

## Supplementary Information

### *syn*-Bimane as a Chelating O-Donor Ligand for Palladium(II)

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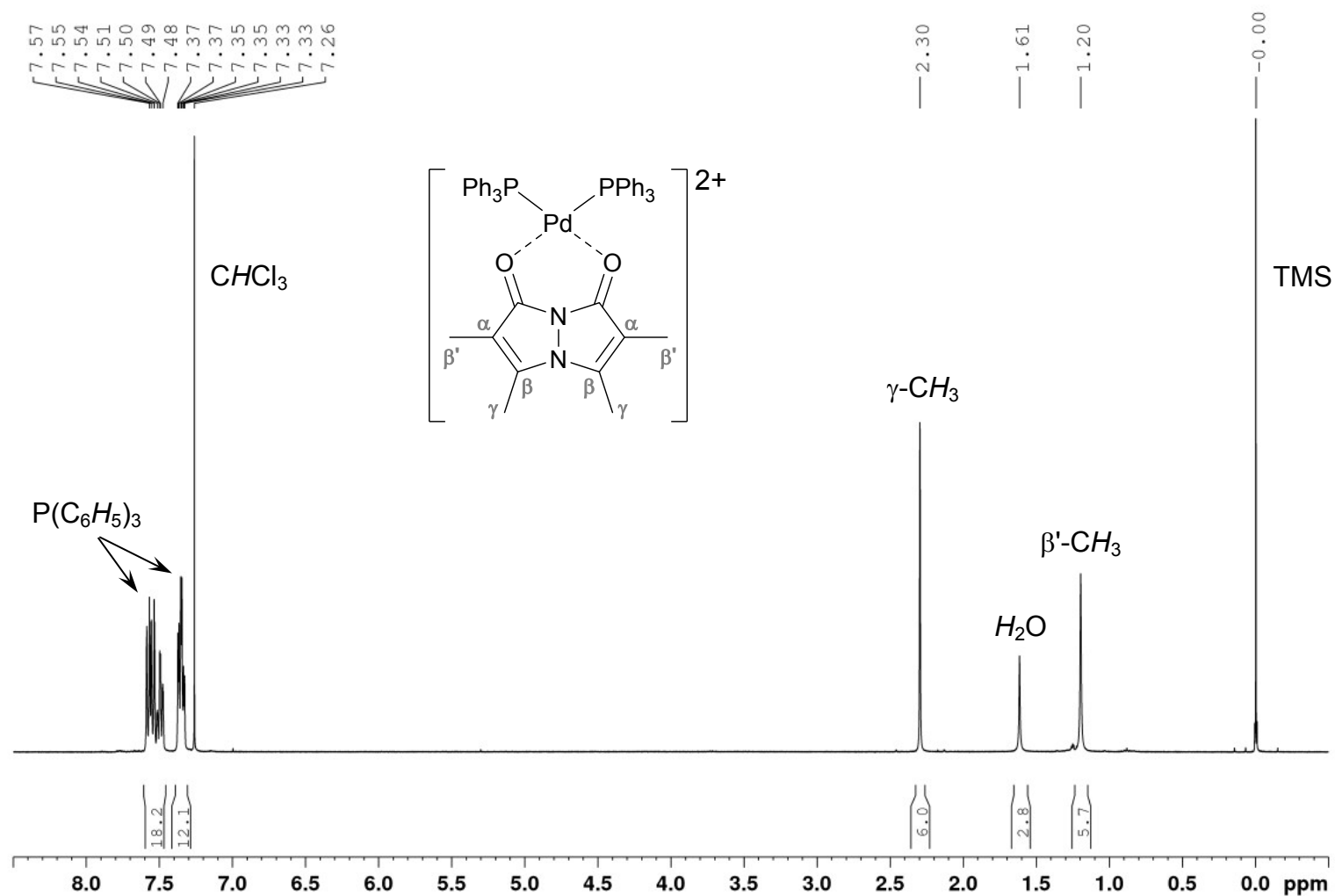
