

Reactivity of a Gold(I)/Platinum(0) Frustrated Lewis Pair with Germanium and Tin Dihalides

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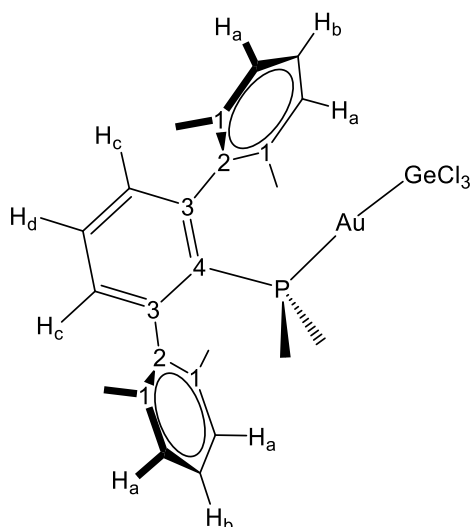
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SUPPORTING INFORMATION

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1. Synthesis and characterization of new compounds



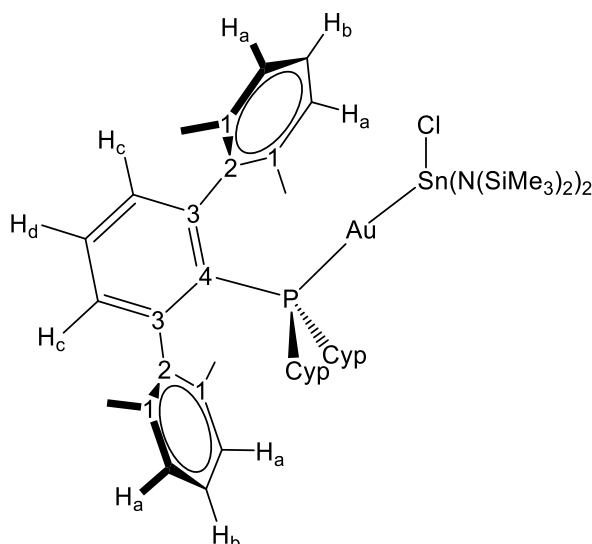
Compound 6^{Xyl}. A solution of (PMe₂Ar^{Xyl2})AuCl (150 mg, 0.26 mmol) in THF (5 mL) was added over a solution of germanium chloride dioxane complex (59 mg, 0.26 mmol) in THF (5 mL). The mixture was stirred for 30 minutes at room temperature. The solvent was then removed under vacuum to give compound 6^{Xyl}, as a fine white powder (169 mg, 90%). Crystals suitable for X-ray analysis were grown by slow diffusion of pentane into a THF solution of 6^{Xyl}.

Anal. Calcd. for C₂₄H₂₇AuCl₃GeP: C, 39.9; H, 3.8. **Found:** C, 39.7; H, 3.8.

¹H NMR (400 MHz, CD₂Cl₂, 25 °C) δ: 7.67 (td, 1 H, ³J_{HH} = 7.6 Hz, ⁵J_{HP} = 1.6 Hz, H_d), 7.28 (m, 6 H, H_a, H_b), 7.16 (dd, 2 H, ³J_{HH} = 7.6 Hz, ⁴J_{HP} = 3.5 Hz, H_c), 2.09 (s, 12 H, Me_{Xyl}), 1.28 (d, 6 H, ²J_{HP} = 9.5 Hz, PMe₂).

¹³C{¹H} NMR (100 MHz, CD₂Cl₂, 25 °C) δ: 147.3 (d, ²J_{CP} = 11 Hz, C₃), 140.5 (d, ³J_{CP} = 5 Hz, C₂), 136.5 (C₁), 133.1 (CH_d), 131.7 (d, ³J_{CP} = 8 Hz, CH_c), 129.4 (CH_b), 128.8 (CH_a), 126.0 (d, ¹J_{CP} = 51 Hz, C₄), 21.8 (Me_{Xyl}), 16.2 (d, ¹J_{CP} = 34 Hz, PMe₂).

³¹P{¹H} NMR (160 MHz, CD₂Cl₂, 25 °C) δ: 6.8.

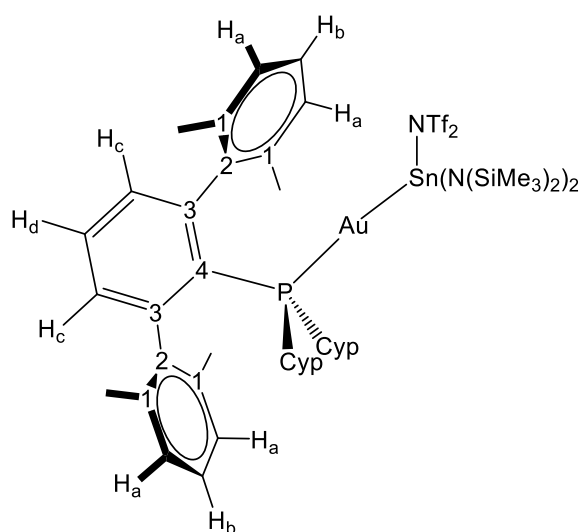


Compound 8^{Cyp}. In a NMR tube, a solution of (PCyp₂Ar^{Xyl2})AuCl (30 mg, 0.04 mmol) in C₆D₆ (0.5 mL) was added tin bis(trimethylsilyl)amide (19 mg, 0.04 mmol). The mixture gives compound 8^{Cyp} after 5 minutes. It can be crystallized by slow diffusion of pentane into a C₆D₆ solution (2:1 by vol.) (23 mg, 51%).

¹H NMR (400 MHz, C₆D₆, 25 °C) δ: 7.29 (t, 2 H, ³J_{HH} = 7.6 Hz, H_b), 7.14 (d, 4 H, ³J_{HH} = 7.6 Hz, H_a), 6.94 (td, 1 H, ³J_{HH} = 7.6 Hz, ⁵J_{HP} = 1.5 Hz, H_d), 6.57 (dd, 2 H, ³J_{HH} = 7.6 Hz, ⁴J_{HP} = 2.7 Hz, H_c), 2.27-2.17 (m, 2 H, PCH), 1.94 (s, 12 H, Me_{Xyl}), 1.8-1.25 (m, 16 H, CH₂), 0.58 (s, 36 H, SiMe₃).

¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C) δ: 148.5 (d, ²J_{CP} = 10 Hz, C₃), 141.1 (d, ³J_{CP} = 4 Hz, C₂), 136.1 (C₁), 136.1 (d, ³J_{CP} = 6 Hz, CH_c), 131.1 (d, ⁴J_{CP} = 2 Hz, CH_d), 129.6 (CH_b), 128.9 (CH_a), 38.9 (d, ¹J_{CP} = 27 Hz, PCH), 35.2 (d, ²J_{CP} = 10 Hz, CH₂), 32.6 (d, ²J_{CP} = 9 Hz, CH₂), 25.1 (d, ²J_{CP} = 10 Hz, CH₂), 24.8 (d, ²J_{CP} = 10 Hz, CH₂), 21.6 (Me_{Xyl}), 7.21 (SiMe₃).

³¹P{¹H} NMR (160 MHz, C₆D₆, 25 °C) δ: 59.9 (²J_{PSn} = 2846 Hz).

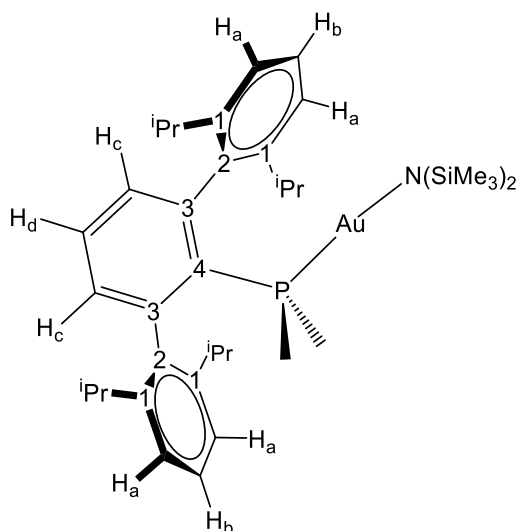


Compound 9^{Cyp}. In a NMR tube, a solution of Au[P(Cyp)₂Ar^{Xyl2}]₂NTf₂ (30 mg, 0.03 mmol) in C₆D₆ (0.5 mL) was added tin bis(trimethylsilyl)amide (14 mg, 0.03 mmol). The mixture gives compound **9^{Cyp}** after 5 minutes. It can be crystallized by slow diffusion of pentane into a C₆D₆ solution (2:1 by vol.) (20 mg, 49%).

¹H NMR (400 MHz, C₆D₆, 25 °C) δ : 7.15 (t, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, H_b), 7.03 (d, 4 H, $^3J_{\text{HH}} = 7.6$ Hz, H_a), 6.93 (td, 1 H, $^3J_{\text{HH}} = 7.6$ Hz, $^5J_{\text{HP}} = 1.5$ Hz, H_d), 6.51 (dd, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, $^4J_{\text{HP}} = 3$ Hz, H_c), 2.35-2.23 (m, 2 H, PCH), 1.91 (s, 12 H, Me_{Xyl}), 1.79-1.25 (m, 16 H, CH₂), 0.49 (s, 36 H, SiMe₃).

¹³C{¹H} NMR (100 MHz, C₆D₆, 25 °C) δ : 147.8 (d, $^2J_{\text{CP}} = 10$ Hz, C₃), 141.5 (d, $^3J_{\text{CP}} = 4$ Hz, C₂), 136.6 (C₁), 132.3 (d, $^3J_{\text{CP}} = 6$ Hz, CH_c), 131.3 (CH_d), 128.7 (CH_b), 128.4 (CH_a), 120.4 (q, $^1J_{\text{CF}} = 323$ Hz, CF₃), 38.9 (d, $^1J_{\text{CP}} = 29$ Hz, PCH), 35.9 (d, $^2J_{\text{CP}} = 10$ Hz, CH₂), 32.8 (d, $^2J_{\text{CP}} = 7$ Hz, CH₂), 25.3 (d, $^2J_{\text{CP}} = 10$ Hz, CH₂), 24.4 (d, $^2J_{\text{CP}} = 10$ Hz, CH₂), 21.6 (Me_{Xyl}), 6.74 ($^1J_{\text{CSi}} = 55$ Hz, $^3J_{\text{CSn}} = 18$ Hz, SiMe₃).

³¹P{¹H} NMR (160 MHz, C₆D₆, 25 °C) δ : 60.0 ($^2J_{\text{PSn}} = 2654$ Hz).

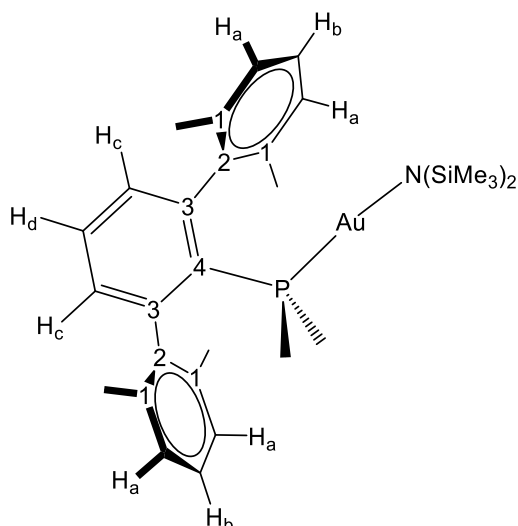


Compound $[\text{PMe}_2\text{Ar}^{\text{Dipp}^2}]\text{Au}[\text{N}(\text{SiMe}_3)_2]$. A solid mixture of compound 5 (30 mg, 0.043 mmol) and $\text{Li}[\text{N}(\text{SiMe}_3)_2]$ (7 mg, 0.043 mmol) was suspended in toluene inside a dry box. The solution was stirred for 30 min, filtered and the solvents evaporated under vacuum. The white residue was washed with pentane to yield $[\text{PMe}_2\text{Ar}^{\text{Dipp}^2}]\text{Au}[\text{N}(\text{SiMe}_3)_2]$ as a white solid (28 mg, 80%).

^1H NMR (400 MHz, C_6D_6 , 25 °C) δ : 7.28 (t, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, H_b), 7.12 (d, 4 H, $^3J_{\text{HH}} = 7.6$ Hz, H_a), 6.93 (m, 2 H, H_c), 6.85 (m, 1 H, H_d), 2.77 (sept, 4 H, $^3J_{\text{HH}} = 6.8$ Hz, $i\text{Pr}(\text{CH})$), 1.39 (d, 12 H, $^3J_{\text{HH}} = 6.8$ Hz, $i\text{Pr}(\text{CH}_3)$), 0.98 (d, 12 H, $^3J_{\text{HH}} = 6.8$ Hz, $i\text{Pr}(\text{CH}_3)$), 0.88 (d, 6 H, $^2J_{\text{HP}} = 10$ Hz, PMe_2), 0.41 (s, 18 H, SiMe_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 25 °C) δ : 146.9 (C_1), 143.8 (d, $^2J_{\text{CP}} = 10$ Hz, C_3), 139.2 (d, $^3J_{\text{CP}} = 5$ Hz, C_2), 132.9 (d, $^3J_{\text{CP}} = 8$ Hz, CH_c), 130.1 (d, $^1J_{\text{CP}} = 46$ Hz, C_4), 129.6 (CH_d), 128.6 (CH_b), 123.6 (CH_a), 31.5 ($i\text{Pr}(\text{CH})$), 25.7 ($i\text{Pr}(\text{CH}_3)$), 23.6 ($i\text{Pr}(\text{CH}_3)$), 18.1 (d, $^1J_{\text{CP}} = 37$ Hz, PMe_2), 6.7 ($^1J_{\text{CSi}} = 38$ Hz, SiMe_3).

$^{31}\text{P}\{^1\text{H}\}$ NMR (160 MHz, C_6D_6 , 25 °C) δ : 3.1.

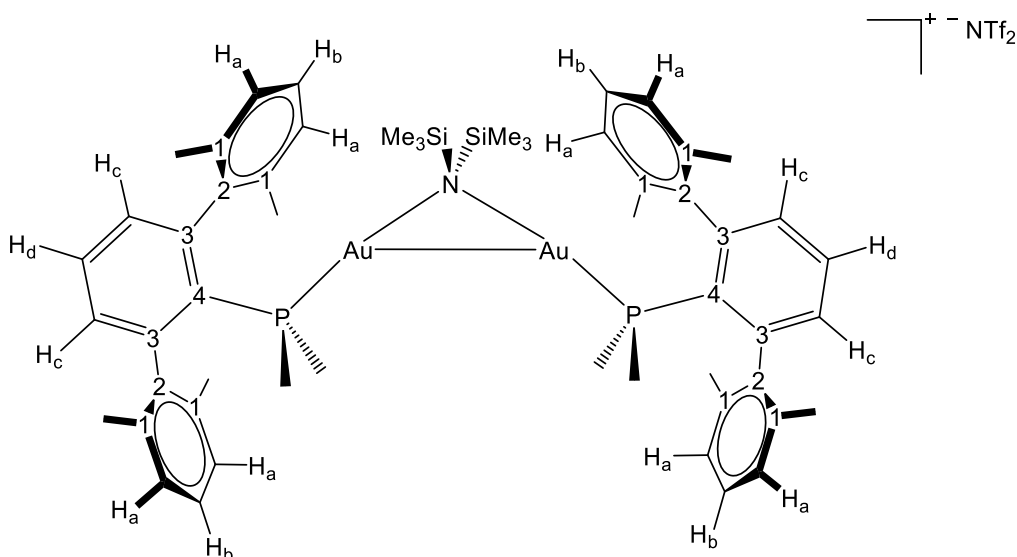


Compound $[\text{PMe}_2\text{Ar}^{\text{Xyl}2}]\text{Au}[\text{N}(\text{SiMe}_3)_2]$. A solid mixture of compound 5^{Xyl} (35 mg, 0.06 mmol) and $\text{Li}[\text{N}(\text{SiMe}_3)_2]$ (10 mg, 0.04 mmol) was suspended in toluene inside a dry box. The solution was stirred for 30 min, filtered and the solvents evaporated under vacuum. The white residue was washed with pentane to yield $[\text{PMe}_2\text{Ar}^{\text{Xyl}2}]\text{Au}[\text{N}(\text{SiMe}_3)_2]$ as a white solid (29 mg, 69%).

^1H NMR (400 MHz, C_6D_6 , 25 °C) δ : 7.08 (t, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, H_b), 6.99 (d, 4 H, $^3J_{\text{HH}} = 7.6$ Hz, H_a), 6.95 (td, 1 H, $^3J_{\text{HH}} = 7.6$ Hz, $^5J_{\text{HP}} = 1.7$ Hz, H_d), 6.58 (dd, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, $^4J_{\text{HP}} = 3.1$ Hz, H_c), 2.11 (s, 12 H, Me_{Xyl}), 0.67 (d, 6 H, $^2J_{\text{HP}} = 9.4$ Hz, PMe_2), 0.48 (s, 18 H, SiMe_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 25 °C) δ : 145.6 (d, $^2J_{\text{CP}} = 9$ Hz, C_3), 141.3 (d, $^3J_{\text{CP}} = 3$ Hz, C_2), 136.5 (C_1), 130.9 (CH_d), 130.8 (CH_c), 129.6 (d, $^1J_{\text{CP}} = 60$ Hz, C_4), 128.7 (CH_b), 128.4 (CH_a), 22.2 (Me_{Xyl}), 17.2 (d, $^1J_{\text{CP}} = 38$ Hz, PMe_2), 6.8 ($^1J_{\text{CSi}} = 53$ Hz, SiMe_3).

$^{31}\text{P}\{^1\text{H}\}$ NMR (160 MHz, C_6D_6 , 25 °C) δ : 1.5.

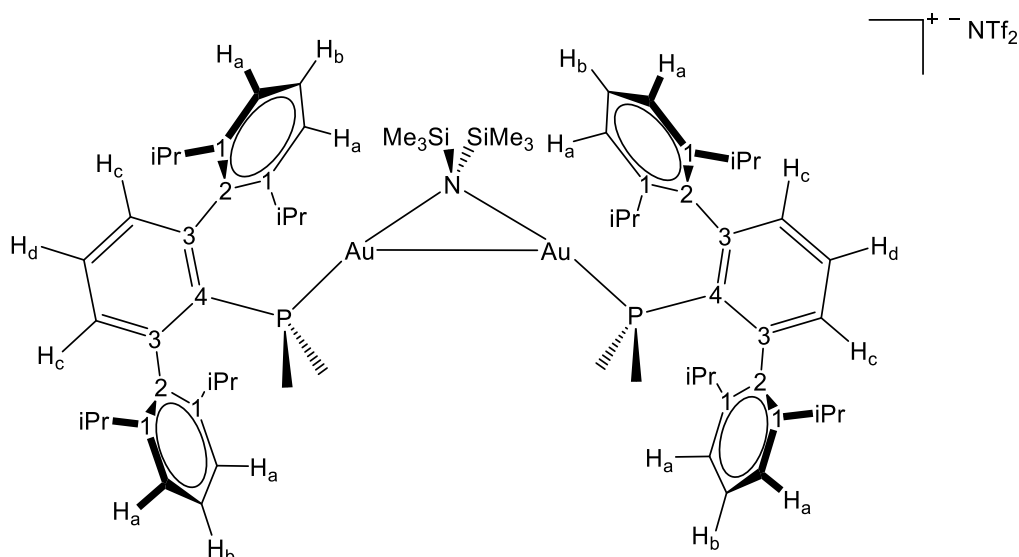


Compound $[\text{Au}_2(\mu\text{-N}(\text{SiMe}_3)_2)(\text{PMe}_2\text{Ar}^{\text{Xyl}2})_2]$. A solid mixture of compounds 1^{Xyl} (35 mg, 0.04 mmol) and $[\text{PMe}_2\text{Ar}^{\text{Xyl}2}]\text{Au}[\text{N}(\text{SiMe}_3)_2]$ (30 mg, 0.04 mmol) was dissolved in toluene inside a dry box. The solution was stirred for 30 min and the solvents evaporated under vacuum. The white residue was washed with pentane to yield $[\text{Au}_2(\mu\text{-N}(\text{SiMe}_3)_2)(\text{PMe}_2\text{Ar}^{\text{Xyl}2})_2]$ as a white solid (44 mg, 88%).

^1H NMR (400 MHz, C_6D_6 , 25 °C) δ : 7.16 (t, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, H_b), 7.03 (d, 4 H, $^3J_{\text{HH}} = 7.6$ Hz, H_a), 6.95 (td, 1 H, $^3J_{\text{HH}} = 7.6$ Hz, $^5J_{\text{HP}} = 1.7$ Hz, H_d), 6.61 (dd, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, $^4J_{\text{HP}} = 3.1$ Hz, H_c), 1.98 (s, 12 H, Me_{Xyl}), 0.87 (d, 6 H, $^2J_{\text{HP}} = 10.0$ Hz, PMe_2), 0.25 (s, 18 H, SiMe_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 25 °C) δ : 146.11 (d, $^2J_{\text{CP}} = 10$ Hz, C_3), 140.8 (C_2), 140.1 (C_1), 136.3 (CH_d), 132.1 (CH_c), 125.4 (d, $^1J_{\text{CP}} = 55$ Hz, C_4), 131.1 (CH_b), 129.1 (CH_a), 120.3 (q, $^1J_{\text{CF}} = 323$ Hz, CF_3), 21.7 (Me_{Xyl}), 17.7 (d, $^1J_{\text{CP}} = 43$ Hz, PMe_2), 6.6 (SiMe_3).

$^{31}\text{P}\{^1\text{H}\}$ NMR (160 MHz, C_6D_6 , 25 °C) δ : -3.4.



Compound $[\text{Au}_2(\mu\text{-N}(\text{SiMe}_3)_2)(\text{PMe}_2\text{Ar}^{\text{Dipp}2})_2]$. A solid mixture of compounds **1** (36 mg, 0.04 mmol) and $[\text{PMe}_2\text{Ar}^{\text{Dipp}2}]\text{Au}[\text{N}(\text{SiMe}_3)_2]$ (32 mg, 0.04 mmol) was dissolved in toluene inside a dry box. The solution was stirred for 30 min and the solvents evaporated under vacuum. The white residue was washed with pentane to yield $[\text{Au}_2(\mu\text{-N}(\text{SiMe}_3)_2)(\text{PMe}_2\text{Ar}^{\text{Dipp}2})_2]$ as a white solid (49 mg, 83%).

^1H NMR (400 MHz, C_6D_6 , 25 °C) δ : 7.31 (t, 2 H, $^3J_{\text{HH}} = 7.6$ Hz, H_b), 7.14 (d, 4 H, $^3J_{\text{HH}} = 7.6$ Hz, H_a), 6.96 (m, 2 H, H_c , H_d), 2.56 (sept, 4 H, $^3J_{\text{HH}} = 6.8$ Hz, $^i\text{Pr}(\text{CH})$), 1.33 (d, 12 H, $^3J_{\text{HH}} = 6.7$ Hz, $^i\text{Pr}(\text{CH}_3)$), 0.95 (d, 12 H, $^3J_{\text{HH}} = 6.6$ Hz, $^i\text{Pr}(\text{CH}_3)$), 0.14 (s, 18 H, SiMe_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6 , 25 °C) δ : 146.6 (C_1), 145.4 (d, $^2J_{\text{CP}} = 10$ Hz, C_3), 138.2 (d, $^3J_{\text{CP}} = 5$ Hz, C_2), 133.3 (d, $^3J_{\text{CP}} = 8$ Hz, CH_c), 130.3 (CH_d), 129.8 (d, $^1J_{\text{CP}} = 47$ Hz, C_4), 127.4 (CH_b), 124.1 (CH_a), 120.5 (q, $^1J_{\text{CF}} = 323$ Hz, CF_3), 31.6 ($^i\text{Pr}(\text{CH})$), 25.5 ($^i\text{Pr}(\text{CH}_3)$), 23.6 ($^i\text{Pr}(\text{CH}_3)$), 19.3 (d, $^1J_{\text{CP}} = 39$ Hz, PMe_2), 7.6 (SiMe_3).

