Supplementary Information for

The Structures of Ring-Expanded NHC supported Copper(I) Triphenylstannyls and Their Phenyl Transfer Reactivity Towards Heterocumulenes.

Rex S. C. Charman,[a] Mary F. Mahon[a], John P. Lowe, and David J. Liptrot[a,]*

[a]*Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY UK.*

Experimental

General Considerations and Starting Materials

All reactions dealing with air- and moisture-sensitive compounds were carried out under argon atmosphere using standard Schlenk line and glovebox techniques. NMR experiments using air sensitive compounds were conducted in J. Young's tap NMR tubes prepared and sealed in a glovebox under argon. Toluene and hexane were purified using an MBraun Solvent Purification System and stored over 4Å molecular sieves. C_6D_6 and d_8-toluene were dried over a potassium mirror prior to vacuum transfer into a sealed ampoule and stored in a glove box under argon. All NMR data, unless otherwise stated, were acquired at 298 K on an Agilent ProPulse or Bruker Avance II+ instrument for ^1H (500 MHz), $^{13}C\{^1H\}$ (126 MHz) and ^{119}Sn (186 MHz). ^1H and ^{13}C NMR spectra were referenced using residual solvent resonances. Mass spectrometry was performed using a Bruker MicrOTOF Electrospray Time-Of-Flight Mass Spectrometer coupled to an Agilent High Performance Liquid Chromatography unit. (6-Mes)CuO^{t}Bu, (6-Dipp)CuO^{t}Bu, and (7-Dipp)CuO^{t}Bu were prepared according to literature procedures.[1]

Synthesis of compound 1, (6-Mes)CuSnPh$_3$

A solution of Ph_3SnH (168 µL, 0.66 mmol) in toluene (10 mL) was added to a stirring suspension of (6-Mes)CuO^{t}Bu (300 mg, 0.66 mmol) in toluene (30 mL) forming a yellow solution. The reaction mixture was left stirring for 1 hour before volatiles were removed *in vacuo* leaving a yellow powder of **1**. Yield 0.403 g (84 %). Single crystals were grown in the glovebox from a saturated solution of **1** in toluene with slow hexane-diffusion.

^1H NMR (500 MHz, C_6D_6) δ 7.66 – 7.58 (m, 6H, SnArH_{meta}), 7.28 – 7.17 (m, 3H, SnArH_{para}), 6.75 (s, 4H, *meta-H*), 2.45 (t, *J* = 5.9 Hz, 4H, NCH_2), 2.17 (s, 6H, *para*-CH_3), 2.06 (s, 12H, *ortho*-CH_3), 1.29 (p, *J* = 5.8 Hz, 2H, NCH2CH_2). ^{13}C NMR (126 MHz, C_6D_6) δ 201.4 (CuC_{ipso}), 151.6 (SnArC_{ipso}), 141.7 (Ar-*C*), 138.7 (Ar-*C*), 138.3 (Ar-*C*), 134.9 (Ar-*C*), 130.0 (Ar-*C*), 127.6 (Ar-*C*), 126.4 (Ar-*C*), 43.4 (NCH_2), 21.1 (*para*-CH_3), 20.5 (NCH_2CH_2), 18.2 (*ortho*-CH_3). ^{119}Sn NMR (186 MHz, C_6D_6) δ -79.1. MS (ESI) Expected: 734.17, found: 729.1762 $[M]^-$ (err [ppm] = -1.86). Analysis calculated for $C_{40}H_{43}CuN_2Sn$ (MW = 734.05 g/mol): Expected: C, 65.45; H, 5.9; N, 3.82 %. Found: C, 62.58; H, 5.61; N, 3.65 %. Despite repeated attempts, we were unable to obtain satisfactory elemental analysis for this compound. This is most likely due to the compound's high sensitivity towards air and moisture and the presence of residual elemental tin.

Synthesis of compound 2, (6-Dipp)CuSnPh$_3$

A solution of Ph_3SnH (142 µL, 0.55 mmol) in toluene (10 mL) was added to a stirring suspension of (6-Dipp)CuO^{t}Bu (300 mg, 0.55 mmol) in toluene (30 mL) forming a yellow solution. The reaction mixture was left stirring for 1 hour before volatiles were removed *in vacuo* leaving a yellow powder of **2**. Yield 0.357 g (79 %). Single crystals were grown in a saturated solution of **2** in toluene at -18 °C.

^1H NMR (500 MHz, C_6D_6) δ 7.57 – 7.47 (m, 6H, SnArH_{meta}), 7.26 – 7.17 (m, 11H, SnArH_{ortho}, SnArH_{para}, *para-H*), 7.06 (d, *J* = 7.8 Hz, 4H, *meta-H*), 2.94 (hept, *J* = 6.8 Hz, 4H, C*H*(CH_3)$_2$), 2.65 (t, *J* = 5.7 Hz, 4H, NCH_2), 1.42 (p, *J* = 5.6 Hz, 2H, NCH_2CH_2), 1.30 (d, *J* = 6.8 Hz, 12H, CH(CH_3)$_2$), 1.13 (d, *J* = 6.9 Hz, 12H,

$CH(CH_3)_2$). ^{13}C NMR (126 MHz, C_6D_6) δ 201.3 (CuC_{ipso}), 151.2 (SnArC_{ipso}), 145.9 (Ar-*C*), 141.1 (Ar-*C*), 138.7 (Ar-*C*), 137.9 (Ar-*C*), 129.6 (Ar-*C*), 129.2 (Ar-*C*), 127.5 (Ar-*C*), 126.3 (Ar-*C*), 124.9 (Ar-*C*), 45.8 (NCH_2), 28.9 ($CH(CH_3)_2$), 25.4 ($CH(CH_3)_2$) , 24.6 ($CH(CH_3)_2$), 20.2 (NCH_2CH_2). ^{119}Sn NMR (186 MHz, C_6D_6) δ -83.1. MS (ESI) Expected: 818.27, found: 819.2915 $[M+H]^+$ (err [ppm] = -3.28). Analysis calculated for $C_{46}H_{55}CuN_2Sn$ (MW = 818.22 g/mol): Expected: C, 67.55; H, 6.78; N, 3.42 %. Found: C, 66.33; H, 6.66; N, 3.40 %. Despite repeated attempts, we were unable to obtain satisfactory elemental analysis for this compound. This is most likely due to the compound's high sensitivity towards air and moisture and the presence of residual elemental tin.

Synthesis of compound 3, (7-Dipp)CuSnPh$_3$

A solution of Ph_3SnH (92 µL, 0.36 mmol) in toluene (10 mL) was added to a stirring suspension of (7-Dipp)CuO^{t}Bu (200 mg, 0.36 mmol) in toluene (30 mL) forming a yellow solution. The reaction mixture was left stirring for 1 hour before volatiles were removed *in vacuo* leaving a beige powder of **3**. Yield 0.231 g (77 %). Single crystals were grown in a saturated solution of **3** in toluene at -18 °C.

^1H NMR (500 MHz, C_6D_6) δ 7.58 – 7.45 (m, 6H, SnArH_{meta}), 7.26 – 7.20 (m, 9H, SnArH_{ortho}, SnArH_{para}), 7.11 – 7.07 (m, 2H, *para-H*), 7.05 (d, *J* = 7.7 Hz, 4H, *meta-H*), 3.25 – 3.19 (m, 4H, NCH_2), 3.13 (hept, *J* = 6.9 Hz, 4H, $CH(CH_3)_2$), 1.62 – 1.57 (m, 4H, NCH_2CH_2), 1.30 (d, *J* = 6.9 Hz, 12H, $CH(CH_3)_2$), 1.14 (d, *J* = 6.9 Hz, 12H, $CH(CH_3)_2$). ^{13}C NMR (126 MHz, C_6D_6) δ 213.3 (CuC_{ipso}), 150.8 (SnArC_{ipso}), 144.8 (Ar-*C*), 143.3 (Ar-*C*), 138.4 (Ar-*C*), 137.5 (Ar-*C*), 128.9 (Ar-*C*), 128.8 (Ar-*C*), 127.0 (Ar-*C*), 125.9 (Ar-*C*), 124.7 (Ar-*C*), 53.2 (NCH_2), 28.6 ($CH(CH_3)_2$), 24.9 ($CH(CH_3)_2$), 24.8 (NCH_2CH_2), 24.3 ($CH(CH_3)_2$). ^{119}Sn NMR (186 MHz, C_6D_6) δ -85.4. MS (ESI) Expected: 832.28, found: 877.2804 $[M+HCOO]^-$ (err [ppm] = -2.90). Due to the failed attempts to obtain satisfactory elemental analysis for compounds **1** and **2**, elemental analysis for compound **3** was not attempted.

Reaction of 1 and di-*p*-tolylcarbodiimide

In a vial in a glovebox, a solution of di-*p*-tolylcarbodiimide (3.3 mg, 15 µmol) in C_6D_6 (0.5 mL) was added to **1** (11 mg, 15 µmol) forming a pale yellow solution. The reaction mixture was transferred to J. Young's tap NMR tube and ^1H and ^{119}Sn NMR was taken after 30 minutes. An aliquot of the reaction was then taken and diluted in acetonitrile (1 mL) for investigation by mass spectrometry. The reaction was repeated and immediately quenched in wet acetonitrile (1 mL) for investigation by mass spectrometry.

^1H NMR (500 MHz, C_6D_6) δ 7.05-7.03 (m, 5H, Ar-H), 6.76 (s, 4H, *meta*-$C\underline{H}_3$), 6.61 (s, 8H, Ar-H), 2.51 (t, J = 5.9 Hz, 4H, $NC\underline{H}_2$), 2.44 (t, J = 5.9 Hz,* = *ca.* 38 % contaminated with compound **1**), 2.18 (s, 12H, *ortho*-$C\underline{H}_3$), 2.11 (s, 6H, *para*-$C\underline{H}_3$), 2.06 (s, 6H, *para*-$C\underline{H}_3$), 1.33 (p, *J* = 5.7 Hz, 2H, $NCH_2C\underline{H}_2$). MS (ESI) Expected for HN(p-Tol)C(=N-p-Tol)Ph: 300.16, found: 301.1703 $[M+H]^+$ (err [ppm] = 1.09).

After immediate quenching in wet acetonitrile: MS (ESI) Expected for HN(p-Tol)C(=N-p-Tol)SnPh$_3$: 574.14, found: 575.1494 $[M+H]^+$ (err [ppm] = -3.07).

Reaction of 10 mol% of 1 with Ph_3SnH and di-*p*-tolylcarbodiimide

In a vial in a glovebox, a solution of di-*p*-tolylcarbodiimide (15 mg, 68 µmol) in C_6D_6 (0.5 mL) was added to **1** (5 mg, 6.8 µmol) forming a pale yellow solution. Ph_3SnH (17 µL, 68 µmol) was then immediately added forming a brown solution. The reaction mixture was transferred to J. Young's tap NMR tube and ^1H and ^{119}Sn NMR was taken after 30 minutes.

Reaction of 10 mol% (6-Mes)CuO^{t}Bu and Ph_3SnH

In a J. Young's tap NMR tube vial in a glovebox, Ph_3SnH (110 µL, 440 µmol) was added to a solution of (6-Mes)CuO^{t}Bu (20 mg, 44 µmol) in C_6D_6 (0.5 mL). Immediate bubbling was observed with concomitant formation of a cream precipitate. ^1H and ^{119}Sn NMR was taken after 30 minutes.

Reaction of 1 and PhNCO

In a vial in a glovebox, a solution of PhNCO (2.7 µL, 25 µmol) in C_6D_6 (0.5 mL) was added to **1** (18 mg, 25 µmol) forming a pale yellow solution. The reaction mixture was transferred to J. Young's tap NMR tube and ^1H and ^{119}Sn NMR was taken after 30 minutes. An aliquot of the reaction was then taken and diluted in acetonitrile (1 mL) for investigation by mass spectrometry. The reaction was repeated and immediately quenched in wet acetonitrile (1 mL) for investigation by mass spectrometry.

^1H NMR (500 MHz, C_6D_6) δ 7.18 – 7.07 (m, 16H, Ar-H with solvent peak included), 6.75 (s, 4H, *meta*-$C\underline{H}_3$), 2.29 (t, J = 5.8 Hz, 4H, $NC\underline{H}_2$), 2.09 (s, 6H, *para*-$C\underline{H}_3$), 1.80 (s, 12H, *ortho*-$C\underline{H}_3$), 1.13 (p, J = 6.1 Hz, 2H, $NCH_2C\underline{H}_2$). MS (ESI) Expected for PhN(H)C(O)Ph: 197.08, found: 198.0914 $[M+H]^+$ (err [ppm] = 0.49).

After immediate quenching in wet acetonitrile: MS (ESI) Expected for $PhN(H)C(O)SnPh_3$: 471.06, found: 494.0531 $[M+Na]^+$ (err [ppm] = 0.76).

Reaction of $IPrCuSnPh_3$ and PhNCO

In a vial in a glovebox, a solution of PhNCO (2.7 µL, 25 µmol) in C_6D_6 (0.5 mL) was added to $IPrCuSnPh_3$ (20 mg, 25 µmol) forming a pale yellow solution. The reaction mixture was transferred to J. Young's tap NMR tube and ^1H and ^{119}Sn NMR was taken after overnight. An aliquot of the reaction was diluted in acetonitrile (1 mL) and investigated by mass spectrometry.

^1H NMR (500 MHz, C_6D_6) δ 7.28 – 7.24 (m, 11H, Ar-$\underline{H}$), 7.08-7.06 (m, *J* = 7.8 Hz, 6H, *para*-$\underline{H}$), 6.26 (s, 2H, $NC\underline{H}_2$), 2.53 (hept, *J* = 7.0 Hz, 6H, $C\underline{H}(CH_3)_2$), 1.29 (d, *J* = 6.9 Hz, 3H, *ca.* 28 % contaminated with $IPrCuSnPh_3$), 1.22 (d, *J* = 6.9 Hz, 12H, $CH(C\underline{H}_3)_2$), 1.04 (d, *J* = 6.9 Hz, 13H, $CH(C\underline{H}_3)_2$). MS (ESI) Expected for PhN(H)C(O)Ph: 197.08, found: 198.0914 $[M+H]^+$ (err [ppm] = 0.47).

Reaction of 10 mol% of 1 with Ph_3SnH and PhNCO

In a vial in a glovebox, a PhNCO (7.4 µL, 68 µmol) was added to a solution of **1** (5 mg, 6.8 mmol) in C_6D_6 forming a pale yellow solution. Ph_3SnH (17.5 µL, 68 µmol) was then immediately added with no change in appearance. The reaction mixture was transferred to J. Young's tap NMR tube and heated overnight at 40 °C forming a colourless solution. ^{1}H and ^{119}Sn NMR was taken and an aliquot of the reaction was diluted in acetonitrile (1 mL) for investigation by mass spectrometry.

MS (ESI) Expected for $(PhNCO)_3$: 357.11, found: 358.1188 $[M+H]^+$ (err [ppm] = 0.29).

Reaction of 1 and PhNCS

In a vial in a glovebox, a solution of PhNCS (2.9 µL, 25 µmol) in C_6D_6 (0.5 mL) was added to **1** (18 mg, 25 µmol) forming a yellow solution. The reaction mixture was transferred to J. Young's tap NMR tube and monitored by ^{1}H and ^{119}Sn NMR spectroscopy after 30 minutes and overnight. An orange solution had formed overnight. Aliquots of the reaction were taken after 30 minutes and overnight. Each aliquot was diluted in acetonitrile (1 mL) for investigation by mass spectrometry.

^{1}H NMR (500 MHz, C_6D_6) δ 7.14 (s, 10H, Ar-$\underline{H}$), 6.80 (s, 4H, *meta*-$\underline{H}$), 2.60 (t, *J* = 5.9 Hz, 4H, $NC\underline{H}_2$), 2.31 (s, 12H, *ortho*-$C\underline{H}_3$), 2.17 (s, 6H, *para*-$C\underline{H}_3$), 1.45 (p, *J* = 5.7 Hz, 2H, $NCH_2C\underline{H}_2$). MS (ESI) Expected for PhN(H)C(S)Ph: 213.06, found: 212.0541 $[M-H]^-$ (err [ppm] = 0.48).

After 30 minutes: MS (ESI) Expected for $PhN(H)C(S)SnPh_3$: 487.04, found: 488.0491 $[M+H]^+$ (err [ppm] = 4.25).

VT-NMR study of reaction of 1 and di-*p*-tolylcarbodiimide

In a vial in a glovebox, a solution of di-*p*-tolylcarbodiimide (9.7 mg, 44 µmol) in d_8-toluene (0.5 mL) was added to **1** (32 mg, 44 µmol) forming a pale yellow solution. The solution was immediately frozen in liquid nitrogen and allowed to thaw in the NMR spectrometer at -50 °C. ^{1}H and ^{119}Sn NMR were taken after 15, 30, and 45 minutes.

VT-NMR study of reaction of 1 and PhNCO

In a vial in a glovebox, PhNCO (4.7 µL, 44 µmol) was added to **1** (32 mg, 44 µmol) in d_8-toluene (0.5 mL) forming a pale yellow solution. The solution was immediately frozen in liquid nitrogen and allowed to thaw in the NMR spectrometer at -50 °C and was heated to -25, 0, and 25 °C. The reaction was monitored by ^{119}Sn NMR at each temperature interval.

X-ray crystallography

The crystals were kept at 150.00(10) K during data collection. Compounds **1** and **2** (CCDC numbers:) were collected with a New Xcalibur EosS2 diffractometer with Mo source (λ = 0.71073). Compound **3** (CCDC numbers:) was collected on RIGAKU SuperNova with Cu source (λ = 1.54184). Using Olex2,[2] the structures were solved with the SHELXT[3] and refined with the ShelXL[3] refinement package using Least Squares minimisation.

