Electronic Supplementary Information to

Strong non-linear effects in the chiroptical properties of the ligand-exchanged Au_{38} and Au_{40} clusters

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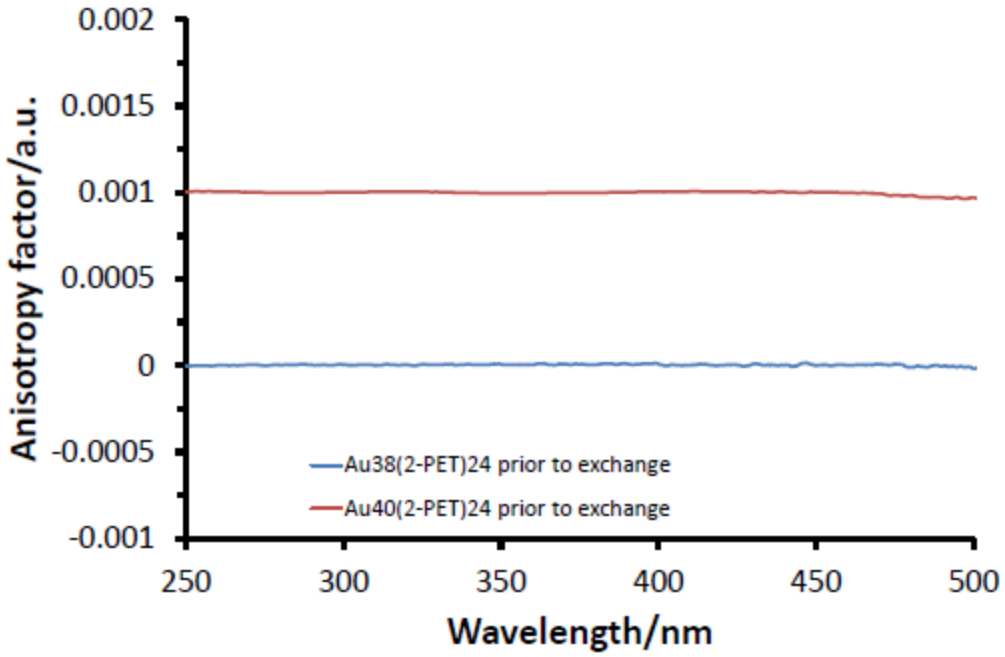

Figure S-1. Anisotropy factors of $Au_{38}(2\text{-PET})_{24}$ (blue) and $Au_{40}(2\text{-PET})_{24}$ (red) prior to exchange with BINAS and CamSH. The trace for Au_{40} is off-set by 0.001 for clarity.

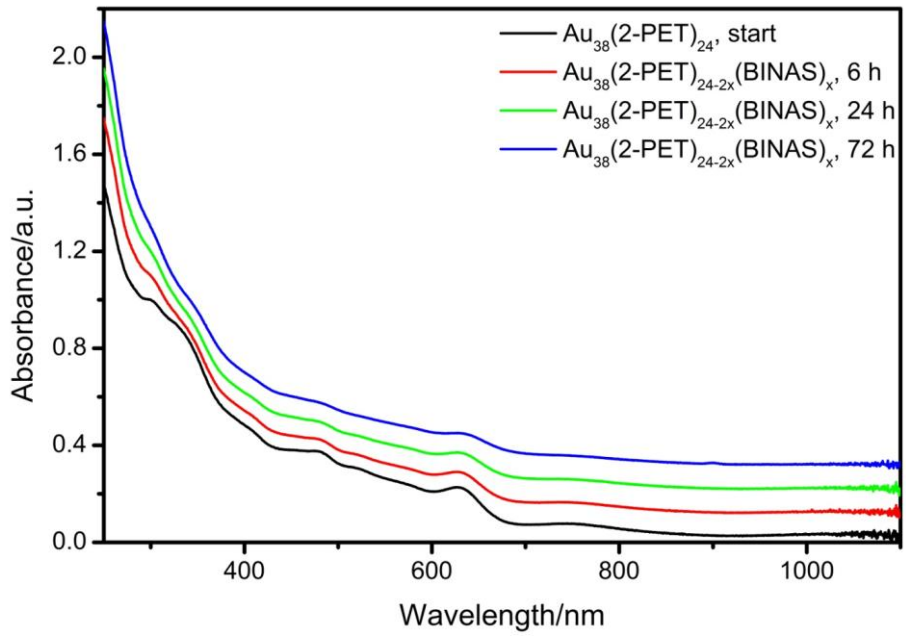

Figure S-2. UV-Vis spectra of $Au_{38}(2\text{-PET})_{24}$ before (black) and after reaction with BINAS. The characteristic features of Au_{38} are maintained, but slightly blurred after long reaction time.

