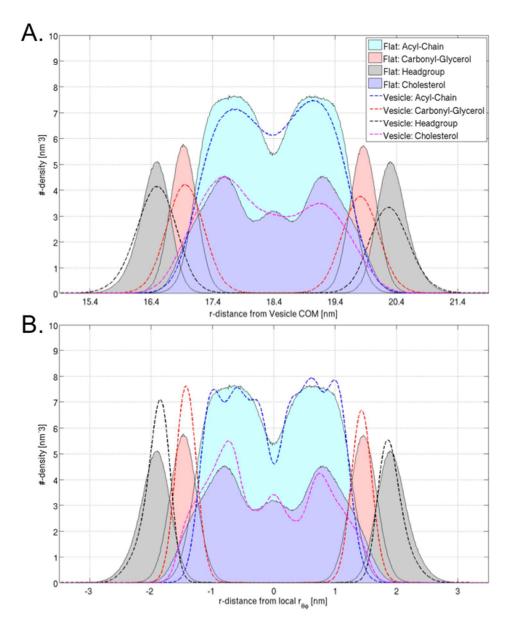
## Determining structural and mechanical properties from

## molecular dynamics simulations of lipid vesicles.

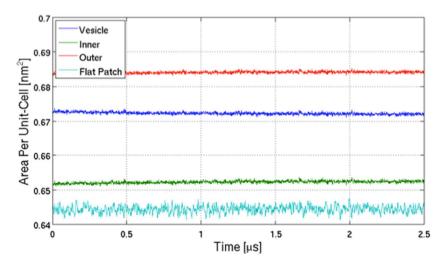
Anthony R. Braun and Jonathan N. Sachs\*

Department of Biomedical Engineering, University of Minnesota, Minneapolis, MN 55455.

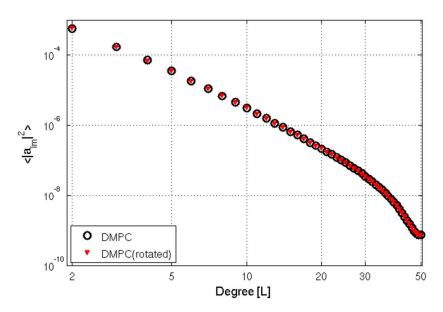


## **Supporting Info**

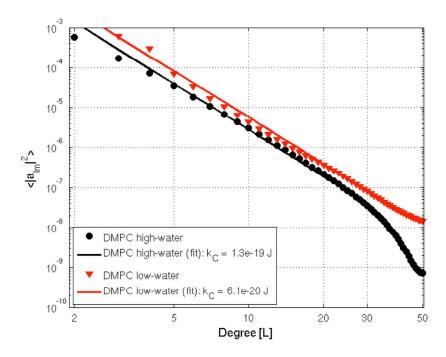
Supplemental Figure 1. A. Comparison of vesicle  $\rho_{rbin}(r)$  and flat-patch undulation corrected number density,  $\rho_{uc}(z)$ , for the DMPC+Cholesterol (30 mol%) system. B. Undulation corrected vesicle,  $\rho_{uc}(r)$  and  $\rho_{uc}(z)$  for DMPC+Cholesterol (30 mol%). Vesicle profiles presented as dashed-lines, flat-patch profiles as filled-distributions.



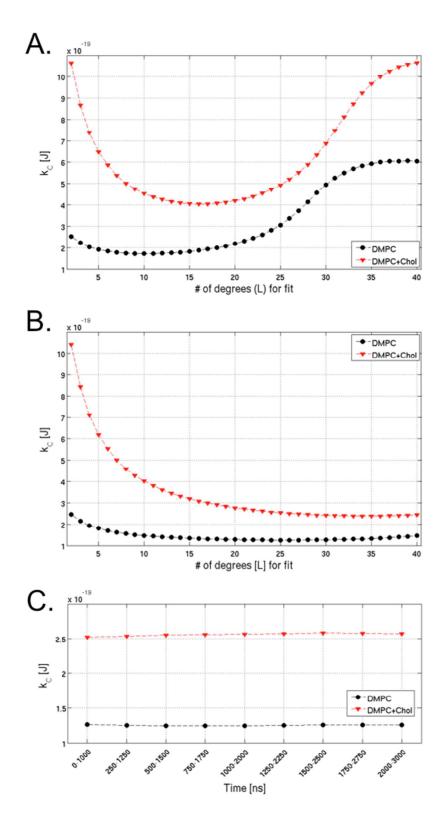
Supplemental Figure 2. Area per lipid trajectory for DMPC+Cholesterol systems. Total vesicle (*blue*), inner monolayer (*green*), outer monolayer (*red*) and flat-patch system (*cyan*).



Supplemental Figure 3. Comparison of SPH fluctuation spectrum of DMPC vesicle and DMPC vesicle rotated 90°. Rotation does not alter the SPHA  $k_c = 1.2536 \times 10^{-19}$  J for the original vesicle (*black*) versus  $k_c = 1.2506 \times 10^{-19}$  J for the rotated vesicle (*red*).



Supplemental Figure 4. Power spectra for both high-water (black) and low-water (red) DMPC vesicle systems.



Supplemental Figure 5. Sensitivity of  $k_c$  to the number of degrees (L) used for the fit for DMPC (*black*) and DMPC+Cholesterol (*red*) systems with a 1.5nm<sup>-1</sup> (A) and 2.5nm<sup>-1</sup> (B) filter cutoffs. C) Time course of  $k_c$  over the simulation time for DMPC (*black*) and DMPC+Cholesterol (*red*) systems.