Modelling the Effects of Electric Fields on Bio-systems workshop

Copenhagen, Denmark, March 28

On March 28, 2014, we were delighted to have the opportunity to organise a workshop on “Modelling the Effects of Electric Fields on Bio-systems” within the activities of WG 1: Basic Mechanism of Electroporation and Modelling, following the Management Committee meeting of our COST Action held in Copenhagen. Most of the main players in Europe have responded favourably to this initiative, the first of its kind, bringing together all the expertise in molecular modelling in a prospective/exploratory one-day meeting.

While some participants were already part of the COST Action, others were not familiar or were not aware of recent progress and current applications of the electroporation-based technologies and treatments. The wonderful dinner party (thanks Julie Gehl), held the evening before the workshop, was a good occasion for them to meet with many distinguished scientists who contributed to the field’s progress. In addition, before proceeding to the core of the working day theme, Damijan Miklavcic kindly agreed to introduce the COST Action, and gave a brief yet exhaustive account of the expertise and the know-how of its members as a kick-off for the workshop. Beside the 7 speakers, the workshop was attended by several members of the COST Action interested in the subject covered, as well as by WG 1 leader, Marie-Pierre Rols, from IPBS (CNRS), France.

The presentations given by the speakers were selected to cover several topics.

First, we started with an exhaustive report on the progress made so far by the community at large using MD simulations to model electroporation of membranes / lipid bilayers.
We then had two contributions, the first addressing the phenomena of lipid translocation driven by electrostatics and proteins, and the second concerning the modulation of membrane phases by electric fields. We then tackled issues related to the methodologies. This included a presentation of recent protocols to perform *in silico* computational electrophysiology, and a discussion about the added value, the perspectives, and the limitations of coarse-grain and hybrid coarse-grain/atomistic modelling of biological membranes and proteins. The final two contributions highlighted very important effects of electric fields on biomaterials, something only recently addressed by the community: a) how, and under what condition(s) electric fields unfold proteins, and b) to what extent such fields may chemically modify molecules, e.g. dissociate water for instance. These two aspects, which we believe are of greatest importance, will likely be more and more often considered in future studies of the effects of intense electric fields in all bio-applications.

All the contributions were followed by exchange between the modellers discussing the many issues that were raised. More importantly, in the discussions that followed this intense and interesting day, the participants agreed that we needed to work more on bringing together the modelling community and the experimentalists, in order to trigger a wide range of collaborations, as it became clear to all attendees that molecular modelling is a necessary tool to understand and characterize many aspects still a matter of debate in the community. A first step in this direction will be to reunite the two fields of expertise (modelling and experiments), and a rendezvous was scheduled for the upcoming meeting of WG 1 that will be held in Toulouse (April 15-16, 2015), which presents a perfect opportunity to do so.

Finally, the participants have also expressed a very strong interest in putting together a large pool of research groups, in order to train researchers in molecular modelling of electroporation within the framework of a Marie Curie Initial Training Network (ITN). Investigation of this prospect will be discussed further and coordinated by the COST Chair, so as to form a part of a larger initiative.

**Forthcoming activities**

**The Third International Conference on Analytical and Nanoanalytical Methods for Biomedical and Environmental Sciences "IC-ANMBES 2014"**

Brasov, June 13-15, 2014

http://icanmbes.unitbv.ro/