Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2017

$Au_{38}Cu_1(2\text{-PET})_{24}$ Nanocluster : Synthesis, Enantioseparation and Luminescence

Rania Kazan, [a] Bei Zhang [a] and Thomas Bürgi* [a]

Department of Physical Chemistry, University of Geneva, 30 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland

E-mail: Thomas.Buergi@unige.ch

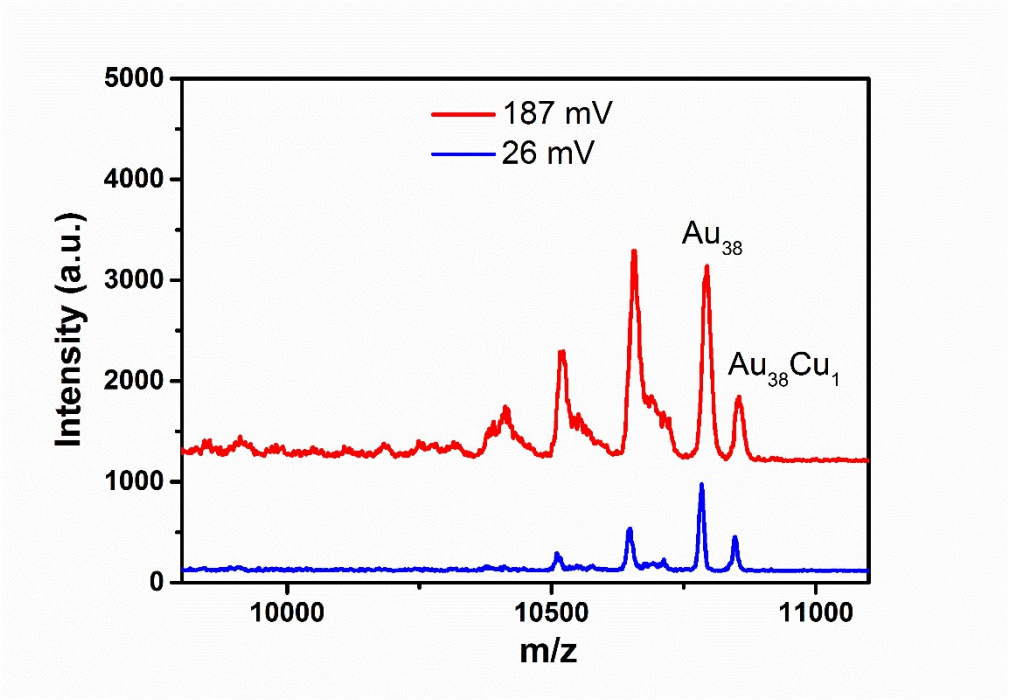

Fig S1. MALDI mass spectra of $Au_{38}Cu_1(2\text{-PET})_{24}$ adduct under different ionization powers.