Table S1. Crystal data and structure refinement details

Identification code	(**1**)	(**2**)	**(3)**
Empirical formula	$C_{40}H_{43}CuN_2Sn$	$C_{46}H_{55}CuN_2Sn$	$C_{47}H_{57}CuN_2Sn$
Formula weight	733.99	818.15	832.17
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/n$	$P2_12_12_1$	$P2_12_12_1$
a/ Å	9.1870(2)	11.9889(3)	12.30344(5)
b/ Å	20.1121(4)	17.2083(4)	16.99760(6)
c/ Å	19.8588(5)	20.1914(4)	20.11837(7)
α/ °	90	90	90
β/ °	101.834(2)	90	90
γ/ °	90	90	90
Volume/ Å^3	3591.32(14)	4165.66(16)	4207.33(3)
Z	4	4	4
ρ_{calc}/ g cm^{-3}	1.358	1.305	1.314
μ/ mm^{-1}	1.316	1.142	5.579
F(000)	1504.0	1696.0	1728.0
Crystal size/ mm^3	0.469 × 0.39 × 0.17	0.324 × 0.307 × 0.117	0.374 × 0.187 × 0.157
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2θ range for data collection/°	5.83 to 58.256	5.782 to 60.782	8.424 to 145.948
Index ranges	$-12 \le h \le 12$, $-27 \le k \le 26$, $-26 \le l \le 26$	$-17 \le h \le 15$, $-24 \le k \le 23$, $-28 \le l \le 26$	$-15 \le h \le 14$, $-21 \le k \le 20$, $-18 \le l \le 24$
Reflections collected	36134	41049	59896
Independent reflections, R_{int}	9300, 0.0298	11265, 0.0291	8355, 0.0222
Data/restraints/*para*meters	9300/0/403	11265/0/459	8355/0/468
Goodness−of−fit on F^2	1.147	1.061	1.086
Final R1, wR2 indexes [I>=2σ (I)]	0.0416, 0.0840	0.0293, 0.0646	0.0177, 0.0461
Final R1, wR2 indexes [all data]	0.0573, 0.0895	0.0368, 0.0679	0.0178, 0.0461
Largest diff. peak/hole / e Å^{-3}	0.92/−0.73	0.66/−0.41	0.42/−0.35
Flack parameter	−	−0.009(5)	−0.0103(10)

In situ reaction monitoring by NMR spectroscopy

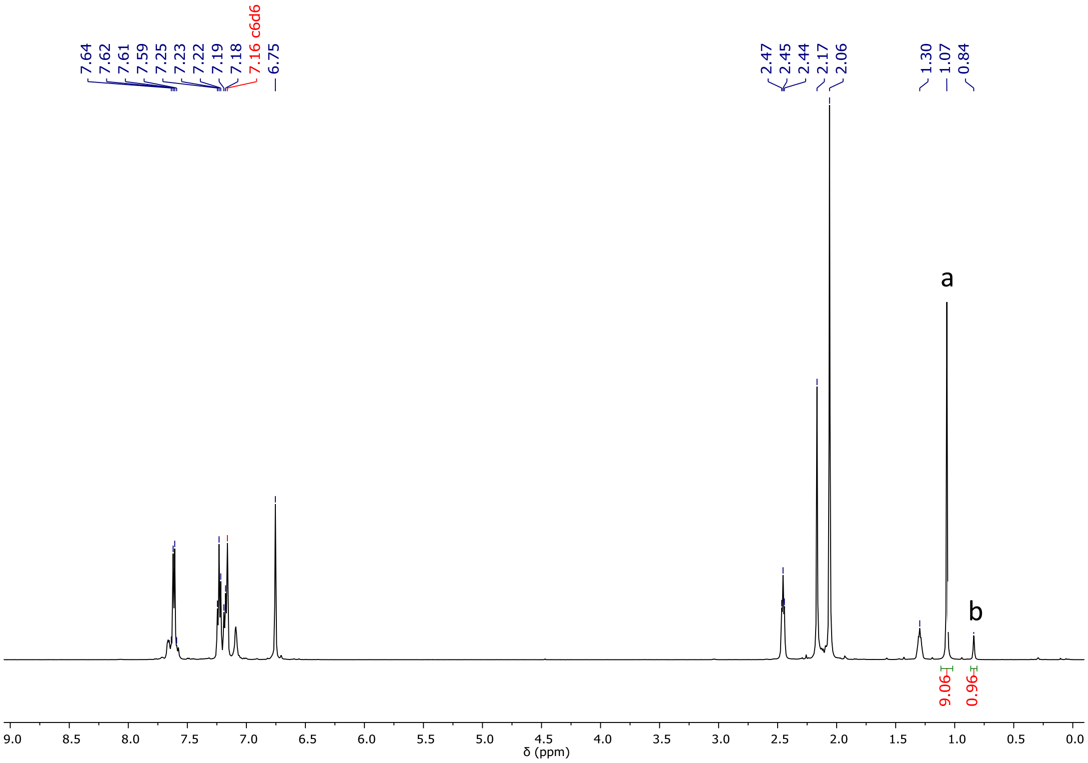

Figure S1. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between (6-Mes)CuO^{t}Bu and Ph$_3$SnH after 30 minutes. **a**, HO$^t\underline{\text{Bu}}$; **b**, $\underline{\text{H}}$O^{t}Bu

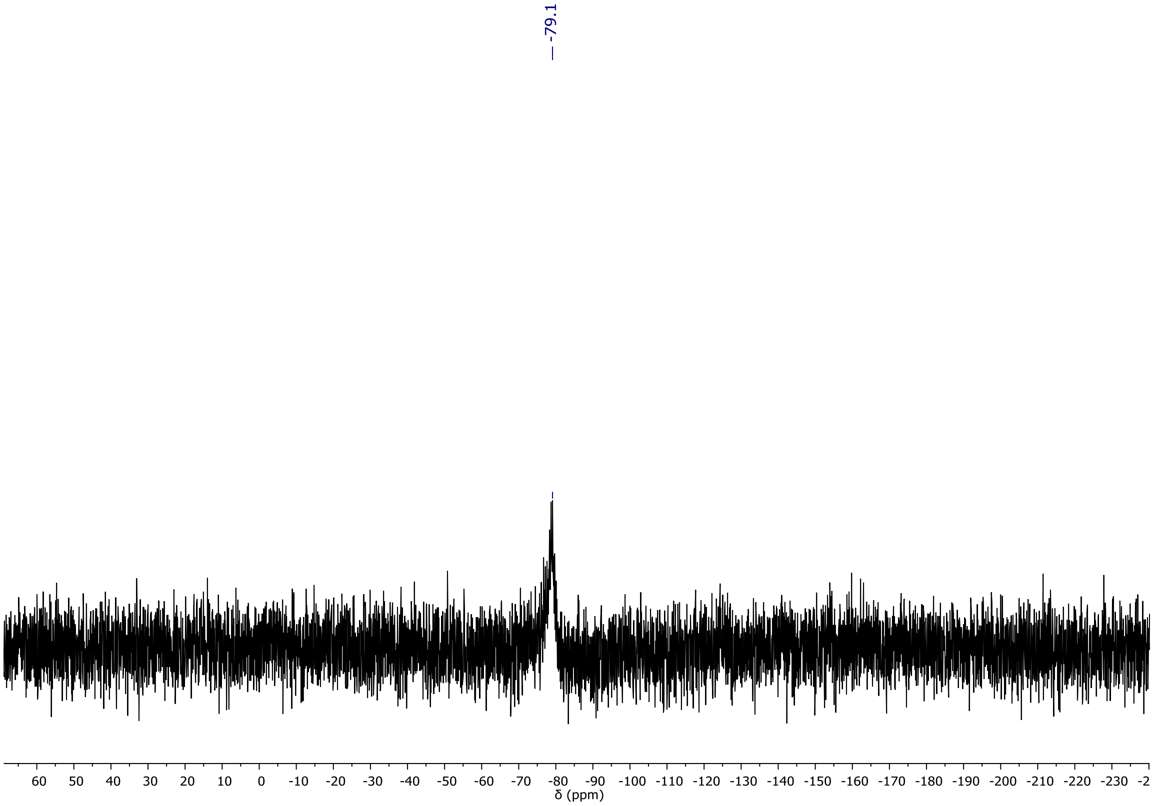

Figure S2. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between (6-Mes)CuO^{t}Bu and Ph$_3$SnH after 30 minutes.

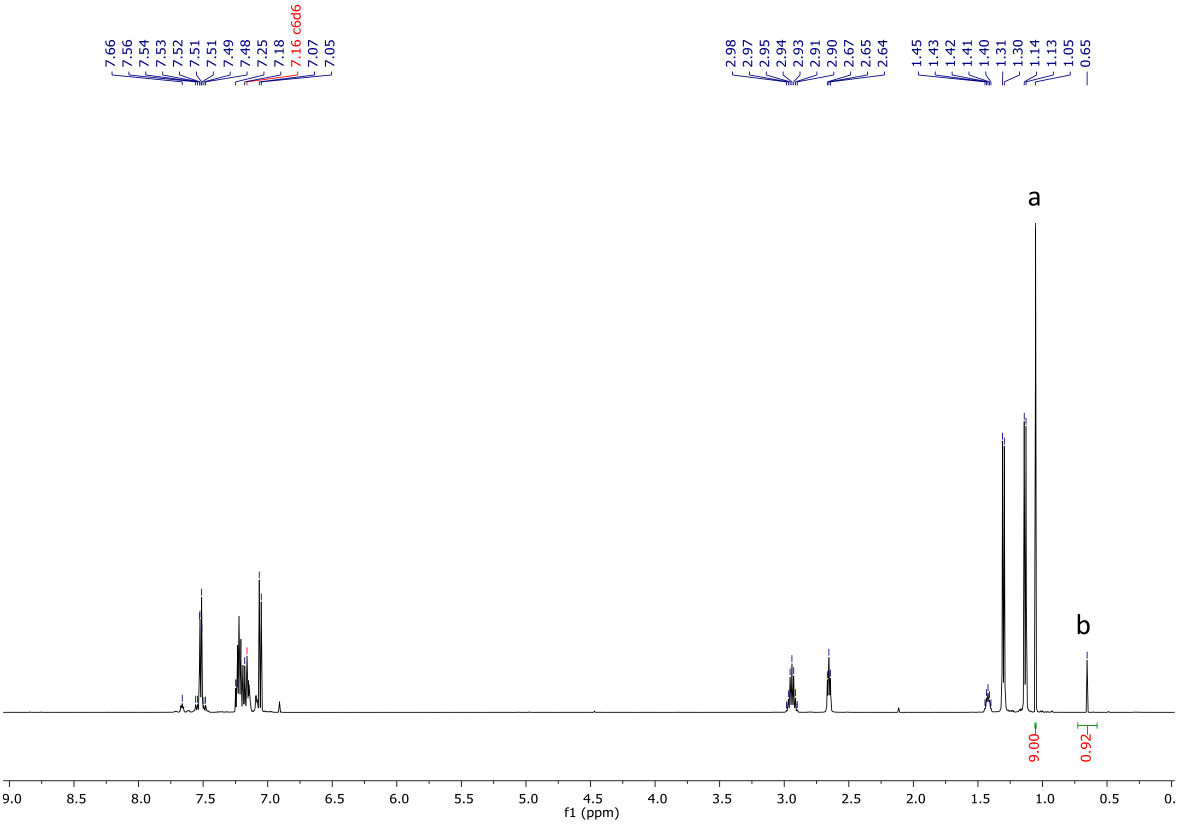

Figure S3. The ^1H NMR spectrum (500 MHz, C_6D_6) of the reaction between (6-Dipp)CuO^{t}Bu and Ph_3SnH after 30 minutes. **a**, HO^t<u>Bu</u>; **b**, <u>H</u>O^{t}Bu

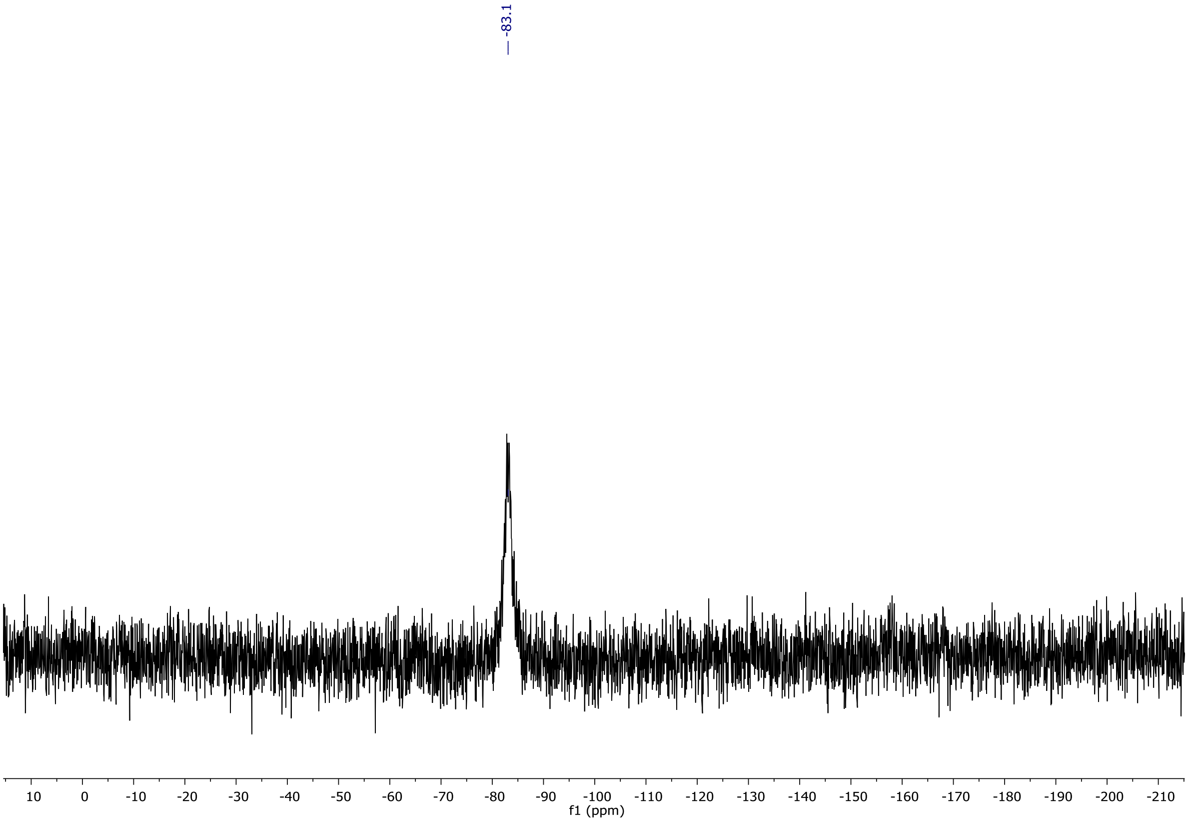

Figure S4. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between (6-Dipp)CuO^{t}Bu and Ph_3SnH after 30 minutes.

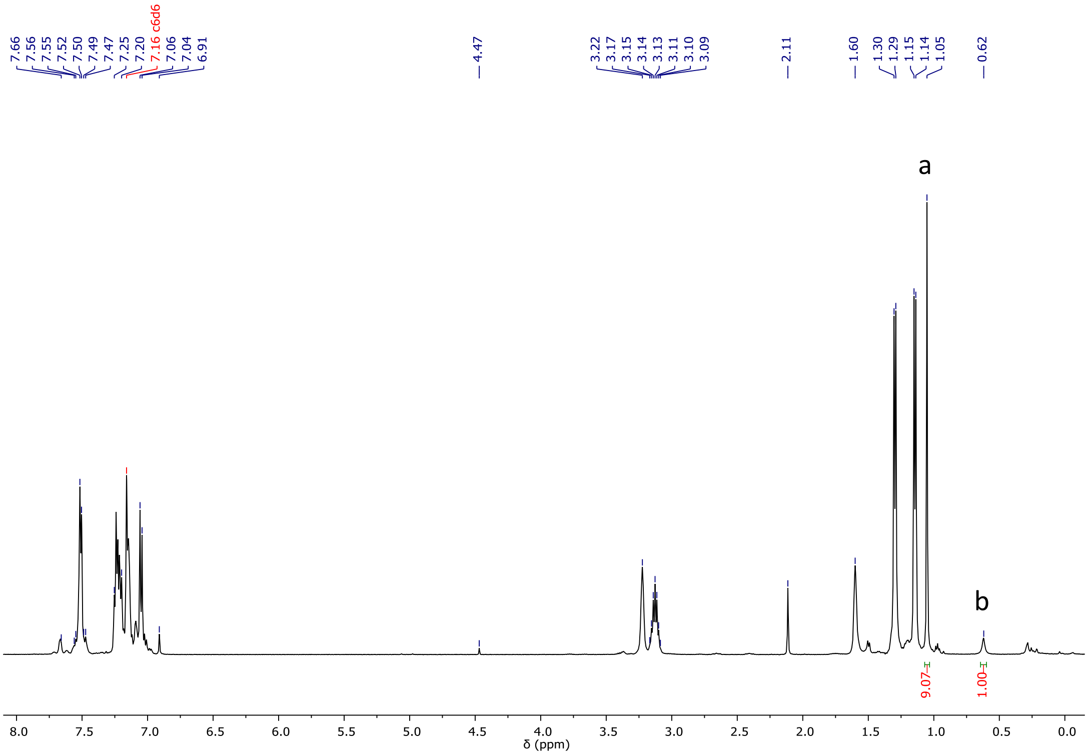

Figure S5. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between (7-Dipp)CuO^{t}Bu and Ph_3SnH after 30 minutes. **a**, HO^{t}<u>Bu</u>; **b**, <u>H</u>O^{t}Bu

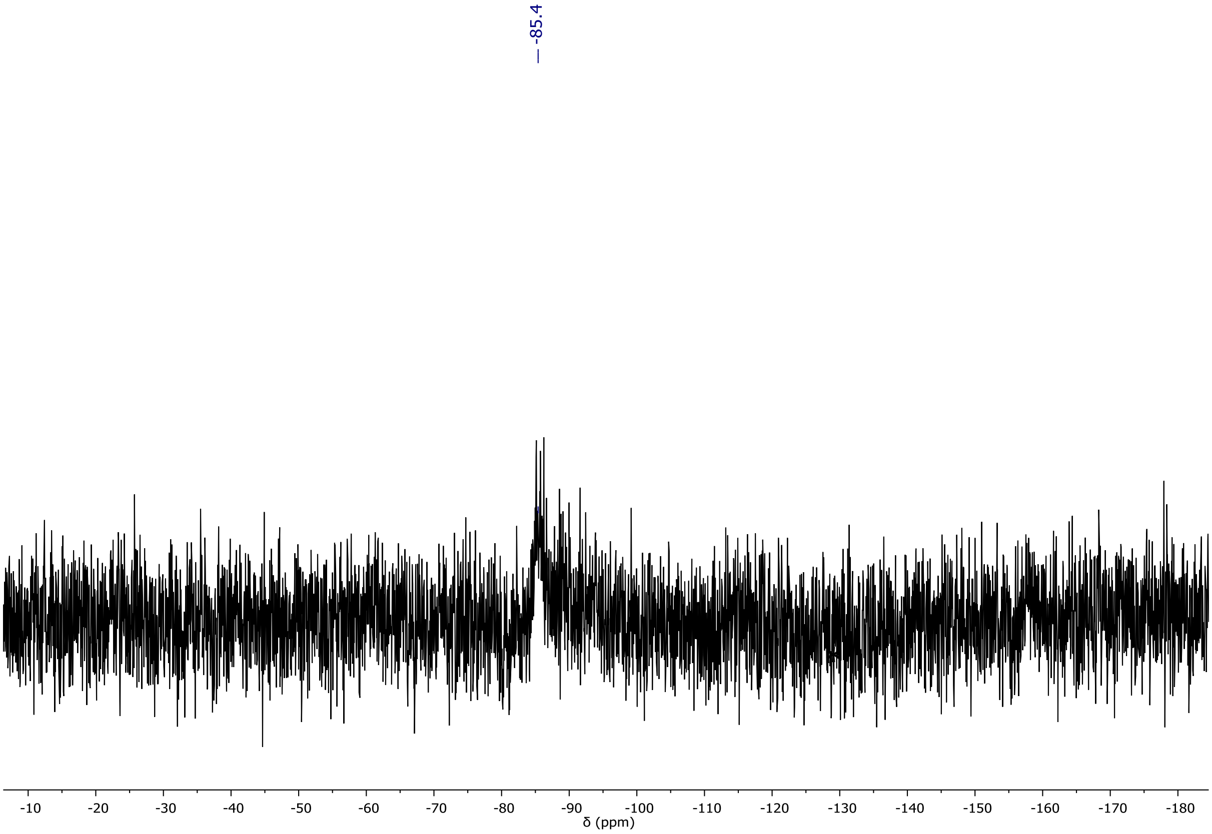

Figure S6. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between (7-Dipp)CuO^{t}Bu and Ph_3SnH after 30 minutes.

