



International Conference on Non-Target Screening (ICNTS 23)

16. – 19. October 2023

**Erding, Germany
and online**

PD Dr. T. Letzel
Dr. Stefan Bieber

Advisory Board:

Dr. Tobias Bader
Dr. Leon Barron
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Prof. Dr. Karl Jobst
Prof. Dr. Herbert Oberacher
Dr. Christine O'Donnell
Prof. Dr. Emma Schymanski
Prof. Dr. Philipp Weller
Dr. Michael Witting

International Conference on Non-Target Screening 2023

In the recent years, there were several very successful workshops and conferences 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' and 'ICNTS 2021' in Erding as well as the 'GC meets NTS' digital in 2020 and 2022.

Again, 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 labs, 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 developer will present their latest results and ideas in keynote lectures, lecture sessions and poster sessions.

The ICNTS 23 is being held as a **hybrid conference** (online and on-site in Erding, Germany) between **16. – 19. October 2023.**

This conference will promote discussion on NTS main topics, such as (order regarding the program agenda):

- **Computational Mass Spectrometry**
- **NTS in Metabolomics**
- **NTS in Food(omics)**
- **GC-MS goes NTS**
- **NTS in 'Materials'**
- **Soft Ionization in NTS**
- **Ion Mobility meets NTS**
- **NTS in Environmental Analysis**
- **NTS in Water Analysis**
- **NTS Harmonization and Reporting Strategies**
- **Commercial Solutions**

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

International Conference on Non-Target Screening 2023

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/icnts23/>

Registration fees:

- online participation 380 €

Registration is possible
for online participation until 30.09.2023.

For further details, please contact:

education@afin-ts.de

Venue:

Stadthalle Erding (City Hall Erding)
Alois-Schießl-Platz 1
D-85435 Erding, Germany
<https://www.stadthalle-erding.de>



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Amtsgericht Augsburg, HRB 32307
Geschäftsführer: Dr. Thomas Letzel und Dr. Stefan Bieber

Program**Monday, 16. October 2023**

- 10:30 Registration and Vendor Exhibition Opening
- 11:30 **Welcome and Introduction**
- 11:45 **What happened since ICNTS 21?**
T. Letzel
(AFIN-TS, Augsburg, DE)
- 12:15 **Modern Programming, Machine Learning and Chemometrics in NTS**
P. Weller
(Mannheim Univ. Appl. Sci. Mannheim, DE)

Subject Area: Computational Mass Spectrometry

Chair: Emma Schymanski

- 12:45 **Multidimensional Non-target Screening and Size-Dependent Fragmentation**
E. Baker
(Univ. of North Carolina at Chapel Hill, US)
- 13:15 **streamFind, a Flexible Workflow Designer for NTS Data Analysis**
J. R. Cunha et al.
(IUTA, Duisburg, DE)
- 13:30 **MLinvitroTox: A Machine Learning Tool for Hazard-Driven Prioritization**
K. Arturi et al.
(Eawag, Dübendorf, CH)
- 13:45 **NTS with a Novel PFAS Prioritization Technique**
B. Bugsel et al.
(University of Tübingen, Tübingen, DE)
- 14:00 Coffee Break / Exhibition
- 14:30 **Modular Open-Access and Open-Source Julia HRMS Toolbox**
D. van Herwerden et al.
(HIMS/CASA, Amsterdam, NL)

- 14:40 **Can Active Learning Improve the Performance of Computational Mass Spectrometry?**
W.-C. Wang et al.
(Stockholm University, Stockholm, SE)
- 14:50 **Spectral quality – Predicting the Quality of MS² Spectra using Machine Learning**
F. Been et al.
(VU Amsterdam, Amsterdam, NL)
- 15:00 **Ranking Candidates for Non-Targeted Feature Identification based on Their Structures**
V. Turkina et al.
(University of Amsterdam, Amsterdam, NL)
- 15:10 **Rapid Non-target Metabolite Structure Annotation with SIRIUS 6**
M. A. Hoffmann et al.
(Friedrich Schiller University, Jena, DE)
- 15:20 **Autoencoders for Extracting Structure and Toxicity Relevant Information**
Y. Kreuzer et al.
(Stockholm University, Stockholm, SE)
- 15:30 **Data Science Enhanced Non-Targeted Analysis for Characterization of Exposome:**
S. Samanipour et al.
(University of Amsterdam, Amsterdam, NL)
- 15:45 **Panel Discussion regarding:**
Computational Mass Spectrometry
- 16:45 Coffee Break / Exhibition

