Supporting Information

Contents

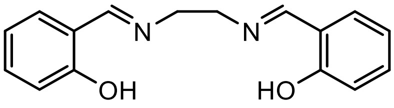
General procedures

Solvents and chemicals were purchased from commercial suppliers (Abcr, Merck, TCI, Lach:ner, Acros). Unless otherwise specified, solvents were dried using automatic drying system PureSolv MD5, or by storing upon activated molecular sieves and degassed by freeze-pump-thaw before use. Glassware was dried and stored in an oven heated up to 180 °C overnight. NMR spectra were measured on Bruker AVANCE-III (400 MHz) at 25 °C. Chemical shifts for ^{1}H are given in δ relative to tetramethylsilane (TMS) and are referenced to residual protium in the NMR solvent ($CDCl_3$: $\delta = 7.26$ ppm, DMSO-d6: $\delta = 2.50$). Chemical shifts for ^{13}C are given in δ relative to TMS and are referenced to the carbon resonances in the solvent ($CDCl_3$: $\delta = 77.0$ ppm, DMSO-d6: $\delta = 39.5$). Peaks of ^{119}Sn NMR spectra are referenced to the external standard peak of tetramethyl-Sn (0 ppm). Peaks of ^{19}F NMR spectra are referenced to the external standard peak of trifluoacetic acid (0 ppm). Mass spectrometry measurements were provided by Service centrum of Mass spectrometry at the Department of Chemistry, Charles University. Ionization method used was ESI positive and the spectra were measured in MeOH. Optimization of catalysts was performed at least in duplicate but generally in triplicate and analyzed by NMR with dibromomethane as the internal standard and structures confirmed by ESI-MS. For determination of total carbon, total nitrogen and total hydrogen were samples weighed into tin capsules (Elemental Microanalysis, 8 × 5 mm) and analysed on elementar analyser with thermal conductivity detector (Flash Smart, Thermo Fisher Scientific, Bremen, Germany).

General synthesis procedure of Schiff base ligands

The general procedure followed synthesis of the ligands according to literature[1]. One equivalent (eq) of the relevant diamine and 2 eq of the relevant salicylaldehyde were dissolved in EtOH. The reaction mixture was refluxed and followed by TLC (hexane : ethyl acetate, 7 : 3). After consumption of the starting materials, the reaction was left to cool down and was placed in a fridge. Solid product was filtrated, washed with ice-cold EtOH and dried in air.

Salen



50 mmol (3.34 mL) of ethylenediamine were used together with 100 mmol (10.52 mL) salicylaldehyde and 210 mL of EtOH. The mixture was refluxed for 90 min. The product was obtained in the form of yellow crystals in 95 % (12.78 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.20 (s, 2H), 8.36 (s, 2H), 7.29 (ddd, J = 8.3, 7.3, 1.7 Hz, 2H), 7.23 (dd, J = 7.7, 1.7 Hz, 2H), 6.94 (dd, J = 8.4, 1.1 Hz, 2H), 6.86 (td, J = 7.5, 1.1 Hz, 2H), 3.95 (s, 4H). ^{13}C NMR (101 MHz, CDCl3) δ 167, 161, 132, 131, 119, 119, 117, 60. ESI + (m/z) for $C_{16}H_{16}N_2O_2^+$ 269.1, calculated 269.3.

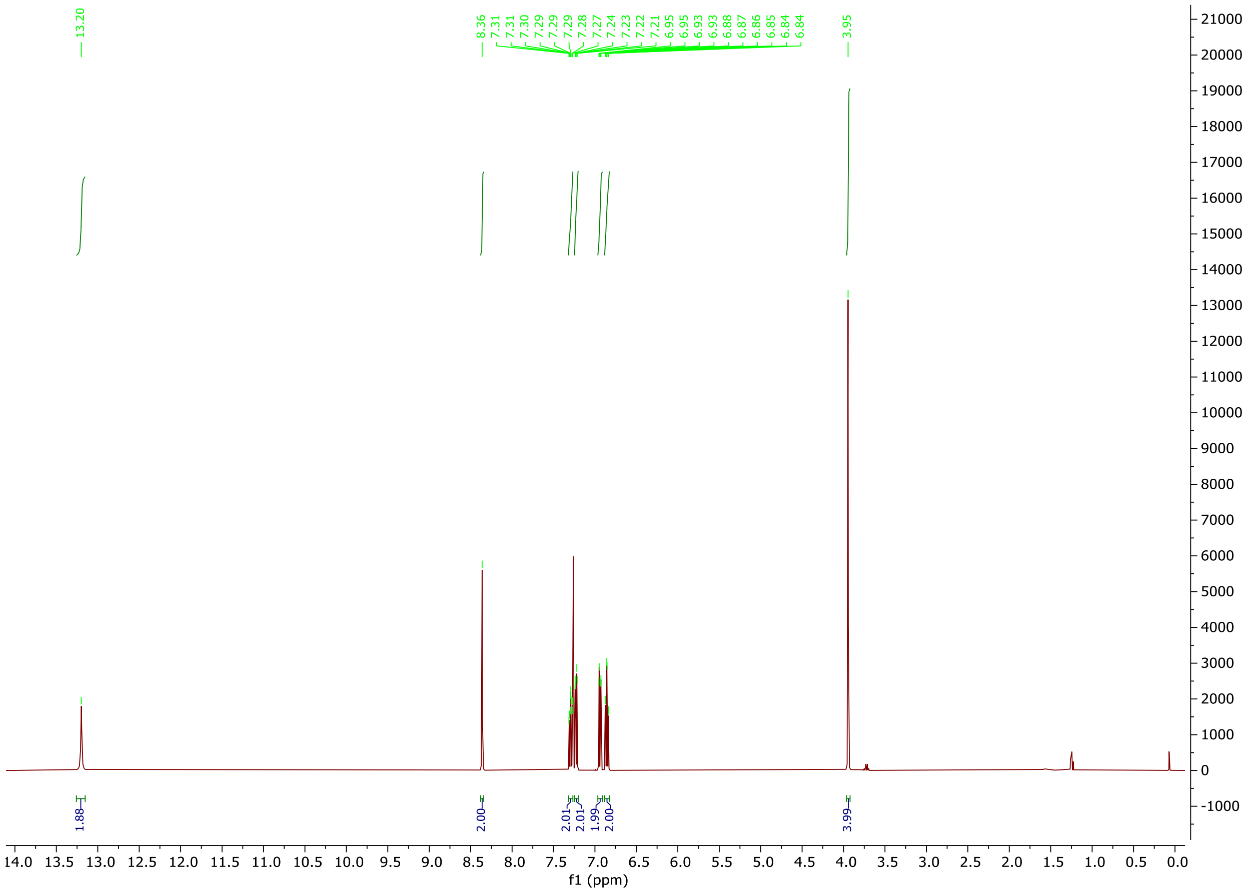


Figure 1: ^{1}H NMR of salen in $CDCl_3$

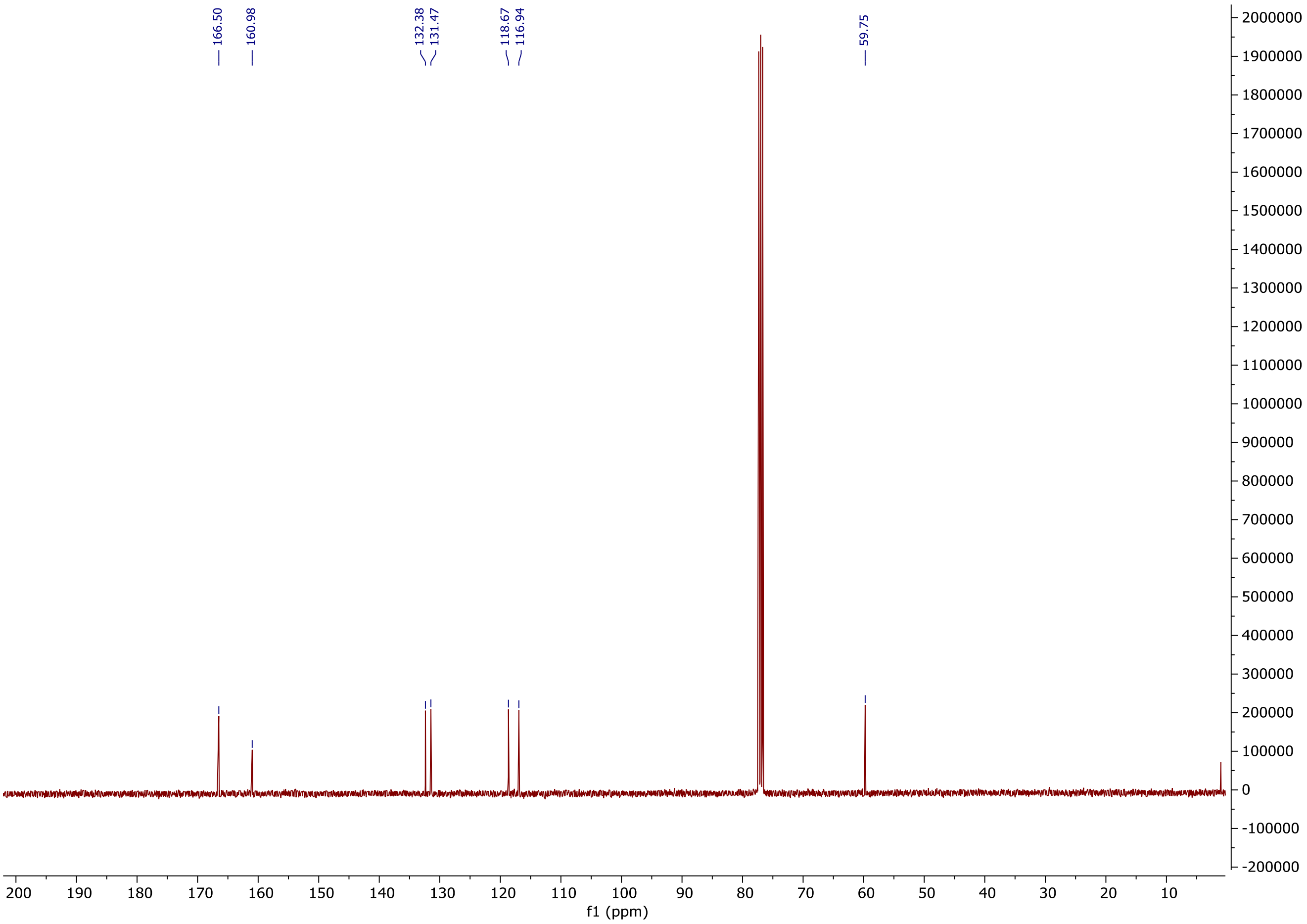


Figure 2: ^{13}C NMR of salen in $CDCl_3$

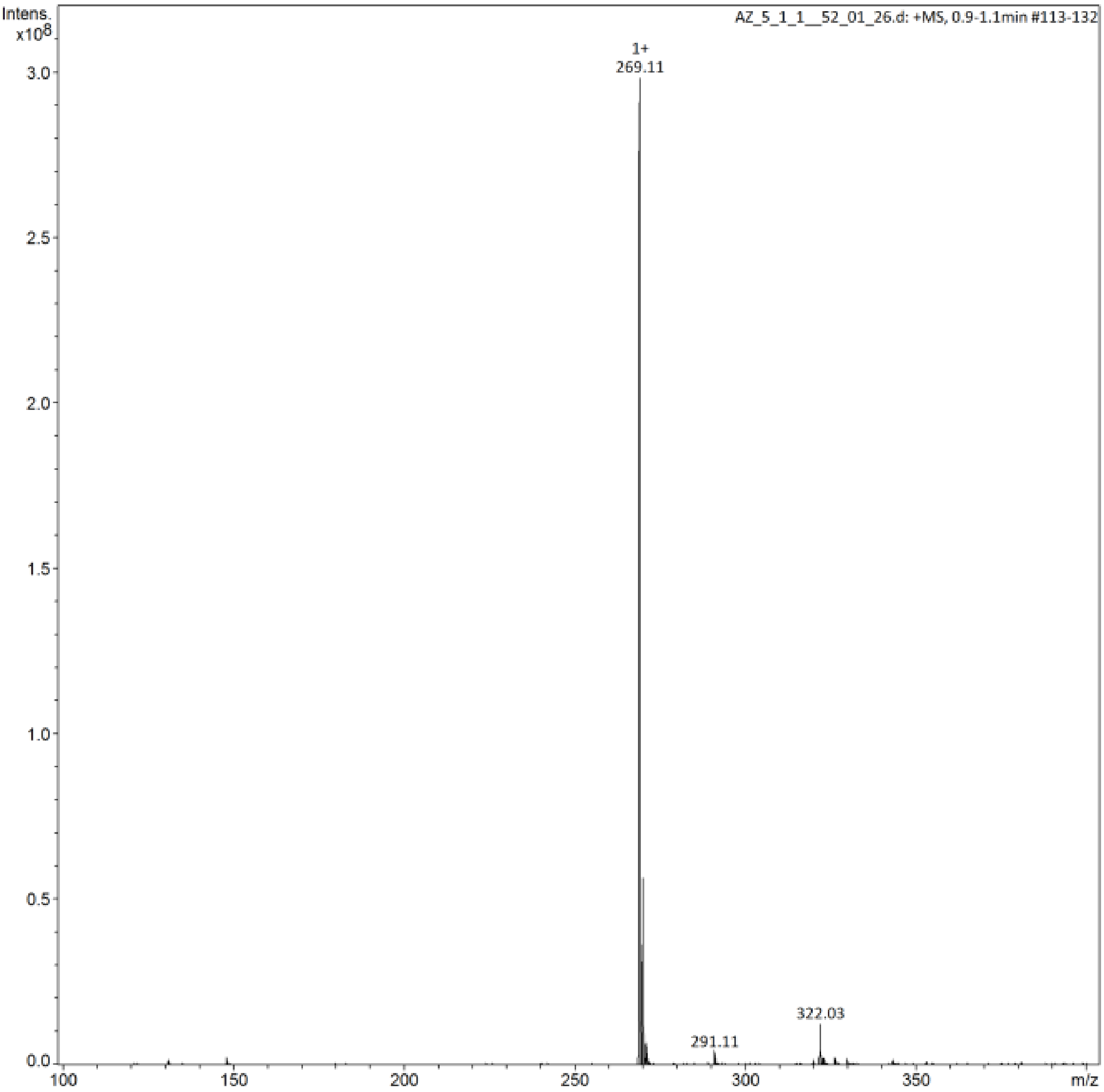
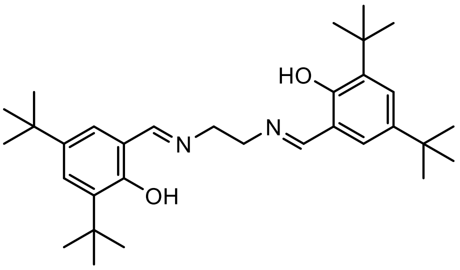


Figure 3: ESI-MS of salen

3,5-di-tert-butyl-salen



25 mmol (1.67 mL) of ethylenediamine was used together with 50 mmol (11.72 g) 3,5-di-tert-butyl-salicylaldehyde and 210 mL of EtOH. The mixture was refluxed for 120 min. The product was obtained in the form of yellow powder in 98 % (12.03 g) yield. ^{1}H NMR (400 MHz, CDCl$_3$) δ 13.63 (s, 1H), 8.38 (s, 2H), 7.36 (d, J = 2.5 Hz, 2H), 7.06 (d, J = 2.4 Hz, 2H), 3.92 (s, 4H), 1.43 (s, 18H), 1.28 (s, 19H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 168, 158, 140, 137, 127, 126, 118, 60, 35, 34, 32,30. ESI + (*m/z*) for $C_{32}H_{48}N_2O_2^+$ 493.4, calculated 493.8.

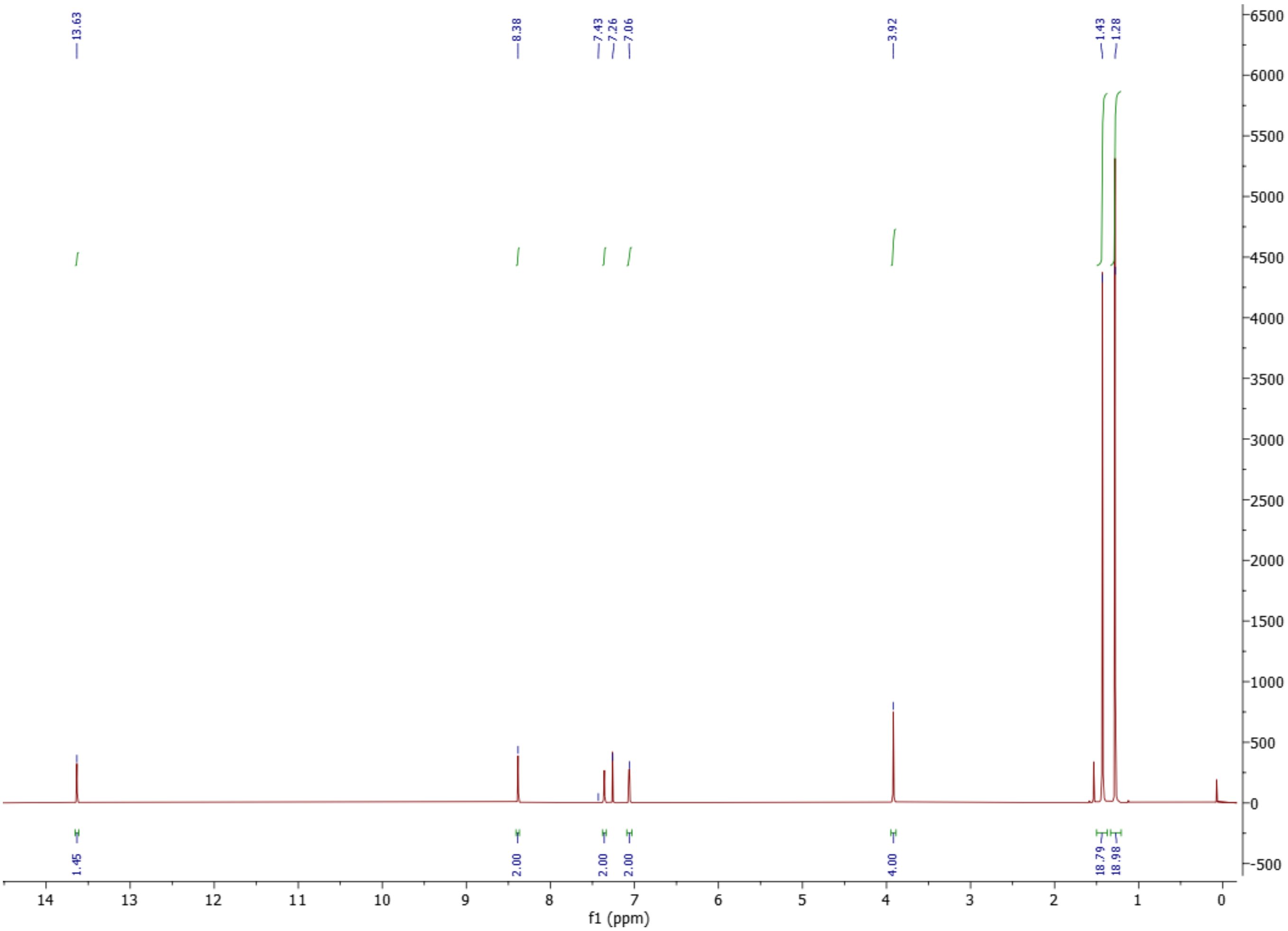


Figure 4: ^{1}H NMR of 3,5-di-tert-butyl-salen in CDCl$_3$

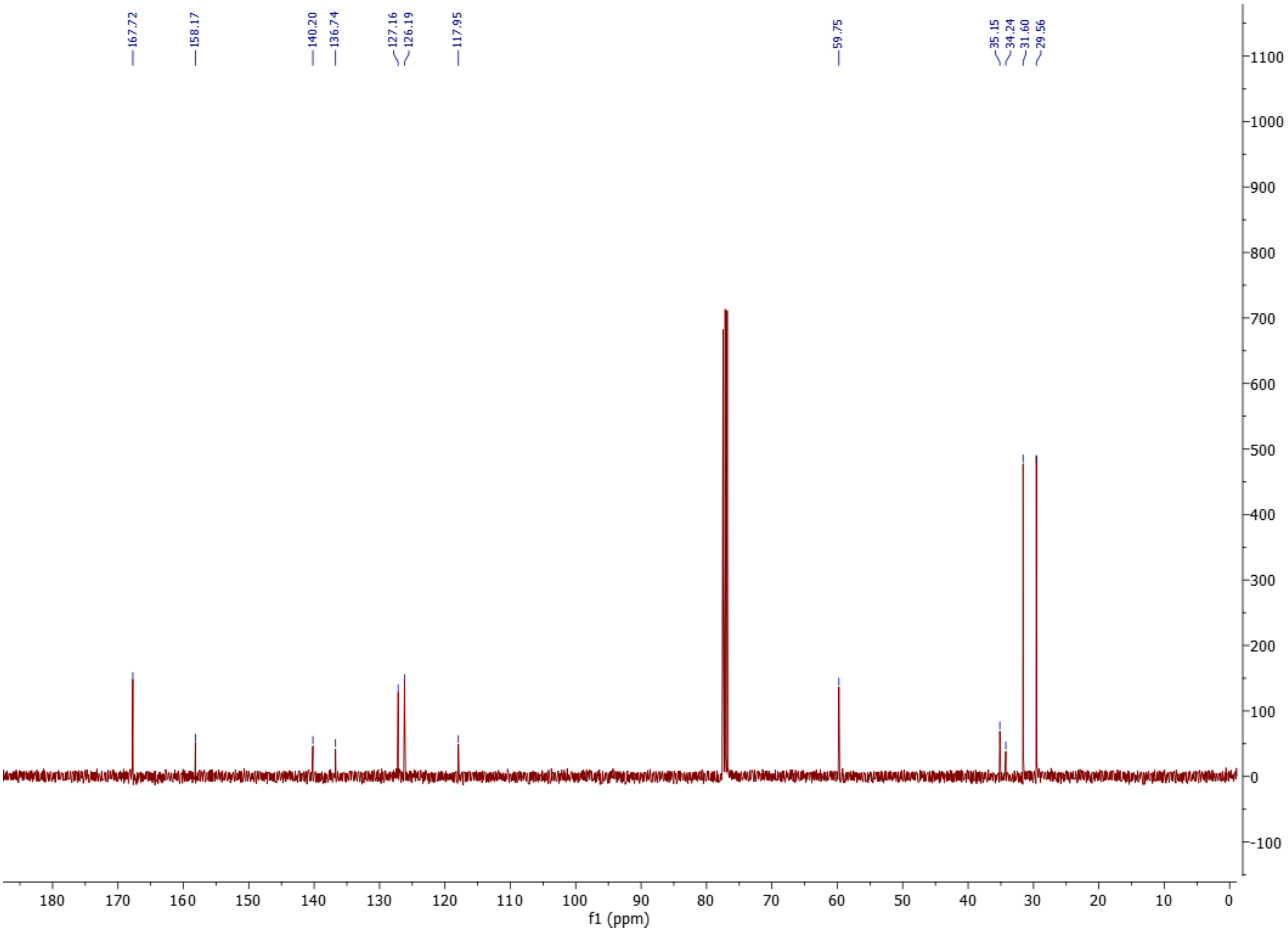


Figure 5: ^{13}C NMR of 3,5-di-tert-butyl-salen in $CDCl_3$

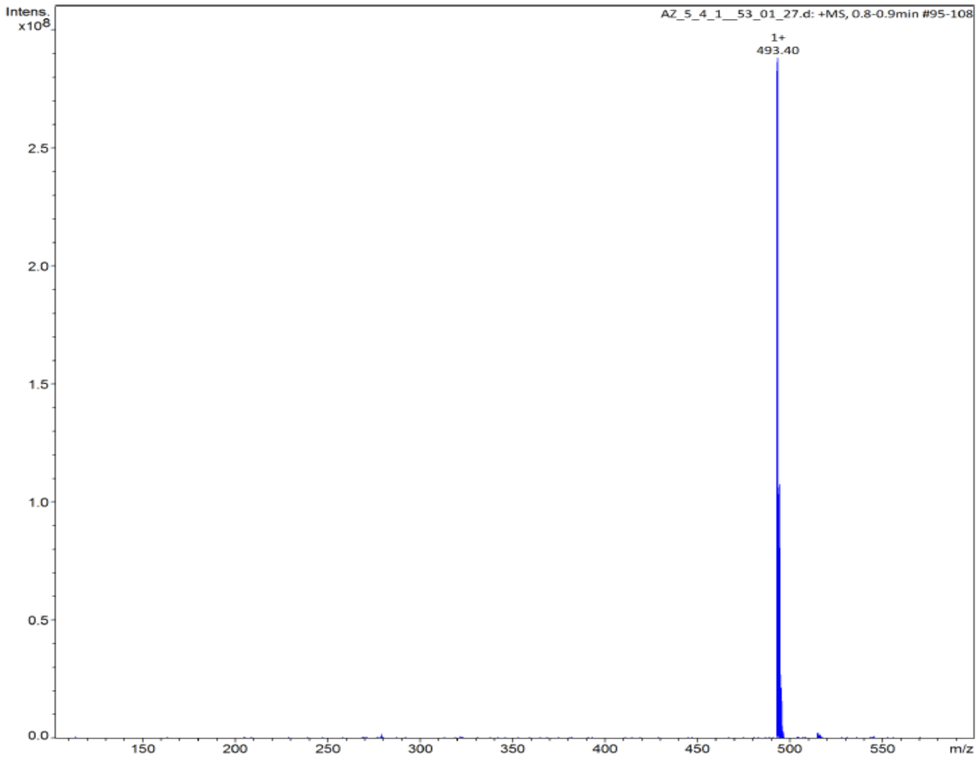
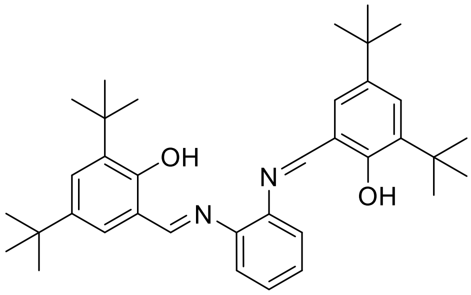


Figure 6: ESI-MS of ^{1}H NMR of 3,5-di-tert-butyl-salen

3,5-di-tert-butyl-salophen



12.5 mmol (1.35 g) of phenylenediamine was used together with 25 mmol (5.86 g) 3,5-di-tert-butyl-salicylaldehyde and 105 mL of EtOH. The mixture was refluxed overnight. The product was obtained in the form of orange powder in 52 % (3.51 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.53 (s, 2H), 8.66 (s, 2H), 7.44 (d, *J* = 2.5 Hz, 2H), 7.31 (dd, *J* = 5.9, 3.4 Hz, 2H), 7.23 (dd, *J* = 5.9, 3.4 Hz, 2H), 7.21 (d, *J* = 2.4 Hz, 2H), 1.43 (s, 18H), 1.32 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165, 159, 143, 140, 137, 128, 127, 127, 120, 119, 35, 34, 32, 30. ESI + (*m/z*) 563.5 for $C_{36}H_{48}N_2O_2Na^+$ and 541.5 for $C_{36}H_{49}N_2O_2^+$, calculated 563.4 for $C_{36}H_{48}N_2O_2Na^+$ and 541.4 for $C_{36}H_{49}N_2O_2^+$.

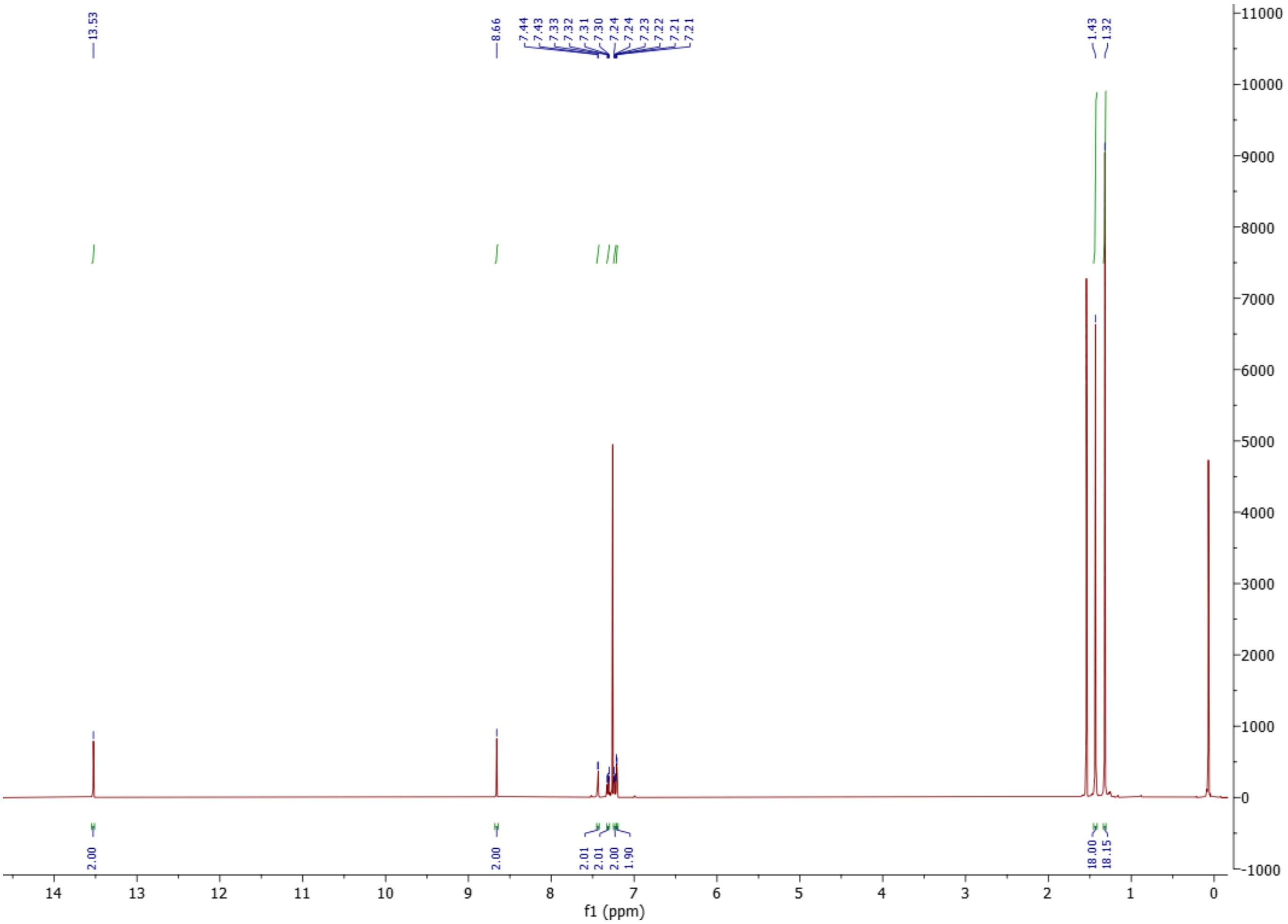


Figure 7: ^{1}H NMR of 3,5-di-tert-butyl-salophen in $CDCl_3$

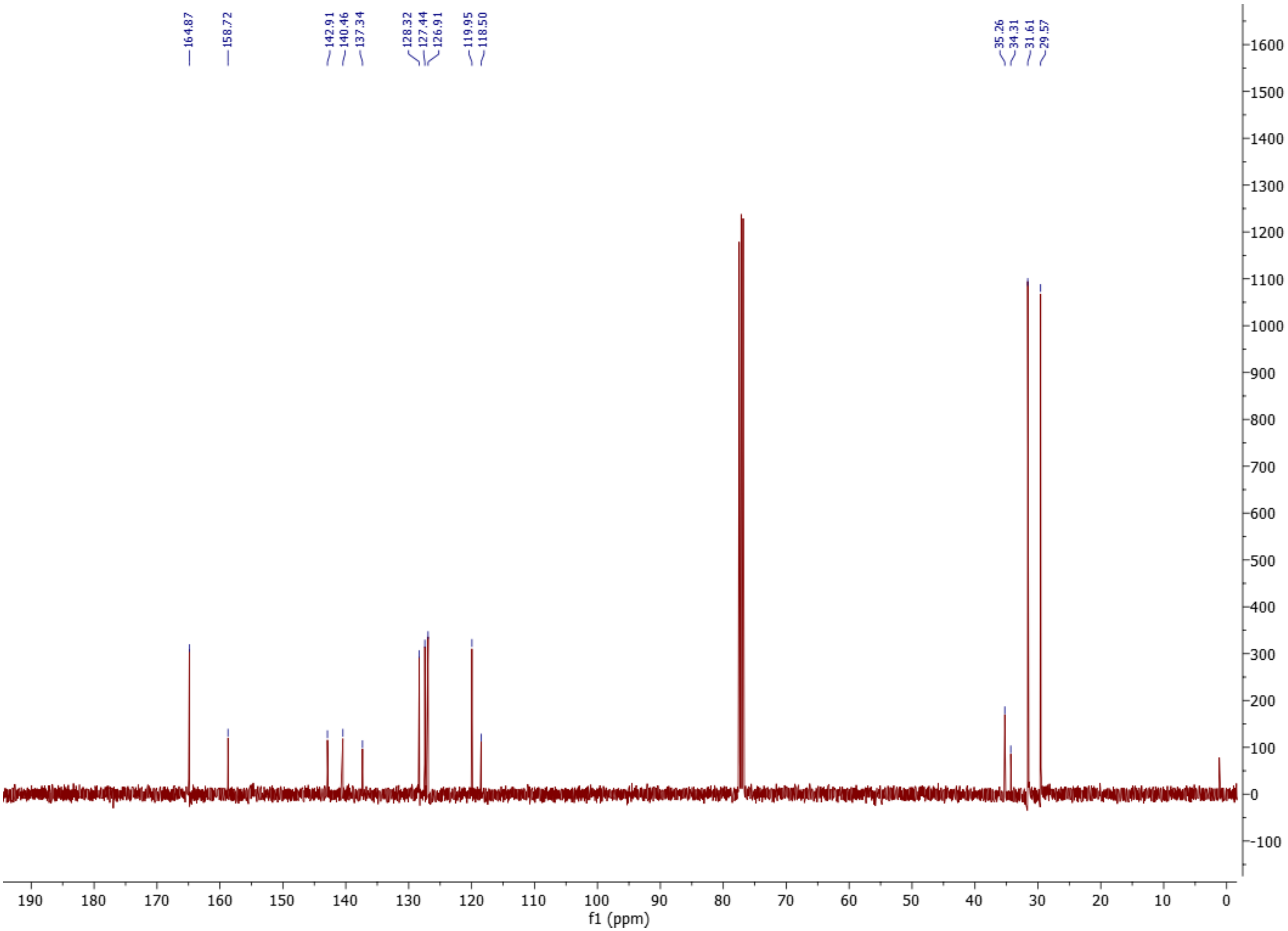


Figure 8: ^{13}C NMR of 3,5-di-tert-butyl-salophen in $CDCl_3$

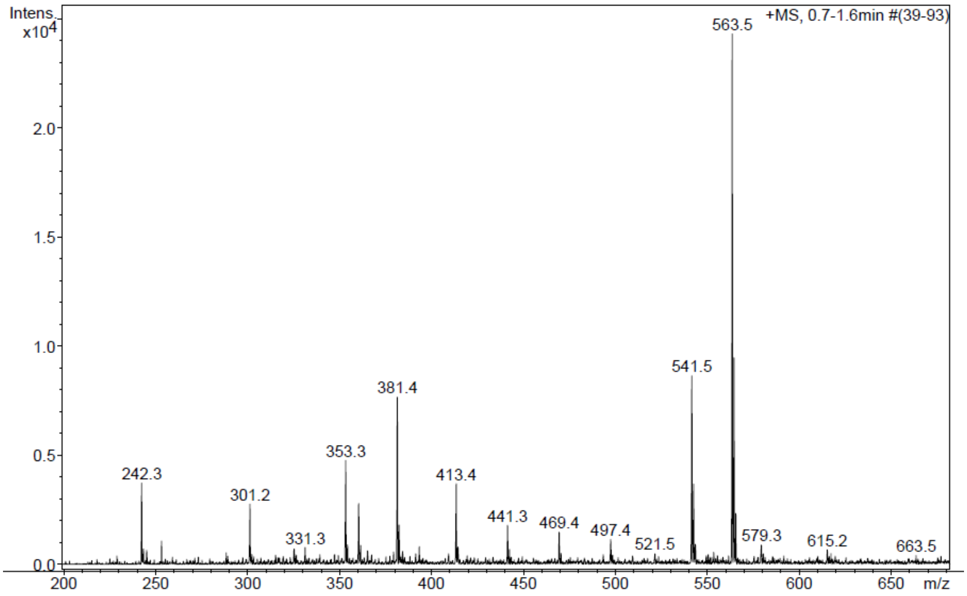


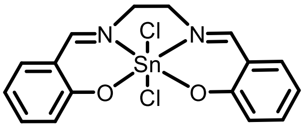
Figure 9: ESI-MS of 3,5-di-tert-butyl-salophen

General synthesis procedure of dichloro-complexes

Complexes [Sn(Salen)Cl_2] and [Sn($^tBu_2$Salen)Cl_2] were prepared according to procedures reported in the literature[2].Complexes [Sn($^tBu_2$Salophen)Cl_2] and [Sn(Salophen)Cl_2] were prepared according to a modified protocol reported for [Sn(Salen)Cl_2].

Reactions were performed in an inert atmosphere of N_2 using Schlenk line apparatus and techniques. Solvents and glassware were dried according to the general procedures. One eq of initial ligand was dissolved in DCM. One eq of $SnCl_4$ was added to the stirring mixture followed by 2 eq of triethylamine. Reactions were followed by NMR and the reaction mixture was left to react at RT until full conversion of the starting materials occured. Reaction work-up was performed in air and is described separately for each complex.

