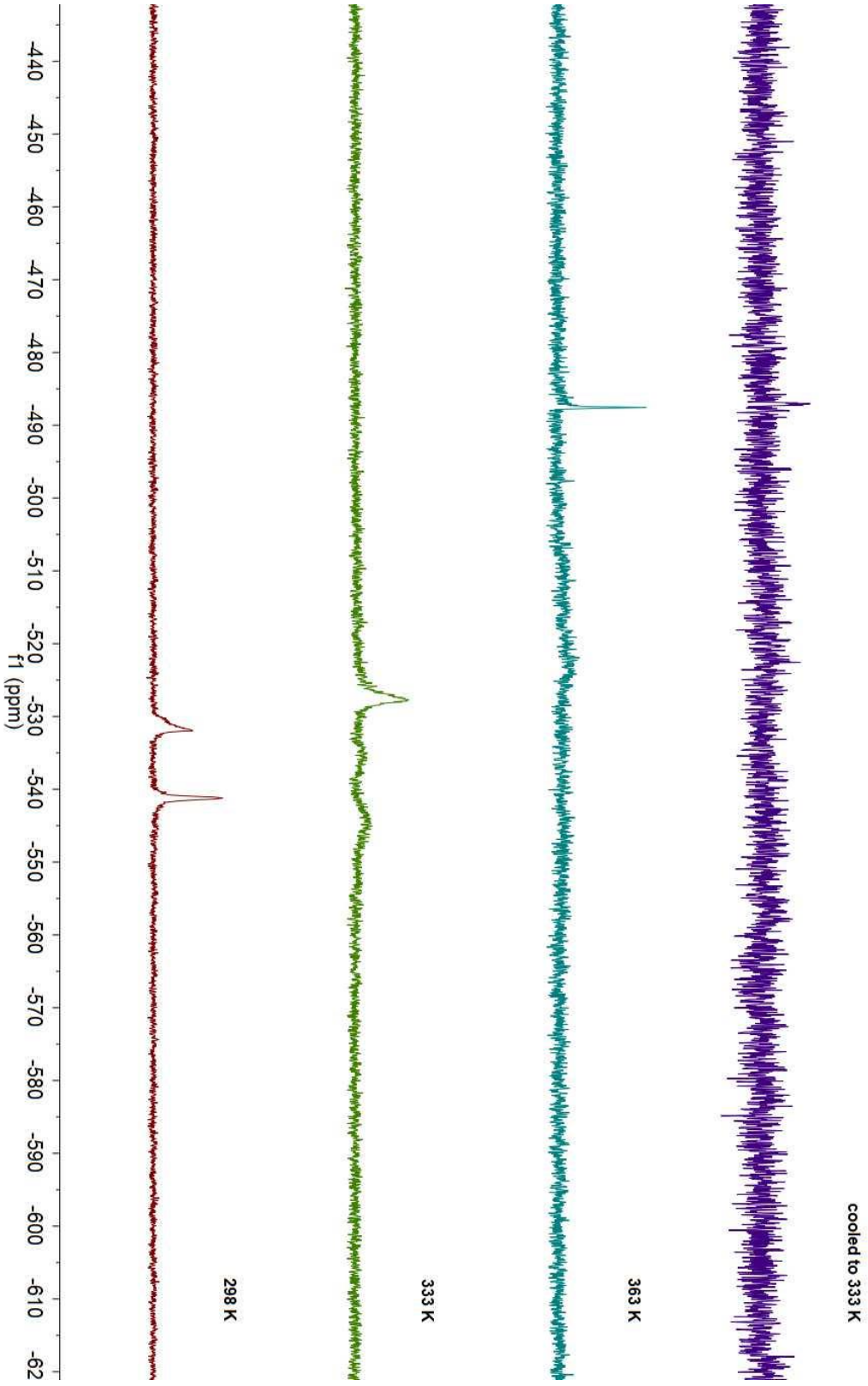


Fig. S56 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) in EtOH at 298, 333 and 363 K (measured unlocked).

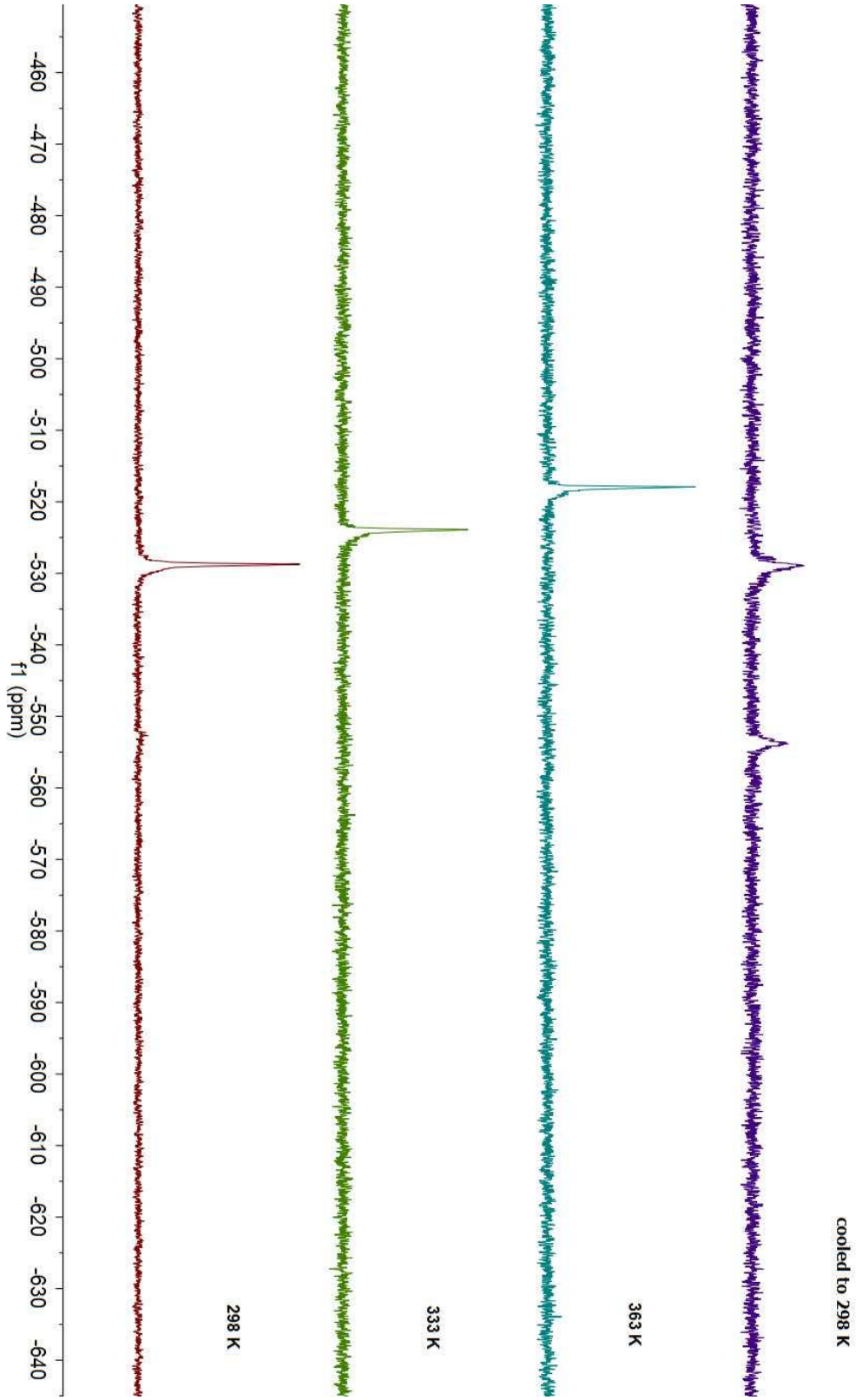


Fig. S57 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) in AcOH:EtOH 1:1 at 298, 333 and 363 K (measured unlocked).

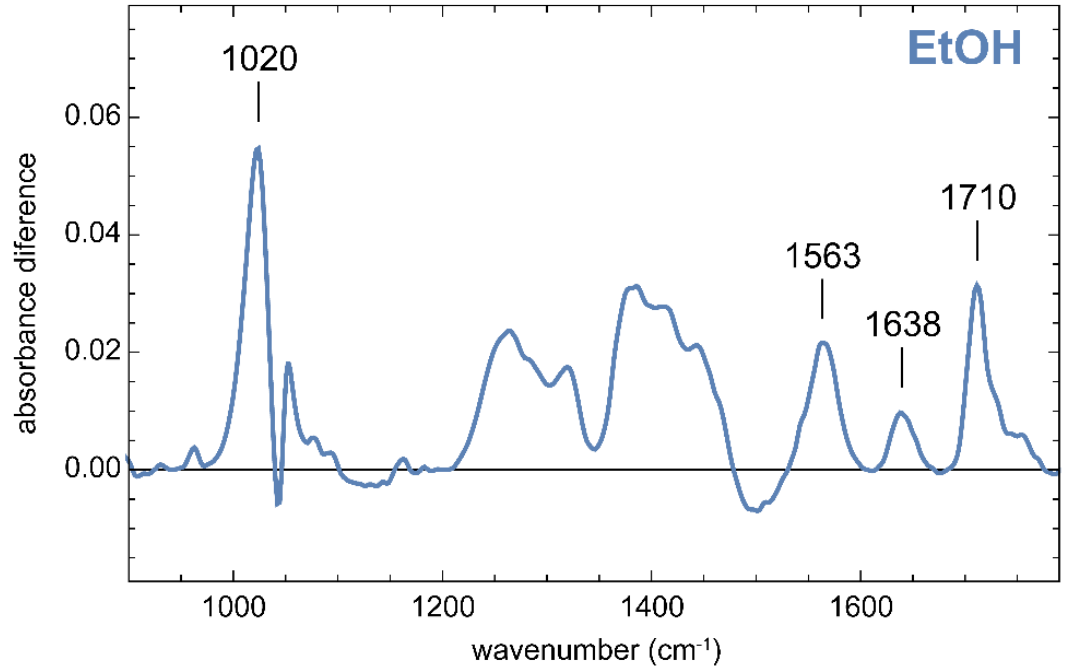


Fig. S58 IR-ATR difference spectrum of **3** in EtOH (minus EtOH)

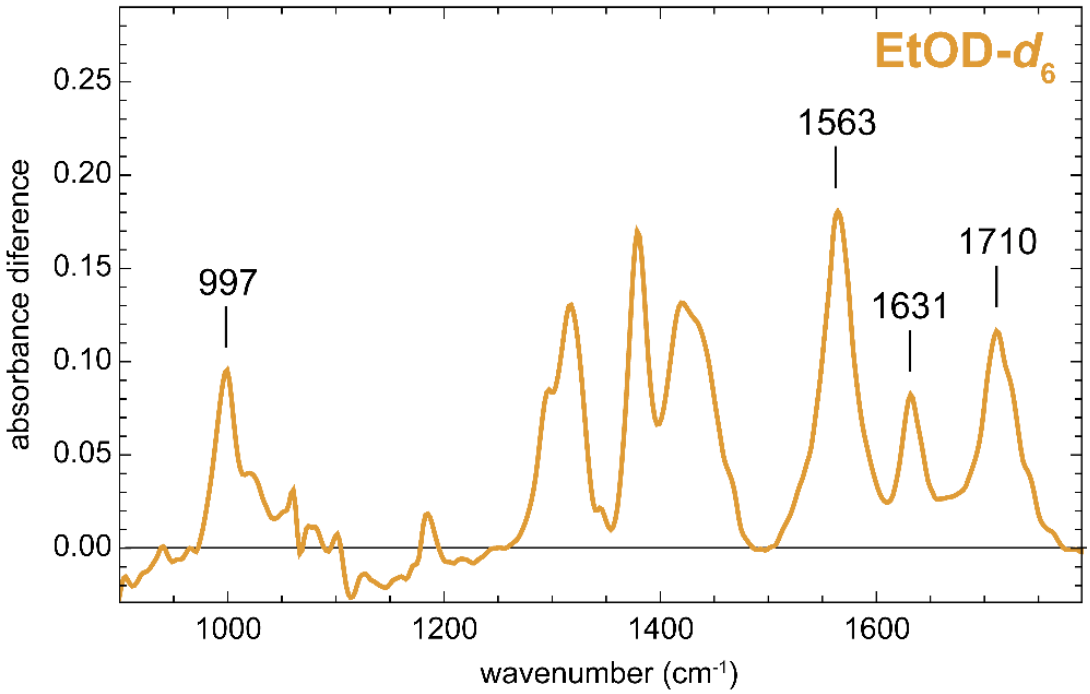


Fig. S59 IR-ATR difference spectrum of **3** in EtOD-d_6 (minus EtOD-d_6)

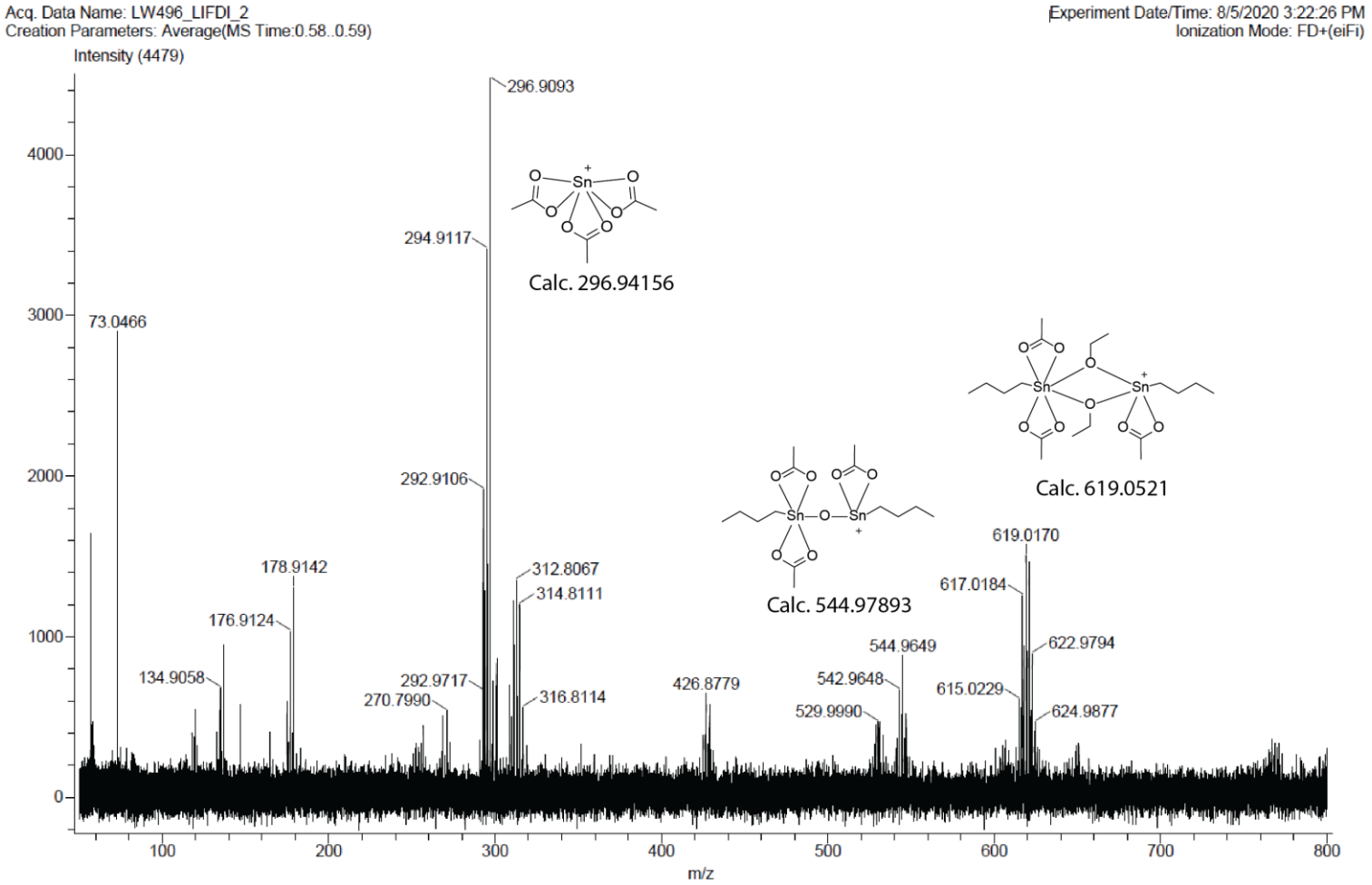


Fig. S60 LIFDI FD-MS spectrum of **3** in EtOH

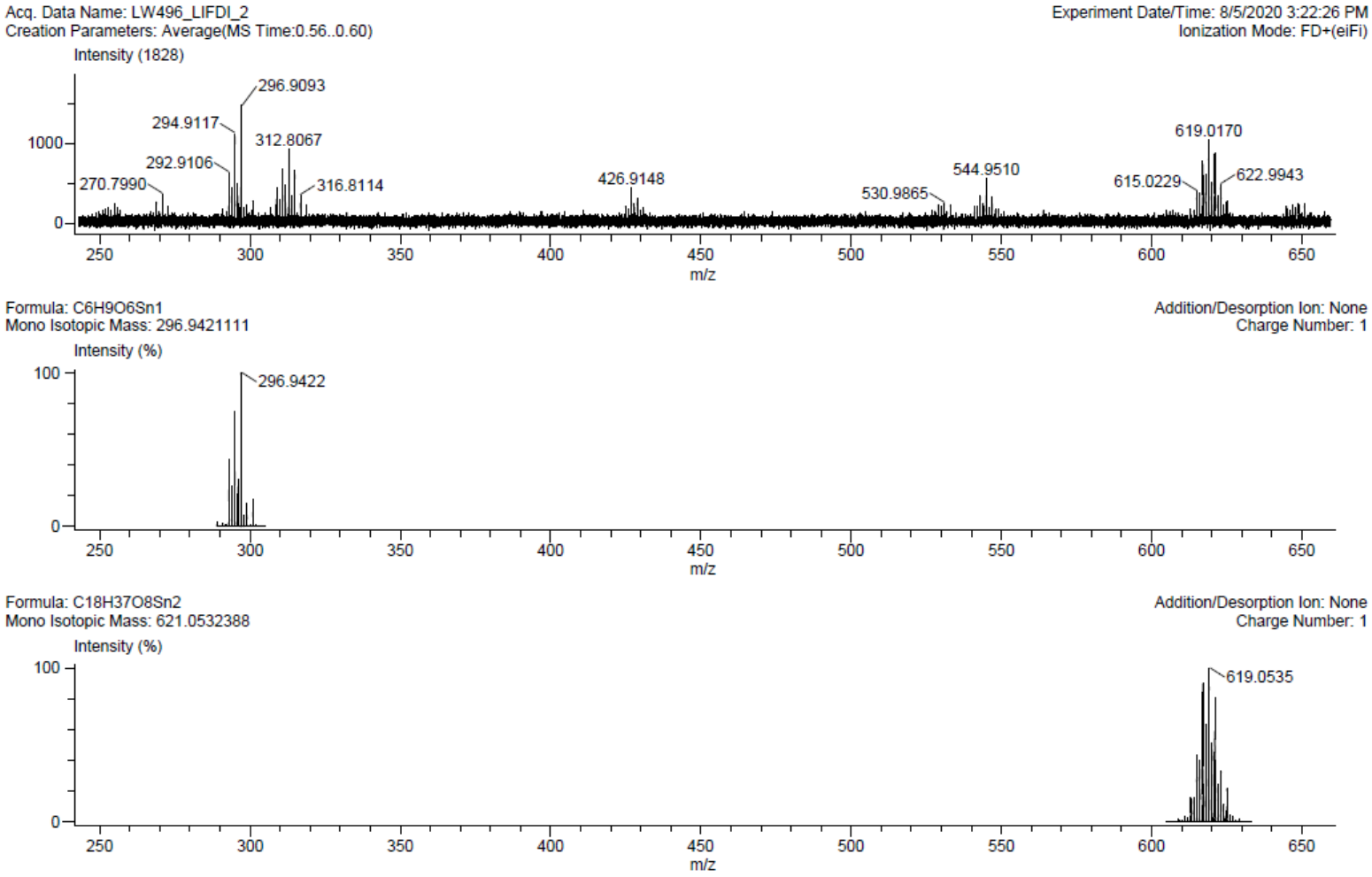


Fig. S61 LIFDI FD-MS spectrum of **3** in EtOH

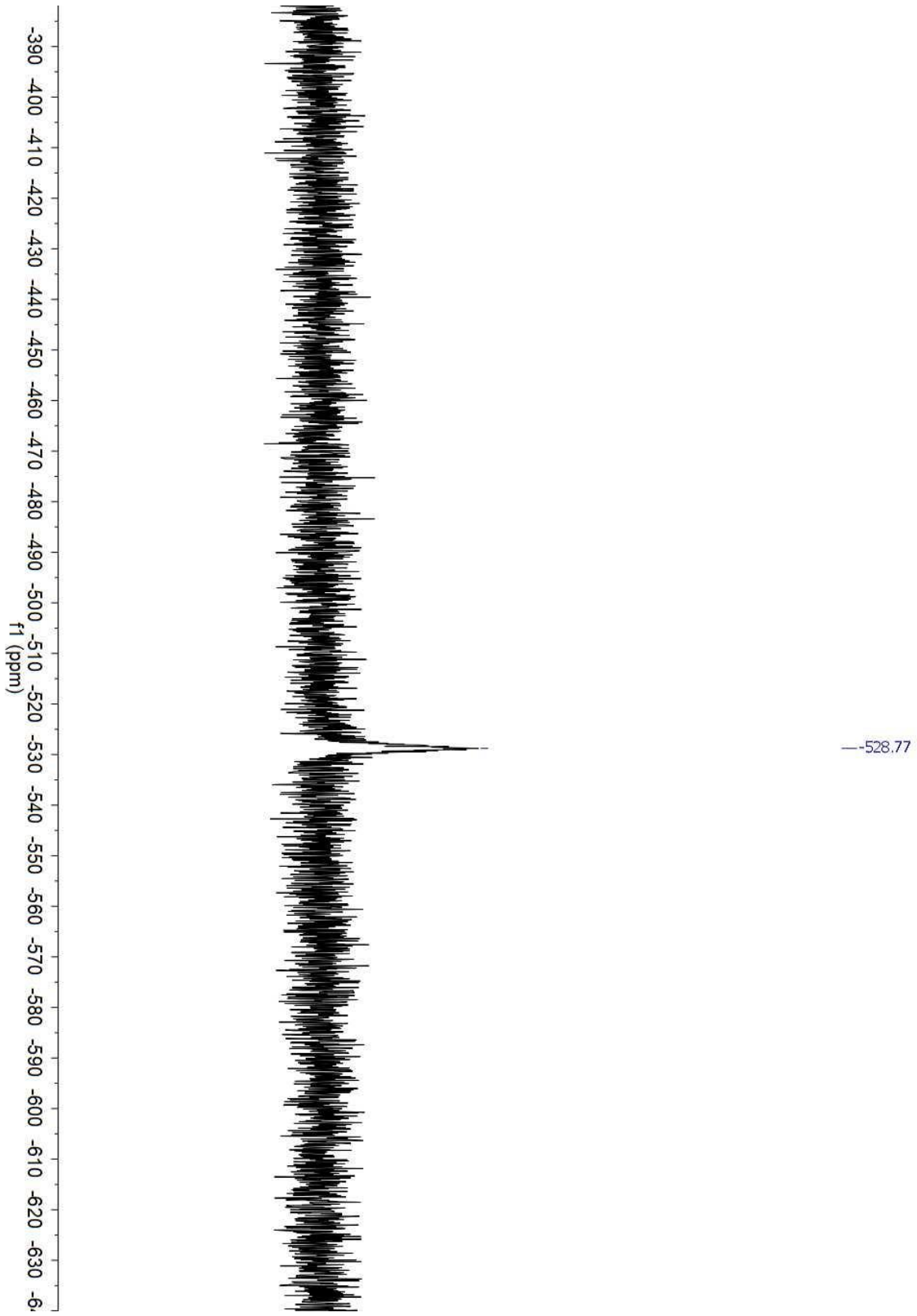


Fig. S62 ^{119}Sn{H} NMR of **5A** in acetic acid (measured unlocked) at 298 K.

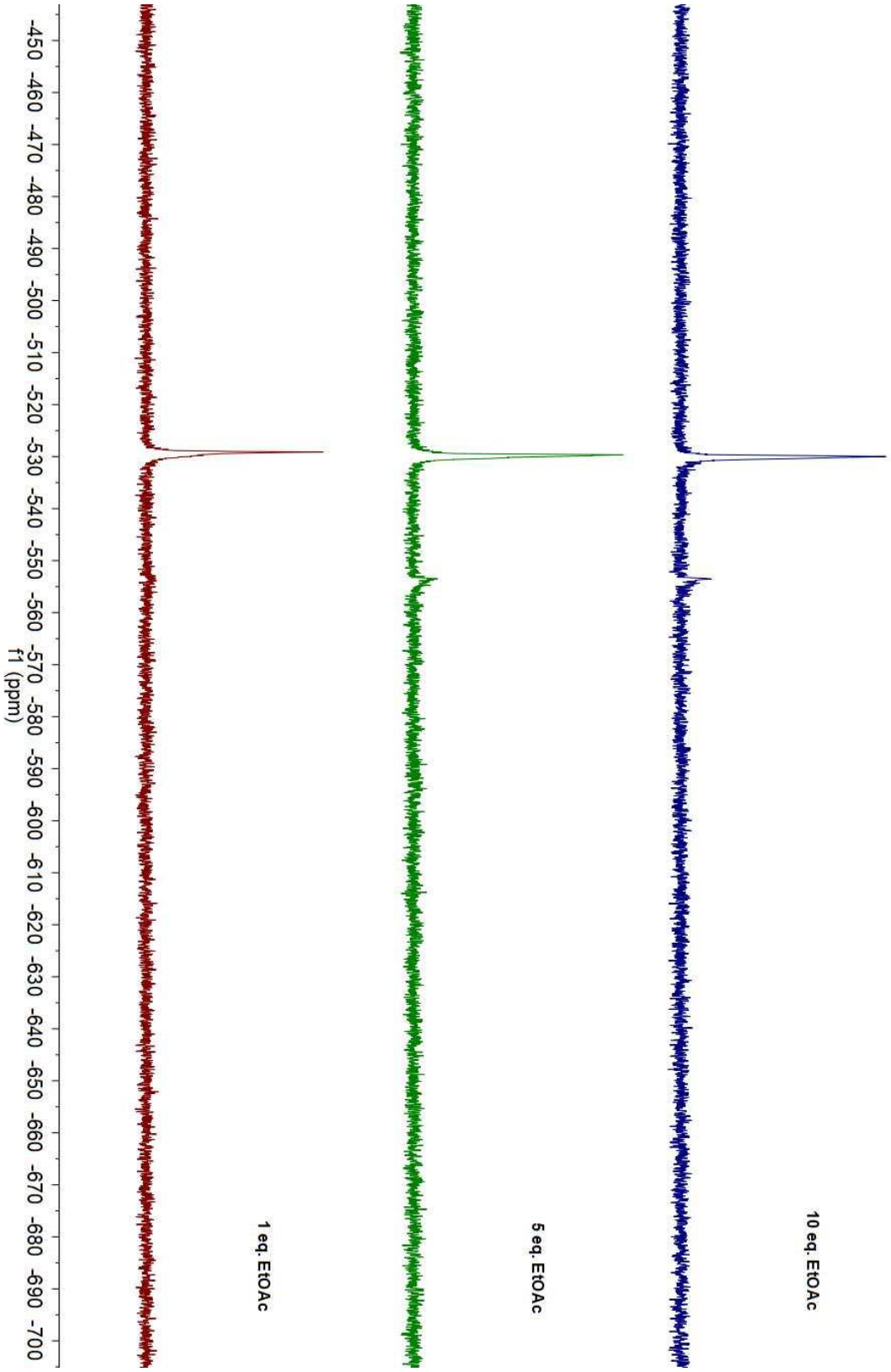


Fig. S63 ^{119}Sn{H} NMR of **3** (0.4 M in Sn) with 1, 5 and 10 equivalents EtOAc at 298K , Acetic acid/EtOH 1:1 (measured unlocked).