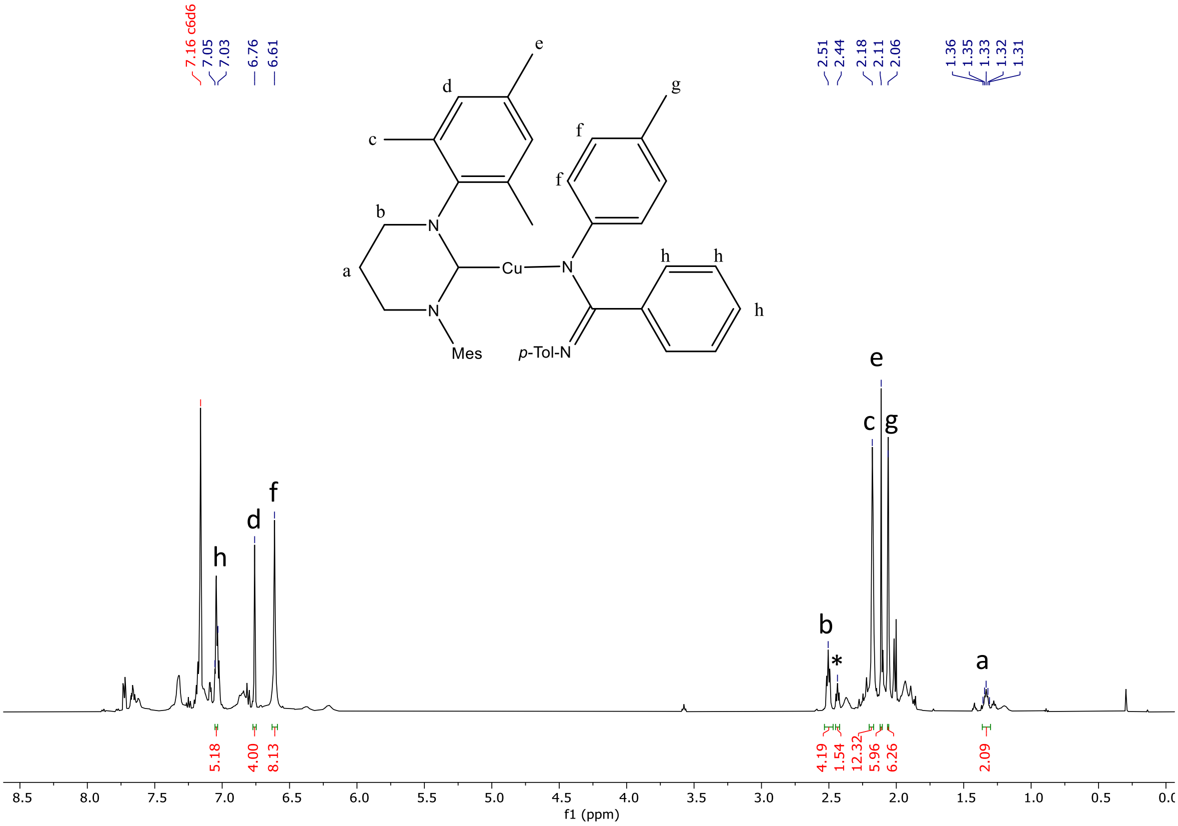

Figure S7. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between **1** and di-*p*-tolylcarbodiimide after 30 minutes. **a**, $NCH_2C\underline{H}_2$; **b**, $NC\underline{H}_2$; **c**, *ortho*-$C\underline{H}_3$; **d**, *meta*-$C\underline{H}_3$; **e**, *para*-$C\underline{H}_3$, **f**, Ar-H; **g**, *para*-$C\underline{H}_3$; **h**, Ar-H; * = *ca.* 38 % contaminated with compound **1**.

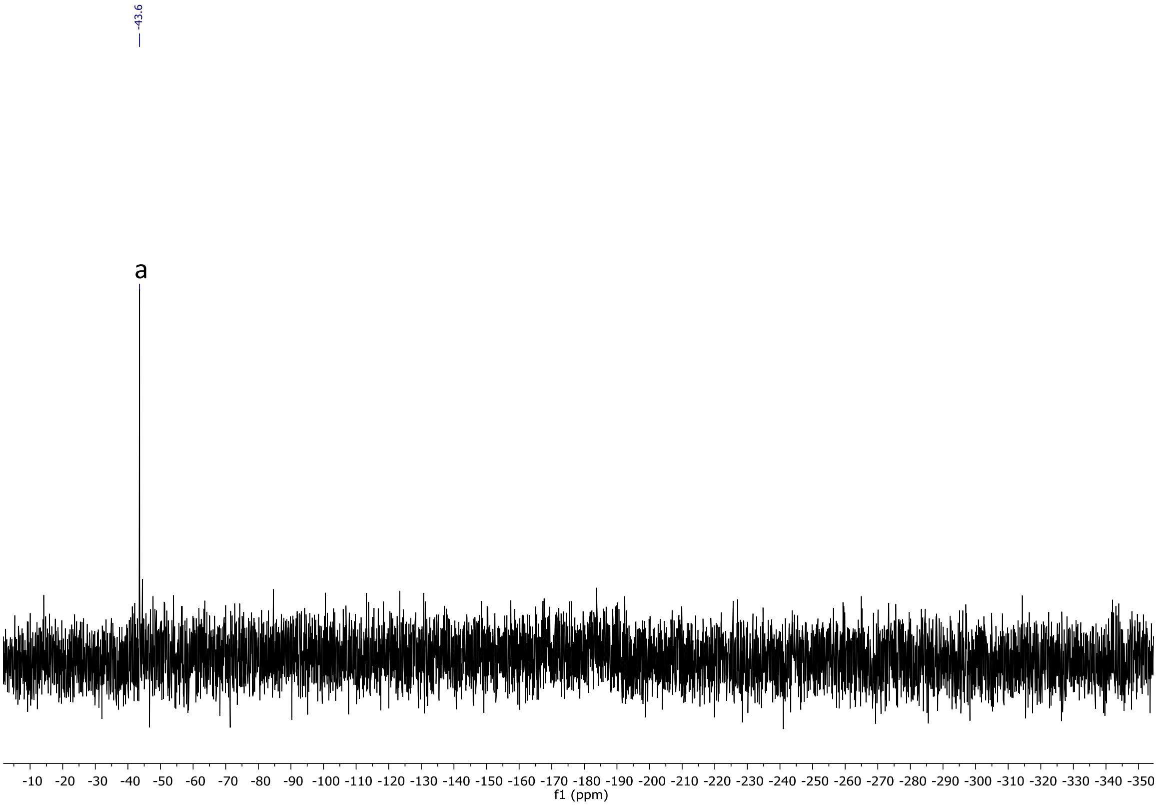

Figure S8. The ^{119}Sn{^{1}H} NMR spectrum (186 MHz, C_6D_6) of the reaction between **1** and di-*p*-tolylcarbodiimide after 30 minutes. **a**, “Ph_2Sn”.[4]

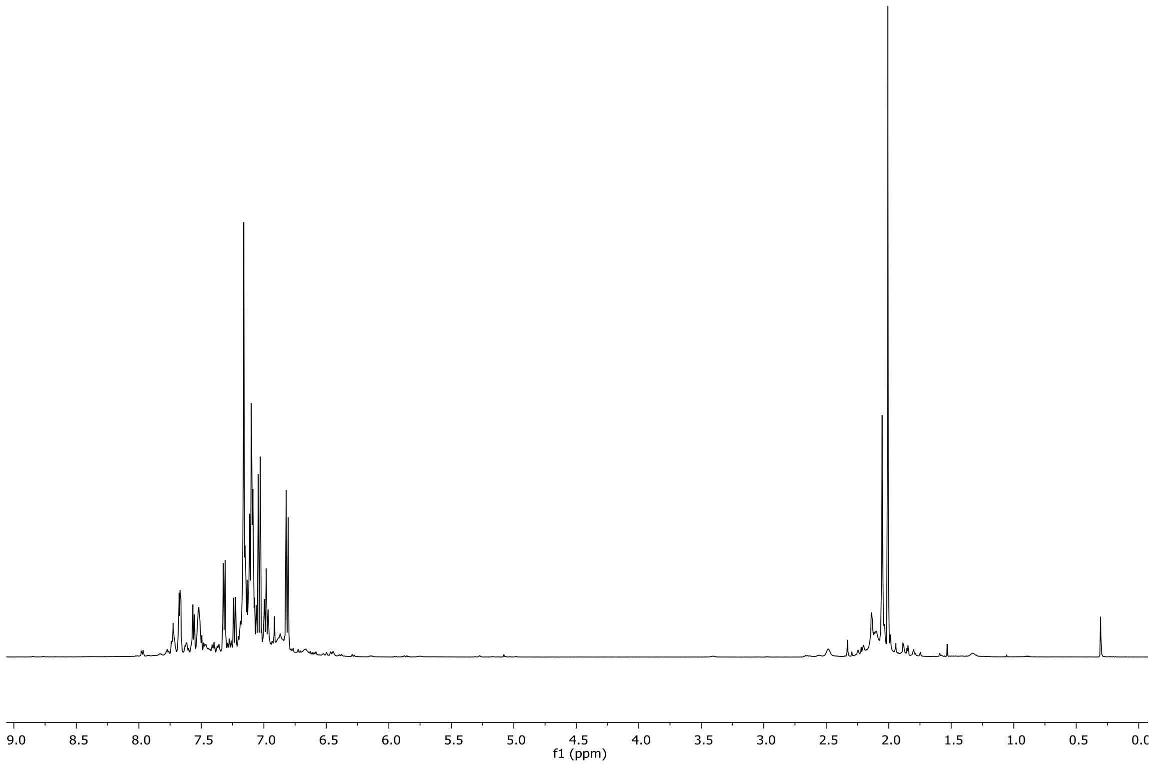

Figure S9. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction with 10 mol% **1**, di-p-tolylcarbodiimide, and Ph_3SnH after 30 minutes.

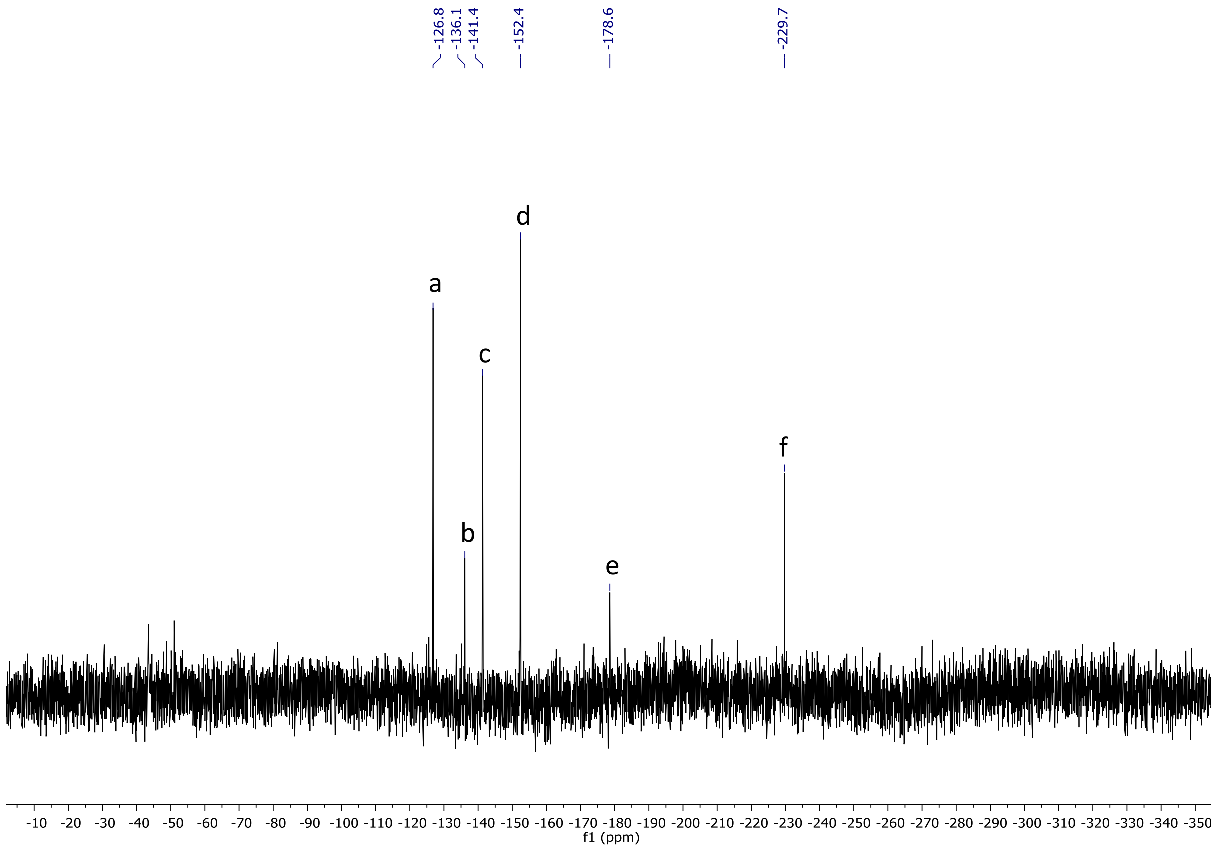

Figure S10. The $^{119}Sn\{^1H\}$ NMR spectrum (186 MHz, C_6D_6) of the reaction with 10 mol% **1,** and di-*p*-tolylcarbodiimide, and Ph_3SnH after 30 minutes. **a**, $Ph_4\underline{Sn}$; **b**, $Ph_3\underline{Sn}Sn(Ph_2)\underline{Sn}Ph_3$; **c**, $Ph_6\underline{Sn}_2$; **d**, un-attributed; **e**, un-attributed; **f**, $Ph_3Sn\underline{Sn}(Ph_2)SnPh_3$.[5]

d

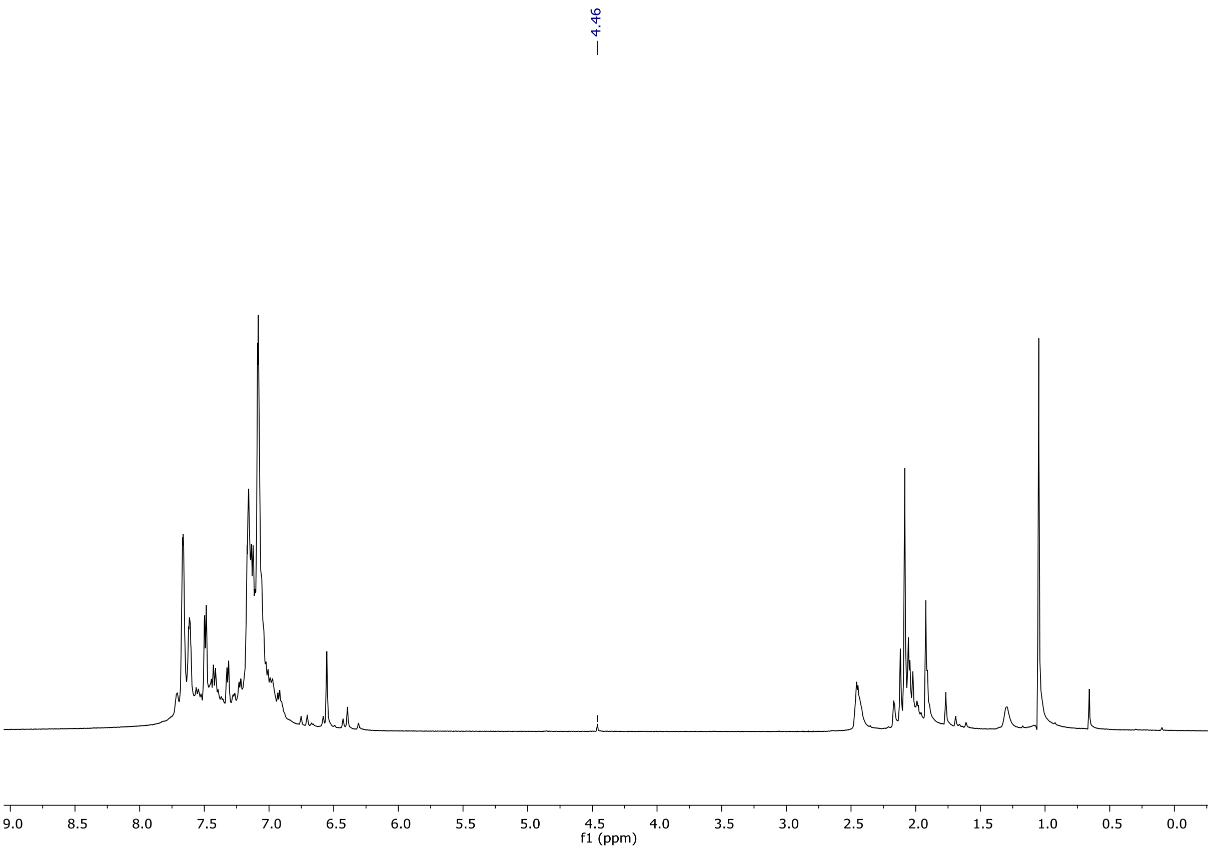

Figure S11. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between 10 mol% (6-Mes)CuO^{t}Bu and Ph_3SnH after 1 hour.

