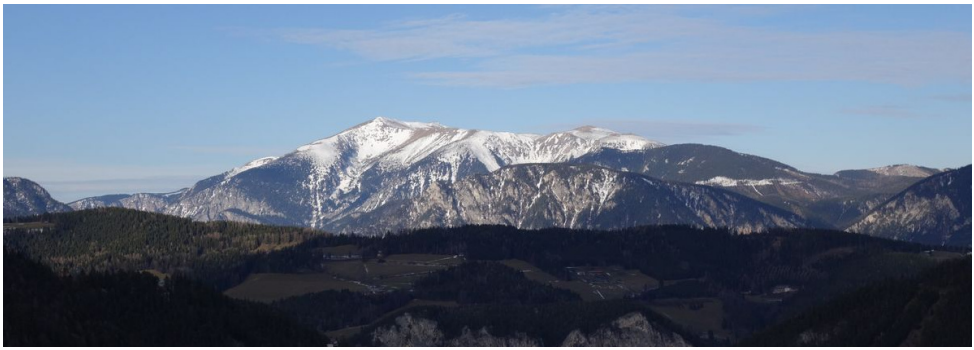

EuBIC Winter School 2017

Programme

10th – 13th January 2017, Sporthotel Semmering, Austria

EuBIC

EuPA
EUROPEAN PROTEOMICS ASSOCIATION

https://www.fh-ooe.at/eubic-ws17

Day 1 – 10. January 2017

Educational Day

Time	Title		
09:10 - 09:30	Opening Welcome & Introduction (Viktoria Dorfer and Marc Vaudel)		
09:30 - 09:45	Coffee Break		
09:45 - 12:00	Developing spectral libraries with Progenesis QI for proteomics, Part I	ELIXIR and de.NBI Hackathon	Introduction to proteomics data analysis, Part I
12:00 - 13:00	Lunch Break		
13:00 - 14:45	Developing spectral libraries with Progenesis QI for proteomics, Part II	ELIXIR and de.NBI Hackathon	Introduction to proteomics data analysis, Part II
14:45 - 15:00	Coffee Break		
15:00 - 19:00	Highlights of the latest developments of the Proteome Discoverer framework	ELIXIR and de.NBI Hackathon	Introduction to proteomics data analysis, Part III
19:00	Dinner		

Day 2 – 11. January 2017

Bioinformatics Challenges in Identification & Quantification

Time	Title	Speaker(s)
09:00 - 09:05	Morning Welcome and Announcements	Viktoria Dorfer and Marc Vaudel
09:05 - 09:55	Constructing community knowledge for peptide identification and quantification	Nuno Bandeira
09:55 - 10:15	Coffee Break	
10:15 - 11:05	Broadening the mission: quality assessment for quantitative and label-dependent MS	David Tabb
11:05 - 12:00	Poster Flash Talks of Young Investigators Part I	
12:00 - 13:00	Lunch Break	
13:00 - 13:50	Developing structural interactomics and its application in cell biology	Fan Liu
13:50 - 14:20	Company Talk	Elixir
14:20 - 14:40	Coffee Break	
14:40 - 18:40	Workshop Session	see workshop descriptions
18:40 - 19:40	Dinner	
19:40	Poster Session & Come together	

Parallel Workshops

Fan Liu	Structural Interactomics by Cross-linking Mass Spectrometry
Nuno Bandeira	Global big data challenge
Qiagen	Ingenuity Pathway Analysis
David Tabb	Proteomics without a genome: leveraging RNA-Seq from non-model organisms

Day 3 – 12. January 2017

Result Interpretation

Time	Title	Speaker(s)
09:00 - 09:05	Morning Welcome and Announcements	Karl Mechtler and Viktoria Dorfer
09:05 - 09:55	Open Data	Lennart Martens
09:55 - 10:15	Coffee Break	
10:15 - 11:05	Issues of LC-MS Quantification	Oliver Kohlbacher
11:05 - 12:00	Poster Flash Talks of Young Investigators Part II	
12:00 - 13:00	Lunch Break	
13:00 - 13:50	Reactome: the statistics behind it	Antonio Fabregat Mundo
13:50 - 14:10	Coffee Break	
14:10 - 18:10	Workshop Session	see workshop descriptions
18:10 - 19:10	Dinner	
from 19:10	Social Event	

Parallel Workshops

Jürgen Cox	on Perseus & MaxQuant
Oliver Kohlbacher	on OpenMS
Antonio Fabregat Mundo	on Reactome & Cytoscape

Day 4 – 13. January 2017

From Proteomics to Multi-Omics in Bioinformatics

Time	Title	Speaker(s)
09:00 - 09:05	Morning Welcome and Announcements	Lennart Martens and Marc Vaudel
09:05 - 09:55	Perseus, systems biology, connection to other omics fields	Jürgen Cox
09:55 - 10:30	Coffee Break & Poster Session	
10:30 - 11:25	Ontologies and Tool Annotations for Automatic Workflow Generation, Data Integration and Visualization in *omics	Magnus Palmblad
11:25 - 12:15	Announcement: Best Flash Talk and Best Poster Award	Viktoria Dorfer and Marc Vaudel
12:15 - 14:00	Lunch , Outlook and Workshop Closing	

Sponsors

Workshop Abstracts

Day 1 – 10. January 2017

Introduction to proteomics data analysis

Harald Barsnes and Marc Vaudel

Mass spectrometry based proteomic experiments generate ever larger datasets and, as a consequence, complex data interpretation challenges. In this course, the concepts and methods required to tackle these challenges will be introduced. The course will focus on protein identification and take the participant from the handling of the raw data to the statistical analysis of the identification data. The course will rely exclusively on free and user friendly software, all of which can be directly applied in your lab upon your return from the Winter School.

