

Supporting material:

**Well-defined coinage metal transfer agents for the synthesis of NHC-based nickel,
rhodium and palladium macrocycles**

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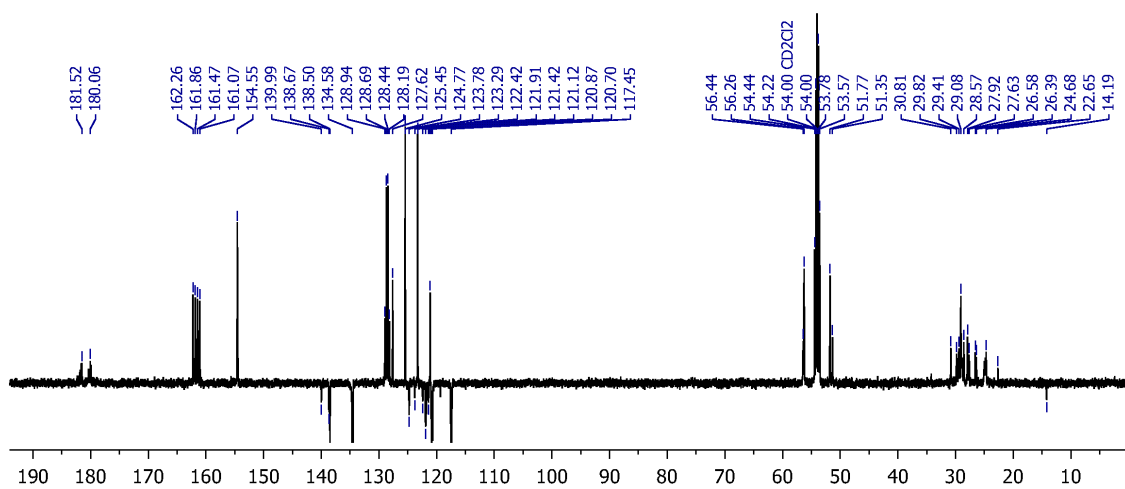
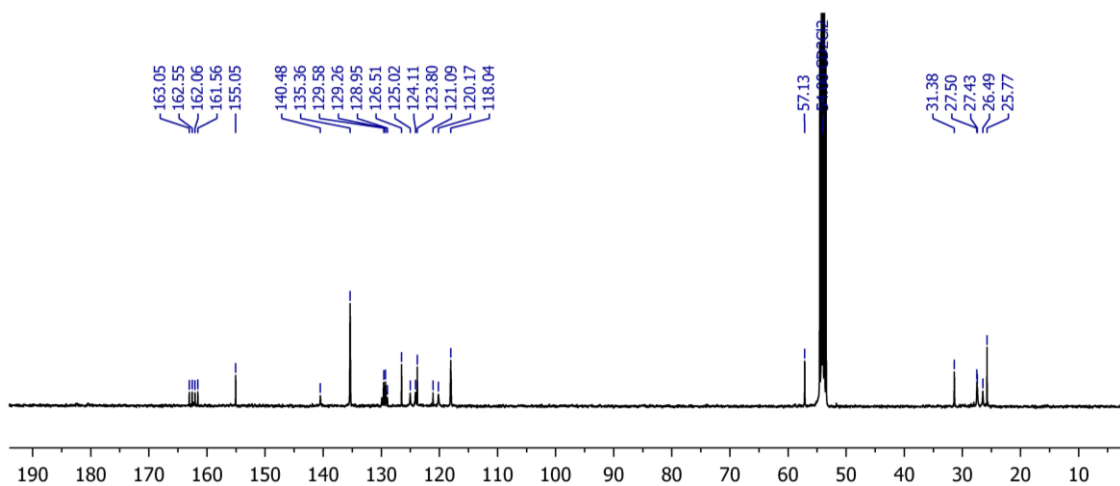
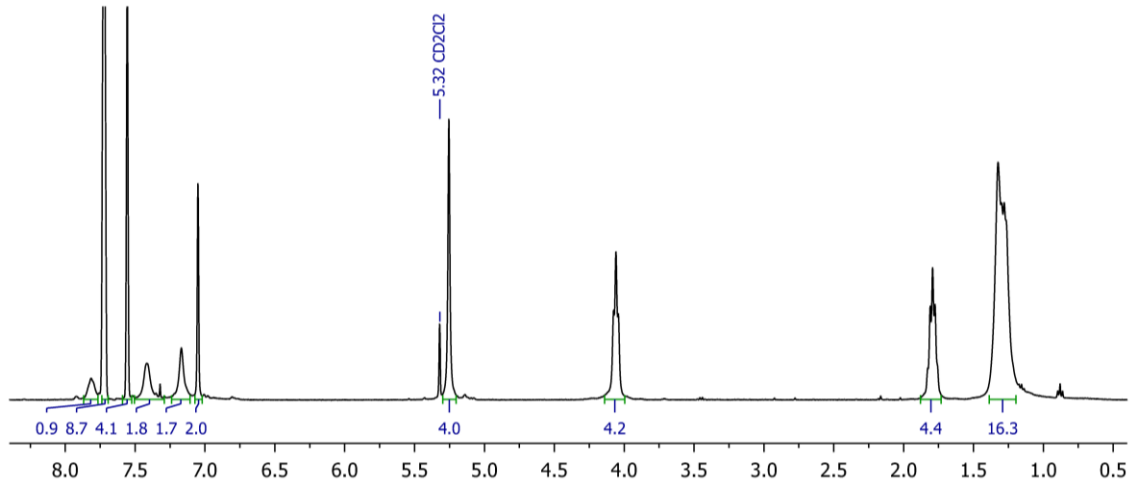
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1. Selected NMR spectra of 2, 3, 4 and 7

1.1. [Ag(1)]₂[BAR^F₄]₂ (2)



