



Analytisches Forschungsinstitut für Non-Target
Screening GmbH

International Conference on Non-Target Screening (ICNTS 21)

04. – 07. October 2021

**Erding, Germany
and online**

**PD Dr. T. Letzel
Dr. Stefan Bieber**

Advisory Board:

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Dr. Michael Witting

International Conference on Non-Target Screening 2021

In the recent years, there were several very successful workshops for Non-Target Screening (NTS), which started in 2016 at the Non-Target meeting in Ascona, continuing with 'SWEMSA 2016' in Garching, many SETAC meetings, ACS, RCS and GDCh events, SWEMSA 2019 in Erding and lastly digital 2020 at the 'Analytica' as well as at the 'GC meets NTS' in early 2021.

Now, Non-Target Screening and its applications are in the focus of its own INTERNATIONAL CONFERENCE

This conference will bring together leading international scientists from various consortia and disciplines. It is the ideal location for free lab, industrial and academic researchers to exchange information with other colleagues internationally, interdisciplinary and inter-professionally. NTS users from all over the world, vendors from the field of instrumental analysis and software developments will present their latest results and ideas in keynote lectures, lecture sessions and poster sessions.

The ICNTS 21 is being held as a **hybrid conference** (online and on-site in Erding, Germany) between **04. – 07. October 2021**.

This conference will promote discussion on NTS main topics, such as:

- **Computational Mass Spectrometry₇**
- **NTS in Metabolomics₇**
- **NTS in Environmental Analysis₇**
- **GC-MS goes NTS₇**
- **NTS in Doping and Forensics₇**
- **Special Chromatography meets NTS₇**
- **Ion Mobility meets NTS₇**
- **NTS in Food(omics)₇**
- **NTS (Guideline) in Water Analysis**
- **NTS Quality and Tox Transfer**
- **Commercial Solutions**

With various instrumental setups and strategies, such as **LC-MS(/MS), GC-MS(/MS), SFC-MS(/MS), Multidimensional Chromatography** and other techniques in NTS like ion mobility, etc.

International Conference on Non-Target Screening 2021

The overall aim of this meeting is to condense, standardize and harmonize various common aspects of NTS, to extend the use and understanding 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

To register, please visit

<https://afin-ts.de/icnts21/>

Registration fees:

- online participation 360 €

Registration is possible for online participation until 26.09.21.

For further details, please contact:

education@afin-ts.de

Venue:

Stadthalle Erding (City Hall Erding)
Alois-Schießl-Platz 1
D-85435 Erding, Germany



AFIN-TS GmbH
Am Mittleren Moos 48
86167 Augsburg
www.afin-ts.de
info@afin-ts.de

Analytisches Forschungsinstitut für Non-Target Screening GmbH
Sitz der Gesellschaft: Wallerstein
Amtsgericht Augsburg, HRB 32307
Geschäftsführer: Dr. Thomas Letzel und Dr. Stefan Bieber

Program**Monday, 04. October 2021**

- 11:00 Registration and Vendor Exhibition
Opening
- 12:00 **Welcome and Introduction**
- 12:15 **What happened since SWEMSA 2019?**
PD Dr. Thomas Letzel
(AFIN-TS, Augsburg, DE)
- 12:45 **Non-Target Screening at the Future Lab**
Dr. Jochen Türk
(IUTA, Duisburg, DE)

Subject Area: Computational Mass Spectrometry

Chair: Assoc. Prof. Dr. Emma Schymanski

- 13:15 **Turbocharging non-target screening workflows using open data in PubChem**
Evan Bolton
(NIH, Bethesda, MD, USA)
- 13:45 **From centroided to profile mode**
Saer Samanipour et al.
(University of Amsterdam, Amsterdam, NL)
- 14:00 **Dynamic binning peak detection for LC-MS**
Xiaodong Feng et al.
(University Medical Center Groningen, Groningen, NL)
- 14:15 **Alternative multivariate approaches to untargeted LC/GC-MS data analysis-**
Andrea Jr Carnoli et al.
(Radboud University, Nijmegen, NL)
- 14:30 Coffee Break / Exhibition
- 14:45 **HaloSeeker, highlight halogenated chemicals in NTS**
Ronan Cariou et al.
(LABERCA, INRAE, Nantes, FR)

- 15:00 **Online Prioritization of Toxic Compounds**
Nienke Meekel et al.
(KWR Water Res. Inst., Nieuwegein, NL)
- 15:15 **patRoom 2.0: Comprehensive NTS workflows incl. automated transformation product screening and other improvements**
Rick Helmus et al.
(UvA-IBED, Amsterdam, NL)
- 15:30 **Panel Discussion regarding:**
Computational Mass Spectrometry
- 16:40 Coffee Break / Exhibition

