Frontiers in Peroxidation of lipid membranes: Key molecular level aspects using computational chemistry

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Biographical sketch

Mounir Tarek is a Senior Research Director at the CNRS-Université de Lorraine. His research involves the use of computational chemistry methods to study membranes, proteins, ion channels and membrane transport proteins. Over the last few years, he studied many aspects of electroporation of cell membranes subject to high electric fields. M. Tarek is a founding member and a member of the Scientific Council of the Europeen Associated Laboratory EBAM 'Pulsed Electric Fields Applications in Biology and Medicine'.

Abstract

Membrane oxidative stress is connected to the emergence of various diseases ranging from inflammation to cancer and ageing. While lipid oxidation is an active field of research, there is an ever-increasing need for understanding the microscopic details involved in its occurrence in cell membranes. Recently, we have been investigating membranes peroxidation in realistic environments using state of the art Quantum Mechanics/Molecular Mechanics modeling. In the spirit of this workshop, we will present our most recent efforts in understanding and characterizing several key steps of the phenomena in order to convey the exquisite predictive power or today's computational techniques and some aspects of the results that could greatly benefit from experimental validation.