

Nontarget2026

Nontarget screening of organic chemicals in the environment

12. April 2026 - 17. April 2026

Congressi Stefano Franscini, Monte Verità, Ascona, Switzerland



Congressi
Stefano Franscini

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aquatic research **ooo**



SCS
Swiss Chemical
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Program

Sunday, 12 April, 2026

17:00 - 17:45

Welcome drink

17:45 – 18:15

Juliane Hollender and Organizers

Welcome and Introduction

Plenary Lecture

Chair Juliane Hollender

18:15 – 19:15

Ed Kolodziej, *University of Washington, USA*

Using Advanced Mass Spectrometry To Identify and Characterize Toxic Chemicals in Roadway Runoff and Vehicle Tires

19:30

Dinner

Monday, 13 April, 2026

Oral Session 1: Analytical frontiers

Chairs Heinz Singer and Lubertus Bijlsma

- 8:30 – 9:00 **Keynote Lecture**
Selina Tisler, *Copenhagen University, Denmark*
NTS strategies for analyzing highly polar compounds, from sample preparation to data treatment
- 9:00 – 9:20 **Juliana Laszakovits**, *ETH Zurich, Switzerland*
New techniques for new unknowns: a case study of chloronitramide
- 9:20 – 9:40 **Richard Jacoby**, *EMBL, Germany*
Microbial Pesticide Biotransformation: Presenting an LC-MS Workflow to Enable Systematic, Large-Scale Measurement of Pesticide Metabolism in Diverse Biological Systems
- 9:40 – 10:00 **Diana Aga**, *University of Buffalo, USA*
Unmasking the Hidden Fluorine Through Integration of Ion-Mobility Spectrometry and F-Nuclear Magnetic Resonance Spectroscopy in NTA Workflows
- 10:00 – 10:30 *Coffee break*
- 10:30 – 11:00 **Keynote Lecture**
Jon Benskin, *Stockholm University, Sweden*
Discovery of a novel class of PFAS in marine mammal blubber by gas chromatography-ion mobility-high resolution mass spectrometry
- 11:00 – 11:20 **Carrie McDonough**, *Carnegie Mellon University, USA*
Prioritizing bioaccumulative PFASs from complex mixtures via biomimetic chromatography and NTA
- 11:20 – 11:40 **Marzieh Shojaei**, *Duke University, USA*
Deep characterization of per and polyfluoroalkyl substances in current and legacy aqueous film-forming foams
- 11:40 – 12:00 **Georg Diekes**, *Federal Institute of Hydrology, Germany*
Critical evaluation of the potential and limitation of non-target screening in suspended particulate matter by GC-HRMS

12:00 – 12:20 **Karl Jobst**, *Memorial University of Newfoundland, Canada*
Are we breathing in sidechain fluoropolymer microplastics?
Insights from non-targeted pyrolysis gas chromatographic ion
mobility mass spectrometry

12:20 – 12:30 **Carmen Brenig**, *CSF*
Welcome Address from Congressi Stefano Franscini

12:30 – 14:00 *Lunch*

Poster sessions

14:30 – 16:00 Poster session – odd numbers posters

16:00 – 16:30 *Coffee break*

16:30 – 18:00 Poster session – even numbers posters

Plenary Lecture

Chair Lee Ferguson

18:15 – 19:15 **Erin Baker**, *University of North Carolina at Chapel Hill, USA*
Integrating Environmental Exposures with Molecular
Responses: Air, Diet, and Beyond

