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Molecular dynamics simulations of membrane proteins

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Abstract

Introduction: Membrane proteins including transporters, channels and receptors, play a critical role in biological systems by controlling the traffic across cell membranes and mediating signal transduction. Determining the structure and function mechanism of these proteins has always been a challenge. Molecular dynamics simulation techniques with recent significant improvements can capture the behavior of biological molecules in atomic detail, shedding light on the biomolecular mechanisms which are difficult to observe experimentally.

Discussion: Molecular dynamics simulation provides researchers with an atomic level microscope to investigate complex function and structure of membrane proteins and phenomena's such as ion penetration in channel proteins, large conformational changes of transporters and also effects of specific mutations in receptor on ligand binding affinity. Despite the increasing application of this tool on this subject, there are some concerning potential issues in these techniques including inadequate sampling timescales and applied approximations which can lead to results that are inconsistent with experimental data.

Conclusion: Although there are still challenges in application, molecular dynamics tools have provided undeniable help in understanding behaviour and structure of membrane proteins and by continues improvement of hardware, software and algorithms, they can play a more substantial role in the future.

Keywords: Molecular dynamics, modeling, protein, membrane

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