[Sn(Salen)Cl_2]



6 mmol, (1.61 g) of salen ligand was used together with 6 mmol (0.70 mL) of $SnCl_4$, 12 mmol (1.67 mL) of Et_3N and 50 mL of DCM. The reaction was stirring for 1h. Product precipitated out of the reaction mixture and was filtrated of. The solid was washed with cold DCM and dried in vacuo. The filtrate was placed in the freezer to crash out the Et3N salt, which was filtered off. The filtrate was overlaid with pentane. Crystallised solid was washed with H_2O, DCM and dried in vacuo. The solid fractions were combined to provide product as a pale-yellow powder in 54 % (1.48 g) yield. (1.12 g) yield. ^{1}H NMR (400 MHz, DMSO-d6) δ 8.79 (s, 2H, *J*(H-Sn) = 88.9), 7.53 (dd, *J* = 8.5, 6.5 Hz, 4H), 7.01 – 6.88 (m, 4H), 4.19 (s, 4H, *J*(H-Sn) = 35.9). ^{13}C NMR (101 MHz, DMSO-d6) δ 172, 165, 137, 136, 122, 119, 118, 51. ^{119}Sn NMR (149 MHz, DMSO-d6) δ −603. ESI + (*m/z*) for $C_{16}H_{14}ClN_2O_2Sn^+$ 421.0, calculated 420.9 for $C_{16}H_{14}ClN_2O_2Sn^+$. IR 1625 cm^{-1} ν(C=N), 1598, 1544, 1436 cm^{-1} ν(C=C)$_{arom}$, 1270 cm^{-1} ν(C-O), 670 cm^{-1} ν(Sn-O), 447 cm^{-1} ν(Sn-N). Elemental. analysis: measured C 41.98%, N 6.16%, H 3.19%; calculated C 42.15%, N 6.14%, H 3.10%

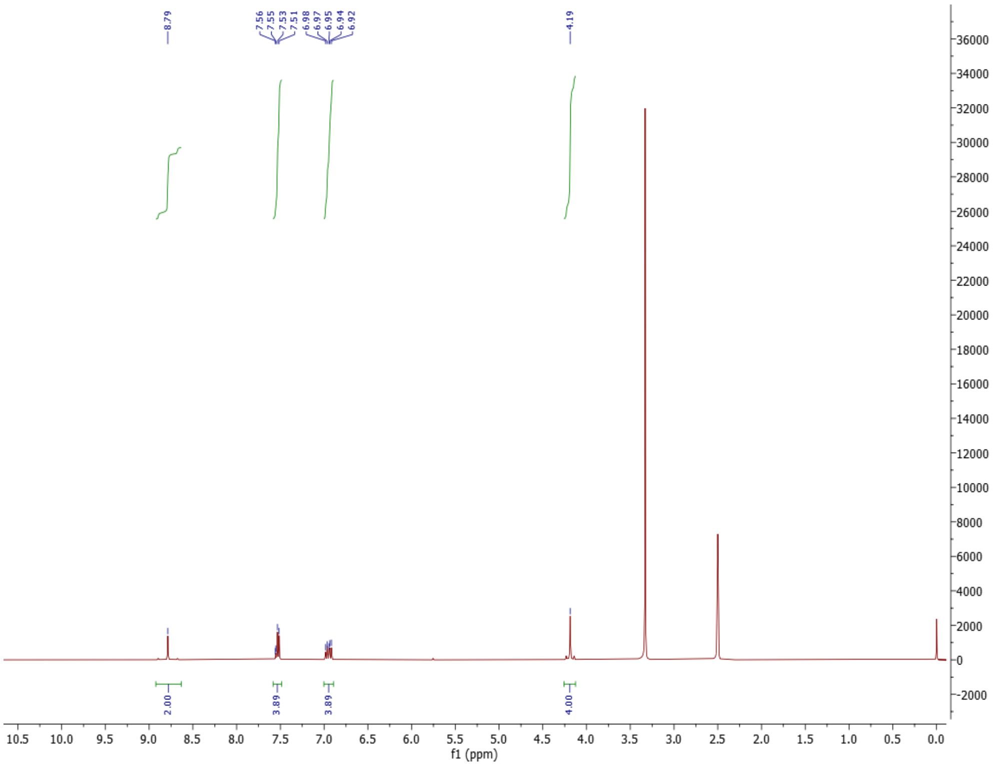


Figure 10: ^{1}H NMR of [Sn(Salen)Cl$_2$] in DMSO-d6

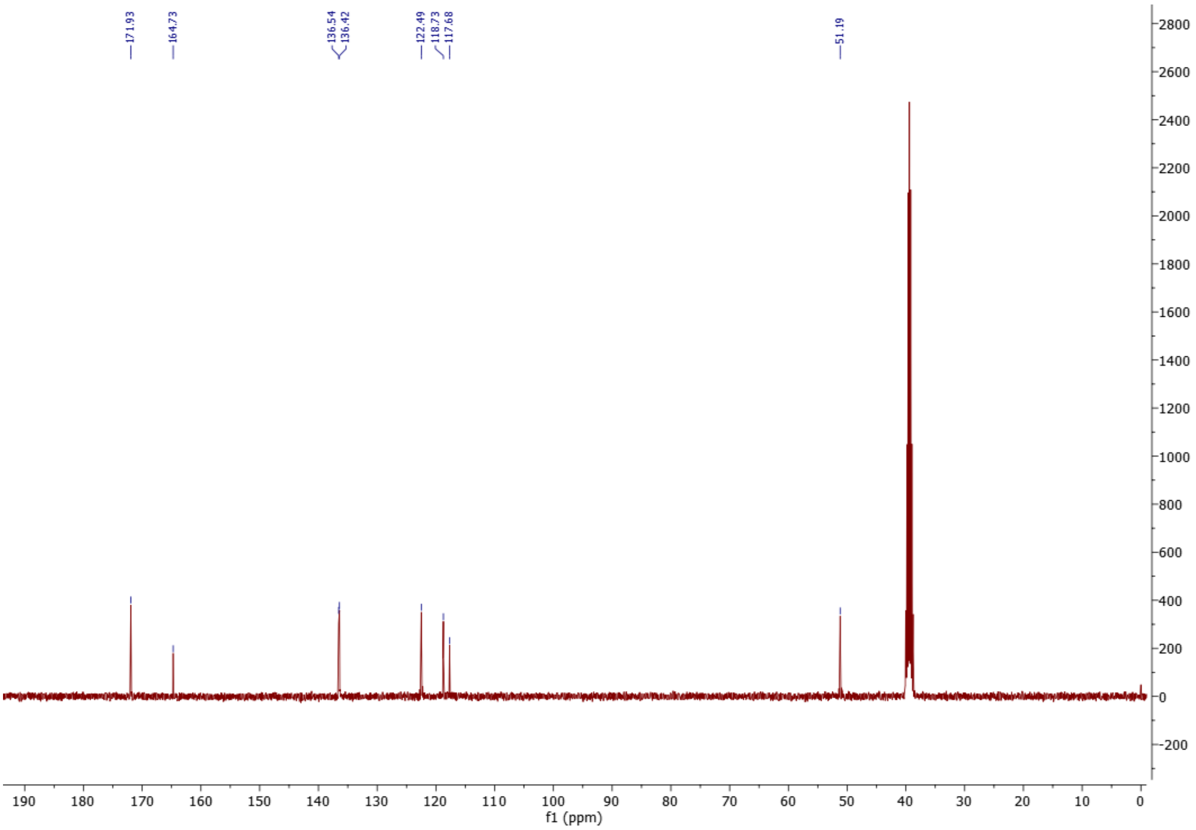


Figure 11: ^{13}C NMR of [Sn(Salen)Cl$_2$]

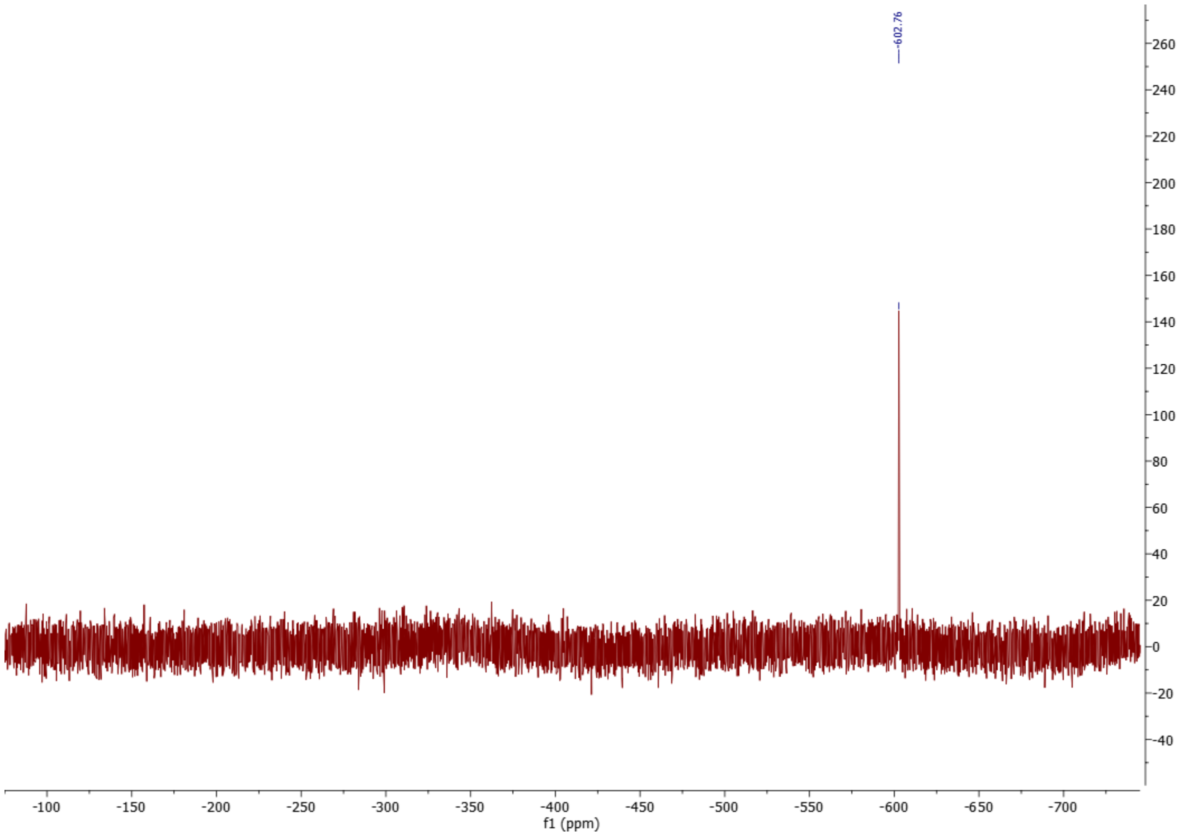


Figure 12: ^{119}Sn NMR of [Sn(Salen)Cl_2]

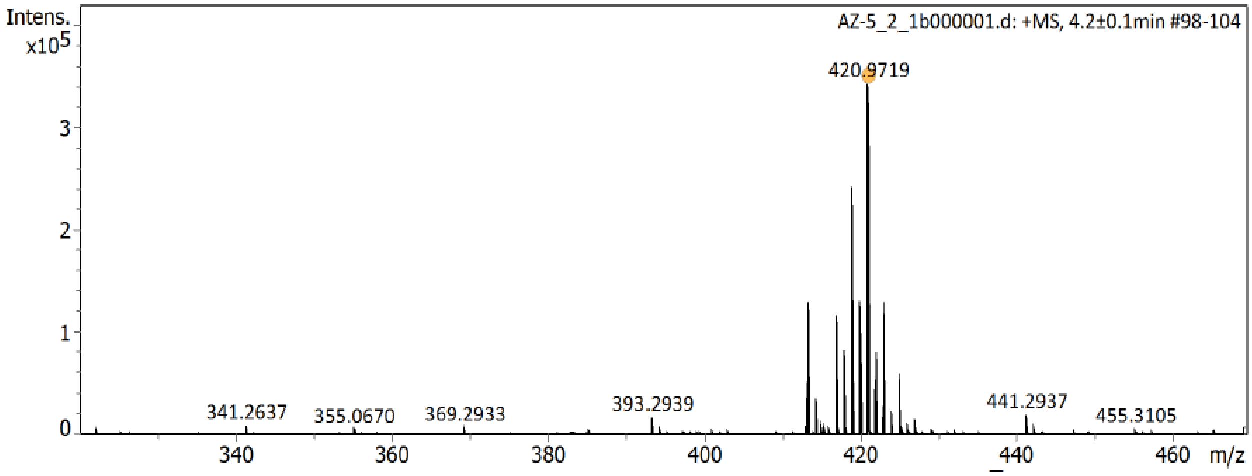
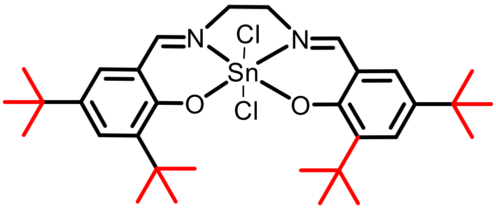


Figure 13: ESI-MS of [Sn(Salen)Cl_2] after loss of chloride during ionization

[Sn(^{t}Bu$_2$Salen)Cl_2]



7 mmol (3.45 g) of 3,5-di-tert-butyl-salen was used together with 7 mmol (0.78 mL) of $SnCl_4$, 14 mmol (1.95 mL) of Et_3N and 40 mL of DCM. The reaction was stirring for 3 hours. The reaction mixture was washed three times with 50 mL of water. The aqueous phase was further washed three times extracted with 15 mL of DCM. Organic phases were combined, dried over $MgSO_4$, filtrated and evaporated. Obtained solid was

washed with cold heptane, redissolved in $CDCl_3$ and dried in vacuo. The product was obtained in the form of yellow powder in 90 % (4.27 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 2H, *J*(H-Sn) = 90.0), 7.61 (d, *J* = 2.6 Hz, 2H), 7.03 (d, *J* = 2.5 Hz, 2H), 4.19 (s, 4H, *J*(H-Sn) = 35.6), 1.51 (s, 17H), 1.30 (s, 18H). ^{13}C NMR (101 MHz, DMSO-d6) δ 172, 162, 141, 140, 131, 118, 51, 35, 34, 31, 29. ^{119}Sn NMR (149 MHz, DMSO-d6) δ -594. ESI + (*m/z*) for $C_{33}H_{49}N_2O_3Sn^+$ 641.2 and for $C_{32}H_{47}N_2O_3Sn^+$ 627.4, calculated 641.3 for $C_{33}H_{49}N_2O_3Sn^+$ after loss of chlorides and attachment of methoxide from MeOH in the measurement and 627.3 for $C_{32}H_{47}N_2O_3Sn^+$ after loss of chlorides and attachment of hydroxide from water in the measurement. IR 1625 cm^{-1} ν(C=N), 1556, 1540, 1436 cm^{-1} ν(C=C)$_{arom}$, 1247 cm^{-1} ν(C-O), 545 cm^{-1} ν(Sn-O), 468 cm^{-1} ν(Sn-N).

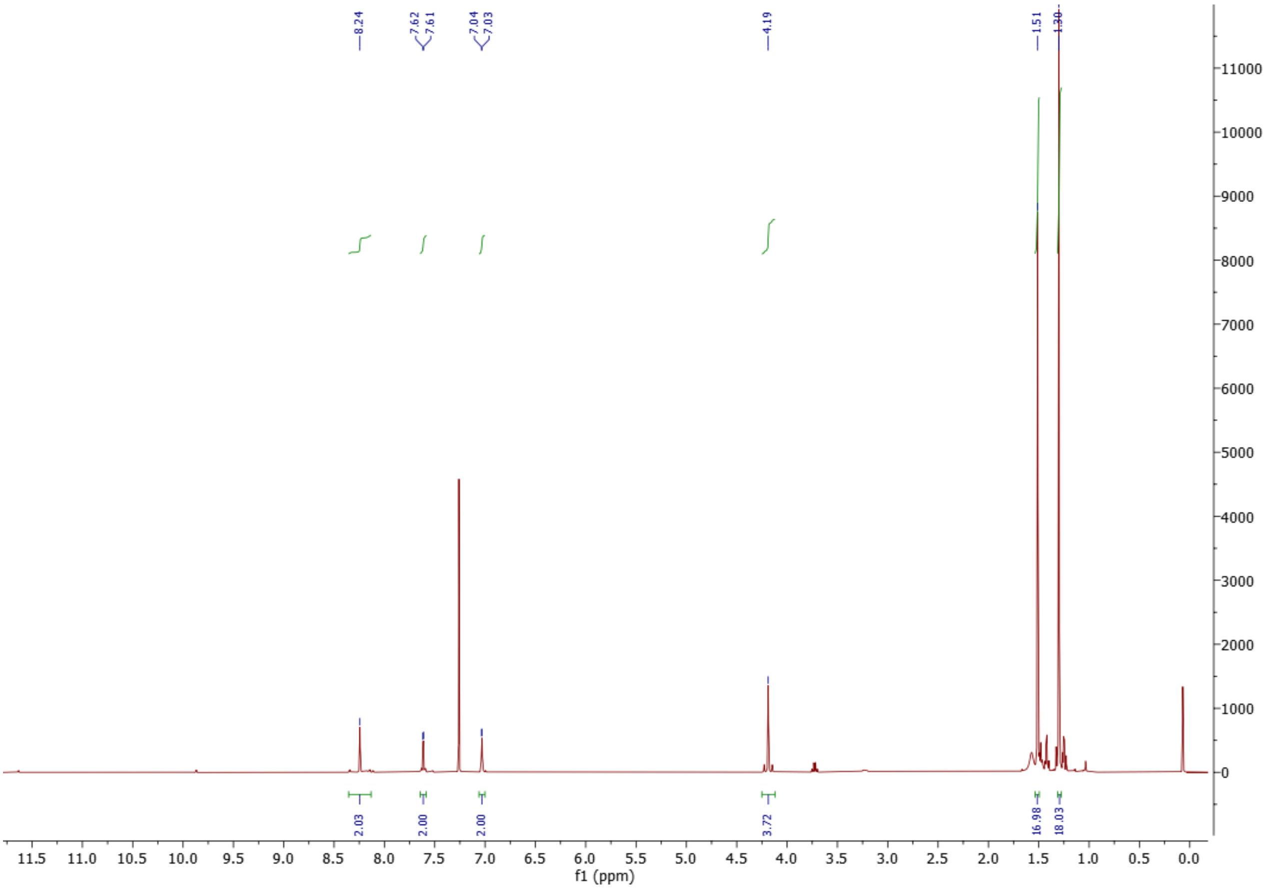


Figure 14: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)Cl$_2$] in $CDCl_3$

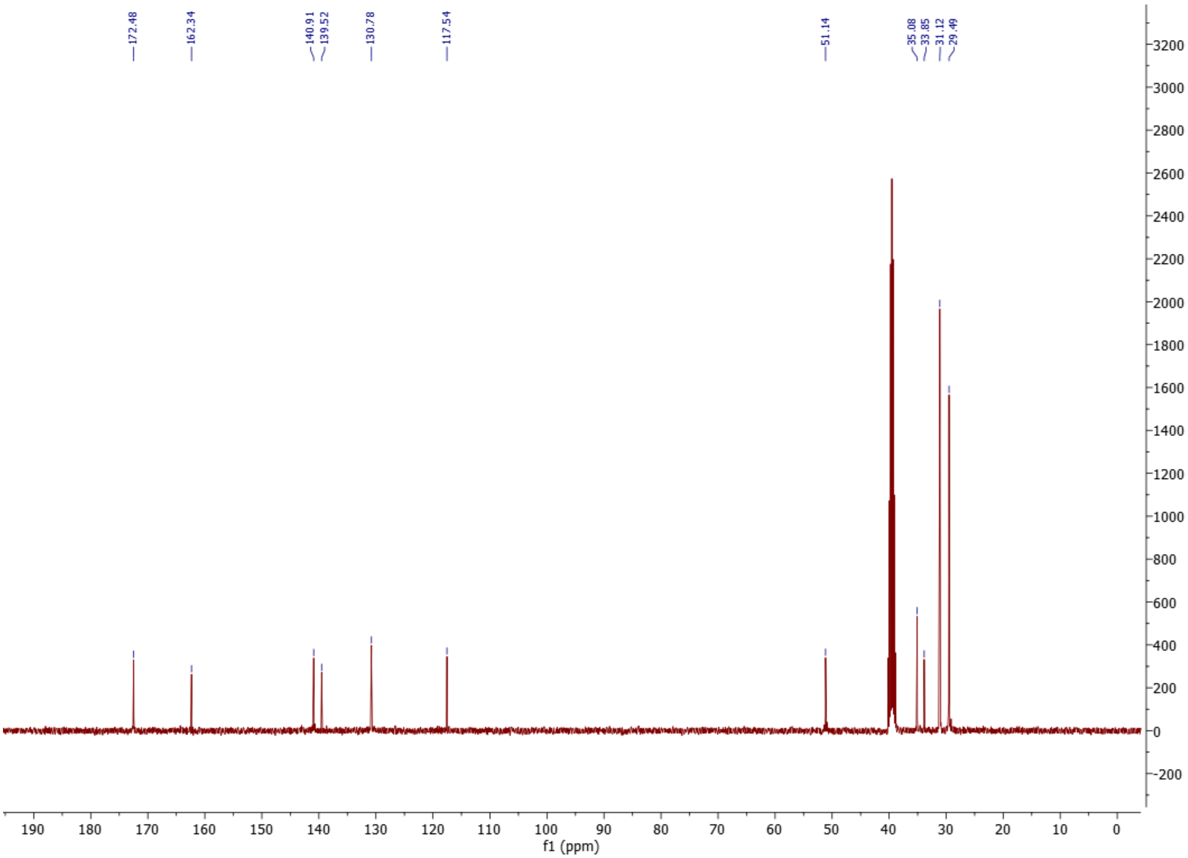


Figure 15: ^{13}C NMR of [Sn(^{t}Bu$_2$Salen)Cl$_2$] in CDCl$_3$

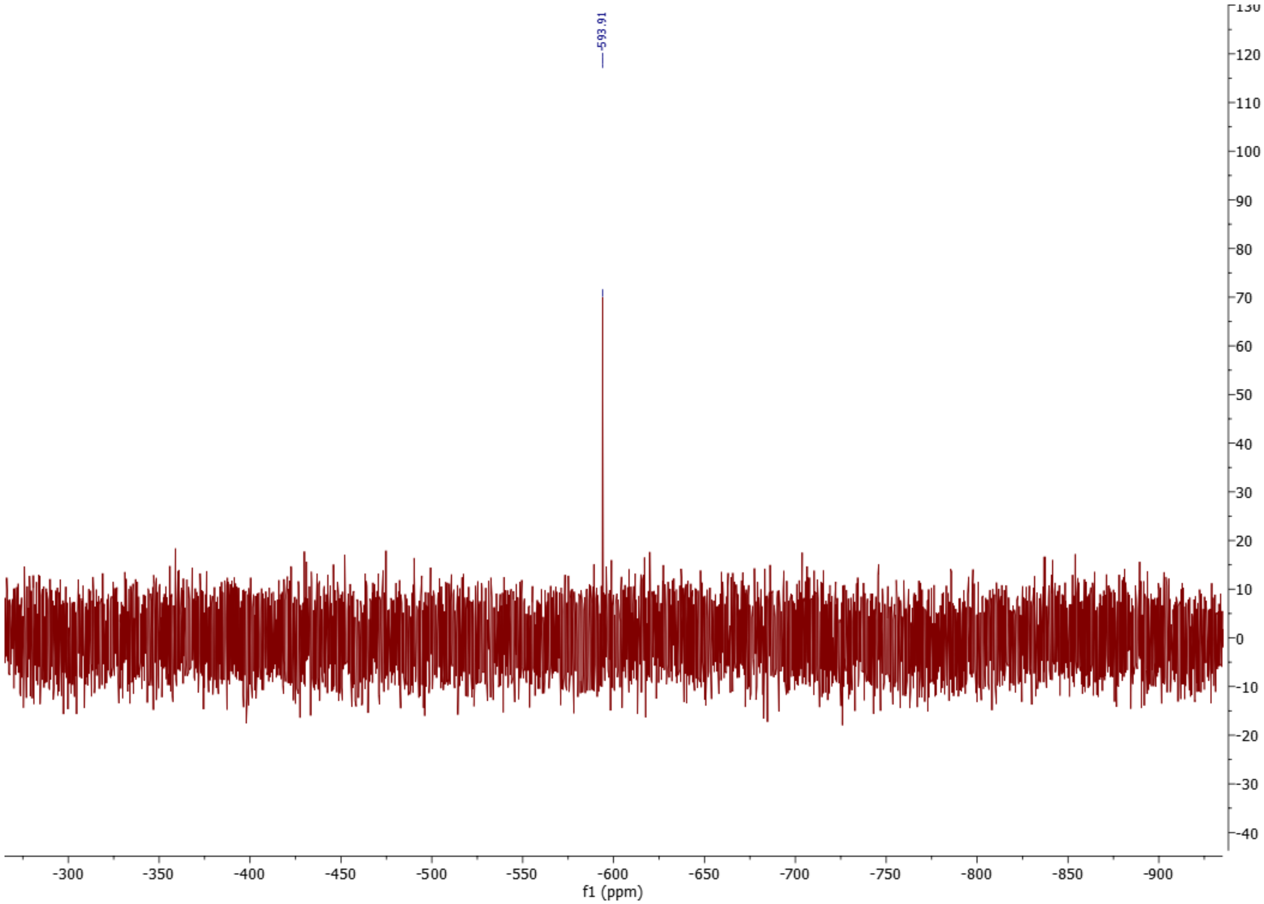


Figure 16: ^{119}Sn NMR of [Sn(^{t}Bu$_2$Salen)Cl$_2$] in CDCl$_3$

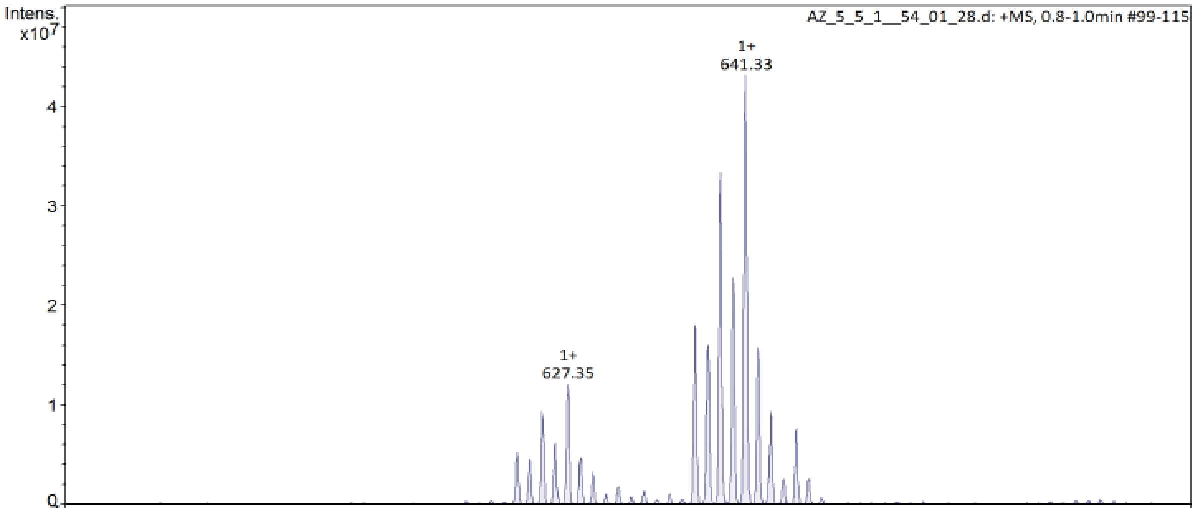
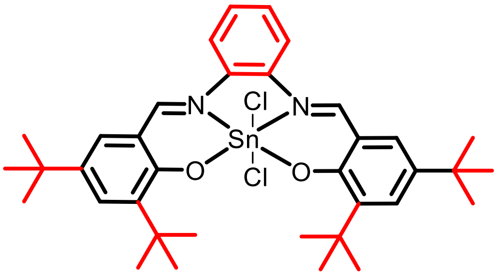


Figure 17: ESI-MS of NMR of [Sn(^{t}Bu$_2$Salen)Cl$_2$]

[Sn(^{t}Bu$_2$Salophen)Cl$_2$]



1 mmol (0.54 g) of 3,5-di-tert-butyl-salophen ligand was used together with 1 mmol of $SnCl_4$ (0.11 mL), 2 mmol (0.28 mL) of Et_3N and 10 mL of DCM. The reaction was stirring for 90 min. The reaction mixture was washed three times with 15 mL of water. The aqueous phase was further washed three times extracted with 30 mL of DCM. Organic phase was dried over $MgSO_4$, filtrated and evaporated. Obtained solid was washed with cold heptane, redissolved in $CDCl_3$ and dried in vacuo. The product was obtained in the form of orange powder in 78 % (0.56 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 2H, J(H-Sn) = 80.0), 7.78 (dd, J = 6.2, 3.4 Hz, 2H), 7.74 – 7.68 (m, 2H), 7.52 (dd, J = 6.2, 3.4 Hz, 2H), 7.19 (d, J = 2.5 Hz, 2H), 1.55 (s, 18H), 1.33 (s, 19H). ^{13}C NMR (101 MHz, DMSO-d6) δ 166, 164, 142, 141, 134, 133, 133, 130, 118, 118, 36, 34, 31, 30. ^{119}Sn NMR (149 MHz, DMSO-d6) δ −589. ESI + (m/z) for $C_{37}H_{49}N_2O_3Sn^+$ 689.3, calculated 689.3 for $C_{37}H_{49}N_2O_3Sn^+$ after loss of chlorides and attachment of methoxide from methanol in the measurement. IR 1602 cm^{-1} ν(C=N), 1581, 1538, 1461 cm^{-1} ν(C=C)$_{\text{arom}}$, 1180 cm^{-1} ν(C-O), 543 cm^{-1} ν(Sn-O), 493 cm^{-1} ν(Sn-N).

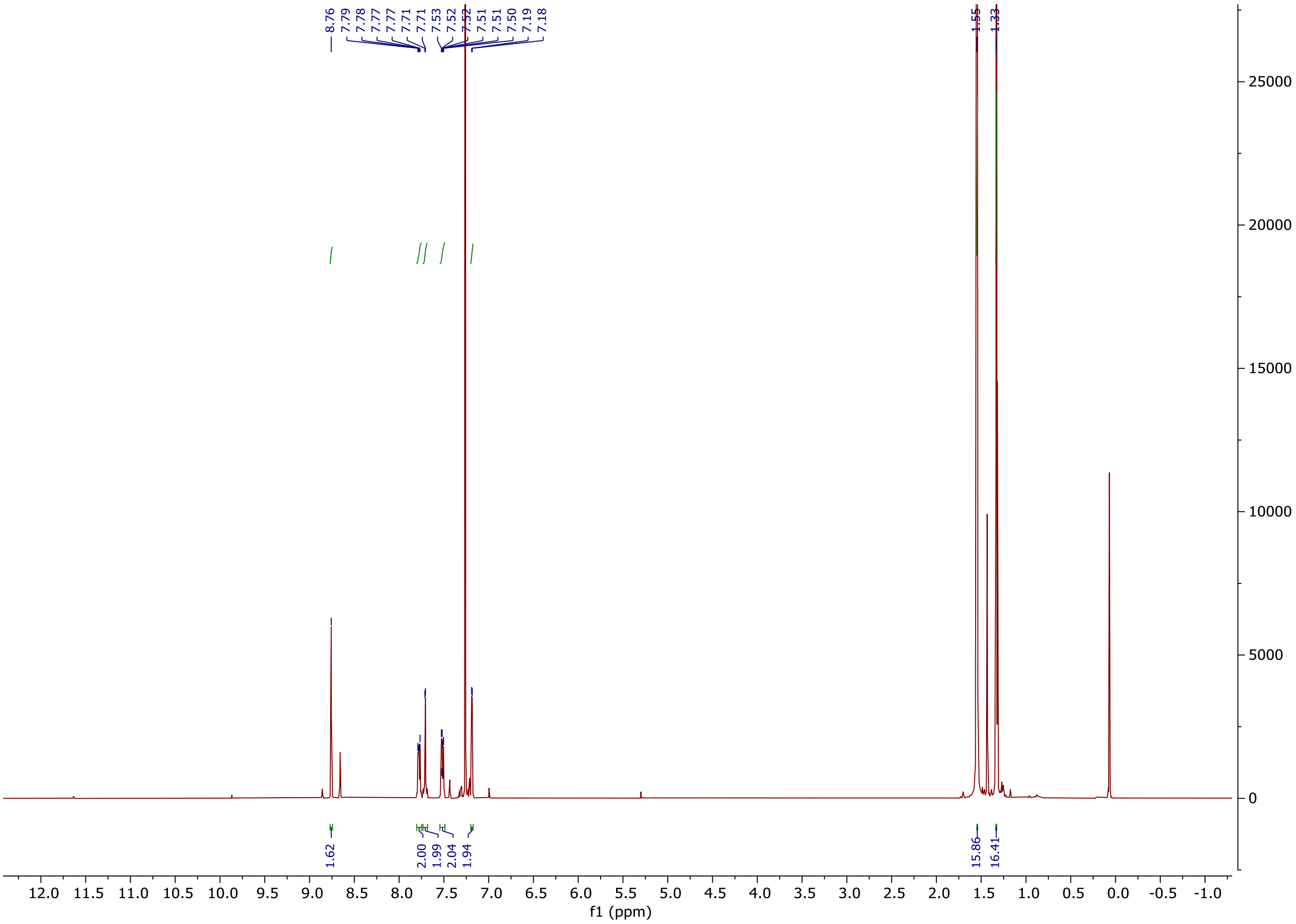


Figure 18: ^{1}H NMR of [Sn(^{t}Bu$_2$Salophen)Cl$_2$] in $CDCl_3$

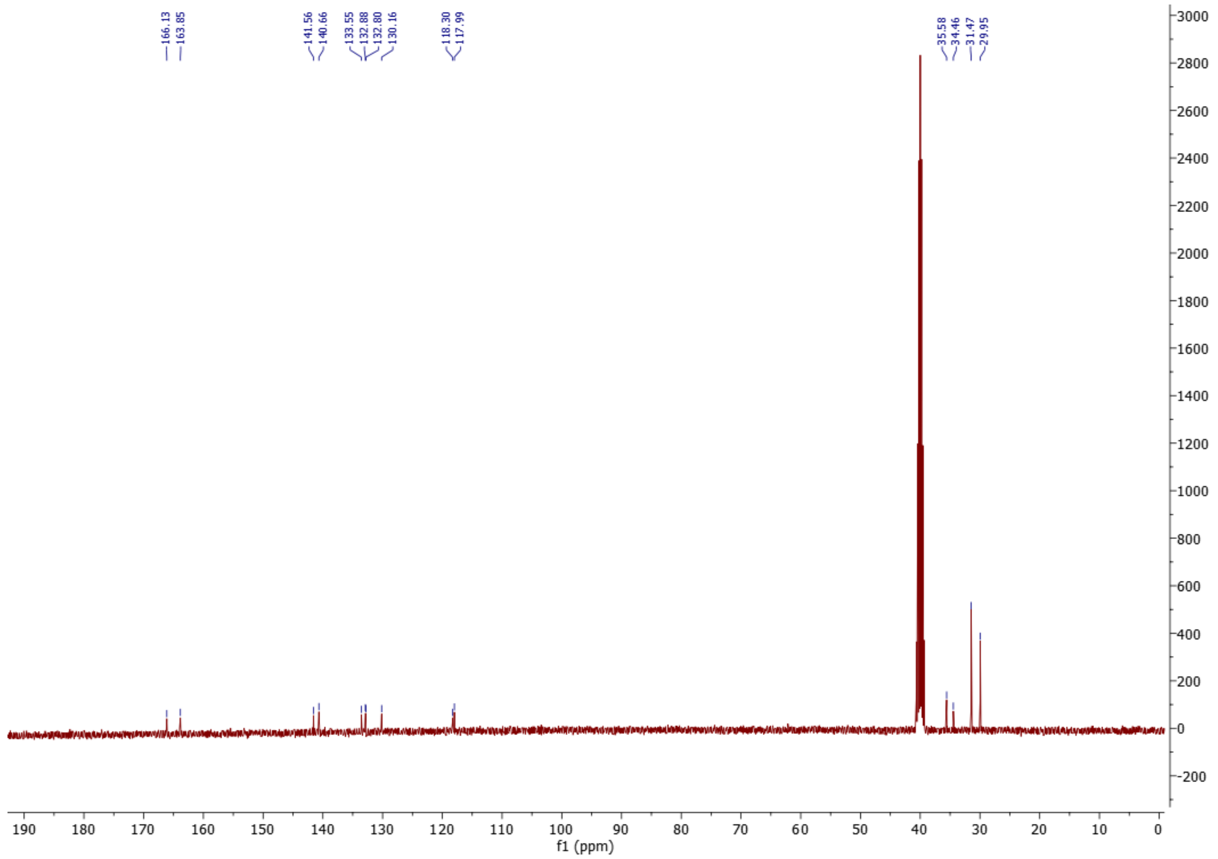


Figure 19: ^{13}C NMR of [Sn(^{t}Bu$_2$Salophen)Cl$_2$] in CDCl$_3$

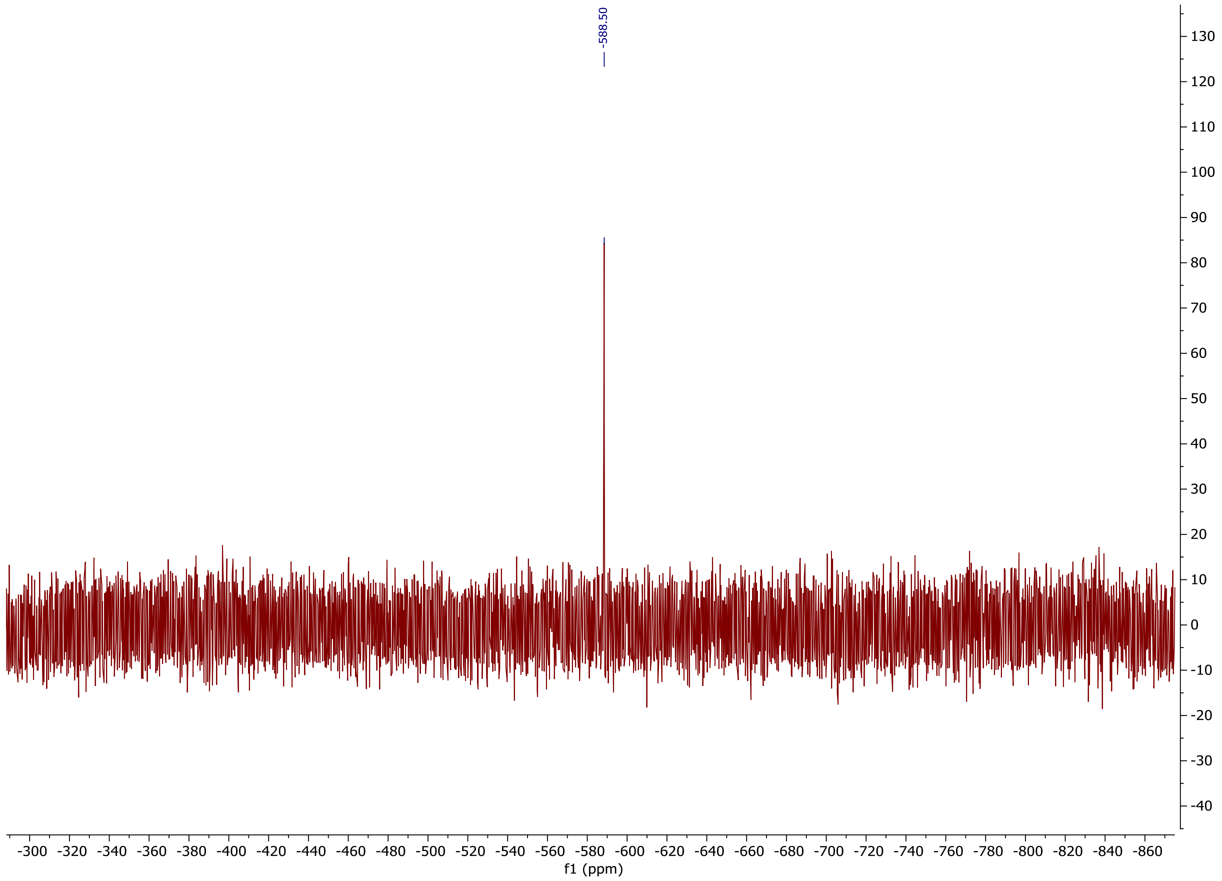


Figure 20: ^{119}Sn NMR of NMR of [Sn(^{t}Bu$_2$Salophen)Cl$_2$] in CDCl$_3$

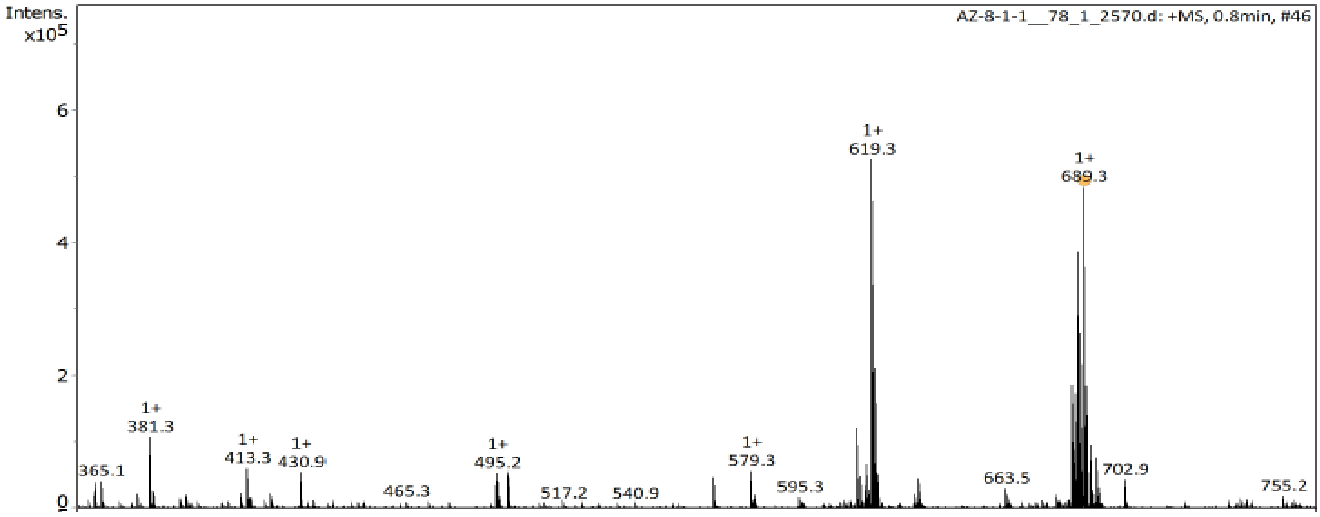
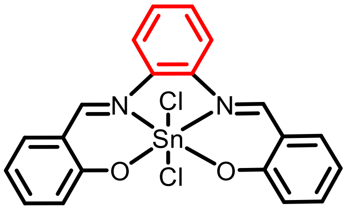


Figure 21: ESI-MS of [Sn(^{t}Bu$_2$Salophen)Cl$_2$]

[Sn(Salophen)Cl$_2$]



1 mmol (0.32 g) of salophen ligand was used together with 1 mmol of $SnCl_4$ (0.11 mL), 2 mmol (0.28 mL) of Et_3N and 10 mL of DCM. The reaction was stirring for 2 hours. Product precipitated out of the reaction mixture and was filtrated off. The filtrate was washed with DCM and dried in vacuo. The product was obtained in the form of orange powder in 93 % (0.47 g) yield. ^{1}H NMR (400 MHz, DMSO-d6) δ 9.50 (s, 2H, *J*(H-Sn) = 85.5), 8.31 – 8.23 (m, 2H), 7.80 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.73 – 7.62 (m, 4H), 7.12 – 7.00 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d6) δ 166, 166, 139, 139, 133, 131, 123, 120, 119, 118. ^{119}Sn NMR (149 MHz, DMSO-d6) δ −592. ESI + (*m/z*) for $C_{21}H_{17}N_2O_3Sn^+$ 465.0, calculated 465.0 for $C_{21}H_{17}N_2O_3Sn^+$ after loss of chlorides and attachment of methoxide from methanol in the measurement. IR 1598 cm^{-1} ν(C=N), 1573. 1535, 1461, ν(C=C)$_{arom}$, 1186 cm^{-1} ν(C-O), 538 cm^{-1} ν(Sn-O), 485 cm^{-1} ν(Sn-N).

