

WORKSHOPS

Young scientists and students are invited to the Conference Workshop (in a frames of School on Genome and Postgenome Medicine supported grant RSF # 15-15-30041) to discover the role of postgenome data and the importance of communication for the modern life science, healthcare and quality of life.

The number of attendees is limited to 30 persons.

We suggest that attendees bring their own laptops. Besides a web browser (Firefox, Safari or Chrome) and a running internet connection, nothing is required (an external mouse will add to your comfort).

October,	30	10:00-12:00	WP1 – Proteoinformatics
October,	30	15:30-17:30	WP2 – How to Work with Human Genome?
October,	31	15:30-17:30	WP3 – Drug Development
October,	31	15:30-17:30	WP4 – Progenesis QI Software
November,	1	15:00-17:00	WP5 – Food Intolerance
November,	1	15:00-17:00	WP6 – Quality control assessment from multi-month data sets

DAY 1: OCTOBER 30, 2017 (Monday)

WP1 10:00-12:00 Room 265

PROTEOINFORMATICS

Speakers: *Veit Schwämmle*, Department of Biochemistry and Molecular Biology, University of Southern Denmark, Denmark;

Julian Uszkoreit, Medizinisches Proteom-Center, Ruhr-University Bochum, Germany

The topics of the workshop are reusable workflows for reproducible analyses of LC-MS proteomics data and the statistical analysis of quantitative LC-MS data.

Reusable workflows for reproducible analyses: We will highlight the importance of not only describing each detail of the wet lab analyses, but also the subsequent data analysis. This can be facilitated by using workflow environments like KNIME and the deposition of the workflows, together with the data, into repositories like PRIDE. In the interest of the time, the hands-on experience will be limited, but we will provide the data and tutorial material online.

Advanced statistical and multi-variate data analysis: We will give an introduction into the basic concepts of the statistical assessment of proteomics data starting with the quantitative protein/peptide measurements. Furthermore, we will show how to apply statistical testing and carry out clustering of protein expression profiles. The novel tool VSclust will be presented which combines statistics and clustering to yield better enrichment of significant features, improved cluster validation and higher output from subsequent data interpretation.

DAY 1: OCTOBER 30, 2017 (Monday)

WP2 15:30-17:30 Room 265

HOW TO WORK WITH HUMAN GENOME?Speaker: *Andrey Afanasiev, IBinom, Russia*

Main topics:

- Genome structure and genetic variability
- Data processing and the construction of the basic analysis pipeline
- Practical application of the gene panels using iBinom – alignment, calling, annotation, and quality control
- Interpretation of the data and bioinformatics predictions

DAY 2: OCTOBER 31, 2017 (Tuesday)

WP3 15:30-17:30 Room 265

**DRUG DEVELOPMENT
CLASSROOM**Speaker: *Andrey Khudoshin, PhD, MBA, Direction of chemical and biological solutions of Elsevier Company in Russia, Iran and CIS countries*

The workshop is targeted at the scientists with basic training in system biology, organic chemistry and pharmacology.

To participate in the workshop, you need to have a laptop with Internet access and a CPU, RAM, video, sufficient for fast work with any Internet sites. Windows 7 and higher, last version of Google Chrome are preferred.

To prepare for the workshop, we also recommend to get acquainted with the instructions and articles on the website of the conference.

The participants of the workshop will conduct an bioinformatic analysis of a large array of experimental data (NGS or microchips) via Pathway Studio platform to identify the biological features of the disease of the patient, including the search for activated cascades of signaling pathways and targets for personalized therapy. With the help of Pathway Studio and Reaxys Medicinal Chemistry, a personalized selection of the drugs acting on the detected targets will be carried out.

DAY 2: OCTOBER 31, 2017 (Tuesday)
 WP4 15:30-17:30 Room 274

PROGENESIS QI SOFTWARE

Speaker: **Paul Goulding**, *Nonlinear Dynamics, UK*

Progenesis® QI for proteomics enables researchers to quantify and identify proteins in complex discovery proteomics experiments using the advantages of label-free analysis. With support for all common vendor data formats and a guided workflow, Progenesis QI Software helps to overcome data analysis challenges, enabling rapid, objective and reliable discovery of proteins of interest from single or fractionated samples.

The workshop will consist of analysis of a simple LC-MS discovery proteomics experiment using Progenesis QI for proteomics software, in order to extract and identify biomarkers for three experimental conditions. This will include automatic data processing (alignment, peak picking and peptide identification) followed by review of the quantitative and statistical results to extract the best candidate biomarkers for each condition. There will be explanation of each analysis step and of the procedures for extracting the biomarkers. Participants who have previously downloaded and installed the software and data set will be able to follow and perform some steps of the analysis on their own laptops.

For more efficient and productive workshop please make yourself familiar with the software <http://www.nonlinear.com/progenesis/qi-for-proteomics/>

DAY 3: NOVEMBER 1, 2017 (Wednesday)
 WP5 15:00-17:00 Room 265

FOOD INTOLERANCE

Speakers: **Arkady Rosensteyn**, *ImmunoHealth Int., New York, U.S.A.*;
Sergey Kondakov, *M.V. Lomonosov Moscow State University, Moscow, Russia*;
Andrey Tarasevich, *Professorial clinic of the Krasnoyarsk state medical university, Krasnoyarsk, Russia*;
Natalia Cherevko, *Siberian State Medical University, Tomsk, Russia*

Demonstration of options of the computer program «ImmunoHealth™ IT»
Marina Rosensteyn, *ImmunoHealth Int., New York, U.S.A.*

The seminar is dedicated to one of the most disputed areas of medicine – food intolerance. The new concept of dietology - interaction of food antigens with the immune system of the person or “immunodietology” is introduced.

The latest achievements in the field of determining the impact of food and the food environment on modern man and, in particular:

- various aspects of interaction of food antigens with immune system;
- determination of criterion norm pathology in immunodietology on the basis of statistically established criteria (program ImmunoHealth);
- features of laboratory diagnostics of IgG using technology of dry spots of blood (DBS) allowing to receive and keep biomaterial long time without cold chain;
- results, showing that immunological approach to creation of personal programs of food allows to customize immune system for non-drug correction of pathological states and in particular to correct mitochondrial dysfunctions.

DAY 3: NOVEMBER 1, 2017 (Wednesday)

WP6 15:00-17:00 Room 274

QUALITY CONTROL ASSESSMENT FROM MULTI-MONTH DATA SETS

Speaker: *David Tabb, Stellenbosch University, South Africa*

Large-scale experiments in proteomics may require weeks or even months of instrument time. Analysis of such sets must extend beyond simple assessment of protein identifications to include more comprehensive quality control data. In this workshop, the group will examine tables of quality control metrics from the ProteoWizard QuaMeter tool in assessing the performance of an Orbitrap over eight months of data collection for the CPTAC colon cancer project. The workshop will examine the generation of metrics, multivariate assessment via robust PCA, the recognition of outliers, and the assessment of batch effects.