Electronic Supplementary Material (ESI) for Materials Advances. This journal is © The Royal Society of Chemistry 2020

## Supplementary information

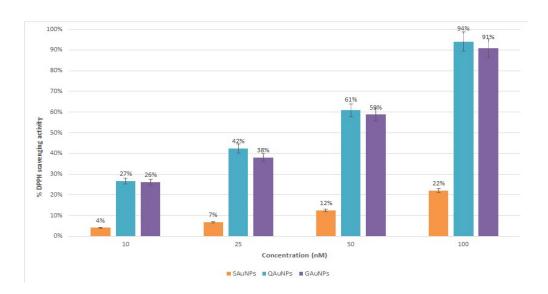


Figure S1: DPPH scavenging activity of SAuNPs, QAuNPs and GAuNPs at different concentrations (10-100 nM).

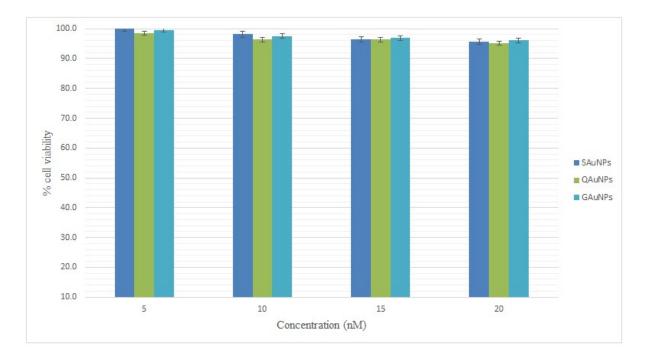


Figure S2: Percentage cell viability of AuNPs at different concentrations (5-20 nM).

## Molecular docking studies

Eighteen hot spots are present in the human serum albumin (PDB ID: 2BXP) structure (figure S4). All the capping molecules were individually docked into HSA to understand their interactions with the amino acid residues.

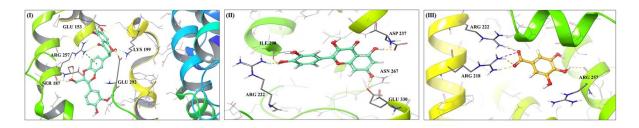


Figure S3. Molecular docking of (I) silymarin (II) quercetin and (III) gallic acid with HSA (PDB: 2BXP) structure.

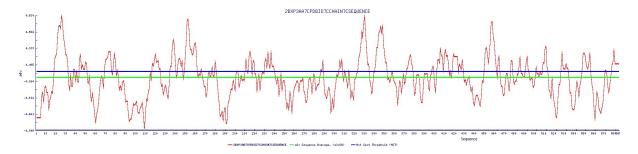


Figure S4. Aggregation prone regions of HSA (PDB: 2BXP) as predicted by Aggrescan online tool. Here, x-axis represents the amino acids and y-axis represents their A3D scores.