Objective: To test a simulation model for accurate characterization of DAPC, a polyunsaturated fatty acid membrane lipid.

Methods: Molecular dynamics simulations using CHARMM, NAMD, and VMD simulation packages. Further data compilation and analysis through scripts for posterior comparison against experimental data.

Results: The adjusted simulation parameters generated accurate sets of data, which were consistent with experimental measurements of area/lipid, NMR spin-lattice relaxation times, and deuterium order parameters of DAPC membranes.

Future Work: To test the simulation parameters on larger systems of molecules and those with DAPC+cholesterol to probe sterol partitioning in the membrane.