

## Introduction

The 'SWEMSA 19' Workshop intends to continue the exciting international dialogue that had started in 2016 at the 'Non-Target Conference 2016' in Ascona and the 'SWEMSA 16' in Garching and is ongoing since in many meetings, workshops, and conferences.

This workshop will extend the discussion in view on Non-Target Screening main topics like the following:

- 'Computational Mass Spectrometry',
- 'NTS in Forensics',
- 'NTS in Food(omics)',
- 'NTS in Metabolomics',
- 'NTS in Commercial Solutions',
- 'NTS (Guideline) in Water Analysis'
- 'NTS in Environmental Analysis'.

This Workshop will bring together leading international scientists from various consortia. SWEMSA intends to inform, combine and harmonize the NTS strategies and workflows from each single discipline to extend the NTS horizon and to give us all the chance to 'have a look over the edge'. Participants of various disciplines like chemistry, food, forensic, informatics, metabolomics and instrumental analysis will jointly discuss latest developments. The program will feature a solution-focused discussion strategy including overview talks and panel discussions in each slot.

The overall aim of this meeting is to condense and harmonize various common aspects of NTS, to extend the use of software and workflow strategies and to learn about the potential of NTS applied in various disciplines. We are looking forward to welcoming you in Erding later this year. Thomas Letzel and Colleagues

## Registration

The total workshop costs of € 195.- cannot be split into days. **Registration until 31.08.19!**

For further details, please contact:

Dr. Linda Bichlmeier PD Dr. Thomas Letzel  
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## Meeting Place

**Stadthalle Erding (City Hall Erding)**

Alois-Schießl-Platz 1, D-85435 Erding, Germany

Further options and information can be found on:

[www.swemsa.eu](http://www.swemsa.eu)

## Program

### Monday, 21<sup>st</sup> October 2019

- 11:00 Registration and Vendor Exhibition Opening (booth visits 11.00-12.00)
- 12:00 **Welcome and Introduction**
- 12:15 **What happened since SWEMSA 2016?**  
PD Dr. Thomas Letzel  
(TUM, Munich, DE)
- 12:45 **Finding small molecules in big data**  
Assoc. Prof. Dr. Emma Schymanski  
(LCSB, Uni.Luxembourg, Belvaux, LU)

#### Subject Area: Computational Mass Spectrometry

Chair: Assoc. Prof. Dr. Emma Schymanski

- 13:15 **patRoom: Open source software platform for MS based NTS in the environment**  
Rick Helmus  
(UvA-IBED, Amsterdam, NL)
- 13:45 **SIRIUS 4 and CSI:FingerID: Turning tandem mass spectra into metabolite structure information**  
Prof. Dr. Sebastian Böcker  
(Friedrich-Schiller-University, Jena, DE)
- 14:15 **Monitoring chemical water quality through integration of non-target and effect-based screening**  
Dr. Andrea Mizzi Brunner  
(KWR, Nieuwegein, NL)
- 14:45 **The ENTACT story: Using US EPA resources to evaluate and enhance non-target workflows**  
Dr. Jon Sobus  
(NERL, US EPA, North Carolina, US)

- 15:15 **Panel Discussion regarding:**  
Computational Mass Spectrometry

- 16:00 **Coffee Break / Exhibition**

#### Subject Area: Non-Target Screening in Forensics

Chair: Prof. Dr. Herbert Oberacher

- 16:30 **Drug use confirmation by non-target LC-MS/MS**  
Prof. Dr. Herbert Oberacher  
(Medical University of Innsbruck, AT)

- 17:00 **Data-driven analysis in forensic toxicology drug screening**  
Dr. Christian Brinch Mollerup  
(University of Copenhagen, DK)
- 17:30 **Metabolite based LC-MS<sup>n</sup> drug screening for routine analysis - a non-targeted low resolution MS workflow**  
Dr. Dirk Wissenbach  
(Rechtsmedizin Jena, DE)
- 18:00 **Panel Discussion regarding:**  
Non-Target Screening in Forensics

#### Evening Lecture

- 18:30 **Surprise Lecture**

#### Evening Event – Vendor Evening

Bavarian Buffet and Drinks

### Tuesday, 22<sup>nd</sup> October 2019

- 08:00 **Welcome and Introduction**

#### Subject Area: Non-Target Screening in Food(omics)

Chair: Prof. Dr. Elke Richling

- 08:05 **Nutrimetabolomics - About the interaction of food with human metabolism**  
Prof. Dr. Sabine E. Kulling  
(Max-Rubner-Institut, Karlsruhe, DE)
- 08:35 **METAVISION: A NMR-based metabolomics platform**  
Dr. Jean-Marie Colet  
(UMONS, Mons, BE)
- 09:05 **Development, validation and accreditation of metabolomics approaches - A chemical risk management study in food**  
Dr. Gaud Dervilly-Pinel  
(LABERCA, Nantes, FR)
- 09:35 **Metabolomics of plasma and urine as a tool: Nutrikinetics of plant polyphenols**  
Prof. Dr. Fulvio Mattivi  
(C3A, San Michele all'Adige, IT)
- 10:05 **Panel Discussion regarding:**  
Non-Target Screening in Food(omics)
- 10:50 **Coffee Break / Exhibition**