ELIXIR and de.NBI Hackathon

Magnus Palmblad, Jon Ison, Niall Beard, Julian Uszkoreit, Gerhard Mayer and Veit Schwaemmle

Do you want to learn about the current European initiatives for computational infrastructure and data standards in life sciences? We aim to make the computational proteomics community an integrative part of these recent developments. The hackathon, kindly sponsored by ELIXIR Denmark and in cooperation with de.NBI, is the first outreach of ELIXIR - the European Infrastructure for Biological Information - to the Proteomics Community. Current ELIXIR efforts for establishing sustainable infrastructures within computational biology will be presented. We will introduce and discuss integration of computational proteomics into ELIXIR and initiation of common projects in both research and training. The main focus is on the bio.tools registry for software annotation, workflow composition, standards for data formats and data uploads. The participants will be engaged in the discussions and task forces to deepen collaborations between ELIXIR, de.NBI and experts in computational proteomics.

Developing spectral libraries with Progenesis QI for proteomics

Waters

Learn how to use Progenesis QI for proteomics to Quantify and Identify the peptides and proteins that are significantly changing in your samples, and how you'll soon be able to develop your own customised spectral libraries to improve

the speed and specificity of your MSe searches. Bring your own laptop and download the demo software and tutorial from `http://www.nonlinear.com/progenesis/qi-for-proteomics/download/`

Highlights of the latest developments of the Proteome Discoverer framework.

Thermo

An overview of the features in the current version, PD 2.1 will be presented with emphasis on the improvements in quantification. Furthermore we will highlight the upcoming new release, including Label Free Quantification and Cross-linking.

This will be an interactive presentation with time for questions and feedback.

Day 2 – 11. January 2017

Structural Interactomics by Cross-linking Mass Spectrometry

Fan Liu

Chemical cross-linking combined with mass spectrometry (XL-MS) has emerged as a powerful approach to investigate protein conformation as well as protein-protein interactions. Especially in recent year, this technique has moved rapidly towards the analysis of very large protein assemblies and heterogeneous mixtures of protein complexes. This course is designed for scientist who is interested in using this technique to probe the structure of various proteins/protein complexes and to discover novel protein-protein interactions. The course will cover most aspects of the XL-MS workflow, including sample preparation, cross-link enrichment, MS data acquisition and cross-link data analysis. Furthermore, attendees will also be provided with practical training on XL-MS data analysis using standalone XlinkX and XlinkX PD node.

Global big data challenge

Nuno Bandeira

This "global big data challenge" workshop will focus on three key aspects of contributing to the global proteomics knowledge base: i) using advanced algorithms for discovery and inspection of post-translational modifications and highly-modified peptides; ii) sharing search results with the community at large

and reviewing results contributed by others; iii) reusing spectral libraries for peptide identification and detection in both DDA and DIA mass spectrometry data. The workshop will cover topics of relevance to both experimentalists (e.g., how to critically inspect search results) and bioinformaticians (e.g., how to share and compare results from new software tools).

IPA workshop

Mario Ricketts and Andre Koper

Ingenuity® Pathway Analysis (IPA®) is a powerful analysis and search tool that helps researchers to uncover the biological significance of 'omics data and to answer critical questions related to their studies. Built on extensive and primarily manually curated scientific content from QIAGEN's distinctive Knowledge Base, IPA's content-aware and causal analytics assists with the identification of canonical pathways, phenotypic effects, networks of interacting molecules and putative upstream drivers that help users interpret various types of 'omics experiments, including measurements of differentially expressed or phosphorylated proteins. The integration of different 'omics data is a strong focus for IPA that allows users to visualize different molecular data together and to gather evidence for a more comprehensive interpretation of experimental data with just a few mouse clicks. IPA has been cited in over 16,000 scientific publications.

This workshop will help the attendees gain an overview of IPA's capabilities and to experience its graphical user interface and approach to the biological interpretation of proteomics and phospho-proteomics datasets with or without accompanying gene expression data. As part of the workshop, we will focus on creating and interpreting IPA analyses and demonstrating tools in IPA to create, visualize and analyze causal effects of automated and user-defined molecular networks. At the end of this 4 hour session, each attendee should be able to upload and analyze their data in IPA in a comprehensive manner. In addition, QIAGEN will provide 14 day IPA trials to every attendee of this IPA workshop at the EuBIC Winterschool 2017.

Proteomics without a genome: leveraging RNA-Seq from non-model organisms

David Tabb

As proteomics spreads to an ever-larger number of applications, some researchers (particularly in agriculture) are hindered by the lack of a high-quality

genome annotation for their species of interest. In this workshop, we will examine methods for preparing a draft proteome sequence database from transcriptomic data collected through high-throughput sequencing (RNA-Seq). These stages include the following:

1. checking the quality of the sequencing reads
2. assembling the transcripts de novo
3. translating the transcripts to amino acids
4. finding nearest annotated taxonomic neighbors
5. annotating sequences by reciprocal BLAST and InterPro

Day 3 – 12. January 2017

MaxQuant/Perseus

Jürgen Cox Description: TBA

Automated processing of quantitative proteomics data with OpenMS

Oliver Kohlbacher and Julianus Pfeuffer

The workshops provides a brief introduction to OpenMS, an open-source software for computational proteomics and metabolomics. Participants will familiarize themselves with the underlying concepts and get to know a few key tools of the OpenMS tool collection. We will construct tailor-made automated data analysis workflows for database search, label-free quantification, data visualization and quality control in proteomics.

These workflows will be applied to selected example data sets. Particpants are encouraged to bring their own data and discuss the analyses required with instructors from the OpenMS team. All software used will be provided and can be installed on particpants' own computers.

Speakers: Antonio

TBA

Antonio Fabregat Mundo

Description: TBA