

# Understanding the Self-Assembly and Phase Behavior of Skin Lipids

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The outermost layer of the skin (the stratum corneum) consists of skin cells embedded in a rich lipid matrix, whose primary role is to provide a barrier to foreign agents entering the body and to water leaving the body. This lipid system is unique in biological membranes in that it is composed of ceramides, cholesterol, and free fatty acids, with phospholipids, which are the major components of most biological membranes, being completely absent. This unique composition enables the lipids of the stratum corneum form highly organized lamella, which in turn are believed to control barrier function. While much is known about the nature of the skin lipids from extensive experimental studies, a clear understanding of how and why these molecules assemble into the structures observed through microscopy and biophysical measurements does not yet exist. In order to probe lipid phase behavior and molecular level arrangement, we are performing molecular simulations with both atomistic and coarse-grained models of key stratum corneum lipids and water. The development and validation of the coarse-grained models will be presented alongside the results of simulation studies for simple mixed lipid systems that provide insight into the lamellar organization and enable us to validate the models developed while working towards the study of more complex stratum corneum systems.