Simulation Studies of Oxidized Lipids in Model Membranes

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Membrane lipids are critical for numerous cellular mechanisms, and alteration of their normal composition may be physiologically detrimental. Of particular interest are the consequences of oxidative stress. Polyunsaturated phosholipids can be fragmented resulting in many different types of oxidized phospholipids. Strongly oxidized acyl chains are thought to show chain reversal and to protrude from the cell surface, as predicted by lipid whisker model, while the second aliphatic chain remains anchored in the hydrophobic part of the membrane. Oxidized lipid species have been associated with many diseases, including Alzheimer's disease or atherosclerosis.

We use molecular dynamics simulations to investigate the behavior of oxidized lipid species in the model membrane POPC. We can clearly observe the proposed chain reversal in highly oxidized species, with the oxidized tail oriented towards the water phase. Interestingly we find that the oxidized lipids “float” above the surround POPC lipids of the bilayer. At the other hand, tails of less strongly oxidized lipid species partition into the hydrophobic-hydrophilic interface of the bilayer. Lipid oxidation does have a oxidation product dependent prominent effect on a number of membrane properties like density profiles, but seems not always to affect other properties like order parameters. Taken together, our data indicate that oxidized lipid molecules can modulate membrane properties and this effects can be observed already at very low concentration.

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