$^{31}\text{P}\{^1\text{H}\}$ NMR (160 MHz, C_6D_6 , 25 °C) δ : -7.8.

2. X-Ray Structural Characterization of new compounds

Crystallographic details. Low-temperature diffraction data were collected either on a Rigaku MicroMax-007HF diffractometer coupled to a Dectris Pilatus3R detector by means of ω -scans (structures **6**, **8^{Cyp}** and $[\text{Au}_2(\mu\text{-N}(\text{SiMe}_3)_2)(\text{PMe}_2\text{Ar}^{\text{Xyl2}})_2]$; Chemistry Department at Yale University) or on a Bruker APEX-II CCD diffractometer by means of ω and ϕ scans (structures **6^{Xyl}**, **13** and **10**; Instituto de Investigaciones Químicas, Sevilla). In both cases data were collected using monochromatic radiation $\lambda(\text{Mo K}\alpha 1) = 0.71073 \text{ \AA}$. The diffraction images collected at the Rigaku instrument were processed and scaled using Rigaku Oxford Diffraction software (CrysAlisPro; Rigaku OD: The Woodlands, TX, 2015), while the ones recorded at the Bruker instrument were reduced (SAINT)^[1] and corrected for Lorentz polarization effects and absorption by multiscan method applied by SADABS.^[2] The structures were solved with SHELXT and was refined against F^2 on all data by full-matrix least squares with SHELXL.³ All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model, unless otherwise noted. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups). In structure **6**, the fluorine of the fluorobenzene is disordered over two positions. The site occupancies were freely refined and fixed near their converged values of 0.70/0.30. Due to the small amount of electron density, the atomic displacement parameter was constrained to the same value of the associated carbon. Structure **6** was solved in P2(1)2(1)2(1) space group and refined as a racemic twin (0.57:0.43). In structure **8^{Cyp}**, $\text{SnClN}(\text{SiMe}_3)_2$ group is disordered over two positions. Nitrogen atoms C5B, C7B, and C8B are common to both models. The site occupancies of the two models were freely refined and converged at nearly equal occupancies. The site occupancies were subsequently fixed at 0.5. A global rigid bond restraint was applied to help the model converge. All disordered hydrogens were placed in geometrically expected positions as riding atoms. In structure **13** the program SQUEEZE was used to compensate for the contribution of disordered solvents, as well as a triflimide anion, contained in voids within the crystal lattice from the diffraction intensities. This procedure was applied to the data file and the submitted model is based on the solvent removed data. Based on the total electron density found in the voids ($672 \text{ e/\AA}^3$), it is likely that one triflimide anion and *ca.* two pentane molecules are present in the unit cell. See "_platon_squeeze_details" in the .cif for more information. In the structure of $[\text{Au}_2(\mu\text{-N}(\text{SiMe}_3)_2)(\text{PMe}_2\text{Ar}^{\text{Xyl2}})_2]$ one xylyl and the triflate groups are disordered in complementing orientations. Their site occupancies were freely refined in linked variables to relative ratios of 0.57/0.43. The minor component is distinguished with the suffix "B". Similarity restraints were applied to all disordered, chemically equivalent bond distances. The structure of compound **10** contains a high degree of disorder that result from the rotation of the 36 *tert*-butyl groups of the phosphine ligands bound to Pt centres, as well as the four phosphonium cations present in the asymmetric unit. In contrast, the position of the heavier atoms (Pt, Sn, P, Cl) was located with very minor deviations, as evinced by the almost identical geometric parameters (bond distances and angles) between the four molecules of **10** has been refined as a 2-component inversion twin. In addition, the program SQUEEZE was used to compensate for the contribution of disordered solvent molecules by the same approach mentioned above. Based on the total electron density found in the voids ($838 \text{ e/\AA}^3$), it is likely that *ca.* 20 dichloromethane molecules are present in the unit cell. The full numbering scheme of all the reported structures can be found in the full details of the X-ray structure determination (CIF), which is included as Supporting Information.

Table S1. Crystal data and structure refinement for compounds **6**, **8^{Cyp}** and **[Au₂(μ-N(SiMe₃)₂)(Pme₂Ar^{Xyl2})₂]**.

	6	8^{Cyp}	[Au₂(μ-N(SiMe₃)₂)(Pme₂Ar^{Xyl2})₂]
formula	C ₃₈ H ₄₈ AuCl ₃ FgeP	C ₄₄ H ₇₅ AuClN ₂ PSi ₄ Sn	C ₅₄ H ₇₂ Au ₂ NP ₂ Si ₂ ·C ₂ F ₆ NO ₄ S ₂
Radiation type	Cu Kα	Mo Kα	Mo Kα
fw	930.64	1126.49	1527.32
cryst.size, mm	0.20 × 0.20 × 0.05	0.20 × 0.20 × 0.04	0.20 × 0.20 × 0.08
crystal system	Monoclinic	Monoclinic	Triclinic
space group	Cc	P2 ₁ /c	P-1
a, Å	13.6626 (3)	14.4337 (7)	12.3889 (2)
b, Å	22.0555 (5)	17.5668 (10)	14.0629 (3)
c, Å	12.6148 (3)	20.4495 (10)	19.0624 (3)
α, deg	90	90	82.064 (2)
β, deg	92.166 (2)	105.385 (5)	78.105 (2)
γ, deg	90	90	72.256 (2)
V, Å ³	3798.57 (15)	4999.2 (5)	3085.10 (10)
T, K	93	93	93
Z	4	4	2
ρ _{calc} , g cm ⁻³	1.627	1.497	1.644
μ, mm ⁻¹ (MoKα)	10.70	3.64	4.97
F(000)	1848	2280	1512
absorption corrections	multi-scan, 0.54-1.00	multi-scan, 0.38-1.00	multi-scan, 0.59-1.00
θ range, deg	3.8 – 66.5	2.9 – 27.5	2.9 – 27.5
no. of rflns measd	67328	57414	139393
R _{int}	0.057	0.060	0.053
no. of rflns unique	6706	11452	14144
no. of params / restraints	419 / 2	562 / 540	850 / 90
R ₁ (I > 2σ(I)) ^a	0.020	0.059	0.019
R ₁ (all data)	0.022	0.079	0.024
wR ₂ (I > 2σ(I))	0.046	0.121	0.044
wR ₂ (all data)	0.046	0.127	0.045
Diff.Fourier.peaks min/max, eÅ ⁻³	0.59 / -0.72	2.23 / -4.76	1.09 / -0.60
CCDC number	1897306	1897307	1897308

Table S2. Crystal data and structure refinement for compounds **6^{xyI}**, **10** and **13**.

	6^{xyI}	10	13
formula	C ₂₄ H ₂₇ AuCl ₃ GeP	C ₃₆ H ₇₈ Cl ₇ P ₃ Pt ₂ Sn ₃	C ₁₈₀ H ₂₈₂ Au ₃ F ₁₂ N ₂ O ₈ P ₈ Pt ₂ S ₄
Radiation type	Mo K α	Mo K α	Mo K α
fw	722.33	1598.29	4187.14
cryst.size, mm	0.20 $\times$ 0.17 $\times$ 0.12	0.40 $\times$ 0.40 $\times$ 0.25	0.20 $\times$ 0.10 $\times$ 0.08
crystal system	Orthorhombic	Orthorhombic	Triclinic
space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	P-1
<i>a</i> , Å	11.9826 (10)	<i>a</i> = 15.0060 (8) Å	12.2275 (4)
<i>b</i> , Å	12.8906 (11)	<i>b</i> = 15.1859 (7) Å	14.0212 (4)
<i>c</i> , Å	16.9382 (14)	<i>c</i> = 29.4759 (16) (6) Å	32.6312 (9)
α , deg	90	90	90.778 (1)
β , deg	90	90	97.949 (2)
γ , deg	90	90	112.880 (1)
<i>V</i> , Å ³	2616.3 (4)	6717.0 (6) Å ³	5090.8 (3)
<i>T</i> , K	193	193	193
<i>Z</i>	4	4	1
ρ_{calc} , g cm ⁻³	1.834	1.580	1.366
μ , mm ⁻¹ (MoK α)	7.13	5.62	3.69
<i>F</i> (000)	1392	3056	2125
absorption corrections	multi-scan, 0.19-0.75	Multi-scan, 0.24-0.14	multi-scan, 0.62-0.75
ϑ range, deg	2.6 – 30.5	1.57 – 25.0	1.7 – 25.0
no. of rflns measd	146074	52412	86632
<i>R</i> _{int}	0.048	0.153	0.029
no. of rflns unique	8002	11487	17919
no. of params / restraints	287 / 0	486 / 432	1026 / 0
<i>R</i> ₁ (<i>I</i> > 2 σ (<i>I</i>)) ^a	0.017	0.065	0.037
<i>R</i> ₁ (all data)	0.018	0.097	0.045
<i>wR</i> ₂ (<i>I</i> > 2 σ (<i>I</i>))	0.041	0.150	0.104
<i>wR</i> ₂ (all data)	0.042	0.159	0.114
Diff.Fourier.peaks min/max, eÅ ⁻³	-1.41 / 0.79	3.11 / -3.04	-3.04 / 5.87
CCDC number	1897309	1897311	1897310

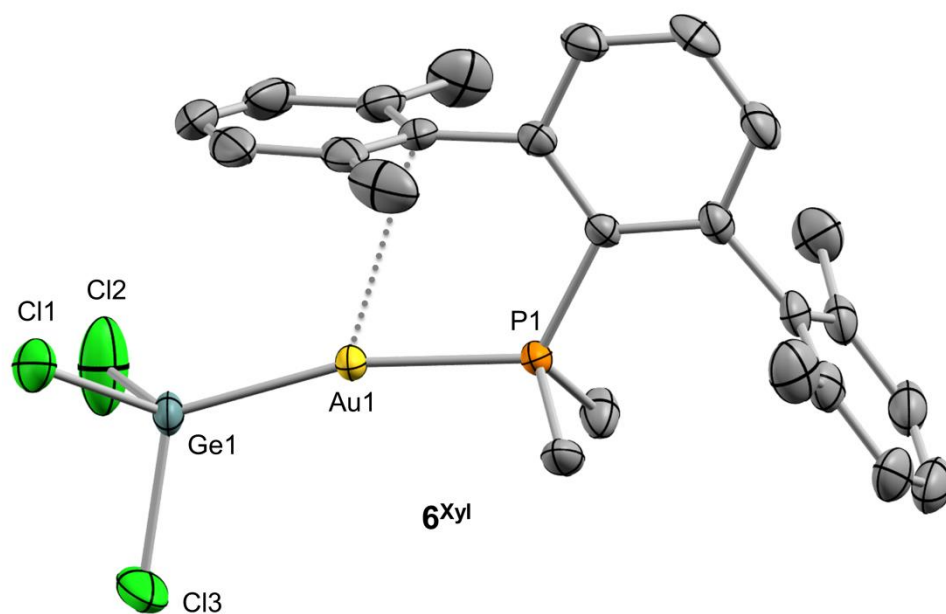


Figure S1. ORTEP diagram of compound 6^{Xyl} ; hydrogen atoms have been excluded for clarity and thermal ellipsoids are set at 50 % probability.

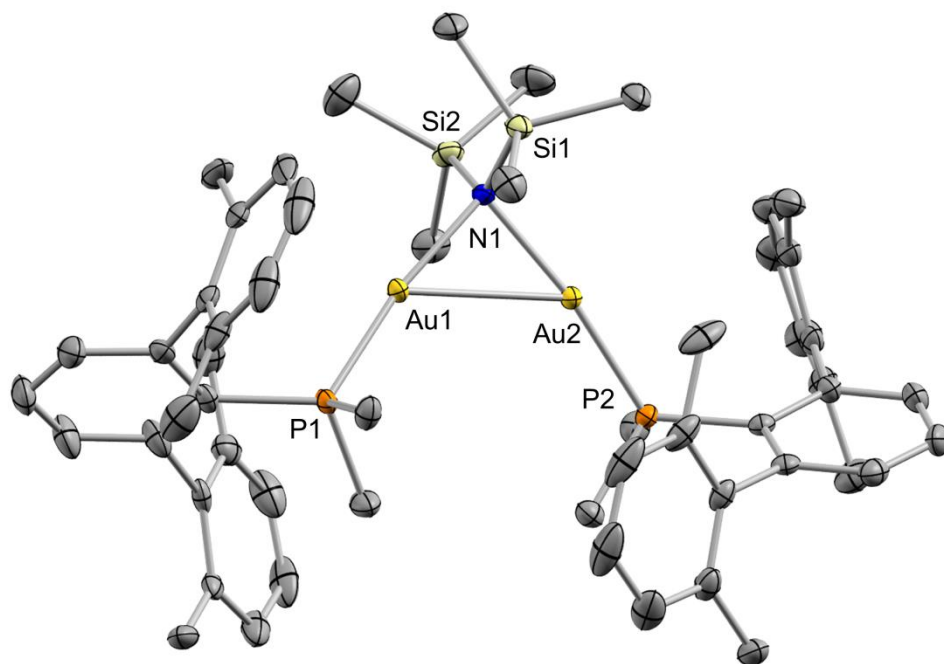


Figure S2. ORTEP diagram of compound $[Au_2(\mu-N(SiMe_3)_2)(PMe_2Ar^{Xyl2})_2]$; hydrogen atoms and the triflimide counteranion have been excluded for clarity. Thermal ellipsoids are set at 50 % probability.

3. Computational details

Calculations were performed at the DFT level with the Gaussian 09 (Revision B.01) program⁴. The ω B97XD⁵ functional was used throughout the computational study, and geometry optimizations were carried out in the gas phase without geometry constraints, using the 6-31G(d,p)⁶ basis set to represent the C, H, P and Cl atoms and the Stuttgart/Dresden Effective Core Potential and its associated basis set (SDD)⁷ to describe the Pt and Sn atoms. The stationary points and its nature as minima were characterized by vibrational analysis. The NMR shieldings were calculated with the Gauge-Independent Atomic Orbital (GIAO)⁸ method at the ω B97XD/6-311+G(2d,p)// ω B97XD/6-31G(d,p) level. The localized molecular orbital study was carried out following the Pipek-Mezey criterion.⁹ The bonding was also investigated by means of the quantum theory of atoms in molecules (QTAIM).¹⁰ The topological analysis of the calculated electron densities was carried out using the Multiwfn program¹¹. The Natural Bond Orbital analysis was performed using the NBOPro 6.0 program.¹²

Table S3. NBOs involved in sigma donation from the Sn atoms to Pt(2).

NBO	Occupancy	Type	Atom	Composition
78	1.54611	LP (1)	Sn 1	s(72.05%)p 0.39(27.95%)
98	1.53720	LP (1)	Sn 7	s(68.40%)p 0.46(31.60%)
109	1.47301	LP (1)	Sn 91	s(57.88%)p 0.73(42.12%)
200	0.35357	LV (1) (non-Lewis)	Pt 6	s(48.88%)p 0.97(47.22%)d 0.08(3.90%)

Table S4. Second Order Perturbation Theory analysis of Fock matrix in NBO basis regarding to the NBOs involved in sigma donation from the Sn atoms to Pt(2).

Donor (L) NBO	Acceptor (NL) NBO	kcal/mol
78. LP (1)Sn 1	200. LV (1)Pt 6	136.27
98. LP (1)Sn 7	200. LV (1)Pt 6	160.06
109. LP (1)Sn 91	200. LV (1)Pt 6	341.23

Table S5. NBOs corresponding to LPs of Pt(2) and a BD* corresponding to Pt(1)-P(1).

NBO	Occupancy	Type	Atoms	Composition
93	1.96101	LP (1)	Pt 6	s(0.00%)p 0.00(0.01%)d 1.00(99.99%)
94	1.95249	LP (2)	Pt 6	s(0.00%)p 1.00(0.02%)d99.99(99.98%)
95	1.95182	LP (3)	Pt 6	s(0.14%)p 0.09(0.01%)d99.99(99.85%)
96	1.94530	LP (4)	Pt 6	s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
97	1.76950	LP (5)	Pt 6	s(1.34%)p 0.04(0.05%)d73.68(98.61%)
205	0.40412	BD*(1) (non-Lewis)	Pt 5- P 12	(81.88%) 0.9049*Pt 5 s(95.43%)p 0.01(0.64%)d 0.04(3.93%) (18.12%) -0.4256* P 12 s(31.91%)p 2.13(67.97%)d 0.00(0.11%)

Table S6. Second Order Perturbation Theory analysis of Fock matrix in NBO basis regarding to the NBOs involved in the Pt-Pt interaction.

Donor (L) NBO	Acceptor (NL) NBO	kcal/mol
97. LP (5)Pt 6	205. BD*(1)Pt 5- P 12	16.90

Table S7. NBOs corresponding to LPs of Pt(1) and LVs corresponding to the Sn atoms of the SnCl₂ units.

NBO	Occupancy	Type	Atoms	Composition
88	1.97142	LP (1)	Pt 5	s(0.15%)p 0.10(0.01%)d99.99(99.84%)
89	1.95868	LP (2)	Pt 5	s(0.03%)p 0.20(0.01%)d99.99(99.96%)
90	1.95719	LP (3)	Pt 5	s(0.04%)p 0.23(0.01%)d99.99(99.95%)
91	1.87229	LP (4)	Pt 5	s(0.01%)p15.89(0.18%)d99.99(99.81%)
92	1.81202	LP (5)	Pt 5	s(3.67%)p 0.02(0.08%)d26.24(96.25%)
199	0.44555	LV (1) (non-Lewis)	Sn 1	s(0.04%)p99.99(99.96%)
201	0.42310	LV (1) (non-Lewis)	Sn 7	s(0.61%)p99.99(99.39%)

Table S8. Second Order Perturbation Theory analysis of Fock matrix in NBO basis regarding to the NBOs involved in the Pt-Sn back-donation.

Donor (L) NBO	Acceptor (NL) NBO	kcal/mol
91. LP (4)Pt 5	199. LV (1)Sn 1	7.91
91. LP (4)Pt 5	201. LV (1)Sn 7	12.71
92. LP (5)Pt 5	201. LV (1)Sn 7	42.88
92. LP (5)Pt 5	199. LV (1)Sn 1	39.34

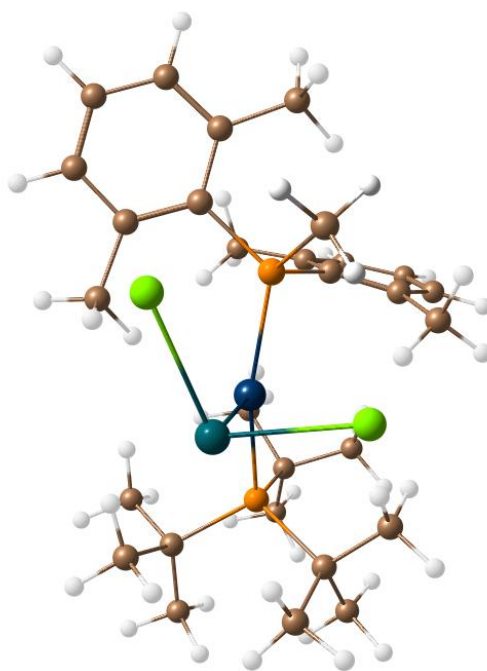


Figure S3. Calculated minimum-energy conformer of complex **15**.

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Complex 10. E (RwB97XD) = -5100.55508957

Sn	0.008698000	-1.182720000	-1.885195000
Cl	0.635829000	-0.630505000	-4.184563000
Cl	0.388375000	-3.602477000	-2.088936000
Cl	0.296841000	3.452848000	-2.116732000
Pt	1.416329000	0.083778000	0.020584000
Pt	-1.349982000	0.019977000	0.021265000
Sn	0.013711000	-1.106773000	1.981028000
Cl	0.528468000	-0.301152000	4.236953000
Cl	0.603181000	-3.449860000	2.398810000
Cl	0.954990000	3.584037000	1.536070000
P	-3.642438000	-0.465574000	-0.010399000
P	3.729596000	-0.050354000	-0.024348000
C	-3.953651000	-2.358625000	-0.244830000
C	-4.540524000	0.437435000	-1.451703000
C	-4.476005000	0.057253000	1.641772000
C	4.459547000	0.296547000	1.712411000
C	4.360534000	1.280517000	-1.248455000
C	4.341224000	-1.771164000	-0.607339000
C	-4.090429000	-0.915750000	2.770769000
H	-4.549585000	-1.900526000	2.673877000
H	-3.007008000	-1.038932000	2.845536000
H	-4.430622000	-0.487441000	3.720228000
C	-3.908374000	1.426426000	2.067745000
H	-2.838721000	1.355837000	2.278713000
H	-4.044111000	2.215811000	1.331053000
H	-4.413770000	1.738366000	2.989444000
C	-6.011254000	0.153241000	1.600126000
H	-6.372160000	0.386555000	2.608916000

H	-6.358599000	0.953285000	0.944940000
H	-6.490019000	-0.776750000	1.290027000
C	-2.940777000	-3.162913000	0.596306000
H	-1.926295000	-3.041393000	0.213628000
H	-2.936792000	-2.906008000	1.654804000
H	-3.191491000	-4.226886000	0.516065000
C	-3.681112000	-2.777011000	-1.700874000
H	-4.434362000	-2.422947000	-2.405546000
H	-2.698657000	-2.443281000	-2.041595000
H	-3.673470000	-3.871347000	-1.749131000
C	-5.372104000	-2.832960000	0.122799000
H	-5.460373000	-3.895392000	-0.133593000
H	-5.575179000	-2.746968000	1.191529000
H	-6.156003000	-2.301389000	-0.418666000
C	-5.929565000	-0.113603000	-1.817766000
H	-6.361912000	0.533717000	-2.590008000
H	-5.891614000	-1.122042000	-2.232596000
H	-6.620342000	-0.114635000	-0.972484000
C	-3.638154000	0.387512000	-2.703052000
H	-2.691906000	0.903444000	-2.523946000
H	-3.413843000	-0.622749000	-3.043926000
H	-4.152344000	0.904501000	-3.521681000
C	-4.699141000	1.931064000	-1.123954000
H	-3.759150000	2.397747000	-0.830155000
H	-5.042173000	2.444690000	-2.029284000
H	-5.437058000	2.127758000	-0.344670000
C	3.455592000	1.262935000	-2.498563000
H	3.446756000	0.314103000	-3.030649000
H	2.422349000	1.522836000	-2.252717000
H	3.815194000	2.029495000	-3.194961000
C	4.178741000	2.678831000	-0.628794000
H	3.165979000	2.835445000	-0.247383000
H	4.894129000	2.888859000	0.169037000
H	4.341703000	3.422606000	-1.416716000
C	5.824200000	1.122189000	-1.689859000
H	6.091963000	1.981691000	-2.316039000
H	6.522239000	1.098077000	-0.850513000
H	5.981534000	0.225440000	-2.292792000
C	5.947944000	0.682935000	1.720052000
H	6.124551000	1.644225000	1.233944000
H	6.274088000	0.784978000	2.762028000
H	6.587583000	-0.065007000	1.247323000
C	4.268051000	-0.931671000	2.620736000
H	3.237438000	-1.295102000	2.613744000
H	4.933011000	-1.759619000	2.369511000
H	4.491014000	-0.633119000	3.650823000
C	3.652533000	1.431036000	2.373312000
H	3.685180000	2.373315000	1.831828000
H	2.600667000	1.165095000	2.498483000
H	4.063714000	1.604862000	3.374761000
C	3.508643000	-2.865511000	0.089994000
H	2.442795000	-2.754533000	-0.113210000
H	3.815044000	-3.839453000	-0.308449000
H	3.638278000	-2.897131000	1.169781000
C	5.832243000	-2.044152000	-0.345547000
H	6.090742000	-3.009115000	-0.797476000