19:30 *Dinner*

Tuesday, 14 April, 2026

Oral Session 2: Computational tools

Chairs Emma Schymanski, Viktoria Turkina

- 8:30 – 9:00 **Keynote Lecture**
Justin van der Hooft, *Wageningen University & Research, the Netherlands*
Structural and Functional Annotation Strategies to Boost Nontarget Screening
- 9:00 – 9:20 **Xander Becking**, *KWR Water Research Institute, the Netherlands*
Retention index alignment algorithm for the alignment of data from different NTS studies without requiring shared standards
- 9:20 – 9:40 **Lucas Ferrando Plo**, *Stockholm University, Sweden*
Uncertainty quantification with conformal prediction in small-molecule collision cross-section machine-learning modeling
- 9:40 – 10:00 **Lapo Renai**, *University of Amsterdam, the Netherlands*
Predicting In Silico Measurable Features and Chemical Coverage Estimates in LC-ESI-HRMS Non-Target Analysis
- 10:00 – 10:30 *Coffee break*
- 10:30 – 11:00 **Keynote Lecture**
Louis-Felix Nothias, *University of Côte d'Azur, France*
From Literature Mining to Self-Evolving Agents: AI Frameworks for Metabolomics and Beyond
- 11:00 – 11:20 **Jonathan Zweigle**, *University of Copenhagen, Denmark*
Non-target screening approaches to unravel the unknown fluorine content in environmental samples
- 11:20 – 11:40 **Iris Hättestrand**, *Stockholm University, Sweden*
Evaluation of generative models for structural elucidation of chemicals from mass spectrometry data
- 11:40 – 12:00 **Kai Kammer**, *Eawag, Switzerland*
NTSuisse: a Web Platform for LC-HRMS Data of Swiss Surface Water
- 12:00 – 12:20 **Bashir Mayahi**, *University of Luxembourg, Luxembourg*
Exploring FAIR Transformation Product Information with FAIR-TPs
- 12:30 – 14:00 *Lunch*

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| 14:00 – 16:00 | Workshops |
| Workshop A | Structure elucidation Organizers: Kai Dührkop, <i>Bright Giant</i> ; Lee Ferguson, <i>Duke University, US</i> ; Viktoriia Turkina, <i>University of Amsterdam, NL</i> |
| Workshop B | Harmonization & NTS portals Organizers: Nicole Bandow, <i>UBA, DE</i> ; Nina Hermens, <i>BFG, DE</i> ; Yasuyuki Zushi, <i>AIST, JP</i> |
| Workshop C | Bioanalytical approaches linked to NTS Organizers: Vittorio Albergamo, <i>New York University, US</i> ; Pablo Gago-Ferrero, <i>IDAEA-CSIC, ES</i> |
| 16:00 – 16:30 | <i>Coffee break</i> |
| 16:30 – 18:00 | Poster session – individual discussions |
| Plenary Lecture | |
| Chair Juliane Hollender | |
| 18:15 – 19:15 | Marja Lamoree , <i>Vrije University Amsterdam, the Netherlands</i> Unravelling key bioactivity drivers in the environment-food-human continuum by High Throughput Effect-Directed Analysis |
| 19:30 | <i>Dinner</i> |

Wednesday, 15 April, 2026

Oral Session 3: Transformation products & PMT substances

Chairs Jonathan Zweigle, July Laszakovits

- 8:30 – 9:00 **Keynote Lecture**
Carsten Prasse, *Johns Hopkins University, USA*
From Molecular Complexity to Environmental Risk: Prioritizing Organic Contaminants in Environmental Mixtures
- 9:00 – 9:20 **Christian Zwiener**, *Tübingen University, Germany*
PFAS in AFFF Contaminated Sites - What Can We Learn from Application of Nontarget Screening and PhotoTOP Assay
- 9:20 – 9:40 **Lubertus Bijlsma**, *University Jaume I, Spain*
Pinpointing Persistent, Mobile and Toxic substances: A prioritized screening strategy for their detection in the water cycle
- 9:40 – 10:00 **Martin Krauss**, *UFZ, Germany*
Tracking transformation of chemicals along a large river course from non-target screening data
- 10:00 – 10:30 *Coffee break*
- 10:30 – 11:00 **Keynote Lecture**
Daniel Zahn, *UFZ, Germany*
Polar chemicals and transformation products – blind spots in nontarget screening?
- 11:00 – 11:20 **Damian Helbling**, *Cornell University, USA*
Nontarget analysis for source tracking of organofluorine-containing chemicals through semiconductor manufacturing processes
- 11:20 – 11:40 **Parviel Chirsir**, *University of Luxembourg, Luxembourg*
Identification of persistent substructures in transformation products with zebrafish embryos using cheminformatics and a suspect screening approach
- 11:40 – 12:00 **Susan Richardson**, *University of South Carolina, USA*
PFAS and DBP Worlds Collide: Discovery of a New Fluorinated Disinfection By-product and Its Precursors in Chlorinated and Chloraminated Drinking Water