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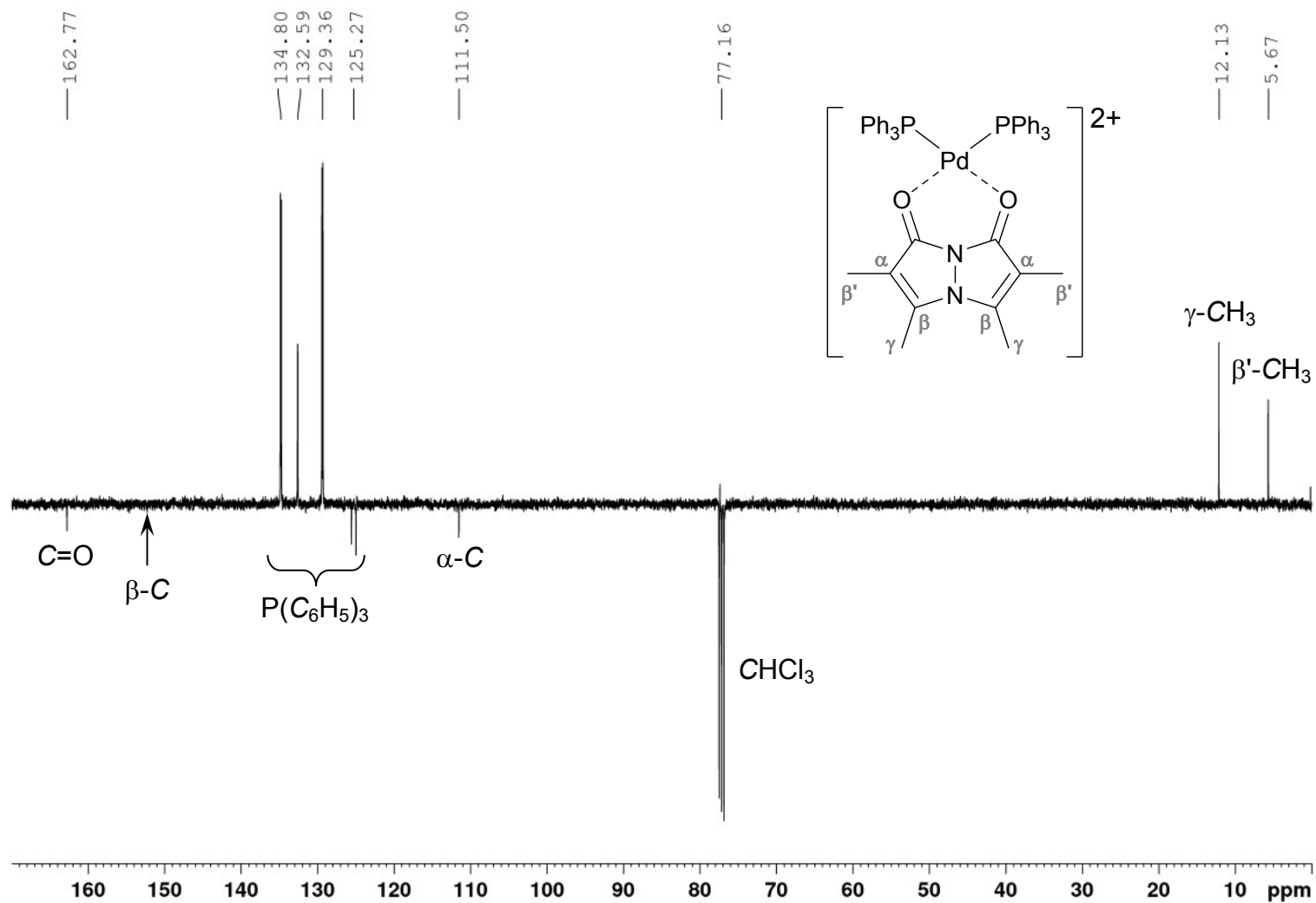
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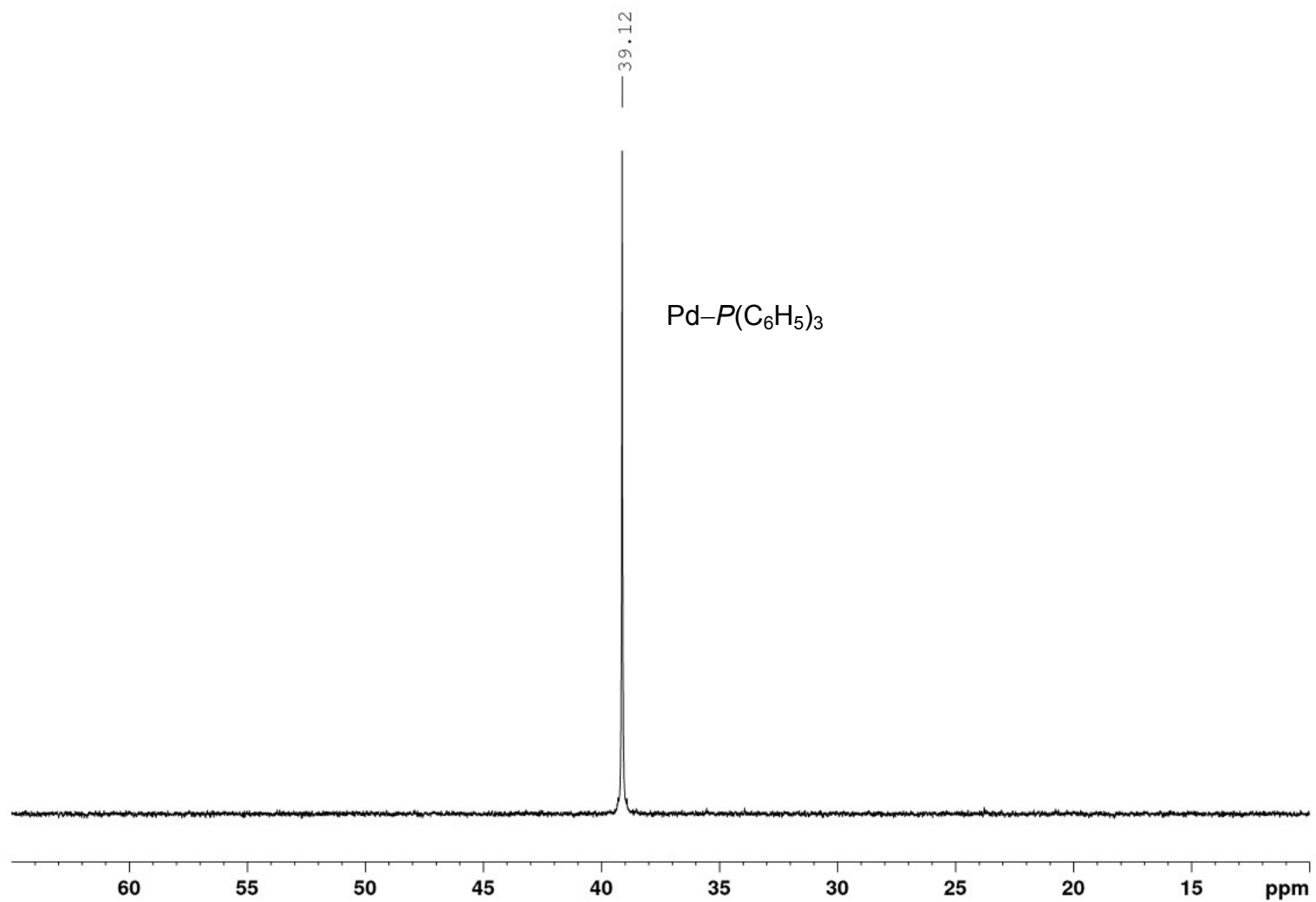
