Atomistic insights into the Protein-functionalized nanoparticles

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Abstract: Protein-functionalized nanoparticles can be used in various pharmaceutical approaches but the choice of nanoparticle size, shape, charge, linking chemistry, protein-labeling site, etc. remains challenging due to their effect on protein structure and function. Here molecular dynamics simulation was used as a functional way to predict atomistic insights into the charge of polystyrene nanoparticle and epidermal growth factor stability as a model of the nanoparticle-protein complex. Our result showed that the epidermal growth factor orientation regarding the conjugation is suitable and the RMSD analysis represents the complex stability during MD simulation.

Keywords: Molecular Dynamics, nanoparticle, conjugation, polystyrene, epidermal growth factor

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