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Implications of Surfactant Hydrophobic Chain Architecture on the Surfactant-Skin Lipid Model Interaction: a Neutron Diffraction Study

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Although surfactants have been widely used in skin care and other related applications, our knowledge about how surfactants interact with stratum corneum (SC) lipids remains limited. Our group has systematically studied how surfactants interact with a lipid SC model by neutron diffraction and molecular dynamics (MD) simulations, focusing on examining the impact of surfactant molecular architecture and surfactant types. The surfactant-SC mixed membrane was constructed by an equimolar mixture of ceramide/cholesterol/fatty acids and surfactant at 1% molar ratio of total lipids. The arrangements of water and surfactant molecules in the membrane were obtained through neutron scattering length density (NSLD) profiles via contrast variation method, mean-while, MD simulation clearly demonstrated the mechanism of hydration change in the surfactant-model SC mixed membrane. Surfactants significantly enhanced the membrane hydration and reduced the amount of phase-separated crystalline cholesterol, showing a strong dependence on surfactant chain length, branching, and double bond. The result clearly demonstrates how surfactant architecture affects its interaction with the SC membrane, providing useful guidance for either choosing an existing surfactant or designing a new one for surfactant-based transdermal application. We have recently extended this system by studying the configuration of zwitterionic, cationic and non-ionic surfactants in model SC membranes by neutron diffraction. The hydration and molecular arrangement change significantly with the type of surfactant.

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