- 12:00 – 12:20 **Frederic Been**, *Vrije University Amsterdam, the Netherlands*
Data-Driven Prioritisation of Transformation Products During
Drinking Water Treatment
- 12:30 – 14:00 *Lunch*
- 14:00 Excursion to Val Verzasca
In case of bad weather: Visit to the Castle of Bellinzona
- 18:00 Conference dinner at the Grotto Broggin

Thursday, 16 April, 2026

Oral Session 4: NTS & hazard assessment

Chairs Jonathan Martin, Lee Ferguson

8:30 – 9:00

Keynote Lecture

Anneli Kruve, *Stockholm University, Sweden (online)*

Quantification in NTS: where are we in 2026?

9:00 – 9:20

Manuel Garcia-Jaramillo, *Oregon State University, USA*

Beyond Detection: Integrating Chemical Prioritization and Zebrafish Bioactivity to Advance Nontarget Drinking Water Surveillance

9:20 – 9:40

Martin Hansen, *DTU Copenhagen, Denmark*

National large-scale soil health study: High-throughput robotics sample preparation and non-target analysis

9:40 – 10:00

Maria Margalef, *Vrije University Amsterdam, the Netherlands*

High-Throughput Effect-Directed Analysis with Multidimensional Chromatography and Ion Mobility HRMS Reveals Transthyretin-Binding Chemicals in Stormwater Ponds

10:00 – 10:30

Coffee break

10:30 – 10:50

Haotian Wang, *UFZ, Germany*

Combining high-resolution fractionation & virtual fractionation by machine learning to enhance identification of bioactive compounds in sediments

10:50 – 11:10

Tom Young, *University of California, Davis, USA*

Comparing Insights Obtained from Application of Diverse Prioritization Schemes to Data from a Broad-Scope Nontarget Analysis of Drinking Water

11:10 – 11:30

Frank Menger, *Stockholm University, Sweden*

Combining AhR Bioassays, LC-HRMS-based non-target screening, and Machine Learning to Identify Hazardous Dyes in Textiles

11:30 – 11:50

Adria Sunyer Caldu, *Stockholm University, Sweden*

A Combined Target/Nontarget Framework to Explore Indoor–Outdoor Differences of Airborne Chemical Exposomes across Europe

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| 11:50 – 12:10 | Frank Wania , <i>University of Toronto Scarborough, Canada</i> Using spatial and temporal trends in the prioritization of features detected in the non-target analysis of XAD-resin based passive air samplers |
| 12:30 – 14:00 | <i>Lunch</i> |
| 14:00 – 16:00 | Workshops |
| Workshop D | Status/Demonstration of NTS processing workflows Organizers: Carolin Huber, <i>Eawag, CH</i> ; Rick Helmus, <i>University of Amsterdam, NL</i> ; Paolo Bonini, <i>oloBion, ES</i> |
| Workshop E | Hazard predictions for NTS prioritisation Organizers: Jonathan Martin, <i>Stockholm University, SE</i> ; Christine Gallampois, <i>Umea University, SE</i> ; Nikiforos Alygizakis, <i>Environmental Institute, SK</i> |
| Workshop F | Analytical approaches to expand the NTS chemical space Organizers: Andrea Brunner, <i>TNO, NL</i> ; Nanna Hjort Vidkjær, <i>GEUS, DK</i> |
| 16:00 – 16:30 | <i>Coffee break</i> |
| 16:30 – 18:00 | Poster session – individual discussions |
| Plenary Lecture Chair Susan Richardson | |
| 18:15 – 19:15 | Timo Niedermeyer , <i>Freie Universität Berlin, Germany</i> Weighing in on Natural Products – Mass Spectrometry in Untargeted and Targeted Specialized Metabolomics |
| 19:30 | <i>Dinner</i> |