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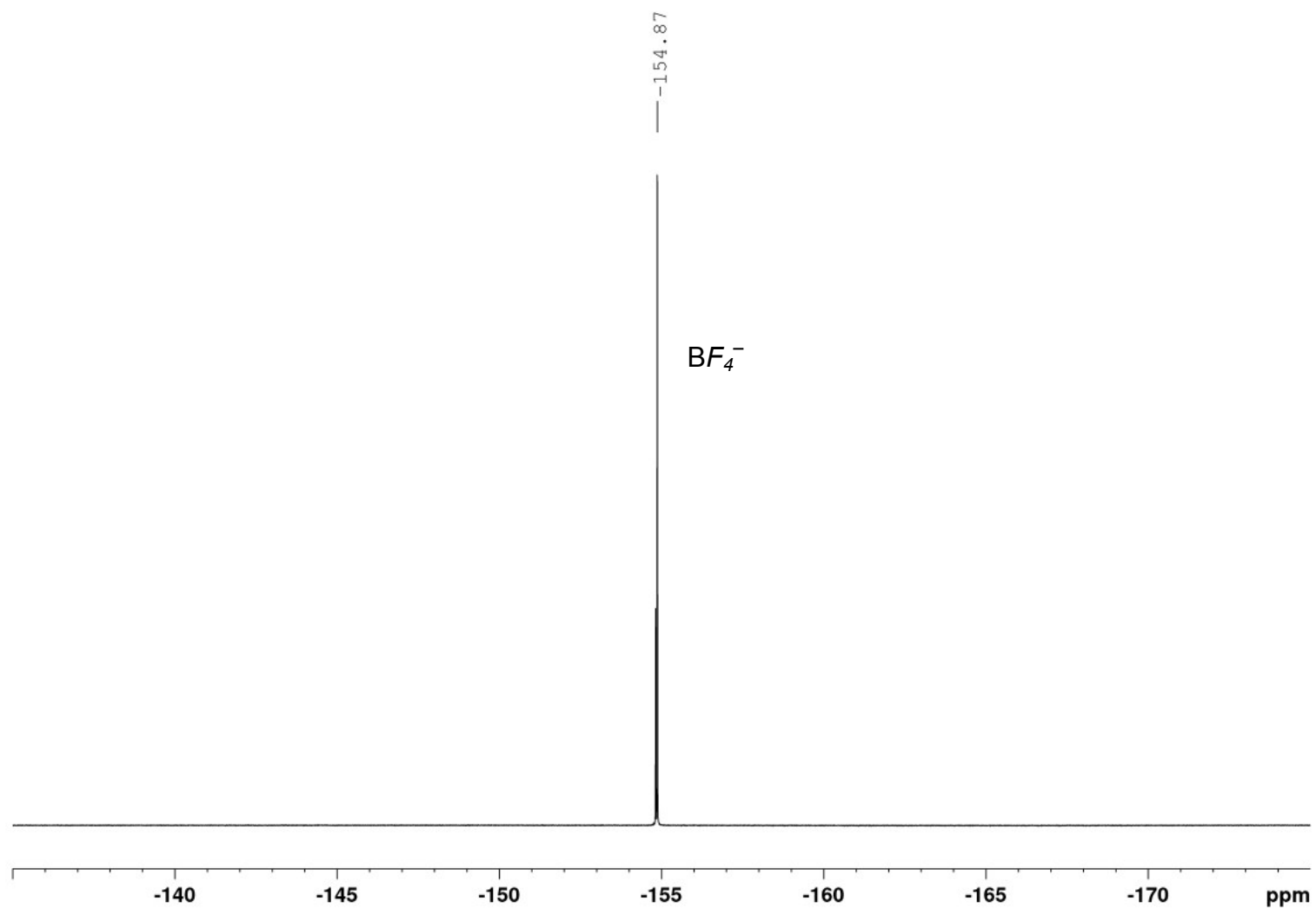
**Figure S1.**  $^1\text{H}$  NMR spectrum of complex **1** in  $\text{CDCl}_3$  (400 MHz, room temperature).



