Barcelona BioMed Conference
Frontiers in dynamics simulations of biological molecules
November 4-6, 2013

Programme

Monday, November 4, 2013

8.30 Registration

9.15 Welcome by Joan J. Guinovart, IRB Barcelona Director

Session I
Chair: Modesto Orozco

9.30 **Michelle Parrinello** (ETH Zurich, Switzerland)
Proteins in Slow Motion

10.15 Short Talk: **Carme Rovira** (Universitat de Barcelona, Spain)
Atomistic simulations of glycosidic bond formation

10.35 Coffee break

11.00 **Ursula Röthlisberger** (EPFL Lausanne, Switzerland)
QM/MM Car-Parrinello Simulations of Biological and Biomimetic Systems

11.45 **Jiali Gao** (University of Minnesota, USA)
Beyond QM/MM: Development of a Quantum Mechanical Force Field

12.30 **Paolo Carloni** (German Research School for Simulation Sciences, Germany)
Multiscale modeling of G-protein coupled receptors

12.50 Visit to posters (Authors from **even** references)

13.30 Lunch (FrescCo, C/ Carme, 16)

Session II
Chair: F. Javier Luque

15.00 **Xavier Salvatella** (Institute for Research in Biomedicine, Spain)
Molecular simulations as a tool to complement experiments probing the structural heterogeneity of proteins

15.45 **Rebecca Wade** (Heildelberg Institute for Theoretical Studies, Germany)
Biomolecular Recognition: Insights from Modeling and Simulation

16.30 Coffee break

17.00 **Adrian Mulholland** (University of Bristol, UK)
Protein dynamics and enzyme catalysis: the ghost in the machine?

18.30 Reception to the participants (Institut d'Estudis Catalans)

Tuesday, November 5, 2013

Session III
Chair: Jiali Gao

9.30 **Helmuth Grubmüller** (Center for Advanced Research in Biotechnology. Maryland University, USA)
Atomistic Simulation of Single Molecule Experiments: Molecular Machines and a Dynasome Perspective

10.15 Short Talk: **Ryoji Takahashi** (Barcelona Supercomputing Center, Spain)
Monte Carlo Free Ligand Diffusion and Absolute Binding Free Energy Calculations

10.35 Coffee break

11.00 **Nikolay Dokholyan** (University of North Carolina at Chapel Hill, USA)
Predicting 3D RNA structure and dynamics using Discrete Molecular Dynamics

11.45 **Victor Guallar** (Barcelona Supercomputing Center, Spain)
Mapping Protein and Ligand-Protein Dynamics with Monte Carlo Techniques

12.30 Short Talk: **Ramon Crehuet** (Institute of Advanced Chemistry of Catalunya, CSIC, Spain)
Simulating Intrinsically Disordered Proteins with coarse-grained methods

12.50 Visit to posters (Authors from **odd** references)

13.30 Lunch (FrescCo, C/ Carme, 16)

Session IV
Chair: Victor Guallar

15.00 **Mark Sansom** (University of Oxford, UK)
Membrane Proteins in Context: Molecular Simulations of Membrane Proteins & their Lipid Interactions

15.45 **F. Javier Luque** (Universitat de Barcelona, Spain)
Disclosing the mechanistic and functional diversity of hemeproteins using molecular simulations

16.30 Coffee break

17.00 **Erik Lindhal** (Center for Biomembrane Research, Sweden)
Heterogeneous Parallel Adaptive Molecular Dynamics & Ensemble Simulation

Wednesday, November 6, 2013

Session V
Chair: Charles A. Laughton

9.30 **Gerhard Hummer** (National Institute of Diabetes and Digestive and Kidney Diseases, USA)
Motions in the molecular machinery powering life

10.15 Short Talk: **Bojan Zagrovic** (University of Vienna, Austria)
X-ray refinement significantly underestimates the level of microscopic heterogeneity in biomolecular crystals

10.35 Coffee break

11.00 **Jonathan W. Essex** (University of Southhampton, UK)
Protein-Ligand Binding by Free Energy Simulations: Issues, Successes and Failures

11.45 **Gianni di Fabritis** (Universitat Pompeu Fabra, Spain)
Intelligent sampling in high-throughput molecular Dynamics

12.30 **Iñaki Tuñón** (Universidad de Valencia, Spain)
Heavy Enzymes: A Meeting Point to Discuss on Dynamical Effects in Catalysis

13.15 **Richard Lavery** (Institute of Biologu and Chemistry of Proteins, France)
Atomistic and coarse-grain studies of biomacromolecules and their interactions: targeting timescale and accuracy

13.00 Concluding remarks: Charles A. Laughton