H	6.487906000	-1.289612000	-0.784746000
H	6.057926000	-2.119315000	0.719753000
C	4.082062000	-1.941351000	-2.115066000
H	4.264386000	-2.989065000	-2.376994000
H	3.046718000	-1.725819000	-2.386377000
H	4.737410000	-1.328237000	-2.735706000
Sn	-0.625495000	2.561069000	-0.030783000
Cl	-2.330171000	4.314108000	0.289301000

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Complex 15. E (RwB97XD) = -2859.80797720

C	-3.695124000	0.259480000	-0.907671000
C	-2.288450000	2.549100000	0.666262000
C	-3.238682000	-0.004558000	2.170504000
C	-4.202983000	-1.190839000	-0.817045000
H	-4.892913000	-1.356095000	0.012065000
H	-4.743685000	-1.418790000	-1.741757000
H	-3.385770000	-1.912233000	-0.744609000
C	-2.918212000	0.348470000	-2.238389000
H	-3.624726000	0.175671000	-3.058564000
H	-2.446568000	1.315098000	-2.405510000
H	-2.143650000	-0.418800000	-2.303650000
C	-4.922773000	1.183937000	-0.974907000
H	-4.660352000	2.213603000	-1.224023000
H	-5.585658000	0.822516000	-1.769211000
H	-5.498732000	1.190283000	-0.047456000
C	-3.001737000	-1.523933000	2.266668000
H	-3.433572000	-2.092029000	1.444266000
H	-1.931954000	-1.744114000	2.309774000
H	-3.457780000	-1.888915000	3.194104000
C	-4.737305000	0.283395000	2.356018000
H	-5.358293000	-0.272931000	1.651770000
H	-5.032921000	-0.032792000	3.363130000
H	-4.978654000	1.343151000	2.261731000
C	-2.471482000	0.597494000	3.361871000
H	-1.390863000	0.467754000	3.248008000
H	-2.689557000	1.654034000	3.523516000
H	-2.773943000	0.063276000	4.269472000
C	-3.486411000	3.292049000	1.278344000
H	-3.291992000	4.369290000	1.219271000
H	-4.423326000	3.101775000	0.753642000
H	-3.630259000	3.051919000	2.333716000
C	-1.993619000	3.140898000	-0.725453000
H	-1.711524000	4.191695000	-0.596685000
H	-1.149360000	2.639732000	-1.207307000
H	-2.853413000	3.116891000	-1.395913000
C	-1.035227000	2.866860000	1.508940000
H	-0.895356000	3.954023000	1.525170000
H	-1.096658000	2.526562000	2.540350000
H	-0.141744000	2.433021000	1.055441000
P	-2.487220000	0.638005000	0.529607000
Pt	-0.294996000	-0.097598000	0.122802000
P	1.929935000	0.057812000	-0.471383000
Sn	-0.582046000	-2.751751000	-0.361593000
Cl	-0.481435000	-2.595013000	-2.875051000

C1	1.736301000	-3.645304000	0.010818000
C	3.313743000	-0.100702000	0.750131000
C	3.076053000	-0.587271000	2.056411000
C	4.628904000	0.258882000	0.369005000
C	4.152665000	-0.721510000	2.935900000
C	5.669334000	0.113145000	1.288855000
C	5.441873000	-0.380949000	2.562608000
H	3.966317000	-1.101653000	3.935719000
H	6.674856000	0.397488000	0.991776000
H	6.262458000	-0.489497000	3.264849000
C	1.852314000	1.841988000	-1.004977000
C	1.332942000	2.144210000	-2.288746000
C	2.159440000	2.899894000	-0.115091000
C	1.252381000	3.478528000	-2.692683000
C	2.052312000	4.217425000	-0.566335000
C	1.628390000	4.513579000	-1.851856000
H	0.860295000	3.699653000	-3.681294000
H	2.297361000	5.023398000	0.119620000
H	1.555773000	5.544798000	-2.182893000
C	2.549073000	2.719527000	1.335685000
H	1.970698000	1.934120000	1.826917000
H	3.605070000	2.465383000	1.457096000
H	2.362497000	3.650674000	1.876587000
C	0.777808000	1.111702000	-3.243704000
H	1.555905000	0.632040000	-3.843075000
H	0.223645000	0.322590000	-2.727406000
H	0.084456000	1.592287000	-3.938070000
C	1.721424000	-0.971974000	2.598543000
H	0.959478000	-0.208263000	2.408057000
H	1.374582000	-1.902068000	2.140253000
H	1.783501000	-1.130995000	3.677831000
C	5.015527000	0.819011000	-0.982456000
H	5.226413000	0.013881000	-1.692790000
H	4.250796000	1.464187000	-1.417138000
H	5.928135000	1.411948000	-0.886882000
C	2.582035000	-0.918748000	-1.888794000
H	1.760929000	-1.353806000	-2.457783000
H	3.204900000	-0.310212000	-2.542525000
H	3.168474000	-1.735791000	-1.465765000

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Complex 2 (int=ultrafine). E(RwB97XD) = -1749.06522363

Pt	0.000166000	0.015476000	0.002385000
P	-2.297184000	0.001607000	-0.000128000
P	2.297362000	0.001561000	-0.000886000
C	-2.994282000	1.744023000	-0.410288000
C	-2.973643000	-0.524974000	1.719285000
C	-2.745589000	0.626906000	2.715717000
C	-2.119151000	-1.100158000	-2.593225000
C	-2.967329000	-1.234048000	-1.309954000
C	-2.759035000	2.033246000	-1.904399000
C	-4.452211000	-1.092336000	-1.677824000
C	-2.154576000	2.798467000	0.342974000
C	-2.718903000	-2.669156000	-0.809594000
C	-2.114774000	-1.694024000	2.248403000

C	2.976943000	-0.466846000	1.733823000
C	2.133431000	0.258450000	2.804626000
C	-4.480413000	1.971506000	-0.095040000
C	-4.453948000	-0.932712000	1.770384000
C	2.993343000	1.729987000	-0.468907000
C	4.462899000	-0.167945000	1.983513000
C	2.964898000	-1.278186000	-1.269326000
C	2.106107000	-2.557970000	-1.175614000
C	2.769922000	2.691202000	0.713198000
C	2.729560000	-1.967717000	1.973303000
C	2.729105000	-0.736872000	-2.691848000
C	4.445592000	-1.662610000	-1.128971000
C	2.144217000	2.304851000	-1.623301000
C	4.476137000	1.780062000	-0.867818000
H	-1.710882000	0.981925000	2.680461000
H	-2.938594000	0.254283000	3.728548000
H	-3.417446000	1.471178000	2.552093000
H	-1.055189000	-1.216632000	-2.366181000
H	-2.419567000	-1.889567000	-3.293342000
H	-2.248747000	-0.146313000	-3.101694000
H	-1.719813000	1.837971000	-2.186783000
H	-2.964150000	3.094107000	-2.090030000
H	-3.419299000	1.460698000	-2.558279000
H	-4.663583000	-0.153265000	-2.194218000
H	-5.111600000	-1.159700000	-0.810297000
H	-4.727101000	-1.903478000	-2.363327000
H	-1.090511000	2.674490000	0.120515000
H	-2.470562000	3.795952000	0.013230000
H	-2.275499000	2.758448000	1.423995000
H	-1.681654000	-2.801758000	-0.486390000
H	-2.904729000	-3.363455000	-1.637453000
H	-3.385300000	-2.957655000	0.005094000
H	-1.054384000	-1.424378000	2.247397000
H	-2.422437000	-1.914421000	3.278093000
H	-2.225725000	-2.610223000	1.670898000
H	2.437765000	-0.105872000	3.793652000
H	2.263153000	1.339205000	2.800965000
H	1.068955000	0.048732000	2.663865000
H	-4.685115000	1.946255000	0.977504000
H	-4.770776000	2.967066000	-0.452896000
H	-5.132729000	1.245039000	-0.583596000
H	-4.733326000	-1.124399000	2.813719000
H	-4.649838000	-1.852078000	1.213986000
H	-5.120608000	-0.155935000	1.390617000
H	4.742154000	-0.555723000	2.971120000
H	4.674480000	0.903634000	1.990519000
H	5.118966000	-0.639743000	1.249488000
H	1.045137000	-2.320252000	-1.297139000
H	2.222109000	-3.090484000	-0.232992000
H	2.409428000	-3.240793000	-1.978948000
H	2.974804000	3.713451000	0.374090000
H	3.436326000	2.493778000	1.554675000
H	1.733316000	2.655122000	1.062450000
H	2.926760000	-2.188956000	3.028810000
H	3.388596000	-2.607395000	1.383694000
H	1.689552000	-2.236064000	1.762640000

H	1.694143000	-0.406063000	-2.823278000
H	3.400869000	0.082646000	-2.952914000
H	2.916662000	-1.546123000	-3.407422000
H	5.112469000	-0.799101000	-1.163486000
H	4.645588000	-2.211016000	-0.205636000
H	4.720792000	-2.323971000	-1.959812000
H	2.460979000	3.338900000	-1.807642000
H	1.082546000	2.303405000	-1.358259000
H	2.254698000	1.757667000	-2.557915000
H	4.766644000	2.826326000	-1.022846000
H	5.134973000	1.368044000	-0.100813000
H	4.671917000	1.252958000	-1.804084000

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Pt (SnCl₂) (PCy₃)₂. E(RwB97XD) = -3137.47045352

Pt	0.056204000	-0.068347000	-0.312492000
Sn	0.145447000	-2.760301000	-0.314333000
Cl	2.227056000	-3.524277000	0.866327000
Cl	-1.337744000	-3.244627000	1.647722000
P	2.265597000	0.545222000	0.002622000
P	-2.251400000	0.217794000	-0.317940000
C	3.639592000	-0.595695000	-0.471219000
H	3.483014000	-1.458300000	0.186738000
C	5.064957000	-0.074650000	-0.245836000
H	5.265303000	0.763617000	-0.927029000
H	5.187753000	0.300939000	0.776350000
C	6.085244000	-1.185624000	-0.519993000
H	7.100429000	-0.801836000	-0.371175000
H	5.937063000	-1.992487000	0.209152000
C	5.928968000	-1.744489000	-1.936801000
H	6.636144000	-2.564728000	-2.098489000
H	6.185188000	-0.959416000	-2.662318000
C	4.496840000	-2.220617000	-2.193833000
H	4.269385000	-3.073735000	-1.542431000
H	4.390573000	-2.567229000	-3.227399000
C	3.479189000	-1.111128000	-1.910363000
H	2.461118000	-1.483659000	-2.070340000
H	3.627449000	-0.288679000	-2.625266000
C	2.524981000	0.940347000	1.798570000
H	3.504578000	1.426016000	1.903676000
C	1.437437000	1.906571000	2.304323000
H	0.459914000	1.434793000	2.142534000
H	1.435392000	2.837717000	1.726552000
C	1.602255000	2.214434000	3.794104000
H	2.552386000	2.742315000	3.956087000
H	0.804425000	2.891355000	4.119112000
C	1.587702000	0.928412000	4.622254000
H	1.727363000	1.154778000	5.684545000
H	0.604002000	0.448884000	4.522916000
C	2.667445000	-0.039186000	4.135331000
H	2.626957000	-0.975684000	4.700079000
H	3.657133000	0.402122000	4.319368000
C	2.517931000	-0.345653000	2.643194000
H	1.572757000	-0.878369000	2.475743000
H	3.311550000	-1.027897000	2.326687000

C	2.618484000	2.119223000	-0.950739000
H	3.089221000	1.752357000	-1.874608000
C	1.335607000	2.862244000	-1.362988000
H	0.656106000	2.171354000	-1.875945000
H	0.812878000	3.208770000	-0.462326000
C	1.642623000	4.060350000	-2.264787000
H	0.712894000	4.586606000	-2.509852000
H	2.057264000	3.694344000	-3.214087000
C	2.643303000	5.016368000	-1.612916000
H	2.882806000	5.839604000	-2.294027000
H	2.185062000	5.464918000	-0.720655000
C	3.918198000	4.275359000	-1.203208000
H	4.613307000	4.958405000	-0.703736000
H	4.428770000	3.905376000	-2.102782000
C	3.603351000	3.092865000	-0.280714000
H	3.162918000	3.480696000	0.645833000
H	4.528347000	2.584030000	0.001862000
C	-2.442853000	2.036615000	-0.739317000
H	-1.718298000	2.165565000	-1.556970000
C	-3.806676000	2.508507000	-1.270727000
H	-4.123520000	1.905458000	-2.126791000
H	-4.573446000	2.389873000	-0.496160000
C	-3.737575000	3.978866000	-1.702557000
H	-3.050399000	4.064458000	-2.555861000
H	-4.720859000	4.305378000	-2.057519000
C	-3.248152000	4.886891000	-0.572858000
H	-3.986186000	4.881546000	0.240665000
H	-3.171739000	5.921286000	-0.924009000
C	-1.900553000	4.405536000	-0.031738000
H	-1.576712000	5.032134000	0.806373000
H	-1.137636000	4.505934000	-0.816386000
C	-1.975593000	2.943122000	0.412406000
H	-1.004524000	2.607730000	0.791186000
H	-2.684051000	2.864885000	1.246249000
C	-3.061326000	-0.154286000	1.303595000
H	-3.105873000	-1.251241000	1.283965000
C	-2.177479000	0.186524000	2.517227000
H	-1.187506000	-0.260185000	2.379418000
H	-2.039105000	1.271459000	2.601333000
C	-2.812028000	-0.347628000	3.803587000
H	-2.818476000	-1.443798000	3.757878000
H	-2.192173000	-0.069352000	4.663189000
C	-4.240009000	0.172425000	3.986072000
H	-4.685365000	-0.249087000	4.893377000
H	-4.215430000	1.263021000	4.122772000
C	-5.109564000	-0.159691000	2.770384000
H	-6.117857000	0.249412000	2.897888000
H	-5.214969000	-1.249342000	2.685893000
C	-4.488389000	0.381777000	1.477900000
H	-4.468771000	1.478444000	1.526928000
H	-5.114078000	0.111855000	0.618797000
C	-3.304477000	-0.624318000	-1.596102000
H	-4.271280000	-0.104317000	-1.610272000
C	-2.642907000	-0.467473000	-2.976974000
H	-2.480333000	0.591834000	-3.208017000
H	-1.648347000	-0.932789000	-2.941719000

C	-3.477219000	-1.121630000	-4.080667000
H	-4.434493000	-0.590415000	-4.175747000
H	-2.963070000	-1.019849000	-5.042193000
C	-3.746788000	-2.594610000	-3.768415000
H	-4.368053000	-3.042783000	-4.550857000
H	-2.794460000	-3.142019000	-3.765160000
C	-4.418610000	-2.747967000	-2.402659000
H	-4.578645000	-3.805782000	-2.171173000
H	-5.410592000	-2.276299000	-2.433576000
C	-3.588594000	-2.101766000	-1.289283000
H	-2.644277000	-2.649340000	-1.189059000
H	-4.108373000	-2.208539000	-0.332808000

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Pt (SnCl₂) (PCy₃) (IMes) . E (RwB97XD) = -3014.39538595

Pt	0.107701000	-0.265057000	-0.158337000
P	-1.312580000	1.559304000	-0.208886000
Cl	1.825131000	-0.672537000	3.290703000
Sn	2.101888000	0.852645000	1.299233000
Cl	1.059059000	2.865196000	2.450027000
N	0.261810000	-3.255287000	-0.194271000
N	2.243950000	-2.534194000	-0.569540000
C	0.982544000	-2.105703000	-0.290395000
C	1.054162000	-4.371576000	-0.401981000
H	0.649712000	-5.369664000	-0.361235000
C	2.303280000	-3.916990000	-0.638842000
H	3.224501000	-4.435044000	-0.847659000
C	3.367616000	-1.672255000	-0.787385000
C	4.392761000	-1.649976000	0.166368000
C	5.449201000	-0.763750000	-0.040967000
H	6.246386000	-0.722181000	0.696575000
C	5.494342000	0.082000000	-1.147954000
C	4.466940000	0.004154000	-2.087050000
H	4.499669000	0.642010000	-2.967087000
C	3.394674000	-0.872552000	-1.935799000
C	4.356824000	-2.530293000	1.388739000
H	5.116666000	-2.215003000	2.106054000
H	4.549428000	-3.578503000	1.136296000
H	3.387416000	-2.475301000	1.892291000
C	6.613224000	1.077565000	-1.311610000
H	6.359599000	2.021508000	-0.817474000
H	6.802146000	1.295359000	-2.366102000
H	7.541295000	0.710861000	-0.865356000
C	2.305186000	-0.925745000	-2.973724000
H	1.447205000	-0.323605000	-2.650993000
H	1.943498000	-1.946526000	-3.128804000
H	2.667208000	-0.535617000	-3.927940000
C	-1.166696000	-3.302426000	-0.058922000
C	-1.926023000	-3.466448000	-1.221032000
C	-3.311604000	-3.544181000	-1.088170000
H	-3.918691000	-3.672897000	-1.980876000
C	-3.931924000	-3.418249000	0.153541000
C	-3.135629000	-3.232879000	1.284499000
H	-3.608628000	-3.127883000	2.257849000
C	-1.745198000	-3.183194000	1.208686000

C	-1.270122000	-3.485057000	-2.576912000
H	-0.776336000	-2.524523000	-2.767858000
H	-2.008906000	-3.651347000	-3.363906000
H	-0.504179000	-4.262097000	-2.657285000
C	-5.433586000	-3.440831000	0.276920000
H	-5.754842000	-4.077860000	1.106027000
H	-5.905094000	-3.808730000	-0.637913000
H	-5.820057000	-2.433744000	0.469782000
C	-0.898824000	-2.985197000	2.433263000
H	-0.124073000	-3.754003000	2.513648000
H	-1.508841000	-3.015250000	3.338321000
H	-0.379828000	-2.022575000	2.402829000
C	-0.593776000	3.197878000	-0.732913000
H	-0.207632000	3.595186000	0.215621000
C	-1.586208000	4.220022000	-1.309345000
H	-1.990691000	3.853761000	-2.262515000
H	-2.437919000	4.357780000	-0.638380000
C	-0.901316000	5.570802000	-1.545568000
H	-1.618379000	6.280142000	-1.973450000
H	-0.584866000	5.983281000	-0.578558000
C	0.319699000	5.429371000	-2.456588000
H	0.814759000	6.398413000	-2.580694000
H	-0.011094000	5.112261000	-3.455771000
C	1.301345000	4.394935000	-1.900928000
H	2.149589000	4.269914000	-2.583020000
H	1.709155000	4.753155000	-0.946411000
C	0.618326000	3.044766000	-1.670529000
H	1.332748000	2.327795000	-1.254593000
H	0.301603000	2.628059000	-2.635316000
C	-2.662168000	1.170680000	-1.432008000
H	-3.346276000	2.030480000	-1.453460000
C	-3.454205000	-0.078019000	-1.007536000
H	-2.761419000	-0.922514000	-0.911190000
H	-3.903939000	0.058540000	-0.021144000
C	-4.544987000	-0.428421000	-2.021477000
H	-5.072343000	-1.330529000	-1.694382000
H	-5.288682000	0.379885000	-2.052077000
C	-3.959246000	-0.631332000	-3.418198000
H	-3.281637000	-1.496020000	-3.396902000
H	-4.749988000	-0.861647000	-4.140350000
C	-3.176382000	0.605840000	-3.858468000
H	-3.868762000	1.452446000	-3.963286000
H	-2.723714000	0.445111000	-4.843067000
C	-2.087534000	0.968988000	-2.845594000
H	-1.564188000	1.868227000	-3.181510000
H	-1.337314000	0.166070000	-2.809148000
C	-2.163548000	1.897029000	1.418282000
H	-1.479270000	2.600174000	1.909394000
C	-2.184382000	0.629214000	2.295092000
H	-2.754548000	-0.169432000	1.801207000
H	-1.163558000	0.253039000	2.409139000
C	-2.780848000	0.910244000	3.674956000
H	-2.822758000	-0.021086000	4.250300000
H	-2.109080000	1.586897000	4.218382000
C	-4.168485000	1.544305000	3.571525000
H	-4.569301000	1.757134000	4.568459000

H	-4.860570000	0.833152000	3.097243000
C	-4.114840000	2.825041000	2.737583000
H	-3.477542000	3.559099000	3.247957000
H	-5.110963000	3.273400000	2.651681000
C	-3.549832000	2.557642000	1.337771000
H	-4.252637000	1.913012000	0.795947000
H	-3.498545000	3.498773000	0.782912000

17

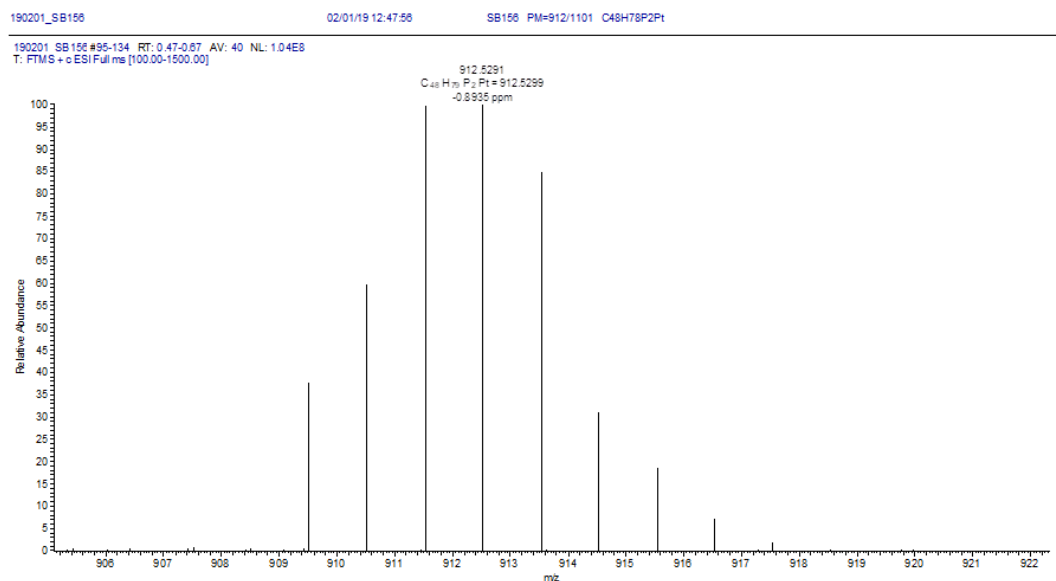
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H	1.557873000	-1.853359000	0.622877000
H	-0.103344000	-2.446632000	0.501679000
H	0.837819000	-2.148908000	-0.965459000
Si	0.000181000	-0.000179000	-0.000510000
C	-0.323584000	0.595611000	1.759390000
H	-0.690959000	1.627194000	1.766633000
H	-1.073973000	-0.028037000	2.256362000
H	0.589187000	0.562378000	2.363351000
C	1.294100000	1.107705000	-0.810213000
H	1.499004000	0.792147000	-1.838532000
H	0.958180000	2.149464000	-0.842039000
H	2.239397000	1.079360000	-0.258167000
C	-1.602170000	0.073662000	-0.992505000
H	-1.444548000	-0.250416000	-2.026480000
H	-2.368474000	-0.574031000	-0.553971000
H	-2.003893000	1.091985000	-1.020166000

