Supporting Information

Preparation of high-yield and ultra-pure Au_{25} nanoclusters: towards their implementation in real-world applications

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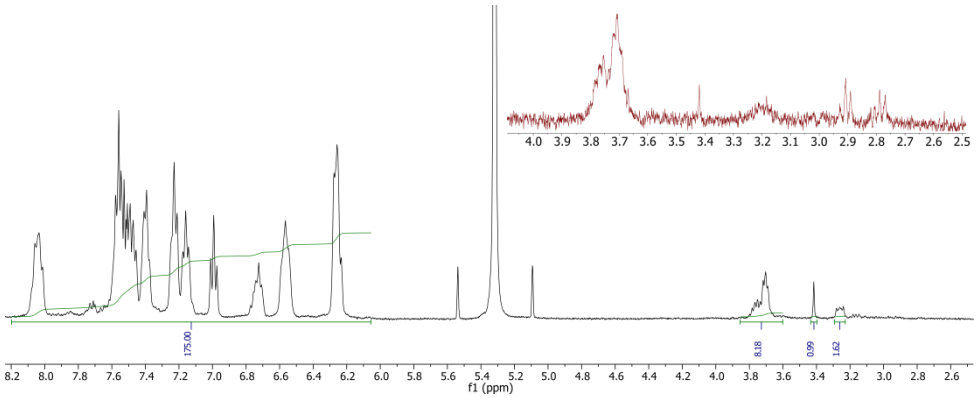

Fig. S1: ^{1}H NMR spectrum of the "purified" Au_{25} nanocluster in CD_2Cl_2. The set of peaks from 6.3 to 8.1 ppm correspond to phenyl groups from PPh_3 and SCH_2CH_2Ph (integral normalized to 175). The inset shows a ^{1}H NMR spectrum of a different sample of Au_{25} NCs in CD_2Cl_2 with unbound SCH_2CH_2Ph present in solution giving rise to two triplets at 2.8 and 2.9 ppm. These signals originate from alpha and beta CH_2 groups in SCH_2CH_2Ph. Proton signals from such alpha/beta group and are known to shift downfield, be broadened or even become undetectable in ^{1}H or ^{13}C NMR spectra upon binding to a Au NC surface.[1] All three effects were observed for the CH_2 groups in Au_{25} NC-bound SCH_2CH_2Ph: We propose that the signal from beta CH_2 is shifted from 2.8 to 3.7 ppm as well as broadened whereas the alpha CH_2 group, closest to the Au core becomes undetectable.

In accordance to a previous report,[2] alpha CH_2 groups of tetraoctylammonium (TOA) molecules are assigned to a signal at 3.25 ppm. Its integral compared to the phenyl regions' is remarkably low compared to a previous report.[2] The singlet at 3.4 ppm is assigned to the CH_3 group of methanol residually present from the purification. [3]

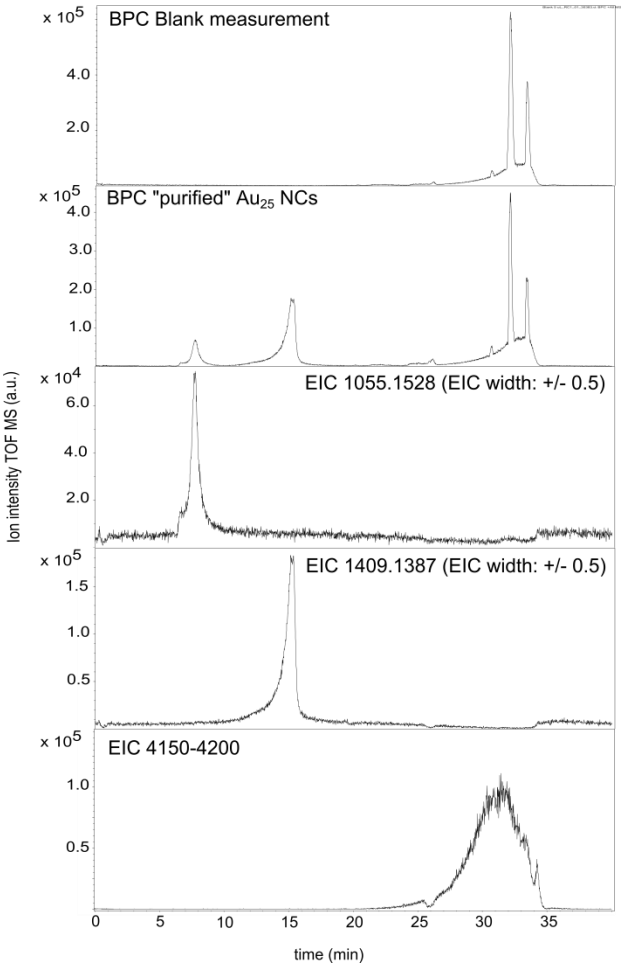

Fig. S2: LC-MS measurement of Au_{25} NCs. Base peak and extracted ion chromatograms (BPC and EIC, respectively) obtained by electrospray ionization mass spectrometry (ESI-MS).

References

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[3] R. Jin, C. Liu, S. Zhao, A. Das, H. Xing, C. Gayathri, Y. Xing, N. L. Rosi, R. R. Gil, and R. Jin, *ACS Nano*, 2015, 9, 8530–8536.