

Scientific Workshop

BioQuant & DKFZ with CIPKEBIP

(Centre of Excellence for Integrated Approaches
in Chemistry and Biology of Proteins, Slovenia)



Tuesday, June 18, 2013, BioQuant-Building, Greenier Saal¹

Draft Agenda

9:30 *Arrival at BioQuant Building*

Welcome by Roland Eils, Introduction of Participants

9:45 *Overview Presentation: Systems Biology and Bioinformatics at BioQuant and DKFZ*

Roland Eils

10:00 *Overview on CIPKEBIP Activities in Slovenia – Part 1*

Livija Tušar: CIPKEBIP and scientific platforms in chemistry and biology of proteins (10 min)

Dušan Turk: High throughput approaches to structural biology of endosomal enzymes, MHC class II molecules, and surface proteins from human pathogens (10 min)

Boris Turk: Proteases in biomedicine: opportunities and challenges (10 min)

Brief Discussion

10:45 *Overview Presentations BioQuant and DKFZ (5 minutes each)*

Holger Erfle: RNAi Screening

Jörg Langowski: Single molecule Fluorescence Spectroscopy

Christian Conrad: intelligent imaging

Benedikt Brors: Cancer Genomics

Marcel Schilling: Systems Biology of Signal Transduction

11:15 *Overview on CIPKEBIP Activities in Slovenia – Part 2*

Robert Zorec: NEUROGLIA: gliotransmission and metabolism (10 min)

Sašo Džeroski: Machine Learning for Systems Biology (10 min)

Enej Kuščer: ACIES BIO – brief info (10 min)

11:45 *Round-Up Discussion*

- Definition of Overlapping Topics
- Potential for Future Collaborations
- Next Steps

12:30 *Departure for Joint Lunch at Restaurant Olive*

14:00 *Short Tour BioQuant Building*

- Intelligent imaging microscopy (Christian Conrad)
- RNAi Screening Facility (Holger Erfle)

14:30 *End of Meeting – Possibility for individual discussions*

¹ BioQuant Building, Im Neuenheimer Feld 267 Greenier-Saal on 7th floor



For Information: Accompanying BioQuant Special Seminar

Date/time: Monday, June 17, 4:00 PM

Location: BioQuant (INF 267) Seminar room ground floor

Speaker: **Saso Dzeroski**

Jozef Stefan Institute (JSI); Centre of Excellence for Integrated Approaches in Chemistry and Biology of Proteins (CIPKEBIP); and Jozef Stefan International Postgraduate School (JSIPS).

Title: **What can Predictive Clustering approaches do for Systems Biologists: Integrating time series, siRNA screening and imaging data using novel Machine Learning methods**

Participants CIPKEBIP (Centre of Excellence for Integrated Approaches in Chemistry and Biology of Proteins, Slovenia)

- Dr. Livija **Tušar**, General Director
- Prof. Dr. **Dušan Turk**, Scientific Director
- Prof. Dr. Boris **Turk**
- Akad. Prof. Dr. Robert **Zorec**
- Prof. Dr. Sašo **Džeroski**
- Dr. Enej **Kuščer**

Participants from DKFZ Heidelberg and BioQuant, Heidelberg University

- Prof. Dr. Roland **Eils**, Division Head Theoretical Bioinformatics and Acting Director of BioQuant - DKFZ and BioQuant
- Dr. Benedikt **Brors**, Group Leader Computational Oncology, eilslabs - DKFZ
- Dr. Christian **Conrad**, Group Leader intelligent imaging, eilslabs - DKFZ and BioQuant
- Dr. Holger **Erfle**, Head RNAi Screening Facility – BioQuant
- Prof. Dr. Jörg **Langowski**, Division Head Biophysics of Macromolecules - DKFZ
- Dr. Matthias **Schlesner**, Group Leader Cancer Genomics, eilslabs - DKFZ
- Dr. Marcel **Schilling**, Senior Postdoc, Division of Systems Biology of Signal Transduction – DKFZ
- Dr. Jan **Eufinger**, Scientific Management, eilslabs – DKFZ



Abstracts of CIPKEBIP Presentations

Dr. Livija Tušar: CIPKEBIP and scientific platforms in chemistry and biology of proteins

CIPKeBiP is a non-profit research organization. CIPKEBIP researchers have expertise in light microscopy, cell, molecular and structural biology, mass spectrometry, biochemistry, biotechnology, bioinformatics, and chemistry. Its goal is to provide scientific platforms for conducting internationally competitive, cutting edge research in the area of life sciences with focus on the studies of proteins in their ex vivo, in situ, and in vitro environments.

