

## Supplementary Material

### Ag and Au complexes of *N*-(2-pyridyl)thiourea: coordination behavior and antiproliferative properties

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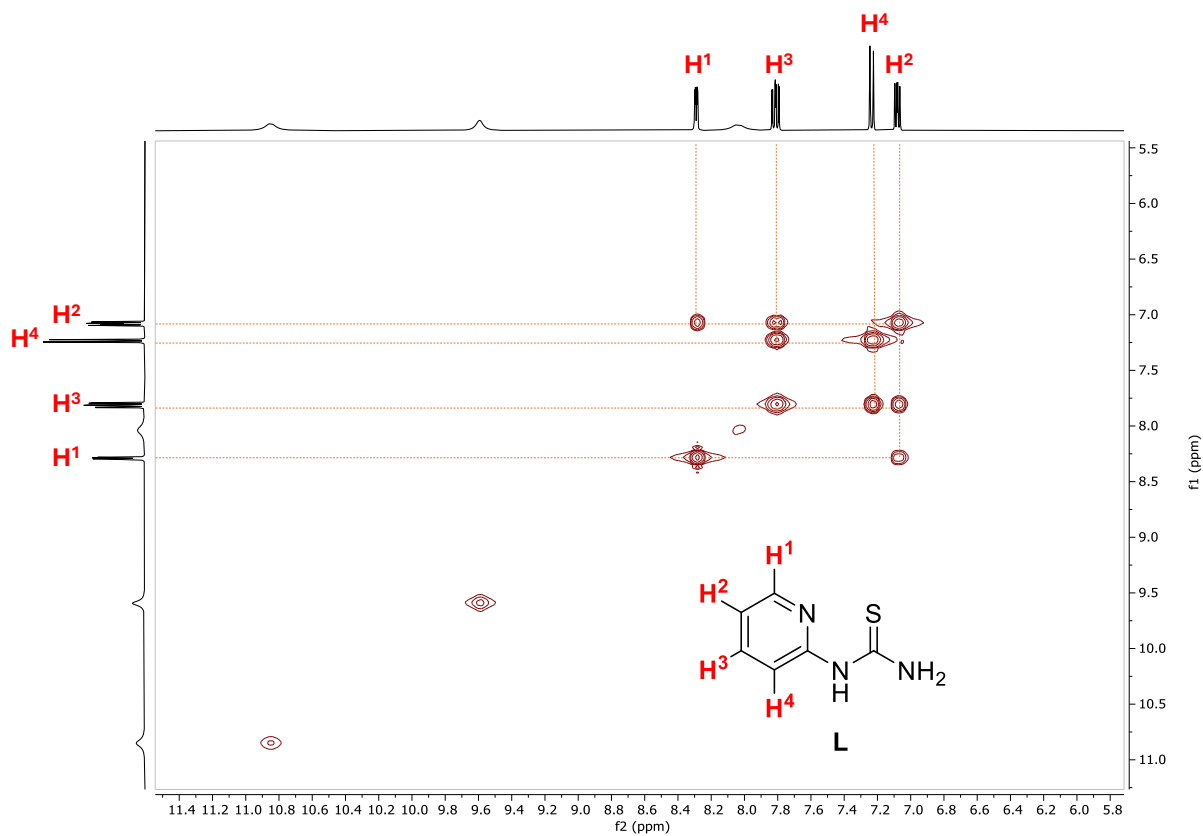
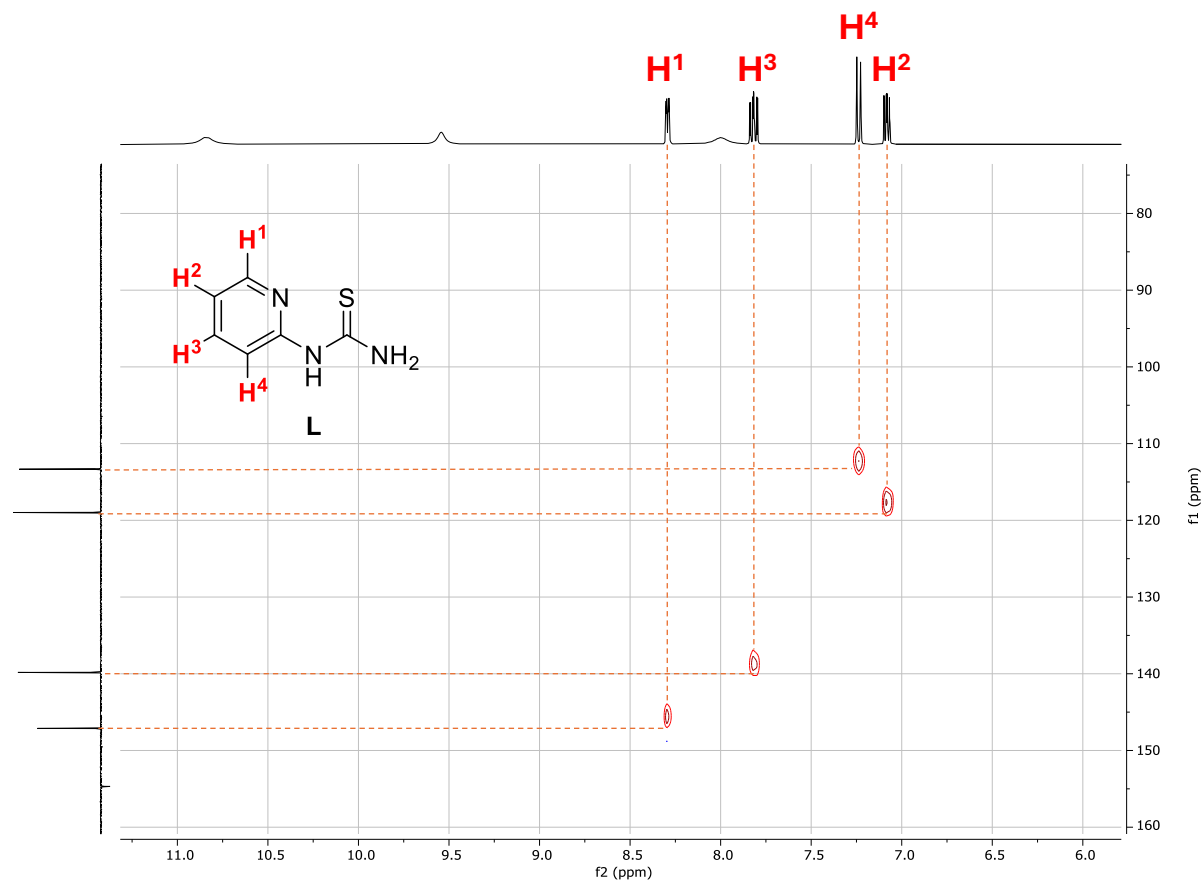
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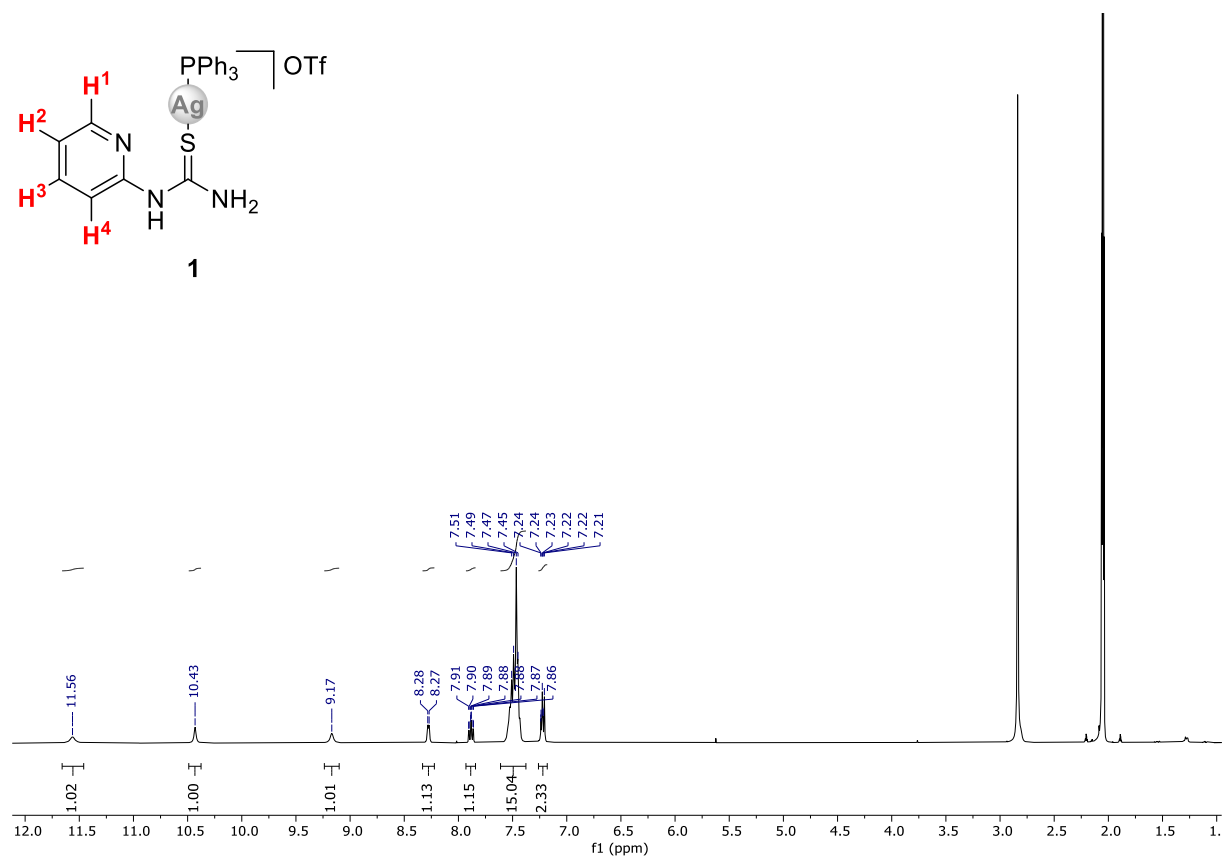
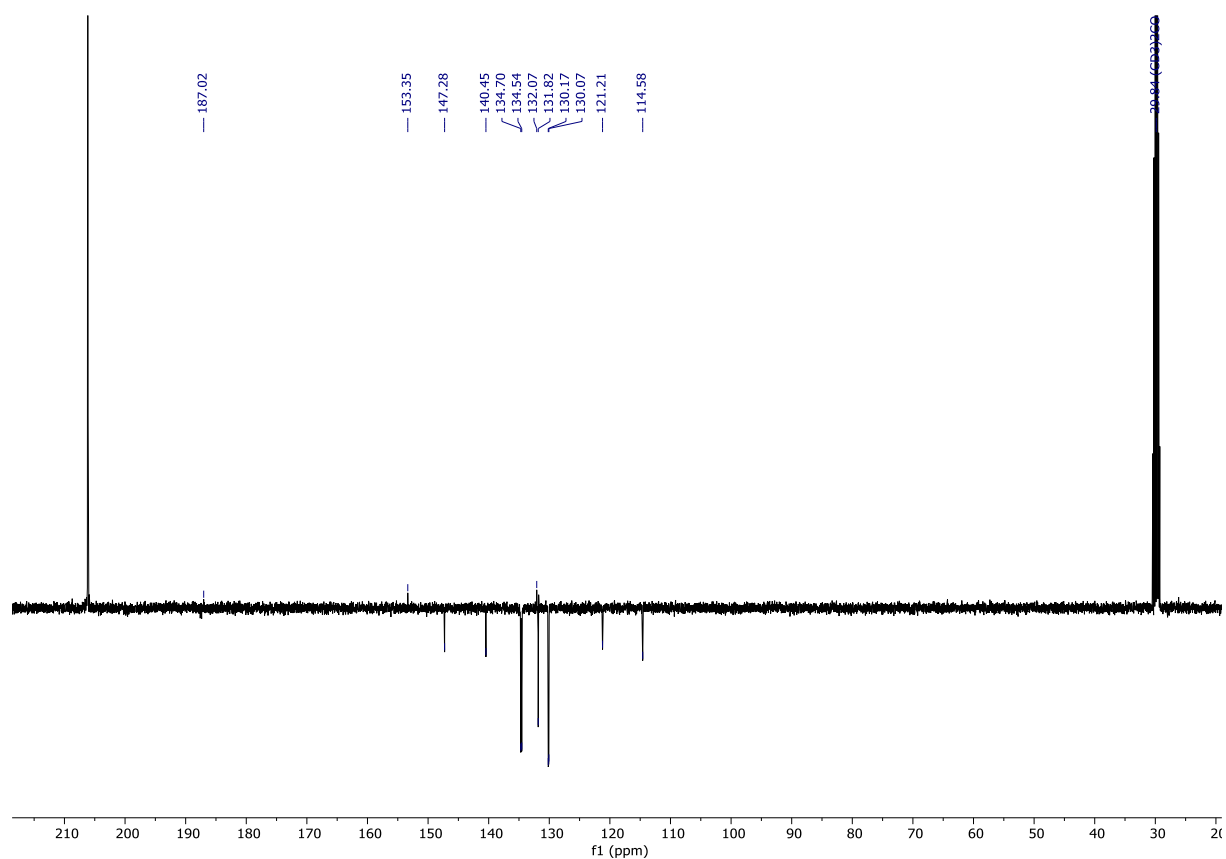
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**Figure S5.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AgL}(\text{PPh}_3)]\text{OTf}$  **1**.**Figure S6.**  $^{13}\text{C}\{^1\text{H}\}$ -APT NMR (100 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AgL}(\text{PPh}_3)]\text{OTf}$  **1**.

