

## Albumin-coated SPIONs: An experimental and theoretical evaluation of protein conformation, binding affinity, and competition with serum proteins.

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### SUPPORTING FIGURES

Figure S1. a) Graphical representation of the mean hydrodynamic diameter and the zeta potential of the C-SPIONs, BSA-C-SPIONs and BSA measured by Zetasizer. B) Procedure followed to obtain BSA-C-SPIONs.

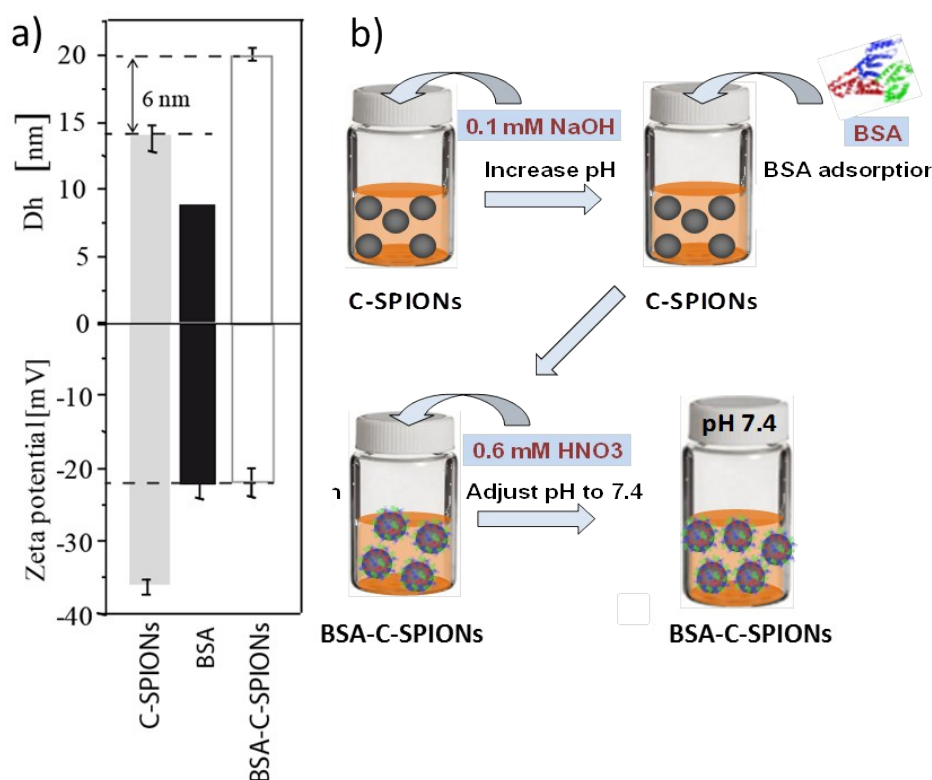


Figure S2. a) The Uv-vis adsorption spectra of collected supernatant after each washing step. b) The calibration curve of the absorbance of a BSA solution measured for different BSA concentration.

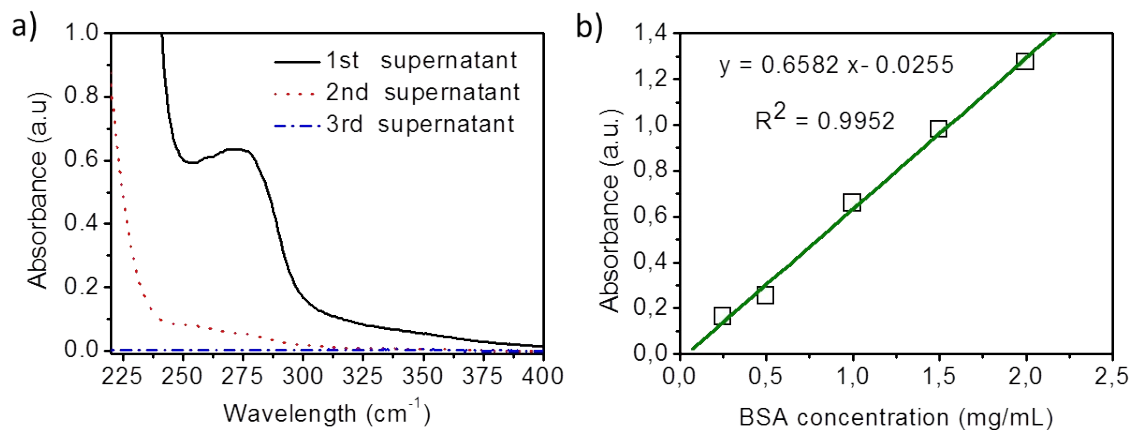


Figure S3. DLS volume-weighted size distribution of BSA in solution, which indicates a hydrodynamic diameter of 8 nm.

