

*Supplementary Materials for*

# **Synthesis and Cytotoxicity Studies of Novel NHC\*- Gold(I) Complexes Derived from Lepidiline A**

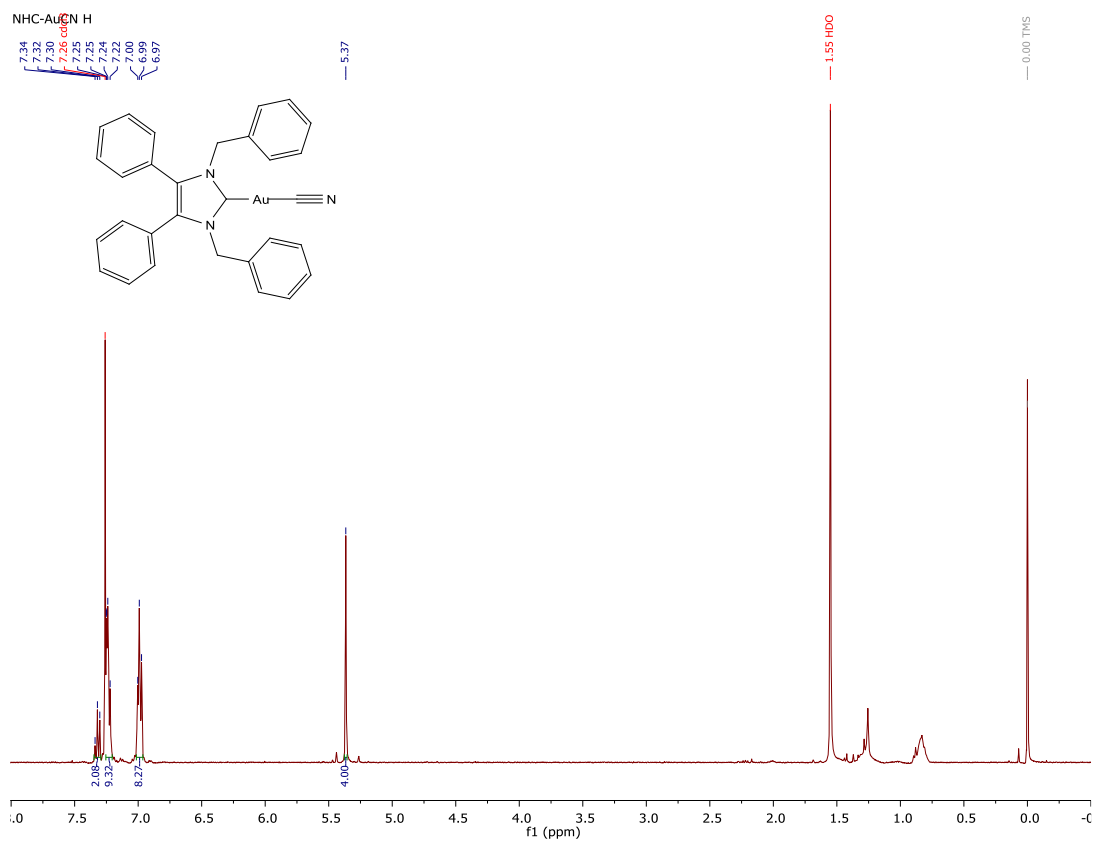
**Danielle Curran <sup>1</sup>, Oyinlola Dada <sup>1</sup>, Helge Müller-Bunz <sup>1</sup>, Matthias Rothemund <sup>2</sup>, Goar Sánchez-Sanz <sup>1,3</sup>, Rainer Schobert <sup>2</sup>, Xiangming Zhu <sup>1</sup> and Matthias Tacke <sup>1,\*</sup>**

<sup>1</sup> School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland

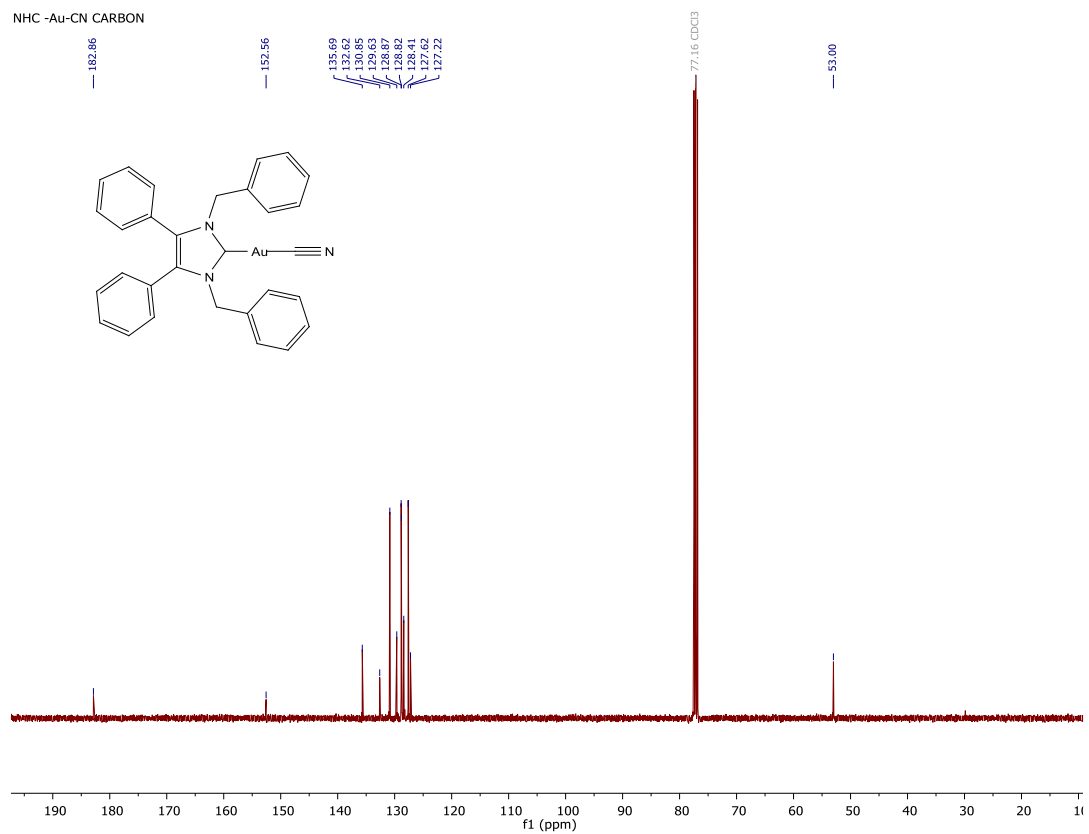
<sup>2</sup> Organic Chemistry Laboratory, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

<sup>3</sup> Irish Centre of High-End Computing, Grand Canal Quay, Dublin 2, Ireland

