

Supporting Information

Size evolution of protein protected gold clusters in solution:

A combined SAXS-MS investigation

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Supporting Information 1

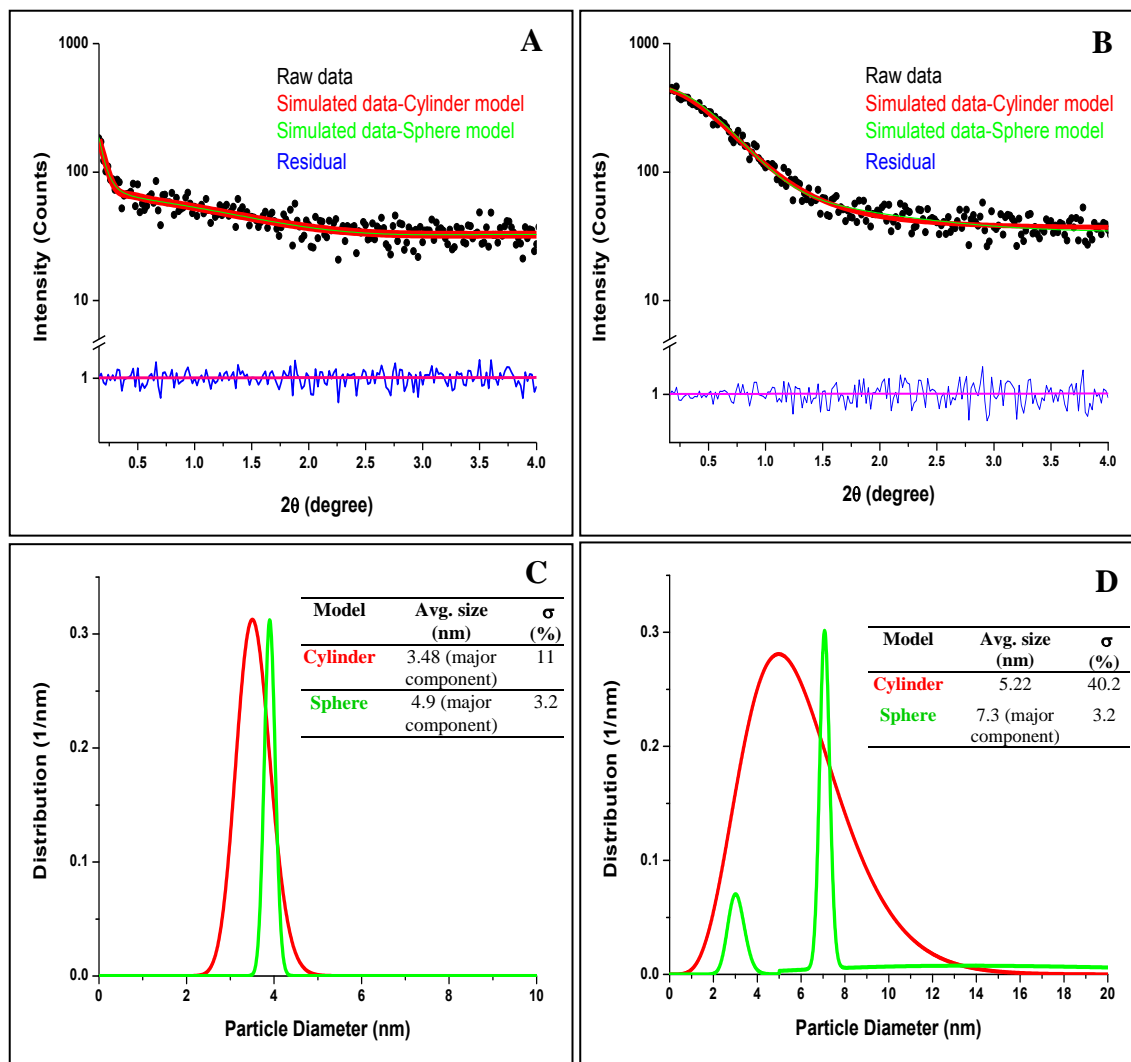


Figure S1: SAXS profiles of freshly prepared aqueous (A) Lyz and (B) BSA solutions evaluated using cylinder and sphere models (same residual factors) are shown for comparison. The corresponding size distribution profiles of (C) Lyz and (D) BSA proteins using the above two models. The average sizes of the proteins are tabulated in the insets of C and D; σ represents normalized dispersion.