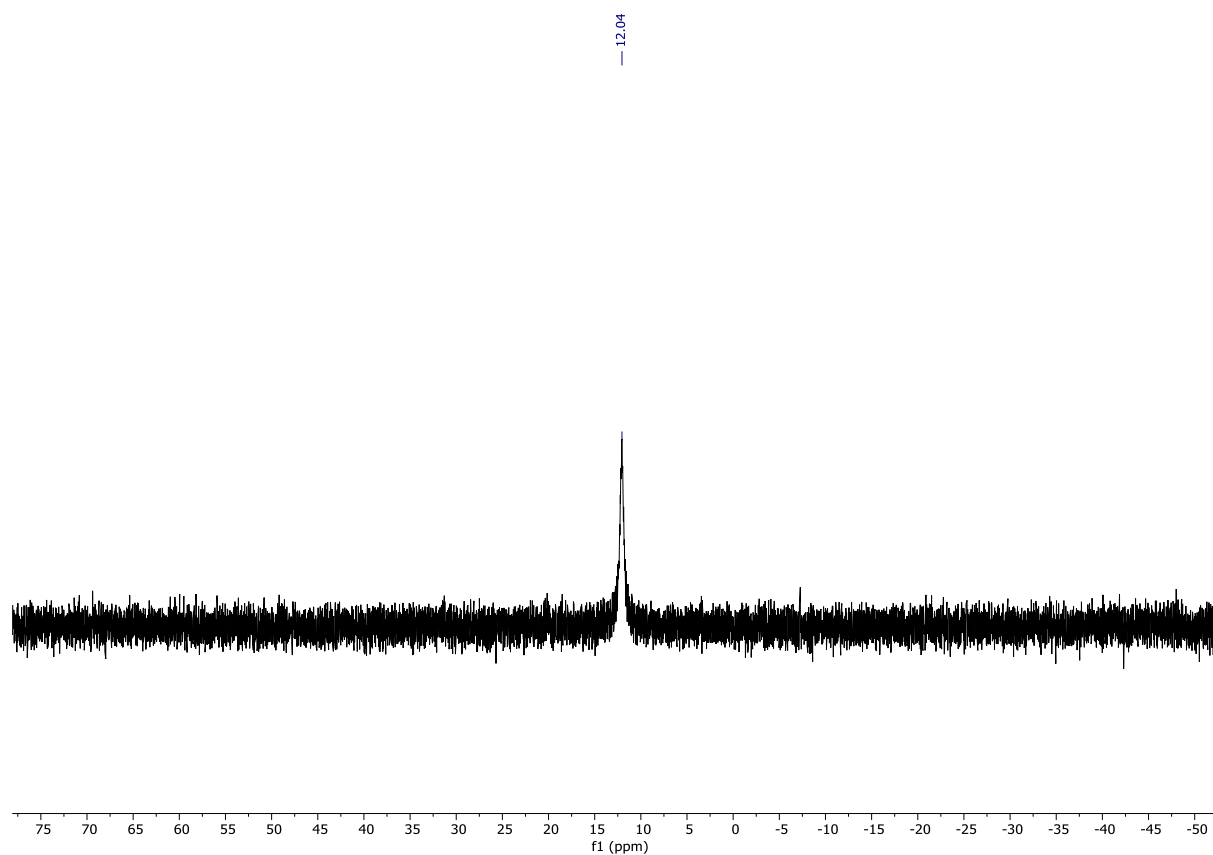
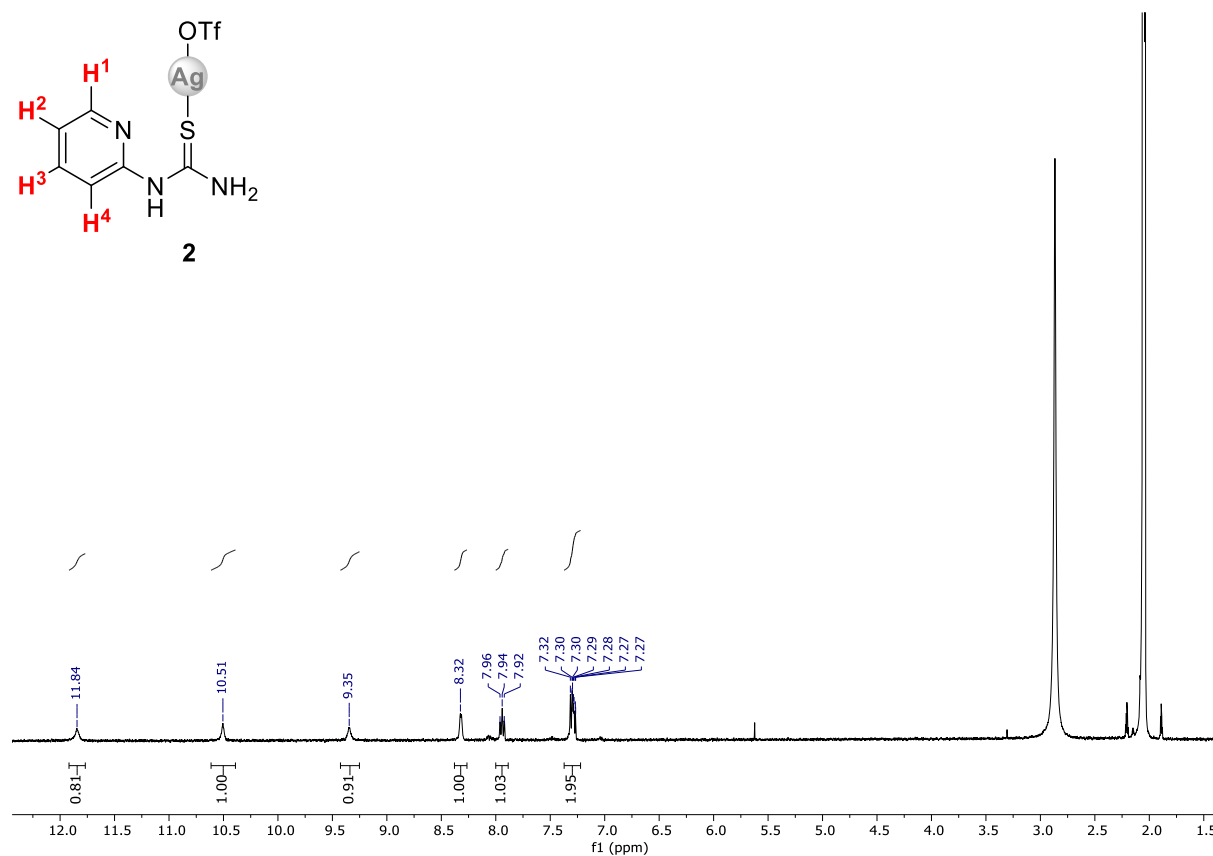
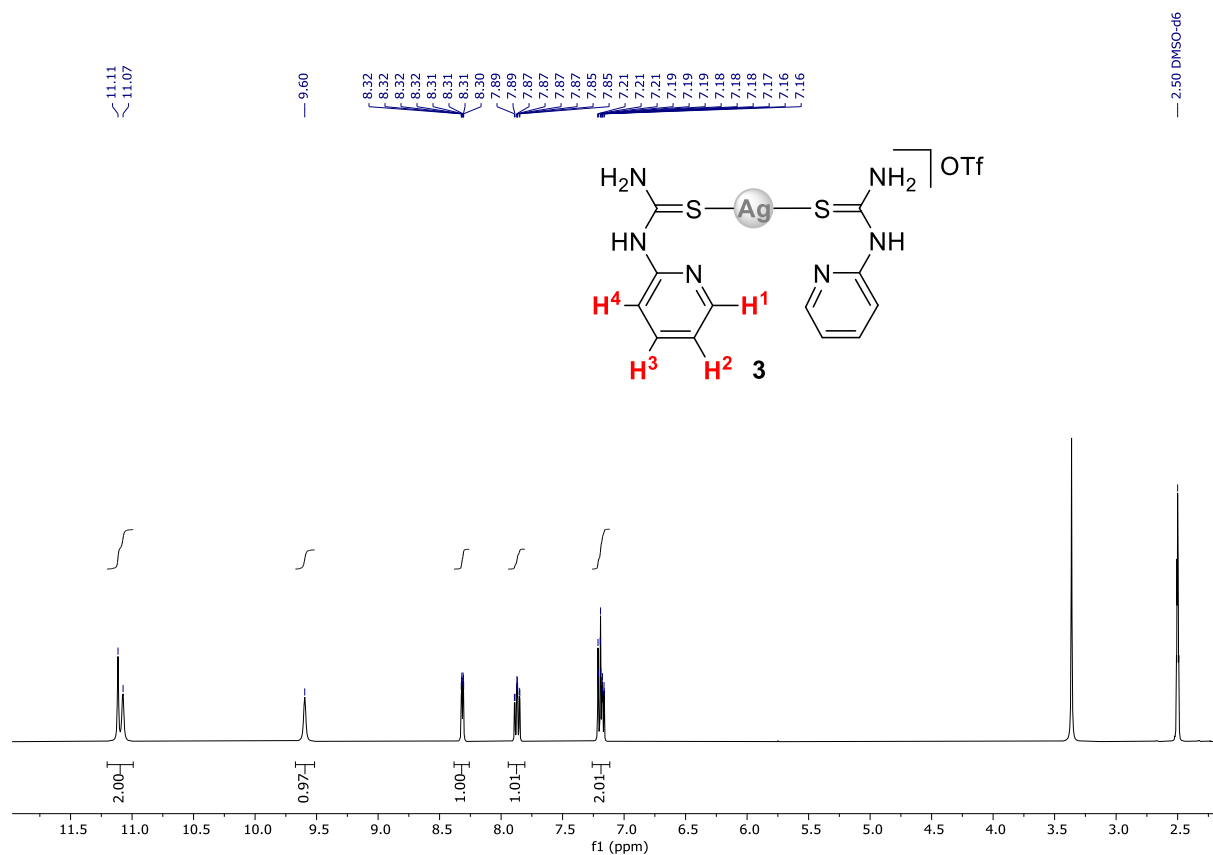
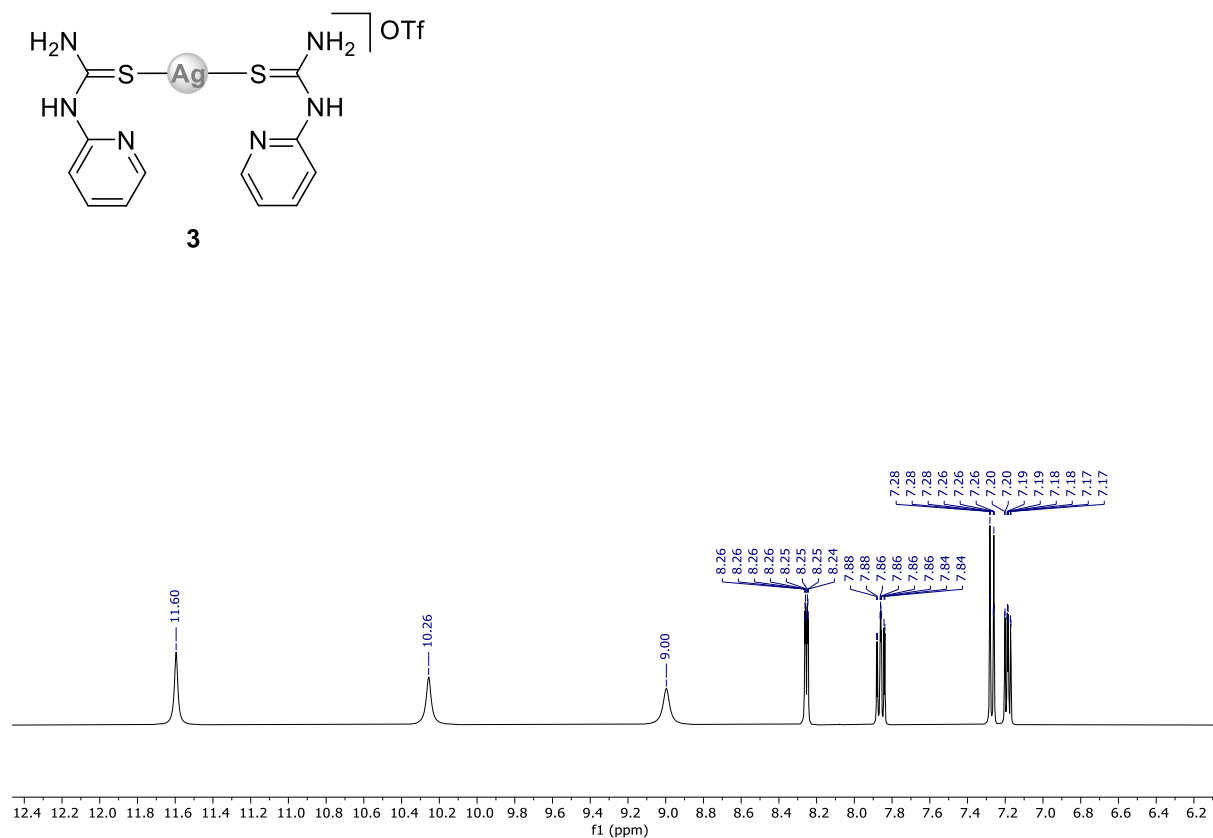
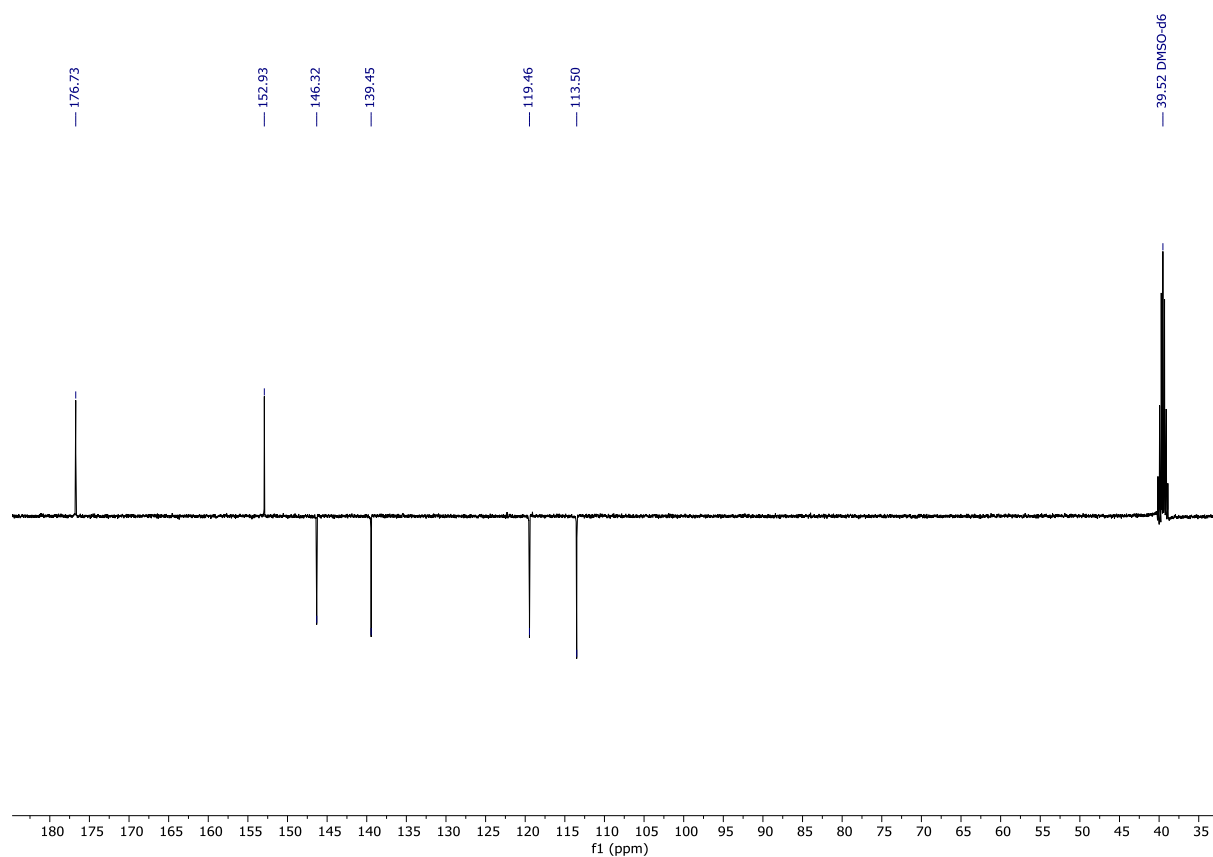
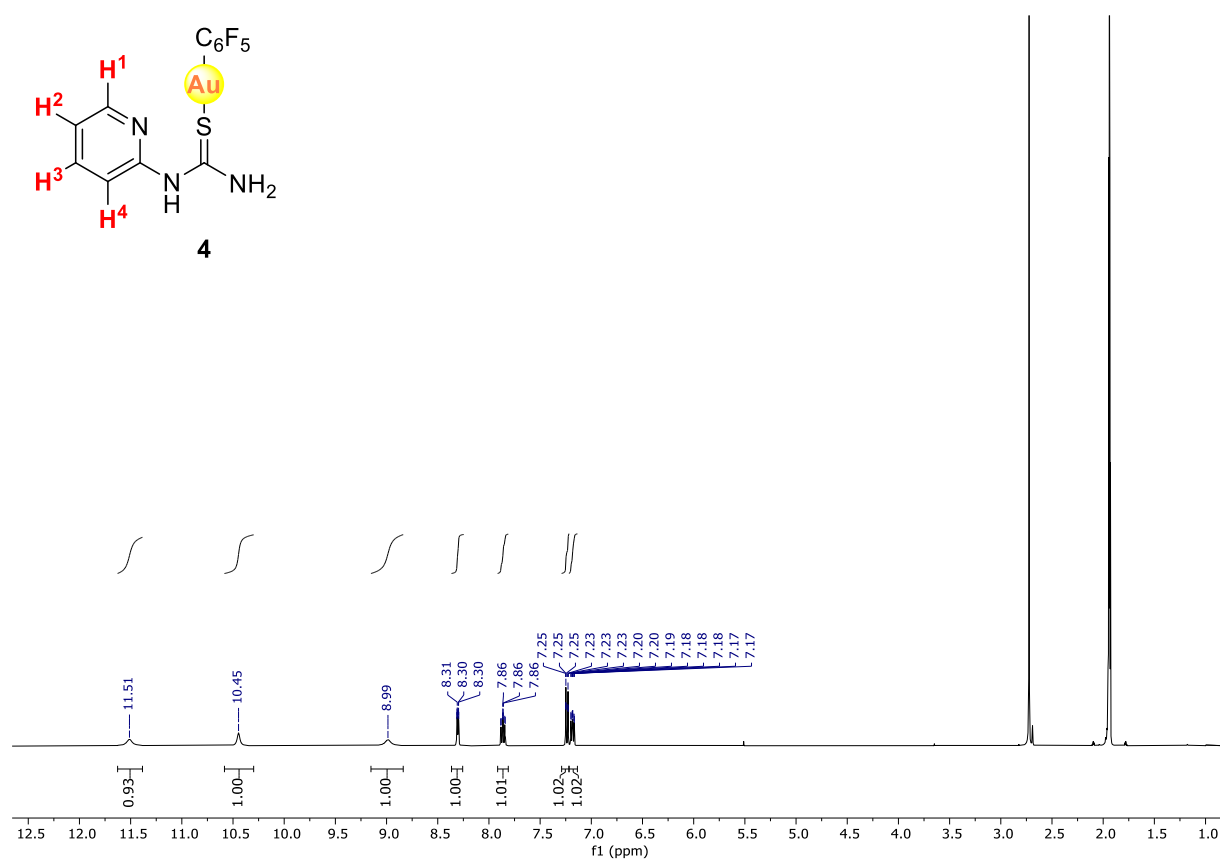
