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Rationalizing the molecular role of natural moisturizing factors in the skin hydration through molecular dynamic simulations

Xerosis or dry skin is a common condition experienced by many. Besides being particularly present during the cold season, various diseases can also lead to localized xerosis. To prevent it, the skin is provided with its own natural moisturizing factors (NMF). NMF are small amino acids or derivatives found in the outermost layer of the skin, the *stratum corneum* (SC). They are often claimed to be highly efficient humectants, increasing the water content to maintain the fluidity of the skin. However, alternative mechanisms have also been proposed, suggesting that NMFs themselves may act as lipid mobility amplifier [1].
This work aims at investigating the effect of four NMF, namely urea (URE), glycerol (GLY), urocanic acid (UCA), and urocanate (UCO) inside an *in silico* SC model[2], considering two different levels of humidity. By using molecular dynamic simulations, we observed an increase in the diffusion of lipid components in the presence of water or NMF. This was accompanied by membrane perturbation, as seen by an increase in conformational changes as well as a decrease in lipid chain ordering. URE, GLY exhibited a similar impact, while UCA exhibited a higher impact on the liquid-like layer of SC. By studying NMF-water intermolecular interactions, we highlighted the role of NMF as a regulator of membrane perturbations, while insuring membrane fluidity. This role may prevent destabilization of the skin membrane in the presence of too high water content.

Session

Computational methods

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