Supporting Information-I

Quantum clusters in cavities: Trapped Au_{15} in cyclodextrins

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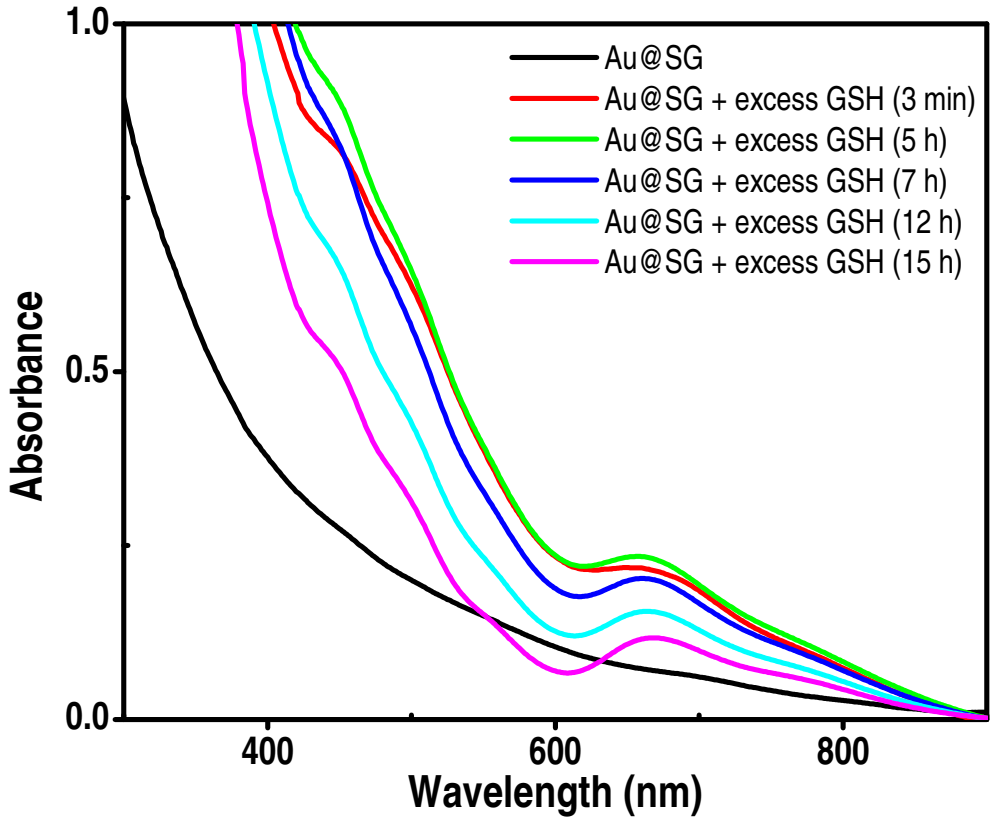

Figure S1. The time dependent UV-Vis spectra taken during the core etching reaction of Au@SG with excess GSH (without CD molecules). As the time progresses, the characteristic optical absorption features of Au_{25} are seen clearly.

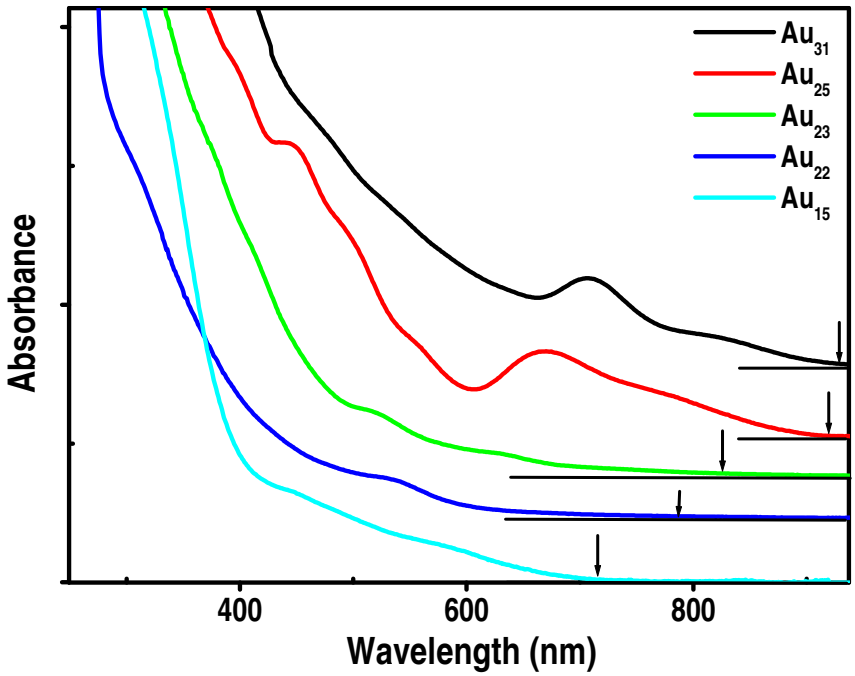

Figure S2. A comparison of the UV-Vis spectra of different –SG protected Au clusters along with the newly formed Au_{15}@αCD. The threshold of absorption is marked.

