Direct Measurement of the Effect of Cholesterol and 6-Ketocholestanol on the Membrane Dipole Electric Field Using Vibrational Stark Effect Spectroscopy Coupled With Molecular Dynamics Simulations

Rebika Shrestha,[†] Cari M. Anderson,[†] Alfredo E. Cardenas,[‖] Ron Elber,[†, ‖]

and Lauren J. Webb*[,†,‡,§]

[†]*Department of Chemistry,* [‡] *Institute for Cell and Molecular Biology,* [§] *Center for Nano- and Molecular Science and Technology, and* [‖] *Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, Texas 78712, United States*

*To whom correspondence should be addressed: lwebb@cm.utexas.edu; 512-471-9361

Supporting Information

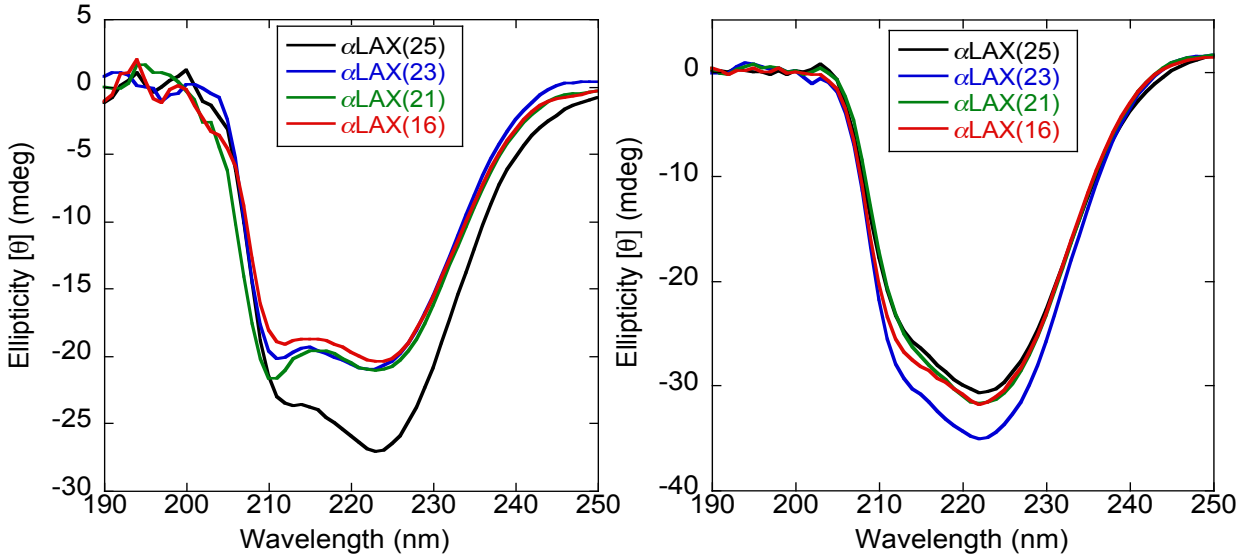

Figure S1. Circular dichroic (CD) spectra of 1 mM peptides: *α*LAX(25) (black), *α*LAX(23) (blue), *α*LAX(21) (green), and *α*LAX(16) (red) inserted in vesicles composed of (a) 30mM DMPC and 20 mol % cholesterol and (b) 30mM DMPC and 20 mol % 6-kc.

