

Frontiers of Electroporation, from Mechanisms to Applications: Unravelling new key molecular level aspects using computational chemistry

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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 electric pulses used in Electroporation Based Technologies and Treatments.