Supporting Information 2

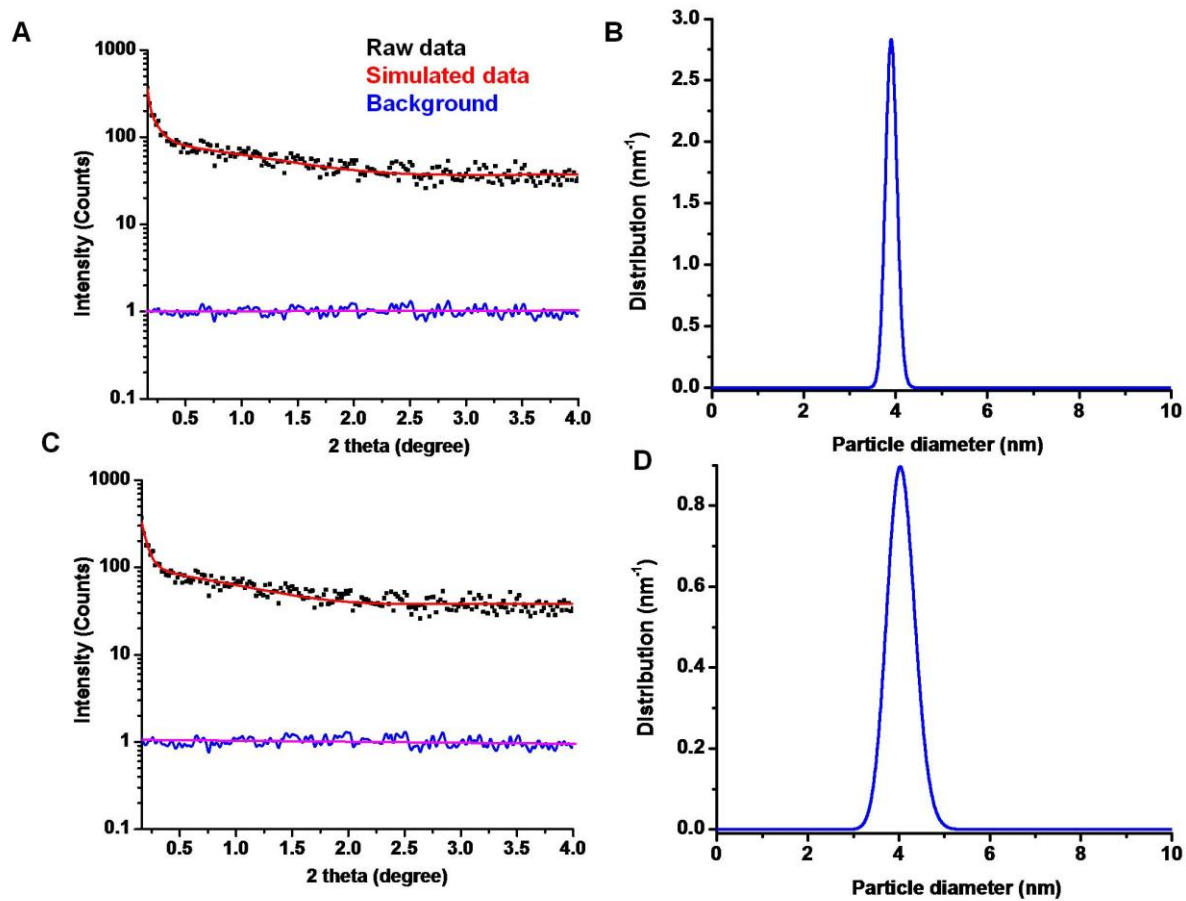


Figure S2: A) SAXS profile of Lyz in water, corresponding size profile is shown in B. C) SAXS profile of Lyz in water after one day, corresponding size profile is shown in D.

