# MOLECULAR MODELING OF LIPID PEROXIDATION

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Molecular dynamics and quantum chemistry studies of interaction between phospholipid, which contains peroxyl radical, and membrane antioxidant -tocopherol (vitamin E) in lipid bilayer is considered in this work. Interplay between oxidized lipid and water-soluble artificial antioxidants is investigated. Influence of oxidized lipid on efficacy of oxygen molecule's penetration into hydrophobic membrane layer is described here too.

Peroxyl radical is positioned in the middle of lipid tail and, it would seem, in hydrophobic membrane layer interior. The chromanol ring of -tocopherol contains polar groups, that is why it seems, that -tocopherol is mainly located in phospholipid heads region. Hydrogen atom, which reduces peroxyl radical, is contained in -tocopherol's chromanol ring. Distance between hydrogen atom and peroxyl radical in such geometry amounts nearly 10 Å. It makes impossible to transfer hydrogen atom to oxidized group. However, established by molecular modeling studies equilibrium states of oxidized phospholipid and -tocopherol in membrane are different from described. Oxidized lipid tail bended thus peroxyl radical locates near polar surface of membrane, and -tocopherol partially settle down into the hydrophobic region. This geometry allows to transfer hydrogen atom between reacting groups.

Moreover, elevation of oxidized lipid tail to membrane surface, nevertheless, don't provide free access from water layer to peroxyl group. That is conflict with well-known fact of effectiveness lipid peroxidation inhibition by water-soluble artificial antioxidants. It proposes penetration of such antioxidants into hydrophobic region of membrane. We revealed, that positive charged water-soluble antioxidant MDL73404 shows the greatest efficacy of interaction with peroxyl groups of membrane lipids in comparison with uncharged chromanol molecule and negative charged antioxidant Trolox. At the same time, MDL molecule spends maximal time for permeation into membrane interior.

Influence of oxidized lipid to membrane permeability for oxygen molecule study show, that changed conformation of oxidized lipid makes membrane deformations, which increase efficacy of oxygen molecule to penetrate into hydrophobic layer. As a result, lipid peroxidation is self-intensify reaction, possibly, not only because the chain process, but facilitation access to reaction place for substrate by product.