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Effect of fullerenol surface chemistry on nanoparticle binding-induced protein misfolding[1] SLAVEN RADIC, PRAVEEN NEDUMPULLY-GOVINDAN, Clemson University, RAN CHEN, Kansas State University, EMPPU SALONEN, Department of Applied Physics, Aalto University, JARED BROWN, Department of Pharmaceutical Sciences, Skaggs School of Pharmacy, University of Colorado Anschutz Medical Campus, PU CHUN KE, FENG DING, Clemson University — Fullerene and its derivatives with different surface chemistry have great potential in biomedical applications. In this study we focus on the effect of hydroxylation - a common strategy for solubilizing and functionalizing these carbon-based nanoparticles - on protein-nanoparticle interactions using a model protein, ubiquitin. We used set of complimentary modeling methods, including docking and molecular dynamics simulations. We found that all derivatives bound to the model protein, but the more hydrophilic nanoparticles with higher number of OH groups bind to the protein surface, stabilizing it, while more hydrophobic ones induced large conformational changes, causing protein denaturation.

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