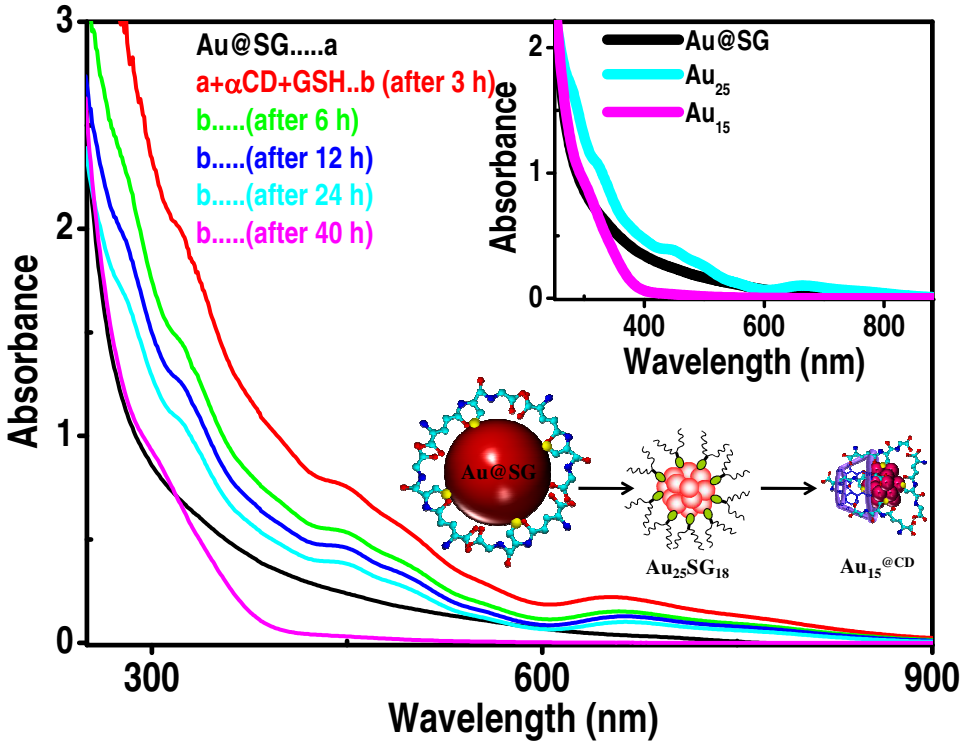

Figure S3. The time dependent UV-Vis spectra taken during the core etching reaction of Au@SG QCs with GSH and CD molecules. During the core reduction, the Au_{25} QCs were formed first, which was then decomposed to Au_{15}. Inset shows the optical absorption features of Au@SG, Au_{25} and Au_{15}.

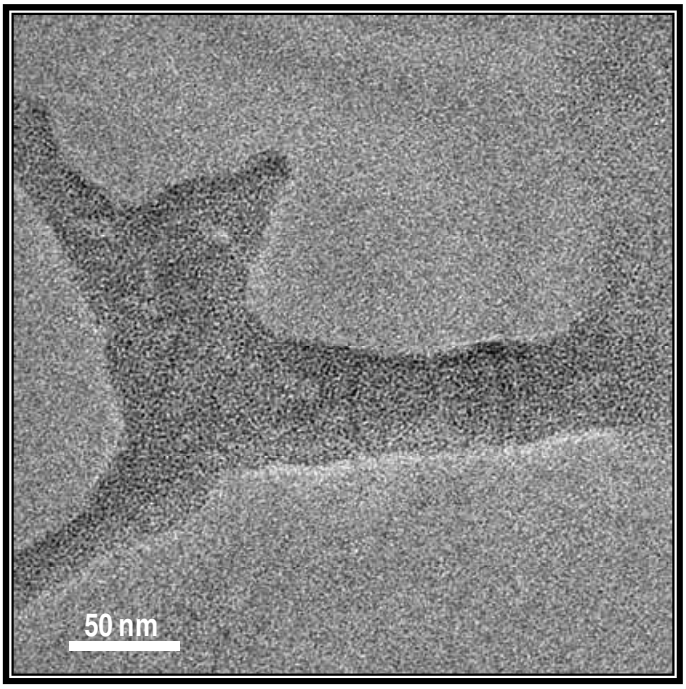

Figure S4. HRTEM image of Au_{15}@CD QCs taken at 100 kV. Here the QCs are embedded within the self-assembled CD structure. The small dots indicate individual QCs. Higher energy of the electron beam or longer exposure even at lower energy lead to aggregation of the cores.