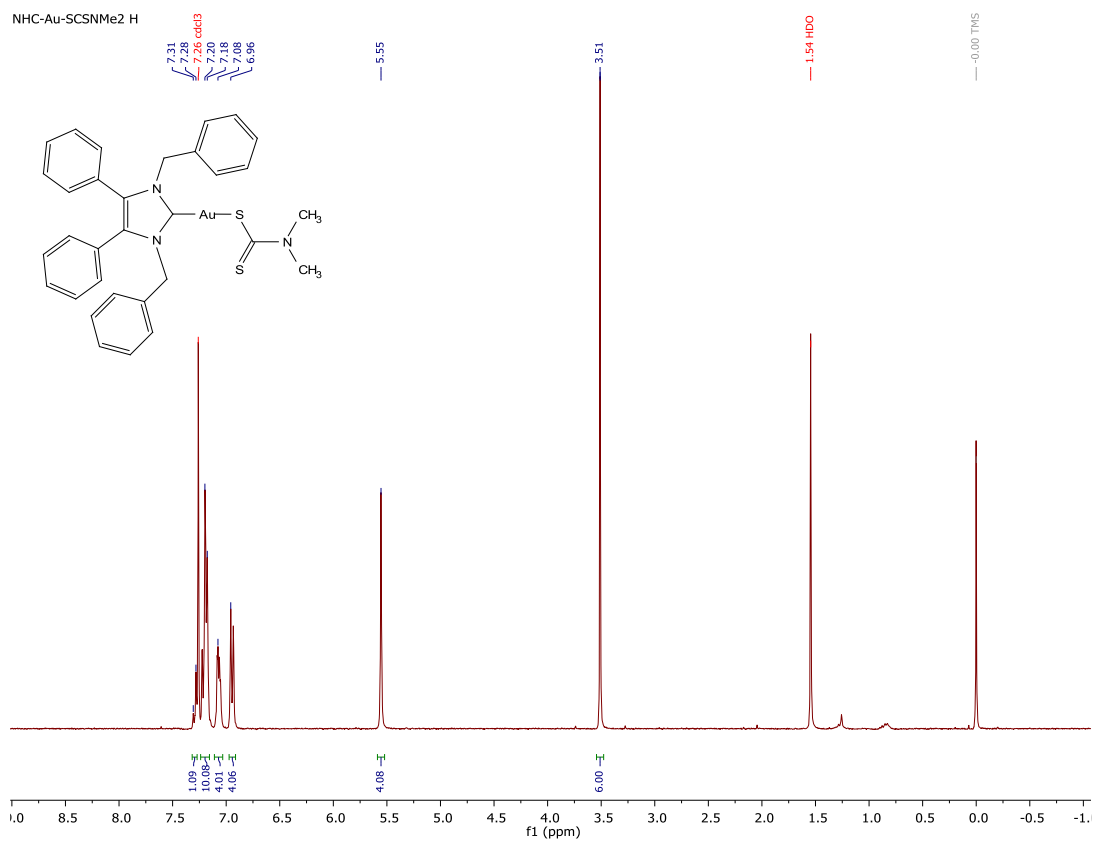
\* Correspondence: matthias.tacke@ucd.ie



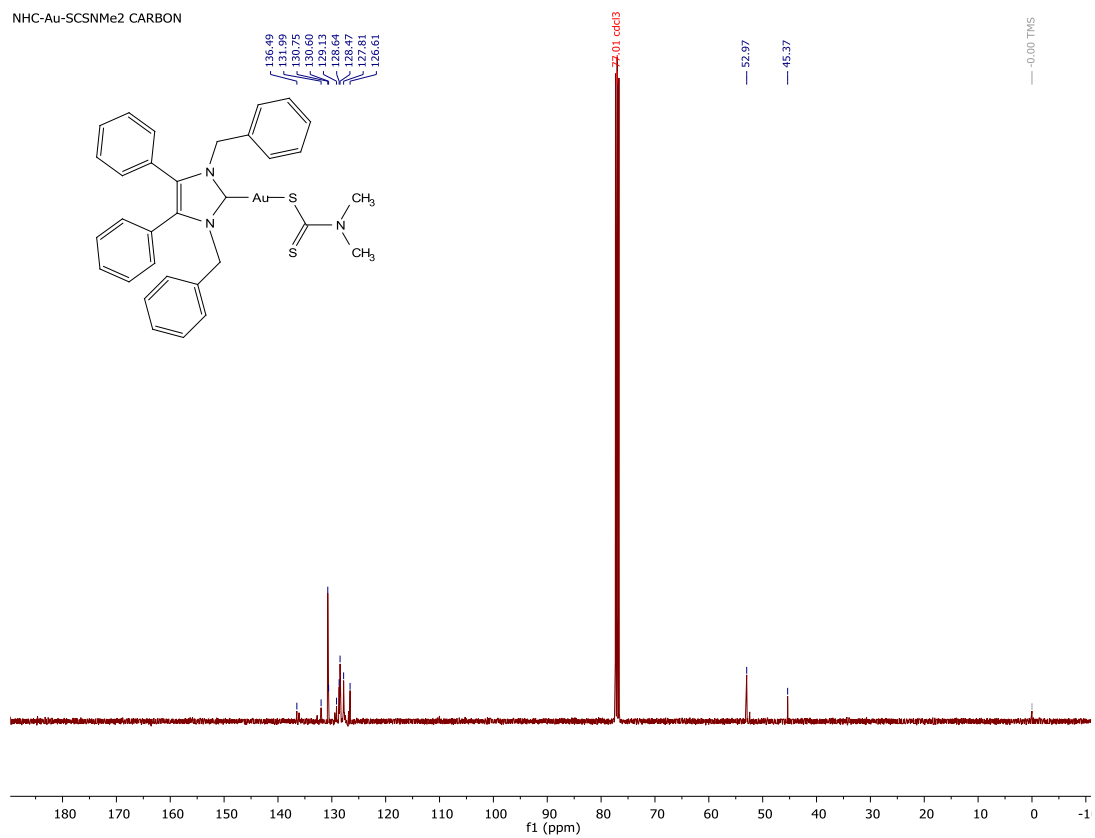
S 1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the new compound 2.



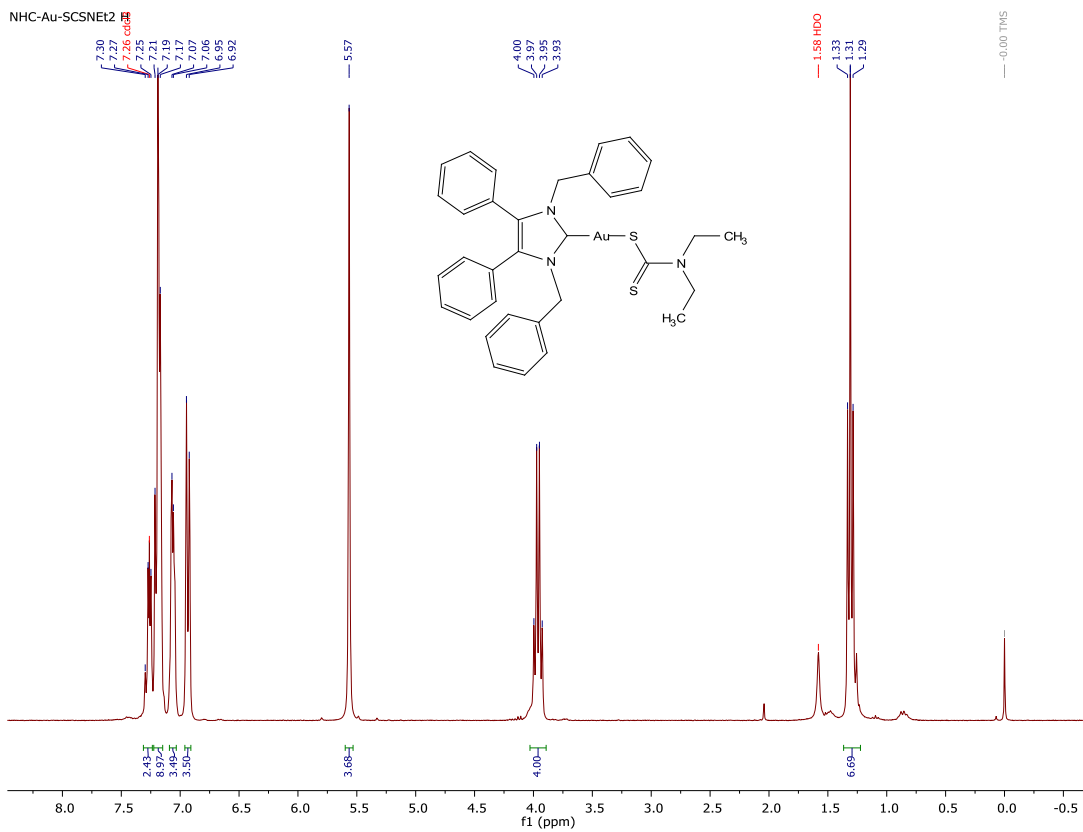
S 2. <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound 2.



