CHEMPHYSCHEM

Supporting Information

Bare Clusters Derived from Protein Templates: Au_{25}^{+}, Au_{38}^{+} and Au_{102}^{+}

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cphc_201200927_sm_miscellaneous_information.pdf

S1. Supporting Information 1

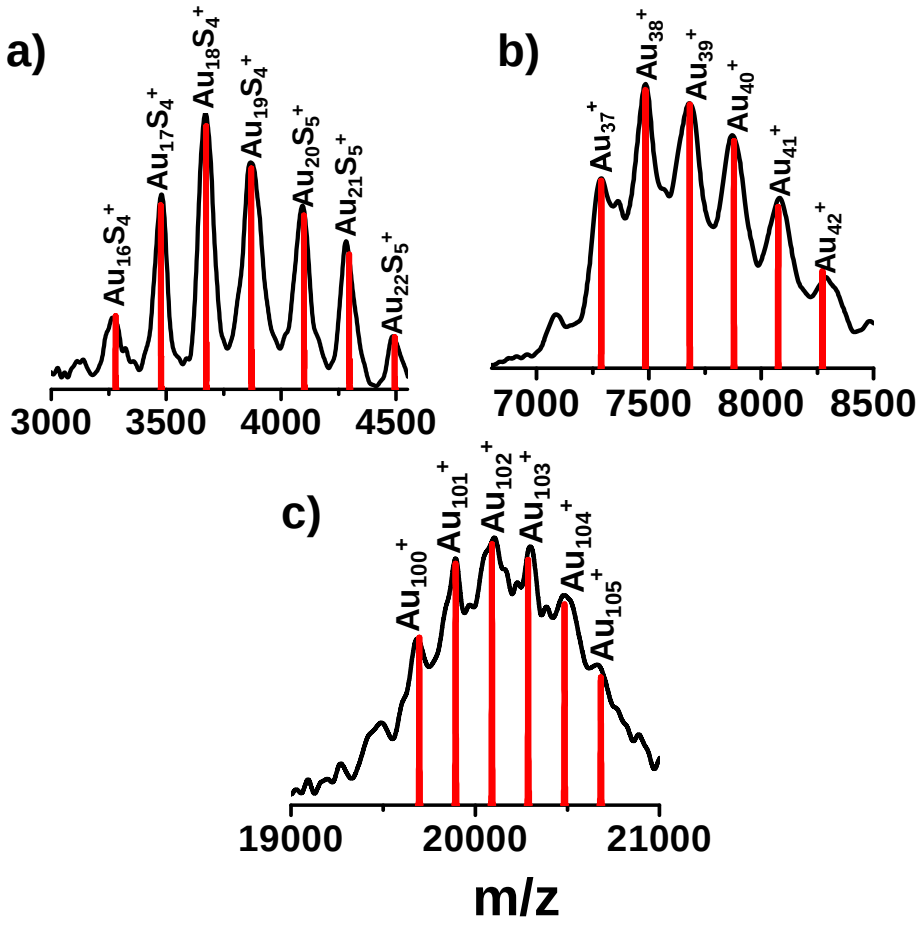

Figure S1. Comparative plot of the theoretical and experimental m/z values of a) $Au_{18}S_{4+m}^+$, b) Au_{38}^+ and c) Au_{102}^+.