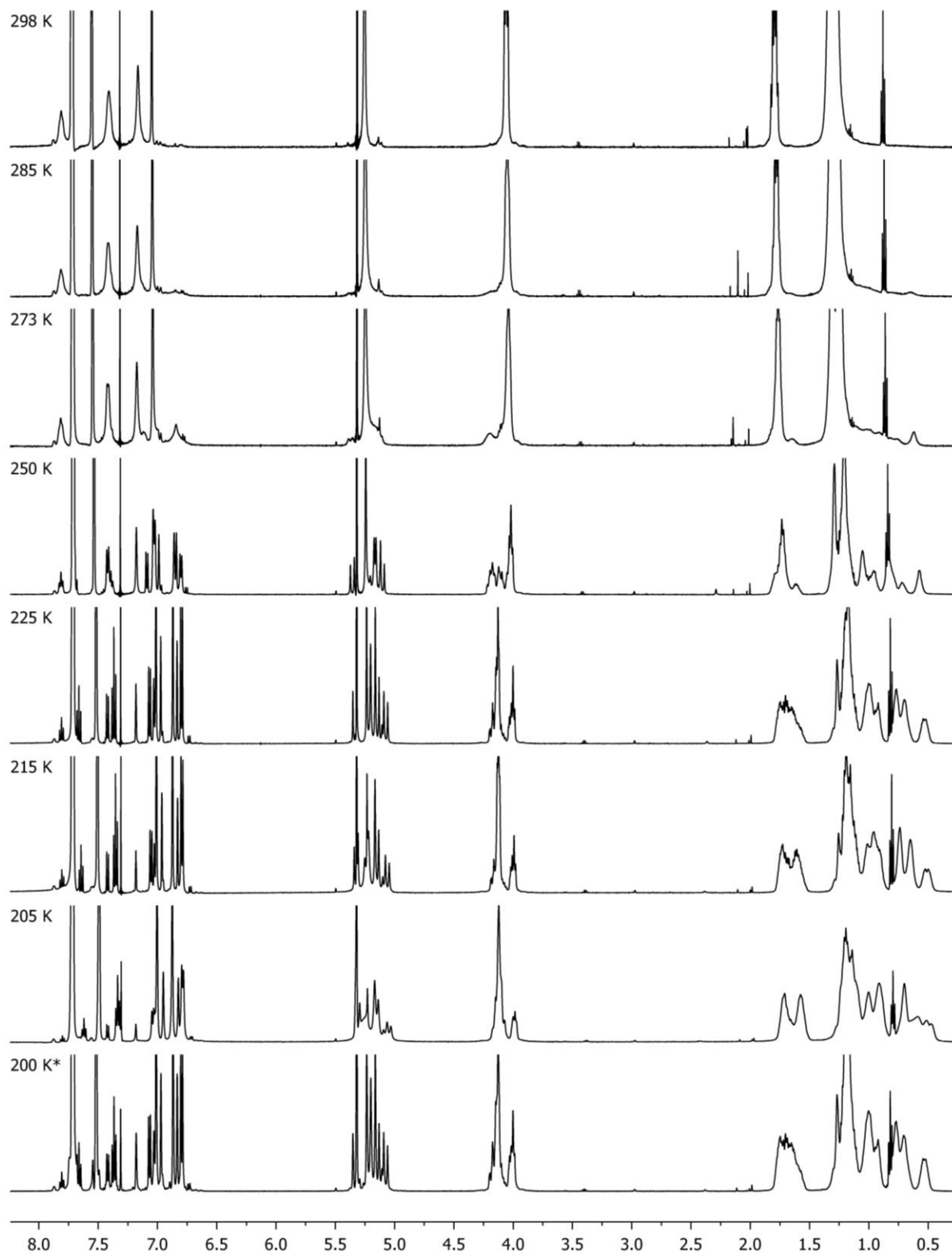


Figure S4: Variable temperature ^1H NMR spectra of **2** (CD_2Cl_2 , 500 MHz, 298-200 K). * = recorded independently from others

1.2. [Cu(1)]₂[Cu₂Br₄] (3)

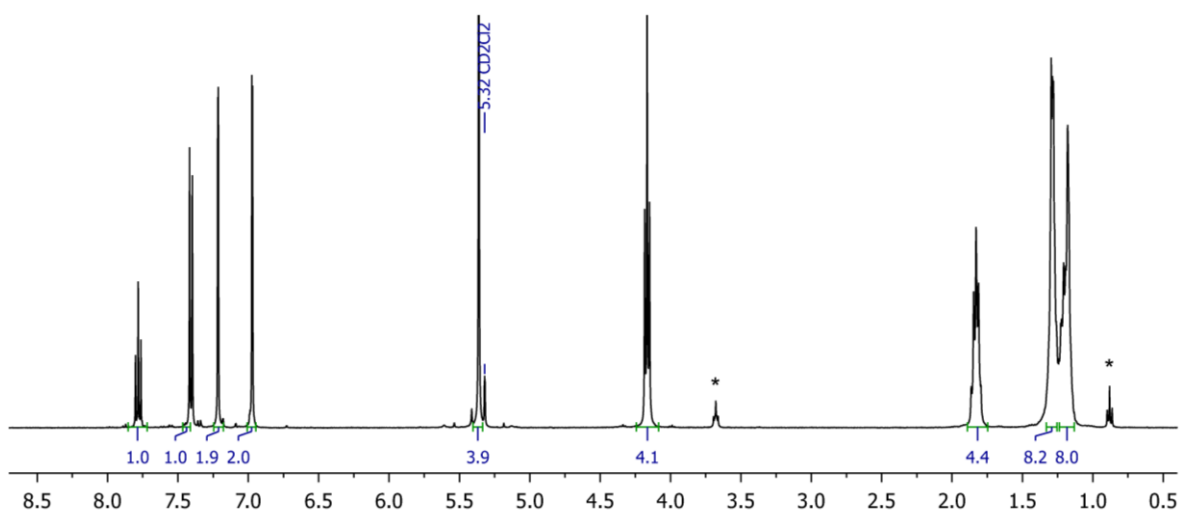


Figure S5: ¹H NMR spectrum of **3** (CD₂Cl₂, 400 MHz). * = THF, pentane.

