

Theoretical Investigation on Prevention of Protein Adsorption by Coated Surface of Cloaking Nanoparticles with Protein Corona Shield

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Nanoparticles are used for drug carriers to minimize the side effects of conventional pharmaceutical agents. However, clinical application is still limited due to the difficulty in controlling the interactions on the interfaces between nanoparticles and biological systems. Here, we present the protein corona shield nanoparticle for preventing the adsorption of substances in the body (i.e., serum albumin). The adsorption of albumin was inhibited by coating fusion protein (GST-HER2-Afb), in which HER2-binding affibody is genetically combined with a glutathione-S-transferase, on silica nanoparticle (NP) surface. Interaction of albumin with silica surface, which were coated with cross-linking polymer, fusion protein, negatively charged fusion protein and glutathione-linked fusion protein were compared via coarse-grained molecular dynamics. The coated structure in which the Afb was exposed on the surface of silica NP was turned out to be the most effective for the NP's cloaking state. We showed that both of electrostatic interactions and the orientation of GST-HER2-Afb on NPs can be important factors of cloaking efficiency.