S2. Supporting information2

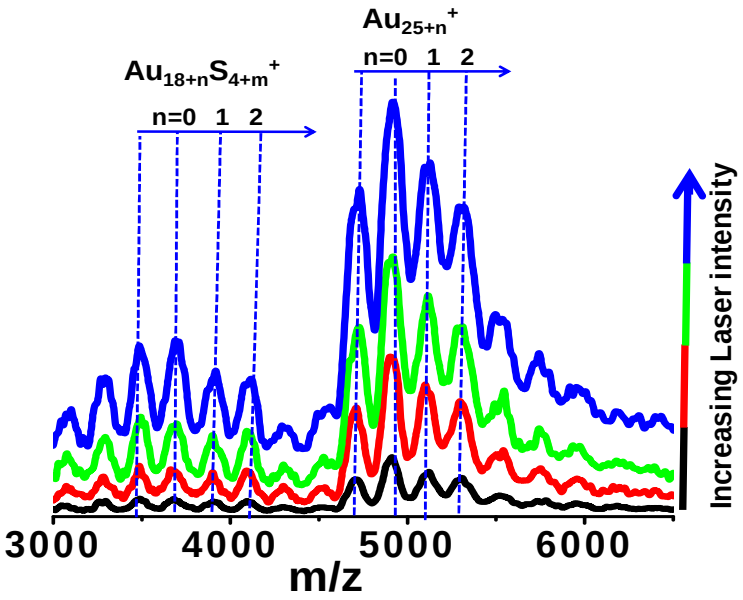

Figure S2. Laser intensity dependence study in MALDI MS with increasing laser intensity in linear positive mode. There is no change in the peak positions with enhanced laser intensity. The spectra were collected for the 1.5 mM Lyz and 5 mM $HAuCl_4.3H_2O$ system in linear positive mode and the laser intensity was varied from 1500 to 1800 (instrumental unit) with an increase of 100 in intensity at each step, plotted in black, red, green and blue, respectively.

S3. Supporting information 3

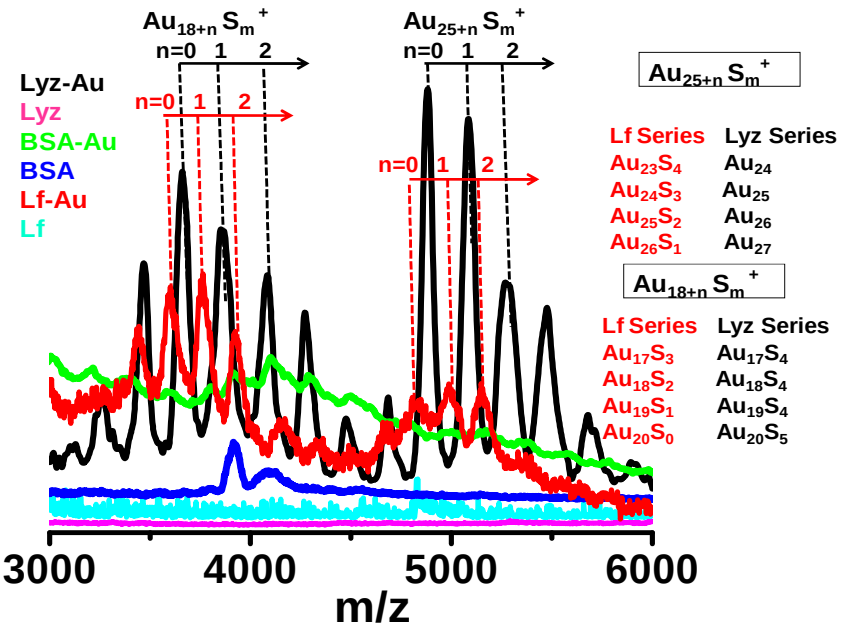

Figure S3. A comparative study of the efficiency of BSA, Lf and Lyz templates for gas phase cluster formation. Spectra show that Lyz is efficient to act as a template for such synthesis.