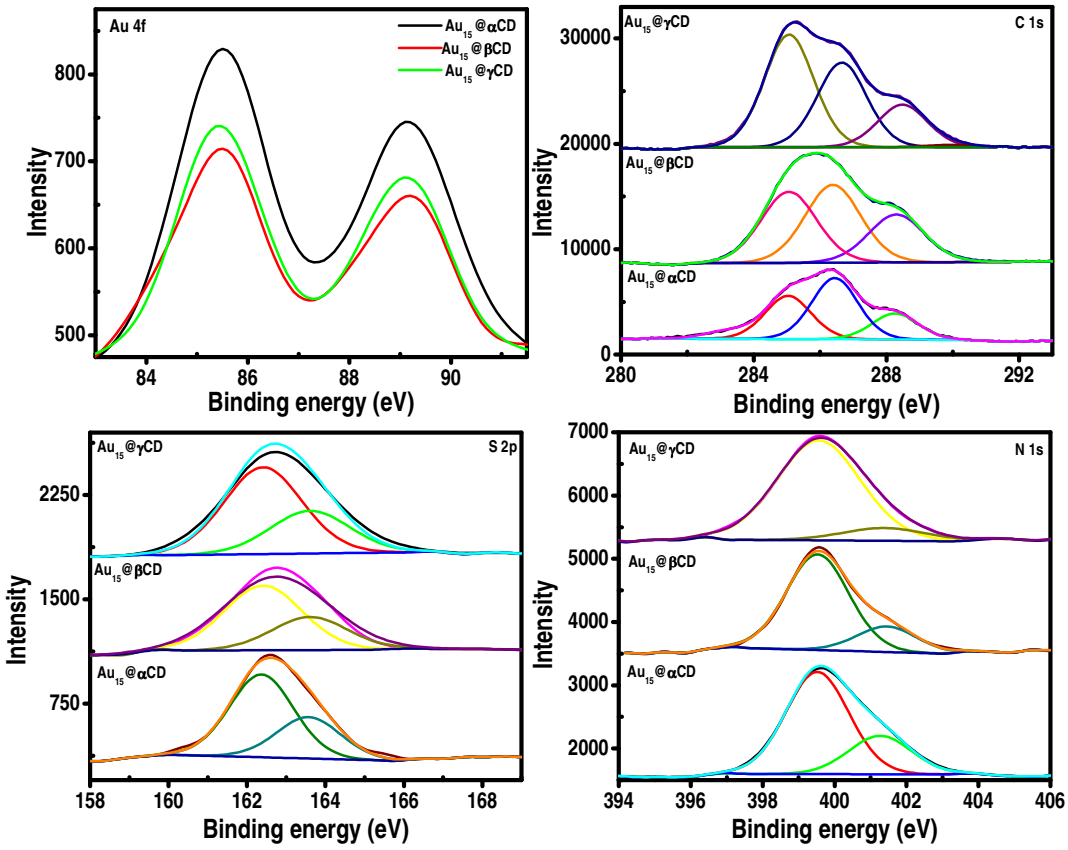

Figure S5. XPS spectra of Au_{15}@αCD, Au_{15}@βCD and Au_{15}@γCD clusters obtained after the CD assisted core etching reaction of Au@SG with excess GSH. C 1s and N 1s are fit into various components. S 2p has been fit into the $p_{3/2}$ and $p_{1/2}$ components.