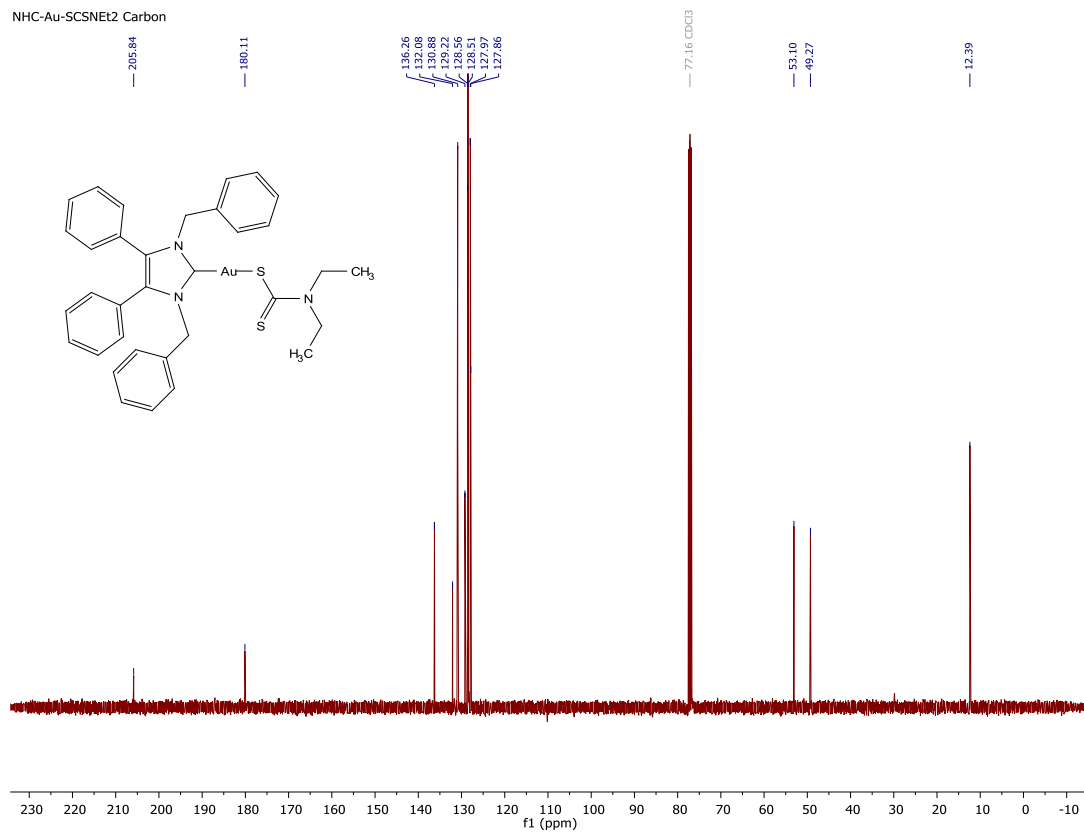
S 3. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of the new compound 3.



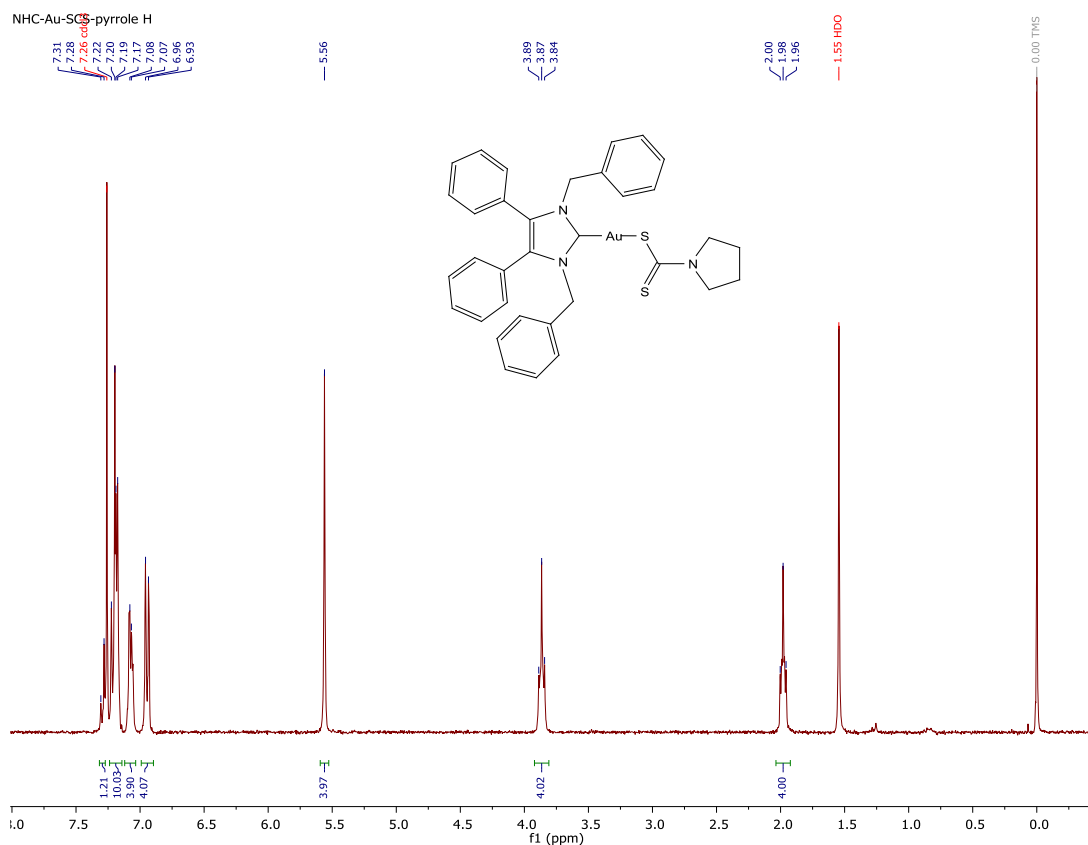
S 4. <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound 3.



