TOWARDS VALIDATING QUATERNARY LIPID MEMBRANE SIMULATIONS

Moiseenko D.Y., Zlenko D.V.

culpritgene@gmail.ru, dvzlenko@gmail.com MSU, Biological Faculty, Department of Biophysics

In order to construct molecular model of reaction center of purple bacteria Rhodobacter sphaeroides we try to reproduce it's native lipid membrane environment. It was shown that there are lipid-binding sites on RC's hydrophobic part, at least some of which bind particular lipid molecules and can influence RC functionality [1, 2]. Here we try to recreate angular lipid environment of RC, including in our simulation all four of it's predominant lipid molecules, namely phosphatydylglycerol (PG), cardiolipin (CL), phosphatydylethanolamine (PE) and phosphatydylcholine (PC).

Our ultimate goal is to find a set of parameters, that would allow us to obtain a reasonable area per lipid (ApL) values in GROMACS OPLS-AA force field simulations of pure and mixed lipid bilayers of different composition. Experimental data we obtain mostly from classical Langmuir experiments with lipid monolayers [3, 4, 5]. It was shown that free energy of lipid mixtures usually depends nonlinearly on bilayer composition. This could be partly explained by tendency of charged lipids to assemble in ordered domains [3]. Hydrogen bonds between ions and water molecules and negatively charged phosphorous groups of PG, CL may account for strong dependency of free energy on ion strength. Upon wide range of concentrations the same nonlinear behavior is observed even in mixtures of zwitterionic lipids like PE and PC, comprising the same set of acyl chains [3]. Acyl chains themselves, their length and presence of double bonds, influence on lipid bilayer thickness in a complicated manner, with interactions of additional methylen groups simply adding to net Van-der-Waals forces but also changing order parameter [4, 5]. Although each of mentioned factors of interaction has it's own distinct nature, all of them affect thermodynamic parameters, including ApL. By comparison of bicomponent lipid mixtures of different compositions we hope to find some general dependencies of ApL on molar fraction. Ideally we hope to find a way to combine those dependencies to get some insight upon how ApL behaves in ternary and quaternary mixtures of these lipids.

References.

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