

Electronic supplementary information (ESI) for Nanoscale
This journal is © The Royal Society of Chemistry 2012

Protein-encapsulated gold cluster aggregates: The case of lysozyme†

Ananya Baksi,^a Paulrajpillai Lourdu Xavier,^a Kamalesh Chaudhary,^{a,b} N. Goswami,^c
S. K. Pal^c and T. Pradeep^{a*}

^aDST Unit of Nanoscience, Department of Chemistry, Indian Institute of Technology Madras,
Chennai-600036, India. *E-mail: pradeep@iitm.ac.in

^bDepartment of Biotechnology, Indian Institute of Technology Madras, Chennai-600036, India

^cUnit of Nanoscience and Technology, Department of Chemical, Biological and Macromolecular
Sciences, Satyendra Nath Bose National Centre for Basic Sciences, Block JD, Sector III, Salt
Lake, Kolkata 700 098, India

Number	Description	Page Number
S1†	<i>Time dependent MALDI MS of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:4</i>	2
S2†	<i>XPS survey spectrum for the as synthesized Au_{QC}@Lyz</i>	3
S3†	<i>EDAX spectrum of as synthesized Au_{QC}@Lyz</i>	4
S4†	<i>Concentration dependent UV-Vis absorption spectra and TEM image of as synthesized Au_{QC}@Lyz</i>	5
S5†	<i>Time dependent MALDI MS of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:5</i>	6
S6†	<i>Time dependent MALDI MS of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:8</i>	7
S7†	<i>Time dependent MALDI MS of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:2.50</i>	8
S8†	<i>Time dependent fluorescence spectra of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:5</i>	9
S9†	<i>Time dependent fluorescence spectra of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:8</i>	10
S10†	<i>Time dependent fluorescence spectra of Au_{QC}@Lyz at Lyz:Au³⁺ ratio of 1:2.50</i>	11
S11†	<i>IR spectra of as synthesized Au_{QC}@Lyz</i>	12

Electronic Supplementary Information 1

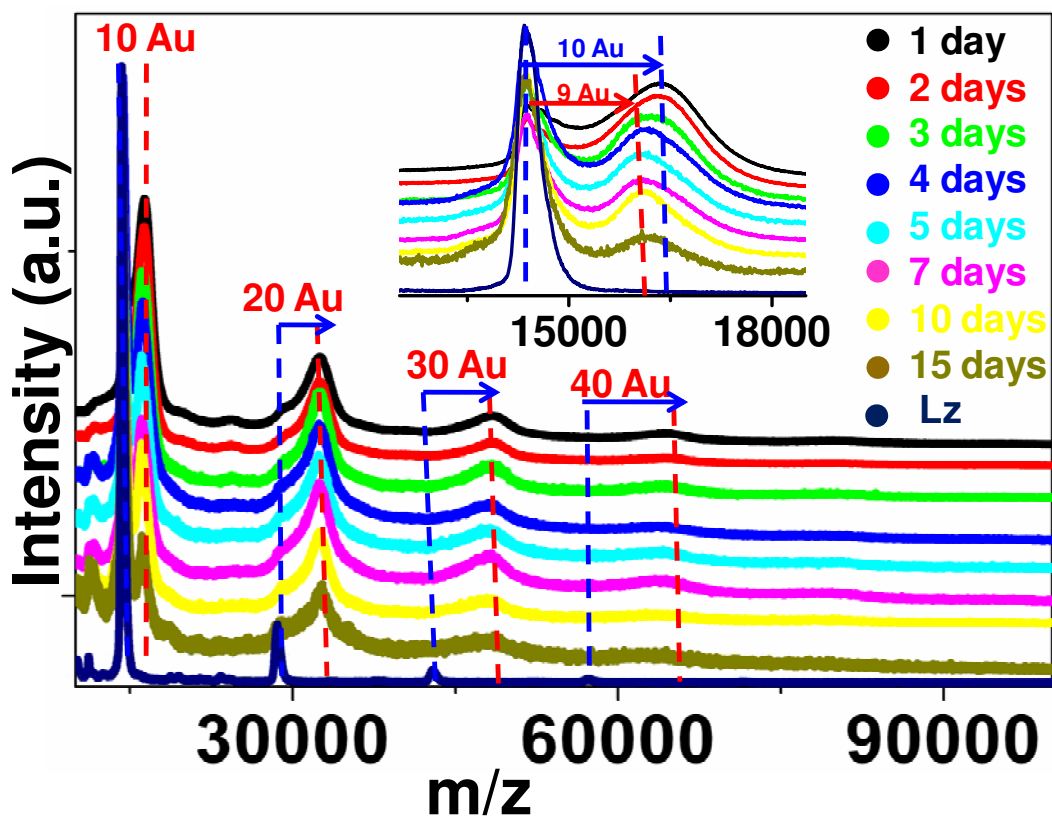


Fig. S1† Time dependent MALDI MS of Lyz: Au³⁺ (molar ratio of 1:4) over 15 days time window. A linear dependence of Au ion uptake is seen for the oligomerized Lyz. While monocation of Au_{QC}@single protein shows a separation of 10 Au atoms from the parent protein peak, oligomerized Lyz show separation of $n \times 10$ (where $n=2, 3, 4, \dots$) from their parent oligomerized Lyz where n is the aggregation number. Inset shows the monomer region.