Subject Area: NTS in Metabolomics

Chair: Michael Witting

- 17:15 **Novel Approaches for Metabolite Identification in LC-MS-based Non-Targeted Metabolomics**
M. Witting
(Helmholtz Munich, Munich, DE)

- 17:45 **Augmented Region of Untargeted Metabolomics MS (AriumMS) of Multi-Platform-based CE-MS and LC-MS data**
A. Haun et al.
(Aalen University, Aalen, DE)
- 18:00 **MetWork Webserver in Clinical Analysis**
E. Bourgoigne et al.
(Université de Paris, Paris, FR)
- 18:15 **PFAS Exposure in Australia**
P. Dewapriya et al.
(University of Queensland, Brisbane, AU)
- 18:30 **Panel Discussion regarding:**
Non-Target Screening in Metabolomics
- 19:30 Break and Vendor Exhibition

Evening Event

- 20:00 **Closing first day**

Tuesday, 17. October 2023

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

Subject Area: NTS in Foodomics

Chair: Andrea Büttner

- 09:05 **NTS and Foodomics**
A. Büttner
(IVV, Freising, D)
- 09:35 **GC-MS/IMS Volatilomics of Coffee Powder and Brewed Coffee**
C. Kiefer et al.
(Mannheim Univ. Appl. Sci. Mannheim, DE)

- 09:50 **Authentication of Raw Nut Products through Untargeted Peptide Profile**
S. Venegas *et al.*
(Friedrich-Alexander-Univ., Erlangen, DE)
- 10:05 **Systematic Monitoring of Thousands PFAS in Biota, Utilizing LC-VIP HESI(-)-TIMS-QTOF MS**
G. Gkotsis *et al.*
(Nat. and Kapodistrian Univ., Athens, GR)
- 10:20 **Panel Discussion regarding:**
Non-Target Screening in Foodomics
- 10:50 Coffee Break / Exhibition

Subject Area: GC-MS goes NTS

Chair: Karl Jobst

- 11:05 **Uncovering Unknown Disinfection By-Products in Water by GCxGC and HRMS**
S. D. Richardson
(Univ. of South Carolina, Columbia, US)
- 11:35 **Applying the Self Adjusting Feature Detection Algorithm to GC-HRMS Data**
L. M. O'Brien *et al.*
(University of Queensland, Brisbane, AU)
- 11:50 **Extraction, Clean-Up, and GCxGC-MS Based NTS of House Dust Samples**
A. Rebryk *et al.*
(Umeå University, Umeå, SE)
- 12:05 **NTS Reveals Fluorotelomer Ethoxylates in Indoor Dust and Industrial Wastewater**
K. Steeves *et al.*
(Mem. Univ. Newfoundland, St. John's, CA)
- 12:20 **Panel Discussion regarding:**
Non-Target Screening with GC-MS
- 12:45 Lunch Break / Exhibition

- Subject Area: NTS in 'Materials', the analytical search**
Chair: Herbert Oberacher
- 13:30 **NTS Using a Combination of High- and Low-Resolution MS Methods: from Recycled Plastics to the Oil Sands**
L. Chibwe
(University of Regina, Saskatchewan, CA)
- 14:00 **Plastic, Water & the Sun – Characterization of Chemicals Leaching**
F. Menger *et al.*
(Helmholtz-Zentr. Hereon, Geesthacht, DE)
- 14:15 **Prioritization and NTS of Emerging Contaminants from Recycled Textiles**
D. Szabo *et al.*
(Stockholm University, Stockholm, SE)
- 14:30 **NTS Survey of California Drinking Water using Point-Of-Use Filters**
S. R. Newton *et al.*
(USEPA, Durham, US)
- 14:45 **Can We Assess the Food-Related Sources of Pesticides in Cohort Studies by Screening for Pesticide Metabolites and Dietary Markers in Urine?**
C. Huber *et al.*
(Helmholtz Centre, Leipzig, DE)
- 15:00 **Novel Identification of Human Pharmaceutical Metabolites in Untreated Wastewater by Wide Scope Suspect Screening**
C. Meyer *et al.*
(Eawag, Dübendorf, CH)
- 15:15 **Panel Discussion regarding:**
Non-Target Screening in Materials
- 16:00 Coffee Break / Exhibition

Subject Area: Commercial NTS Solutions by GC-MS(/MS) Vendors and Others
Chair: Thomas Letzel

