Lipid Reorientation in the Cell Membrane Bilayer: Fe (II) Effect

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Abstract

In the molecular membrane, phospholipids perform the forming, retaining, labile alteration, and the transfer of the barrier layer functions. Under normal physiological conditions, direct permeability through the membrane without exposure from the outside is practically impossible. Induced effects from outside (uncontrolled discharge of electricity, electroporation, formation of acidic, alkaline media, localization of aggressive metal ions) allow cell membrane damage through lipid conformational and destructive processes.

To understand the dynamics of the hole formation and the progression of the hole closing in the membrane layer at the lowest molecular level, modeling of the structure of phospholipids and Fe(II) ion associates by quantum molecular theory methods was performed. It has been found that metal ion fixation to the lipid chain is insignificant to form lipid conformational movement. Similarly, metal ion fixation in the case of the $-N(CH_3)_3$ head in the lipid head group is not formed. The iron ion binds two lipid molecules in the orthophosphoric region, forming an energetically stable bridge between orthophosphoric fragments. As a result of this process, the lipid aliphatic chains change their conformation - a curved chain around the metal ion centre is formed from a straight structure. A typical molecular charge redistribution during excitation was determined and described. It is stated that due to the energetically favourable Fe^{2+} ion position, one lipid becomes a charge donor and the other – a charge acceptor.

Keywords

Fe(II) ion; lipid-Fe-lipid associate; complex stability, electroporation.