Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Binding of Cytoskeletal Proteins with Silver Nanoparticles

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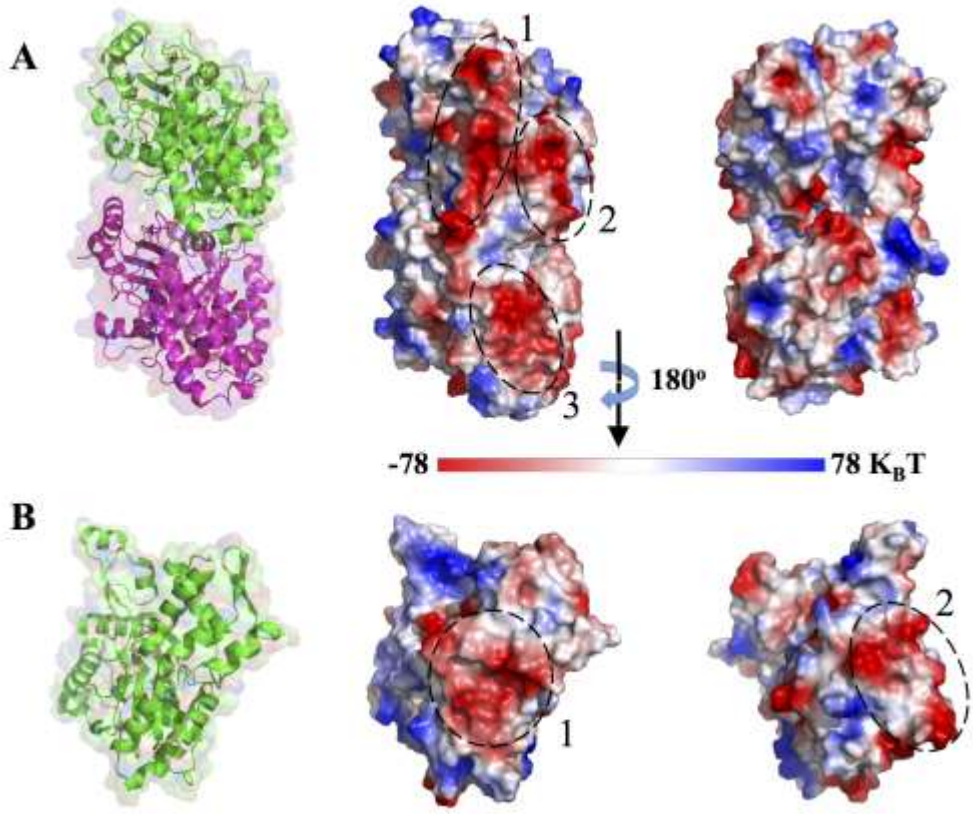
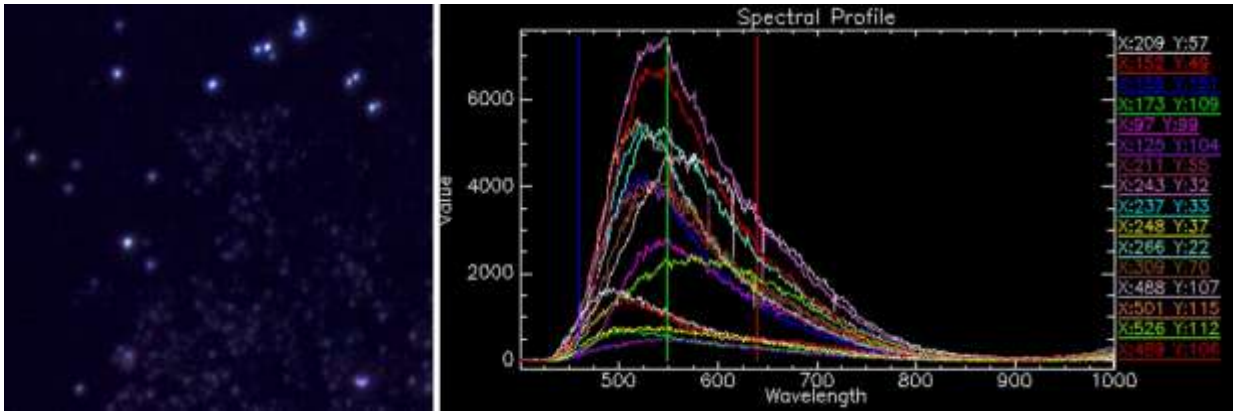


Fig. S1 Structures and potential NP-binding sites of Tubulin dimer (A) and Actin (B). The left panels correspond to the 3D structures in cartoon representations. The molecular surfaces are shown with high transparency. The alpha- and beta-tubulin molecules are colored differently. The middle panels illustrate the electrostatic potentials (computed using PyMol, www.pymol.org) on the corresponding molecular surface, where red corresponds to negative energy and blue denotes positive electrostatic potential. The right panels show the same surfaces from a different view point. Based on previous experimental[1] and computational[2,3] studies, AgNP has a preference to bind the negatively charged protein surfaces. We highlighted the NP-binding clusters with dashed circles, corresponding to well-defined surface patches featuring low

electrostatic potentials. Specifically, for tubulin dimer (A), cluster 1 on alpha-tubulin consists of residues 386, 392, 396, 415, 423, 429, 433, and 439, cluster 2 on alpha-tubulin consists of residues 155, 196, 414, 417, 420, 424, 431, and 434, and cluster 3 on beta-tubulin consists of residues 110, 113, 159, 196, 411, 414, 417, 420, 427, and 431. For actin (B), cluster 1 consists of residues 222, 224, 259, 265, 270, 276, and 316 while cluster 2 consists of residues 51, 80, 83, 99, 100, 125, 363, and 364, respectively.