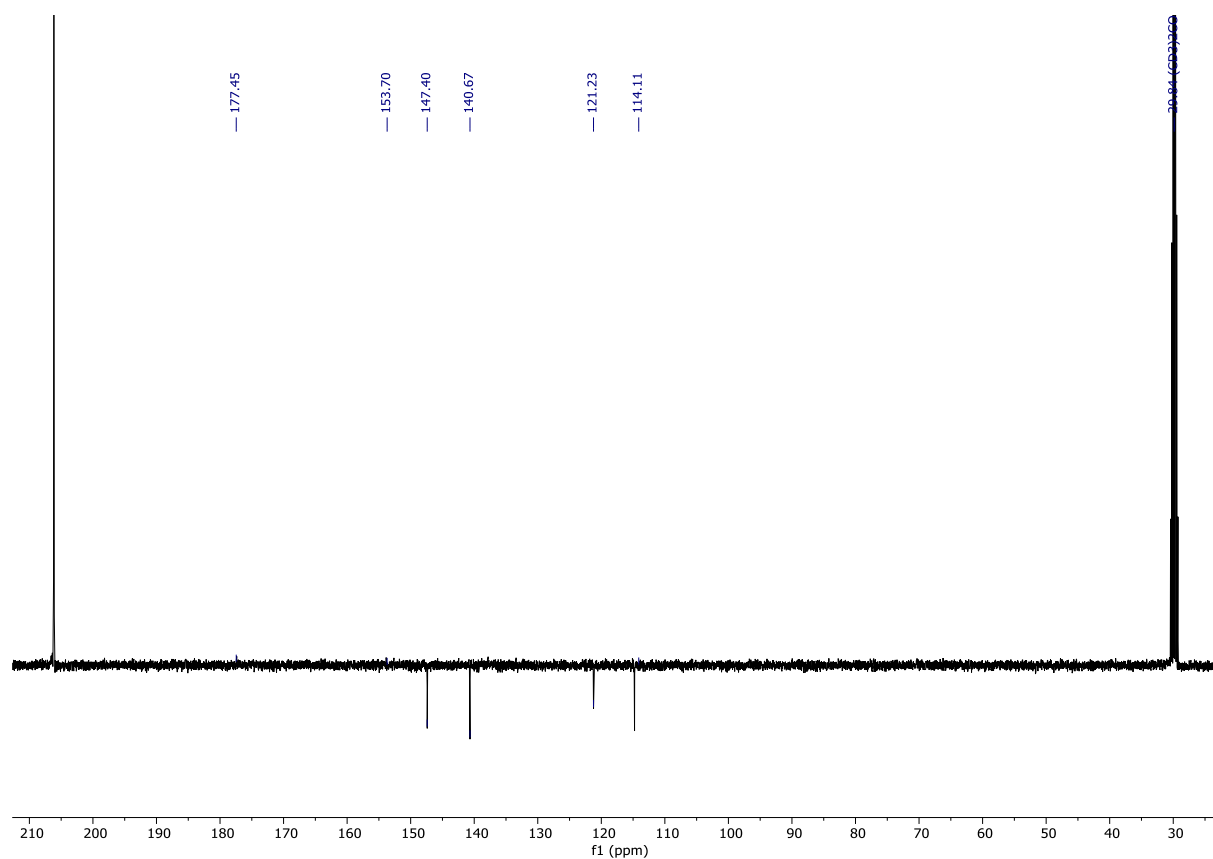
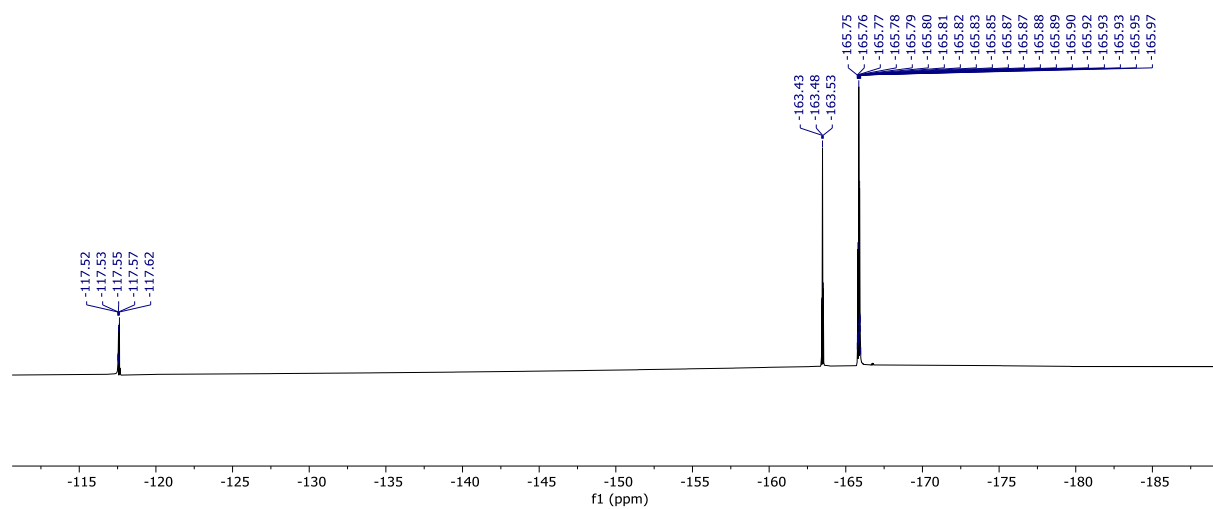
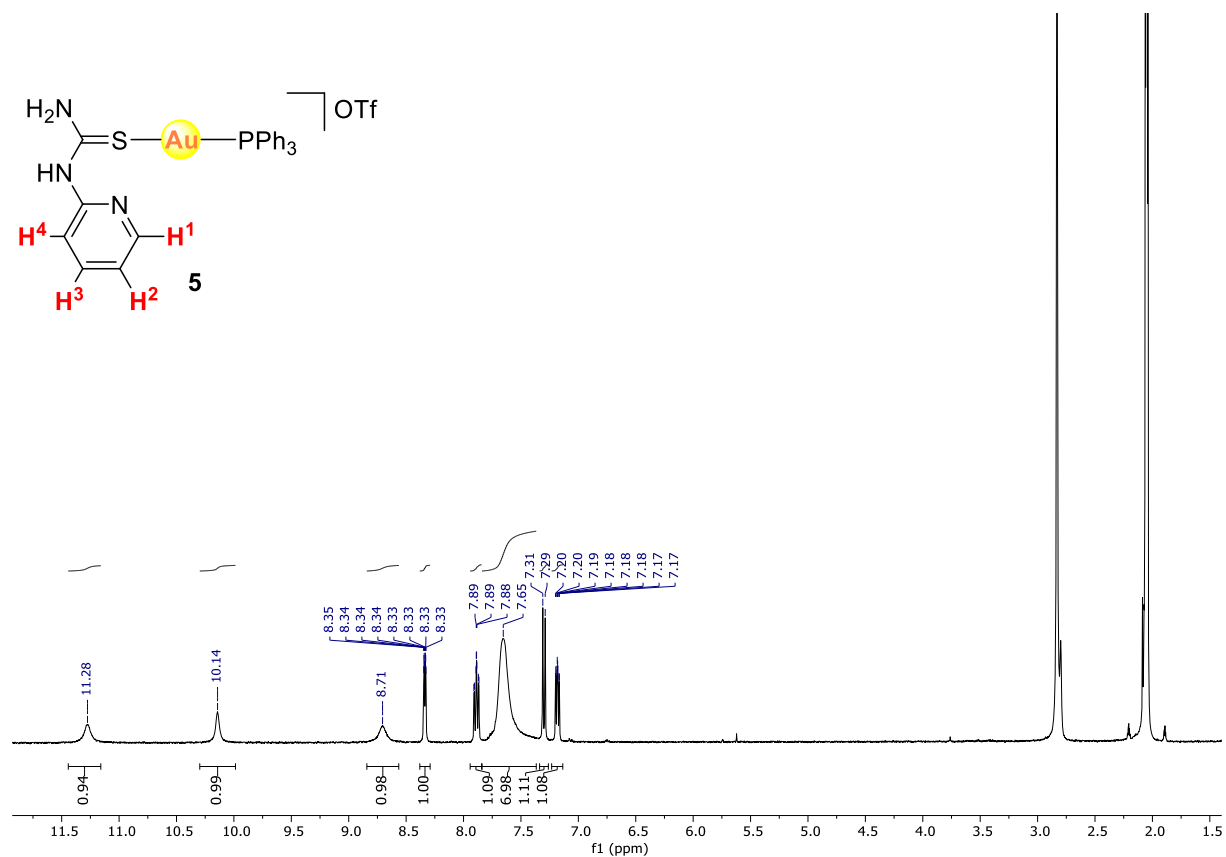
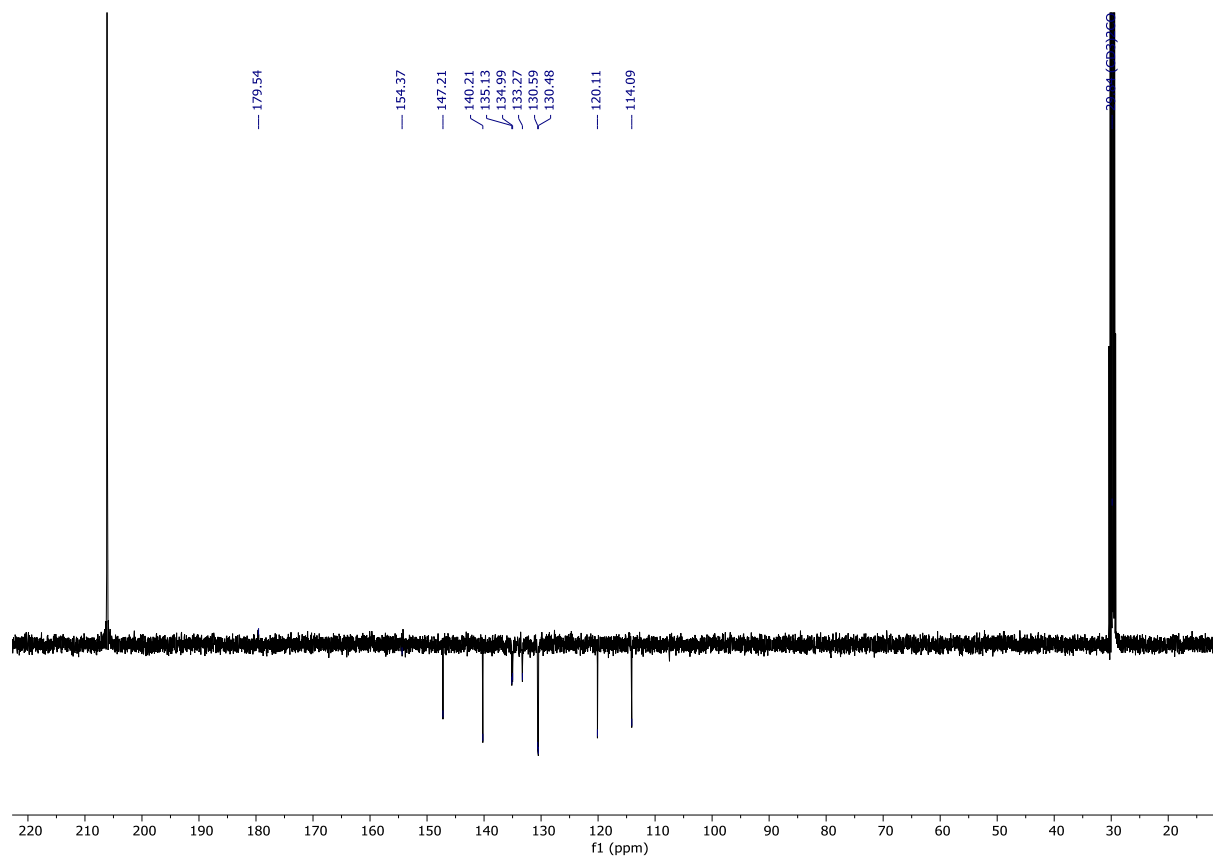
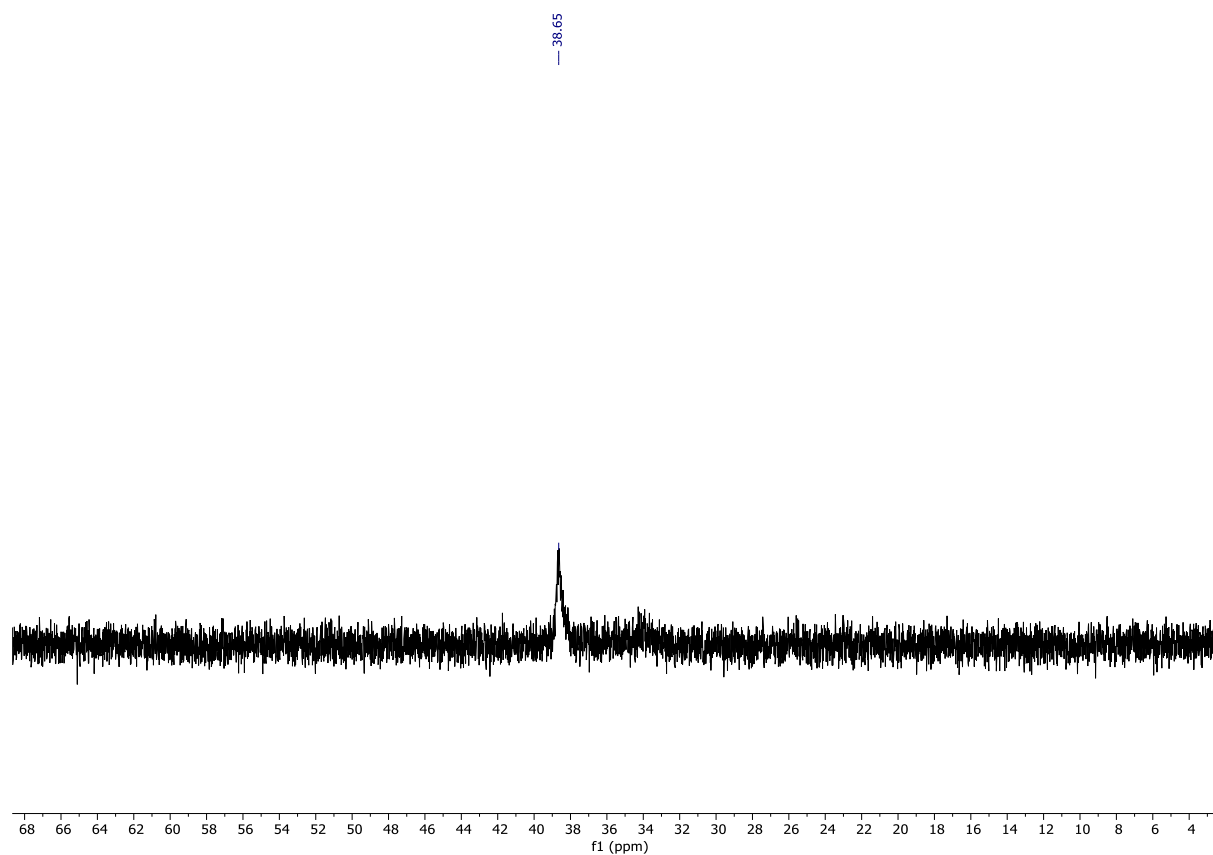
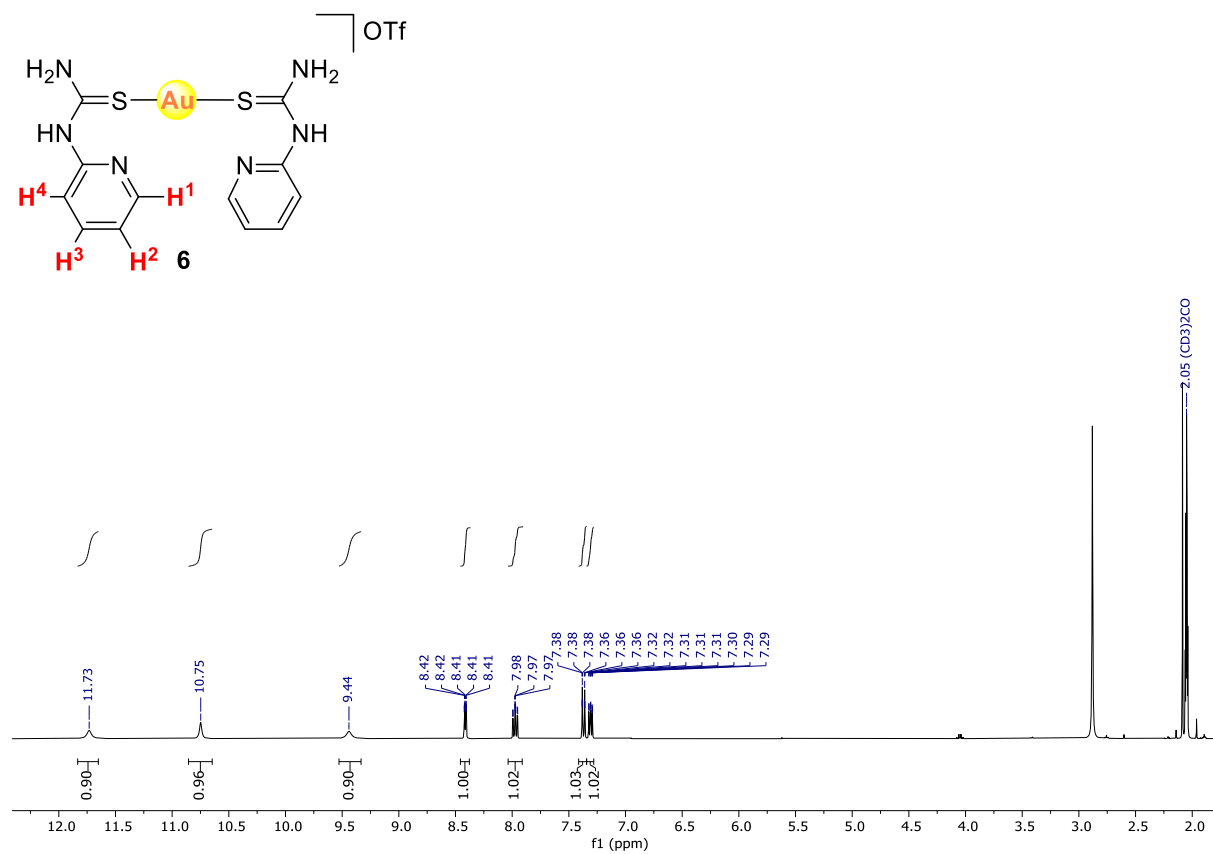
**Figure S7.**  $^{31}\text{P}\{^1\text{H}\}$  NMR (ppm) (162 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AgL}(\text{PPh}_3)]\text{OTf}$  **1**.**Figure S8.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AgL}(\text{OTf})]$  **2**.