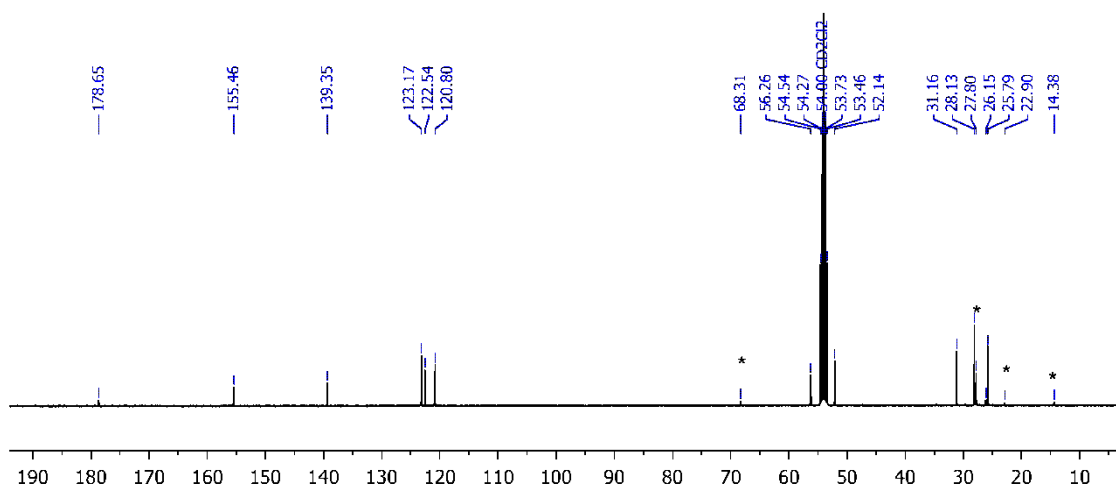


Figure S6: ¹³C{¹H} NMR spectrum of **3** (CD₂Cl₂, 101 MHz). * = THF, pentane.

1.3. [Cu(1)][BAR^F₄] (4)

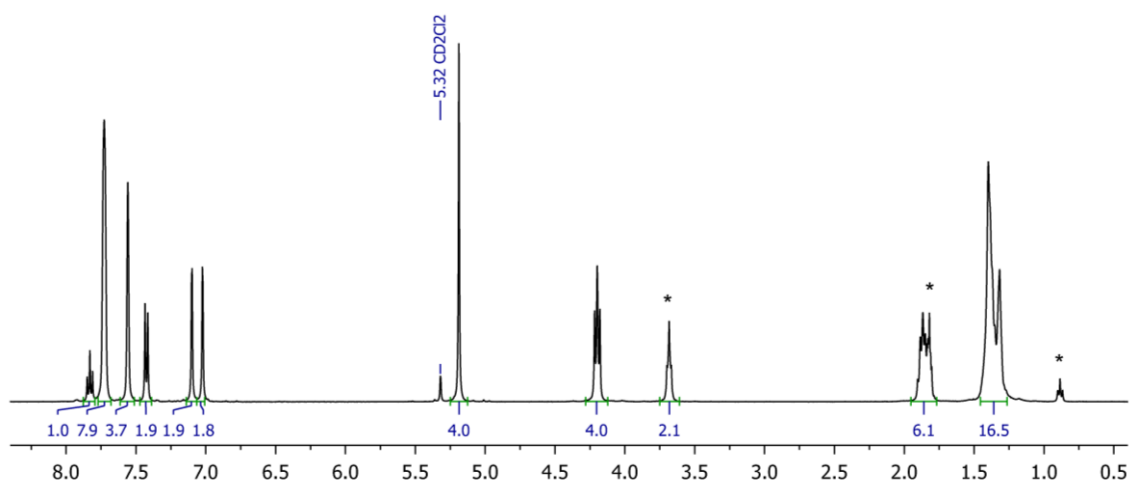


Figure S7: ¹H NMR spectrum of 4 (CD₂Cl₂, 400 MHz). * = THF, pentane.

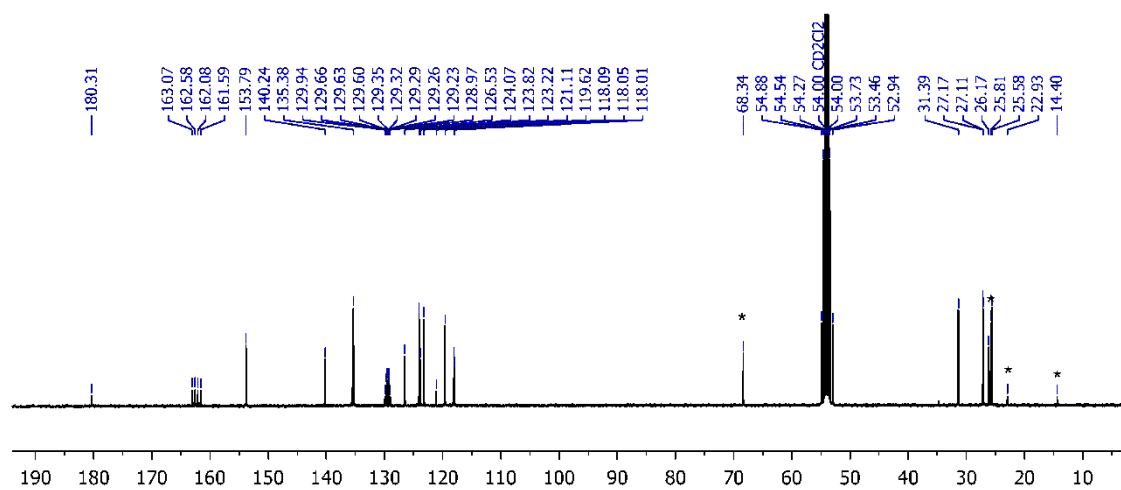


Figure S8: ¹³C{¹H} NMR spectrum of 4 (CD₂Cl₂, 101 MHz). * = THF, pentane.

1.4. [Ni(**1**)][BAr^F₄] (**7**)

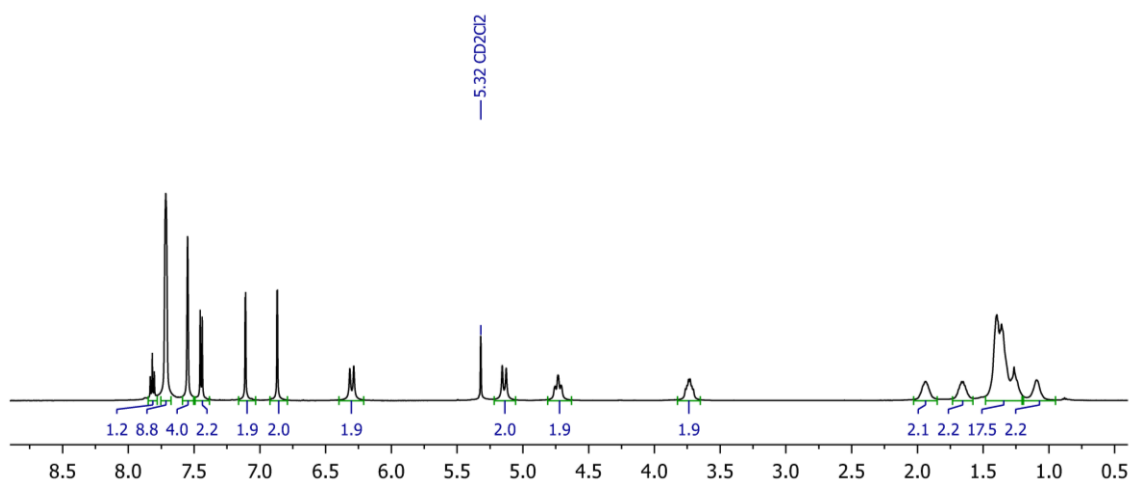


Figure S9: ¹H NMR spectrum of **7** (CD₂Cl₂, 500 MHz).