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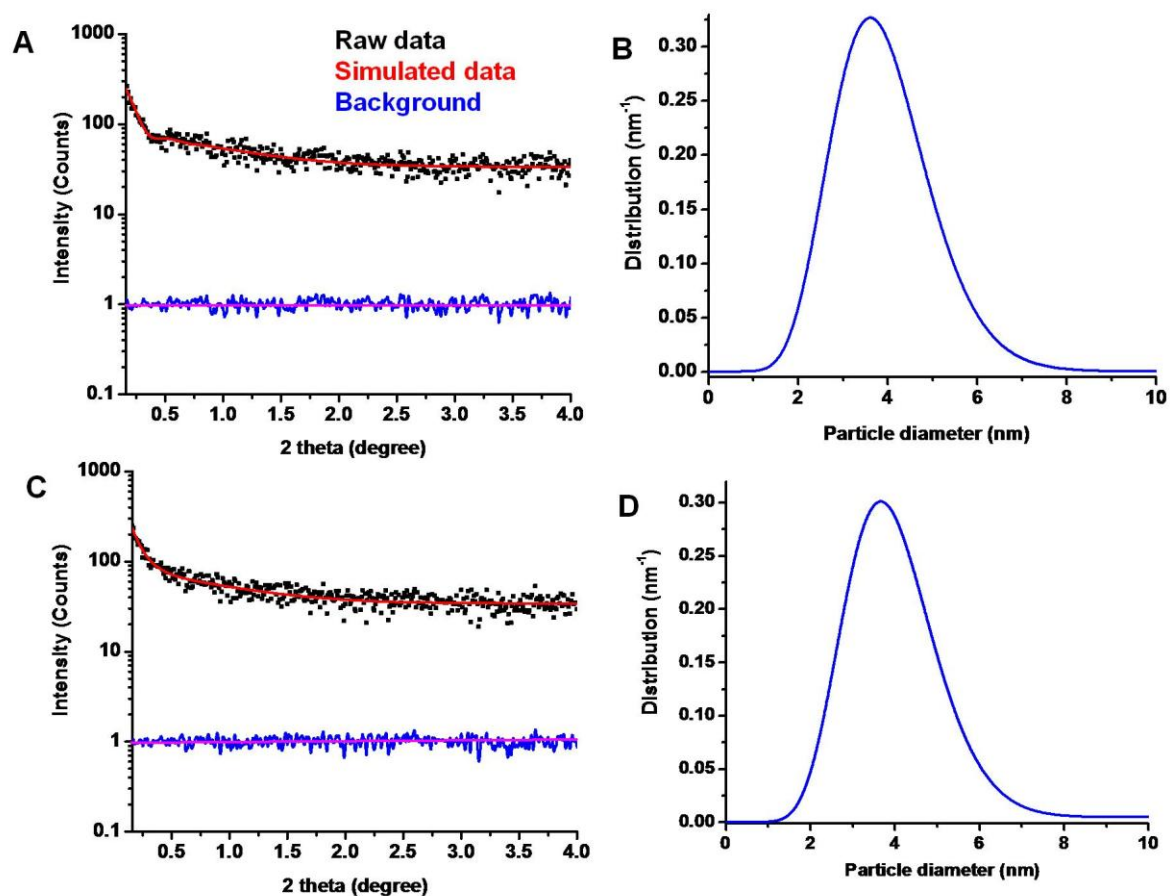


Figure S3: A) SAXS profile of Lyz in presence of NaOH at pH 12, corresponding size profile is shown in B. C) SAXS profile of Lyz in presence of NaOH at pH 12 after one day, corresponding size profile is shown in D.

