Lipid monolayers as membrane models for cancer and infection: a synergic *in-vitro/in-silico* study

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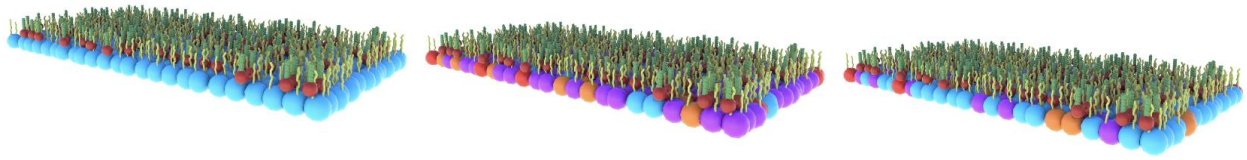
Abstract

Lipid membranes are highly complex and dynamic systems formed by hundreds of different types of lipids combined in specific ratios. Many pathological cells exhibit significant alterations in the lipid composition of their membranes when compared to healthy cells. For example, lipid profile singularities have been found in cancer, bacterial and viral infections and even in senescent cells [1].

All the properties of a cell membrane (the internal structure, the dynamic correlation between different lipids, and the thermodynamic stability of the whole system) are endowed by its molecular composition. Mechanical perturbations could irreversibly destroy the cell or could be transitory if the membrane spontaneously repairs itself. Thus, the vulnerability of pathological membranes to certain perturbations could be exploited as a therapeutic strategy. However, the connection between membrane composition and the associated properties is poorly understood.

Lipid monolayers have been extensively used as minimalistic models for cell membranes, being lipidic composition essential for the determination of their structure and mechanical properties. Particularly, the determination of adsorption isotherms for Langmuir monolayers can be easily performed by both computational and experimental methods [2, 3]. Molecular Dynamics (MD) simulations at atomic scale can provide high resolution results not available through wet-lab experiments [4], realizing the synergistic potential of a combined *in-silico*/*in-vitro* approach in the characterization of the mechanical membrane destabilization process.

In this work, the results obtained from MD simulations and Langmuir trough experiments will be presented, aiming to understand the response of different models of bacteria and cancer cells to mechanical efforts.



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