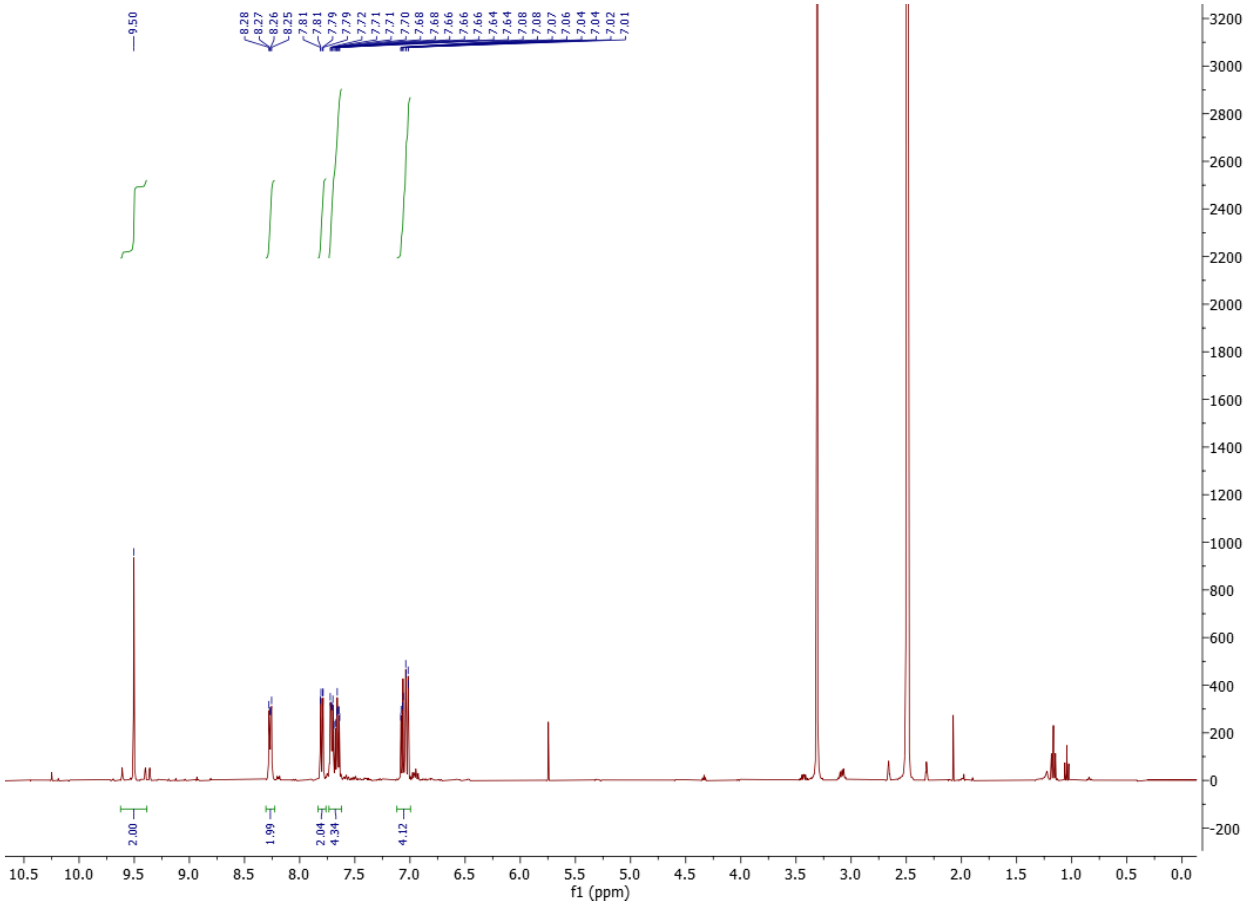


Figure 22: ^{1}H NMR of [Sn(Salophen)Cl$_2$] in DMSO-d6

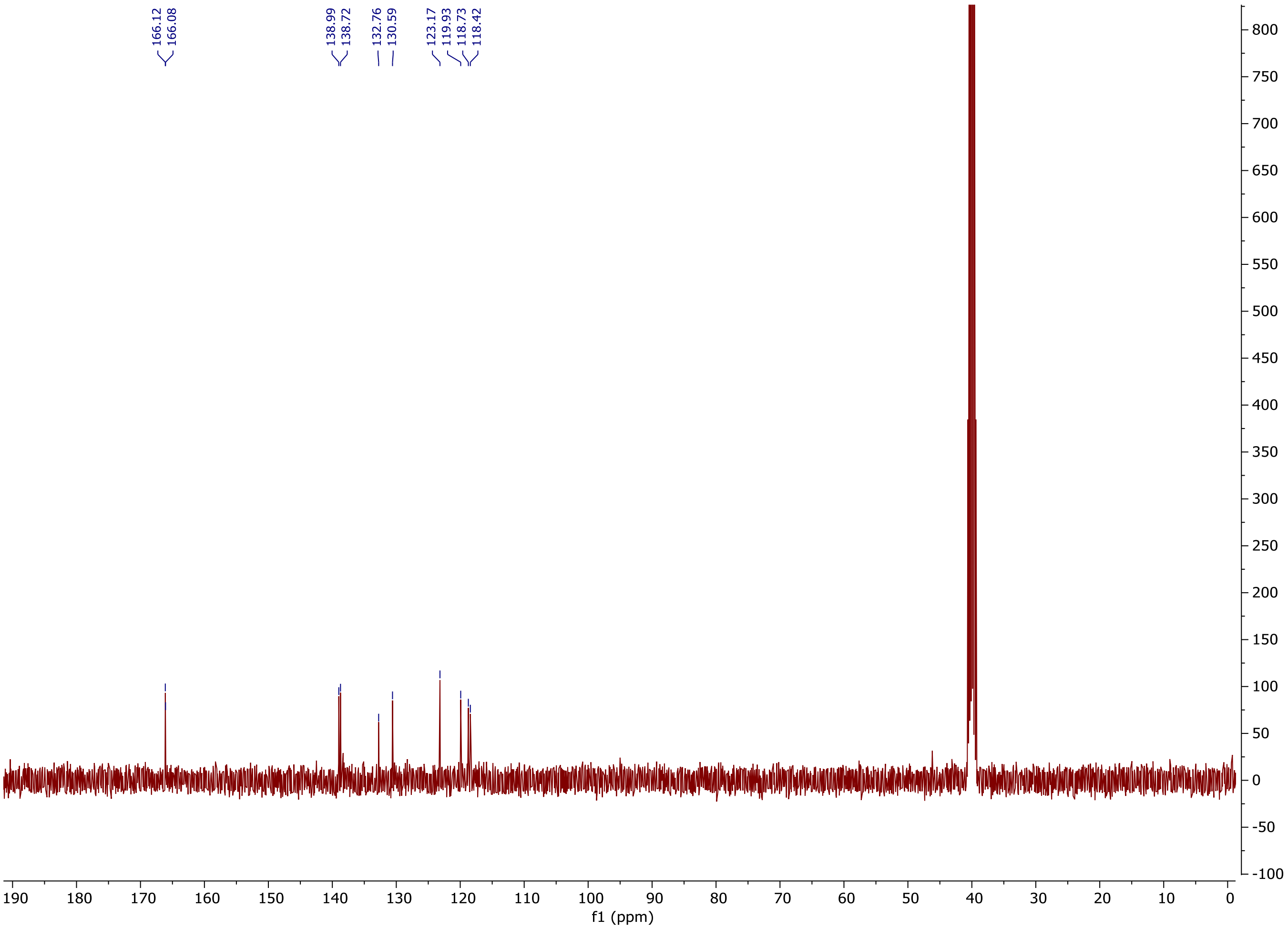


Figure 23: ^{13}C NMR of [Sn(Salophen)Cl$_2$] in DMSO-d6

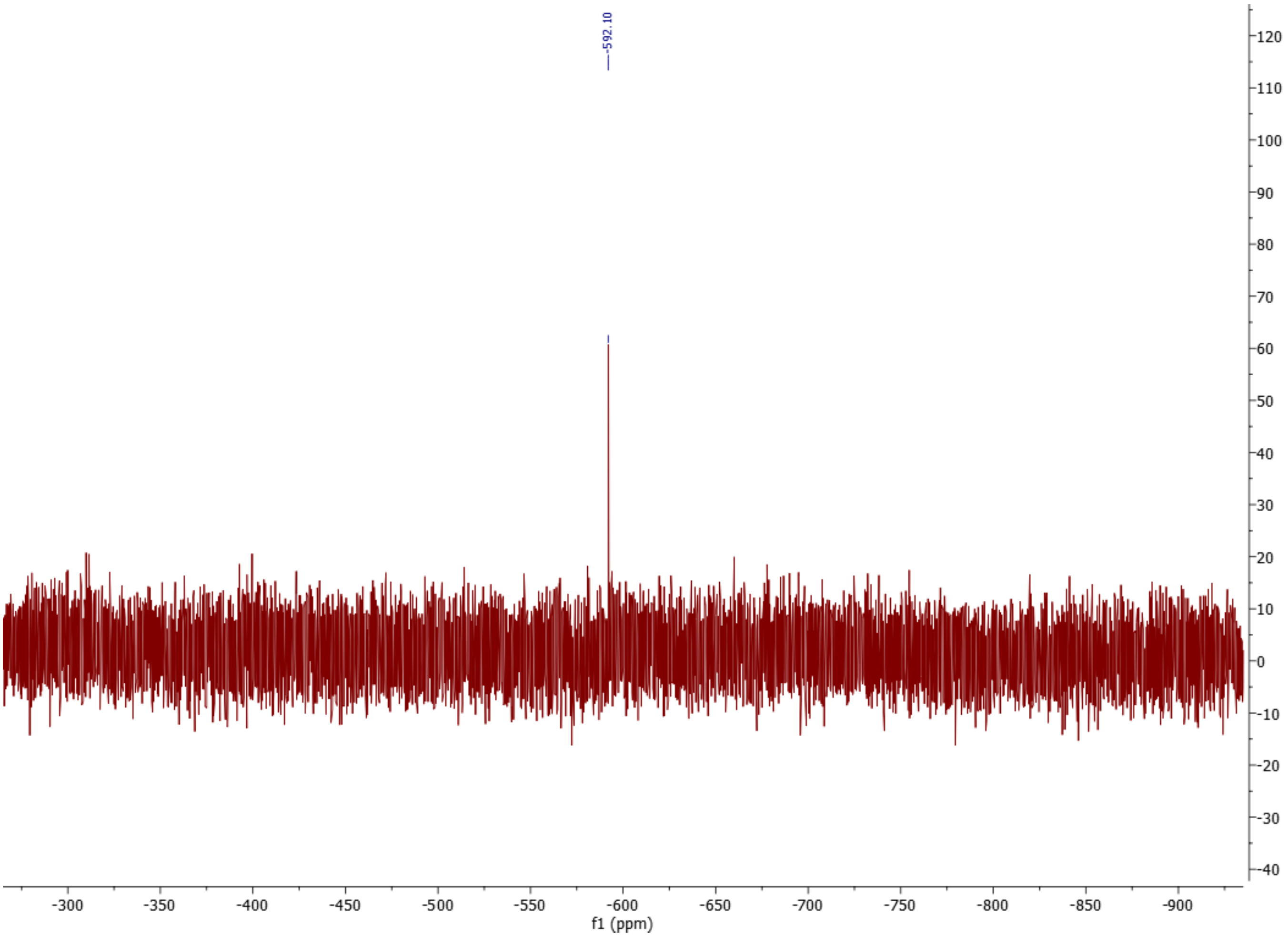


Figure 24: ^{119}Sn NMR of [Sn(Salophen)Cl_2] in DMSO-d6

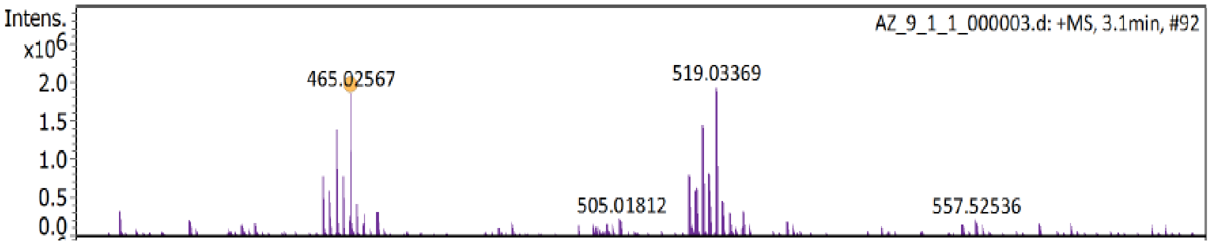


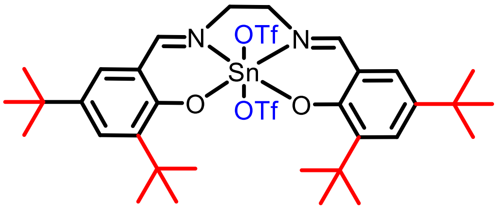
Figure 25: ESI-MS of [Sn(Salophen)Cl_2], additional peak at 519.0 represents loss of both chlorides, attachment of two methoxides and ionization via additional sodium ion.

General synthesis procedure of triflate containing complexes

[Sn(^{t}Bu$_2$Salen)(OTf)$_2$] was prepared according to procedures reported in the literature[3]. [Sn(^{t}Bu$_2$Salen)Cl(OTf)] complex was prepared by adjustment of the stoichiometry in the preparative procedure of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] complex .

Reactions were performed in an inert atmosphere of N_2 using Schlenk line apparatus and techniques. Solvents and glassware were dried according to the general procedure mentioned above. The starting complex was dried in vacuo before use, AgOTf was heated up by heat gun under vacuum for 5 min before use. 1 eq of [Sn(^{t}Bu$_2$Salen)Cl_2] was dissolved in DCM. For the synthesis if [Sn(^{t}Bu$_2$Salen)Cl(OTf)] and [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] 1 eq and 2 eq of AgOTf were added respectively against flow of nitrogen gas to the stirring solution. Reaction flasks were wrapped in aluminum foil. Reactions were followed by NMR and the reaction mixture was left to react at RT until full conversion of starting material. Reaction mixtures were separated from formatted solid waste by filtration via canula. The solid fractions were washed with DCM. The solvent was evaporated, and the solid products were dried in vacuo. Products were stored and manipulated under an inert atmosphere.

[Sn(^{t}Bu$_2$Salen)(OTf)$_2$]



1 mmol (0.68 g) of [Sn(^{t}Bu$_2$Salen)Cl$_2$] was used together with 2 mmol (0.51 g) AgOTf and 125 mL of DCM. The reaction was stirred overnight. The reaction mixture was filtered via cannula and the precipitated waste was washed two times with 8 mL of DCM. After evaporation of the solvent the product was obtained in the form of yellow powder in 76 % (0.69 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 2H, *J*(H-Sn) = 110.5), 7.73 (d, *J* = 2.6 Hz, 2H), 7.13 (d, *J* = 2.6 Hz, 2H), 4.35 (s, 4H, *J*(H-Sn) = 40.4), 1.48 (s, 18H), 1.33 (s, 18H). ^{13}C NMR (101 MHz, DMSO-d6) δ 177, 162, 142, 141, 132, 132, 117, 51, 35, 34, 31, 30. ^{119}Sn NMR (149 MHz, DMSO-d6) δ −622. ^{19}F NMR (376 MHz, DMSO-d6) δ −77.75. ESI + (*m/z*) for $C_{33}H_{49}N_2O_3Sn^+$ 641.3, calculated 641.3 for $C_{33}H_{49}N_2O_3Sn^+$ after loss of triflate ligands and attachment of methoxide from the measurement. IR 1608 cm^{-1} ν(C=N), 1542. 1438, 1346, ν(C=C)$_{arom}$, 1176 cm^{-1} ν(C-O), 630 cm^{-1} ν(Sn-O), 512 cm^{-1} ν(Sn-N).

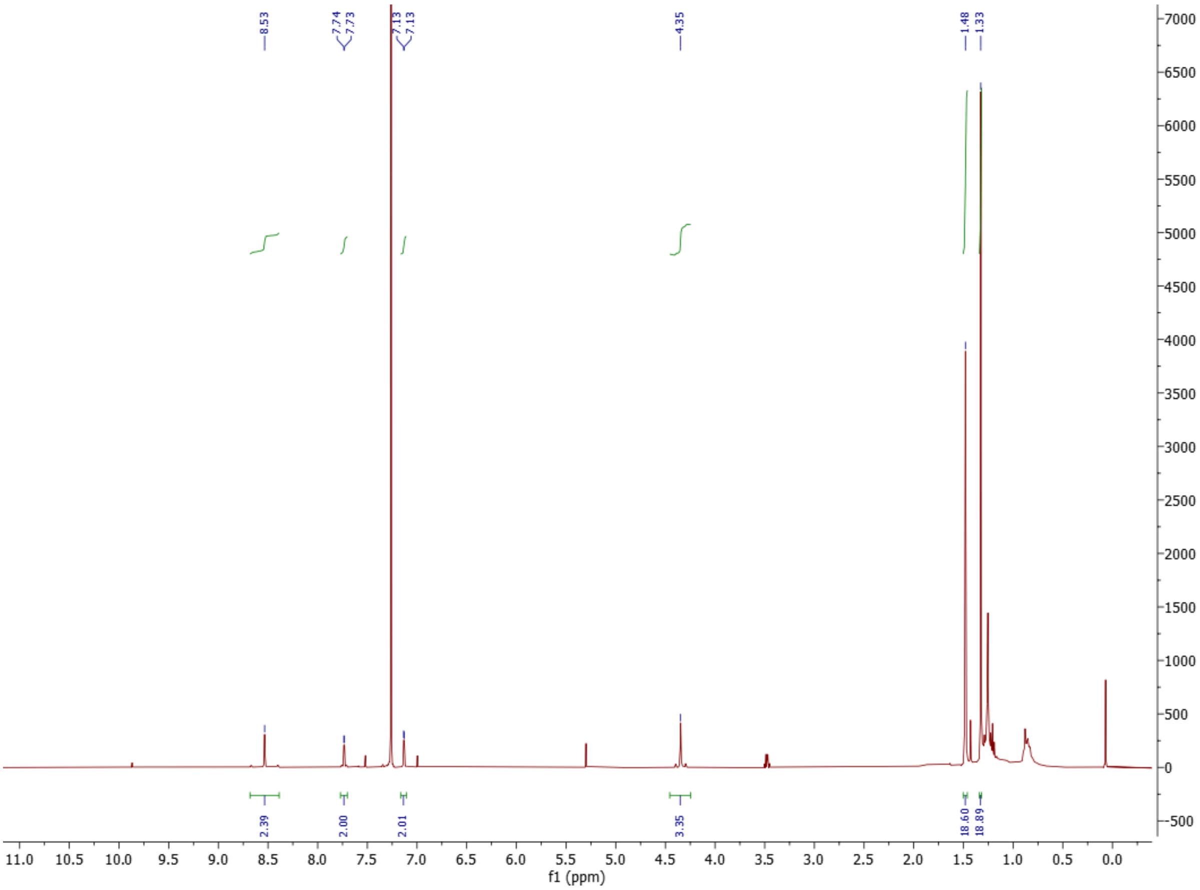


Figure 26: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in $CDCl_3$.

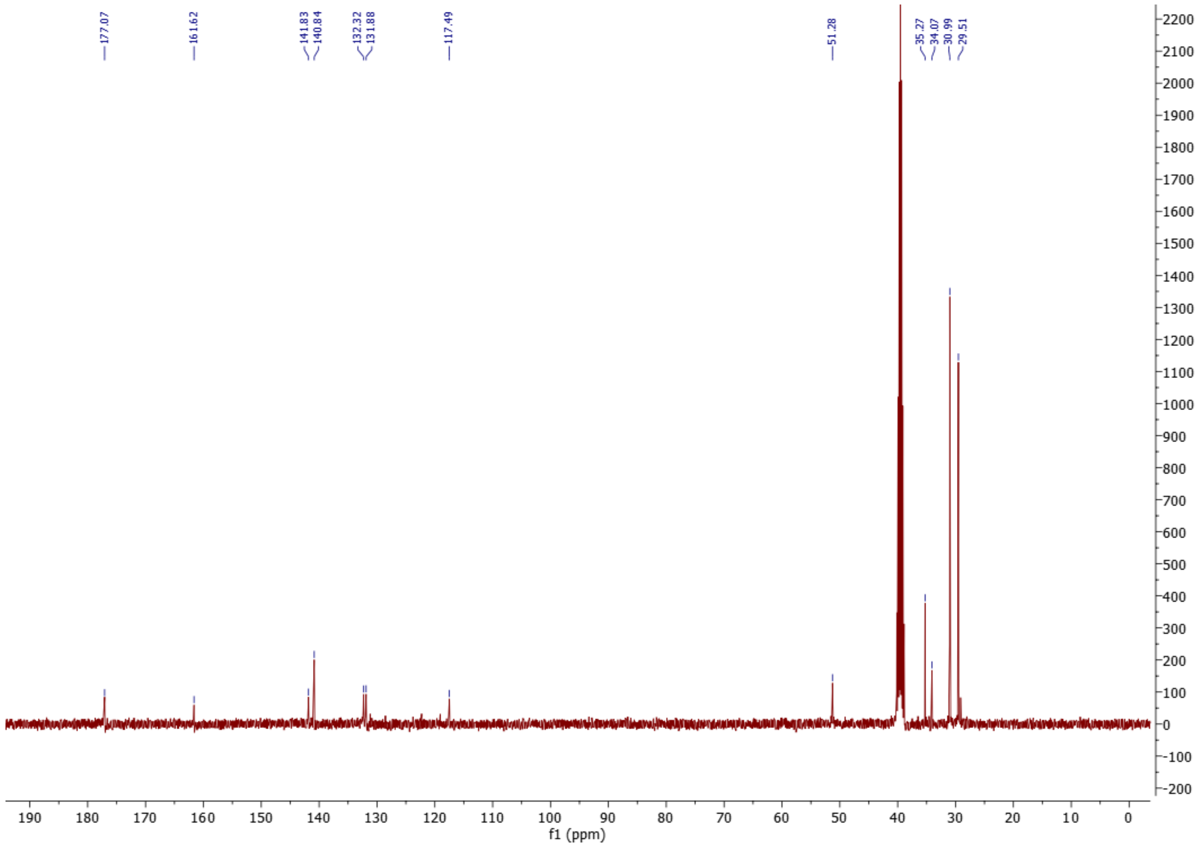


Figure 27: ^{13}C NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in CDCl$_3$.

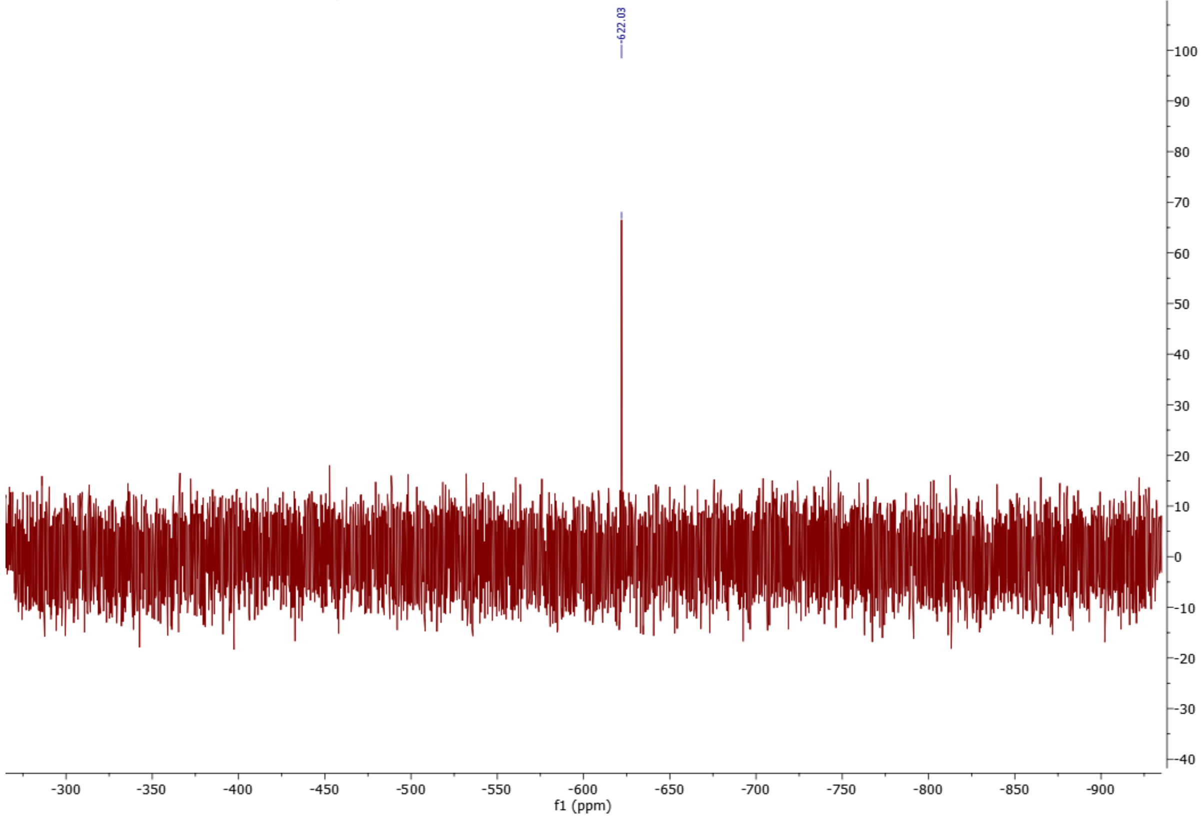


Figure 28: ^{119}Sn NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in CDCl$_3$.

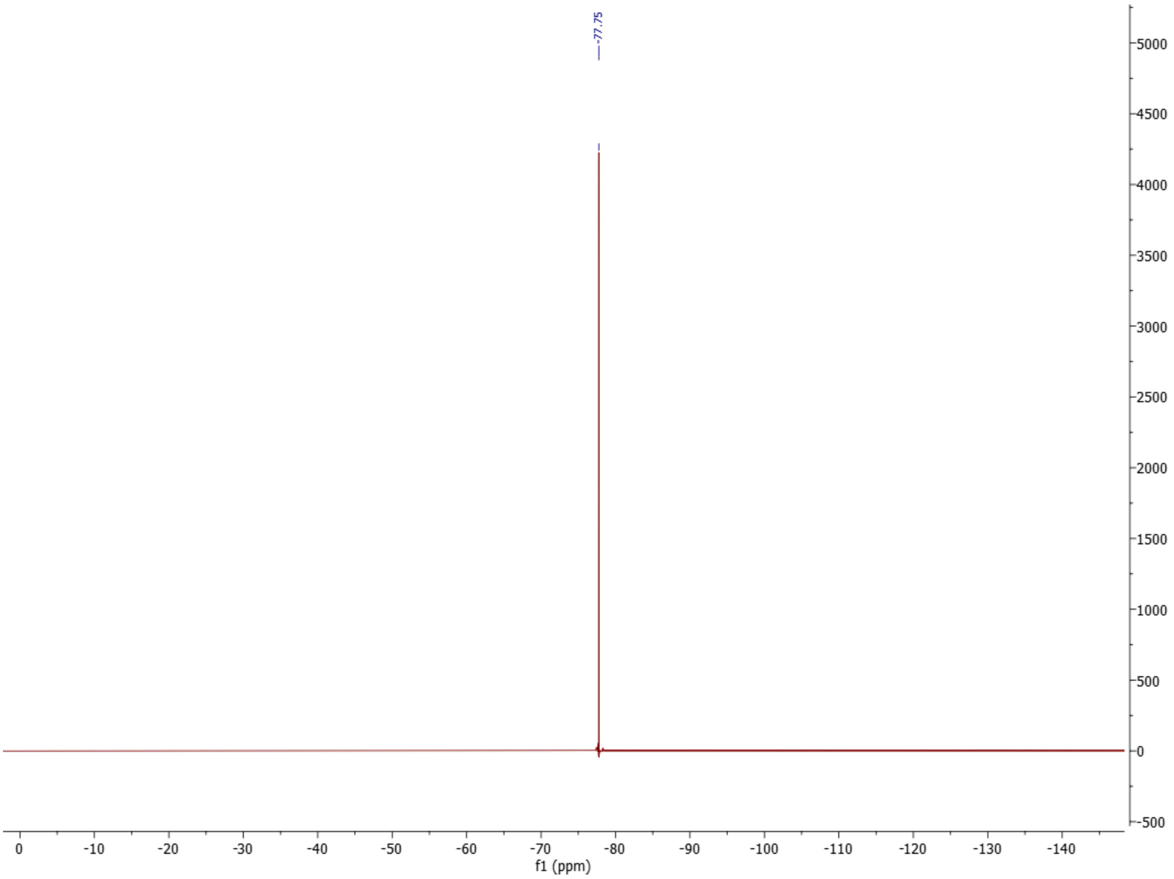


Figure 29: ^{19}F NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in CDCl$_3$.

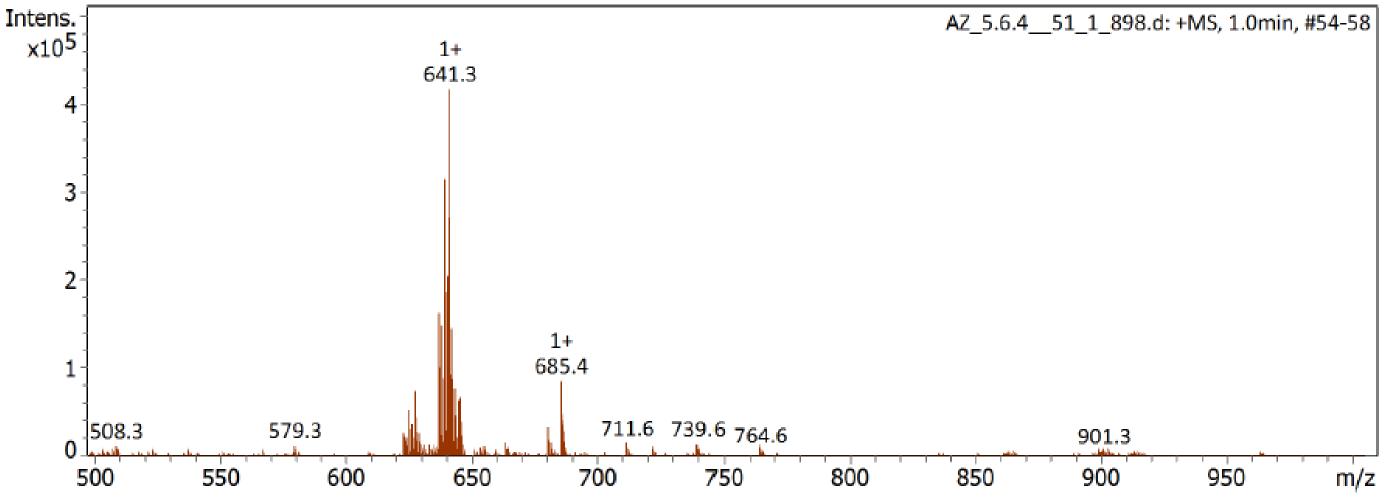
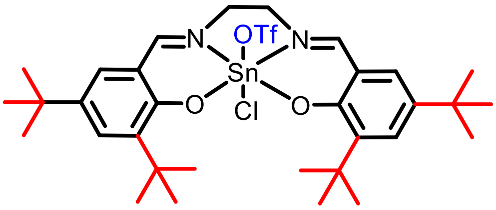


Figure 30: ESI-MS of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$].

[Sn(^{t}Bu$_2$Salen)Cl(OTf)]



0.5 mmol (0.34 g) of [Sn(^{t}Bu$_2$Salen)Cl$_2$] was used together with 0.5 mmol (0.13 g) AgOTf and 40 mL of DCM. The reaction was stirred for 5 days. The reaction mixture was filtered via cannula and the precipitated waste was washed three times with 2 mL of DCM. After evaporation of the solvent, the product was obtained in the form of yellow powder in 99 % (0.39 g) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 2H, *J*(H-Sn) = 95.4), 7.71 – 7.61 (m, 2H), 7.10 (d, *J* = 2.5 Hz, 2H), 4.47 – 4.25 (m, 2H), 4.24 – 4.00 (m, 2H), 1.48 (s, 18H), 1.31 (s, 20H). ^{13}C NMR (101 MHz, DMSO-d6) δ 175, 162, 141, 141, 132, 131, 118, 51, 35, 34, 31, 30. ^{119}Sn NMR (149 MHz, DMSO-d6) δ −595. ^{19}F NMR (376 MHz, DMSO-d6) δ −77.76. ESI + (*m/z*) for $C_{32}H_{46}ClN_2O_2Sn^+$ and $C_{33}H_{49}N_2O_3Sn^+$ 641.3, calculated 641.3 for $C_{33}H_{49}N_2O_3Sn^+$ after loss of the triflate and chloride ligands and attachment of methoxide from the measurement. IR 1610 cm^{-1} ν(C=N), 1540. 1461, 1440, ν(C=C)$_{arom}$, 1240 cm^{-1} ν(C-O), 626 cm^{-1} ν(Sn-O), 547 cm^{-1} ν(Sn-N).

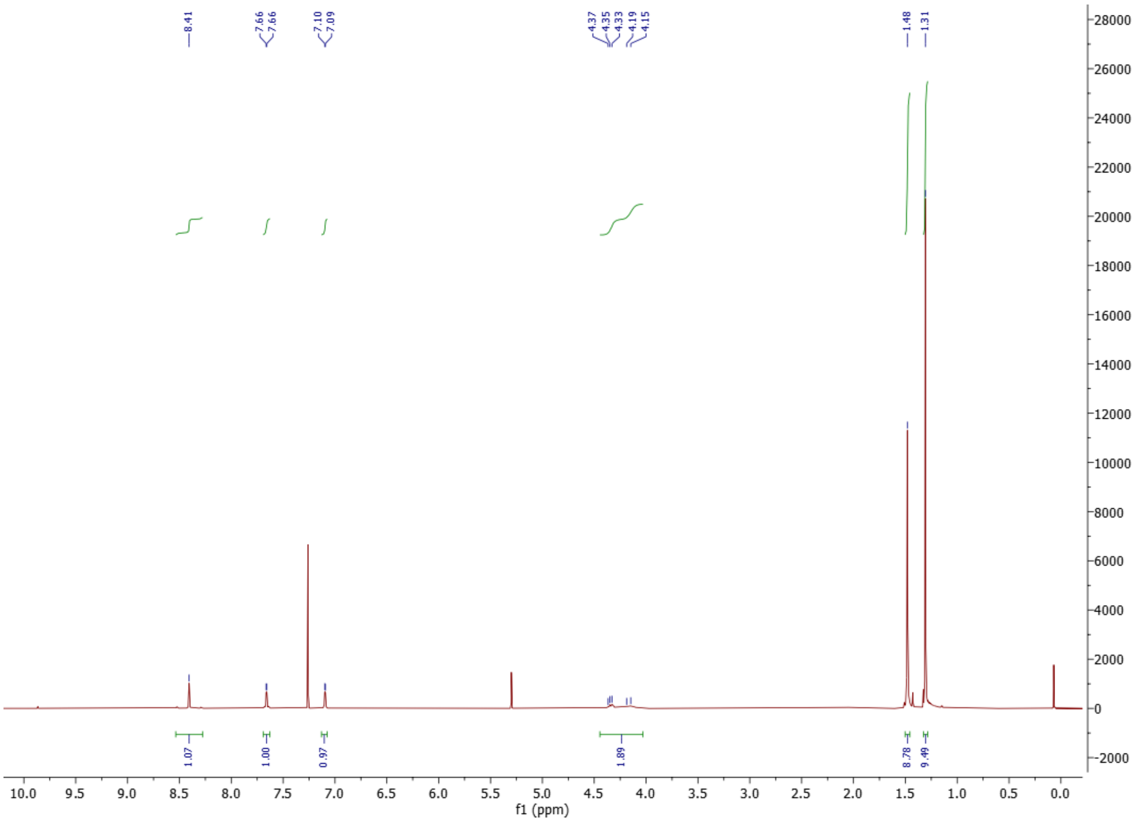


Figure 31: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)Cl(OTf)] in $CDCl_3$

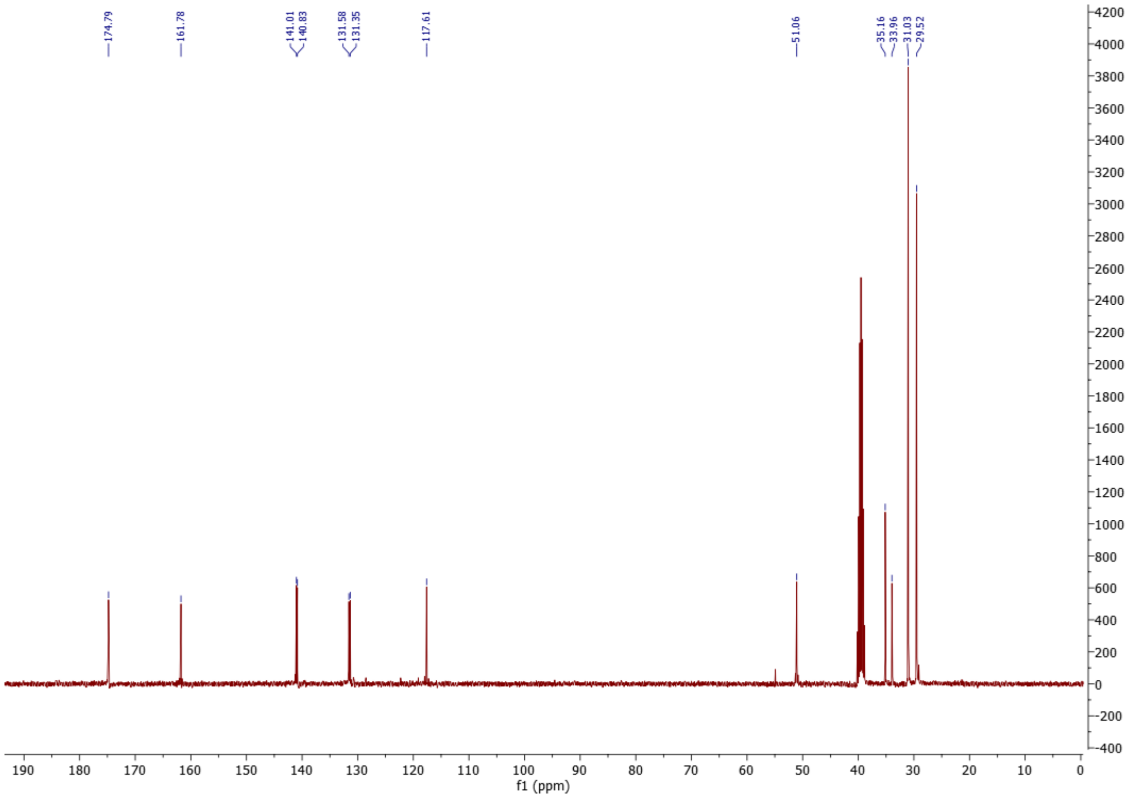


Figure 32: ^{13}C NMR of [Sn(^{t}Bu$_2$Salen)Cl(OTf)] in $CDCl_3$

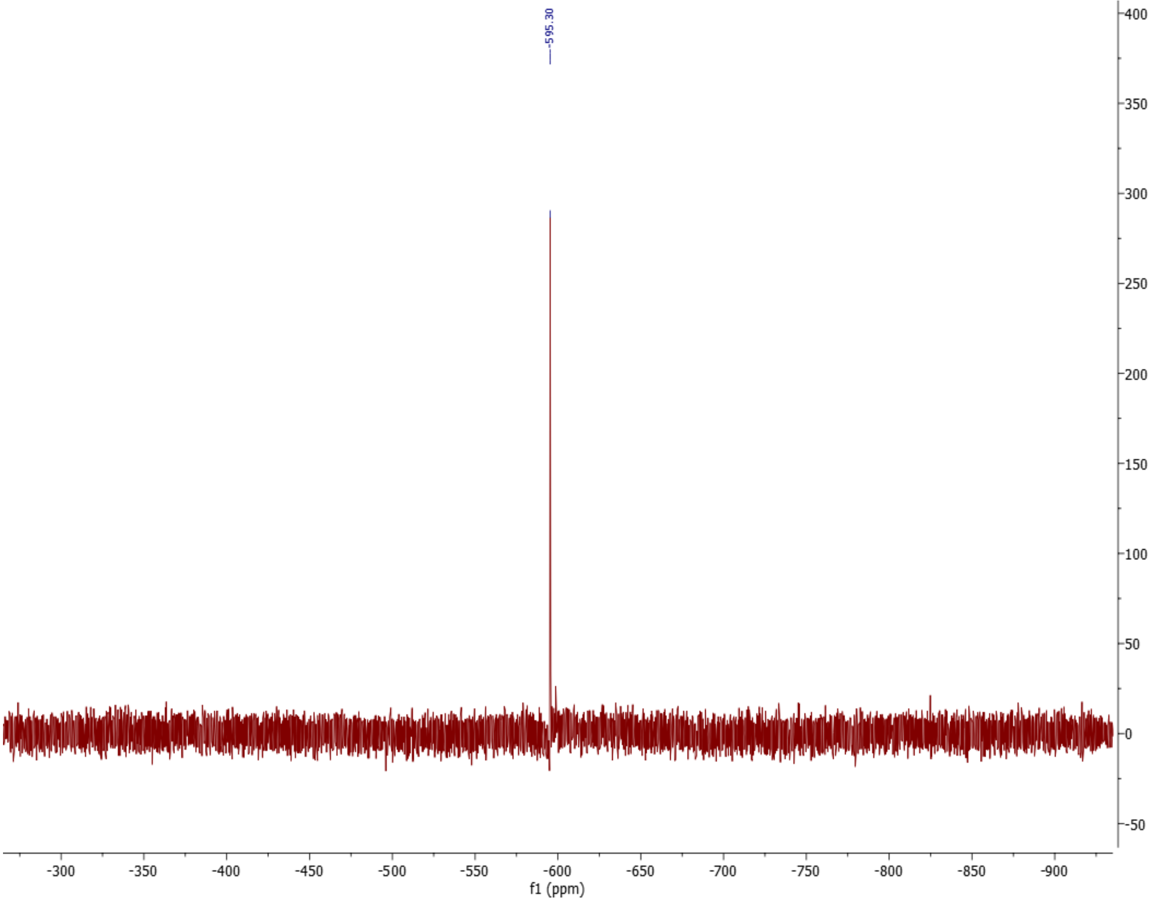


Figure 33: 119Sn NMR of [Sn(^{t}Bu$_2$Salen)Cl(OTf)] in $CDCl_3$

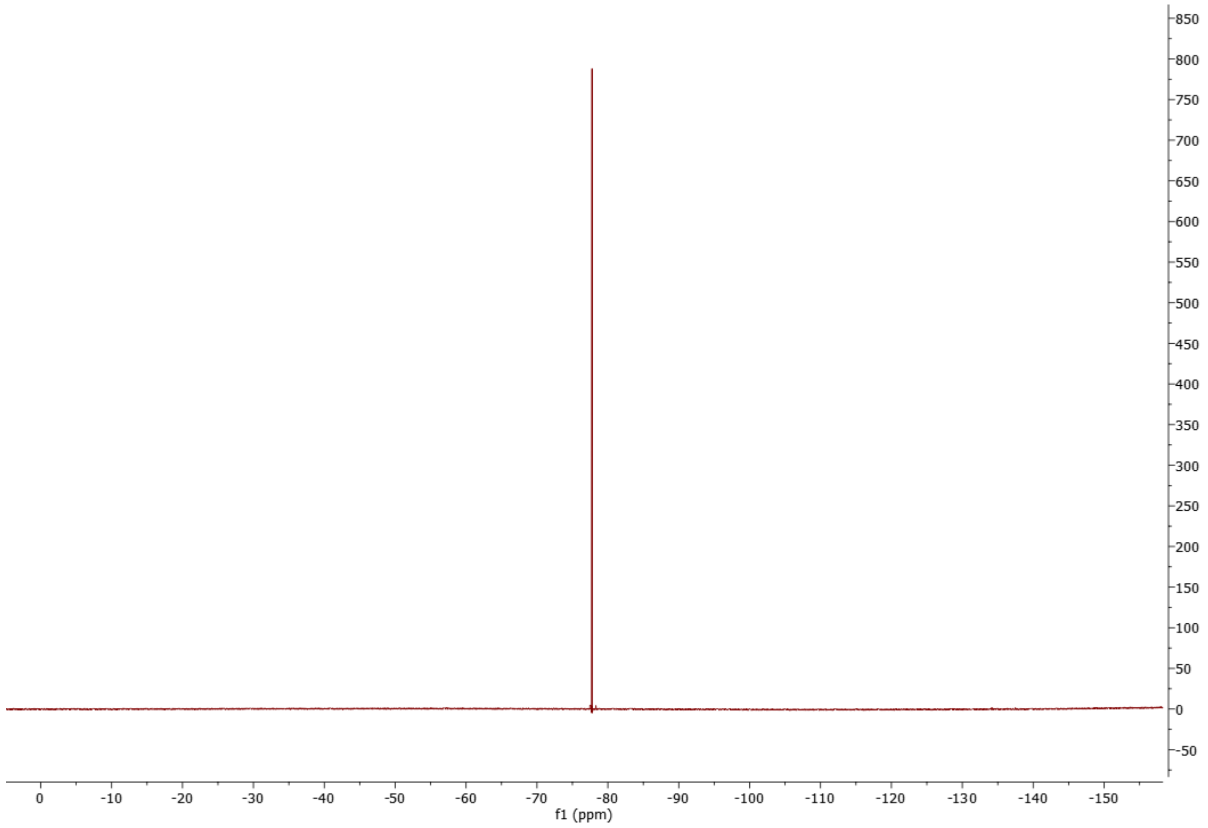


Figure 34: ^{19}F NMR of [Sn(^{t}Bu$_2$Salen)Cl(OTf)] in $CDCl_3$

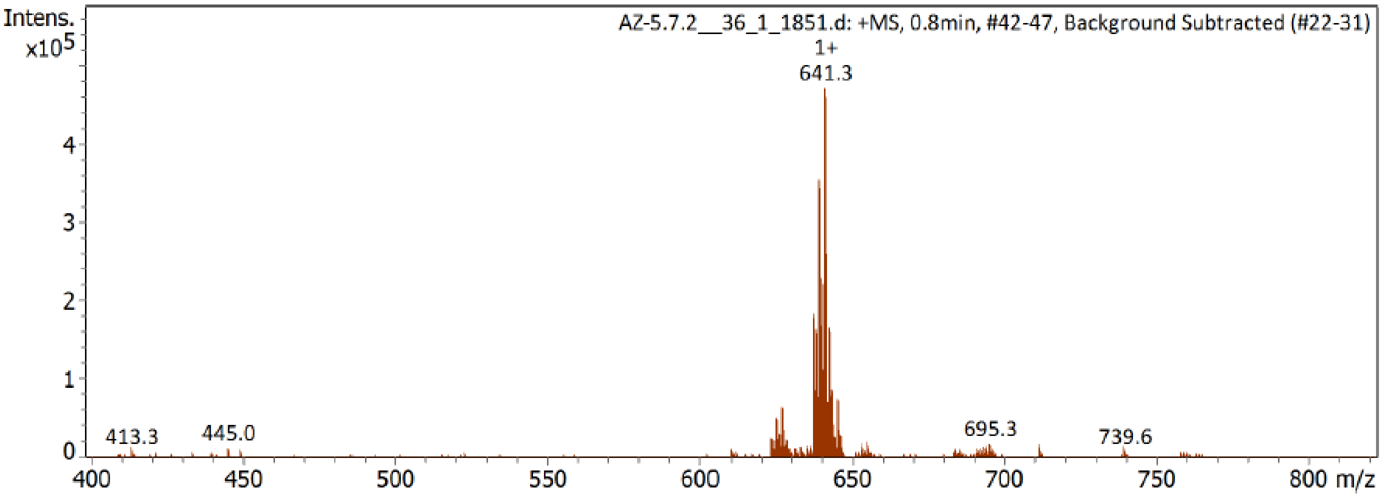


Figure 35: ESI-MS of [Sn(^{t}Bu$_2$Salen)Cl(OTf)]

Gutmann-Beckett acidity measurements

The ^{31}P NMR experiments were performed under inert atmosphere in dry $CDCl_3$. A stock solution of Et_3PO (c = 0.13 M, 0.1 mL) was added to a solution of complex with each measurement. The measurements were repeated with increasing quantity of the measured complex until the ppm of ^{31}P signal of Et_3PO stopped shifting. The acceptance numbers (ANs) were calculated according to Equation 1. Experimental data and calculated values are displayed in **Error! Reference source not found.**.

$$AN = 2.21 \cdot (\delta_{\mathrm{sample}} - 41) \tag{1}$$

Table 1:NMR shifts and calculated values for Gutmann-Beckett acidity measurements.

Complex	δ [ppm]	AN
[Sn(^{t}Bu$_2$Salen)(OTf)$_2$]	78.8	83.6
[Sn(^{t}Bu$_2$Salen)Cl(OTf)]	73.5	71.8

Activation of HD gas

Activation of HD gas was performed in high pressure sapphire NMR tubes. The desired complex [Sn(^{t}Bu$_2$Salen)(OTf)$_2$], [Sn(^{t}Bu$_2$Salen)Cl(OTf)] or [Sn(^{t}Bu$_2$Salen)Cl$_2$] (0.01mmol) was dissolved in THF-d8 or CDCl3 (0.4 mL) and the NMR tube was pressurized with HD gas (10 bar). ^{1}H NMR and ^{2}D NMR were measured immediately then again after 4 hours and 17 hours. Activation of HD was observed with [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] and [Sn(^{t}Bu$_2$Salen)Cl(OTf)] in THF-d$_8$ but not in CDCl$_3$ confirming the necessity of the basic solvent, which acts as the FLP partner of the complex.

