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Supplemental Information

Influence of Cholesterol on the Oxygen Permeability of Membranes: Insight from Atomistic Simulations

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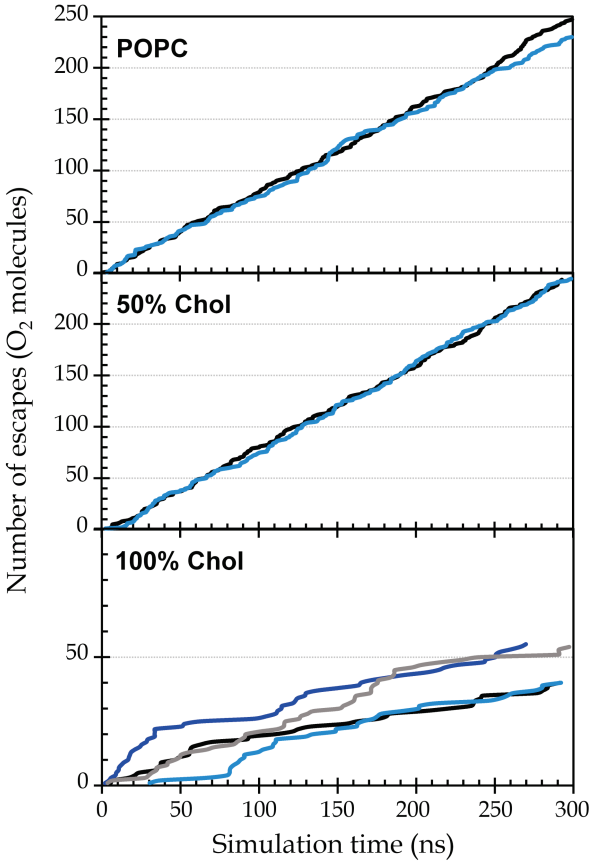

FIGURE S1 Plots of O_2 molecule escapes over time for the pure POPC, 50% cholesterol, and 100% cholesterol simulation systems. For this analysis, O_2 coordinates were sampled every 10 ps. Each line represents an independent trajectory. The linearity of the plots demonstrates convergence within individual trajectories, and the overlap of the lines demonstrates convergence across independent simulations. 100% cholesterol is somewhat less well-converged than the others but is still approximately linear. Note the difference in the *y*-axis scale for 100% cholesterol.

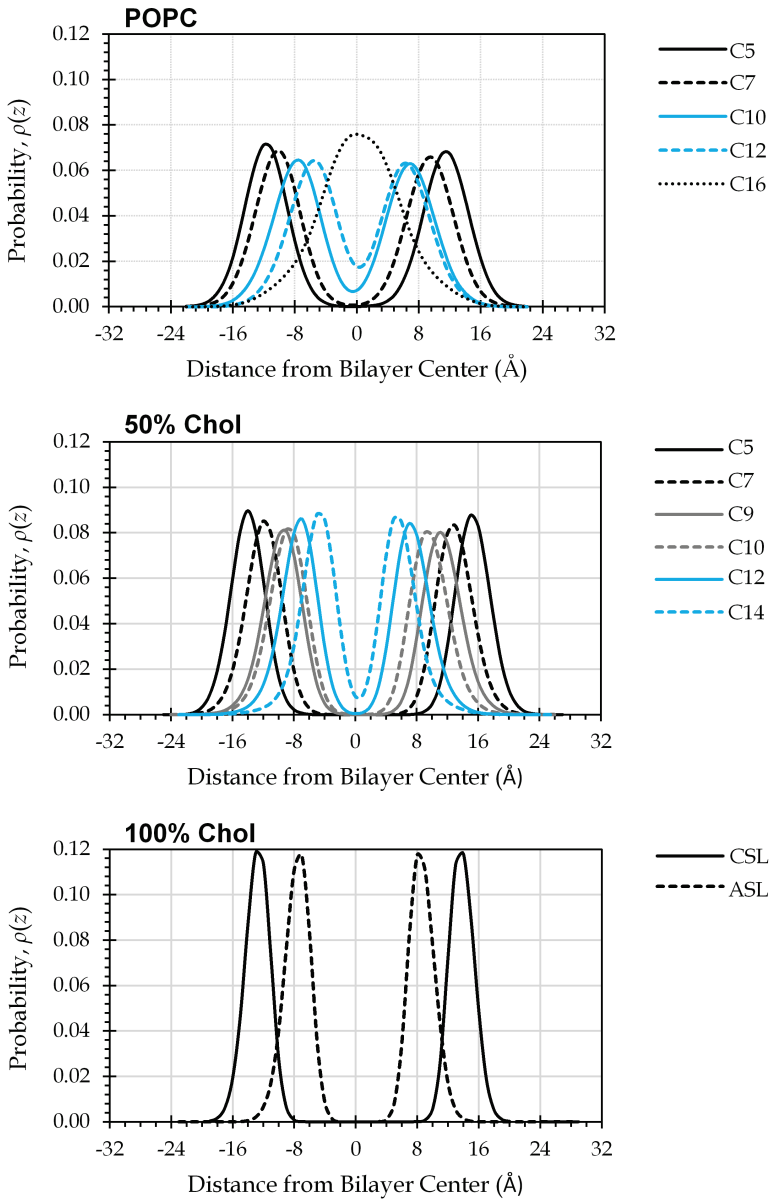

FIGURE S2. Representative probability distribution curves for "probe" atoms. Used to generate the discrete oxygen transport parameter data, W_i, plotted in Fig. 3 of the manuscript.

