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Molecular Dynamics as a tool for in silico screening of skin permeability

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Abstract

Prediction of skin permeability can have manifold applications ranging from drug delivery to toxicity prediction. Along with the semi-empirical or mechanistic models proposed in the last decades, molecular dynamics simulations have recently become a fruitful tool for investigating membrane permeability, in particular as they allow the involved mechanisms to be modelled at a molecular level. Despite their significant structural complexity, molecular dynamics simulations can also be utilized to study permeation through the lipid matrix that characterizes the stratum corneum. In this work, Steered Molecular Dynamics simulations are performed on a suitably developed stratum corneum lipid matrix model. Regardless of their actual tortuous path within