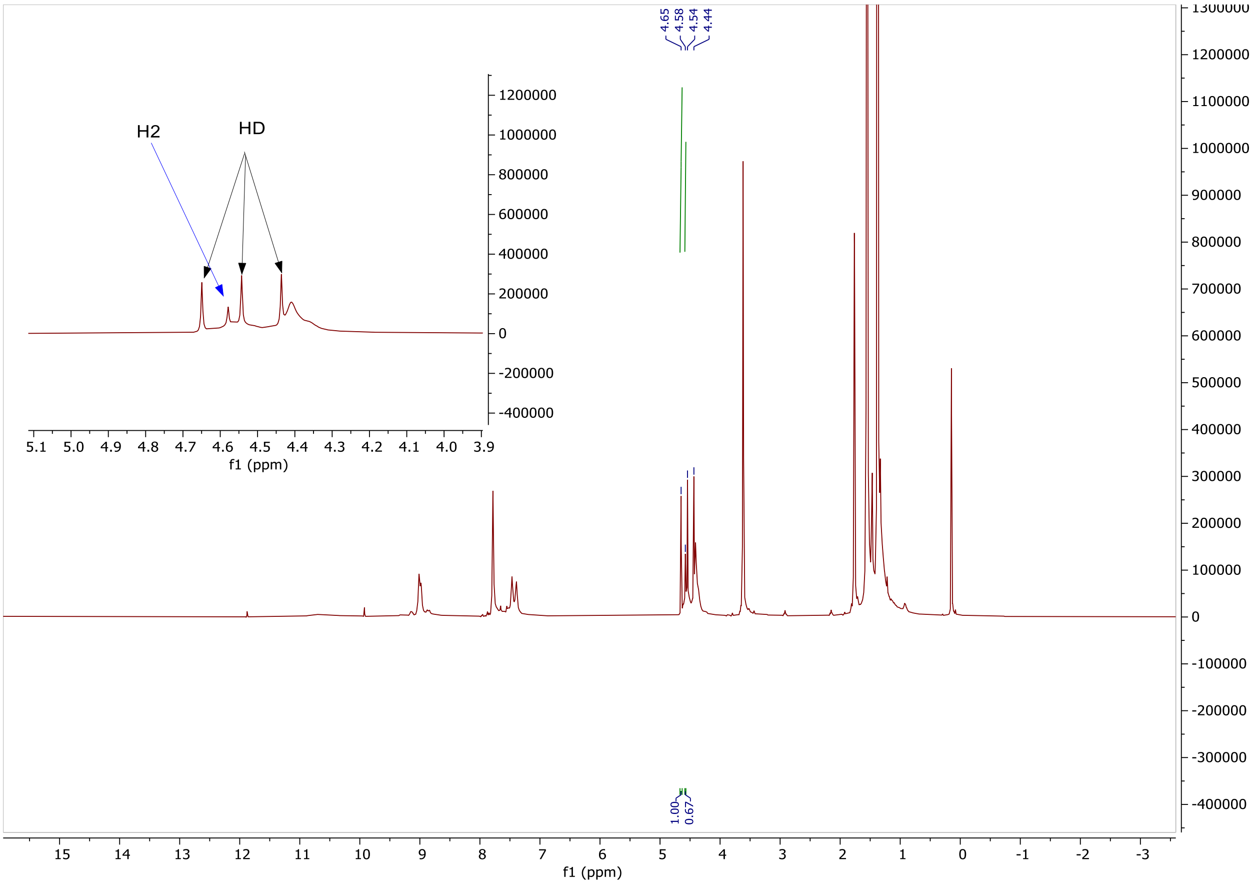


Figure 36: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in THF-d8 with HD gas at time 0 hrs

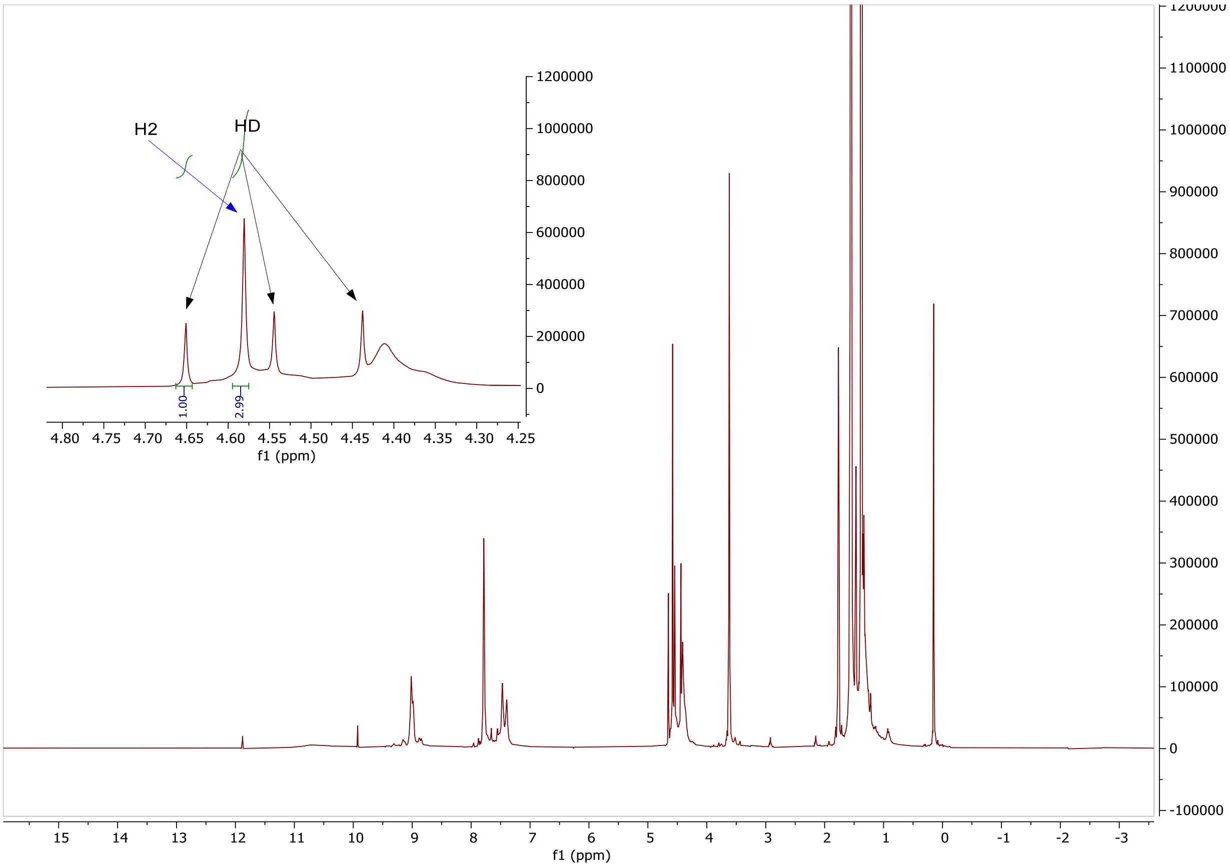


Figure 37: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in THF-d_8 with HD gas after 17 hrs at 25°C

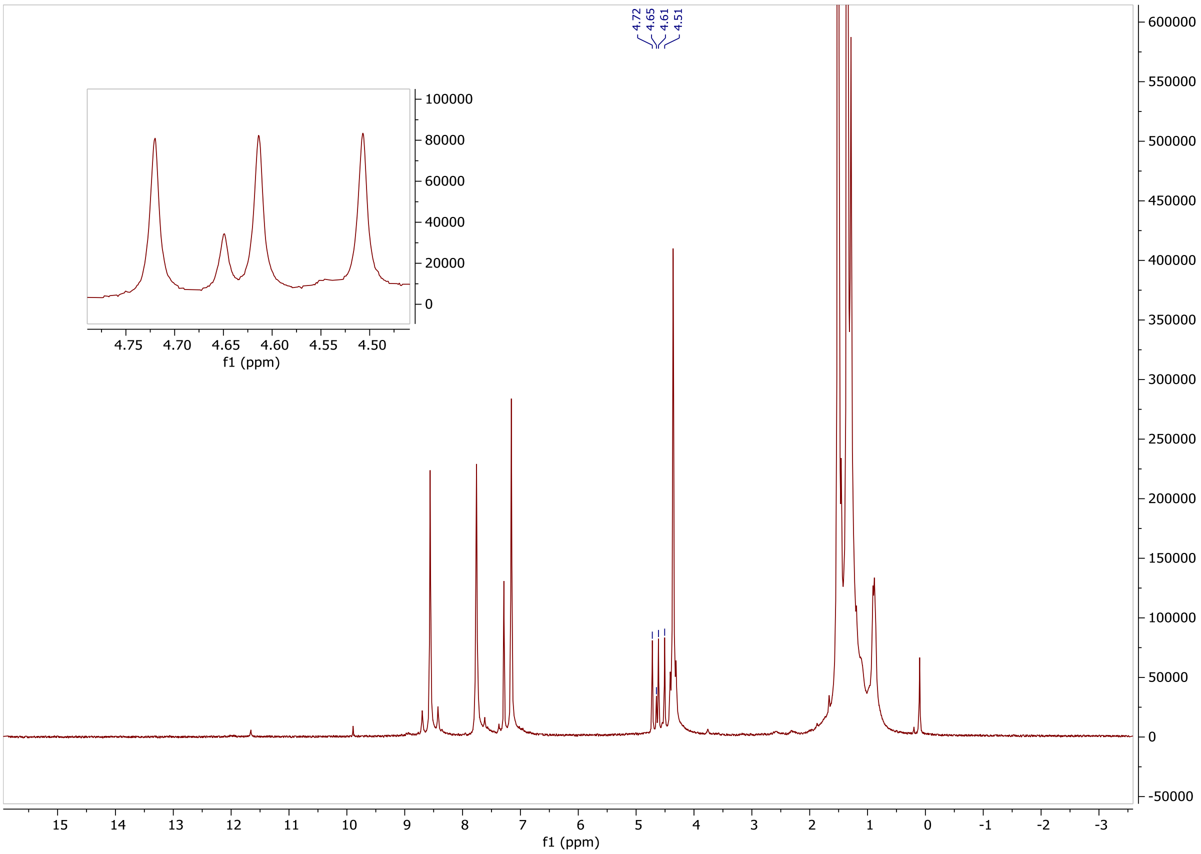


Figure 38: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in $CDCl_3$ with HD gas at time 0 hrs

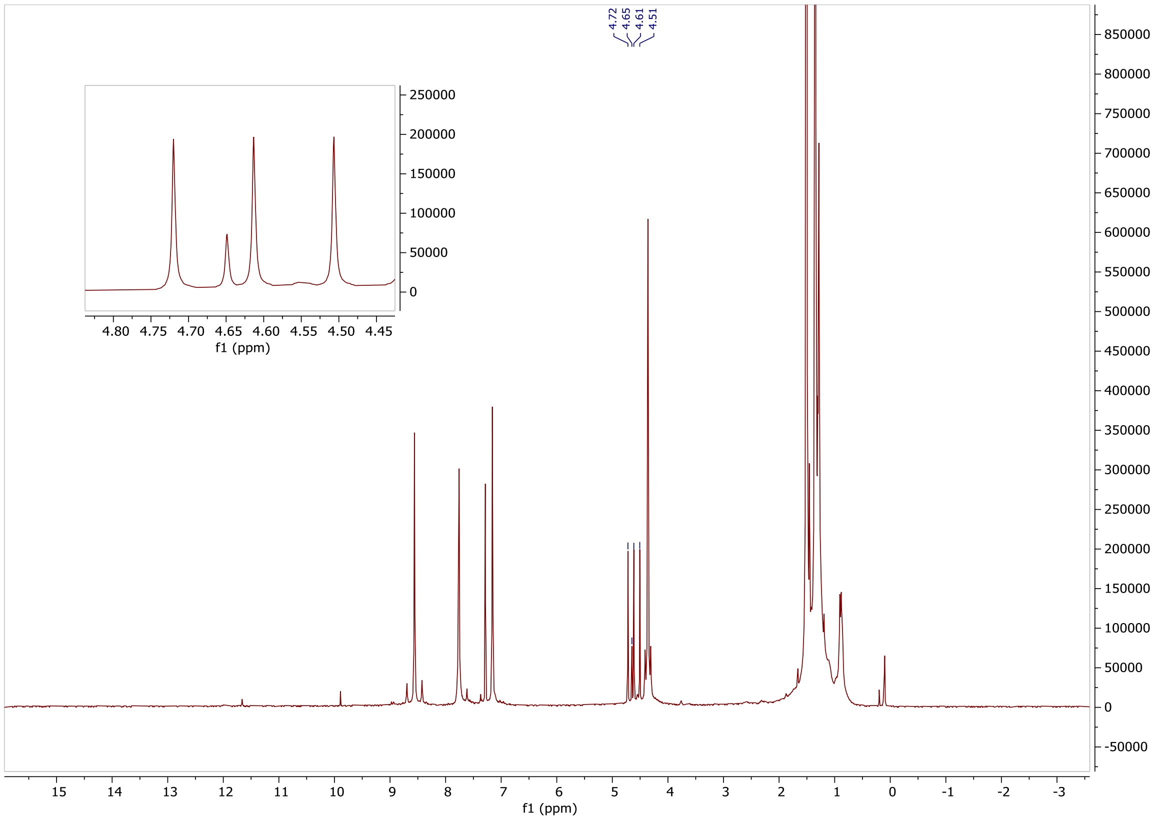


Figure 39: ^{1}H NMR of [Sn(^{t}Bu$_2$Salen)(OTf)$_2$] in $CDCl_3$ with HD gas after 17 hrs at 25°C

Catalyst screening

In glove box, Salen-Sn compounds (0.5 mmol) and imine (1 mmol) were dissolved in sulfolane (4 mL) in a steel autoclave. The autoclave was then sealed and purged 3 times with the 50 bar H_2. The temperature and stirring rate were set using the Spec view program on Parr 5000 series multi reactor system. T = 0 was defined as the time the heating starts. The heating was turned off 2 hours before the end of the stated reaction time and allowed to cool down under pressure over the course of the remaining 2 hours of the test i.e., for a reaction time of 17 hours the heating was turned off after 16 hours and the reaction was depressurized after the 17-hour mark. Dibromomethane (1 mmol) or in earlier tests dichloromethane was added to the reactor, stirred and an aliquot was taken for ^{1}H NMR analysis in $CDCl_3$. The conversion of imine and the yield of product were quantified by ^{1}H NMR analysis with the added Dibromo methane as the internal standard. Other reaction products were quantified by their respective CH_2 signal in ^{1}H NMR and structures confirmed by ESI spectra.

Table 2: Catalytic- test reproducibility

ENTRY	CATALYST	SOLVENT	TEMPERATURE	YIELD (cycle 1, 2, 3)
1	**[Sn(Salen)Cl$_2$]** **(2-Cl2)**	sulfolane	180	50, 54, 56
2	**[Sn(^{t}Bu$_2$Salen) Cl$_2$]** **(1-Cl2)**	sulfolane	180	25, 30, 31
3	**[Sn(^{t}Bu$_2$Salen)Cl(OTf)]** **(1-Cl(OTf)**	sulfolane	180	47, 50, 50
4	**[Sn(^{t}Bu$_2$Salen)(OTf)$_2$]** **([1-(OTf)2)**	sulfolane	180	9, 10, 11
5	**[Sn(^{t}Bu$_2$Salophen)Cl$_2$]** **(4-Cl2)**	sulfolane	180	30, 24, 31
6	**[Sn(Salophen)Cl$_2$]** **(3-Cl2)**	sulfolane	180	41, 45, 41

Example of Reproducibility results using [Sn(Salen)Cl$_2$]

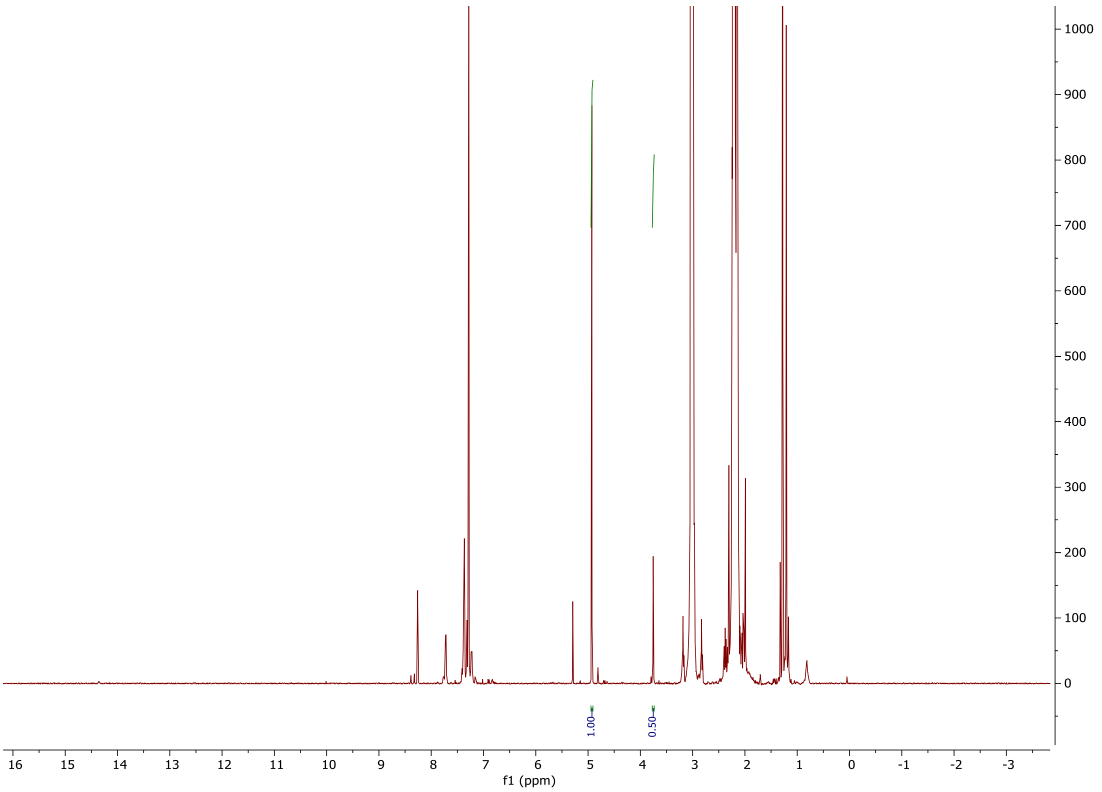


Figure 40: ^{1}H NMR of catalytic test 1 with [Sn(Salen)Cl$_2$] with CH$_2$Br$_2$ as internal standard

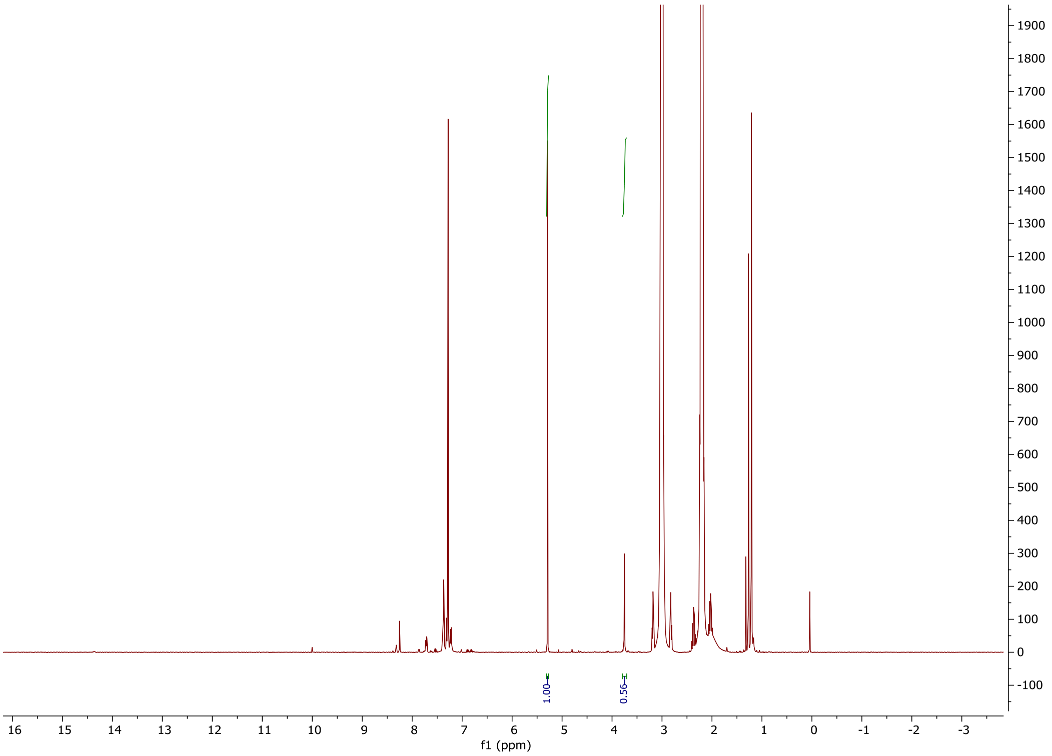


Figure 41: ^{1}H NMR of catalytic test 2 with [Sn(Salen)Cl$_2$] with DCM as internal standard

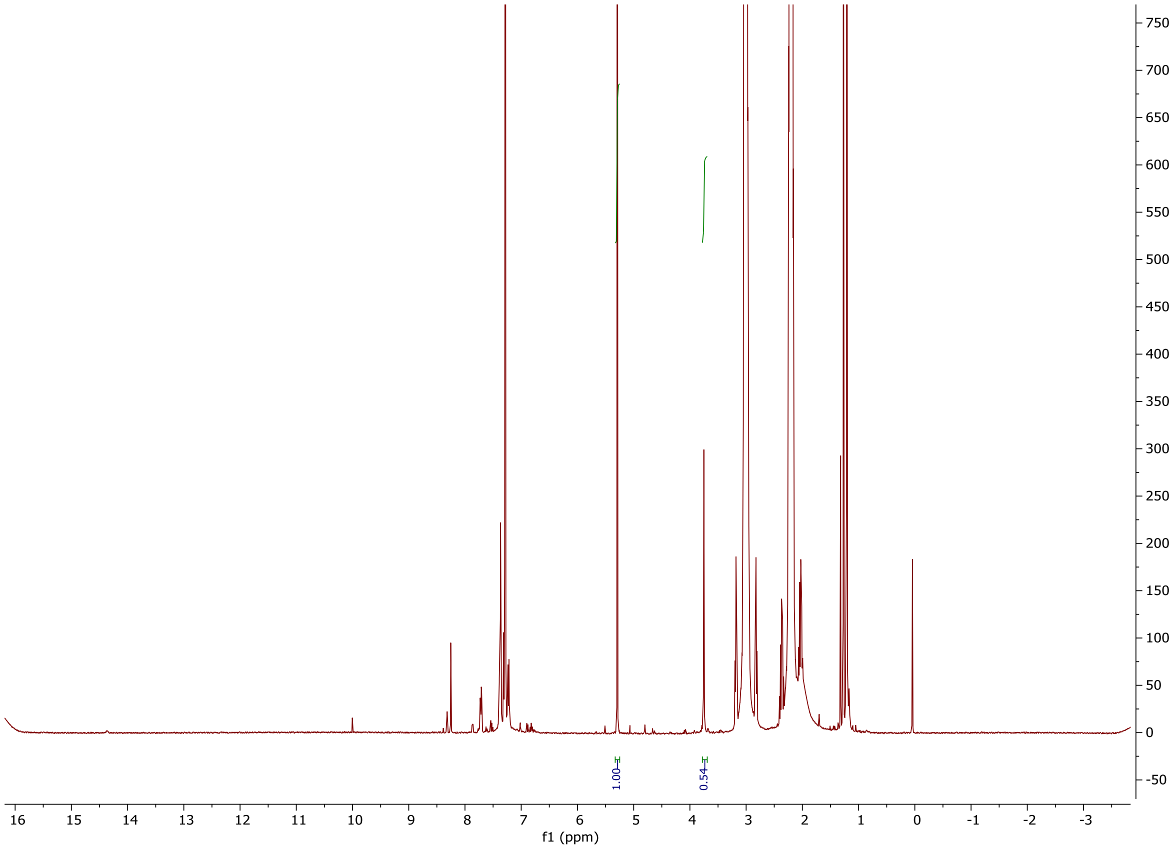


Figure 42: ^{1}H NMR of catalytic test 3 with [Sn(Salen)Cl$_2$] with DCM as internal standard

Solvent screening

To determine the effect of different solvents, catalytic reduction of imine was carried out at 50 bar H_2 with toluene and 2,4,6-trimethylpyridine and the corresponding reproducible values are reported here.

Table 3: Solvent screening

CATALYST	SOLVENT	TEMPERATURE	YIELD
[Sn(Salen)Cl_2] **(2-Cl2)**	sulfolane	180	50,54,56
[Sn(Salen)Cl_2] **(2-Cl2)**	toluene	180	98,98,99
[Sn(Salen)Cl_2] **(2-Cl2)**	2,4,6-trimethylpyridine	180	83,85,87
[Sn(^{t}Bu_2Salen)Cl_2] **(1-Cl2)**	toluene	180	80,85,86
[Sn(^{t}Bu_2Salen)Cl(OTf)] **(1-Cl(OTf)**	toluene	180	85,86,87
[Sn(^{t}Bu_2Salen)$(OTf)_2$] **([1-(OTf)2)**	toluene	180	27,30,32

Reproducibility test of [Sn(Salen)Cl_2] in toluene

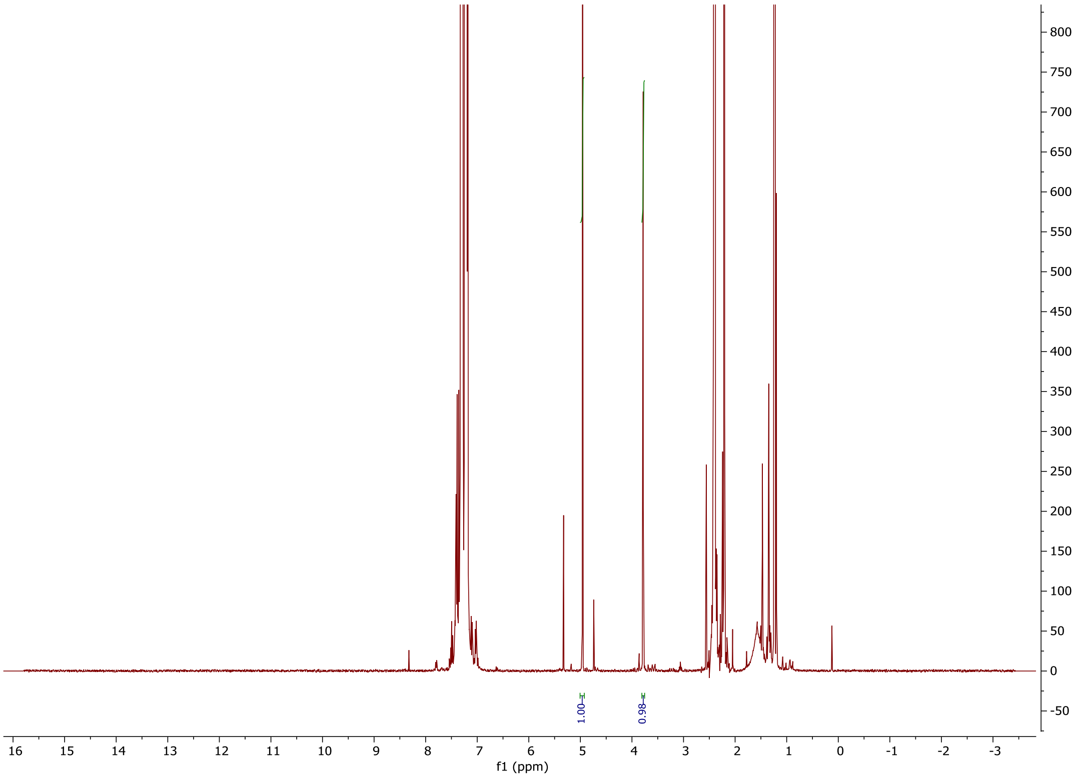


Figure 43: ^{1}H NMR of catalytic test-1 of [Sn(Salen)Cl_2] in toluene, measured in $CDCl_3$

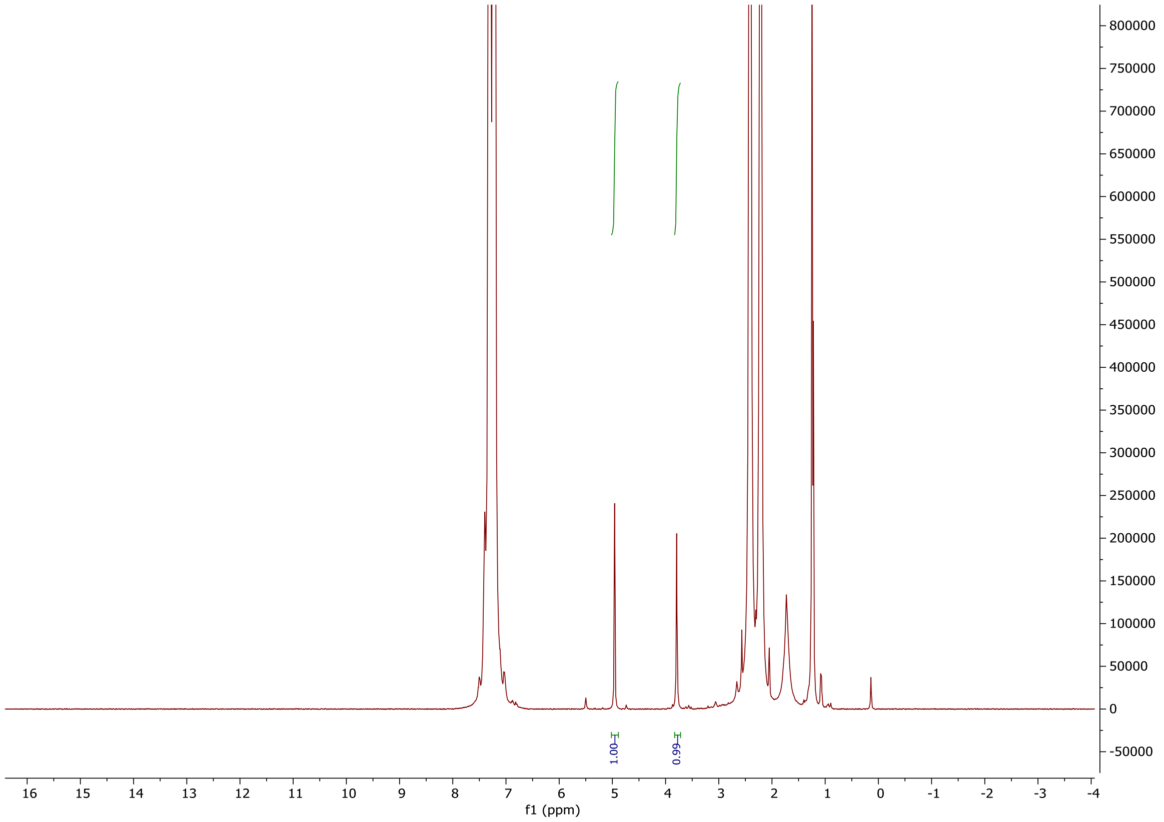


Figure 44: ^{1}H NMR of catalytic test-2 of [Sn(Salen)Cl$_2$] in toluene, measured in CDCl$_3$

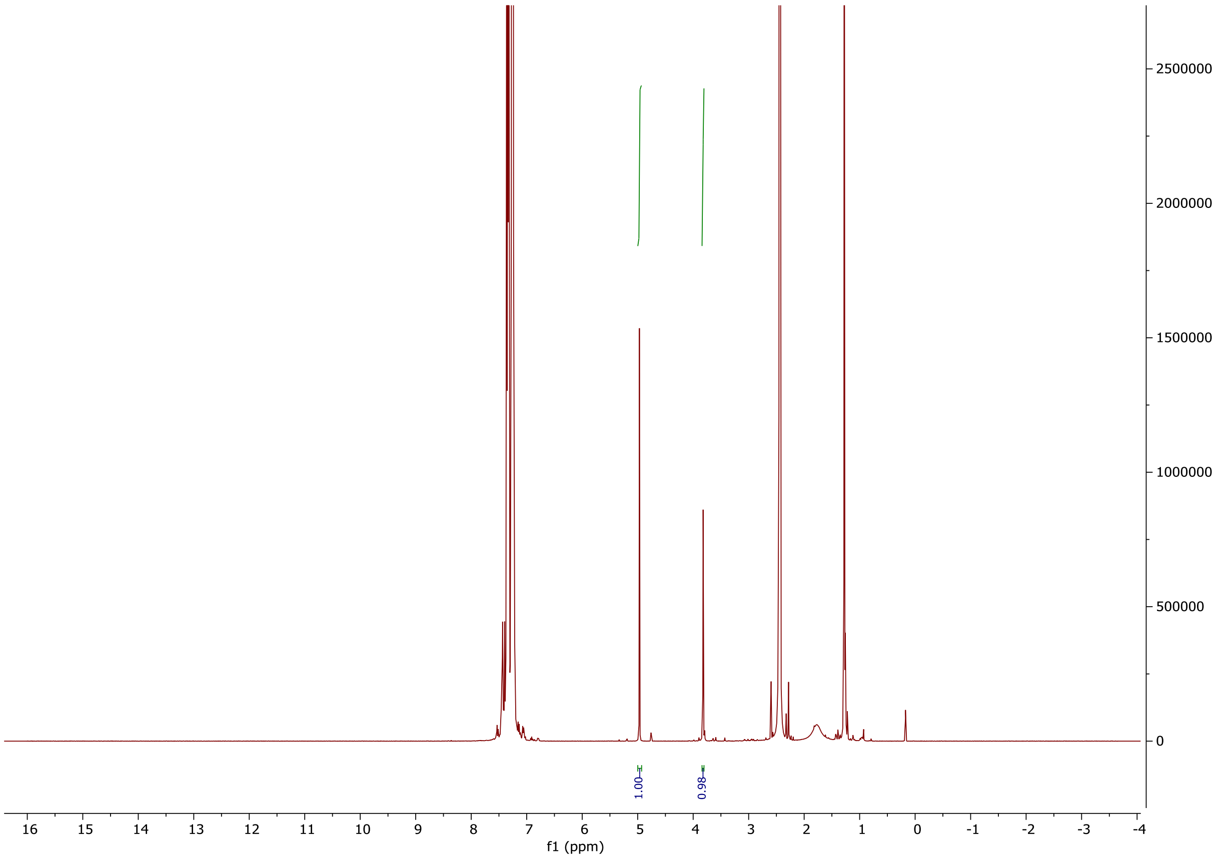


Figure 45: ^{1}H NMR of catalytic test-3 of [Sn(Salen)Cl$_2$] in toluene, measured in CDCl$_3$

Temperature screening

Table 4: Temperature screening

CATALYST	SOLVENT	TEMPERATURE	YIELD
[Sn(Salen)Cl_2] **(2-Cl2)**	Toluene	180	98,98,99
[Sn(Salen)Cl_2] **(2-Cl2)**	Toluene	150	25,26,30
[Sn(Salen)Cl_2] **(2-Cl2)**	2,4,6-trimethylpyridine	180	83,85,87
[Sn(Salen)Cl_2] **(2-Cl2)**	2,4,6-trimethylpyridine	150	25,25,28
[Sn(^{t}Bu_2Salen)Cl_2] **(1-Cl2)**	toluene	180	80,85,86
[Sn(^{t}Bu_2Salen)Cl_2] **(1-Cl2)**	toluene	150	NR
[Sn(^{t}Bu_2Salen)Cl(OTf)] **(1-Cl(OTf)**	toluene	150	NR

Screening of the catalyst 2-Cl_2 with /without the added product(N-benzyl-2-methylpropan-2-amine)

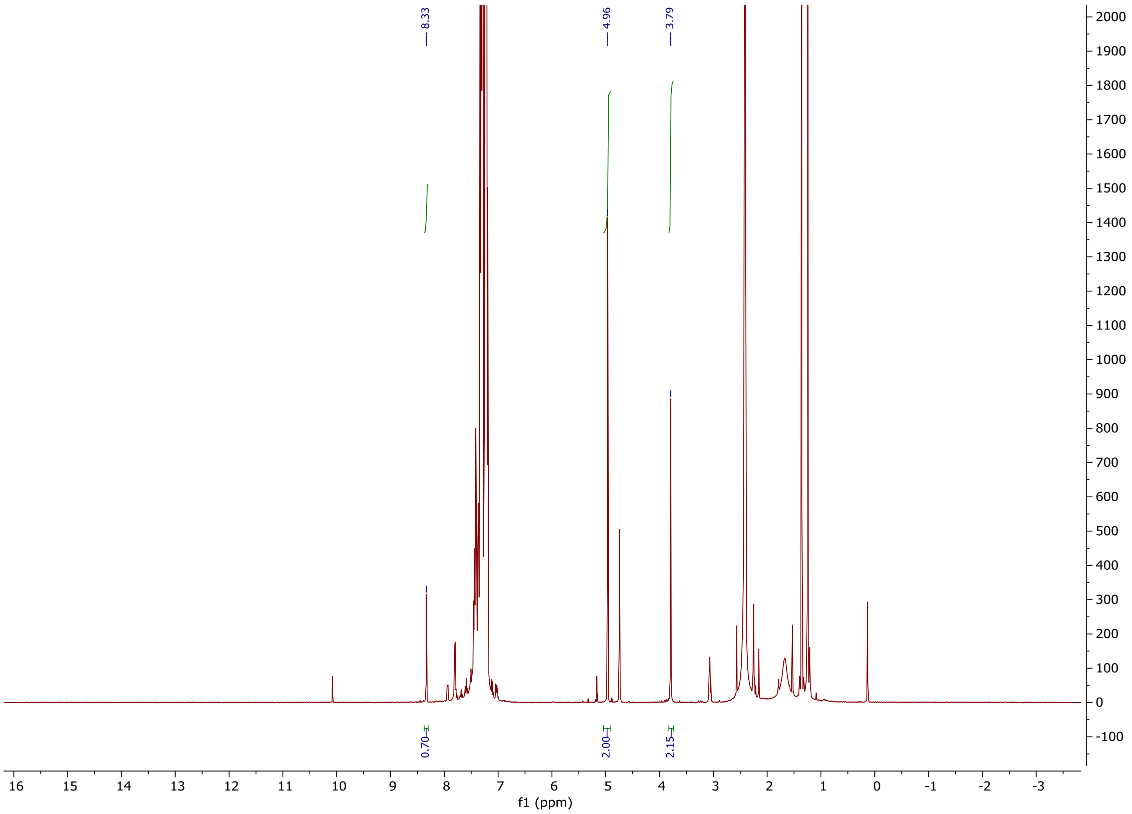


Figure 46: Test with 1mmole of added product using dibromo methane as internal standard

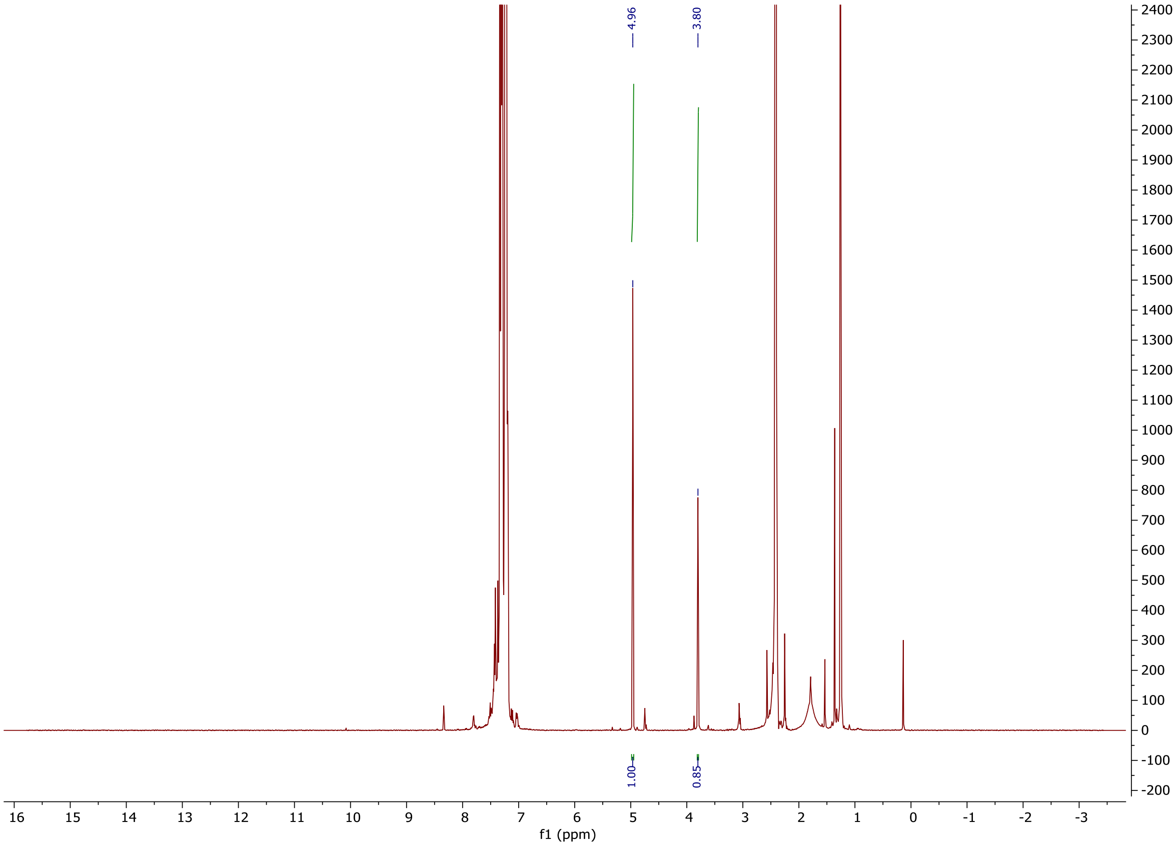


Figure 47: Test without the added product using dibromo methane as internal standard

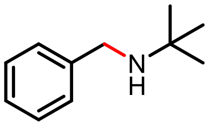
Substrate scope

General procedure for imine synthesis[4–8]

Different substituted Benzaldehydes were added to a Schlenk flask. 2eq of the respective amine was added dropwise under N_2 atmosphere in the presence of molecular sieves. the reaction was kept stirring overnight at room temperature. Next day the excess amine was evaporated under reduced pressure. It was then kept under vacuum overnight to obtain analytically pure imine.

N-benzyl-2-methylpropan-2-amine

The corresponding imine was synthesized according to the reported procedures from literature.[4] Imine characterization: ^1H NMR (400 MHz, Chloroform-*d*) δ 8.34 (s, 1H), 7.91 – 7.77 (m, 2H), 7.57 – 7.40 (m, 3H), 1.37 (S,9H).



