

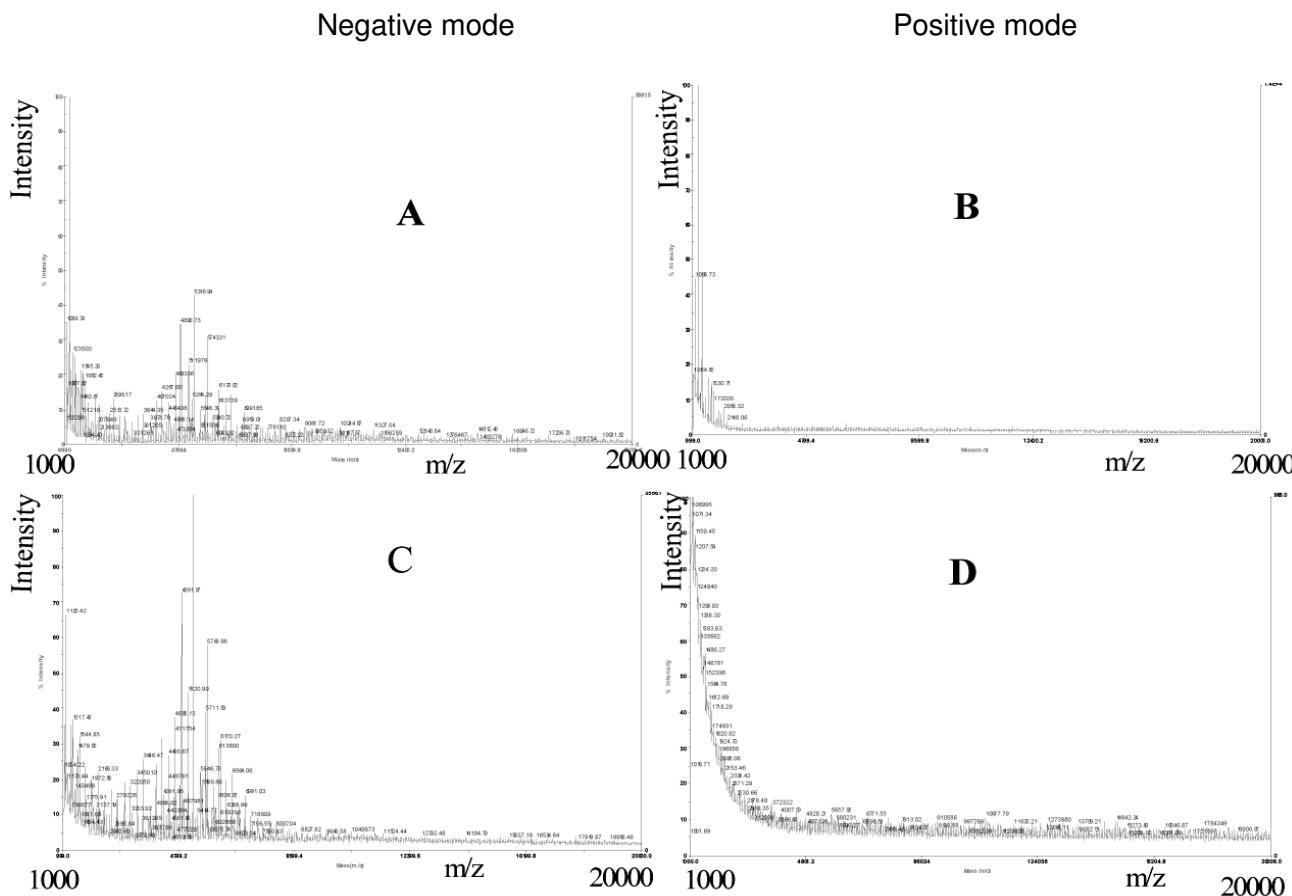
## **Supporting Information:**

# Probing the Structure and Charge State of Glutathione-Capped $\text{Au}_{25}(\text{SG})_{18}$ Clusters by NMR and Mass Spectrometry