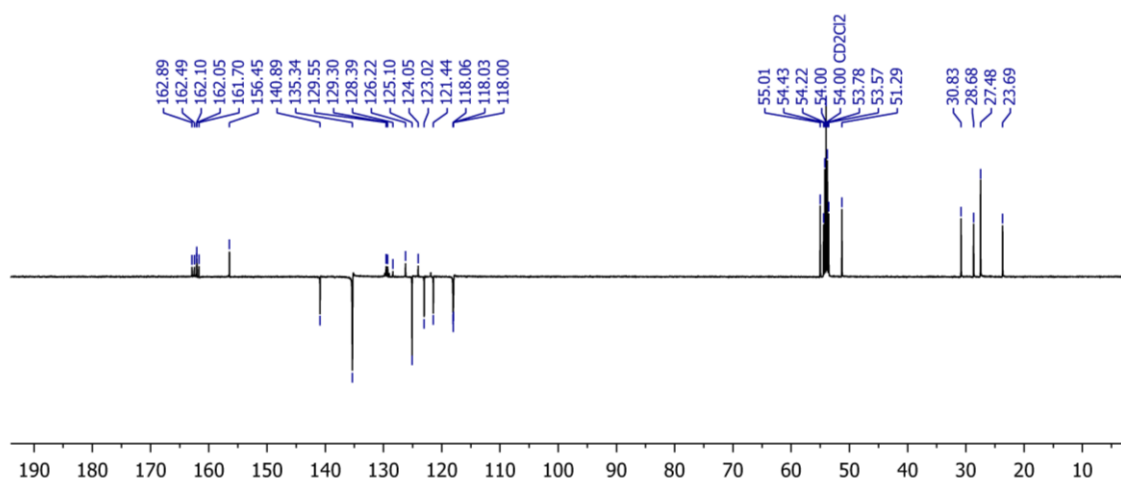


Figure S10: ¹³C{¹H} APT NMR spectrum of **7** (CD₂Cl₂, 126 MHz).

2. NMR-scale Transmetalation Reactions of **2** and **4**

2.1. Reaction of **2** with $[\text{PdCl}_2(\text{NMe}_2)_2]$ to give **5**

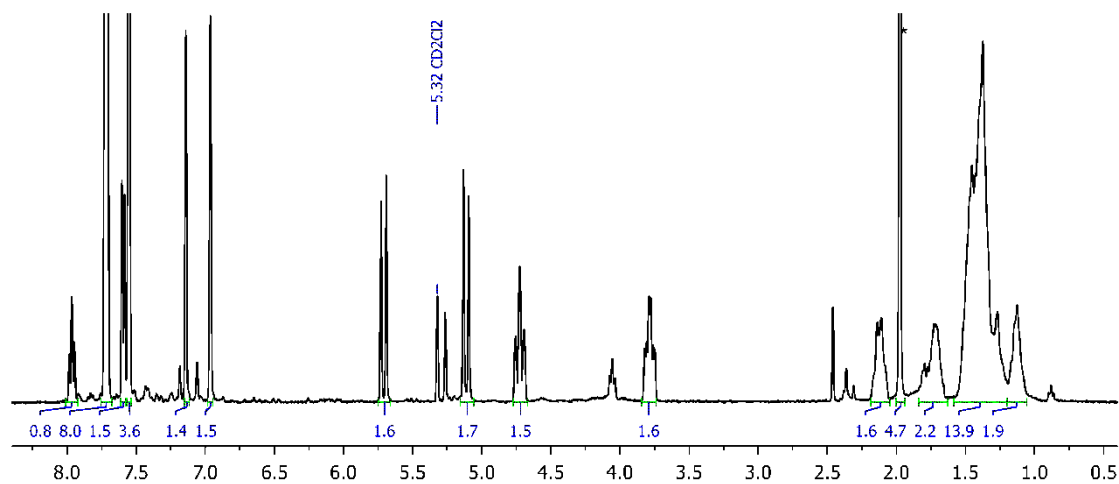


Figure S11: ^1H NMR spectrum of *in situ* reaction of **2** and $[\text{PdCl}_2(\text{NMe}_2)_2]$ at 20°C after 0.5 h (CD_2Cl_2 , 400 MHz). * = MeCN.

2.2. Reaction of **4** with $[\text{PdCl}_2(\text{NMe}_2)_2]$ to give **5**

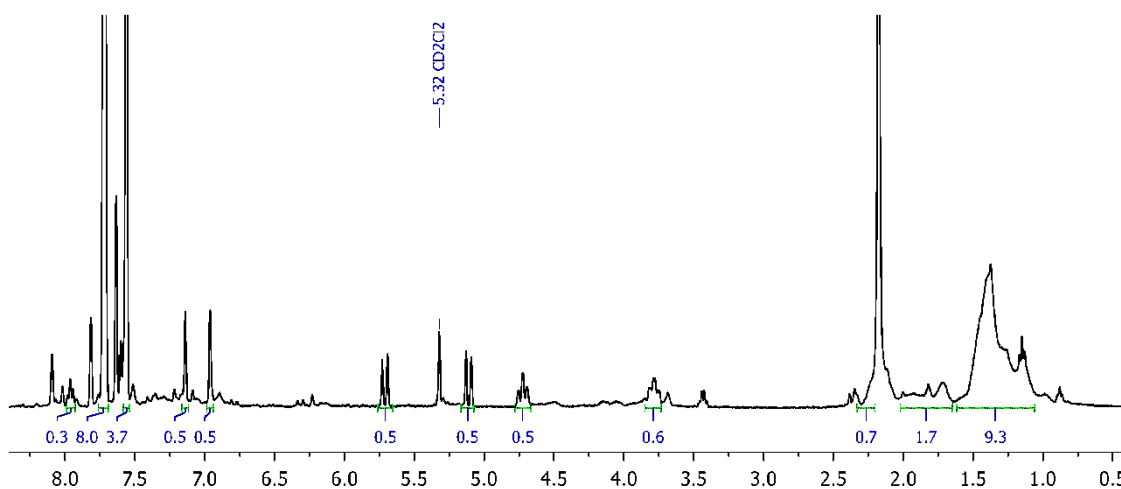


Figure S12: ^1H NMR spectrum of *in situ* reaction of **4** and $[\text{PdCl}_2(\text{MeCN})_2]$ at 20°C after 0.5 h (CD_2Cl_2 , 400 MHz). * = MeCN.

