# Supplementary Information

## Synthesis, crystal structure and spectral studies of silver(I) cyclohexyldiphenylphosphine complexes: Towards the biological evaluation on malignant and non-malignant cells

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## 1. Spectral data ($^{1}H$, $^{13}C$, $^{31}P$ NMR and FTIR) for complexes 1–6

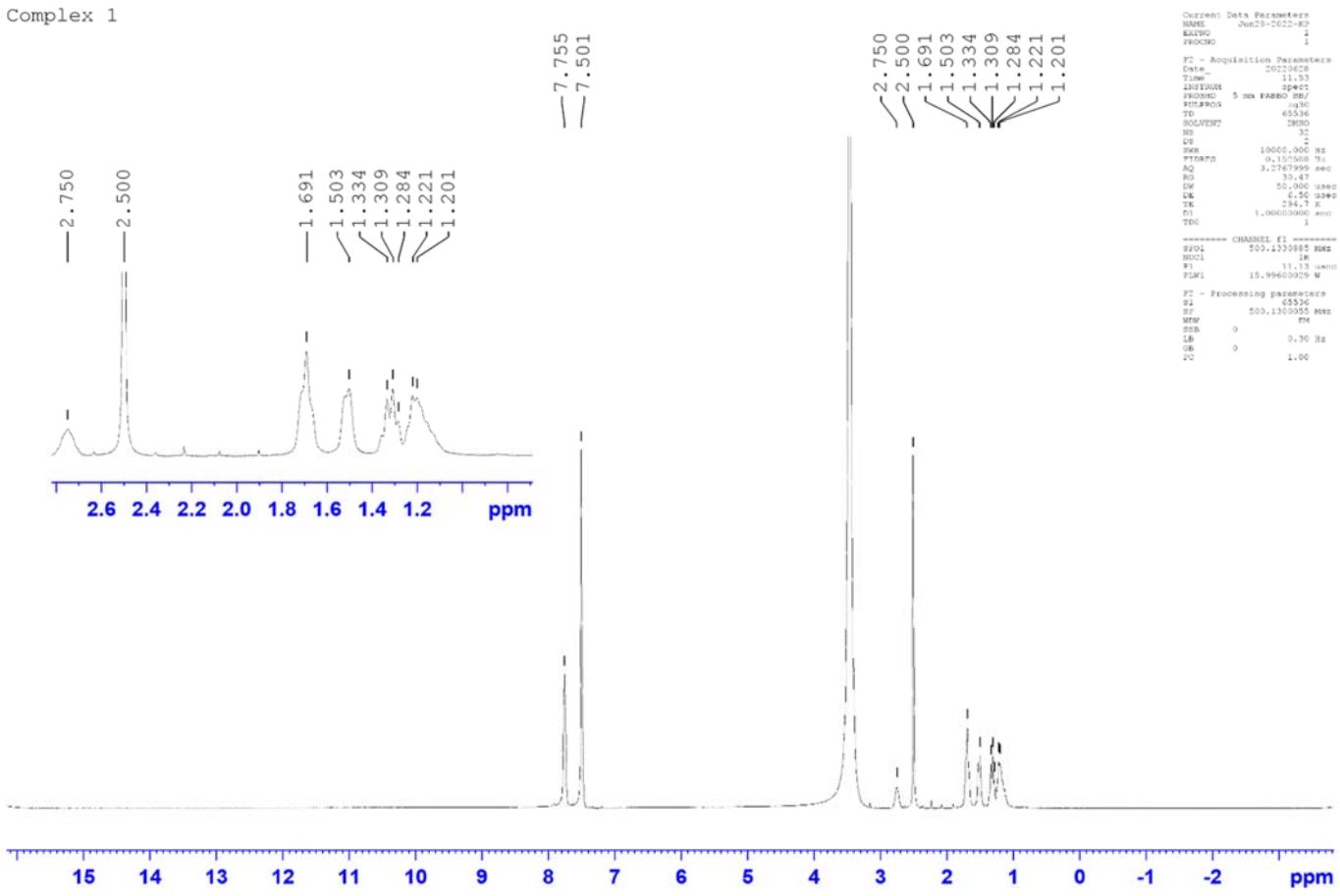



**Figure S1:** $^{1}H$-NMR spectrum of complex **1**.

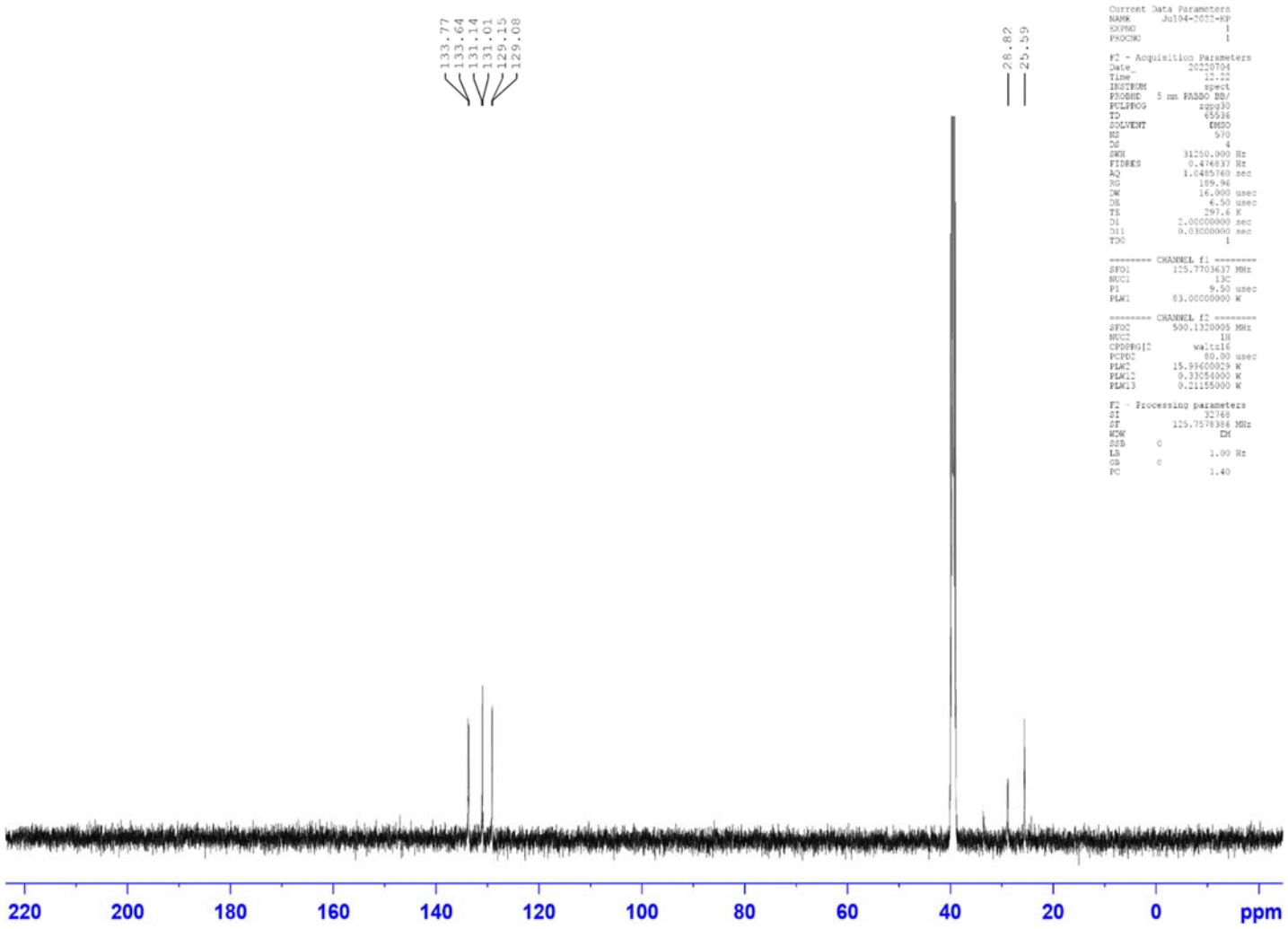



**Figure S2:** $^{13}C\{H\}$-NMR spectrum of complex **1**.

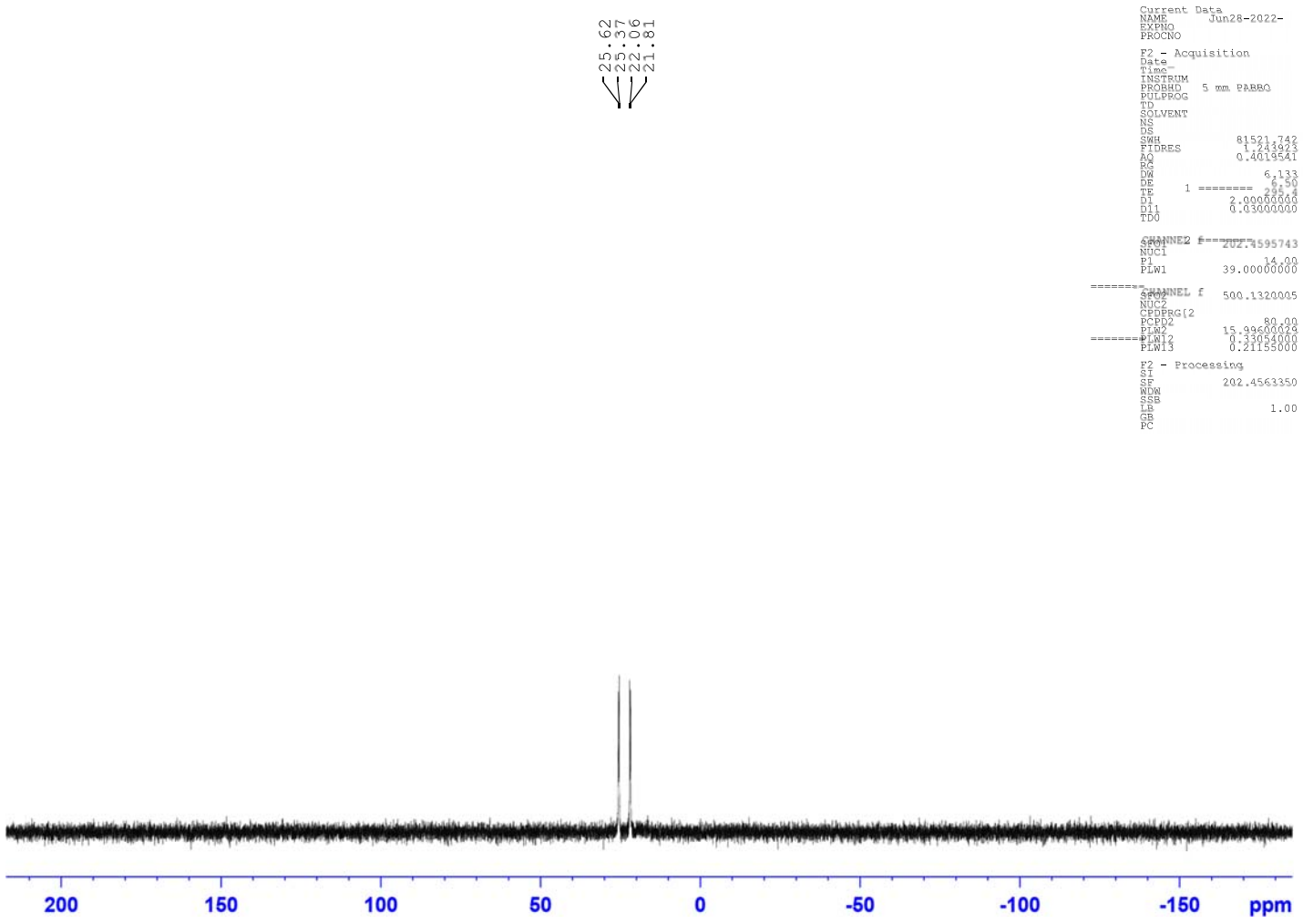