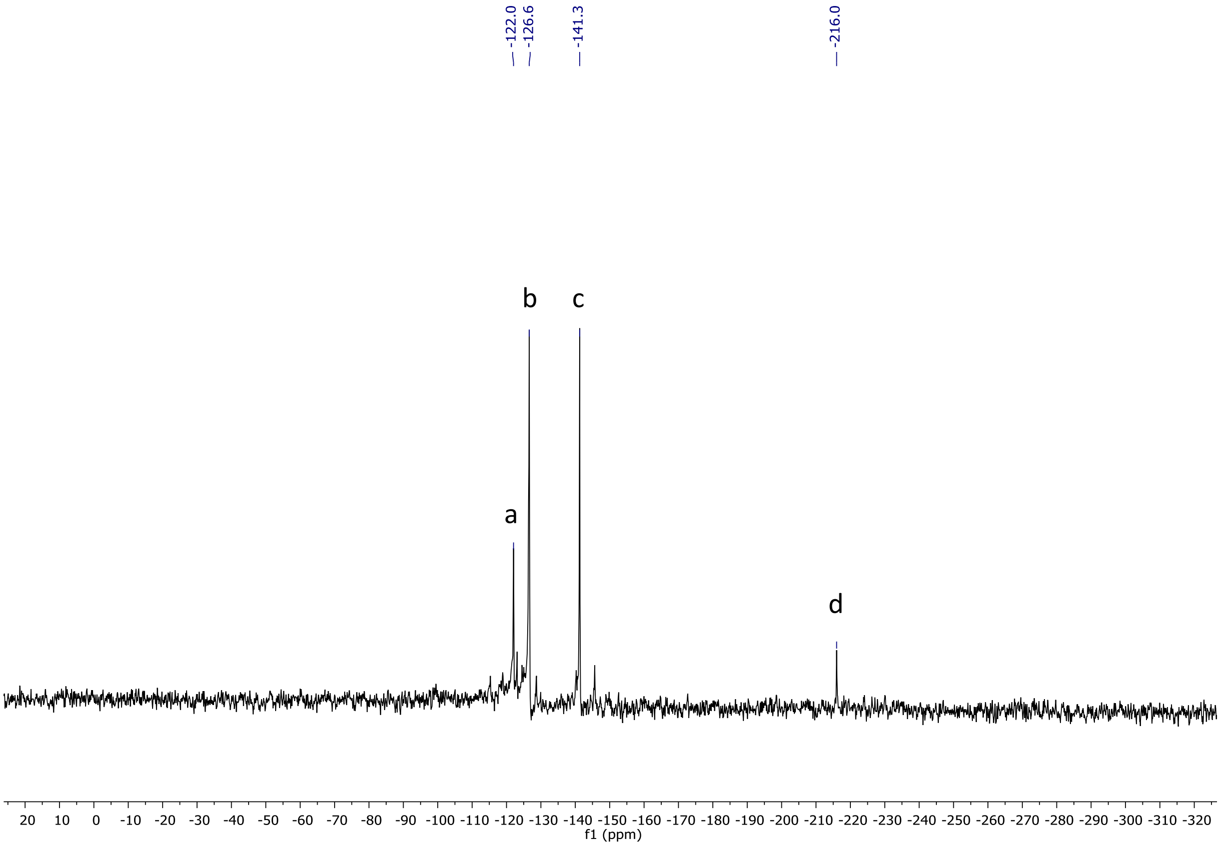

Figure S12. The ^{119}Sn{^{1}H} NMR spectrum (186 MHz, C_6D_6) of the reaction between 10 mol% (6-Mes)CuO^{t}Bu and Ph_3SnH after 1 hour. **a**, Unattributed; **b**, $Ph_4\underline{Sn}$; **c**, $Ph_6\underline{Sn}_2$; **d**, $(Ph_2\underline{Sn})_6$.[5]

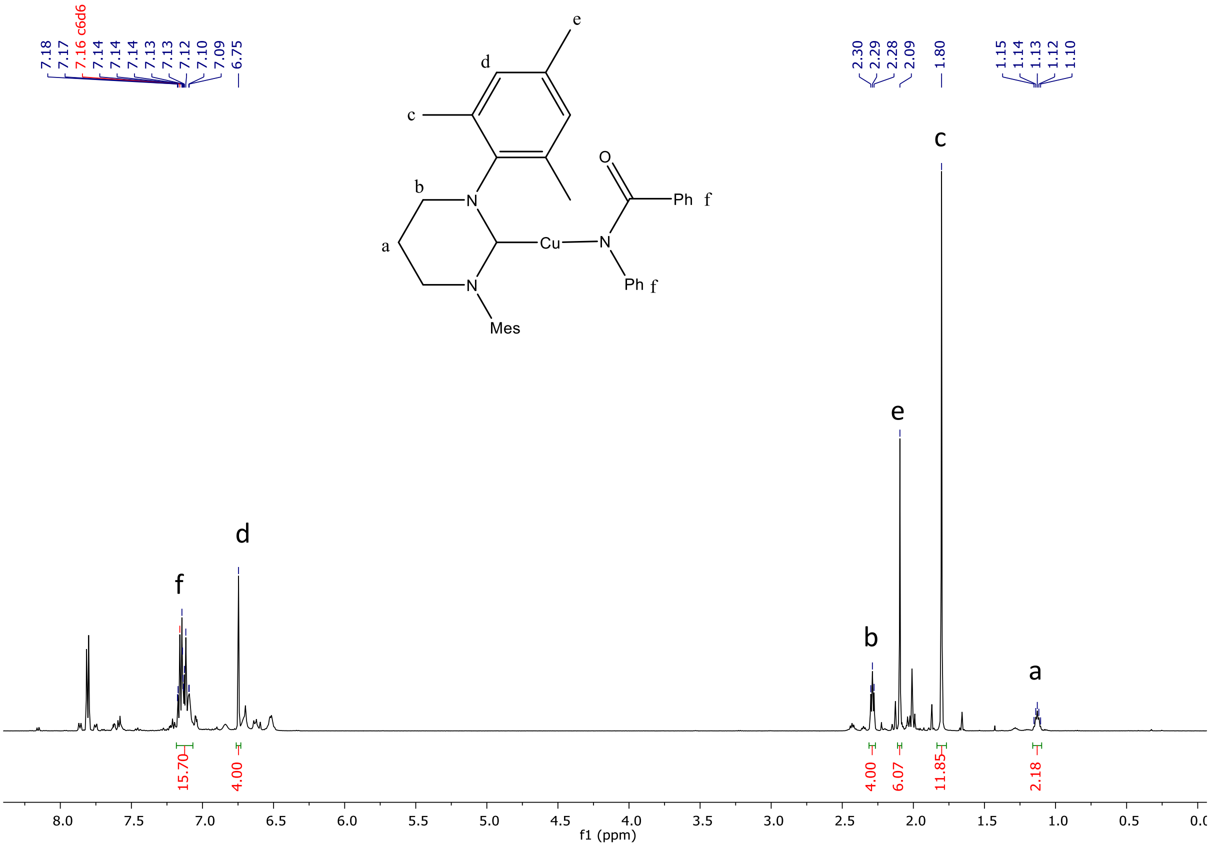

Figure S13. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between **1** and PhNCO after 30 minutes. **a**, $NCH_2C\underline{H}_2$; **b**, $NC\underline{H}_2$; **c**, *ortho*-$C\underline{H}_3$; **d**, *meta*-$C\underline{H}_3$; **e**, *para*-$C\underline{H}_3$, **f**, Ar-H (solvent peak included)

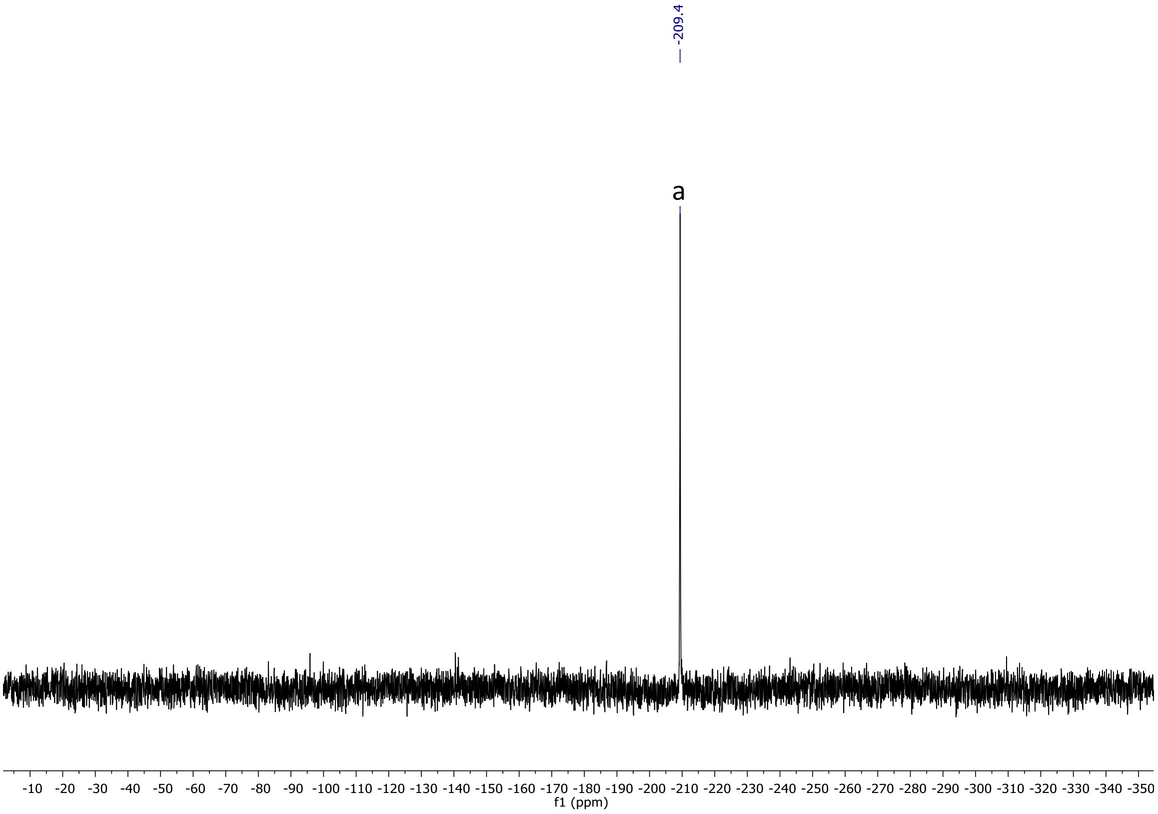

Figure S14. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between **1** and PhNCO after 30 minutes. **a**, $(Ph_2\underline{Sn})_6$.[5]

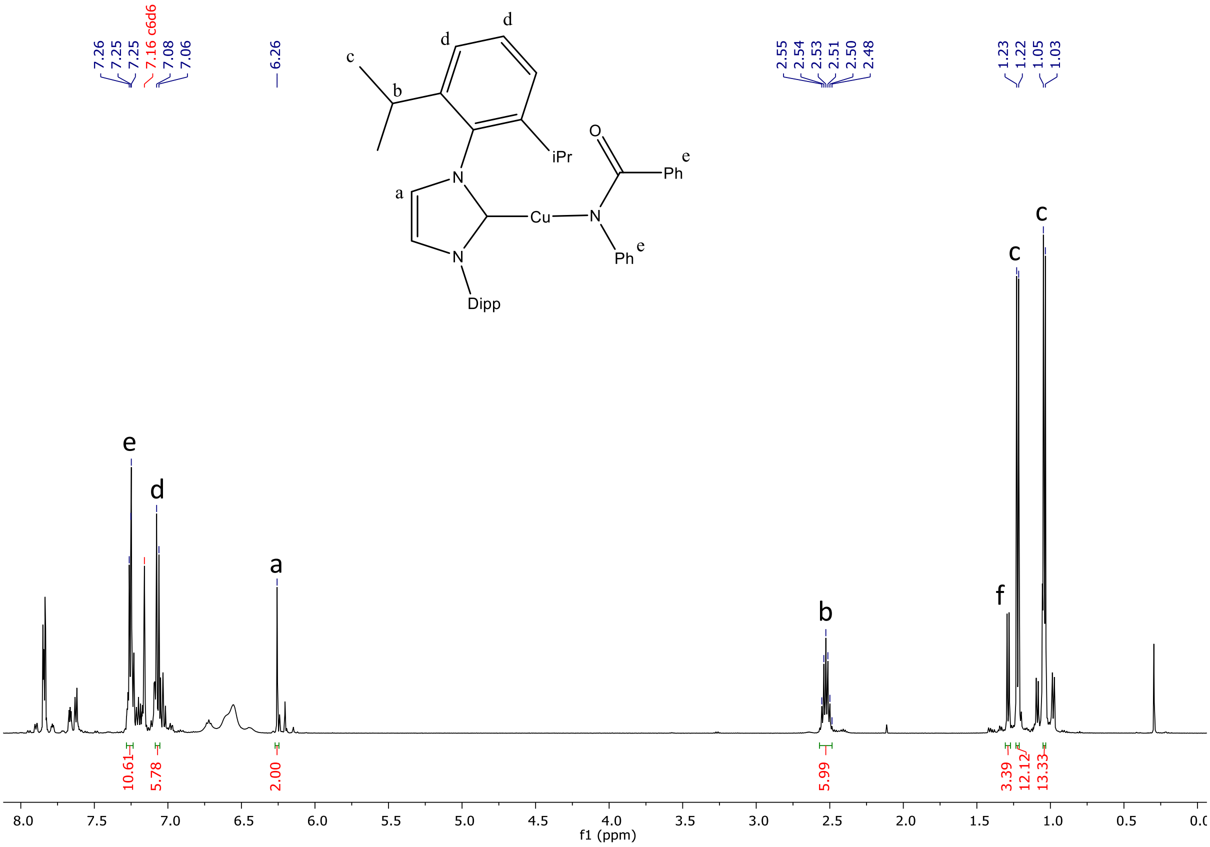

Figure S15. The ^1H NMR spectrum (500 MHz, C_6D_6) of the reaction between $IPrCuSnPh_3$ and PhNCO after overnight. **a**, $NC\underline{H}_2$; **b**, $C\underline{H}(CH_3)_2$; **c**, $CH(C\underline{H}_3)_2$; **d**, *para*-H̲, *meta*-H̲; **e**, Ar-H; **f**, *ca.* 28% contaminated with $IPrCuSnPh_3$.

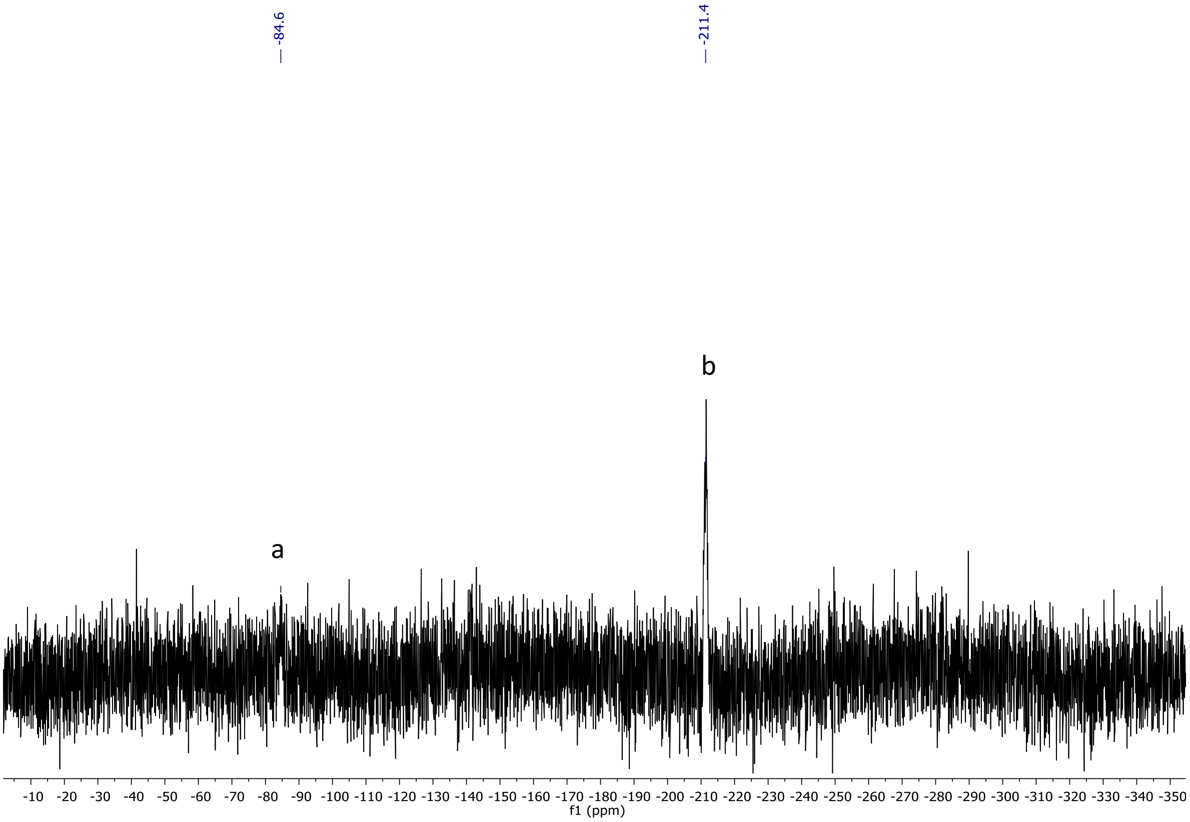

Figure S16. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between $IPrCuSnPh_3$ and PhNCO after overnight. **a**, $IPrCu\underline{Sn}Ph_3$; **b**, $(Ph_2\underline{Sn})_6$.[5]

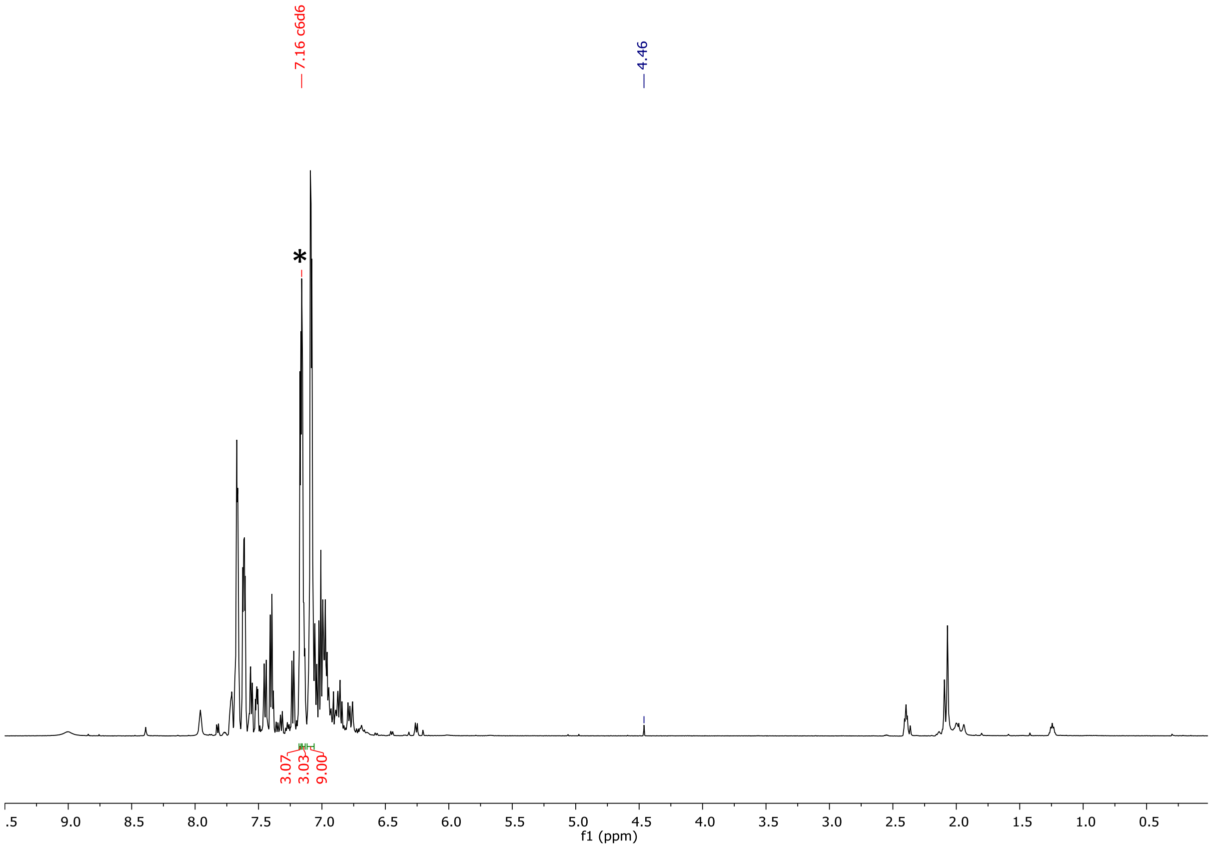

Figure S17. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between 10 mol% **1**, PhNCO, and Ph_3SnH after overnight heating at 40 °C. ***** = N,N',N"-triphenylisocyanurate, Solvent overlapped.

