



Barcelona BioMed Conference Macromolecular Dynamics October 24-26, 2011

INSTITUTE
FOR RESEARCH
IN BIOMEDICINE

Programme

Monday, October 24, 2011

8.30 Registration

9.00 Welcome

Session I:

Chair: Xavier Salvatella, ICREA and IRB Barcelona (Barcelona, Spain)

9.15 **Hashim Al-Hashimi**
Excited state structures of nucleic acids

10.00 **Robert Best**
Elementary time scales for protein folding: simulation versus experiment

10.45 Short talk: **Alessandro Barducci**
Determination of protein multimerization free-energy landscape using explicit-solvent MD simulations

11.05 Coffee break and poster session

11.35 **Modesto Orozco**
Pushing the frontier of theoretical methods for dynamics simulation

12.20 **Ben Schuler**
Protein Folding Dynamics from Single Molecule Spectroscopy

13.05 Short talk: **Mats Wikström**
Biophysical and structural studies of a novel SUMO-binding Zinc finger motif involved in the response to DNA double-strand breaks

13.25 - 15.00 Lunch (FresCo, C/ Carme, 16)

Session II:

Chair: Arthur G. Palmer, Columbia University (NY, USA)

15.00 **Dorothee Kern**
Surfing an enzyme's energy landscape

15.45 **Kresten Lindorff-Larsen**

Using Molecular Dynamics Simulations to Describe How Fast-Folding Proteins Fold

16.30 Coffee break and poster session

17.00 **Frans Mulder**

Isotope labeling approaches for protein dynamics studies by NMR spectroscopy and neutron scattering

17.45 **Rafael Bruschweiler**

Toward Protein Boltzmann Ensembles by NMR and Computation

18.30 Poster Session (odd numbers)

Tuesday, October 25, 2011

Session III:

Chair: Christian Griesinger, Max Planck Institute for Biophysical Chemistry
(Göttingen, Germany)

9.00 **Sergi Garcia-Manyes**

Conformational dynamics in the folding trajectory of a single protein under force

9.45 **Bert de Groot**

Detection of functional modes in protein dynamics

10.30 Short talk: **Clemens Kaminski**

In situ studies of protein aggregation kinetics with multiparametric and superresolution imaging

10.50 Coffee break and poster session

11.15 **Pau Bernadó**

Characterization of Large-Amplitude Motions in Proteins by Small-Angle X-ray
Scattering

12.00 **Arthur G Palmer**

Protein dynamics from NMR spectroscopy and MD simulations

12.45 Short talk: **Oscar Millet**

Insights on the 'Venus flytrap mechanism': solution structure and segmental motion of periplasmic binding proteins

13.05 Lunch (FresCo, C/ Carne, 16)

Session IV:

Chair: Ruth Nussinov, Tel Aviv University (Tel Aviv, Israel) and NCI (Bethesda, MD, USA)

15.00 **G. Marius Clore**

Exploring Sparsely-Populated States of Macromolecules by Paramagnetic and Diamagnetic NMR

15.45 **Lila M. Gierasch**

The allosteric mechanism of Hsp70 molecular chaperones

16.30 Coffee break and poster session

17.00 **Mikael Akke**

Dynamics and thermodynamics of ligand binding to the carbohydrate recognition domain of Galectin-3

17.45 Short talk: **Donghan Lee**

Molecular recognition kinetics within inaccessible time window

18.05 Poster session (even numbers)

20.30 **Speakers dinner**

Wednesday, October 26, 2011

Session V:

Chair: Michele Vendruscolo, University of Cambridge (Cambridge, UK)

9.00 **Christian Griesinger**

Globular and domain dynamics from NMR

9.45 **Francesco Gervasio**

Understanding the DGF-flip in cSrc and Abl tyrosine kinases through experimentally-validated free energy calculations

10.30 Short talk: **Nico Van Nuland**

Molecular recognition in TA modules couples allostery and intrinsic disorder

10.50 Coffee break and poster session

11.15 Short talk: **Carlo Camilloni**

Determination of Secondary Structure Populations in Disordered States of Proteins using NMR Chemical Shifts

11.35 **Ruth Nussinov**

Allostery and Conformational Control in Signaling: The Ubiquitin E3 Ligases

12.20 **Martin Blackledge**

Towards a Unified Description of Proteins Motions on Multiple Timescales

13.05 Concluding remarks