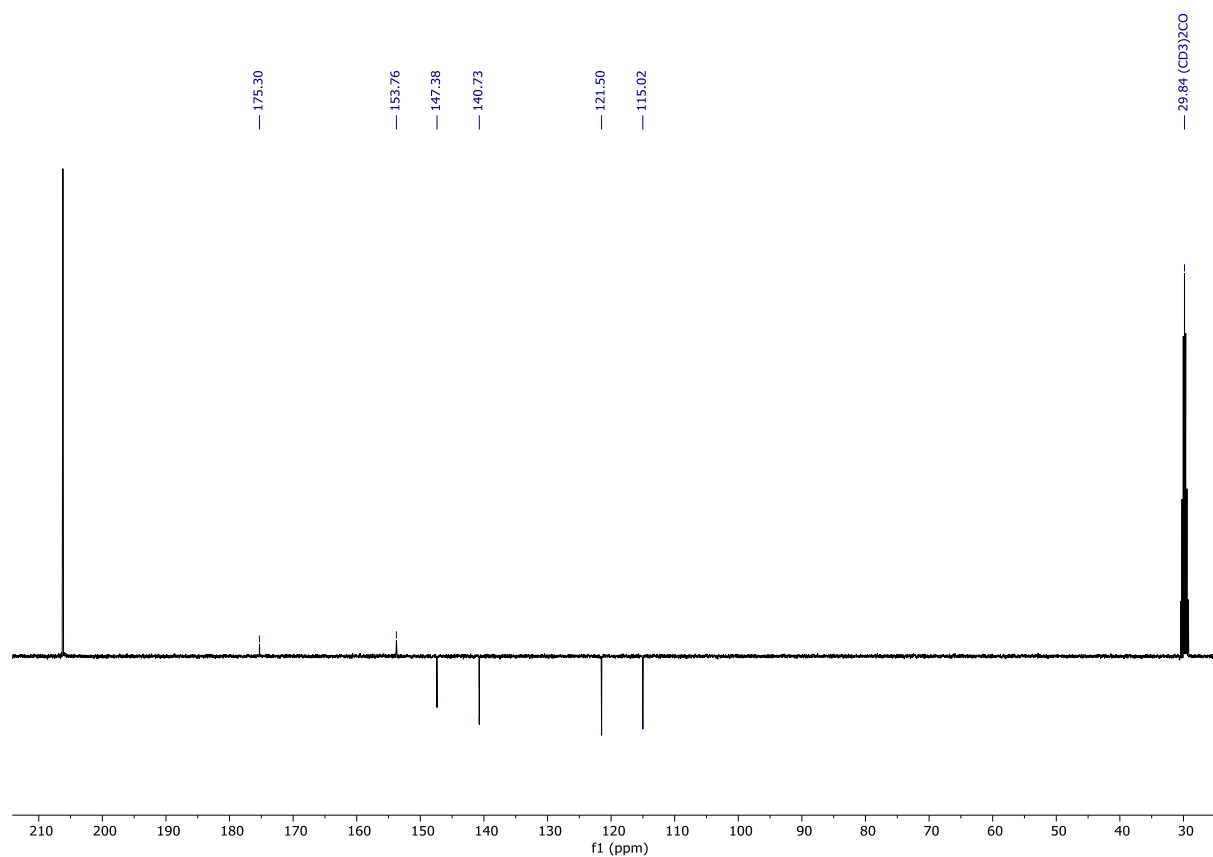
Figure S9.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex  $[\text{AgL}_2](\text{OTf})$  **3**.Figure S10.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AgL}_2](\text{OTf})$  **3**.