Electronic Supplementary Information 2

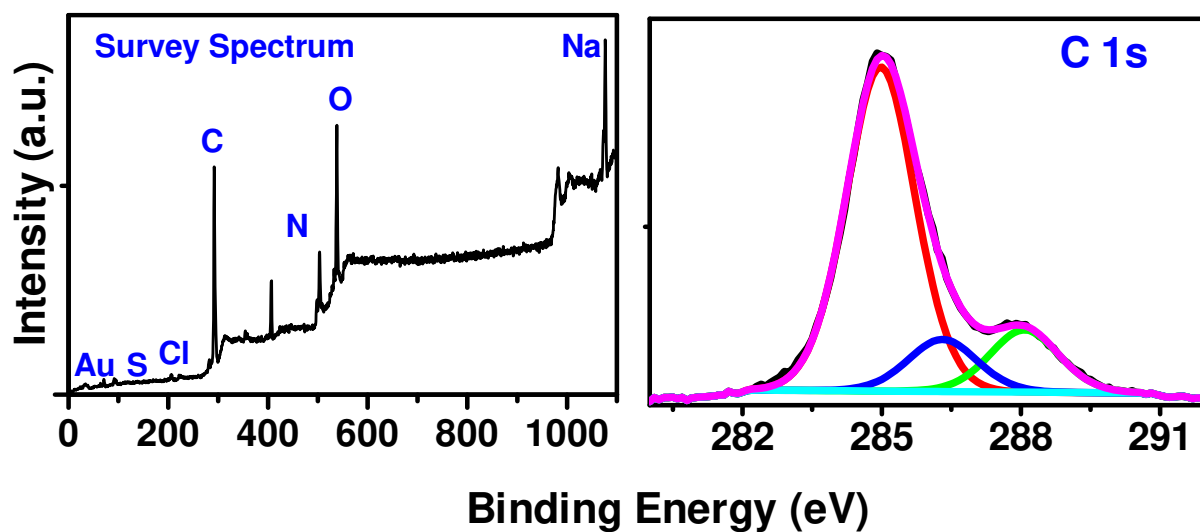


Fig. S2† The survey spectrum is characterized by peaks due to carbon, oxygen, nitrogen, sodium, chlorine, gold and sulphur. Carbon 1s binding energy for the main peak is taken to be 285 eV and other binding energy values have been determined.