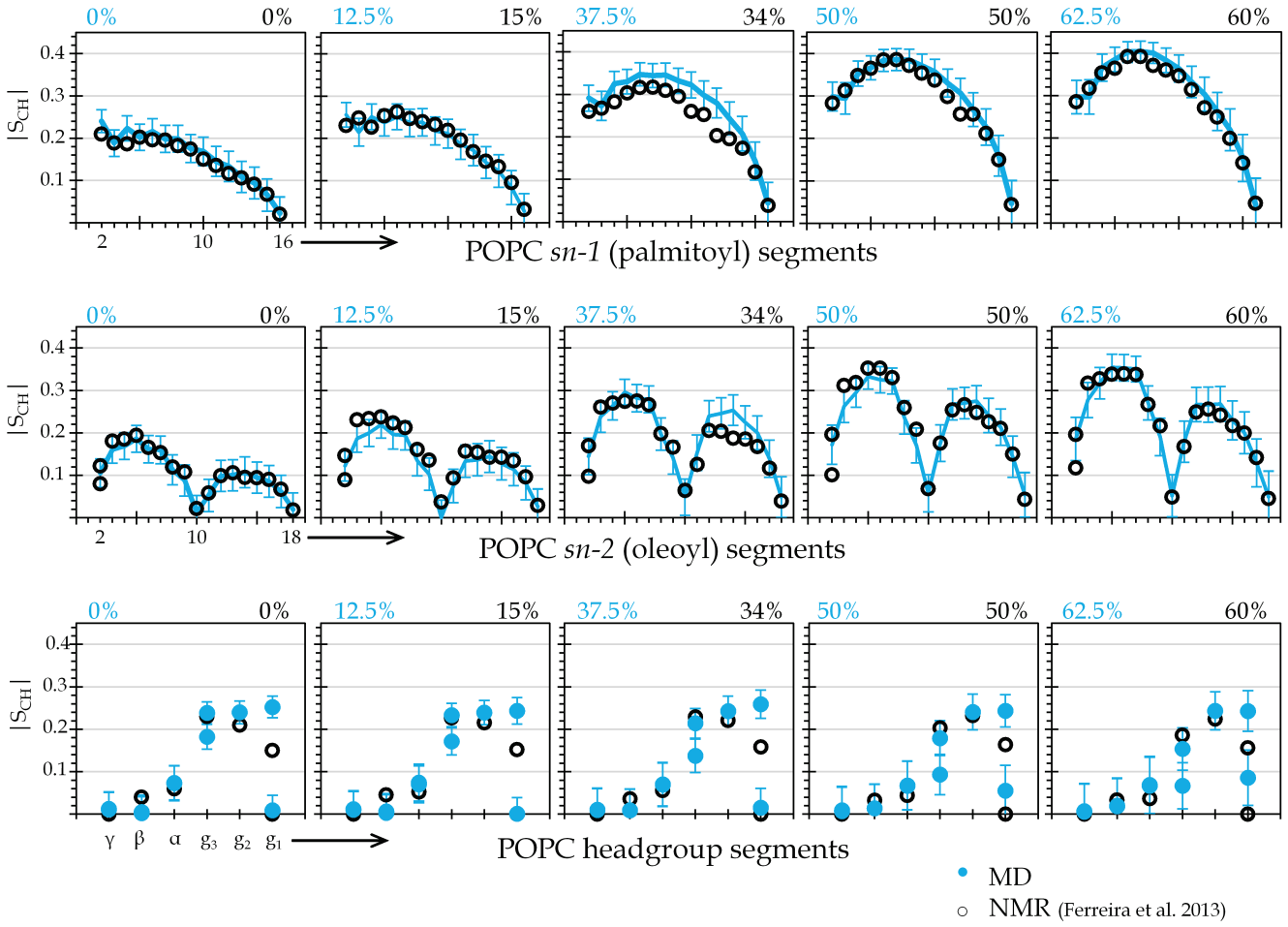

Figure S3 Order parameter magnitude $|S_{CH}|$ for individual carbon atoms in POPC *sn-1* (palmitoyl tail), *sn-2* (oleoyl tail), and headgroup. Data are shown for one 300 ns trajectory (at 310 K) per bilayer composition. Error bars indicate the standard deviation calculated by the AmberTools program CPPTRAJ. The NMR data were reported by Ferreira and colleagues from ^{1}H-^{13}C solid-state NMR experiments at 300 K (1). Percentage values above each plot denote cholesterol content for MD (blue) and NMR (black) bilayers.

SUPPORTING REFERENCES

1. Ferreira, T.M., F. Coreta-Gomes, O.H.S. Ollila, M.J. Moreno, W.L.C. Vaz, and D. Topgaard. 2013. Cholesterol and POPC segmental order parameters in lipid membranes: Solid state ^{1}H-^{13}C NMR and MD simulation studies. Phys. Chem. Chem. Phys. PCCP. 15: 1976–89.