Supporting Information

Effect of Fullerenol Surface Chemistry on Nanoparticle Binding-induced Protein Misfolding

Slaven Radic\textsuperscript{1,*}, Praveen Nedumpully-Govindan\textsuperscript{1,2,*}, Ran Chen\textsuperscript{1}, Emppu Salonen\textsuperscript{2}, Jared M. Brown\textsuperscript{3}, Pu Chun Ke\textsuperscript{1}, and Feng Ding\textsuperscript{1}

\textsuperscript{1}Department of Physics and Astronomy, Clemson University, Clemson, SC 29634, USA
\textsuperscript{2}Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland
\textsuperscript{3}Department of Pharmaceutical Sciences, Skaggs School of Pharmacy, University of Colorado Anschutz Medical Campus, Aurora, CO 80045, USA

*These authors contributed equally

Address correspondence to: fding@clemson.edu

Figure S1. The binding sites of C\textsubscript{60}(OH)\textsubscript{20} fullerenol on ubiquitin as predicted by docking simulations. The residues that make direct contact with ubiquitin include Phe45, Asn60, Gln 62 and Ser65 at site 1 (A), and Leu71, Leu73, Gly75 and Gly76 at site 2 (B), which are highlighted by depicting in stick representation. The C\textsubscript{60} fullerene bind predominantly to site 1.
Figure S2. Stern-Volmer plot of fluorescence quenching of ubiquitin in the presence of fullerene $C_{60}(OH)_{20}$. 

\[ \frac{I_0}{I} = 6.54 \times 10^4 \times C + 1.15 \]

\[ R^2 = 0.98 \]
Figure S3. Isothermal titration calorimetry of $C_{60}(OH)_{20}$ fullerenol into ubiquitin.
Figure S4. Representative RMSD plots of ubiquitin without any nanoparticles from DMD simulations. The three trajectories (A-C) are taken from three independent simulations.
Figure S5. Protein heavy atom RMSD fluctuations in MD simulations in the cases of ubiquitin-alone (black), ubiquitin with C$_{60}$ fullerene (red) and ubiquitin with C$_{60}$(OH)$_{20}$ fullerenol (green).
Figure S6. Circular dichroism spectra of ubiquitin and ubiquitin-fullerenol solutions.