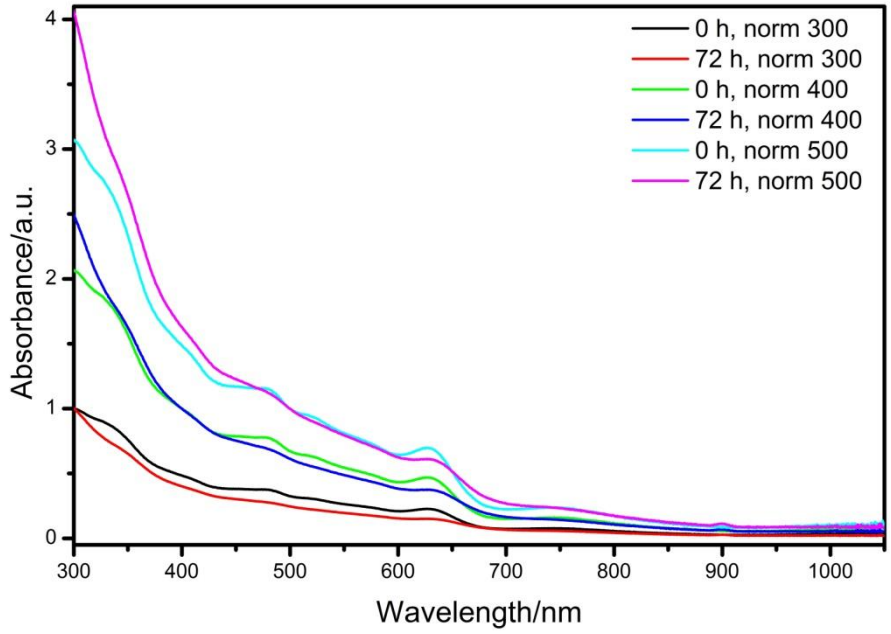

Figure S-3. UV-Vis spectra of $Au_{38}(2\text{-PET})_{24}$ before and after exchange with BINAS (72 h). The spectra are normalized at 300, 400 and 500 nm, respectively. This highlights that a) the spectra seem less defined as an effect of the normalization (at 300 nm) due to BINAS absorbance and b) partial covering of the cluster with BINAS leads to slightly altered absorption features (e.g., compare the 629 nm transition).

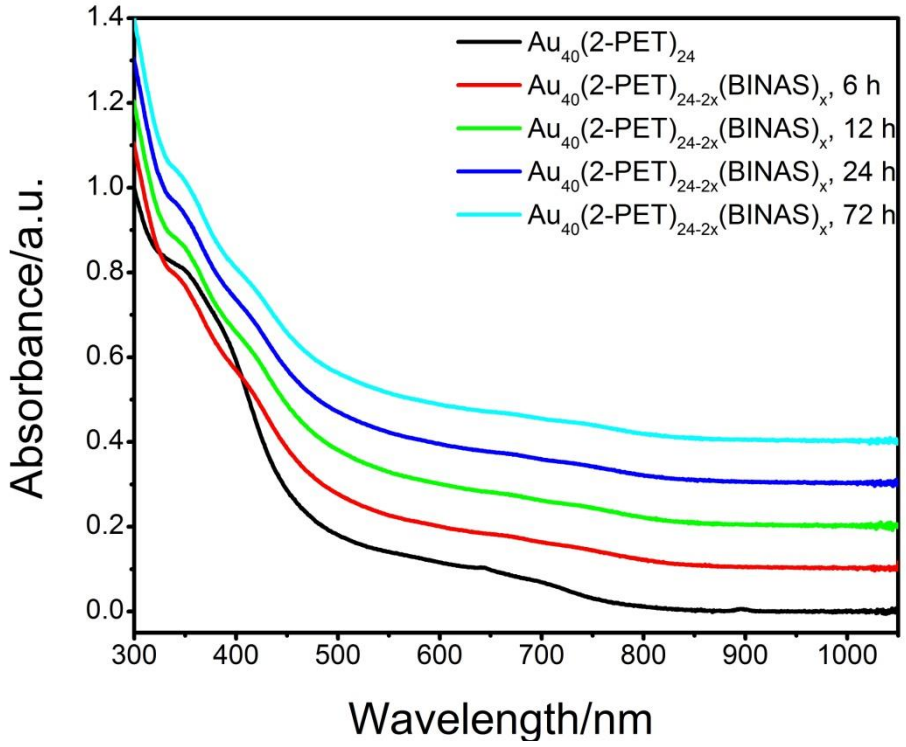

Figure S-4. UV-Vis spectra of $Au_{40}(2\text{-PET})_{24\text{-}2x}(BINAS)_x$ before (black) and after 6, 12 24 and 72 h of ligand exchange. The characteristic features are maintained, but blurred at longer reaction times.

