Workshops - Overview

There will be a list to sign up to the different workshops on site, so we can re-assign the rooms if necessary according to the number of interested participants.

Monday, May 30th, 2016, 16:30 – 18:00

1. New hyphenation techniques (Eranos, max. 42)
Heinz Singer (Eawag, CH), Lee Ferguson (Duke Uni, US), Felix Hernandez (UJI, ES)

2. Full scan (MS1) data processing (Pioda, max. 30)
Steffen Neumann (IPB Halle, DE), Martin Loos (Eawag, CH)

3. Suspect screening in the environment (Auditorium, max. 70)
Juliane Hollender (Eawag, CH), Emma Schymanski (Eawag, CH)

Tuesday, May 31st, 2016, 16:30 – 18:00

4. Statistics-based prioritization (Eranos, max. 42)
Jennifer Schollée (Eawag, CH), Gordon Getzinger (Duke Uni., US)

5. Demonstration: Workflows (I) (Pioda, max. 30)
Uwe Schmitt (ETH, CH), Martin Krauss (UFZ, DE), Heinz Singer (Eawag, CH)

6. MS/MS libraries and in silico methods (Auditorium, max. 70)
Emma Schymanski (Eawag, CH), Steffen Neumann (IPB Halle, DE)

Thursday, June 2nd, 2016, 14:00 – 15:30

7. Experimental approaches and toxicity (Eranos, max. 42)
Lee Ferguson (Duke Uni., US), Marja Lamorée (VU, NL), Martin Krauss (UFZ, DE)

8. Demonstration: Workflows (II) (Pioda, max. 30)
Aurea Chiaia-Hernandez (Eawag, CH), Thomas Letzel (TUM, DE), Pablo Gago-Ferrero (UoA, GR / SLU, SE)

9. Identification of transformation products (Auditorium, max. 70)
Michael Stravs (Eawag, CH), Jennifer Schollée (Eawag, CH), Juliane Hollender (Eawag, CH)

Thursday, June 2nd, 2016, 16:00 – 17:30

10. Retention time prediction (Auditorium, max. 70)
Martin Krauss (UFZ, DE), Nikos Thomaidis (Uni. Athens, GR)

11. Demonstration: MS/MS ID workflows (Pioda, max. 30)
Christoph Ruttkies (IPB Halle, DE), Steffen Neumann (IPB Halle, DE)

12. Workshop(s) on demand (Eranos, max. 42, or other rooms)
Decided on site – please contact the organisers to propose potential topics.

1. New hyphenation techniques

Heinz Singer (Eawag, CH), Lee Ferguson (Duke Uni, US), Felix Hernandez (UJI, ES)

Workshop #1 - New hyphenation techniques		**Minutes (Presentation+Discussion)**
Introduction		
Topic overview and setting the scene	Felix Hernandez	5
Vendor presentations		
Capillary electrophoresis coupled to Mass Spectrometry (SelexIon)	Jianru Stahl-Zeng (ABSciex)	5
Drift Tube Ion Mobility coupled to Quadrupole Time-of-Flight Mass spectrometer	Thomas Glauner (Agilent)	5
Fusion Orbitrap Mass Spectrometers coupled to Liquid Chromatograph and /or Ion Chromatography	Frans Schoutsen (Thermo)	5
Travelling Wave Ion Mobility coupled to Quadrupole Time-of-Flight Mass spectrometer	Eric Van Beelen (Waters)	5
User presentations		
Multidimensional Gas Chromatography (GCxGC) coupled to High Resolution Mass Spectrometry	Peter Haglund	5+5
Gas Chromatography coupled to Time-of-Flight Mass spectrometry via Atmospheric Pressure Chemical Ionization	Pablo Lara-Martin	5+5
Gas Chromatography coupled to Orbitrap via Electron Impact Ionization	Tobias Schulze	5+5
Two-dimensional Liquid Chromatography coupled to Orbitrap	Lee Ferguson	5+5
Supercritical Fluid Chromatography coupled to Time-of-Flight Mass spectrometry	Sofia Veloutsou	5+5
Discussion and Conclusions		
Emerging Hyphenation Techniques for non-target Screening	Discussion with all	15