2.3. Reaction of **2** with $[\text{Rh}(\text{CO})_2\text{Cl}]_2$ to give **6**

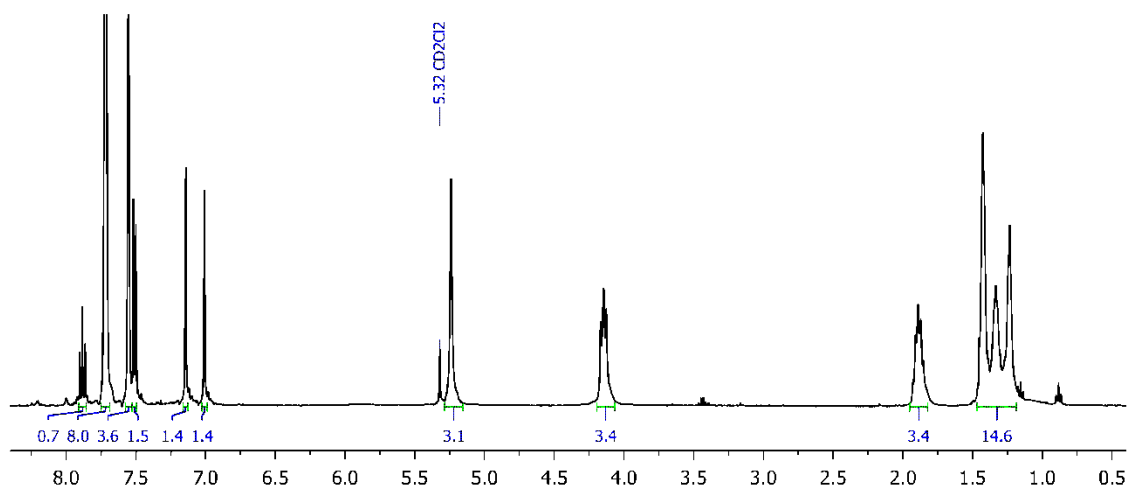


Figure S13: ^1H NMR spectrum of *in situ* reaction of **2** and $[\text{Rh}(\text{CO})_2\text{Cl}]_2$ at 20°C after 0.5 h (CD_2Cl_2 , 400 MHz).

2.4. Reaction of **4** with $[\text{Rh}(\text{CO})_2\text{Cl}]_2$ to give **6**

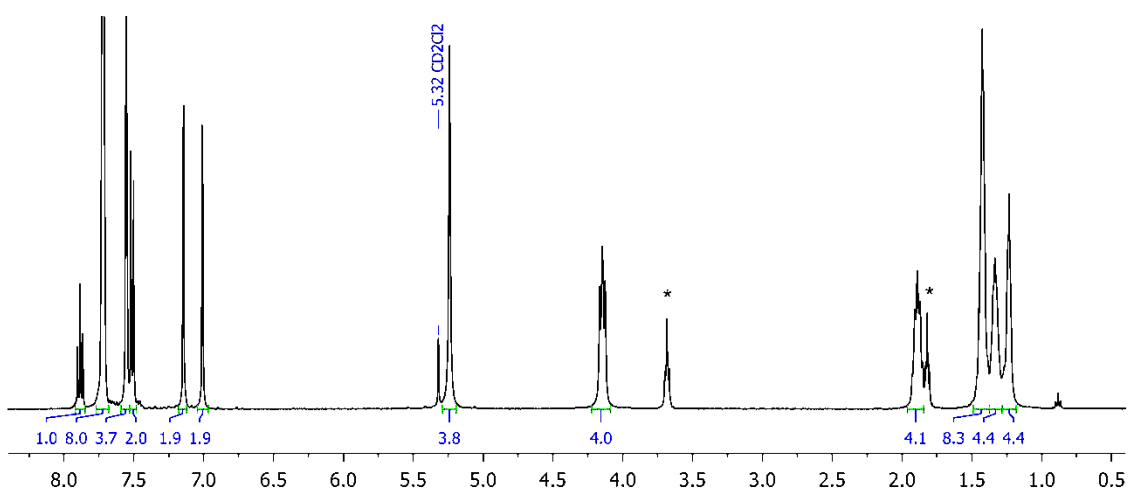


Figure S14: ^1H NMR spectrum of *in situ* reaction of **4** and $[\text{Rh}(\text{CO})_2\text{Cl}]_2$ at 20°C after 0.5 h (CD_2Cl_2 , 400 MHz). * = THF

2.5. Reactions of **2** with $[\text{NiCl}_2(\text{glyme})]$ to give **7**

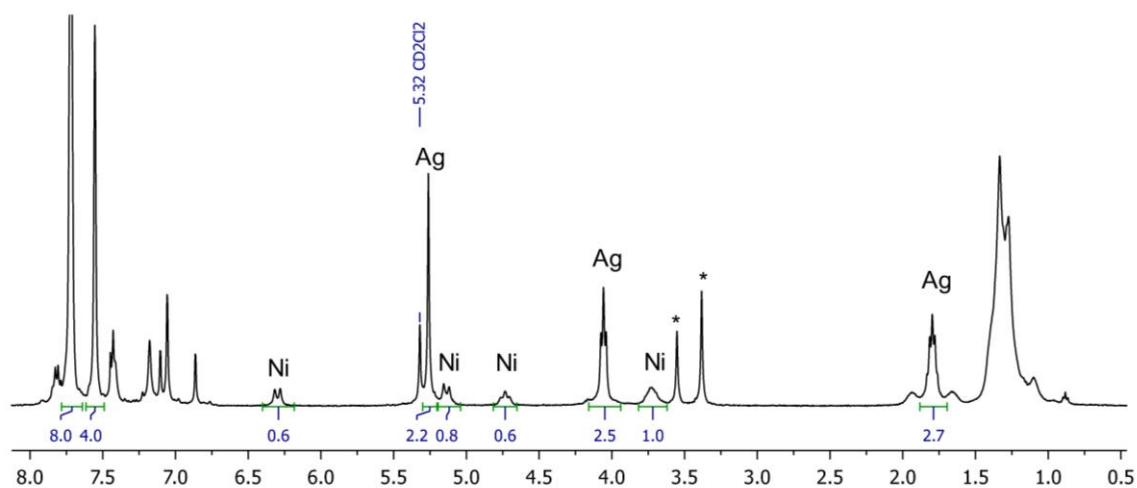


Figure S15: ^1H NMR spectrum of *in situ* reaction of **2** and $[\text{NiCl}_2(\text{glyme})]$ at 20°C after 20 h (CD_2Cl_2 , 400 MHz). * = glyme.

