Insight into the Molecular Dynamic Simulation Studies of Reactive Oxygen Species in Native and Oxidized skin membrane

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Non-enzymaticlipid peroxidation of the skin-lipid bilayer causes perturbations that affectthe biomembrane structure, function, and permeability of reactive oxygenspecies (ROS). Inthis study, we investigated the molecular dynamics simulations (MDS) on native andeffect of lipid peroxidation on the bilayer structural properties and permeabilityof various ROS skin-lipid bilayer membranes. Native skin-lipid bilayers are composedof ceramide, cholesterol, and free fatty acid in almost equal molar ratio(1:1:1). Dynamic distribution studies on ROS, i.e. $H_2O_2$and O_2 ($^1O_2$ by analogy), revealed that thesespecies interact with cholesterol as a primary target in lipid peroxidation of skin-lipidbilayer. The oxidized skin-lipid bilayer was composed of ceramide, cholesterol,free fatty acid, and 5α-hydroperoxycholesterol (5α-CH).The simulation showed that, upon oxidation, the oxidized group (-OOH) of 5α-CHmigrates towards the aqueous phase and the backbone of 5α-CH tilts, which causesthe membrane to expand laterally. Measurements of the permeability of H_2O_2,HO_2, HO, and O_2 ROS along the oxidized skin-lipid bilayerrevealed a decreased breaching barrier for all the species as the degree ofperoxidation increased, with a resulting easy passage across the membrane. Thisstudy helps to understand oxidative stress at the atomic level. To ourknowledge, this is the first reported MDS study on oxidized skin-lipid bilayerand permeability of ROS.

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