Possible discussion points

- Pros and cons (limitations and opportunities) of the presented hyphenation technique
  for non-target screening of environmental contaminants
- Additional and orthogonal information to established approaches (LC-ESI-HRMS)
- - Requirements for a successful application (sample preparation, concentration range, matrix, etc)
- Consequences for workflow and software (established software workflows available)
- Suitable for which kind of environmental samples: water, sediment and biota

2. Full scan (MS1) data processing

Steffen Neumann (IPB Halle, DE), Martin Loos (Eawag, CH)

The workshop demonstrates the use of mass spectrometry analysis tools implemented in the R statistical programming environment. We will showcase the two toolsets xcms and enviMass as well as related R packages and interfaces for MS1 data processing in nontarget analysis, based on a representative environmental dataset. A focus will be on typical concepts and processes underlying the use of R packages, accompanied by workshop demos. Times given are approximations.

Workshop #2 - Full scan (MS1) data processing		**Minutes (Presentation+Discussion)**
Introduction		
Common terminology, TOF vs. Orbitrap, enviPat	Steffen Neumann Martin Loos	~20
XCMS		
Recent developments (MTBLS2 profiling package)	Steffen Neumann	~20
Pre-processing		
Peak picking with centwave	Steffen Neumann	~10
Peak picking with enviPick	Martin Loos	~10
enviMass R package	Martin Loos	~10
nontarget R package	Martin Loos	~10
Discussion and Conclusions		
Wrap-up / Questions	Steffen Neumann Martin Loos	~10

A first block briefly introduces common terminology, highlights the heterogeneity of (LC-)MS data in a comparison of TOF and Orbitrap measurements and lists widespread processing steps and open-source data formats. The webtool enviPat is used to demonstrate the influence of instrument resolution on measurable data.

A second block focuses on xcms, highlighting recent developments such as automatized workflow parameterization and the MTBLS2 profiling package.

A third block details two peak picking algorithms (centwave, enviPick) and subsequent preprocessing, filtering (blind, replicates), target screening and profiling steps as available in the R enviMass package. A further grouping of remaining nontarget peaks for ESI adducts and isotopologue peaks and homologue series relations is demonstrated using the R nontarget package, as well as a recently developed webtool. Certain pitfalls and problems in integrating R functions to workflows are explicitly addressed and the general data structures for the computational handling of LC-MS information outlined.

3. Suspect screening in the environment

Juliane Hollender (Eawag, CH), Emma Schymanski (Eawag, CH)

The goal of this workshop is to use the short (5 min each) presentations to stimulate discussion on different approaches as well as the pros and cons of suspect screening!

Workshop #3 - Suspect screening in the environment		**Minutes (Presentation+Discussion)**
Introduction		
Short Introduction	Juliane Hollender	5
User presentations		
Definition of suspect screening, presentation of Norman platform for suspect list exchange	Emma Schymanski	5
Suspect screening for CECs in plant material	Ana Martinez	5
NormaNews – first results	Kevin Thomas	5
STOFF-IDENT for suspect screening	Sylvia Grosse	5
Suspect screening in a routine lab (LR-MS)	Peter Tarabek	5
Exposure & hazard index for prioritization of suspects	Stellan Fischer	5
Suspect screening with REACH compounds	Ton van Leerdam	5
A US perspective on suspect screening	Amy Pochodylo	5
US EPA's benchmark suspect screening using ToxCast chemicals	Elin Ulrich	5
Discussion and Conclusions		
Discussion and Questions	Discussion with all	45

Possible discussion points

- Who is doing suspect screening? Who wants to do it?
- Did you compile your own list? On which data? Consumption data, European lists, Country-specific lists? How many lists do you use in your lab? Only 1, < 5, <10? Transformation products? How do you obtain identifiers?
- For which matrix are you using suspect screening? Surface water, wastewater, sediment, soil, treatment steps (before, after), lab experiments. Are there too many false positives in heavier matrices? Certain sample types better to increase true positives?
- Are you intending to use Norman lists? If so, what are the minimum requirements apart from molecular ion (structures, fragments, RT, ionization, identifier CAS v InChI)
- How many suspects become targets in your lab over time? 1 per year, 10 per year, 100 per year?