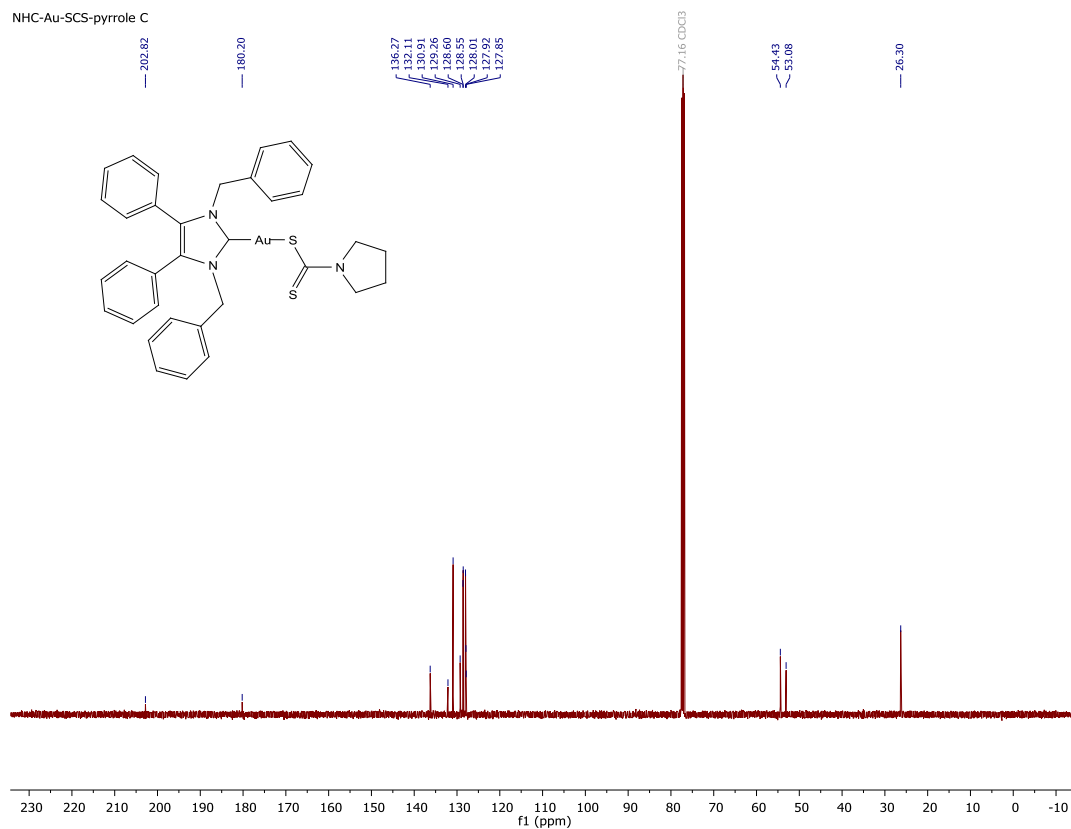
S 5.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound 4.



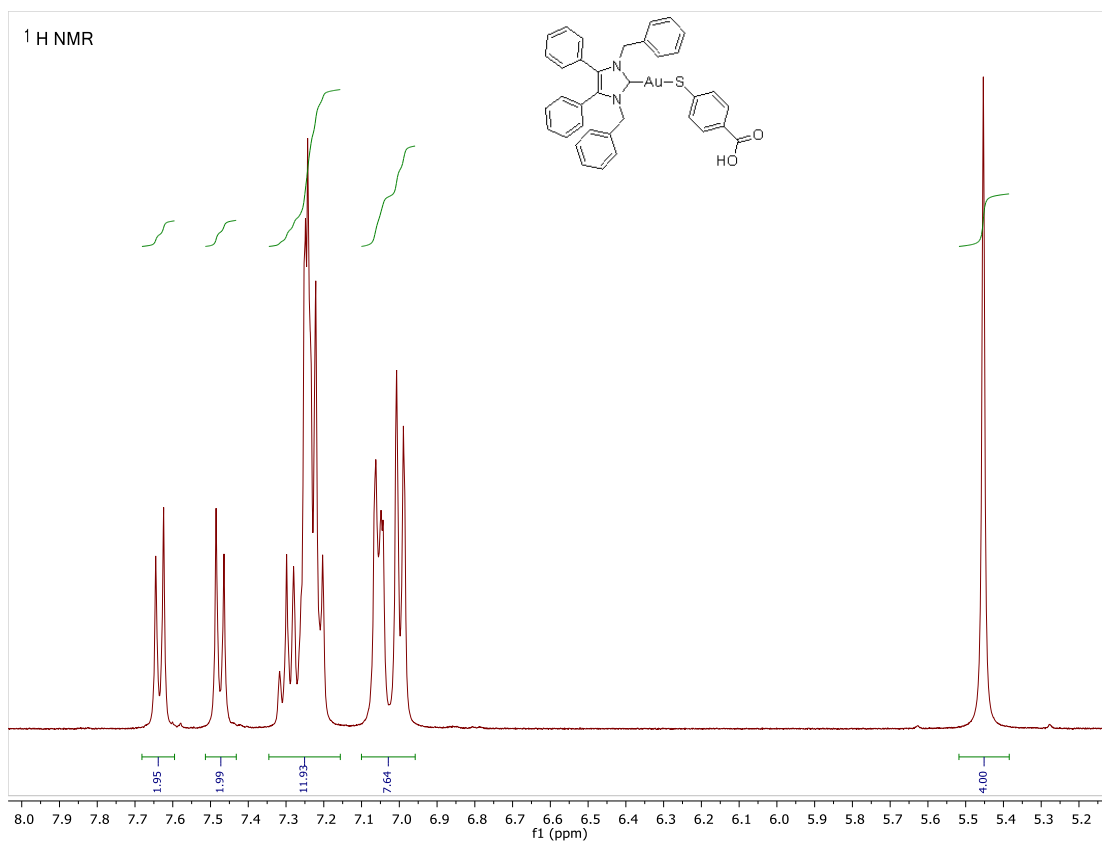
S 6.  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound 4.



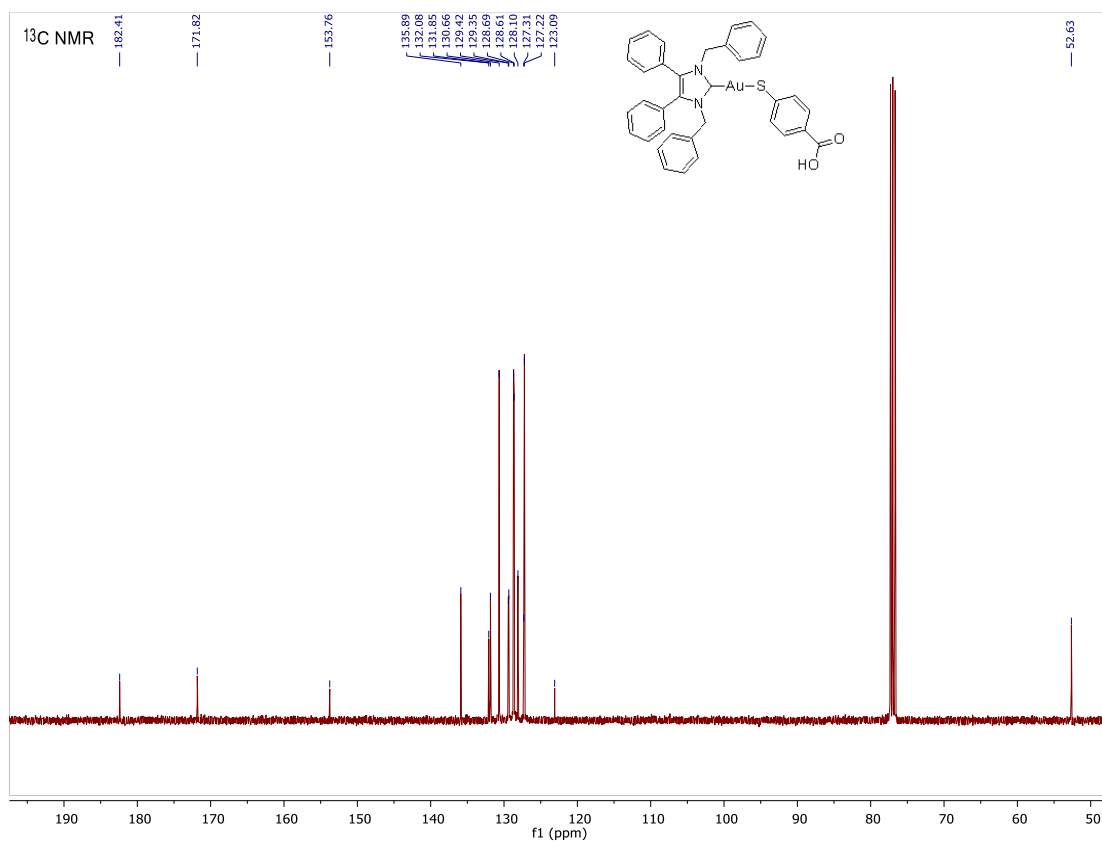
S 7.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound 5.