4. High resolution mass spectra of compounds 14 and 15



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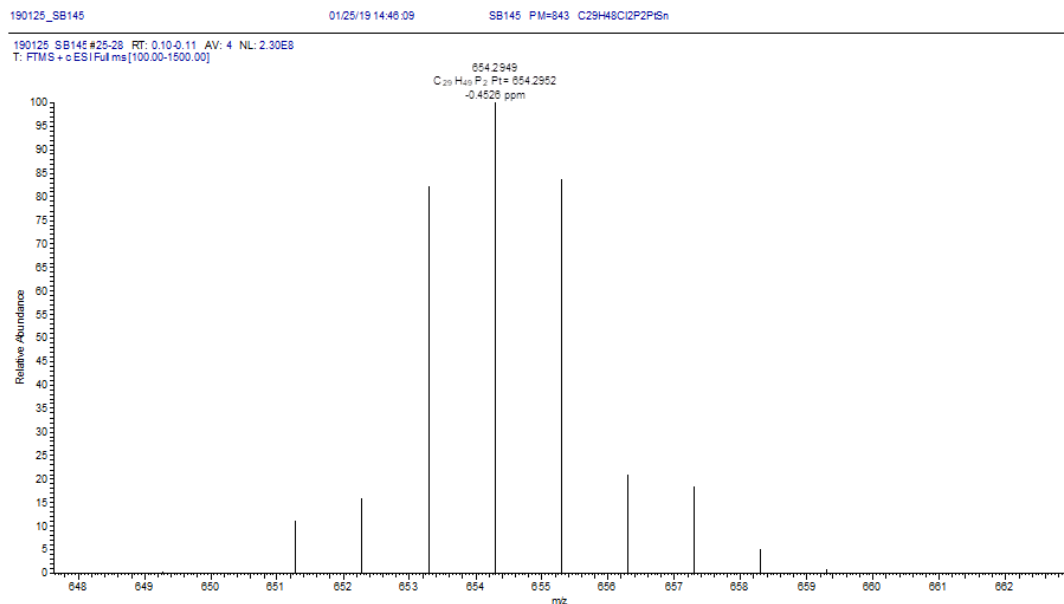


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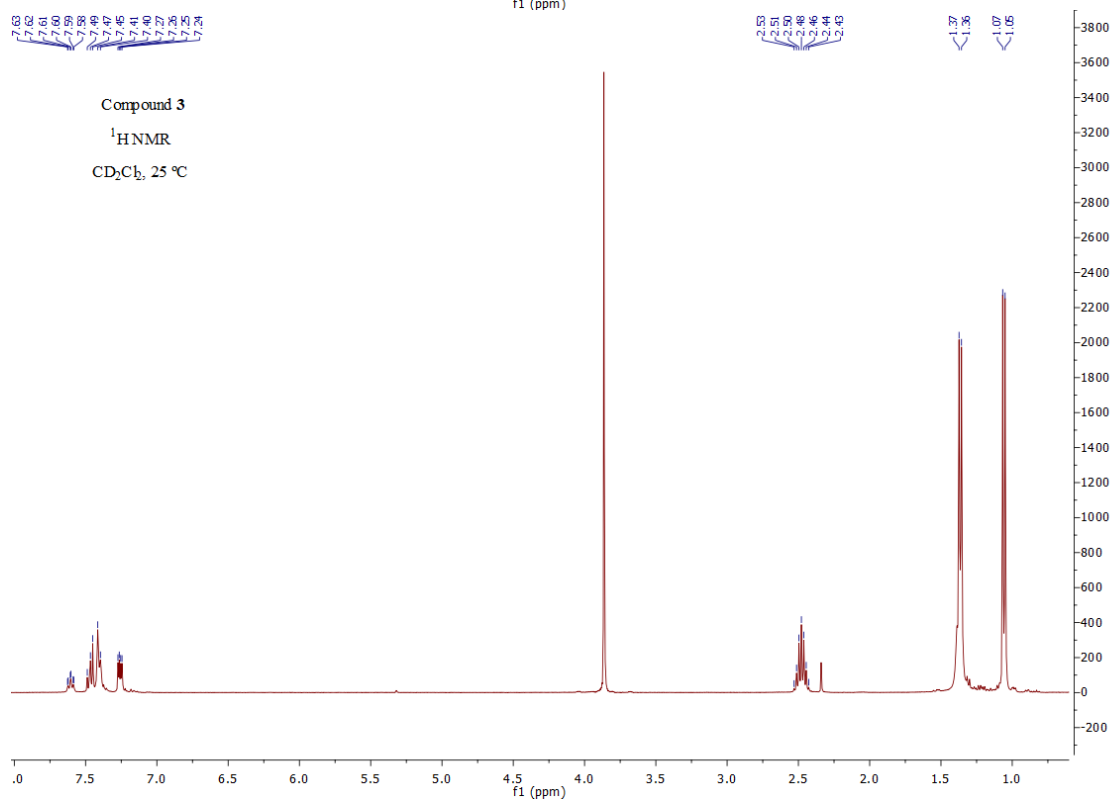
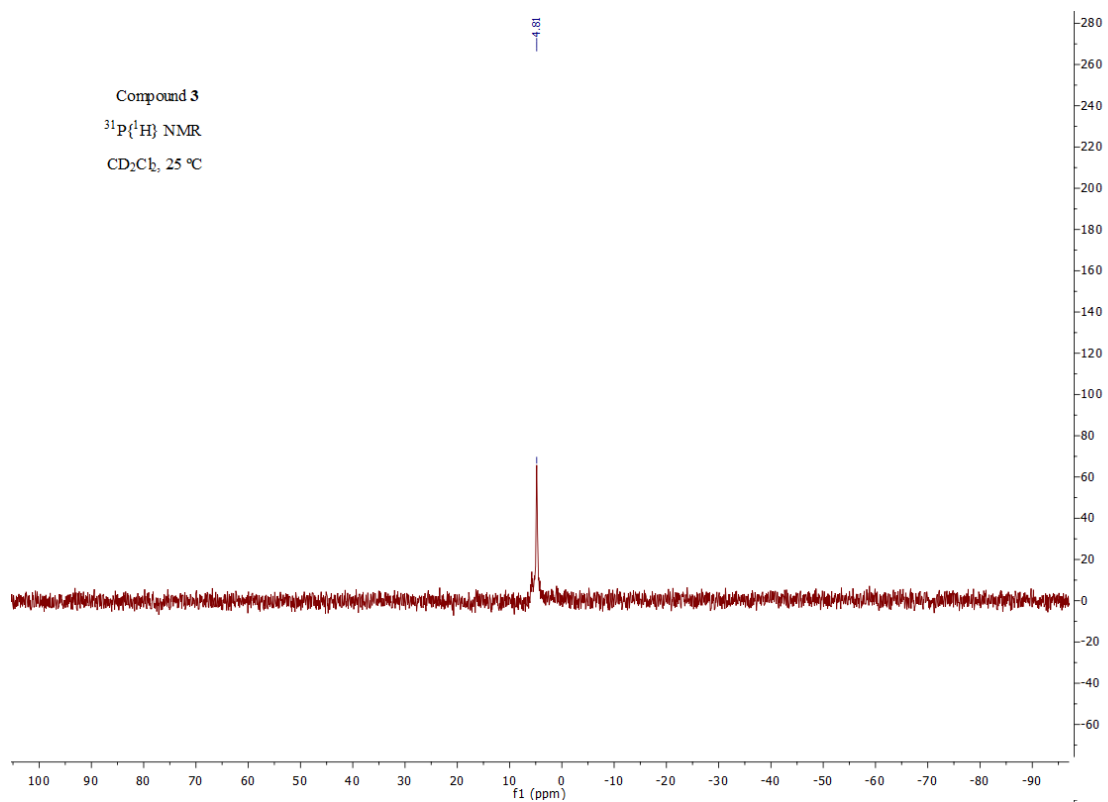


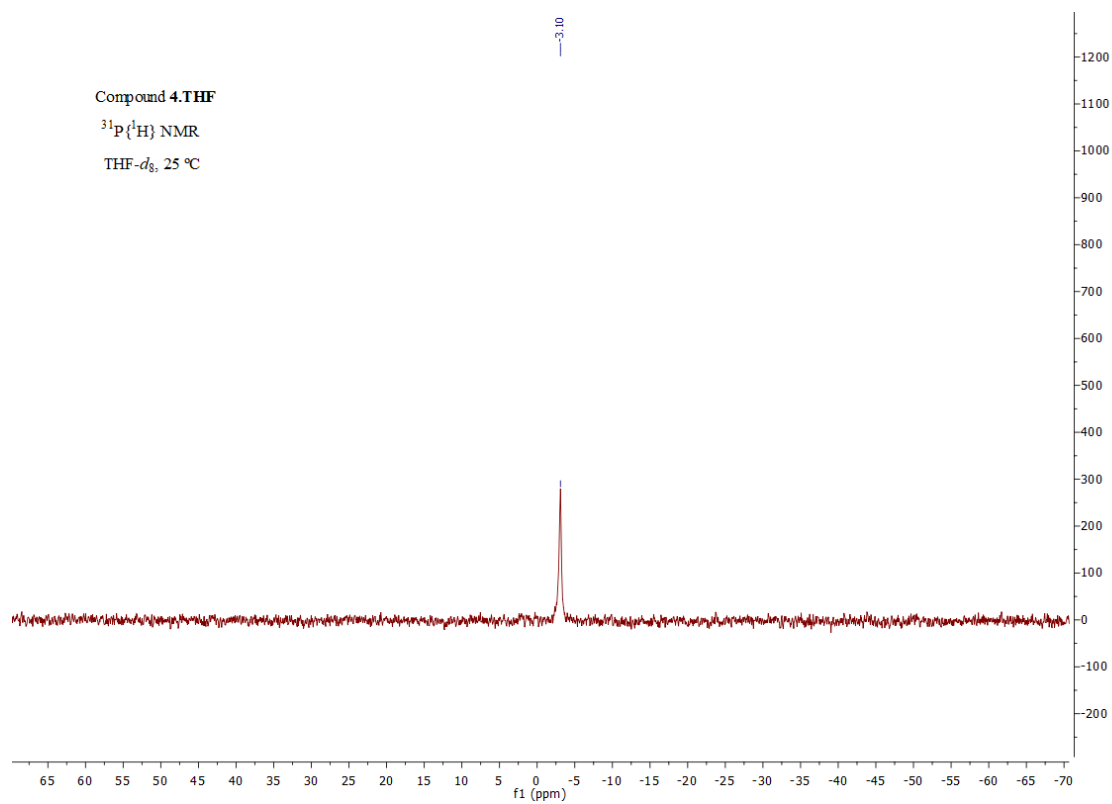
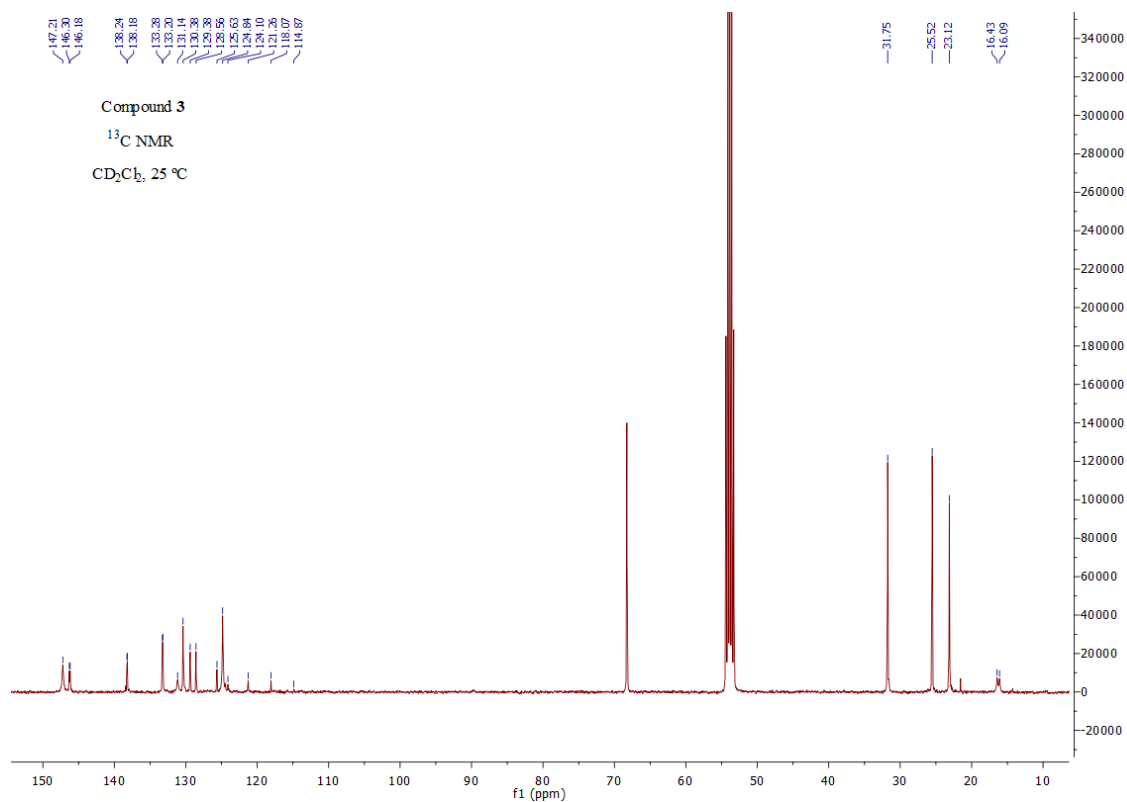
SGIEspectrometría de Masas
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 PGC07FT06-EPM
 Rev.: 01

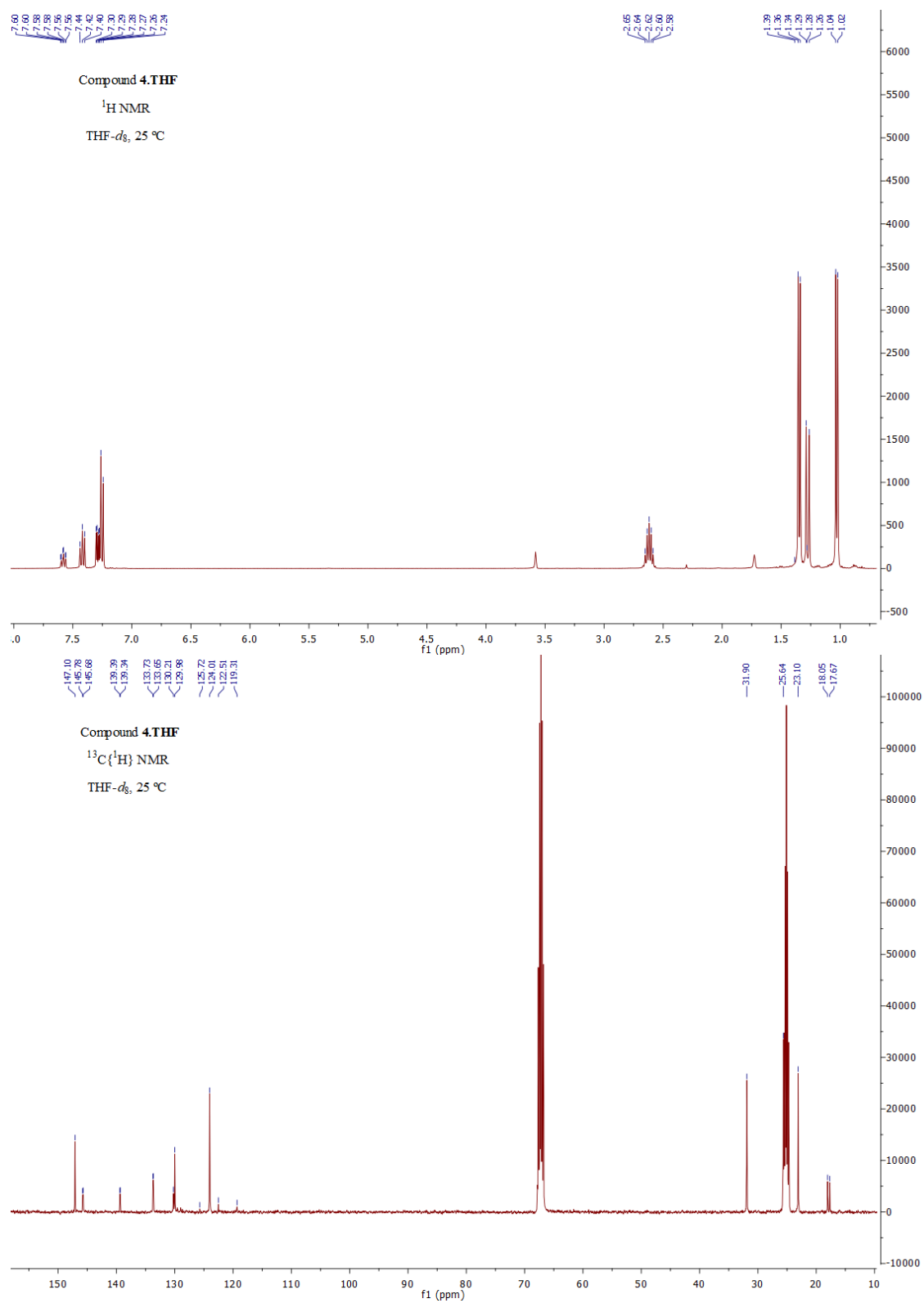
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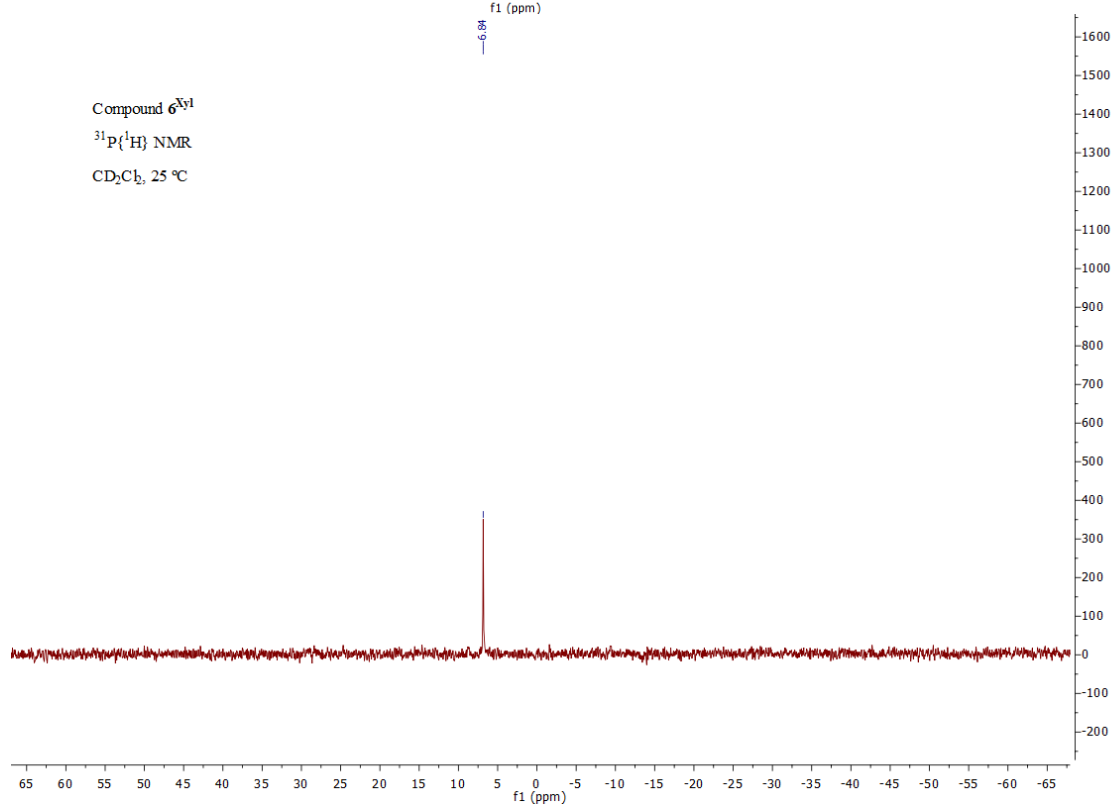
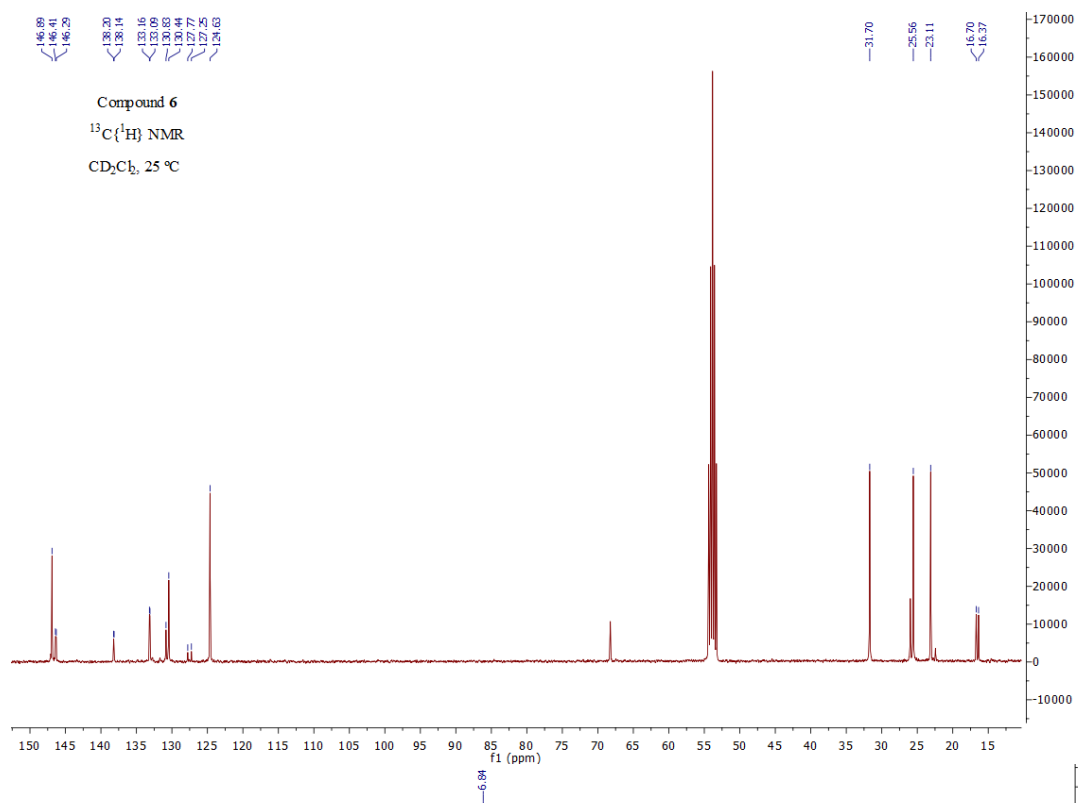