**Figure S11.**  $^{13}\text{C}\{^1\text{H}\}$ -APT NMR (100 MHz,  $\text{DMSO-}d_6$ ) spectrum of complex  $[\text{AgL}_2](\text{OTf})$  **3**.**Figure S12.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{Au}(\text{C}_6\text{F}_5)\text{L}]$  **4**.

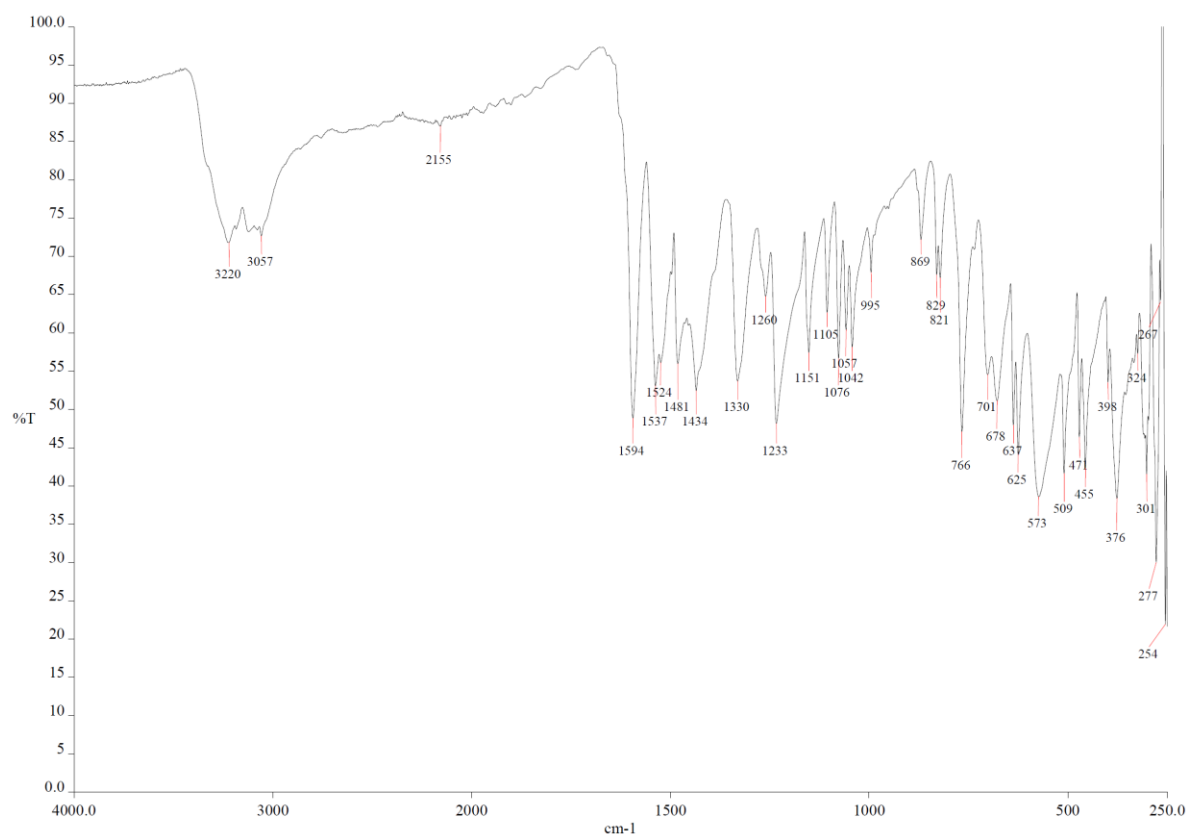
**Figure S13.**  $^{13}\text{C}\{^1\text{H}\}$ -APT NMR (100 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{Au}(\text{C}_6\text{F}_5)\text{L}]$  **4**.**Figure S14.**  $^{19}\text{F}$  NMR (376 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{Au}(\text{C}_6\text{F}_5)\text{L}]$  **4**.