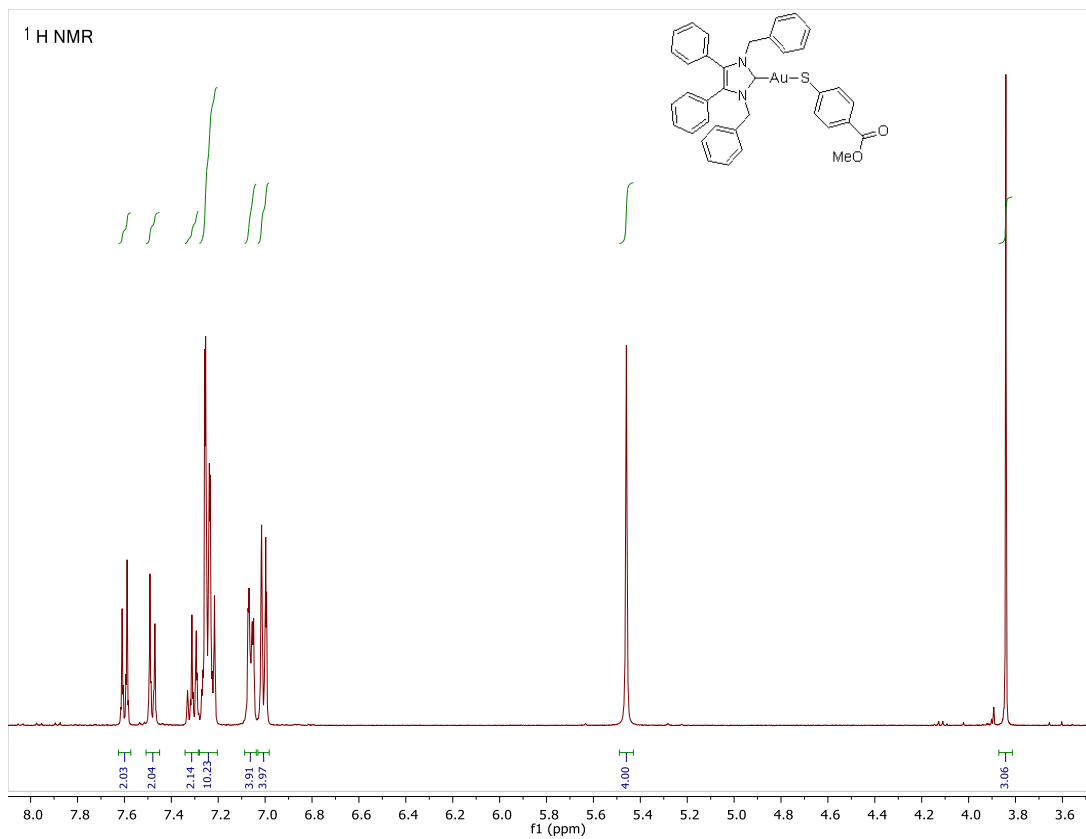
S 8.  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of the new compound 5.



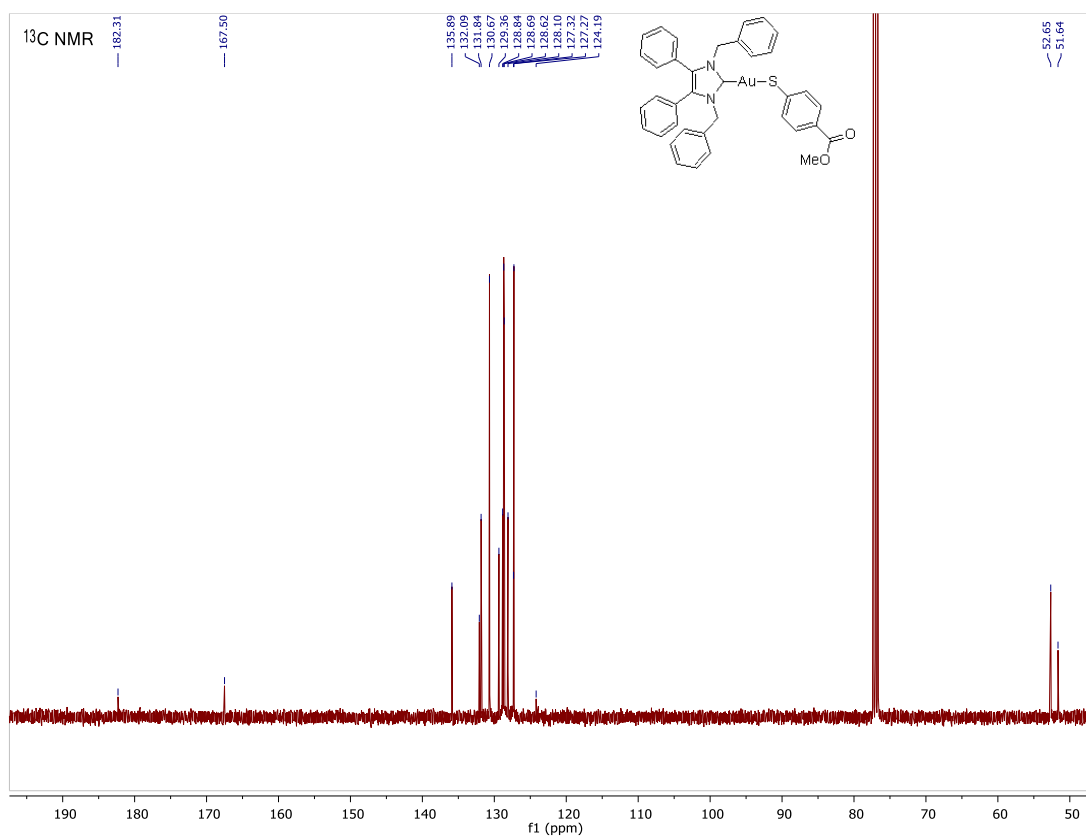
**S 9.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the new compound **12**.



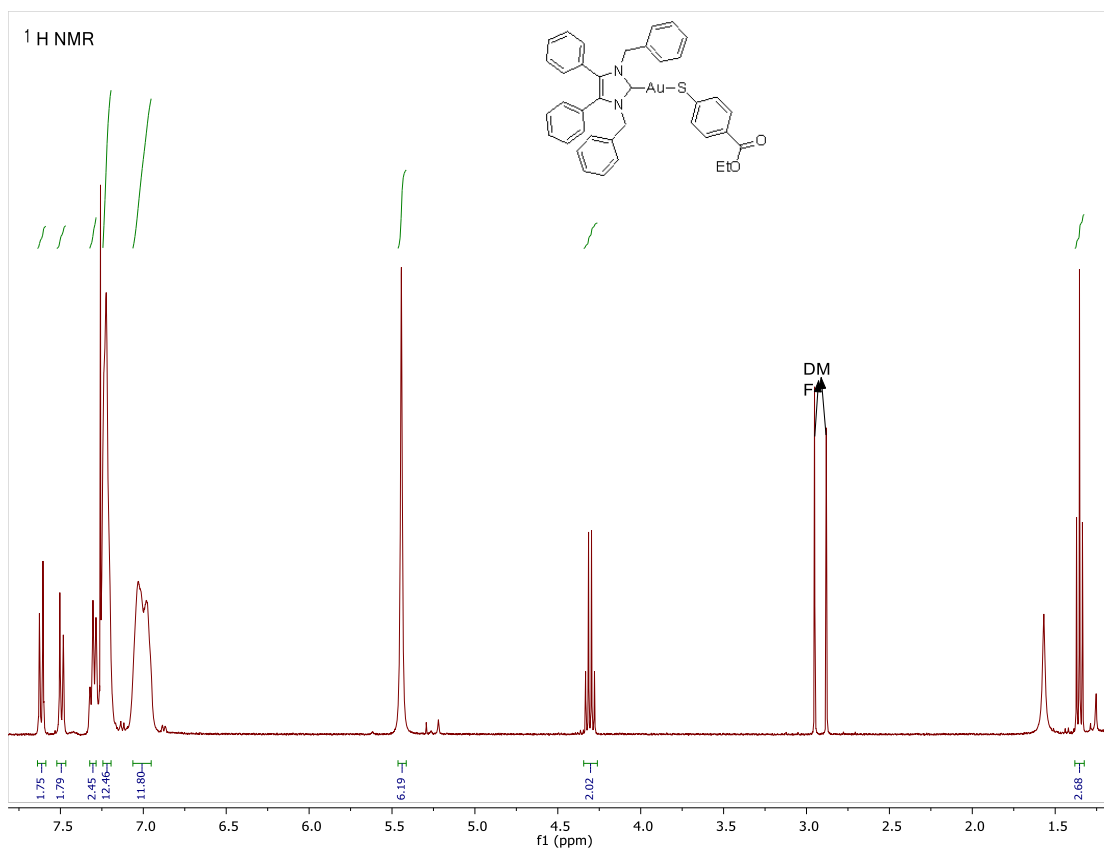
**S 10.** <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound **12**.