4. Statistics-based prioritization

Jennifer Schollée (Eawag, CH), Gordon Getzinger (Duke Uni., US)

This workshop will give an overview of the current statistical methods in use in nontarget screening. Available vendor and open source software will be discussed. Four users will present practical feedback on their respective tools followed by opportunity to discuss.

Workshop #4 - Statsitics-based prioritization		**Minutes (Presentation+Discussion)**
Introduction		
Introduction to statistical methods	Jennifer Schollée	15
Overview of software and implementation	Gordon Getzinger	10
User presentations		
Significance testing (univariate)	Christoph Moschet	5+10
Time trend analysis (univariate)	Merle Plassman	5+10
Pairwise comparison (univariate)	Gordon Getzinger	5+10
Principal component analysis (multivariate)	Karina Knuksmark	5+10
Discussion and Conclusions		
Wrap-up	Discussion with all	5

5. Demonstration: Workflows (I)

Uwe Schmitt (ETH, CH), Martin Krauss (UFZ, DE), Heinz Singer (Eawag, CH), Tobias Bader (Landeswasserversorgung Langenau)

Workflow tools set themselves apart from analysis tools provided as programming libraries in some aspects. In particular one-click installers and graphical user interfaces allow data analysis for researchers having no or little programming skills.

We will demonstrate the tools „envipy“ and „MZmine“ in this presentation and show how interactive data analyisis can increase confidence in the computed results.

Workshop #5 - Demonstration: Workflows (I)		**Minutes (Presentation+Discussion)**
Envipy		
Envipy – concepts	Uwe Schmitt	10
Envipy – algorithms	Uwe Schmitt	10
Envipy – case study	Tobias Bader	15
Envipy – Q & A	Uwe Schmitt, Tobias Bader, Heinz Singer	10
MZmine		
Presentation of MZmine features and demonstration of a typical MZmine nontarget screening workflow	Martin Krauss	25
MZmine – Q & A	Martin Krauss	20

6. MS/MS libraries and in silico methods

Emma Schymanski (Eawag, CH), Steffen Neumann (IPB Halle, DE)

The aim of this workshop is to provide an overview of small molecule identification with MS/MS data. Many spectral libraries, ranging from public data, to commercial and in-house libraries, are available to experimentalists and this workshop will cover basic features and the overlap of several libraries. The discussion will include how various libraries and different spectral similarity functions will perform for different purposes and how the choice can affect the outcomes.

An alternative for small molecule identification are in silico tools, which score candidate structures against the spectral data. In recent years, several options were developed, and the concepts behind some of the major approaches will be introduced.

The Critical Assessment of Small Molecule Identification (CASMI) contest has acted as a forum to compare various identification approaches since 2012, where participants have to identify unknown (to them) compounds from MS/MS spectral data. Several of the current top in silico tools participated in the 2016 CASMI contest, showing that identification approaches have improved immensely since the first contest.

Workshop #6 - MS/MS libraries and in silico methods		**Minutes (Presentation+Discussion)**
Introduction		
Welcome and Introduction	Emma Schymanski	5
User presentations		
Overview MS/MS libraries	Emma Schymanski	25
Overview in silico tools	Steffen Neumann	20
Results and insights from CASMI 2016	Steffen Neumann	20
Discussion and Conclusions		
Discussion / Question time	Discussion with all	15
Wrap-up and Summary	Emma Schymanski Steffen Neumann	5

7. Experimental approaches and toxicity

Lee Ferguson (Duke Uni., US), Marja Lamorée (VU, NL), Martin Krauss (UFZ, DE)

Goal: Discussion of the most current approaches for incorporating experimental approaches and toxicity information to identify and prioritize contaminants in non-targeted analysis.

Workshop #7 - Experimental approaches and toxicity		**Minutes (Presentation+Discussion)**
Introduction		
Topic overview and setting the scene	Lee Ferguson	10
User presentations		
Analyte ionization in ESI/APCI/APPI as evidence for structural identification	Martin Krauss	5+5
TBD	TBD	5+5
New strategies for effects-directed analysis	Marja Lamorée	5+5
Combining HRMS with invertebrate toxicity to identify causative stressors in aquatic systems	Christoph Moschet	5+5
Discussion and Conclusions		
Frontiers in experimental approaches and toxicity measurement applied to non-targeted analysis	Discussion with all	40

Possible discussion points

- What are the most relevant experimental data that can be combined with mass spectrometry measurements for compound ID?
- How best can high-content, high-throughput effects screening be performed in concert with HRMS for enhanced prioritization
- Which endpoints are most relevant for conducting effects-directed analysis?