**Figure S3:** $^{31}P\{H\}$-NMR spectrum of complex **1**.

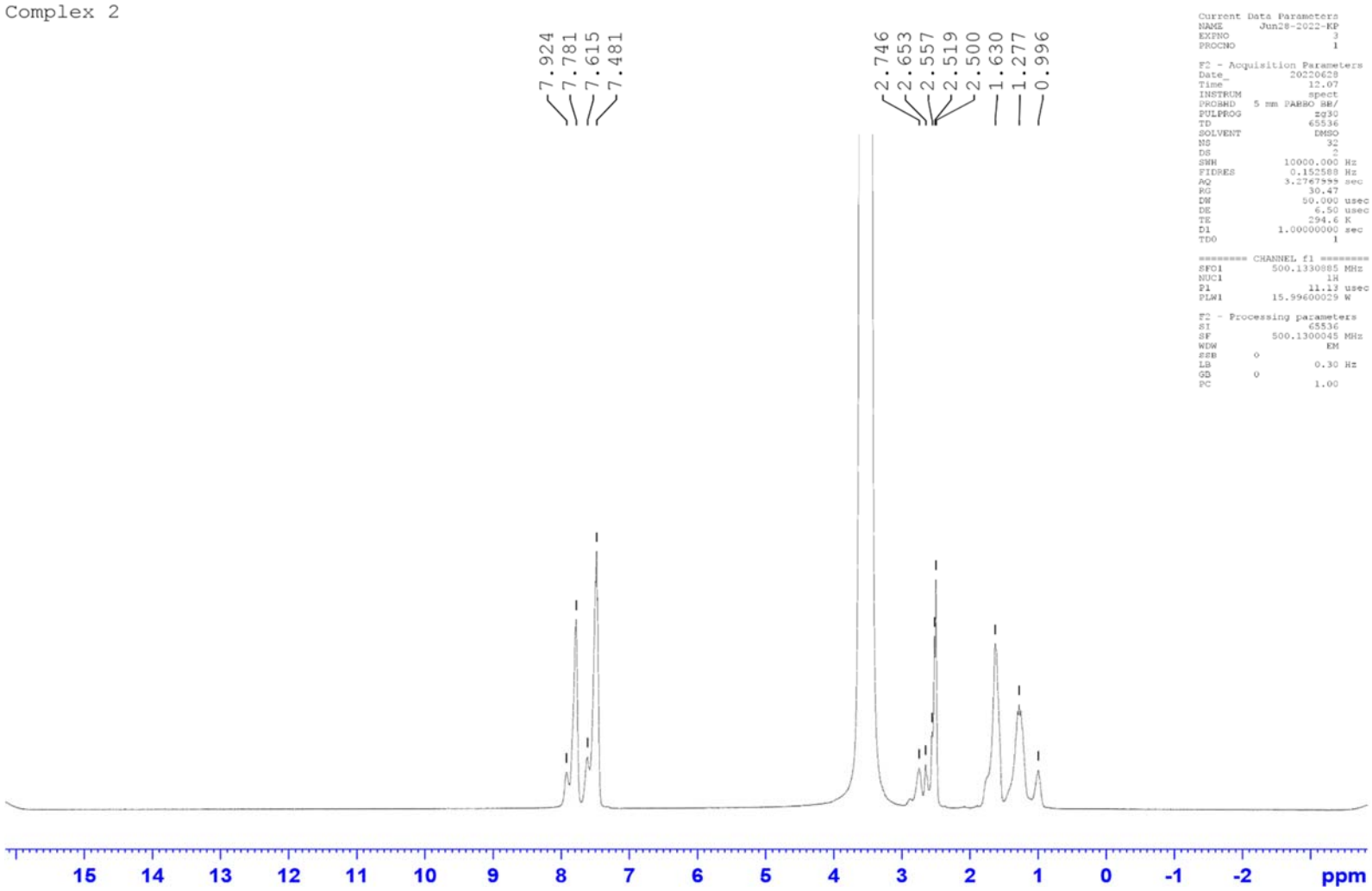



**Figure S4:** $^{1}$H-NMR spectrum of complex **2**.

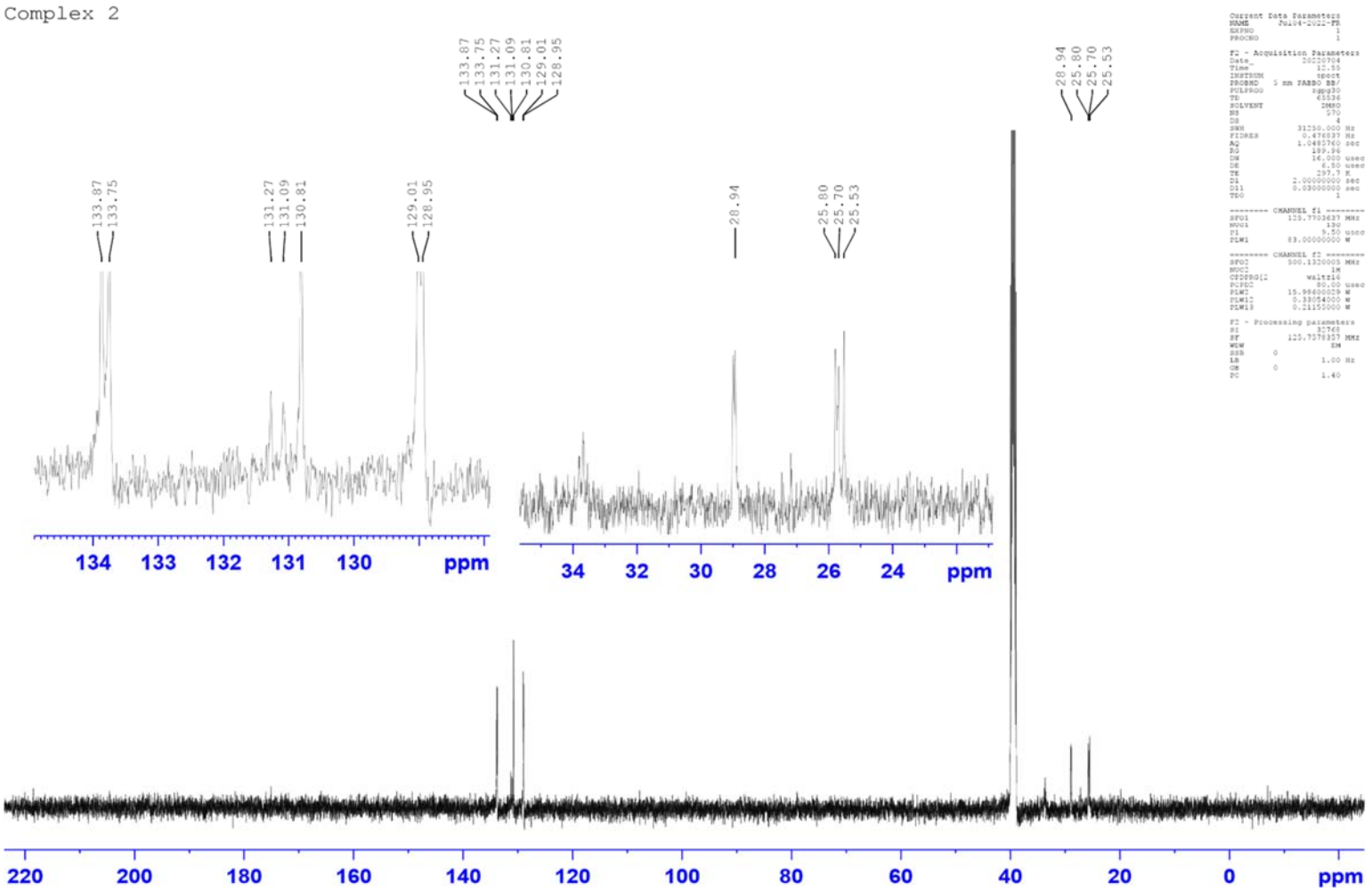



**Figure S5:** $^{13}C\{H\}$-NMR spectrum of complex **2**.

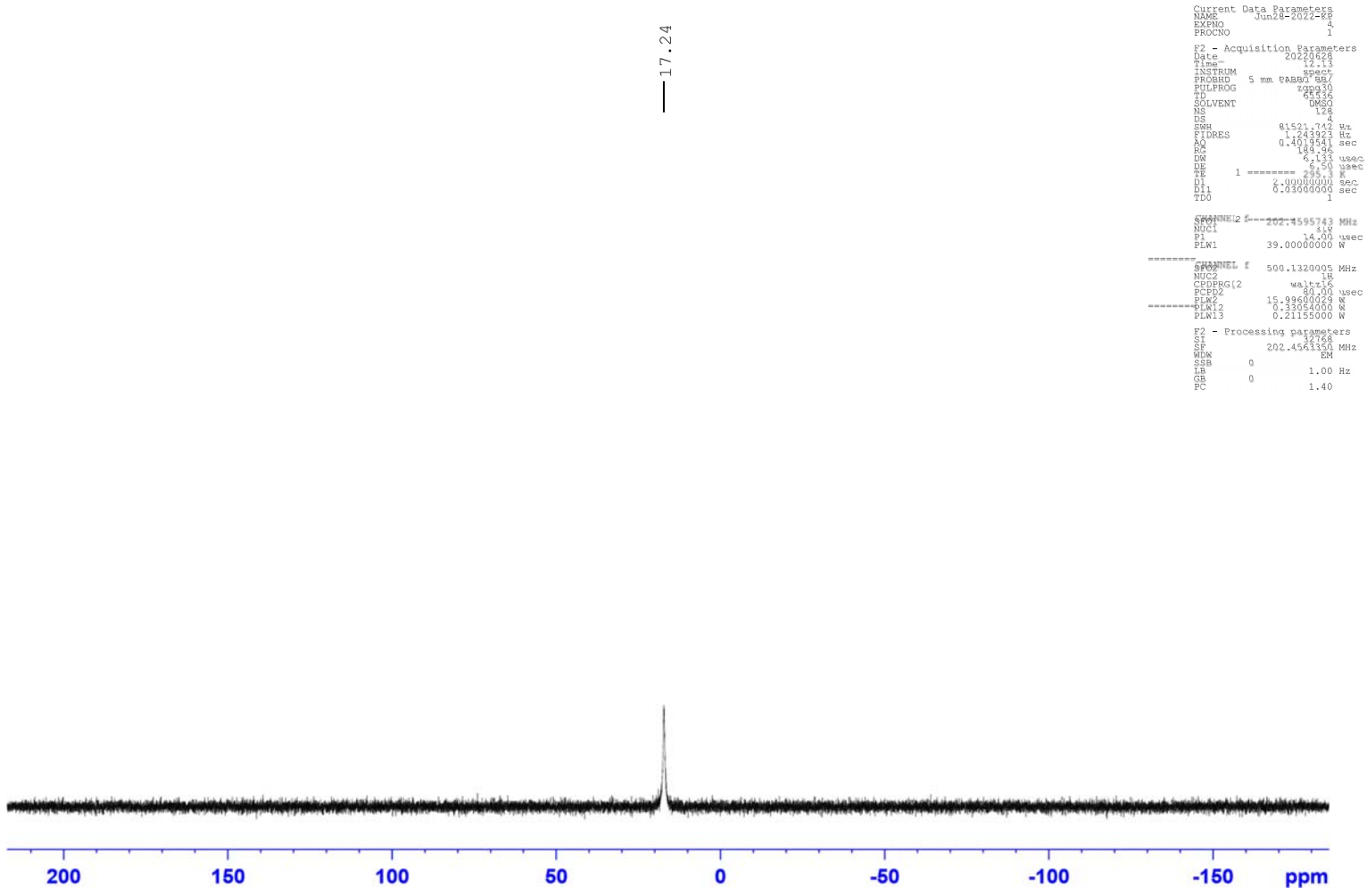



**Figure S6:** $^{31}P\{H\}$-NMR spectrum of complex **2**.

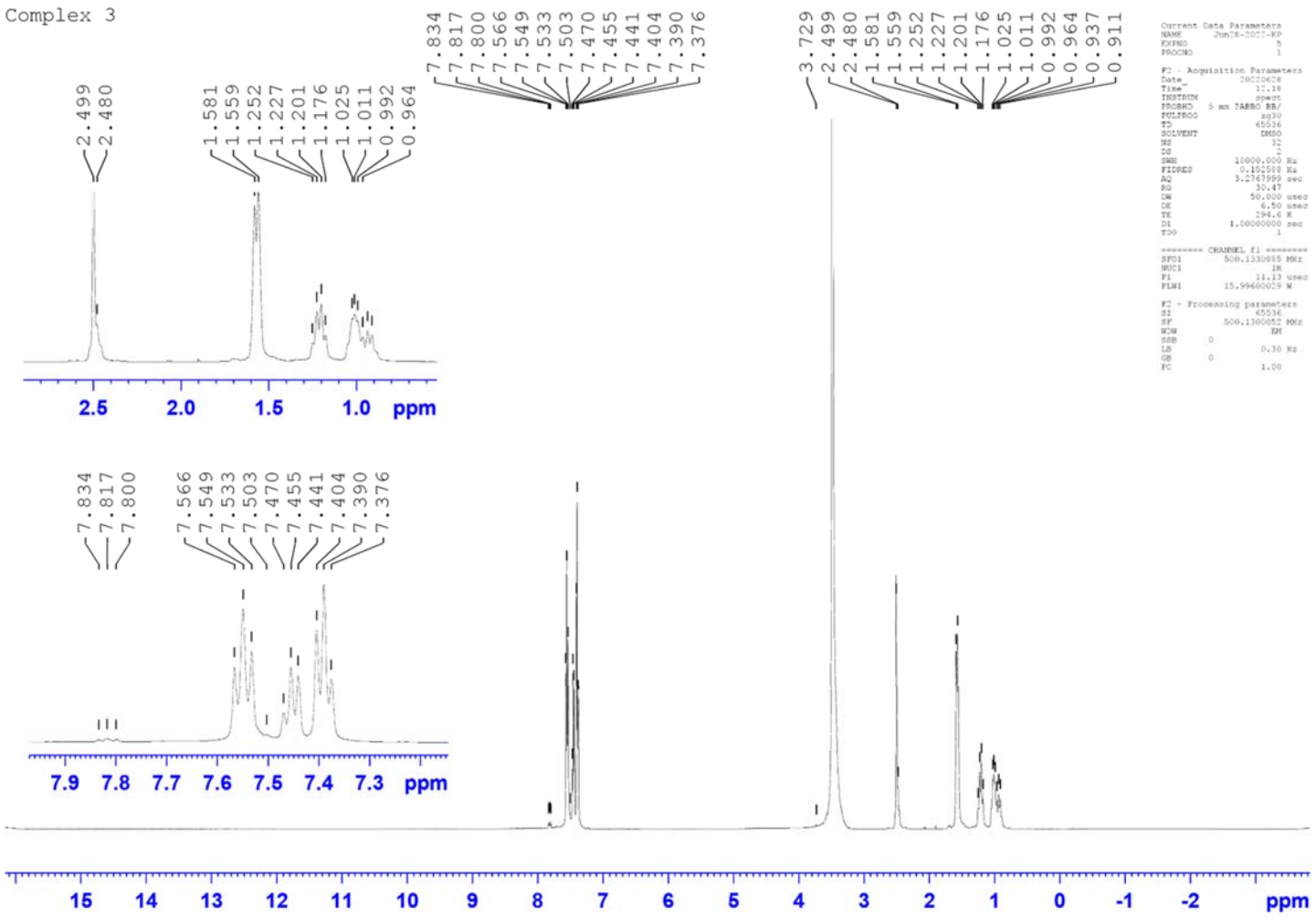



**Figure S7:** $^{1}$H-NMR spectrum of complex **3**.

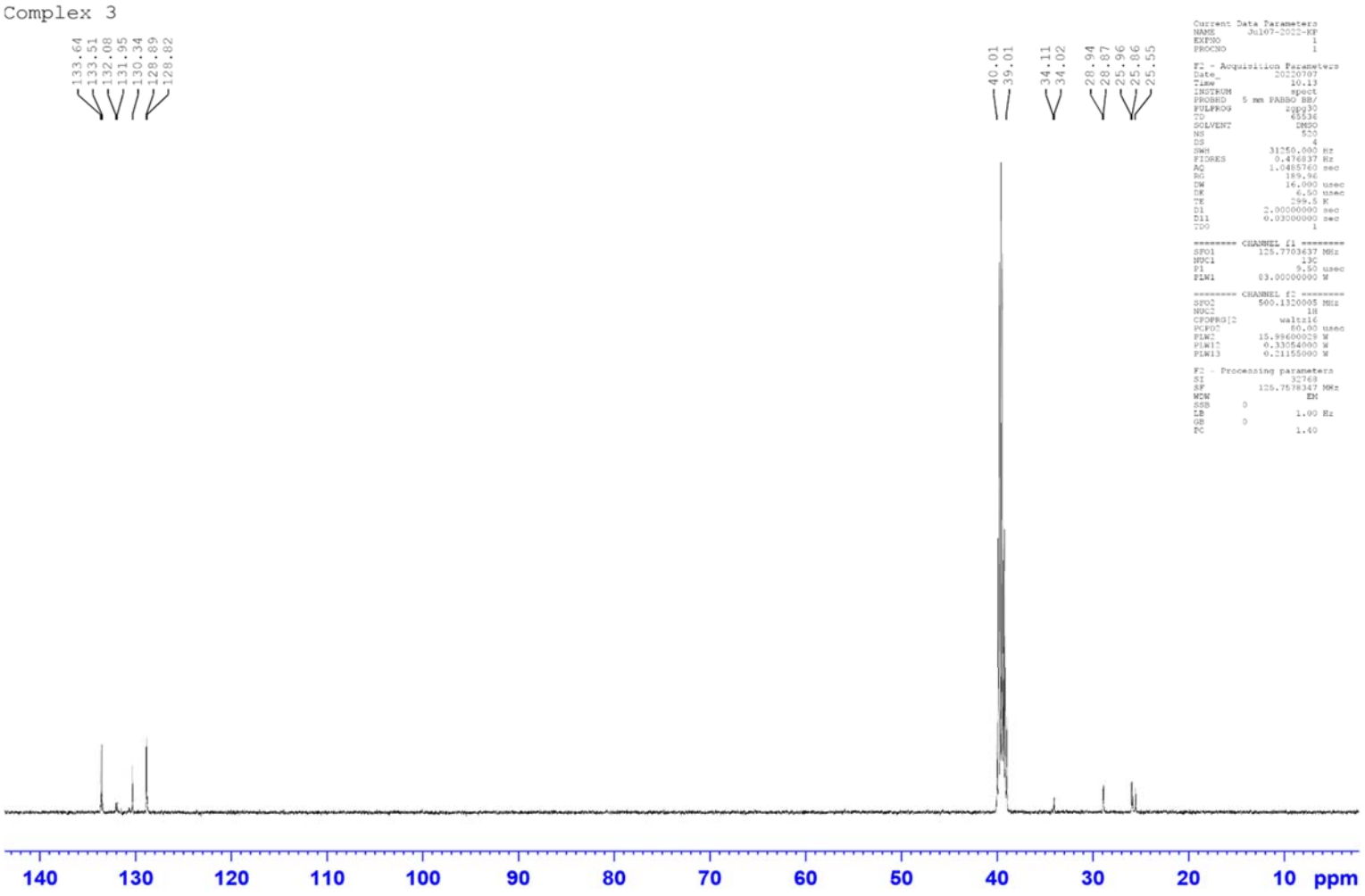



**Figure S8:** $^{13}C\{H\}$-NMR spectrum of complex **3**.

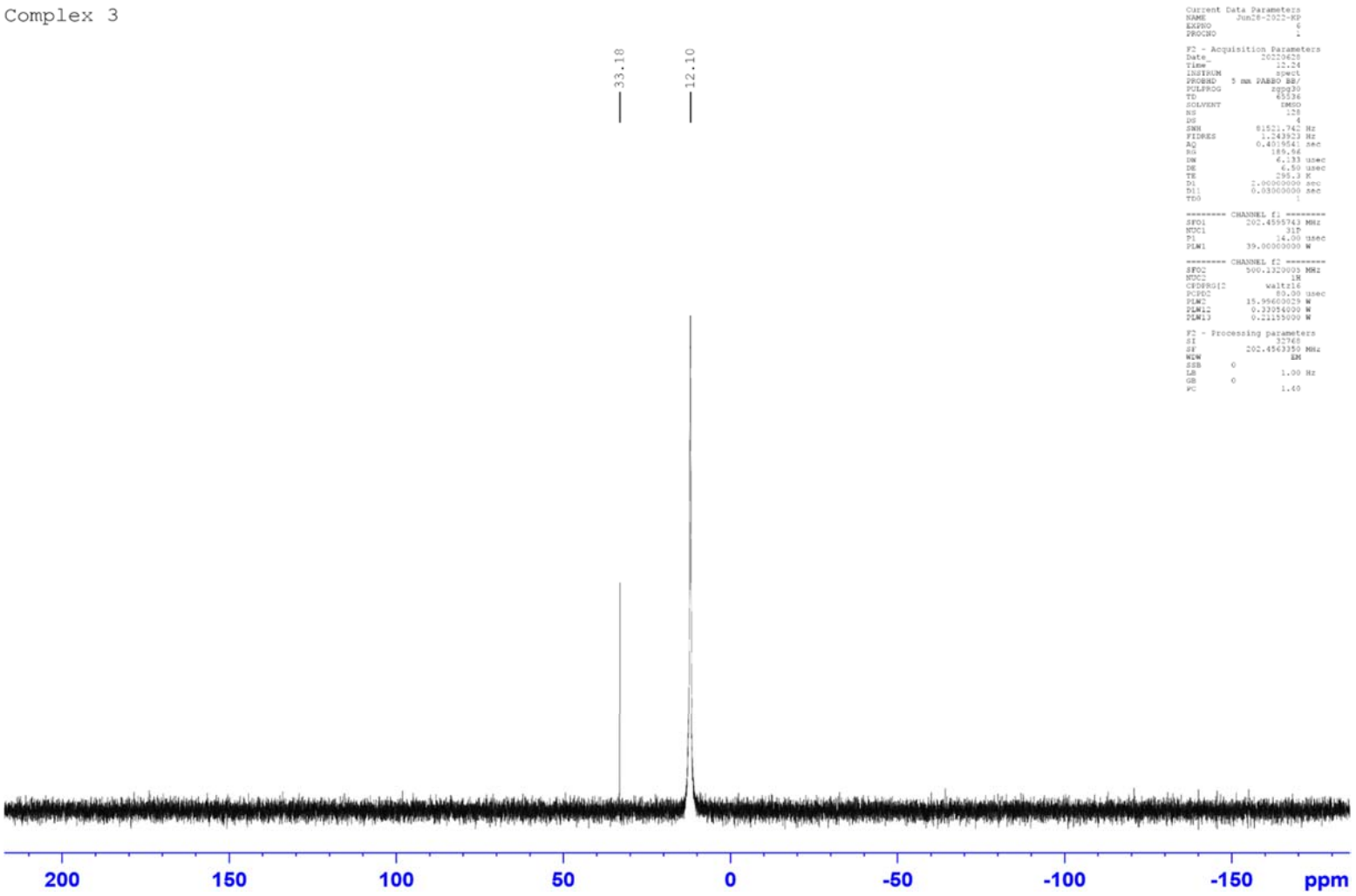