- 16:30 **NTS Workflow Presentations (Commercial GC-MS/MS Solutions)**
(e.g., Gerstel, Lablicate, Leco, SepSolv, TOFWERK)
- 17:30 **Panel Discussion regarding:**
NTS Vendor Solutions- Past, Presence and Future
- 18:30 **Poster Session and Exhibition**
Presenting Posters with even numbers

Evening Event

- 19:30 **General meeting 'FOR-IDENT Club'**
- 20:00 **VIP-Evening Event**
(‘Vendor Informs Participants Event’ in the City Hall Erding)
- 21:30 **Closing second day**

Wednesday, 18. October 2023

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

Subject Area: Soft Ionization in NTS

Chair: Philipp Weller

- 09:05 **API Techniques: The Last Frontier for NTS Approaches by GC-MS**
J. F. Ayala-Cabrera
(PiE-UPV/EHU, Plentzia, ES)
- 09:35 **NTS of Environmental Contaminants in a Colony of Glaucous Gulls using GC-HRAM MS (EI/NCI)**
M. Harju *et al.*
(NILU, Tromsø, NO)

- 09:50 **DART-HRMS to differentiate black truffle species**
K. Losso et *al.*
(Leopold-Franzens University Innsbruck AT)
- 10:05 **Advantages in NTS Using Medium Pressure Chemical Ionization Including Fast Reactant Switching**
S. Bräkling et *al.*
(University of Wuppertal, Wuppertal, DE)
- 10:20 **NTS of Industrial Wastewater Samples Using HS-SPME and GC-TOFMS with Parallel Chem. and Electron Ionization**
L. K. Tintrop et *al.*
(University of Duisburg-Essen, Essen, DE)
- 10:35 **Panel Discussion regarding:**
Soft Ionization in NTS
- 11:00 [Coffee Break / Exhibition](#)

Subject Area: Ion Mobility meets NTS

Chair: Lubertus Bijlsma

- 11:15 **Ion Mobility MS in NTS: Advantages and Limitations in the Food Safety and Natural Toxins Fields**
L. Righetti
(Wageningen University, Wageningen, NL)
- 11:45 **Prediction of CCS Values and their Utility Across Different Instrumental Platforms**
A. Celma et *al.*
(Swedish Uni. of Agric. Sci., Uppsala, SE)
- 11:55 **Implementation of Ion-Mobility Spectrometry Derived CCS-m/z Trendlines in the Identification of QACs**
L. Belova et *al.*
(University of Antwerp, Antwerp, BE)
- 12:05 [Lunch Break / Exhibition](#)

- 13:00 **Comprehensive Two-Dimensional GC Coupled to IMS for Three-Dimensional Separation of Complex Samples**
R. Frey et *al.*
(Mannheim Uni. Appl. Sci. Mannheim, DE)
- 13:10 **Python-Based Chemometric Data Analysis for Non-Targeted GC-IMS Exhaust Gas Monitoring of Fermentation Processes**
J. Christmann et *al.*
(Mannheim Uni. Appl. Sci. Mannheim, DE)
- 13:20 **Extended Non-Target Authenticity Screening of Citrus Juices and Oils Based on Chiral HS-GC-MS-IMS**
L. Bodenbender et *al.*
(Mannheim Uni. Appl. Sci. Mannheim, DE)
- 13:30 **Panel Discussion regarding:**
Ion Mobility meets NTS
- 13:50 [Coffee Break / Exhibition](#)

Subject Area: NTS in Environmental Analysis

Chair: Leon Barron

- 14:05 **Combining NTS, Wastewater-Based Epidemiology and Census as a Technique to Identify Population and Demographic Markers**
J. O'Brien et *al.*
(University of Queensland, Saint Lucia, AU)
- 14:35 **Detection of Thyroid Hormone System Disrupting Compounds in House Dust and Cat Serum Using Effect-Directed Analysis**
J. Meijer et *al.*
(VU Amsterdam, Amsterdam, NL)
- 14:50 **NTS of Surface Water Samples to Identify Exposome-Related Pollutants: A Case Study from Luxembourg**
D. Aurich et *al.*
(University of Luxembourg, Belvaux, LU)