**Figure S2.**  $^{13}\text{C}\{^1\text{H}\}$  DEPTQ NMR spectrum of complex **1** in  $\text{CDCl}_3$  (101 MHz, room temperature).



**Figure S3.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of complex **1** in  $\text{CDCl}_3$  (162 MHz, room temperature).



**Figure S4.**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of complex **1** in  $\text{CDCl}_3$  (376 MHz, room temperature).

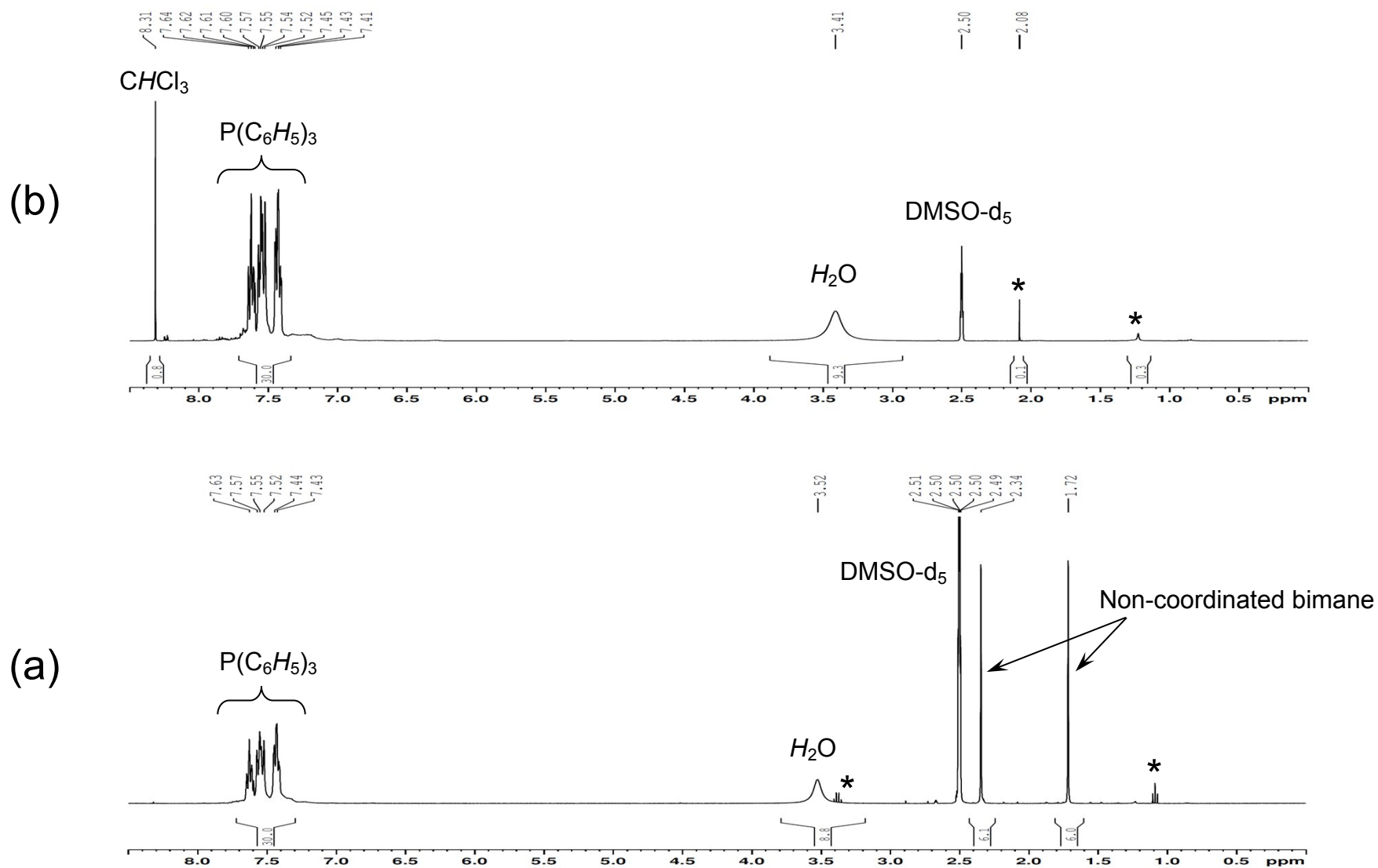
## Synthesis of $[\text{Pd}(\text{PPh}_3)_2(\text{solvent})_2](\text{BF}_4)_2$

