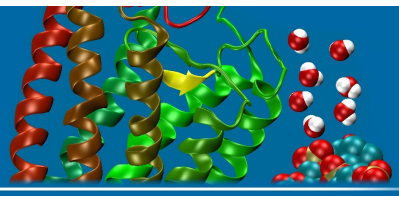
Structural Biology *of* Membrane Proteins



E-bulletin of Marie-Curie Integrated Training Network - SBMPs

May 2012

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Conferences and workshops related to membrane proteins in 2012:

CNRS School:

Expression, purification and stabilization of membrane proteins for structural analysis

October 1st to 4th, 2012

"Les Cèdres", Grasse, France

http://membraneproteinsschool.ipbs.fr/index.html

Description:

This course will cover key topics in the area of membrane protein expression, purification and stabilization for structural analysis. The programme is divided into plenary lectures of invited speakers, communications and round tables. The school is limited to 50 participants and will take place in the village "Les Cèdres" of Grasse, which provides excellent facilities. We will have the great pleasure to invite you to attend this CNRS school.

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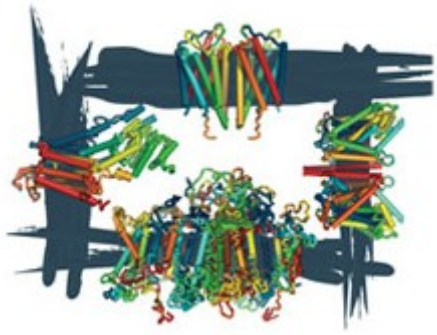
The NIH Roadmap to Membrane Protein Structures:

The 4th Membrane Protein Technologies Meeting

November 28-30, 2012

Westin Hotel, San Francisco, USA

http://rmi2012.org/index.html



Description:

Previous NIH Roadmap to Membrane Protein Structures meetings have been very successful in generating open exchange and sharing of technologies, materials, and ideas focused on targeting membrane protein structure determination. This 4th meeting in the series provides a unique opportunity for all investigators engaged in developing and applying new technologies for structural biology of membrane proteins and complexes to focus on technologies that facilitate membrane protein structure determination, and recent structures of membrane proteins. This meeting will include all investigators supported by the NIH common fund program for structural biology, and invites all PSI member membrane protein groups, and all investigators of membrane protein structure to participate fully.

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Centre Européen de Calcul Atomique et Moléculaire:

Protein Folding: Integrating theory, simulation and experiment

September 3 - 6, 2012

CECAM-ETHZ, Zurich, Switzerland

http://www.cecam.org/workshop-0-781.html

Description:

While the general principles guiding protein folding have now been established, a complete understanding of folding dynamics at the atomistic level remains an important unsolved challenge. Significant discrepancies between different simulations, and between simulation, theory and experiment indicate the need for closer communication between these areas. Examples include differences between folding mechanisms predicted by simulations with different energy functions, differences between mechanism deduced from simulations and from experiment, and the suggestion that the "folding funnel", a central concept in protein folding theory, may not capture mechanism seen in simulations.

These emerging differences indicate that there are important challenges still to be overcome. Novel experimental and theoretical methods, however, are increasingly promising to bridge this gap; from the simulation side, by being able to tackle longer time scales, from the theoretical side through the development of more detailed models, and from the experimental side, by obtaining higher resolution spatial and temporal information. In fact, it is precisely because of the development of these methods, that many of the controversial issues mentioned above have been identified. We therefore believe that the time is right for bringing together the leading scientists from each of these areas in order to bridge the gaps between the different disciplines.

Simulation: Advances in computer simulation have of course been driven by the ever-increasing available computer power, now extended to specialized machines for molecular simulation, and the exploitation of low-cost consumer devices (e.g. graphics processing units) for this purpose. These advances have seen simulations on a microsecond, and even millisecond, time scale becoming possible,

making connections with experiment more feasible. In addition, however, recent years have seen the increased use of enhanced sampling methods for extending the accessible range of folding simulations; examples include replica-exchange molecular dynamics (REMD) and Markov-State Models. While these advances help to solve the sampling problem, inaccuracies in the energy functions used are also becoming evident. Recent work in optimizing energy functions has yielded significant improvements to the accuracy of folding simulations. Notably, many of these advances have been driven by direct comparison with experimental data.

Theory: Early theories of protein folding focused on the qualitative aspects of the problem, i.e. resolving Levinthal's Paradox, and explaining the origin of cooperative two-state folding in small proteins. Modern theory seeks to explain experimental observations for specific proteins, ideally in a predictive fashion. By constructing simple analytic models for folding, insights may be gained which would be hard to obtain directly from experiments. A particularly promising, but relatively unexploited, area, is the use of such theories to bridge experiment and simulation. Theoretical models are important for interpreting single molecule experiments, allowing the observations to be interpreted in terms of either one-dimensional or multidimensional landscapes. In the other direction, theory can assist in the construction of such free energy landscapes and associated dynamics.

Experiment: New experiments are increasingly yielding quantitative information that can be quantitatively compared with simulation. Ultrafast spectroscopy experiments on fast-folding proteins and protein fragments provide information on relaxation processes occurring on time scales that can be directly probed by simulation. Single molecule experiments make it possible to study the properties and interconversion of different folded, unfolded and partially folded or misfolded species. This removes the problem of ensemble averaging – as a result, comparison with simulation can be much more direct. In addition, single molecule "pulling" experiments allow the energy landscape of proteins to be probed in a different way by application of a mechanical pulling force.

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The information about new **conferences**, **courses** and **workshops** related to membrane proteins as well as some important news related to **SBMPs** (including meetings, publications etc.) please send to ***Slawomir Filipek*** *(*sfilipek@chem.uw.edu.pl*)*.

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