Program

ISQBP 2012 President's Meeting

Långholmen, Stockholm
June 17 - 20, 2012

Sunday June 17th

11.00 – 12.50 **Registration and brunch**

Advances in Methodology I

12.50 – 13.00 **Introduction**

13.00 – 13.40 **Drug discovery accelerated by computational methods**
William L. Jorgensen

13.40 – 14.20 **A multiscale approach to characterize macromolecular dynamics and functions**
Cecilia Clementi

14.20 – 14.40 **Bio&pharma modeling across spatial & temporal scales**
Aatto Laaksonen

14.40 – 15.00 **Hydration entropy from molecular dynamics**
Roland Huber

15.00 – 15.30 **Coffee**

15.30 – 16.10 **Constant pH simulations of proteins and nucleic acids**
Charles L. Brooks III

16.10 – 16.50 **Structured continuum electrostatic calculation of free energy**
Montgomery Pettitt

16.50 – 17.10 **Implosion-based mapping procedure between all-atom and coarse-grained normal modes**
An Ghysels

17.10 – 17.30 **MD simulations of biomolecular machines with an eye to drug design**
Giorgio Colombo

Monday June 18th

Nucleic Acid Simulations

08.30 – 09.10 **Exploring the dynamics and interactions of the ribosomal A-site**
Joanna Trylska

09.10 – 09.50 **Contribution of the 2'-hydroxyl to the conformational properties of RNA**
Alexander D. MacKerell Jr

09.50 – 10.20 **Coffee**

10.20 – 11.00 **Convergence, salt, and force field dependence in simulations of nucleic acids**
Thomas E. Cheatham III

11.00 – 11.20 **Virus swelling and prediction of genome location in virus capsids**

David van der Spoel

11.20 – 11.40 **A structural and dynamical model of human telomerase**
Samuel Flores

11.40 – 13.30 **Lunch**

13.30 – 14.10 **Insights into gene expression and packaging from computer simulation**
Wilma Olson

14.10 – 14.50 *President's Award Lecture*
Probing DNA recognition mechanisms
Richard Lavery

Advances in Methodology II

14.50 – 15.10 **Challenges for molecular simulation on heterogeneous architectures**
Berk Hess

15.10 – 15.30 **The power of N: Collective ensemble-based simulation methods for complex biological events**
Kwangho Nam

15.30 – 18.00 **Poster session**

Tuesday June 19th

Protein Simulations

08.30 – 09.10 **Interfacial binding sites of peripheral membrane proteins: Insights from computations and experiments**
Nathalie Reuter

09.10 – 09.30 **Capturing large conformational changes of the human serotonin transporter by un-biased MD simulations.**
Birgit Schiøtt

09.30 – 09.50 **Membrane-bound cytochromes P450 in action: A general framework to simulate proteins with a single trans-membrane anchor**
Vlad Cojocaru

09.50 – 10.20 **Coffee**

10.20 – 11.00 **Transition path for conformational activation of Src -like kinase domains**
Carol Post

11.00 – 11.40 *Loew Memorial Lecture*
Cold-adaptation of enzyme reaction rates
Johan Åqvist

11.40 – 13.15 **Lunch**

13.15 – 14.00 **ISQBP Business meeting**

14.00 – 14.40 **Analyzing biomacromolecular flexibility: From fuzzy constraint networks to entropically dominated allostery**
Holger Gohlke

14.40 – 15.00 **Defining independently moving domains based on sets of biomolecular conformations**

Julia Romanowska

15.00 – 15.20 **Interface dynamics explain assembly dependancy of influenza neuraminidase catalytic activity**
Susanne von Grafenstein

15.20 – 15.40 **Coffee**

15.40 – 16.20 **Characterization of free energy landscapes of proteins using NMR spectroscopy**
Michele Vendruscolo

16.20 – 16.40 **Two transition routes for PrP misfolding at pH 4.5**
Julian Garrec

16.40 – 17.00 **Simulation of the excited state chromophore-protein interplay in fluorescent Proteins**
Gabriella Jonasson

18:30 – 21:30 **Boat excursion and dinner on M/S Östanå I**
Departure: Långholmen
Return: Långholmen

Wednesday June 20th

QM/MM Methods

08.30 – 09.10 **Computer simulation of photochemistry in the condensed phase: Photoisomerization and excitation energy transfer**
Gerrit Groenhof

09.10 – 09.30 **Active state dynamics and catalytic mechanism of sortase a enzymes**
Leif Eriksson

09.30 – 09.50 **Comparison of QM-only and QM/MM models for the mechanism of tungsten-dependent acetylene hydratase**
Rong-Zhen Liao

09.50 – 10.20 **Coffee**

10.20 – 11.00 **Mechanism for natural and artificial water oxidation**
Per Siegbahn

11.00 – 11.40 **Computational photochemistry of flavoproteins**
Tatiana Domratcheva

11.40 – 12.00 **Computational enzyme design strategies: The curious case of Diels-Alderases**
Mats Linder

12.00 – 12.20 **Remote cofactor control of active site properties in hydrogen converting enzymes**
Matthias Stein

12.20 – 12.30 **Closing remarks**

12.30 – 13.30 **Lunch**