Friday, 17 April, 2026

Oral Session 5: Applications

Chairs: Nicole Bandow, Emma Schymanski

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| 8:30 – 9:00 | Keynote Lecture Tobias Bader , <i>LUBW, Germany</i> River-to-Tap Surveillance in a Large-Scale Water Supply: Practical Challenges and Insights from Routine Non-Target Screening |
| 9:00 – 9:20 | Aline Reis de Carvalho , <i>VITO, Belgium</i> Creating NTAF: The Non-Target Analysis Platform of Flanders to Enhance Environmental Governance |
| 9:20 – 9:40 | Eric Winter , <i>UBA, Germany</i> NTS Can Support the Transformation of Water Monitoring and Regulatory Decision-Making in Chemicals Management |
| 9:40 – 10:00 | Teofana Chonova , <i>Eawag, Switzerland</i> From high-frequency NTS monitoring to enhanced source elucidation: advancing the characterization of industrial emissions in the Rhine |
| 10:00 – 10:20 | Roman Grabic , <i>University of South Boemia, Czech Republic</i> Nontargeted analysis workflow as a tool for management of contaminants of emerging concern in river basins |
| 10:30 – 11:00 | <i>Coffee break</i> |
| 11:00 – 11:40 | Workshops reports & discussion |
| 11:40 – 12:00 | Lee Ferguson and Juliane Hollender Wrap up |
| 12:00 – 13:30 | <i>Lunch and departure</i> |

Posters (alphabetical order)

1. Lena Aisch, *Eawag, Switzerland*

Using machine learning for the prioritization of non-target screening features across both electrospray ionization modes: a case study with suspended particulate matter samples

2. Vittorio Albergamo, *NYU Grossman School of Medicine, USA*

Integrating Non-Targeted Screening for Chemical Exposure Assessment in Humans and Consumer Products

3. Isabelle André, *ISCR - Rennes, France*

Monitoring the chemical quality of wastewater by combining passive integrative sampling and untargeted mass spectrometry analysis

4. Nicole Bandow, *Umweltbundesamt, Germany*

The Strategic Role of Ion Mobility–Enhanced Non-Target Screening in Future Chemical Regulation

5. Nicole Bandow, *Umweltbundesamt, Germany*

Advancing Non-Targeted Screening for Regulatory Applications: Insights from the European Partnership PARC

6. Joseph Beaney, *University of Bath, UK*

Establishing an Effect-Directed Analysis Workflow for Assessing Environmental Risks of Hazardous Chemicals and Their Mixtures

7. Samia Boudah, *L'Oréal R&I, France*

Advanced Characterization of Environmental Pollutant Metabolism in Human Skin

8. Jolien Bridelance, *Flemish Environment Agency (VMM), Belgium*

Graphical PowerBI report of screening results in Flanders

9. Andrea Mizzi Brunner, *TNO, the Netherlands*

Comprehensive Characterization of Tunnel Airborne Particulate Matter: Insights from EASVOLEE Using GC-MS and LC-HRMS Non-Target Screening

10. Teofana Chonova, *Eawag, Switzerland*

Insights from the workshop Today and Tomorrow of Non-Target Screening Portals

11. Konstantina Diamanti, *National and Kapodistrian University of Athens, Greece*

Investigating the comparability of experimental CCS values across different instrumental platforms