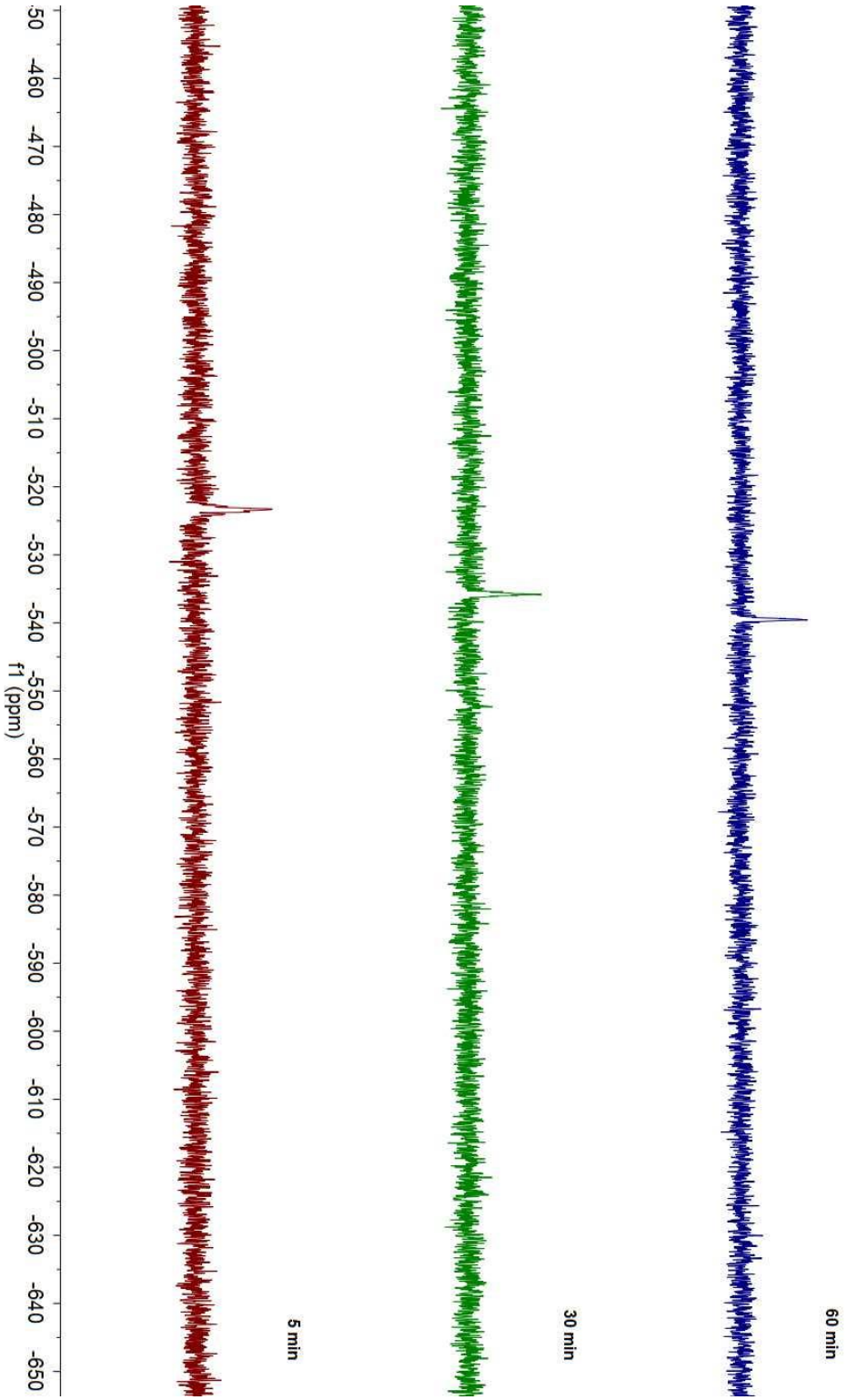


Fig. S64 ^{119}Sn{H} NMR of esterification reaction catalyzed by **3** (0.4 M in Sn) at 5, 30 and 60 min., Acetic acid/Ethanol ratio 1:1 (measured unlocked at 363 K).

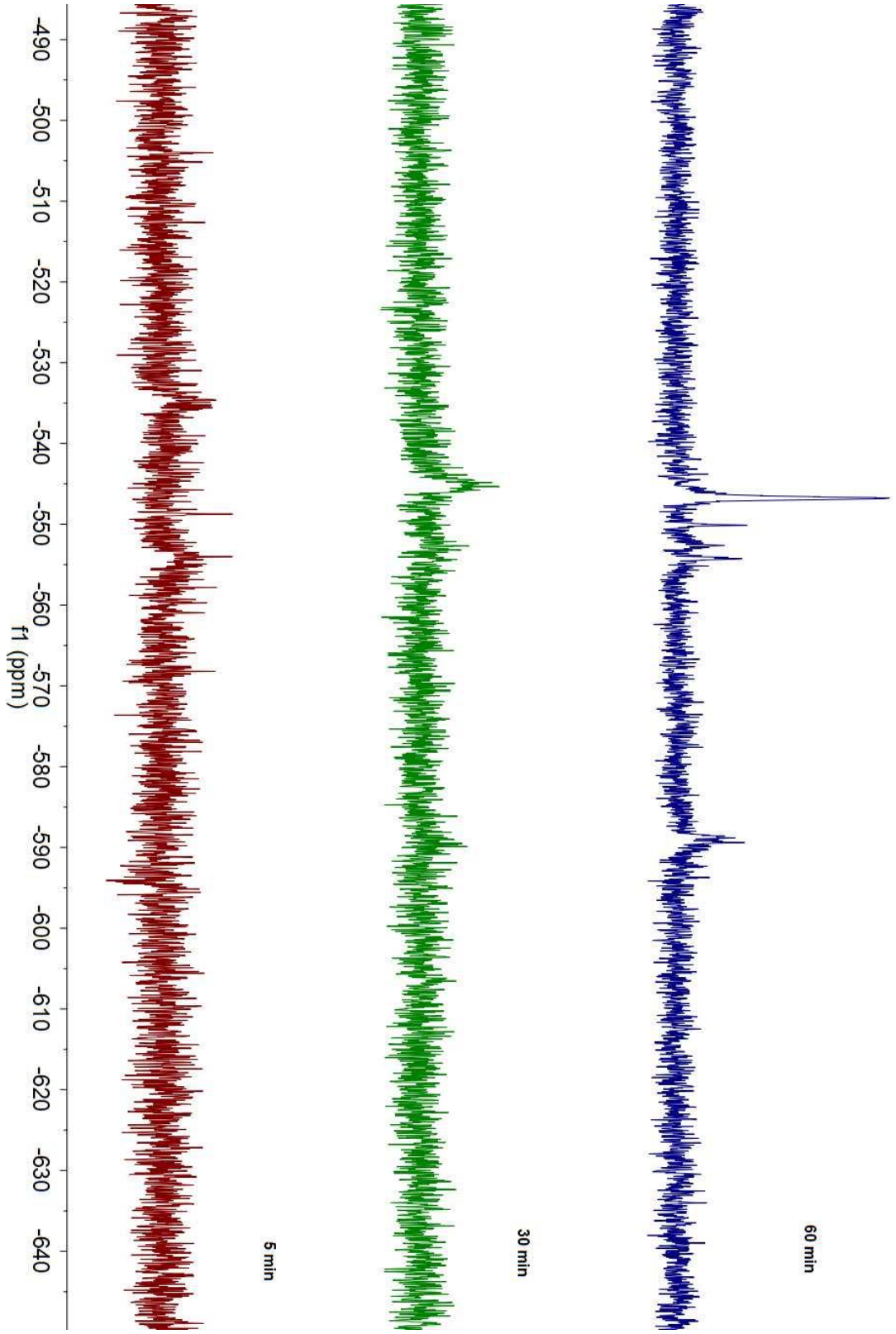


Fig. S65 ^{119}Sn{H} NMR of esterification reaction catalyzed by **3** (0.4 M in Sn) at 5, 30 and 60 min., Acetic acid/Ethanol ratio 1:1 (measured unlocked at 298 K).

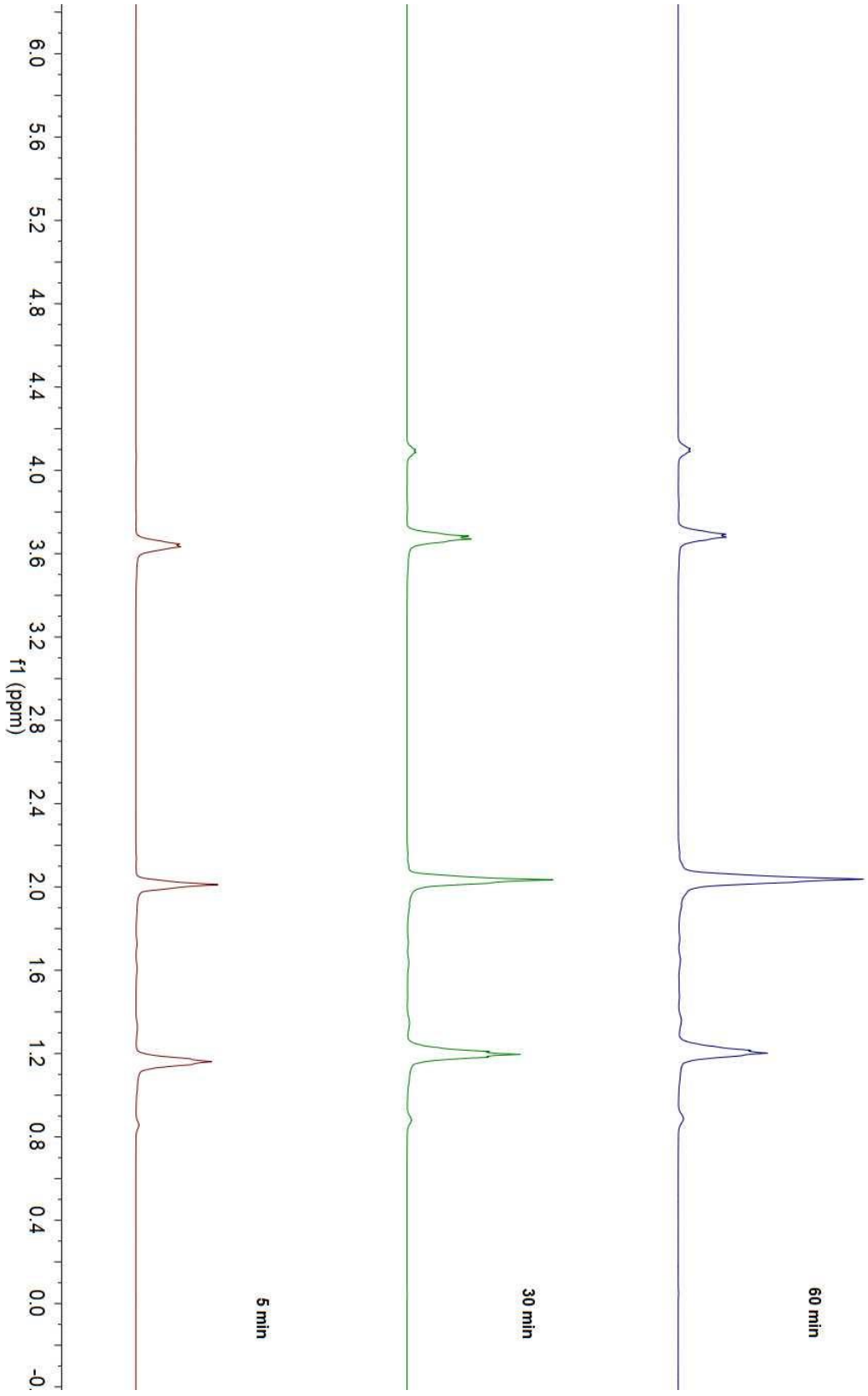


Fig. S66 ^{1}H NMR of esterification reaction catalyzed by **3** (0.4 M in Sn) at 5, 30 and 60 min, $CDCl_3$ at 298 K.

DFT calculations of catalytic cycle

Geometry optimizations were performed using the BP86 functional, def2-TZVP basisset, disp3 dispersion corrections and an M5 grid. Energies were subsequently refined with single point calculations using the M06-2x functional, def2-TZVP basisset for H,C,O and def2-QZVPP basisset for Sn, disp3 dispersion corrections and grid 7.

3 (BuSnOAc3)
E (Hartree) = -1057.65425127
G_{298} (Hartree) = -1057.42411

35

Sn	0.7231258	-0.3570411	0.2664018
C	-1.4013969	-0.3947614	0.6298516
H	-1.5140085	-0.1264522	1.6892622
H	-1.6943923	-1.4450902	0.4961566
C	-2.1683320	0.5478801	-0.2964211
H	-1.9829267	0.2808836	-1.3500221
H	-1.7990414	1.5802597	-0.1792716
C	-3.6810477	0.5197825	-0.0290657
H	-4.0493347	-0.5126343	-0.1512670
H	-3.8657870	0.7873931	1.0248681
C	-4.4598779	1.4630687	-0.9497091
H	-4.1268009	2.5041654	-0.8224547
H	-5.5389642	1.4282727	-0.7428794
H	-4.3117791	1.1957061	-2.0068971
O	0.8672980	-0.1132877	-1.9082572
C	0.7666289	-1.3734475	-2.1691009
O	0.6417063	-2.2019169	-1.2213986
C	0.8223938	-1.8179598	-3.6054015
H	1.8614981	-1.7303623	-3.9538671
H	0.2097469	-1.1555881	-4.2288910
H	0.4959597	-2.8579269	-3.7016870
O	2.8260684	-0.8399552	0.3712253
C	2.6483375	-1.7804822	1.2427370
O	1.4777259	-2.0379637	1.6454045
C	3.8465991	-2.5180245	1.7649566
H	4.5459953	-2.7278717	0.9473354
H	3.5402253	-3.4415316	2.2650773
H	4.3610149	-1.8693354	2.4885734
O	1.1775117	1.7881718	0.2292181
C	1.3345412	1.8938482	1.5062240
O	1.1992871	0.8738208	2.2417336
C	1.6970372	3.2378036	2.0775717
H	1.1035790	4.0248657	1.5970014
H	2.7542961	3.4357407	1.8494141
H	1.5551126	3.2479701	3.1625784

C1
E (Hartree) = -1967.22056833
G_{298} (Hartree) = -1966.69469

72

Sn	-1.1750517	-1.5077447	0.1217112
Sn	0.6167556	1.4336205	-0.1886009
O	-1.1067431	0.5249504	0.7384761
C	-1.8898595	1.1721446	1.7581368
H	-2.9050067	0.7491512	1.7239654
H	-1.9715132	2.2356118	1.4731499
C	-1.2988439	1.0231317	3.1533352
H	-1.9136488	1.5809272	3.8760384
H	-0.2708788	1.4066365	3.1917946
H	-1.2720480	-0.0337323	3.4450328
C	0.7481808	3.3598193	0.7935738
H	0.3369225	3.1935352	1.7989798
H	1.8321808	3.5148112	0.8981597
C	0.0674994	4.5177756	0.0727549
H	-1.0036337	4.3025198	-0.0673719
H	0.4858013	4.6287040	-0.9416704
C	0.2258020	5.8474237	0.8259172
H	-0.1910573	5.7380160	1.8413827
H	1.2993824	6.0629653	0.9582913
C	-0.4549194	7.0157459	0.1078700
H	-1.5339344	6.8331034	-0.0092078
H	-0.0331640	7.1604870	-0.8984571
H	-0.3318895	7.9578045	0.6609619
C	-1.1528444	-3.4913203	-0.7582679
H	-1.1390323	-4.1458589	0.1252287
H	-0.1722632	-3.5793498	-1.2441273
C	-2.3050788	-3.8172640	-1.7007288
H	-2.3371145	-3.0960861	-2.5330399
H	-3.2678373	-3.7098291	-1.1731048
C	-2.2058121	-5.2411191	-2.2691739
H	-2.1835127	-5.9633309	-1.4358769
H	-1.2424020	-5.3518485	-2.7949220
C	-3.3583238	-5.5774853	-3.2194345
H	-3.2710310	-6.5992437	-3.6155743
H	-3.3794196	-4.8858732	-4.0753190
H	-4.3290775	-5.4987607	-2.7065376
O	0.3163026	-0.4841810	-1.0200455
C	1.2358528	-1.1425727	-1.9203084
H	2.1157376	-0.4949360	-2.0269765
H	1.5693489	-2.0769490	-1.4425737
C	0.5766996	-1.3832897	-3.2680191
H	0.2881422	-0.4279882	-3.7258497
H	-0.3254366	-2.0031919	-3.1712720
H	1.2768215	-1.8966709	-3.9437992
O	2.7725680	0.8290415	-0.1437689
O	1.1359879	2.0268088	-2.2904137
C	2.7108229	0.3459309	1.0469629

C	-0.0865484	2.3001331	-2.5830940
O	-0.9929620	2.1532034	-1.7094873
O	1.6353339	0.4498179	1.7105892
C	3.8899958	-0.3930398	1.6116425
H	3.6714688	-1.4639516	1.4789852
H	3.9870060	-0.1964556	2.6857015
H	4.8126266	-0.1407318	1.0796250
C	-0.4256384	2.7619755	-3.9750239
H	-1.3361691	3.3704193	-3.9652687
H	-0.6147430	1.8713448	-4.5928354
H	0.4133012	3.3116795	-4.4157456
O	-3.3283716	-1.4664958	0.7141647
O	1.2649773	-2.5061730	1.0297947
C	0.6412049	-2.3332683	2.0898327
C	-3.6916375	-1.0024486	-0.4315156
O	-0.6187414	-1.9617538	2.1182584
O	-2.8187908	-0.7465237	-1.3152964
C	-5.1495691	-0.7497746	-0.7032434
H	-5.7807546	-1.2564571	0.0333990
H	-5.3993247	-1.0718573	-1.7209923
H	-5.3266238	0.3339946	-0.6458106
C	1.2887466	-2.4802168	3.4452065
H	0.5878877	-2.8954406	4.1787225
H	1.5667957	-1.4668513	3.7710187
H	2.1920988	-3.0951685	3.3750905

D

E (Hartree) = -1212.69468234

G_{298} (Hartree) = -1212.38798

44

Sn	1.8104067	-1.5972640	0.7734893
C	0.9686832	-1.5491728	2.7540247
H	0.4853217	-2.5312047	2.8463582
H	1.8443104	-1.5232896	3.4192284
C	0.0044498	-0.4004203	3.0224038
H	0.5236954	0.5648203	2.9061949
H	-0.8033705	-0.4010689	2.2736515
C	-0.6062414	-0.4729448	4.4302918
H	-1.1333240	-1.4349331	4.5454079
H	0.2047298	-0.4770413	5.1780360
C	-1.5683062	0.6839319	4.7134658
H	-2.3998777	0.6915099	3.9926613
H	-1.9990320	0.6141411	5.7225305
H	-1.0540280	1.6538403	4.6347636
O	-0.9465034	-0.9774687	-1.4703793
C	-0.9478118	-2.1662395	-0.9035727
C	-1.8159674	-3.1752573	-1.5971184
H	-2.6609893	-2.6962537	-2.1035487
H	-1.1956434	-3.6762959	-2.3555929
H	-2.1559013	-3.9302152	-0.8810197
O	-0.2929762	-2.4690172	0.1090989
O	2.4200579	-3.8137856	1.0109347
O	0.4950971	0.5987417	0.0426852
C	1.5977541	1.1527937	0.3261270
C	1.7506632	2.6447440	0.1593286
H	1.4185172	2.9342036	-0.8459226
H	1.0889045	3.1476334	0.8785876
H	2.7847698	2.9601700	0.3279691
O	2.5931656	0.4846973	0.7838706
C	4.7169160	-4.4515814	1.4108041
C	3.6205093	-3.4428872	1.1996922
H	4.3017288	-5.4126797	1.7304766
H	5.2401832	-4.5931875	0.4538156
H	5.4458379	-4.0755231	2.1379565
O	3.9148973	-2.1899286	1.1900461
O	2.0304700	-1.7601251	-1.1985816
H	2.3758167	-1.6640938	-3.8085071
H	3.6611525	-2.6675227	-3.0923932
C	3.0427452	-0.9978572	-1.8586986
H	2.7103930	0.0504318	-1.9955835
H	3.9751379	-0.9659549	-1.2663847
C	3.3014383	-1.6366370	-3.2163206
H	4.0572259	-1.0641724	-3.7752531
H	-0.3271429	-0.3520270	-0.9686652

E

E (Hartree) = -1367.74338859

G_{298} (Hartree) = -1367.35884

53

Sn	1.8937423	-1.6167227	0.6656502
C	0.9029226	-1.4500340	2.5732705
H	0.5961378	-2.4840913	2.7832804
H	1.7056511	-1.1726401	3.2717409
C	-0.2703880	-0.4799564	2.6266758
H	0.0708341	0.5446686	2.4092062
H	-1.0051989	-0.7265275	1.8428388
C	-0.9746520	-0.4942759	3.9923094
H	-1.3249870	-1.5178730	4.2063855
H	-0.2418225	-0.2508275	4.7797769
C	-2.1517557	0.4825516	4.0564694
H	-2.9073570	0.2417033	3.2934379
H	-2.6458223	0.4558522	5.0380663
H	-1.8184139	1.5159951	3.8770131
O	-1.3845526	-1.0129476	-1.0415776
C	-1.0418924	-2.2681907	-0.8073217
C	-1.9582326	-3.2770851	-1.4222324
H	-2.9788762	-2.8885563	-1.5102564
H	-1.5586823	-3.4601385	-2.4314573
H	-1.9310423	-4.2110310	-0.8523117
O	-0.0560214	-2.6174555	-0.1333597
O	2.5039827	-3.7872040	1.0824437
O	0.6674697	0.3842083	-0.2469502
C	1.6905342	1.0662387	0.0797982
C	1.7251716	2.5455985	-0.2006374

H	1.6114219	2.7049917	-1.2815640
H	0.8690523	3.0268014	0.2910395
H	2.6611603	2.9917531	0.1480855
O	2.6883333	0.5032116	0.6427709
C	4.7445267	-4.3846214	1.7578544
C	3.6761349	-3.3943569	1.3831589
H	4.2971745	-5.3000995	2.1587936
H	5.3037536	-4.6421135	0.8462926
H	5.4463624	-3.9411285	2.4727645
O	3.9607055	-2.1414512	1.3429076
O	2.4301089	-1.8982354	-1.2452737
H	3.3278946	-2.1185573	-3.7245944
H	4.4968422	-2.8829789	-2.6226573
C	3.5159024	-1.1388855	-1.7979374
H	3.1473832	-0.1531640	-2.1419093
H	4.2885061	-0.9523745	-1.0334625
C	4.0990547	-1.9186728	-2.9673331
H	4.9137040	-1.3491017	-3.4391421
H	-0.6633397	-0.3850788	-0.7284937
O	0.5337269	-2.2474687	-3.1779032
H	1.2380420	-2.2604507	-2.4778909
C	0.4834331	-0.9139751	-3.6866279
H	1.3408677	-0.7239339	-4.3642622
H	0.5572875	-0.1825488	-2.8592250
C	-0.8241316	-0.7269745	-4.4375637
H	-0.8815710	0.2772747	-4.8823428
H	-1.6746293	-0.8550245	-3.7537522
H	-0.9094732	-1.4690240	-5.2442957

F

E (Hartree) = -1367.72899995

G_{298} (Hartree) = -1367.34013

53

Sn	1.7132527	-1.9067619	0.8728723
H	3.1806616	-1.8723538	5.1943517
H	3.3169350	-0.1373951	4.8287790
C	3.5650679	-1.1413173	4.4677246
C	2.8974670	-1.4070705	3.1472834
H	-3.6909038	-1.1002784	2.9199195
O	1.7746772	-0.8567035	2.8742496
H	-3.1918670	-2.2251155	4.2048736
C	-2.9300599	-1.2917454	3.6879471
H	-2.9622500	-0.4699857	4.4189635
H	-0.7785347	-1.5572282	3.8497009
C	-1.5429970	-1.3924930	3.0754325
H	-0.1097720	-3.2187270	2.3072799
H	-1.2514235	-0.4765721	2.5408196
O	-1.2661682	-3.4703522	0.1596633
C	-1.3452071	-2.1916173	0.7156721
C	-2.5989939	-1.4579233	0.2469146
H	-3.4792500	-2.0759006	0.4576982
H	-2.6978918	-0.4797980	0.7337067
H	-2.5145504	-1.3027292	-0.8353528
O	-0.2404432	-1.4083747	0.4848527
H	3.6075825	-4.3972299	-2.4748222
O	3.4344378	-2.2026255	2.3039461
H	3.6370042	-0.6094083	-4.4099627
C	0.3365229	-5.6855805	3.1155957
H	-0.7356577	-5.4492924	3.1683395
H	0.4388912	-6.7653849	2.9343162
O	-1.4625705	-2.5236365	2.1696612
H	4.6488465	-1.2747314	4.3855138
O	0.7058924	-3.6459280	-1.6777476
O	2.4497297	-3.5492218	-0.2340350
C	1.8482867	-3.9696615	-1.3231153
C	2.6961520	-4.9164020	-2.1475669
H	3.0133100	-5.7644640	-1.5256764
H	2.1344629	-5.2722225	-3.0165964
H	0.7996263	-5.4485214	4.0832656
O	0.8910479	-3.4823428	2.2628122
H	-0.5969680	-3.4400516	-0.5795646
C	0.9985126	-4.9079156	1.9924994
H	2.0720190	-5.1197514	1.9169801
H	0.5203294	-5.1267662	1.0261119
C	2.5639938	-0.3211397	-0.3239421
H	1.9673149	0.5645868	-0.0624207
H	3.5902078	-0.1722079	0.0410994
C	2.5192807	-0.6157240	-1.8226836
H	3.1268923	-1.5082261	-2.0476015
H	1.4905963	-0.8637846	-2.1304427
C	3.0319708	0.5593741	-2.6681428
H	2.4189284	1.4508872	-2.4538198
H	4.0591763	0.8111366	-2.3538208
C	3.0053399	0.2592984	-4.1693170
H	1.9840079	0.0280890	-4.5073313
H	3.3700984	1.1124563	-4.7590447

G

E (Hartree) = -1367.72692446

G_{298} (Hartree) = -1367.33846

53

Sn	1.7937266	-2.0204824	0.8955821
H	3.0729426	-2.2257370	5.2783439
H	3.3599890	-0.5023331	4.9635365
C	3.5482553	-1.5139668	4.5873610
C	2.9203898	-1.6945377	3.2332967
H	-3.6605970	-0.3189127	2.1902841
O	1.8220100	-1.1023781	2.9556623
H	-3.2915407	-0.9397032	3.8161594
C	-2.9487960	-0.2587048	3.0250138
H	-2.9643453	0.7682108	3.4208257
H	-0.8247251	-0.5379120	3.4047740
C	-1.5429583	-0.6323882	2.5764576
H	0.0360099	-3.8337090	1.7112870

H	-1.1849349	0.0261535	1.7694023
O	-1.1591755	-3.6597294	0.7319742
C	-1.2660543	-2.2253818	0.7662016
C	-2.4310080	-1.7706160	-0.1119992
H	-3.3519091	-2.2544854	0.2330000
H	-2.5414528	-0.6800023	-0.0614125
H	-2.2312301	-2.0528599	-1.1529679
O	-0.1078580	-1.6097935	0.3100623
H	2.9123201	-4.0838304	-3.0701963
O	3.4696843	-2.4593488	2.3665948
H	3.1697910	-0.0636234	-4.3315862
C	1.1262113	-5.9082321	3.1992477
H	0.0404138	-6.0610273	3.1269768
H	1.6137532	-6.8941799	3.1865551
O	-1.4932159	-2.0075960	2.1507970
H	4.6213302	-1.7274205	4.5489284
O	0.4940069	-4.3929698	-1.2170434
O	2.4501878	-3.4827930	-0.4898260
C	1.7192722	-4.2129951	-1.2961660
C	2.5269440	-4.8662759	-2.4009726
H	3.3958043	-5.3845905	-1.9747082
H	1.9039405	-5.5629512	-2.9704483
H	1.3450536	-5.4213178	4.1589420
O	0.9977910	-3.7558302	2.0833227
H	-0.6424666	-3.8927025	-0.1025249
C	1.6323635	-5.0647651	2.0425437
H	2.7122438	-4.8842706	2.1104774
H	1.4168312	-5.5410340	1.0734160
C	2.7647295	-0.3839536	-0.1263530
H	2.4126426	0.5235143	0.3854564
H	3.8402267	-0.4967345	0.0717180
C	2.4515154	-0.3568896	-1.6222005
H	2.7904931	-1.2958183	-2.0903596
H	1.3609280	-0.3127462	-1.7761442
C	3.1134672	0.8287708	-2.3398973
H	2.7724697	1.7687370	-1.8739112
H	4.2040963	0.7855748	-2.1789396
C	2.8098248	0.8533676	-3.8404384
H	1.7267182	0.9225445	-4.0230562
H	3.2893234	1.7092814	-4.3366156

H

E (Hartree) = -1367.73966714

G_{298} (Hartree) = -1367.35541

53

Sn	1.5431359	-2.3172166	0.5894149
H	4.8432118	0.1898424	2.5901410
H	4.3481890	1.3800720	1.3562468
C	4.6089922	0.3302795	1.5247009
C	3.4521139	-0.5685876	1.1741979
H	-0.0528077	1.2855212	1.2069757
O	2.2689739	-0.1184591	1.1129562
H	-1.1815345	2.1434767	2.3094942
C	-0.2964360	1.4945026	2.2548110
H	0.5588326	2.0285429	2.6915381
H	-0.7495326	0.3862683	4.0763449
C	-0.5177771	0.2042475	3.0198833
H	-0.4634265	-3.2464438	2.8712503
H	0.3396428	-0.4762926	2.9477351
O	-1.3155831	-3.7410997	2.8053107
C	-1.6211959	-1.2081320	1.4207073
C	-2.9256483	-1.8204060	1.0073883
H	-3.4336844	-2.2362474	1.8831947
H	-3.5598999	-1.0395490	0.5604180
H	-2.7350816	-2.6036762	0.2683065
O	-0.5874761	-1.2942049	0.7444210
H	0.8108126	-6.6551752	-0.9886839
O	3.6828551	-1.8165556	0.9559635
H	4.6228487	-1.3197188	-4.1563314
C	1.8681089	-3.1526098	4.7801251
H	0.8171951	-3.3031160	5.0650340
H	2.4912833	-3.8253857	5.3880378
O	-1.7178553	-0.4970593	2.5375693
H	5.4984257	0.0490918	0.9489851
O	0.1135950	-4.2693593	0.3129864
O	2.3262187	-4.3908325	0.3346888
C	1.1760360	-4.9596883	0.2478049
C	1.1081117	-6.4521426	0.0502580
H	2.0785242	-6.9194259	0.2445475
H	0.3354527	-6.8759626	0.7034703
H	2.1467383	-2.1143536	5.0089632
O	1.2135126	-2.5465779	2.5604670
H	-1.1830953	-4.2145655	1.9619117
C	2.0630987	-3.4423091	3.2998067
H	3.1177682	-3.3061705	3.0069987
H	1.7911288	-4.4911542	3.0800197
C	1.3690786	-1.8219299	-1.4959755
H	0.5419729	-2.4479867	-1.8568096
H	1.0485891	-0.7718941	-1.5045728
C	2.6650241	-2.0533074	-2.2663632
H	3.4747204	-1.4365397	-1.8430857
H	2.9938143	-3.0994508	-2.1521142
C	2.5154716	-1.7302646	-3.7612235
H	1.7091157	-2.3519242	-4.1856241
H	2.1853415	-0.6837429	-3.8732776
C	3.8116300	-1.9538756	-4.5448647
H	4.1446437	-2.9998996	-4.4675810
H	3.6842872	-1.7197250	-5.6114351

I

E (Hartree) = -1291.29479770

G_{298} (Hartree) = -1290.93451

50

Sn	1.5293310	-2.3686922	0.5382068

H	5.0036488	-0.0739516	2.5049317
H	4.5910093	1.1560579	1.2756772
C	4.7699094	0.0891798	1.4428417
C	3.5451038	-0.7182977	1.0965868
H	-0.7461389	1.4722980	0.8371599
O	2.4125950	-0.1695742	0.9637637
H	-1.7605103	2.1506876	2.1481186
C	-0.7618865	1.7702043	1.8921100
H	-0.0352550	2.5836502	2.0292760
H	-0.3688958	0.8823146	3.8425989
C	-0.3760008	0.6034970	2.7817442
C	3.9642911	-1.5022954	-4.4571143
H	0.5973441	0.1794820	2.5062113
H	4.5038487	-2.4558392	-4.3532642
C	-1.3129635	-1.3069123	1.6956582
C	-2.2560736	-2.4645195	1.8059616
H	-2.9341966	-2.3638703	2.6588697
H	-2.8149786	-2.5664959	0.8675100
H	-1.6382902	-3.3679257	1.9094283
O	-0.5533020	-1.1365970	0.7325447
H	1.4676464	-6.7792809	-0.8353949
O	3.6742150	-1.9924392	0.9507759
H	4.6007375	-0.7140956	-4.0270018
C	1.4523381	-3.1110102	4.7472487
H	0.3751615	-3.0241877	4.9487370
H	1.8713032	-3.8841542	5.4088223
O	-1.3778838	-0.4712538	2.7296658
H	5.6300584	-0.2592272	0.8585516
O	0.0066775	-4.2608658	0.2934582
O	2.2148663	-4.4654074	0.3496069
C	1.0389825	-4.9885363	0.2513548
C	0.9436609	-6.4843171	0.0839458
H	1.4568739	-6.9759074	0.9211663
H	-0.1013122	-6.8058692	0.0390430
H	1.9248754	-2.1485443	4.9885443
O	1.0917455	-2.4480972	2.4850319
H	3.8529549	-1.2945421	-5.5309791
C	1.6908653	-3.4667648	3.2861451
H	2.7740058	-3.5504788	3.0824230
H	1.2405071	-4.4537736	3.0606420
C	1.3771305	-1.8921573	-1.5531839
H	0.7131172	-2.6649696	-1.9642134
H	0.8573648	-0.9260741	-1.5794929
C	2.7342094	-1.8519824	-2.2478915
H	3.3715006	-1.0800089	-1.7860626
H	3.2653432	-2.8080760	-2.1088849
C	2.6069809	-1.5588742	-3.7509920
H	1.9742640	-2.3328920	-4.2170797
H	2.0726886	-0.6037060	-3.8881061

TS_E_F

E (Hartree) = -1367.72328923

G_{298} (Hartree) = -1367.33750

53

Sn	1.7084406	-1.9711158	0.7818381
H	2.9451440	-1.5780372	5.1887585
H	3.0734690	0.1230443	4.6915520
C	3.3609556	-0.9008827	4.4280924
C	2.7800754	-1.2844570	3.0931660
H	-3.5185368	-1.3704760	3.3669491
O	1.6480263	-0.8095113	2.7311271
H	-2.9816893	-2.7167933	4.3978126
C	-2.7152993	-1.7160067	4.0308991
H	-2.6637075	-1.0330505	4.8920266
H	-0.5740856	-2.0804049	3.9854677
C	-1.3783794	-1.7496524	3.3102344
H	-0.2492604	-3.2188867	2.1411016
H	-1.0731438	-0.7626094	2.9309867
O	-1.5074721	-3.1764434	-0.0670897
C	-1.4041307	-2.0324665	0.7031489
C	-2.6798266	-1.2164223	0.6057097
H	-3.5488393	-1.8561192	0.7947859
H	-2.6627969	-0.3770525	1.3094867
H	-2.7381567	-0.8172309	-0.4146249
O	-0.2965017	-1.3054812	0.5759803
H	2.6237687	-4.5278161	-3.0194311
O	3.3960485	-2.0979384	2.3309991
H	4.1835233	-0.7118678	-4.3081126
C	0.3932591	-5.6582395	3.0306245
H	-0.6848550	-5.4501535	3.0763318
H	0.5303308	-6.7442962	2.9257352
O	-1.4138897	-2.6921359	2.2072751
H	4.4500193	-1.0148857	4.4223210
O	1.0288105	-3.3544187	-1.0916181
O	2.9870411	-3.6424543	-0.1166105
C	2.1511690	-3.9560435	-1.0264978
C	2.4961156	-5.0130725	-2.0413996
H	3.4179948	-5.5354969	-1.7687600
H	1.6625117	-5.7205947	-2.1349992
H	0.8541424	-5.3380721	3.9750161
O	0.8568154	-3.5124435	2.0227288
H	-0.6361938	-3.3373685	-0.5019787
C	1.0310145	-4.9357237	1.8552427
H	2.1102851	-5.1295662	1.7994321
H	0.5686790	-5.2550581	0.9051682
C	2.5647611	-0.3861482	-0.4113785
H	1.8781262	0.4566599	-0.2487881
H	3.5246314	-0.1594175	0.0741737
C	2.7325387	-0.7138065	-1.8916910
H	3.3982525	-1.5852417	-2.0105935
H	1.7635777	-1.0042030	-2.3278542
C	3.3134149	0.4646986	-2.6881038

H 2.6483545 1.3374214 -2.5763500
H 4.2808883 0.7581811 -2.2469422
C 3.4969128 0.1378548 -4.1726828
H 2.5375674 -0.1336164 -4.6388147
H 3.9093102 0.9927284 -4.7274984

TS_F_G

E (Hartree) = -1367.72670226

G_{298} (Hartree) = -1367.33864

53

Sn 1.4634398 -2.6026314 0.1983441
H 5.5479389 -4.4272781 1.1031320
H 5.9441567 -3.5404880 -0.3838616
C 5.2339994 -4.2436426 0.0649662
C 3.8550069 -3.6468649 0.0986503
H 2.8606753 2.2018691 3.1463820
O 3.7080009 -2.3869698 0.2647632
H 3.9858122 1.1408788 4.0256985
C 3.6766165 1.4764308 3.0261677
H 4.5286892 1.9884329 2.5536983
H 4.0658375 -0.4195077 2.0326251
C 3.2382483 0.2898438 2.1798389
H 1.7036426 -2.4141240 2.8854873
H 2.9090006 0.6022107 1.1764569
O 0.1589302 -1.2544482 3.0689560
C 0.8783304 -0.3718136 2.2313117
C 0.2912846 1.0382859 2.2825485
H 0.2723543 1.3790529 3.3241228
H 0.8842919 1.7312410 1.6721713
H -0.7311624 1.0099538 1.8869589
O 0.8978187 -0.7849453 0.9018040
H -2.6234349 -4.4603342 -0.6471675
O 2.8253157 -4.3967752 -0.0128259
H -2.5480984 -1.8903236 -3.8540754
C 1.8982731 -4.6750509 4.3196169
H 1.7771571 -3.8268230 5.0080278
H 1.4125116 -5.5524276 4.7710946
O 2.1837005 -0.4444091 2.8336436
H 5.2301541 -5.1976542 -0.4720982
O -1.6073211 -2.7078611 1.6554546
O -0.1867607 -3.9051879 0.3446097
C -1.3593371 -3.6339981 0.8724575
C -2.4431595 -4.5968252 0.4286491
H -2.1070869 -5.6321988 0.5715262
H -3.3681647 -4.4122564 0.9835771
H 2.9701583 -4.8870630 4.2086235
O 1.9371051 -3.2318988 2.3615510
H -0.5467538 -1.6957292 2.5119983
C 1.2654302 -4.3708718 2.9742916
H 1.3856498 -5.1968335 2.2630250
H 0.1936842 -4.1434357 3.0768593
C 1.2015392 -2.1560157 -1.8985897
H 1.8981401 -1.3306680 -2.1050975
H 1.5422512 -3.0439353 -2.4499470
C -0.2422090 -1.7830820 -2.2360236
H -0.9113369 -2.6259334 -1.9953260
H -0.5694677 -0.9405909 -1.6049663
C -0.4234751 -1.4079022 -3.7142707
H 0.2404871 -0.5605180 -3.9546057
H -0.0872600 -2.2486089 -4.3445840
C -1.8712287 -1.0465124 -4.0572941
H -2.2180692 -0.1926614 -3.4559359
H -1.9807281 -0.7771830 -5.1175197

TS_G_H

E (Hartree) = -1367.71757450

G_{298} (Hartree) = -1367.33426

53

Sn 1.1560935 -2.2204224 0.4812546
H 5.3306296 -4.1358228 0.6983787
H 5.5593341 -3.0901700 -0.7198050
C 4.8972846 -3.8364825 -0.2673106
C 3.5380596 -3.2448964 -0.0070695
H 3.6747663 0.6361825 1.1743275
O 3.4180591 -2.0037616 0.2610086
H 4.1923345 1.8128209 2.4214261
C 4.1012580 0.7448741 2.1778820
H 5.1072455 0.2995238 2.1758183
H 3.6505201 0.1064293 4.2091859
C 3.2236941 0.0384439 3.1981112
H 0.9567057 -2.0139898 3.0921565
H 3.1052708 -1.0235864 2.9431555
O 0.2902784 -1.0434468 3.4814569
C 0.9030295 0.1814275 2.5416210
C -0.2310167 1.1903321 2.5042851
H -0.4911189 1.5193070 3.5165583
H 0.1050270 2.0521265 1.9140545
H -1.1024487 0.7426032 2.0110105
O 1.2514877 -0.3210199 1.3608487
H -3.3673369 -3.5136165 0.2964772
O 2.4994667 -3.9902259 -0.0323004
H 2.2509976 -2.9778336 -5.1329563
C 2.0608545 -4.4737247 4.1953462
H 1.8152760 -3.7564264 4.9912217
H 1.8538976 -5.4877168 4.5680383
O 1.9265168 0.6817647 3.3115944
H 4.8159473 -4.7269329 -0.8995250
O -1.2118702 -2.0390956 1.3849871
O -0.3978739 -3.8563791 0.4106367
C -1.3667114 -3.2255191 0.9645656
C -2.7072141 -3.9091261 1.0821562
H -2.6107866 -4.9917280 0.9516281
H -3.1663682 -3.6712663 2.0491561
H 3.1344124 -4.3936079 3.9768132

O 1.5337610 -2.8594126 2.4794881
H -0.5604951 -1.2621514 3.0315513
C 1.2428022 -4.1958249 2.9451713
H 1.4880806 -4.8954654 2.1348276
H 0.1618260 -4.2873505 3.1517382
C 0.6674523 -1.5072867 -1.4931435
H -0.4230402 -1.3690919 -1.4745146
H 1.1420592 -0.5184724 -1.5564423
C 1.1130908 -2.4488830 -2.6075074
H 2.2091024 -2.5701202 -2.5831864
H 0.6937734 -3.4555068 -2.4461423
C 0.6990428 -1.9437914 -3.9981715
H -0.3978521 -1.8301962 -4.0275747
H 1.1149418 -0.9341590 -4.1547207
C 1.1551731 -2.8752757 -5.1244783
H 0.7299838 -3.8827844 -5.0005810
H 0.8464156 -2.4992481 -6.1103624

AcOH
E (Hartree) = -229.08763661
G_{298} (Hartree) = -229.05148

8
H 0.5170707 0.7603004 -1.5407461
C 0.4285750 0.7414128 -0.4510412
H 1.4250609 0.7871242 0.0093646
H -0.1328423 1.6181216 -0.1006074
C -0.2724943 -0.5214547 -0.0240313
O -0.6678006 -1.4046882 -0.7560963
O -0.4202092 -0.5680652 1.3358422
H -0.8783601 -1.4127509 1.5283156

EtOH
E (Hartree) = -155.02653332
G_{298} (Hartree) = -154.97101

9
C -0.0775664 0.1462435 1.0080721
H 0.9570154 0.1180282 1.3771402
H -0.6012351 -0.7439334 1.3833051
H -0.5701749 1.0400122 1.4169312
C -0.0977324 0.1727871 -0.5093930
H 0.4208321 1.0779174 -0.8805994
H -1.1420669 0.2129614 -0.8752548
O 0.5592818 -1.0174081 -0.9743118
H 0.5506464 -1.0076084 -1.9458897

EtOAc
E (Hartree) = -307.69216119
G_{298} (Hartree) = -307.60321

14
C -0.1007697 0.0947965 0.9158948
O -0.1270237 -1.1114384 1.5470228
O -0.1433365 0.2256544 -0.2915027
C 0.0189722 1.2233235 1.9117515
H 1.0865441 1.4230603 2.0865829
H -0.4419817 0.9669742 2.8724769
H -0.4342624 2.1265374 1.4896953
C -0.1913669 -2.2732847 0.6709247
H 0.6725574 -2.2490813 -0.0101340
H -1.0995625 -2.1983616 0.0542527
C -0.1944352 -3.5044754 1.5534576
H 0.7180735 -3.5529125 2.1629651
H -0.2423691 -4.4087355 0.9304301
H -1.0620397 -3.5030570 2.2271822

H2O
E (Hartree) = -76.42584221
G_{298} (Hartree) = -76.42235

3
H 0.0000000 0.7673526 0.1988264
O 0.0000000 0.0000000 -0.3966527
H 0.0000000 -0.7673526 0.1988264

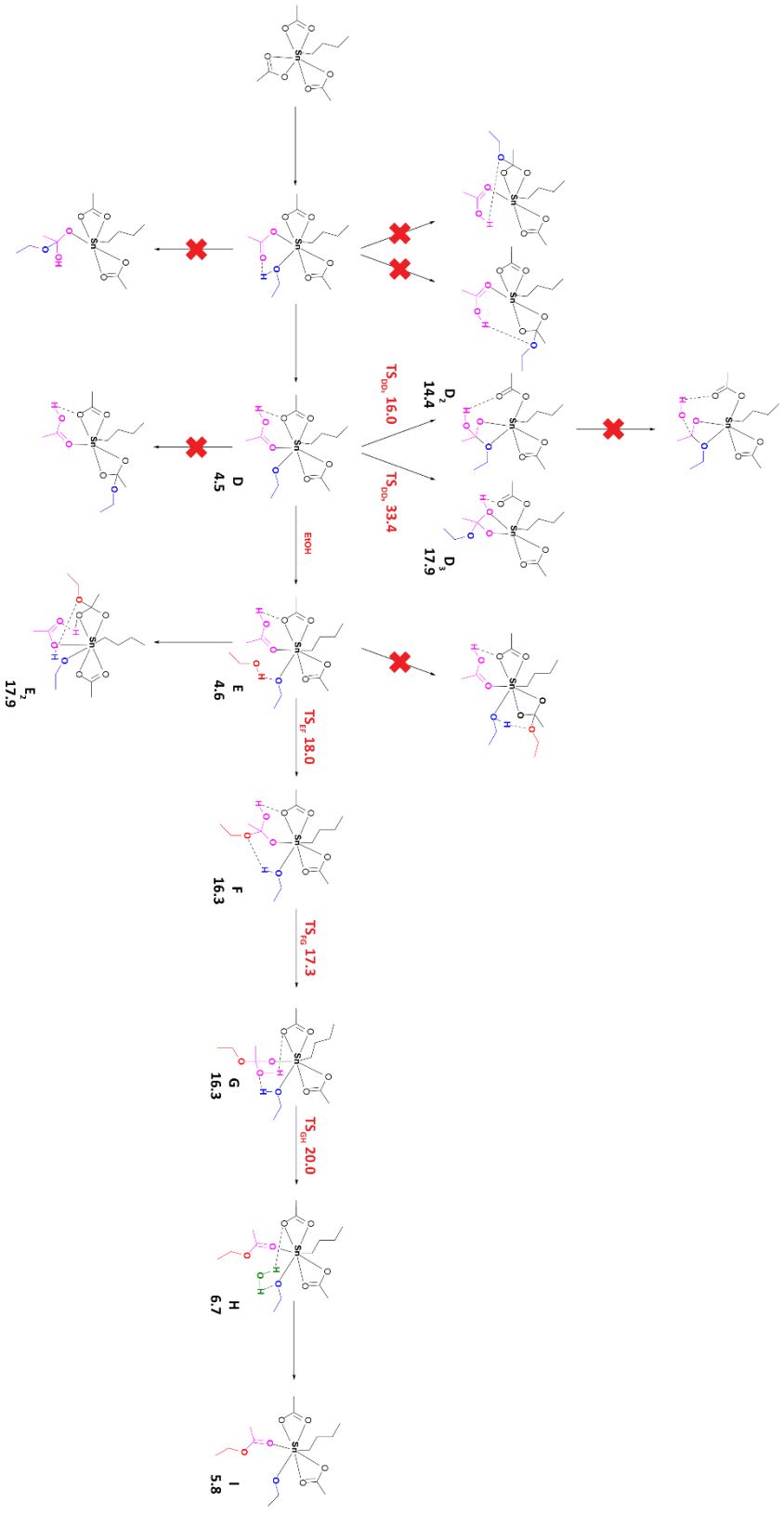


Fig. S67 Alternative pathways and structures from catalytic cycle. Free energy values are given in kcal mol^{-1} relative to *n*-BuSn(OAc)$_3$.

Alternative structures / pathways with *trans*-$BuSnOAc_3$

Besides the calculated catalytic cycle, we have also explored possible side paths and alternatives for this catalytic cycle. Figure S63 shows the alternative structures, with the corresponding XYZ coordinates and (free) energies below.

D_2
E (Hartree) = -1212.68214516
G_{298} (Hartree) = -1212.37217

44
Sn 1.5251219 -1.7317124 0.9120843
C 0.9249431 -1.5805032 2.9793588
H 0.1338524 -2.3359399 3.0907137
H 1.7906121 -1.8965731 3.5790166
C 0.4410857 -0.1796246 3.3560315
H 1.2581300 0.5477684 3.2185571
H -0.3669842 0.1392744 2.6772076
C -0.0595443 -0.1047000 4.8058602
H -0.8842208 -0.8245697 4.9399449
H 0.7463601 -0.4313244 5.4847905
C -0.5285166 1.3005175 5.1924763
H -1.3491241 1.6360278 4.5407467
H -0.8884631 1.3345494 6.2305716
H 0.2897518 2.0305035 5.0972379
O -0.5155219 -0.9987214 -1.9151003
C 0.0322527 -2.1197863 -1.3581255
C -0.2402109 -3.3375646 -2.2145610
H 0.0659766 -3.1552673 -3.2523042
H 0.3020019 -4.1961249 -1.8055023
H -1.3184583 -3.5384896 -2.1950171
O -0.2093030 -2.2892208 -0.0306100
O 2.3055865 -3.8850190 0.9375914
O 0.0936152 0.9419183 -0.0844161
C 1.2676709 1.1778326 0.2384504
C 1.8122135 2.5907266 0.2789852
H 1.1012274 3.2862363 -0.1774311
H 1.9813396 2.8748079 1.3275439
H 2.7830165 2.6372530 -0.2309242
O 2.1457522 0.2676043 0.5882139
C 4.6772178 -4.3652744 0.8937683
C 3.4955950 -3.4392788 0.9300976
H 4.3895679 -5.3730495 1.2085667
H 5.0452512 -4.4067144 -0.1418883
H 5.4869892 -3.9722986 1.5193070
O 3.6895104 -2.1668274 0.9265980
O 1.6295773 -1.9556253 -1.3221036
H 4.0492919 -2.3021188 -2.3920696
H 4.1159847 -0.9186283 -1.2707063
C 2.2374604 -1.1179736 -2.3280827
H 1.8514560 -1.4527862 -3.3038657
H 1.9209206 -0.0735008 -2.1852129
C 3.7461809 -1.2560045 -2.2471635
H 4.2158441 -0.6451283 -3.0314283
H -0.4514686 -0.2745568 -1.2315609

D_3
E (Hartree) = -1212.67657590
G_{298} (Hartree) = -1212.36671

44
Sn 1.8742494 -1.5974223 1.0687228
C 0.9970700 -1.2465506 3.0001836
H 1.2964218 -2.1109599 3.6100825
H 1.5285991 -0.3629386 3.3810918
C -0.5144745 -1.0448846 2.9571478
H -0.7713843 -0.2252092 2.2686748
H -1.0057546 -1.9432384 2.5487286
C -1.0940262 -0.7407572 4.3470664
H -0.8341101 -1.5606586 5.0378430
H -0.6087946 0.1644366 4.7490659
C -2.6123823 -0.5466721 4.3165768
H -3.1191341 -1.4510891 3.9475394
H -3.0095916 -0.3236319 5.3169591
H -2.8907195 0.2830313 3.6499608
O -1.0781415 -0.7573888 -0.3368348
C -0.7564776 -1.9470775 -0.4924676
C -1.6462963 -2.8908548 -1.2704071
H -2.6627928 -2.4885325 -1.3305722
H -1.2385814 -2.9744093 -2.2889211
H -1.6426630 -3.8930748 -0.8259861
O 0.3457681 -2.5108668 -0.0535842
O 2.8449464 -3.5046145 0.9483159
O 1.0943428 0.5511246 0.2253828
C 2.1000507 0.3684193 -0.7874007
C 2.8721723 1.6611245 -1.0080197
H 2.1942024 2.4310151 -1.3947320
H 3.3085657 1.9922877 -0.0586107
H 3.6828325 1.4882058 -1.7267654
O 2.9582096 -0.6377990 -0.3252744
C 4.9449530 -4.2307997 1.8655435
C 3.8858736 -3.1835424 1.6615887
H 4.4812149 -5.1899728 2.1266529
H 5.4802631 -4.3715646 0.9156355
H 5.6531988 -3.9160218 2.6376702
O 3.9837821 -2.0242540 2.1408573
O 1.3715491 -0.0370545 -1.9384614
H 0.3579345 -1.1022560 -4.1007274
H 1.1053806 -2.4027325 -3.1337462
C 2.1549208 -0.5211031 -3.0423519
H 2.4259396 0.3251611 -3.6995723

H	3.0808929	-0.9821504	-2.6640095
C	1.3139269	-1.5436087	-3.7862455
H	1.8435914	-1.9012906	-4.6809103
H	0.1945880	0.1967971	-0.1134998

E_2

E (Hartree) = -1367.72530352

G_{298} (Hartree) = -1367.33768

53

Sn	1.3497222	-2.1632048	-0.3913455
O	1.8901462	1.0702682	1.0958531
C	0.6327634	0.4951535	1.1035733
C	-0.4210561	1.5910719	1.0421882
H	-0.3046300	2.1384268	0.0992959
H	-1.4174078	1.1382350	1.0845299
H	-0.8401845	-6.1985632	-0.0246187
O	1.2633931	-4.4206942	-0.5872236
O	-0.6187636	-3.2667592	-0.6733764
C	-0.0057651	-4.3849233	-0.7462119
C	-0.7647712	-5.6616582	-0.9817866
H	-1.7720409	-5.4542726	-1.3553348
O	0.4090653	-0.4256564	0.1165912
H	-0.2115689	-6.3039759	-1.6770378
O	3.3896524	-2.3626848	0.1043973
C	4.0179008	-1.8172403	1.1142162
C	5.3439494	-2.4799122	1.4269039
H	5.1466137	-3.4780135	1.8440665
H	5.9235660	-2.6221498	0.5057209
H	5.9091293	-1.8835860	2.1500260
O	3.6076786	-0.8587589	1.7857891
H	-0.2896799	2.2908091	1.8772045
H	-0.0241618	0.8582876	4.0807978
H	1.5992758	1.1428796	3.3836894
C	1.4538178	-0.6719475	4.5557438
C	0.8552654	0.3707124	3.6262420
H	1.7634276	-0.2040413	5.5010681
H	2.3336813	-1.1321520	4.0853899
H	0.7208892	-1.4570025	4.7943175
O	1.1033609	-2.6158869	1.7871247
H	2.5593326	0.3445279	1.2725696
C	0.3519366	-3.6741881	2.4288367
H	-0.5071661	-3.9507476	1.7979058
H	-0.0502293	-3.2595881	3.3662313
C	1.2631078	-4.8572697	2.6969146
H	0.7003608	-5.6671577	3.1839165
H	2.0898688	-4.5612334	3.3564031
H	1.6822519	-5.2361569	1.7557744
O	0.4360418	-0.2744243	2.4042081
H	0.8175595	-1.6764516	2.1435095
C	1.6791540	-1.6563176	-2.4626846
H	2.0642853	-2.5558373	-2.9628702
H	0.6793608	-1.4295870	-2.8596291
C	2.6293584	-0.4643670	-2.5795847
H	2.2753695	0.3636830	-1.9424514
H	3.6240378	-0.7436815	-2.1947317
C	2.7695039	0.0377188	-4.0243857
H	3.1027861	-0.7941945	-4.6676940
H	1.7755547	0.3356887	-4.3984035
C	3.7436368	1.2128195	-4.1463849
H	4.7527979	0.9252837	-3.8145686
H	3.8203486	1.5688472	-5.1837333
H	3.4197526	2.0594638	-3.5226987

TS_D_D_2

E (Hartree) = -1212.67965769

G_{298} (Hartree) = -1212.36959

44

Sn	1.5552907	-1.7168086	0.8918641
C	0.9871294	-1.5701929	2.9674445
H	0.2937586	-2.4096907	3.1195905
H	1.8966027	-1.7609767	3.5550216
C	0.3471808	-0.2248949	3.3111417
H	1.0711338	0.5883992	3.1382618
H	-0.5028761	-0.0245617	2.6382261
C	-0.1371894	-0.1638117	4.7673514
H	-0.8686600	-0.9713706	4.9376968
H	0.7120930	-0.3723699	5.4399634
C	-0.7631240	1.1875179	5.1224235
H	-1.6281224	1.4035804	4.4775761
H	-1.1077148	1.2108607	6.1660534
H	-0.0389739	2.0057892	4.9900912
O	-0.5762068	-0.9681670	-1.8528695
C	-0.1054752	-2.0910985	-1.2705750
C	-0.3820806	-3.3230627	-2.0969659
H	-0.0717193	-3.1682084	-3.1373869
H	0.1484217	-4.1773009	-1.6652162
H	-1.4633933	-3.5132983	-2.0759948
O	-0.2759271	-2.2067662	0.0552207
O	2.3175866	-3.8743823	0.9370542
O	0.1249805	1.0259938	-0.1923232
C	1.2745495	1.2302952	0.2278487
C	1.8155370	2.6372376	0.3814391
H	1.1395818	3.3594312	-0.0866331
H	1.9104364	2.8648386	1.4529487
H	2.8201935	2.7055921	-0.0551130
O	2.1258199	0.3014758	0.5910032
C	4.6843135	-4.3758032	0.8924489
C	3.5117085	-3.4380617	0.9233869
H	4.3862357	-5.3802596	1.2081649
H	5.0554426	-4.4217585	-0.1419622
H	5.4957675	-3.9894853	1.5200672
O	3.7191327	-2.1677219	0.9089753
O	1.6067964	-1.9837567	-1.2769296
H	3.9399384	-2.4481123	-2.4976232

H 4.1717998 -1.1005156 -1.3543730
C 2.2146915 -1.1569416 -2.2842711
H 1.7495464 -1.4368920 -3.2433275
H 1.9782795 -0.0968166 -2.1008305
C 3.7159557 -1.3886574 -2.3102912
H 4.1717378 -0.7886786 -3.1113054
H -0.4467515 -0.2161401 -1.1984135

TS_D_D_3
E (Hartree) = -1212.64982699
G_{298} (Hartree) = -1212.34192

44
Sn 1.7287777 -1.4527926 0.9341397
C 1.0850751 -1.4789220 2.9901406
H 1.0608632 -2.5398971 3.2785841
H 1.8923982 -0.9799909 3.5436961
C -0.2676424 -0.7948680 3.1702527
H -0.2165102 0.2435617 2.8048106
H -1.0263154 -1.2994873 2.5499943
C -0.7287971 -0.7972713 4.6358500
H -0.7770446 -1.8379488 4.9988734
H 0.0311277 -0.2914106 5.2548806
C -2.0881206 -0.1177962 4.8231266
H -2.8680003 -0.6254108 4.2354367
H -2.4018943 -0.1274234 5.8766858
H -2.0544002 0.9309458 4.4915937
O -0.9928983 -0.7514248 -1.2235269
C -0.9444358 -1.9006603 -0.7237837
C -1.9432151 -2.9489057 -1.1664941
H -2.6926774 -2.5113050 -1.8335207
H -1.4047371 -3.7537816 -1.6862185
H -2.4258783 -3.3966814 -0.2879240
O -0.0991241 -2.3147850 0.1687967
O 2.4717729 -3.4465900 0.3914011
O 0.6401092 0.5606871 0.1150729
C 1.9620887 0.6969052 -0.3227801
C 2.2185797 1.8503329 -1.2565482
H 1.5595842 1.7931486 -2.1303671
H 2.0023047 2.7742282 -0.7047999
H 3.2683934 1.8659869 -1.5685417
O 2.7892526 0.4608961 0.6630581
C 4.6653217 -4.3735356 0.7349599
C 3.6629953 -3.2593717 0.8587313
H 4.2033532 -5.3286295 1.0126324
H 4.9683857 -4.4482274 -0.3196384
H 5.5466264 -4.1712982 1.3508035
O 3.9581349 -2.1473508 1.3777816
O 2.0256775 -0.7530843 -1.2043952
H 2.3399306 -2.2496195 -3.4048489
H 2.9218972 -3.1614859 -1.9920080
C 3.2679775 -1.0208278 -1.8842266
H 3.4526315 -0.1843764 -2.5779244
H 4.0990350 -1.0473754 -1.1582155
C 3.1460557 -2.3222147 -2.6624895
H 4.0882393 -2.5323674 -3.1898867
H -0.0319870 0.1265445 -0.5884349

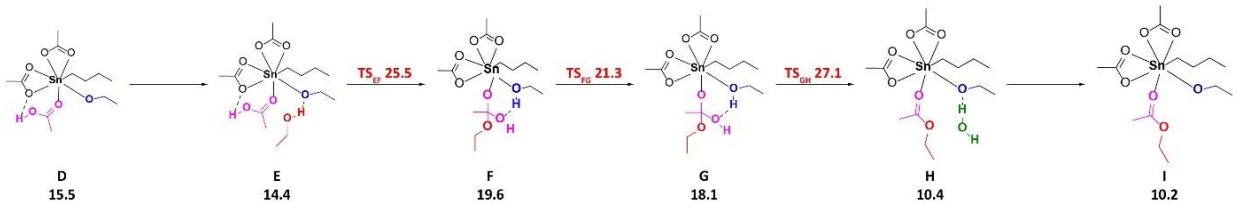


Fig. S68 Catalytic cycle for reactivity of one of the acetates *cis* to the *n*-butyl tail. Free energy values are given in kcal mol^{-1} relative to *n*-BuSn(OAc)$_3$.

