Coarse-Grained Simulations of the Self-Assembly of Skin-Relevant Lipid Structures

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Overview

Stratum corneum:
- Outermost layer of skin; controls barrier properties
- Composed of flattened dead skin cells held together with lipid lamellar structures
- Known lipid composition including ceramides, cholesterol, and free fatty acids
- Molecular structural details are unknown

Coarse-Grained Models

CG models treat groups of atoms as single interaction sites, known as CG beads. Groups of atoms are "mapped" to CG beads. The mappings used in these simulations are as follows:

Water: 4:1; each blue bead of water represents 4 water molecules

Ceramides (CER NS): equal-chain (C16) and unequal-chain (C24)

Cholesterol (CHOL):
- 3:1 tails; each tail bead represents 3 carbon atoms
- 4-bead headgroup, including individual OH group beads

Mixed Lipid Simulations

1:1 C24:C16 Mixture

Attempts to simulate self-assembly of a C24:C16 stacked system were unsuccessful. The ceramides formed cylindrical structures instead of the expected flat layers after heating.

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References


Molecular modeling:
- Precise control over lipid concentration, easily visualized
- Atomic models: useful, but slow kinetics can yield results influenced by the initial configuration - fixed with self-assembly
- Self-assembly: formation of physically-relevant lamellar structures for use in future simulations and structure analysis
- Inefficently-large computation times preclude modeling of self-assembly using atomic models

Self-Assembly Process

Self-assembly is useful in that the resulting lamellar structures are representative of those found in the body, making them more useful in analysis than arbitrarily chosen structures. The self-assembly simulations shown here follow the following process:

a) Begin with an already-formed lamellar structure
b) Increase simulation temperature to destroy structural order
c) Return to skin temperature and allow lamellae to reform
d) Promote faster lamellae formation by compressing and expanding the system

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References