The following research infrastructure / scientific platforms are established:

- High resolution and super-resolution light microscopy for visualization of molecules and their interactions in cells or in tissues and organisms.
- Mass spectrometry for analysis of protein composition in complex samples and analysis and identification of individual biological molecules and their modifications.
- Protein and structure production high throughput platform for analysis of molecular mechanisms from biochemical to atomic resolution studies (3D crystal structures, kinetics of interactions and properties of biologically active molecules - proteins and small organic molecules).
- Platform for development of biologically active organic molecules based on biological and chemical synthesis.
- Computational analysis of complex biological and other experimental data with the purpose of descriptive and predictive modeling, knowledge extraction and integration, as well as optimization of experimental approaches and technological processes.

Prof. Dr. Dušan Turk: High throughput approaches to structural biology of endosomal enzymes, MHC class II molecules, and surface proteins from human pathogens

In the processes of adaptive immunity antigenic determinants are made recognizable by the immune system. An important part of the process is taking part in endosomal compartments, where foreign proteins are degraded to fragments, which can bind to MHC class II molecules for later presentation at the surface of antigen presenting cells. We have established expression systems in *Escherichia coli*, insect and mammalian cell lines by adopting approaches from the large high throughput labs. Approximately 50 human enzymes and MHC class II molecules, 50 surface and host interaction proteins from *Staphylococcus aureus*, and lately 20 from *Clostridium difficile* were selected for protein production, structure determination and further biochemical analysis. Within the last 3 years we were able to produce a number of proteins and a small number of structures.

Prof. Dr. Boris Turk: Proteases in biomedicine: opportunities and challenges

Proteases control a great variety of physiological processes that are critical for life, including the immune response, cell cycle, cell death, wound healing, food digestion and protein and organelle recycling. Their action is strictly controlled. Imbalances in their activities have been found to be critical in a number of pathologies, such as cardiovascular diseases, inflammation, cancer, osteoporosis, as well as in neglected diseases such as malaria and Chagas' disease, thereby making proteases suitable and valuable drug targets. A number of small molecule drugs targeting proteases are already on the market and many more are in development, supporting this view. Several recent strategies in protease research based on chemical biology, proteomics and nanotechnologies will be presented. This includes development of activity-based probes for in vivo imaging of proteases as a strategy for early diagnostics and monitoring of diseases, proteomics-based discovery of protease-based biomarkers and development of targeted drug delivery systems, which can decrease toxicity of the drugs and improve their bioavailability. Moreover, all these approaches provide major opportunities for identification of protease signaling pathways, which is of highest biomedical interest.



Prof. Dr. Robert Zorec: NEUROGLIA: gliotransmission and metabolism

Astrocytes, the most abundant glial cells in the mammalian brain, play an active role in information processing. Their special form of excitability modulates network function via gliotransmission and metabolic neuronal support. We are studying how these processes can be manipulated in view of treating neurological pathophysiological states.

Prof. Dr. Sašo Džeroski: Machine Learning for Systems Biology

Two major machine learning approaches, relevant for applications in systems biology, will be presented. These include methods for analyzing structured data, in particular structured-output prediction, and methods for learning the dynamics of biological networks, including network structure and reaction kinetics. Example applications include finding drug targets and modeling the dynamics of endosome maturation.

Dr. Enej Kuščer: ACIESBIO---BRIEF INFO

ACIES BIO is a biotechnology research SME working primarily in the field of pharmaceutical, environmental and food industries. ACIESBIO collaborates with industrial partners on development and improvement of microbial strains and bioprocesses, especially in the field of secondary metabolite biosynthesis. Our activities on strain development and biosynthetic processes is complemented also by our expertise in synthetic organic chemistry, allowing us to offer a comprehensive service, covering all key development steps for efficient production of biosynthetic natural products or their semi---synthetic derivatives. In addition to providing services to industrial clients, ACIES BIO also runs its own Drug discovery programme, researching for novel secondary metabolite compounds with a particular focus on antibacterial, antifungal, anti---cancer, anti---inflammatory and neuroregenerative applications.

