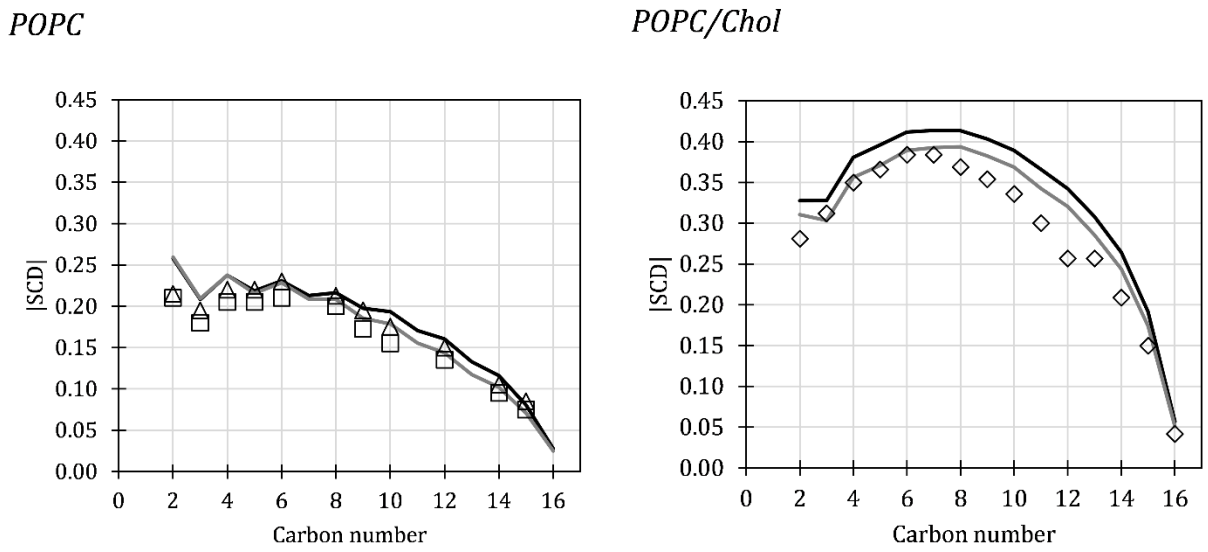
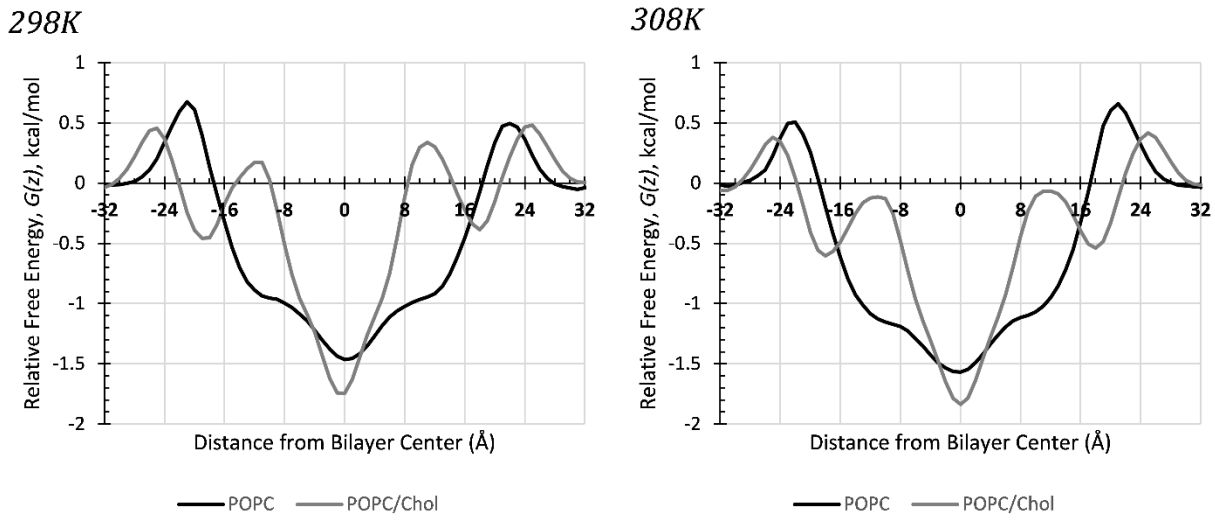
Supplemental Information