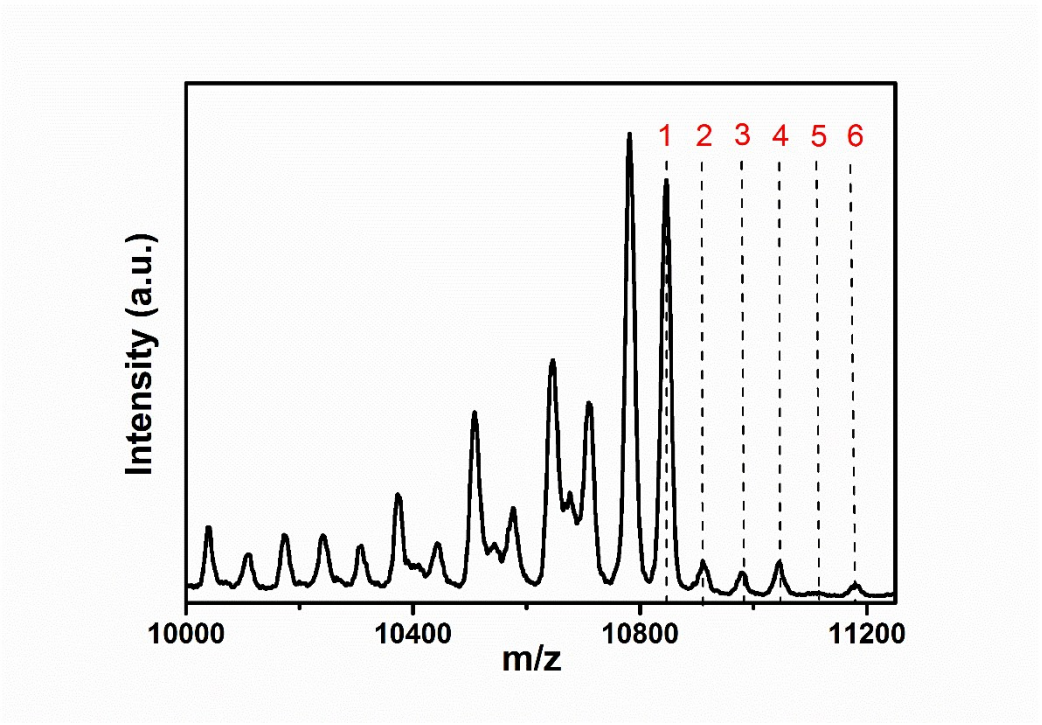

Fig S2. MALDI mass spectrum of $Au_{38}Cu_x(2\text{-PET})_{24}$ adduct nanoclusters, the number of copper atoms incorporated is marked in red above the corresponding peak.

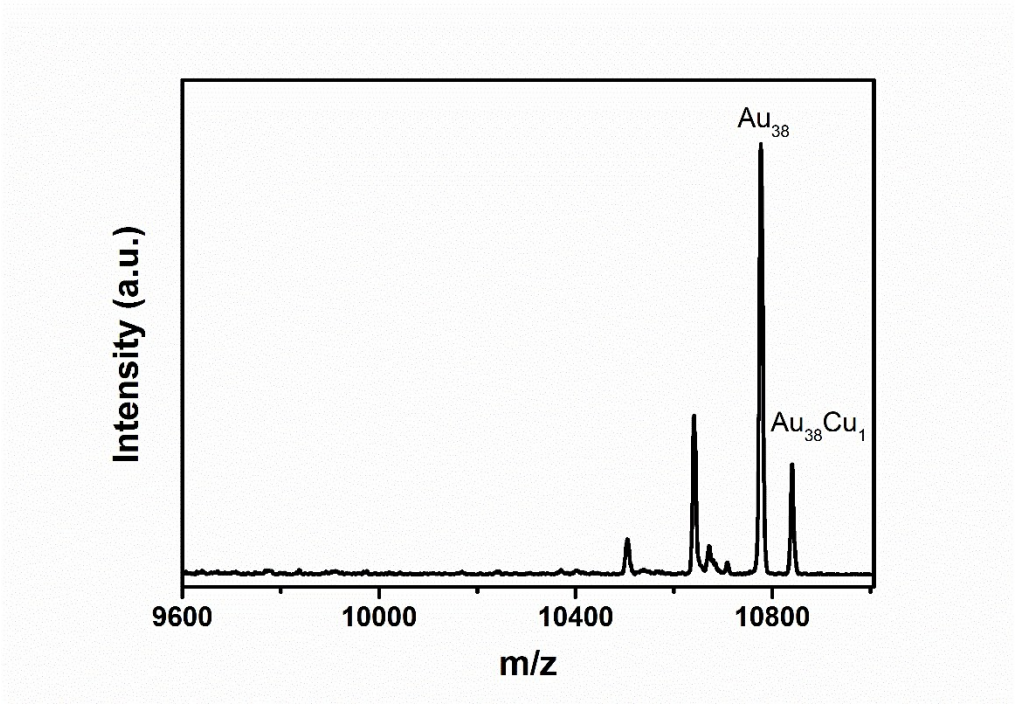

Fig S3. MALDI mass spectrum of the bimetallic cluster synthesized after increasing the Au: Cu mass ratio to 1: 1.3.

