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An atomistic model of the human stratum corneum lipid matrix transport

Content

The stratum corneum (SC) layer of the human skin is the outermost and primary barrier against chemical topical exposure. The ability of a chemical to pass the SC is a key point for risk assessment and development of cosmetic ingredients. From neutron diffraction data, the SC peaks comprise a short periodicity phase (SPP) with a repeat distance of 6 nm, and a long periodicity phase (LPP) with a repeat distance of 13 nm. The LPP captures long-scale dynamics and can be represented as a sandwich model by Bouwstra.
Here we present a simulation model of the LPP with a mixture of three ceramides (Ceramides 1, 2, and 3), cholesterol, and lignoceric acid and we investigate whether the use of solute-penetration enhancers (known as pro-penetrant) (ex. dipropylene glycol -DPG-) significantly alter the barrier properties of these skin models. In our model, we find that DPG increases the hydrogen-bonding profile and, by consequence, reduces the lipid diffusivity in the lateral direction (DL) by one order of magnitude. Using multi-microsecond constant-velocity steered molecular dynamics of several solutes (hydrophilic and hydrophobic, ...) we expect to be able to construct a chemical profile model of the human stratum corneum of broad applicability in Cosmetics.

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