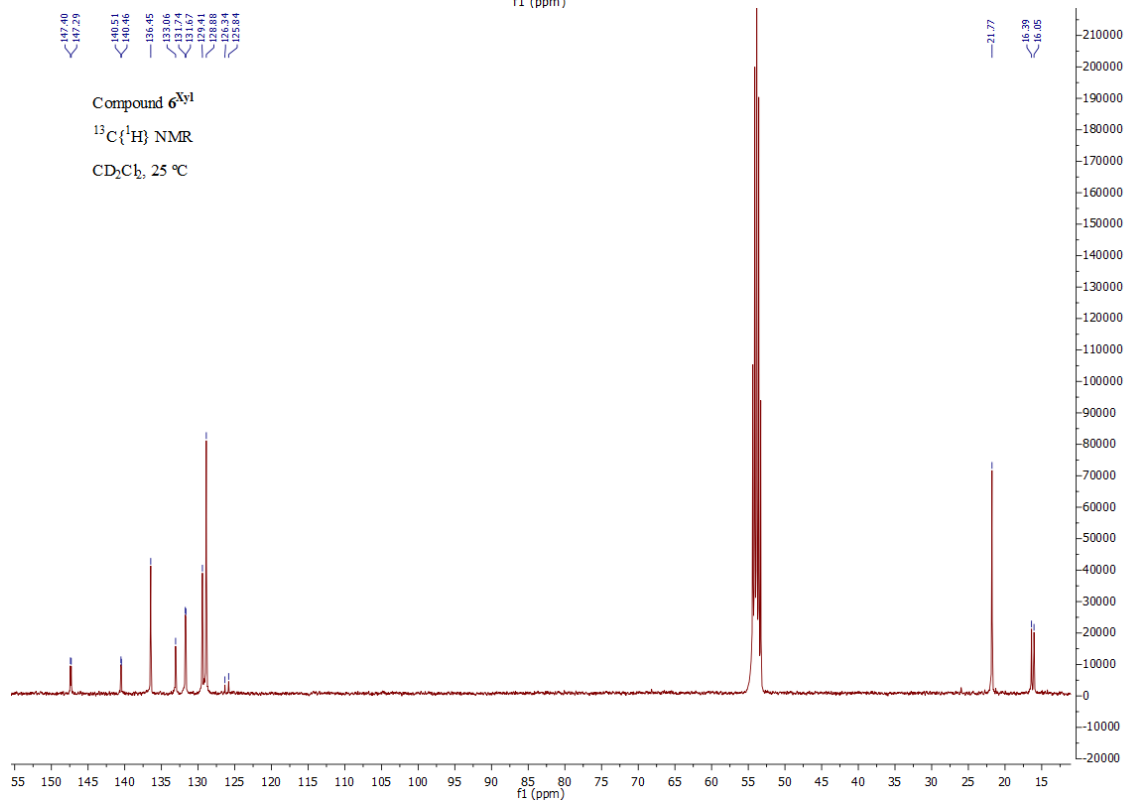
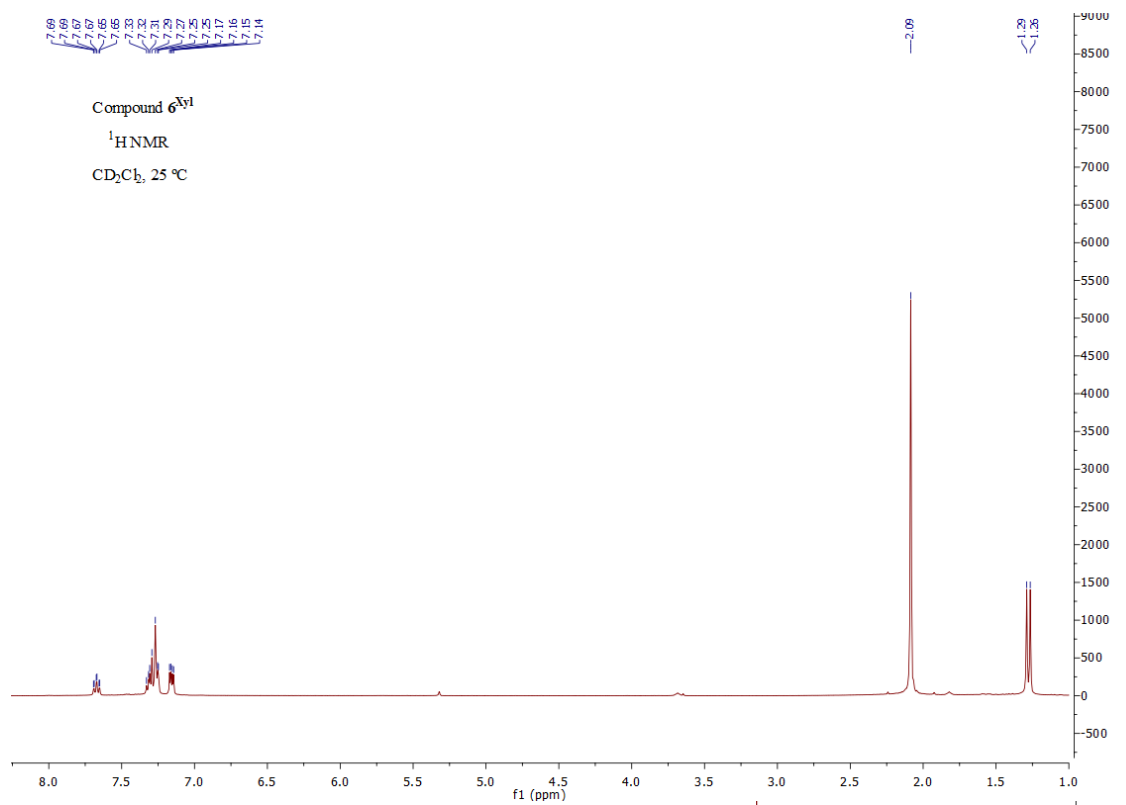
5. NMR spectra of new compounds

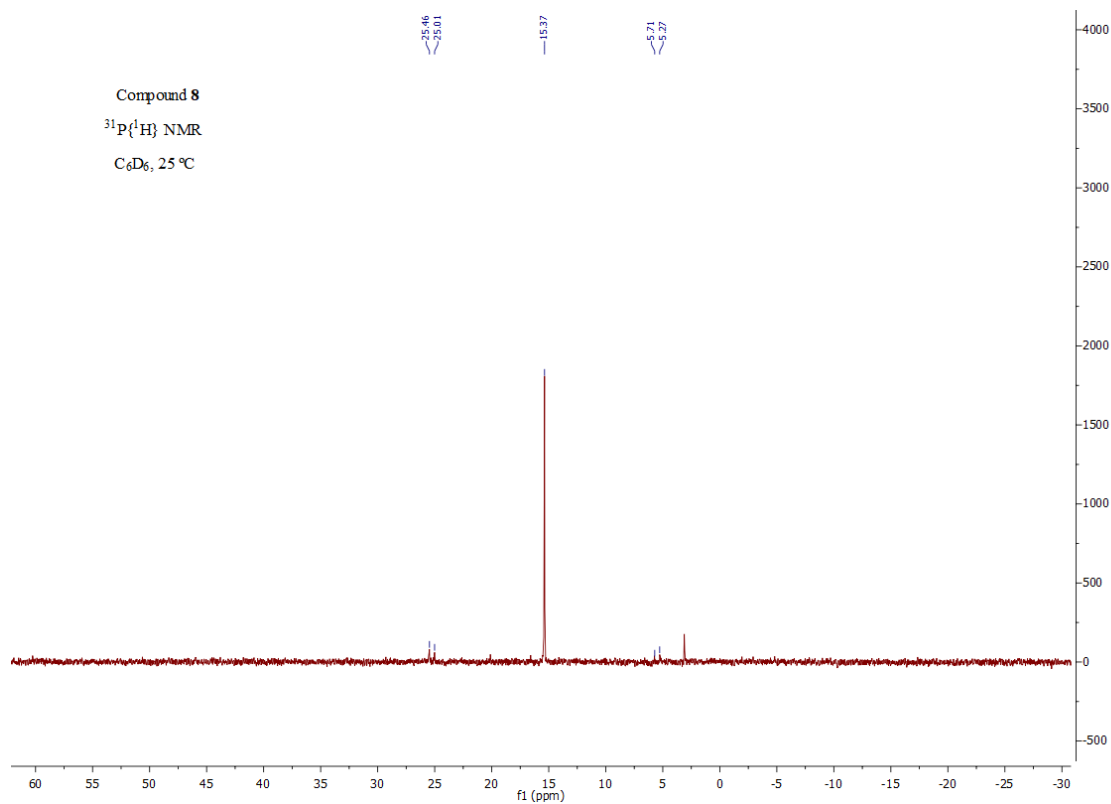
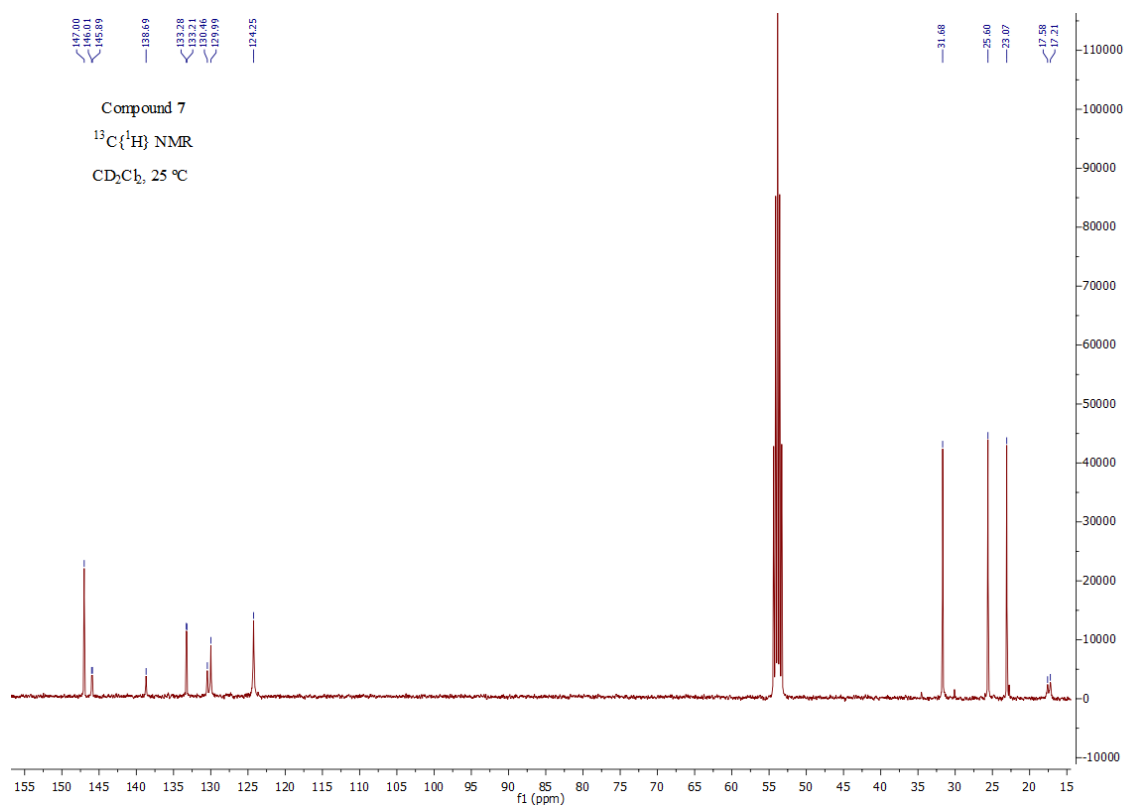


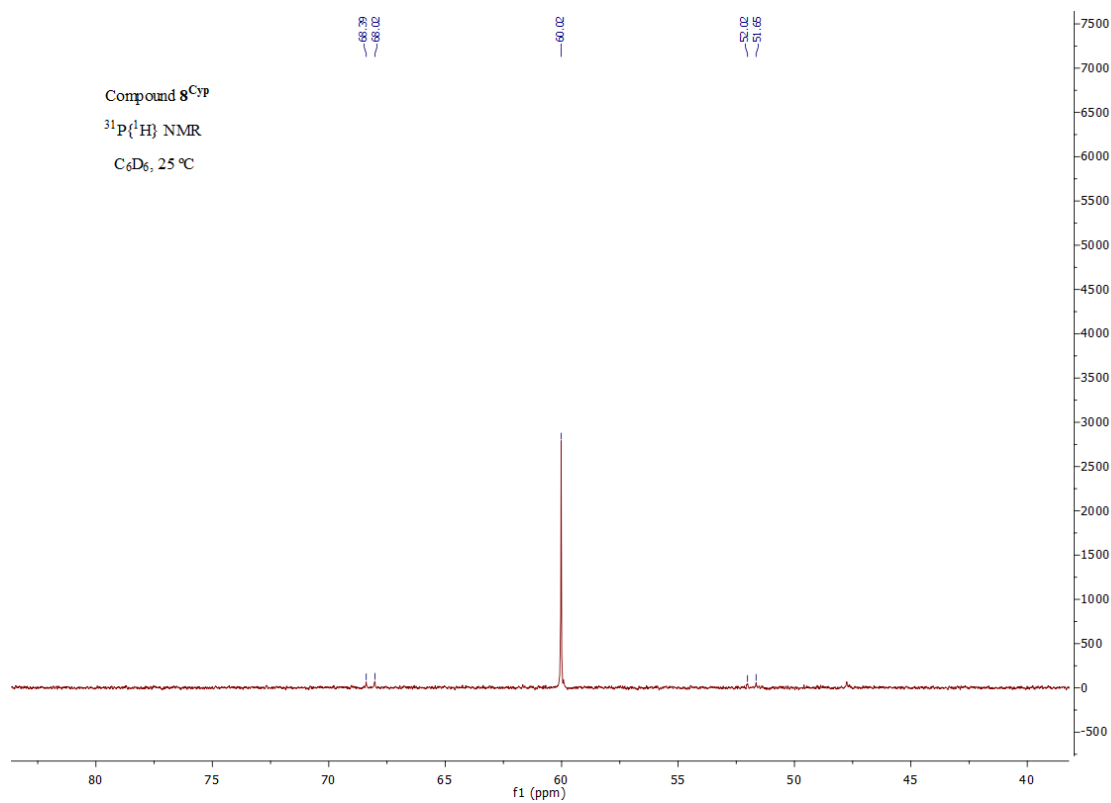
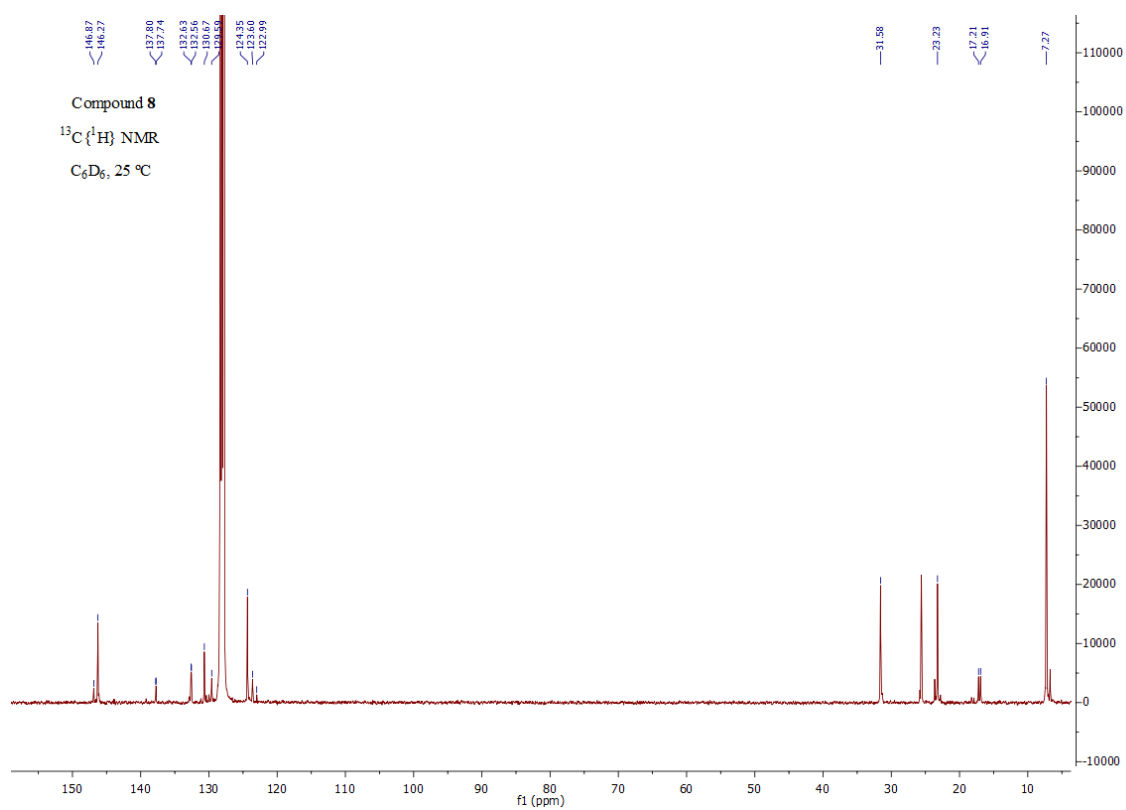


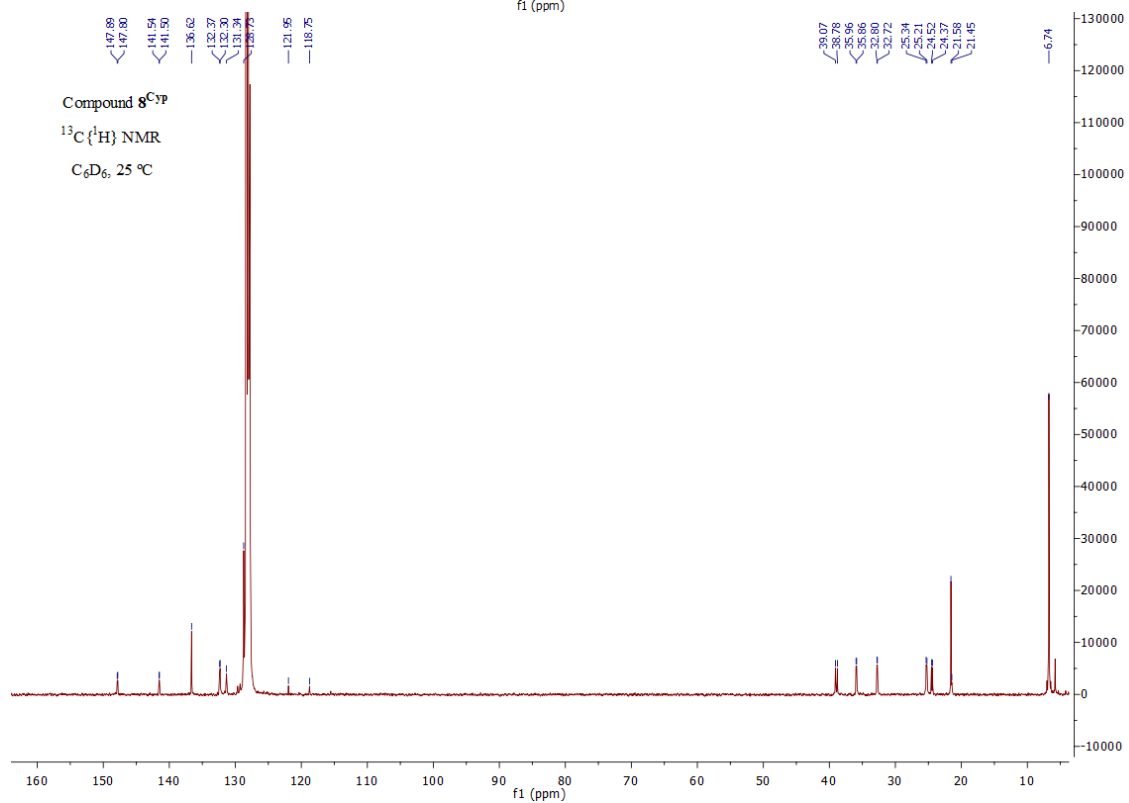
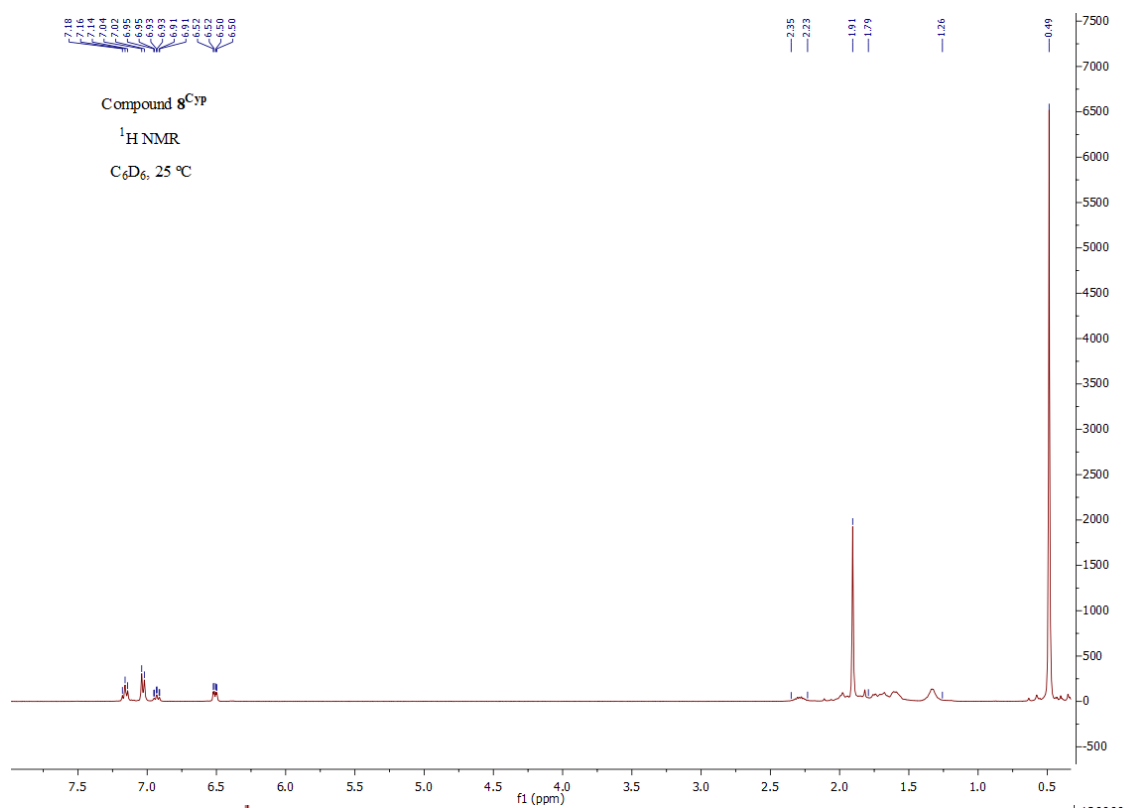


