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Structure and dynamics of lipid bilayer membranes – comparison of EPR and molecular dynamics simulation results

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Results of molecular dynamics (MD) simulation of fully hydrated dimyristoylphosphatidylcholine membranes in the liquid-crystalline phase are compared to these obtained by electron paramagnetic resonance (EPR) spin labeling method. There is an excellent agreement between the results in the case of polarity profiles across the membrane and diffusion of small molecules both in the membrane interior and water phase. There is, however, only partial agreement between the order parameter profiles obtained by EPR and those obtained by nuclear magnetic resonance and MD simulation. This indicates that the use of bulky assemblies as probes has limitations. The polarity profile obtained by MD simulation as well as EPR spin labeling method indicate certain amount of water to be present in the hydrophobic, hydrocarbon region of the membrane. Both methods also show that with lipid bilayer membrane in the liquid-crystalline phase nitric oxide (NO) diffuse about as readily as in water even though the macroscopic viscosity is about 100 times grater. A new and most interesting result, demonstrated by MD simulation, is that NO diffusion in the lipid bilayer is isotropic. Earlier, a similar result was obtained for molecular oxygen diffusion using an EPR spin labeling method (Kusumi, Subczyński & Hyde, 1982).