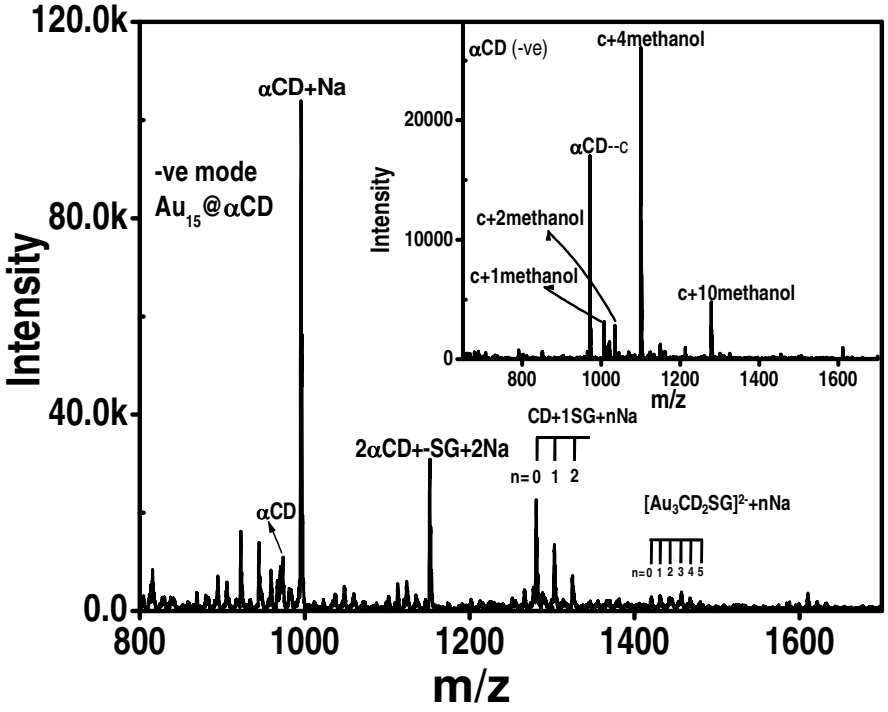

Figure S6. ESI-MS of Au_{15}@αCD cluster in 1:1 water/methanol mixture. Inset shows the ESI-MS of pure αCD molecule.

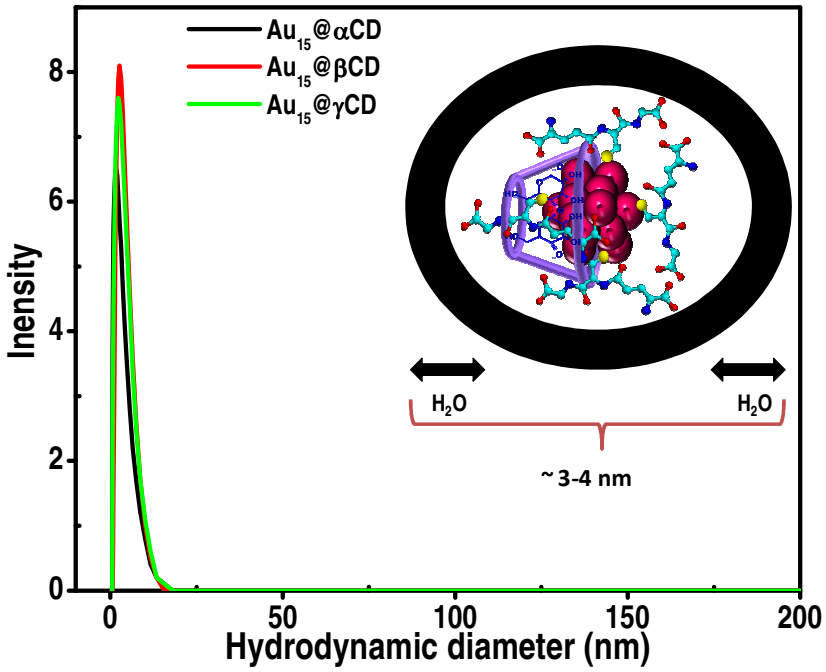

Figure S7. DLS of Au_{15}@αCD, Au_{15}@βCD and Au_{15}@γCD clusters in water with an average diameter of 3-4 nm (with water of hydration). Inset shows the possible orientation of cluster in the CD cavity.