Alternative structures / pathways with *cis*-BuSnOAc$_3$

In the proposed catalytic cycle the acetate *trans* to the n-butyl tail reacts towards the ester. We have also explored the reactivity of one of the acetates *cis* to the n-butyl tail (Figure S64) and found this pathway to be higher in free energy. The corresponding structures and (free) energies can be found below.

D

E (Hartree) = -1212.67756285

G_{298} (Hartree) = -1212.37039

44

Sn	1.5962172	-2.1664733	0.5117154
C	2.7291086	-1.7166497	2.3114579
H	1.9363971	-1.5813826	3.0625357
H	3.2553862	-2.6530746	2.5482677
C	3.6748595	-0.5242954	2.2401097
H	4.4327537	-0.6933825	1.4596935
H	3.1187288	0.3790948	1.9397820
C	4.3774465	-0.2562089	3.5802331
H	3.6173432	-0.0896874	4.3620828
H	4.9348404	-1.1586582	3.8827889
C	5.3271442	0.9430761	3.5152502
H	4.7850125	1.8616788	3.2435423
H	5.8226261	1.1199056	4.4805847
H	6.1112042	0.7851576	2.7592654
O	-1.6865066	-2.4089287	-0.7405876
C	-1.5860488	-1.6857529	0.3590847
C	-2.9062288	-1.3396564	0.9815669
H	-3.2098023	-2.1889919	1.6118748
H	-2.8006204	-0.4538612	1.6151212
H	-3.6762392	-1.1909098	0.2163212
O	-0.5191937	-1.3144879	0.8742247
H	1.5142043	-3.9370922	-3.7735813
O	1.5661534	-0.1036433	-0.3249055
C	2.7113325	-0.1754093	-0.9140553
C	3.2373490	1.0580085	-1.6042267
H	2.4195769	1.6061489	-2.0861241
H	3.6802439	1.7154352	-0.8416863
H	4.0116085	0.7906385	-2.3305196
O	3.3808044	-1.2432494	-0.8790526
O	0.8222691	-2.7367852	-1.4914053
O	2.5300745	-3.9547425	-0.7882925
C	1.6505776	-3.7361733	-1.6504643
C	1.5003337	-4.5801722	-2.8839706
H	2.2991373	-5.3253030	-2.9388616
H	0.5230906	-5.0825972	-2.8548816
H	1.3077799	-4.0103034	3.8070087
O	0.4800672	-3.7330887	1.2153989
H	-0.7687650	-2.6401321	-1.0994712
C	1.1367226	-4.8453386	1.8062643
H	2.2276162	-4.8432687	1.6101526
H	0.7539520	-5.7707452	1.3329267
C	0.8851493	-4.8971592	3.3119762
H	-0.1950033	-4.9161187	3.5153998
H	1.3411914	-5.7942579	3.7598751

E

E (Hartree) = -1367.72796828

G_{298} (Hartree) = -1367.34326

53

Sn	1.6070045	-2.1711986	0.5001897
C	2.6624435	-1.6846684	2.3311212
H	1.8375053	-1.6034427	3.0546952
H	3.2329822	-2.5924141	2.5759635
C	3.5398410	-0.4400044	2.2924475
H	4.3253344	-0.5594908	1.5296277
H	2.9410838	0.4333826	1.9863978
C	4.1957595	-0.1476126	3.6510789
H	3.4095336	-0.0313482	4.4158666
H	4.7953083	-1.0208878	3.9585112
C	5.0784453	1.1030458	3.6189671
H	4.4927040	1.9928482	3.3422113
H	5.5401061	1.2971761	4.5975721
H	5.8881427	0.9961483	2.8812267
O	-1.7164568	-2.3127643	-0.6816208
C	-1.5528381	-1.5697805	0.3949730
C	-2.8248165	-1.0044821	0.9413222
H	-3.4940117	-1.8399378	1.1785096
H	-2.6197086	-0.4214011	1.8425317
H	-3.3031026	-0.3745720	0.1786169
O	-0.4475789	-1.3080062	0.9109074

H	1.3115232	-3.9822260	-3.7534483
O	1.5973039	-0.1117694	-0.3928637
C	2.7536072	-0.2318513	-0.9419460
C	3.3469498	0.9559087	-1.6545763
H	2.5642568	1.5191623	-2.1755114
H	3.7940579	1.6194682	-0.8997897
H	4.1298803	0.6364777	-2.3497843
O	3.3895996	-1.3223712	-0.8496846
O	0.7680249	-2.7740618	-1.4418856
O	2.4964748	-4.0069426	-0.8245280
C	1.5798527	-3.7837338	-1.6416825
C	1.3538285	-4.6252372	-2.8648050
H	2.1477919	-5.3702027	-2.9687055
H	0.3806210	-5.1284155	-2.7748892
H	1.3531759	-4.4026561	3.8297763
O	0.5814379	-3.7925971	1.3015402
H	-0.8246030	-2.6203230	-1.0405988
C	1.3141407	-4.9428552	1.7298681
H	2.4004093	-4.8072820	1.5744445
H	1.0261463	-5.8065330	1.1019505
C	1.0411558	-5.2478744	3.1985497
H	-0.0308446	-5.4244871	3.3649460
H	1.5953967	-6.1435378	3.5185286
O	-1.8371007	-3.5250667	2.4797574
H	-0.9572750	-3.6685973	2.0275320
C	-1.5866533	-2.7697009	3.6616553
H	-1.1324841	-1.7895064	3.4094280
H	-0.8650011	-3.2942532	4.3177699
C	-2.8992320	-2.5681350	4.4020301
H	-2.7431448	-1.9947811	5.3275805
H	-3.3431724	-3.5392268	4.6624297
H	-3.6206179	-2.0236270	3.7759516

F

E (Hartree) = -1367.72271909

G_{298} (Hartree) = -1367.33494

53

Sn	1.5330238	-1.9848189	0.4746126
C	2.7030982	-1.6910518	2.2610438
H	1.9662971	-1.7735075	3.0728645
H	3.3557081	-2.5731060	2.2996578
C	3.4759251	-0.3776618	2.2950457
H	4.1765731	-0.3359877	1.4459275
H	2.7884116	0.4752355	2.1728547
C	4.2633354	-0.2058503	3.6037069
H	3.5642931	-0.2485187	4.4558990
H	4.9492298	-1.0606351	3.7266066
C	5.0533162	1.1050496	3.6447142
H	4.3837121	1.9733566	3.5500484
H	5.6096830	1.2117962	4.5868125
H	5.7791046	1.1542816	2.8189553
O	-1.6699653	-3.2084685	0.0462637
C	-1.5285234	-2.1629103	0.9852196
C	-2.7804943	-1.2911054	0.9736558
H	-3.6658057	-1.9188884	1.1275880
H	-2.7280389	-0.5170563	1.7490604
H	-2.8437592	-0.8006222	-0.0047316
O	-0.4164402	-1.3966873	0.8255512
H	1.9335366	-4.2081068	-3.5023553
O	1.5776484	0.0103992	-0.4374298
C	2.7159021	-0.1221422	-1.0318653
C	3.2601628	1.0564444	-1.7960458
H	2.4932409	1.4364791	-2.4830008
H	3.4909909	1.8625717	-1.0854921
H	4.1647403	0.7784863	-2.3451907
O	3.3477757	-1.2108221	-0.9486306
O	0.9053191	-2.9877446	-1.2959753
O	2.7335307	-3.9866880	-0.5304239
C	1.8458325	-3.9044882	-1.3958241
C	1.7704204	-4.8078242	-2.5961577
H	2.5288179	-5.5931703	-2.5299731
H	0.7667656	-5.2467186	-2.6699366
H	0.5252434	-6.1764852	3.2120592
O	0.8161621	-3.9723253	1.6901944
H	-0.9374917	-3.1245575	-0.5990871
C	0.6852443	-5.3337057	1.2218480
H	1.7032010	-5.6907214	1.0246188
H	0.1219844	-5.3423399	0.2718808
C	-0.0242508	-6.1881758	2.2603648
H	-1.0428380	-5.8142010	2.4363668
H	-0.0956448	-7.2289955	1.9119935
O	-1.4687489	-2.9314171	2.2746924
H	-0.1143094	-3.6659973	1.9746567
C	-1.3018613	-2.1381932	3.4713859
H	-0.9985598	-1.1160208	3.1954898
H	-0.4617278	-2.5842130	4.0297065
C	-2.5655216	-2.1532183	4.3179177
H	-2.4034786	-1.5997953	5.2551160
H	-2.8461737	-3.1851705	4.5690030
H	-3.4052433	-1.6899321	3.7836886

G

E (Hartree) = -1367.72492749

G_{298} (Hartree) = -1367.33732

53

Sn	0.9984525	-2.8633125	0.6851689
C	0.9436586	-2.8682685	2.8409216
H	0.0264811	-2.3241751	3.1025108
H	0.8078066	-3.9300150	3.0854898
C	2.1814832	-2.2626971	3.4893187
H	3.0831195	-2.8030663	3.1592082
H	2.2973187	-1.2163861	3.1658605
C	2.1099609	-2.3066563	5.0236694
H	1.2050801	-1.7721812	5.3589735

H	1.9874359	-3.3526039	5.3506216
C	3.3484336	-1.6957247	5.6847253
H	3.4734577	-0.6421803	5.3916149
H	3.2819646	-1.7332591	6.7814300
H	4.2608439	-2.2335200	5.3855335
O	-1.1595054	-0.3514324	1.3426969
C	0.0051651	-0.0413234	0.4980397
C	-0.3781126	1.1126915	-0.4265239
H	-0.6811242	1.9857344	0.1636024
H	0.4657968	1.3759748	-1.0758869
H	-1.2145399	0.7898878	-1.0572152
O	0.3586986	-1.1197437	-0.2346196
H	1.3351560	-6.3496122	-2.1941763
O	3.0038573	-2.1696716	0.2003057
C	3.6670706	-3.2573529	0.4566237
C	5.1643193	-3.2056257	0.2783922
H	5.4000141	-2.8792258	-0.7431649
H	5.5835293	-2.4570957	0.9649310
H	5.6105949	-4.1847043	0.4766906
O	3.0742549	-4.2912490	0.8443788
O	0.8008915	-3.8595007	-1.1469633
O	0.2873363	-5.2988719	0.4682181
C	0.4673294	-5.0634884	-0.7394393
C	0.3319640	-6.1094810	-1.8144719
H	-0.1296759	-7.0144589	-1.4085479
H	-0.2531783	-5.7159983	-2.6550770
H	-4.1154233	-3.3750994	0.8334360
O	-1.4468024	-2.9816588	0.9161882
H	-0.9588742	0.0306708	2.2169801
C	-2.2508785	-3.2275109	-0.2622406
H	-2.1626457	-4.3049084	-0.4568964
H	-1.8204542	-2.6829811	-1.1192462
C	-3.6988362	-2.8300875	-0.0247305
H	-3.7784002	-1.7513245	0.1744351
H	-4.3073036	-3.0573980	-0.9124483
O	0.9795305	0.3327117	1.4948785
H	-1.5213368	-2.0080310	1.1300987
C	2.2595558	0.7754393	0.9877005
H	2.3744248	0.4454135	-0.0551789
H	3.0226211	0.2327764	1.5645623
C	2.4285321	2.2787257	1.1483714
H	3.4396137	2.5807823	0.8361428
H	2.2918631	2.5706505	2.1990931
H	1.7020070	2.8336447	0.5402026

H

E (Hartree) = -1367.73022078

G_{298} (Hartree) = -1367.34953

53

Sn	1.8274444	-2.6960199	0.4980546
C	2.2146109	-1.8375937	2.4394507
H	1.2848493	-2.0551641	2.9844991
H	3.0340565	-2.4487656	2.8412469
C	2.5383874	-0.3481452	2.4220569
H	3.5186965	-0.1774445	1.9500501
H	1.7957469	0.1914090	1.8149961
C	2.5309299	0.2471288	3.8386007
H	1.5463923	0.0552319	4.2973893
H	3.2706416	-0.2805807	4.4639302
C	2.8188929	1.7504166	3.8438349
H	2.0655217	2.2960202	3.2551852
H	2.8090056	2.1612797	4.8635918
H	3.8038083	1.9674844	3.4034416
O	-0.8794836	-3.5155150	3.1778989
C	-1.4067003	-0.9379144	0.8992313
C	-1.8918071	-1.3350555	-0.4642293
H	-2.9091974	-0.9810448	-0.6600116
H	-1.1817268	-0.9740985	-1.2166179
H	-1.8699325	-2.4341241	-0.4991903
O	-0.2292292	-0.9298368	1.2356415
H	5.1274588	-5.4041069	-1.1633071
O	1.4107029	-1.3882832	-1.1753928
C	2.6248761	-0.9561730	-1.3194568
C	2.8930358	0.0246363	-2.4287286
H	2.7492404	-0.4855352	-3.3914747
H	2.1682575	0.8472326	-2.3804186
H	3.9152208	0.4088276	-2.3644819
O	3.5372228	-1.3638348	-0.5519915
O	2.5658330	-4.0664410	-1.1006331
O	3.3184948	-4.4560841	0.9370164
C	3.3083233	-4.7423450	-0.2991441
C	4.1699262	-5.8452100	-0.8492578
H	4.3715131	-6.5945952	-0.0767743
H	3.6994441	-6.3003084	-1.7276409
H	1.2155665	-6.1932881	0.9791025
O	0.0884936	-3.7285628	0.6118903
H	-0.3358726	-4.1582159	3.6605575
C	-0.2130608	-4.9445976	-0.0801435
H	0.3019452	-4.9790404	-1.0537003
H	-1.2992789	-4.9320268	-0.2848410
C	0.1393667	-6.1702311	0.7561497
H	-0.4080081	-6.1496385	1.7096754
H	-0.1282611	-7.0963172	0.2246888
O	-2.4073063	-0.6196905	1.7396320
H	-0.5764495	-3.6045634	2.2348832
C	-2.0183310	-0.3778358	3.1339311
H	-1.3318316	-1.1806366	3.4365018
H	-2.9631281	-0.4889325	3.6803138
C	-1.4207803	1.0059183	3.3241195
H	-1.2409591	1.1815993	4.3948419
H	-2.1047144	1.7852504	2.9596334
H	-0.4636445	1.0936580	2.7959137

I

E (Hartree) = -1291.28693566

G_{298} (Hartree) = -1290.92749

50

Sn	1.9461807	-3.0148047	0.6857330
C	2.1990274	-2.2164331	2.6698866
H	1.2560884	-2.4863007	3.1640613
H	3.0267642	-2.7766806	3.1260890
C	2.4238803	-0.7065582	2.6852248
H	3.4116257	-0.4591972	2.2656274
H	1.6774119	-0.2161144	2.0420412
C	2.2841907	-0.1158903	4.0940809
H	1.2907579	-0.3860821	4.4861560
H	3.0271257	-0.5796980	4.7648243
C	2.4466448	1.4063833	4.1022310
H	1.6851155	1.8812005	3.4644251
H	2.3410403	1.8201269	5.1153065
H	3.4341071	1.7050664	3.7181899
H	-0.0011707	2.8996676	1.3653151
C	-1.5051278	-0.9305341	1.5985330
C	-2.0493968	-2.1418373	0.8947235
H	-3.1463103	-2.1503445	0.9407860
H	-1.7515490	-2.0990567	-0.1613028
H	-1.6244832	-3.0425408	1.3472485
O	-0.6735864	-0.9424736	2.4890660
H	5.4931754	-4.7049300	-1.6566655
O	0.8132116	-1.5224080	-0.4757216
C	1.8631316	-0.8471704	-0.8060243
C	1.7129846	0.3767070	-1.6670035
H	2.2721463	0.2224981	-2.5995854
H	0.6607655	0.5766174	-1.8884294
H	2.1614369	1.2360606	-1.1520611
O	3.0038808	-1.2220060	-0.4065023
O	2.5198648	-3.9248756	-1.3294754
O	3.7955626	-4.2445744	0.4442164
C	3.5644354	-4.4291904	-0.8040067
C	4.5308030	-5.2340158	-1.6255834
H	4.7045016	-6.2017161	-1.1376281
H	4.1532377	-5.3796637	-2.6417927
H	1.4951570	-6.4161492	-0.6244308
O	0.4765730	-4.3466116	0.8813043
H	-0.5443792	2.0741669	-0.1196583
C	-0.1212070	-5.0249896	-0.2251658
H	0.0147459	-4.4665118	-1.1682027
H	-1.2091269	-5.0636832	-0.0296901
C	0.4253188	-6.4401550	-0.3737310
H	0.3031864	-6.9963308	0.5661805
H	-0.1030402	-6.9811469	-1.1739831
O	-2.0656834	0.2116480	1.1114532
H	0.4760187	1.2108606	1.0627017
C	-1.5788418	1.4577771	1.6828913
H	-1.3761161	1.3076192	2.7525137
H	-2.4164209	2.1574944	1.5645318
C	-0.3377786	1.9385727	0.9503929

TS_E_F

E (Hartree) = -1367.70971905

G_{298} (Hartree) = -1367.32556

53

Sn	1.5620898	-2.0348709	0.5091387
C	2.6992374	-1.6183564	2.2923283
H	1.9389015	-1.6613909	3.0855175
H	3.3603013	-2.4888030	2.4057980
C	3.4627958	-0.2994193	2.2731638
H	4.1868537	-0.3004641	1.4427886
H	2.7719531	0.5377127	2.0816845
C	4.2107079	-0.0441480	3.5911593
H	3.4876653	-0.0446425	4.4241886
H	4.9004039	-0.8831567	3.7833098
C	4.9878047	1.2750295	3.5785367
H	4.3134281	2.1293365	3.4153166
H	5.5163489	1.4417336	4.5279602
H	5.7362658	1.2843853	2.7717179
O	-1.7598738	-2.7176922	-0.2289085
C	-1.5326379	-1.8840437	0.8231490
C	-2.7487924	-1.0453542	1.1315372
H	-3.6423907	-1.6765458	1.1653565
H	-2.6187191	-0.5132294	2.0792750
H	-2.8525672	-0.3048763	0.3267583
O	-0.3796946	-1.2770847	0.9329789
H	1.7619667	-4.1594708	-3.5484669
O	1.6040338	-0.0550524	-0.4877072
C	2.7532245	-0.2064917	-1.0495866
C	3.3232191	0.9459822	-1.8361441
H	2.5438082	1.3944456	-2.4640042
H	3.6612852	1.7162228	-1.1279282
H	4.1722569	0.6179868	-2.4437798
O	3.3869717	-1.2904409	-0.9137899
O	0.8161800	-2.9335944	-1.3003943
O	2.6306143	-3.9925086	-0.5969521
C	1.7208715	-3.8770496	-1.4392341
C	1.5963871	-4.7643425	-2.6460566
H	2.3312520	-5.5732234	-2.6024930
H	0.5784107	-5.1709906	-2.7065620
H	0.7053882	-5.6657393	3.4942294
O	0.6742253	-3.7920871	1.5769654
H	-0.9032042	-2.9367304	-0.6694064
C	0.8315612	-5.2033394	1.3821637
H	1.9038632	-5.4245643	1.2866353
H	0.3478964	-5.5112805	0.4349297
C	0.2202918	-5.9621251	2.5533868
H	-0.8556710	-5.7531987	2.6356795
H	0.3537228	-7.0457971	2.4198814

O -1.5603485 -3.0947658 2.1622293
H -0.4465371 -3.5280892 1.8610825
C -1.3949076 -2.5497948 3.4799907
H -1.0220285 -1.5111822 3.4060632
H -0.6041572 -3.1305018 3.9870722
C -2.6934922 -2.6235313 4.2692641
H -2.5498523 -2.2304212 5.2869781
H -3.0358014 -3.6648397 4.3435275
H -3.4859989 -2.0390538 3.7832079

TS_F_G
E (Hartree) = -1367.71868953
G_{298} (Hartree) = -1367.33226

53
Sn 1.4419181 -1.9863809 0.4295322
C 2.6284195 -1.8542102 2.2232064
H 1.9038523 -2.0506415 3.0254805
H 3.3117522 -2.7113438 2.1540965
C 3.3624191 -0.5291740 2.3910023
H 4.0512704 -0.3750916 1.5452390
H 2.6484606 0.3104947 2.3678666
C 4.1597213 -0.4750333 3.7038854
H 3.4722334 -0.6314014 4.5520905
H 4.8722874 -1.3164381 3.7274085
C 4.9107726 0.8473923 3.8801884
H 4.2146421 1.6997893 3.8858825
H 5.4747032 0.8687336 4.8235992
H 5.6249958 1.0079605 3.0585506
O -1.6666381 -3.4095899 0.3713945
C -1.6021087 -2.1493930 1.0912273
C -2.8591002 -1.3234713 0.8140888
H -3.7467768 -1.9095099 1.0787321
H -2.8337525 -0.3984260 1.4044281
H -2.8931760 -1.0507781 -0.2481367
O -0.4998864 -1.4130431 0.7549225
H 1.9442304 -3.9452147 -3.6638988
O 1.5201011 0.0398572 -0.3704939
C 2.6735901 -0.0443708 -0.9517481
C 3.2094936 1.1912733 -1.6280128
H 2.4481990 1.6026880 -2.3030803
H 3.4138645 1.9534860 -0.8629985
H 4.1280776 0.9641217 -2.1772451
O 3.3173561 -1.1249192 -0.9266881
O 0.8790939 -2.9303566 -1.3734698
O 2.7372229 -3.9497911 -0.6893965
C 1.8433702 -3.8138655 -1.5384889
C 1.7816891 -4.6188431 -2.8110161
H 2.5495309 -5.3979541 -2.8051654
H 0.7843135 -5.0621680 -2.9292849
H 0.9124272 -5.9465478 3.4331742
O 0.7303441 -4.0897492 1.4931632
H -1.3256586 -3.2168899 -0.5243816
C 1.2003628 -5.4472204 1.3457479
H 2.2949275 -5.3942365 1.3885871
H 0.9323654 -5.8311467 0.3461713
C 0.6304037 -6.3313779 2.4436809
H -0.4671633 -6.3673429 2.3884361
H 1.0131890 -7.3580617 2.3436758
O -1.5830910 -2.6432371 2.4349922
H -0.2483401 -4.0636926 1.3186129
C -1.3086477 -1.6720261 3.4562458
H -0.9716356 -0.7282118 2.9989172
H -0.4645460 -2.0645380 4.0479332
C -2.5267249 -1.4617851 4.3458004
H -2.2868988 -0.7719148 5.1691749
H -2.8552876 -2.4168572 4.7781744
H -3.3634602 -1.0398053 3.7726829

TS_G_H
E (Hartree) = -1367.70572668
G_{298} (Hartree) = -1367.32302

53
Sn 1.7756359 -2.3671534 0.6537748
C 2.8271202 -1.6222111 2.3751945
H 2.1749364 -1.8976788 3.2156576
H 3.7459697 -2.2222196 2.4287838
C 3.1157224 -0.1253461 2.3182607
H 3.7506410 0.0974078 1.4459379
H 2.1796825 0.4385699 2.1731389
C 3.8163494 0.3794946 3.5891315
H 3.1847622 0.1541416 4.4650673
H 4.7526210 -0.1854826 3.7330879
C 4.1172923 1.8797651 3.5377209
H 3.1924148 2.4646767 3.4195861
H 4.6170315 2.2238666 4.4545856
H 4.7726257 2.1216744 2.6873302
O -1.4252711 -3.9165253 1.1831244
C -1.3530381 -2.1113029 0.7723173
C -1.6668487 -2.2130144 -0.6971061
H -2.6875407 -2.5808045 -0.8416375
H -1.5616006 -1.2092356 -1.1325678
H -0.9572136 -2.8889442 -1.1834781
O -0.1863544 -1.7314909 1.1832640
H 2.9942057 -4.6785877 -3.0555634
O 1.5433799 -0.6028415 -0.6215302
C 2.7382066 -0.5351145 -1.1224098
C 3.0184916 0.6041763 -2.0732052
H 2.2848015 0.5898922 -2.8899723
H 2.8936492 1.5566213 -1.5396902
H 4.0344168 0.5318484 -2.4733267
O 3.6147416 -1.3762086 -0.8129813
O 1.3781287 -3.5127246 -1.1178433
O 3.2281013 -4.1506548 -0.0815416
C 2.4379537 -4.2665846 -1.0489244

C	2.6704628	-5.2422286	-2.1689381
H	3.4481829	-5.9611623	-1.8947597
H	1.7353489	-5.7554826	-2.4241560
H	0.8368545	-5.7410275	3.8867852
O	0.9163667	-4.0858311	1.7903892
H	-2.0304777	-3.9509601	1.9437293
C	1.3817145	-5.4433394	1.8104004
H	2.4685808	-5.4341435	1.9735756
H	1.2028784	-5.9220131	0.8296812
C	0.6695894	-6.2186523	2.9112448
H	-0.4129661	-6.2578481	2.7227775
H	1.0454046	-7.2515827	2.9585497
O	-2.4174346	-1.6108528	1.4731699
H	-0.2287634	-4.0629706	1.5617193
C	-2.1412064	-1.1836217	2.8312003
H	-1.4688046	-0.3133588	2.8048230
H	-1.6141198	-1.9902012	3.3676968
C	-3.4731531	-0.8516454	3.4741212
H	-3.3154195	-0.5054804	4.5053780
H	-4.1297891	-1.7321835	3.5001967
H	-3.9858027	-0.0560065	2.9166569

NMR-calculated structures

Geometry optimizations were performed using the BP86 functional, def2-TZVP basisset, disp3 dispersion corrections and an M5 grid. NMR shielding constants were calculated using the B3LYP functional, def2-TZVP basisset for H,C,O and TZVPPall for Sn and grid 5.