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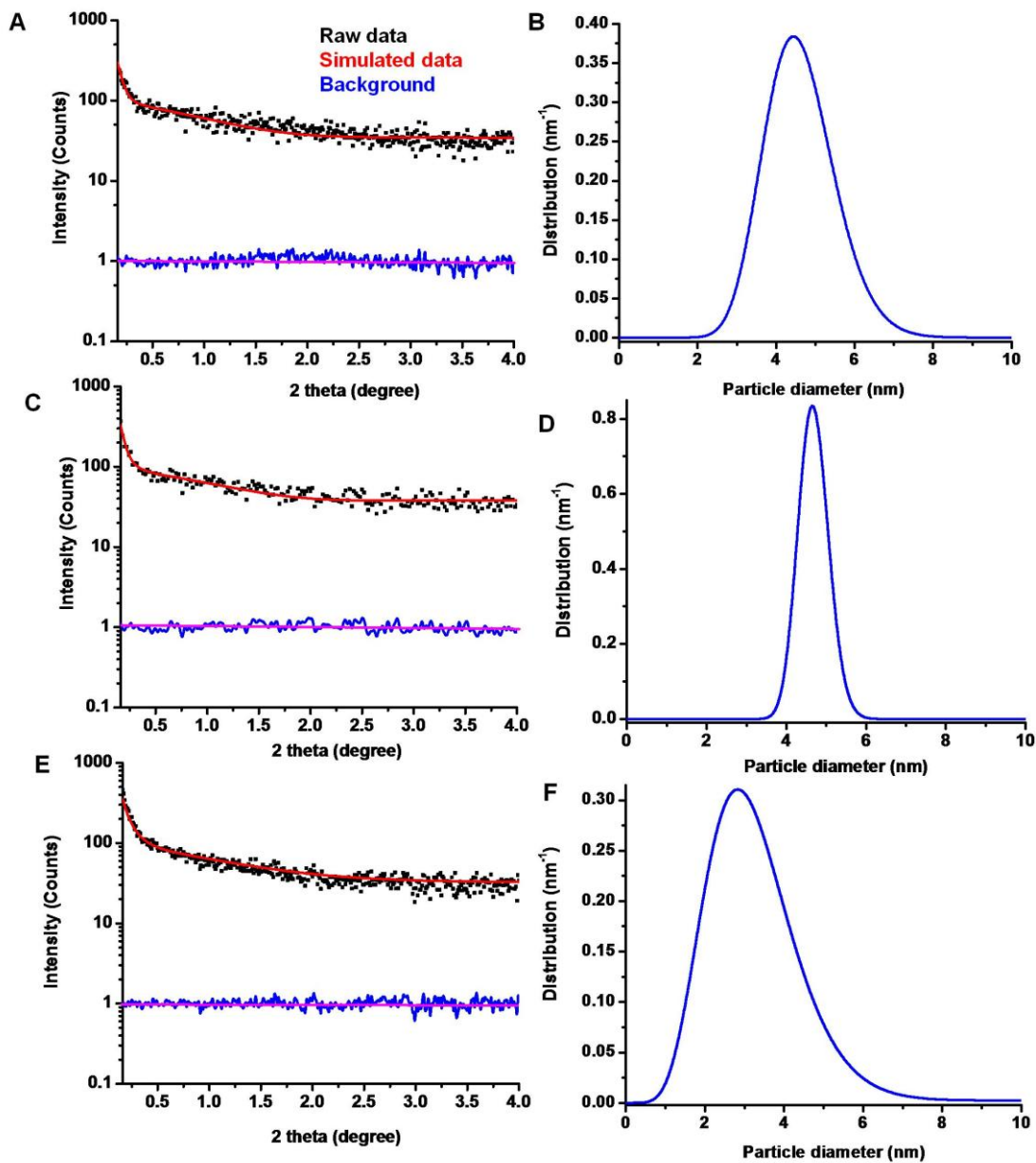


Figure S4: A) SAXS profile of Au⁺-Lyz, corresponding size profile is shown in B. C) SAXS profile of Au⁺-Lyz after 24 h, corresponding size profile is shown in D. After 48 hours of incubation, nanoparticles form. The SAXS profile is shown in E and the corresponding size profile in F is showing overall decrease in protein size after nanoparticle formation.

