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Simulations of Structural Transformations in Ceramide Phases from fitting structures to CEMOVIS image data

The stratum corneum is the outermost layer of human skin and primary barrier towards the environment. The main component is stacked layers of saturated long-chain ceramides, free fatty acids and cholesterol, but we do not yet know the molecular structure or formation details. Here, I will present our work on new methods to fit models to low-resolution cryo-EM microscopy vitreous section (CEMOVIS) data, in particular by generating molecular models and using cryo-EM simulation to generate electron diffraction micrographs that can be compared directly to experimental data, and iteratively use these to improve the models. This has enabled us to create a number of alternative models, compare how they fit existing experimental data, and also use coarse-grained simulations to understand the formation process where cubic phases turn into bilayers depending on the lipid composition. These types of models can be highly useful tools for understanding the barrier properties, and we are currently combining it with free energy calculations to explore rapid prediction of permeation properties from CEMOVIS-derived models, which could have important applications in developing new generations of skin-permeating drugs.

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