SnMe4
E (Hartree) = -374.15744462
G_{298} (Hartree) = -374.05362
Shielding = 2581.0
Calculated NMR shift = 0.0

17

Sn	0.0001777	0.0000003	1.0001302
C	0.0004642	-0.0000015	-1.1702273
H	0.5158778	-0.8925267	-1.5480717
H	0.5158862	0.8925180	-1.5480735
H	-1.0300162	0.0000029	-1.5485234
C	2.0464487	0.0000022	1.7237012
H	2.5746925	-0.8925318	1.3639920
H	2.0590890	-0.0000050	2.8213615
H	2.5746872	0.8925442	1.3640038
C	-1.0231171	1.7720390	1.7236061
H	-0.5149851	2.6757282	1.3628448
H	-1.0286128	1.7836726	2.8212550
H	-2.0604456	1.7824175	1.3646432
C	-1.0231140	-1.7720395	1.7236081
H	-0.5149780	-2.6757281	1.3628513
H	-2.0604413	-1.7824225	1.3646419
H	-1.0286133	-1.7836700	2.8212570

BuSnOAc3
E (Hartree) = -1058.27129812
G_{298} (Hartree) = -1058.05933
Shielding = 3178.2
Calculated NMR shift = -597.2

35

Sn	0.7231258	-0.3570411	0.2664018
C	-1.4013969	-0.3947614	0.6298516
H	-1.5140085	-0.1264522	1.6892622
H	-1.6943923	-1.4450902	0.4961566
C	-2.1683320	0.5478801	-0.2964211
H	-1.9829267	0.2808836	-1.3500221
H	-1.7990414	1.5802597	-0.1792716
C	-3.6810477	0.5197825	-0.0290657
H	-4.0493347	-0.5126343	-0.1512670
H	-3.8657870	0.7873931	1.0248681
C	-4.4598779	1.4630687	-0.9497091
H	-4.1268009	2.5041654	-0.8224547
H	-5.5389642	1.4282727	-0.7428794
H	-4.3117791	1.1957061	-2.0068971
O	0.8672980	-0.1132877	-1.9082572
C	0.7666289	-1.3734475	-2.1691009
O	0.6417063	-2.2019169	-1.2213986
C	0.8223938	-1.8179598	-3.6054015
H	1.8614981	-1.7303623	-3.9538671
H	0.2097469	-1.1555881	-4.2288910
H	0.4959597	-2.8579269	-3.7016870
O	2.8260684	-0.8399552	0.3712253
C	2.6483375	-1.7804822	1.2427370
O	1.4777259	-2.0379637	1.6454045
C	3.8465991	-2.5180245	1.7649566
H	4.5459953	-2.7278717	0.9473354
H	3.5402253	-3.4415316	2.2650773
H	4.3610149	-1.8693354	2.4885734
O	1.1775117	1.7881718	0.2292181
C	1.3345412	1.8938482	1.5062240
O	1.1992871	0.8738208	2.2417336
C	1.6970372	3.2378036	2.0775717
H	1.1035790	4.0248657	1.5970014
H	2.7542961	3.4357407	1.8494141
H	1.5551126	3.2479701	3.1625784

BuSnOOAc_6_drum
E (Hartree) = -4058.00828937
G_{298} (Hartree) = -4057.10449
Shielding = 3122.4
Calculated NMR shift = -541.4
132

Sn	4.9208107	12.1590337	2.2878421
Sn	7.9546822	12.3762823	1.2123772
Sn	5.5748178	9.3425993	0.8686883
O	6.1672554	13.4756326	1.1692156
O	6.5690504	10.9181294	1.8804158
O	4.0772599	10.8246521	0.8792039
O	5.9980833	12.9039514	4.0612439
O	8.1570455	12.9398988	3.3403439
C	7.2451779	13.1095741	4.2106480
C	7.6768813	13.6326028	5.5641019
H	8.7587674	13.5311868	5.6962465
H	7.1331468	13.1096471	6.3599469
H	7.4076775	14.6974965	5.6212498
O	9.0504922	14.2869103	1.0386103
O	7.6971018	15.4948639	-0.3368226
C	8.7299206	15.3317224	0.3881028
C	9.6946455	16.4960875	0.4609130
H	10.4416204	16.3683775	-0.3367019
H	10.2190157	16.5016722	1.4227692
H	9.1699428	17.4424223	0.2907554
O	4.8681681	8.7235198	2.8704667
O	4.2556306	10.7079334	3.8049918
C	4.3716940	9.4397798	3.7967343
C	3.8348318	8.7069328	5.0077303
H	3.9189056	9.3310339	5.9041684
H	4.3532961	7.7513173	5.1409596
H	2.7686857	8.4987222	4.8331495
C	3.2825170	13.5340014	2.4999019
H	2.8015630	13.5189812	1.5102580
H	2.5744767	13.1001938	3.2193040
C	3.7299041	14.9432396	2.8815734
H	4.1276482	14.9423666	3.9090780
H	4.5687943	15.2545101	2.2375464
C	2.5995374	15.9731630	2.7635489
H	1.7542849	15.6686358	3.4037015
H	2.2135039	15.9613789	1.7301888
C	3.0537754	17.3870552	3.1307108
H	3.3860071	17.4367828	4.1786719
H	2.2482559	18.1230217	2.9964651
H	3.8999262	17.7001504	2.5010820
C	9.7296216	11.1631049	1.1722490
H	10.1224647	11.1695525	2.1988244
H	9.3525571	10.1503631	0.9673897
C	10.7716724	11.6218155	0.1525032
H	11.1049998	12.6381866	0.4115399
H	10.3109557	11.7012389	-0.8460654
C	11.9942897	10.6884299	0.0783618
H	12.7643756	11.1661819	-0.5498533
H	12.4350864	10.5928538	1.0853987
C	11.6821543	9.2980542	-0.4832675
H	10.9364204	8.7675490	0.1274731
H	12.5822871	8.6677634	-0.5188975
H	11.2813564	9.3670275	-1.5052272
C	7.2034076	7.9326301	0.8515041
H	7.9386651	8.3538962	0.1481156
H	7.6297501	7.9936559	1.8630610
C	6.8276942	6.5021008	0.4729567
H	6.3992180	6.4822374	-0.5430042
H	6.0308004	6.1341494	1.1384118
C	8.0258945	5.5446669	0.5373255
H	8.8140335	5.9034939	-0.1449556
H	8.4602940	5.5800892	1.5507575
C	7.6516210	4.1031061	0.1845926
H	6.8922378	3.7114863	0.8783835
H	8.5239921	3.4354734	0.2284761
H	7.2343460	4.0397783	-0.8317580
Sn	6.7869543	11.2159025	-2.2878592
Sn	3.7530868	10.9986457	-1.2123921
Sn	6.1329480	14.0323325	-0.8686997
O	5.5405158	9.8992942	-1.1692337
O	5.1387134	12.4568063	-1.8804218
O	7.6305096	12.5502768	-0.8792193
O	5.7096713	10.4709863	-4.0612704
O	3.5507177	10.4350398	-3.3403493
C	4.4625855	10.2653075	-4.2106454
C	4.0308304	9.7420869	-5.5640074
H	2.9491673	9.8450976	-5.6967806
H	4.5758331	10.2635625	-6.3599418
H	4.2982571	8.6766877	-5.6201835
O	2.6572828	9.0880116	-1.0386213
O	4.0106819	7.8800529	0.3367984
C	2.9778722	8.0431875	-0.3881414
C	2.0131253	6.8788396	-0.4609450
H	1.2658884	7.0068025	0.3363834
H	1.4890552	6.8730423	-1.4229654
H	2.5377246	5.9325217	-0.2903876
O	6.8395713	14.6514210	-2.8704888
O	7.4521084	12.6670052	-3.8050079
C	7.3360351	13.9351597	-3.7967584
C	7.8728436	14.6679841	-5.0077917
H	7.7884188	14.0439802	-5.9042664
H	7.3546085	15.6237481	-5.1408348
H	8.9390872	14.8758713	-4.8334217
C	8.4252523	9.8409489	-2.4999973
H	8.9062220	9.8559224	-1.5103602
H	9.1332785	10.2748043	-3.2193846
C	7.9778798	8.4317297	-2.8817579
H	7.5801202	8.4326741	-3.9092565
H	7.1390047	8.1203964	-2.2377418
C	9.1082654	7.4018149	-2.7638331
H	9.9535082	7.7064135	-3.4039652
H	9.4943069	7.4135129	-1.7304750
C	8.6540487	5.9879485	-3.1311218
H	8.3218135	5.9383116	-4.1790869
H	9.4595809	5.2519821	-2.9969459
H	7.8079048	5.6747826	-2.5015187

C	1.9781454	12.2118184	-1.1722471
H	1.5852943	12.2053745	-2.1988196
H	2.3552093	13.2245605	-0.9673867
C	0.9361036	11.7531034	-0.1524940
H	0.6027772	10.7367315	-0.4115296
H	1.3968290	11.6736797	0.8460707
C	-0.2865154	12.6864856	-0.0783410
H	-1.0565935	12.2087320	0.5498829
H	-0.7273233	12.7820595	-1.0853734
C	0.0256217	14.0768629	0.4832833
H	0.7713437	14.6073716	-0.1274694
H	-0.8745134	14.7071499	0.5189252
H	0.4264353	14.0078928	1.5052371
C	4.5043621	15.4423054	-0.8514487
H	3.7690970	15.0209846	-0.1481006
H	4.0780296	15.3813601	-1.8630147
C	4.8800685	16.8728013	-0.4727682
H	5.3085500	16.8925696	0.5431925
H	5.6769556	17.2408227	-1.1381930
C	3.6818615	17.8302338	-0.5370332
H	2.8937344	17.4713383	0.1452267
H	3.2474492	17.7949032	-1.5504631
C	4.0561298	19.2717644	-0.1841722
H	4.8154955	19.6634560	-0.8779421
H	3.1837524	19.9393945	-0.2279774
H	4.4734244	19.3350004	0.8321762

BuSnOOAc_6_ladder
E (Hartree) = -4821.95489604
G_{298} (Hartree) = -4820.87803
Shielding = 3151.9, 3198.0, 3293.7
Calculated NMR shift = -570.9, -617.0, -712.8

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Sn	-1.9637271	1.6554254	0.2333684
Sn	-0.6575856	1.6982687	3.2297551
Sn	-1.9151605	4.8794496	2.0038688
O	-0.3564035	0.9170192	1.3250361
O	-1.9189302	2.8590267	2.0295420
O	-3.2338276	0.2424978	1.4108260
O	-2.3954302	0.3792754	3.5195560
O	-0.5931359	2.9762545	-0.8792772
O	-1.7598320	4.8154994	-0.2832017
O	1.0279547	2.9944745	2.8212766
O	0.3289478	4.6881603	1.4869963
O	-1.2800652	2.9026479	4.9333429
O	-1.0249453	4.9797265	4.0639526
C	-3.7011080	2.1981831	-0.9209006
C	-4.5699922	0.9908348	-1.2681307
C	-5.6796212	1.3316613	-2.2711984
C	0.4732094	0.4132077	4.5338500
C	1.6697550	1.0739451	5.2082900
C	2.3801615	0.1321229	6.1909132
C	-1.7608653	7.0189801	1.9088086
C	-2.6954334	7.7332128	2.8774906
C	-2.5098260	9.2579182	2.8419768
C	-3.1659103	-0.1080413	2.6292003
C	-0.8916926	4.2182918	-0.9841620
C	1.1669064	3.8113936	1.8410840
C	-1.2035015	4.1774733	5.0259784
H	-3.2863225	2.6807959	-1.8181525
H	-4.2302031	2.9665502	-0.3427007
H	-5.0195992	0.5839155	-0.3496302
H	-3.9572768	0.1734272	-1.6825922
H	-5.2223136	1.6953361	-3.2063384
H	-6.2837183	2.1679211	-1.8814414
H	0.7714769	-0.4422449	3.9106066
H	-0.2703965	0.0598227	5.2616902
H	1.3476414	1.9809608	5.7460368
H	2.3867819	1.4163425	4.4473277
H	2.6372653	-0.8061865	5.6704639
H	1.6793521	-0.1497104	6.9947993
H	-1.9618586	7.2661209	0.8584211
H	-0.7017333	7.2106954	2.1282358
H	-3.7445059	7.4937428	2.6378646
H	-2.5255663	7.3673263	3.9024518
H	-2.6734910	9.6197814	1.8128110
H	-1.4619926	9.4990454	3.0882021
O	-1.2677843	0.0465298	-0.9092785
Sn	0.3392453	-0.6922552	0.1827534
Sn	-0.9663966	-0.7348340	-2.8138200
O	0.2945019	-1.8958774	-1.6134653
O	1.6096924	0.7205305	-0.9947578
O	-1.0321836	-2.0121406	1.2950449
C	2.0764438	-1.2352549	1.3371769
O	0.7716794	0.5837196	-3.1036401
O	-2.6518115	-2.0314654	-2.4057041
O	-0.3448571	-1.9395540	-4.5173187
C	-2.0971137	0.5499991	-4.1182186
Sn	0.2903515	-3.9163302	-1.5884201
C	1.5420173	1.0710466	-2.2131199
C	-0.7333946	-3.2541658	1.4002192
C	2.9453811	-0.0280434	1.6847254
H	1.6614712	-1.7179338	2.2343060
H	2.6055409	-2.0036225	0.7589864
C	-2.7909945	-2.8481522	-1.4253642
C	-0.4223356	-3.2142763	-4.6108590
C	-3.2932467	-0.1111253	-4.7930110
H	-2.3958057	1.4053972	-3.4951112
H	-1.3533708	0.9035219	-4.8458507
O	0.1352602	-3.8511263	0.6998016
O	-1.9533924	-3.7253697	-1.0714620
O	-0.5982162	-4.0174712	-3.6491702
C	0.1333280	-6.0557247	-1.4940982
C	4.0547722	-0.3690979	2.6879794
H	3.3952273	0.3789325	0.7663715

H	2.3326560	0.7893614	2.0991681
C	-4.0033841	0.8302633	-5.7762417
H	-2.9707250	-1.0182426	-5.3303396
H	-4.0105489	-0.4534311	-4.0322662
C	1.0976857	-6.7712914	-2.4320409
H	0.3014326	-6.3012989	-0.4376190
H	-0.9183350	-6.2475042	-1.7466881
H	3.5972570	-0.7330044	3.6229290
H	4.6589807	-1.2052433	2.2981550
H	-4.2609420	1.7686713	-5.2561993
H	-3.3022496	1.1120069	-6.5798753
C	0.9130985	-8.2961695	-2.3981701
H	2.1386944	-6.5299217	-2.1609357
H	0.9587680	-6.4085045	-3.4627576
H	1.0457831	-8.6550203	-1.3635257
H	-0.1264187	-8.5393761	-2.6755701
C	-0.2652488	-3.8012420	-5.9932412
H	0.7871895	-4.1047177	-6.0973251
H	-0.5005575	-3.0656446	-6.7693780
H	-0.8871423	-4.6979649	-6.0961156
C	2.4654946	2.1898603	-2.6386360
H	3.4743077	2.0136836	-2.2450906
H	2.0894017	3.1169982	-2.1841532
H	2.4871208	2.2974400	-3.7275836
C	-0.1307051	5.0139876	-2.0174431
H	0.7904025	5.3732545	-1.5337648
H	-0.7123376	5.8864935	-2.3336624
H	0.1421148	4.3911629	-2.8766628
C	2.4268483	3.6576333	1.0259912
H	3.2758347	3.3849438	1.6635767
H	2.6420236	4.5603617	0.4442849
H	2.2413077	2.8138476	0.3402614
C	-1.4948354	-4.0498138	2.4332158
H	-0.9127839	-4.9216215	2.7506070
H	-2.4151071	-4.4101901	1.9487729
H	-1.7690787	-3.4267046	3.2917711
C	-4.0894504	-1.2267357	3.0548969
H	-3.7141163	-2.1538223	2.5996818
H	-5.0985064	-1.0499433	2.6622382
H	-4.1103176	-1.3347646	4.1438127
C	-1.3649205	4.7660484	6.4071327
H	-1.1383985	4.0297241	7.1851561
H	-2.4159779	5.0763669	6.5047327
H	-0.7381040	5.6590579	6.5128454
C	-4.0506505	-2.6936530	-0.6100007
H	-4.2659350	-3.5960305	-0.0277942
H	-4.8997350	-2.4210706	-1.2475098
H	-3.8647281	-1.8495558	0.0752432
C	1.8836958	-9.0267772	-3.3301207
H	2.9285866	-8.8212447	-3.0519535
H	1.7495607	-8.7015340	-4.3729554
H	1.7357015	-10.1157456	-3.2962337
C	3.6452714	0.7520298	6.7890246
H	4.3711372	0.9967808	5.9992005
H	4.1362490	0.0698471	7.4978127
H	3.4130578	1.6845269	7.3256986
C	4.9553336	0.8322793	2.9864815
H	5.7333456	0.5860494	3.7232732
H	4.3691238	1.6734964	3.3870748
H	5.4569973	1.1859368	2.0726496
C	-3.4505298	9.9873258	3.8050319
H	-3.2848500	9.6593428	4.8424698
H	-4.5037138	9.7836266	3.5585818
H	-3.3023394	11.0762075	3.7692885
C	-5.2680743	0.2099086	-6.3747807
H	-5.0354018	-0.7226909	-6.9110785
H	-5.7588637	0.8917788	-7.0839992
H	-5.9942639	-0.0347781	-5.5852359
C	-6.5802833	0.1302374	-2.5691958
H	-5.9941682	-0.7111504	-2.9695691
H	-7.3583577	0.3762722	-3.3059870
H	-7.0818697	-0.2230894	-1.6551937
O	-4.0948267	4.7061370	1.3101140
C	-4.5340177	4.6396601	2.5100057
O	-3.7281450	4.7391908	3.4869594
C	-6.0040962	4.4093599	2.7486087
H	-6.2889151	4.7248511	3.7576340
H	-6.1988335	3.3313602	2.6491141
H	-6.6008748	4.9303699	1.9910813
O	2.4702504	-3.7444979	-0.8932609
C	2.9095476	-3.6779776	-2.0930300
O	2.1035364	-3.7763179	-3.0700702
C	4.3794308	-3.4478996	-2.3329220
H	4.9767085	-3.9379127	-1.5556420
H	4.5666120	-2.3655801	-2.2731576
H	4.6696265	-3.7964712	-3.3295939

BuSnOAc2_muO_dimer_v2

E (Hartree) = -1734.58617316

G_{298} (Hartree) = -1734.22566

Shielding = 3027.4, 3039.4

Calculated NMR shift = -446.4, -458.4

Correlated to experiment = -404.8, -415.4

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Sn	0.2388879	1.5157056	-1.0314152
C	-1.3104803	2.4437806	0.1551141
H	-1.0908320	3.5208961	0.1233585
H	-1.1443481	2.0748680	1.1769815
C	-2.7138140	2.1250060	-0.3515171
H	-2.8621226	1.0342554	-0.3608023
H	-2.8280352	2.4669523	-1.3932989
C	-3.8033371	2.7693627	0.5177822
H	-3.6858242	2.4180730	1.5567650
H	-3.6516714	3.8618578	0.5433167
C	-5.2159874	2.4527886	0.0189478

H -5.3633948 2.8189730 -1.0084856
H -5.9840897 2.9168599 0.6541416
H -5.3975054 1.3672534 0.0122182
O 1.0023592 0.4386792 -2.8489083
C -0.0649948 -0.2489761 -2.9342827
O -1.0204992 -0.0300286 -2.1069995
C -0.2006355 -1.3364503 -3.9609276
H -0.0405803 -2.2994497 -3.4540346
H 0.5454834 -1.2211060 -4.7530200
H -1.2152511 -1.3392035 -4.3763873
O 1.3877554 0.3453902 0.0766900
O 1.6896564 3.0636931 -1.4457224
C 1.0186280 3.6163379 -2.4084840
O -0.0996121 3.1453108 -2.7543567
C 1.6252507 4.8108939 -3.0932451
H 0.9000980 5.2814792 -3.7639772
H 2.4967623 4.4742506 -3.6725601
H 1.9858930 5.5279380 -2.3451370
Sn 0.8050415 -0.9339965 1.4608665
C 2.5664705 -2.1131660 1.8515692
H 3.2349597 -1.4637453 2.4360885
H 2.2372054 -2.9408870 2.4941671
C 3.2192939 -2.5924398 0.5545646
H 3.4505208 -1.7297699 -0.0909752
H 2.5100214 -3.2183395 -0.0122031
C 4.5025773 -3.3962663 0.8126143
H 5.2144604 -2.7675483 1.3737616
H 4.2686283 -4.2533246 1.4667255
C 5.1556490 -3.8916674 -0.4805903
H 5.4194432 -3.0490003 -1.1372922
H 4.4726546 -4.5473802 -1.0417894
H 6.0743278 -4.4601649 -0.2771691
O 0.4703902 0.4810210 3.0866914
O -0.3328218 -2.4698388 0.2489356
C -1.4013320 -1.7739621 0.3353233
O -1.3728062 -0.6732388 0.9903840
C -2.6632036 -2.2052097 -0.3471496
H -2.6510874 -3.2816153 -0.5450957
H -2.7079137 -1.6581880 -1.3005784
H -3.5355127 -1.9245851 0.2537859
C -0.0839799 -0.3817529 3.8778009
O -0.2143057 -1.5833744 3.5107377
C -0.5832879 0.0940560 5.2146023
H -1.5330488 0.6254005 5.0560374
H 0.1260623 0.8049040 5.6545670
H -0.7571656 -0.7533114 5.8848663

BuSnOAc2_muOH_dimer_v2
E (Hartree) = -1811.07880581
G_{298} (Hartree) = -1810.69645
Shielding = 3113.1, 3083.7
Calculated NMR shift = -532.1, -502.7
Correlated to experiment = -480.1, -454.3

60
Sn -1.2658634 1.1265181 -0.2033982
C -2.9947662 0.0229794 0.4350051
H -2.6824759 -0.4383138 1.3813481
H -3.1085413 -0.7613299 -0.3257103
C -4.2422014 0.8868838 0.5914696
H -4.4841555 1.3872886 -0.3610052
H -4.0519522 1.6791750 1.3319349
C -5.4555077 0.0603954 1.0459055
H -5.6420430 -0.7446776 0.3150375
H -5.2118239 -0.4385999 1.9985542
C -6.7161541 0.9128821 1.2133244
H -6.5594212 1.7046755 1.9612242
H -7.5730053 0.3067275 1.5406515
H -6.9923608 1.4011203 0.2663438
O 0.0849672 2.0557120 -1.7979386
C -0.9351950 2.3509659 -2.5080253
O -2.0988361 1.9984543 -2.1128061
C -0.7726398 3.1273080 -3.7841324
H 0.2116674 2.9423397 -4.2275222
H -0.8441648 4.1971456 -3.5387693
H -1.5742356 2.8822857 -4.4889390
O -1.1437394 3.0893085 0.5231863
C -1.4772961 3.1438037 1.8065681
O -1.8294290 2.1586919 2.4568067
C -1.3835360 4.5368572 2.3925249
H -2.0555019 5.2120796 1.8450288
H -0.3625249 4.9219993 2.2668858
H -1.6522631 4.5180372 3.4531642
Sn 1.1623359 -1.2464240 -0.0909210
O 2.2321340 -0.4726691 -1.7627809
O 0.7487018 -3.2808143 -0.9171501
C -0.1869317 -3.4647179 -0.0588048
O -0.4513721 -2.5535792 0.7976075
C -0.9846903 -4.7370996 -0.0841928
H -0.3638469 -5.5725879 -0.4257192
H -1.8059254 -4.6059530 -0.8042956
H -1.4163002 -4.9412316 0.9011216
C 2.8354620 0.6569981 -1.4514119
C 3.4678203 1.3765383 -2.6181599
H 2.6904898 2.0265367 -3.0471210
H 3.8033875 0.6756970 -3.3907147
H 4.2924712 2.0077359 -2.2703418
O -0.5051245 -0.6741632 -1.3078010
O 0.4419464 0.5212317 0.9046883
H -0.0961290 -0.3913298 -2.1482749
H 1.2042884 1.1301165 0.7481999
C 2.7377436 -1.8250091 1.2670119
H 2.3522450 -2.7133226 1.7877043
H 2.8047857 -0.9963638 1.9852940
C 4.0701351 -2.0904299 0.5710833
H 4.4008688 -1.1823491 0.0426296

H	3.9533928	-2.8734789	-0.1966578
C	5.1650020	-2.5174558	1.5607992
H	4.8379485	-3.4262108	2.0936148
H	5.2786170	-1.7350734	2.3297179
C	6.5100693	-2.7721799	0.8753393
H	7.2801825	-3.0764410	1.5983968
H	6.8695504	-1.8668984	0.3632420
H	6.4250873	-3.5683480	0.1202682
O	2.8636536	1.1255631	-0.3020880

BuSnOAc2_OEt_2HOEt

E (Hartree) = -1294.44472184

G_{298} (Hartree) = -1294.06782

Shielding = 3130.4

Calculated NMR shift = -549.4

Correlated to experiment = -495.4

54

Sn	0.6716767	-0.9652124	0.0615455
C	-0.6890301	-1.1159702	1.7433643
H	-1.6966011	-1.0873139	1.3036210
H	-0.5175438	-2.1364188	2.1159466
C	-0.5134791	-0.0759632	2.8486342
H	0.5285659	-0.0704405	3.2057268
H	-0.6986083	0.9367001	2.4540004
C	-1.4561218	-0.3211568	4.0362088
H	-2.4985435	-0.3255411	3.6750514
H	-1.2692144	-1.3301137	4.4411728
C	-1.2937776	0.7226211	5.1446044
H	-1.5047936	1.7351336	4.7678896
H	-1.9745845	0.5298910	5.9860279
H	-0.2658519	0.7241329	5.5379561
O	1.2245573	-3.4341825	-2.2429654
C	0.0360364	-3.3367551	-1.8527068
C	-0.9769371	-4.3846299	-2.2549202
H	-0.5417256	-5.0877836	-2.9718221
H	-1.3040430	-4.9256261	-1.3558599
H	-1.8633753	-3.8980922	-2.6825235
O	-0.4372068	-2.3846729	-1.1079009
O	1.7753669	-2.7511250	0.7306125
O	0.2174591	0.6904692	-1.0123819
C	-0.3080158	1.8435436	-0.3641810
C	-1.8316979	1.8258166	-0.2694773
H	-2.2694557	1.6848379	-1.2673796
H	-2.1801510	1.0052879	0.3740923
H	-2.2088682	2.7715946	0.1498549
C	3.4924222	-4.2360130	1.4047488
C	2.9369833	-2.8355137	1.2806813
H	2.7622091	-4.8784202	1.9141913
H	3.6363672	-4.6463811	0.3954519
H	4.4424375	-4.2327913	1.9481514
O	3.6143382	-1.8595208	1.7066039
O	2.2339553	-1.2546034	-1.5114687
O	2.2742794	0.1454902	1.1418541
H	2.9055979	-0.6724005	1.4536830
H	1.9448792	-2.2137928	-1.8481314
C	3.1008013	1.1393746	0.4886602
H	3.8326342	0.6273972	-0.1576581
H	2.4397773	1.7363512	-0.1540557
C	3.7904642	2.0009405	1.5325147
H	4.4451203	1.3909178	2.1701914
H	3.0481664	2.4985744	2.1713069
H	4.4050091	2.7717219	1.0442623
C	2.4251768	-0.3802239	-2.6610500
H	3.4279529	-0.6077183	-3.0583637
H	2.4219510	0.6445332	-2.2737882
C	1.3546261	-0.5461618	-3.7274520
H	1.3410422	-1.5698534	-4.1246606
H	1.5582317	0.1442835	-4.5592269
H	0.3695958	-0.3037711	-3.3084421
H	0.1285339	1.9835577	0.6457551
H	0.0104113	2.7199922	-0.9599500

BuSnOAc2_OEt_cis

E (Hartree) = -984.16573768

G_{298} (Hartree) = -983.93564

Shielding = 3037.8

Calculated NMR shift = -456.9

Correlated to experiment = -414.0

36

Sn	1.8080951	-1.6480839	-0.9479669
C	2.6057136	-1.3860587	1.0480355
H	2.4621438	-2.3599307	1.5362811
H	3.6870890	-1.2168289	0.9379526
C	1.9156813	-0.2500147	1.8034238
H	2.0244975	0.6983633	1.2511516
H	0.8319276	-0.4425567	1.8619554
C	2.4734167	-0.0671536	3.2229335
H	2.3598311	-1.0128491	3.7790671
H	3.5582059	0.1241106	3.1624419
C	1.7866292	1.0701785	3.9837213
H	0.7061127	0.8852385	4.0796007
H	2.1986402	1.1852097	4.9963730
H	1.9127758	2.0293143	3.4590191
O	0.2948819	-2.3086103	-2.4281490
C	-0.6355096	-2.2425140	-1.5551273
C	-2.0517668	-2.5852234	-1.9141389
H	-2.1301392	-2.8761934	-2.9654500
H	-2.3963716	-3.4024672	-1.2665415
H	-2.6906710	-1.7150621	-1.7131598
O	-0.3446563	-1.8790988	-0.3620867
O	2.1779807	-3.9635109	-0.9287244
O	1.7561621	0.1481330	-1.8152972
C	2.8468829	1.0434671	-1.5958299
C	2.3083136	2.4574598	-1.4198282

H 1.7196370 2.7488134 -2.3006459
H 1.6530931 2.5118642 -0.5384472
H 3.1306133 3.1782795 -1.2929593
C 3.9473332 -4.9103996 -2.2800080
C 3.1341749 -3.7683158 -1.7368044
H 3.8088455 -5.8079797 -1.6694622
H 3.6041677 -5.1171059 -3.3042099
H 5.0059940 -4.6307137 -2.3345830
O 3.4117490 -2.5683803 -2.1267578
H 3.4463624 0.7668587 -0.7031170
H 3.5371640 1.0017609 -2.4596621

BuSnOAc2OEt_dimer
E (Hartree) = -1968.37751782
G_{298} (Hartree) = -1967.88883
Shielding = 3144.0
Calculated NMR shift = -563.0
Correlated to experiment = -507.3

72
Sn -1.0868024 -1.9227100 0.0206898
Sn 0.5660468 1.1044740 -0.2713053
O -0.6330741 0.0521109 1.0474649
C -1.2191281 0.5450240 2.2674542
H -1.9607359 -0.2026113 2.5862277
H -1.7794656 1.4677402 2.0527546
C -0.1700766 0.7665535 3.3466828
H -0.6554572 1.1145205 4.2711875
H 0.5649849 1.5189349 3.0330029
H 0.3662964 -0.1665960 3.5672473
C 0.1049921 1.5896881 -2.3196134
H 0.7270265 0.8826414 -2.8855208
H -0.9486539 1.3064259 -2.4336137
C 0.3893945 3.0406104 -2.6809588
H 1.4301216 3.2993020 -2.4277486
H -0.2595519 3.7069401 -2.0912927
C 0.1521715 3.3135419 -4.1751740
H 0.8021723 2.6510898 -4.7710985
H -0.8845683 3.0394774 -4.4327206
C 0.4132307 4.7741249 -4.5531061
H 1.4497573 5.0627321 -4.3219648
H -0.2513949 5.4507382 -3.9947970
H 0.2466742 4.9502147 -5.6255778
C -0.4214222 -2.9384976 1.8028280
H -0.6611059 -4.0012494 1.6692584
H -1.0751500 -2.5337412 2.5892346
C 1.0535198 -2.6713692 2.0905350
H 1.2828979 -1.6038679 1.9426920
H 1.6809873 -3.2227537 1.3706219
C 1.4630904 -3.0678684 3.5157945
H 1.2568220 -4.1391042 3.6774929
H 0.8274434 -2.5222741 4.2339736
C 2.9372072 -2.7643582 3.7959903
H 3.2189379 -3.0330271 4.8239684
H 3.1470162 -1.6933719 3.6547903
H 3.5926613 -3.3241389 3.1113609
O 0.6762829 -1.0562011 -0.8553081
C 1.9889157 -1.5952554 -1.1044613
H 2.5049377 -0.8759040 -1.7646545
H 2.5555537 -1.6320070 -0.1577495
C 1.9782369 -2.9643929 -1.7610963
H 1.3897578 -2.9555391 -2.6862756
H 1.5472141 -3.7293362 -1.1014224
H 3.0134360 -3.2555926 -1.9954993
O 2.9244548 1.6815779 -0.8321566
O 0.4196049 2.9470448 0.7975387
C 3.1880802 1.1906267 0.2923662
C -0.7820938 3.4412523 0.6020390
O -1.6669680 2.8342070 -0.0227716
O 2.2379689 0.6957109 1.0275753
C 4.5897732 1.1194482 0.8368057
H 4.9016273 0.0656211 0.8702931
H 4.6083021 1.4995056 1.8660951
H 5.2786976 1.6866976 0.2039782
C -1.0024156 4.8113980 1.2045818
H -2.0252818 5.1516991 1.0163886
H -0.2827323 5.5200848 0.7726232
H -0.8095694 4.7716878 2.2853086
O -3.2253921 -0.9479803 0.6284624
O -0.9482139 -3.4073824 -1.5961486
C -2.0580559 -4.0182064 -1.3285497
C -3.1686962 -0.3908653 -0.4928253
O -2.7720942 -3.6371533 -0.3647735
O -2.1789550 -0.6676446 -1.3011373
C -4.1531211 0.6479565 -0.9374080
H -5.0835140 0.5639061 -0.3674767
H -4.3408124 0.5703290 -2.0144470
H -3.6886863 1.6268440 -0.7379432
C -2.4625463 -5.1680474 -2.2144136
H -3.2687617 -5.7455688 -1.7518200
H -1.5962206 -5.8061835 -2.4267714
H -2.8145780 -4.7596824 -3.1727066