Electronic Supplementary Information 3

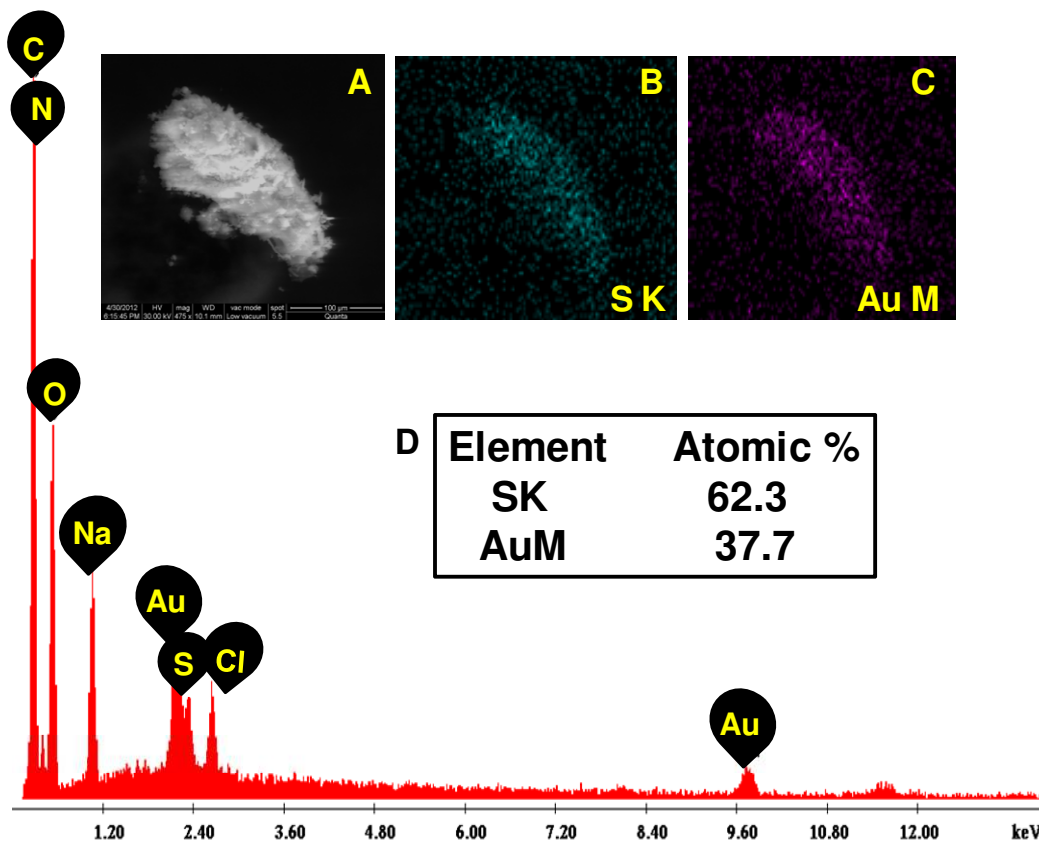


Fig. S3† SEM EDAX spectra of AuQC@Lyz using Lyz: Au³⁺ ratio 1:4. Inset A, is the SEM image of the sample. B and C are EDAX mapping of SK and AuM corresponding to A. D is the quantification of S and Au in the sample.

Electronic Supplementary Information 4

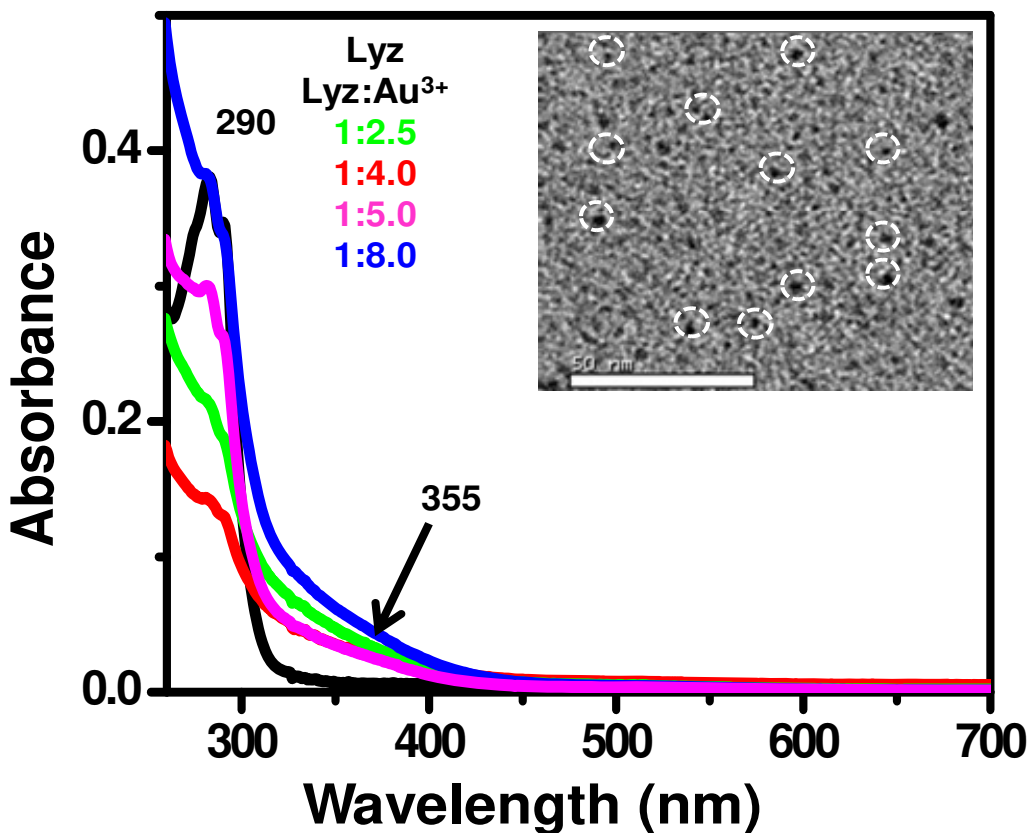


Fig. S4† Concentration dependent UV-Vis spectra of as-synthesized AuQC@Lyz. The peak at 290 nm is assigned to the protein. A characteristic hump near 355 nm is also seen. There is no specific feature of cluster core in these spectra. In the inset, HRTEM image is shown, clusters are sized between 1.1 ± 0.1 nm. There is no feature corresponding to the formation of bigger plasmonic nanoparticles.