Estimating the percentage of the adduct present in the bimetallic cluster after increasing the Au: Cu mass ratio to 1: 1.3

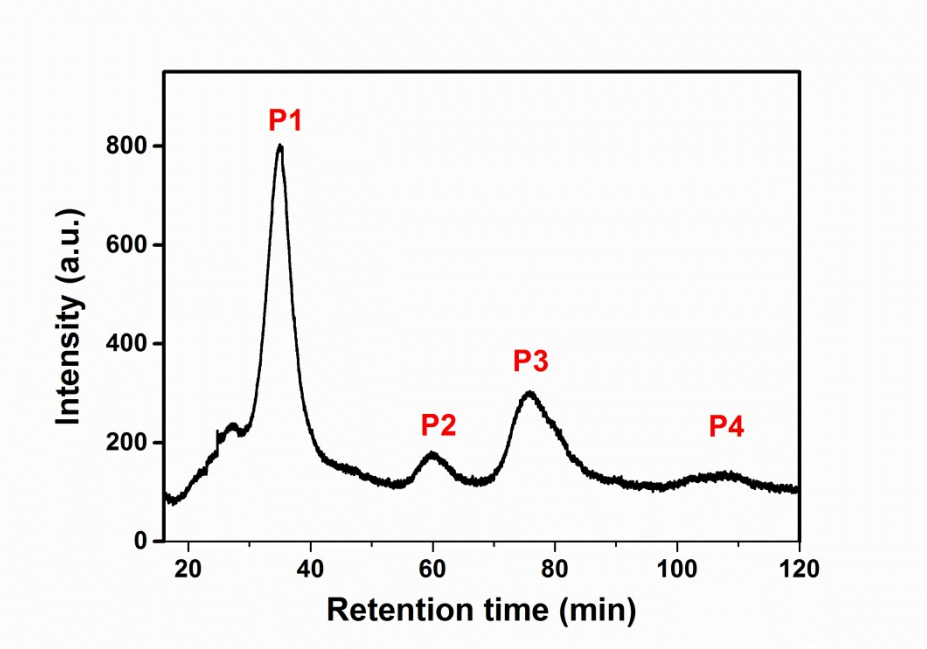

Fig S4. HPLC chromatogram of the bimetallic cluster synthesized after increasing the Au: Cu mass ratio to 1: 1.3. The different peaks are denoted as P1, P2, P3 and P4 respectively.

Table **S1:** Relative areas of P1, P2, P3 and P4 in the HPLC chromatogram (Fig. S4†) of the bimetallic cluster synthesized after increasing the Au: Cu mass ratio to 1: 1.3.

Peak	Area %
P1	58.8
P2	6.6
P3	29
P4	5.5

The percentage of the adduct present in the sample is calculated from the E2 enantiomers (Table S1) as below:

$$Amount\ of\ adduct\ in\ sample\ (\%) = \frac{(area\%\ P2\ +\ area\%\ P4)}{(area\ \%\ P2 + area\ \%\ P3 +\ area\ \%\ P4)} (1)$$

The content of the crude sample is ~29 % $Au_{38}Cu_1$ and ~71 % Au_{38}.