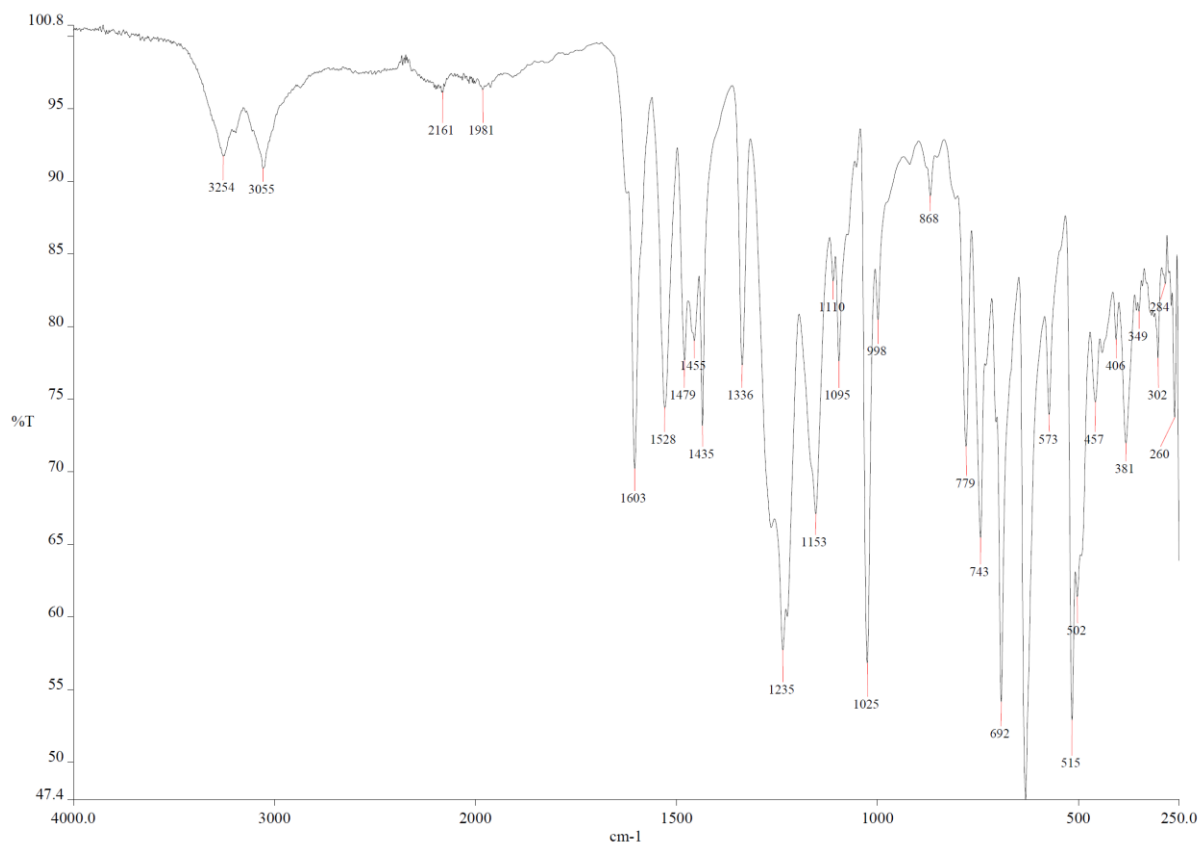
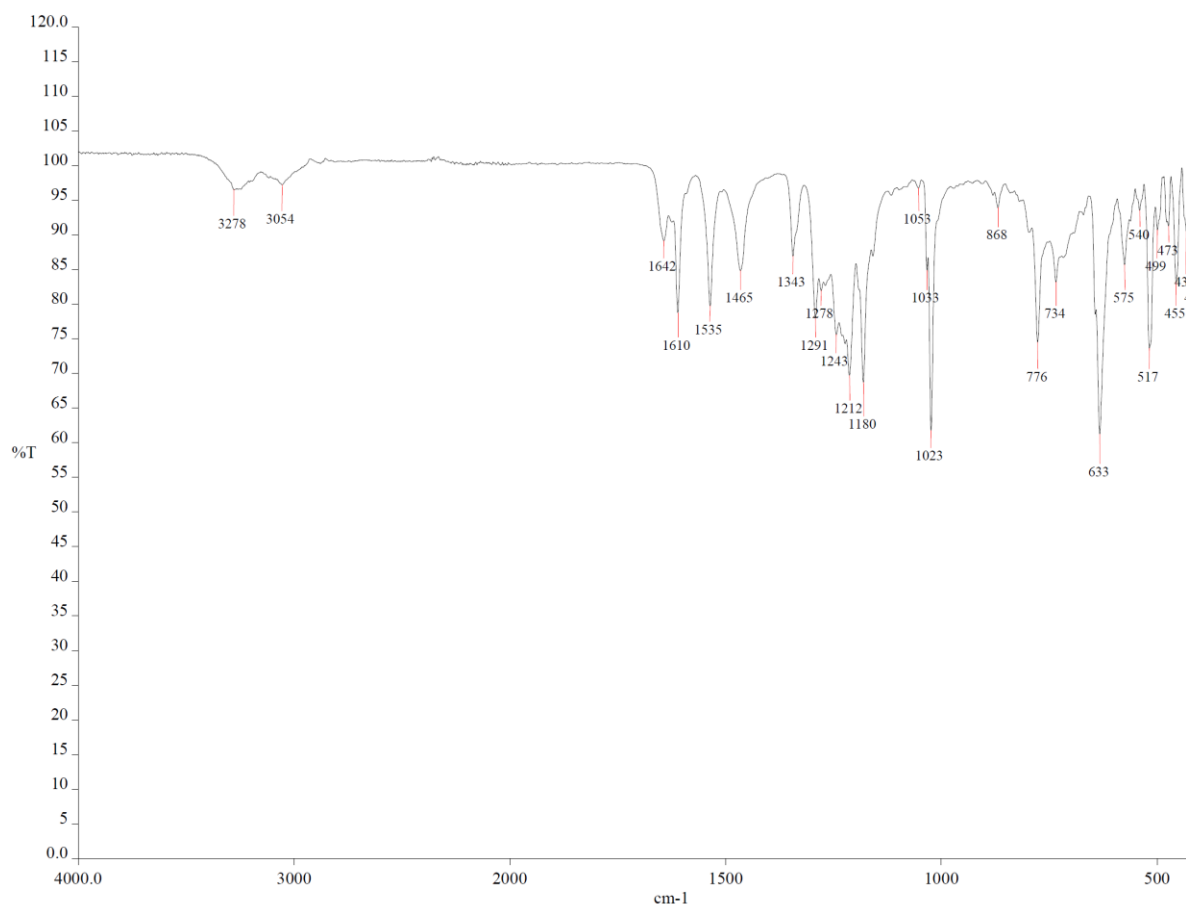
**Figure S15.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AuL}(\text{PPh}_3)]\text{OTf}$  5.**Figure S16.**  $^{13}\text{C}\{^1\text{H}\}$ -APT NMR (100 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AuL}(\text{PPh}_3)]\text{OTf}$  5.