- 15:05 **NTA of Contaminants in Freshwater Sediments: Extraction, Optimization and Application in the Rhone River**
T. Ducrocq et *al.*
(INRAE, Villeurbanne, FR)
- 15:20 **NTS via Fragment Mass Differences and Kendrick Mass Defect: Application to Highly PFAS-Contaminated Soil in Germany**
J. Zweigle et *al.*
(University of Tübingen, Tübingen, DE)
- 15:35 **Panel Discussion regarding:**
Non-Target Screening in Environmental Analysis
- 16:05 [Coffee Break / Exhibition](#)

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

Chair: Thomas Letzel

- 16:20 **NTS Workflow Presentations (Commercial LC-MS/MS Solutions)**
(e.g., Agilent, Bruker, Sciex, Plasmion, ThermoFisher)
- 17:10 **Panel Discussion regarding:**
NTS Vendor Solutions- Past, Presence and Future
- 18:10 **Poster Session / Exhibition**
Presenting Posters with odd number
- 19:10 **Closing third day**

Evening Event

- 19:15 Sight Seeing Tour in Erding
- 20:15 **Evening Event**
local event in Erding (Gasthaus zur Post)

Thursday, 19. October 202309:00 **Welcome and Introduction****Subject Area: NTS in Water Analysis**

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

Chair: Tobias Bader

09:05 **Introduction German Expert Committee NTS**K. Jewell
(BfG, DE)09:15 **NTS Guideline for Water Analysis 2.0**W. Schulz
(Aalen Univ. of Applied Sciences, Aalen, DE)09:45 **NTS Workflow for the Characterization of Monitoring Sites in the Context of Regulatory Water Monitoring in Saxony**T. Köppe
(Federal Inst. of Hydrology, Koblenz, DE)10:00 **LC-HRMS NTS in the Monitoring Strategy of Rijkswaterstaat in the Rhine, as Part of the ICPR Rhine Project.**M. Pijnappels et al.
(Rijkswaterstaat, Lelystad, NL)10:15 **NTSuisse: Towards a LC-HRMS Data Processing Platform for Swiss Water Stakeholders**J. Boog et al.
(Eawag, Dübendorf, CH)10:30 Coffee Break11:00 **Suspect and NTS for Metabolites of New Psychoactive Substances in Wastewater**R. Bade et al.
(University of Queensland, Brisbane, AU)11:15 **Selective Extraction of Acidic Contaminants in Drinking Water by SAX-SPE and RP-WAX LC-HRMS**D. Ciccarelli et al.
(Imperial College London, London, UK)11:30 **Non-Targeted Detection of Micropollutants in Groundwater Wells Used for Drinking Water Production**M.Y. Nanusha et al.
(Aarhus University, Aarhus, DK)11:45 **Panel Discussion regarding:**
NTS in Water Analysis12:15 Lunch Break / Exhibition**Subject Area: NTS Harmonization and Reporting Strategies**

Chair: Christine O'Donnell

13:00 **SRT from BP4NTA**C. O'Donnell
(CFSAN, FDA, Maryland, US)13:30 **When is Enough Actually Enough-How Does the Number of Replicates Influence the Quality of NTA Results?**K. E. Butler et al.
(University of Maryland, College Park, US)13:45 **Structural Alerts for Prioritization of Potentially Toxic Substances in NTS**N. Meekel et al.
(KWR Res. Institute, Nieuwegein, NL)14:00 **Predicting LoDs Based on the Ionization Efficiency Values for Reporting and Harmonization in NTS Using LC/ESI/HRMS**A. Souihi et al.
(Stockholm University, Stockholm, SE)14:10 **Machine Learning Tools Can Pinpoint Urgent Water Pollutants**H. Sepman et al.
(Stockholm University, Stockholm, SE)14:20 **Evaluation of Quantification Approaches Without Analytical Standards in NTS Using LC/ESI/HRMS**L. Malm et al.
(Stockholm University, Stockholm, SE)14:30 Coffee Break14:50 **Enhanced Data Evaluation in NTS: Uncovering Uncertainties through a Multi-Workflow Approach**G. Renner et al.
(Univ. Duisburg-Essen, Essen, DE)15:00 **Next Generation of Data Processing for NTS: User-Independent and Data Quality-Based**M. Reuschenbach et al.
(Univ. Duisburg-Essen, Essen, DE)15:10 **From Data to Reliable Conclusions- Prioritization of Emerging Contaminants and Transformation Products in the Environment**S. Tisler et al.
(Univ. of Copenhagen, Frederiksberg C, DK)15:25 **Panel Discussion regarding:**
NTS Harmonization and Reporting Strategies16:00 **Wrap Up and Conclusion**16:10 **Closing last day**

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