S4. Supporting Information 4

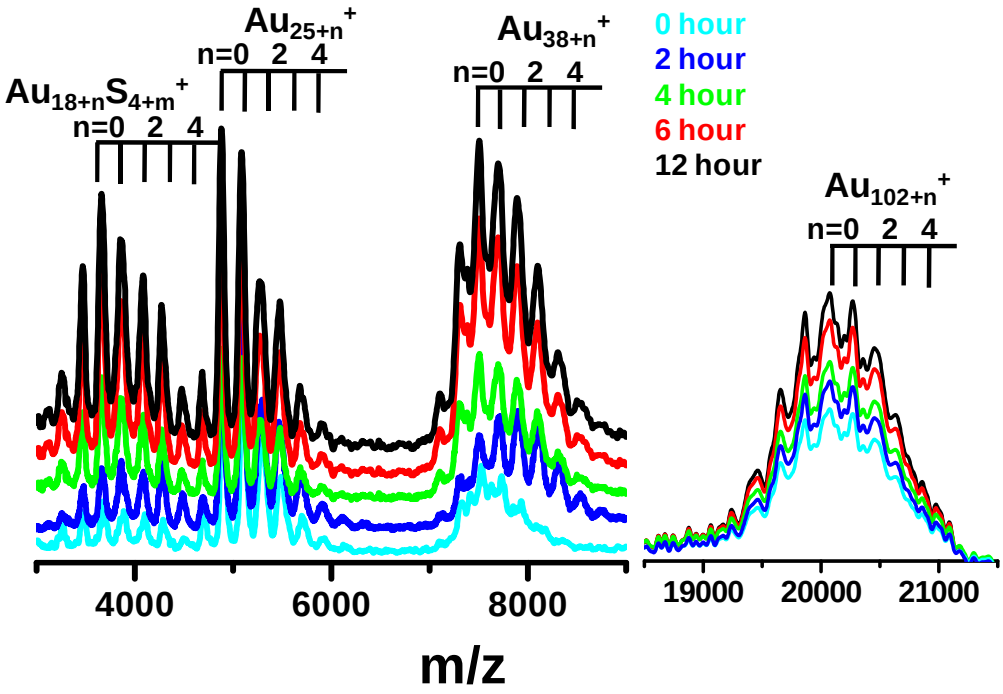

Figure S4. Time dependent MALDI MS study of the as prepared precursor. There is a significant change in the Au_{38} region. At starting, the peaks were appearing along with $(Lyz\text{-}Au_n)^{2+}$ but upon longer time, only cluster related peaks get enhanced.