To a suspension of 50 mg (0.071 mmol) of  $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$  in 1.5 ml of chloroform were added 28 mg (0.144 mmol) of  $\text{AgBF}_4$ , and the resulting mixture was stirred in the dark, at room temperature, for 15 min. The reaction mixture was then filtered through a cotton plug to remove  $\text{AgCl}$ . The resulting clear solution was divided into two portions, and the solvent was removed under vacuum. This quantitatively yielded the product as two samples of a solid residue. One sample was dissolved in  $\text{DMSO-d}_6$  to afford  $[\text{Pd}(\text{PPh}_3)_2(\text{DMSO-d}_6)_2](\text{BF}_4)_2$ , and the second sample was dissolved in  $\text{CD}_3\text{CN}$  to afford  $[\text{Pd}(\text{PPh}_3)_2(\text{CD}_3\text{CN})_2](\text{BF}_4)_2$ . The  $^1\text{H}$  and  $^{31}\text{P}$  NMR spectra of these complexes are presented below (Figures S5-8),<sup>1,2</sup> alongside the NMR spectra of complex **1** in the same solvents.

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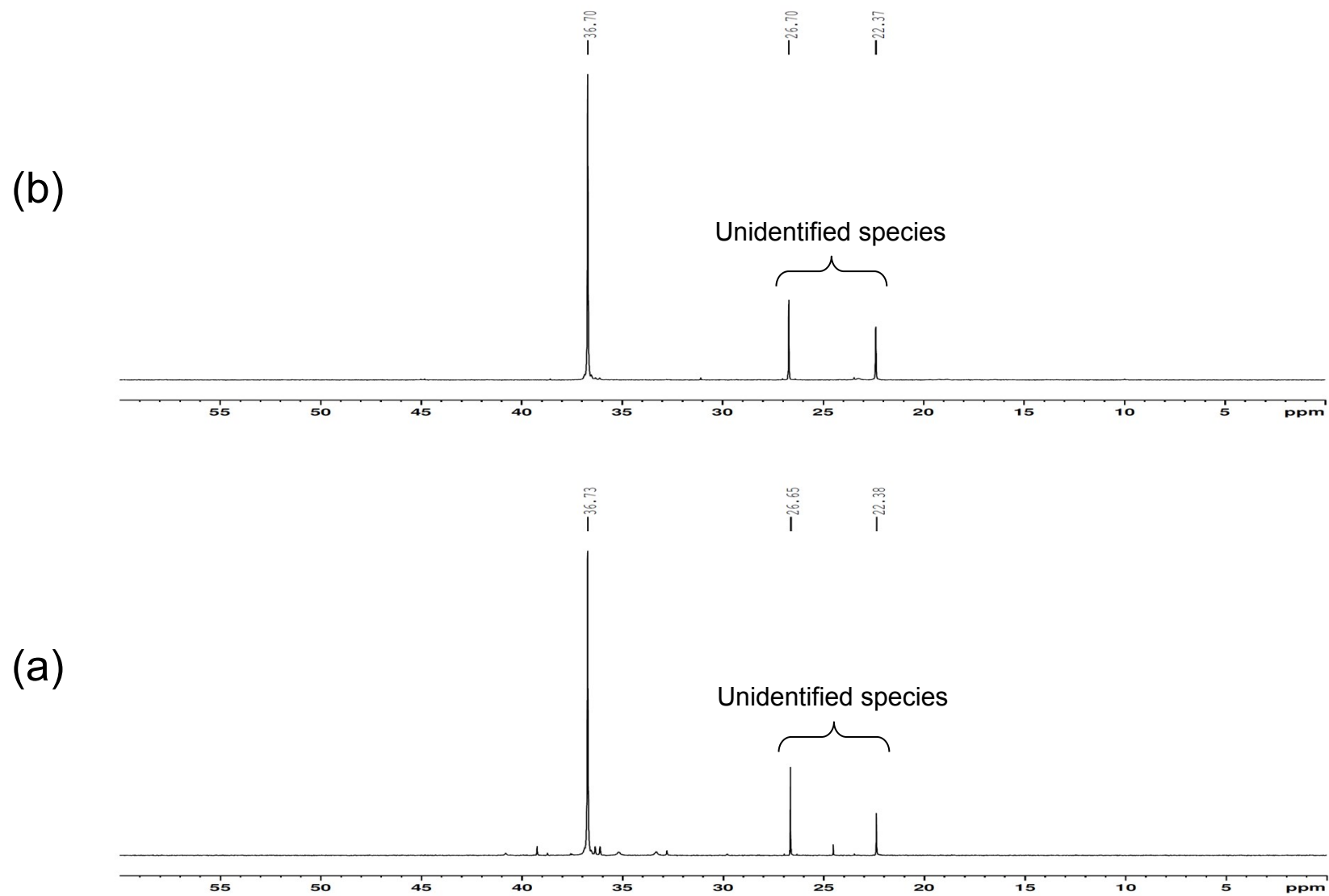
<sup>1</sup> The complex  $[\text{Pd}(\text{PPh}_3)_2(\text{CH}_3\text{CN})_2](\text{BF}_4)_2$  has been previously reported by Lai and Sen, but the available NMR data was collected under conditions that are different from the present work. See: T.-W. Lai, A. Sen, *Organometallics*, 1984, **3**, 866.