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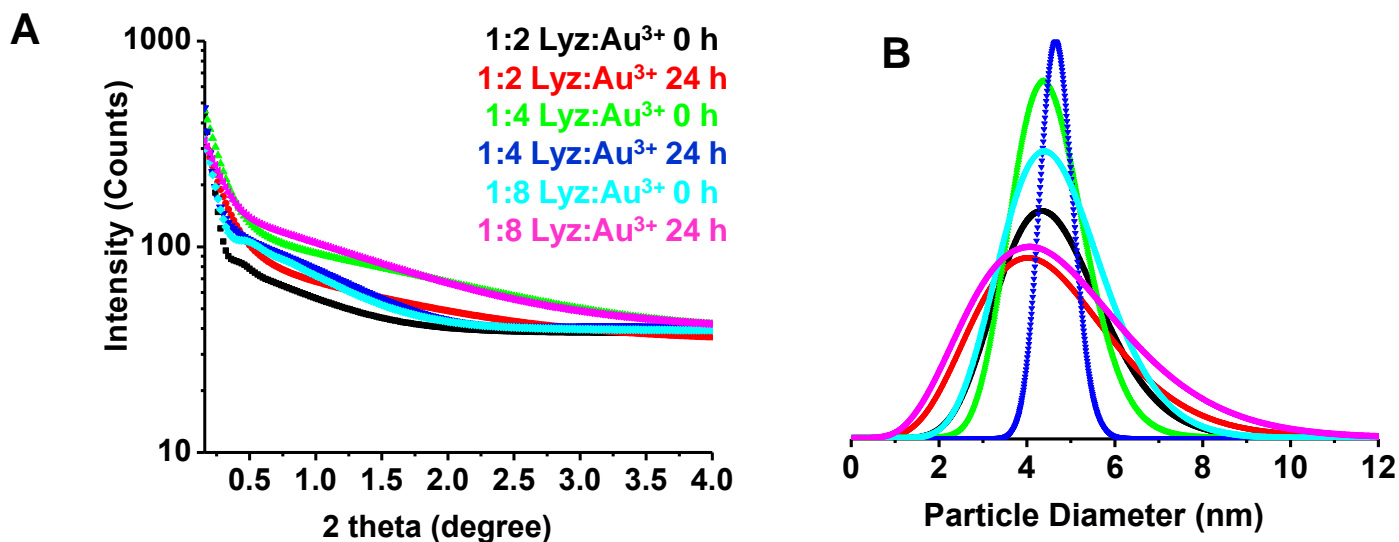


Figure S5: A) Time and concentration dependent SAXS profile of Au_{QC}@Lyz and the corresponding size profile is shown in B.

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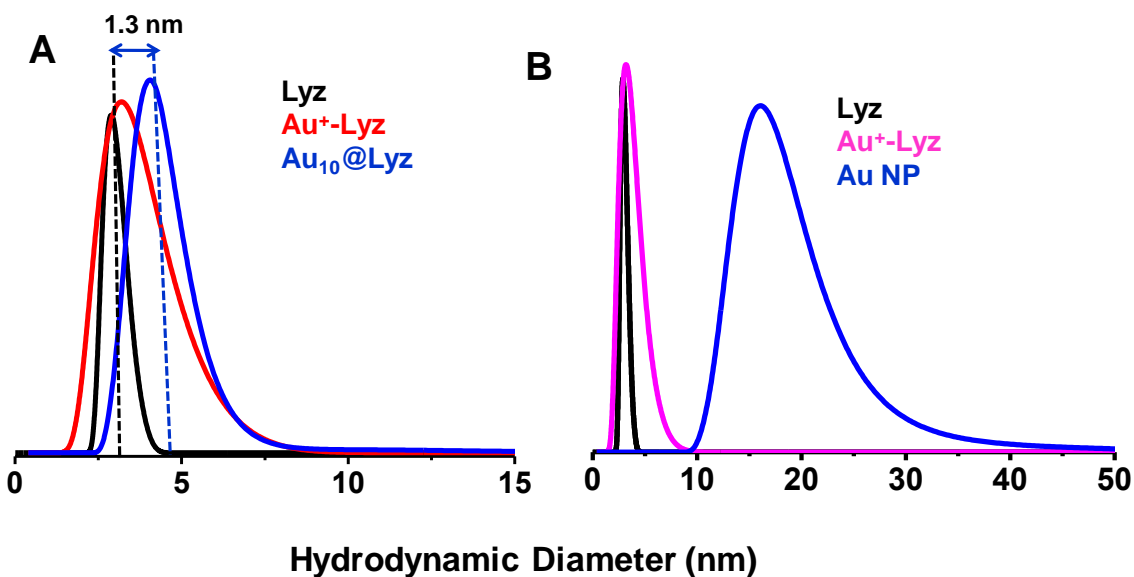


Figure S6: A) DLS data of Lyz, Au⁺-Lyz adduct and Au₁₀@Lyz showing presence of 1.3 nm cluster core. B) Time dependent growth of Au⁺-Lyz adduct lead to

nanoparticle formation and the corresponding size of nanoparticle was observed by DLS study.

