

**Supplementary Figure S1: 2D SEDFIT screen capture.** The  $c(s, t/f_0)$  model was applied to fit ~70 AUC scans for Au<sub>144</sub>(SR)<sub>60</sub>.



## Supplementary Figure S2: TEM micrographs of PDT-NPs and MUS-NPs. Transmission electron microscope (TEM) images illustrating the availability of information by this

method.



Supplementary Figure S3: ESI-MS time-of-flight (TOF) spectra. ESI-MS TOF for  $Au_{25}(SCH_2CH_2Ph)_{18}$ ,  $Au_{38}(SCH_2CH_2Ph)_{24}$ , and  $Au_{144}(SCH_2CH_2Ph)_{60}$  nanoclusters.