BuSnOAc2OEt_dimer_cis_v2
E (Hartree) = -1968.37555858
G_{298} (Hartree) = -1967.88820
Shielding = 3156.9
Calculated NMR shift = -575.9
Correlated to experiment = -518.7

72
Sn -1.0983934 -2.0242529 0.1491406
Sn 0.9513497 0.8300157 0.0109013
O -0.6078161 -0.0222883 1.0815298
C -1.3134612 0.5704971 2.1892107
H -2.0796847 -0.1536951 2.5031195

H	-1.8417004	1.4662642	1.8334314
C	-0.3781994	0.8935514	3.3456492
H	-0.9559611	1.2798240	4.1985262
H	0.3540000	1.6629455	3.0613251
H	0.1624922	-0.0056044	3.6764000
C	-0.5593539	-2.9276055	2.0334058
H	-0.8539899	-3.9828488	1.9620558
H	-1.1969881	-2.4370768	2.7826565
C	0.9243923	-2.7369312	2.3340971
H	1.1909118	-1.6752647	2.2217210
H	1.5350092	-3.2794362	1.5933823
C	1.3124580	-3.1910586	3.7476737
H	1.0636408	-4.2578228	3.8749557
H	0.6953415	-2.6435497	4.4804998
C	2.7967350	-2.9577647	4.0423767
H	3.0623236	-3.2684766	5.0627591
H	3.0555696	-1.8931101	3.9356755
H	3.4320545	-3.5221247	3.3431146
O	0.7605018	-1.2492545	-0.6184050
C	1.6086030	-1.8492753	-1.6187038
H	2.5656989	-1.3006606	-1.6024779
H	1.8092404	-2.8877961	-1.3128337
C	1.0095108	-1.8211126	-3.0174150
H	0.7652382	-0.7979402	-3.3247201
H	0.0905069	-2.4173241	-3.0557437
H	1.7300830	-2.2406240	-3.7355230
O	0.5983234	2.8232445	0.5813624
C	-0.5606353	3.4387419	0.3691799
O	-1.6027909	2.8880691	0.0249779
C	-0.4685144	4.9351445	0.6156229
H	-1.4490844	5.4023389	0.4794677
H	0.2581748	5.3773905	-0.0800712
H	-0.0975207	5.1236289	1.6322869
O	-3.1762560	-0.9563634	0.4485899
O	-0.5953961	-3.7765672	-1.1566479
C	-1.7562173	-4.3240382	-1.0308186
C	-3.0290742	-0.5253130	-0.7283127
O	-2.6494080	-3.7574399	-0.3394480
O	-2.0284589	-0.9542459	-1.4381808
C	-3.9087591	0.5361979	-1.3090896
H	-4.8866876	0.5403811	-0.8175878
H	-4.0061990	0.4149762	-2.3933602
H	-3.3988520	1.4933159	-1.1101254
C	-2.0149857	-5.6312741	-1.7330913
H	-2.9603871	-6.0699453	-1.3999046
H	-1.1819120	-6.3228784	-1.5556515
H	-2.0614713	-5.4434285	-2.8152580
C	2.7350217	0.5467900	1.1928002
H	3.1821930	-0.3866605	0.8213041
H	2.3770194	0.3636448	2.2167913
C	3.7075295	1.7218668	1.1295751
H	3.2068134	2.6406350	1.4751066
H	4.0003659	1.9088667	0.0840430
C	4.9673188	1.4791053	1.9743457
H	5.4641913	0.5576882	1.6260117
H	4.6710217	1.2889930	3.0200549
C	5.9499195	2.6518613	1.9186873
H	5.4821631	3.5761400	2.2900664
H	6.2805146	2.8407535	0.8861592
H	6.8448263	2.4601849	2.5280584
O	0.0549387	1.3469207	-1.9037443
C	1.1731952	1.5688268	-2.5024711
C	1.1435650	2.0621799	-3.9224881
H	2.0846381	1.8253703	-4.4290358
H	1.0191734	3.1547239	-3.9024606
H	0.2882873	1.6347794	-4.4576634
O	2.2653029	1.3871949	-1.8858659

BuSnOAc2OEt_dimer_trans

E (Hartree) = -1968.38386672

G_{298} (Hartree) = -1967.89195

Shielding = 3175.9

Calculated NMR shift = -594.9

Correlated to experiment = -535.4

72

Sn	-1.1750517	-1.5077447	0.1217112
Sn	0.6167556	1.4336205	-0.1886009
O	-1.1067431	0.5249504	0.7384761
C	-1.8898595	1.1721446	1.7581368
H	-2.9050067	0.7491512	1.7239654
H	-1.9715132	2.2356118	1.4731499
C	-1.2988439	1.0231317	3.1533352
H	-1.9136488	1.5809272	3.8760384
H	-0.2708788	1.4066365	3.1917946
H	-1.2720480	-0.0337323	3.4450328
C	0.7481808	3.3598193	0.7935738
H	0.3369225	3.1935352	1.7989798
H	1.8321808	3.5148112	0.8981597
C	0.0674994	4.5177756	0.0727549
H	-1.0036337	4.3025198	-0.0673719
H	0.4858013	4.6287040	-0.9416704
C	0.2258020	5.8474237	0.8259172
H	-0.1910573	5.7380160	1.8413827
H	1.2993824	6.0629653	0.9582913
C	-0.4549194	7.0157459	0.1078700
H	-1.5339344	6.8331034	-0.0092078
H	-0.0331640	7.1604870	-0.8984571
H	-0.3318895	7.9578045	0.6609619
C	-1.1528444	-3.4913203	-0.7582679
H	-1.1390323	-4.1458589	0.1252287
H	-0.1722632	-3.5793498	-1.2441273
C	-2.3050788	-3.8172640	-1.7007288
H	-2.3371145	-3.0960861	-2.5330399
H	-3.2678373	-3.7098291	-1.1731048
C	-2.2058121	-5.2411191	-2.2691739

H	-2.1835127	-5.9633309	-1.4358769
H	-1.2424020	-5.3518485	-2.7949220
C	-3.3583238	-5.5774853	-3.2194345
H	-3.2710310	-6.5992437	-3.6155743
H	-3.3794196	-4.8858732	-4.0753190
H	-4.3290775	-5.4987607	-2.7065376
O	0.3163026	-0.4841810	-1.0200455
C	1.2358528	-1.1425727	-1.9203084
H	2.1157376	-0.4949360	-2.0269765
H	1.5693489	-2.0769490	-1.4425737
C	0.5766996	-1.3832897	-3.2680191
H	0.2881422	-0.4279882	-3.7258497
H	-0.3254366	-2.0031919	-3.1712720
H	1.2768215	-1.8966709	-3.9437992
O	2.7725680	0.8290415	-0.1437689
O	1.1359879	2.0268088	-2.2904137
C	2.7108229	0.3459309	1.0469629
C	-0.0865484	2.3001331	-2.5830940
O	-0.9929620	2.1532034	-1.7094873
O	1.6353339	0.4498179	1.7105892
C	3.8899958	-0.3930398	1.6116425
H	3.6714688	-1.4639516	1.4789852
H	3.9870060	-0.1964556	2.6857015
H	4.8126266	-0.1407318	1.0796250
C	-0.4256384	2.7619755	-3.9750239
H	-1.3361691	3.3704193	-3.9652687
H	-0.6147430	1.8713448	-4.5928354
H	0.4133012	3.3116795	-4.4157456
O	-3.3283716	-1.4664958	0.7141647
O	1.2649773	-2.5061730	1.0297947
C	0.6412049	-2.3332683	2.0898327
C	-3.6916375	-1.0024486	-0.4315156
O	-0.6187414	-1.9617538	2.1182584
O	-2.8187908	-0.7465237	-1.3152964
C	-5.1495691	-0.7497746	-0.7032434
H	-5.7807546	-1.2564571	0.0333990
H	-5.3993247	-1.0718573	-1.7209923
H	-5.3266238	0.3339946	-0.6458106
C	1.2887466	-2.4802168	3.4452065
H	0.5878877	-2.8954406	4.1787225
H	1.5667957	-1.4668513	3.7710187
H	2.1920988	-3.0951685	3.3750905

BuSnOAc2OEt_dimer_trans_v2

E (Hartree) = -1968.37833442

G_{298} (Hartree) = -1967.88635

Shielding = 3170.6

Calculated NMR shift = -589.7

Correlated to experiment = -530.7

72

Sn	-1.4202762	-1.3021459	-0.0091827
Sn	0.6487267	1.4601393	-0.2451328
O	-1.2180007	0.7463709	0.5773231
C	-1.9270945	1.3837527	1.6523816
H	-2.9970966	1.1419327	1.5449673
H	-1.8380516	2.4739998	1.5088460
C	-1.4140579	0.9725244	3.0260284
H	-1.9981507	1.4752290	3.8115913
H	-0.3550066	1.2351692	3.1432321
H	-1.4963486	-0.1147695	3.1616294
C	0.8167426	3.3851211	0.7340047
H	0.4545975	3.2166490	1.7582642
H	1.9027531	3.5509341	0.7877269
C	0.0940713	4.5362451	0.0429365
H	-0.9769861	4.3034718	-0.0720893
H	0.4819384	4.6621795	-0.9815842
C	0.2476368	5.8631214	0.8015521
H	-0.1436926	5.7400341	1.8256647
H	1.3204512	6.0948274	0.9108719
C	-0.4679667	7.0254270	0.1079829
H	-1.5459741	6.8254622	0.0122996
H	-0.0703339	7.1853747	-0.9057069
H	-0.3490718	7.9648434	0.6664684
O	0.2637348	-0.4918757	-1.0058438
C	1.1769095	-1.2685442	-1.8374888
H	2.1973863	-0.9885964	-1.5480609
H	1.0386991	-2.3200520	-1.5615928
C	0.9381989	-1.0265259	-3.3196233
H	1.2580297	-0.0184264	-3.6103802
H	-0.1222525	-1.1462753	-3.5763298
H	1.5256560	-1.7520435	-3.9026416
O	2.7684236	0.7866024	-0.0999197
O	1.3157458	2.0646378	-2.2935054
C	2.6411938	0.3137406	1.0902652
C	0.1206046	2.3435894	-2.6804972
O	-0.8494495	2.1891029	-1.8802473
O	1.5275472	0.4248273	1.6888618
C	3.7919242	-0.4109684	1.7242520
H	3.6363788	-1.4795593	1.5077472
H	3.7810850	-0.2750909	2.8113523
H	4.7463971	-0.0908587	1.2940013
C	-0.1057757	2.8080358	-4.0927057
H	-1.0226789	3.4026660	-4.1605224
H	-0.2257095	1.9137201	-4.7226485
H	0.7600204	3.3700936	-4.4595473
O	1.4982698	-2.6496421	0.8400028
C	0.7462463	-2.4456587	1.7867059
O	-0.5252351	-2.0691002	1.6864351
O	-2.2823733	-1.4491231	-2.2202304
C	1.1887981	-2.5649574	3.2315503
H	0.4222961	-3.0594744	3.8409716
H	1.3186793	-1.5421630	3.6144034
H	2.1398700	-3.1038391	3.2957677
C	-3.4540730	-1.5071517	0.7074991
H	-3.3835612	-1.3343439	1.7913583

H	-4.0231982	-0.6831170	0.2546975
C	-4.0808901	-2.8638217	0.3952467
H	-3.4480116	-3.6780298	0.7843465
H	-4.1340432	-3.0113950	-0.6959703
C	-5.4949641	-3.0009203	0.9800165
H	-5.4478443	-2.8617297	2.0731102
H	-6.1256941	-2.1825513	0.5936845
C	-6.1387235	-4.3516206	0.6556372
H	-5.5367787	-5.1822822	1.0541203
H	-6.2250102	-4.4972394	-0.4319061
H	-7.1474399	-4.4321192	1.0851682
C	-1.8953367	-2.6540495	-2.2289186
O	-1.2484871	-3.1360149	-1.2204089
C	-2.1497241	-3.5539850	-3.4073693
H	-1.1915477	-3.7376728	-3.9141784
H	-2.8491695	-3.0877648	-4.1075965
H	-2.5299314	-4.5233255	-3.0621436

BuSnOAc2_OEt_HOEt_trans

E (Hartree) = -1139.30418608

G_{298} (Hartree) = -1139.00363

Shielding = 3092.2

Calculated NMR shift = -511.2

Correlated to experiment = -461.8

45

Sn	1.6823994	-1.7021789	0.6006578
C	0.8416281	-1.6464555	2.5987017
H	0.4823839	-2.6697352	2.7767430
H	1.6813973	-1.4590082	3.2840509
C	-0.2722448	-0.6115765	2.7526995
H	0.1013023	0.3942384	2.4985719
H	-1.0779699	-0.8245427	2.0319844
C	-0.8558757	-0.5816729	4.1729849
H	-1.2354521	-1.5854231	4.4276644
H	-0.0464437	-0.3697150	4.8918733
C	-1.9737754	0.4525324	4.3299798
H	-2.8055123	0.2423040	3.6406672
H	-2.3787967	0.4595599	5.3520402
H	-1.6081393	1.4663496	4.1069954
O	0.1622497	-2.1436967	-2.5131401
C	-0.6065064	-2.1152033	-1.5249876
C	-2.1037606	-2.1496953	-1.7262496
H	-2.3475020	-2.2867936	-2.7841611
H	-2.5384349	-2.9583682	-1.1245042
H	-2.5337503	-1.2056903	-1.3634313
O	-0.2322051	-2.0550526	-0.2804886
O	2.2675040	-3.9058871	0.7915223
O	1.9838120	0.2216919	0.1023297
C	2.5628873	1.0953794	1.0680274
C	1.9130088	2.4691174	0.9597338
H	2.0353742	2.8664468	-0.0575766
H	0.8360987	2.4010452	1.1711683
H	2.3676852	3.1770978	1.6696258
C	4.5171559	-4.6128724	1.3080807
C	3.4655656	-3.5664700	1.0592753
H	4.0569381	-5.5617061	1.6012733
H	5.0727601	-4.7665160	0.3714199
H	5.2272832	-4.2673941	2.0678192
O	3.7896546	-2.3241454	1.0951424
O	2.4203207	-2.1360296	-1.4413227
H	3.0980576	-2.0039901	-4.0631694
H	4.3457416	-2.8887521	-3.1476762
C	3.4173075	-1.2674278	-2.0476513
H	2.9807382	-0.2714227	-2.2105241
H	4.2225664	-1.1656718	-1.3079367
C	3.9163280	-1.8955549	-3.3373145
H	4.6916063	-1.2590989	-3.7887537
H	1.5341375	-2.1456550	-2.0139569
H	2.4428428	0.7132959	2.1030092
H	3.6536342	1.1753434	0.8928028

BuSnOAc2_OEt_trans

E (Hartree) = -984.16581754

G_{298} (Hartree) = -983.93681

Shielding = 3003.9

Calculated NMR shift = -422.9

Correlated to experiment = -384.2

36

Sn	1.6166617	-1.6663294	0.5453804
C	0.1408949	-2.0997478	2.0602696
H	-0.6391256	-2.6812056	1.5485718
H	0.6639173	-2.7653605	2.7604652
C	-0.4281341	-0.8548137	2.7380042
H	0.3818610	-0.2572624	3.1883098
H	-0.9133788	-0.2107760	1.9883293
C	-1.4515052	-1.2126791	3.8269567
H	-2.2637779	-1.8058707	3.3748521
H	-0.9732543	-1.8669638	4.5748153
C	-2.0329450	0.0254038	4.5147471
H	-2.5402570	0.6787104	3.7889900
H	-2.7651924	-0.2497096	5.2868591
H	-1.2418100	0.6178425	4.9985973
O	2.8082304	-3.6412506	1.2272479
O	-0.1632432	-0.1590019	-0.5056454
C	0.6464245	0.7444337	-0.2008933
C	0.3650717	2.2034474	-0.4507265
H	-0.5400362	2.3214013	-1.0538829
H	0.2342414	2.7100367	0.5160200
H	1.2252438	2.6691510	-0.9484094
O	1.7866880	0.4607705	0.3722875
C	4.9914219	-3.3434129	2.2318480
C	3.7080657	-2.8541899	1.6190866
H	4.9150603	-4.4041280	2.4889631
H	5.7989114	-3.2051618	1.4985075

H 5.2425735 -2.7426938 3.1146731
O 3.5509255 -1.5689445 1.4855385
O 2.0581098 -2.3127391 -1.2654703
H 2.1174476 -3.1955138 -3.7482314
H 3.6041587 -2.2718609 -3.4178185
C 1.8354201 -1.5017977 -2.4300932
H 0.7549496 -1.3919884 -2.6245417
H 2.2492565 -0.4852327 -2.2914873
C 2.5243779 -2.1855980 -3.6015617
H 2.3697465 -1.6079644 -4.5255585

BuSnOAc3_2H2O_ciscis
E (Hartree) = -1211.24518307
G_{298} (Hartree) = -1210.99012
Shielding = 3219.8
Calculated NMR shift = -638.8
Correlated to experiment = -573.9

41
Sn -3.4215904 -3.8381356 -2.4293292
C -3.4295573 -2.3585502 -0.8635848
H -4.3873150 -2.5078725 -0.3477254
H -2.6144318 -2.6855691 -0.2013240
C -3.2383593 -0.9256288 -1.3486384
H -2.3163401 -0.8424344 -1.9469768
H -4.0652937 -0.6449596 -2.0206007
C -3.1717831 0.0767293 -0.1861006
H -4.0897596 -0.0087057 0.4193663
H -2.3374034 -0.1984327 0.4804218
C -2.9973854 1.5193566 -0.6683753
H -3.8382649 1.8260546 -1.3089700
H -2.9447311 2.2231147 0.1744223
H -2.0745335 1.6297715 -1.2573490
O -4.7430585 -5.3557512 -1.2025720
C -3.6843823 -5.9820427 -0.8851866
C -3.7375302 -7.2138052 -0.0214567
H -4.7203842 -7.3188173 0.4481394
H -3.5416574 -8.0908267 -0.6550540
H -2.9454087 -7.1737186 0.7361244
O -2.5473935 -5.5715873 -1.3166455
C -3.6364521 -6.8070103 -5.6771604
O -3.7699544 -2.3533386 -4.1214172
C -2.9181948 -1.5555319 -4.6907521
C -3.5236890 -0.5221220 -5.6171712
H -4.2321012 -0.9997974 -6.3065122
H -4.0887843 0.2035187 -5.0141821
H -2.7405389 0.0008913 -6.1749911
O -1.6809014 -1.5836457 -4.5055109
H -4.2491168 -7.5291833 -5.1211267
O -1.3509100 -3.6687975 -3.0691226
H -4.3064714 -6.2660978 -6.3599048
H -2.8625366 -7.3270017 -6.2499739
O -1.7744020 -5.6558093 -4.6895042
H -1.3031368 -4.4636903 -3.7056454
O -3.8835892 -5.2080607 -3.9562649
H -1.3483891 -2.8161836 -3.6639400
C -3.0028455 -5.8249169 -4.7143824
H -6.1020166 -4.2700147 -3.1310521
O -5.7698660 -3.3829602 -2.9004635
H -5.5456754 -2.9284985 -3.7451548

BuSnOAc3_2H2O_ciscis_v2
E (Hartree) = -1211.24839126
G_{298} (Hartree) = -1210.99452
Shielding = 3260.5
Calculated NMR shift = -679.6
Correlated to experiment = -609.8

41
Sn -3.3663473 -3.7773716 -2.4609968
C -3.1375558 -2.3262416 -0.8863731
H -3.7537736 -2.7285118 -0.0695768
H -2.0802804 -2.3876132 -0.5938136
C -3.5598127 -0.9150980 -1.2834477
H -2.9339172 -0.5552451 -2.1153731
H -4.5948056 -0.9245867 -1.6619867
C -3.4614611 0.0719979 -0.1100812
H -4.1011541 -0.2831338 0.7152436
H -2.4295436 0.0705027 0.2797594
C -3.8658757 1.4947891 -0.5052996
H -4.9014993 1.5223938 -0.8763067
H -3.7957201 2.1860867 0.3465798
H -3.2173702 1.8819822 -1.3057408
O -4.6503737 -5.2999756 -1.2398447
C -3.5967820 -5.9485250 -0.9383221
C -3.6699902 -7.1873783 -0.0858227
H -4.6445731 -7.2664195 0.4057577
H -3.5191493 -8.0633714 -0.7330172
H -2.8592953 -7.1814711 0.6527084
O -2.4616577 -5.5528912 -1.3760351
C -3.5000137 -6.8487845 -5.6340491
O -3.0856630 -2.2691122 -4.1351741
C -3.9126433 -1.8466232 -5.0345858
C -3.2986166 -1.0319235 -6.1525278
H -2.7422512 -0.1859967 -5.7270319
H -2.5774380 -1.6548239 -6.6998089
H -4.0709419 -0.6685002 -6.8375191
O -5.1507365 -2.0639924 -5.0328990
H -4.0531492 -7.5929625 -5.0442207
O -1.1777028 -3.7438250 -3.1075059
H -4.2270167 -6.3409786 -6.2814064
H -2.7333191 -7.3469681 -6.2353051
O -1.6252709 -5.7558593 -4.6090253
H -1.1927571 -4.6026076 -3.6878214
O -3.7376281 -5.1372655 -4.0264959
H -1.2235836 -3.0116610 -3.7580599

C -2.8644079 -5.8476860 -4.6945693
H -6.0018213 -4.0684613 -2.9111367
O -5.5001759 -3.2352879 -2.8672375
H -5.4779252 -2.7765991 -3.8306312

BuSnOAc3_2H2O_cistrans
E (Hartree) = -1211.24760366
G_{298} (Hartree) = -1210.99259
Shielding = 3232.6
Calculated NMR shift = -651.7
Correlated to experiment = -585.2

41
Sn 1.2580066 -1.5392628 0.6598159
C 0.1641179 -1.7229437 2.5000005
H -0.7434659 -2.2750327 2.2187209
H 0.7905402 -2.3718606 3.1281209
C -0.1474449 -0.3883184 3.1702465
H 0.7863978 0.1589344 3.3743587
H -0.7294744 0.2460690 2.4834445
C -0.9279894 -0.5697007 4.4810998
H -1.8621435 -1.1184979 4.2738379
H -0.3440599 -1.2073288 5.1661431
C -1.2494731 0.7637996 5.1613687
H -1.8563909 1.4056243 4.5049992
H -1.8082263 0.6164484 6.0966688
H -0.3286481 1.3155942 5.4034276
O 0.6041575 -2.5174007 -2.5702594
C -0.3764118 -2.8111015 -1.7702251
C -1.5518911 -3.5026245 -2.4045031
H -1.2194612 -4.1601244 -3.2156356
H -2.1166854 -4.0598453 -1.6505185
H -2.2097674 -2.7346017 -2.8378474
O -0.4081653 -2.5355648 -0.5447032
O 1.9290701 -3.6993605 0.4910028
O 0.0125166 0.1924742 -0.0340033
C 0.4667760 1.2270507 -0.6507237
C -0.5744667 2.1391920 -1.2636721
H -0.9693664 1.6576186 -2.1704227
H -1.4147809 2.2739414 -0.5714294
H -0.1330760 3.1038082 -1.5341339
O 1.6947583 1.5023159 -0.7869839
C 4.0247541 -4.6170394 1.2449113
C 3.0408588 -3.4878512 1.0881649
H 3.4986285 -5.5711864 1.3613628
H 4.6276977 -4.6719831 0.3264965
H 4.6954196 -4.4317105 2.0905584
O 3.3142212 -2.3246750 1.5255540
O 2.2504323 -1.3484834 -1.1434839
H 1.3862819 -1.9846768 -2.0084260
H 2.2819995 -0.3852753 -1.3389791
O 2.5380374 0.2863476 1.3234044
H 2.3938062 0.8853652 0.5051093
H 3.4499103 -0.0581339 1.3021329

BuSnOAc3_2H2O_cistrans_v2
E (Hartree) = -1211.25655815
G_{298} (Hartree) = -1211.00018
Shielding = 3156.2
Calculated NMR shift = -575.3
Correlated to experiment = -518.1

41
Sn 0.8953737 -1.6196153 0.5432745
C -0.1805023 -1.7126071 2.4036642
H -1.1016479 -2.2702671 2.1840277
H 0.4484114 -2.3313794 3.0599928
C -0.4613973 -0.3363605 3.0053062
H 0.4816196 0.2213915 3.1270457
H -1.0796755 0.2551203 2.3114160
C -1.1711578 -0.4301032 4.3642253
H -2.1093611 -0.9978240 4.2444640
H -0.5459994 -1.0152904 5.0595272
C -1.4695051 0.9453934 4.9667945
H -2.1192666 1.5351161 4.3025195
H -1.9745134 0.8597800 5.9393879
H -0.5430706 1.5194035 5.1188383
O 0.3411171 -2.6944942 -2.6688407
C -0.4626716 -3.1391842 -1.8182073
C -1.6150885 -4.0167242 -2.2474534
H -1.5570658 -4.2308936 -3.3190551
H -1.6018743 -4.9494561 -1.6684637
H -2.5599410 -3.5047755 -2.0180184
O -0.4098059 -2.9104012 -0.5367973
O 2.2539395 -3.2398691 0.8954358
O -0.1413282 0.1360711 -0.1936953
C 0.4502988 1.1438222 -0.7623102
C -0.4412648 2.3354243 -1.0267074
H -1.2614253 2.0326654 -1.6919118
H -0.8953142 2.6692824 -0.0840997
H 0.1300080 3.1497097 -1.4824381
O 1.6642627 1.1679186 -1.0869113
C 4.2907738 -4.4525629 0.9436419
C 3.5442581 -3.1416795 1.0188839
H 3.7457963 -5.2358302 1.4839314
H 4.3439525 -4.7543974 -0.1126835
H 5.3066604 -4.3397109 1.3351850
O 4.1814356 -2.0726059 1.1793855
O 2.0350313 -1.4569846 -1.2999106
H 2.0328852 -0.4638504 -1.4583370
O 2.4887300 -0.2420205 1.2512693
H 2.5884189 0.4325101 0.5403527
H 3.3136918 -0.9203285 1.2159842
H 1.3942119 -1.9263928 -1.9977130

BuSnOAc3_2H2O_cistrans_v3
E (Hartree) = -1211.24591626
G_{298} (Hartree) = -1210.99116
Shielding = 3183.0
Calculated NMR shift = -602.1
Correlated to experiment = -541.6

41

Sn	1.4541193	-1.4843133	0.6895511
C	0.1026662	-1.6550098	2.3498544
H	-0.8491675	-1.9548709	1.8920119
H	0.4924580	-2.4969839	2.9393011
C	-0.0133717	-0.3702081	3.1640754
H	0.9732427	-0.0779752	3.5577435
H	-0.3406366	0.4542608	2.5112181
C	-1.0016744	-0.5179055	4.3314772
H	-1.9893800	-0.8079511	3.9348558
H	-0.6762497	-1.3487846	4.9801622
C	-1.1291959	0.7651863	5.1571256
H	-1.4792800	1.6023767	4.5345284
H	-1.8402126	0.6431490	5.9867312
H	-0.1586379	1.0559308	5.5869521
O	0.7900030	-2.8493098	-2.5491569
C	-0.2885787	-2.9627973	-1.8141432
C	-1.3225810	-3.9133612	-2.3528991
H	-1.3029565	-3.9405993	-3.4482309
H	-1.0751317	-4.9191186	-1.9814763
H	-2.3160418	-3.6432769	-1.9801659
O	-0.4684807	-2.3601193	-0.7346895
O	1.7817513	-3.7669728	0.4267754
O	2.3591295	1.4529849	-0.6130426
C	2.8586288	1.2618847	0.5271688
C	3.8651383	2.2382335	1.0937547
H	3.9851693	3.0993690	0.4292589
H	3.5398150	2.5651401	2.0902054
H	4.8280518	1.7240500	1.2203704
O	2.5823524	0.2579158	1.2974509
C	3.7432593	-4.8723634	1.3049030
C	2.8687012	-3.6688524	1.0815659
H	3.1499511	-5.7921877	1.2708974
H	4.4852937	-4.9071575	0.4938131
H	4.2823688	-4.7848892	2.2545979
O	3.2347105	-2.5266942	1.5370363
O	2.3015549	-1.4019871	-1.1620434
H	1.4759844	-2.2105424	-2.0477201
H	2.4480507	-0.4525657	-1.3668038
O	0.0493507	0.3175886	-0.1104044
H	0.7992397	0.8760555	-0.4931978
H	-0.4244141	-0.1053283	-0.8494122