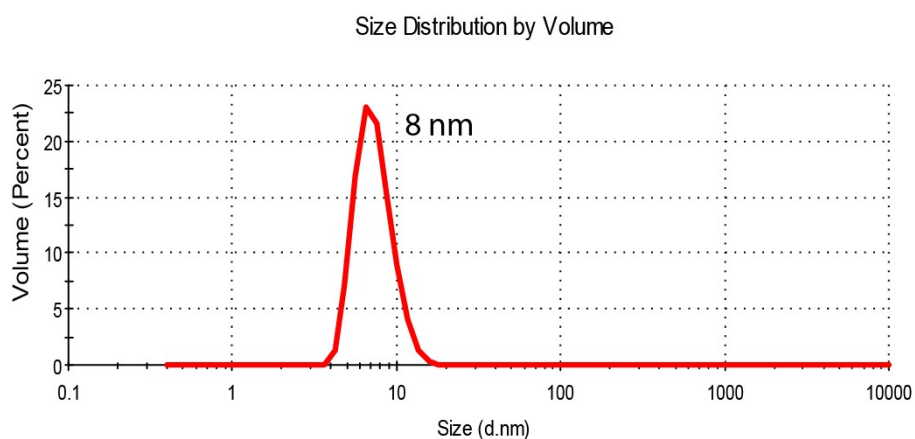


Figure S4. High-resolution XPS a) Fe 2p and b) S 2p spectra of C-SPIONs (gray) and BSA-SPIONs (black) and c) N 1s spectra of C-SPIONs (gray) and BSA-SPIONs (black).

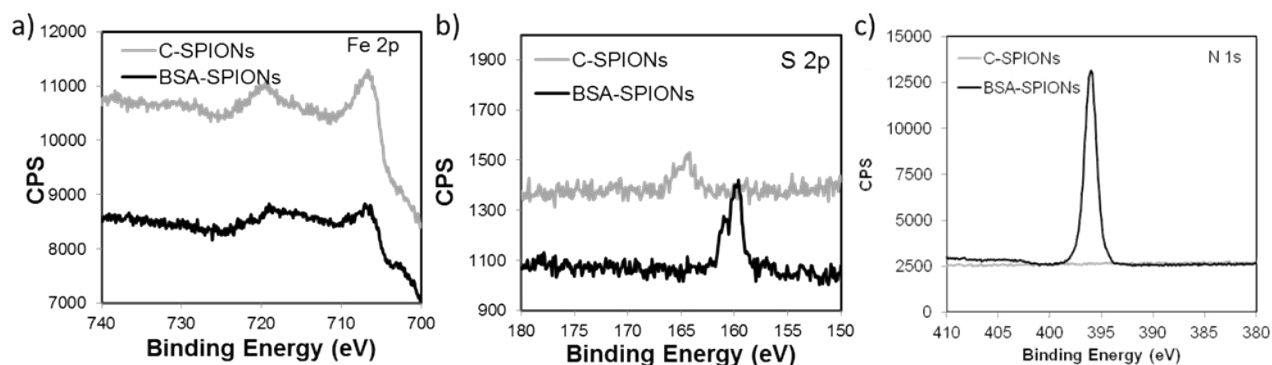


Figure S5. Fluorescence spectra of C-SPIONs with increasing concentrations at pH 7.4.

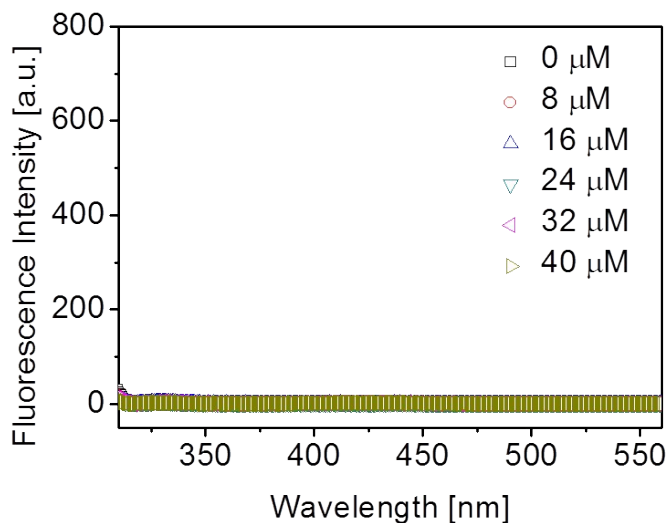


Figure S6. a) Stern–Volmer plots for the  $4 \times 10^{-6}$  M BSA in the presence of increasing concentrations of C-SPIONs; b) in logarithmic scale.