**Figure S9:** $^{31}P\{H\}$-NMR spectrum of complex **3**.

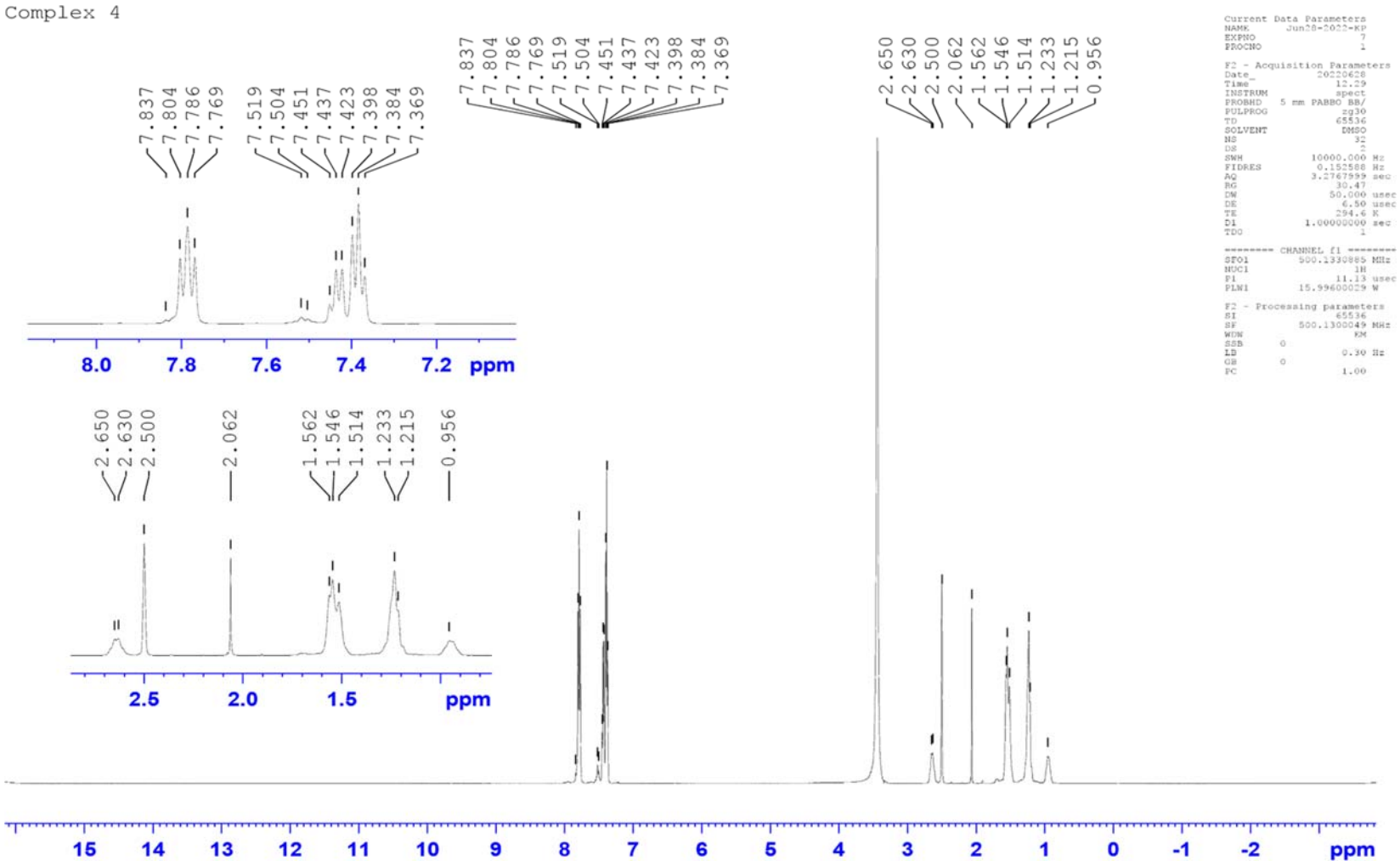



**Figure S10:** $^{1}$H-NMR spectrum of complex **4**.

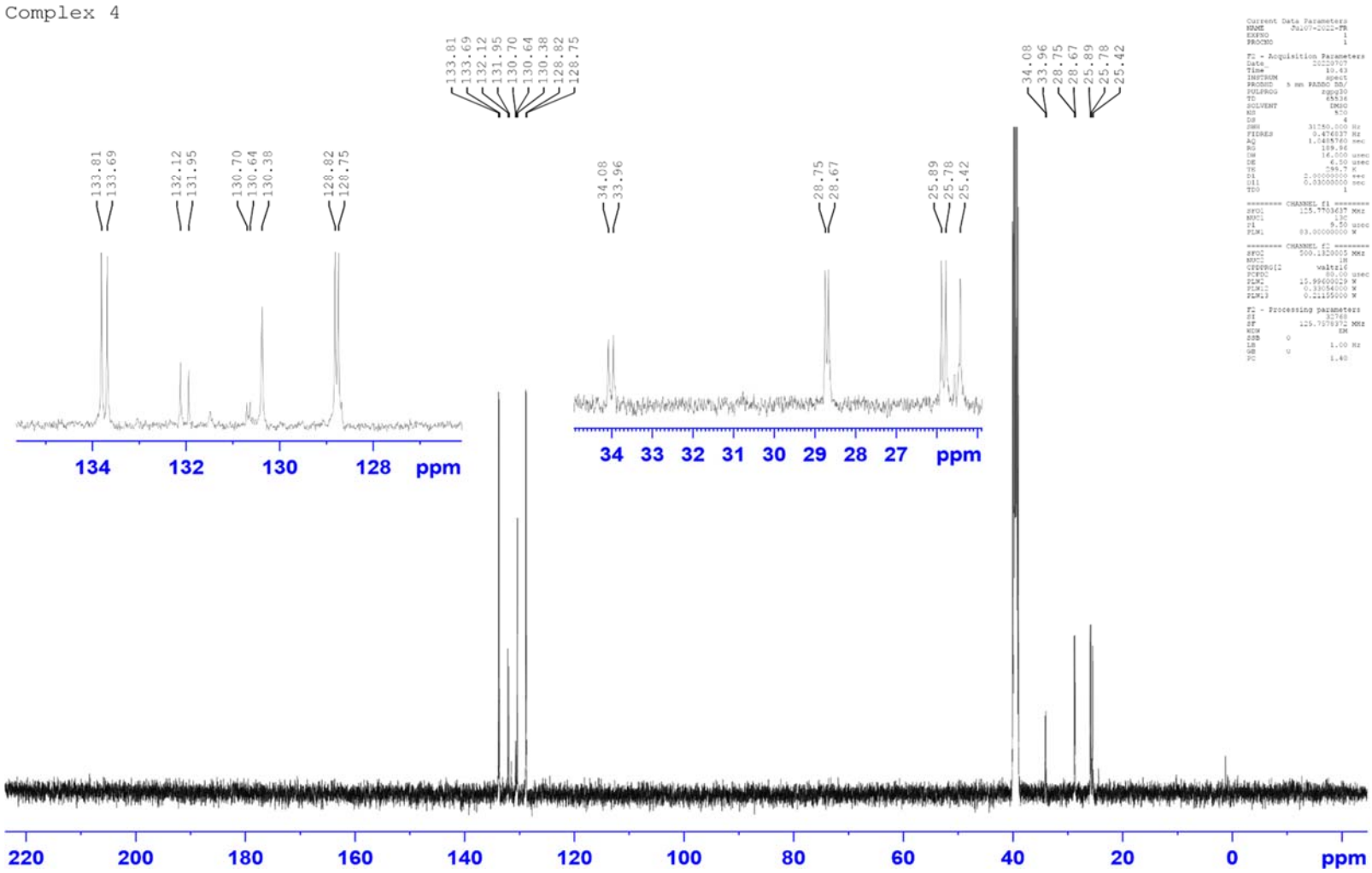



**Figure S11:** $^{13}C\{H\}$-NMR spectrum of complex **4**.

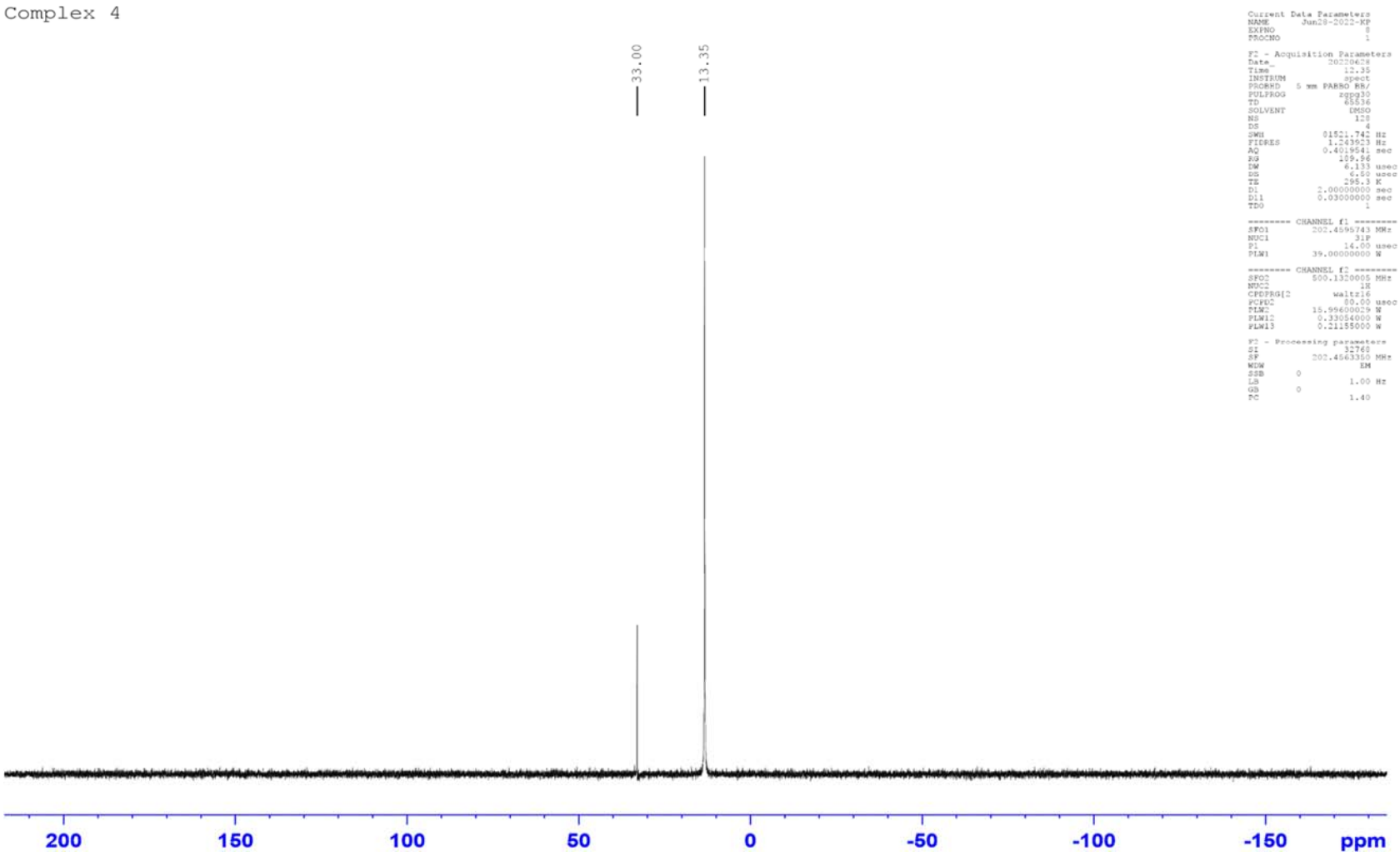



**Figure S12:** $^{31}P\{H\}$-NMR spectrum of complex **4**.

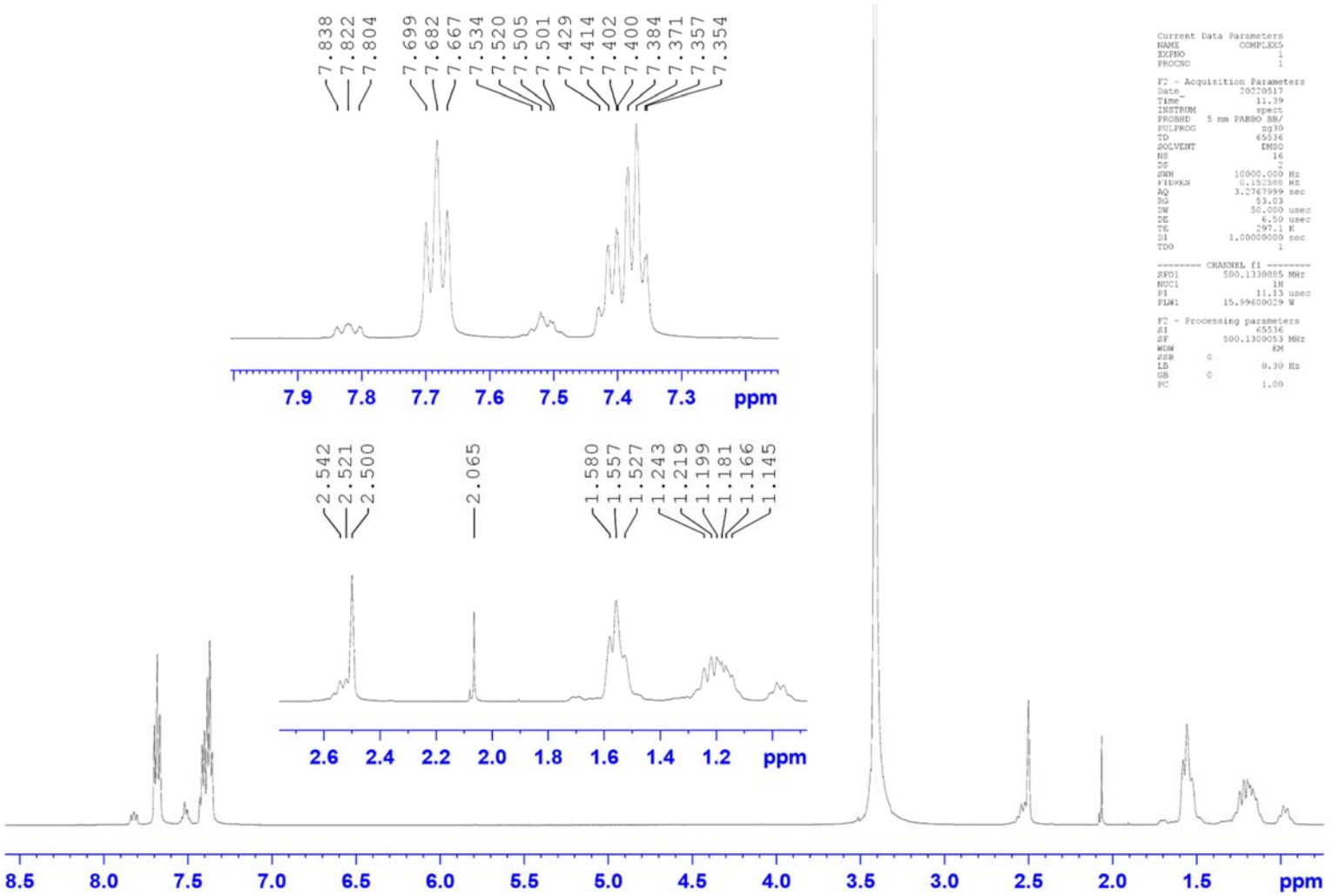



**Figure S13:** $^{1}$H-NMR spectrum of complex **5**.

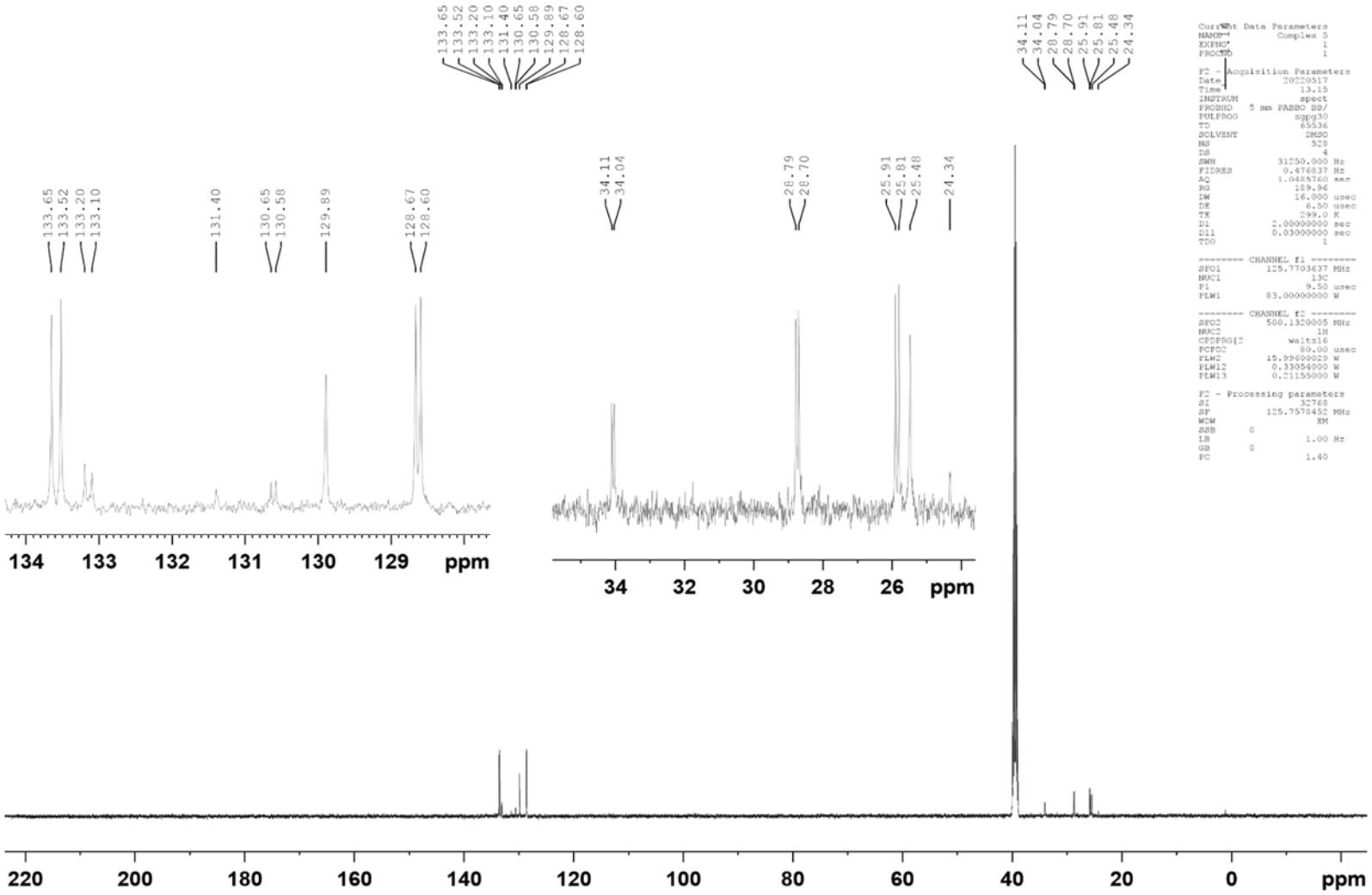
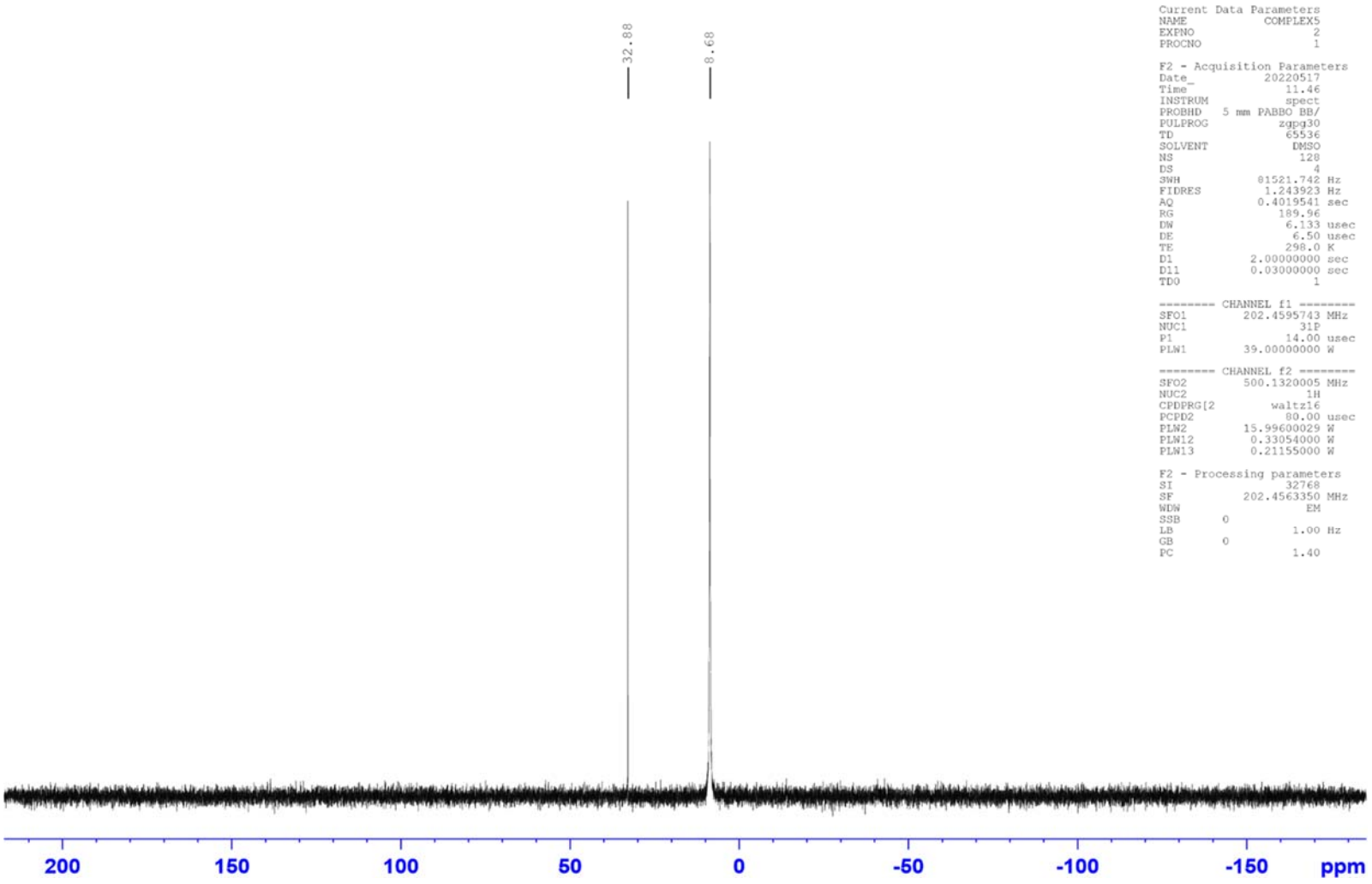



**Figure S14:** $^{13}C\{H\}$-NMR spectrum of complex **5**.

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PROCNO                       1

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TD                        65536
SOLVENT                   DMSO
NS                          128
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FIDRES              1.243923 Hz
AQ                  0.4019541 sec
RG                      189.96
DW                       6.133 usec
DE                       6.50 usec
TE                      298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                          1

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NUC1                      31P
P1                      14.00 usec
PLW1             39.00000000 W

======== CHANNEL f2 ========
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NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   80.00 usec
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PLW12             0.33054000 W
PLW13             0.21155000 W

F2 - Processing parameters
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WDW                         EM
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**Figure S15:** $^{31}P\{H\}$-NMR spectrum of complex **5**.

