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Comparison of the conformation and the dynamics of saturated and mono-unsaturated hydrocarbon chains of phosphatidylcholines

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The conformations and dynamics of hydrocarbon chains of 1-palmitoyl-2-oleoyl-phosphatydylcholine (POPC) molecules in the POPC membrane were compared with those of dimyristoyl-phosphatidylcholine (DMPC) molecules in the DMPC membrane. The main difference between these two phospholipids is that POPC has a double bond in *cis* conformation between C9 and C10 in the β-chain, whereas all C-C bonds of DMPC are saturated. The double bond in *cis* conformation affects both populations and lifetimes of conformational states in the β-chain whereas those in the γ-chain are only weakly affected. The strongest effect of the double bond is on its nearest neighbor torsion angles. For most of the time, these angles have neither a *trans* nor a *gauche* conformation and so are in energetically non-optimal states. The rigid bend in the β-chain might affect the diffusion of the POPC molecules in the membrane plane differently from that in the plane perpendicular to it.