8. Demonstration: Workflows (II)

Aurea Chiaia-Hernandez (Eawag, CH), Thomas Letzel (TUM, DE), Pablo Gago-Ferrero (UoA, GR / SLU, SE)

Workshop #8 - Demonstration: Workflows (II)		**Minutes (Presentation+Discussion)**
XCMS-online		
XCMS-online demonstration using environmental samples	Pablo Gago Ferrero	30
FOR-IDENT		
FOR-IDENT online demonstration	Thomas Letzel	30
Discussion and Conclustions		
Discussion / Question time	Discussion with all	35

9. Identification of transformation products

Michael Stravs (Eawag, CH), Jennifer Schollée (Eawag, CH), Juliane Hollender (Eawag, CH)

This workshop focuses on transformation product identification, encompassing transformation product prediction, experimental approaches, and data analysis. We welcome in particular the discussion of methods and pitfalls rather than results.

Workshop #9 - Identification of transformation products		**Minutes (Presentation+Discussion)**
Pathway prediction		
TBD	TBD	5+5
Eawag-PPS / enviPath	Kathrin Fenner	5+5
User presentations		
Combining HRMS and isotope labeling approaches	Quiguo Fu	5+5
Using electrochemistry to elucidate micropollutant transformation	Sascha Lege	5+5
Automation of transformation product identification	Rick Helmus	5+5
MS2 spectra similarity of TP pairs	Jennifer Schollée	5+5
Discussion and Conclusions		
Reality check and confidence levels	Michele Stravs	10
open discussion	Discussion with all	20

10. Retention time prediction

Martin Krauss (UFZ, DE), Nikos Thomaidis (Uni. Athens, GR)

Goal: Discuss current approaches for RT prediction and indexing and suggest a strategy how to move on with development and harmonization

Workshop #10 - Retention time prediction		**Minutes (Presentation+Discussion)**
User presentations		
Setting the scene: RT prediction/indexing in nontarget/suspect screening and compound identification	Martin Krauss	5+5
The Retention Time Index in StoffIdent – Experiences with its application	Thomas Letzel	5+5
A modular approach for a wide-scope and transferable RT prediction/indexing for NORMAN to facilitate data exchange	Nikos Thomaidis	5+5
Discussion and Conclusions		
Emerging Hyphenation Techniques for non-target Screening	Discussion with all	50
Wrap-up and Conclusions	Martin Krauss / Nikos Thomaidis	10

Possible discussion points

- Balancing complexity of models and ease of use
- How can we implement a RT prediction/indexing system to allow a harmonization among different methods/groups?
- How should calibration compound sets for RT prediction models look like?

11. Demonstration: MS/MS ID workflows

Christoph Ruttkies (IPB Halle, DE), Steffen Neumann (IPB Halle, DE)

Small molecule identification from MS/MS data is one of the very time consuming tasks in nontarget screening. In silico fragmentation tools have come a long way in the past years. In this workshop, we will focus on MetFrag and different available options (web application, command line, R package). We also demonstrate the use of different components in the scoring function.

Call for participant data: if you want us to work live on your data, please prepare your MS/MS spectrum as peak list and contact us before Thursday.

Workshop #11 - Demonstration: MS/MS ID workflows		**Minutes (Presentation+Discussion)**
Introduction		
Welcome and Introduction	Steffen Neumann	5
User presentations		
Steps (training, candidate retrieval, scoring, post processing)	Steffen Neumann	15
Demo CFM-ID with selected CASMI Challenge(s)	Christoph Ruttkies	10
Demo MetFrag with selected CASMI Challenge(s), scoring options	Christoph Ruttkies	10
Different options: command line, R package	Christoph Ruttkies	10
Time for experimenting, own data, etc.	Steffen Neumann Christoph Ruttkies	30
Discussion and Conclusions		
Wrap-up and Summary	Steffen Neumann Christoph Ruttkies	5