12. Jonas Dietrich, *Wageningen University and Research, the Netherlands*

Spectral alerts for prioritizing contaminant class during nontarget screening

13. Victoria Eriksson, *Linköping University, Sweden*

Enhancing nontarget screening of wastewater micropollutants using ammonium fluoride additive and multi-fractionation solid-phase extraction

14. Ben Faill, *University of Bath, UK*

Transitioning from targeted analysis to high-resolution mass spectrometry for a comprehensive water-based epidemiology workflow

15. Pablo Gago Ferrero, *IDAEE-CSIC, Spain*

Nontarget HRMS profiling of the glioblastoma chemical exposome and its potential links to air pollution

16. Christine Gallampois, *Umeå University, Sweden*

Identification of chemicals in Baltic Sea sediments prioritized from non-target screening by Machine Learning-based toxicity prediction

17. Fanshu Geng, *Cornell University, USA*

Integrating suspect and nontarget screening to elucidate biotransformation products and pathways of polyfluoroalkyl substances

18. Rick Helmus, *University of Amsterdam, the Netherlands*

patRoon 3.0: Enhanced non-target analysis workflows with ion mobility separation and other major improvements

19. Nina Hermes, *Bundesanstalt für Gewässerkunde, Germany*

A time series analysis approach to evaluate non-target screening data for the prioritization of discontinuously discharged compounds

20. Daniel Höhn, *Universität Duisburg-Essen, Germany*

Fully Automated Feature Detection Workflow for Non-Target Screening with HPLC-HRMS

21. Joelle Houriet, *Swiss Federal Institut for Metrology (METAS), Switzerland*

Multilaboratory Untargeted Mass Spectrometry Metabolomics Collaboration to Identify Bottlenecks and Comprehensively Annotate A Single Dataset

22. Heewon Jang, *Changwon National University, South Korea*

Characterizing Pharmaceuticals and Their Transformation Products under Anoxic and Aerobic Conditions: A Non-Target Screening Approach

23. Susana Kimura, *University of Calgary, Canada*

From Micropollutant to DBP Driver: The Unexpected Reactivity of 1-Chlorobenzotriazole in Water Disinfection

24. Christoph Kornpointner, *Environment Agency Austria, Austria*

Non-Target Screening based Clustering Analysis of Chemical Fingerprints in Austrian Surface Waters

- 25. Christoph Kornpointner**, *Environment Agency Austria, Austria*
Non-target screening of surface water samples from Austrian rivers and lakes
- 26. Futoshi Kurisu**, *The University of Tokyo, Japan*
Prioritizing emerging contaminants in secondary treated wastewater based on removal efficiency and potential ecological toxicity using non-target screening approach
- 27. Francesc Labad Roig**, *GEUS - Geological Survey of Denmark and Greenland, Denmark*
Revealing Groundwater Chemical Fingerprints by applying Non-Target Screening: Samsø Island as a Case Study (Denmark)
- 28. Aina Lara**, *oloBion, Spain*
Anchoring Retention-Time Prediction for Environmental Non-Target Screening Using a Standard Metabolite Library
- 29. Theodora Lee**, *National Environment Agency Singapore, Singapore*
From Detection to Decision: A Non-Targeted Analysis Framework for Prioritising Contaminants in Urban Waterways.
- 30. Thomas Letzel**, *Analytisches Forschungsinstitut für Non-Target Screening GmbH, Germany*
Non-Target Screening in (chemical) process monitoring and (retrospective) data handling concepts
- 31. Haizhou Liu**, *University of California - Riverside, USA*
UV Direct Photolysis of PFAS Compounds: Degradation Mechanisms and Transformation Products
- 32. Martin Loos**, *enviBee GmbH, Switzerland*
Machine learning for the non-targeted detection of industrial micropollutants
- 33. Maria Margalef**, *Vrije Universiteit Amsterdam, the Netherlands*
High-Throughput Effect-Directed Analysis in Water Samples from the Upper Rhine to identify chemicals with Transthyretin binding properties
- 34. Giulia Martella**, *Eawag, Switzerland*
Developing an Non targeted DNA Adductomics Workflow Using Astral HRMS: Integrating MS², Multi-Software Analysis, and Homolog Pattern Recognition
- 35. Fanny Mathiaux**, *INRAE, France*
Application of non-target screening methodology to dissolved organic matter characterisation in small watersheds as a novel strategy for chemical pressure assessment in surface freshwaters
- 36. Carrie McDonough**, *Carnegie Mellon University, USA*
Known and novel per/polyfluoroalkyl substances in contact lenses