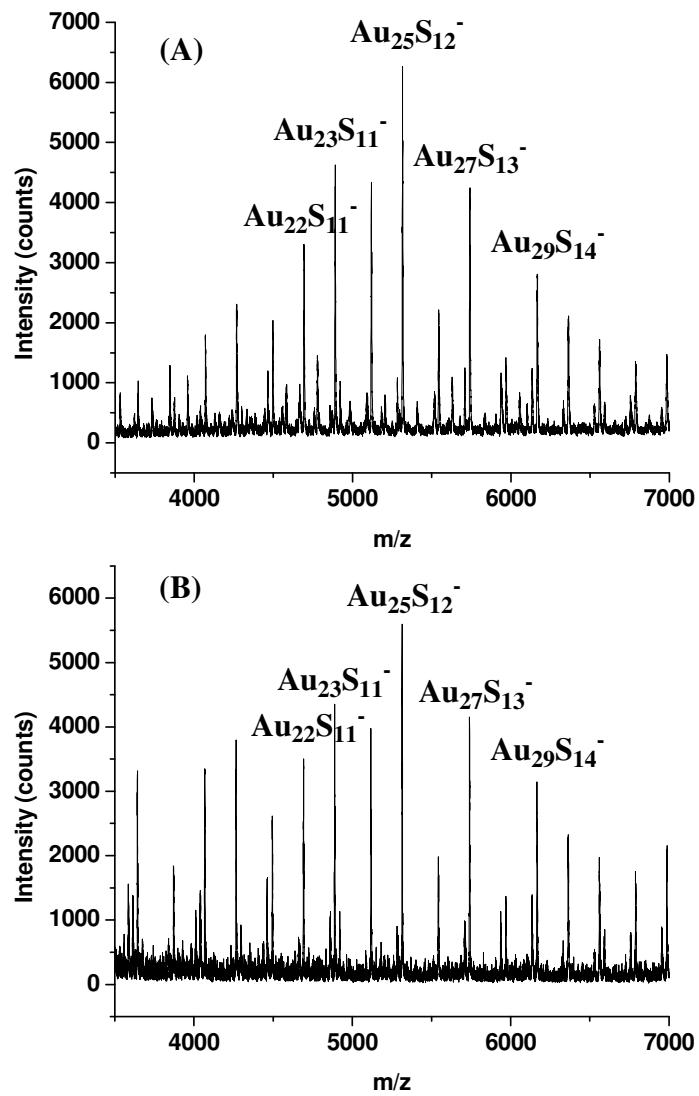
Zhiqun Wu, Chakicherla Gayathri, Roberto R. Gil, and Rongchao Jin <sup>\*</sup>

*Department of Chemistry, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213.*

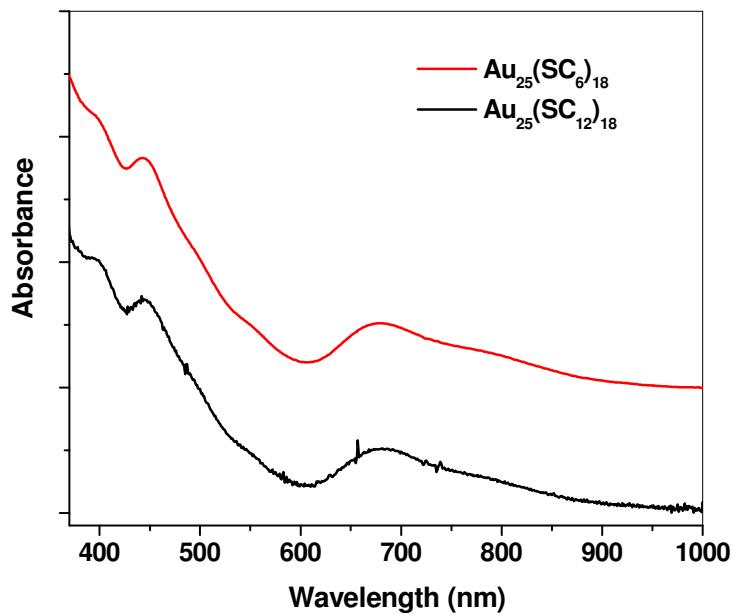
## 1. Supporting Figure S1–S3



**Figure S1.** Laser desorption ionization (LDI) MS spectra of phenylethylthiolate and glutathione capped  $\text{Au}_{25}$  clusters.  $\text{Au}_{25}(\text{SCH}_2\text{CH}_2\text{Ph})_{18}$  in the negative ion mode (A) and positive ion mode (B);  $\text{Au}_{25}(\text{SG})_{18}$  in the negative ion mode (C) and positive ion mode (D).



**Figure S2.** Laser desorption ionization (LDI) MS spectra of  $\text{Au}_{25}(\text{SC}_6\text{H}_{13})_{18}$  (A) and  $\text{Au}_{25}(\text{SC}_{12}\text{H}_{25})_{18}$  (B). Both spectra were collected in the negative mode.



**Figure S3.** The UV-vis absorption spectra of  $\text{Au}_{25}(\text{SC}_6\text{H}_{13})_{18}$  (red profile) and  $\text{Au}_{25}(\text{SC}_{12}\text{H}_{25})_{18}$  (black profile). The spectra are shifted for clarity.