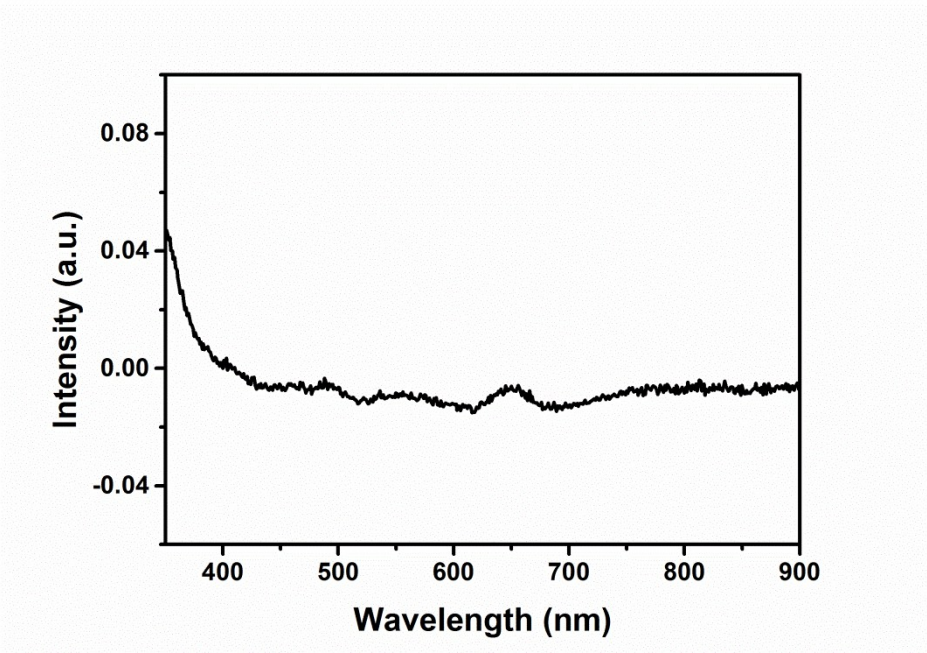

Fig S5. Difference spectrum obtained by subtracting the UV-Vis spectrum of the crude sample containing a mixture of Au_{38} and $Au_{38}Cu_1$ nanoclusters from the spectrum of pure Au_{38} nanocluster (Fig. S8†).

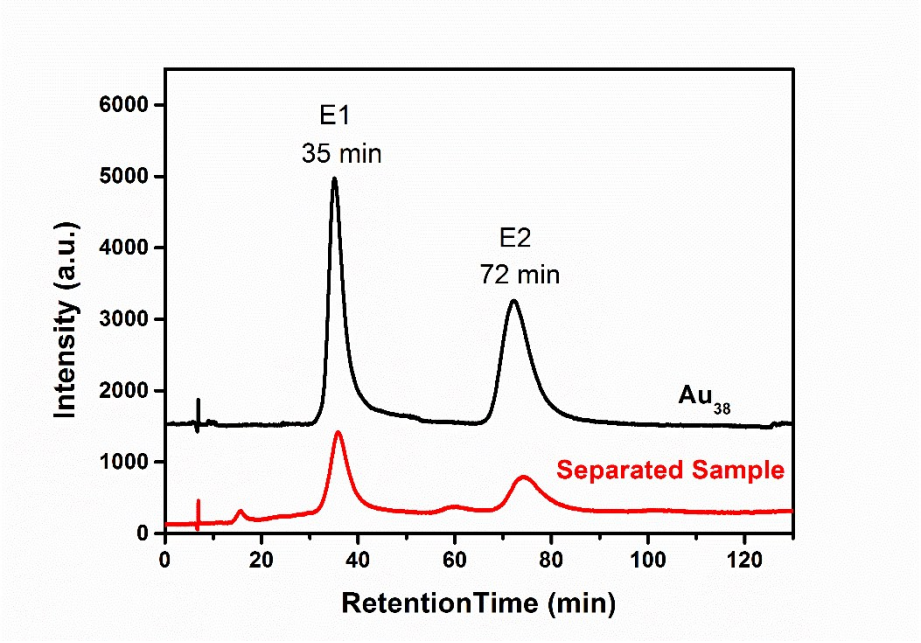

Fig S6. HPLC chromatograms of the separation of rac-$Au_{38}(2\text{-PET})_{24}$ (black) and the reaction mixture obtained after purification by SEC (red); E1 and E2 represent the 1st and 2nd enantiomer of Au_{38}.