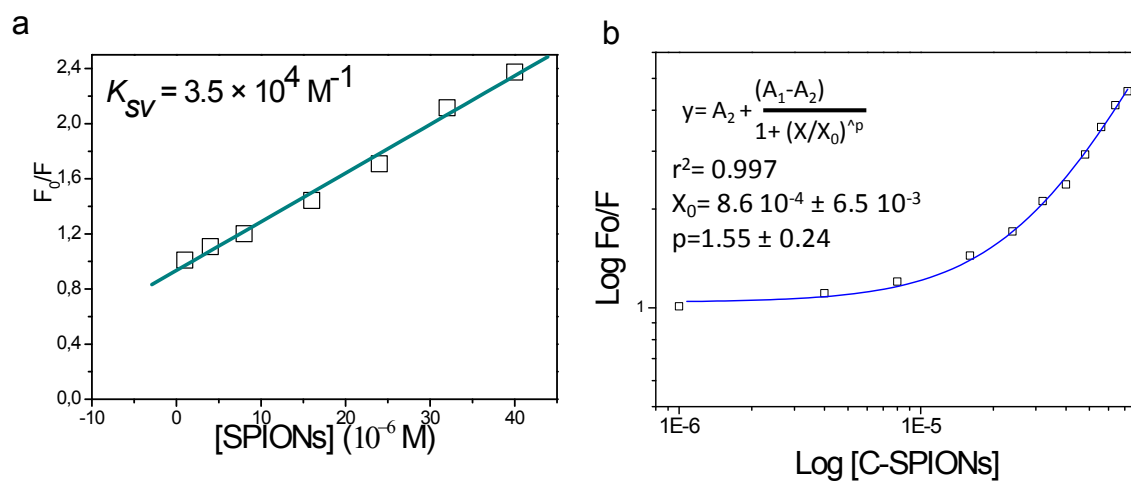


Figure S7. Plot of the evolution of the solvent accessible surface area (SASA) in Å<sup>2</sup> during the adsorption of a BSA protein onto a clean NP surface as a function of time. The three values for the SASA corresponding to the snapshots in Figure 6 are indicated.

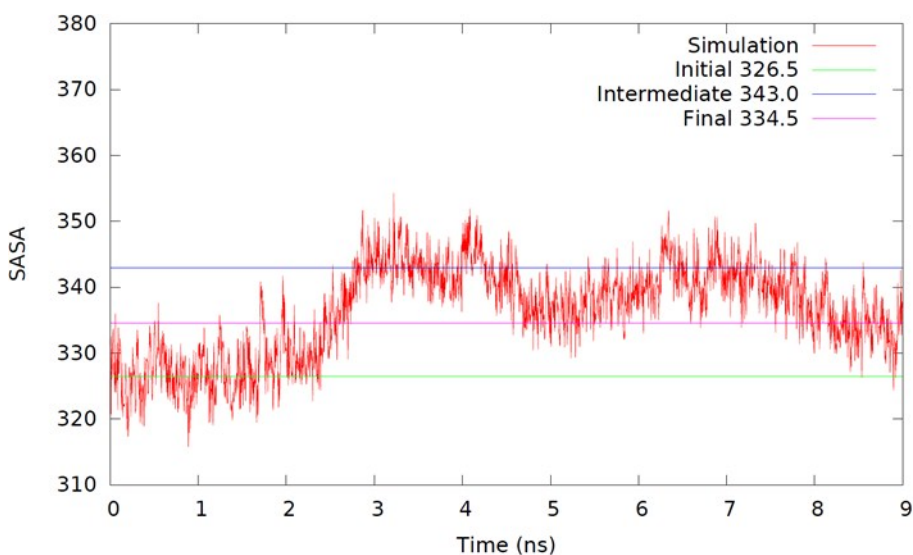


Table S1. Polydispersity values of the DLS of the increase of  $D_h$  of C-SPIONs upon BSA incubation at room temperature for 1 h for concentrations ranging from 0.1–100  $\mu\text{M}$  BSA

[BSA] ( $\mu\text{M}$ )	0	0,1	1	2	6	8	10	20	30	50
$D_h$ (nm)	15.8± 0.2	16.4± 0.1	17.1±0 .03	18.2± 0.4	20.4± 0.4	21.2± 0.5	22± 0.1	23.04± 0.3	23.0± 0.6	22.8± 0.4
PDI	0.16	0.17	0.16	0.18	0.2	0.2	0.2	0.21	0.26	0.28

Table S2. CD calculated using Kd2 and the mean residual ellipticity of 583 residues; no difference was seen. (<https://cbdm.uni-mainz.de/andrade/>)

	BSA (%)	BSA-SPIONs (%)
$\alpha$ helix	68.04	68.12
$\beta$ strand	8.4	7.85