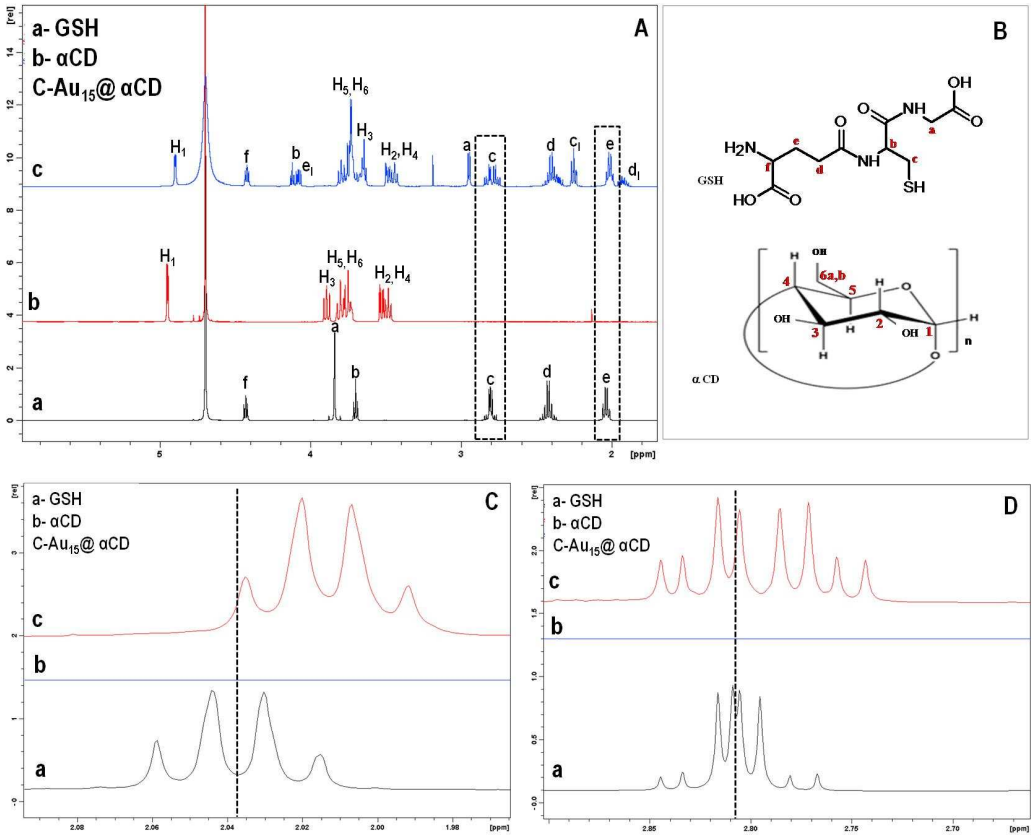

Figure S8. (A) ^{1}H NMR of Au_{15}@αCD along with those of pure GSH and αCD. (B) Molecular structures of GSH and CD are given. (C and D) Expanded views of '*c*' and '*e*' regions, respectively of -SG, in the three systems.

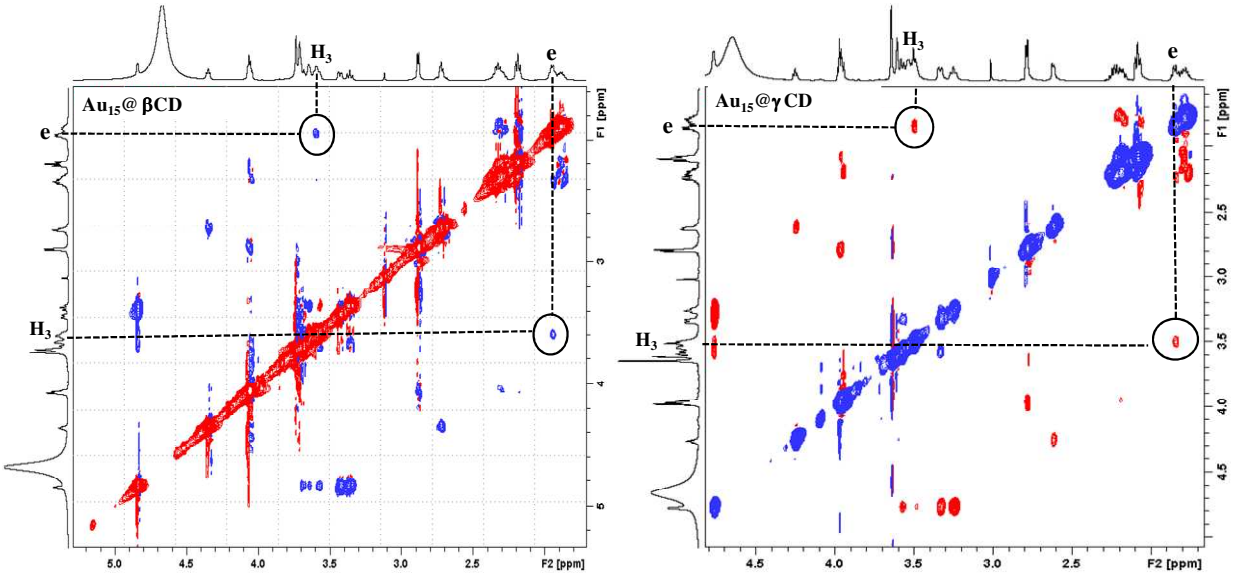

Figure S9. ROESY spectra of Au_{15}@βCD and Au_{15}@γCD clusters in D_2O at 25 °C with a mixing time of 200 ms. Cross peaks between proton '*e*' of glutathione (-SG) ligand and 'H_3' proton of CD are marked.