Developing Coarse Grained Models for Skin Lipids

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The top layer of the skin, known as the stratum corneum (SC), acts as a barrier to foreign agents entering the body and to water leaving the body. Diffusion across the SC occurs through a complex lipid matrix that is a mixture of ceramides, cholesterol, and free fatty acids, embedded between dead skin cells (corneocytes). Although the lipid matrix is known to have a periodic repeat structure the exact molecular-level arrangement of the SC lipids is unknown and cannot be determined from experimental studies. In order to probe the molecular level arrangement, we are developing coarse-grained models of the SC lipids that will allow us to simulate complex mixed lipid systems and study their structural characteristics on timescales accessible to molecular dynamics simulations. Coarse-grained models allow molecular simulations to be performed on larger spatial and temporal scales than is possible through atomistic simulation and are necessary to study the self-assembly of mixed lipid systems. We have developed a coarse-grained force field for the key SC lipids and water using the method formulated by Reith, Pütz, and Müller-Plathe (RPM) [1,2]. The RPM method allows for the CG models developed to match the structural behavior seen in the atomistic simulations through optimization of the CG potential against radial distribution function data for the atomistic system. The development and validation of the CG models developed will be presented.