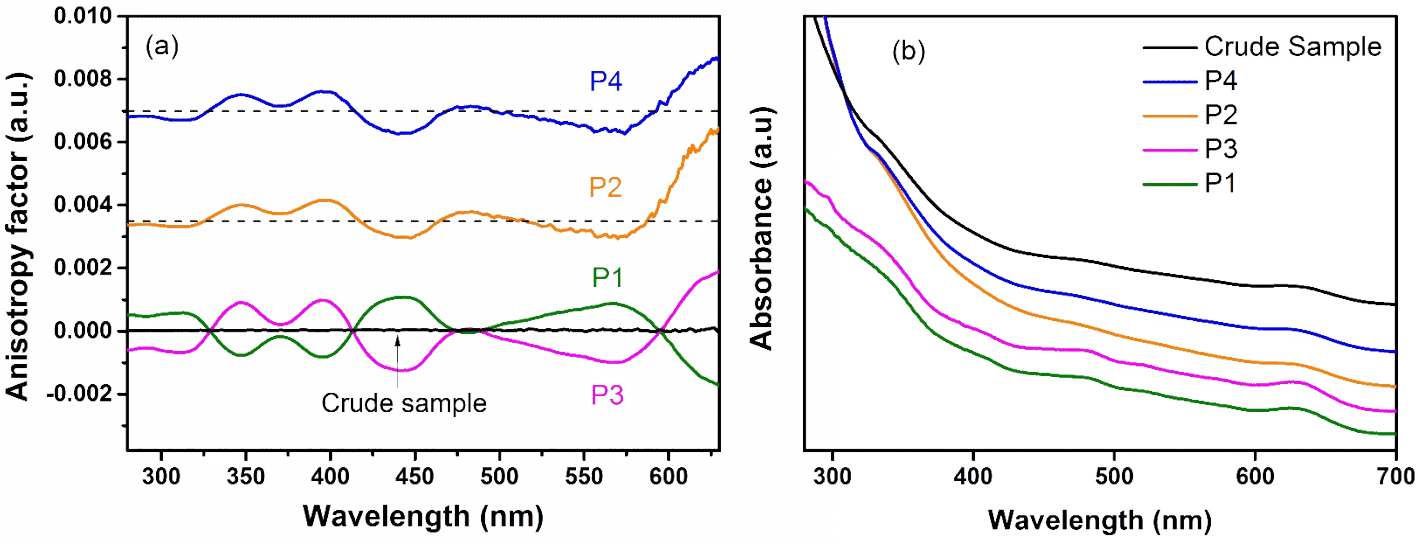

Fig S7. Anisotropy factor (a) and UV-Vis spectra of the crude sample and the collected HPLC peaks (b). The spectra were normalized at 400 nm and off-set vertically for clarity.

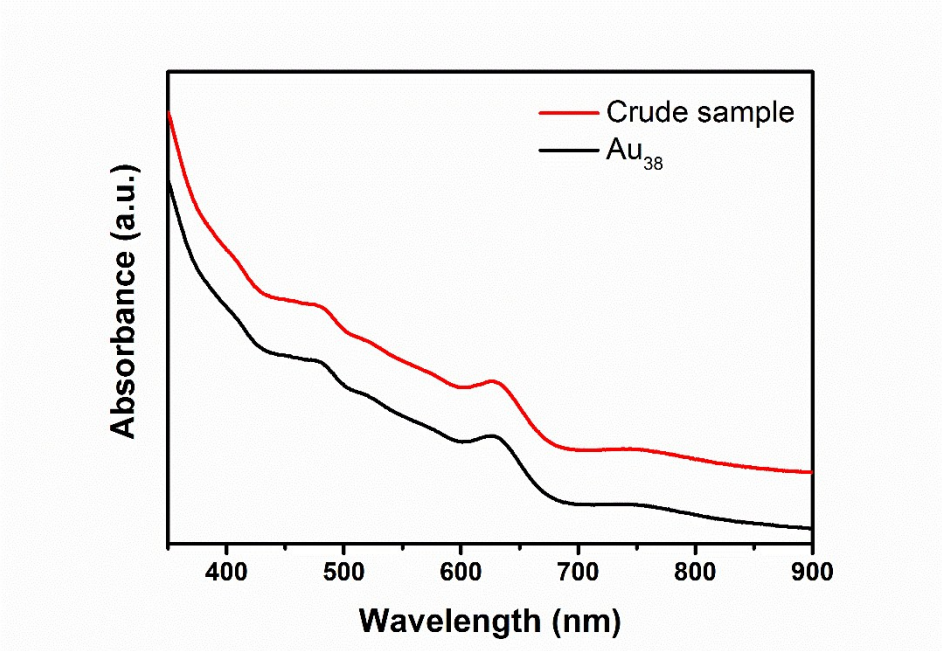

Fig S8. UV-Vis spectra of the purified $Au_{38}(2\text{-PET})_{24}$ nanocluster (black) and the crude sample containing $Au_{38}Cu_1(2\text{-PET})_{24}$ adduct (red). The two samples have the same absorbance at 480 nm (excitation wavelength) and hence the same concentration.

