Curvature-sensing of cardiolipin in a buckled membrane

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***Short Abstract* — We perform coarse-grained simulations of a lipid bilayer consisting of POPG, POPE and CL, with proportions corresponding to *E. Coli*. This membrane is buckled with different compression factors and the CL concentration is also varied. We then obtain quantitative measures of CL localisation as a function of the curvature of the membrane, and we also quantify the clustering of the CL. We then relate our simulation results to theoretical results of elasticity theory.**

***Keywords* — Membrane curvature, lipid localisation.**

I. Extended abstract

THE spatial organisation of lipids and proteins within the cell membrane is a fundamental question of cell biology which has received a substantial amount of attention recently. This localisation is often critical to function of cell processes or to maintain the membrane's shape. The effects of cardiolipin localisation has important consequences, for example, in the membrane insertion of antimicrobial peptides [1] or amphipathic helices in general [2]. Recently, it has been experimentally [3] show that cardiolipin localises to negative curvature regions in *E. Coli* membranes. Ref, [4] presents an elegant theory of how cardiolipin above certain critical concentration forms microdomains that localise in the cell poles, through cell-wall mediated interactions. These same results were obtained through numerical simulations in [5].

Here, we present the results of coarse-grained molecular dynamics simulations of a buckled lipid bilayer with the lipid constitution of an *E. Coli* cell membrane. We obtain quantitative results of cardiolipin localisation and clustering as a function of the membrane's curvature. We also develop an elasticity theory based on Helfrich's model [6], relating the intrinsic and spontaneous curvature of cardiolipin and the membrane to the membrane's free energy and entropy. We then compare our theoretical results to those of numerical simulations. Finally, we relate the effects of the cardiolipin localisation to the curvature sensing ability of some proteins containing amphipathic helices.

References

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