Introduction

The 'SWEMSA 16' Workshop intends to continue the exciting dialogue that was started earlier this year at the 'Non-Target Conference 2016' in Ascona.

This workshop will focus on the following topics:

- '**Open access platforms in Non-Target Screening (NTS)'**,
- '**Commercial software solutions in NTS'**,
- '**Holistic NTS workflows and solutions**',
- '**NTS in epidemiology, toxicology, molecule degradation in environmental analysis'**,
- **'NTS and linkages to different disciplines'.**

This Workshop will bring together international leading scientists from the NORMAN initiative, ESSEM COST Action ES1307, ESSEM COST Action ES1202, NEREUS-COST Action ES1403 and many other international consortia. SWEMSA combines and intends to harmonize for the first time analytical topics of the NORMAN and the three environmental COST Action initiatives. Participants from these consortia and various other disciplines like chemistry, food, forensic, informatics, toxicology and instrumental analysis will jointly discuss latest developments.

The program will feature a solution-focused discussion strategy including flip chart discussions, online TED talks, panel discussions and overview talks.

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 Garching later this year.

Thomas Letzel and Jörg E. Drewes

Registration

https://www.sww.bgu.tum.de/veranstaltungen/swemsa-2016/ The total workshop costs of € 175.- cannot be split into days.   Registration until 25.09.16!
For further details, please contact:
Gudrun Lampart   Prof. Dr. Thomas Letzel
g.lampart@tum.de   T.Letzel@tum.de

Program

Wednesday, 2nd November 2016

13:00   **Welcome and Introduction**
Prof. Dr. Thomas Letzel
(TUM, Munich, Germany)

13:15   **enviPath–Towards an essential resource for environmental metabolomics**
PD Dr. Kathrin Fenner
(Eawag, Zürich, Switzerland)

Subject Area: COST / NORMAN Action Themes
Chairman: Prof. Dr.-Ing. Jörg E. Drewes
13:45   **Potential of HRMS (LC-QTOF MS) in wastewater drug testing**
Dr. Lubertus Bijlsma
(University Jaume I, Castellón, Spain)

14:15   **Moving away from EIC-based screening workflows in HRMS: The rise of spectral analysis and meta-data**
Dr. Malcolm Reid
(NIVA, Oslo, Norway)

14:45   **Employment of PCA for comparing the formation of degradation products when applying AOPs after biological treatment**
Dr. Giuseppe Mascolo
(National Research Council, Bari, Italy)

15:15   **Coffee Break** (with 'flip chart' discussion)

Subject Area: Open Access/Source Software in Instrumental (Environmental) Analysis
Chairman: Prof. Dr. Frank Lesske
16:00   **The History of**
a) EnviPy (R tool)
Dr. Uwe Schmitt
(ETH, Zürich, Switzerland)

b) FOR-IDENT (Vaadin tool)
Marco Luthardt
(HSWT, Freising, Germany)

c) OpenChrom (Eclipse tool)
Dr. Philip Wenig
(Lablicate, Hamburg, Germany)

17:30   **STOFF-IDENT and other open access chemical databases**
Dr. Marion Letzel
(LfU, Wielenbach, Germany)

18:00   **Myths and truths about small molecular identification with tandem MS databases**
Prof. Dr. Herbert Oberacher
(Medical University, Innsbruck, Austria)

Evening Lecture by TUM Water Cluster:
18:30   **Towards the development of resilient water systems**
Prof. Dr.-Ing. Jörg E. Drewes
(TUM, Munich, Germany)

Evening Event
Buffet and drinks at the IAS

Thursday, 3rd November 2016

08:45   **Welcome and Introduction**
Prof. Dr. Thomas Letzel
(TUM, Munich, Germany)

Subject Area: Open Access/Source Software in Analysis of Various Disciplines
Chairman: Dr. Jaroslav Slobodnik
09:00   **Open access software, workflows and databases for metabolite identification in non-targeted metabolomics**
Dr. Michael Witting,
(Helmholtz Centre, Munich, Germany)

09:30   **Developments and challenges in suspect and non-target screening of air**
Dr. Pawel Rostkowski
(NILU, Kjeller, Norway)

10:00   **Coffee Break** (with 'nomenclature' survey)

10:30   **Targeted and non-targeted drug screening in whole blood by UHPLC-TOF-MS**
Christian Brinch Mollerup
(University, Kopenhagen,Denmark)

11:00   **Targeted, semi-targeted and non-targeted screening approaches for food analysis**
n.n.

