# Supporting Information

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

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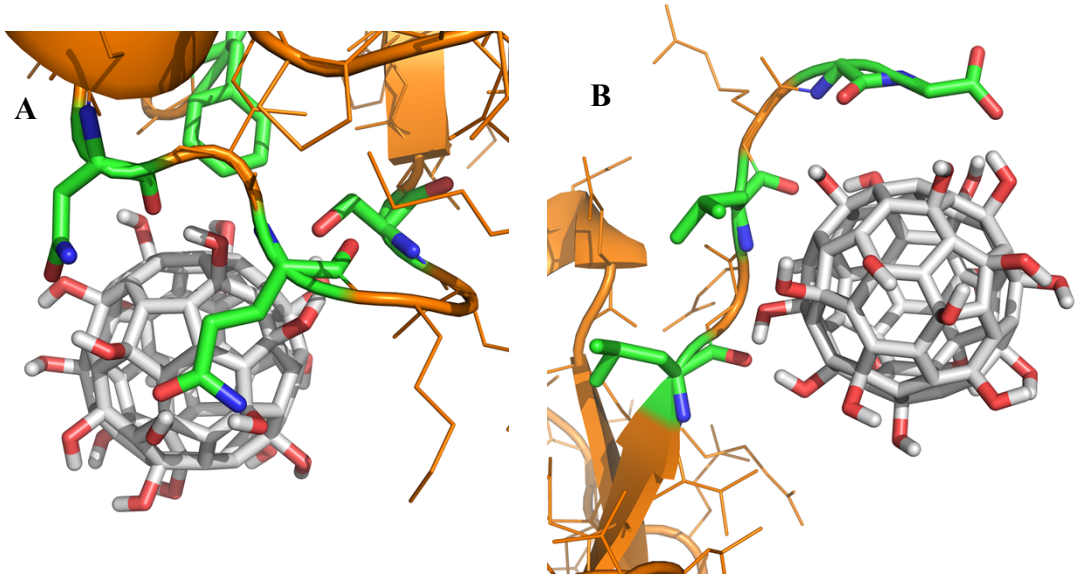


**Figure S1.** The binding sites of $C_{60}(OH)_{20}$ fullerenol on ubiquitin as predicted by docking simulations. The residues that make direct contact with ubiquitin include Phe45, Asn60, Gln 62 and Ser65 at site 1 (A), and Leu71, Leu73, Gly75 and Gly76 at site 2 (B), which are highlighted by depicting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