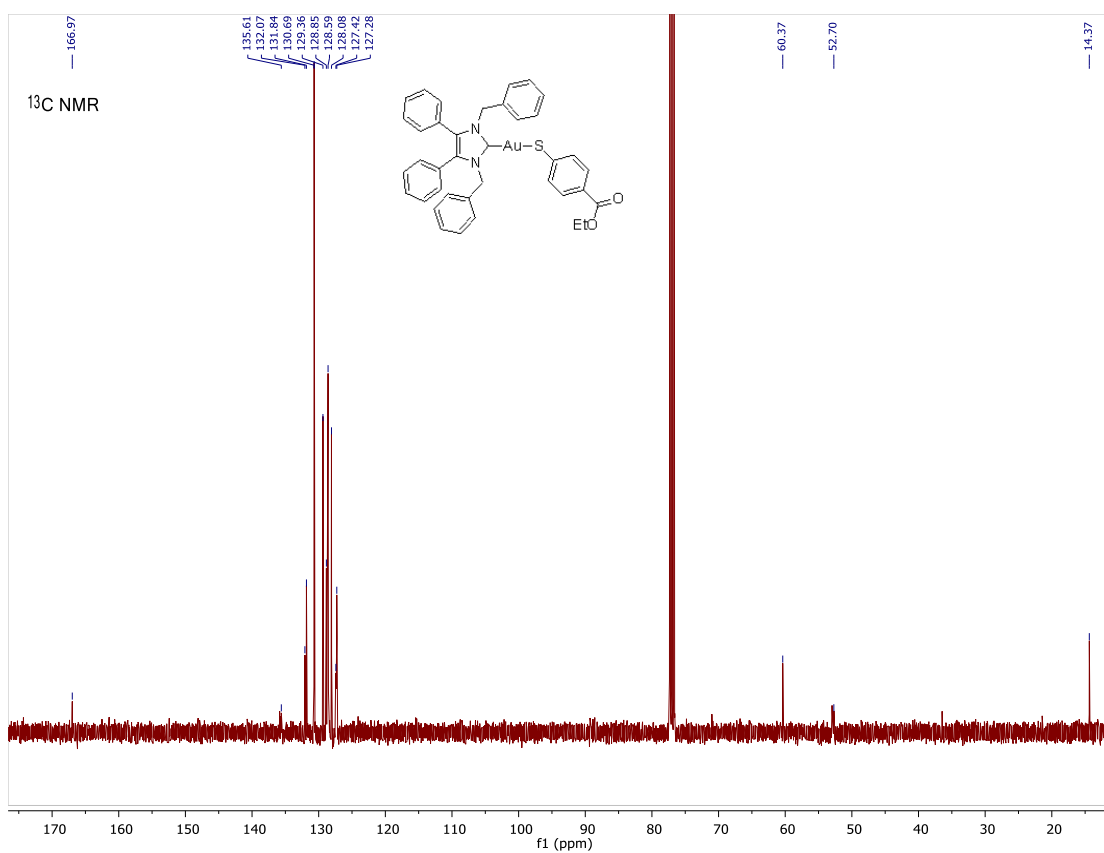
**S 11.** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the new compound **13**.