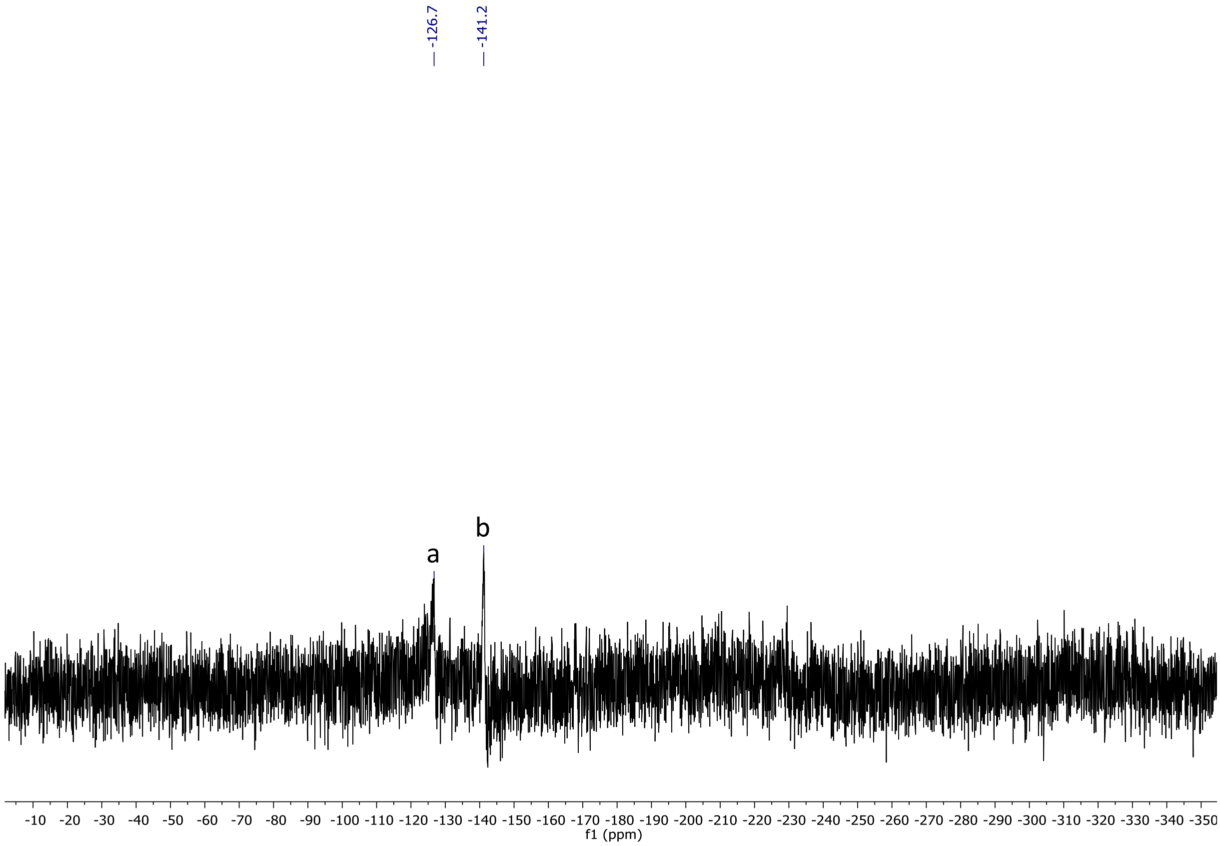

Figure S18. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between 10 mol% **1**, PhNCO, and Ph_3SnH after overnight heating at 40 °C. **a**, $Ph_4\underline{Sn}$; **b**, $Ph_6\underline{Sn_2}$.[5]

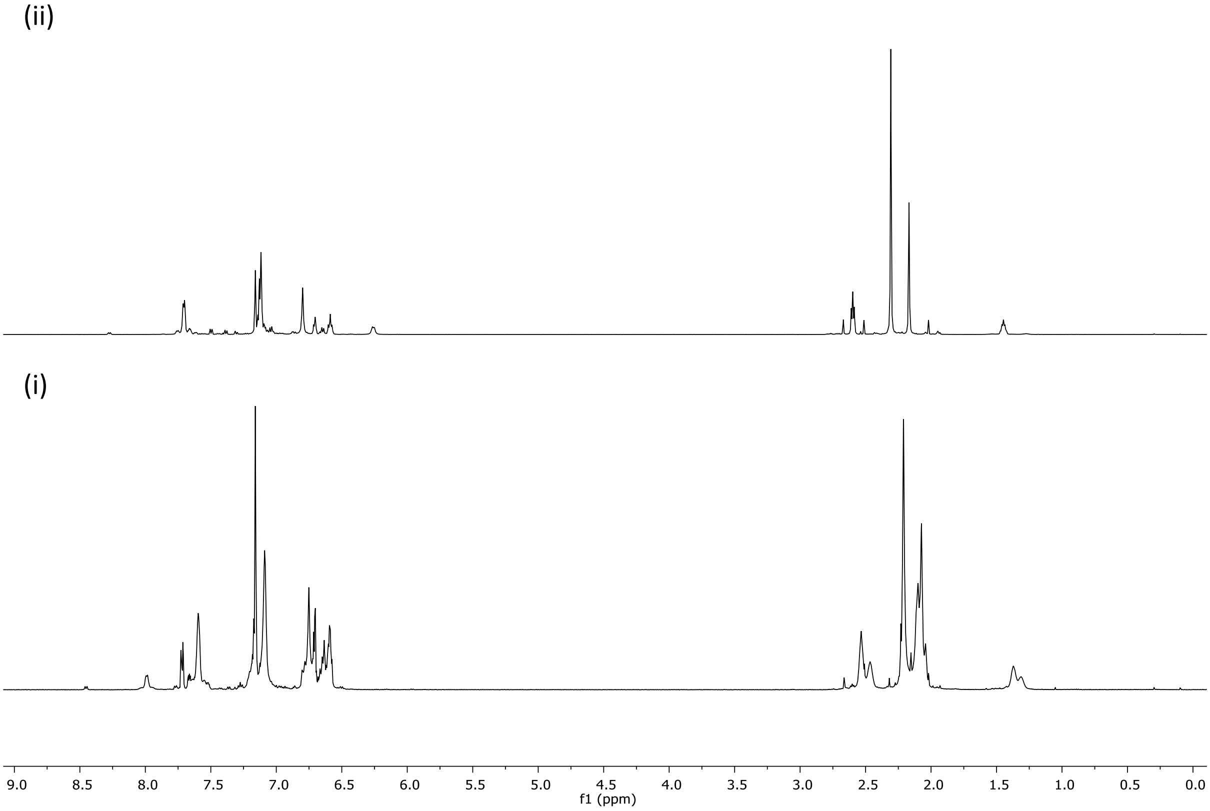

Figure S19. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between **1** and PhNCS after (i) 30 minutes and (ii) overnight.

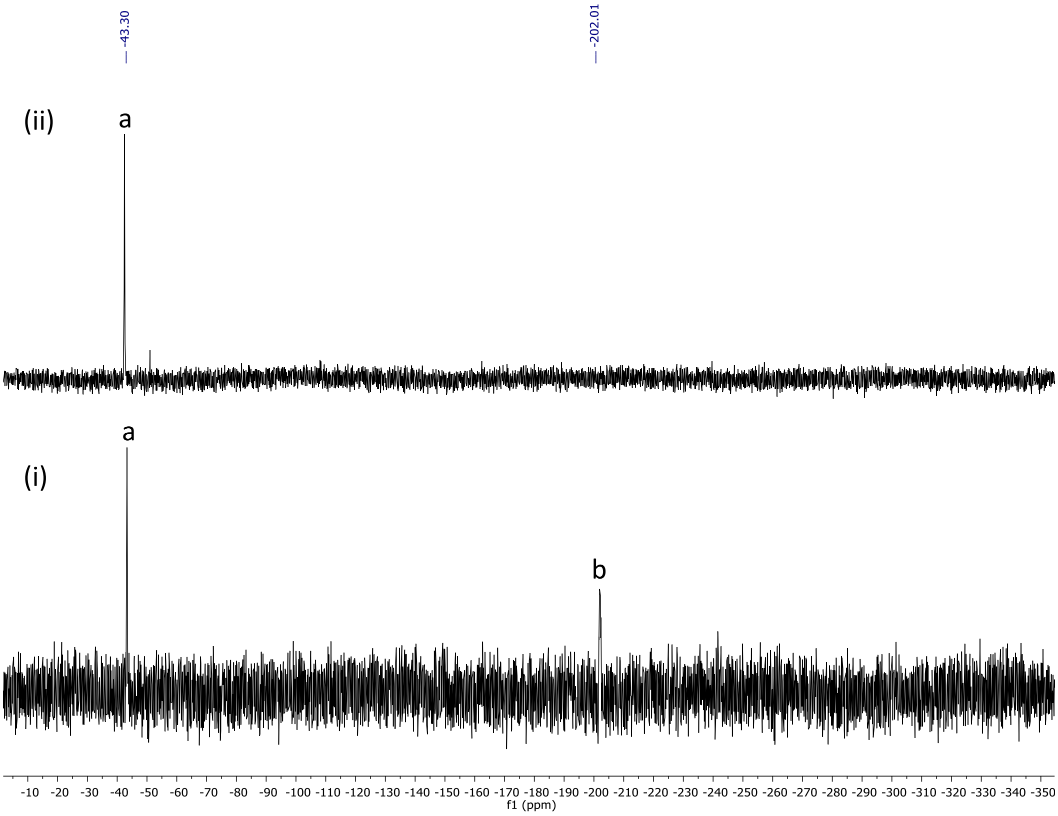

Figure S20. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of the reaction between **1** and PhNCS after (i) 30 minutes and (ii) overnight. **a**, $(Ph_2\underline{Sn})_n$;[4] **b**, (6-Mes)CuN(Ph)C(S)$\underline{Sn}Ph_3$.

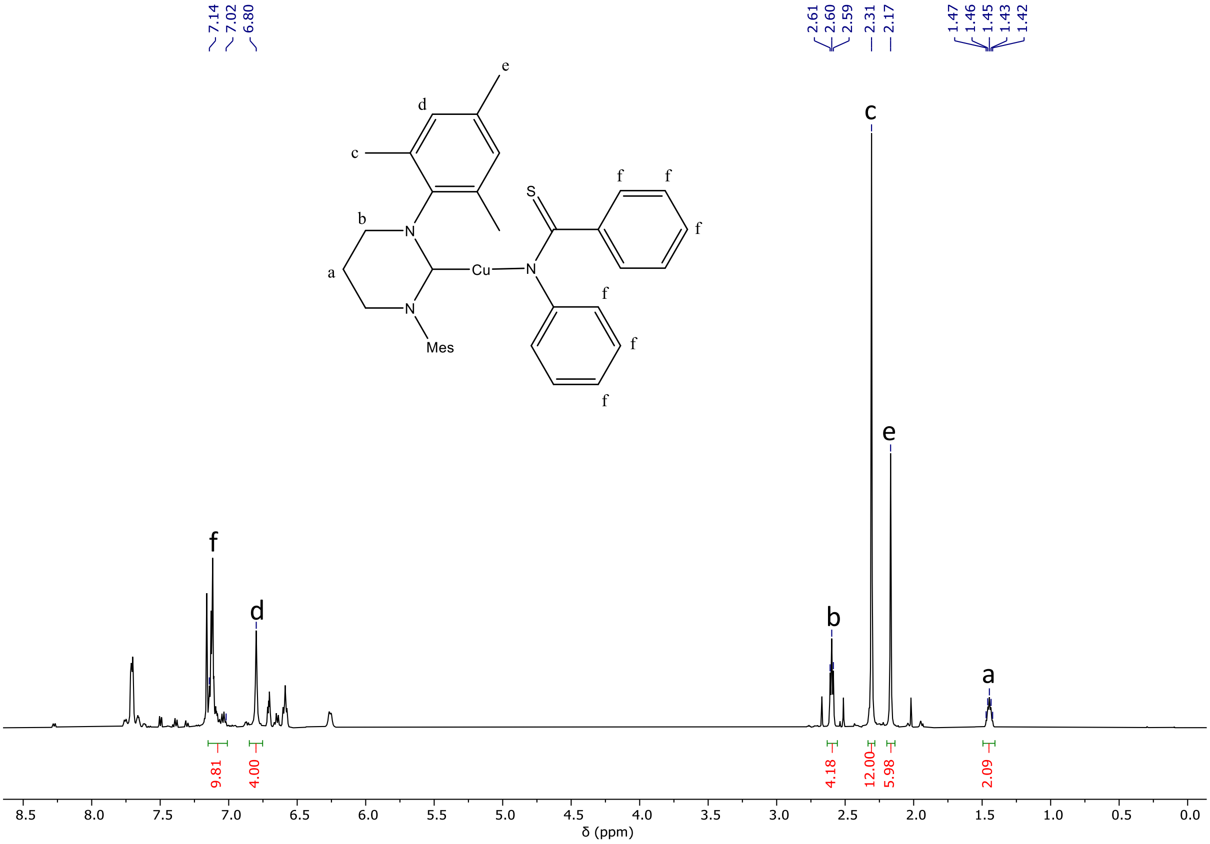

Figure S21. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of the reaction between **1** and PhNCS after overnight. **a**, $NC\underline{H}_2$; **b**, $NCH_2C\underline{H}_2$; **c**, *ortho*-$C\underline{H}_3$; **d**, meta-$\underline{H}$; **e**, *para*-$C\underline{H}_3$; **f**, Ar-H.

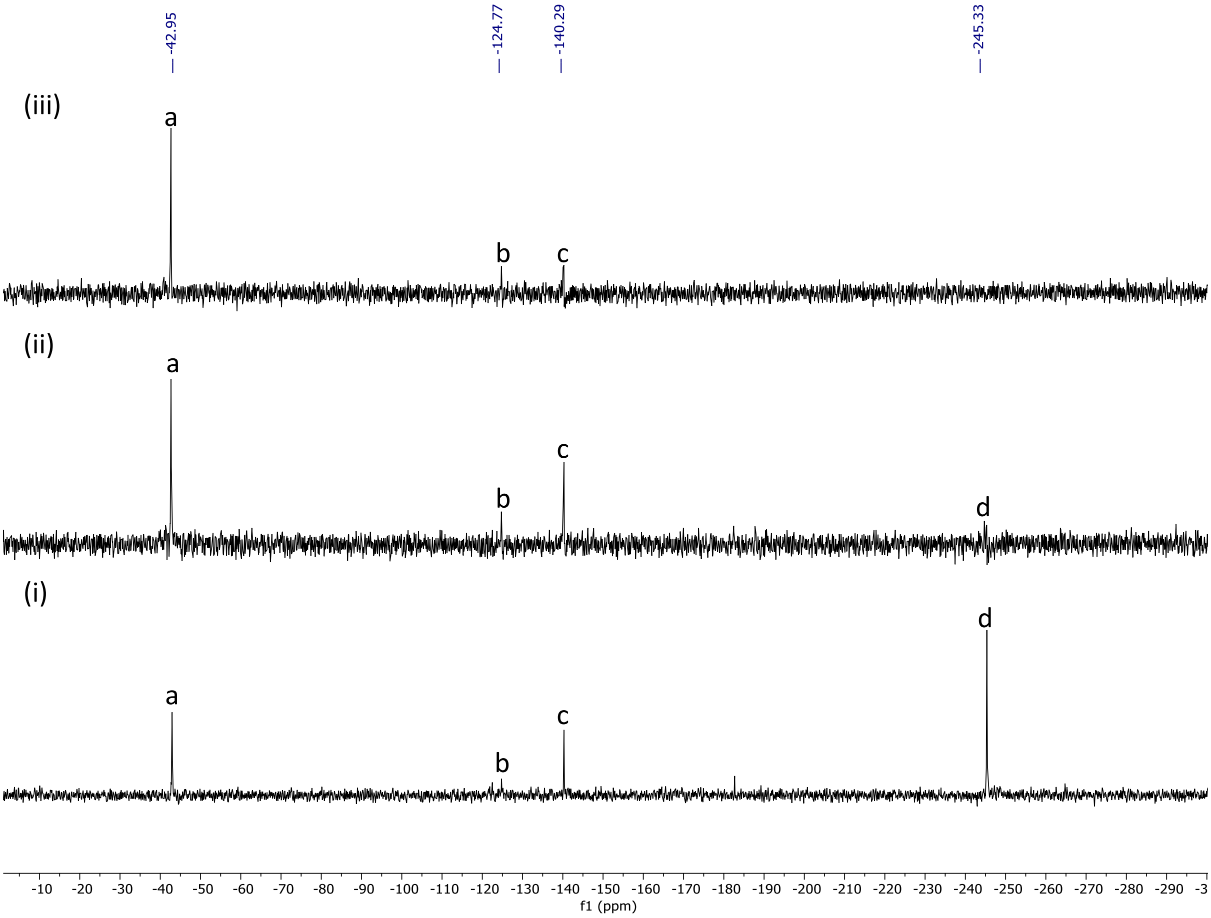

Figure S22. The ^{119}Sn NMR spectra (186 MHz, d_8-toluene) of the reaction between **1** and di-*p*-tolylcarbodiimide at -50 °C. (i) 15 min, (ii) 30 min, and (iii) 45 minutes. **a (**$Ph_2\underline{Sn})_n$;[4] **b** $SnPh_4$; **c** Sn_2Ph_6;[5] **d** (6-Mes)CuN(*p*-Tol)C(=N-*p*-Tol)$SnPh_3$

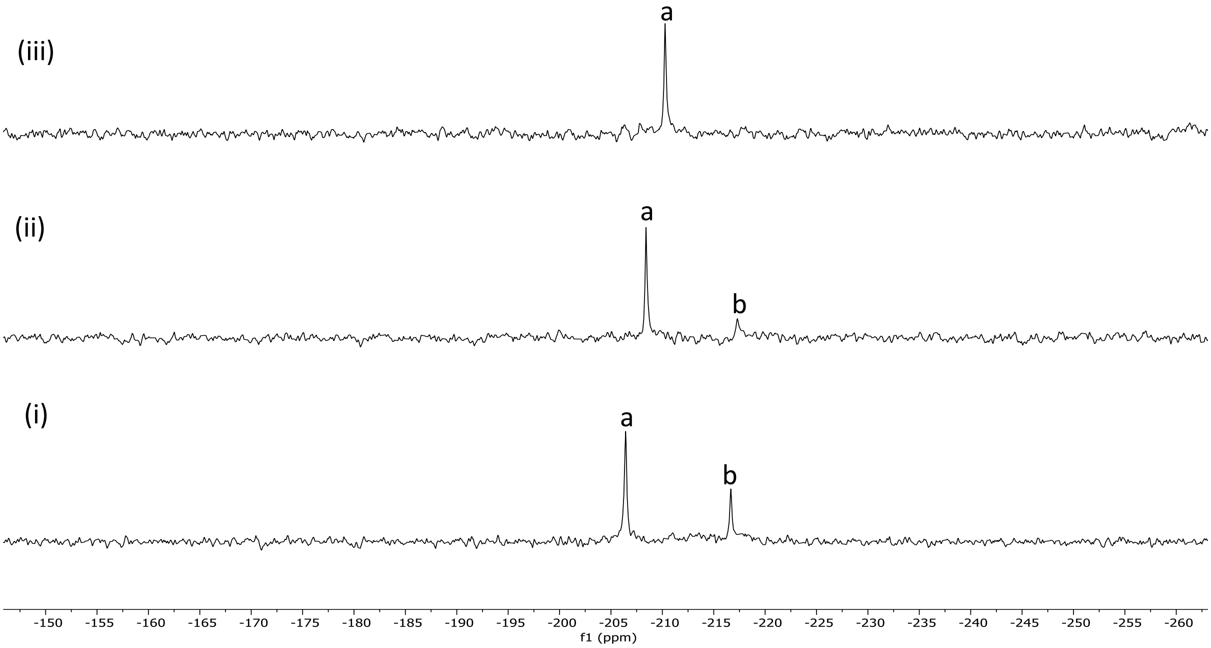

Figure S23. The ^{119}Sn NMR spectra (186 MHz, d_8-toluene) of the reaction between **1** and PhNCO with increasing temperature (i) -50 °C, (ii) -25 °C, and (iii) 0 °C. **a**, $(Ph_2\underline{Sn})_6$;[5] **b**, (6-Mes)CuN(Ph)C(=O)$SnPh_3$.