^1H NMR (400MHz, $CDCl_3$): Product peak at 3.78 ppm All other product peaks were obscured by reaction solvent. ESI(+H): expected 163.3 (M+H), found 162.0

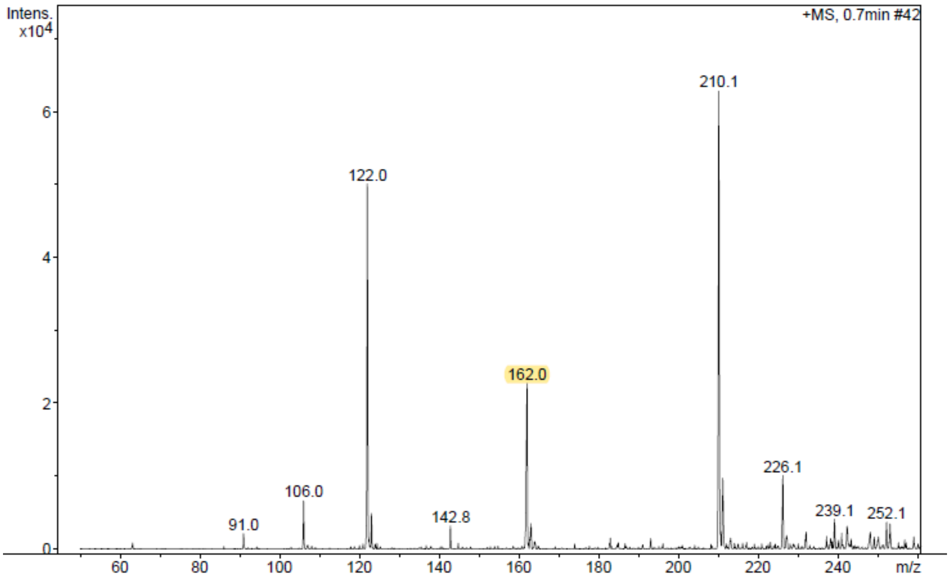


Figure 48:ESI-MS of N-benzyl-2-methylpropan-2-amine

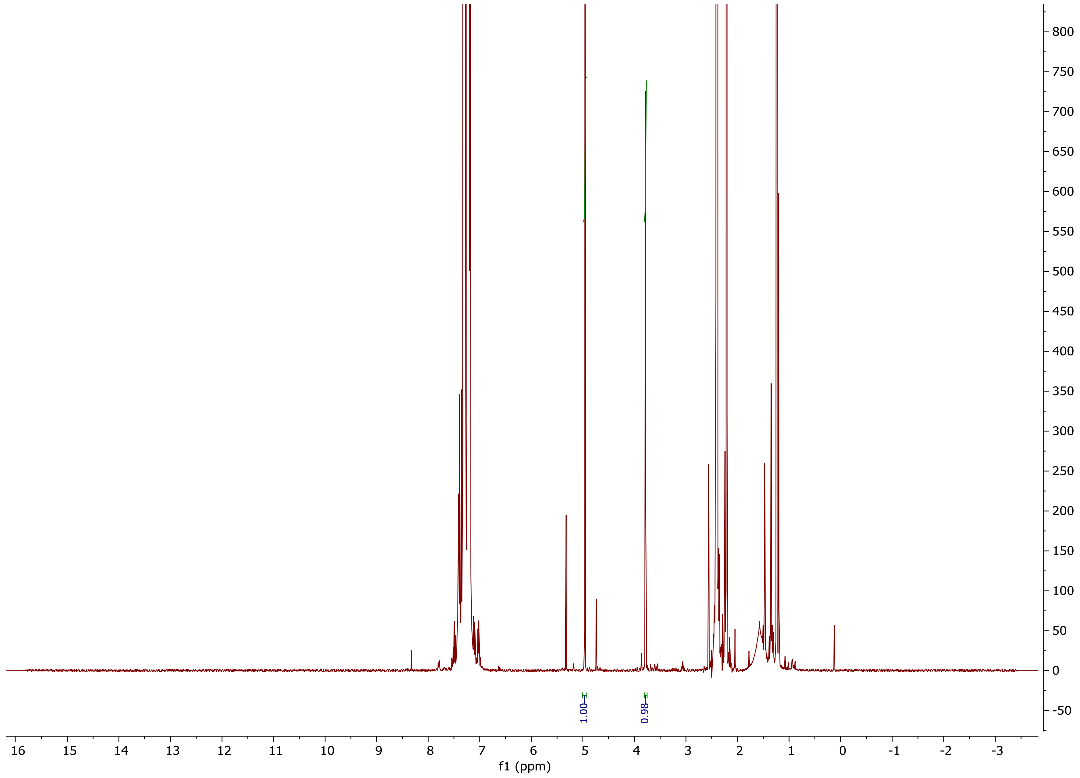
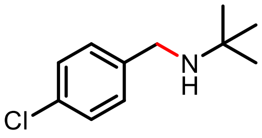


Figure 49:^{1}H NMR IN CDCl$_3$ FOR N-benzyl-2-methylpropan-2-amine using CH$_2$Br$_2$ as internal standard

2. N-(4-chlorobenzyl)-2-methylpropan-2-amine

The corresponding imine was synthesized according to the reported procedure.[4] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-d) δ 8.25 (s, 1H), 7.73 – 7.67 (m, 2H), 7.41 – 7.36 (m, 2H), 1.31(s,9H)



^{1}H NMR (400MHz, CDCl$_3$): product peak 3.75ppm (-CH2 peak). All other product peaks were obscured by reaction solvent. ESI(+H): expected 198.09, found 198.1(M+H)

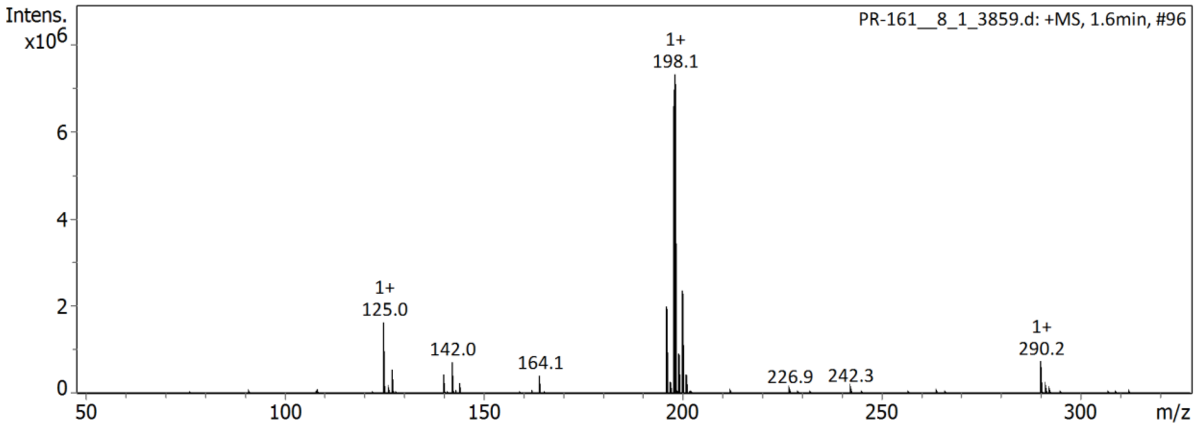


Figure 50: ESI-MS of N-(4-chlorobenzyl)-2-methylpropan-2-amine

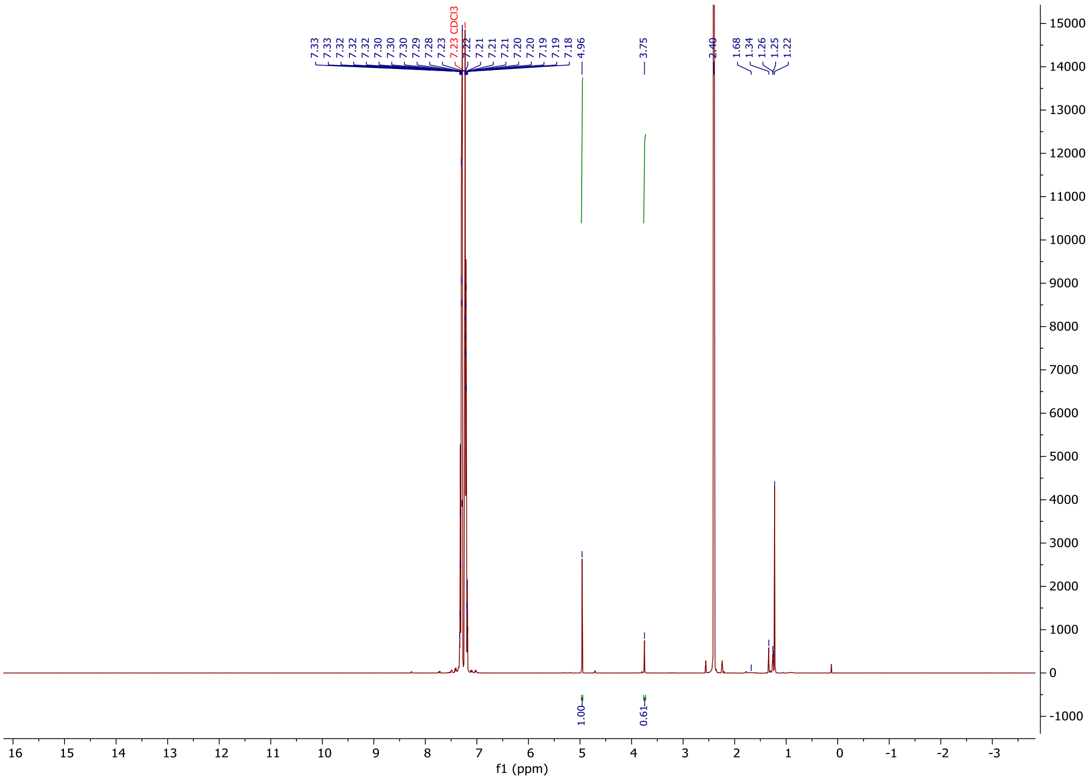
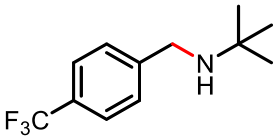


Figure 51:NMR of N-(4-chlorobenzyl)-2-methylpropan-2-amine with CH_2Br_2 as internal standard

3. 2-methyl-N-(4-(trifluoromethyl)benzyl)propan-2-amine

The corresponding imine was synthesized according to the reported procedure.[4] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (s, 1H), 7.87 (d, *J* = 8.1 Hz, 2H), 7.65 (d, *J* = 8.1 Hz, 2H), 1.32 (s, 9H).



^{1}H NMR (400MHz,$CDCl_3$) Product peak at 3.83 ppm. All other product peaks were obscured by reaction solvent. ESI(+H): Expected 232.12, found 232.1(M+H)

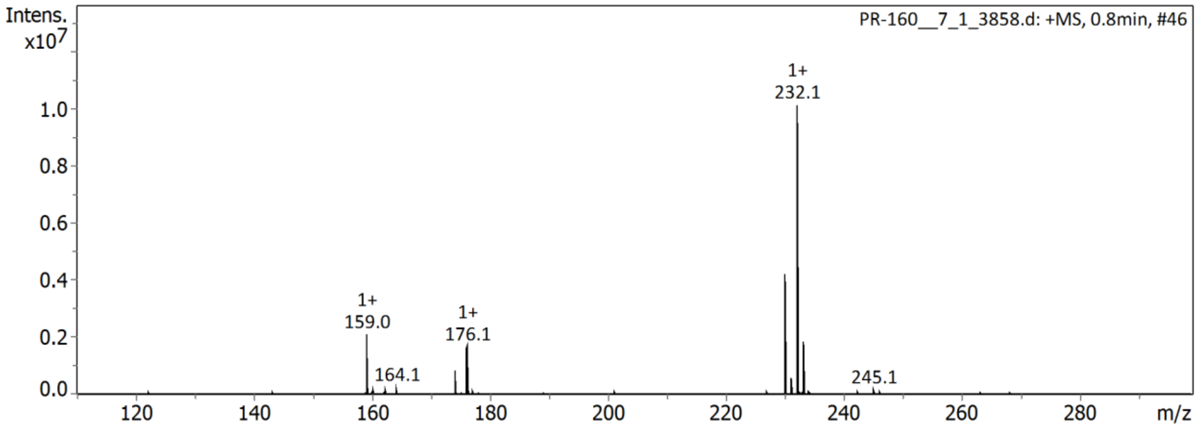


Figure 52:ESI-MS of 2-methyl-N-(4-(trifluoromethyl)benzyl)propan-2-amine

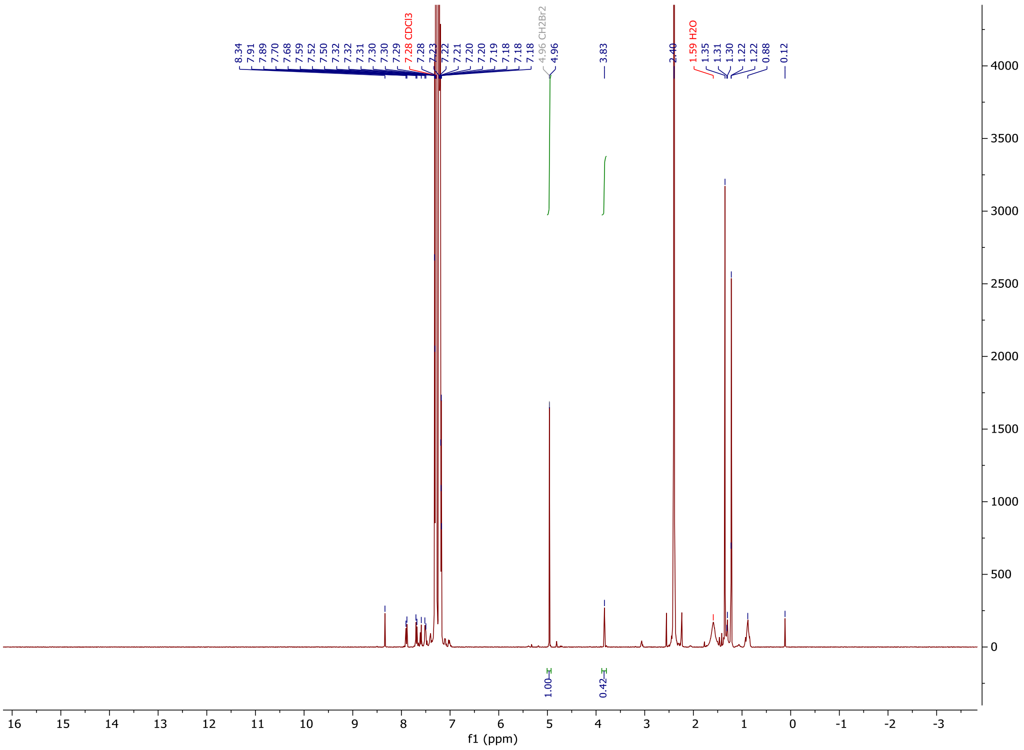


Figure 53: NMR of-2-methyl-N-(4-(trifluoromethyl)benzyl)propan-2-amine with CH_2Br_2 as internal standard

Catalytic test at increased H_2-pressure(75bar)

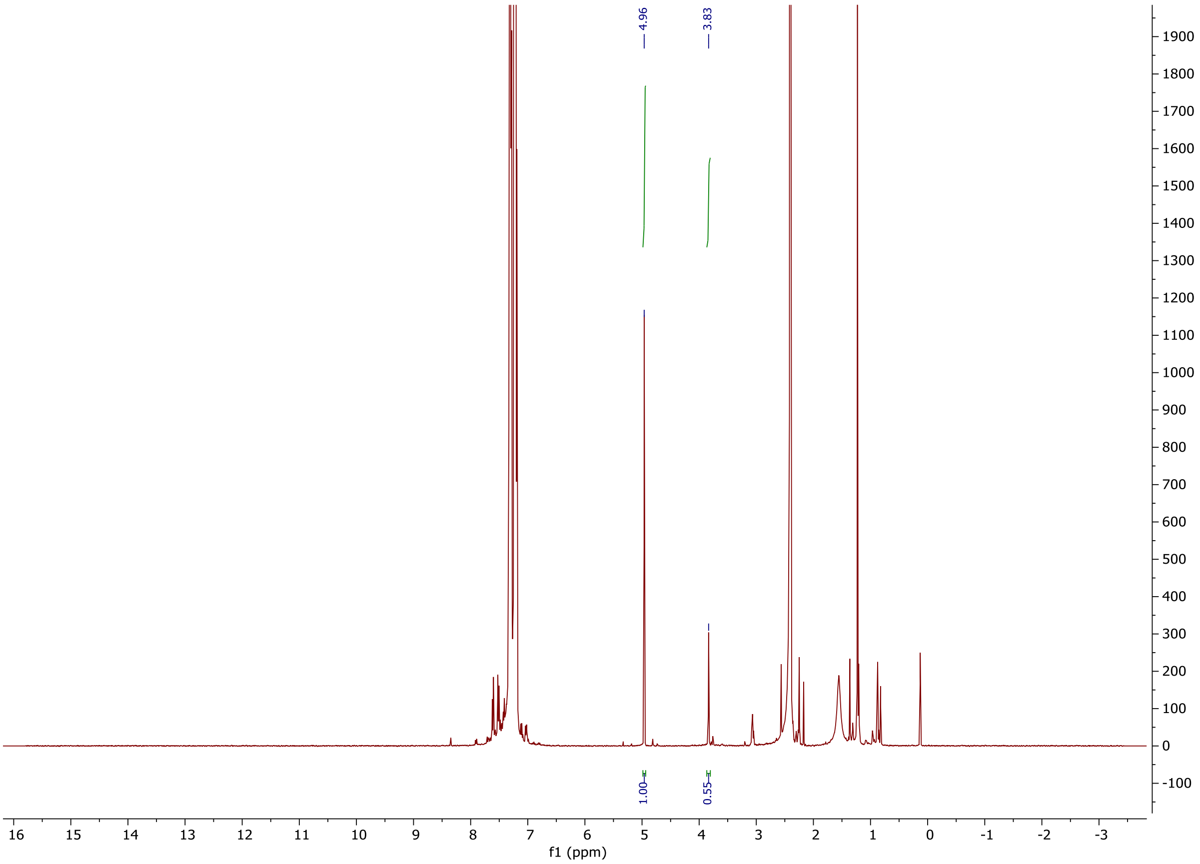


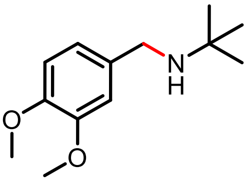
Figure 54:NMR of-2-methyl-N-(4-(trifluoromethyl)benzyl)propan-2-amine with CH_2Br_2 as internal standard at 75bar H_2 pressure

4. 2-methyl-N-(4-nitrobenzyl)propan-2-amine

The corresponding imine was synthesized according to the reported procedure.[5] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (s, 1H), 8.30 – 8.25 (m, 2H), 7.97 – 7.89 (m, 2H), 1.34 (s, 9H). Reduction of the imine was not observed.

5.N-(3,4-dimethoxybenzyl)-2-methylpropan-2-amine

The corresponding imine was synthesized according to the reported procedure.[4] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 1.7 Hz, 1H), 7.49 – 7.39 (m, 1H), 7.15 (dt, *J* = 8.2, 1.8 Hz, 1H), 6.85 (dd, *J* = 8.2, 1.6 Hz, 1H), 3.95 – 3.91 (m, 4H), 3.88 (d, *J* = 2.0 Hz, 3H), 1.27 (d, *J* = 1.9 Hz, 9H).



^{1}H NMR(400MHz,$CDCl_3$): product peak at 3.72ppm. All other product peaks were obscured by reaction solvent. ESI(+H): expected 224.15 found 224.2 (M+H)

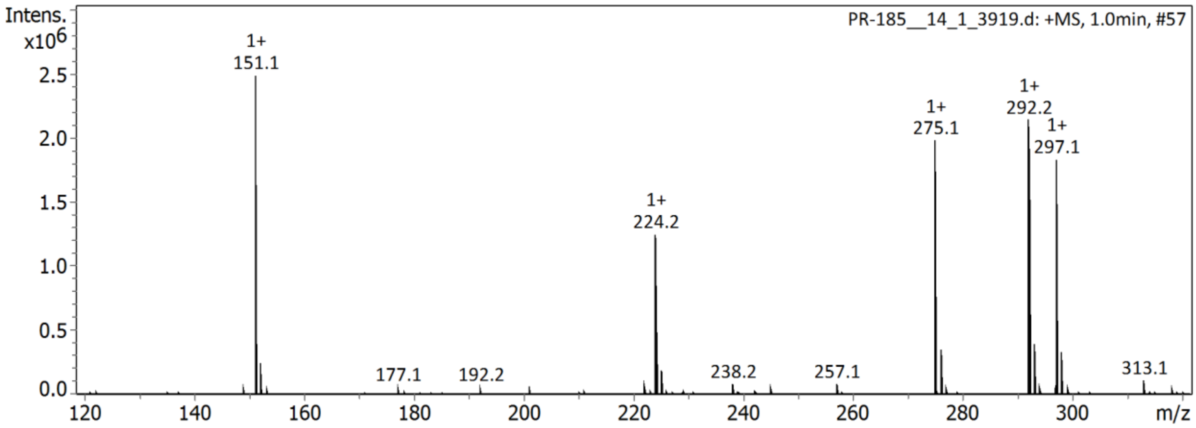


Figure 55: ESI-MS of N-(3,4-dimethoxybenzyl)-2-methylpropan-2-amine

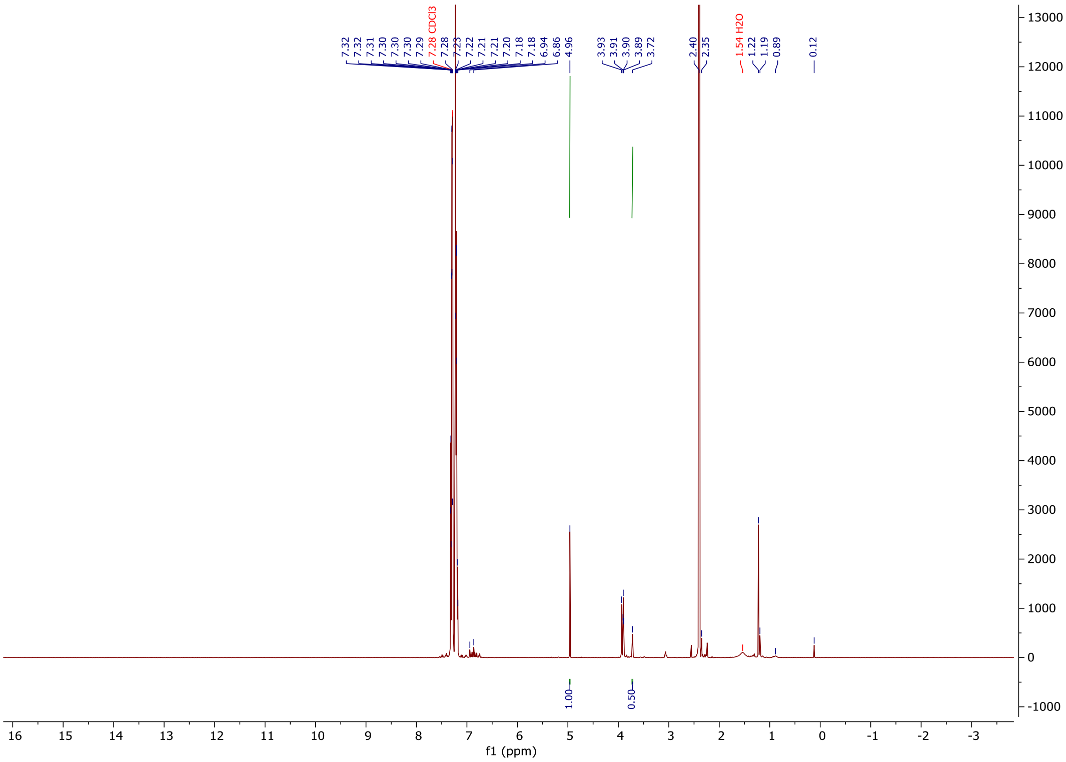
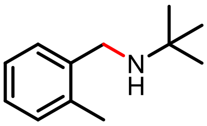


Figure 56: ^{1}H NMR of-N-(3,4-dimethoxybenzyl)-2-methylpropan-2-amine with CH_2Br_2 as internal standard

6. 2-methyl-N-(2-methylbenzyl)propan-2-amine

The corresponding imine was synthesized according to the reported procedure.[4] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.59 (s, 1H), 7.85 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.33 – 7.23 (m, 2H), 7.17 (ddt, *J* = 7.6, 1.6, 0.7 Hz, 1H), 2.50 (s, 3H), 1.32 (s, 9H).



^{1}H NMR (400MHz, $CDCl_3$): Product peak at 3.77ppm. All other product peaks were obscured by reaction solvent. ESI(+H): Expected 177.15, found 177.

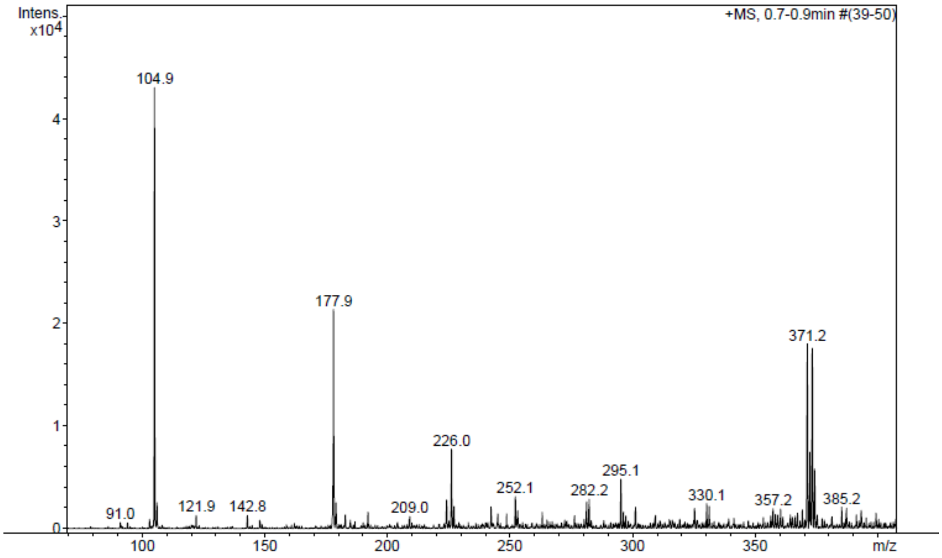


Figure 57: ESI-MS of 2-methyl-N-(2-methylbenzyl)propan-2-amine

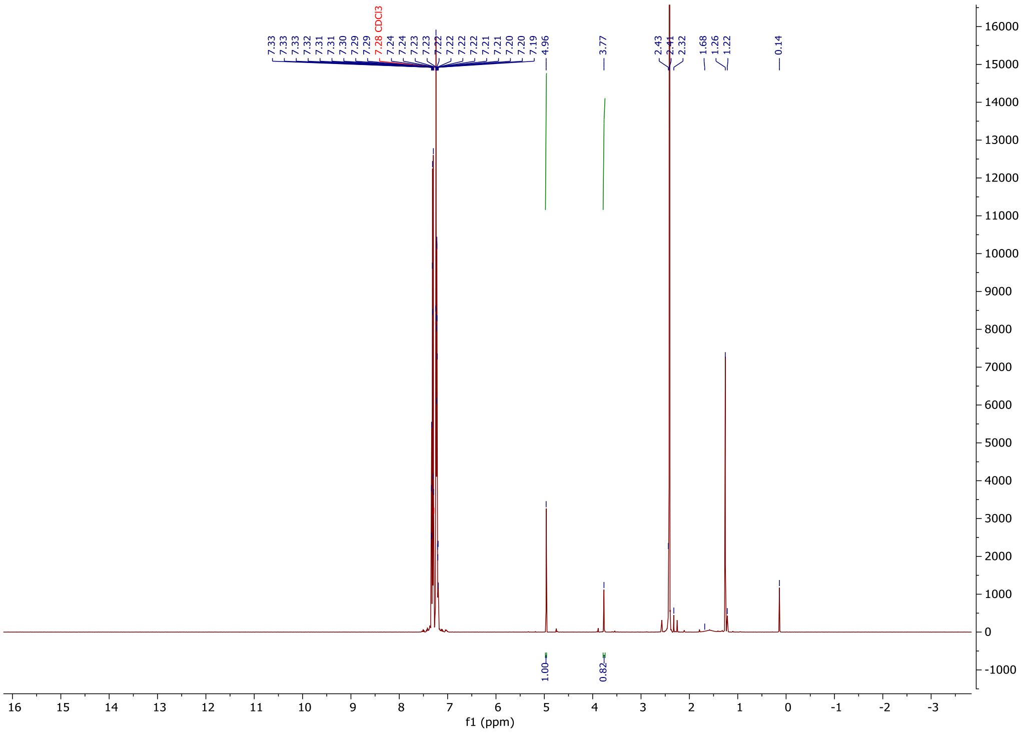
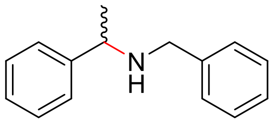


Figure 58: NMR of-2-methyl-N-(2-methylbenzyl)propan-2-aminewith CH_2Br_2 as internal standard

7. N-benzyl-1-phenylethan-1-amine

The corresponding imine was synthesized according to the modified reported procedure.[9] Reaction was performed in an inert atmosphere of N_2 using Schlenk line apparatus and techniques. Solvents and glassware were dried according to the general procedure mentioned above. Molecular sieves (3A) were activated in vacuo by heating up to 300 °C for 5 minutes with a heat gun and leaving to cool down, the cycle was repeated three times.

To the activated molecular sieves was added toluene (10 mL) followed by 1 eq of acetophenone (20 mmol, 2.33 mL) and 1.2 eq of benzylamine (24 mmol, 2.62 mL). The reaction was stirred at RT and followed by NMR. After 44 h only approx. 33 % conversion was observed. The reaction mixture was heated up to 70 °C and stirred for 4 days. The molecular sieves were filtered off and washed with toluene (3 x 2 mL). The solvent was evaporated in vacuo. Resulting pale yellow liquid was mixed with pentane, overlaid with diethylether and placed in a freezer to crystallise. Crystals were filtered off, washed with diethylether, redissolved in chloroform and dried in vacuo. The filtrate was mixed with water and placed in a fridge to provide a second fraction of crystals. These crystals were filtered off, washed with water and dried in vacuo. The fractions were combined to provide product as yellow solid in 56 % (2.34 g) yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.83 (m, 2H), 7.46 – 7.15 (m, 10H), 4.75 (s, 2H), 2.34 (s, 3H). ESI + (*m/z*) for $C_{15}H_{15}N^+$ 210.1.



^{1}H NMR(400MHz,CDCl$_3$): product peak at 1.38ppm. All other product peaks were obscured by reaction solvent. GC-MS retention time was 16.9 -17.0 minutes; EI (*m/z*) 211.

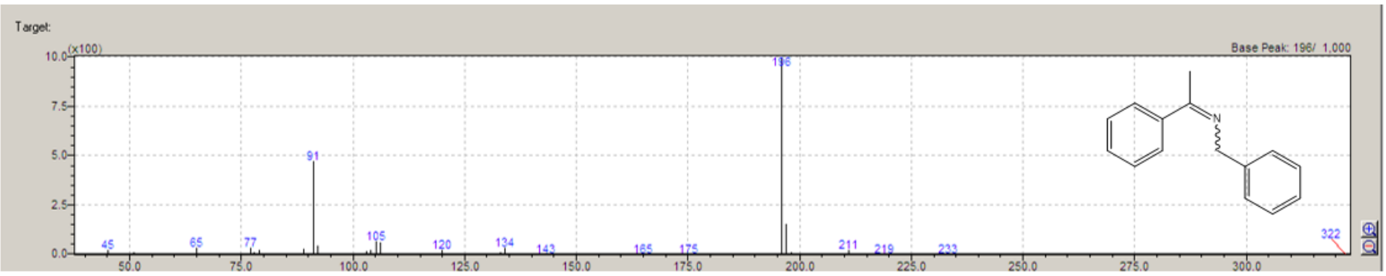


Figure 59 :GC-MS spectra of N-benzyl-1-phenylethan-1-amine

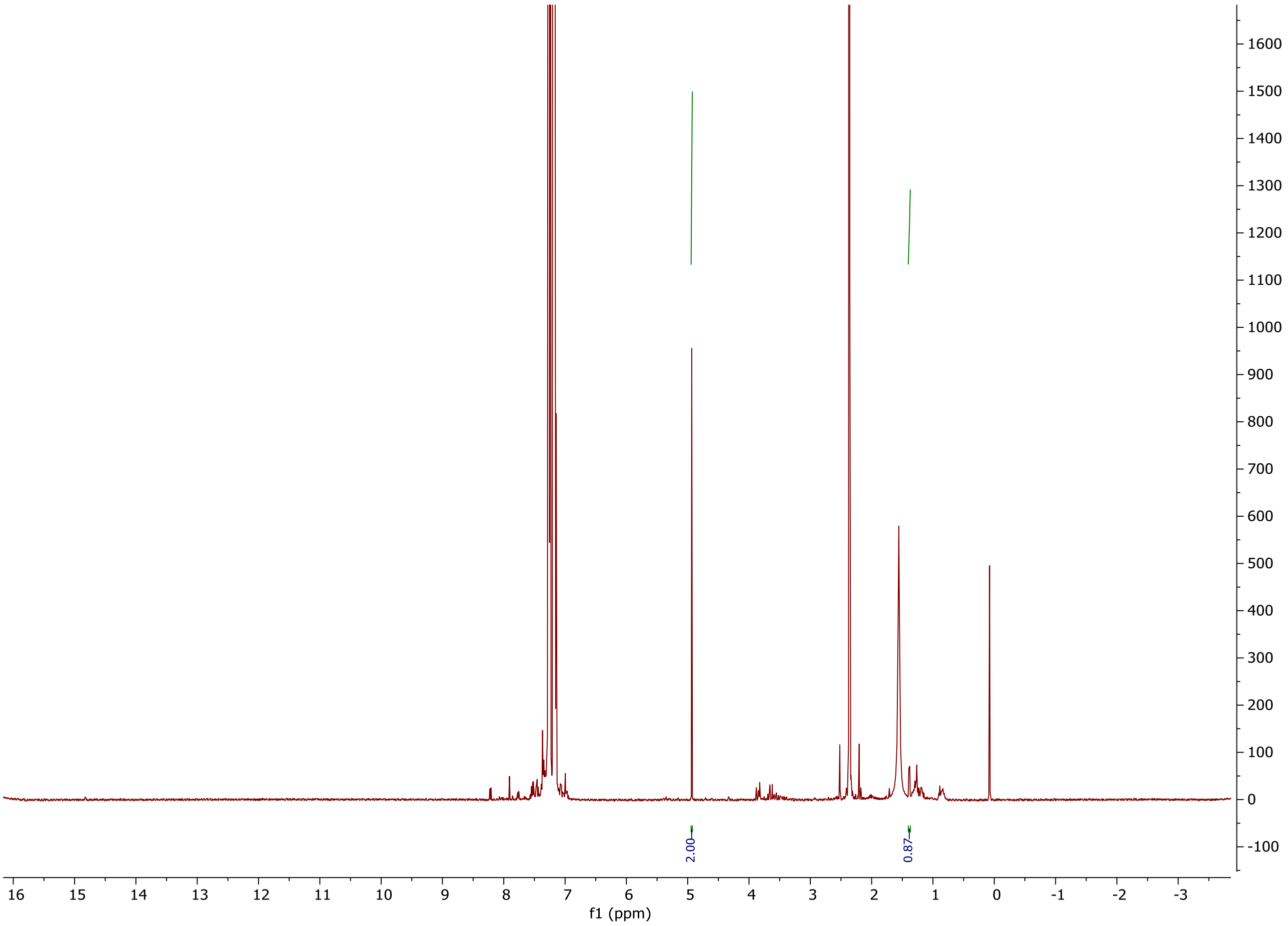
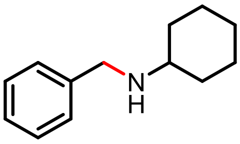


Figure 60: ^{1}H NMR of N-benzyl-1-phenylethan-1-amine using CH_2Br_2 as internal standard

8. N-benzylcyclohexanamine

The corresponding imine was synthesized according to the reported procedure.[6] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.79 – 7.70 (m, 2H), 7.40 (ddt, *J* = 5.7, 3.9, 2.0 Hz, 3H), 3.20 (tt, *J* = 10.5, 4.1 Hz, 1H), 1.87-1.81(m,2H), 1.77 – 1.67 (m, 3H), 1.59 (dd, *J* = 7.0, 5.1 Hz, 2H), 1.41 – 1.31 (m, 2H), 1.30 – 1.22 (m, 1H).



^{1}H NMR(400MHz,$CDCl_3$): product peak at 3.86 ppm. All other product peaks were obscured by reaction solvent.

ESI(+H): expected 190.15, found 190(M+H)

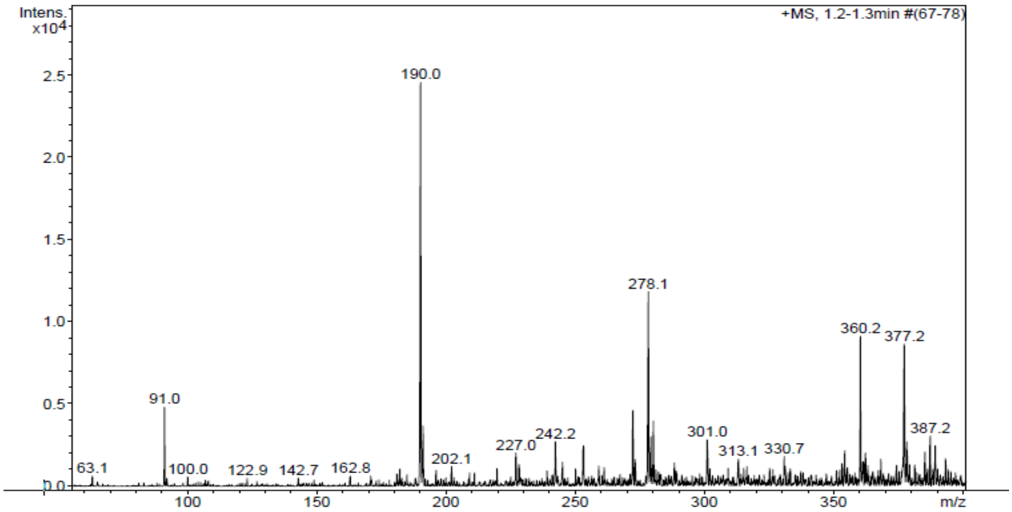


Figure 61: ESI-MS of - N-benzylcyclohexanamine

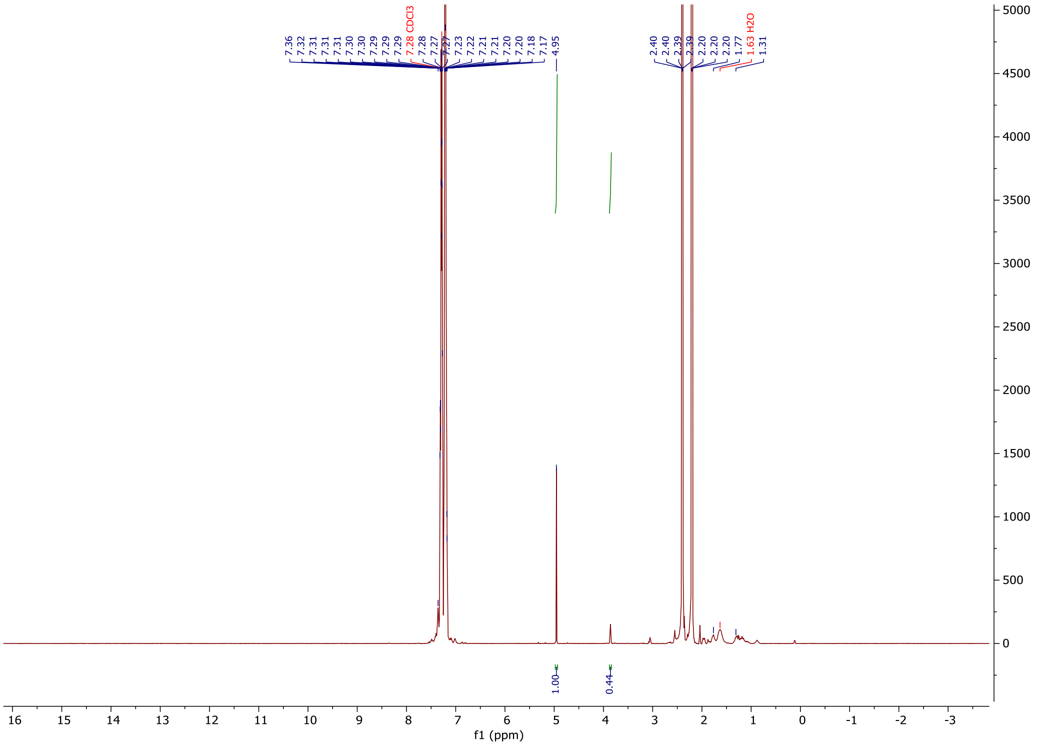
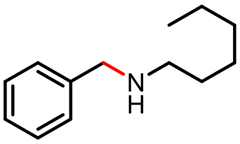


Figure 62: NMR of- N-benzylcyclohexanamine with CH_2Br_2 as internal standard

9. N-benzylhexan-1-amine

The corresponding imine was synthesized according to the reported procedure.[6]

Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 – 8.14 (m, 1H), 7.65 (dp, *J* = 9.6, 3.6, 2.9 Hz, 2H), 7.35 (ddt, *J* = 6.7, 4.1, 2.1 Hz, 3H), 3.53 (tt, *J* = 7.0, 3.6 Hz, 2H), 1.63 (ddd, *J* = 9.9, 6.9, 3.5 Hz, 2H), 1.30 – 1.21 (m, 6H), 0.82 (dt, *J* = 7.9, 4.4 Hz, 3H).



^{1}H NMR(400MHz,$CDCl_3$): product peak at 3.86 ppm. All other product peaks were obscured by reaction solvent. ESI(+H): expected 192.16, found 192 (M+H)

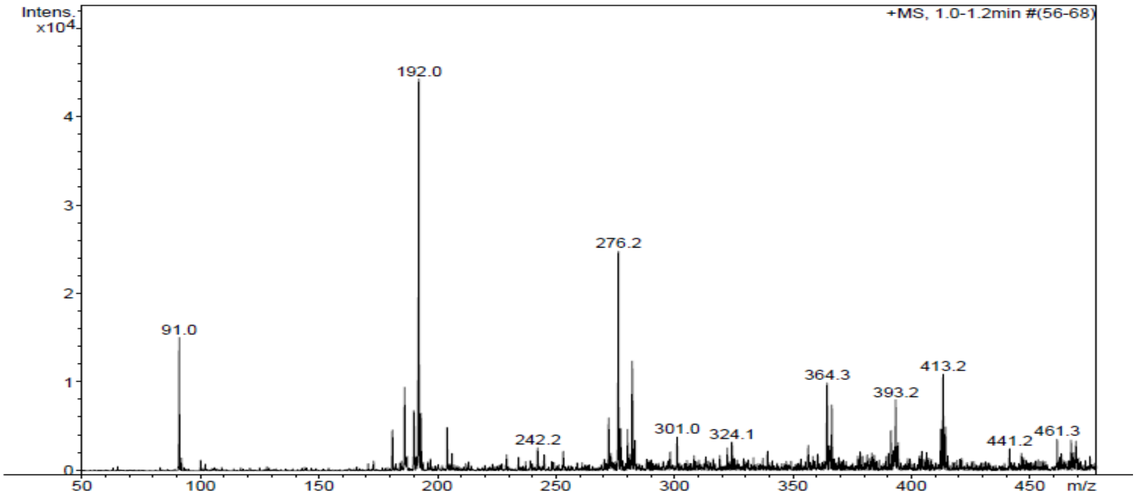


Figure 63: ESI-MS of N-benzylhexan-1-amine

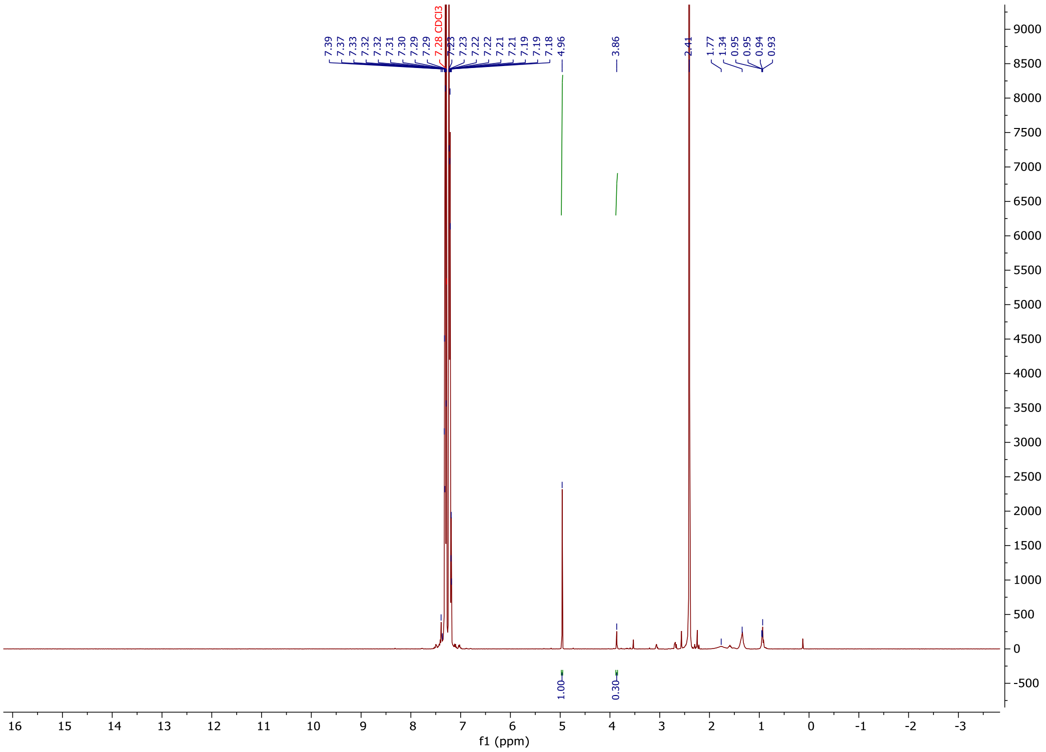


Figure 64: NMR of-N-benzylhexan-1-aminewith CH_2Br_2 as internal standard

48h catalytic test

^{1}H NMR(400MHz,$CDCl_3$): product peak at 3.86 ppm. All other product peaks were obscured by reaction solvent. GC-MS retention time was 13.5-13.6 minutes; EI (*m/z*) 191.