Electronic Supplementary Information 5

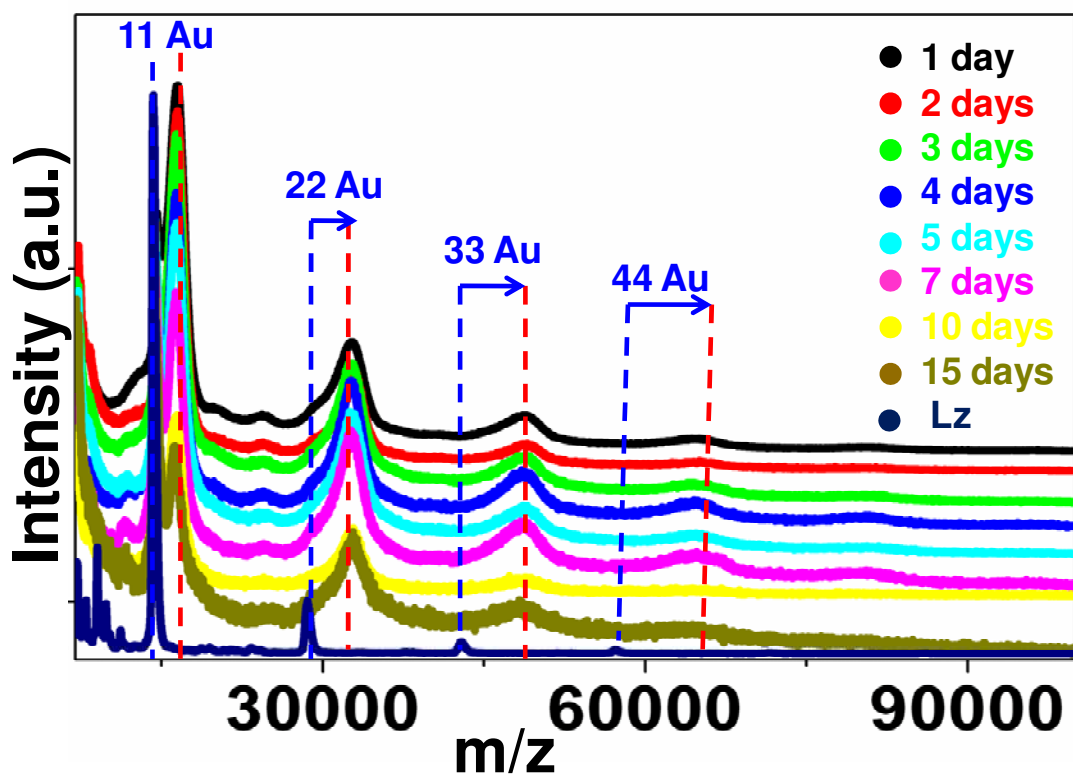


Fig. S5† Time dependent MALDI MS of Lyz: Au³⁺ (molar ratio 1:5) over 15 days time window.

A linear dependence of Au uptake is seen for the oligomers. While monomer shows a separation of 11 Au atoms from the parent protein peak, oligomers show separation of $n \times 11$ (where $n = 2, 3, 4 \dots$).