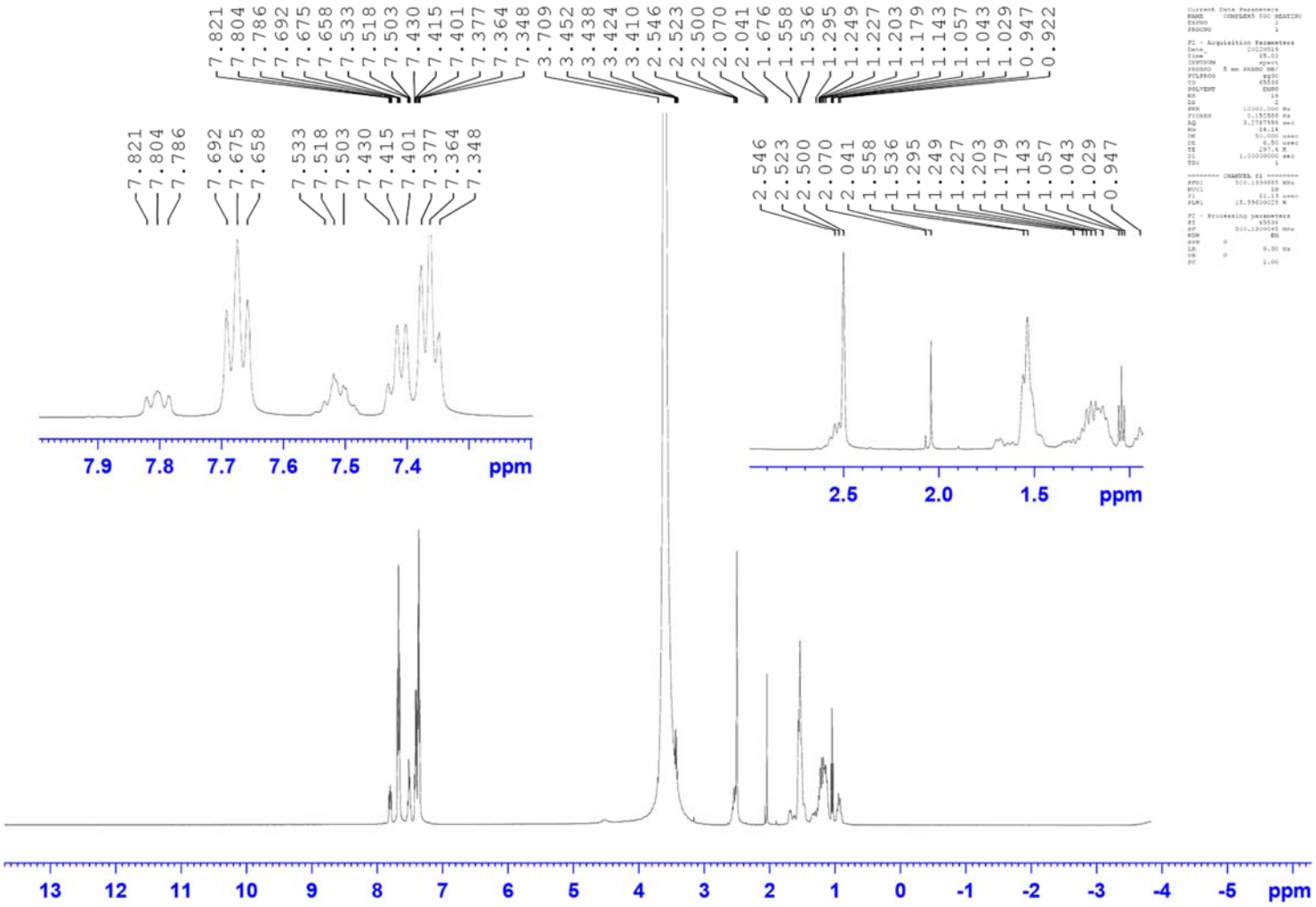


**Figure S16:** $^{1}$H-NMR spectrum of complex **5** after heat treatment (1 hour at 70°C).

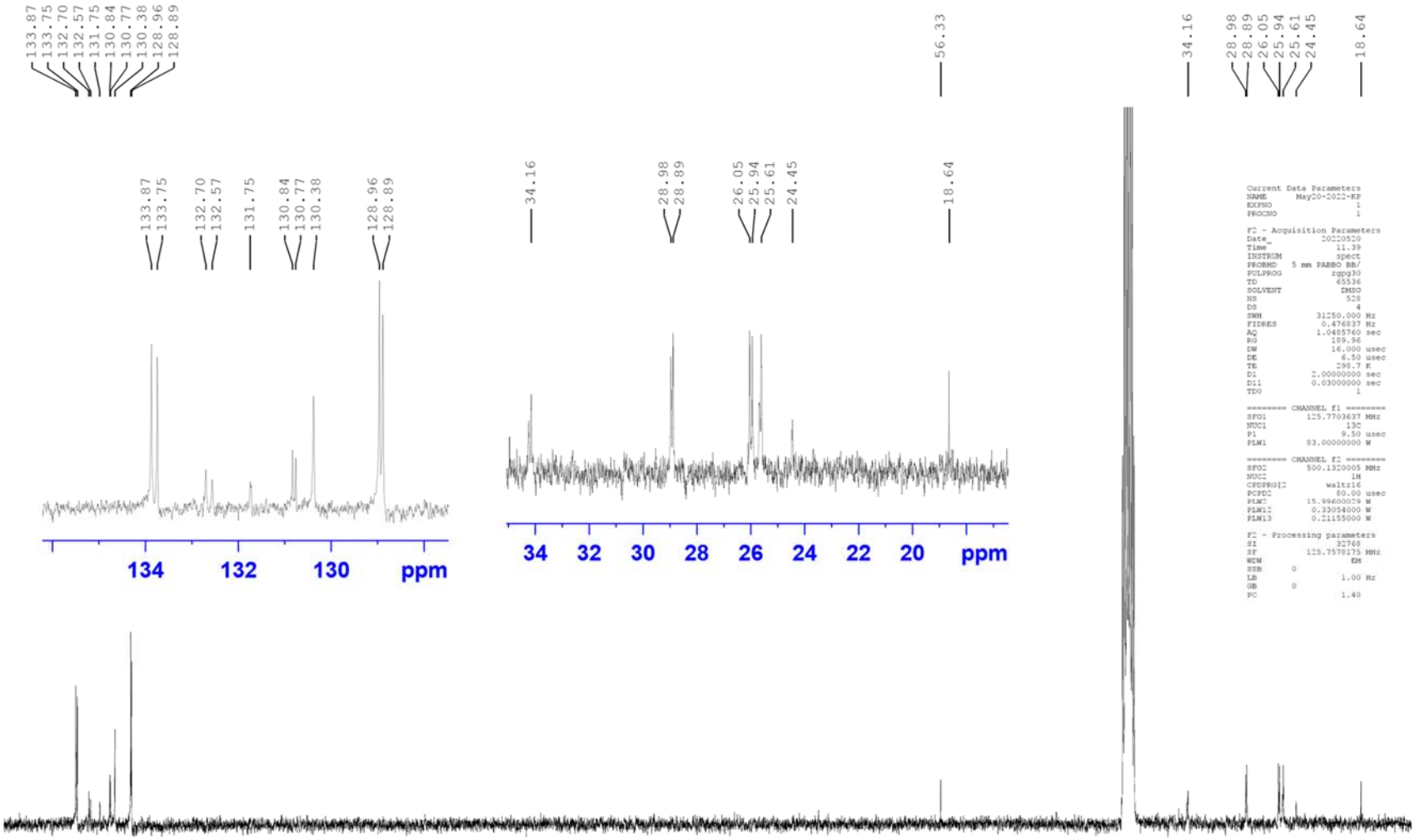


**Figure S17:** $^{13}C\{H\}$-NMR spectrum of complex **5** after heat treatment (1 hour at 70°C).

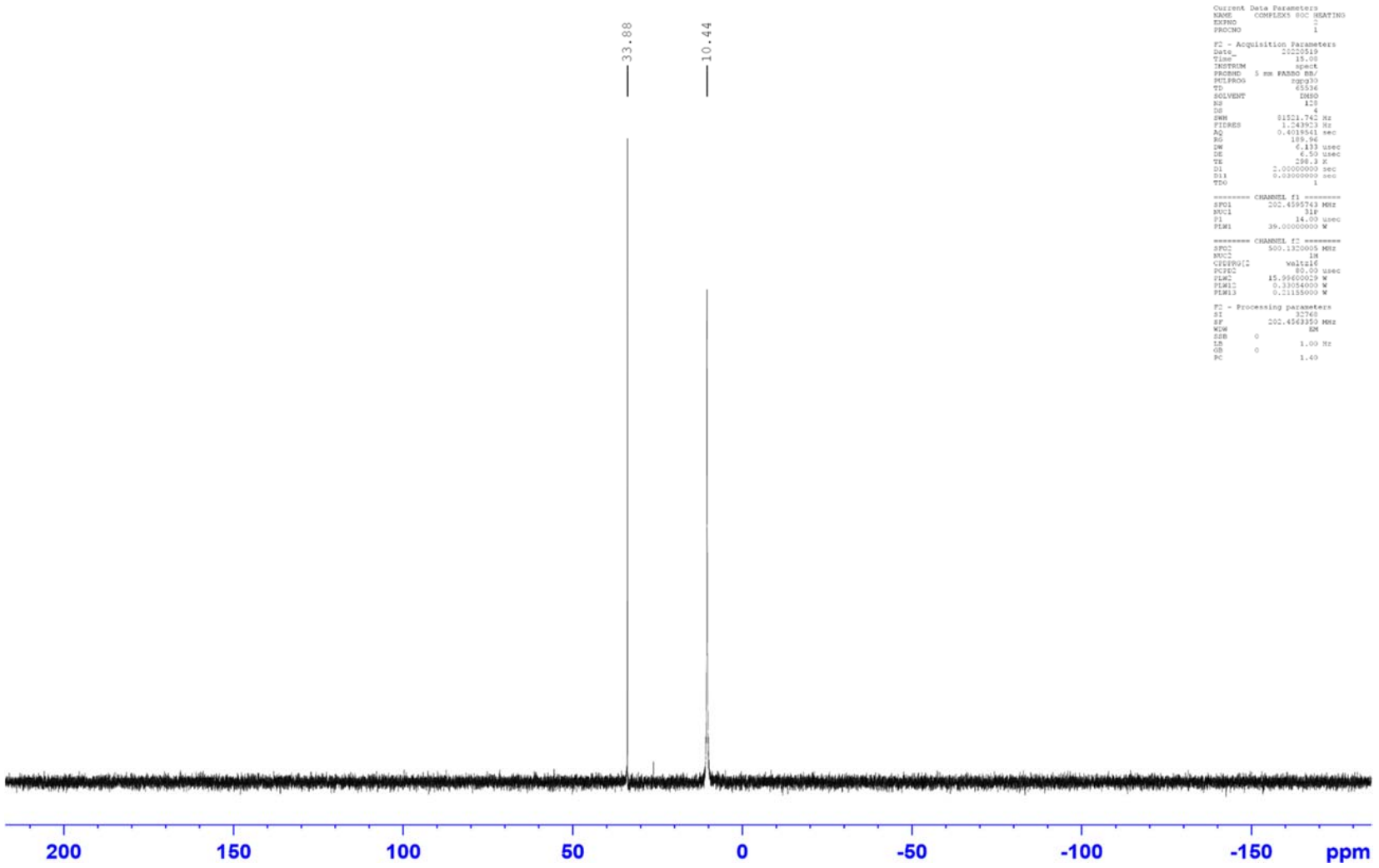


**Figure S18:** $^{31}P\{H\}$-NMR spectrum of complex **5** after heat treatment (1 hour at 70°C).

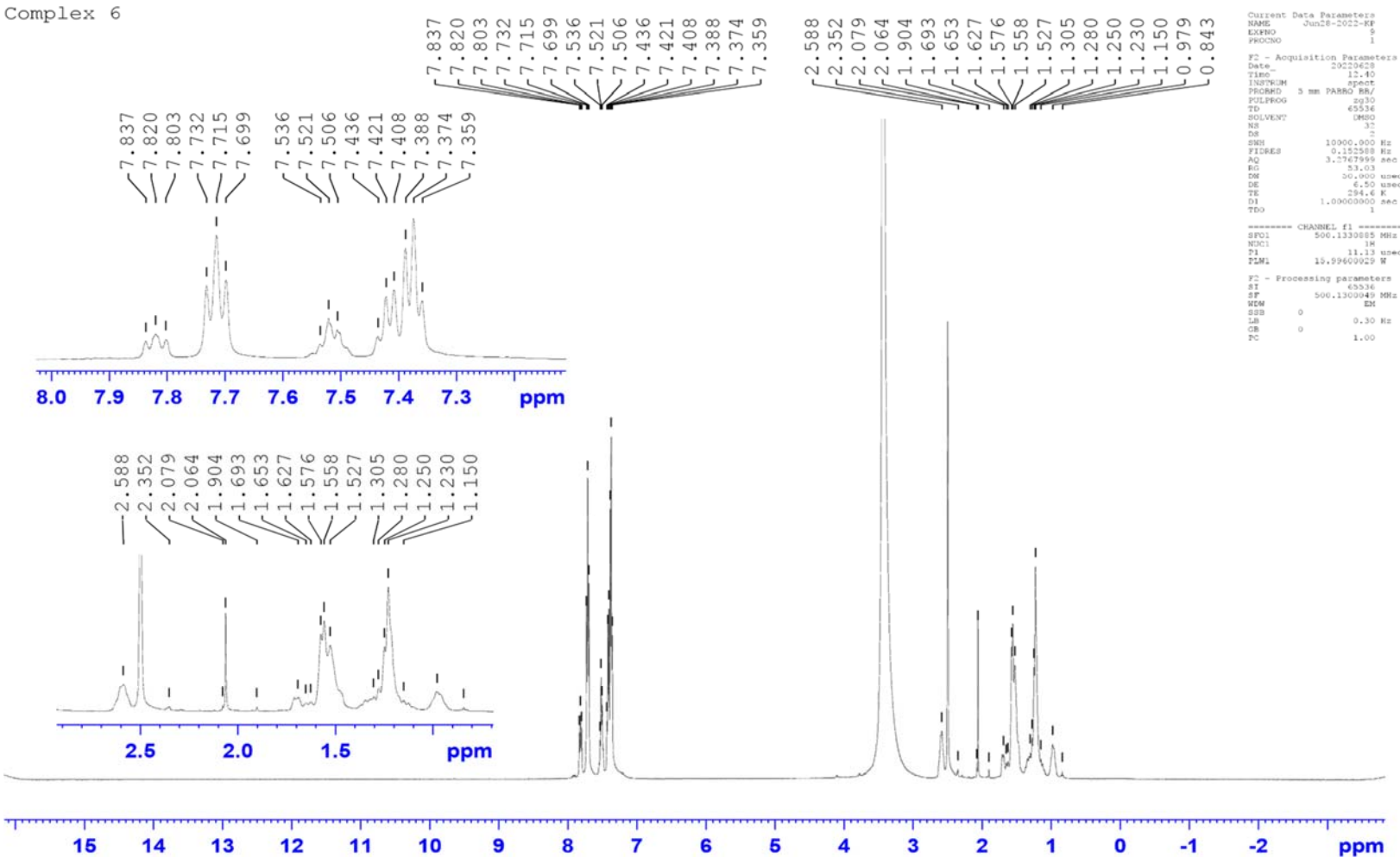


**Figure S19:** $^{1}$H-NMR spectrum of complex **6**.

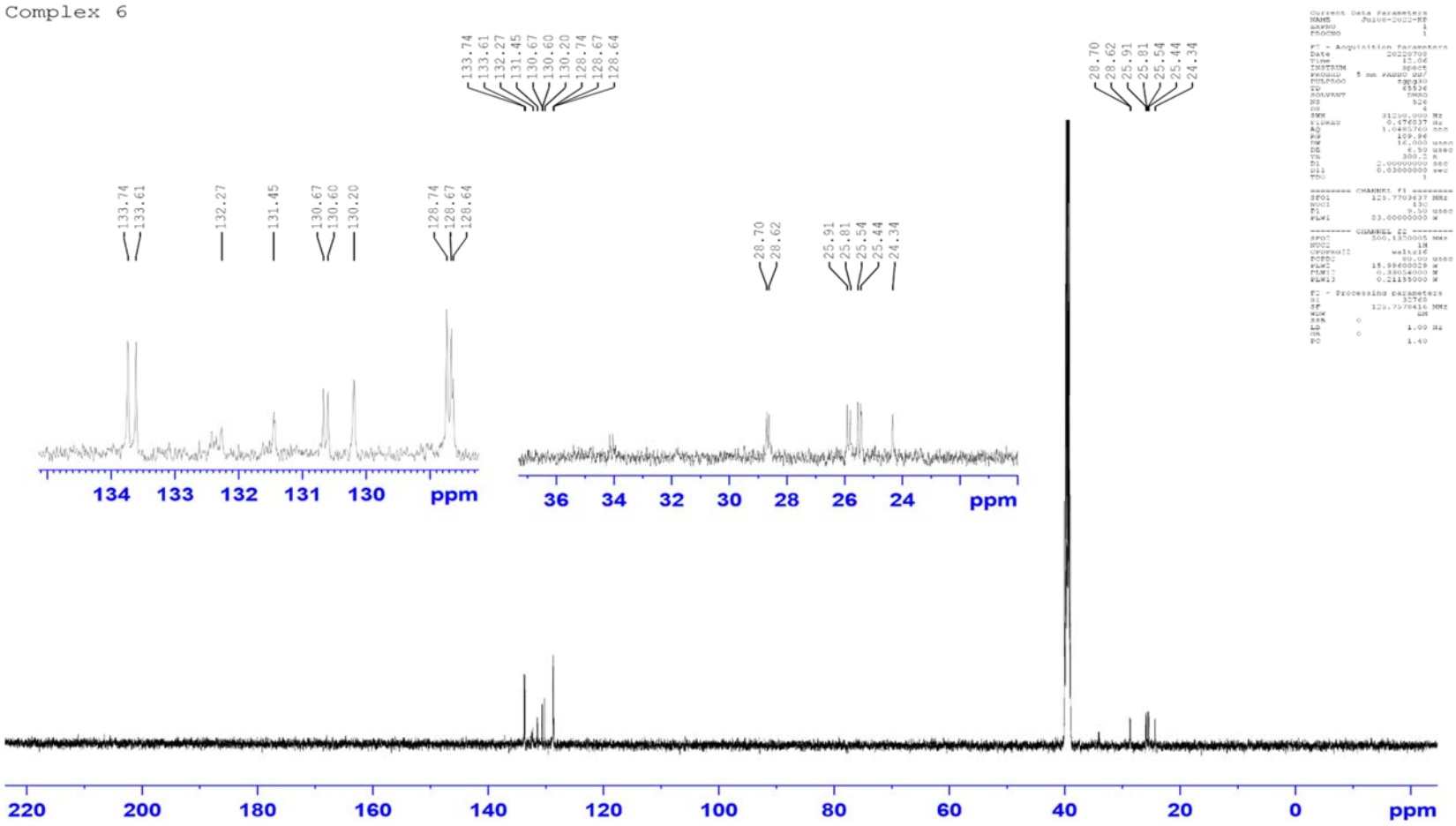


**Figure S20:** $^{13}C\{H\}$-NMR spectrum of complex **6**.

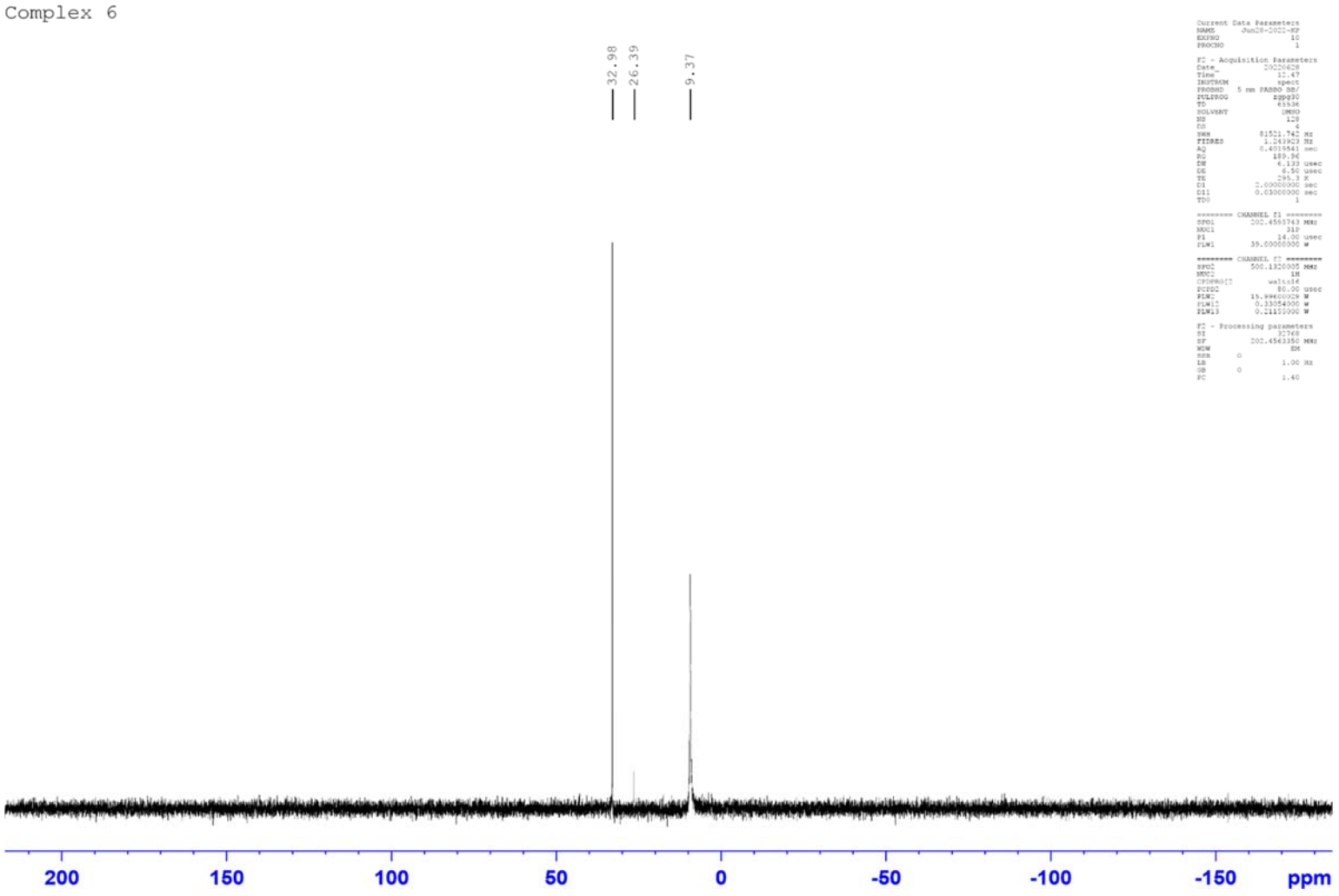


**Figure S21:** $^{31}P\{H\}$-NMR spectrum of complex **6**.

## 2. Crystallographic data and structure refinement parameters (Tables S1, S2).

**Table S1.** Crystal data and structure refinement for **5**, **5'** and **6**.

| Complex | 5 | 5' | 6 |
|---|---|---|---|
| **Emp. Formula** | $C_{56}H_{66}NP_3ClAg$ | $C_{109.89}H_{128.66}N_{1.11}P_6Cl_2Ag_2$ | $C_{56}H_{66}NP_3BrAg$ |
| **CCDC Identifier** | 1480482 | 2205381 | 2183297 |
| **Form. Weight (g.mol$^{-1}$)** | 989.32 | 3874.96 | 1033.78 |
| **Crystal system** | Triclinic | Triclinic | Triclinic |
| **Space group** | *P*-1 | *P*-1 | *P*-1 |
| **Crystal 23escry.** | Colorless block | colorless block | colorless block |
| **a (Å)** | 10.72080(2) | 13.36190(10) | 10.8451(2) |
| **b (Å)** | 13.2344(2) | 15.0591(2) | 13.2804(2) |
| **c (Å)** | 18.2606(2) | 23.8992(2) | 18.2297(3) |
| **α (°)** | 87.1300(10) | 90.5030(10) | 87.0380(10) |
| **β (°)** | 88.4400(10) | 90.7230(10) | 88.7920(10) |
| **γ (°)** | 72.1430(10) | 91.0590(10) | 71.843(2) |
| **Volume (Å$^3$)** | 2462.77(5) | 4807.55(8) | 2491.47(8) |
| **Z** | 2 | 2 | 2 |
| **Abs. coeff. (m.mm$^{-1}$)** | 0.599 | 0.612 | 1.340 |
