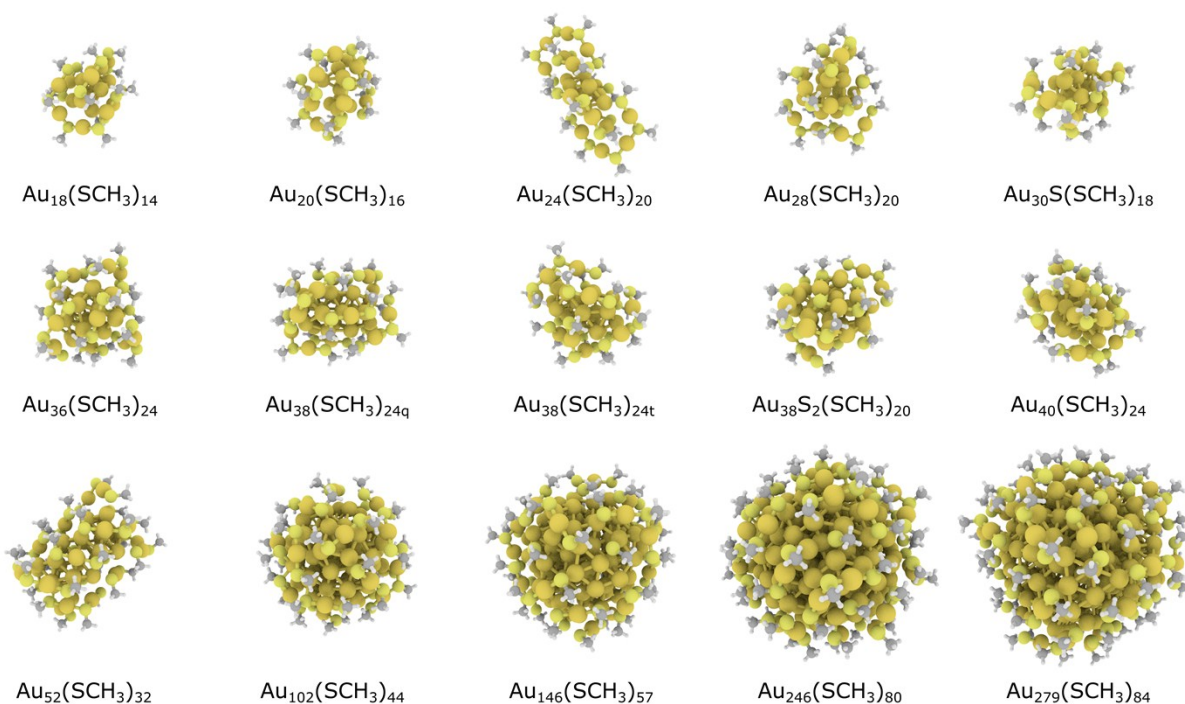


## Supporting Information for “Structure-property Relationships on Thiolate-protected Gold Nanoclusters”

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**Figure S1:** Fully optimized structures of Au NC ranging from  $\text{Au}_{18}(\text{SR})_{14}$  to  $\text{Au}_{279}(\text{SR})_{84}$ , where the R groups have been simulated with methyl ligands. White, gray, yellow, and gold correspond to hydrogen, carbon, sulfur, and gold atoms, respectively.