Electronic Supplementary Information 6

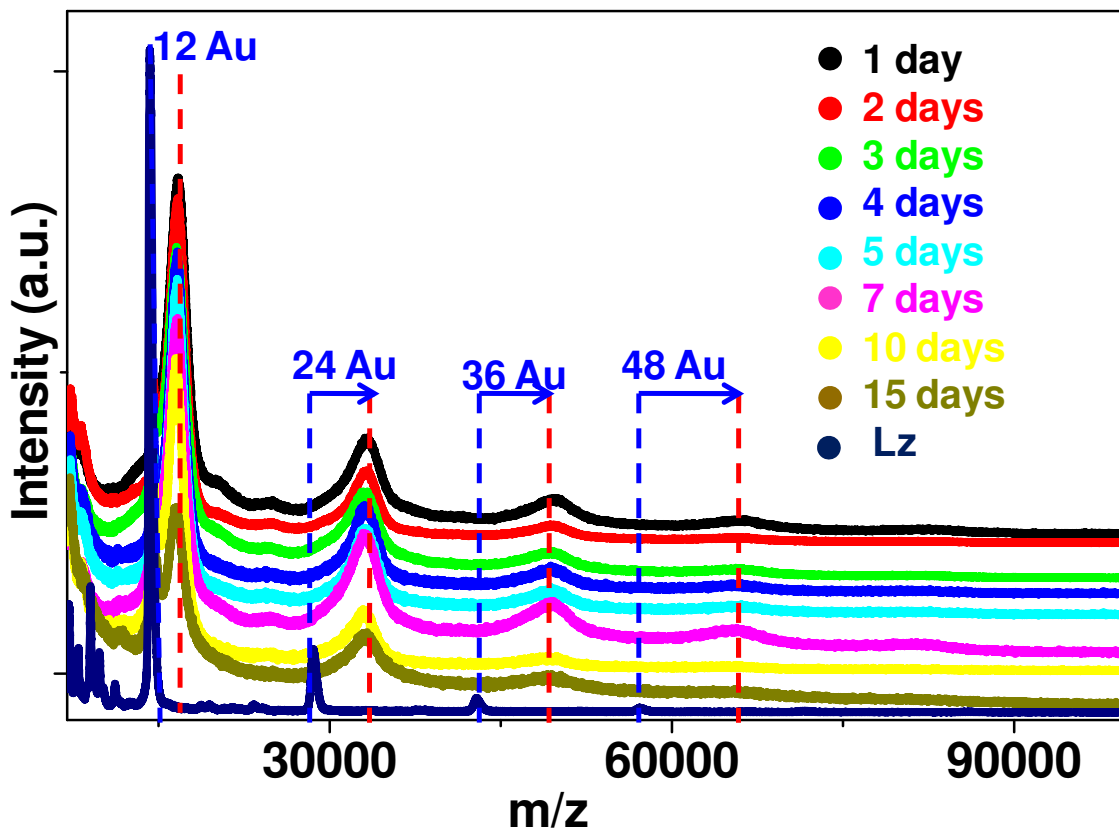


Fig. S6† Time dependent MALDI MS of Lyz: Au³⁺ (1:8 molar ratio) over 15 days time window. A linear dependence of Au uptake is seen for the oligomers. While monomer shows a separation of 12 Au atoms from the parent protein peak, oligomers show separation of $n \times 12$ (where $n=2, 3, 4, \dots$).

Electronic Supplementary Information 7

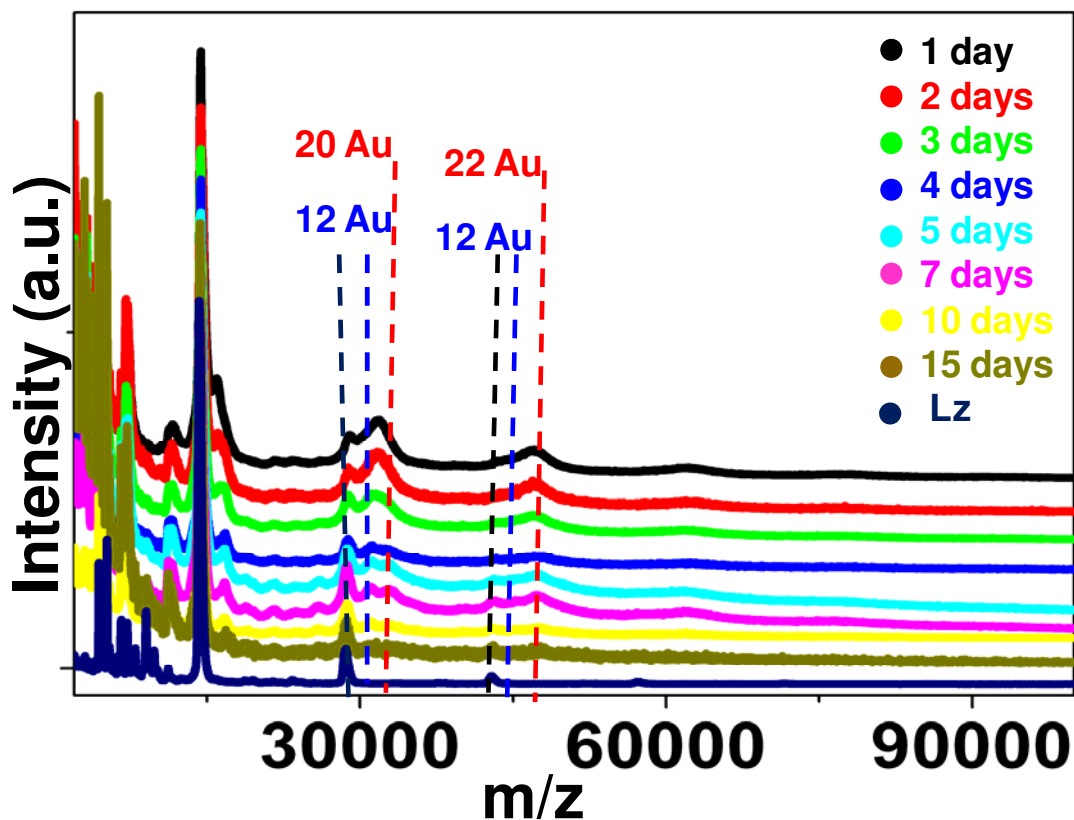


Fig. S7† Time dependent MALDI MS of Lyz: Au³⁺ (1:2.5molar ratio) over 15 days time window. A linear dependence of Au uptake is seen for the oligomers. While monomer shows a separation of 10 Au atoms, after 5 days the peak shifts to 12 Au atoms. In the dimer and trimer regions two distinct peaks appear. For dimer, peaks are separated by 12 and 20 Au atoms while in trimer, peaks are separated by 12 and 22 Au atoms.