**Figure S17.**  $^{31}\text{P}\{^1\text{H}\}$  NMR (ppm) (162 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AuL}(\text{PPh}_3)]\text{OTf}$  **5**.**Figure S18.**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AuL}_2]\text{OTf}$  **6**.

**Figure S19.**  $^{13}\text{C}\{^1\text{H}\}$ -APT NMR (100 MHz,  $\text{CD}_3\text{C}(\text{O})\text{CD}_3$ ) spectrum of complex  $[\text{AuL}_2]\text{OTf}$  **6**.

## 2.- IR spectra of complexes 1-6 and ligand L

**Figure S20.** IR spectrum of L

**Figure S21.** IR spectrum of complex [AgL(PPh<sub>3</sub>)OTf] 1**Figure S22.** IR spectrum of complex [AgL(OTf)] 2

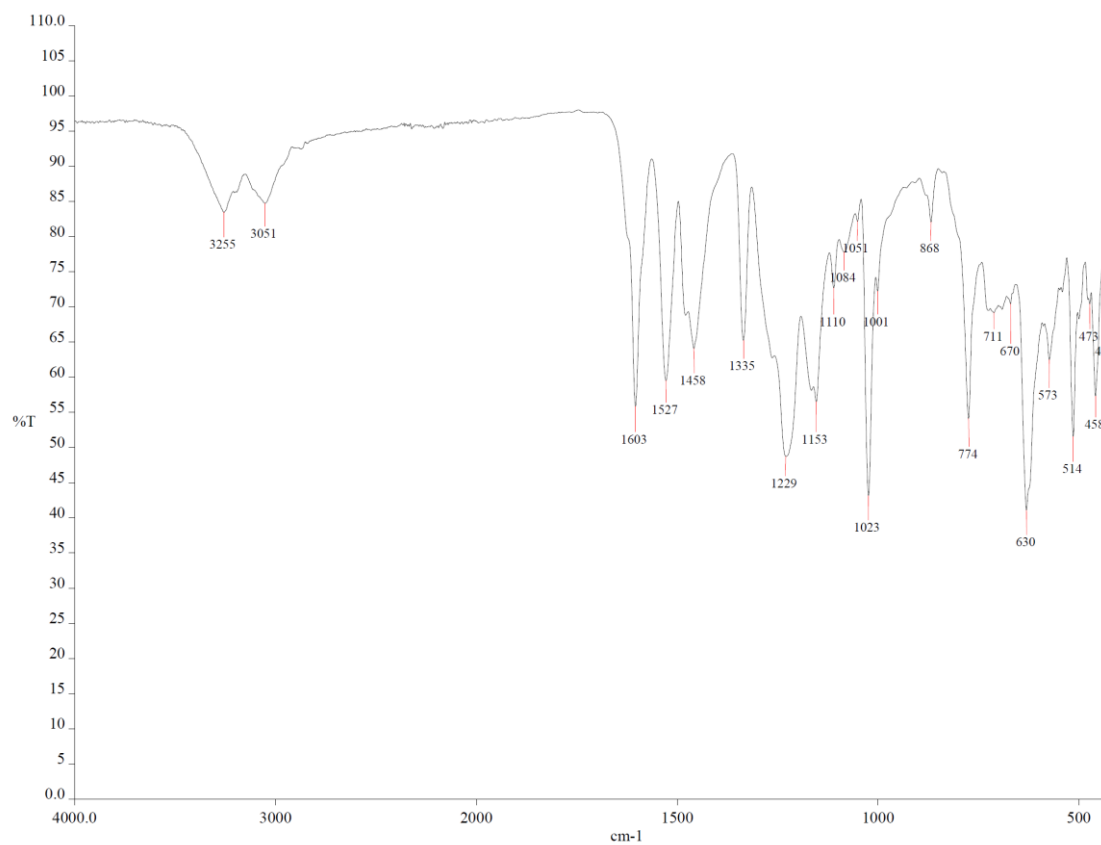
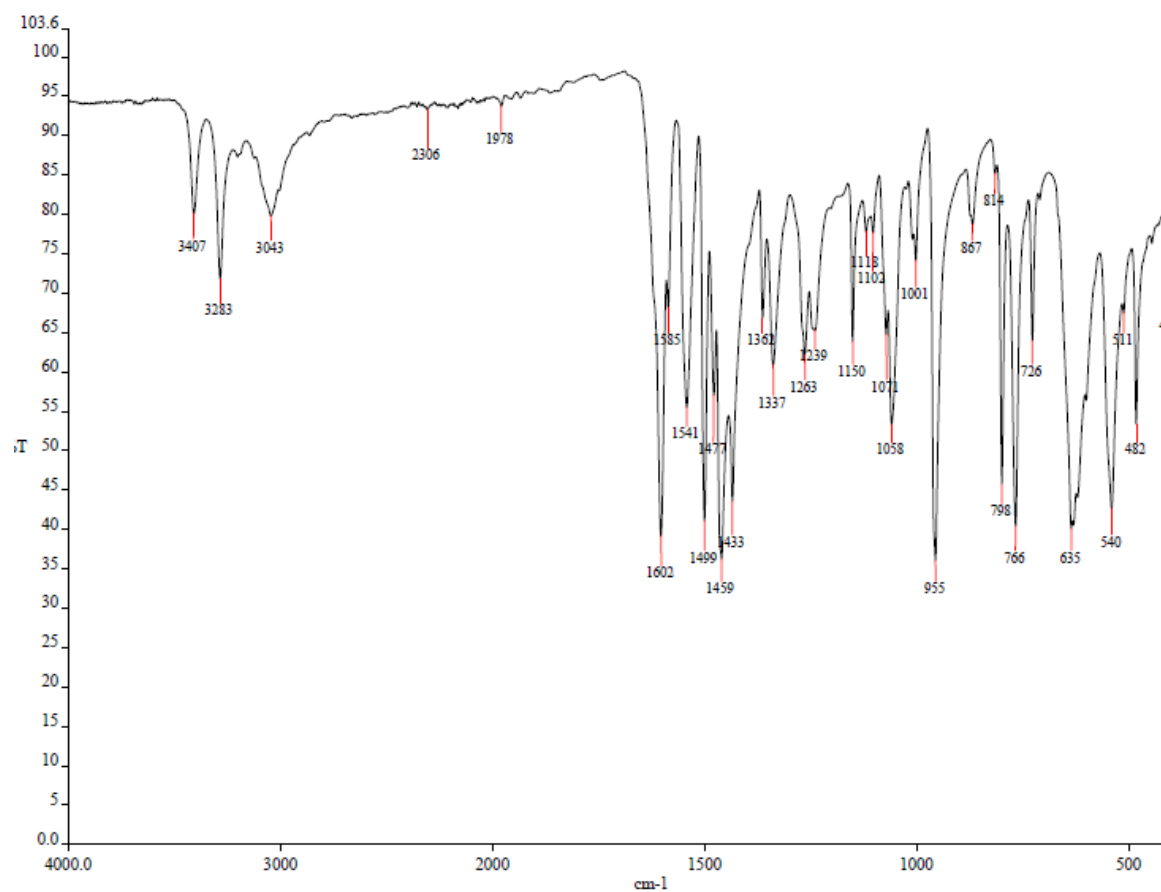
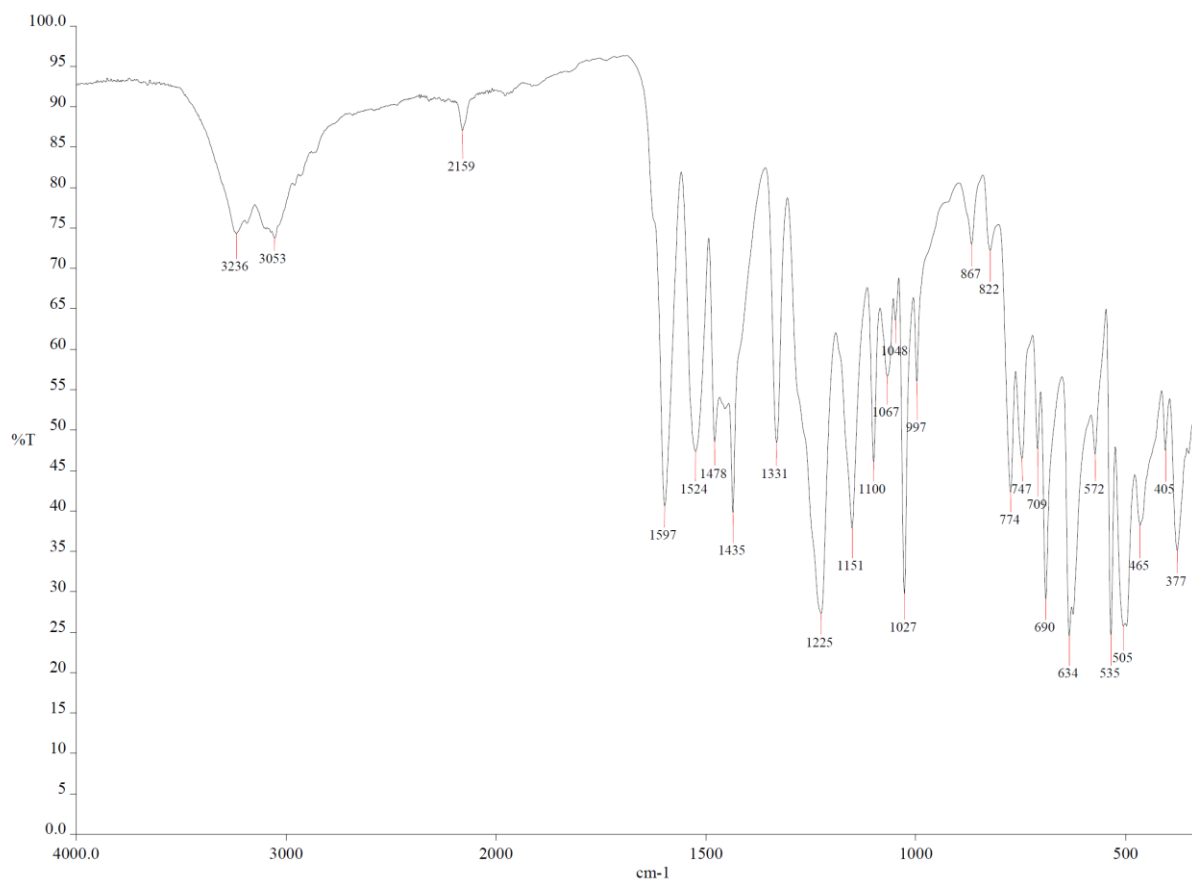
**Figure S23.** IR spectrum of complex  $[\text{AgL}_2](\text{OTf})$  **3****Figure S24.** IR spectrum of complex  $[\text{Au}(\text{C}_6\text{F}_5)\text{L}]$  **4**

Figure S25. IR spectrum of complex  $[\text{AuL}(\text{PPh}_3)]\text{OTf } 5$ Figure S26. IR spectrum of complex  $[\text{AuL}_2]\text{OTf } 6$ 