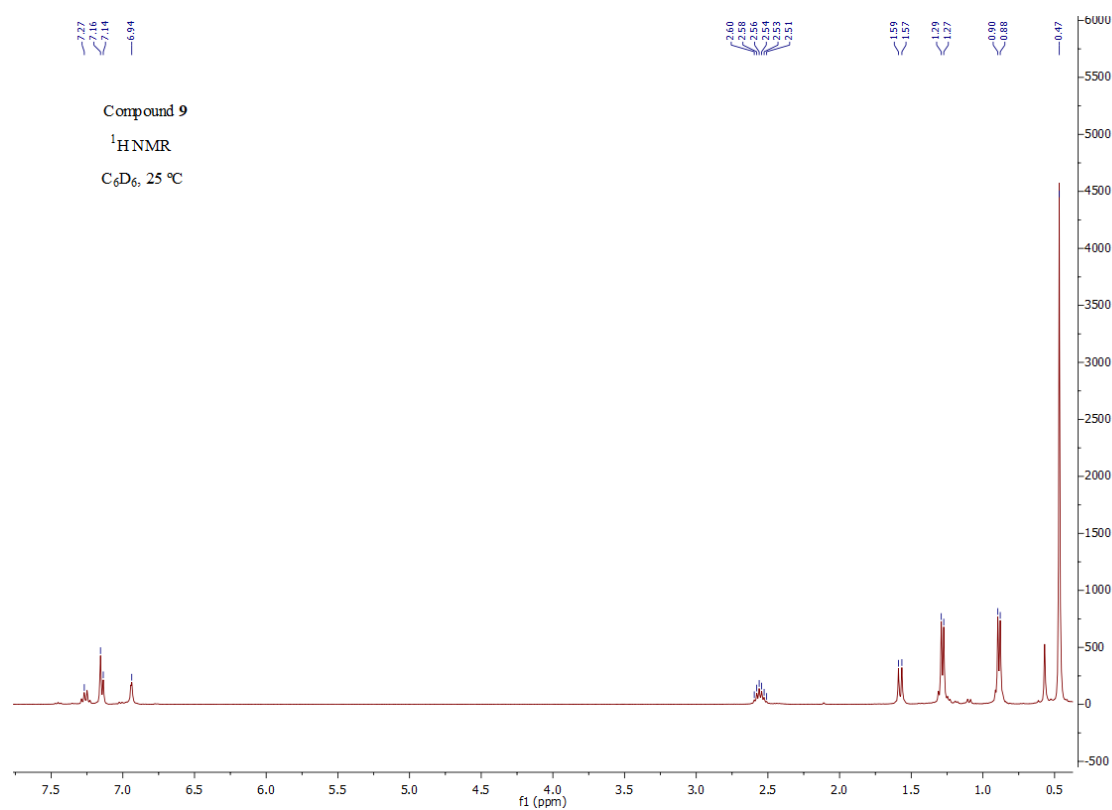
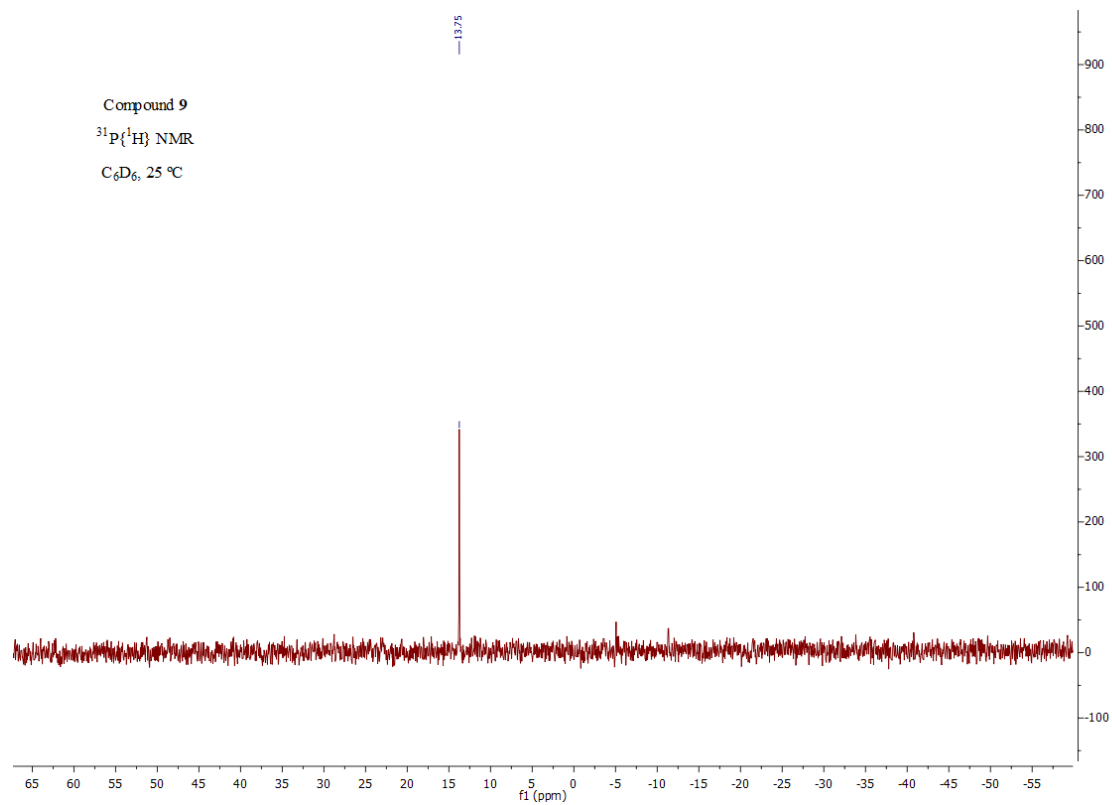


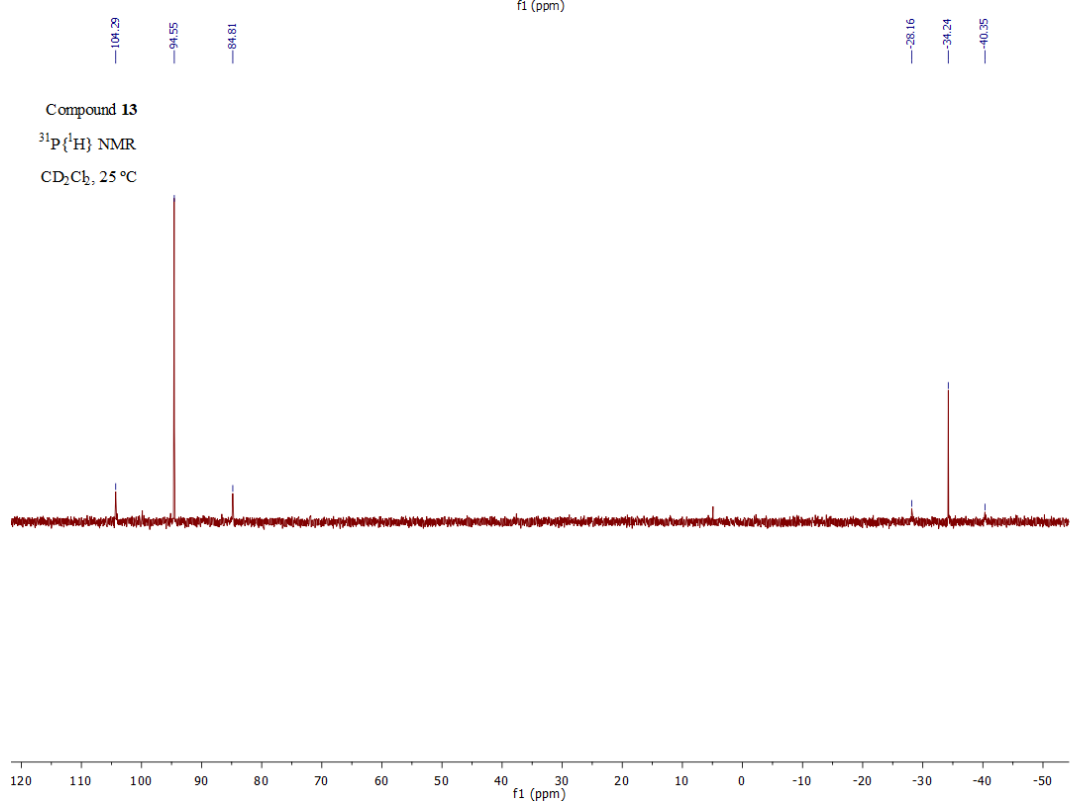
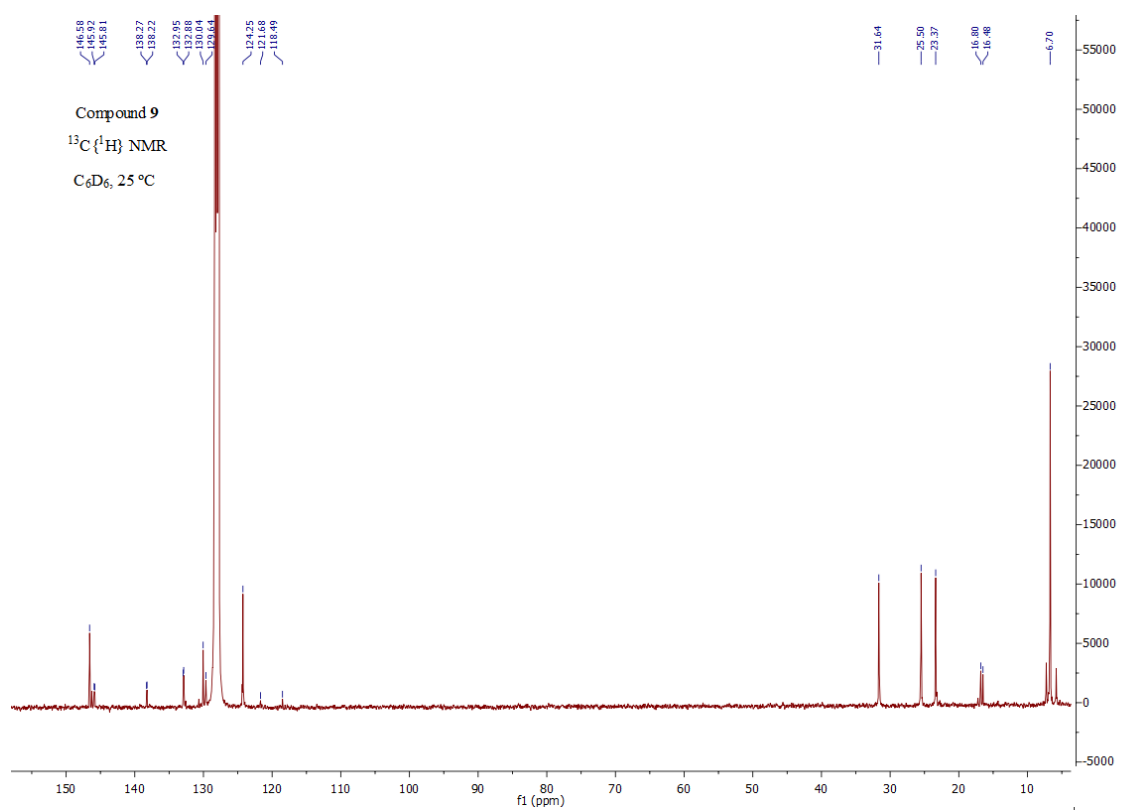


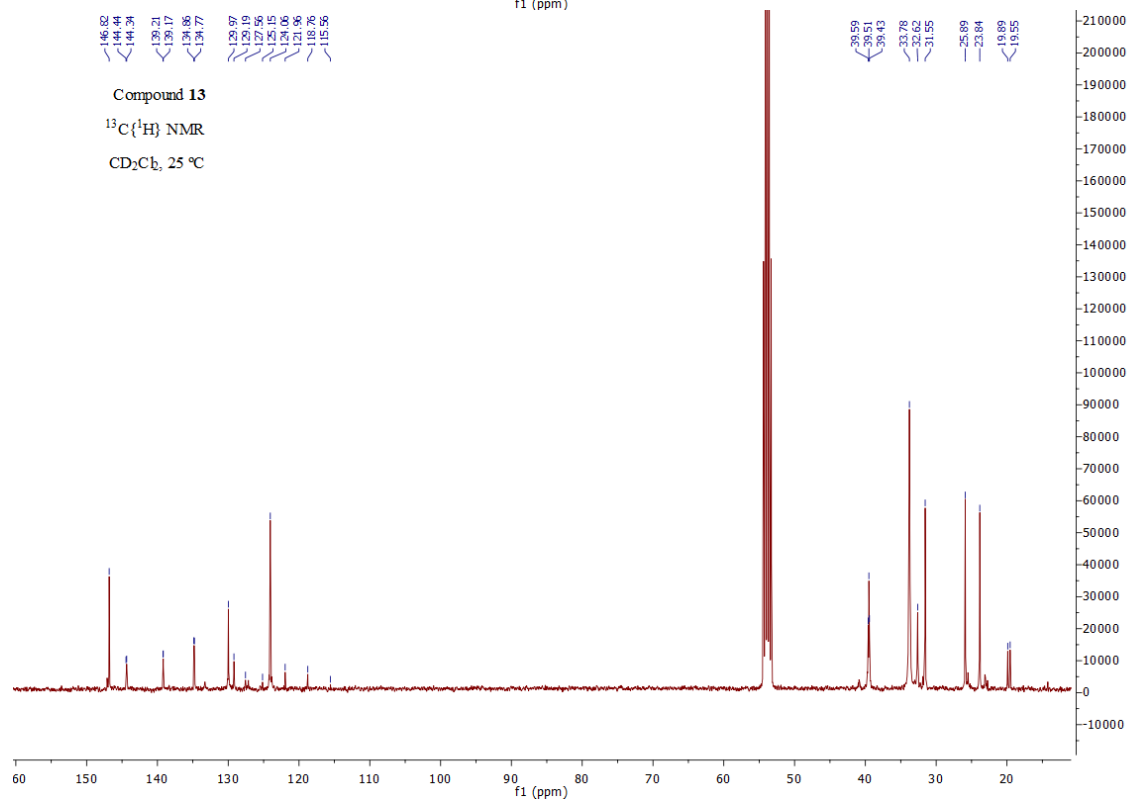
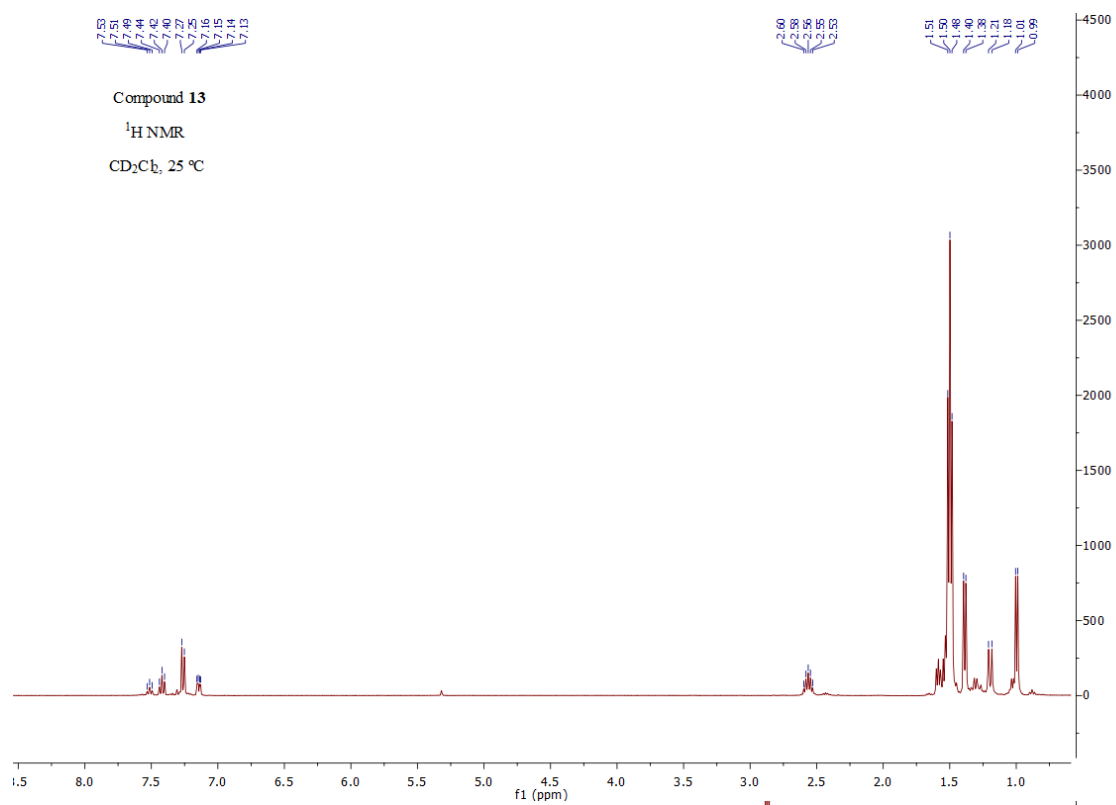


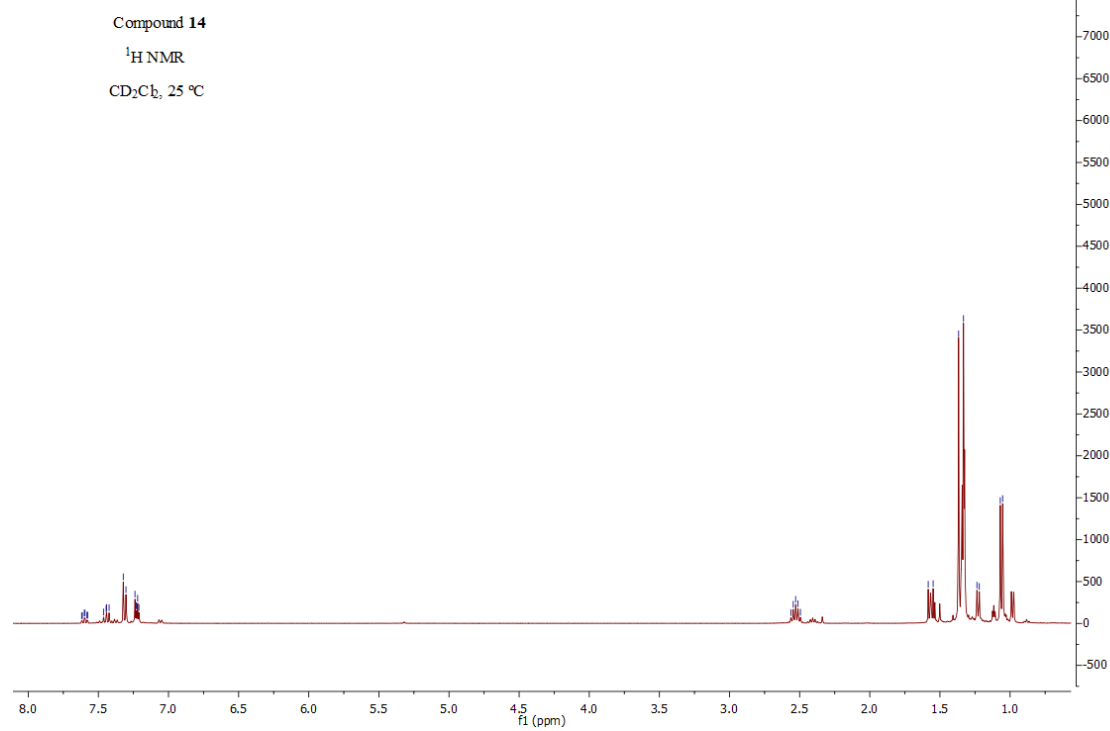
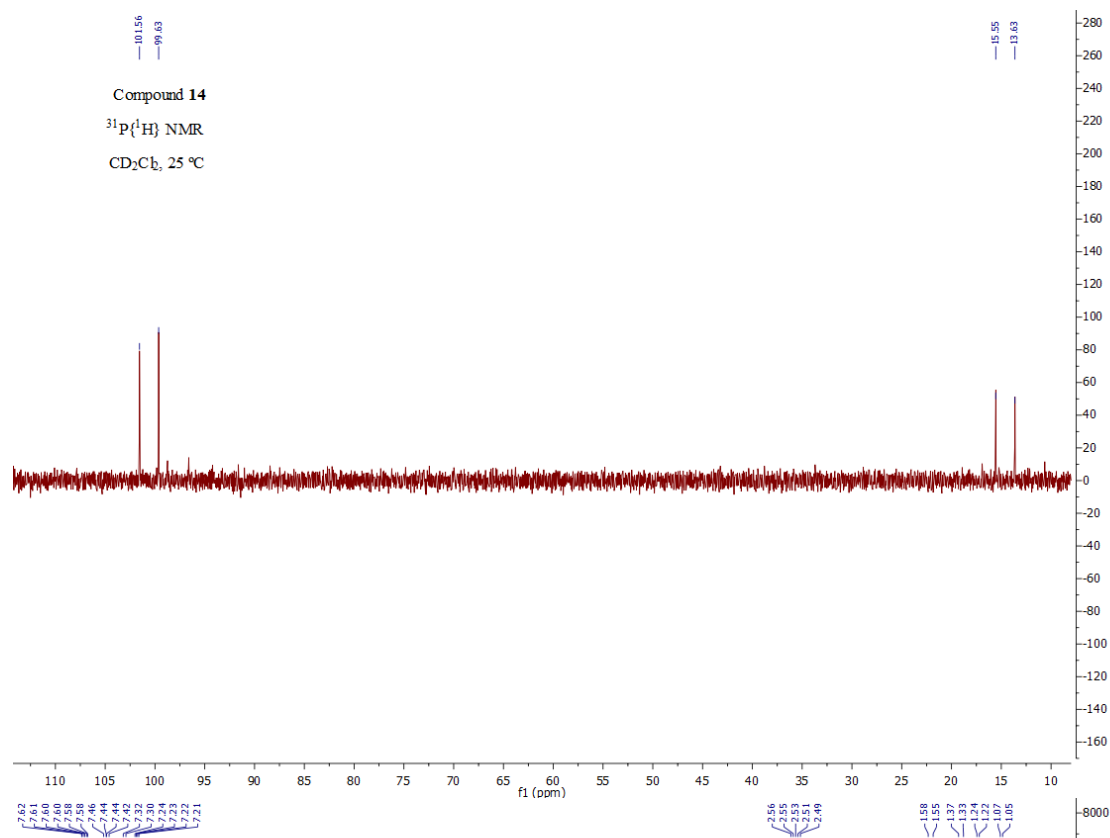