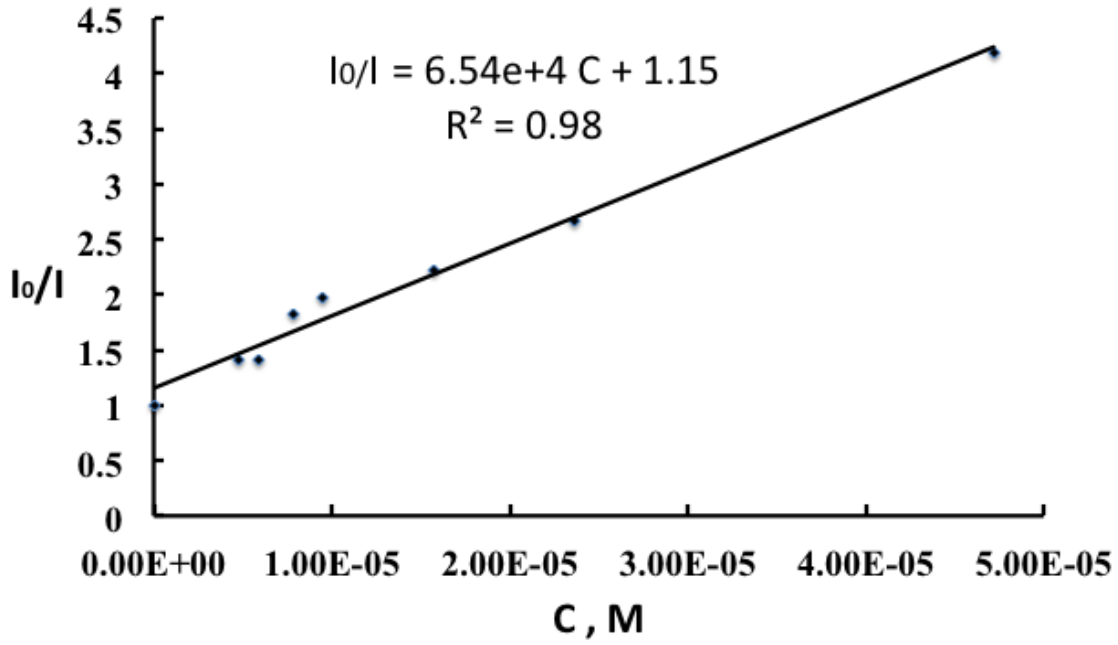


**Figure S2.** Stern-Volmer plot of fluorescence quenching of ubiquitin in the presence of fullerenol $C_{60}(OH)_{20}$.

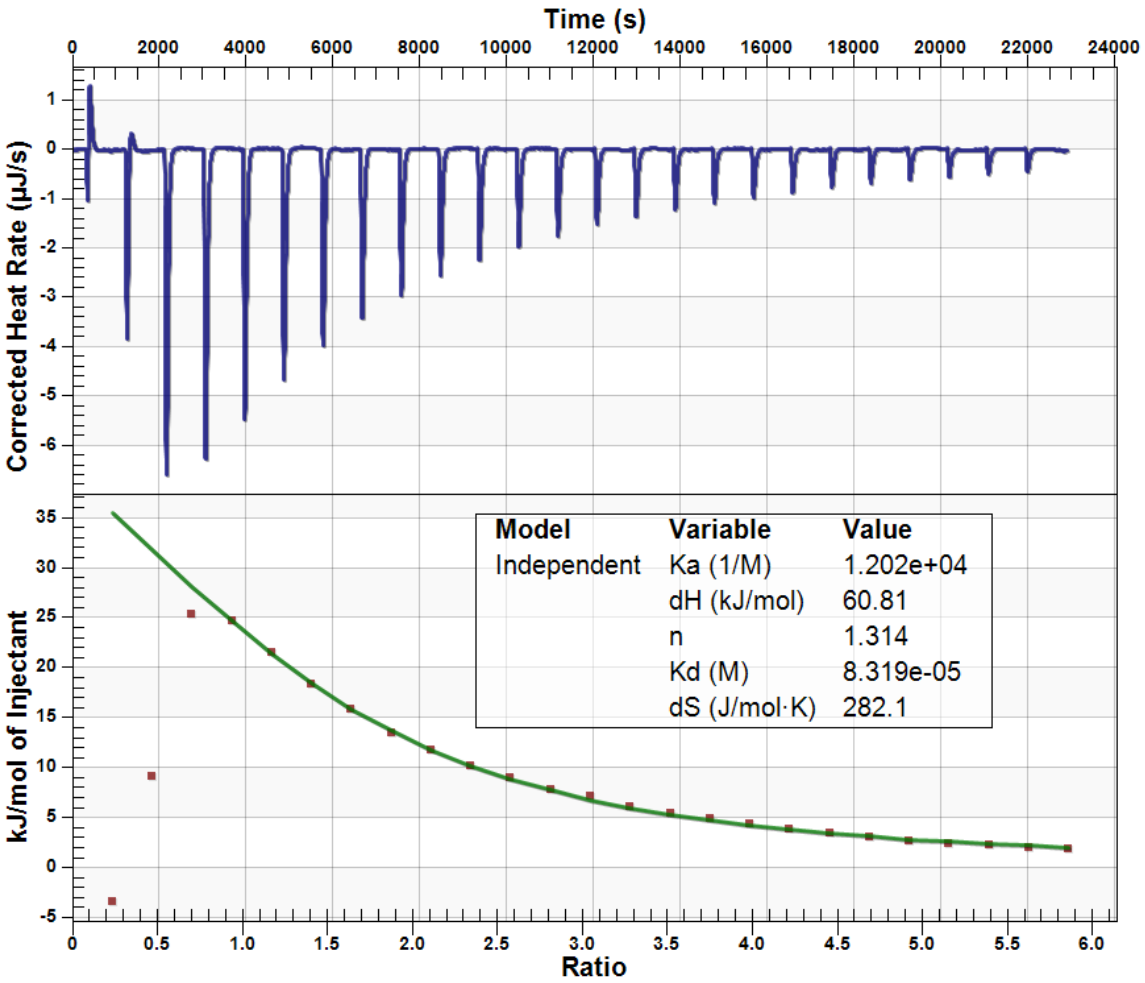


**Figure S3.** Isothermal titration calorimetry of $C_{60}(OH)_{20}$ fullerenol into ubiquitin.

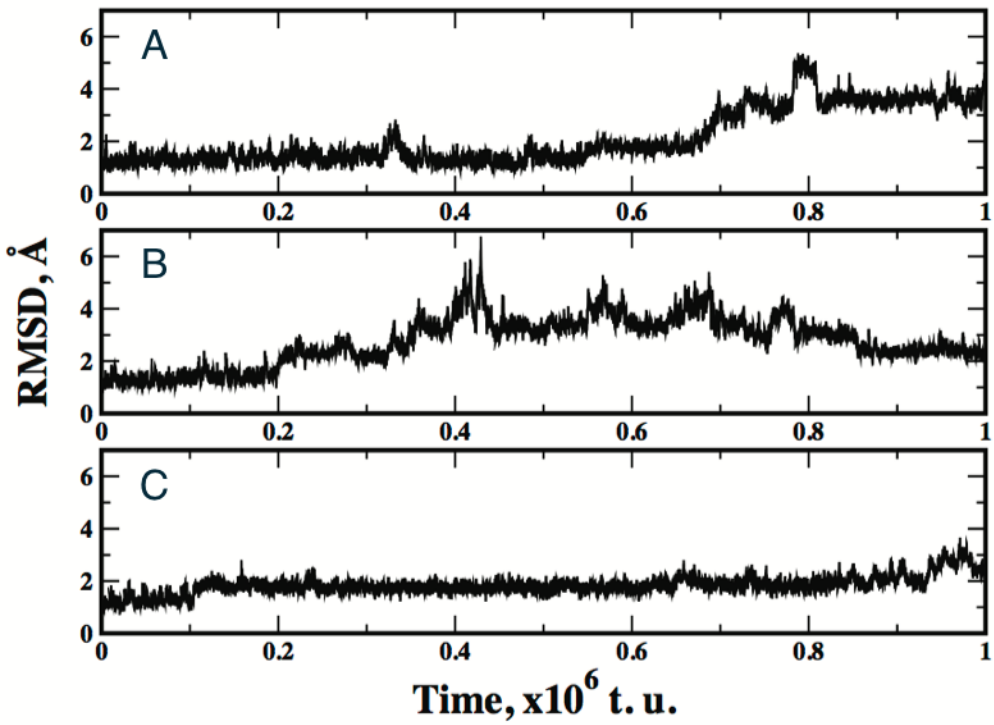


**Figure S4.** Representative RMSD plots of ubiquitin without any nanoparticles from DMD simulations. The three trajectories (A-C) are taken from three independent simulations.