<sup>2</sup> The complex  $[\text{Pd}(\text{PPh}_3)_2(\text{DMSO})_2](\text{PF}_6)_2$  has been reported by Wilkinson *et al.*, but the available NMR data was collected under conditions that are different from the present work. See: F. R. Hartley, S. G. Murray, A. Wilkinson, *Inorg. Chem.*, 1989, **28**, 549.

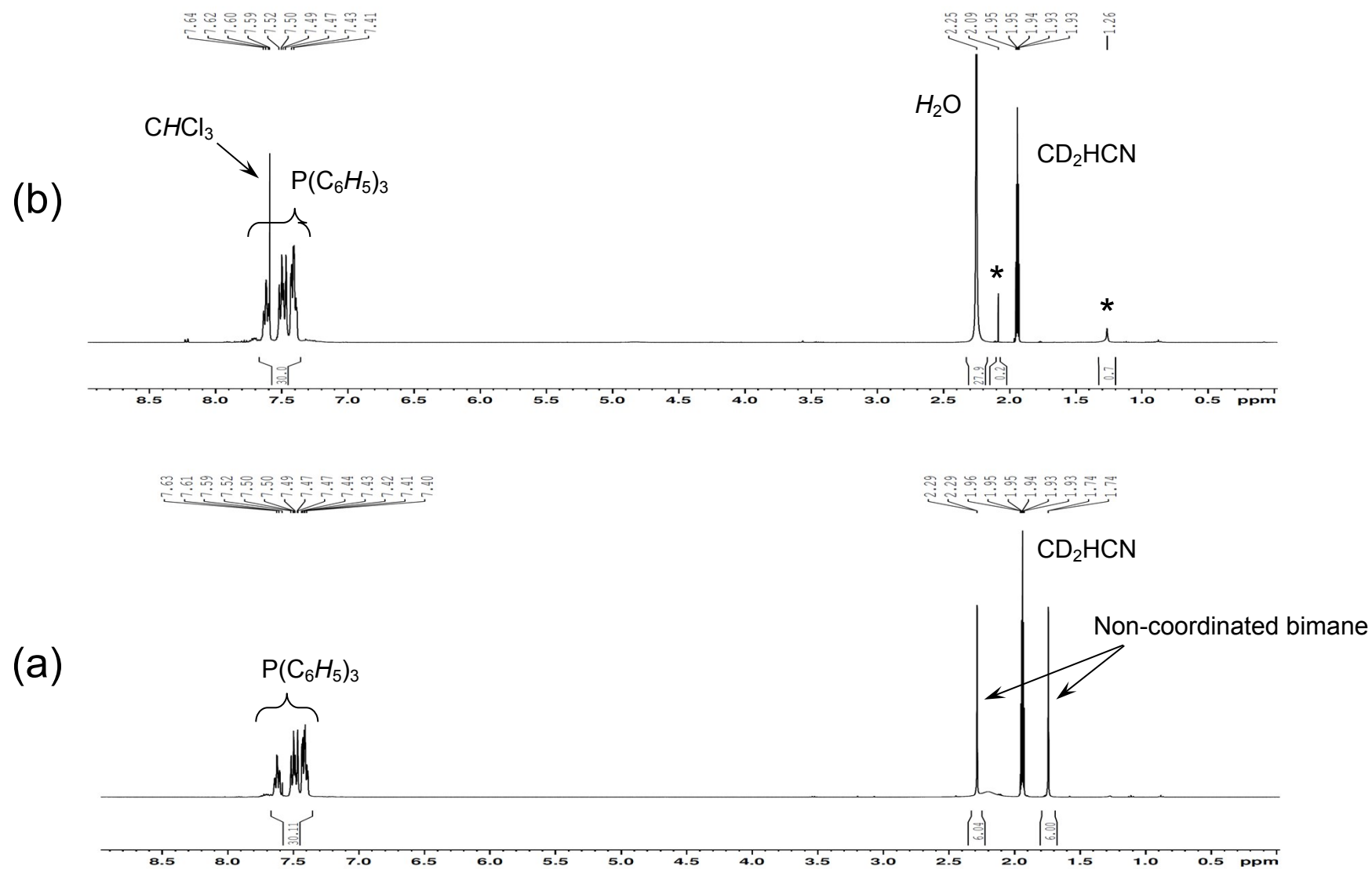


**Figure S5.**  $^1\text{H}$  NMR spectra of complex **1** (a) and  $[\text{Pd}(\text{PPh}_3)_2(\text{DMSO-d}_6)_2](\text{BF}_4)_2$  (b) in  $\text{DMSO-d}_6$  (400 MHz, room temperature). Trace adventitious impurities are marked with asterisks (\*).