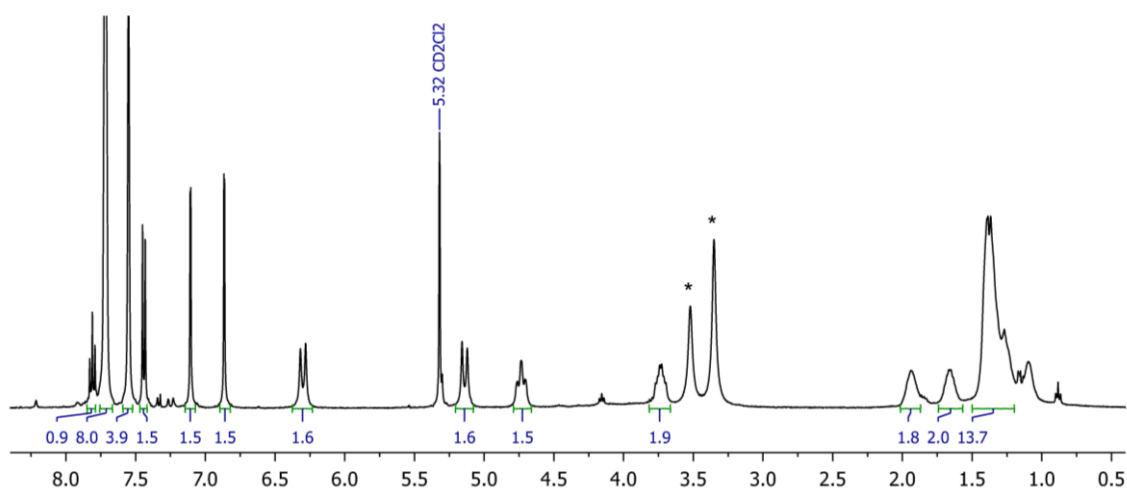


Figure S16: ^1H NMR spectrum of *in situ* reaction of **2** and $[\text{NiCl}_2(\text{glyme})]$ at 40°C after 20 h (CD_2Cl_2 , 400 MHz). * = glyme.

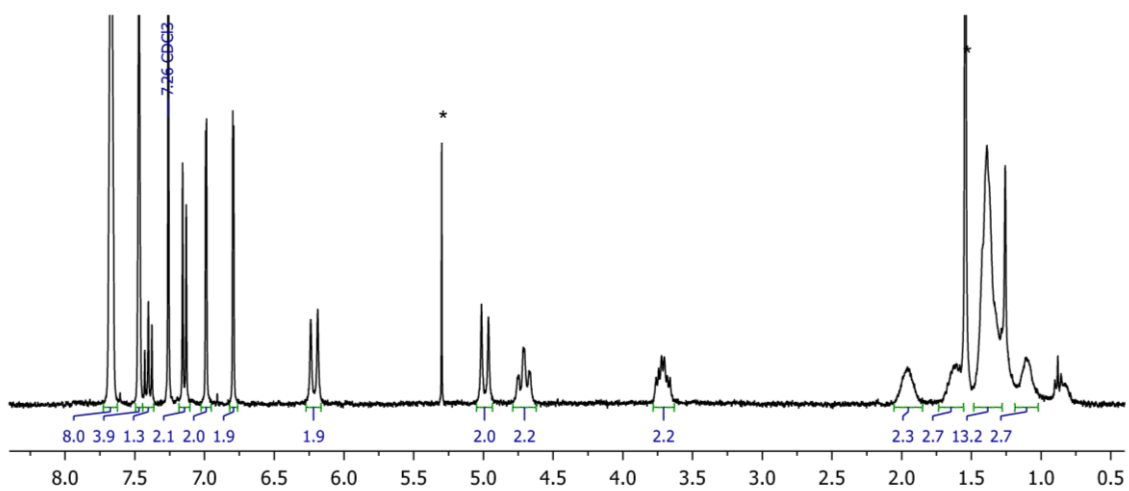
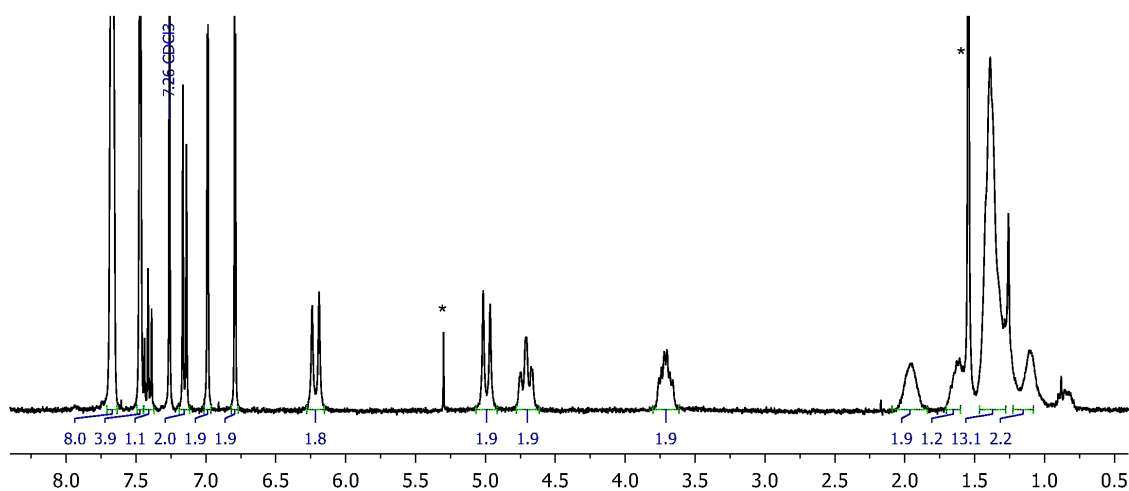
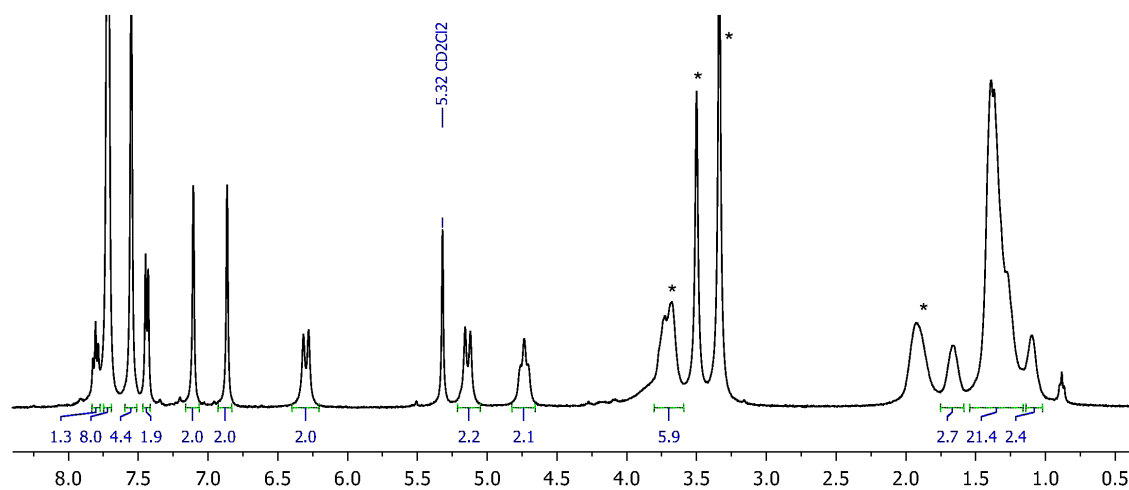
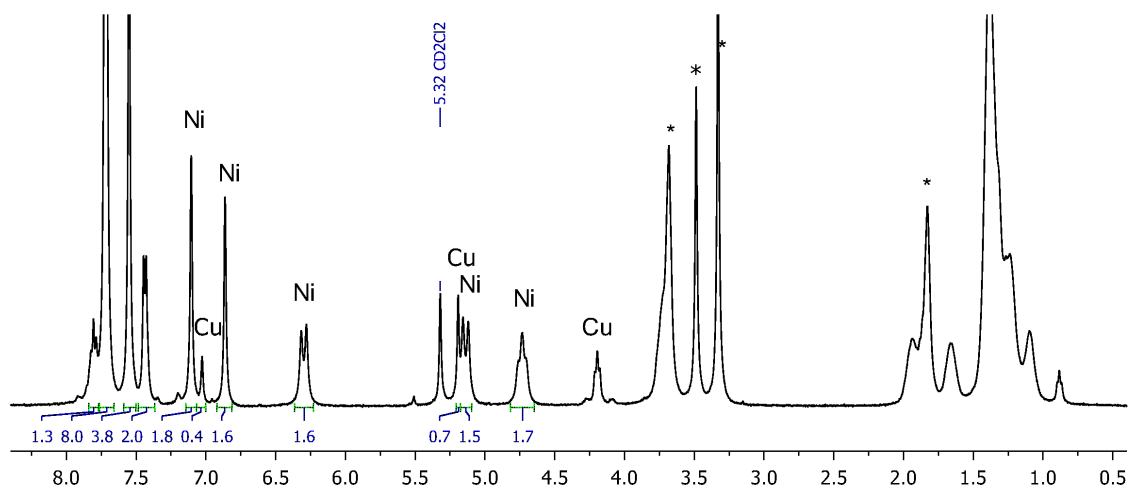