| **F(000)** | 1036.0 | 2027.5 | 1072.0 |
| **Independent refl.** | 13199 | 25676 | 13250 |
| **Completeness (%)** | 99.9 | 99.9 | 99.9 |
| **Data/Restr/Para** | 13199/0/548 | 25676/36/1105 | 13250/0/548 |
| **Goodness of fit on F$^2$** | 1.070 | 1.061 | 1.069 |
| **Final $R_1$ indexes** | 0.0320 | 0.0289 | 0.0362 |
| **w$R_2$ indices (all data)** | 0.0809 | 0.0702 | 0.0921 |
| **Largest diffr. Peak and hole (e.Å$^{-3}$)** | 1.21/-1.02 | 0.49/-0.44 | 1.41/-1.24 |

**Table S2.** Selected bond lengths and angles for **5**, **5'** and **6**.

| Description | 5 | 5'[a] | 6 |
|---|---|---|---|
| **Ag1-P1** | 2.5356(4) | 2.5258(4) | 2.5375(6) |
| **Ag1-P2** | 2.5262(4) | 2.5209(4) | 2.5336(6) |
| **Ag1-P3** | 2.5283(4) | 2.5155(4) | 2.5321(6) |
| **Ag-X**[b] | 2.6124(4) | 2.5746(4) | 2.7239(2) |
| **P1-$C_{Cy}$** | 1.8462(19) | 1.8573(15) | 1.843(2) |
| **P1-$C_{Ph}$** | 1.8486(17) | 1.8269(15) | 1.8517(13) |
| **P1-$C_{Ph}$** | 1.8256(17) | 1.8276(16) | 1.828(2) |
| **Ag1-P1-$C_{Cy}$** | 115.57(6) | 119.13(5) | 115.46(8) |
| **Ag1-P1-$C_{Ph}$** | 116.33(4) | 112.06(5) | 117.54(6) |
| **Ag1-P1-$C_{Ph}$** | 112.15(5) | 112.26(5) | 115.46(8) |
| **X-Ag1-P1** | 105.267(15) | 105.592(13) | 105.050(14) |
| **P1-Ag1-P2** | 111.758(15) | 110.104(13) | 112.813(19) |
| **P1-Ag1-P3** | 112.645(14) | 112.930(13) | 112.036(19) |
| **P2-Ag1-P3** | 116.565(15) | 117.165(13) | 116.732(19) |
| **X-Ag1-P1-$C_{Cy}$**[b] | 67.65(14) | -62.95(15) | 67.64(10) |
| **X-Ag1-P1-$C_{Ph}$**[b] | -50.18(15) | 57.90(16) | -50.42(13) |
| **X-Ag1-P1-$C_{Ph}$**[b] | -171.42(15) | 173.79(15) | -171.73(15) |
| **P1-Ag1-P2-$C_{Cy}$** | 175.60(17) | 51.82(16) | -50.43(12) |
| **P1-Ag1-P2-$C_{Ph}$** | 56.28(15) | -72.14(15) | -169.29(12) |
| **P1-Ag1-P2-$C_{Ph}$** | -65.43(17) | 171.66(17) | 71.55(15) |

[a] Data of only one molecule is shown. [b] X = halide (Cl, Br).