Estimation of the intrinsic fluorescence of $Au_{38}Cu_1(2\text{-PET})_{24}$ relative to $Au_{38}(2\text{-PET})_{24}$

The content of the crude sample is ~25 % $Au_{38}Cu_1$ and ~75 % Au_{38} as determined from HPLC (Table 1) using equation 1 The following relations were used to estimate the intrinsic $Au_{38}Cu_1$ luminescence compared to Au_{38}:

$$D_{Sample}\ \alpha\ [Sample].IF_{Sample} \quad (2)$$

$$2 \times D_{Au38} = D_{crude\ sample} \quad (3)$$

$$[Au_{38}] = [CuAu_{38}]_{crude\ sample} + [Au_{38}]_{crude\ sample} \quad (4)$$

Where D is the integrated area under the emission spectra and IF is the intrinsic fluorescence. Here we assume that the peak area is proportional to the concentration and to the intrinsic fluorescence of a species (equation 2). The crude sample containing Au_{38} (75 %) and $Au_{38}Cu_1$ (25 %) shows stronger fluorescence by a factor of two compared to the Au_{38} sample (equation 3). The concentration of cluster is identical for the Au_{38} sample and the crude sample, as determined by absorption spectroscopy (equation 4). This set of equations allows one to determine the relative intrinsic fluorescence of $Au_{38}Cu_1$ and Au_{38} (IF $Au_{38}Cu_1$/ IFAu_{38}), which is around five.

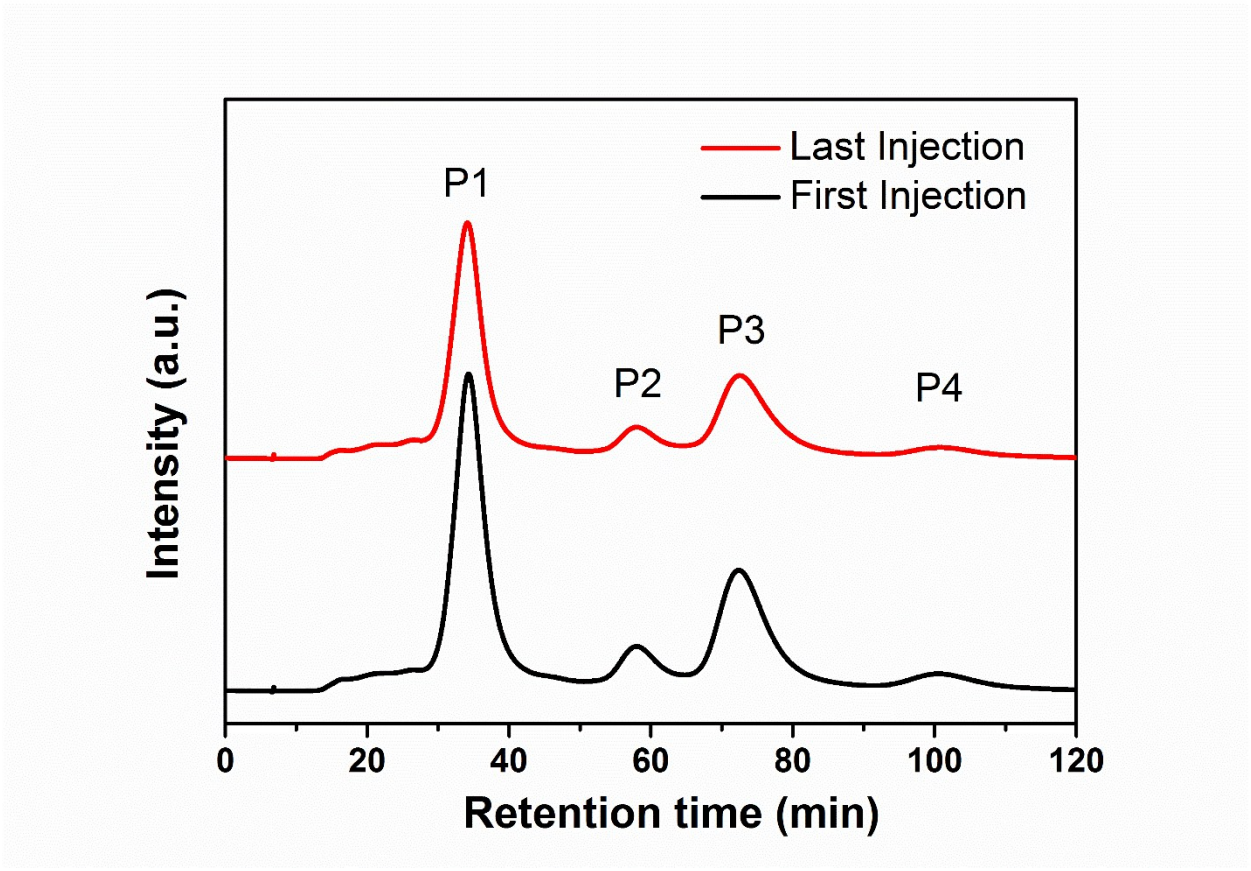

Fig S9. HPLC chromatograms of the unseparated sample. The time between the first and last injection is 12 hours.