Subject Area: NTS in Metabolomics

Chair: Dr. Michael Witting

- 17:15 **Metabolomics by non-target LC-MS/MS**
Warwick Dunn
(University of Birmingham, Birmingham, UK)
- 17:45 **Variable Selection in Untargeted Metabolomics and the Danger of Sparsity**
Gerjen H. Tinnevelt et al.
(Radboud University, Nijmegen, NL)
- 18:00 **A multi-lab NTS approach for SS of pesticide metabolites in human urine**
Arjen Lommen et al.
(WFSR, Wageningen, NL)
- 18:15 **NTS on thyroid hormone system disrupting compounds on the mouse plasma metabolome**
Rikke Poulsen et al.
(Aarhus University, Roskilde, DK)
- 18:30 **Panel Discussion regarding:**
Non-Target Screening in Metabolomics
- 19:10 Break

Evening Lecture

- 19:30 **Science & Society: How to think about a complex relationship**
Sophia Rossmann
(TUM, Munich, DE)
- 20:00 **Evening Event – Vendor Evening**
Bavarian Buffet and Drinks

Tuesday, 05. October 2021

- 08:30 Registration and Vendor Exhibition
- 09:00 **Welcome and Introduction**

Subject Area: NTS in Environmental Analysis

Chair: Dr. Leon Barron

- 09:05 **Machine-learning assisted emerging contaminant screening of passive sampler and invertebrate extracts**
Leon Barron et al.
(Imperial College London, London, UK)
- 09:35 **Online database and analysis platform f. NTS data for chemical water monitoring**
Ina Fettig et al.
(UBA, Dessau-Roßlau, DE)
- 09:55 **Posidonia oceanica Seagrass: A Comprehensive Array Using HRMS**
Marina Astudillo-Pascual
(University of Almeria, Almeria, ES)
- 10:10 **Prediction of disinfection byproduct formation during water treatment (in NTS)**
Maria Jose Farre et al.
(ICRA, Girona, ES)

- 10:25 **Detection of non-conventional halogenated disinfection by-products**
Josep Sanchis et al.
(ICRA, Girona, ES)
- 10:40 Coffee Break / Exhibition
- 11:00 **Evaluation of the human exposure to organic chemicals and potential use of sew. sludge to prioritize haz. substances**
Ruben Gil-Solsona et al.
(IEAWR, Barcelona, ES)
- 11:20 **Panel Discussion regarding:**
Non-Target Screening in Environment
- 12:20 Lunch Break / Exhibition

Subject Area: GC-MS goes NTS

Chair: Prof. Dr. Karl Jobst

- 13:20 **NTS with GC-APCI-MS and computational chemistry**
Karl J. Jobst et al.
(MUNL, St. John's, CA)
- 13:50 **A time-trend study in the Baltic top consumers using NTS workflow**
Andriy Rebryk et al.
(Umeå University, Umeå, SE)
- 14:10 **NTS of semi-volatile compounds by GC - HT proton transfer reaction MS**
Vera Reinstadler et al.
(Medical University of Innsbruck, AT)

Subject Area: NTS in Doping

Chair: Prof. Dr. Herbert Oberacher

- 14:30 **New challenges in doping controls**
Andreas Thomas
(German Sport University Cologne, DE)
- 15:00 **Panel Discussion regarding:**
NTS with GC-MS as well as NTS in Doping
- 15:40 Coffee Break / Exhibition

- Subject Area: Commercial NTS Solutions by GC-MS(/MS) Vendors and Others**
Chair: PD Dr. Thomas Letzel
- 16:00 **NTS Workflow Presentations (Commercial GC-MS/MS Solutions)**
(e.g., Gerstel, Lablicate, Leco, MSCi, SepSolv, TOFWERK)
- 16:50 **Panel Discussion regarding:**
NTS Vendor Solutions- Past, Presence and Future
- 17:50 **Poster Session and Exhibition**
Presenting Posters with even numbers

Evening Lecture

- 18:50 **Individual Presentation Techniques**
Stefan Moser
(Stefan Moser Prozess Optimierung, Nussdorf, DE)
- 19:20 **Evening Event**
local event in Erding (incl. sightseeing)

Wednesday, 06. October 2021

- 08:30 Registration and Vendor Exhibition
- 09:00 **Welcome and Introduction**

Subject Area: Special Chromatography meets NTS

Chair: Dr. Jochen Türk

- 09:05 **Exploring different chromatographic modes for the determination of contaminants of emerging concern in water**
Jose B. Quintana et al.
(Universidade de Santiago de Compostela, ES)

- 09:25 **Column switching for automated online enrichment and separation of polar and nonpolar analytes**
Kjell Kochale et al.
(IUTA, Duisburg, DE)
- 09:40 **NTS for plant protection product characterization: Use of chromatographic techniques-HRMS**
Roberto Romero-González et al.
(University of Almería, ES)
- 09:55 **Suspect screening strategies to identify transformation products after uptake by Pak Choi vegetable**
Adria Sunyer-Caldú et al.
(CSIC, Barcelona, ES)
- 10:10 **Panel Discussion regarding:**
Special Chromatography meets NTS
- 10:50 Coffee Break / Exhibition