NMR spectra of Compounds 1-3

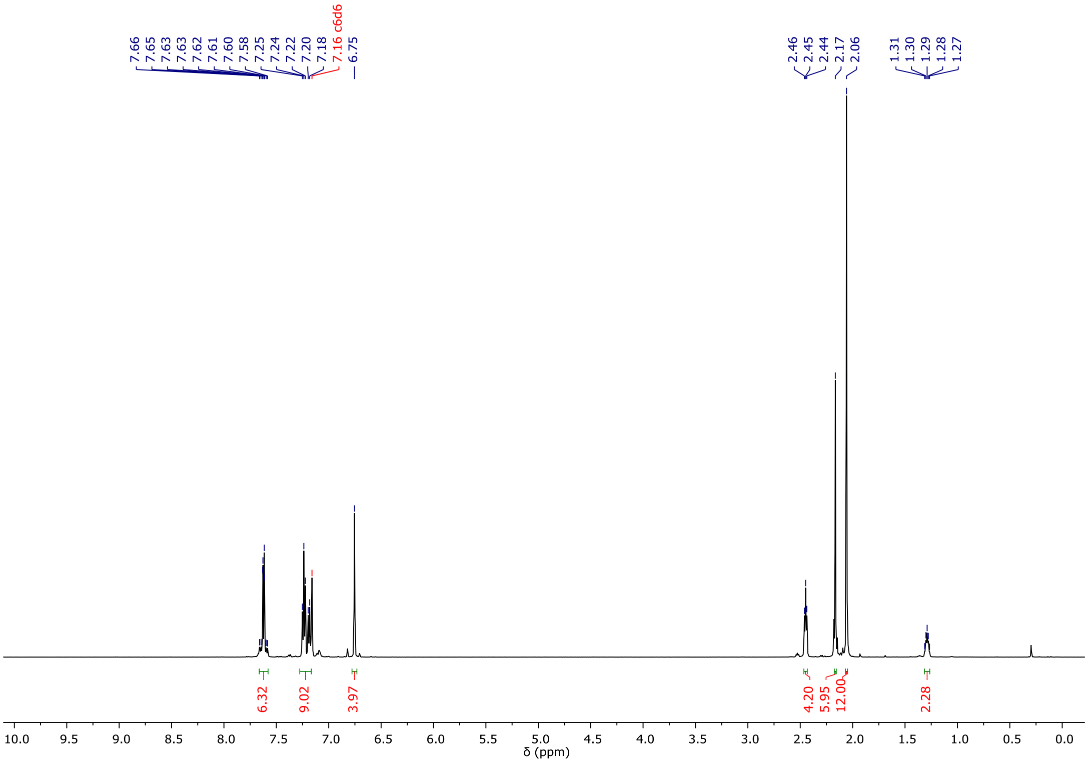

Figure S24. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of compound **1**.

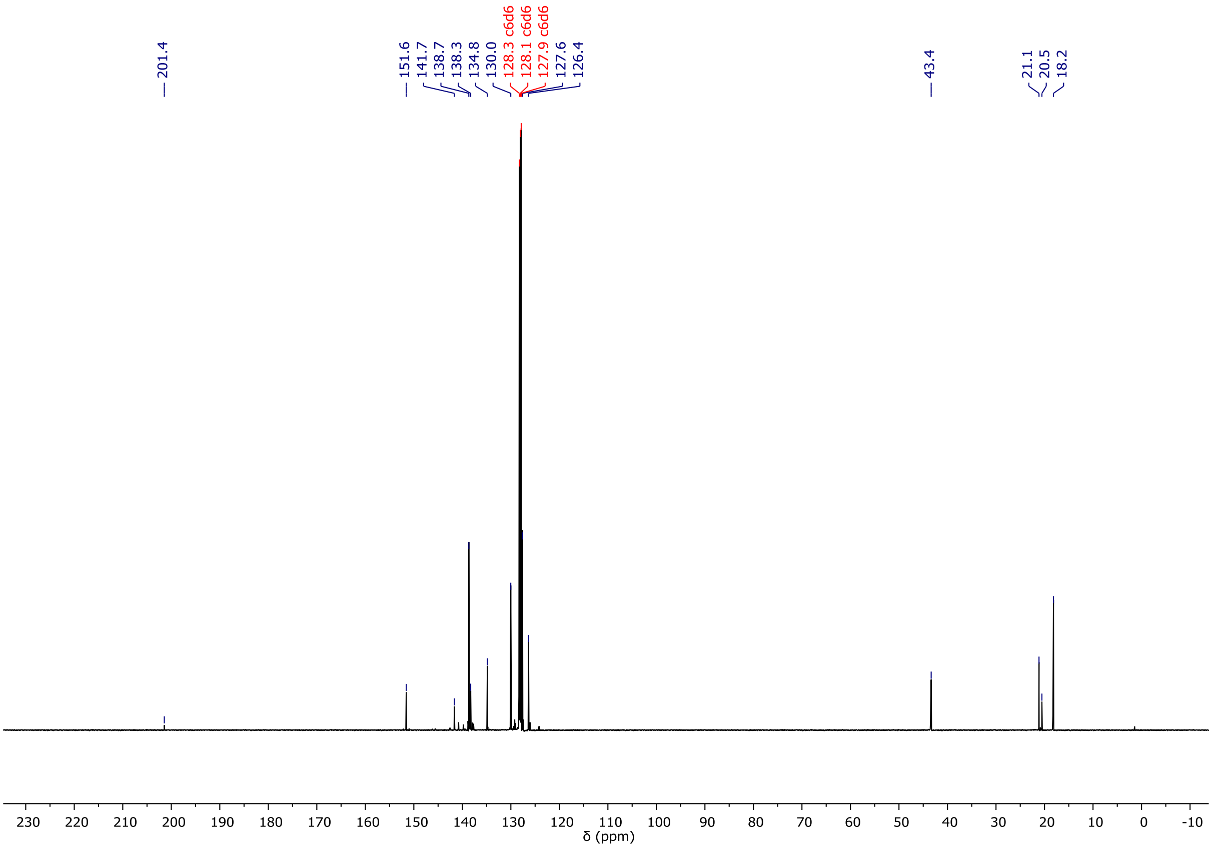

Figure S25. The $^{13}C\{^1H\}$ NMR spectrum (126 MHz, C_6D_6) of compound **1**.

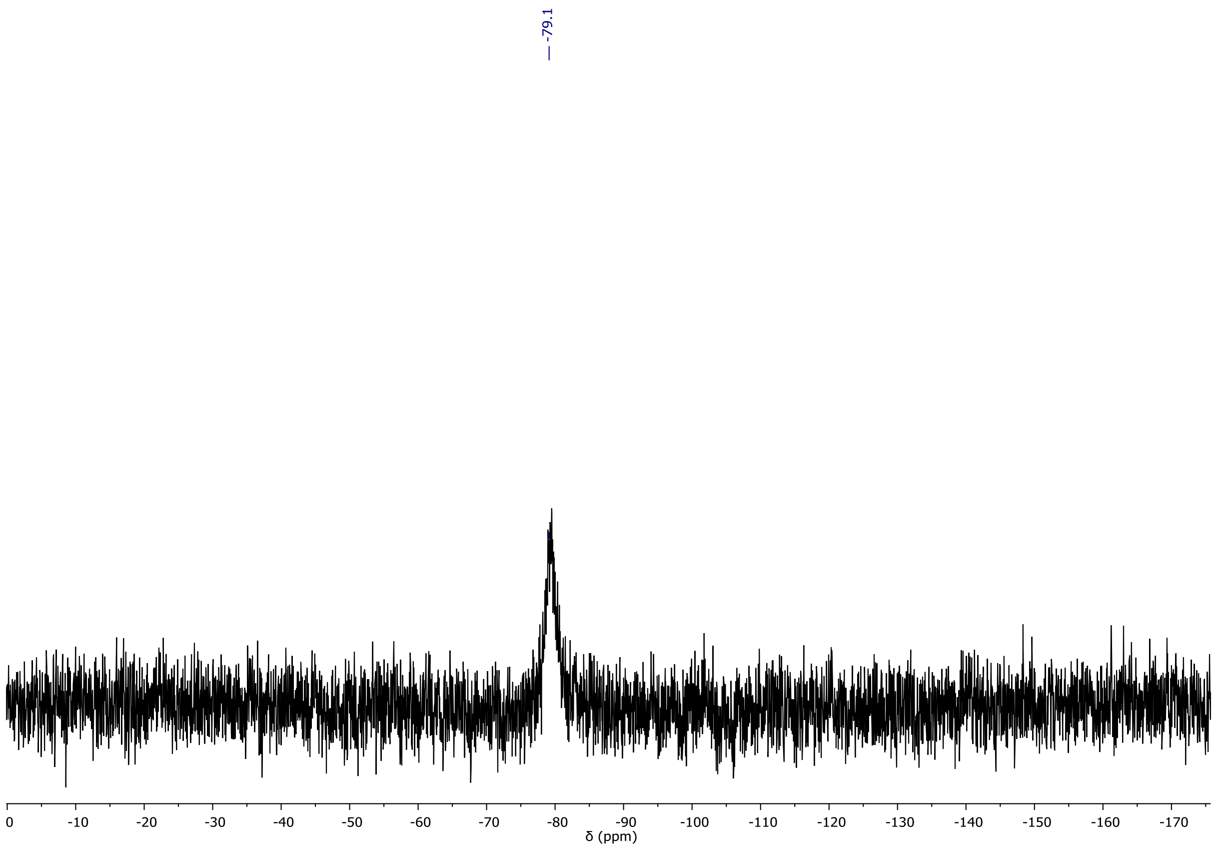

Figure S26. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of compound **1**.

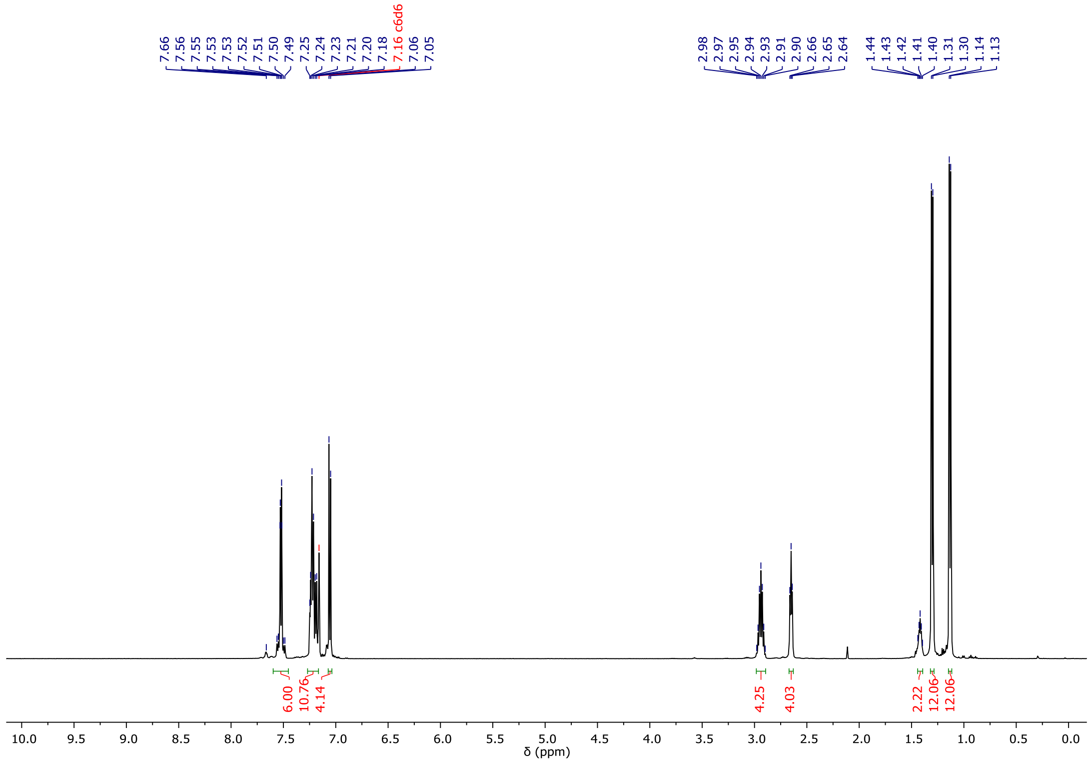

Figure S27. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of compound **2**.

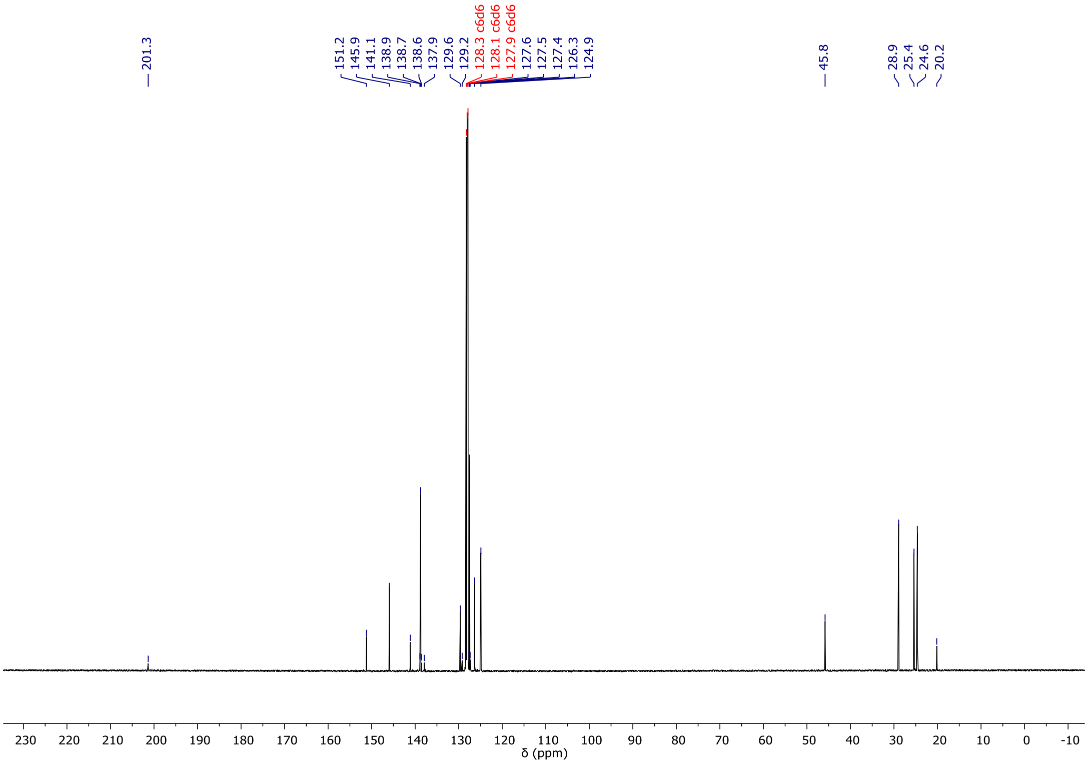

Figure S28. The $^{13}C\{^1H\}$ NMR spectrum (126 MHz, C_6D_6) of compound **2**.