11:30   Panel Discussion regarding:
Common NTS solutions initiated from different disciplines

12:30   **Lunch Break**

Program

Subject Area: Commercial NTS Solutions by LC-MS(/MS) Vendors and others
Chairman: Prof. Dr. Thomas Letzel

13:30 **NTS Workflow Presentations (Commercial Solutions)**
(e.g., Agilent, Bruker, Sciex, Shimadzu, Thermo, Waters, ACD/Labs)

15:00 Panel Discussion regarding:
Commercial NTS Solutions-Past, Presence and Future

16:00 **Coffee Break** (with 'LC-MS' survey)

Subject Area: Public Domain NTS Solutions using Open Access/Source Software
Chairman: Dr. Manfred Sengl

16:30 **Structure identification using HRMS data and the EPA CompTox Dashboard**
Dr. Antony Williams
(EPA, North Carolina, USA)

17:00 **Computational MS from the R/Bioconductor Open Source world to the cloud.**
Dr. Steffen Neumann
(IPB, Halle, Germany)

17:30 **Retention time indexing and modelling**
Prof. Dr. Thomas Letzel
(TUM, Munich, Germany)

18:00 Panel Discussion regarding:
Public Domain NTS Solutions-Past, Presence and Future

Evening Event
Restaurant in Garching

Friday, 4th November 2016

08:45 **Welcome and Introduction**
Prof. Dr. Thomas Letzel
(TUM, Munich, Germany)

Subject Area: NTS in Water analysis - Do we need any Harmonization?
Chairman:

09:00 organized by the 'FA Non Target Screening' (German Water Chemistry Society)
NTS-applications in water analysis: Approaches for contaminants and TPs
Prof. Dr. Christian Zwiener
(University, Tübingen, Germany)

Results of two interlaboratory studies
Thomas Lucke
(LW, Langenau, Germany)
Guidance for NTS in water analysis
Dr. Wolfgang Schulz
(LW, Langenau, Germany)

10:00 Panel Discussion regarding:
NTS in Water Analysis - Harmonization

11:00 **Coffee Break** (Wrap Up Break)

11:30 **Wrap Up and Conclusions**

12:30 **Optional:**
-13:30 **Live Presentations of NTS software**

Meeting Place

Technical University of Munich
Institute for Advanced Study
Lichtenbergstraße 2 a
85748 Garching, Germany

By Public Transportation from Munich Main Station:
From Munich Central Station (Hauptbahnhof) take the U4 (eastbound towards 'Arabellapark') to Odeonsplatz Station. At Odeonsplatz change from the U4 line to the U6 line (northbound towards 'Garching Forschungsgelände'. Exit at the final stop 'Garching Forschungsgelände'. Once at the final stop, use the exit 'Lichtenbergstrasse'. You can see the IAS building right in front of you (walking distance about 200m) **approx. 30 min**

By Car from the Airport:
Coming from Munich Airport merge onto the autobahn A92 toward Munich. At the interchange "Neufahrn" keep right and follow the signs for A9 toward Munich. Take exit "Garching Nord" toward Forschungszentrum/TUM. Alternatively, take the A92 as above, then exit at "Freising Süd" for highway B11 toward Munich. Take exit "Hochschul- und Forschungszentrum / TUM", Zufahrt Nord". **approx. 20-30 min**

Further options can be found at: http://www.tum-ias.de/fileadmin/material_ias/pdf/general_IAS/TUM-IAS_Directions/TUM-IAS_travel_contact_Garching_English_AKTUELL.pdf

Closest Hotels:
- Hotel IBIS München Garching
- Hotel König Ludwig II. Garching
- Hotel am Park, Garching
- Hotel Motel One München – Garching
- Hotel Garni Maria's Inn, Garching
or others close to the U6 line stations (close to Garching)

2.- 4. November 2016

Garching / Munich

Non-Target Screening
embedded in
(Open Access) Platforms
and its role
in various disciplines

Prof. Dr. T. Letzel
Prof. Dr.-Ing. J.E. Drewes

S W E M S A 16
(Solutions and Workflows in Environmental Molecular Screening and Analysis)

An international, interdisciplinary workshop in kind collaboration with:

with participation of members from

ESSEM COST Action ES1307 (http://score-cost.eu/)
ESSEM COST Action ES1202 (http://www.water2020.eu/)
NEREUS-COST Action ES 1403 (http://www.nereus-cost.eu)