## Subject Area: Non-Target Screening in Metabolomics

Chair: Dr. Michael Witting

11:10 **Handling and processing of metabolomics data with Bioconductor's MSnbase and xcms packages**  
Dr. Johannes Rainer,  
(Eurac Research, Bolzano, IT)

11:40 **Metabolome mining and annotation strategies to decipher complex mixtures**  
Dr. Justin van der Hoof  
(Wageningen University, Wageningen, NL)

12:10 **Network based solutions to improve metabolic profile interpretation**  
Dr. Fabien Jourdan  
(INRA, Toulouse, FR)

12:40 **Panel Discussion regarding:**  
Non-Target Screening in Metabolomics

13:10 **Lunch Break / Exhibition**

## Subject Area: Commercial NTS Solutions by LC-MS/MS Vendors and Others

Chair: PD Dr. Thomas Letzel

14:10 **NTS Workflow Presentations (Commercial LC(GC)-MS/MS Solutions)**  
(e.g., Agilent, Bruker, Leco, Sciex, Thermo-fisher, Waters)

15:40 **Panel Discussion regarding:**  
NTS Vendor Solutions- Past, Presence and Future

16:40 **Coffee Break / Exhibition**

## Subject Area: Commercial NTS Solutions by Software Developer

Chair: PD Dr. Thomas Letzel

17:10 **NTS Workflow Presentations (Vendor-independent Software Solutions)**  
(e.g., EnviMass, Lablicate, etc.)

17:40 **Panel Discussion regarding:**  
NTS Software Solutions- Past, Presence and Future

## Evening Event

local event in Erding (incl. sightseeing)

## Wednesday, 23<sup>th</sup> October 2019

08:00 **Welcome and Introduction**

## Subject Area: NTS (Guideline) in Water Analysis

Chair: Prof. Dr. Torsten C. Schmidt

08:05 organized by the 'FA Non Target Screening' (German Water Chemistry Society)  
**Suspect and non-target screening in water resources**

Prof. Dr. Torsten C. Schmidt, (Univ. Duisburg-Essen & IWW Water Centre, DE)  
**Assessment of water treatment processes by NTS**

Dr. Tobias Bader (LW, Langenau, DE)  
**Data Platform for NTS analysis of Rhine water**

Dr. Steffen Ruppe (ICPR, EG-SANA and AUE, Basel, CH)  
**A first guideline towards standardization of non-target screening**

Dr. Wolfgang Schulz (LW, Langenau, DE)

09:50 **Panel Discussion regarding:**  
NTS in Water Analysis - Guideline

10:20 **Coffee Break / Exhibition**

## Subject Area: NTS in Environmental Analysis

Chair: Dr. Jaroslav Slobodnik

10:45 Organized by the 'NORMAN network'  
**Overview on NTS activities in NORMAN**  
Prof. Dr. Julianne Hollender, (Eawag, CH)  
**Retention Time Index**  
Prof. Dr. Nikos Thomaidis, (Uni Athens, GR)

**NORMAN MassBank**  
Dr. Tobias Schulze, (UFZ, DE)

**NORMAN Digital Sample Freezing Platform**  
Dr. Nikiforos Alygizakis, (EI, SK)

**NORMAN guideline for NTS**  
Dr. Martin Krauss, (UFZ, DE)

12:30 **Panel Discussion regarding:**  
Harmonization and application of NTS in Europe

13:00 **Wrap Up and Conclusion**

13:15 **Optional:**

-14:15 **Live Presentations of NTS software**

21. - 23. October 2019

Erding / Munich



# Non-Target Screening embedded in (Open Access) Platforms and Multi- disciplinary Applications

PD Dr. T. Letzel

**Advisory Board:**

Valeria Dulio

Prof. Dr. Herbert Oberacher

Prof. Dr. Elke Richling

Prof. Dr. Torsten Schmidt

Dr. Wolfgang Schulz

Assoc. Prof. Dr. Emma Schymanski

Dr. Michael Witting

## S W E M S A 19

(Solutions and Workflows

in (Environmental) Molecular Screening  
and Analysis)

An international, interdisciplinary workshop realized  
in kind collaboration and our funding by:

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