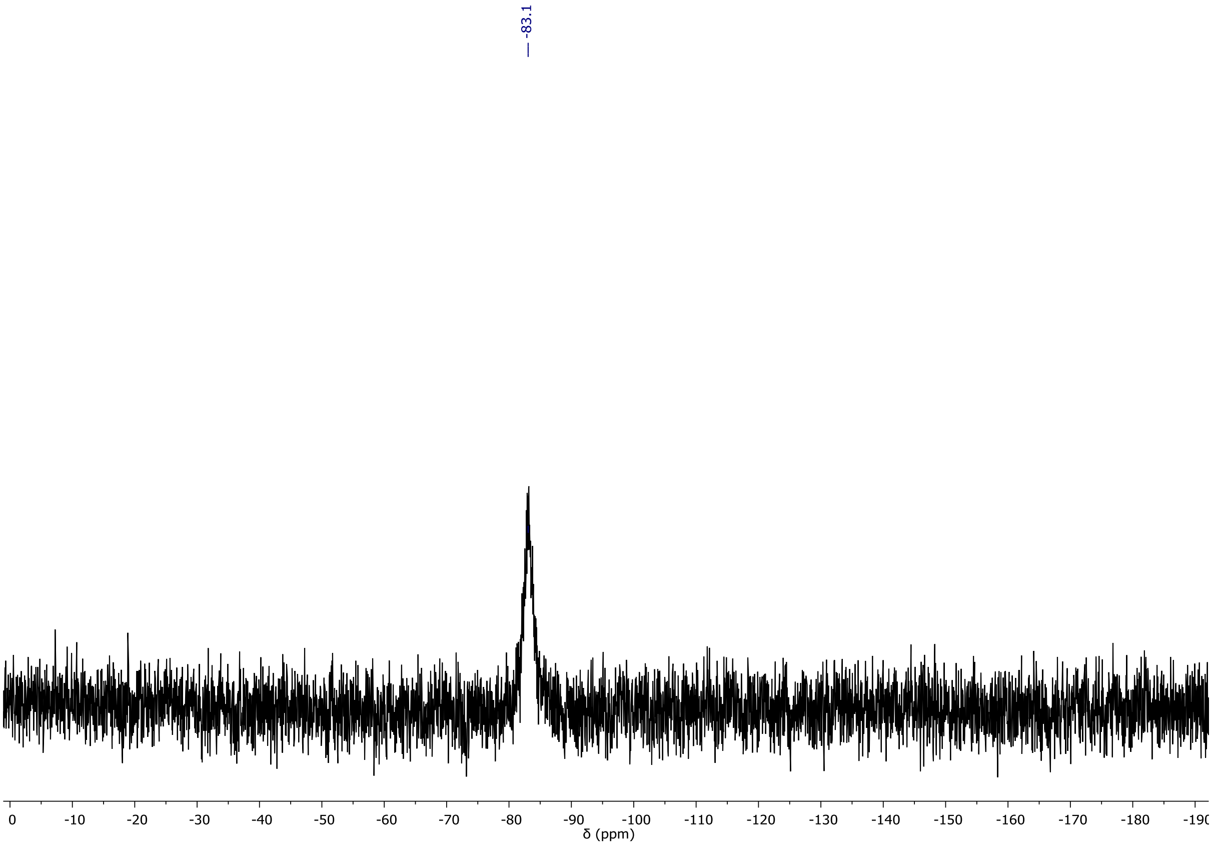

Figure S29. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of compound **2**.

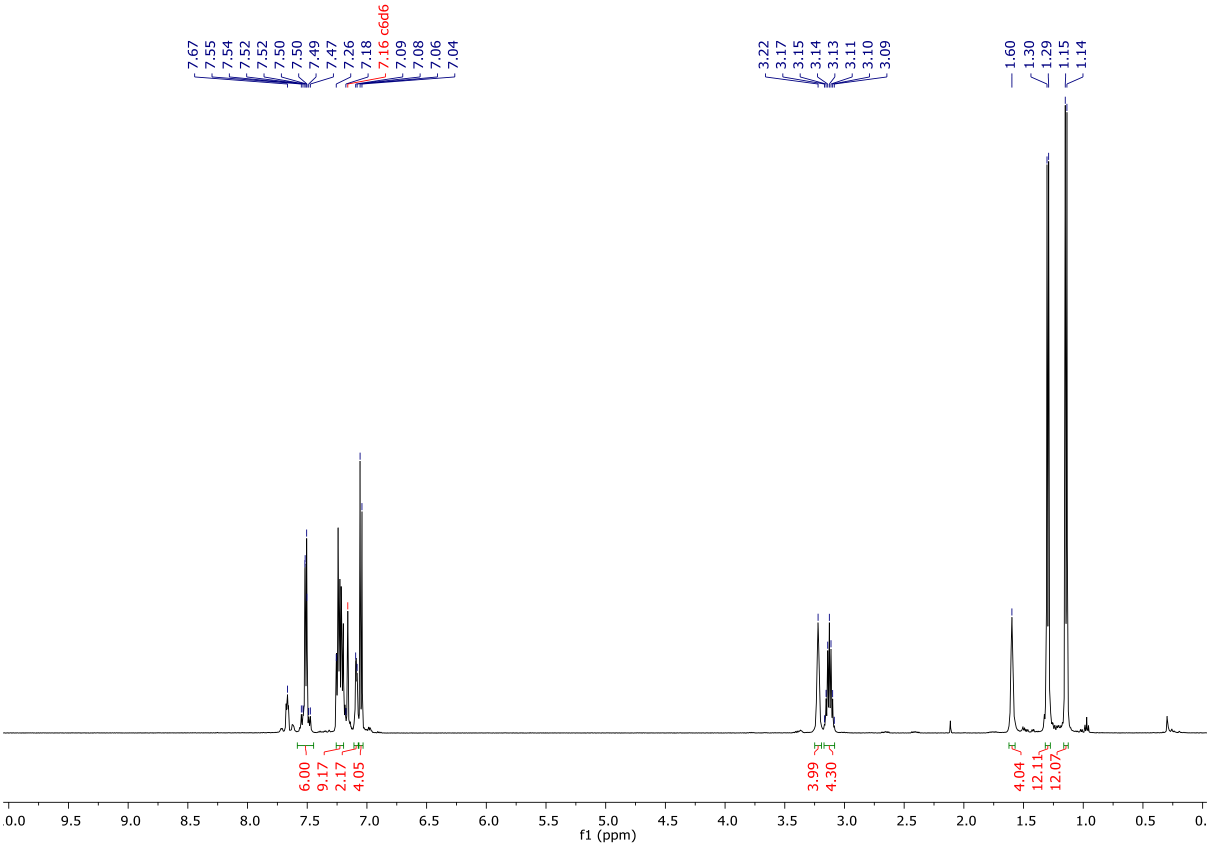

Figure S30. The ^{1}H NMR spectrum (500 MHz, C_6D_6) of compound **3**.

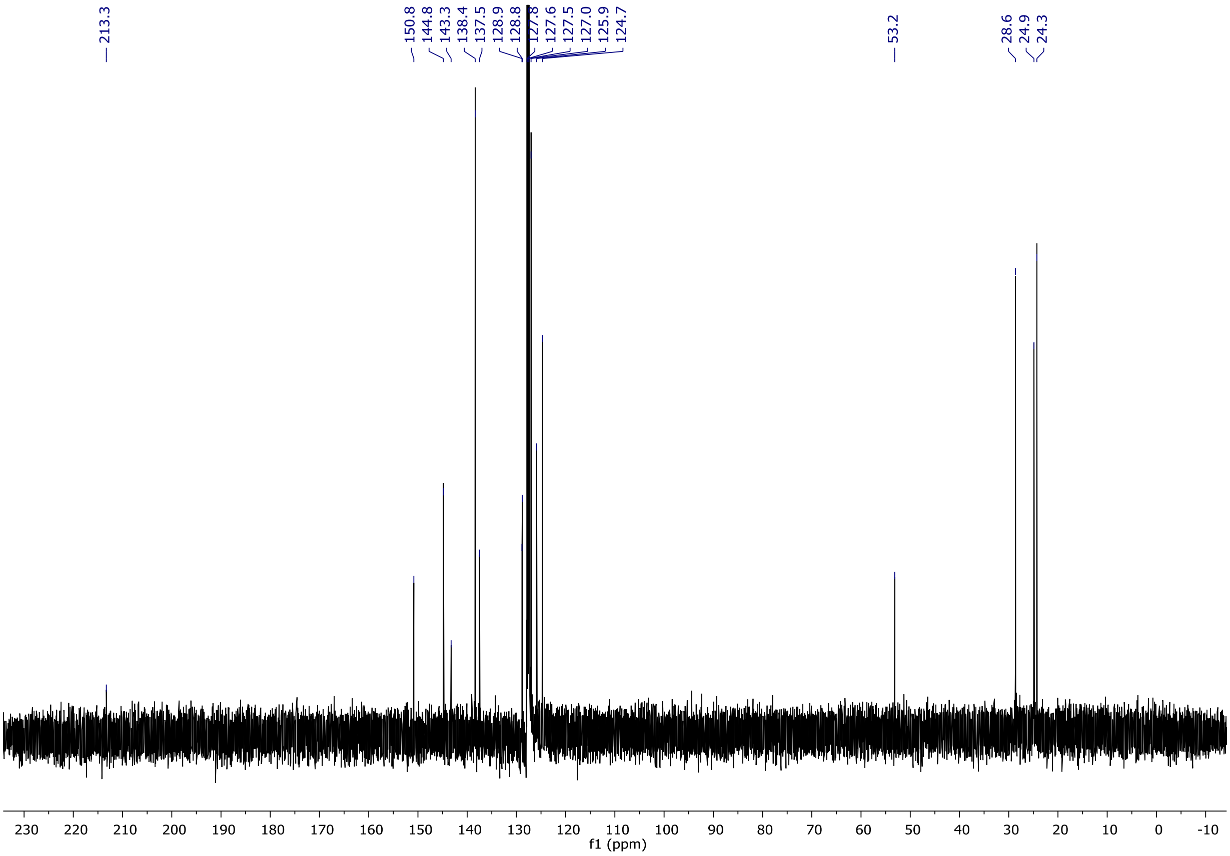

Figure S31. The $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of compound **3**.

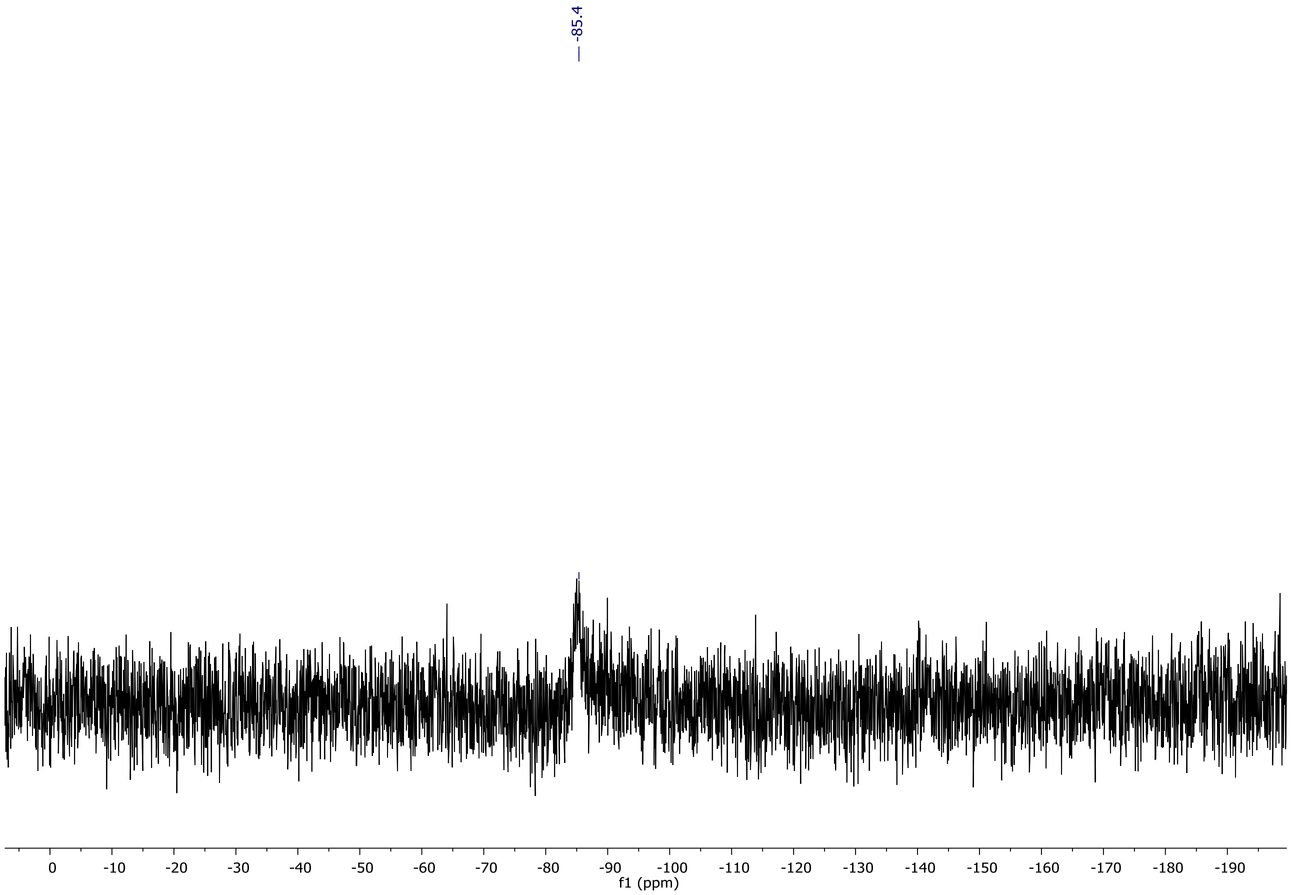

Figure S32. The ^{119}Sn NMR spectrum (186 MHz, C_6D_6) of compound **3**.

Mass Spectrometry Data

Compound 1

Walkup MS Report

Data File	RC168_Neg_5mins_MS_21217.d	**Sample Name**	RC168
Sample Type	Sample	**Position**	P1-A2
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Neg_5mins_MS.m	**Acquired Time**	05/08/2021 13:34:18
IRM Calibration Status	Success	**DA Method**	Neg_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	6MesCuSnPh3	**Walkup Method**	Neg_5Mins_C18
Formula	C40 H43 Cu N2 Sn	**Walkup Method Description**	Negative mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

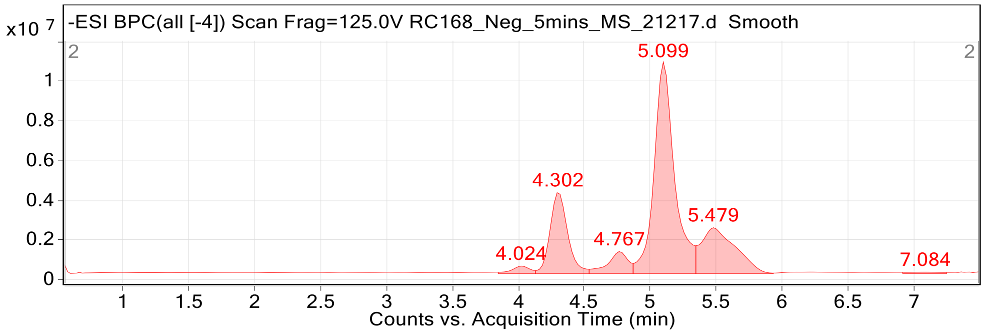

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
4.02	3563153	3.09	1.68	1033.9836	0.144
4.30	37986120	32.95	17.95	441.0134	0.141
4.77	11826134	10.26	5.59	194.0813	0.158
5.10	115292316	100.00	54.47	311.2025	0.160
5.48	41688935	36.16	19.69	473.3039	0.244
7.08	1320165	1.15	0.62	1033.9839	0.266

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C40 H43 Cu N2 Sn	5.57	729.1762	726.1757	726.1770	-1.86	64.68

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

Compound 2

Walkup MS Report

Data File	6DippCuSnPh3_Pos_5mins_MS_21855.d	**Sample Name**	6DippCuSnPh3
Sample Type	Sample	**Position**	P1-A2
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Pos_5mins_MS.m	**Acquired Time**	8/26/2021 4:08:36 PM
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description		**Walkup Method**	Pos_5Mins_C18
Formula	C46H55CuN2Sn	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

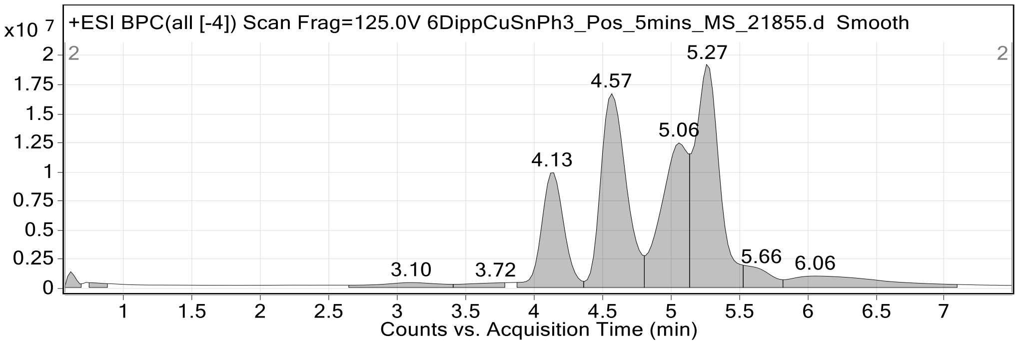

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.62	5701828	2.39	0.68	194.1178	0.070
0.79	3012643	1.26	0.36	116.1071	0.110
3.10	14039235	5.89	1.68	194.1179	0.460
3.72	7710998	3.24	0.92	116.9862	0.300
4.13	112960084	47.40	13.48	351.0206	0.170
4.57	216912726	91.02	25.89	508.2771	0.200
5.06	166618557	69.91	19.88	421.3240	0.200
5.27	238325279	100.00	28.44	421.3292	0.180
5.66	23808792	9.99	2.84	325.2936	0.250
6.06	48891187	20.51	5.83	116.9864	0.730

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C46 H55 Cu N2 Sn	4.77	819.2915	810.2683	810.2709	-3.28	63.40

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

---

Compound 3

Walkup MS Report

Data File	7DippCuSnph3_Neg_LoopInjection_MS_unbiased_21748.d	**Sample Name**	7DippCuSnph3
Sample Type	Sample	**Position**	P1-A3
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Neg_LoopInjection_MS_unbiased.m	**Acquired Time**	23/08/2021 17:33:55
IRM Calibration Status	Success	**DA Method**	Neg_LoopInjection_MS_unbiased.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	7DippCuSnPh3	**Walkup Method**	Neg_LoopInjection_unbiased
Formula	C47H57CuN2Sn	**Walkup Method Description**	Negative mode loop injection with unbiased isotope model
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

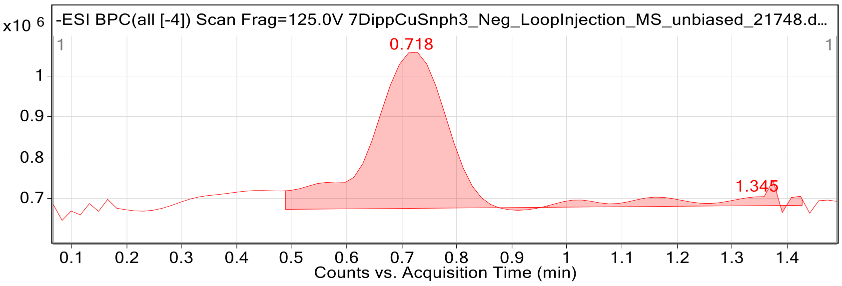

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.72	3604628	100.00	89.63	1033.9782	0.182
1.35	416930	11.57	10.37	1033.9782	0.222

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C47 H57 Cu N2 Sn	0.69	877.2804	824.2842	824.2866	-2.90	91.25

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

1 and di-p-tolylcarbodiimide immediately quencl

Walkup MS Report

Data File	RC283_Pos_5mins_MS_24218.d	**Sample Name**	RC283
Sample Type	Sample	**Position**	P1-A1
Instrument Name	6545 QTof	**User Name**	Rex Charman
Acq Method	Pos_5mins_MS.m	**Acquired Time**	06/12/2021 10:44:02
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	6MesCuSnPh3 + (p-tol)NCN(p-tol) after immediate quenching with wet acetonitrile (1 mL)	**Walkup Method**	Pos_5Mins_C18
Formula	C33H30N2Sn	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

