Study interactions between inhaled nanoparticles and pulmonary surfactant using molecular dynamics simulations

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Abstract

Respiratory system is the most important way for the nanoparticles in the environment getting into the human body. Interaction with the pulmonary surfactant film, being the first line of host defense, represents the initial nano-bio interaction in the lungs. Such interaction determines the fate of the inhaled nanoparticles and their potential therapeutic or toxicological effect. Despite considerable progress in optimizing physicochemical properties of nanoparticles for improved delivery and targeting, the mechanisms by which inhaled nanoparticles interact with the pulmonary surfactant are still largely unknown. As it is hard to experimentally observe the molecular behavior in complex biological environment, we investigated the interaction between inhaled nanoparticles and pulmonary surfactant using molecular dynamics simulation. We developed a coarse-grained model for the pulmonary surfactant that contains different lipids and protein fractions, simulated the translocation of nanoparticles through the pulmonary surfactant film, investigated the mechanisms of toxicity caused by the nanoparticles, and unveiled the structure and molecular conformation of the pulmonary surfactant corona formed on nanoparticles of representative surface properties. Our simulation results shed light on understanding the molecular mechanism of nano-bio interactions in the respiratory system.

Keywords: Pulmonary surfactant; Nanoparticle; Biomolecular corona; Nanotoxicology; Molecular dynamics simulation