Electronic Supplementary Information 8

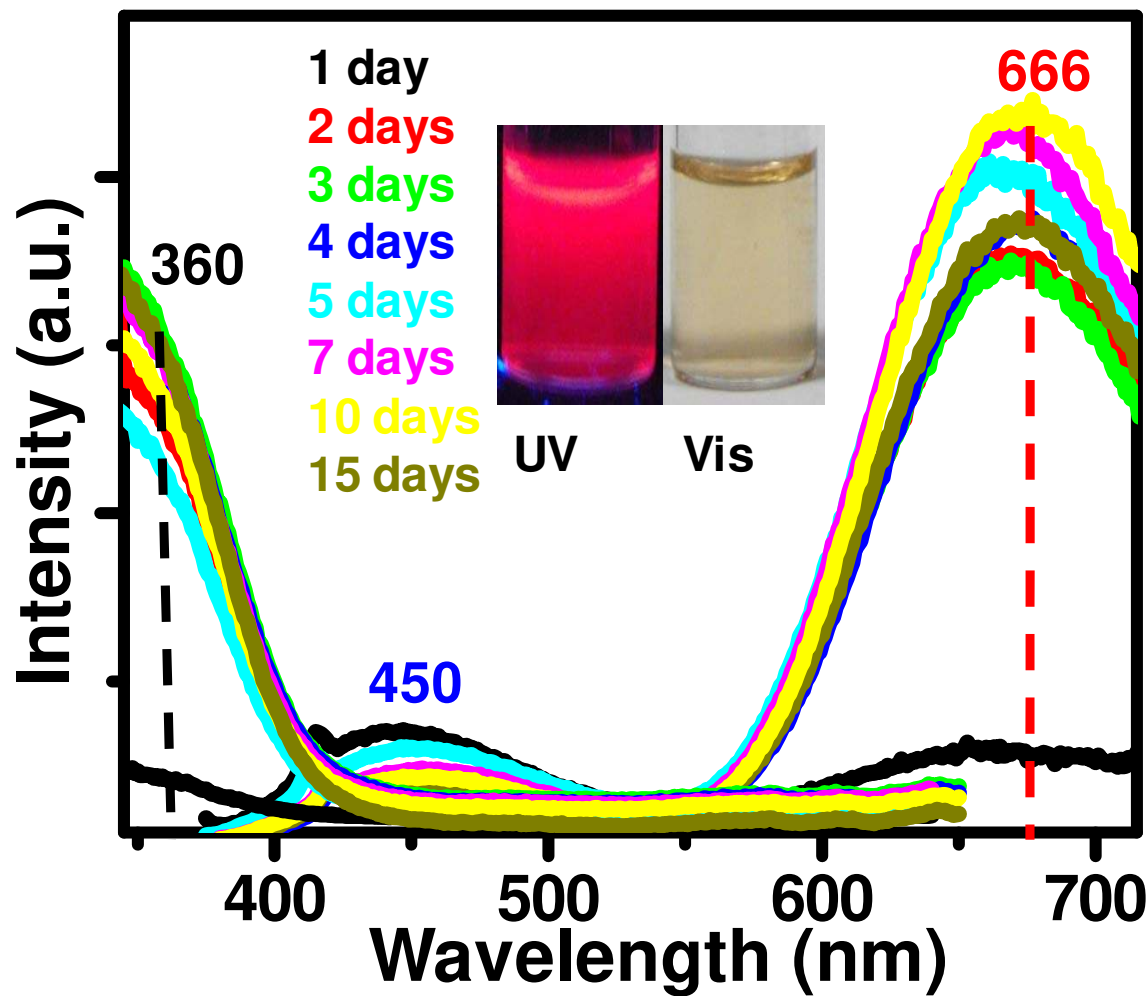


Fig. S8† Time dependent luminescence spectra of Lyz: Au³⁺ (1:5 molar ratio) over 15 days time window. Upon exciting at 360 nm, the cluster emits at 666 nm. Insets show the photographs of the sample under ultra-violet and visible light.

