Atomistic simulations of skin lipids: effect of product ingredients

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Abstract

The stratum corneum (SC), the outermost layer of the skin is the only 10-20 micron thick but provides the main barrier against water loss and penetration of external substances and pathogens. According to the 'brick and mortar' model, the SC consists of flattened protein-rich corneocytes surrounded by extracellular lipid matrix. The three main components of the SC lipid phase are ceramides, cholesterol, and free fatty acids, with the ceramides being the most responsible for the skin lipid bilayer rigidity and the barrier properties. Specific ingredients are often used in personal care industry. We investigate their structural and mechanical effects on the extracellular lipid matrix.

Atomistic models are used to probe the role of specific lipid species in maintaining the structural stability of the SC extracellular lipid matrix and to investigate the role of specific interactions, e.g. hydrogen bonding networks, in the overall SC lipid cohesion.