VII CONGRESO NACIONAL DE NANOTECNOLOGÍA
12 AL 15 DE NOVIEMBRE 2023
PUCÓN, CHILE

Exploring the influence of traction speeds on nanoparticle penetration through molecular simulation

Luis Espinoza Arcos
Centro de Bioinformática y Simulación Molecular (CBSM), Universidad de Talca, Talca, Chile
Horacio Poblete Vilches
Centro de Bioinformática y Simulación Molecular (CBSM), Universidad de Talca, Talca, Chile
Cristian Vilos-Ortiz
Facultad de Medicina, Universidad de Talca, Talca, Chile.

Understanding the atomic-level mechanisms of nanoparticle (NP) penetration into cells is crucial for optimizing their biomedical applications and assessing potential biological effects. Today, it exist the need to investigate NP-cell interactions at the atomic level, highlighting the importance of advanced characterization techniques such as molecular simulations. Obtaining insights into NP internalization and intracellular fate will facilitate the design of safe and effective nanomaterials for targeted drug delivery and diagnostics.

In this study, our focus is on investigating the mechanical properties of biomimetic nanoparticles (NPs) and their interaction with cell membranes, with a specifically on cellular uptake. The intricate interactions between nanoparticles and lipid membranes play a crucial role in several biological processes and hold significant potential for future applications in nanomedicine. To investigate these interactions, we will employ coarse-grained models and molecular dynamics simulations utilizing the Martini 2 force field. Two membrane bilayer models will be constructed using 2-oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine (POPC) and cholesterol (CHOL). The nanoparticles under investigation consist of gold molecules, collectively forming a nano-biointerface [1]. Our objective is to assess the impact of different traction speeds on nanoparticle penetration through coarse-grained molecular simulations. Nanoparticles will be placed near a lipid membrane bilayer, and their movement along the Z axis will be simulated using varying traction speeds. We will evaluate the membrane deformation and pore closure during the penetration process to understand how different speeds affect these factors. The most promising simulation result from lipid membrane extraction will be selected, and umbrella sampling with GROMACS 2018.2 will be employed to calculate the free energy profile in different membrane models [2]. This analysis will provide insights into nanoparticle-membrane interactions under various conditions, contributing to our understanding of lipid membrane properties and their interactions with nanoparticles at different speeds.

Acknowledgments

Thanks to the Nano-biomaterials Laboratory, ND3 Lab. This work was supported by Fondecyt Regular Nº 1211143 and 1201147.

References

[1] Salassi S. et al. (2021), doi.org/10.1021/acs.jctc.1c00627
[2] Hoffman C. et al. (2020), doi.org/10.1038/s41597-020-0391-0