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Decoding Skin Stratum Corneum Bio-interface through Computational Modeling

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Abstract

Effective transdermal delivery of active ingredients remains a significant challenge due to the formidable barrier properties of the stratum corneum (SC). Understanding molecular-level transport mechanisms across the SC lipid bilayer is essential for rational design of skin-penetrating formulations. Here, we present computational insights from two molecular dynamics (MD) simulation studies focusing on strategies to enhance skin permeation. In the first study, we investigated the effect of palmitoylation on short polar peptides. The simulations revealed that conjugation with a palmitoyl chain markedly increased the peptides' affinity toward the hydrophobic SC lipid bilayer and facilitated their penetration efficiency through the SC. This highlights lipidation as a viable approach to overcome the limited permeability of polar bioactive peptides. In the second study, we explored the interactions between niacinamide, a widely used skin-brightening agent, and other co-applied actives. MD simulations demonstrated that certain agents could alter bilayer structure and fluidity, thereby lowering the energetic barrier for niacinamide transport. These results suggest a synergistic strategy, where pairing niacinamide with specific actives enhances its penetration efficiency without chemical modification. Together, these studies underscore the power of MD simulations in elucidating transport mechanisms of skin actives and guiding formulation design. Our findings provide a computational foundation for developing more effective transdermal and cosmetic delivery systems.

Keywords:

Stratum corneum Skin permeation Transdermal delivery Lipid bilayer Molecular simulation