**S 12.** <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound **13**.

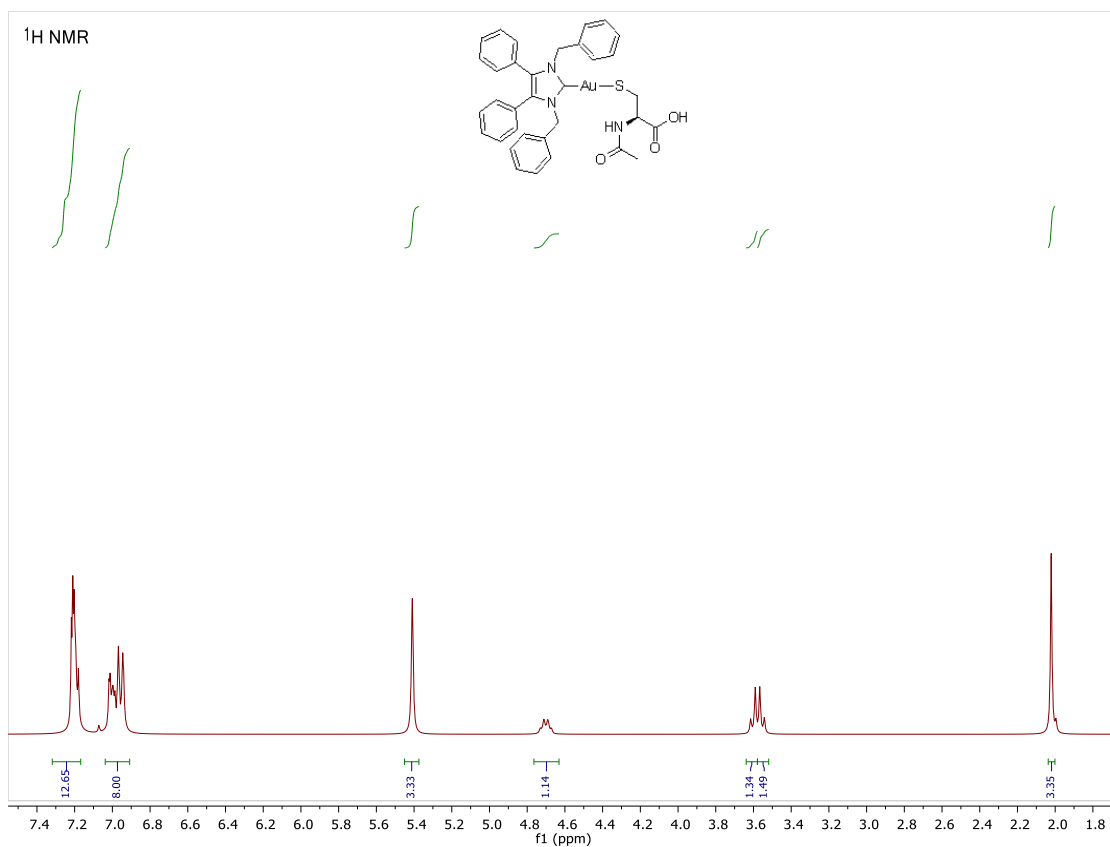


**S 13.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of the new compound **14**.

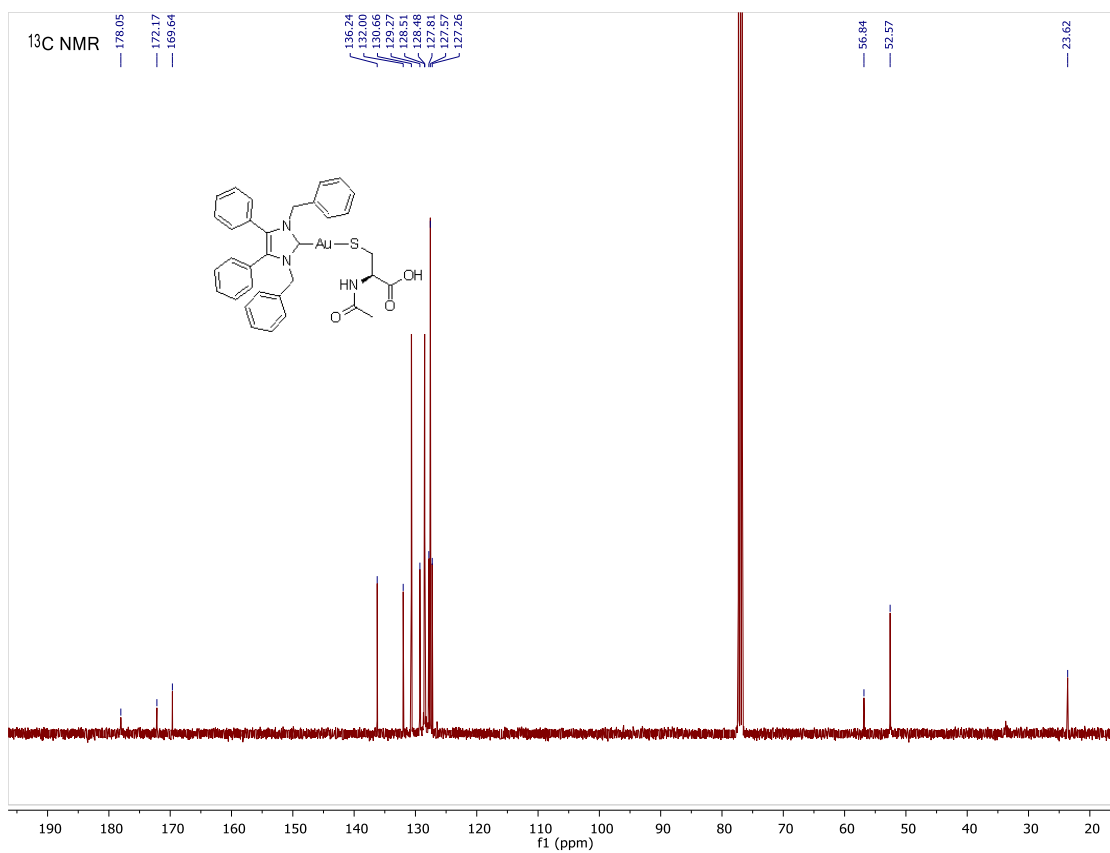


**S 14.** <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound **14**.

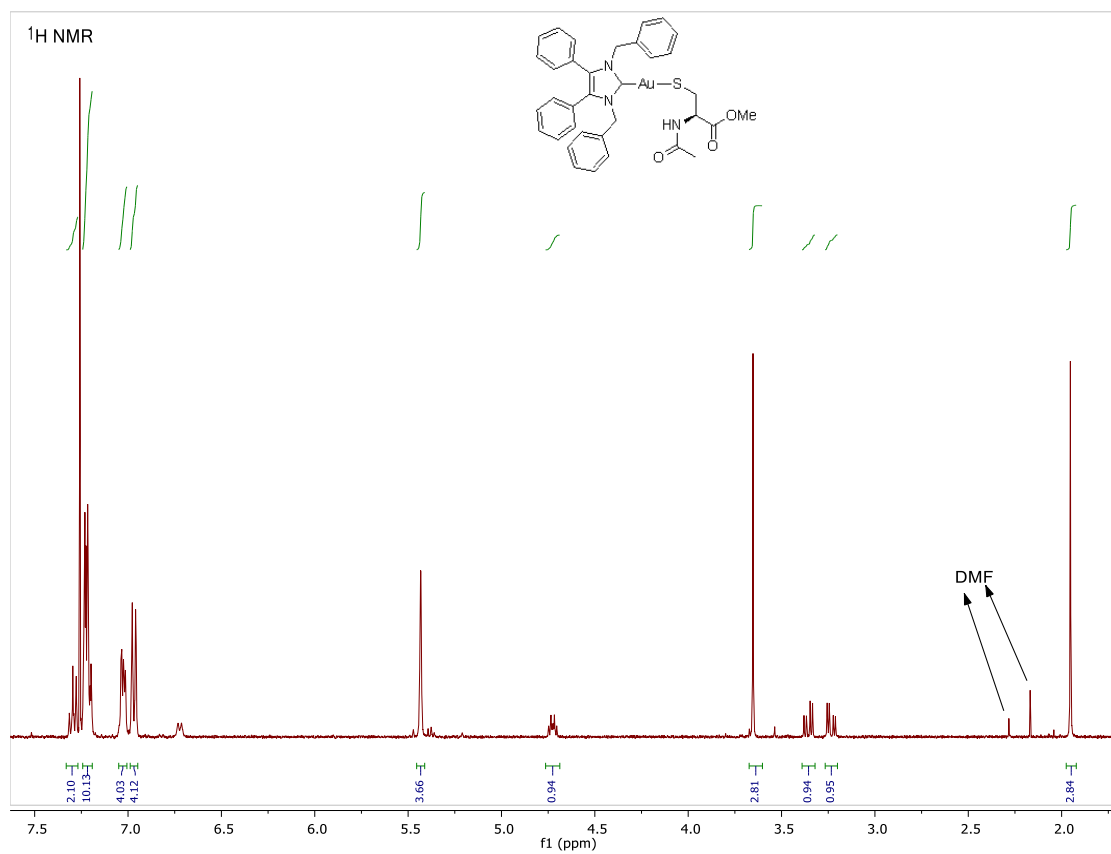




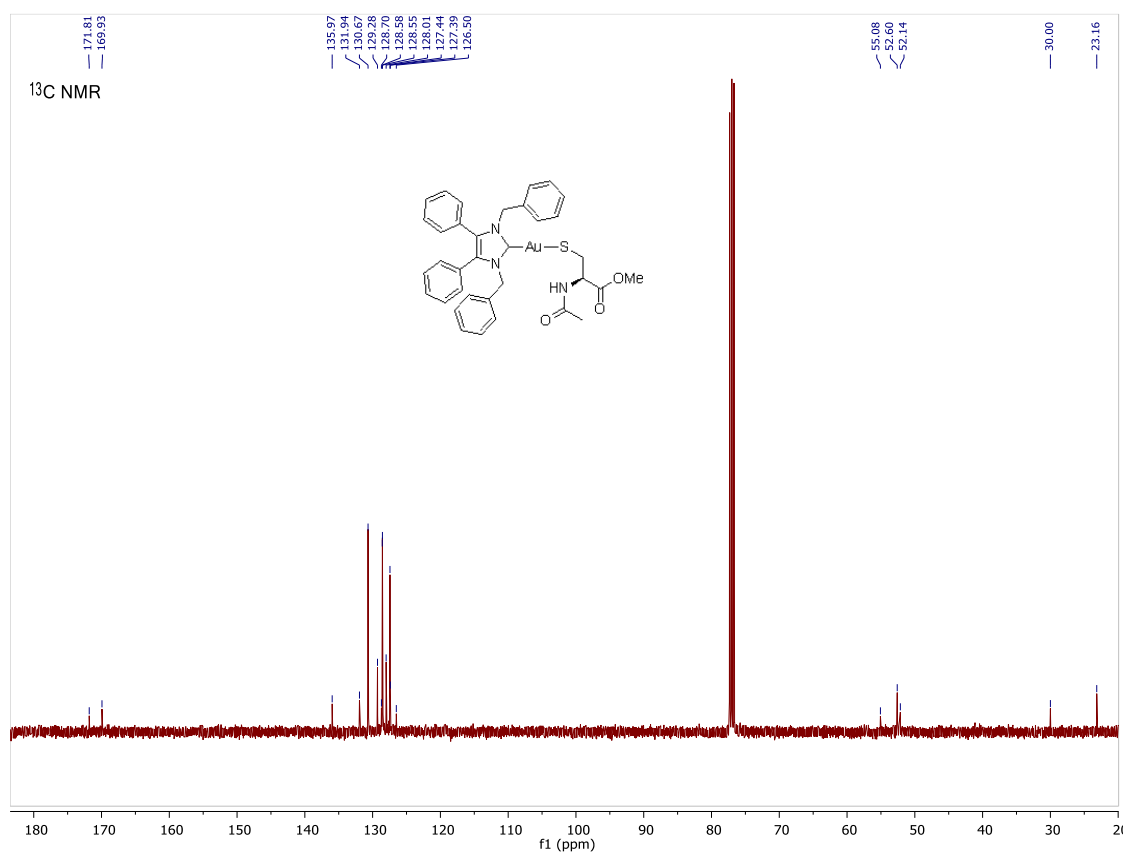
**S 15.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of the new compound 15.