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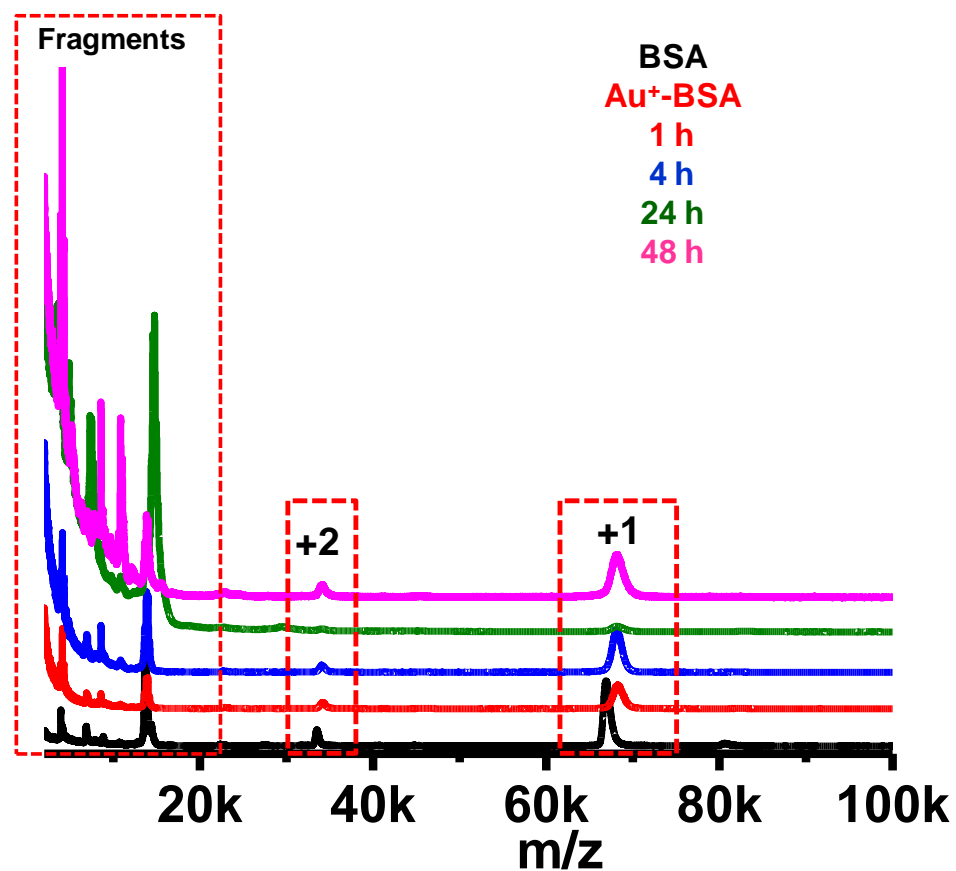


Figure S7: Time dependent MALDI MS of Au⁺-Lyz showing increase in fragmentations at lower mass region (<m/z 20k).

