

Effects of Local Anesthetics on a Phospholipid Bilayer : A Comparative Molecular Dynamics Simulation Study with Anesthetic Molecules of Different Strengths of Action

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Abstract - Local anesthetics provoke reversible blockade of nerves by interaction with sodium channels in nerve membranes. On their route to the specific receptor sites, these molecules have to encounter the lipid bilayer. Effects of uncharged local anesthetics (LA) on a fully hydrated 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine (POPC) bilayer in liquid crystal phase have been investigated with molecular dynamics (MD) simulation scheme. Using two different LA molecules, Benzocaine (BZC) and Lidocaine (LDC), in low anesthetic concentration, comparisons have been made for their dynamical behavior in the membrane as well as their effect on membrane lipids. The differences in the mobility of the two anesthetics and the extent of increase of order in the interior of lipid bilayer have clearly been shown. The diffusion coefficient for two anesthetics in lipid environment was calculated which are comparable to experimentally determined values.