- 37. Yamini Mittal**, *University of Luxembourg, Luxembourg*
Comprehensive assessment of micropollutants in stormwater runoff from industrial and urban sites using target and non-target screening
- 38. Michael Mohr**, *Landeswasserversorgung, Germany*
Automated near-real time monitoring of micropollutants as an early warning system for drinking water resources
- 39. Catherine Mullins**, *Emory University, USA*
Optimization of Rapid LCMS Methods for Comprehensive Exposome Profiling
- 40. Jeong-Eun Oh**, *Pusan National University, South Korea*
Identification of persistent mobile chemicals and ultrashort chain perfluoroalkyl substances in full-scale drinking water treatment plants by target and suspect screening analysis
- 41. Emma Palm**, *University of Luxembourg, Luxembourg*
Non-target Analysis of Transformation Products in Drinking Water in and around Luxembourg
- 42. Jessica Patrone**, *CSIC, Spain*
Integrative Non-Target Molecular Profiling of Oceanic Dissolved Organic Matter (DOM) and Microbial Communities Across Depth and Latitude
- 43. Racchana Ramamurthy**, *McGill University, Canada*
Expanding PFAS Chemical Space: Challenges and Advances in Non-Target Screening of Polymeric PFAS
- 44. Stefan Reimann**, *Empa, Switzerland*
Expanding Atmospheric Surveillance: Non-Target Screening and Open Spectral Databases for Persistent Halogenated Compounds
- 45. Anna Rojewska**, *University of Gdańsk, Poland*
Integrating targeted and non-target screening to evaluate groundwater quality and drinking-water treatment performance
- 46. Jorg Roosma**, *TNO, the Netherlands*
From Volatiles to Unknowns: Non-Target Analysis of Plastics in Recycling
- 47. Franziska Schanbacher**, *Institut für Pharmazie, Germany*
From a Single Toxin to a Toxin Network: A Fast-Track HRMS2 Strategy for Uncovering Aetokthonotoxin Congeners
- 48. Leonardo Soto**, *Norwegian University of Science and Technology (NTNU), Norway*
Automated Prediction of the Endocrine Disruptive Potency of Chemicals detected with LC/ESI/HRMS based on Mass Spectral Networks

49. Viktoriia Turkina, *University of Amsterdam, the Netherlands*
Enhancing Compound Identification in NTA through Informed Use of Spectral Databases

50. Yutaro Uehara, *The University of Tokyo, Japan*
Suspect screening of emerging contaminants in the watershed of Laguna de Bay, the Philippines with a local chemical inventory list using direct large-volume injection coupled with LC-HRMS

51. Nanna Hjort Vidkjær, *GEUS - Geological Survey of Denmark and Greenland, Denmark*
Aquaplexus – Developing Non-Target Screening Methods for Comprehensive Danish Groundwater Monitoring

52. Milena Voll, *UFZ Leipzig, Germany*
Integrating Transformation Product Analysis into High Throughput Persistence Testing

53. Frank Wania, *University of Toronto Scarborough, Canada*
Using model-predicted hazard metrics to prioritize features in non-target analysis

54. Yasuyuki Zushi, *National Institute of Advanced Industrial Science and Technology, Japan*
An LC-HRMS/MS Spectral Search System Enabling Compound Identification with Higher Confidence