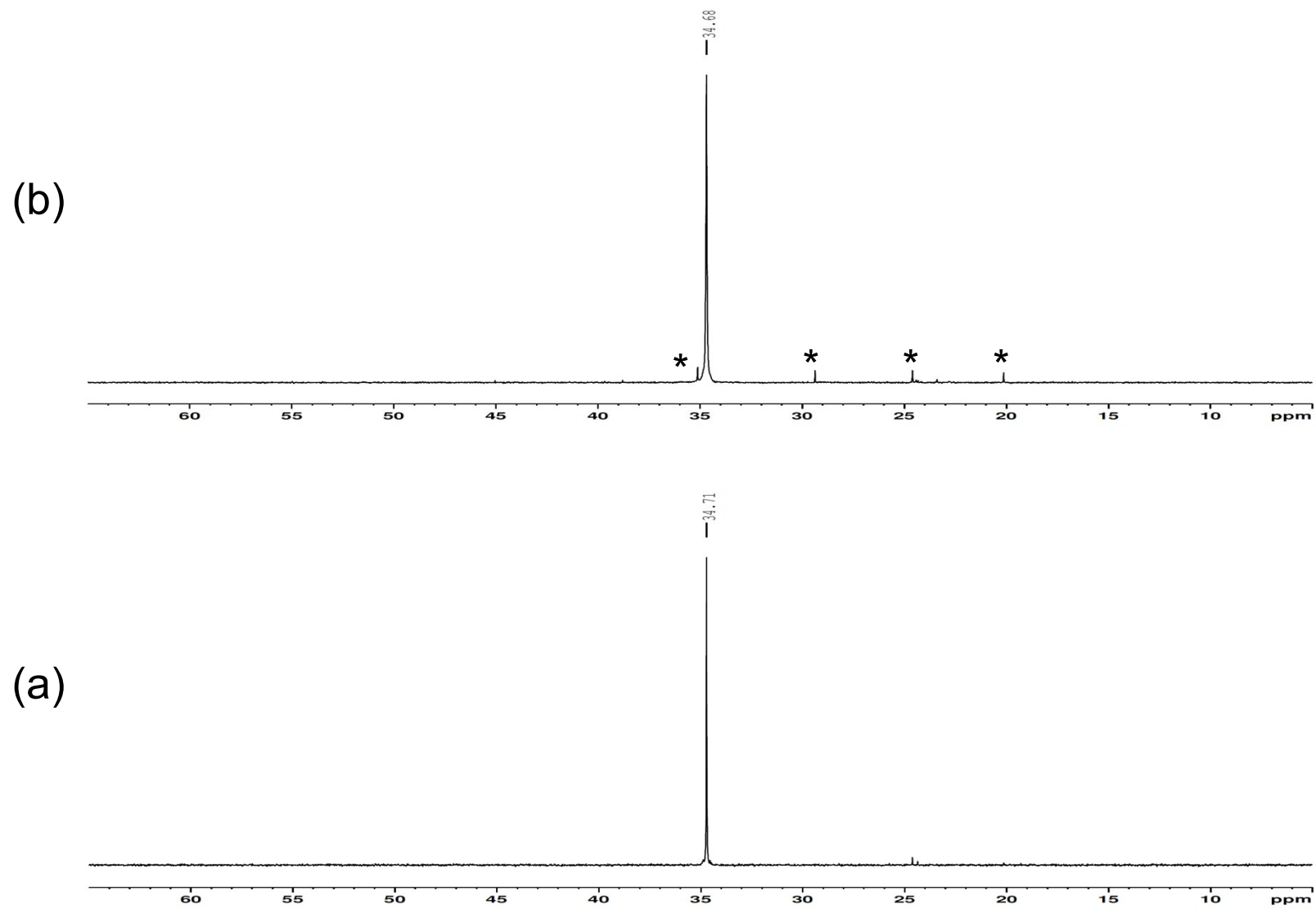




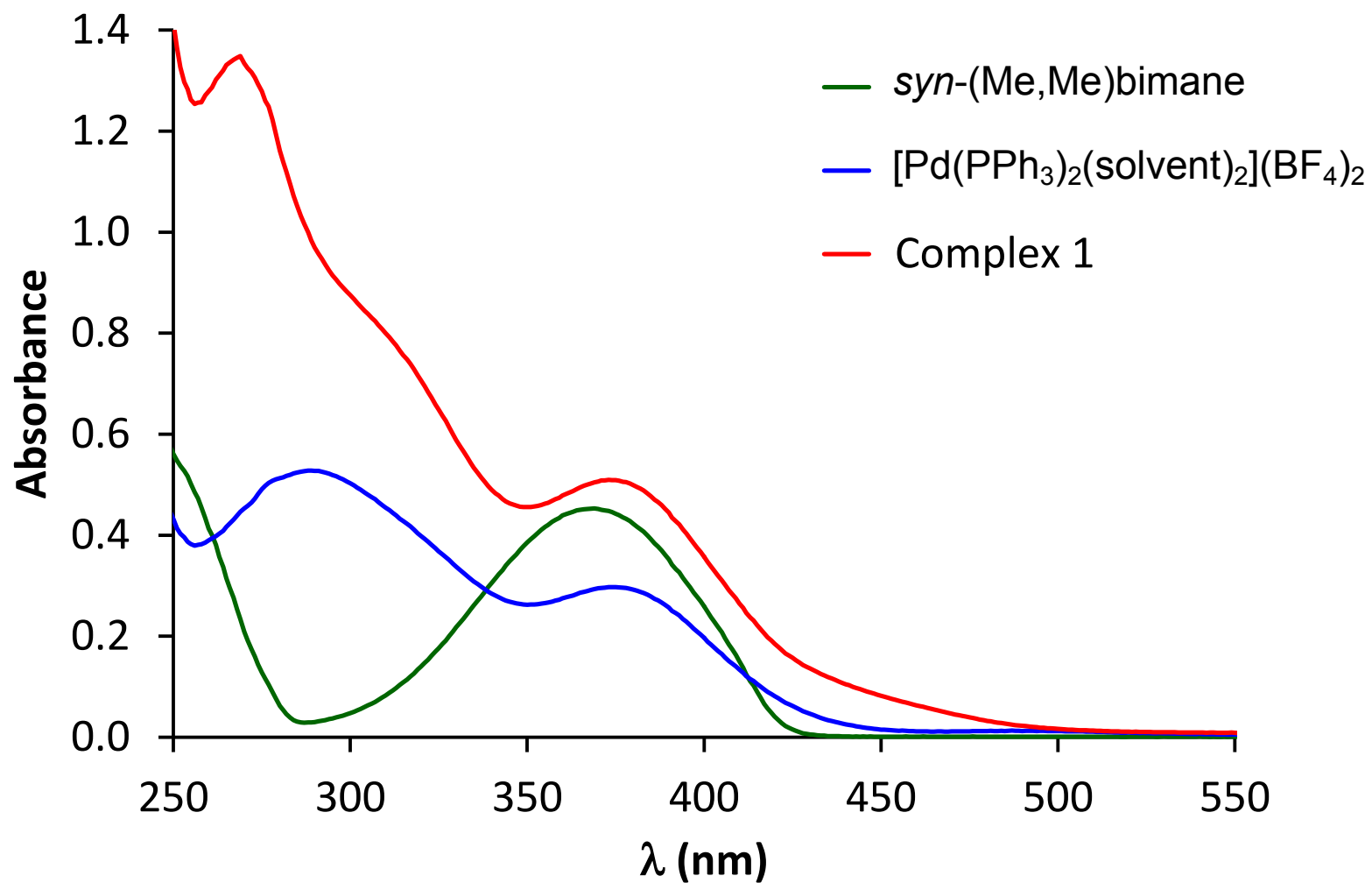
**Figure S6.**  $^{31}\text{P}$  NMR spectra of complex **1** (a) and  $[\text{Pd}(\text{PPh}_3)_2(\text{DMSO-d}_6)_2](\text{BF}_4)_2$  (b) in  $\text{DMSO-d}_6$  (162 MHz, room temperature).



**Figure S7.** <sup>1</sup>H NMR spectra of complex **1** (a) and [Pd(PPh<sub>3</sub>)<sub>2</sub>(CD<sub>3</sub>CN)<sub>2</sub>](BF<sub>4</sub>)<sub>2</sub> (b) in CD<sub>3</sub>CN (400 MHz, room temperature). Trace adventitious impurities are marked with asterisks (\*).



**Figure S8.**  $^{31}\text{P}$  NMR spectra of complex **1** (a) and  $[\text{Pd}(\text{PPh}_3)_2(\text{CD}_3\text{CN})_2](\text{BF}_4)_2$  (b) in  $\text{CD}_3\text{CN}$  (162 MHz, room temperature). Unidentified species are marked with asterisks (\*).



**Figure S9.** UV-vis spectra of *syn*-(Me,Me)bimane,  $[\text{Pd}(\text{PPh}_3)_2(\text{solvent})_n](\text{BF}_4)_2$  (solvent =  $\text{CHCl}_3$ , adventitious  $\text{H}_2\text{O}$ ;  $n = 0-2$ ), and complex **1** in  $\text{CHCl}_3$  (50  $\mu\text{M}$ , room temperature).