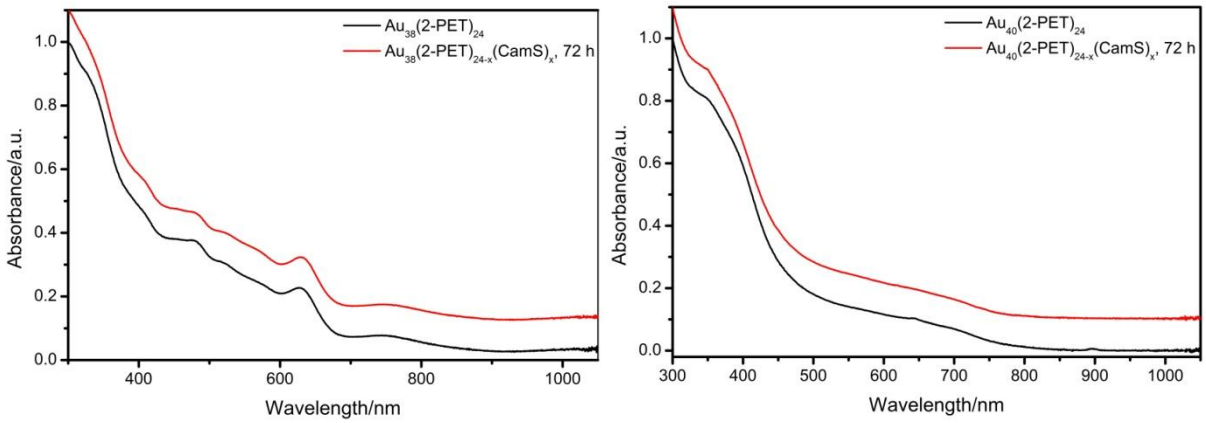

Figure S-5. UV-Vis spectra of $Au_{38}(2\text{-PET})_{24}$ (left) and $Au_{40}(2\text{-PET})_{24}$ (right) before and after exchange with camphorthiol (72 h). The features of the spectra are maintained.

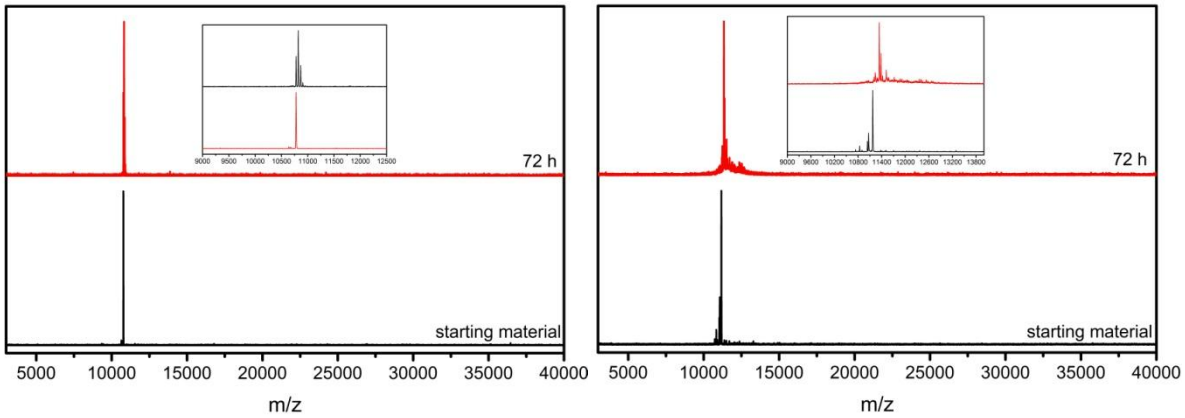

Figure S-6. MALDI mass spectra of $Au_{38}(2\text{-PET})_{24}$ (left) and $Au_{40}(2\text{-PET})_{24}$ (right) before and after exchange with BINAS. For Au_{38}, no hints of decomposition are observed; for Au_{40}, small impurities in the mass range of 12,000 – 14,000 Da are visible. These impurities are ignored in the discussion as they are a) not assigned yet and b) very weak in overall intensity (< 5 % overall intensity). Insets show the region from 9,000 to 12,000 Da (for Au_{38}) and 9,000 to 14,000 Da (for Au_{40}), respectively.