S5. Supporting Information 5

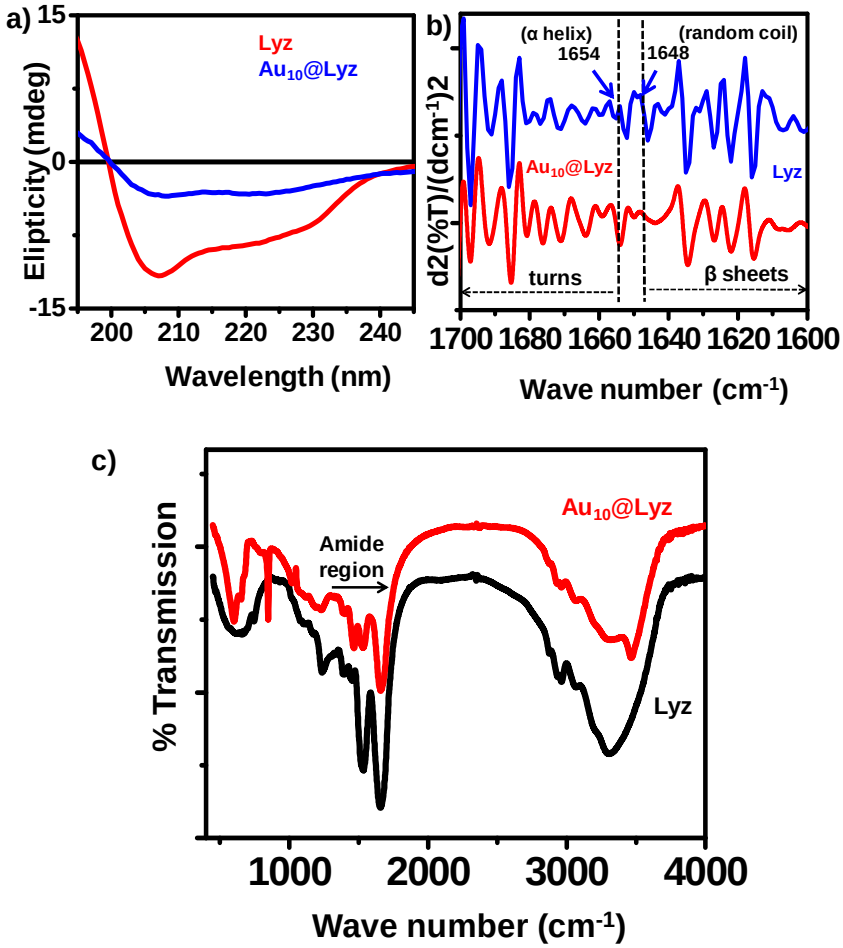

Figure S5: a) CD spectra of Lyz and as prepared Au_{10}@Lyz showing a clear change in ellipticity of the spectra, which indicates a huge change in the alpha helical structure. (b) Double derivative of the infrared (IR) spectra shows the disappearance of the peak at 1654 cm^{-1} in the case of Au_{QC}@Lyz. c) Infrared (IR) spectra of Lyz and Au_{QC}@Lyz showing significant change in the amide region (from the published work of the authors, ref. 6i).

S6. Supporting information 6

In this section we give the weights of the angular momentum components (S, P, S, …..,,I) for the wave functions whose iso-surface images are shown in Figures 5, 7 and 8. In each case, we give the energy ($E-E_F$) of the state and the weights.

Table of weights for Figure 5: Au_{38} (cysteine)$_4$

$E-E_F$ (eV)	S	P	D	F	G	H	I
0.48	0.000	0.015	0.018	0.010	0.577	0.008	0.022
-0.27	0.001	0.144	0.011	0.213	0.058	0.020	0.017
-0.99	0.004	0.004	0.019	0.344	0.027	0.020	0.023

Tables of weights for figures 7 and 8 in the manuscript, corresponding to Au_{102}+, Au_{38}^+, and Au_{25}^+

Au_{102}^+ (Figure 7)

$E-E_F$ (eV)	S	P	D	F	G	H	I
-8.65	0.949	0.008	0.013	0.001	0.003	0.006	0.003
-8.03	0.000	0.946	0.001	0.012	0.001	0.003	0.002
-7.11	0.001	0.006	0.843	0.031	0.014	0.004	0.007
-7.02	0.820	0.004	0.039	0.004	0.017	0.014	0.007
-6.65	0.000	0.054	0.002	0.601	0.004	0.090	0.033
-6.43	0.016	0.444	0.028	0.084	0.073	0.035	0.040
-1.74	0.000	0.001	0.003	0.017	0.151	0.014	0.019
-1.13	0.041	0.002	0.262	0.007	0.027	0.073	0.070

-1.07	0.000	0.000	0.030	0.012	0.015	0.403	0.014
-0.71	0.210	0.006	0.126	0.011	0.030	0.114	0.088
-0.08	0.001	0.021	0.002	0.399	0.004	0.028	0.133

Au_{38}^{+} (Figure 8)

$E-E_F$ (eV)	S	P	D	F	G	H	I
-0.31	0.002	0.014	0.084	0.014	0.387	0.007	0.041
-0.79	0.006	0.002	0.010	0.539	0.021	0.026	0.027
-2.84	0.004	0.010	0.021	0.017	0.047	0.066	0.043
-5.95	0.002	0.060	0.541	0.044	0.052	0.027	0.021
-6.31	0.479	0.019	0.061	0.143	0.051	0.013	0.033
-6.72	0.000	0.762	0.096	0.022	0.009	0.015	0.006
-7.59	0.864	0.020	0.011	0.050	0.015	0.003	0.006

Au_{25}^{+} (Figure 8)

$E-E_F$ (eV)	S	P	D	F	G	H	I
-0.07	0.000	0.009	0.031	0.436	0.073	0.020	0.031
-0.99	0.000	0.065	0.279	0.031	0.012	0.061	0.031