How wettable is the skin surface?

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Abstract

Water is a vital need for human beings and loss of water must be carefully controlled[1]. This regulation function is mainly performed by our skin, where water is distributed inhomogeneously, with a strong concentration gradient across the epidermis (from 80% to 15% grams of water per total grams of wet tissue[2]), resulting in a very low water content near the surface.
The skin surface is coated with a mixture of sebaceous lipids (the sebum oil) and epidermis lipids that can detach from the outermost layer of the skin, the stratum corneum. The properties of these lipid molecules are fundamental to maintaining the low permeability of the skin and to preventing water loss and penetration. Specifically, the sebum oil has been shown to play a key role in regulating the hydration of the skin and its waterproofing properties. The sebum also provides antimicrobial properties and assists in the transport of antioxidants[3]. A microscopic understanding of the properties of the skin surface is essential to explain the performance of the skin as an external barrier for molecule penetration, as well as to design strategies for transdermal drug delivery.

Molecular dynamics is an increasingly powerful tool for studying the structure and functionality of biomembranes and has already been successfully applied to investigate the properties of complex structures like skin lipid mixtures[4,5].
Here we present a molecular dynamics simulations study of a representative sebum triglyceride (TG). TG interacts with water in a complex manner, adopting a characteristic "trident" configuration at the water-TG interface, with the glycerol groups facing the water phase. The interaction between water molecules and TG oxygen atoms enables water to penetrate through the sebum, which may contribute to its role in water regulation.
We further quantify the structural and mechanical properties of a stratum corneum bilayer in the presence of TG, and evaluate the degree of penetration of TG into the membrane structure.
Finally, we quantify the wettability of the skin surface, showing that the stratum corneum bilayer features a low affinity for water. Contact angle computations indicate contact angles > 90°.

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