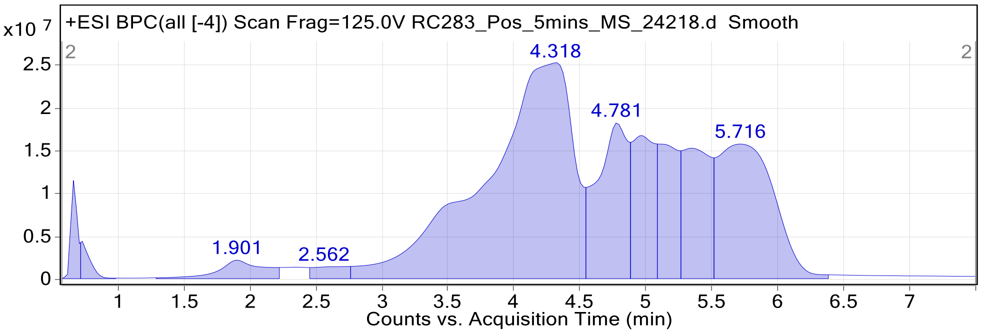

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.67	40339458	3.40	1.51	144.9814	0.064
0.72	20454386	1.72	0.77	144.9811	0.078
1.90	51829830	4.37	1.94	108.0799	0.314
2.56	25517390	2.15	0.96	108.0799	0.259
4.32	1186228860	100.00	44.41	321.2365	0.589
4.78	292519704	24.66	10.95	500.2123	0.221
4.97	197955183	16.69	7.41	673.4456	0.165
5.18	165340310	13.94	6.19	321.2310	0.158
5.35	223100666	18.81	8.35	321.2310	0.218
5.72	467664038	39.42	17.51	321.2311	0.475

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C33 H30 N2 Sn	4.28	575.1494	566.1440	566.1457	-3.07	64.15

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

1 and di-*p*-tolylcarbodiimide after hours

Walkup MS Report

Data File	RC193_Pos_5mins_MS_21775.d	**Sample Name**	RC193
Sample Type	Sample	**Position**	P1-A3
Instrument Name	6545 QTof	**User Name**	Laura English
Acq Method	Pos_5mins_MS.m	**Acquired Time**	8/24/2021 4:04:05 PM
IRM Calibration Status	🟩 Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	RC193 - C21H20N2	**Walkup Method**	Pos_5Mins_C18
Formula	C21H20N2	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

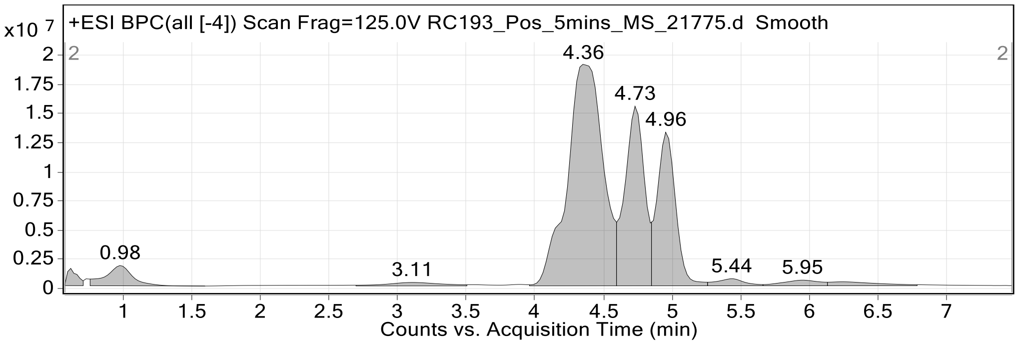

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.62	7457646	2.16	1.08	194.1179	0.080
0.98	23793281	6.91	3.46	225.1388	0.190
3.11	8395207	2.44	1.22	922.0090	0.410
4.36	344493708	100.00	50.10	321.2347	0.270
4.73	153228187	44.48	22.28	543.3586	0.150
4.96	124136599	36.03	18.05	337.2308	0.140
5.44	8658314	2.51	1.26	353.2669	0.200
5.95	9053976	2.63	1.32	125.9865	0.270
6.24	8450105	2.45	1.23	922.0107	0.360

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C21 H20 N2	4.16	301.1703	300.1630	300.1626	1.09	99.21

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

1 and phenyl isocyanate immediately quench

Walkup MS Report

Data File	RC284_Pos_5mins_MS_24268.d	**Sample Name**	RC284
Sample Type	Sample	**Position**	P1-C4
Instrument Name	6545 QTof	**User Name**	Rex Charman
Acq Method	Pos_5mins_MS.m	**Acquired Time**	12/6/2021 1:15:54 PM
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	6MesCuSnPh3 + PhNCO, after immediate quenching with wet acetonitrile	**Walkup Method**	Pos_5Mins_C18
Formula	C25H21NOSn	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

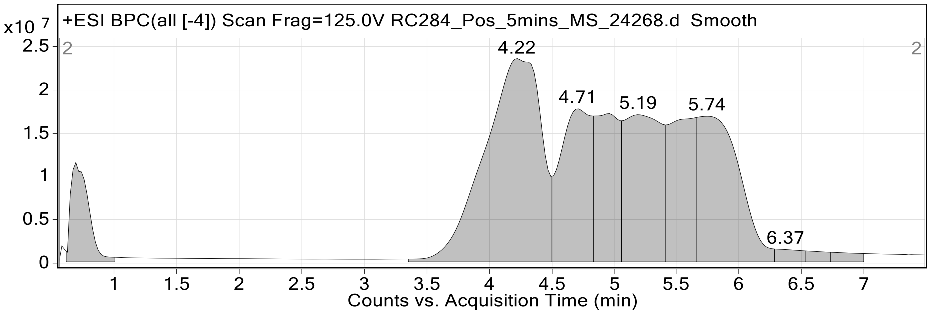

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.69	114879329	15.39	4.73	144.9813	0.140
4.22	746362715	100.00	30.72	321.2334	0.420
4.71	306886689	41.12	12.63	321.2311	0.250
4.95	225090884	30.16	9.26	673.4443	0.170
5.19	351586829	47.11	14.47	321.2308	0.310
5.52	237368520	31.80	9.77	321.2307	0.210
5.74	395892932	53.04	16.29	321.2308	0.390
6.37	20465789	2.74	0.84	337.2239	0.210
6.59	14378769	1.93	0.59	337.2236	0.160
6.75	16652255	2.23	0.69	337.2238	0.210

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)	Error flag
Cpd 1: C25 H21 N O Sn	0.58	494.0531	463.0675	463.0671	0.76	71.15	No H adduct

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

1 and phenyl isocyanate after hours

walkup MS Report

Data File	6MesCuSnPh3 + PhNCO_Pos_5mins_MS_21586.d	**Sample Name**	6MesCuSnPh3 + PhNCO
Sample Type	Sample	**Position**	P1-A3
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Pos_5mins_MS.m	**Acquired Time**	8/20/2021 6:57:49 PM
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	HN(Ph)C(O)Ph	**Walkup Method**	Pos_5Mins_C18
Formula	C13H11NO	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

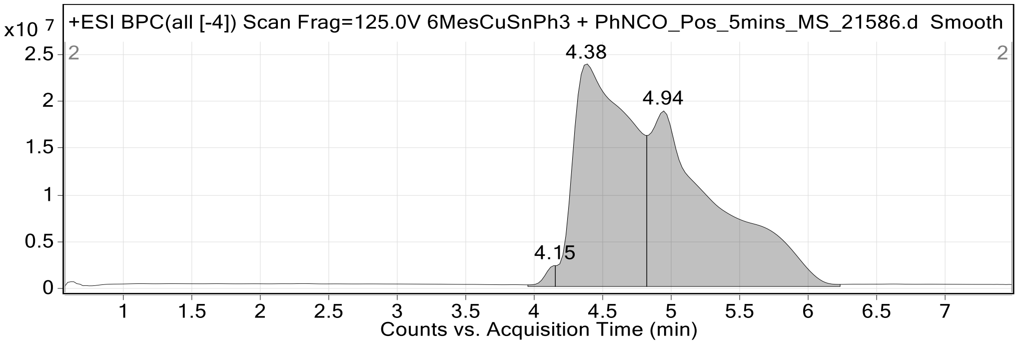

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
4.15	11734672	1.72	0.86	356.2124	0.080
4.38	682533166	100.00	50.25	321.2376	0.390
4.94	663909035	97.27	48.88	337.2317	0.450

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C13 H11 N O	4.41	198.0914	197.0842	197.0841	0.49	99.37

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

IPrCuSnPh3 + PhNCO after hours

Walkup MS Report

Data File	IprCuSnPh3 + PhNCO_Pos_5mins_MS_21582.d	**Sample Name**	IprCuSnPh3 + PhNCO
Sample Type	Sample	**Position**	P1-A2
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Pos_5mins_MS.m	**Acquired Time**	8/20/2021 6:49:26 PM
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	HN(Ph)C(O)Ph	**Walkup Method**	Pos_5Mins_C18
Formula	C13H11NO	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

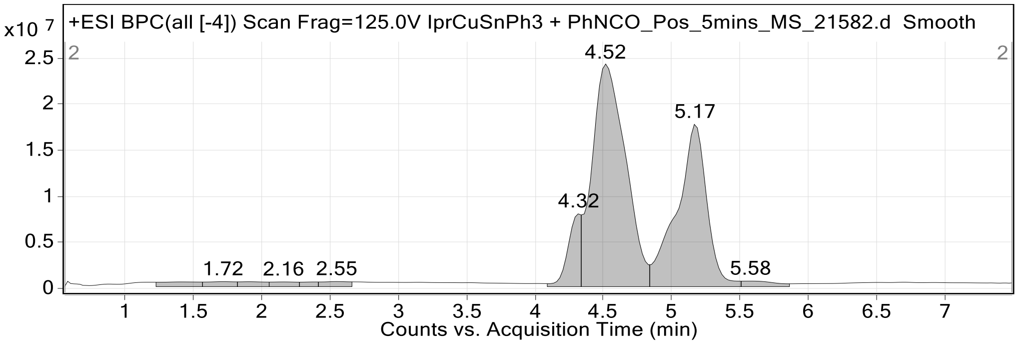

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
1.42	10176856	2.47	1.29	101.0042	0.270
1.72	7996225	1.94	1.02	101.0039	0.210
1.91	7176305	1.74	0.91	101.0039	0.180
2.16	6669473	1.62	0.85	101.0037	0.190
2.40	4144636	1.01	0.53	101.0038	0.120
2.55	7802049	1.90	0.99	101.0035	0.200
4.32	50962331	12.38	6.47	351.0205	0.100
4.52	411599473	100.00	52.28	389.3022	0.250
5.17	270428449	65.70	34.35	405.2953	0.220
5.58	10372874	2.52	1.32	389.2963	0.260

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C13 H11 N O	4.41	198.0914	197.0842	197.0841	0.47	99.51

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

PhNCO + Ph3SnH with 10 mol% **1**

Walkup MS Report

Data File	RC184_Pos_5mins_MS_21531.d	**Sample Name**	RC184
Sample Type	Sample	**Position**	P1-A3
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Pos_5mins_MS.m	**Acquired Time**	19/08/2021 15:50:02
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	(PhNCO)3	**Walkup Method**	Pos_5Mins_C18
Formula	C21H15N3O3	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

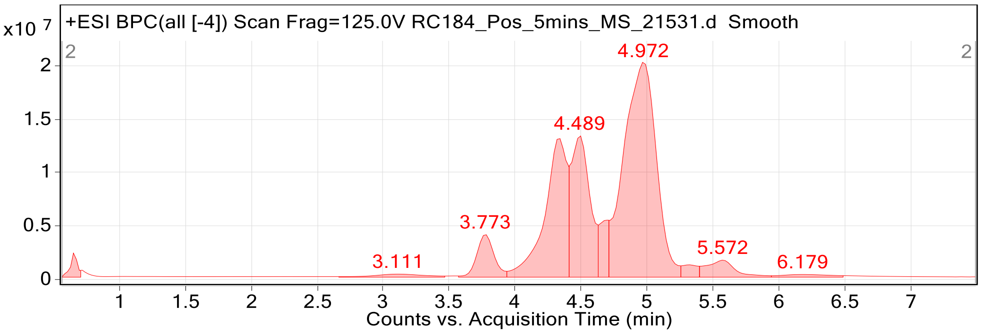

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.66	8375296	2.44	1.13	123.0915	0.061
3.11	7708273	2.24	1.04	922.0078	0.397
3.77	36354397	10.58	4.89	122.0600	0.139
4.33	152699047	44.43	20.56	321.2341	0.170
4.49	128889487	37.50	17.35	440.2729	0.147
4.70	25044997	7.29	3.37	342.1240	0.065
4.97	343683561	100.00	46.27	337.2311	0.246
5.32	9323880	2.71	1.26	400.2384	0.114
5.57	24381139	7.09	3.28	351.0192	0.212
6.18	6385758	1.86	0.86	922.0085	0.408

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C21 H15 N3 O3	4.36	358.1188	357.1114	357.1113	0.29	96.94

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

1 and phenyl isothiocyanate after 30 minutes

Walkup MS Report

Data File	RC285_Pos_5mins_MS_24224.d	**Sample Name**	RC285
Sample Type	Sample	**Position**	P1-A4
Instrument Name	6545 QTof	**User Name**	Rex Charman
Acq Method	Pos_5mins_MS.m	**Acquired Time**	06/12/2021 11:25:49
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	6MesCuSnPh3 + PhNCS, after 30 minutes, orange solution.	**Walkup Method**	Pos_5Mins_C18
Formula	C25H21NSnS	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

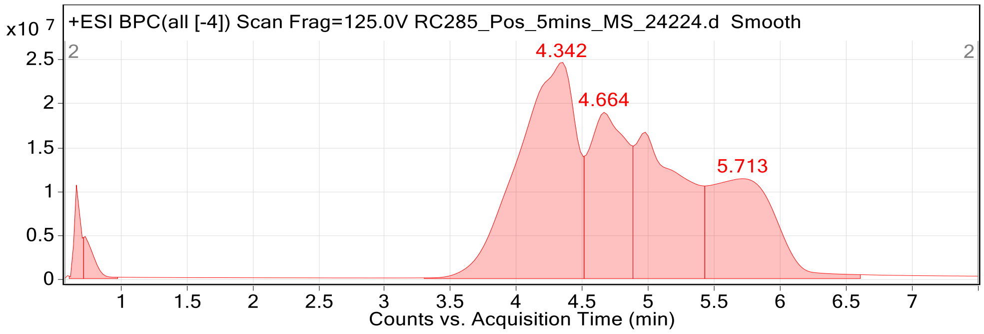

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.67	35393388	4.66	1.76	144.9815	0.055
0.72	24814410	3.27	1.23	144.9812	0.086
4.34	759039911	100.00	37.69	321.2354	0.400
4.66	370275236	48.78	18.38	486.1966	0.269
4.97	425038382	56.00	21.10	673.4462	0.331
5.71	399517377	52.63	19.84	321.2304	0.537

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C25 H21 N S Sn	5.45	488.0491	479.0463	479.0443	4.25	68.09

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

1 and phenyl isothiocyanate after 16 hrs

Walkup MS Report

Data File	RC194_Neg_5mins_MS_21878.d	**Sample Name**	RC194
Sample Type	Sample	**Position**	P1-B1
Instrument Name	6545 QTof	**User Name**	Thomas Horsley Downie
Acq Method	Neg_5mins_MS.m	**Acquired Time**	8/27/2021 1:32:43 PM
IRM Calibration Status	Success	**DA Method**	Neg_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description	After overnight RT - orange solution	**Walkup Method**	Neg_5Mins_C18
Formula	C13H11NS	**Walkup Method Description**	Negative mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

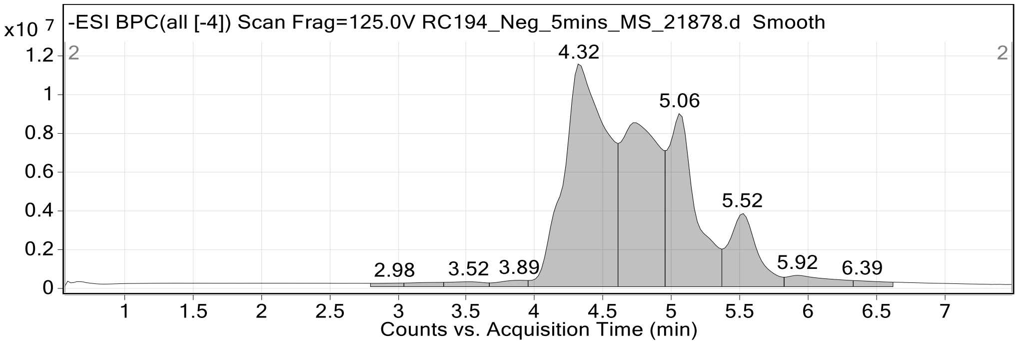

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
2.98	2634082	1.05	0.42	134.8656	0.190
3.20	3648504	1.46	0.58	134.8655	0.240
3.52	4693033	1.87	0.75	134.8657	0.280
3.89	4798245	1.91	0.76	134.8657	0.220
4.32	250645116	100.00	39.94	441.0167	0.290
4.73	161914350	64.60	25.80	441.0165	0.290
5.06	125953000	50.25	20.07	311.2032	0.200
5.52	54922585	21.91	8.75	293.1799	0.210
5.92	13637659	5.44	2.17	134.8662	0.310
6.39	4754301	1.90	0.76	134.8660	0.210

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C13 H11 N S	4.55	212.0541	213.0613	213.0612	0.48	98.77

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

---

References

1. L. R. Collins, I. M. Riddlestone, M. F. Mahon, M. K. Whittlesey, *Chem. - Eur. J.*, 2015, **21**, 14075 –14084; J. W. Hall, D. M. L. Unson, P. Brunel, L. R. Collins, M. K. Cybulski, M. F. Mahon, and M. K. Whittlesey, *Organometallics*, 2018, **37**, 3102–3110; A. J. Jordan, C. M. Wyss, J. Bacsa, and J. P. Sadighi, *Organometallics*, 2016, **35**, 5, 613–616.
2. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
3. G. Sheldrick, *Acta Cryst. A*, 2015, **71**, 3-8.
4. K. X. Bhattacharyya, J. A. Akana, D. S. Laitar, J. M. Berlin, and J. P. Sadighi, *Organometallics*, 2008, **27**, 12, 2682–2684
5. B. Wrackmeyer, *Annu. Rep. NMR Spectrosc.*, 1999, **38**, 203–264; N. R. Neale and T. D. Tilley, J. Am. Chem. Soc., 2005, **127**, 14745-14755; U. Englich, K. Ruhlandt-Senge, F. Uhlig, *J. Organomet. Chem.*, 2000, **613**, 139-147.