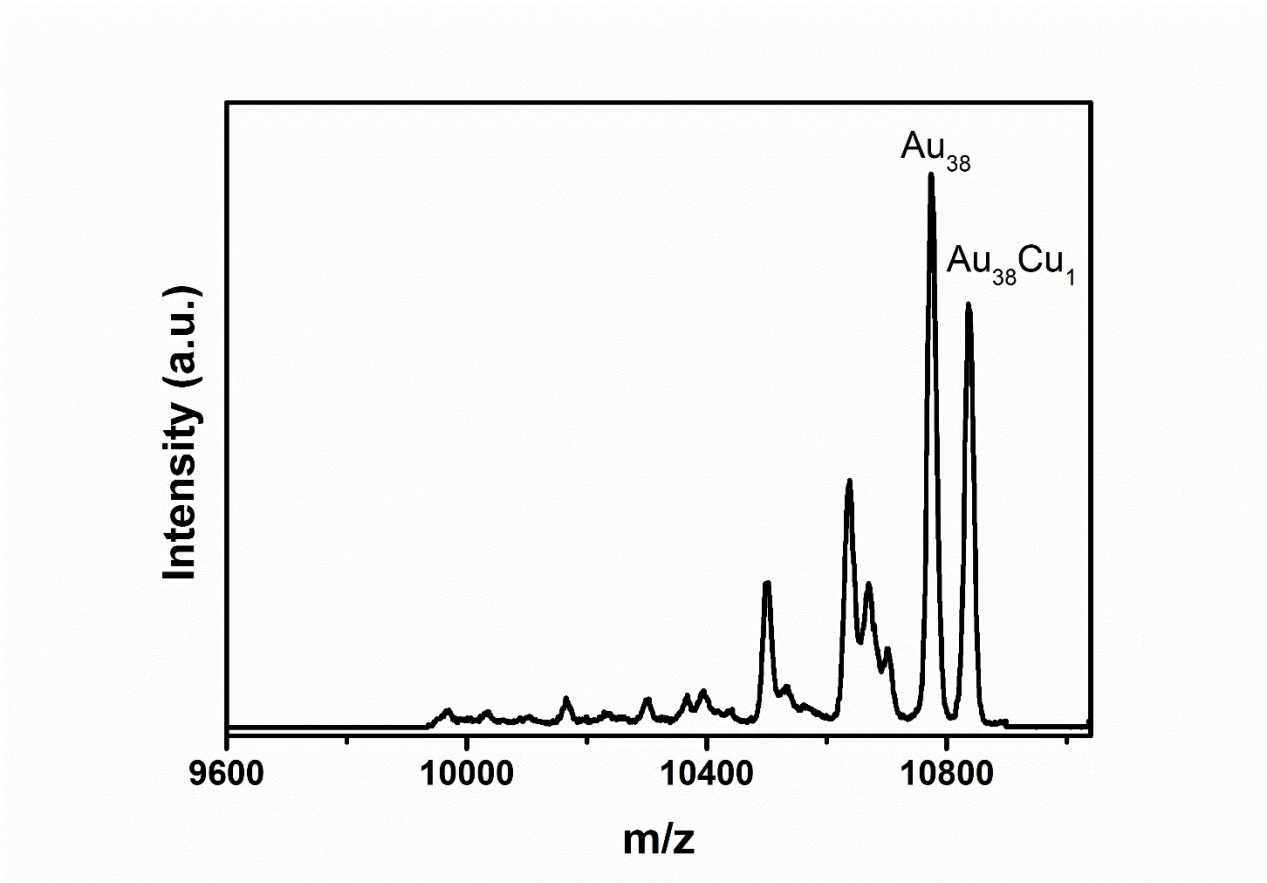

Fig S10. MALDI mass spectrum of the mixture containing $Au_{38}Cu_1(2\text{-PET})_{24}$ adduct after stirring in solution for four days.