BuSnOAc3_2H2O_Hbonded
E (Hartree) = -1211.23587170
G_{298} (Hartree) = -1210.98426
Shielding = 3182.5
Calculated NMR shift = -601.5
Correlated to experiment = -541.6

41

Sn	-0.4844157	-0.4773495	-0.2816903
C	-1.2375343	-0.5017346	1.7384039
H	-2.2333698	-0.9611349	1.6669843
H	-0.5717883	-1.1959984	2.2702853
C	-1.2727898	0.8838643	2.3791652
H	-0.2711617	1.3442288	2.3600035
H	-1.9347873	1.5477253	1.7986341
C	-1.7718884	0.8322111	3.8317761
H	-2.7724752	0.3688240	3.8576497
H	-1.1106511	0.1703618	4.4156393
C	-1.8197398	2.2188910	4.4787640
H	-2.5012375	2.8870863	3.9305819
H	-2.1695046	2.1649690	5.5193896
H	-0.8242830	2.6869858	4.4805134
O	-0.1639305	-0.8195977	-2.3875161
C	-1.1849113	-1.6078861	-2.4864589
C	-1.4968941	-2.2298772	-3.8140394
H	-0.6862490	-2.9245411	-4.0747403
H	-2.4478229	-2.7683372	-3.7740300
H	-1.5243581	-1.4510797	-4.5865581
O	-1.8840970	-1.8385806	-1.4548366
O	0.6874623	-2.5296984	-0.0367673
O	0.0774126	1.6565760	-0.5458363
C	-1.1077871	2.0205180	-0.9077198
C	-1.3697857	3.4733906	-1.1808578
H	-1.2061641	4.0439213	-0.2560208
H	-0.6479304	3.8399997	-1.9222953
H	-2.3930709	3.6238626	-1.5363189
O	-2.0146057	1.1436077	-1.0098732
C	3.0711633	-2.5288821	0.4033914
C	1.7518032	-1.8705857	0.1207319
H	3.0337610	-2.9621447	1.4134251
H	3.2244637	-3.3561352	-0.3007359
H	3.8916753	-1.8049185	0.3453025
O	1.6971663	-0.5748499	0.0520390
O	4.3324222	0.7730433	-0.2618461
H	4.0720298	1.4876527	0.3503579
H	3.4669111	0.4047004	-0.5214332
O	2.1380497	1.9639801	1.5229076
H	1.5414710	2.1851265	0.7793859
H	2.1924147	0.9924504	1.4519239

BuSnOAc3_2H2O_Hbonded_v2
E (Hartree) = -1211.23645089
G_{298} (Hartree) = -1210.98643
Shielding = 3182.9
Calculated NMR shift = -602.0
Correlated to experiment = -541.6

41

Sn	-0.2972163	-0.3368523	-0.2477794
C	-0.8355612	-0.3688705	1.8363262
H	-1.4728107	-1.2595412	1.9365193
H	0.1296415	-0.5499468	2.3298789
C	-1.4814663	0.9228276	2.3205636
H	-0.8050872	1.7721850	2.1301838
H	-2.4124264	1.1202010	1.7659733
C	-1.7866949	0.8679550	3.8261197
H	-2.4502099	0.0112334	4.0292312
H	-0.8503349	0.6734036	4.3741386
C	-2.4291724	2.1601462	4.3366990
H	-3.3773056	2.3641395	3.8160931
H	-2.6432499	2.1038812	5.4134648
H	-1.7654412	3.0224371	4.1717912
O	-0.2257025	-0.7647898	-2.3623856
C	-1.2924196	-1.4942756	-2.3555082
C	-1.7356378	-2.1490419	-3.6295976
H	-1.1541118	-3.0740901	-3.7568934
H	-2.7983316	-2.4051297	-3.5779172
H	-1.5272753	-1.4981806	-4.4859908
O	-1.9202158	-1.6557452	-1.2671205
O	0.6979168	-2.5211618	-0.0996803
O	0.3323264	1.7542615	-0.6196553
C	-0.8627253	2.1594919	-0.9007561
C	-1.0890858	3.6180121	-1.1784507
H	-1.0094307	4.1691968	-0.2302612
H	-0.3074999	3.9970324	-1.8480156
H	-2.0824440	3.7798157	-1.6071420
O	-1.8112626	1.3229409	-0.9134637
C	3.0969981	-2.7355452	0.1300074
C	1.8283507	-1.9536673	-0.0657426
H	3.3361993	-2.7397148	1.2039939
H	2.9631428	-3.7710639	-0.1993412
H	3.9281064	-2.2572158	-0.4001971
O	1.8952949	-0.6692346	-0.1744646
O	2.0091590	1.5437878	1.7940116
H	1.5842579	2.0506888	1.0766809
H	2.4089400	0.8010986	1.3039102
H	-2.2280310	-3.1721607	0.2203280
O	-1.8402039	-3.5737907	1.0193942
H	-0.8869794	-3.5707178	0.8130542

BuSnOAc3_2H2O_trans_uncoord
E (Hartree) = -1211.24385816
G_{298} (Hartree) = -1210.98834
Shielding = 3197.7
Calculated NMR shift = -616.8
Correlated to experiment = -554.5

41

Sn	-0.1607635	-0.5814856	-0.5203419
C	-1.4587393	-0.4970926	1.2010554
H	-2.4060271	-0.1077981	0.8020284
H	-1.6024480	-1.5442368	1.5025850
C	-0.9141370	0.3719560	2.3297164
H	0.0485134	-0.0305032	2.6866565
H	-0.7033122	1.3809391	1.9409063
C	-1.8770544	0.4820080	3.5200959
H	-2.8440122	0.8785052	3.1684570
H	-2.0833158	-0.5249878	3.9196259
C	-1.3192282	1.3797888	4.6282043
H	-1.1427410	2.4011739	4.2561569
H	-2.0091969	1.4530158	5.4805669
H	-0.3612865	0.9918175	5.0078650
O	-1.0312522	-2.4427347	-1.4251175
C	-1.8863006	-1.7886223	-2.1217975
C	-2.9084261	-2.5356943	-2.9357142
H	-2.4926464	-3.4831794	-3.2962253
H	-3.7632740	-2.7673538	-2.2832554
H	-3.2655413	-1.9185715	-3.7667895
O	-1.8773864	-0.5138410	-2.0994706
O	1.3631000	-1.9984156	0.3513240
O	-0.3687140	1.7190664	-0.5777707
C	0.4999428	2.5188640	-1.0077031
C	0.5020005	3.9422666	-0.5480113
H	-0.5253826	4.2890566	-0.3915917
H	1.0217022	3.9444927	0.4258695
H	1.0401606	4.5886402	-1.2488434
O	1.4627493	2.1784601	-1.8222738
C	3.3866430	-1.3765102	1.5146802
C	2.1068463	-1.0618412	0.7935861
H	3.3367955	-2.3670063	1.9787707
H	4.1999387	-1.3798548	0.7741544
H	3.6079268	-0.6005325	2.2562523
O	1.7602569	0.1543620	0.5983585
O	1.0788239	-0.2976239	-2.1327056
H	0.5550755	-0.4693484	-2.9360927
H	1.3796595	1.1400198	-2.0268374
O	1.9030125	2.5067798	2.1386709
H	1.2311658	2.3100166	2.8114918
H	1.9463598	1.6814742	1.6019703

BuSnOAc3_2H2O_trans_uncoord_v2
E (Hartree) = -1211.24312227
G_{298} (Hartree) = -1210.98979
Shielding = 3200.0
Calculated NMR shift = -619.0
Correlated to experiment = -556.5

41

Sn	0.0558309	-0.2115708	-0.3800630
C	-1.3927778	-0.0066062	1.2017584
H	-1.9206704	0.9283765	0.9699976
H	-2.0647845	-0.8606329	1.0414232
C	-0.8004752	-0.0236503	2.6054211
H	-0.2444405	-0.9623828	2.7589152
H	-0.0785936	0.7991493	2.7301216
C	-1.8875625	0.0814678	3.6859940
H	-2.4639630	1.0093165	3.5319924
H	-2.5982500	-0.7513123	3.5585404
C	-1.3075516	0.0580571	5.1027129
H	-0.6089135	0.8942913	5.2588586
H	-2.0974938	0.1341676	5.8635384
H	-0.7552147	-0.8759123	5.2860123
O	-0.8570929	-2.0696638	-1.3654949
C	-1.7139831	-1.3755686	-2.0339617
C	-2.7619922	-2.0936309	-2.8418126
H	-2.3084035	-2.9268989	-3.3924223
H	-3.5010134	-2.5220110	-2.1491180
H	-3.2671891	-1.4039529	-3.5248323
O	-1.6741875	-0.1101840	-1.9858193
O	1.3930280	-1.7501614	0.6344382
O	0.0295469	2.0151849	-0.8032468
C	0.4431517	2.6146747	-1.8294502
C	0.2108287	4.0928825	-1.9646744
H	-0.6893319	4.3860115	-1.4149667
H	1.0724053	4.6151188	-1.5224045
H	0.1426629	4.3790206	-3.0198787
O	1.0991770	2.0517852	-2.7985527
C	3.3408393	-1.1959083	1.9423681
C	2.1554533	-0.8264560	1.0953656
H	3.0450205	-1.9385164	2.6937048
H	4.0970505	-1.6637428	1.2959717
H	3.7695184	-0.3100761	2.4204954
O	1.9032496	0.3904058	0.8194937
O	1.3622028	-0.2606043	-1.9801213
H	1.1315468	-1.0274363	-2.5335599
H	1.2468916	0.9999563	-2.5561494
H	-1.1318674	-3.2701910	0.3024750
O	-0.9829862	-3.3858450	1.2608096
H	-0.0496658	-3.1149511	1.3491207

BuSnOAc3_2HOEt_ciscis
E (Hartree) = -1368.54428602
G_{298} (Hartree) = -1368.18841
Shielding = 3276.0
Calculated NMR shift = -695.1
Correlated to experiment = -623.4

53

Sn	-3.4383138	-3.8736032	-2.5178947
C	-3.1792859	-2.3379032	-1.0235522
H	-3.7931857	-2.6890228	-0.1823147
H	-2.1198138	-2.4017408	-0.7378190
C	-3.5809695	-0.9394540	-1.4817791
H	-2.9691404	-0.6331875	-2.3460956
H	-4.6237608	-0.9393400	-1.8380098
C	-3.4327718	0.1062050	-0.3662498
H	-4.0571457	-0.1925076	0.4922633
H	-2.3912334	0.1036723	-0.0025074
C	-3.8208515	1.5138407	-0.8269586
H	-4.8647607	1.5416671	-1.1737624
H	-3.7158230	2.2482289	-0.0156243
H	-3.1860988	1.8450216	-1.6629915
O	-4.3642377	-5.4311851	-1.0660848
C	-3.2273711	-5.9779036	-0.8840059
C	-3.0918681	-7.1726847	0.0240414
H	-3.9383457	-7.2338146	0.7158932
H	-3.0784854	-8.0785099	-0.5997602
H	-2.1416574	-7.1290569	0.5689047
O	-2.2020660	-5.5219095	-1.4895365
C	-3.5209733	-6.8989666	-5.7300386
O	-3.5278680	-2.4863006	-4.2677759
C	-4.4608332	-1.7282598	-4.7312367
C	-4.0416943	-0.8156828	-5.8656891
H	-3.3186346	-0.0823086	-5.4811625
H	-3.5323949	-1.3992549	-6.6436479
H	-4.9067137	-0.2916217	-6.2845174
O	-5.6463272	-1.6871755	-4.3098052
H	-4.0191709	-7.6756342	-5.1347419
O	-1.2561392	-3.6935141	-3.2366654
H	-4.2911366	-6.4191055	-6.3495183
H	-2.7515515	-7.3442962	-6.3681769
O	-1.6969601	-5.5902736	-4.8823800
H	-1.2703128	-4.4768275	-3.9054075
O	-3.7741376	-5.3380011	-3.9823214
C	-2.9085845	-5.8661230	-4.8079389
O	-5.6571381	-3.5364911	-2.6243843
H	-5.7555439	-2.7354894	-3.3034032
C	-6.6071836	-4.5709642	-2.9869745
H	-6.4641081	-4.8373051	-4.0469433
H	-6.3575238	-5.4477447	-2.3779842
C	-8.0220243	-4.0846880	-2.7201560
H	-8.2523271	-3.1957810	-3.3244726

H -8.1467796 -3.8270907 -1.6594866
H -8.7468935 -4.8718084 -2.9760969
C -0.6651925 -2.5332042 -3.8644888
H -0.9407286 -1.6685082 -3.2436100
H -1.1119912 -2.3803049 -4.8581245
C 0.8441559 -2.6983005 -3.9404728
H 1.1081143 -3.5669530 -4.5601501
H 1.2708820 -2.8463985 -2.9392276
H 1.3019009 -1.8044343 -4.3901571

BuSnOAc3_2HOEt_ciscis_v2
E (Hartree) = -1368.54266104
G_{298} (Hartree) = -1368.18787
Shielding = 3270.9
Calculated NMR shift = -690.0
Correlated to experiment = -618.9

53
Sn -3.4998167 -3.6411005 -2.5481373
C -3.2897305 -2.1190159 -1.0299399
H -4.1738475 -2.2391173 -0.3890956
H -2.3947993 -2.4097824 -0.4611663
C -3.1792211 -0.7105207 -1.6053061
H -2.3528756 -0.6628619 -2.3329128
H -4.0963564 -0.4611420 -2.1637126
C -2.9582761 0.3496523 -0.5154754
H -3.7849743 0.2971504 0.2128492
H -2.0396779 0.1068404 0.0450123
C -2.8595197 1.7662566 -1.0879565
H -3.7793007 2.0384109 -1.6273684
H -2.7012610 2.5124561 -0.2962768
H -2.0226130 1.8473030 -1.7980725
C -3.8207601 -7.2737026 -5.0184445
O -3.7016482 -2.3459816 -4.2955225
C -4.6418842 -1.5458600 -4.6647251
C -4.2841394 -0.6308228 -5.8158869
H -3.5712258 0.1227926 -5.4511349
H -3.7800711 -1.2008712 -6.6060562
H -5.1761405 -0.1289710 -6.2044432
O -5.7845052 -1.4622503 -4.1392798
H -4.4535239 -6.8366891 -5.8013417
O -4.3582031 -5.1436715 -0.9637069
H -2.7816455 -7.2187069 -5.3722842
H -4.0949522 -8.3175472 -4.8369734
O -4.1597934 -7.0300913 -2.6554439
H -4.2551327 -6.0069302 -1.5164776
O -3.7983062 -5.1810097 -3.9338363
C -3.9411605 -6.4674127 -3.7444756
O -5.7597653 -3.3783086 -2.5363678
H -5.8766584 -2.5433001 -3.1739000
C -6.6804233 -4.4125486 -2.9540144
H -6.5024417 -4.6574589 -4.0149494
H -6.4472809 -5.3013455 -2.3535923
C -8.1128230 -3.9558649 -2.7298131
H -8.3340447 -3.0590374 -3.3254134
H -8.2793017 -3.7197548 -1.6699720
H -8.8149399 -4.7489786 -3.0266126
C -3.7688644 -5.3124664 0.3454078
H -3.9346835 -4.3661643 0.8803384
H -2.6836467 -5.4683242 0.2459454
C -4.4295368 -6.4720922 1.0743773
H -4.2633854 -7.4147240 0.5338576
H -5.5121481 -6.3094332 1.1656947
H -4.0043600 -6.5776137 2.0833325
O -1.4098043 -3.4362739 -3.3646073
C -0.9132307 -4.3630225 -2.6347104
O -1.6587351 -5.0084958 -1.8359360
C 0.5639500 -4.6544639 -2.7175822
H 1.0946701 -3.9457175 -2.0650036
H 0.9249534 -4.5035647 -3.7412056
H 0.7758624 -5.6718499 -2.3726822

BuSnOAc3_2HOEt_cistrans
E (Hartree) = -1368.54500001
G_{298} (Hartree) = -1368.18808
Shielding = 3230.5
Calculated NMR shift = -649.6
Correlated to experiment = -583.4

53
Sn 1.3410436 -1.5760883 0.5900590
C 0.2079487 -1.7869555 2.4082386
H -0.7959664 -2.0598380 2.0575736
H 0.6506701 -2.6485750 2.9270466
C 0.2051884 -0.5243953 3.2640761
H 1.2347055 -0.2652254 3.5595447
H -0.1703687 0.3292245 2.6765574
C -0.6580519 -0.6792412 4.5254787
H -1.6896297 -0.9314451 4.2275980
H -0.2903965 -1.5369550 5.1137092
C -0.6609980 0.5830248 5.3921669
H -1.0464049 1.4468576 4.8297165
H -1.2869551 0.4579789 6.2872735
H 0.3568725 0.8342746 5.7271808
O 0.6103292 -3.1456484 -2.4980679
C -0.3548785 -3.3454320 -1.6350497
C -1.3869095 -4.3534232 -2.0595006
H -1.5388352 -4.3265993 -3.1445791
H -1.0110734 -5.3526062 -1.7933918
H -2.3262112 -4.1817459 -1.5241632
O -0.4407051 -2.7721485 -0.5302544
O 1.9413966 -3.8325420 0.4235532
O 1.1005071 2.0074510 0.6519763
C 2.1580263 1.4993367 1.1097268
C 3.2121060 2.3990088 1.7187537
H 2.9601388 3.4530556 1.5649259

H	3.2756811	2.1874756	2.7955475
H	4.1935325	2.1672007	1.2853505
O	2.4457422	0.2424518	1.1222693
C	4.0989560	-4.6427153	1.1447167
C	3.0666983	-3.5625314	0.9515169
H	3.6157249	-5.6169535	1.2763693
H	4.7197446	-4.6864822	0.2377481
H	4.7495761	-4.4077250	1.9940980
O	3.3346717	-2.3607287	1.3003601
O	2.0788798	-1.5081235	-1.3203408
H	1.2943471	-2.4380911	-2.0831345
O	-0.2007782	0.0131276	-0.0896488
H	0.2615438	0.9146531	0.1896766
C	2.6136659	-0.2984266	-1.8797355
H	3.5986450	-0.1018598	-1.4256266
H	1.9634441	0.5606554	-1.6388866
C	2.7321833	-0.4624640	-3.3870645
H	3.3769268	-1.3173021	-3.6341898
H	3.1667059	0.4424257	-3.8358971
H	1.7451217	-0.6321971	-3.8410993
C	-0.8011310	0.1392223	-1.3943176
H	-0.3075269	-0.5645865	-2.0825876
H	-0.6047439	1.1580146	-1.7678148
C	-2.2923124	-0.1405127	-1.3144515
H	-2.4598084	-1.1471714	-0.9094472
H	-2.7507105	-0.0796731	-2.3130930
H	-2.7883281	0.5869693	-0.6574668

BuSnOAc3_2HOEt_cistrans_v1_1
E (Hartree) = -1368.54608114
G_{298} (Hartree) = -1368.18860
Shielding = 3227.9
Calculated NMR shift = -646.9
Correlated to experiment = -581.1

53

Sn	1.3158517	-1.5676192	0.6311917
C	0.1683014	-1.7909021	2.4388321
H	-0.8321965	-2.0634592	2.0779879
H	0.6076813	-2.6549961	2.9563967
C	0.1553701	-0.5340419	3.3027043
H	1.1814826	-0.2755220	3.6102610
H	-0.2149324	0.3232730	2.7171975
C	-0.7209868	-0.6979693	4.5539317
H	-1.7489968	-0.9495787	4.2434124
H	-0.3585792	-1.5590436	5.1404831
C	-0.7349699	0.5587295	5.4285017
H	-1.1156284	1.4255232	4.8674053
H	-1.3705518	0.4270764	6.3158860
H	0.2788093	0.8092493	5.7760921
O	0.6444565	-3.1084146	-2.4752037
C	-0.3268228	-3.3211192	-1.6260482
C	-1.3558838	-4.3239734	-2.0699984
H	-1.5002434	-4.2825986	-3.1555918
H	-0.9815480	-5.3264567	-1.8145048
H	-2.2989665	-4.1595806	-1.5390555
O	-0.4251865	-2.7630739	-0.5122511
O	1.9575941	-3.8083483	0.4646429
O	1.0568999	2.0235979	0.7188953
C	2.1180164	1.5181424	1.1706128
C	3.1839881	2.4190829	1.7556186
H	2.8949682	3.4713311	1.6707203
H	3.3373059	2.1548697	2.8110025
H	4.1355665	2.2404808	1.2369738
O	2.4051347	0.2609630	1.1858328
C	4.1246535	-4.5868992	1.1918877
C	3.0748434	-3.5233259	1.0027684
H	3.6579832	-5.5701709	1.3160468
H	4.7479371	-4.6142091	0.2859132
H	4.7694140	-4.3462567	2.0441159
O	3.3187154	-2.3203163	1.3632692
O	2.0828448	-1.4914294	-1.2724914
H	1.3294410	-2.4015070	-2.0344725
O	-0.2130289	0.0211650	-0.0588042
H	0.2337612	0.9242835	0.2392519
C	2.6284579	-0.2923680	-1.8459760
H	2.1002875	0.5940637	-1.4560061
C	-0.7903603	0.1582704	-1.3734785
H	-0.2797879	-0.5345857	-2.0598899
H	-0.5920699	1.1820153	-1.7312914
C	-2.2810725	-0.1304758	-1.3229491
H	-2.4503080	-1.1432654	-0.9342271
H	-2.7223648	-0.0584691	-2.3284066
H	-2.7925062	0.5855065	-0.6651502
H	2.4244144	-0.3381813	-2.9295882
C	4.1222600	-0.1884791	-1.5773555
H	4.6494474	-1.0524492	-2.0045157
H	4.3083146	-0.1678023	-0.4953266
H	4.5307895	0.7292644	-2.0272532

BuSnOAc3_2HOEt_cistrans_v2
E (Hartree) = -1368.54117728
G_{298} (Hartree) = -1368.18175
Shielding = 3155.6
Calculated NMR shift = -574.6
Correlated to experiment = -517.5

53

Sn	0.7896470	-1.2360082	0.3251032
C	-0.2096578	-1.3656518	2.2307199
H	-1.0575104	-2.0475624	2.0736959
H	0.5243601	-1.8637746	2.8799784
C	-0.6378717	-0.0094220	2.7830319
H	0.2208435	0.6802866	2.7996910
H	-1.3803188	0.4535073	2.1124300
C	-1.2350295	-0.1154089	4.1939366

H	-2.0945622	-0.8066537	4.1748529
H	-0.4897184	-0.5723061	4.8665812
C	-1.6711313	1.2431823	4.7493627
H	-2.4363684	1.7055245	4.1075419
H	-2.0920640	1.1504157	5.7607769
H	-0.8203128	1.9390460	4.8009849
O	1.0345160	-3.2436399	-2.3983126
C	-0.0340808	-3.3951775	-1.7460040
C	-0.9663183	-4.5269329	-2.1070281
H	-0.6971617	-4.9566026	-3.0769621
H	-0.8852223	-5.3019059	-1.3311911
H	-2.0047565	-4.1736616	-2.1113302
O	-0.4182714	-2.6557861	-0.7596533
O	1.9774728	-3.0578459	0.5818754
O	-0.4277070	0.2039402	-0.6383721
C	-0.3264769	1.4874059	-0.3463501
C	-1.4069151	2.3261295	-1.0041937
H	-1.3412451	2.2181845	-2.0959813
H	-2.3967198	1.9574935	-0.7026872
H	-1.2936234	3.3778811	-0.7239647
O	0.5482431	1.9741181	0.3707532
C	3.7652404	-4.6013784	0.7527311
C	3.2225681	-3.1979112	0.8969253
H	3.1411985	-5.2977336	1.3284998
H	3.6960896	-4.8993510	-0.3026134
H	4.8046590	-4.6534383	1.0912869
O	3.9773168	-2.2749445	1.2994416
O	2.0277241	-1.1691827	-1.4812470
O	2.5445439	-0.2467176	1.2499750
H	3.2156338	-1.0750496	1.3239401
H	1.6914452	-2.0873372	-1.9522905
C	3.3098706	0.9328257	0.8748692
H	4.3127765	0.5936162	0.5700629
H	2.8195588	1.4069844	0.0179683
C	3.3634046	1.8947297	2.0454514
H	3.8159075	1.4164419	2.9251897
H	2.3471324	2.2249613	2.2946710
H	3.9621566	2.7797085	1.7828156
C	2.0255368	-0.0674622	-2.4320658
H	3.0380364	-0.0307604	-2.8640049
H	1.8693597	0.8562364	-1.8591998
C	0.9669746	-0.2190375	-3.5128422
H	1.1283368	-1.1307034	-4.1035208
H	1.0113616	0.6446332	-4.1923353
H	-0.0328714	-0.2609051	-3.0619936

BuSnOAc3_2HOEt_cistrans_v2_1

E (Hartree) = -1368.54247711

G_{298} (Hartree) = -1368.18724

Shielding = 3160.2

Calculated NMR shift = -579.2

Correlated to experiment = -521.6

53			
Sn	0.8209160	-1.1797616	0.3334331
C	-0.1632883	-1.3751477	2.2414546
H	-0.8936918	-2.1881020	2.1236451
H	0.6320350	-1.7142089	2.9211901
C	-0.8026800	-0.0709505	2.7124760
H	-0.0581205	0.7413520	2.6961301
H	-1.5971852	0.2302475	2.0097525
C	-1.3986649	-0.1866906	4.1230328
H	-2.1366351	-1.0066572	4.1397714
H	-0.6014166	-0.4775980	4.8275528
C	-2.0555336	1.1147345	4.5910018
H	-2.8766478	1.4069074	3.9187897
H	-2.4705440	1.0168424	5.6043416
H	-1.3288916	1.9409942	4.6027717
O	1.1389836	-2.9967731	-2.5128817
C	0.0996519	-3.2673103	-1.8496076
C	-0.7778219	-4.4143944	-2.2901814
H	-0.5105359	-4.7410407	-3.3000859
H	-0.6341151	-5.2486694	-1.5884274
H	-1.8336845	-4.1211798	-2.2410204
O	-0.2927805	-2.6442721	-0.7906487
O	2.1194125	-2.9336780	0.5614649
O	-0.5030046	0.1918903	-0.5788124
C	-0.4075975	1.4899226	-0.3553985
C	-1.6212378	2.2614495	-0.8407429
H	-1.8640620	1.9799300	-1.8735577
H	-2.4869574	1.9915968	-0.2192334
H	-1.4398808	3.3382912	-0.7677650
O	0.5506896	2.0386844	0.1898014
C	3.7643495	-4.4443276	1.3489931
C	3.1494847	-3.0621470	1.3302894
H	3.0105173	-5.1739747	1.6742853
H	4.0625326	-4.7193613	0.3281809
H	4.6308821	-4.4744246	2.0168500
O	3.6508798	-2.1474694	2.0352635
O	2.0790721	-0.9868381	-1.4357044
O	2.4635303	-0.0555461	1.3384160
H	3.0066640	-0.8856501	1.7142768
H	1.7701720	-1.8996434	-1.9533538
C	3.4110518	0.8557072	0.7182040
H	3.9400551	0.3273575	-0.0922113
H	2.8095692	1.6658237	0.2910627
C	4.3799582	1.3730498	1.7674976
H	4.9572353	0.5505436	2.2128796
H	3.8363991	1.8945411	2.5667817
H	5.0862120	2.0801107	1.3079842
C	1.9316954	0.1236334	-2.3668488
H	1.9102263	1.0460524	-1.7729285
H	0.9648012	0.0324821	-2.8861319
C	3.0961419	0.1094701	-3.3401647
H	4.0503530	0.1995808	-2.8032000
H	3.0098106	0.9518945	-4.0418996

H 3.1096951 -0.8232728 -3.9207685

BuSnOAc3_2HOEt_trans_uncoord
E (Hartree) = -1368.54227888
G_{298} (Hartree) = -1368.18810
Shielding = 3222.2
Calculated NMR shift = -641.2
Correlated to experiment = -576.0

53
Sn 1.7973393 -1.3167801 0.6847204
C 0.5899653 -1.6504251 2.4457852
H 0.1114622 -2.6208509 2.2553839
H 1.3270417 -1.7767192 3.2523985
C -0.4224902 -0.5541591 2.7602770
H 0.0966221 0.4096009 2.8960794
H -1.1092821 -0.4185196 1.9097135
C -1.2392903 -0.8596369 4.0254120
H -1.7627216 -1.8213759 3.8928865
H -0.5512058 -1.0001581 4.8758037
C -2.2509175 0.2423173 4.3521781
H -2.9647163 0.3814694 3.5259183
H -2.8280541 0.0058969 5.2574914
H -1.7452519 1.2056678 4.5195879
O 1.2535565 -2.4824490 -2.5781143
C 0.3717045 -2.9191565 -1.7316864
C -0.7322494 -3.7580104 -2.3122567
H -0.3158426 -4.4925506 -3.0125493
H -1.2967670 -4.2537908 -1.5172229
H -1.4052290 -3.1013870 -2.8824754
O 0.3887543 -2.6743468 -0.4986278
O 2.8732074 -3.3123480 0.9110530
O 0.3695122 0.2612595 -0.2761873
C 1.0298082 1.1893702 0.2915699
C 0.5716818 2.6200356 0.2011048
H 0.0192226 2.7880219 -0.7296294
H -0.1084744 2.8131274 1.0440949
H 1.4231812 3.3039531 0.2846355
O 2.0787693 0.9024537 0.9708624
C 5.0973531 -3.5029576 1.8278160
C 3.8791899 -2.7228503 1.4354774
H 4.8169573 -4.5045945 2.1719730
H 5.6995384 -3.6028965 0.9115044
H 5.6780526 -2.9689755 2.5868512
O 3.8473925 -1.4491974 1.5836817
O 2.8200588 -1.2255091 -1.1617142
H 3.3553057 -0.6459830 -3.7419118
H 4.8817691 -0.9454534 -2.8706766
C 3.3456521 0.0229872 -1.6769848
H 2.5178163 0.7368162 -1.8206853
H 4.0334729 0.4424342 -0.9280491
C 4.0536690 -0.2356369 -2.9984483
H 4.4560424 0.7089102 -3.3929547
H 1.9921719 -1.8789838 -2.0222815
O 5.0035905 -3.0582845 -1.4144662
H 4.2895286 -2.4064984 -1.2319249
C 4.3582564 -4.2421683 -1.9022800
H 3.8082443 -4.0230447 -2.8380396
H 3.6213075 -4.6030505 -1.1609219
C 5.4229769 -5.2956615 -2.1523401
H 4.9726127 -6.2207599 -2.5402587
H 5.9545325 -5.5339462 -1.2197610
H 6.1601721 -4.9332057 -2.8828117