(a)



(b)

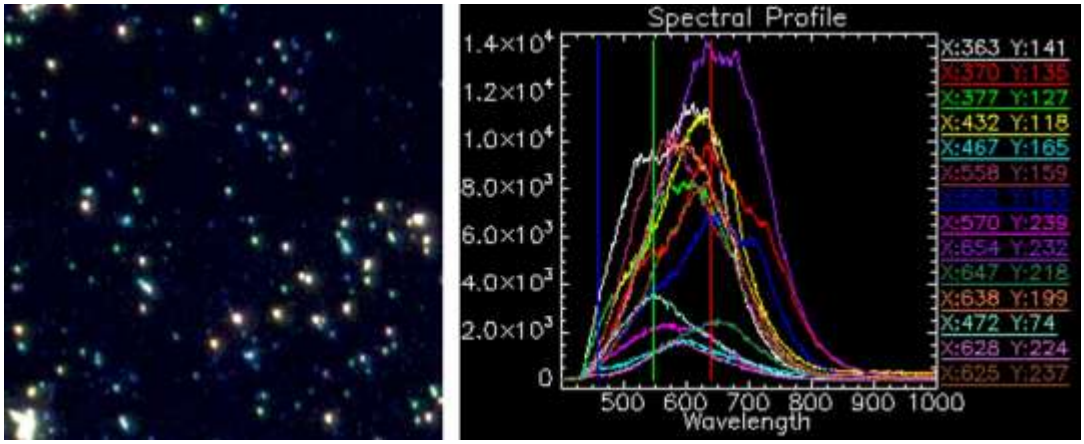


Fig. S2 (A, B) Exemplary CytoViva images and their corresponding hyperspectra for actin-AgNP and tubulin-AgNP at 2 h, respectively. (B) The double-shoulder spectra for tubulin-AgNP indicate an aggregation-induced quadrupole resonance that is different from the primary resonance in electron oscillation.

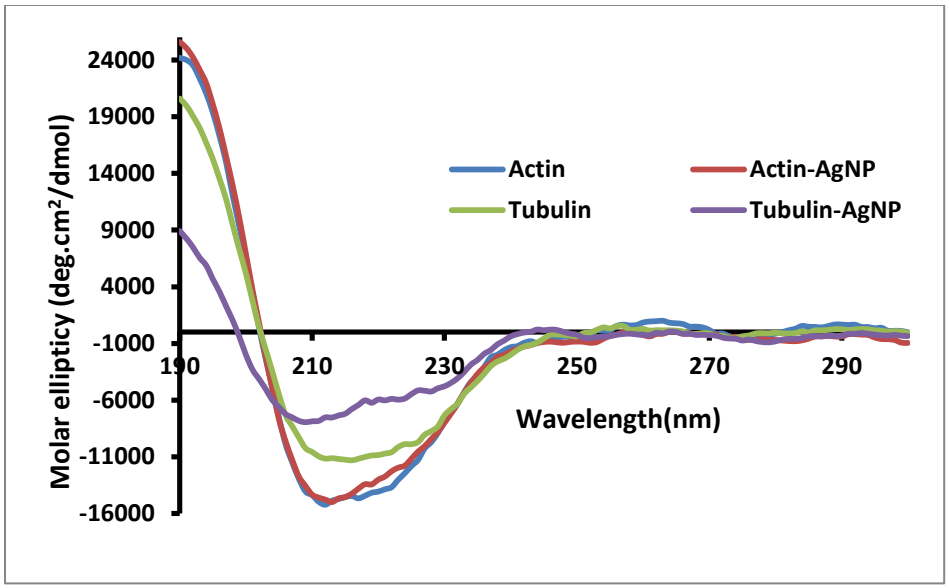


Fig. S3 Circular dichroism spectra of cytoskeletal protein (0.25 mg/ml) and cytoskeletal protein mixed with AgNPs (0.05 mg/ml).

Secondary structure percentages	Actin	Actin-AgNPs	Tubulin	Tubulin-AgNPs
Helix	38	29	35	29
Sheet	25	34	21	22
Turns	16	17	16	20
Others	21	20	28	29

Table. S1 Secondary structure percentages of cytoskeletal protein (0.25 mg/ml) and cytoskeletal protein mixed with AgNPs (0.05 mg/ml) (derived from the CD measurement).

References:

1. L. Calzolai, F. Franchini, D. Gilliland, and F. Rossi, *Nano Lett*. 2010, **10**, 3101-3105.

2 . F. Ding, S. Radic, R. Chen, P. Chen, N. K. Geitner, J. M. Brown, and P. C. Ke, *Nanoscale*, 2013 (DOI: 10.1039/c3nr02147e).

3. A. Kakinen, F. Ding, P. Chen, M. Mortimer, A. Kahru, and P. C. Ke, *Nanotechnology* 2013, **34**, 345101.