BIOMOL STRUCT

GUEST LECTURE SERIES

FRONTIERS OF ELECTROPORATION, FROM MECHANISMS TO APPLICATIONS: UNRAVELING NEW KEY MOLECULAR LEVEL ASPECTS USING COMPUTATIONAL CHEMISTRY

Mounir Tarek, PhD

Senior Research Director (Chemistry)
Centre National de La Recherche Scientifique (CNRS),
Université de Lorraine, Nancy, France

Thursday, 11.11.2021, 13:00
BioMolStruct students & faculty:
MC1.F.05.016 (UR Pathology 01, tract F, 5th floor), MED CAMPUS Graz

For all other attendees via Webex:
https://medunigraz.webex.com/medunigraz/j.php?MTID=m812164e1d8256fed6e015dfe7edbfb0d

Biographical sketch

Mounir Tarek is a Senior Research Director at the CNRS-Université de Lorraine, recipient of a Ph.D. in Physics from the University of Paris in 1994. He joined the CNRS after a four-years tenure at the National Institute of Standards and Technology (Gaithersburg Maryland USA) following three years tenure at the University of Pennsylvania, Philadelphia, USA. His research focus and expertise lies in the study of cell membranes transport processes. It involves the use of computational chemistry methods to study membranes, proteins, ion channels and membrane transport proteins.

Abstract

The application of short and intense electric pulses enables to transiently alter the properties of cell membranes, making them permeable to a wide range of chemical species. This phenomenon is routinely used in a range of medical applications as well in biotechnology and industrial processing. Few years ago, pioneering MD simulations have been conducted in order to model the effect of electric fields on membranes, providing perhaps the first molecular model of the electroporation process of lipid bilayers. Our knowledge however about all occurring processes is still sketchy. In this contribution we show how we harness the capabilities of computational resources and the predictive power of advanced atomistic and quantum level molecular dynamics techniques to decipher key steps in several physical and biophysical and chemical processes occurring at the cell membranes when these are subject to voltage gradients of magnitude and duration equivalent to those generated by electric pulses used in Electroporation Based Technologies and Treatments.