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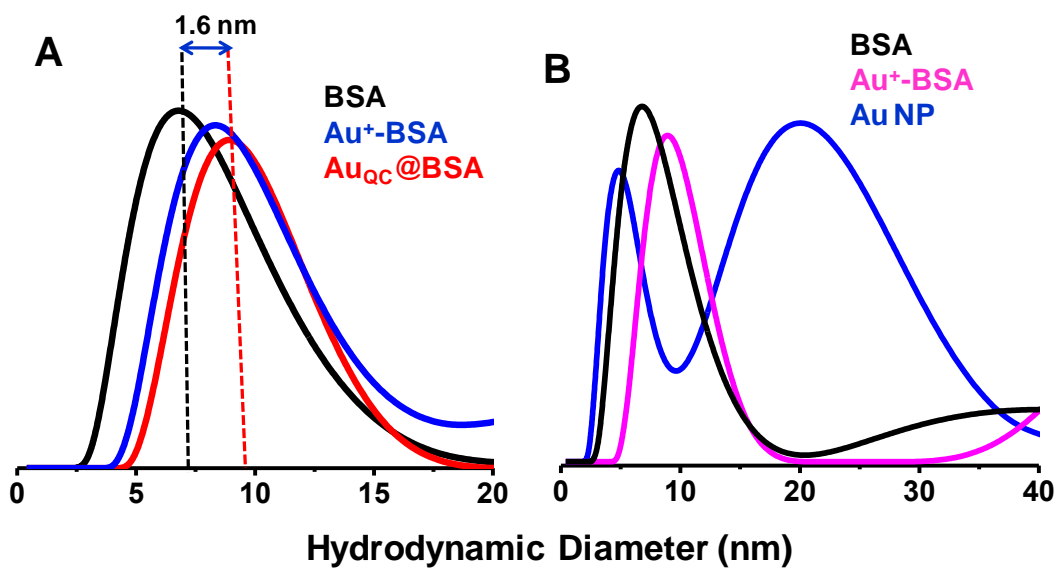


Figure S8: A) DLS data of BSA, Au⁺-BSA adduct and Au₁₀@BSA showing presence of 1.3 nm cluster core. B) Time dependent growth of Au⁺-BSA adduct leads to nanoparticle formation and the corresponding size of nanoparticle was observed by DLS study. After nanoparticle formation, the size of the protein decreases.

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Table S1: Details of SAXS parameters of Lyz and Au⁺-Lyz at different conditions.

	Sample	Particle Size (nm)	Normalized Distribution (%)	Volume (%)	R Factor (%)
1	Lyz (0 h)	03.9 37.1	03.2 31.4	88.86 11.14	4.54
2	Lyz (24 h)	04.0 62.8	07.3 20.9	68.12 31.88	3.82
3	Lyz+NaOH (0 h)	03.9 28.5	27.9 03.2	86.52 13.48	4.14
4	Lyz+NaOH (24 h)	04.0 26.9	27.4 61.1	78.85 21.15	4.54
5	Lyz+Au ³⁺ (0 h)	04.6 37.9	19.3 23.7	84.34 15.66	6.25
6	Lyz+Au ³⁺ (24 h)	04.7 42.2	08.1 28.1	79.10 21.90	3.99
7	Lyz+Au ³⁺ (48 h) Nanoparticles	03.3 39.8	35.2 69.3	83.57 16.43	4.19
8	Lyz+Au ³⁺ (high concentration) (0 h)	04.7 30.3	25.0 03.2	88.07 18.93	3.84

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Table S2: Details of SAXS parameters of Au_{QC}@protein at different conditions.

	Sample	Particle Size (nm)	Normalized Distribution (%)	Volume (%)	R Factor (%)
1	Lyz+Au ³⁺ + NaOH (0 h) (1:4 Lyz: Au ³⁺)	04.5 34.8	18.7 30.5	78.87 21.13	4.00
2	Lyz+Au ³⁺ + NaOH (24 h) (1:4 Lyz: Au ³⁺)	04.7 42.2	08.1 28.1	79.04 20.96	3.99
3	Lyz+Au ³⁺ + NaOH (48 h) (1:4 Lyz: Au ³⁺)	04.7 33.0	31.3 43.7	81.57 18.43	4.18
4	Lyz+Au ³⁺ + NaOH (0 h) (1:2 Lyz: Au ³⁺)	04.6 34.2	26.0 12.7	70.63 29.37	4.11
5	Lyz+Au ³⁺ + NaOH (24 h) (1:2 Lyz: Au ³⁺)	04.6 34.0	35.4 38.2	73.43 26.57	4.59
6	Lyz+Au ³⁺ + NaOH (0 h) (1:8 Lyz: Au ³⁺)	04.9 36.6	31.1 27.5	81.59 18.47	4.14
7	Lyz+Au ³⁺ + NaOH (24 hr) (1:8 Lyz: Au ³⁺)	04.8 32.4	39.7 23.1	88.36 11.64	4.02