Electronic Supplementary Information 9

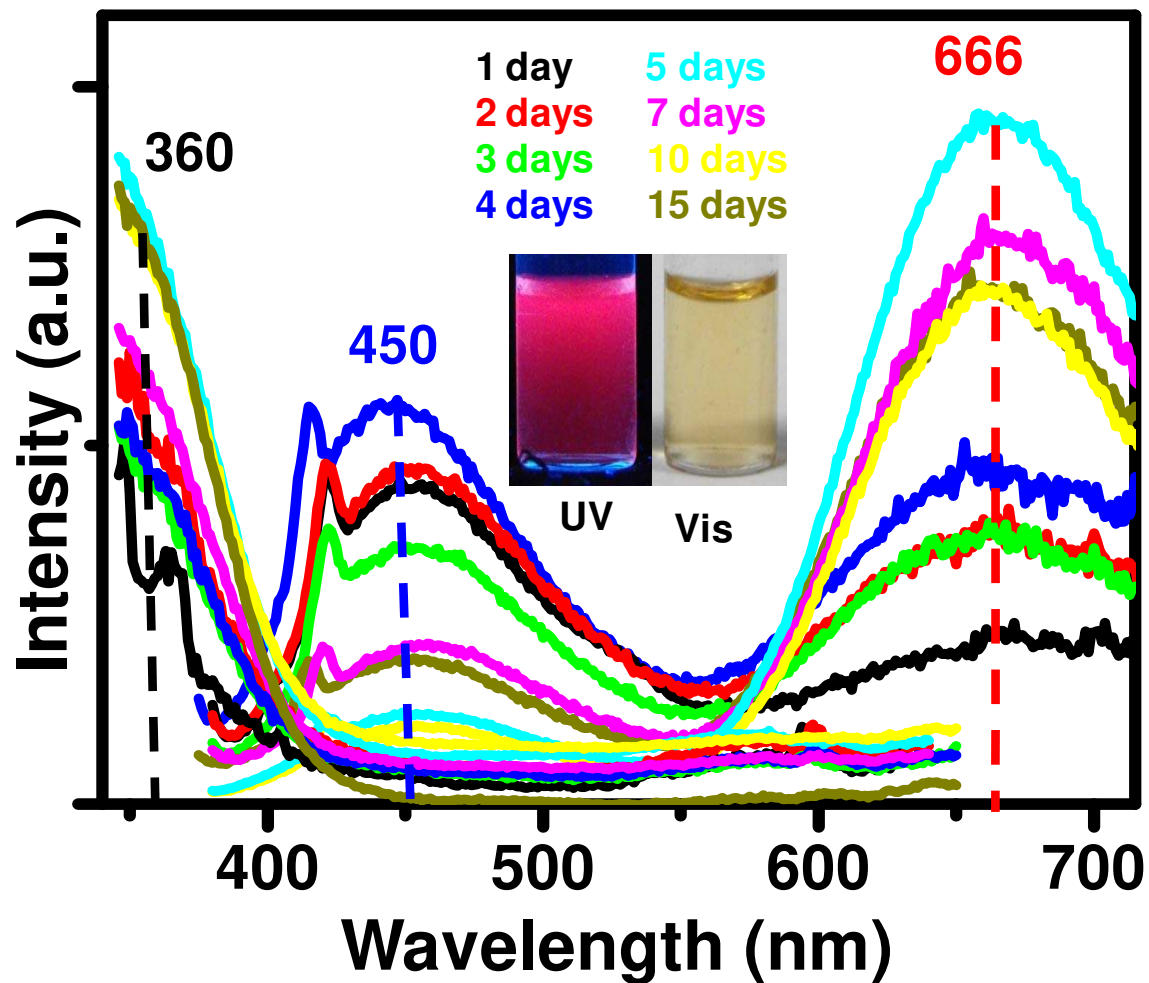


Fig. S9† Time dependent luminescence spectra of Lyz: Au³⁺ (1:8molar ratio) over 15 days time window. Upon exciting at 360 nm the cluster emits at 666 nm. Insets show the photographs of the sample under ultra-violet and visible light.

