On the Determination of Lipid Monolayer Langmuir Isotherms via Molecular Dynamics. Too big of a stretch?

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Lipid cellular membranes constitute a common factor to all known Life on Planet Earth. It is this commonness, and yet their distinctions based on cell type, organism, or age[1] what makes them attractive targets for a wide range of treatments. Therefore, it is of paramount importance to understand how these ubiquitous structures react to different stimuli. Specifically, their mechanical properties are of great interest in the pharmaceutical field, as the permeation of drugs is dependent on them.

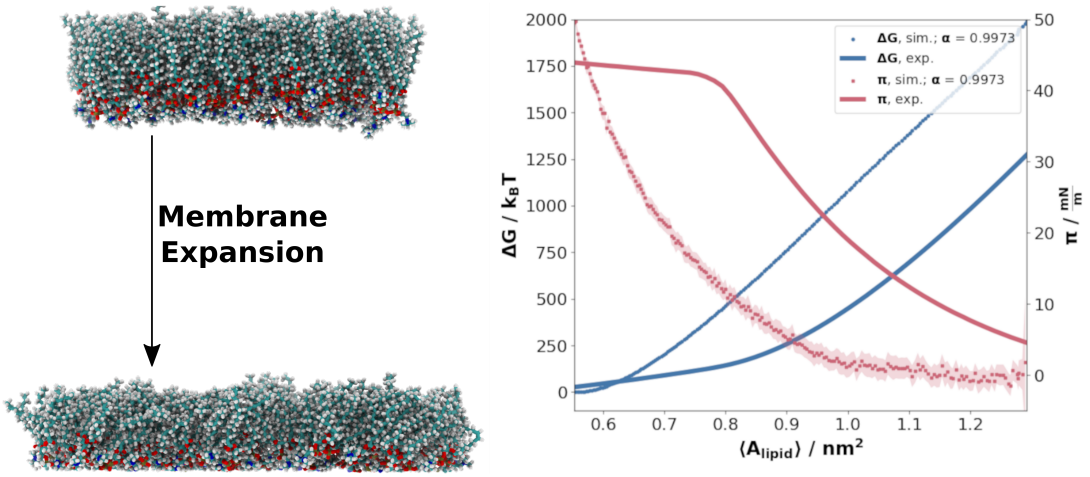

Figure 1: Selected snapshots of simulations (left) plus results from our simulation method and Langmuir Trough experiment (right)

Traditionally, the in-plane expansion of lipid membranes has been studied with wet lab techniques, being the determination of Langmuir Isotherms for monolayers as membrane models a gold standard at that[2]. On the other hand, Molecular Dynamics has proven to be an invaluable tool at giving insight on the molecular mechanisms that govern the mechanics of lipid membranes[3]. In this work we attempt to design new simulation protocols to mimic Langmuir trough experiments using Umbrella Sampling MD. Our results point to agreements, but also to differences, to typical results obtained in a lab; and help to shed light on the nanoscopic-scale processes that are involved in membrane mechanics, while paving the way towards new approaches for their study with *in-silico* techniques.

References

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