**3. Fully labeled figures of the molecular structures of 5, 5' and 6.**

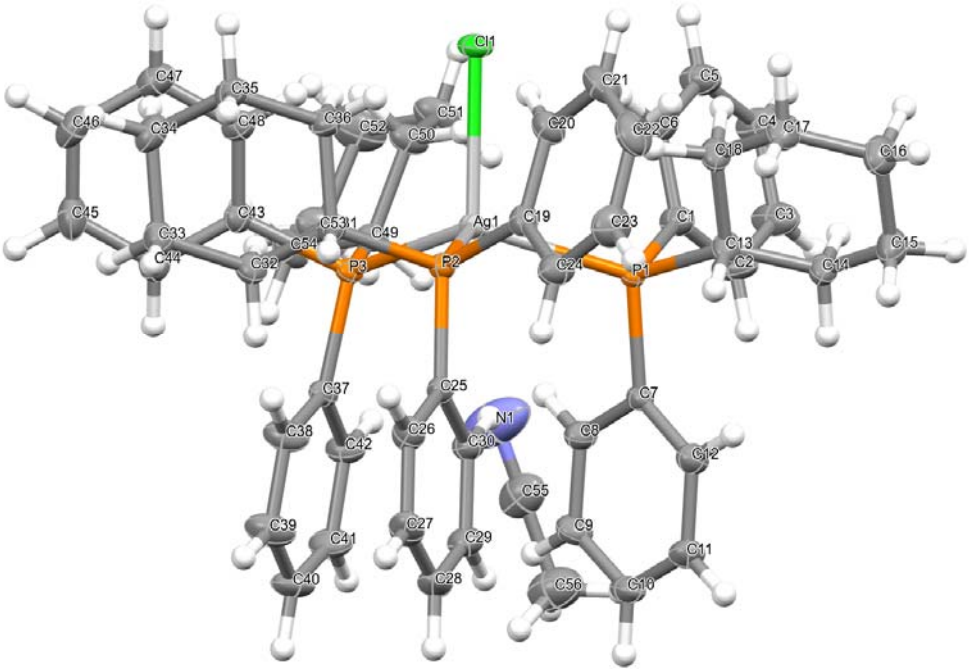


**Figure S22:** Molecular structure of complex **5** with thermal ellispoids drawn at 50% probability level.

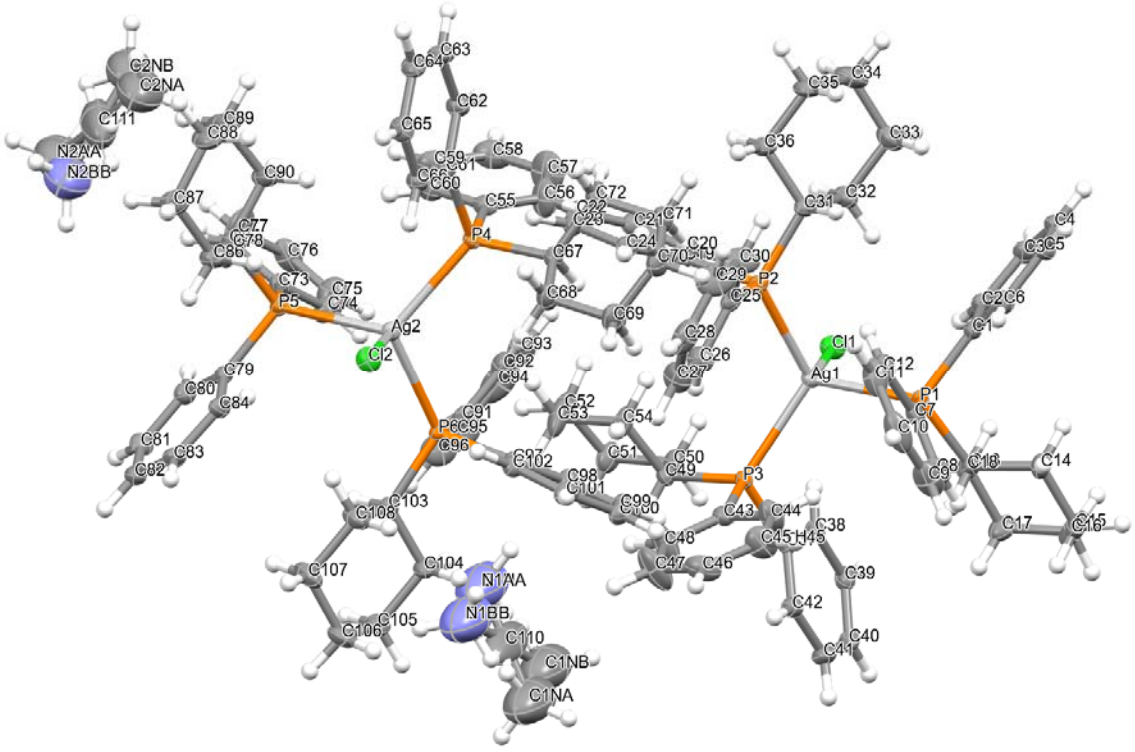


**Figure S23:** Molecular structure of complex **5'** with thermal ellispoids drawn at 50% probability level.

Complementary to the discussion in the main text, the structure of 5' contained two unique complex molecules, as well as a disordered acetonitrile molecule (featured as two half molecules - each with an sp-hybridized carbon on a special position - over two sites as indicated in **Figure S24**) in the asymmetric unit. In the grown structure, each of the half acetonitrile molecules feature as a full positionally disordered molecule (See figure below) that appears as an "X" over two positions. As part of adequately modeling the disorder each nitrogen and methyl carbon atom was modelled to occupy alternating positions according to the (refined) free variables 0.47792 ($CH_3CN$ molecule 1) and 0.40905 ($CH_3CN$ molecule 2). This means that within $CH_3CN$ molecule 1 the methyl carbon atom occupies the indicated site with a capacity of 48% (and the nitrogen within the same configuration on the opposite end at 48%), while the nitrogen atom occupies the same site (as an alternative configuration) for the remaining 52% (and the methyl carbon within the same alternatice configuration on the opposite end at 52%). Similarly, within $CH_3CN$ molecule 2 the methyl carbon atom occupies the indicated site with a capacity of 41% (and the nitrogen within the same configuration on the opposite end at 41%), while the nitrogen atom occupies the same site (as an alternative configuration) for the remaining 59% (and the methyl carbon within the same alternatice configuration on the opposite end at 59%).

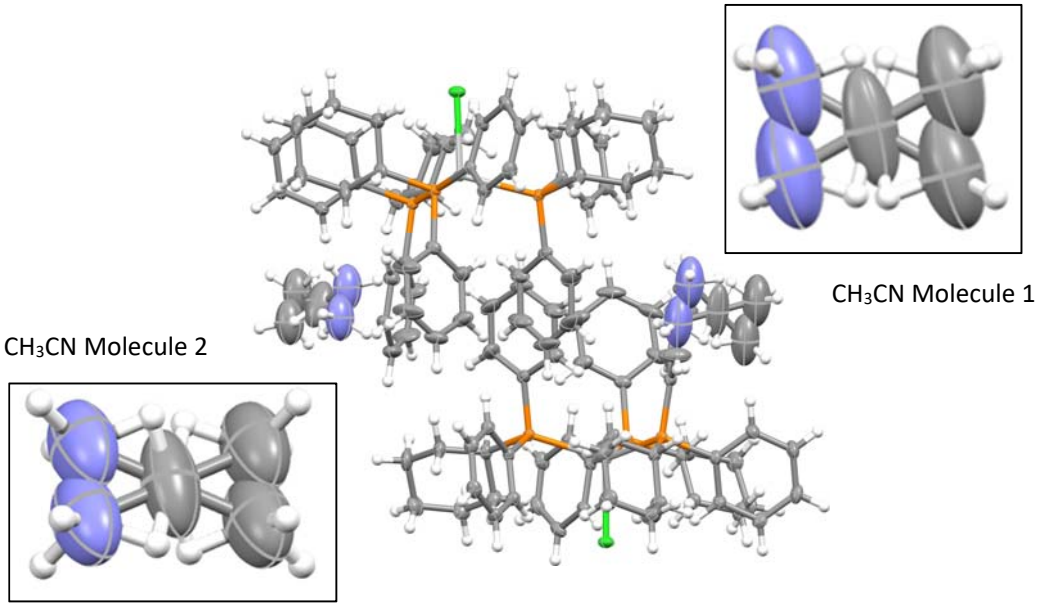


**Figure S24:** Molecular structure of complex **5'**, with thermal ellispoids drawn at 50% probability level.

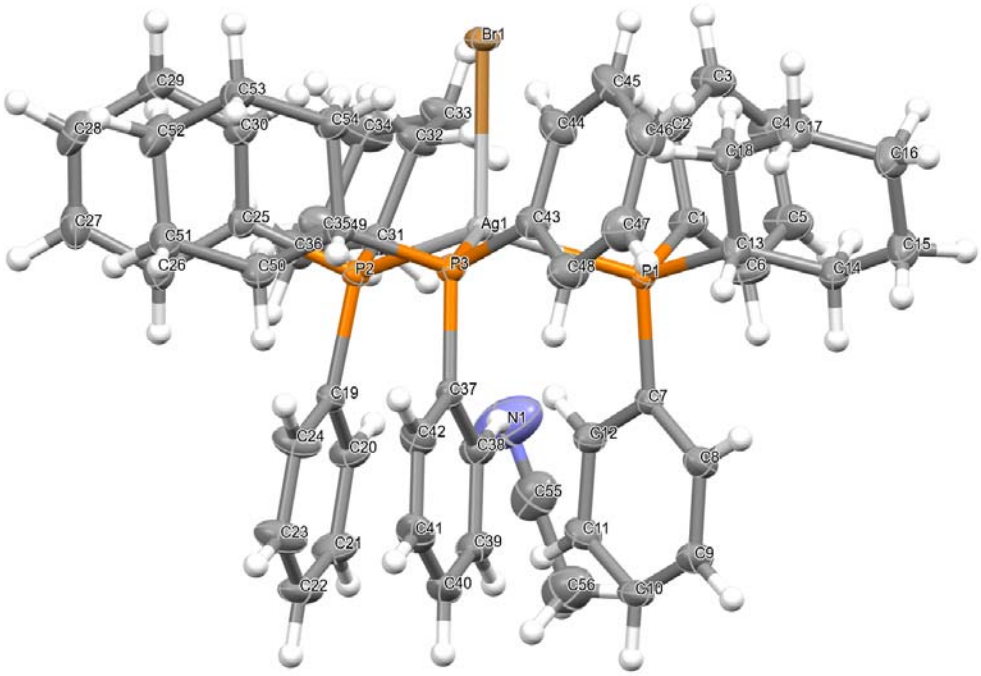


**Figure S25:** Molecular structure of complex **6** with thermal ellispoids drawn at 50% probability level.