Figure S17: ^1H NMR spectrum of isolated **7** from **2** (CDCl_3 , 300 MHz). * = CH_2Cl_2 , H_2O

2.6. Reactions of **4** with $[\text{NiCl}_2(\text{glyme})]$ to give **7**



3. High Resolution Mass Spectra of 2, 3, 4 and 7

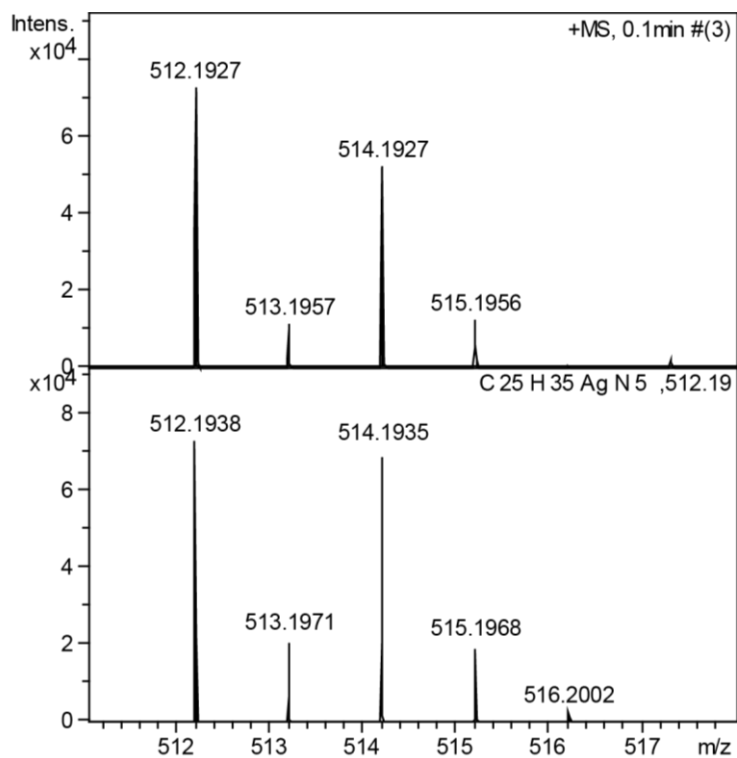


Figure S21: ESI-MS spectrum of 2.