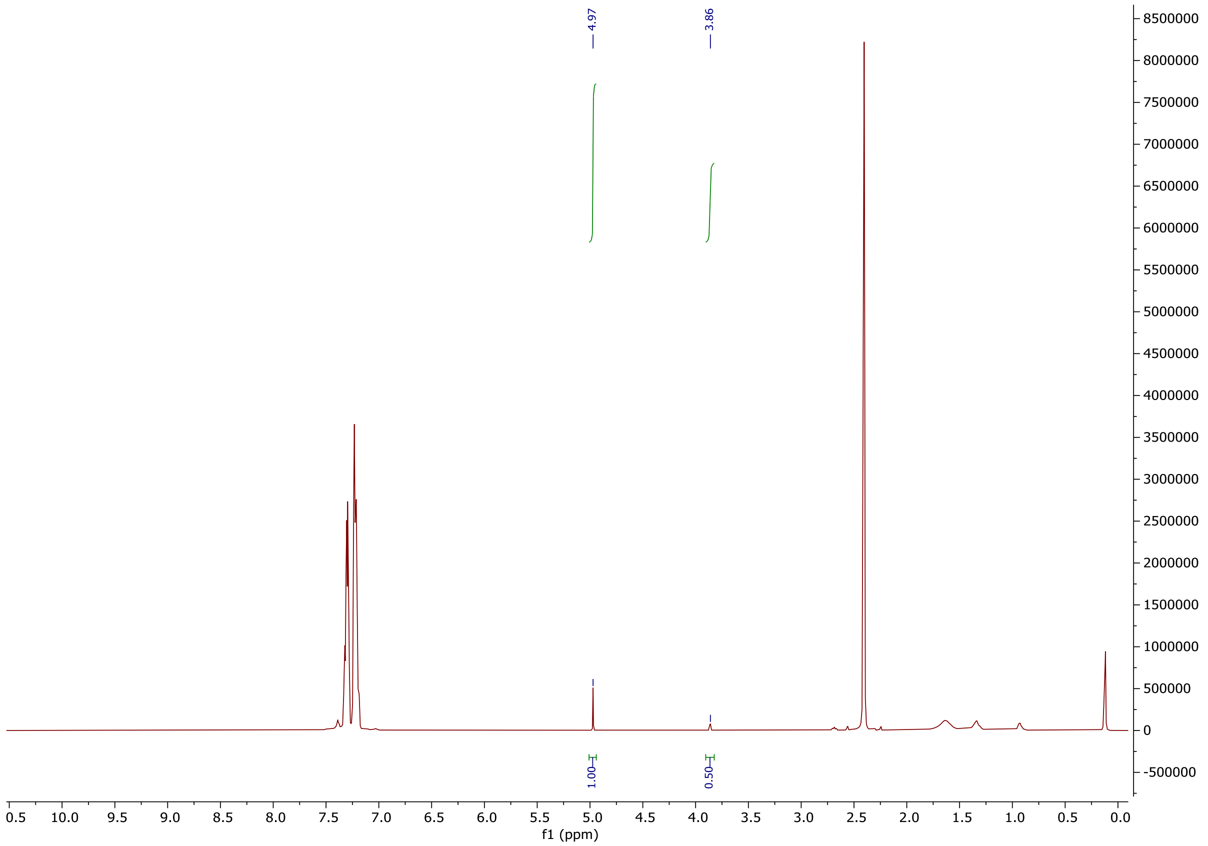


Figure 65:NMR of-N-benzylhexan-1-amine with CH_2Br_2 as internal standard, 48h test

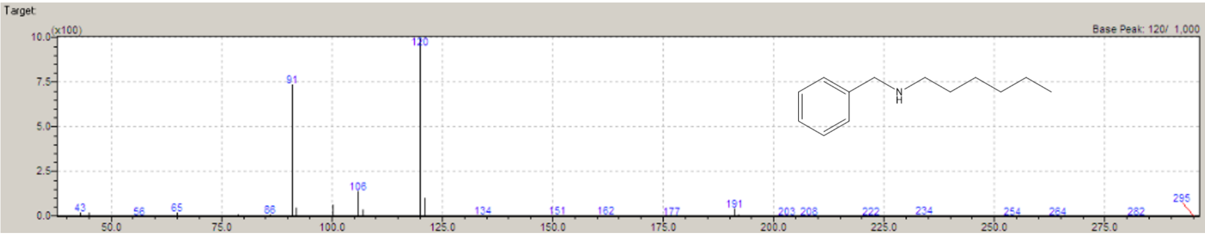


Figure 66: *GC*-*MS* spectra *of N*-benzylhexan-*1*-amine, 48 h test

10% mol of catalyst test

^{1}H NMR(400MHz,$CDCl_3$): product peak at 3.83 ppm. All other product peaks were obscured by reaction solvent. ESI(+H) expected: 192.2; found 192.1 (M+H).

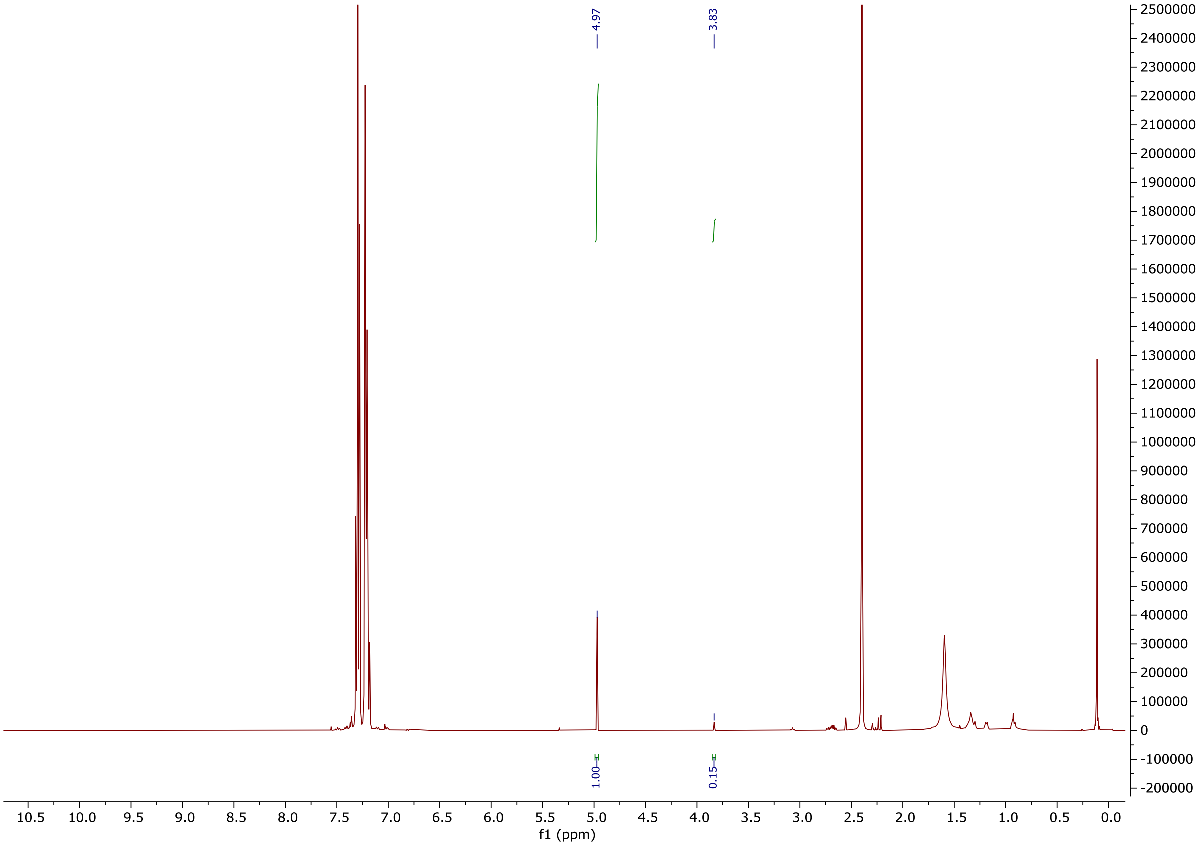


Figure 67: NMR of-N-benzylhexan-1-amine with CH_2Br_2 as internal standard, 10% mmol of catalyst

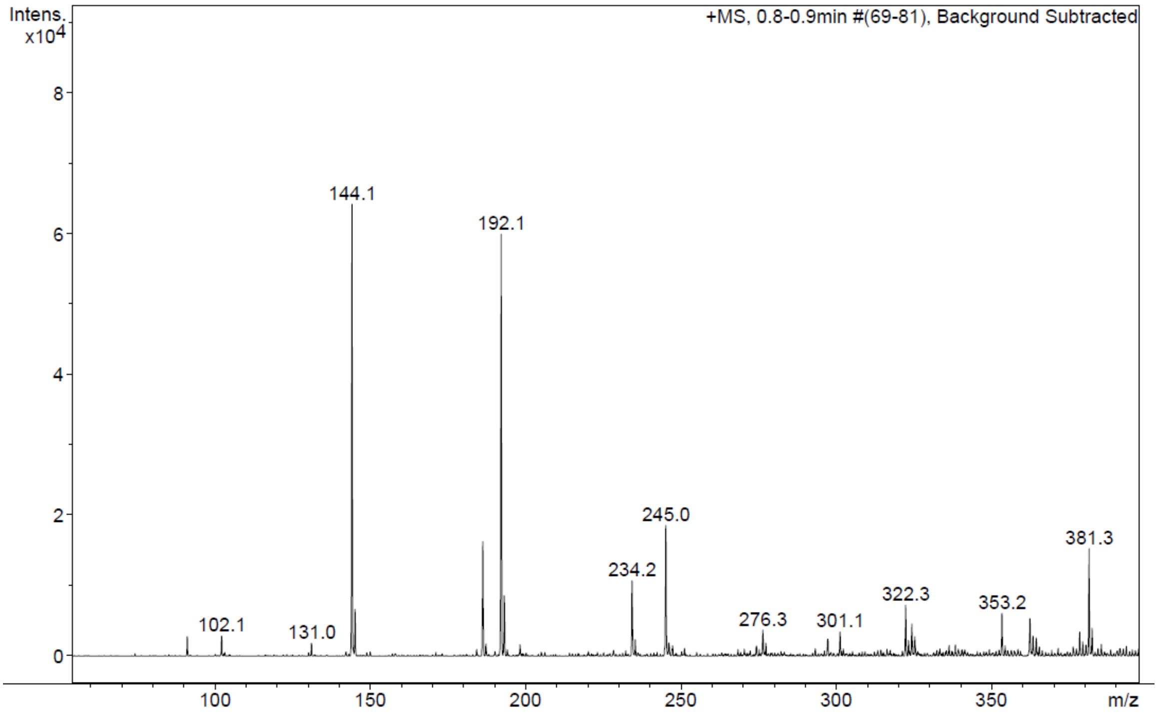


Figure 68: ESI-MS spectra of N-benzylhexan-1-amine, 10 % mmol of catalyst

2,5% mol of catalyst test

^1H NMR(400MHz,$CDCl_3$): product peak at 3.84 ppm. All other product peaks were obscured by reaction solvent. ESI(+H) expected: 192.2; found 192.0 (M+H).

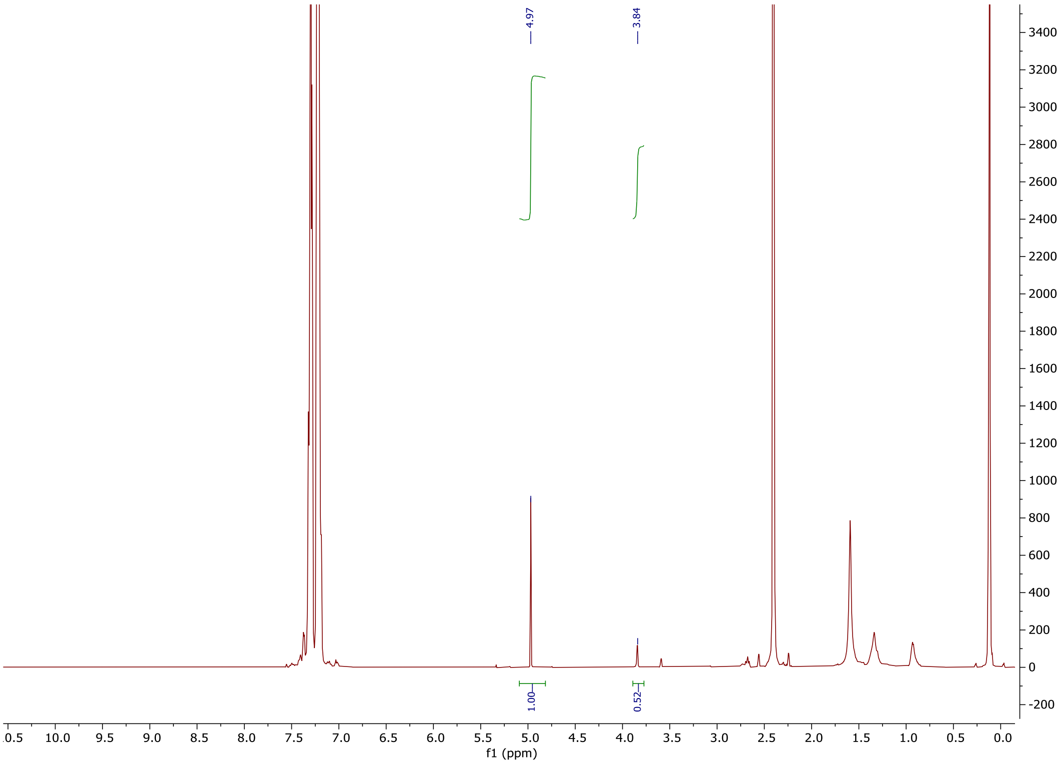


Figure 69: NMR of-N-benzylhexan-1-amine with CH_2Br_2 as internal standard, 2.5 % mmol of catalyst

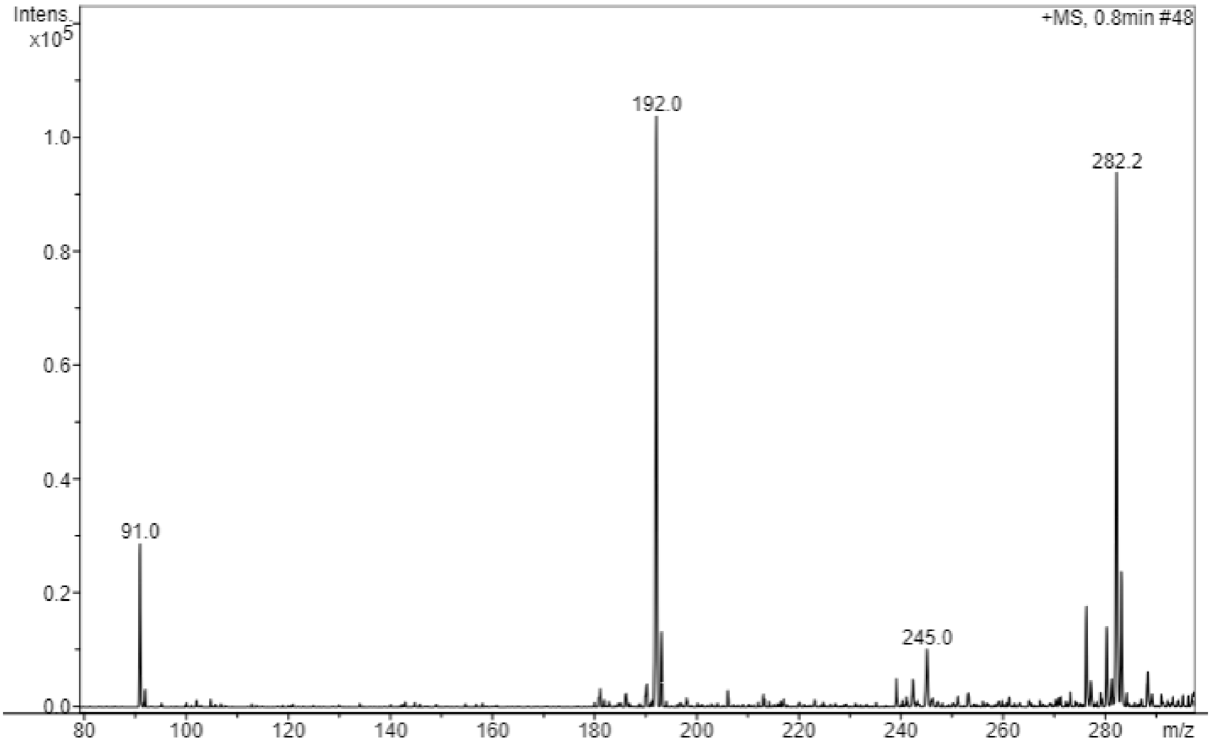
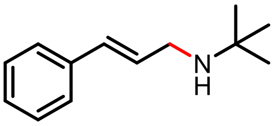


Figure 70 :ESI-MS spectra of N-benzylhexan-1-amine, 2.5 % mmol of catalyst.

10.(E)-N-(tert-butyl)-3-phenylprop-2-en-1-amine

The corresponding imine was synthesized according to the reported procedure.[8] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (t, *J* = 4.1 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.40 – 7.22 (m, 3H), 6.92 (d, *J* = 4.1 Hz, 2H), 2.47 – 2.24 (m, 2H), 1.24 (s, 9H).



^{1}H NMR(400MHz,$CDCl_3$): Product peak at 3.77ppm. All other product peaks were obscured by reaction solvent. ESI(+H): expected 190.15, found 190(M+H)

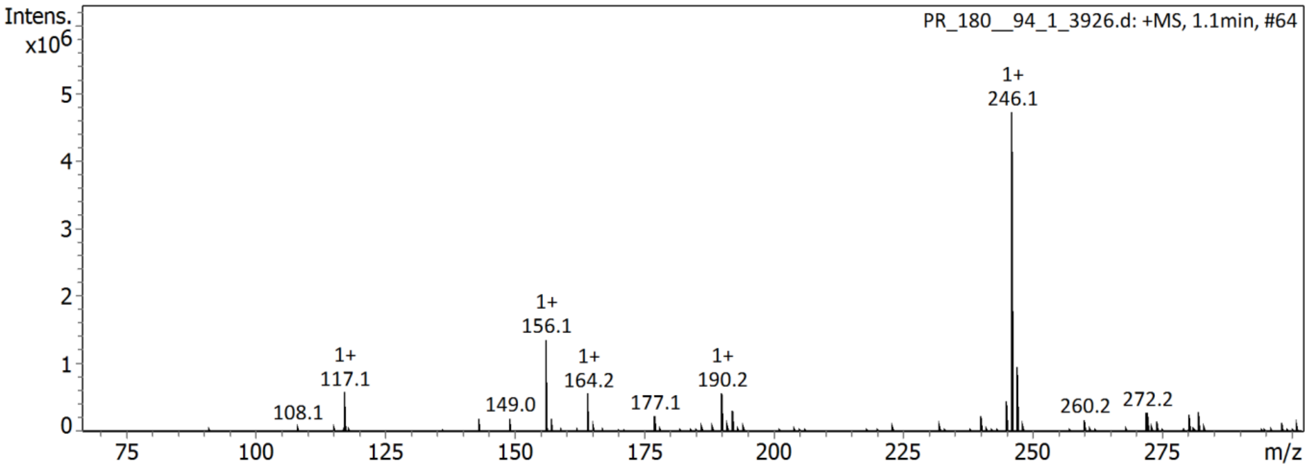


Figure 71: ESI-MS of -(E)-N-(tert-butyl)-3-phenylprop-2-en-1-amine

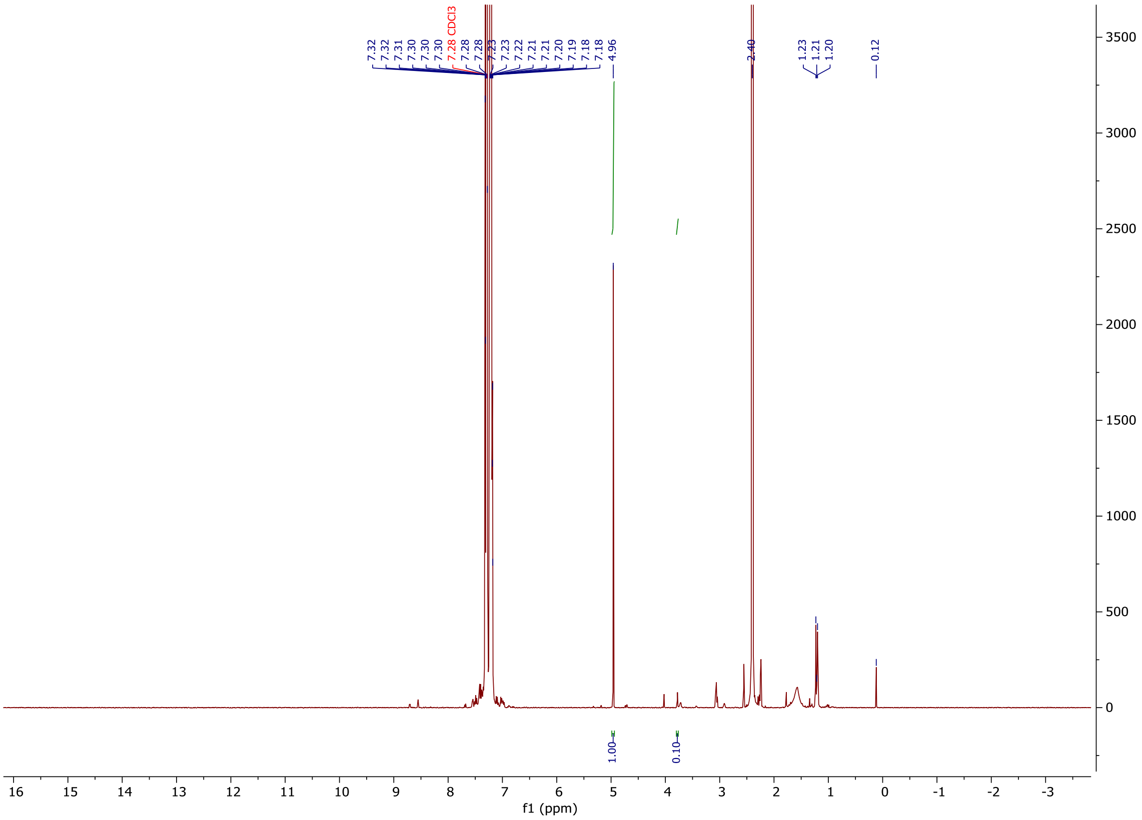
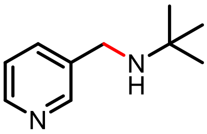


Figure 72: NMR of-(E)-N-(tert-butyl)-3-phenylprop-2-en-1-aminewith CH_2Br_2 as internal standard

11.2-methyl-N-(pyridin-3-ylmethyl)propan-2-amine

The corresponding imine was synthesized according to the reported procedure.[7] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 (t, *J* = 2.2 Hz, 1H), 8.50 (ddd, *J* = 4.7, 3.0, 1.4 Hz, 1H), 8.26 – 8.16 (m, 1H), 8.04 (dp, *J* = 7.9, 2.0 Hz, 1H), 1.33 – 1.16 (m, 9H).



^{1}H NMR(400MHz,CDCl$_3$): product peak at 3.79ppm. All other product peaks were obscured by reaction solvent. ESI(+H): expected 165. Found 165 (M+H)

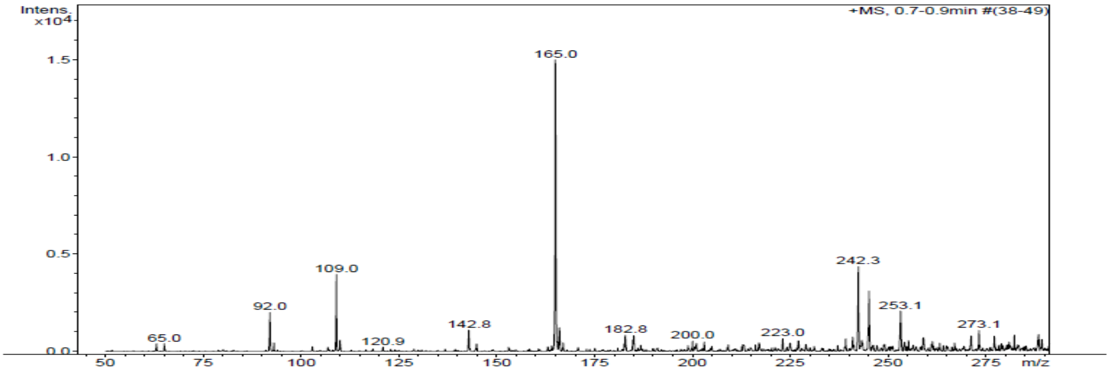


Figure 73: ESI-MS of 2-methyl-N-(pyridin-3-ylmethyl)propan-2-amine

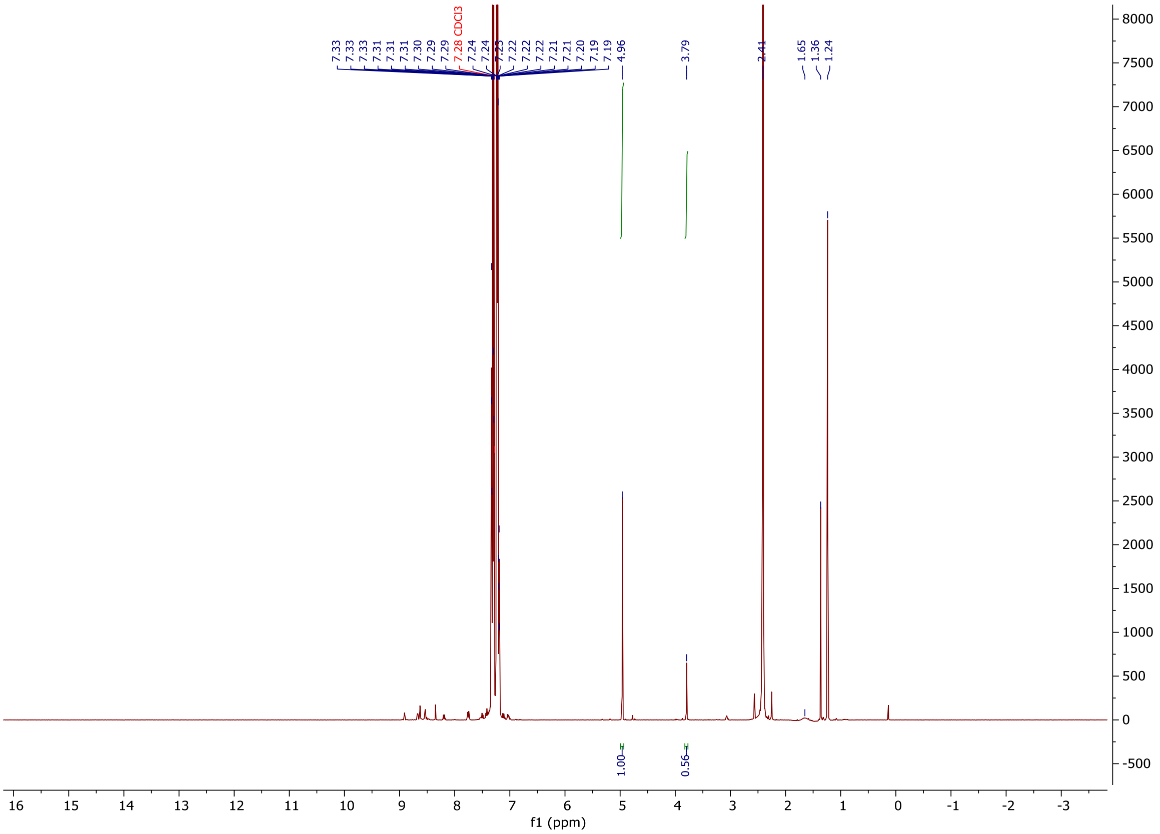
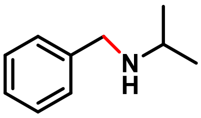


Figure 74: NMR of 2-methyl-N-(pyridin-3-ylmethyl)propan-2-amine with CH_2Br_2 as internal standard

12. N-benzylpropan-2-amine

The corresponding imine was synthesized according to the reported procedure.[10] Imine characterization: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.72 – 7.75 (m, 2H), 7.39-7.41 (m, 3H), 3.51-3.59 (m,1H),1.24-1.31 (d,6H).



^{1}H NMR(400MHz,$CDCl_3$): product peak at 3.84ppm. All other product peaks were obscured by reaction solvent. GC-MS(+H): 149

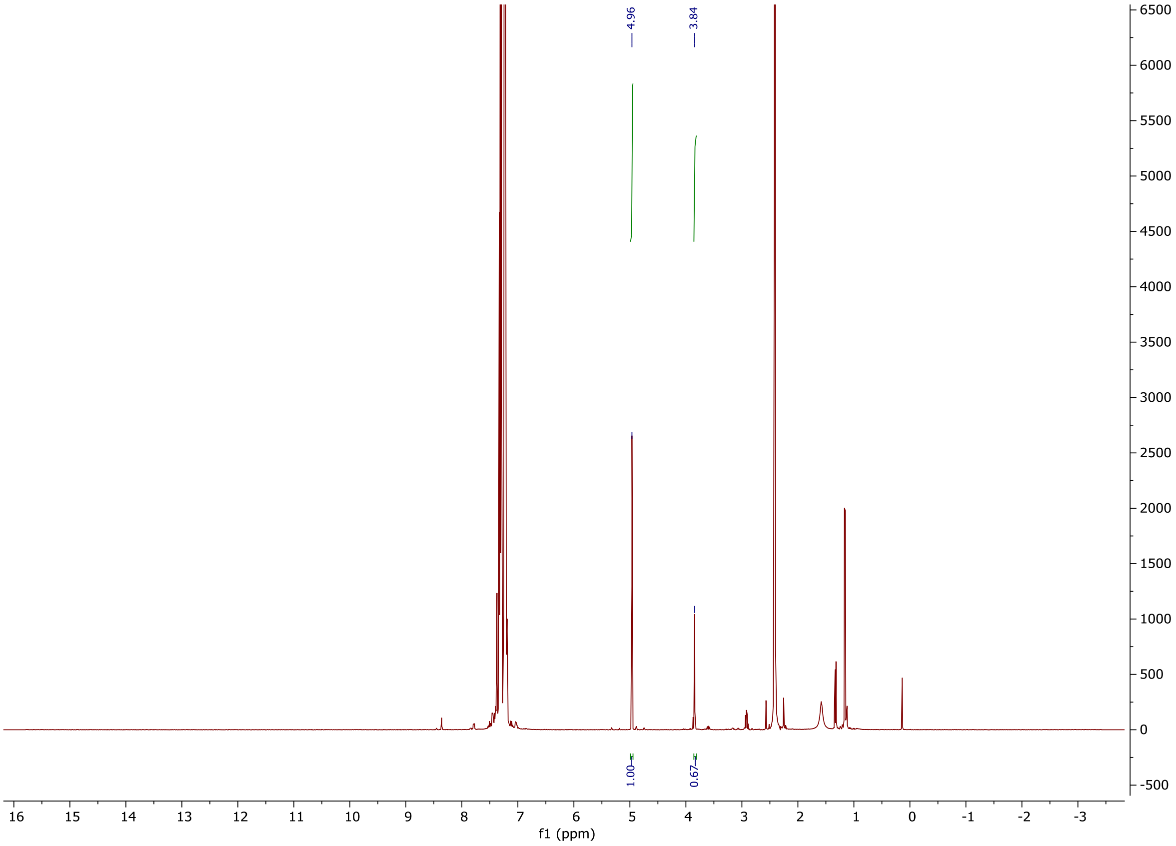


Figure 75: NMR of N-benzylpropan-2-amine with CH_2Br_2 as internal standard

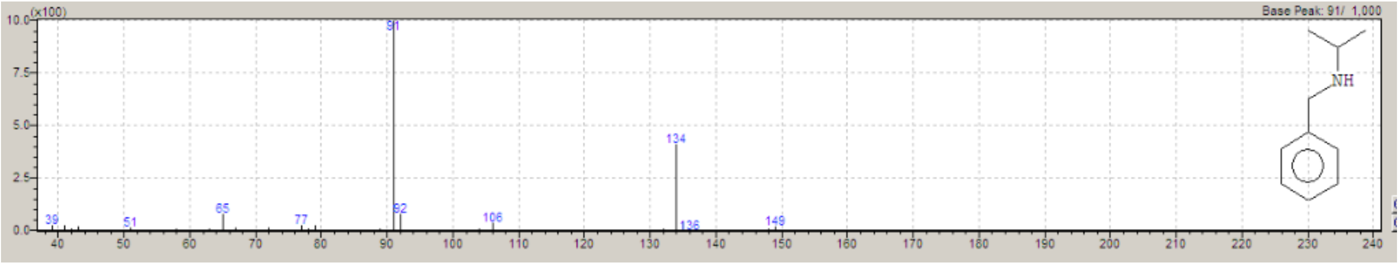
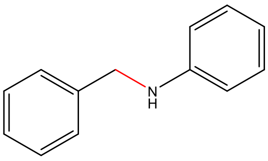


Figure 76: GC-MS of N-benzylpropan-2-amine

13 N-benzylaniline

The corresponding imine was synthesized according to the following synthesis. 10 mmol (1.02 mL) of benzaldehyde was dissolved in 50 mL of toluene. To the stirring solution was added 12 mmol (1.09 mL) of aniline. The mixture was refluxed in Dean-Stark apparatus overnight. After evaporation of the solvent, the crude mixture was heated to 80 °C in vacuum for 30 minutes. The product was obtained as a brown solid (94 % yield) NMR corresponds with literature.[11] ^1H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.99 – 7.85 (m, 2H), 7.53 – 7.44 (m, 3H), 7.44 – 7.35 (m, 2H), 7.25 – 7.20 (m, 3H). GC-MS retention time was 17.8-18 minutes; EI (*m/z*) 181.



^1H NMR(400MHz,$CDCl_3$): product peak at 4.40 ppm, 6.70-6.78 ppm, 6.80-6.85 ppm. All other product peaks were obscured by reaction solvent. GC-MS retention time was 19.5 -19.7 minutes; EI (*m/z*) 183.

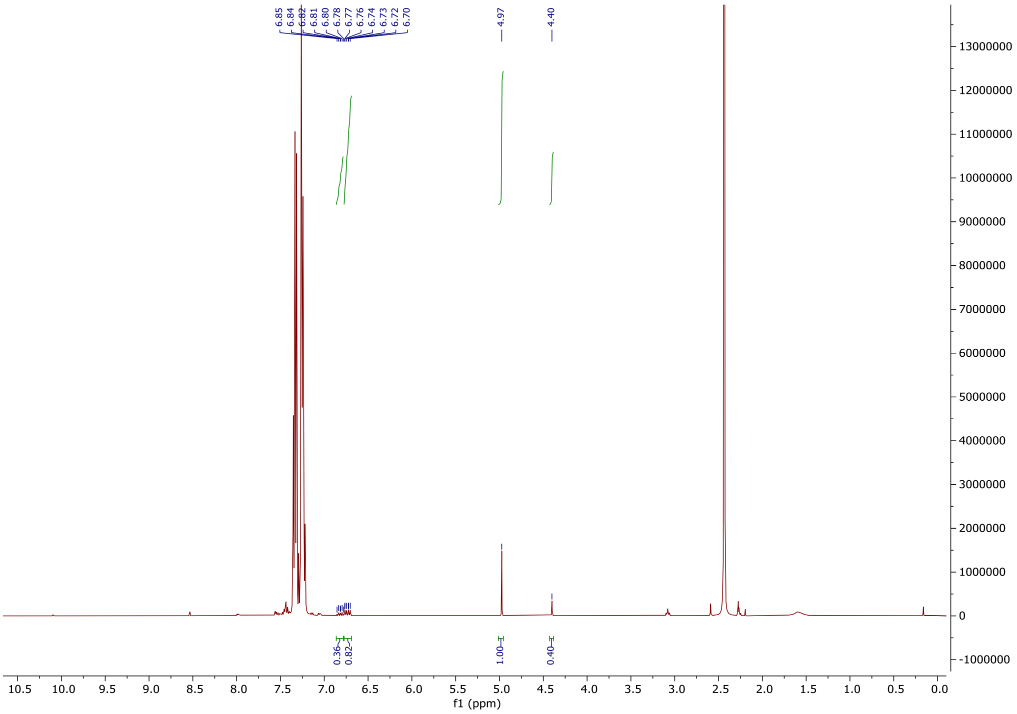


Figure 77: NMR of-N-benzylaniline with CH2Br2 as internal standard

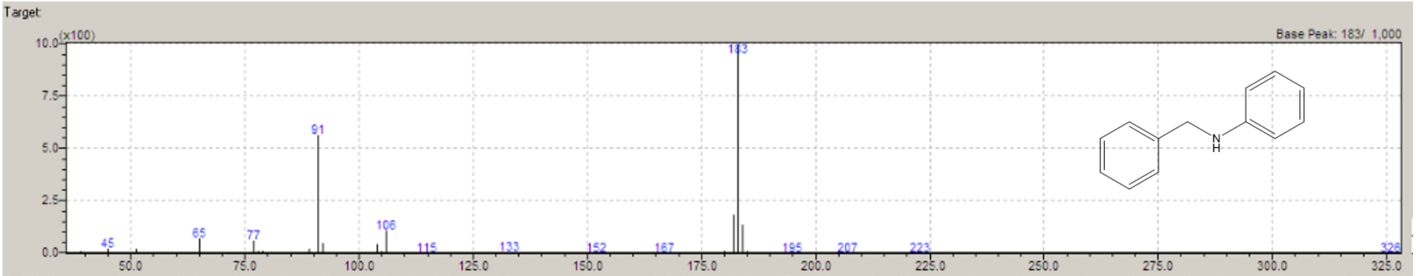


Figure 78: GC-MS spectra of N-benyzlaniline

48h catalytic test

^1H NMR(400MHz,$CDCl_3$): product peak at 4.38 ppm, 6.68-6.74 ppm, 6.76-6.82 ppm. All other product peaks were obscured by reaction solvent. GC-MS retention time was 19.6 -19.7 minutes; EI (*m/z*) 183.

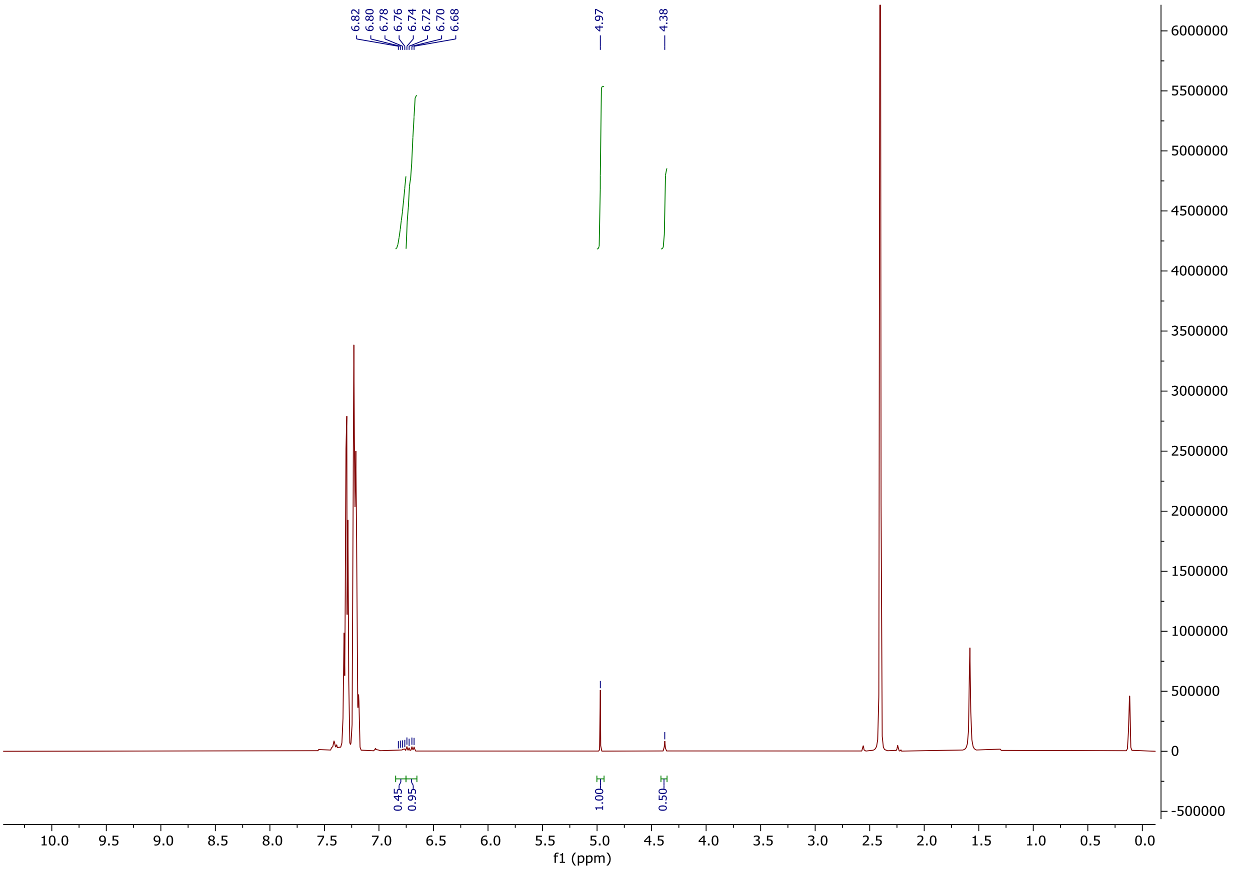


Figure 79: NMR of-N-benzylaniline with CH_2Br_2 as internal standard, 48h test

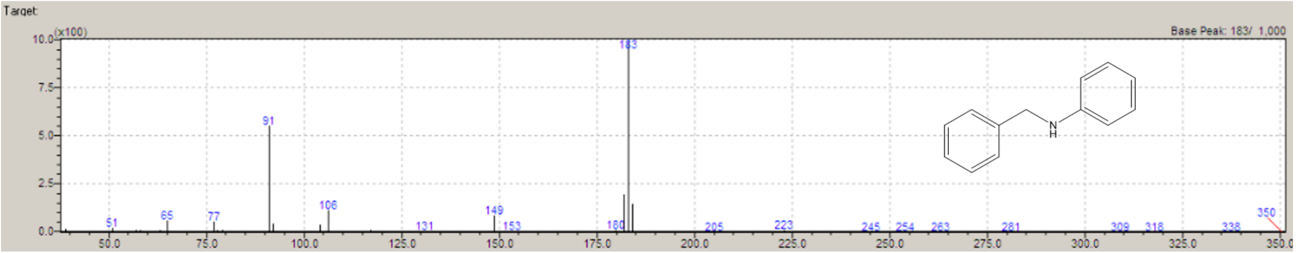


Figure 80:GC-MS spectra of N-benyzlaniline, 48 h test

10 % mol of catalyst test

^{1}H NMR(400MHz,$CDCl_3$): product peak at 4.39 ppm, 6.60-6.75 ppm, 6.78-6.83 ppm. All other product peaks were obscured by reaction solvent. GC-MS retention time was 19.6 -19.8 minutes; EI (*m/z*) 183.