Electronic Supplementary Information 10

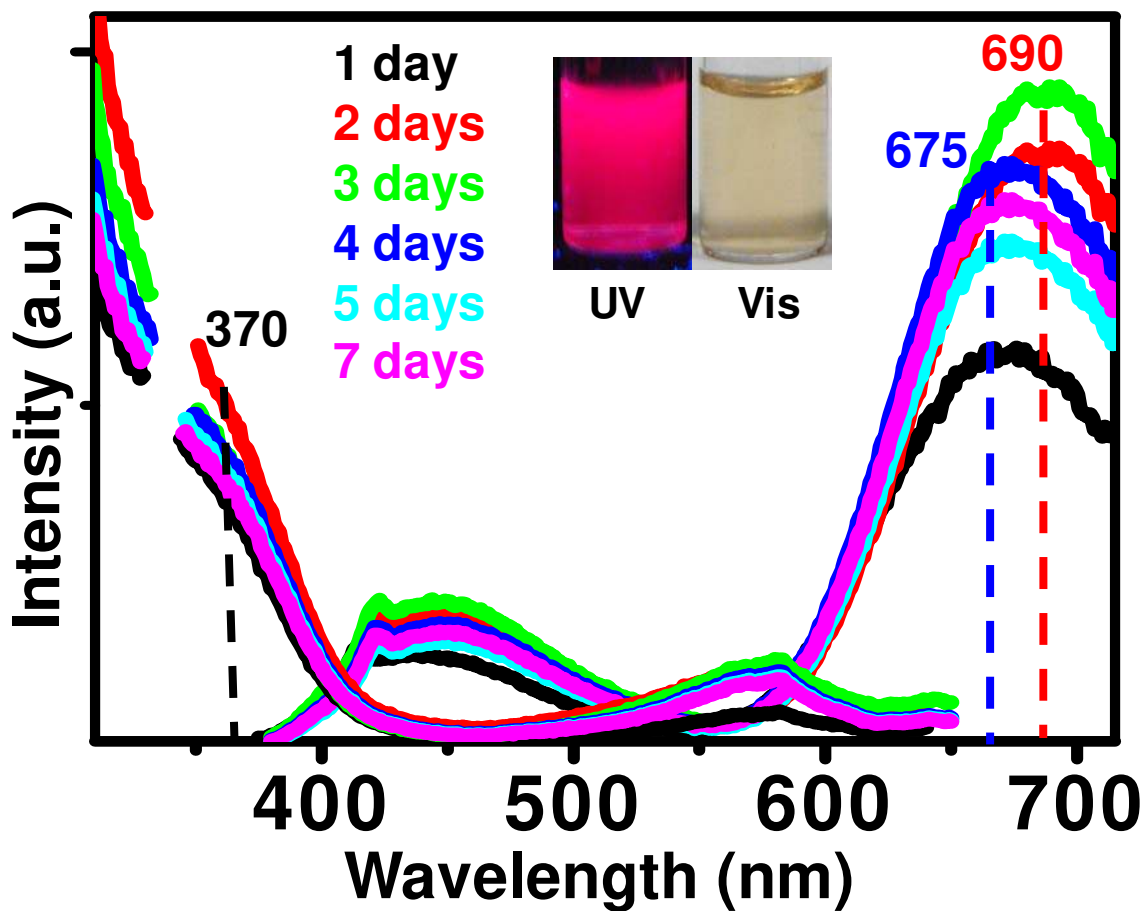


Fig. S10† Time dependent luminescence spectra of Lyz: Au³⁺ (1:2.5 molar ratio) over 7 days time window. Upon exciting at 370 nm the cluster emits at 690 nm which again blue shifts to 675 nm upon longer time. Insets show the photographs of the sample under ultra-violet and visible light. Calculated quantum yield is 15.2%.

Electronic Supplementary Information 11

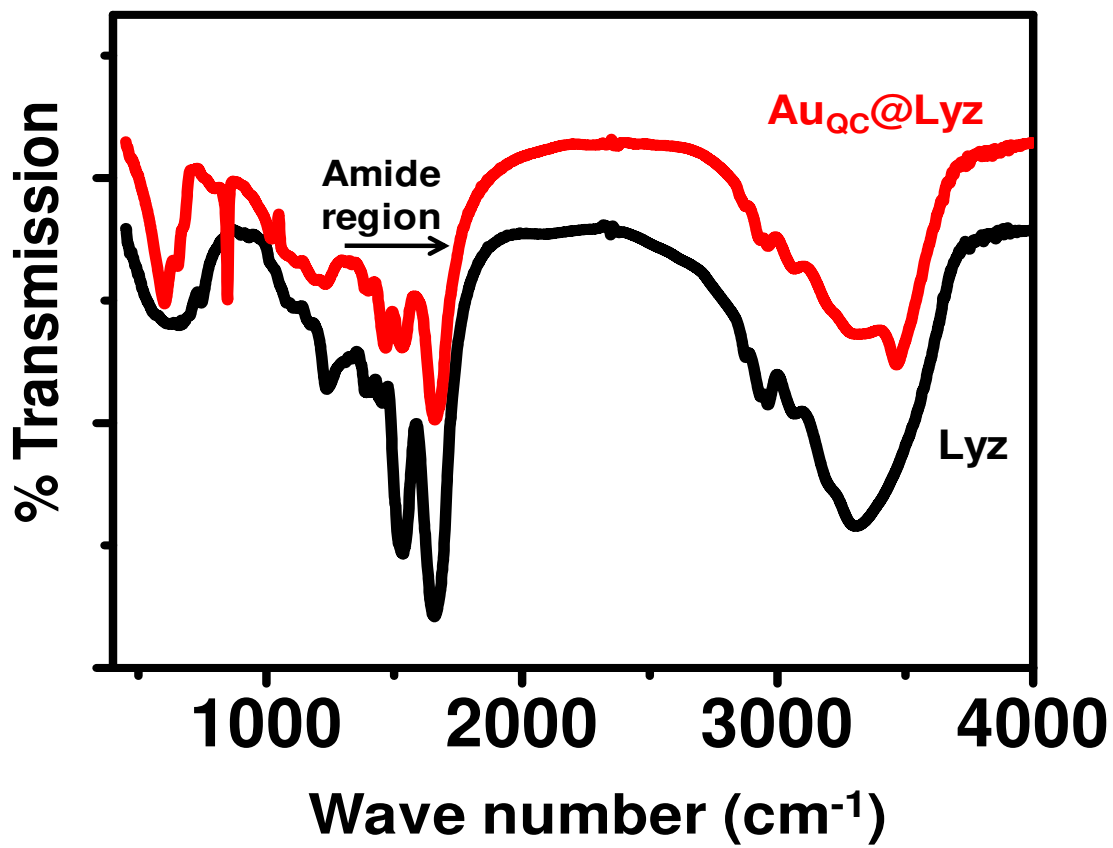


Fig. S11† Infrared (IR) spectra of Lyz and $\text{Au}_{\text{QC}}@\text{Lyz}$ showing significant change in the amide region.