BuSnOAc3_H2O_cis
E (Hartree) = -1134.75578961
G_{298} (Hartree) = -1134.52347
Shielding = 3180.0
Calculated NMR shift = -599.0
Correlated to experiment = -538.9

38
Sn 1.5952239 -0.8086215 0.4991477
C 0.5560927 -2.1300464 1.8463319
H 0.6717789 -1.6422283 2.8244497
H -0.4971196 -2.0452272 1.5444864
C 1.0549931 -3.5703737 1.8363396
H 0.9426942 -3.9972942 0.8270416
H 2.1314201 -3.6041884 2.0708421
C 0.2932734 -4.4506995 2.8399299
H 0.4010709 -4.0243057 3.8512708
H -0.7837800 -4.4158335 2.6054336
C 0.7802325 -5.9021955 2.8329780
H 1.8482944 -5.9622058 3.0915835
H 0.2253775 -6.5170827 3.5557390
H 0.6533269 -6.3565800 1.8387064
O 2.3916811 2.2810670 1.8289682
C 3.2730756 1.3978237 1.9232619
C 4.6607262 1.7544867 2.4054487
H 4.6981828 2.7975932 2.7344170
H 4.9529130 1.0819788 3.2225229
H 5.3728201 1.5943231 1.5838529
O 3.1172297 0.1361617 1.6378651
H 1.1403425 0.7204360 -3.7562917
O 3.3250615 -2.0309009 -0.0829952
C 2.7151786 -2.6892311 -1.0114459
C 3.4793752 -3.7605645 -1.7433340
H 4.4315987 -3.3520478 -2.1050507
H 3.7170655 -4.5695473 -1.0383837
H 2.8901805 -4.1574309 -2.5753937
O 1.5047582 -2.4401376 -1.2730744
O 1.9560529 0.4937171 -1.1234551
O -0.2086053 -0.0155900 -1.1402640
C 0.7705637 0.5525021 -1.6720517
C 0.6673171 1.3179900 -2.9638660
H -0.3814321 1.4935166 -3.2213638

H 1.2171119 2.2643412 -2.8904725
H -0.2926799 1.2008515 0.7697675
O 0.3343792 0.8955898 1.4500584
H 1.0832249 1.6149539 1.5839997

BuSnOAc3_H2O_cis_EA
E (Hartree) = -1134.75927165
G_{298} (Hartree) = -1134.52740
Shielding = 3228.3
Calculated NMR shift = -647.4
Correlated to experiment = -581.4

38
Sn 0.7199673 0.0950165 0.1854059
C -1.3035133 0.8435946 0.3538972
H -1.2089020 1.9312407 0.2230099
H -1.5869633 0.6402045 1.3961763
C -2.2859200 0.2281812 -0.6386278
H -2.3075009 -0.8670771 -0.5195407
H -1.9465822 0.4211697 -1.6701560
C -3.7093640 0.7819841 -0.4715102
H -4.0533079 0.5871261 0.5581644
H -3.6867880 1.8789438 -0.5848759
C -4.6968939 0.1762737 -1.4726423
H -4.3892235 0.3876841 -2.5080154
H -5.7100855 0.5800906 -1.3357641
H -4.7531598 -0.9169887 -1.3598736
O 0.7966129 -0.0150233 -2.0593318
C 0.4374470 -1.2427027 -2.0485622
O 0.2472716 -1.8345387 -0.9330485
C 0.2065314 -1.9783757 -3.3393474
H 0.6659557 -1.4476173 -4.1786520
H -0.8781027 -2.0456077 -3.5073231
H 0.5934256 -3.0011994 -3.2616846
O 2.7094938 -0.6231684 0.0978760
C 3.1911292 -1.7298920 0.5880947
C 4.5912899 -2.0484490 0.1147899
H 4.5625869 -2.2530393 -0.9646295
H 4.9864839 -2.9190734 0.6472295
H 5.2417408 -1.1766507 0.2622481
O 1.7349436 2.0628351 -0.0584232
C 1.8957781 2.2376416 1.2010408
O 1.4845940 1.3545758 2.0211552
C 2.5946488 3.4771883 1.6903029
H 2.3815653 4.3235825 1.0278822
H 3.6782455 3.2902851 1.6623940
H 2.3065511 3.7017928 2.7225973
O 0.4668898 -1.3185625 1.9374826
O 2.6041224 -2.5022842 1.3779417
H 1.3122711 -1.9321267 1.7766657
H 0.6887611 -0.7760340 2.7176541

BuSnOAc3_H2O_trans
E (Hartree) = -1134.75965206
G_{298} (Hartree) = -1134.52764
Shielding = 3200.2
Calculated NMR shift = -619.2
Correlated to experiment = -556.7

38
Sn 1.4336972 -1.7548512 0.5214900
C 0.3831611 -1.7925228 2.4078618
H -0.3617131 -2.5900314 2.2812358
H 1.1432236 -2.1347945 3.1251452
C -0.2480889 -0.4693482 2.8282081
H 0.5221453 0.3189909 2.8731569
H -0.9786708 -0.1441798 2.0710089
C -0.9430668 -0.5629068 4.1952118
H -1.7125053 -1.3520929 4.1552819
H -0.2104561 -0.8876505 4.9530391
C -1.5795907 0.7624175 4.6224602
H -2.3350270 1.0911804 3.8927363
H -2.0733312 0.6776336 5.6010230
H -0.8226399 1.5579690 4.6971990
O 0.2148106 -2.3916632 -2.6611327
C -0.6003267 -2.7724141 -1.7255419
C -1.9651793 -3.2103784 -2.1778708
H -1.9325034 -3.5998756 -3.2009690
H -2.3719277 -3.9534224 -1.4838075
H -2.6237175 -2.3290160 -2.1624509
O -0.3273581 -2.7759715 -0.4972735
O 2.1422854 -3.9098133 0.7036248
O 0.1844879 0.0945395 -0.3096227
C 1.1240823 0.8607388 0.0600890
C 0.9910483 2.3567478 -0.0575189
H 0.3123929 2.6190172 -0.8761182
H 0.5601014 2.7335912 0.8819193
H 1.9723793 2.8245630 -0.1924686
O 2.1960647 0.3668379 0.5740414
C 4.3507917 -4.5075350 1.4728699
C 3.2708814 -3.5120713 1.1475801
H 3.9111781 -5.4526345 1.8100483
H 4.9191515 -4.7044678 0.5519189
H 5.0379717 -4.1016528 2.2227986
O 3.4896239 -2.2590394 1.2932530
O 2.2450138 -1.8303589 -1.3841724
H 1.1574844 -2.0846081 -2.1977603
H 2.7151258 -0.9919265 -1.5384937

BuSnOAc3_HOAc
E (Hartree) = -1287.48774787
G_{298} (Hartree) = -1287.22569
Shielding = 3226.5
Calculated NMR shift = -645.6
Correlated to experiment = -579.9

43

Sn	2.2255109	-2.2381375	0.5066319
C	1.2215041	-2.5775086	2.3850822
H	0.2245935	-2.9230150	2.0763899
H	1.7561361	-3.4349189	2.8127229
C	1.1719118	-1.3624675	3.3019504
H	2.1960006	-1.0379902	3.5480756
H	0.6895486	-0.5130433	2.7922180
C	0.4179800	-1.6635139	4.6075215
H	-0.6075904	-1.9895717	4.3661908
H	0.8991804	-2.5163225	5.1141458
C	0.3720268	-0.4563638	5.5481215
H	-0.1280128	0.3994584	5.0696047
H	-0.1721466	-0.6875216	6.4749232
H	1.3868516	-0.1343448	5.8268998
O	-0.0221842	-3.0864600	-2.2195785
C	-0.1757713	-1.8957105	-1.7084842
C	-1.0939451	-0.9785466	-2.4655939
H	-1.8752204	-1.5438830	-2.9852277
H	-1.5232951	-0.2338649	-1.7876996
H	-0.4925745	-0.4483511	-3.2193015
O	0.3951374	-1.4846186	-0.6712146
H	5.8329761	-2.3515840	-2.2403192
O	2.2966912	0.0038461	0.5564941
C	3.4053071	0.0386733	1.2019935
C	3.9610095	1.3703343	1.6330541
H	3.7717757	2.1286159	0.8646589
H	3.4361197	1.6804518	2.5486062
H	5.0307990	1.2898664	1.8508548
O	3.9992168	-1.0432518	1.4971314
O	3.2722208	-2.0669662	-1.3666189
O	4.1170872	-3.5093358	0.0770580
C	4.1715441	-2.9480549	-1.0500859
C	5.2475905	-3.2612318	-2.0492807
H	5.9006855	-4.0541826	-1.6740603
H	4.7866375	-3.5612253	-2.9994909
H	-0.1649695	-6.1172327	-1.0993478
O	1.4103186	-4.0866465	-0.4789367
H	0.6073747	-3.6471114	-1.5604195
C	1.4008338	-5.2785216	0.1313552
O	1.8116030	-5.4534840	1.2675293
H	0.7915919	-7.3218395	-0.1701790
C	0.8374316	-6.3875527	-0.7381089
H	1.4781238	-6.5213844	-1.6212289

BuSnOAc3_HOAc_uncoord
E (Hartree) = -1287.49249303
G_{298} (Hartree) = -1287.22824
Shielding = 3086.3
Calculated NMR shift = -505.3
Correlated to experiment = -456.6

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Sn	2.5464611	-1.8954416	0.0994431
C	3.1160138	-2.5142547	2.0874541
H	3.0021965	-3.6061718	2.0640145
H	4.1829718	-2.2638447	2.1704187
C	2.2596342	-1.8754497	3.1778931
H	2.4701301	-0.7965341	3.2454076
H	1.1907998	-1.9772771	2.9392095
C	2.4937782	-2.5442807	4.5400743
H	2.2843373	-3.6213237	4.4371520
H	3.5559484	-2.4521128	4.8246254
C	1.5962902	-1.9491068	5.6280838
H	0.5368628	-2.0714369	5.3591748
H	1.7612220	-2.4401452	6.5978456
H	1.7892907	-0.8732542	5.7589338
O	1.6628584	-5.0351585	-0.1705216
C	2.4467330	-4.6838723	-1.0627044
C	2.8933787	-5.6478503	-2.1414021
H	2.5063125	-6.6510767	-1.9391526
H	2.5231423	-5.2933391	-3.1134861
H	3.9896903	-5.6632646	-2.1977286
O	2.9649443	-3.4837396	-1.1980483
H	5.0357358	1.3399213	-1.9804641
O	0.3923218	-1.9528559	-0.0817789
C	0.2309586	-0.7787892	0.4455357
C	-1.1588569	-0.2959168	0.7135644
H	-1.7925845	-0.4792100	-0.1627900
H	-1.5580205	-0.8957686	1.5466783
H	-1.1566715	0.7644456	0.9812896
O	1.2576796	-0.0996663	0.7516566
O	2.5817395	-0.7199905	-1.7936337
O	4.3554830	-0.7302538	-0.4882531
C	3.7750838	-0.3327702	-1.5613146
C	4.5011303	0.5544998	-2.5277693
H	5.2508240	-0.0518548	-3.0560624
H	3.8079245	0.9870604	-3.2550208
H	-0.9196960	-4.2136015	-0.1606559
O	0.5018659	-4.2353761	2.0973848
H	0.8479225	-4.6354830	1.2498593
C	-0.7573116	-3.7699171	1.9417859
O	-1.2195658	-2.9828877	2.7494465
H	-2.4672011	-3.7850512	0.6469696
C	-1.5172373	-4.3173599	0.7537988
H	-1.7124243	-5.3882988	0.9111083

BuSnOAc3_HOEt_cis
E (Hartree) = -1213.40406601
G_{298} (Hartree) = -1213.12071
Shielding = 3201.4
Calculated NMR shift = -620.5
Correlated to experiment = -557.8

44

Sn	0.6265222	0.1837749	0.2227647
C	-1.4847948	0.3559472	0.6159007
H	-1.5762018	1.3305745	1.1145864
H	-1.6832926	-0.4305284	1.3572516
C	-2.3693112	0.2312814	-0.6192184
H	-2.2114140	-0.7504377	-1.0936599
H	-2.0877594	0.9884141	-1.3689982
C	-3.8598410	0.3884988	-0.2789682
H	-4.1399710	-0.3686991	0.4724836
H	-4.0210038	1.3693565	0.1989153
C	-4.7595385	0.2559988	-1.5106697
H	-4.5144204	1.0206357	-2.2633015
H	-5.8210924	0.3710034	-1.2492883
H	-4.6357480	-0.7289415	-1.9858229
O	0.6916525	0.2006062	-1.9718442
C	0.4211898	-1.0507633	-2.1453525
O	0.2550336	-1.8065918	-1.1504161
C	0.2905022	-1.5558931	-3.5590649
H	1.1560627	-1.2312847	-4.1503180
H	-0.6036680	-1.1057958	-4.0130573
H	0.2004498	-2.6462432	-3.5737853
O	2.6341282	-0.5056752	0.3057151
C	2.4348111	-1.5350782	1.0811117
O	1.2887842	-1.7683265	1.5311941
C	3.6206307	-2.4079172	1.3851923
H	3.9035517	-2.9435319	0.4680686
H	3.3735127	-3.1306449	2.1682659
H	4.4757926	-1.7879706	1.6821090
O	1.2793593	2.1711155	-0.1868095
C	2.1359877	2.9398239	0.4196254
O	2.5438486	2.7890028	1.5929954
C	2.6319861	4.0962843	-0.4192246
H	1.7749203	4.6701107	-0.7962758
H	3.1657199	3.6997942	-1.2938476
H	3.2943654	4.7415057	0.1662400
O	0.9479371	1.0193248	2.3833852
H	1.6744682	1.7420869	2.1937624
C	1.1675190	0.3793813	3.6577821
H	2.0218414	-0.3147648	3.5913000
H	1.4261108	1.1692383	4.3822449
C	-0.0869646	-0.3567716	4.0880516
H	-0.3077862	-1.1770852	3.3933483
H	-0.9437738	0.3305619	4.1179036
H	0.0508935	-0.7863771	5.0907248

BuSnOAc3_HOEt_cis_EA
E (Hartree) = -1213.40863748
G_{298} (Hartree) = -1213.12536
Shielding = 3227.5
Calculated NMR shift = -646.5
Correlated to experiment = -580.7

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Sn	0.7050022	0.2130229	0.2037072
C	-1.3122991	0.9928294	0.2607389
H	-1.2182298	2.0321127	-0.0856842
H	-1.5806273	1.0060876	1.3267588
C	-2.3105684	0.1933712	-0.5708626
H	-2.3214425	-0.8578274	-0.2416375
H	-1.9928282	0.1808129	-1.6271031
C	-3.7332829	0.7673599	-0.4889838
H	-4.0561556	0.7823676	0.5657222
H	-3.7184461	1.8195064	-0.8197605
C	-4.7374267	-0.0272077	-1.3284306
H	-4.4511622	-0.0262060	-2.3912402
H	-5.7500314	0.3943962	-1.2543645
H	-4.7852751	-1.0761580	-0.9992676
O	0.8710535	0.0649421	-2.0374099
C	0.5009227	-1.1596236	-2.0286095
O	0.2565490	-1.7368336	-0.9180359
C	0.3213254	-1.9066056	-3.3222100
H	0.8514170	-1.4055012	-4.1381251
H	-0.7524565	-1.9338580	-3.5577517
H	0.6632928	-2.9417197	-3.2083540
O	2.6742365	-0.5472505	0.2653023
C	3.0777029	-1.7003814	0.7242225
C	4.5188103	-2.0129290	0.3866872
H	4.6219178	-2.0938683	-0.7042485
H	4.8288007	-2.9485327	0.8623583
H	5.1625409	-1.1850914	0.7120299
O	1.7622010	2.1555269	-0.1317656
C	1.8654105	2.4029266	1.1193084
O	1.4048717	1.5720862	1.9688601
C	2.5552309	3.6598584	1.5765457
H	2.4480970	4.4523713	0.8282158
H	3.6266306	3.4378063	1.6890885
H	2.1668614	3.9800657	2.5492418
O	0.2716579	-1.2400881	1.8828360
C	0.1378646	-0.8633797	3.2771224
H	-0.3032161	0.1431047	3.2940959
H	-0.5838311	-1.5623898	3.7306465
C	1.4616349	-0.8787312	4.0247961
H	2.1599627	-0.1611022	3.5762322
H	1.9158052	-1.8788739	4.0065954
H	1.2955886	-0.5933037	5.0738942
O	2.3945093	-2.5099756	1.3849943
H	1.0703812	-1.8961169	1.7508440

BuSnOAc3_HOEt_trans
E (Hartree) = -1213.40959478
G_{298} (Hartree) = -1213.12710
Shielding = 3235.3
Calculated NMR shift = -654.4
Correlated to experiment = -587.6

44

Sn	1.3841693	-1.7482225	0.5451447
C	0.4276851	-1.7515087	2.4815368
H	-0.2313363	-2.6302424	2.4477417
H	1.2418211	-1.9511663	3.1932382
C	-0.3305856	-0.4718688	2.8207749
H	0.3591795	0.3886888	2.8046919
H	-1.0939626	-0.2692161	2.0526611
C	-1.0056928	-0.5403642	4.1991651
H	-1.6970872	-1.3994185	4.2192602
H	-0.2407641	-0.7449758	4.9670835
C	-1.7623394	0.7440490	4.5483697
H	-2.5491050	0.9528587	3.8075935
H	-2.2409877	0.6762271	5.5357377
H	-1.0836277	1.6105015	4.5640985
O	0.2077408	-2.4305281	-2.6217624
C	-0.5930095	-2.7414721	-1.6909392
C	-1.9881091	-3.1939148	-2.0491863
H	-2.0654413	-3.4051808	-3.1203693
H	-2.2580117	-4.0775293	-1.4577436
H	-2.6909821	-2.3911108	-1.7838049
O	-0.3212869	-2.6972112	-0.4361851
O	2.1026715	-3.9092458	0.7074555
O	0.3002541	0.1217862	-0.3217320
C	1.2291899	0.8728056	0.1176514
C	1.1232666	2.3691210	-0.0127203
H	0.5839400	2.6348458	-0.9286504
H	0.5439443	2.7456164	0.8432669
H	2.1152824	2.8321595	0.0098109
O	2.2447388	0.3535443	0.6987048
C	4.3571713	-4.5146068	1.3161937
C	3.2645466	-3.5140055	1.0526128
H	3.9435103	-5.4115415	1.7910492
H	4.7861913	-4.8140849	0.3487304
H	5.1489162	-4.0737967	1.9305108
O	3.5038705	-2.2604635	1.1514442
O	2.2569532	-1.8752496	-1.4141742
H	3.0725400	-1.6673106	-3.9759919
H	4.3910017	-2.3168828	-2.9669054
C	3.1391441	-0.8669064	-1.9600472
H	2.5599216	0.0436050	-2.1897036
H	3.8674994	-0.6205674	-1.1763895
C	3.8146218	-1.4132519	-3.2062954
H	4.4997469	-0.6606643	-3.6232578
H	1.3762276	-2.0917969	-2.0638275

BuSnOAc3_Kappa_1
E (Hartree) = -1058.26803698
G_{298} (Hartree) = -1058.05909
Shielding = 3093.5
Calculated NMR shift = -512.5
Correlated to experiment = -462.9

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Sn	2.4745659	-1.9156347	0.0475807
C	3.2571516	-1.9815825	2.0498727
H	4.0835550	-2.7031911	1.9884529
H	3.6713338	-0.9772321	2.2122266
C	2.2052758	-2.3693588	3.0812538
H	1.3909952	-1.6269857	3.0788473
H	1.7580976	-3.3394554	2.8128967
C	2.7987971	-2.4601873	4.4965307
H	3.6165107	-3.2002473	4.4986700
H	3.2579597	-1.4929198	4.7610628
C	1.7505719	-2.8419171	5.5451508
H	1.2981089	-3.8178917	5.3136920
H	2.1910018	-2.9053504	6.5504062
H	0.9387728	-2.0997644	5.5803226
O	1.9986317	-4.3993806	0.4322762
C	2.3867940	-4.4845682	-0.7503137
C	2.4284554	-5.7848195	-1.5093886
H	2.1999868	-6.6225812	-0.8440680
H	1.6892115	-5.7437622	-2.3215493
H	3.4153030	-5.9158623	-1.9715084
O	2.7764508	-3.4187542	-1.4064915
H	5.8053700	0.5284467	-2.2611230
O	0.3807230	-1.9199834	-0.2958553
C	0.0537186	-0.8148899	0.3225877
C	-1.4012150	-0.4296905	0.2889096
H	-1.6944501	-0.2368027	-0.7522546
H	-2.0128854	-1.2663118	0.6510198
H	-1.5749235	0.4633209	0.8962854
O	0.9249220	-0.1287971	0.9008715
O	2.7498315	-0.4332359	-1.4610731
O	4.6898125	-1.1714967	-0.6851766
C	4.0527176	-0.4294019	-1.4721165
C	4.7318689	0.4739229	-2.4644693
H	4.5695766	0.0680738	-3.4731091
H	4.2781443	1.4722910	-2.4344592

BuSnOAc3_muEtOH2_dimer
E (Hartree) = -2426.83033253
G_{298} (Hartree) = -2426.23207
Shielding = 3162.2, 3132.3
Calculated NMR shift = -581.2, -551.3
Correlated to experiment = -523.3, -497.0

88

Sn	-1.4068814	0.9202007	-0.3777069
C	-3.5103692	0.8328393	-0.8600754
H	-3.9384834	0.1835161	-0.0820688
H	-3.5508105	0.3084661	-1.8245149
C	-4.1985133	2.1920235	-0.8963502
H	-3.7428291	2.8245480	-1.6747387
H	-4.0325373	2.7091433	0.0604860
C	-5.7071989	2.0681890	-1.1564715
H	-5.8733090	1.5362034	-2.1090750
H	-6.1572797	1.4381702	-0.3705291
C	-6.4088601	3.4287242	-1.1927856
H	-6.2791297	3.9627522	-0.2394891
H	-7.4880855	3.3241608	-1.3758042
H	-5.9933072	4.0661965	-1.9880322
O	0.3859982	-0.7266979	-3.0561233
C	-0.4245029	0.2072915	-3.4522172
O	-1.0575896	0.9873733	-2.7060007
C	-0.5726703	0.3326464	-4.9520453
H	-0.9584514	-0.6125477	-5.3595432
H	0.4134630	0.5071694	-5.4034764
H	-1.2520501	1.1517581	-5.2050442
O	-1.2078907	3.0175123	-0.3507421
C	-0.6765540	3.5758538	0.7147473
O	0.2199491	3.0420004	1.3818779
C	-1.2681110	4.9171508	1.0727089
H	-2.1845891	4.7108123	1.6460499
H	-1.5494582	5.4797035	0.1748720
H	-0.5759243	5.4907494	1.6980930
Sn	0.9567988	-1.4016236	-0.9620174
C	1.4033092	-2.1804160	0.9981431
H	0.5442017	-1.8317364	1.5911055
H	1.3919255	-3.2756138	0.9253653
C	2.7218503	-1.6374804	1.5423998
H	2.7338560	-0.5382069	1.4977208
H	3.5612732	-2.0052179	0.9304815
C	2.9436682	-2.0534526	3.0048270
H	2.1164488	-1.6506704	3.6127159
H	2.8889592	-3.1525102	3.0881675
C	4.2784112	-1.5442875	3.5539810
H	4.3176237	-0.4476370	3.4910004
H	5.1236178	-1.9531442	2.9792184
H	4.4181362	-1.8372056	4.6051949
O	0.7316768	2.4061795	3.8764544
O	0.5676852	-3.3728824	-1.9991540
C	1.0738526	-3.7188698	-3.0930587
O	1.2924544	-2.8900074	-4.0867685
C	1.4977826	-5.1316257	-3.3204761
H	0.8211259	-5.8156640	-2.7970342
H	2.4948365	-5.2202380	-2.8609744
H	1.5647588	-5.3698797	-4.3866519
C	1.7794143	1.5710199	3.9716573
O	2.5761246	1.3584381	3.0711724
C	1.8437615	0.9098623	5.3303522
H	1.7355510	1.6556365	6.1286759
H	2.7870571	0.3659688	5.4368852
H	1.0044496	0.2053467	5.4252497
O	-1.1428854	-1.2465074	-0.8023862
O	0.7143540	0.6460326	-0.5188041
H	0.9634319	-1.9482181	-3.8192976
C	-1.9259198	-2.2622351	-0.1482466
H	-2.4806299	-1.8009847	0.6853680
H	-1.2532668	-3.0137918	0.2986307
C	-2.8641894	-2.9198968	-1.1471554
H	-2.2864895	-3.3823210	-1.9589645
H	-3.5468275	-2.1767714	-1.5815799
H	-3.4664874	-3.6990385	-0.6563648
C	1.5868282	1.6613052	-1.1026319
H	1.8177616	1.3691136	-2.1392690
H	1.0168604	2.5973921	-1.1287384
C	2.8443890	1.8140419	-0.2729487
H	3.4468892	2.6434519	-0.6743683
H	3.4541697	0.9012952	-0.3160183
H	2.5897013	2.0274772	0.7718064
H	0.6317622	2.7354907	2.9243325
O	3.4987364	-3.1875801	-1.5610760
C	3.7215192	-2.0189770	-1.8790299
O	2.8089308	-1.0572730	-1.8879628
C	5.0904843	-1.5230555	-2.2985684
H	5.7907615	-2.3607605	-2.3733962
H	5.4518569	-0.8016876	-1.5517971
H	5.0231038	-0.9914281	-3.2567602
O	-2.7284135	1.8643985	2.0752027
C	-2.0049832	0.9318574	2.4404764
O	-1.2044546	0.2725235	1.6217629
C	-1.9496536	0.4685618	3.8797131
H	-1.2422444	1.1265476	4.4044328
H	-1.5951033	-0.5654697	3.9591997
H	-2.9366269	0.5805163	4.3428054

References

1 V. Chandrasekhar, C. G. Schmid, S. D. Burton, J. M. Holmes, R. O. Day, R. R. Holmes, *Inorg. Chem.*, 1987, **26**, 1050–1056.

2 H. H. Anderson, *Inorg. Chem.*, 1964, **3**, 912–914.

3 J. D. Kennedy, W. Mcfarlane, P. J. Smith, F. Raymond, L. Smith, *J. Chem. Soc. Perkin Trans. 2*, 1973, 1785–1788.

4 R. R. Holmes, C. G. Schmid, V. Chandrasekhar, R. O. Day, J. M. Holmes, *J. Am. Chem. Soc.*, 1987, **109**, 1408–1414.

5 TURBOMOLE Version 7.3.1 (TURBOMOLE Gmbh, Karlsruhe, Germany).

6 R. Baer, M. Haeser, M. Horn, H. Koelmel, C. *Chem. Phys. Lett.* 1989, **162**, 165–169.

7 PQS version 2.4, 2001, Parallel Quantum Solutions, Fayetteville, Arkansas, USA (the Baker optimizer is available separately from PQS upon request).

8 J. Baker, *J. Comput. Chem.* 1986, **7**, 385–395.

9 P. H. M. Budzelaar, *J. Comput. Chem.* 2007, **28**, 2226–2236.

10 A. D. Becke*, Phys. Rev. A*. 1988, **38**, 3098–3110.

11 J. P. Perdew, *Phys. Rev. B.* 1986, **33**, 8822–8824.

12 J. P. Perdew, *Phys. Rev. B.* 1986, **34**, 7406–7406.

13 F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297−3305.

14 F. Weigend, M. Haser, H. Patzelt, R. Ahlrichs, *Phys. Lett.* 1998, **294**, 143−152.

15 S. Grimme, J. Antony, S. Ehrlich, J. Krieg, *J. Chem. Phys.* 2010, **132**, 154104−154119.

16 B. Kamenar, M. Bruvo, Izv. Jug. Cent. Krist., Ser. A 1967, **2**, 60 / CCDC 1100657

17 Y. Zhao, D. G. Truhlar*, Theor. Chem. Acc.* 2008, **120**, 215−241.

18 Y. Zhao, D.G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157−167.

19 U. Ekstrom, L. Visscher, R. Bast, A.J. Thorvaldsen, K.J. Ruud, *Chem. Theor. Comp.* 2010, **6**, 1971–1980.

20 C. Müller, D. M. Andrada, I. Bischoff, M. Zimmer, V. Huch, N. Steinbrück, A. Schäfer, *Organometallics*, 2019, **38**, 1052−1061.

21 M. Haser, R. Ahlrichs, H.P. Baron, P. Weis, H. Horn, *Theoret. Chim. Acta*, 1992, **83**, 455–470.

22 A.D. Becke, *J. Chem. Phys*. 1993, **98**, 5648–5652.

23 C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.

24 S.H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* 1980, **58**, 1200–1211.

25 P.J. Stephens, F.J. Devlin, C.F. Chabalowski, M.J. Frisch, *Phys. Chem.* 1994, **98**, 11623–11627.