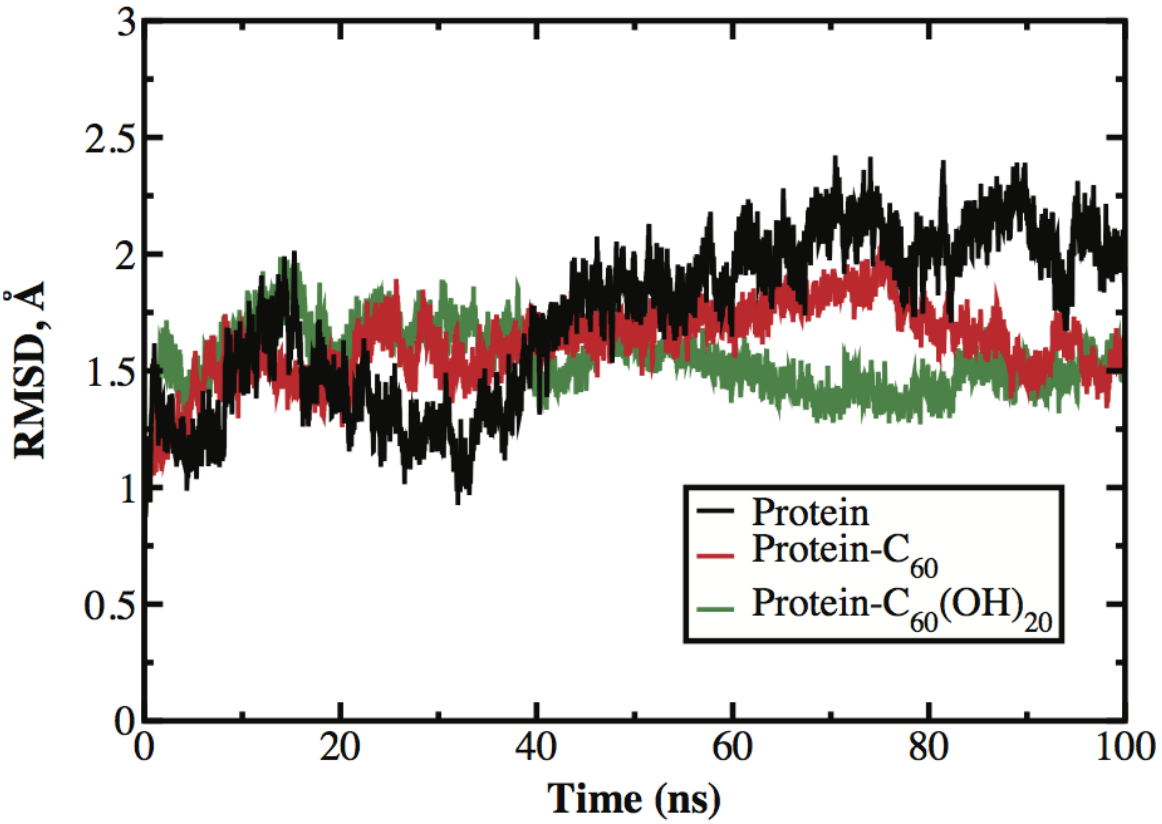


**Figure S5.** Protein heavy atom RMSD fluctuations in MD simulations in the cases of ubiquitin-alone (black), ubiquitin with $C_{60}$ fullerene (red) and ubiquitin with $C_{60}(OH)_{20}$ fullerenol (green).

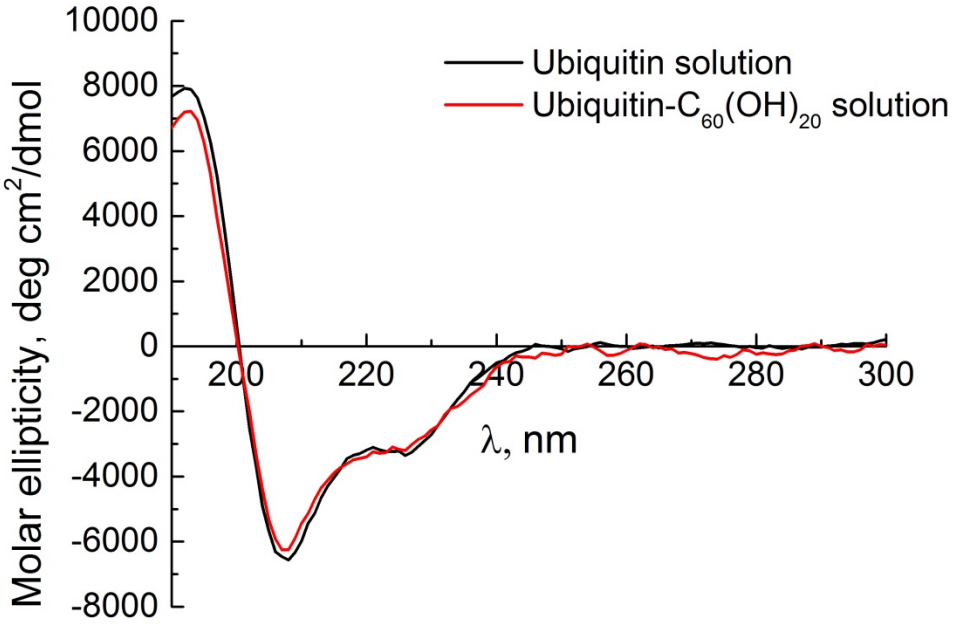


**Figure S6.** Circular dichroism spectra of ubiquitin and ubiquitin-fullerenol solutions.