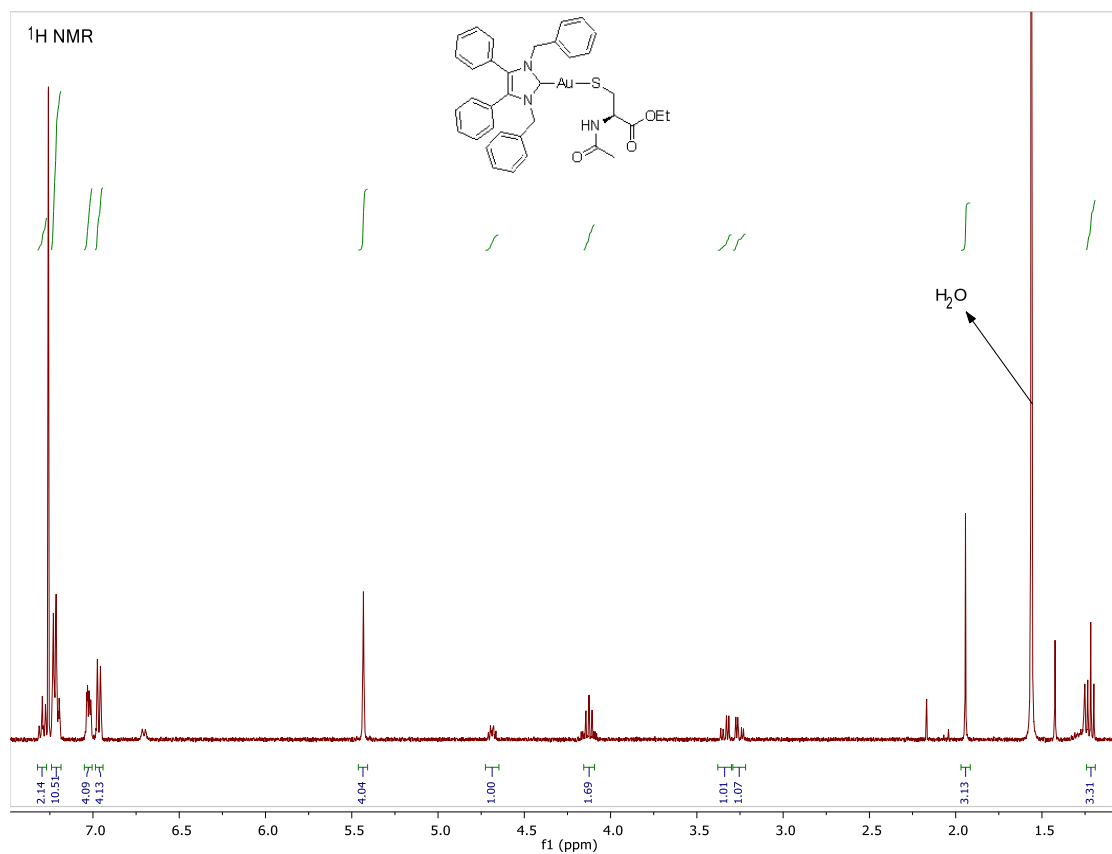
**S 16.** <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound 15.



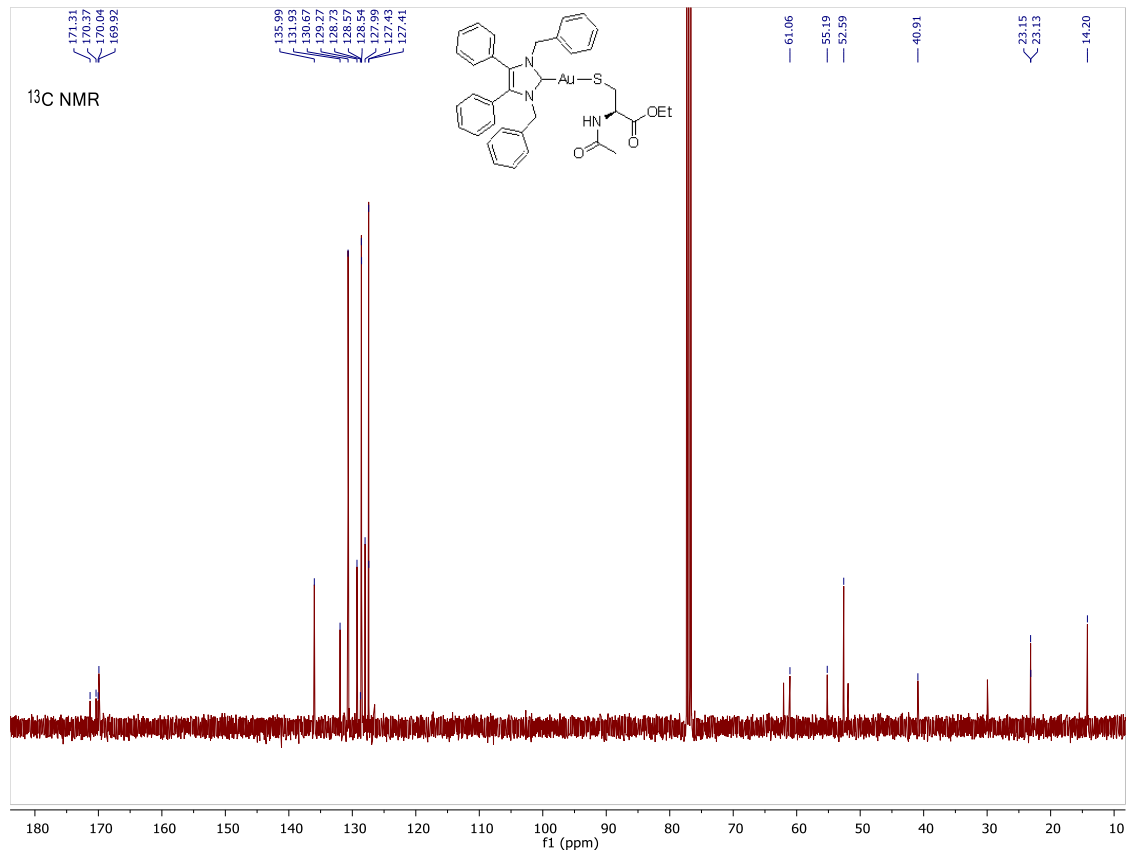
S 17. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of the new compound 16.



S 18. <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound 16.



S 19. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of the new compound 17.



S 20. <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) spectrum of the new compound 17.