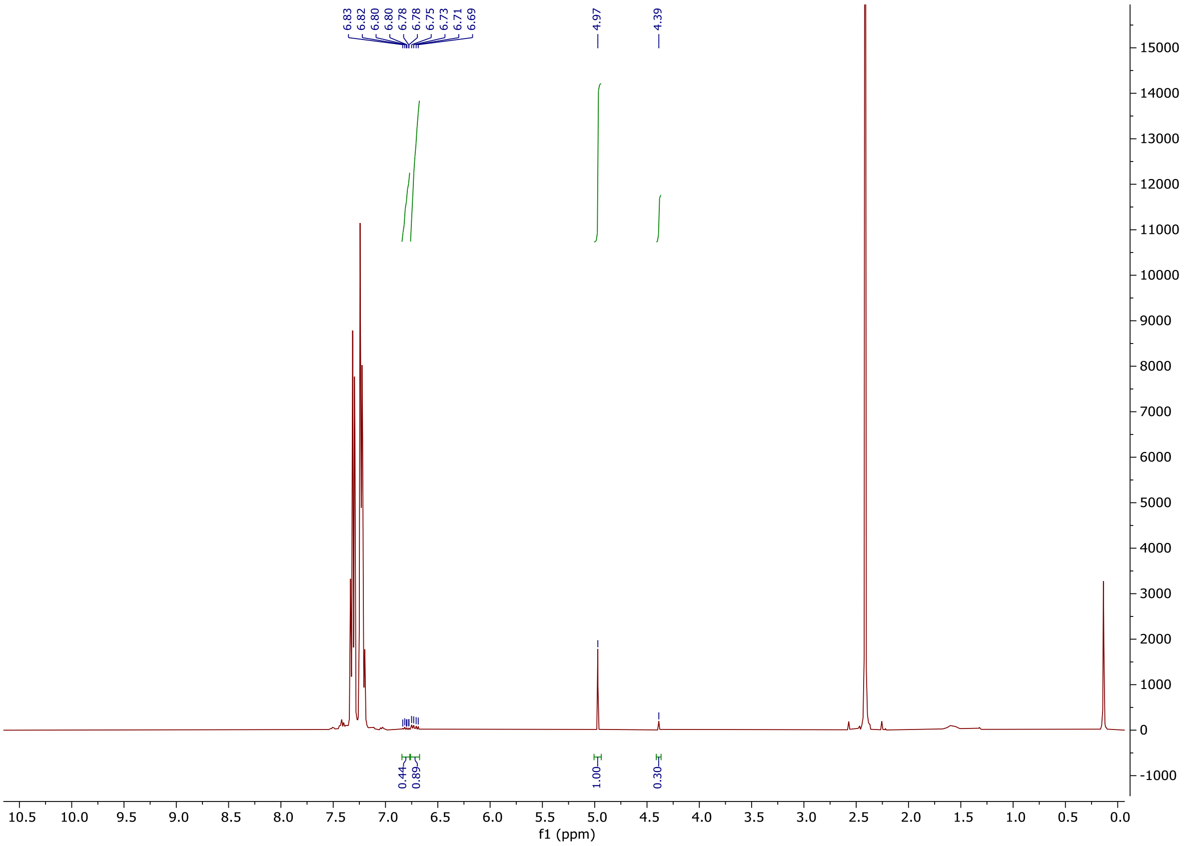


Figure 81: NMR of-N-benzylaniline with CH_2Br_2 as internal standard, 10 % mmol catalyst test

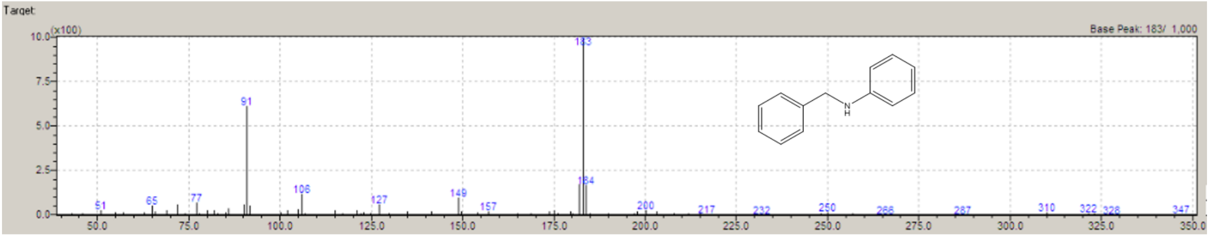


Figure 82: GC-MS spectra of N-benyzlaniline, 10% mmol catalyst test

2,5 % mol of catalyst test

^{1}H NMR(400MHz,$CDCl_3$): product peak at 4.38 ppm, 6.68-6.74 ppm, 6.76-6.82 ppm. All other product peaks were obscured by reaction solvent. GC-MS retention time was 19.7 -19.8 minutes; EI (*m/z*) 183.

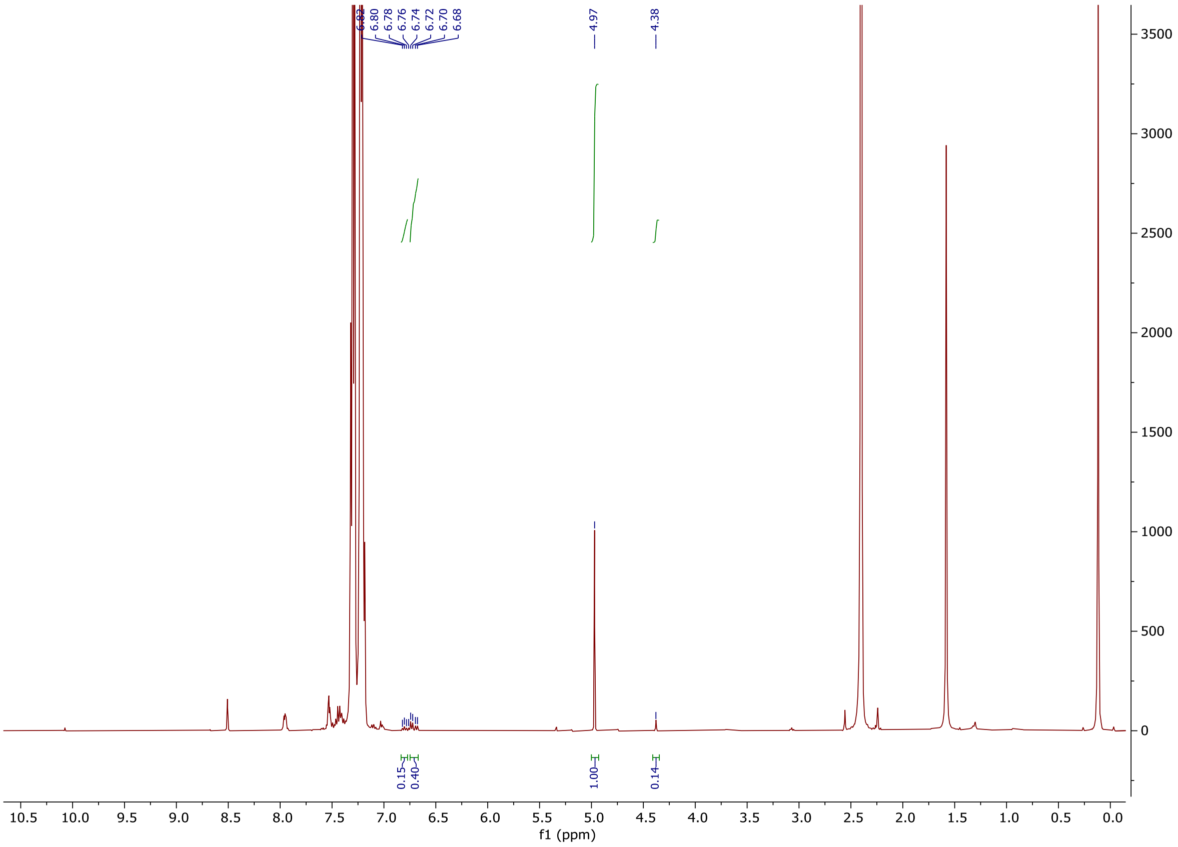


Figure 83: NMR of-N-benzylaniline with CH_2Br_2 as internal standard, 2.5 % mmol catalyst test.

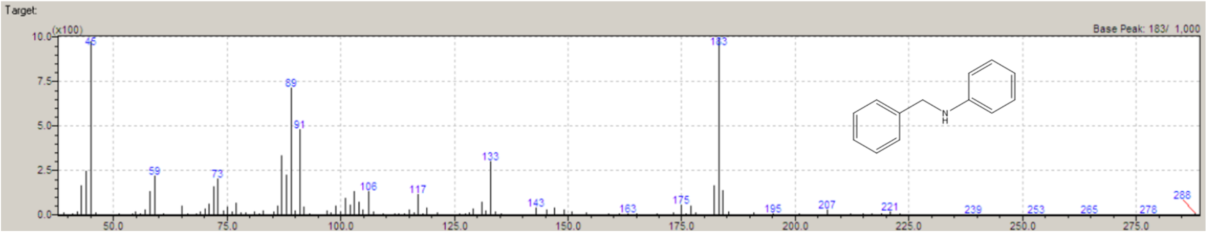
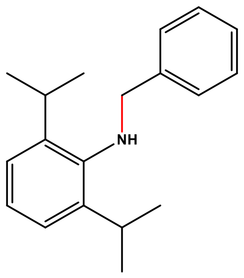


Figure 84:GC-MS spectra of N-benyzlaniline, 2.5 % mmol catalyst test

14 2 N-benzyl-2,6-diisopropylaniline

The corresponding imine was synthesized according to the following synthesis. 12 mmol of 2,4,-diisopropylaniline (2.26 mL) was added to the stirring solution of 10 mmol of benzaldehyde (1,02 mL). The mixture was refluxed in a Dean-Stark apparatus for 4 days. After evaporation of the solvent, the crude product was purified by distilling out the remaining starting material from reaction mixture. Product was obtained as brown oil, 2.42 g, 91 % yield. NMR corresponds with literature.[12] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.20 (s, 1H), 7.96 – 7.87 (m, 2H), 7.57 – 7.45 (m, 3H), 7.19 – 7.09 (m, 3H), 2.98 (hept, J = 6.9 Hz, 2H), 1.17 (d, J = 6.9 Hz, 12H). GC-MS retention time was 17.8-17.9 minutes; EI (m/z) 265.



^{1}H NMR(400MHz,CDCl$_3$): product peak at 4.10 ppm, 1.30 (d, *J* = 8 Hz). All other product peaks were obscured by reaction solvent. GC-MS retention time was 17.4-17.5 minutes; EI (*m/z*) 267.

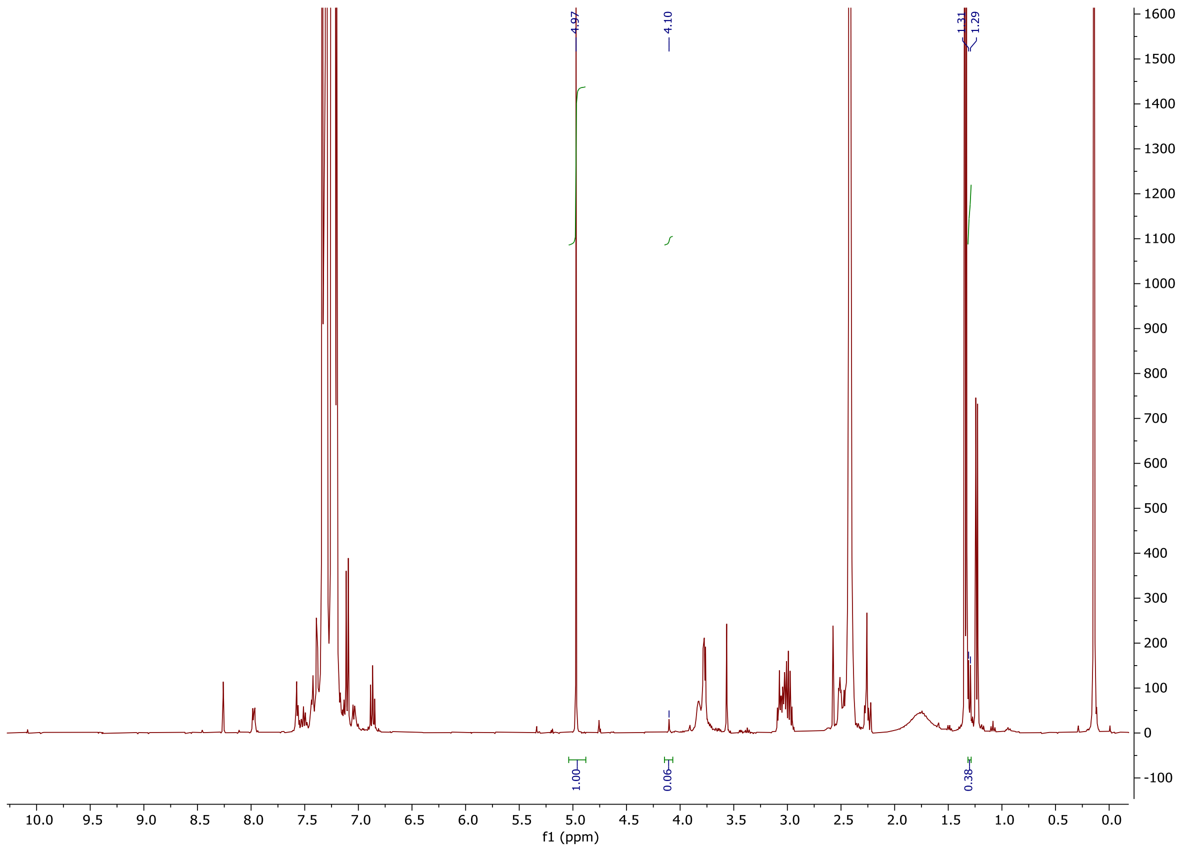


Figure 85:NMR of N-benzyl-2,6-diisopropylaniline with CH$_2$Br$_2$ as internal standard

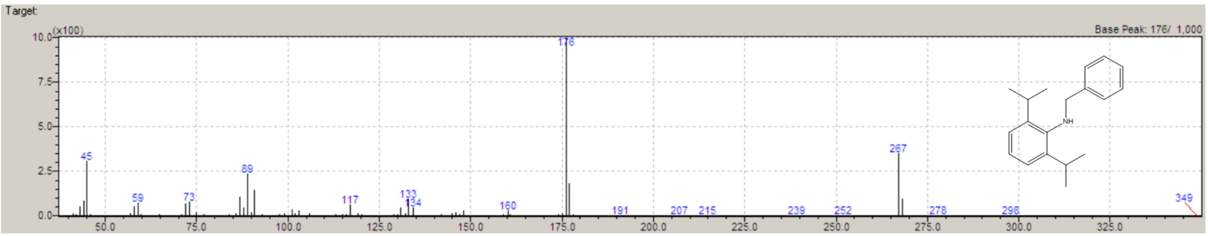
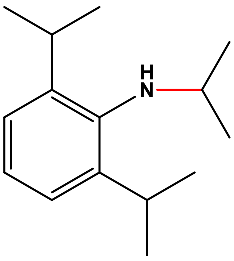


Figure 86: GC-MS spectra of N-benzyl-2,6-diisopropylaniline

15 N,2,6-triisopropylaniline

The corresponding imine was synthesized according to the modified reported procedure.[13] 10 mmol of 2,4-diisopropylaniline (1.89 mL) was refluxed in 50 mL of acetone over 5 g of 3A molecular sieves for six days. Crude product was purified by distillation (120 °C, 100 mbar) to obtain colorless oil, 0.27 g, 12 % yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.11-7.02 (m, 3H), 2.93 (hept, J = 6.8 Hz, 23H), 1.29 (s, 6H), 1.26 (d, J = 2.1 Hz, 12H). GC-MS retention time was 11.5-11.6 minutes; EI (m/z) 217.



^{1}H NMR(400MHz,$CDCl_3$): product peak at 1.29 ppm (d, J = 8 Hz). All other product peaks were obscured by reaction solvent. GC-MS retention time was 11.0-11.1 minutes; EI (*m/z*) 219.

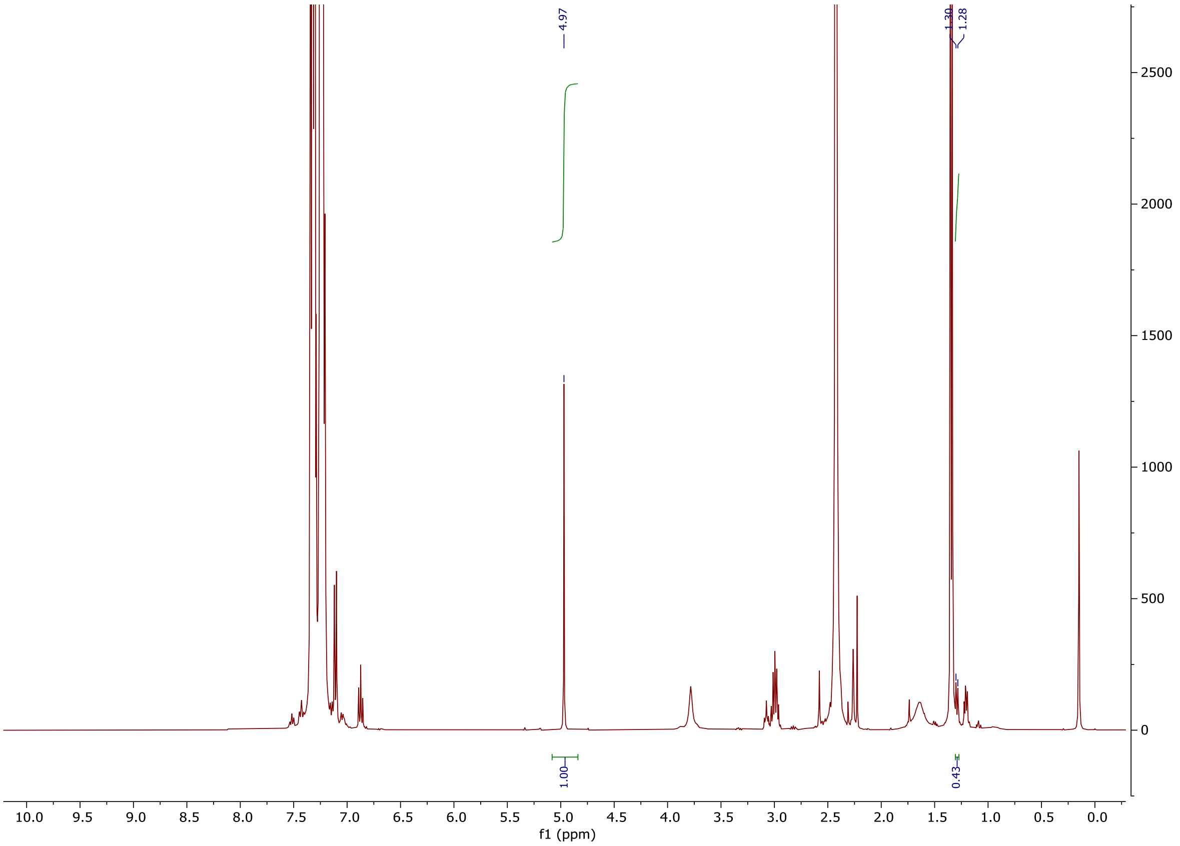


Figure 87: NMR of N,2,6-triisopropylaniline with CH_2Br_2 as internal standard

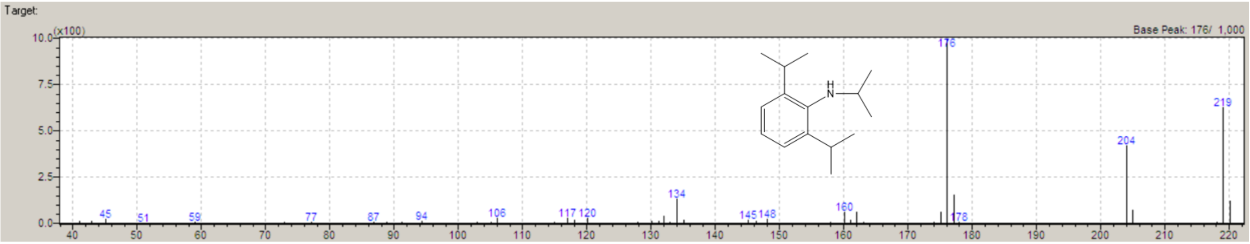


Figure 88: GC-MS spectra of N,2,6-triisopropylaniline

Crystal structure of[Sn(Salen)Cl_2] and [Sn(^{t}Bu_2Salophen)Cl_2] complexes

The crystals of [Sn(Salen)Cl_2] were obtained by evaporation of its dichloromethane solution under reduced pressure and the crystals of partially solvated [Sn(^{t}Bu_2Salophen)Cl_2] were prepared by diffusion of hexane vapors into its dichloromethane solution. The selected crystals were mounted onto goniometer heads of a Bruker D8 VENTURE Kappa Duo diffractometer with a PHOTON100 detector and an IμS microfocus sealed tube source, equipped with Cryostream Cooler (Oxford Cryostreams). Full-set diffraction data ($\pm h$, $\pm k$, $\pm l$, $2\theta \leq 55°$) were collected at 120(2) K using monochromated MoK_α radiation (λ = 0.71073 Å) and reduced using the software of the diffractometer (SAINT[14]). The data were corrected for absorption using methods incorporated in the diffractometer software (SADABS[15]).

The structures were solved by direct methods with SHEXT-2018[16] and refined by weighted full-matrix least-squares against F^2 using SHELXL-2019.[17] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were located on the difference electron density maps and refined as riding atoms with their U_{iso}(H) fixed to a 1.2 multiple of U_{eq} of their bond partners with the exception of the hydrogen atoms of the tert-butyl groups in the structure of partially solvated [Sn(^{t}Bu_2Salophen)Cl_2] which were placed in the theoretical positions and refined as riding atoms with their U_{iso}(H) fixed to a 1.5 multiple of U_{eq} of their bond partners. Two of the four tert-butyl groups (carbon atoms C21 – C24 and C25 – C28) in the structure of partially solvated [Sn(^{t}Bu_2Salophen)Cl_2] were refined disordered over two positions mutually rotated around the pivotal bond to their quaternary carbon atoms (C21 and C25, respectively). The positions were restrained to be equivalent with relative occupancy ratios refined as 3:1 and 1:1, respectively. Additionally, rigid-bond restraints had to be applied to the anisotropic displacement parameters of the carbon atoms of the disordered tert-butyl groups to prevent them from becoming negative.

In the structure of partially solvated [Sn(^{t}Bu_2Salophen)Cl_2], a disordered dichloromethane molecule could not be satisfactorily modeled with full occupancy and was removed from the refinement using the PLATON SQUEEZE[18] routine which removed electron density amounting to a total of 21 electrons from a solvent accessible void of the potential volume of 262 Å^3 per unit cell. After the final cycle of refinement of the structure of [Sn(^{t}Bu_2Salophen)Cl_2], the residual difference electron density map maximum of 1.84 e·Å^{-3} was located in the vicinity of the tin atom and the residual difference electron density map minimum of −1.30 e·Å^{-3} was located in the vicinity of one of the disordered tert-butyl groups.

Selected structure solution parameters are listed in Table 5. All geometric calculations and graphics were calculated and plotted using PLATON[19] software. Displacement ellipsoid ORTEP[20] plots are contained in the Figure 89. The complex [Sn(Salen)Cl_2] crystallized in monoclinic system with space group *Cc* and 4 formula units in the unit cell (Figure 90). The partially solvated complex [Sn(^{t}Bu_2Salophen)Cl_2] crystallized in triclinic system with space group *P*−1 and 2 formula units in the unit cell (Figure 91). The respective selected valence parameters in the structures of [Sn(Salen)Cl_2] and

[Sn(^{t}Bu$_2$Salophen)Cl$_2$] are listed in Table 6 and Table 7. The values related to the atoms in refined positions are rounded with respect to their estimated standard deviations that are provided with one decimal place. The corresponding crystallographic information files for [Sn(Salen)Cl$_2$] and [Sn(^{t}Bu$_2$Salophen)Cl$_2$] can be accessed in Cambridge Crystallographic Data Centre at https://www.ccdc.cam.ac.uk/structures/ under submission codes CCDC-2330171 and CCDC-2333521, respectively.

Table 5: Basic crystallographic data and structure refinement details for the crystals of [Sn(Salen)Cl_2] and [Sn($^tBu_2$Salophen)Cl_2].

Structure code	[Sn(Salen)Cl_2]	[Sn($^tBu_2$Salophen)Cl_2] (solvated)
Empirical formula	$C_{16}H_{14}Cl_2N_2O_2Sn$	$C_{36}H_{46}Cl_2N_2O_2Sn$
Formula weight [g·mol^{-1}]	455.90	728.34
Crystal system	monoclinic	triclinic
Space group	*Cc*	*P*−1
a [Å]	10.7059(4)	11.2684(8)
b [Å]	14.2716(4)	13.0888(9)
c [Å]	10.8582(3)	13.536(1)
α [°]		75.089(3)
β [°]	101.977(1)	75.968(3)
γ [°]		88.152(3)
V [Å^3]	1622.91(9)	1870.6(2)
Z	4	2
F(000)	896	752
Calculated density [g·cm^3]	1.866	1.293
μ(Mo Kα) [mm^{-1}]	1.913	0.857
crystal size [mm]	0.032 x 0.032 x 0.134	0.054 x 0.078 x 0.162
θ range [°]	2.412–27.481	1.864–28.426
Collected diffractions	17662	124490
Independent diffractions	3720	9370
Observed[a] diffractions	3687	8716
R_{int}[b] [%]	3.11	5.26
Number of parameters	208	462
R, wR[c] (observed) [%]	1.47, 3.09	4.53, 10.46
R, wR[c] (all data) [%]	1.48, 3.09	4.93, 10.66
Goodness of fit[d]	1.071	1.149
$\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e·Å^{-3})	−0.379, 0.288	−1.296, 1.841
Flack parameter	−0.013(9)	
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$; where $P = (F_o^2 + 2F_c^2)/3$.	
	a = 0.0089	a = 0.0296
	b = 0.3295	b = 5.4616

[a] $I > 2\sigma(I)$

[b] $R_{int} = \Sigma|F_o^2 - F_{o,mean}^2|/\Sigma F_o^2$

[c] $R(F) = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR(F^2) = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma w(F_o^2)^2]^{1/2}$

[d] $S = [\Sigma(w(F_o^2 - F_c^2)^2)/(N_{diffrns} - N_{par})]^{1/2}$

Table 6: List of selected bond lengths and angles in [Sn(Salen)Cl_2].

bond	value [Å]	angle	value [°]	torsion	value [°]
Sn1-O1	2.012(2)	O1-Sn1-O2	102.17(8)	C3-N1-C1-C2	144.6(3)
Sn1-O2	2.013(2)	O1-Sn1-N1	91.15(8)	Sn1-N1-C1-C2	-31.7(3)
Sn1-N1	2.142(2)	O2-Sn1-N1	166.34(8)	C4-N2-C2-C1	144.9(3)
Sn1-N2	2.145(2)	O1-Sn1-N2	169.11(9)	Sn1-N2-C2-C1	-34.1(3)
Sn1-Cl2	2.4190(8)	O2-Sn1-N2	88.69(9)	N1-C1-C2-N2	42.2(3)
Sn1-Cl1	2.4237(8)	N1-Sn1-N2	78.05(9)	C1-N1-C3-C6	177.1(3)
O1-C5	1.345(3)	O1-Sn1-Cl2	89.33(7)	Sn1-N1-C3-C6	-6.9(5)
O2-C11	1.345(3)	O2-Sn1-Cl2	92.54(7)	C2-N2-C4-C12	177.7(3)
N1-C3	1.277(4)	N1-Sn1-Cl2	90.60(7)	Sn1-N2-C4-C12	-3.5(4)
N1-C1	1.466(4)	N2-Sn1-Cl2	89.35(7)	Sn1-O1-C5-C10	-167.5(2)
N2-C4	1.285(4)	O1-Sn1-Cl1	89.43(6)	Sn1-O1-C5-C6	14.7(4)
N2-C2	1.464(4)	O2-Sn1-Cl1	90.68(7)	O1-C5-C6-C7	179.2(3)
C1-C2	1.529(4)	N1-Sn1-Cl1	86.39(7)	O1-C5-C6-C3	1.5(5)
C3-C6	1.446(4)	N2-Sn1-Cl1	91.29(7)	N1-C3-C6-C7	176.8(3)
C4-C12	1.440(4)	Cl2-Sn1-Cl1	176.72(3)	N1-C3-C6-C5	-5.4(5)
C5-C10	1.398(4)	C5-O1-Sn1	124.5(2)	Sn1-O2-C11-C16	-156.0(2)
C5-C6	1.418(4)	C11-O2-Sn1	124.7(2)	Sn1-O2-C11-C12	26.9(4)
C6-C7	1.412(4)	C3-N1-C1	122.8(3)	O2-C11-C12-C4	-2.8(5)
C7-C8	1.371(4)	C3-N1-Sn1	122.8(2)	N2-C4-C12-C13	171.5(3)
C8-C9	1.394(4)	C1-N1-Sn1	114.3(2)	N2-C4-C12-C11	-9.4(5)
C9-C10	1.379(4)	C4-N2-C2	122.0(2)		
C11-C16	1.395(4)	C4-N2-Sn1	124.1(2)		
C11-C12	1.419(4)	C2-N2-Sn1	113.9(2)		
C12-C13	1.408(4)	N1-C1-C2	109.7(2)		
C13-C14	1.377(5)	N2-C2-C1	109.5(2)		
C14-C15	1.391(5)	N1-C3-C6	126.5(3)		
C15-C16	1.377(4)	N2-C4-C12	125.9(3)		

Table 7: List of selected bond lengths and angles in [Sn(^{t}Bu$_2$Salophen)Cl$_2$].

bond	value [Å]	angle	value [°]	torsion	value [°]
Sn1-O1	1.996(2)	O1-Sn1-O2	104.20(9)	C3-N1-C1-C20	-14.1(5)
Sn1-O2	1.999(2)	O1-Sn1-N2	166.13(9)	Sn1-N1-C1-C20	178.7(3)
Sn1-N2	2.146(3)	O2-Sn1-N2	89.19(9)	C3-N1-C1-C2	166.8(3)
Sn1-N1	2.150(3)	O1-Sn1-N1	89.4(1)	Sn1-N1-C1-C2	-0.4(4)
Sn1-Cl1	2.4136(9)	O2-Sn1-N1	166.1(1)	N1-C1-C2-C17	-178.4(3)
Sn1-Cl2	2.4287(9)	N2-Sn1-N1	77.4(1)	C20-C1-C2-N2	-177.9(3)
O1-C5	1.338(4)	O1-Sn1-Cl1	91.08(8)	N1-C1-C2-N2	1.2(4)
O2-C11	1.337(4)	O2-Sn1-Cl1	89.54(7)	C4-N2-C2-C17	-14.9(5)
N1-C3	1.305(4)	N2-Sn1-Cl1	92.65(7)	Sn1-N2-C2-C1	178.1(3)
N1-C1	1.416(4)	N1-Sn1-Cl1	87.21(8)	C4-N2-C2-C	165.5(3)
N2-C4	1.301(4)	O1-Sn1-Cl2	89.24(8)	Sn1-N2-C2-C1	-1.4(4)
N2-C2	1.420(4)	O2-Sn1-Cl2	90.25(7)	C1-N1-C3-C6	-174.1(3)
C1-C20	1.399(5)	N2-Sn1-Cl2	87.06(7)	Sn1-N1-C3-C6	-7.8(5)
C1-C2	1.411(4)	N1-Sn1-Cl2	92.93(8)	C2-N2-C4-C12	-172.6(3)
C2-C17	1.390(5)	Cl1-Sn1-Cl2	179.65(3)	Sn1-N2-C4-C12	-6.6(4)
C3-C6	1.421(5)	C5-O1-Sn1	127.5(2)	Sn1-O1-C5-C10	-157.8(2)
C4-C12	1.432(4)	C11-O2-Sn1	126.0(2)	Sn1-O1-C5-C6	24.8(4)
C5-C10	1.406(5)	C3-N1-C1	122.8(3)	N1-C3-C6-C7	176.8(3)
C5-C6	1.422(5)	C3-N1-Sn1	121.4(2)	N1-C3-C6-C5	-1.5(6)
C6-C7	1.421(4)	C1-N1-Sn1	114.5(2)	O1-C5-C6-C7	175.2(3)
C7-C8	1.361(6)	C4-N2-C2	122.1(3)	O1-C5-C6-C3	-6.5(5)
C8-C9	1.399(5)	C4-N2-Sn1	122.0(2)	O1-C5-C10-C9	-175.3(3)
C8-C21	1.548(5)	C2-N2-Sn1	114.6(2)	O1-C5-C10-C29	5.5(5)
C9-C10	1.396(5)	C20-C1-N1	124.1(3)	Sn1-O2-C11-C12	30.0(4)
C10-C29	1.547(5)	C2-C1-N1	116.8(3)	Sn1-O2-C11-C16	-153.8(2)
C11-C12	1.415(5)	C17-C2-N2	124.0(3)	O2-C11-C12-C13	172.6(3)
C11-C16	1.416(4)	C1-C2-N2	116.7(3)	O2-C11-C12-C4	-9.0(5)
C12-C13	1.416(4)	N1-C3-C6	127.9(3)	N2-C4-C12-C11	-2.7(5)
C13-C14	1.373(5)	N2-C4-C12	127.1(3)	N2-C4-C12-C13	175.9(3)
C14-C15	1.400(5)	O1-C5-C10	118.4(3)	O2-C11-C16-C15	-173.6(3)
C14-C25	1.538(5)	O1-C5-C6	122.1(3)	O2-C11-C16-C33	6.2(4)
C15-C16	1.393(5)	O2-C11-C12	122.4(3)	N2-C2-C17-C18	178.7(3)
C16-C33	1.546(5)	O2-C11-C16	118.3(3)	N1-C1-C20-C19	179.5(3)
C17-C18	1.375(5)				
C18-C19	1.389(6)				
C19-C20	1.369(6)				

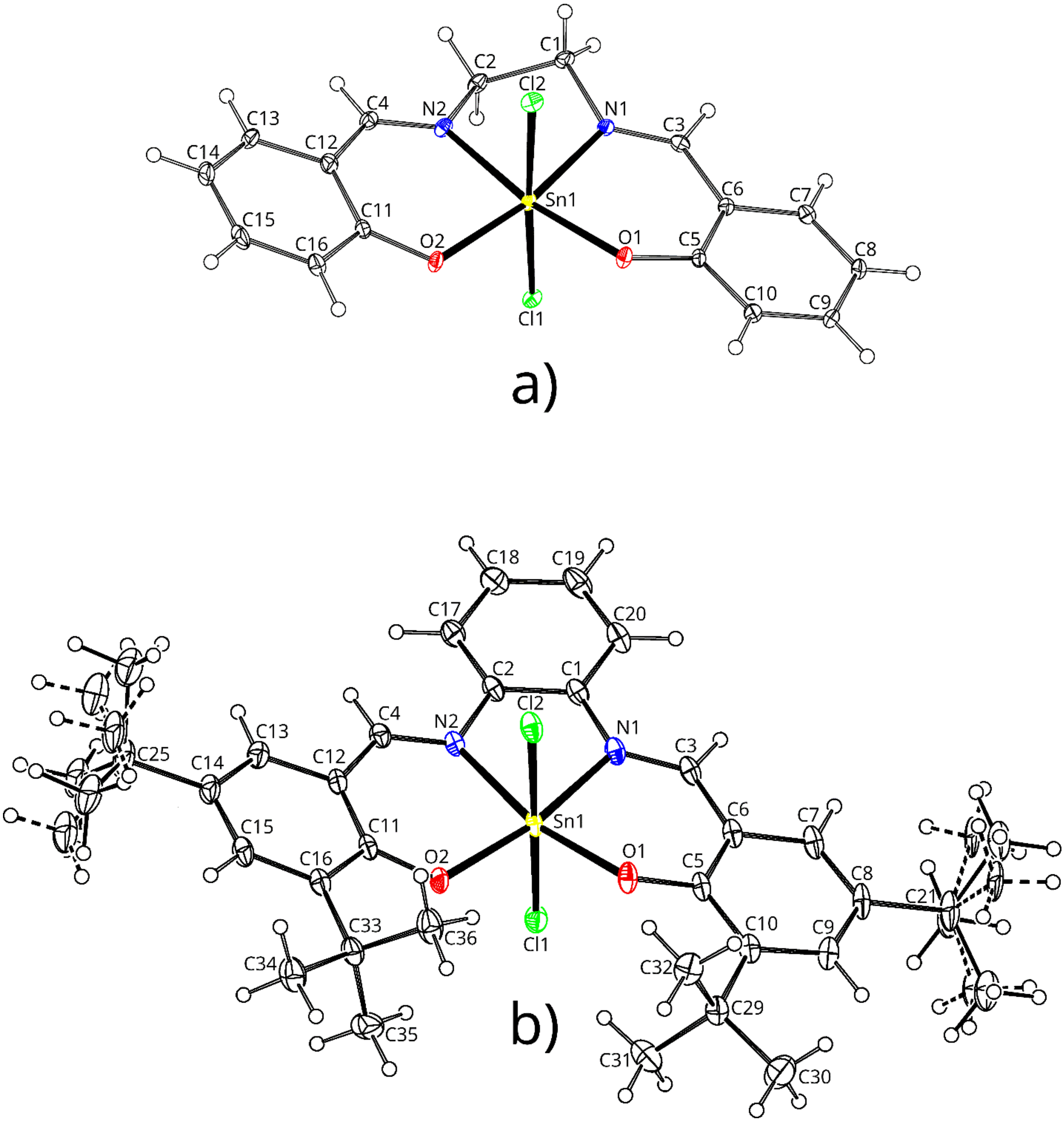


Figure 89: a) View of the molecular structure of [Sn(Salen)Cl$_2$]. b) View of the molecular structure of [Sn(^{t}Bu$_2$Salophen)Cl$_2$]. Thermal displacement elipsoids are plotted at the 30 % probability level. Applied colors: C – black, H – black contour, Cl – green, N – blue, O – red, Sn – yellow.

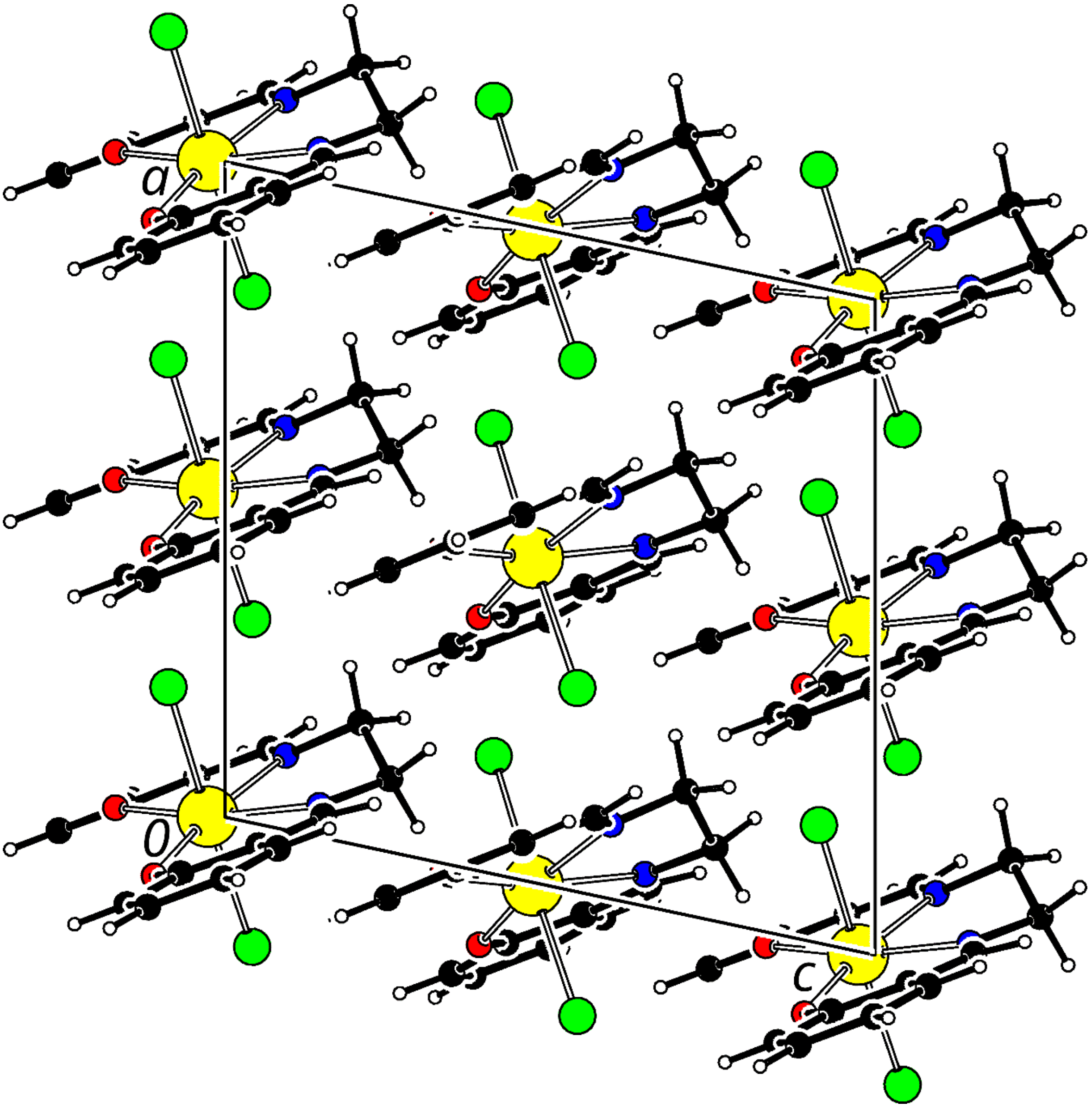


Figure 90: Crystal packing of [Sn(Salen)Cl_2] viewed along the axis *b*. The unit cell is outlined by the solid line. Applied colors: C – black, H – black contour, Cl – green, N – blue, O – red, Sn – yellow.

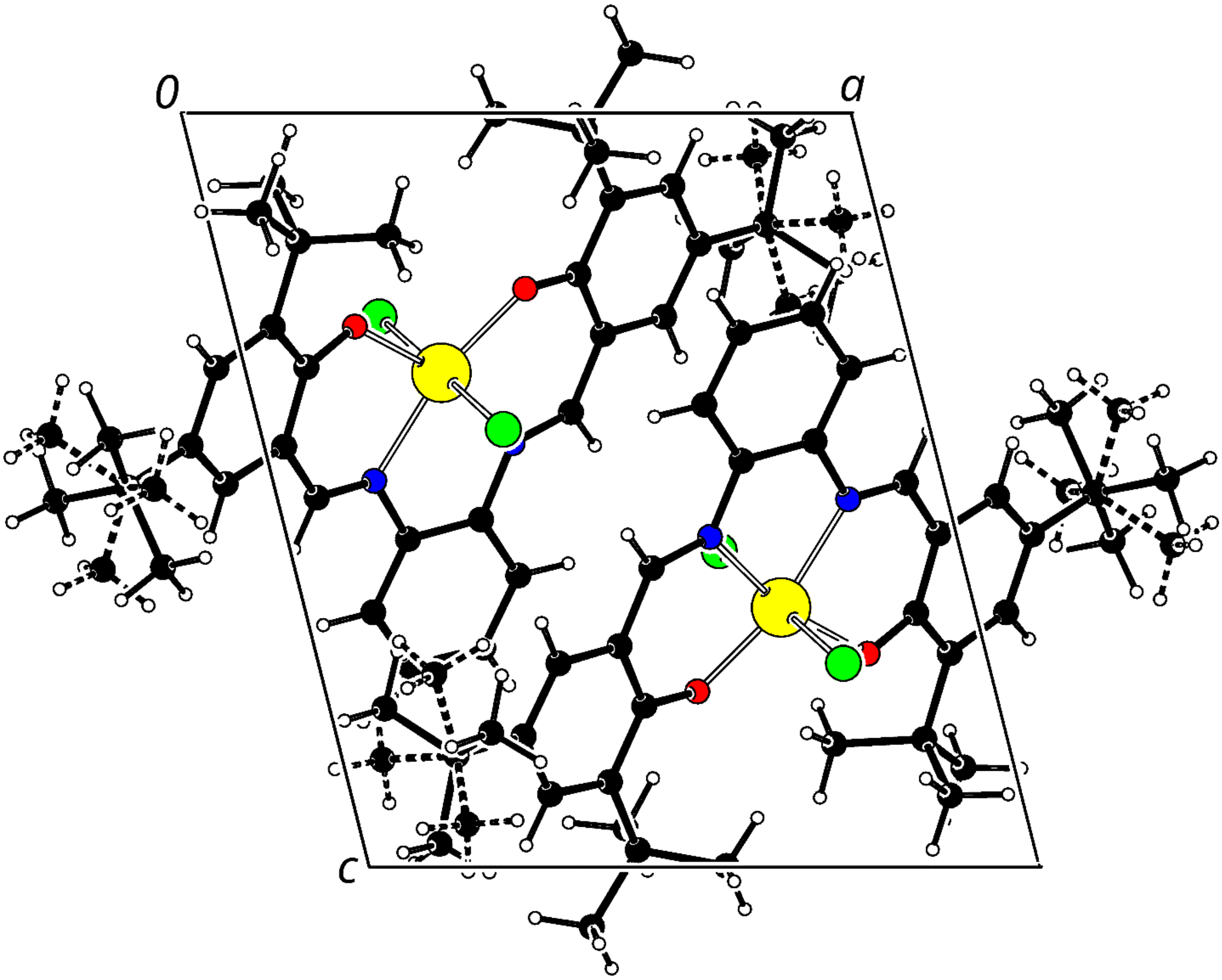


Figure 91: Crystal packing of [Sn(^{t}Bu$_2$Salophen)Cl$_2$] viewed along the axis *b*. The unit cell is outlined by the solid line. Applied colors: C – black, H – black contour, Cl – green, N – blue, O – red, Sn – yellow.