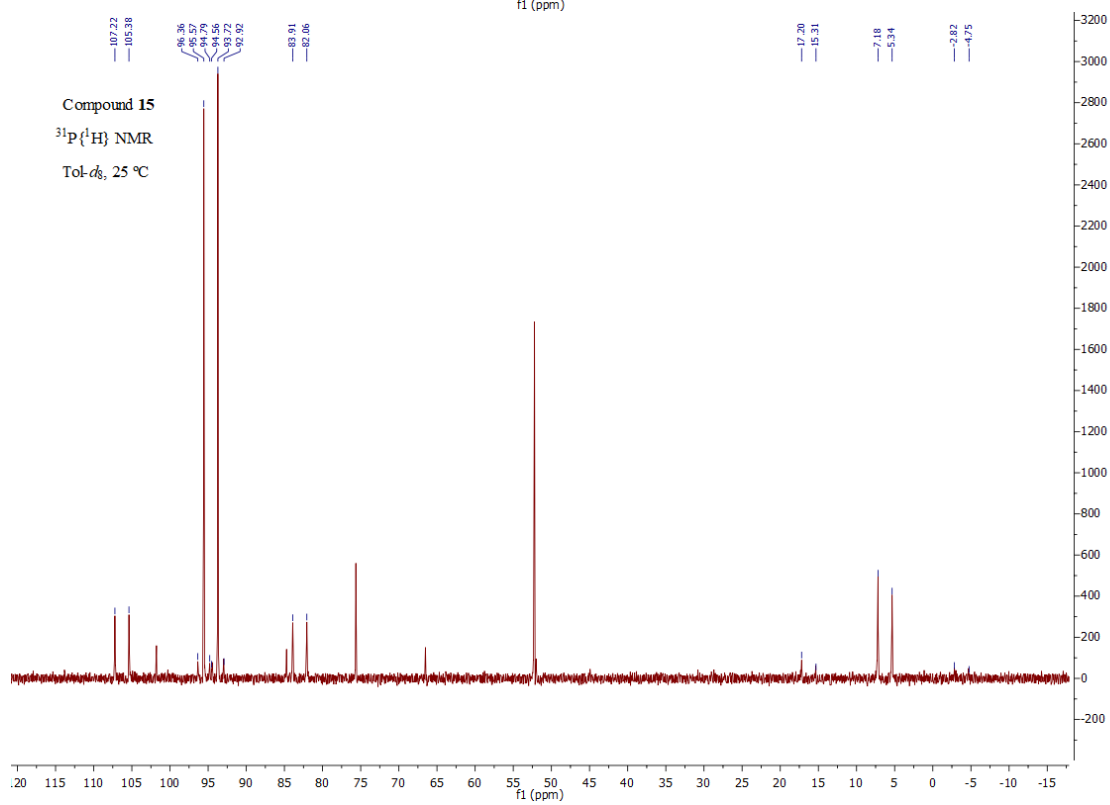
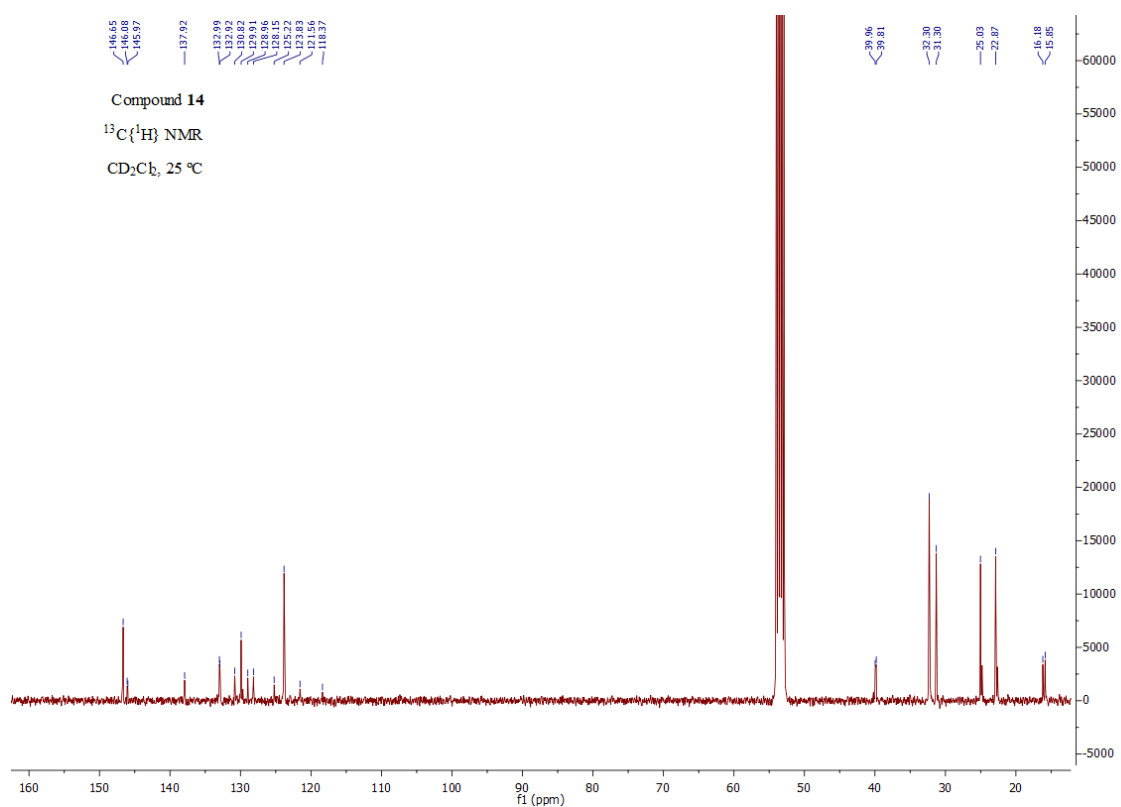


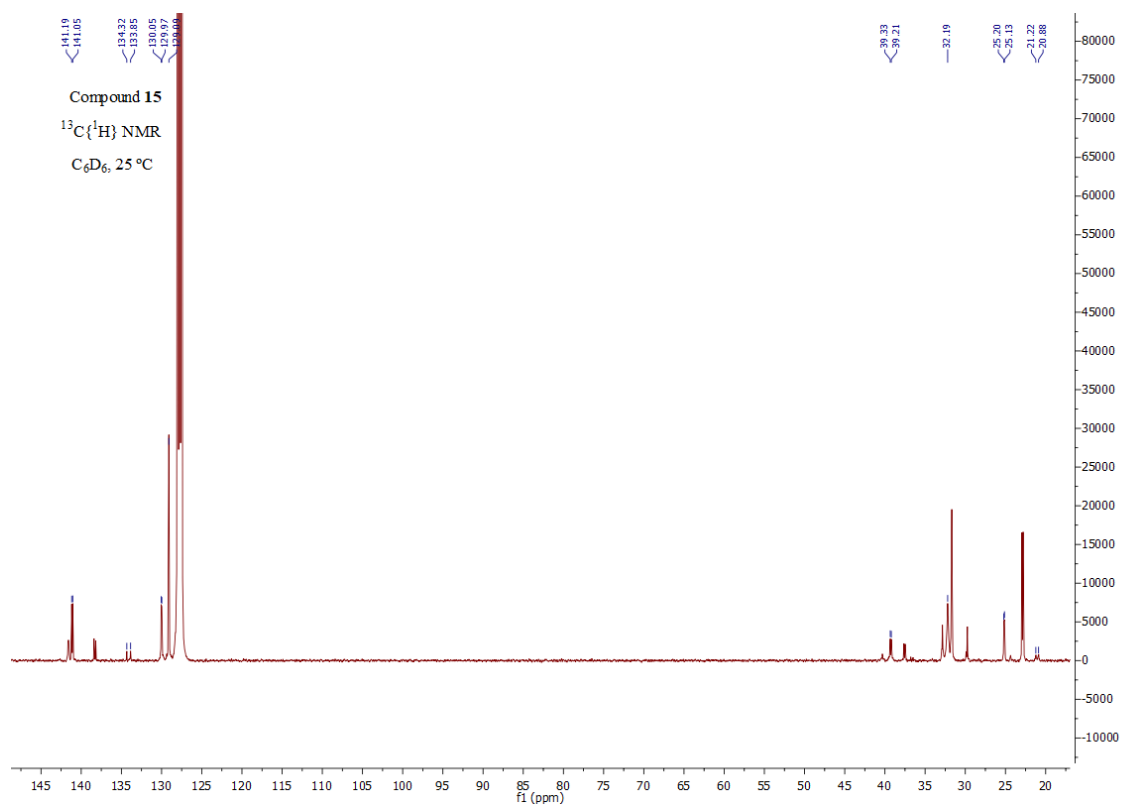
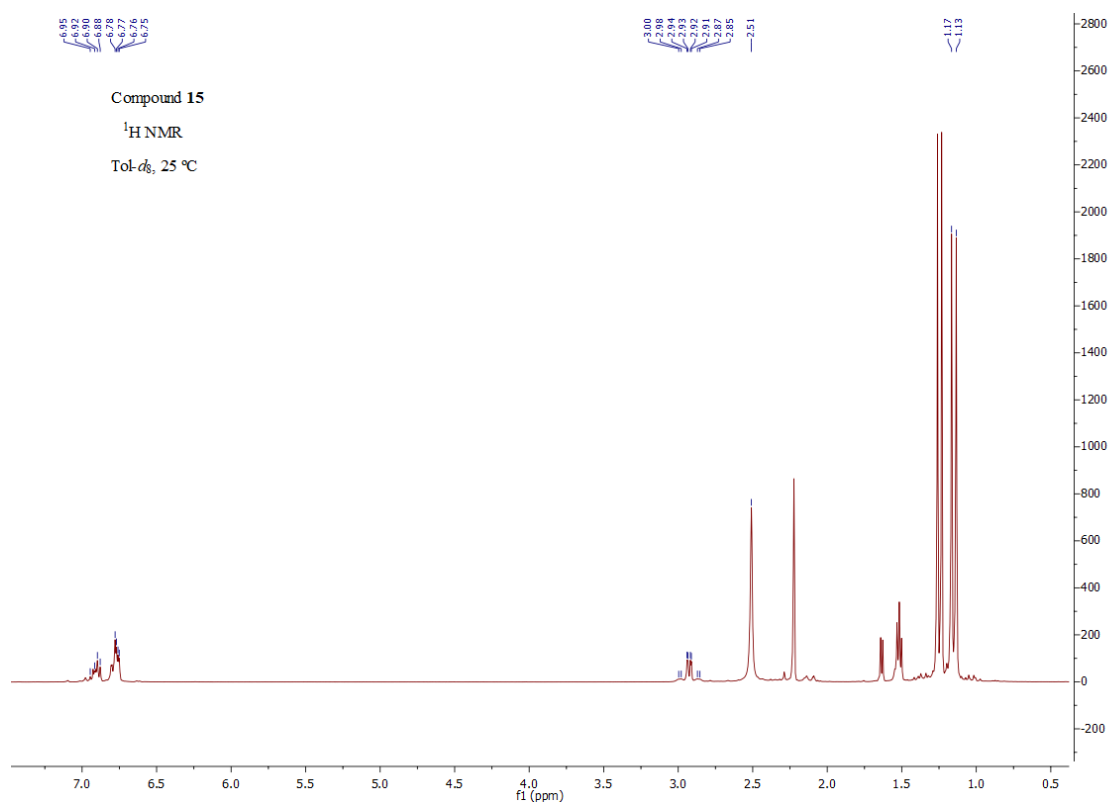


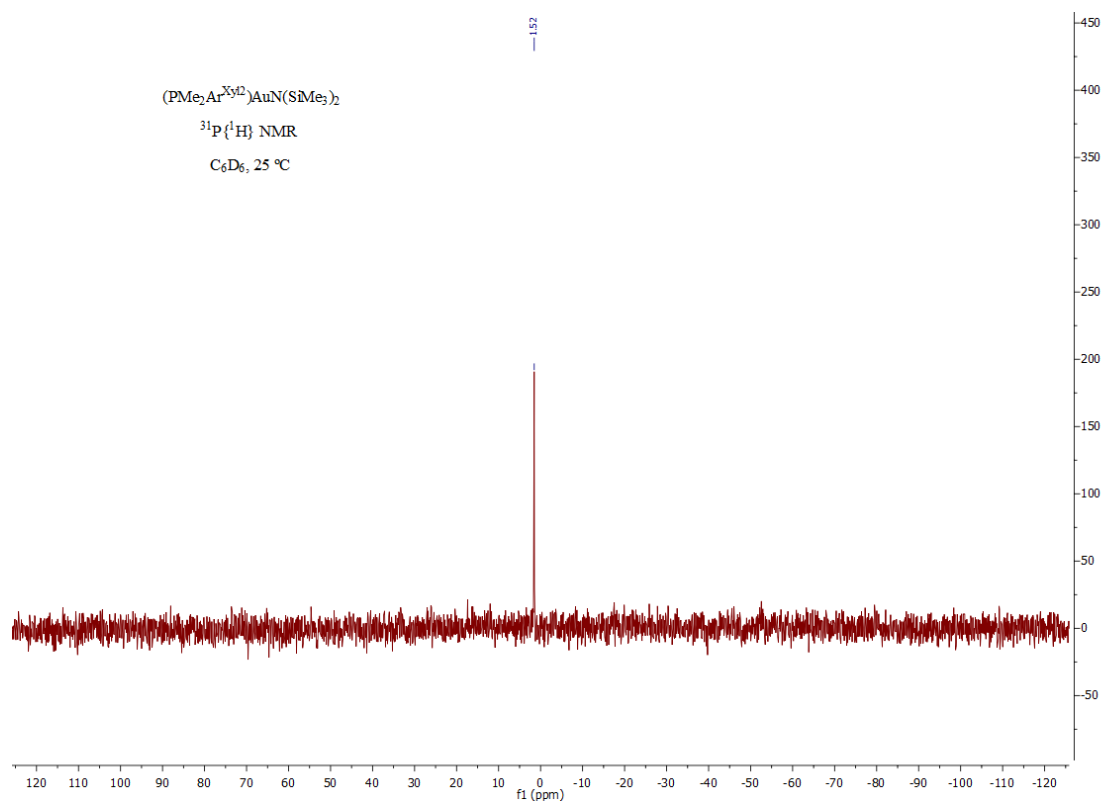
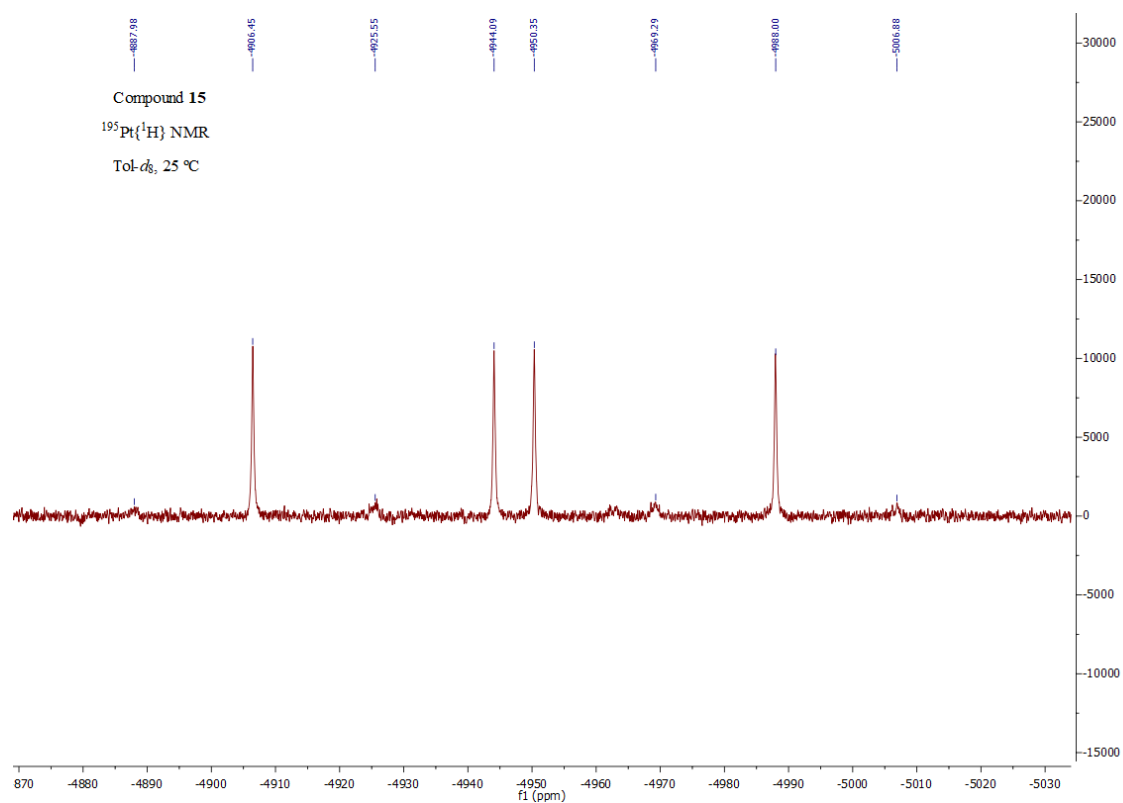


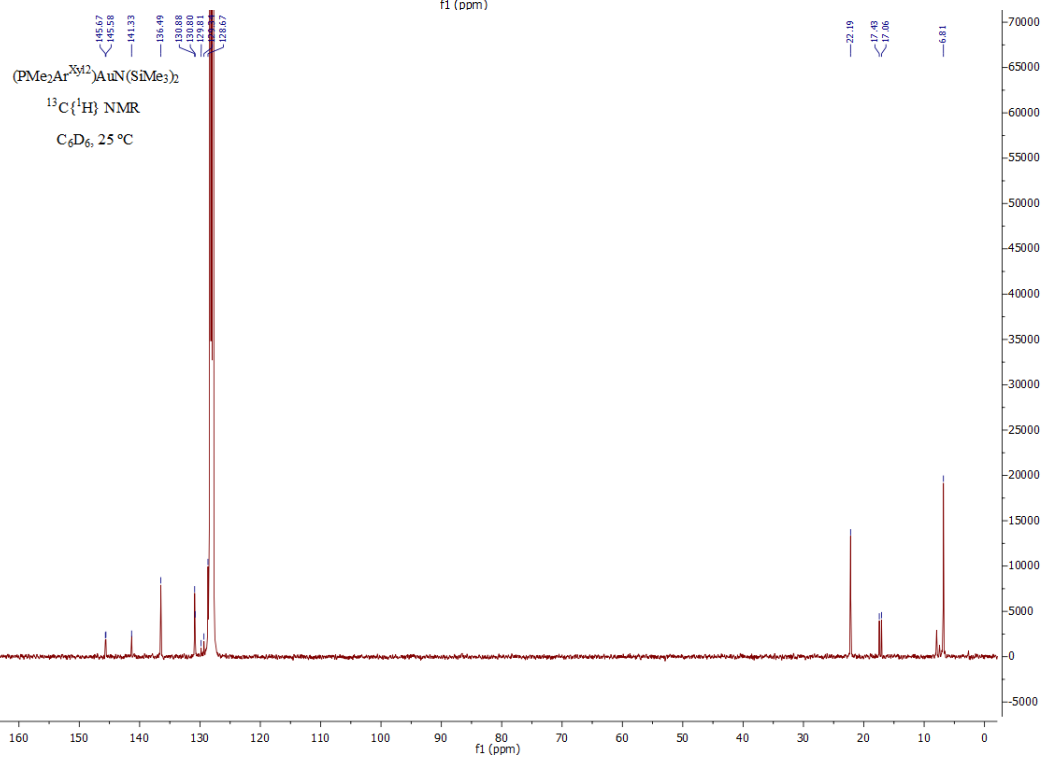
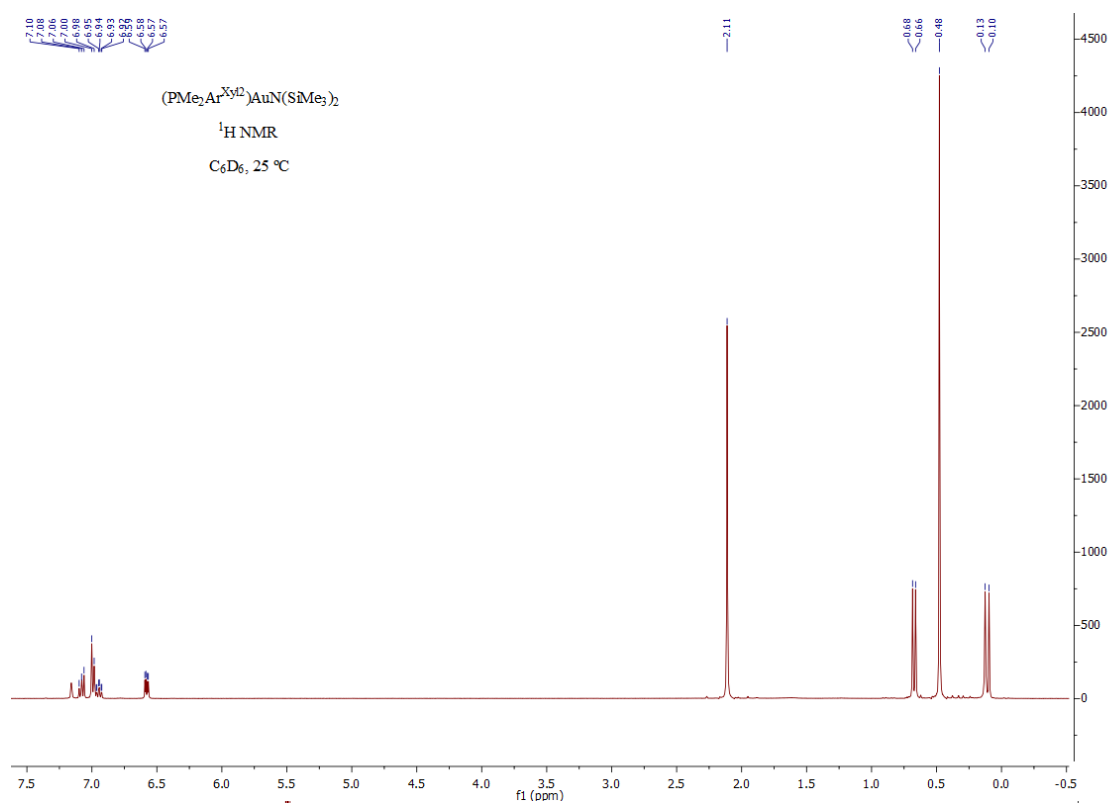