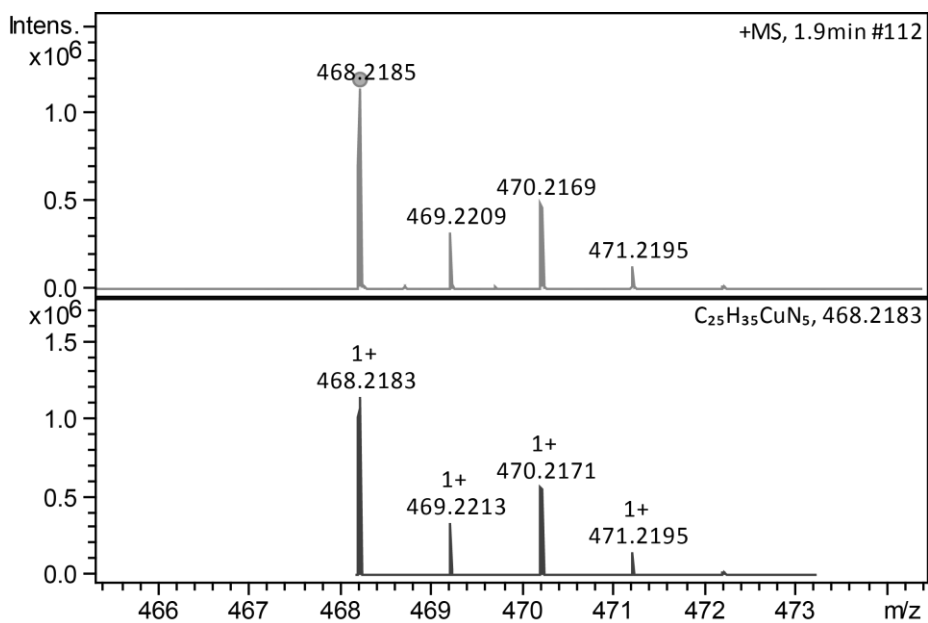


Figure S22: ESI-MS spectrum of 3.

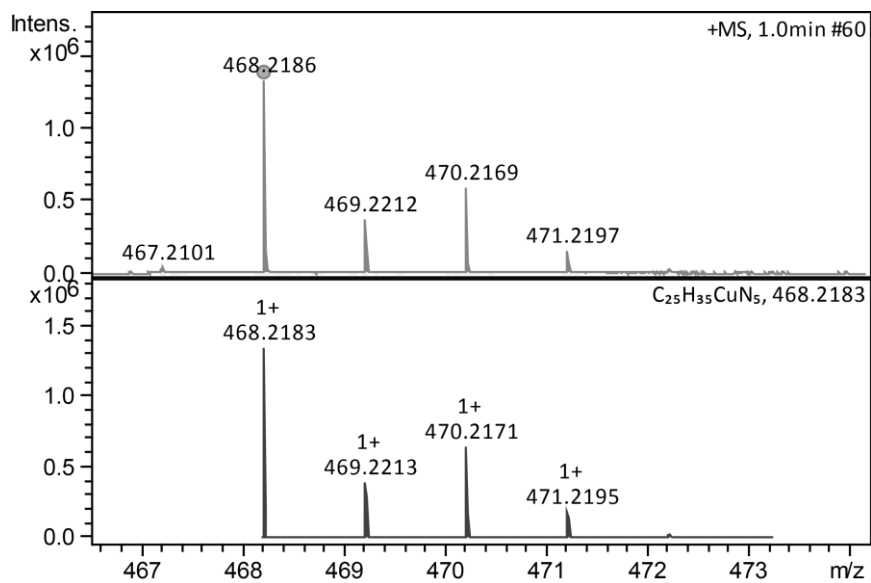


Figure S23: ESI-MS spectrum of 4.

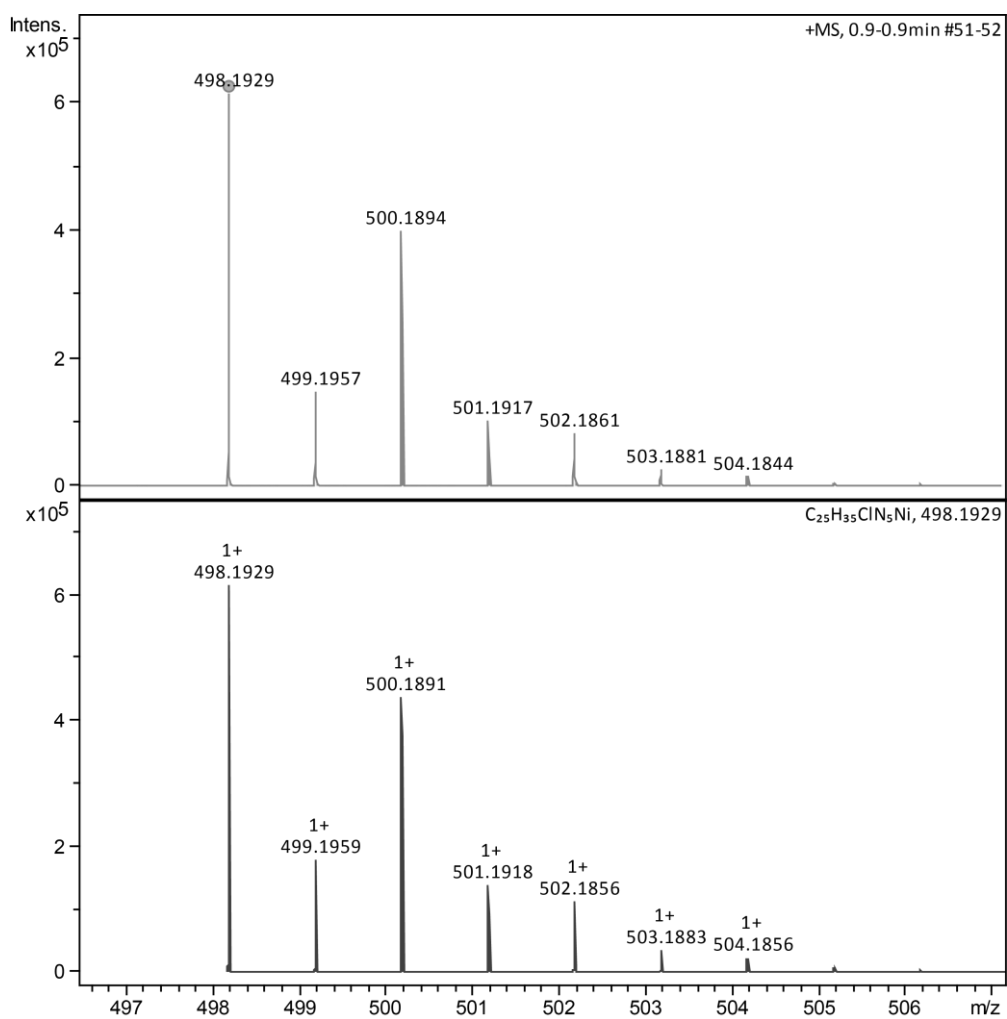


Figure S24: ESI-MS spectrum of 7.