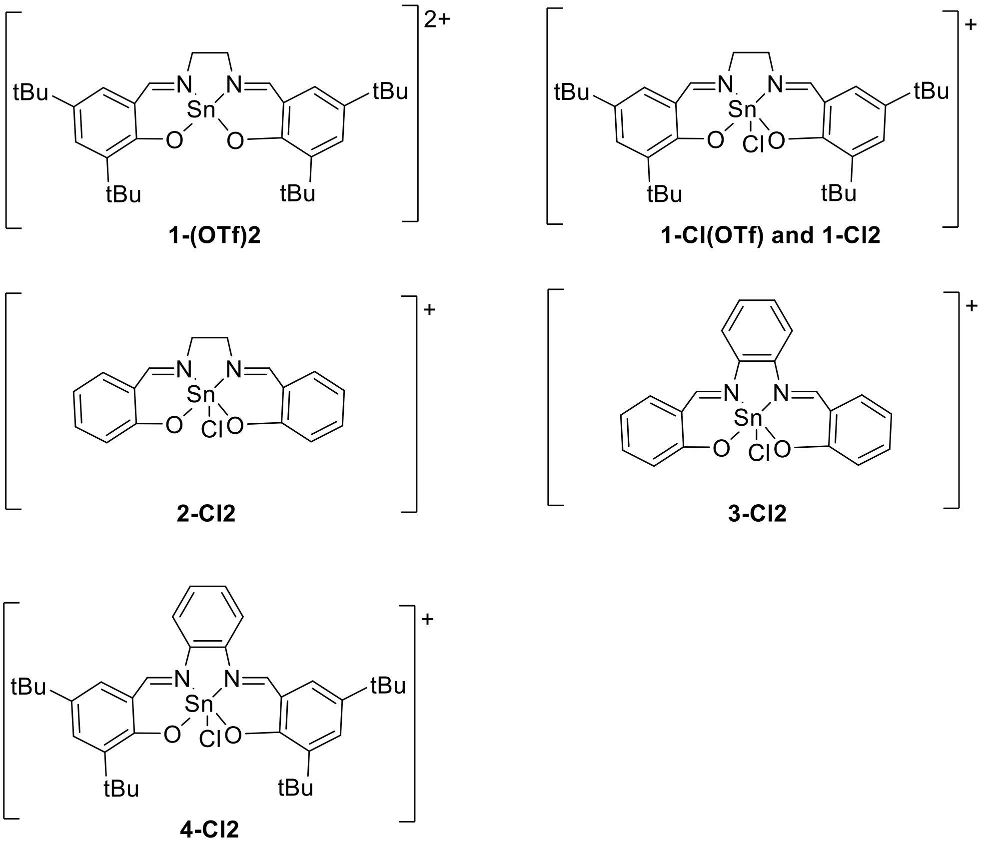
Computational Details

The HIA values were calculated following a protocol validated by Greb et al[20] as follows.

Structure optimization of all involved LAs and the corresponding [LA-H] counterpart (see Figure 91) was performed at the threefold-corrected PBEh-3c/def2-mSVP level of theory as implemented in ORCA 5.0 software. Considering that the sixth ligand should be released to have a vacant active site, the calculations were carried out using the corresponding cations of the LAs. In the case of the LA with the two triflate ligands (1-OTf2), those ligands were not considered since the interaction with the Tin center is weak. In all cases, the structures were confirmed as local minima through normal analysis using frequency calculations. Zero-point energies and thermal corrections at 298 K were obtained at the same level of theory and subsequently used.

Previously optimized geometries were utilized for single-point calculations at the DSD-PBEP86-D3BJ / def2-QZVP level of theory which has been demonstrated to be suitable for HIA[20]. In all DFT calculations, the "resolution-of identity" and "chain of spheres" approximation in the form of RIJCOSX was used in combination with auxiliary basis sets (autoaux). In particular, the def2/C auxiliary basis set was applied. These electronic energies were combined with ZPE/Thermal corrections from the previous step, to obtain the total enthalpies of the Lewis acids and their hydride adducts.

The HIA values were calculated with isodesmic anchoring to the CCSD(T)/CBS values of the trimethylsilylium (TMS) system (924 kJ/mol). The isodesmic reaction corresponds to the calculation of the reaction enthalpy LA(+) + TMS−H→LA−H + TMS(+) and subtracting the CCSD(T)/CBS value of TMS−H→TMS(+) + H-. By doing so, a final absolute HIA is obtained.



1-(OTf)2

1-Cl(OTf) and 1-Cl2

2-Cl2

3-Cl2

4-Cl2

Figure 92:Chemical struture of LAs considered in the HIA analysis. 1-Cl(OTf) and 1-Cl2 were considered as the same structure since both of them result in the same LA (cation).

To analyze the preorientation of the catalyst for the most active LA (2-Cl2), the frustrated Lewis Pair arising from the interaction between the model Imine and 2-Cl2 was optimized.

Different structures were considered as initial guesses, and only the lowest energy structure was selected for the final Lewis pair shown in Figure 93. As can be noted, in the absence of t-Bu group Tin center can interact with the imine nitrogen ($R_{Sn\text{-}N}$= 2.33 A)

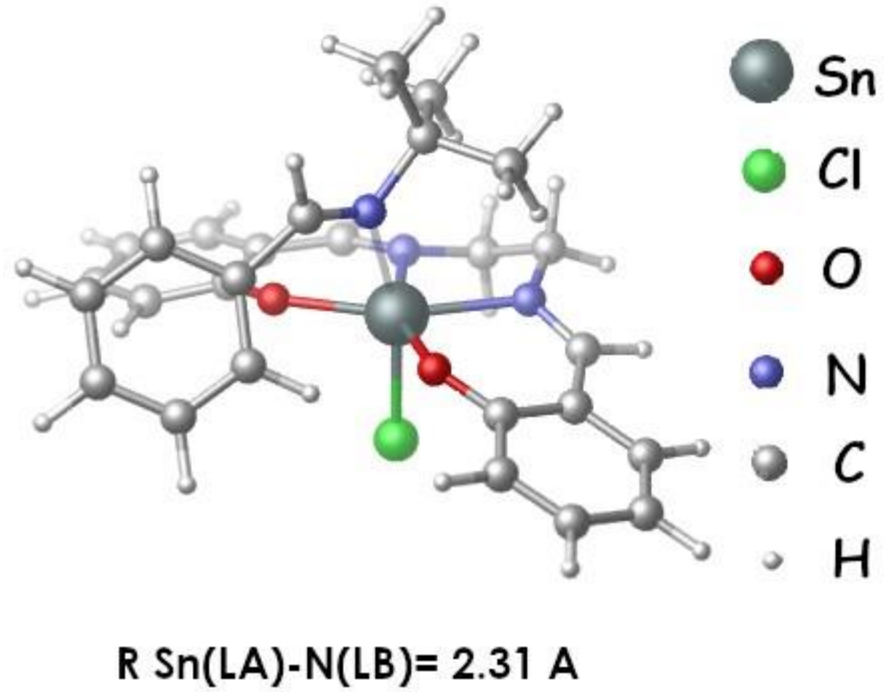


Figure 93:Optimized structure corresponding to imine 2-Cl2 FLP.

Cartesian Coordinates for optimized structures corresponding to LAs and LAHs

1-OTf2

```
   83
FINAL HEAT OF FORMATION = -1716.682832
 C    -0.020962     0.541833     0.072488
 C     0.032333     0.368341     1.459036
 C     1.261519     0.012721     2.098304
 C     2.431302    -0.151135     1.318881
 C     2.416270     0.009432    -0.046311
 C     1.178664     0.347048    -0.618060
 O    -1.094349     0.548688     2.164175
Sn    -1.461707     0.246645     4.033208
 C     1.437090    -0.170659     3.484664
 N     0.526184    -0.117997     4.430298
 C     0.804897    -0.230782     5.856914
 C    -0.137300     0.707083     6.624762
 N    -1.477479     0.599223     6.061123
 C    -2.587773     0.613696     6.764144
 C    -3.908946     0.424917     6.310440
 C    -4.289800     0.120867     4.965442
 C    -5.636045    -0.064503     4.634455
 C    -6.549882     0.065096     5.683891
 C    -6.236928     0.355697     7.021903
 C    -4.904534     0.527423     7.311210
 O    -3.376299     0.014170     3.989189
 H     1.846354     0.039367     6.071573
 H     0.660395    -1.271663     6.183481
 H    -0.138849     0.437487     7.688309
 H     0.212453     1.747457     6.549501
 H     2.462935    -0.371852     3.817038
 H    -2.469819     0.781934     7.841682
```

H	3.356683	-0.413440	1.831892
C	3.691956	-0.163009	-0.869208
H	1.150006	0.470831	-1.695469
C	-1.310712	0.915116	-0.676243
H	-4.586586	0.749216	8.329867
C	-7.296723	0.445629	8.117348
H	-7.598585	-0.071104	5.441194
C	-6.114168	-0.371441	3.205943
C	-7.639676	-0.513059	3.157023
C	-5.739272	0.784123	2.262930
C	-5.520791	-1.700865	2.711546
H	-6.160175	0.598102	1.267564
H	-6.156368	1.735547	2.614815
H	-4.661130	0.912751	2.129855
H	-7.949313	-0.727689	2.128751
H	-8.011275	-1.339560	3.775029
H	-8.159385	0.405329	3.455790
H	-5.943326	-1.946265	1.730285
H	-4.433881	-1.678335	2.591246
H	-5.773397	-2.527013	3.386973
C	-8.713060	0.425507	7.541527
C	-7.118842	-0.761882	9.049411
C	-7.110227	1.748328	8.906352
H	-7.878757	1.832943	9.683126
H	-6.143274	1.800521	9.421365
H	-7.197268	2.630782	8.261004
H	-7.870111	-0.744532	9.847897
H	-7.233271	-1.709465	8.509304
H	-6.134646	-0.771551	9.534403
H	-9.442956	0.539369	8.349995
H	-8.888453	1.247477	6.836047
H	-8.952725	-0.519161	7.037658
C	-1.057145	1.032126	-2.183606
C	-2.375822	-0.177171	-0.481889
C	-1.830303	2.281216	-0.199168
H	-2.707136	2.569252	-0.791224
H	-2.141161	2.290471	0.849320
H	-1.076388	3.065286	-0.339262
H	-1.990765	1.307693	-2.685424
H	-0.326026	1.810991	-2.431308
H	-0.726398	0.088464	-2.634859
H	-3.255272	0.057677	-1.092617
H	-2.006755	-1.156514	-0.809879
H	-2.725568	-0.270883	0.550407
C	3.433220	0.019757	-2.364688
C	4.713638	0.889393	-0.414663
C	4.253360	-1.572546	-0.633878
H	5.638174	0.798011	-0.996601
H	4.335153	1.908704	-0.557224
H	4.991427	0.779970	0.641066
H	4.369551	-0.104004	-2.919233
H	2.729409	-0.720759	-2.765258
H	3.057259	1.021555	-2.606648
H	5.157407	-1.725796	-1.234159
H	4.537277	-1.745479	0.411620
H	3.533182	-2.348757	-0.918862

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 84
FINAL HEAT OF FORMATION = -1717.675836
 C    -0.103585     0.540632     0.012609
 C    -0.040447     0.689204     1.417478
 C     1.190825     0.425524     2.083193
 C     2.325804     0.009493     1.351821
 C     2.292624    -0.126782    -0.012927
 C     1.061786     0.150744    -0.634748
 O    -1.113258     1.031734     2.086633
Sn    -1.348982     1.874648     3.887537
 N     0.517462     0.930169     4.384415
 C     1.349258     0.483628     3.491668
 O    -3.197630     1.149348     3.944901
 C    -4.138511     1.228154     4.865373
 C    -3.822491     1.412031     6.239389
 C    -4.843570     1.445941     7.208646
 C    -6.169792     1.339041     6.863360
 C    -6.442890     1.157691     5.498672
 C    -5.491009     1.085363     4.486972
 C    -2.490972     1.526794     6.735018
 N    -1.412307     1.674104     6.042200
 C    -0.087509     1.712843     6.610144
 C     0.797814     0.767548     5.802085
 H    -0.082335     1.425156     7.670321
 H     0.306224     2.740687     6.554217
 H     1.856929     0.959625     6.022838
 H     0.584163    -0.270880     6.098042
 H    -2.385719     1.489316     7.828556
 H     2.304206     0.090704     3.867581
 H    -4.551817     1.570161     8.252327
 C    -7.261342     1.390886     7.931777
 H    -7.483257     1.062948     5.207707
 C    -5.906476     0.852992     3.026708
 H     3.240767    -0.203193     1.906200
 C     3.526023    -0.591562    -0.787525
 H     1.016244     0.045755    -1.713210
 C    -1.396153     0.801140    -0.774147
 C    -1.185067     0.582567    -2.276161
 C    -2.499171    -0.170118    -0.325346
 C    -1.852798     2.257503    -0.590904
 H    -2.125040     0.771233    -2.806475
 H    -0.437257     1.262218    -2.703880
 H    -0.888619    -0.446271    -2.514228
 H    -3.401192    -0.014999    -0.930809
 H    -2.187622    -1.212385    -0.466535
 H    -2.785828    -0.041679     0.721258
 H    -2.719336     2.461500    -1.232134
 H    -2.155621     2.485524     0.434300
 H    -1.062259     2.961815    -0.878629
 C    -7.431591     0.786962     2.887947
 C    -5.427224     2.003834     2.126360
 C    -5.346387    -0.489069     2.530554
 H    -5.671319    -0.669471     1.498083
 H    -4.253907    -0.526247     2.540185
 H    -5.719384    -1.321091     3.140507
 H    -5.838393     1.880280     1.116719
 H    -5.775392     2.974288     2.501778
 H    -4.340462     2.045486     2.019544
 H    -7.694839     0.613982     1.838407
 H    -7.873268    -0.035426     3.463700
 H    -7.922929     1.720078     3.190869
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 C     3.299726    -0.558700    -2.299509
 C     4.715304     0.320977    -0.459906
 C     3.853736    -2.033184    -0.373819
 H     4.729856    -2.402861    -0.921006
 H     4.081379    -2.114466     0.696286
 H     3.018618    -2.712097    -0.585595
 H     4.209855    -0.880957    -2.817987
 H     2.497659    -1.235202    -2.618817
 H     3.061810     0.448355    -2.664874
 H     5.605362     0.006615    -1.018605
 H     4.507269     1.364244    -0.726714
 H     4.984944     0.297262     0.603025
 C    -8.662509     1.369812     7.320696
 C    -7.108197     0.170950     8.850240
 C    -7.111404     2.679801     8.750482
 H    -9.416285     1.447335     8.112279
 H    -8.829326     2.209591     6.634711
 H    -8.869082     0.439798     6.776613
 H    -7.891445     2.743711     9.519135
 H    -6.148332     2.735348     9.272006
 H    -7.196276     3.570503     8.116074
 H    -7.882783     0.166651     9.627381
 H    -7.196266    -0.765996     8.286961
 H    -6.137942     0.156807     9.361914
 H    -1.212404     3.536632     3.656810
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1-Cl2

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   84
FINAL HEAT OF FORMATION = -2176.834085
 C    -0.091713     0.555175     0.016238
 C    -0.025777     0.691010     1.419305
 C     1.200759     0.417199     2.089187
 C     2.328720    -0.016414     1.357236
 C     2.288655    -0.165234    -0.006443
 C     1.065077     0.136362    -0.629988
 O    -1.106274     1.030370     2.085594
Sn    -1.341444     1.801187     3.893754
 N     0.538852     0.939842     4.388650
 C     1.374657     0.501807     3.494321
 O    -3.214530     1.189949     3.923166
 C    -4.149472     1.260374     4.853727
 C    -3.824916     1.452936     6.224936
 C    -4.842258     1.471120     7.200582
 C    -6.167371     1.328987     6.864491
 C    -6.445560     1.146479     5.500970
 C    -5.500054     1.098265     4.481664
 C    -2.496352     1.597005     6.715963
 N    -1.410623     1.703138     6.022219
 C    -0.083995     1.797598     6.584908
 C     0.829434     0.846656     5.811002
Cl    -1.082427     4.074155     3.608428
 H    -0.072989     1.545841     7.653687
 H     0.276089     2.833886     6.488643
 H     1.881247     1.086310     6.017383
 H     0.652700    -0.185683     6.149383
 H    -2.393353     1.618965     7.809516
 H     2.344702     0.145267     3.866437
 H    -4.547580     1.605989     8.241905
 C    -7.253951     1.340609     7.939198
 H    -7.485622     1.029583     5.217137
 C    -5.922508     0.863992     3.023739
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 H     3.243029    -0.235006     1.909983
 C     3.510749    -0.662525    -0.777899
 H     1.017326     0.029700    -1.708190
 C    -1.373452     0.862631    -0.771214
 C    -1.165765     0.644554    -2.273834
 C    -2.514765    -0.069599    -0.333718
 C    -1.772341     2.334996    -0.579801
 H    -2.095933     0.874788    -2.804761
 H    -0.390677     1.297251    -2.694503
 H    -0.910011    -0.393878    -2.517940
 H    -3.401035     0.115077    -0.953599
 H    -2.238279    -1.122881    -0.466525
 H    -2.815040     0.073731     0.706945
 H    -2.647160     2.568520    -1.199376
 H    -2.037359     2.580952     0.451597
 H    -0.964020     3.008426    -0.890371
 C    -7.447710     0.777401     2.895854
 C    -5.464939     2.024754     2.125049
 C    -5.349804    -0.470388     2.520400
 H    -5.682423    -0.652342     1.490783
 H    -4.256932    -0.495275     2.518077
 H    -5.707003    -1.308209     3.131929
 H    -5.867410     1.889340     1.113473
 H    -5.839468     2.986209     2.497667
 H    -4.379170     2.096881     2.026644
 H    -7.715562     0.608353     1.846918
 H    -7.874085    -0.055413     3.468206
 H    -7.949453     1.701685     3.208379
 C     3.281731    -0.639601    -2.289603
 C     4.718619     0.228913    -0.460001
 C     3.807836    -2.106721    -0.350136
 H     4.675389    -2.499711    -0.894418
 H     4.034784    -2.183058     0.720499
 H     2.958227    -2.769481    -0.555282
 H     4.183307    -0.986837    -2.806733
 H     2.464119    -1.301447    -2.600090
 H     3.065417     0.368874    -2.664147
 H     5.600482    -0.107045    -1.018872
 H     4.530196     1.274039    -0.733658
 H     4.990778     0.207297     0.602320
 C    -8.658145     1.305158     7.334719
 C    -7.072796     0.104097     8.830290
 C    -7.124484     2.614262     8.784430
 H    -9.408280     1.353545     8.131935
 H    -8.844573     2.154401     6.665670
 H    -8.851259     0.381562     6.775065
 H    -7.903862     2.647072     9.555528
 H    -6.161952     2.676047     9.306114
 H    -7.226879     3.516417     8.169301
 H    -7.843254     0.069006     9.610799
 H    -7.147034    -0.822416     8.247961
 H    -6.099692     0.097158     9.336734
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   85
FINAL HEAT OF FORMATION = -2177.630033
 C     0.018980    -0.178883     0.032139
 C     0.012002    -0.143782     1.458404
 C     1.218280     0.006966     2.179130
 C     2.428114     0.144683     1.553483
 C     2.409961     0.100063     0.142475
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C	1.282180	-0.067611	-0.633304
C	-1.156834	-0.347879	2.260863
N	-2.383313	-0.388709	1.885471
C	-3.460420	-0.712100	2.784789
C	-4.670072	0.157474	2.449389
N	-4.905927	0.112037	1.028269
Sn	-3.046426	0.039877	-0.183274
O	-1.049144	-0.337539	-0.668125
C	3.751298	0.327360	2.291667
C	4.352979	1.689139	1.918819
C	1.366117	-0.142002	-2.163163
C	2.814988	-0.021117	-2.646915
C	-6.079137	-0.048702	0.534300
C	-6.465409	-0.141730	-0.842085
C	-7.837580	-0.375938	-1.056569
C	-8.376527	-0.492416	-2.314305
C	-7.469493	-0.400828	-3.384044
C	-6.109017	-0.175137	-3.258101
C	-5.573427	0.000463	-1.948374
C	-9.877972	-0.713411	-2.506155
C	-10.270600	-0.730958	-3.984195
O	-4.329436	0.320754	-1.797241
C	-5.201414	-0.120368	-4.493456
C	-5.992451	-0.368312	-5.782791
Cl	-3.396853	-2.309783	-0.478565
C	-10.283002	-2.055896	-1.882816
C	-10.652662	0.423064	-1.823920
C	-4.129483	-1.219153	-4.408551
C	-4.546912	1.264041	-4.629179
C	4.723098	-0.790957	1.890775
C	0.836388	-1.497385	-2.660576
C	0.580536	1.011177	-2.809030
H	-2.726722	1.713924	-0.126877
H	3.363820	0.200627	-0.370104
H	-0.956162	-0.492927	3.334235
H	-3.170966	-0.575068	3.838263
H	-3.728578	-1.771267	2.647924
H	-5.549120	-0.177819	3.021066
H	-4.464832	1.197669	2.750003
H	-6.914066	-0.140764	1.246525
H	-8.477693	-0.458684	-0.176158
H	-7.865598	-0.515627	-4.387263
H	1.151896	0.011705	3.266448
C	3.566603	0.277727	3.808013
H	-11.735025	0.291241	-1.953857
H	-10.460727	0.468915	-0.745112
H	-10.380576	1.397878	-2.246844
H	-10.008588	0.206223	-4.490450
H	-9.796161	-1.553970	-4.532684
H	-11.354976	-0.861742	-4.083166
H	-9.742914	-2.888735	-2.349213
H	-10.072427	-2.092057	-0.806916
H	-11.358341	-2.238379	-2.010370
H	-5.308149	2.050851	-4.708557
H	-3.895265	1.508613	-3.787754
H	-3.939739	1.302307	-5.543492
H	-6.480313	-1.351116	-5.794760
H	-6.761091	0.395047	-5.958000
H	-5.310815	-0.339244	-6.641069
H	-3.466779	-1.108557	-3.547644
H	-4.591928	-2.211743	-4.340596
H	-3.506106	-1.204336	-5.312179

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 H    -0.491497     0.960358    -2.606235
 H     0.947649     1.983570    -2.456618
 H     0.708325     0.986393    -3.899381
 H     3.270687     0.938909    -2.373056
 H     3.452980    -0.824846    -2.258465
 H     2.844077    -0.089582    -3.740723
 H     1.414804    -2.324148    -2.228828
 H    -0.215018    -1.660214    -2.413115
 H     0.937556    -1.561213    -3.752225
 H     3.678540     2.508391     2.196283
 H     5.309885     1.852204     2.432183
 H     4.544377     1.773708     0.842268
 H     4.316081    -1.778586     2.140188
 H     4.940447    -0.787774     0.816254
 H     5.681783    -0.681242     2.414473
 H     4.534226     0.390119     4.311956
 H     2.919330     1.084531     4.174459
 H     3.138397    -0.676776     4.138543
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2-Cl2

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   36
FINAL HEAT OF FORMATION = -1549.534518
 C    -0.072075     0.258713     0.007665
 C    -0.035349     0.317858     1.406166
 C     1.194582     0.034441     2.064210
 C     2.333494    -0.302944     1.292807
 C     2.278835    -0.341747    -0.074708
 C     1.061703    -0.057406    -0.710441
 O    -1.147079     0.597455     2.045406
Sn    -1.361693     1.357222     3.868084
 N     0.477614     0.381010     4.367275
 C     1.343523     0.009120     3.475228
 O    -3.295999     0.951114     3.864365
 C    -4.191012     1.117565     4.817016
 C    -3.865592     1.249179     6.195174
 C    -4.906264     1.380773     7.144069
 C    -6.221436     1.405651     6.759570
 C    -6.528078     1.281960     5.398654
 C    -5.539949     1.134718     4.446861
 C    -2.535476     1.231843     6.699706
 N    -1.446200     1.216168     6.004771
 C    -0.122703     1.180209     6.585089
 C     0.720186     0.189312     5.787264
Cl    -0.942799     3.606529     3.634386
 H    -0.151081     0.886556     7.642677
 H     0.322894     2.186054     6.535143
 H     1.783633     0.318223     6.030006
 H     0.441153    -0.838631     6.064424
 H    -2.433982     1.235638     7.793761
 H     2.303565    -0.375363     3.846499
 H    -4.646185     1.471816     8.199031
 H    -7.013126     1.518053     7.496451
 H    -7.569135     1.302086     5.078563
 H    -5.789735     1.035413     3.392206
 H     3.267225    -0.531144     1.807364
 H     3.160406    -0.594696    -0.658651
 H     1.005363    -0.086645    -1.797995
 H    -1.012845     0.473416    -0.495775
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2H-Cl2

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   37
FINAL HEAT OF FORMATION = -1550.335286
 C     0.126272    -0.025364    -0.066292
 C     0.065344    -0.109025     1.343592
 C     1.286194     0.086067     2.060488
 C     2.477657     0.341306     1.348287
 C     2.504442     0.420160    -0.020570
 C     1.305767     0.231126    -0.723018
 O    -1.064028    -0.399273     1.896478
Sn    -1.701660     0.025816     3.827792
 N     0.462690    -0.128395     4.341420
 C     1.407256     0.010699     3.486661
 O    -3.737390     0.455526     3.952341
 C    -4.434174     0.978339     4.898151
 C    -3.935044     1.306406     6.198114
 C    -4.814718     1.849631     7.162360
 C    -6.141492     2.069829     6.900413
 C    -6.628110     1.754716     5.622521
 C    -5.805884     1.234415     4.653933
 C    -2.567648     1.184417     6.606656
 N    -1.576655     0.697005     5.953202
 C    -0.224129     0.838964     6.444516
 C     0.688460    -0.175211     5.761083
Cl    -1.321212     2.342902     3.324245
 H    -0.172961     0.716313     7.537229
 H     0.133259     1.853044     6.206571
 H     1.738423     0.030839     6.020154
 H     0.455669    -1.187543     6.128333
 H    -2.358968     1.588491     7.609814
 H     2.437226     0.085314     3.870112
 H    -4.411738     2.100595     8.144810
 H    -6.798938     2.485928     7.660130
 H    -7.678355     1.928250     5.388585
 H    -6.190874     0.996566     3.663771
 H     3.399663     0.480537     1.914966
 H     3.432975     0.622421    -0.549396
 H     1.304595     0.288189    -1.811405
 H    -0.800343    -0.171060    -0.618800
 H    -2.011660    -1.616341     4.145359
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3-Cl2

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   40
FINAL HEAT OF FORMATION = -1701.525111
 C    -0.001057    -0.019616     0.006302
 C    -0.000926    -0.036486     1.397815
 C     1.220542    -0.026903     2.095633
 C     2.418867     0.002112     1.388572
 C     2.404741     0.050987     0.004871
 C     1.197318     0.039525    -0.684711
 N    -1.159513    -0.099724     2.187662
 C    -2.334250     0.290495     1.784702
 C    -3.548173     0.269472     2.513188
 C    -3.652536    -0.123141     3.877001
 C    -4.909180    -0.068359     4.493738
 C    -6.016961     0.356010     3.791509
 C    -5.928715     0.750680     2.448378
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 C    -4.709422     0.709266     1.828548
 O    -2.629162    -0.506200     4.600830
Sn    -0.748925    -0.917805     4.130747
Cl    -0.509928    -3.172960     3.800776
 N     1.128060    -0.086261     3.494904
 C     2.070414     0.298979     4.305736
 C     2.056083     0.272081     5.721950
 C     0.931770    -0.116923     6.503198
 C     1.037121    -0.068676     7.899050
 C     2.207460     0.342839     8.499457
 C     3.323086     0.731665     7.743223
 C     3.238103     0.699939     6.377796
 O    -0.213452    -0.493548     5.988767
 H    -2.401578     0.703028     0.771281
 H     2.981315     0.707581     3.852682
 H    -4.618278     1.015522     0.786257
 H    -6.981503     0.387096     4.296960
 H     4.091884     1.004933     5.772513
 H     2.261368     0.367799     9.587167
 H     3.373001    -0.034945     1.910850
 H     3.345320     0.072998    -0.541538
 H     1.189564     0.052017    -1.772688
 H    -0.934382    -0.074857    -0.551017
 H     4.236269     1.057073     8.235323
 H     0.174257    -0.362335     8.493676
 H    -4.988084    -0.365231     5.537831
 H    -6.813350     1.086508     1.912848
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3H-Cl2

```
   41
FINAL HEAT OF FORMATION = -1702.329125
 C    -0.037692    -0.365327    -0.018766
 C     0.035127    -0.334351     1.393082
 C     1.180083     0.294818     1.976350
 C     2.174093     0.846777     1.135701
 C     2.071987     0.806011    -0.229596
 C     0.947794     0.187235    -0.799713
 O    -0.894047    -0.900337     2.081388
Sn    -1.559805    -0.355415     3.991127
 N     0.616236     0.057432     4.337422
 C     1.416507     0.389862     3.378597
 O    -3.609223    -0.249375     4.409844
 C    -4.222058     0.690494     5.042748
 C    -3.631561     1.437234     6.110650
 C    -4.400547     2.410934     6.788481
 C    -5.700241     2.673834     6.444931
 C    -6.276210     1.943873     5.392976
 C    -5.565442     0.983898     4.714202
 C    -2.293516     1.261928     6.569072
 N    -1.369431     0.527192     6.043924
 C    -0.093400     0.401497     6.589604
 C     0.959524     0.153463     5.684624
Cl    -1.743335     1.876006     3.142713
 C     2.254129    -0.018066     6.170877
 H    -2.030744     1.851028     7.459001
 H     2.389430     0.820222     3.654718
 H    -3.933946     2.967965     7.602427
 H    -7.308799     2.141041     5.105117
 H     3.040866     1.319632     1.599647
 H     0.850699     0.144675    -1.884437
 C     2.514001     0.082847     7.528748
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 H     3.063808    -0.257609     5.483363
 H     3.529277    -0.057123     7.895016
 C     1.476727     0.327175     8.420223
 C     0.179174     0.470649     7.954507
 H     1.673797     0.380100     9.489274
 H    -0.634945     0.614134     8.663354
 H     2.844617     1.240945    -0.859410
 H    -0.908327    -0.839572    -0.468280
 H    -6.019229     0.423868     3.898500
 H    -6.274603     3.431104     6.973523
 H    -1.544933    -1.980156     4.465761
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4-Cl2

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   88
FINAL HEAT OF FORMATION = -2328.824669
 C    -0.100197     0.270705     0.047094
 C     0.024969     0.476810     1.436235
 C     1.299835     0.322201     2.050791
 C     2.419805    -0.058682     1.279199
 C     2.326686    -0.263050    -0.074558
 C     1.054708    -0.081540    -0.644035
 O    -1.046120     0.757954     2.150196
Sn    -1.236772     1.661202     3.896346
 N     0.726411     0.929590     4.348548
 C     1.543945     0.487831     3.436263
 O    -3.176757     1.278192     3.858170
 C    -4.096694     1.293401     4.797206
 C    -3.748022     1.161019     6.171280
 C    -4.757879     1.074377     7.155916
 C    -6.088657     1.148471     6.831548
 C    -6.387682     1.322362     5.468534
 C    -5.457278     1.400135     4.438679
 C    -2.420531     1.109806     6.657484
 N    -1.308586     1.267210     5.994667
 C    -0.034672     1.247644     6.583045
 C     1.051266     1.064475     5.706208
Cl    -0.949972     3.930281     3.654037
 C     2.348920     1.057025     6.212041
 H    -2.330200     0.919674     7.732541
 H     2.548890     0.200816     3.764812
 H    -4.446830     0.959158     8.194837
 C    -7.162804     1.069780     7.915616
 H    -7.434417     1.402253     5.196053
 C    -5.902288     1.602775     2.983772
 H     3.374664    -0.180170     1.791767
 C     3.556048    -0.659284    -0.891786
 H     0.963428    -0.236105    -1.713517
 C    -1.447017     0.399588    -0.678472
 C    -1.282221     0.202876    -2.189338
 C    -2.410546    -0.688014    -0.177843
 C    -2.058119     1.796141    -0.471260
 H    -2.258173     0.300419    -2.677333
 H    -0.622271     0.953067    -2.642921
 H    -0.900256    -0.792125    -2.447563
 H    -3.369335    -0.612358    -0.705948
 H    -2.009132    -1.690311    -0.371471
 H    -2.621518    -0.609906     0.891896
 H    -2.934201     1.913902    -1.120291
 H    -2.396208     1.973195     0.552551
 H    -1.347468     2.588014    -0.737974
 C    -7.427049     1.717115     2.881272
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 C    -5.317170     2.911477     2.428200
 C    -5.477779     0.406304     2.118887
 H    -5.850544     0.537169     1.095171
 H    -4.394128     0.285155     2.056330
 H    -5.903298    -0.529072     2.503139
 H    -5.684302     3.078362     1.408057
 H    -5.630439     3.772081     3.032067
 H    -4.225420     2.915843     2.378852
 H    -7.710438     1.873601     1.834461
 H    -7.941996     0.808198     3.216275
 H    -7.825785     2.567382     3.448276
 C     3.208696    -0.922036    -2.357265
 C     4.585040     0.477924    -0.827900
 C     4.165743    -1.939497    -0.304531
 H     5.043793    -2.247839    -0.885218
 H     4.501348    -1.809384     0.731650
 H     3.449595    -2.770051    -0.318981
 H     4.108668    -1.225549    -2.903930
 H     2.476643    -1.731109    -2.473073
 H     2.816397    -0.031053    -2.863059
 H     5.480308     0.219851    -1.406554
 H     4.179423     1.410477    -1.238429
 H     4.912198     0.683707     0.198696
 C    -8.573317     1.075695     7.326165
 C    -6.979487    -0.225286     8.717651
 C    -7.014578     2.282504     8.844607
 H    -9.313047     0.979936     8.128850
 H    -8.802199     2.007674     6.794455
 H    -8.739300     0.239475     6.635716
 H    -7.780798     2.268056     9.629654
 H    -6.039437     2.303304     9.346556
 H    -7.120699     3.224156     8.292519
 H    -7.746031    -0.307924     9.497877
 H    -7.062077    -1.110692     8.075671
 H    -6.007334    -0.272171     9.223075
 C     2.568265     1.208508     7.569950
 H     3.204995     0.948953     5.549459
 H     3.586038     1.200448     7.954437
 C     1.495820     1.397835     8.434763
 C     0.202795     1.431413     7.943155
 H     1.669916     1.541421     9.499128
 H    -0.618236     1.622404     8.631264
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4H-Cl2

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   41
FINAL HEAT OF FORMATION = -1702.329125
 C    -0.037692    -0.365327    -0.018766
 C     0.035127    -0.334351     1.393082
 C     1.180083     0.294818     1.976350
 C     2.174093     0.846777     1.135701
 C     2.071987     0.806011    -0.229596
 C     0.947794     0.187235    -0.799713
 O    -0.894047    -0.900337     2.081388
Sn    -1.559805    -0.355415     3.991127
 N     0.616236     0.057432     4.337422
 C     1.416507     0.389862     3.378597
 O    -3.609223    -0.249375     4.409844
 C    -4.222058     0.690494     5.042748
 C    -3.631561     1.437234     6.110650
 C    -4.400547     2.410934     6.788481
 C    -5.700241     2.673834     6.444931
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 C    -6.276210     1.943873     5.392976
 C    -5.565442     0.983898     4.714202
 C    -2.293516     1.261928     6.569072
 N    -1.369431     0.527192     6.043924
 C    -0.093400     0.401497     6.589604
 C     0.959524     0.153463     5.684624
Cl    -1.743335     1.876006     3.142713
 C     2.254129    -0.018066     6.170877
 H    -2.030744     1.851028     7.459001
 H     2.389430     0.820222     3.654718
 H    -3.933946     2.967965     7.602427
 H    -7.308799     2.141041     5.105117
 H     3.040866     1.319632     1.599647
 H     0.850699     0.144675    -1.884437
 C     2.514001     0.082847     7.528748
 H     3.063808    -0.257609     5.483363
 H     3.529277    -0.057123     7.895016
 C     1.476727     0.327175     8.420223
 C     0.179174     0.470649     7.954507
 H     1.673797     0.380100     9.489274
 H    -0.634945     0.614134     8.663354
 H     2.844617     1.240945    -0.859410
 H    -0.908327    -0.839572    -0.468280
 H    -6.019229     0.423868     3.898500
 H    -6.274603     3.431104     6.973523
 H    -1.544933    -1.980156     4.465761
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TMS+

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   13
FINAL HEAT OF FORMATION =  -408.284834
Si    -0.043591    -0.486428    -0.183527
 C    -1.867947    -0.464270    -0.158945
 H    -2.290777     0.542850    -0.088465
 H    -2.256511    -0.951068    -1.066748
 H    -2.238794    -1.068051     0.683213
 C     0.846011    -2.076967    -0.275218
 H     1.555417    -2.162100     0.561776
 H     0.183281    -2.948101    -0.272137
 H     1.460472    -2.102913    -1.188729
 C     0.889853     1.080013    -0.106053
 H     0.569800     1.751328    -0.917001
 H     0.645534     1.607152     0.829458
 H     1.974591     0.944492    -0.160410
```

TMSH

```
   14
FINAL HEAT OF FORMATION =  -409.174447
 C     0.009921    -0.016622    -0.011280
Si     0.020436    -0.036781     1.868811
 C     1.789078    -0.016980     2.506879
 H    -0.682460     1.181946     2.366578
 C    -0.880030    -1.559142     2.507054
 H    -1.013341    -0.010644    -0.406111
 H     0.521838     0.869889    -0.405207
 H     0.517491    -0.900681    -0.417770
 H    -0.391663    -2.479822     2.163163
 H    -0.897200    -1.583243     3.603592
 H    -1.920121    -1.585902     2.159664
 H     2.330842     0.871004     2.158803
 H     1.821290    -0.014435     3.603309
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 H     2.342861    -0.899299     2.161362
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Imine---2-Cl2 FLP

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   63
FINAL HEAT OF FORMATION =     0.000000
 C    -0.439373     0.072860     0.095662
 C    -0.282034     0.162974     1.486164
 C     1.029878     0.084542     2.028097
 C     2.136252    -0.007987     1.149935
 C     1.963691    -0.042398    -0.212065
 C     0.661746    -0.022110    -0.725994
 O    -1.344732     0.291735     2.224744
Sn    -1.687932    -0.022239     4.197527
Cl    -1.643163    -2.383395     3.936168
 C     1.314714    -0.067461     3.415571
 N     0.497548    -0.037507     4.415914
 C     0.959991    -0.504808     5.712170
 C     0.009880    -0.047779     6.806251
 N    -1.347462    -0.257870     6.376994
 C    -2.188764    -0.899182     7.113006
 C    -3.546389    -1.206042     6.815790
 C    -4.211305    -0.774305     5.637675
 C    -5.540190    -1.171270     5.448316
 C    -6.192795    -1.933015     6.398465
 C    -5.553214    -2.341468     7.571195
 C    -4.242690    -1.981478     7.766428
 O    -3.648482     0.019932     4.754556
 H     1.974216    -0.138809     5.926005
 H     1.002587    -1.604090     5.697382
 H     0.229338    -0.587858     7.737821
 H     0.162306     1.020891     7.020784
 H     2.367702    -0.284034     3.644155
 H    -1.829529    -1.256366     8.088903
 H     3.140105    -0.071003     1.569579
 H     2.823945    -0.111144    -0.872609
 H     0.511259    -0.093570    -1.801877
 H    -1.454126     0.088462    -0.290857
 H    -3.722069    -2.299199     8.669524
 H    -6.080029    -2.939119     8.310531
 H    -7.228161    -2.221571     6.223658
 H    -6.056743    -0.872468     4.538879
 N    -2.143561     2.252778     3.991154
 C    -2.775655     2.684194     2.973213
 H    -2.875933     3.769948     2.880813
 C    -3.396845     1.994678     1.827996
 C    -2.987936     2.415793     0.558948
 C    -4.448259     1.097572     1.955408
 C    -3.575177     1.881382    -0.568952
 H    -2.187788     3.148960     0.450912
 C    -5.057547     0.589339     0.809907
 H    -4.818393     0.815804     2.933191
 C    -4.618439     0.964551    -0.447151
 H    -3.234901     2.173640    -1.560819
 H    -5.891537    -0.102515     0.911308
 H    -5.092603     0.560837    -1.339318
 C    -1.684884     3.256712     5.008976
 C    -2.040642     4.706057     4.666864
 H    -3.121809     4.869686     4.588830
 H    -1.684430     5.346356     5.479138
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H	-1.557106	5.062247	3.749943
C	-0.162384	3.171318	5.091947
H	0.219583	3.925067	5.788422
H	0.209944	2.205402	5.433493
H	0.294602	3.360257	4.113013
C	-2.365616	2.919491	6.334705
H	-2.220780	1.888434	6.656999
H	-1.971045	3.571213	7.122423
H	-3.446637	3.086004	6.273961

Imine---2-Cl2 FLP

63

C	-0.369007	0.127899	0.068805
C	-0.203901	0.160762	1.463641
C	1.105756	0.008335	1.994483
C	2.202969	-0.128001	1.110922
C	2.024014	-0.131793	-0.248085
C	0.723704	-0.017060	-0.757649
O	-1.252921	0.321694	2.213612
Sn	-1.611698	-0.057345	4.176538
Cl	-1.587186	-2.404508	3.863846
C	1.385068	-0.146822	3.379656
N	0.573222	-0.085836	4.384019
C	1.036299	-0.564568	5.675882
C	0.086128	-0.123326	6.776002
N	-1.276420	-0.302544	6.339389
C	-2.140338	-0.885608	7.102050
C	-3.517255	-1.130243	6.845290
C	-4.183801	-0.725720	5.657728
C	-5.552722	-1.011661	5.538721
C	-6.229715	-1.653239	6.554487
C	-5.582420	-2.048633	7.731025
C	-4.242977	-1.788947	7.863359
O	-3.590500	-0.069147	4.697437
H	2.048044	-0.195187	5.894954
H	1.084210	-1.663371	5.650528
H	0.293087	-0.694432	7.691330
H	0.254737	0.935397	7.023914
H	2.431394	-0.394373	3.607821
H	-1.782887	-1.228717	8.083101
H	3.203355	-0.247981	1.526515
H	2.874244	-0.241068	-0.916095
H	0.573558	-0.055028	-1.835138
H	-1.378928	0.221090	-0.323491
H	-3.718531	-2.092154	8.769392
H	-6.131039	-2.553801	8.521663
H	-7.292378	-1.857994	6.433057
H	-6.073928	-0.714573	4.630634
N	-2.181914	2.177110	3.991731
C	-2.869149	2.599336	3.000424
H	-3.050525	3.676758	2.968844
C	-3.445759	1.956196	1.814063
C	-3.275922	2.680337	0.628990
C	-4.206839	0.787634	1.799078
C	-3.792362	2.208222	-0.564406
H	-2.734468	3.627009	0.638716
C	-4.753529	0.340303	0.605376
H	-4.407414	0.245077	2.715537
C	-4.538860	1.035627	-0.576732

H	-3.639078	2.762041	-1.488803
H	-5.363175	-0.561259	0.603480
H	-4.971595	0.677082	-1.508772
C	-1.781401	3.179977	5.034594
C	-2.132419	4.627197	4.676717
H	-3.212019	4.802147	4.603841
H	-1.764280	5.274977	5.477877
H	-1.652323	4.965264	3.751300
C	-0.264483	3.111524	5.185006
H	0.075632	3.820547	5.946864
H	0.102951	2.127577	5.476836
H	0.232295	3.366993	4.241514
C	-2.515093	2.836119	6.330796
H	-2.340759	1.818678	6.681500
H	-2.191445	3.516248	7.126649
H	-3.597107	2.956842	6.209412

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