Subject Area: Ion Mobility meets NTS

Chair: Dr. Lubertus Bijlsma

- 11:15 **Ion mobility separations: the additional value to HRMS screening strategies**
Lubertus Bijlsma
(University Jaume I, Castello, ES)
- 11:45 **Prospects for ion mobility-MS in addressing small molecule questions**
Tim Causon et al.
(BOKU, Vienna, AT)
- 12:00 Lunch Break / Exhibition
- 13:00 **Ion Mobility-HRMS for Screening of CECs - Database Compilation and Application to Plastics Samples**
Lidia Belova et al.
(University of Antwerp, Antwerp, BE)

13:15 **Enhancing Spec. Quality / Peak Annotation in Biota with Ion Mobility Separation**

Frank Menger et al.
(Swedish University of Agricultural Sciences, Uppsala SE)

13:30 **Panel Discussion regarding:**
Ion Mobility meets NTS

Subject Area: NTS in Foodomics

Chair: Prof. Dr. Elke Richling

14:10 **NTS and Suspect Screening Analyses for Food Safety Applications: Data Quality and Implemented Approaches**

Ann L. Knolhoff
(US FDA, MD, USA)

14:40 **Simplifying and adapting to changes in the analysis of food contaminants with GC HRMS(/MS)**

Jim Garvey. (Department of Agriculture, Food and the Marine, Celbridge, Ireland)

14:55 **Optimizing the acquisition and data-processing workflow in suspect screening of antibiotics in archive matrices using LC-HRMS**

Rosalie Nijssen et al.
(WFSR, Wageningen, NL)

15:10 **Panel Discussion regarding:**
Non-Target Screening in Food(omics)

15:40 Coffee Break / Exhibition

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

Chair: PD Dr. Thomas Letzel

16:00 **NTS Workflow Presentations (Commercial LC-MS/MS Solutions)**
(e.g., Agilent, Bruker, Sciex, Shimadzu, ThermoFisher, Waters)

17:00 **Panel Discussion regarding:**
NTS Vendor Solutions- Past, Presence and Future

18:00 **Inaugural meeting 'FOR-IDENT Club'**

19:00 **Poster Session / Exhibition**
Presenting Posters with odd number

19:30 **VIP-Evening Event**
(‘Vendor Informs Participants Event’ in the City Hall Erding)

Thursday, 07. October 2021

08:30 Registration and Vendor Exhibition

09:00 **Welcome and Introduction**

Subject Area: NTS in Water Analysis

organized by the ‘FA Non Target Screening’ (German Water Chemistry Society)

Chair: Prof. Dr. Torsten C. Schmidt

09:05 **Introduction**
Prof. Dr. Torsten C. Schmidt, (Univ. Duisburg-Essen & IWW Water Centre, DE)

09:15 **Screening Strategies for PFAS to Protect Groundwater and Drinking Water**
Christian Zwiener
(Univ. Tübingen, DE)

09:35 **NTS workflow to assess the fate of nitrosamine precursors and formation of transformations during wastewater ozonation**
J. Ricardo Cunha
(IUTA, Duisburg, DE)

09:55 **How to survive the NTS data chaos in water analysis; examples and recommendations**
Toni Köppe
(BfG, Koblenz, DE)

10:15 **Relevant Feature or False-Positive? - A new approach to describe reliabilities of individual NTS features**
Gerrit Renner
(Univ. Duisburg-Essen, DE)

10:35 **NTS goes ISO**
Michael Petri
(BWV, Stuttgart, DE)

10:55 **Panel Discussion regarding:**
NTS in Water Analysis

11:20 Coffee Break / Exhibition

Subject Area: NTS Quality and Tox Transfer

Chair: Dr. Thomas Letzel

11:40 **Predicting concentration and toxicity for suspects in non-targeted screening allows pinpointing the relevant contaminants**
Anneli Kruve et al.
(Stockholm University, Stockholm, SE)

12:10 **LC-TWIMS-HRMS analysis combined to in silico structure prediction and QSAR-based genotoxicity assessment for the comprehensive discovery and prioritization of transformation products before further toxicological testing**
Sylvain Merel et al.
(INRAE, Villeurbanne, FR)

12:25 **Evaluating and correcting the matrix effect in LC-ESI-HRMS for reliable NTS**
Selina Tisler et al.
(University of Copenhagen, Frederiksberg C, DK)

- 12:40 **Pipelines And Systems for Threshold Avoiding Quantification of LC-MS/MS data (PASTAQ)**
Alejandro Sanchez Brotons et al.
(University of Groningen, Groningen, NL)
- 12:55 **Benchmarking of open-access tandem mass spectral libraries**
Michael Sasse et al.
(University of Innsbruck, Innsbruck, AT)
- 13:10 **Development and Implementation of a Standard Quality Control Mixture for Assessing Non-Targeted LC-HRMS Method Performance**
Christine. M. Fisher et al.
(US FDA, MD, USA)
- 13:25 **Panel Discussion regarding: NTS Quality and Tox Transfer**
- 14:25 **Wrap Up and Conclusion**

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