## A comprehensive investigation of the differential interaction of

## Human Serum Albumin with Gold nanoparticles based on the

## variation in morphology and surface functionalization

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## **Supplementary Information**

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Figure S1 UV-visible spectra of (A) CTAB-AuNSs (B) PEG-AuNSs (C) CTAB-AuNRs (D) PEG-AuNRs.



**Figure S2 (A)** UV–visible and **(B)** Fluorescence spectra for **(a)** HSA **(b)** HSA+CTAB-AuNSs 80 μM **(c)** HSA+CTAB-AuNRs 80 μM **(d)** CTAB



**Figure S3** UV–visible spectra for (**A**) HSA+CTAB-AuNSs 40 μM (**B**) HSA+CTAB-AuNSs 80 μM (**C**) HSA+CTAB-AuNRs 40 μM (**d**) HSA+CTAB-AuNRs 80 μM (Main spectra shows increase in HSA peak; Inset shows decrease in AuNP peak upon nanoparticle consumption for complex formation).



**Figure S4** Plot showing the inverse of A–A<sub>0</sub> versus the inverse of nanoparticle concentration for (A) CTAB-AuNSs (B) CTAB-AuNRs (C) PEG-AuNSs (D) PEG-AuNRs.



Figure S5 Arrhenius plot for (A) CTAB-AuNSs (B) CTAB-AuNRs (C) PEG-AuNSs (D) PEG-AuNRs.



**Figure S6** Effect of denaturant concentration on the emission wavelength of HSA before and after interaction with (**A**) CTAB-AuNSs (**B**) CTAB-AuNRs (**C**) PEG-AuNSs (**D**) PEG-AuNRs at 0, 40, and 80 μM.



**Figure S7** UV–visible spectra for (**A**) PEG-AuNSs 40  $\mu$ M (**B**) PEG-AuNSs 80  $\mu$ M (**C**) PEG AuNRs 40  $\mu$ M (**d**) PEG-AuNRs 80  $\mu$ M (Main spectra shows increase in HSA peak; Inset shows decrease in AuNP peak upon nanoparticle consumption for complex formation).



**Figure S8 (A–B)** Stern–Volmer plot (at 298, 308, and 318 K) and **(C–D)** double logarithmic plot (298 K) for HSA interacted with PEG-modified AuNSs and AuNRs.

Table S1: Protein concentrations in interacted samples before and after centrifugation

Sample	Reading 1 <sup>a</sup> (µM)	Reading 2 <sup>b</sup> (µM)	Reading 3 <sup>c</sup> (µM)	Reading 4 <sup>d</sup> (µM)
HSA control	99.0±0.7	93.3±1.7	5.7±1.2	_
CTAB AuNS 40	97.6±1.2	72.1±0.7	25.5±0.9	19.7±1.9
CTAB AuNS 80	97.2±0.8	70.7±0.4	26.5±0.4	20.8±1.3
CTAB AuNR 40	96.5±0.5	70.3±1.0	26.2±0.7	20.5±0.8
CTAB AuNR 80	97.2±0.5	66.8±0.8	30.4±1.1	24.7±1.2
PEG AuNS 40	99.3±0.4	85.3±0.6	14.0±0.6	8.3±0.7
PEG AuNS 80	98.3±0.8	84.6±0.5	13.7±0.4	7.9±1.4
PEG AuNR 40	98.1±0.4	80.9±0.3	17.2±0.3	11.5±1.2
PEG AuNR 80	98.4±1.1	80.2±0.5	18.1±1.4	12.4±1.1

a – Protein concentrations estimated in 1-h interacted sample before centrifuge b – Protein concentrations estimated for supernatant in 1-h interacted sample before centrifuge

c – Protein concentration in pellet (c=a–b)

d – Protein concentration estimated to be involved in complex formation (d=Reading 3 for sample – Reading 3 for control)