Probing Electroporation in Lipid Bilayers: Insights from Molecular Dynamics Simulations

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Abstract

Electroporation is a critical phenomenon in cellular processes, where applied electric fields induce transient pores in lipid bilayers, facilitating molecular transport. This study aims to elucidate the underlying mechanisms of electroporation at the molecular level, using advanced molecular dynamics simulations to model the effects of specific electric field strengths ranging from 10 to 100 MV/m on various lipid bilayer compositions. By systematically varying the electric field intensity and lipid types, we investigated the dynamics of lipid rearrangements, pore formation, and stabilization. Our simulations revealed that fields exceeding 50 MV/m significantly enhanced pore formation, with distinct differences observed based on lipid saturation and headgroup structure. Furthermore, we characterized the critical transition points for pore emergence, highlighting the role of lipid packing and hydrophobic mismatches in modulating electroporation susceptibility. These findings provide a comprehensive understanding of how electric fields interact with lipid membranes, offering insights that could enhance applications in drug delivery and gene therapy. The results underscore the importance of optimizing electric field parameters for efficient electroporation, paving the way for future experimental validations and practical applications in biotechnology and membrane biophysics.

Keywords: Electroporation, Molecular Dynamics, Lipid Bilayers, Electric fields, Pore Formation, Membrane Permeability