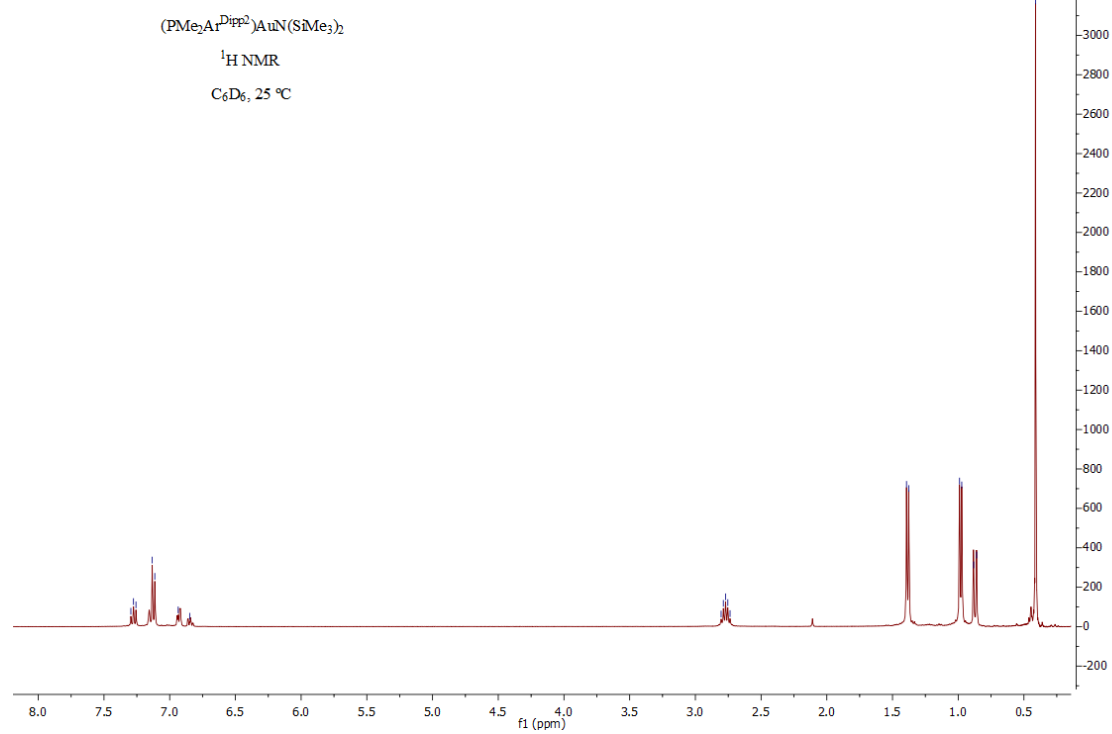
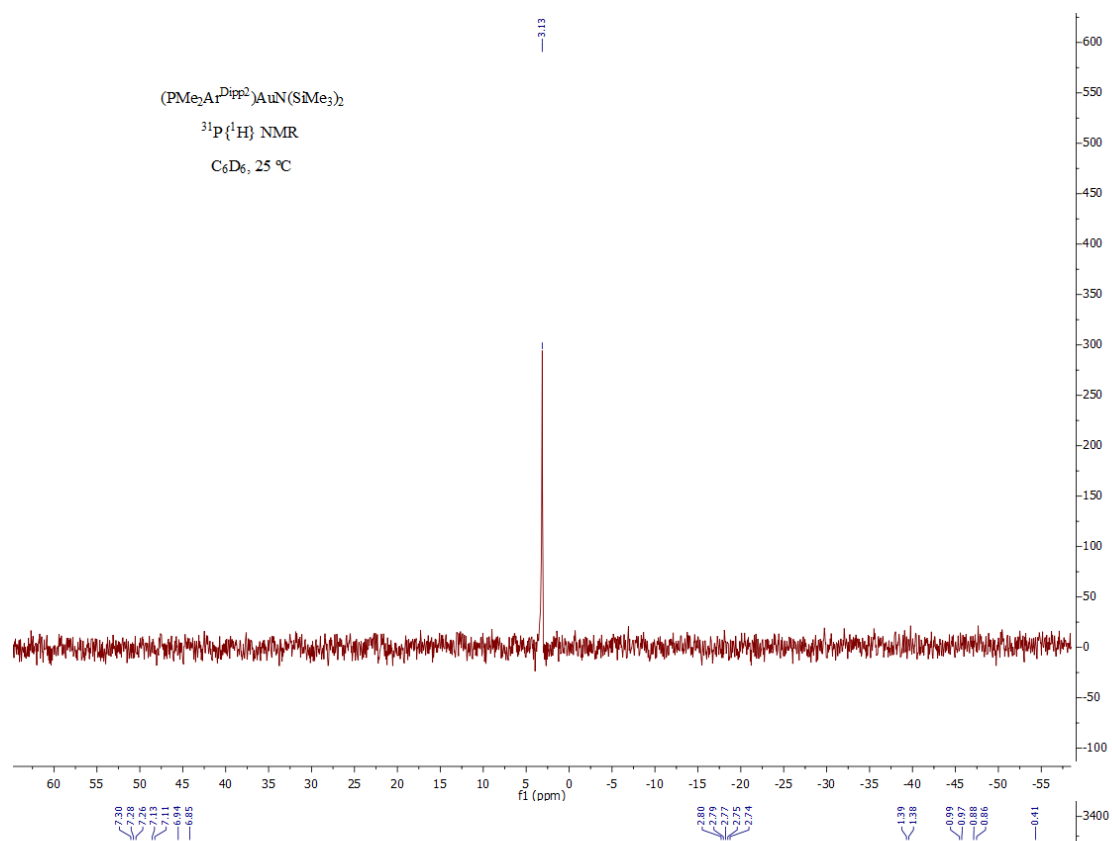


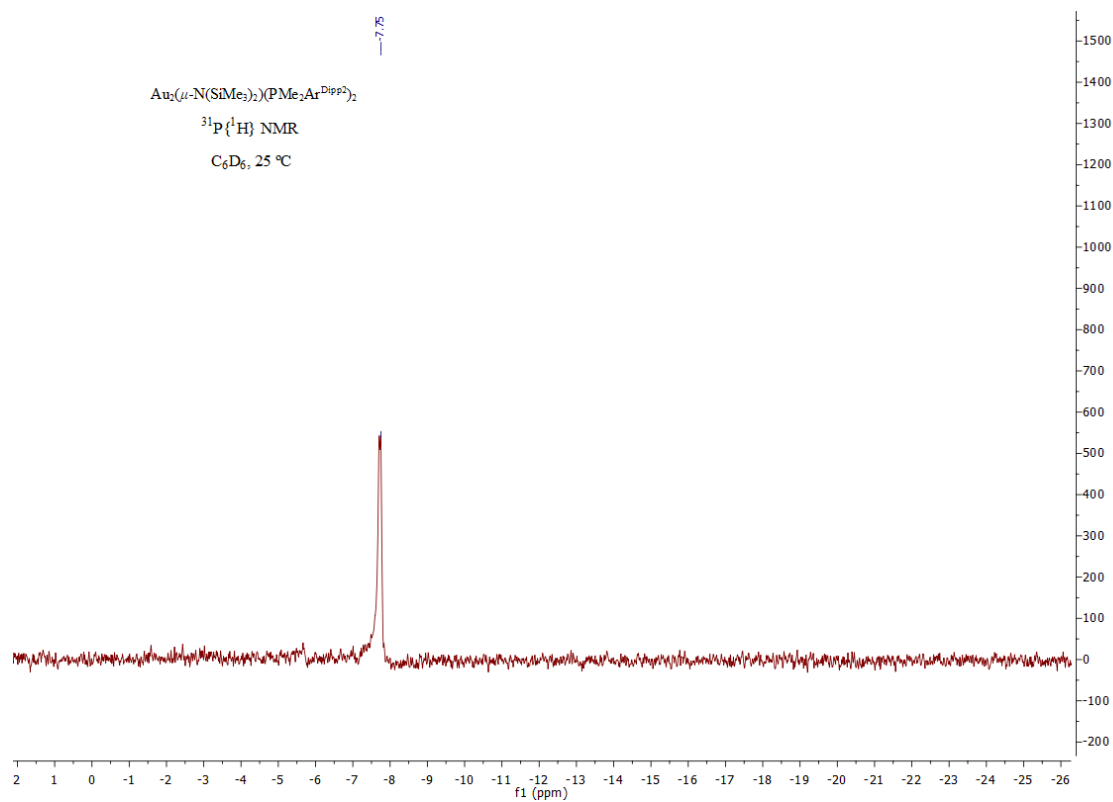
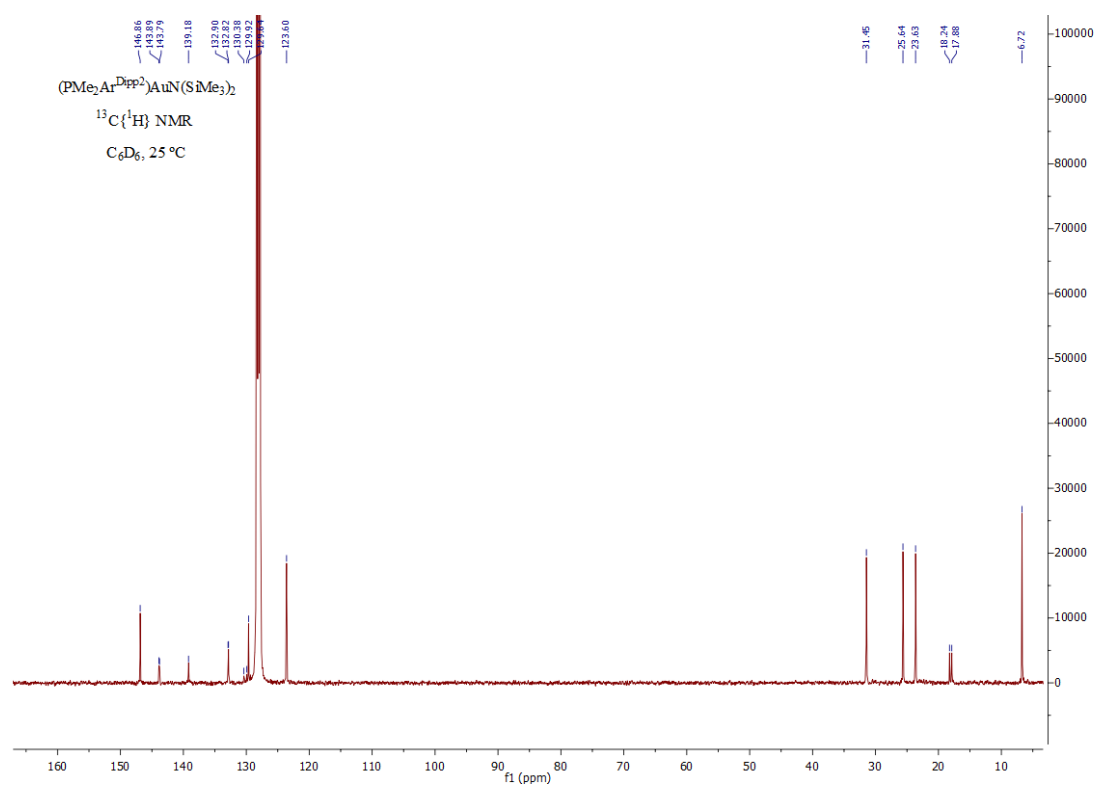


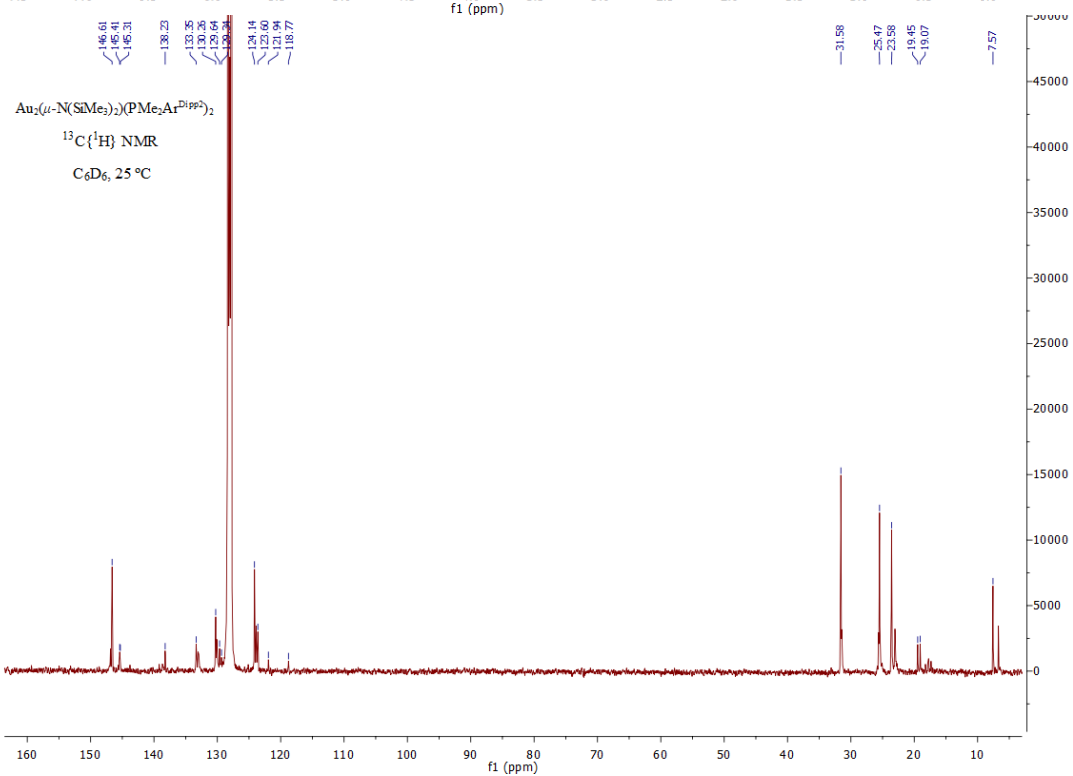
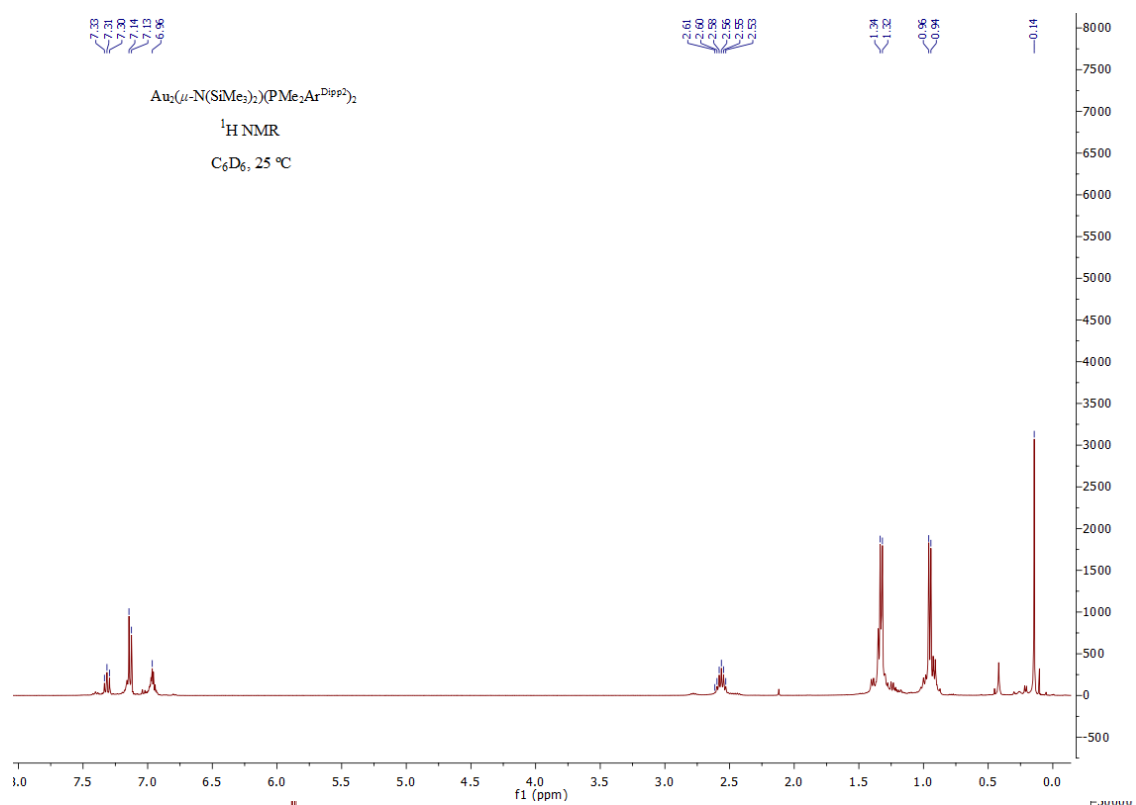


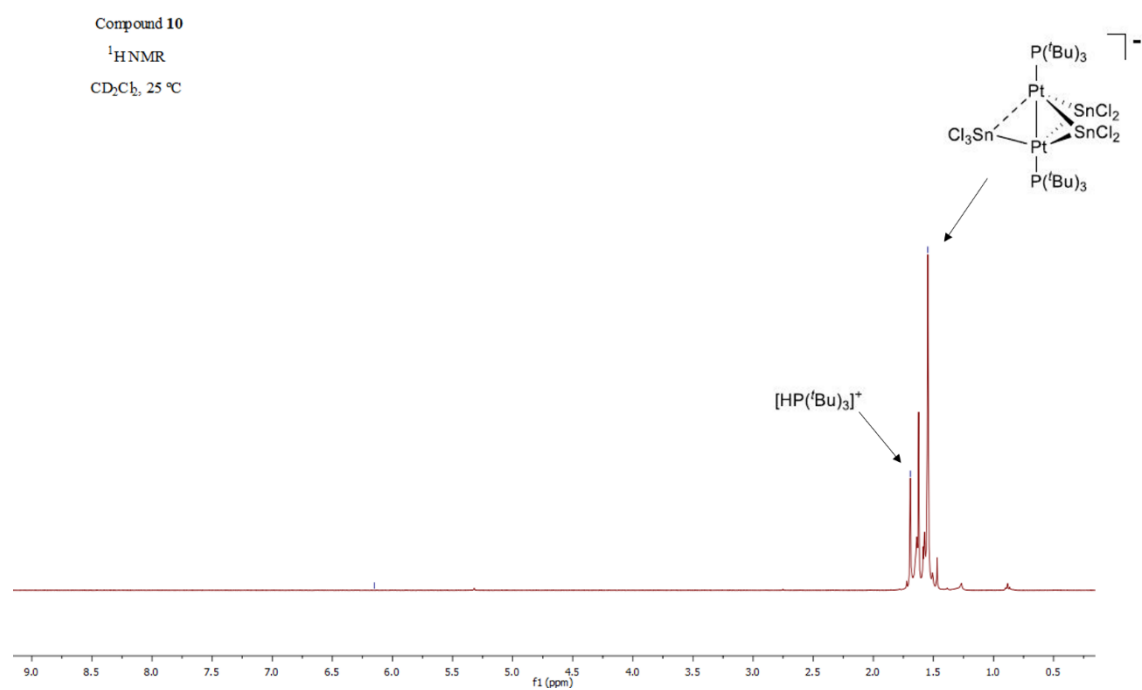
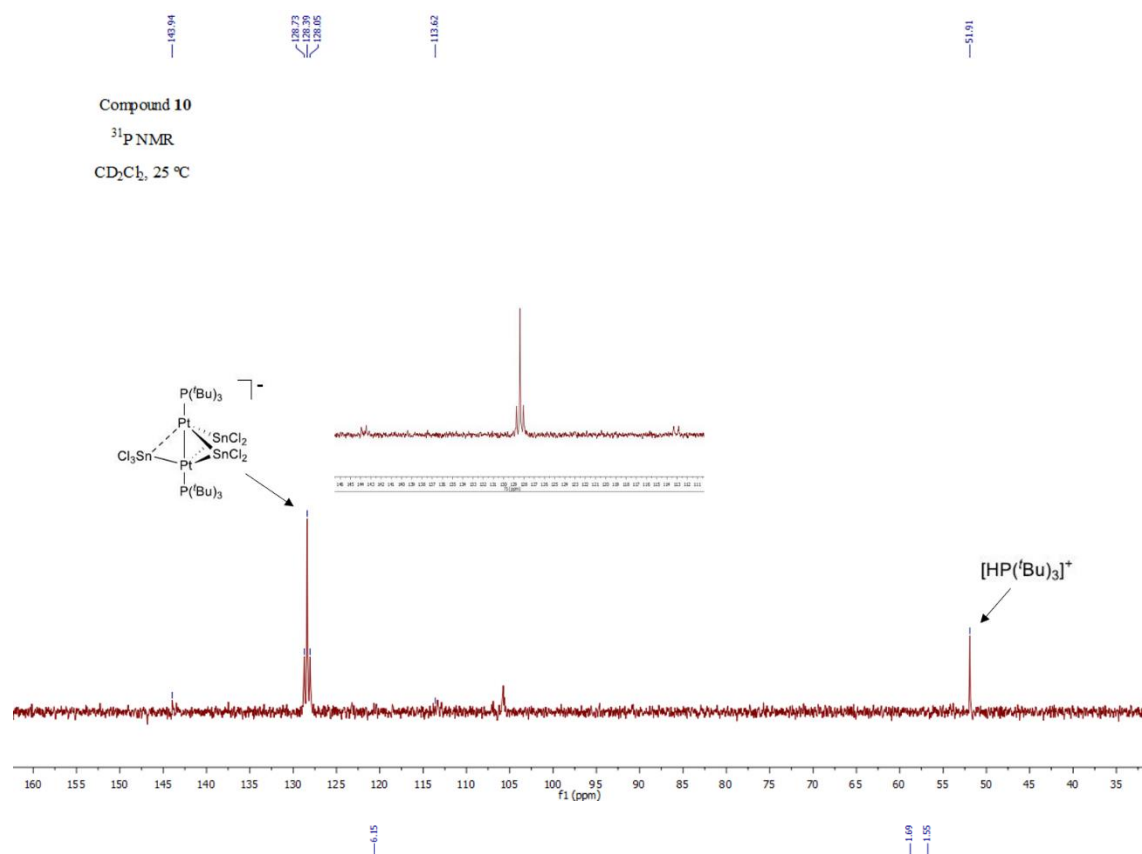


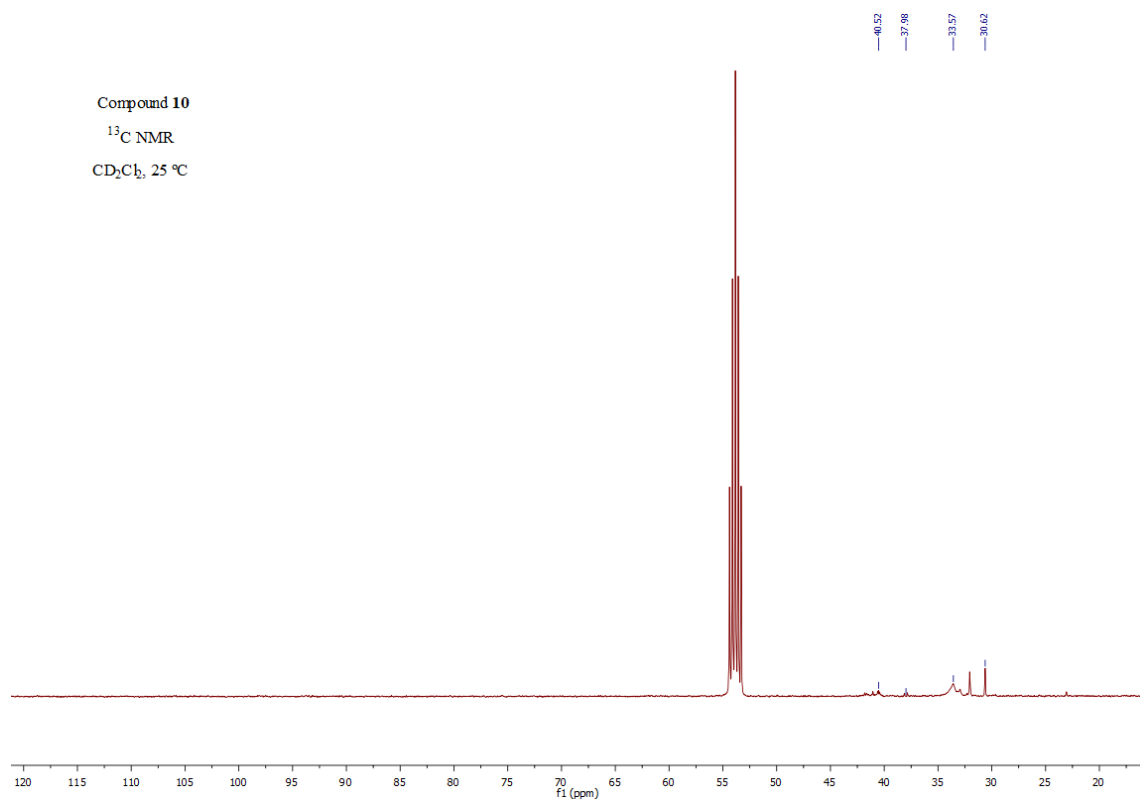












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