# Program

**Monday, 21st October 2019**

<table>
<thead>
<tr>
<th>Time</th>
<th>Activity</th>
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<tbody>
<tr>
<td>11:00</td>
<td>Registration and Vendor Exhibition Opening (booth visits 11.00-12.00)</td>
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<tr>
<td>12:00</td>
<td>Welcome and Introduction</td>
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<tr>
<td>12:15</td>
<td>What happened since SWEMSA 2016?</td>
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<tr>
<td>12:15</td>
<td>PD Dr. Thomas Letzel (TUM, Munich, DE)</td>
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<tr>
<td>12:45</td>
<td>Finding small molecules in big data</td>
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<td>13:15</td>
<td>patRoom: Open source software platform for MS based NTS in the environment</td>
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<td>13:15</td>
<td>Rick Helmus (UvA-IBED, Amsterdam, NL)</td>
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<td>13:45</td>
<td>SIRIUS 4 and CSI:FingerID: Turning tandem mass spectra into metabolite structure information</td>
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<td>13:45</td>
<td>Prof. Dr. Sebastian Böcker (Friedrich-Schiller-University, Jena, DE)</td>
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<td>14:15</td>
<td>Monitoring chemical water quality through integration of non-target and effect-based screening</td>
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<td>14:15</td>
<td>Dr. Andrea Mizzi Brunner (KWR, Nieuwegein, NL)</td>
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<td>14:45</td>
<td>The ENTACT story: Using US EPA resources to evaluate and enhance non-target workflows</td>
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<td>14:45</td>
<td>Dr. Jon Sobus (NERL, US EPA, North Carolina, US)</td>
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<tr>
<td>15:15</td>
<td>Panel Discussion regarding: Computational Mass Spectrometry</td>
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<tr>
<td>16:00</td>
<td>Coffee Break / Exhibition</td>
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**Tuesday, 22nd October 2019**

<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
<td>08:00</td>
<td>Welcome and Introduction</td>
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<tr>
<td>08:05</td>
<td>Nutr metabolomics - About the interaction of food with human metabolism</td>
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<td>08:05</td>
<td>Prof. Dr. Sabine E. Kulling (Max-Rubner-Institut, Karlsruhe, DE)</td>
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<td>08:35</td>
<td>METAVISION: A NMR-based metabonomics platform</td>
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<td>08:35</td>
<td>Dr. Jean-Marie Colet (UMONS, Mons, BE)</td>
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<td>09:05</td>
<td>Development, validation and accreditation of metabonomics approaches - A chemical risk management study in food</td>
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<td>09:05</td>
<td>Dr. Gaud Dervilly-Pinel (LABERCA, Nantes, FR)</td>
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<td>09:35</td>
<td>Metabolomics of plasma and urine as a tool: Nutrikinetics of plant polyphenols</td>
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<td>09:35</td>
<td>Prof. Dr. Fulvio Mattivi (C3A, San Michele all’Adige, IT)</td>
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<tr>
<td>10:05</td>
<td>Panel Discussion regarding: Non-Target Screening in Food(omics)</td>
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<tr>
<td>10:50</td>
<td>Coffee Break / Exhibition</td>
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# 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 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
info@swemsa.eu tech@swemsa.eu

# 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
Wednesday, 23rd 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
Optional:
Live Presentations of NTS software

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 Hooft (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)
Panel Discussion regarding:
NTS Vendor Solutions- Past, Presence and Future
15:40 Coffee Break / Exhibition

Subject Area: Commercial NTS Software Developer Workshop
Chair: PD Dr. Thomas Letzel
17:10 NTS Workflow Presentations (Vendor-independent Software Solutions)
(e.g., Lablicate, Looscomputing, etc.)
Panel Discussion regarding:
NTS Software Solutions- Past, Presence and Future
17:40 Evening Event
local event in Erding (incl. sightseeing)

S W E M S A 19
(Solutions and Workflows in (Environmental) Molecular Screening and Analysis)
An international, interdisciplinary workshop in kind collaboration and
realized by:
with:
our sponsors:
and our funding partner: