Title: Molecular modeling of lipid membranes with fluorescent probes

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Abstract: We studied biological membranes with fluorescent probes. First part of the work describes the properties of lipid bilayer consisting of DPPC (dipalmitoylphosphatidylcholine) and various cholesterol concentrations (5 mol % and 20 mol %). The properties are studied via the free probe – DPH (diphenylhexatriene) which is in various concentrations randomly immersed into both layers of the membrane. Second part of this work studies the properties of DOPC (dioleoylphosphatidylcholine) membrane via pyrene probes attached to 4^{th}, 6^{th}, 8^{th}, and 10^{th} carbon atom in both acyl chains of the host lipid and compares how the membrane properties differ based on the various pyrene positions. Here we focused also on dimerization rate of pyrene probes based on their position and the relationship with lateral pressure profile.

Keywords: molecular simulation, membrane, fluorescent probes, lipids, lateral pressure profile