Atomistic simulations modify interpretation of spin-label oximetry data. Part 1: intensified water–lipid interfacial resistances

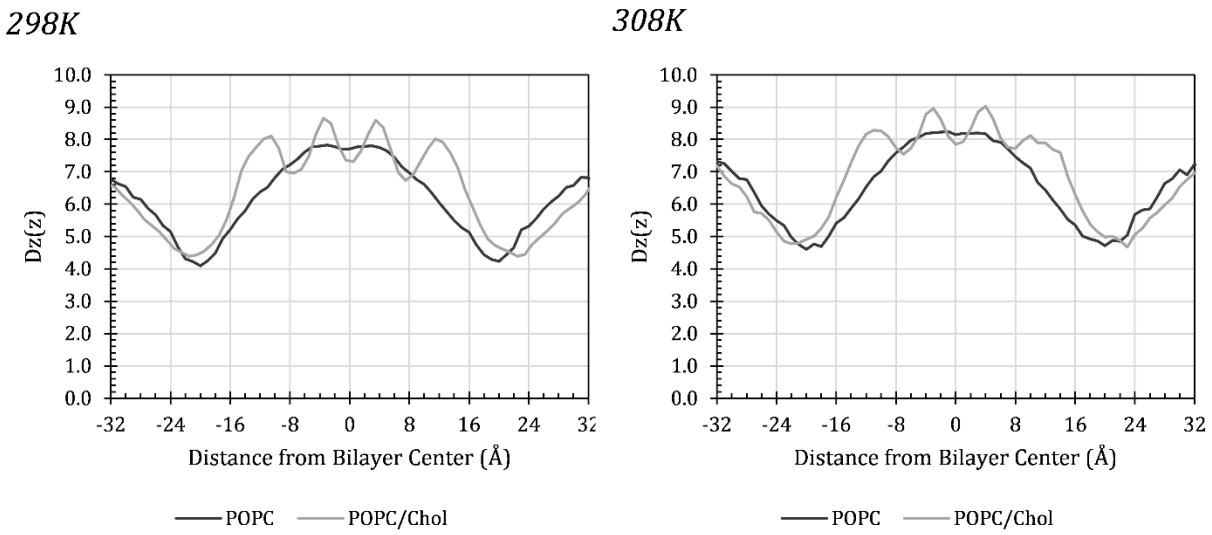
Gary Angles, Angela Hail, Rachel J. Dotson, and Sally C. Pias



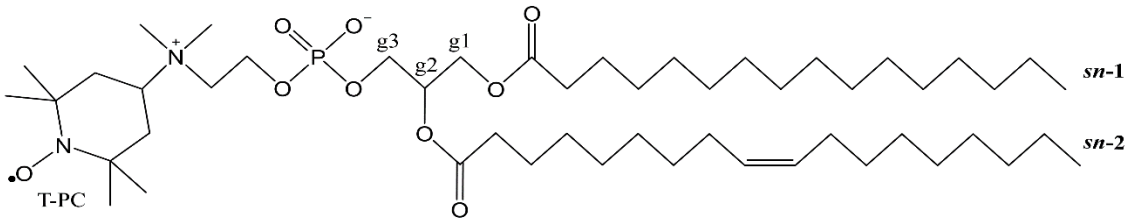
SI Figure 1 Comparison of carbon-wise simulation and experimental order parameters, $|S_{CD}|$, for the *sn*-1 palmitoyl tail of POPC, in bilayers composed of POPC alone (*left*) or POPC/chol (*right*). Simulation order parameters shown for 298K (*black lines*) and for 308K (*gray lines*). Experimental order parameters shown for POPC at 293K [67] (*triangles*) and 300K [67] (*squares*) and for POPC/chol at 300K [69] (*diamonds*).



SI Figure 2 Free energy profiles for POPC (*black lines*) and POPC/chol *(gray lines*) at 298K (*left*) and 308K (*right*).



SI Figure 3 Diffusion coefficient ($D_z(z)$) profiles for POPC (*black lines*) and POPC/chol *(gray lines*) at 298K (*left*) and 308K (*right*).



SI Figure 4 Molecular structure of the modified POPC lipid used in EPR work to probe oxygen levels in the bilayer-water interfacial region, *via* the bulky and largely hydrophobic tempo-phosphocholine (T-PC) spin-label [38]