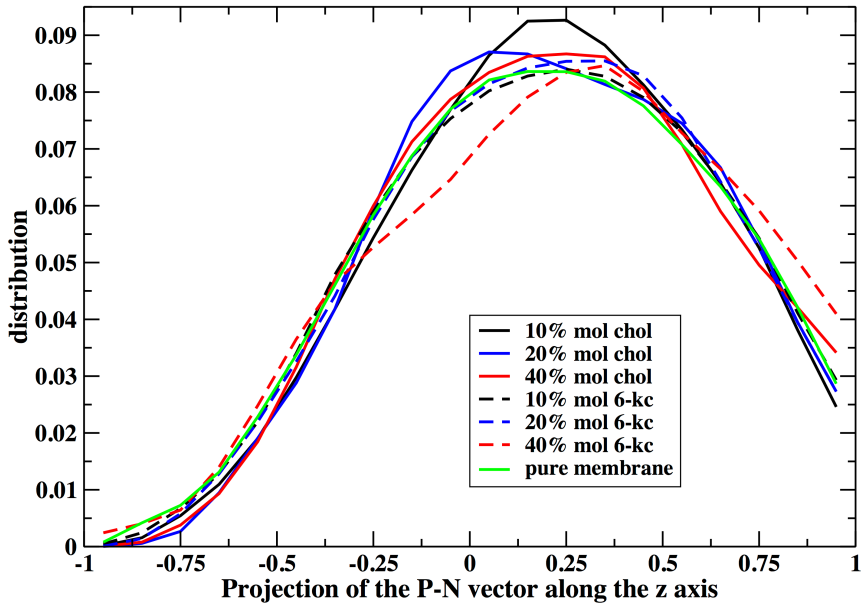

Figure S2. The projection of the vector between the phosphate atom and the nitrogen of the choline group along the normal to the membrane. Note the high similarity of the different distributions (with the exception of 40% mol 6-kc). It is therefore unlikely that the reorientation of the phospholipid alone can explain the variation in electric field that we observe as a function of sterols content.

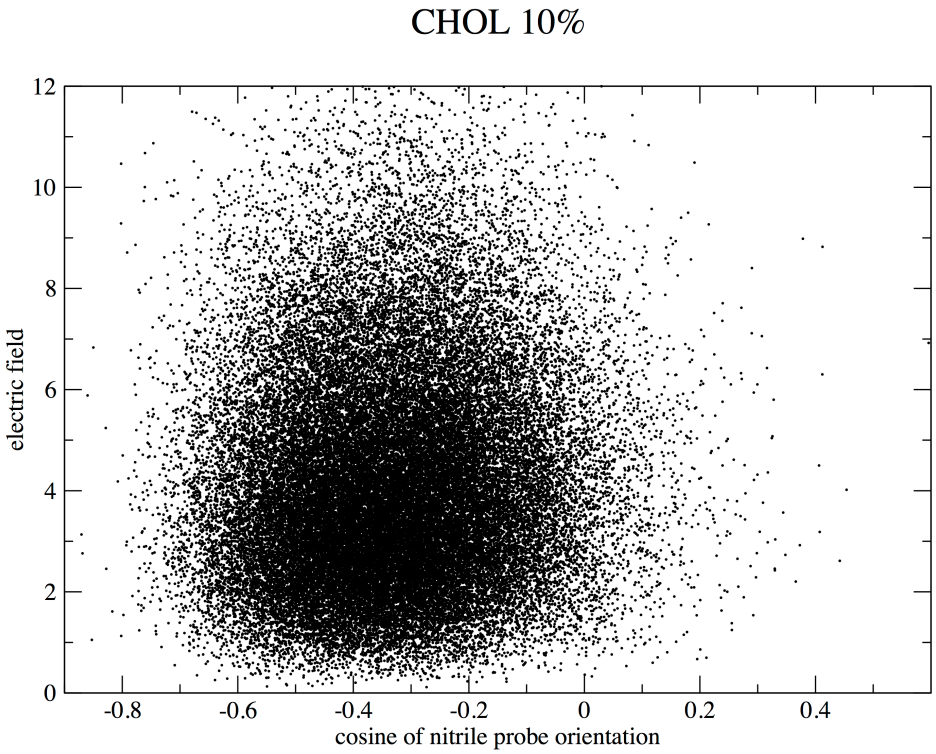

Figure S3. Scatter plot of the orientation of the nitrile bond probe and the membrane electric field. The calculated correlation coefficient is 0.06, supporting our hypothesis that the two are uncorrelated.