Nontarget2026
Nontarget screening of organic chemicals in the environment

12. April 2026 - 17. April 2026
Congressi Stefano Franscini, Monte Verità, Ascona, Switzerland

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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*

14:00 – 16:00	**Workshops** Workshops programs are at the end of this document
Workshop A	**Structure elucidation** Organizers: Kai Dührkop, *Bright Giant*; Lee Ferguson*, Duke University, US*; Viktoriia Turkina, *University of Amsterdam, NL*
Workshop B	**Harmonization & NTS portals** Organizers: Nicole Bandow, *UBA, DE*; Nina Hermens, *BFG, DE*; Yasuyuki Zushi, *AIST, JP*
Workshop C	**Bioanalytical approaches linked to NTS** Organizers: Vittorio Albergamo, *New York University, US*; Pablo Gago-Ferrero, *IDAEA-CSIC, ES*
16:00 – 16:30	*Coffee break*
16:30 – 18:00	Poster session – individual discussions

Plenary Lecture

Chair Juliane Hollender

18:15 – 19:15	**Marja Lamoree**, *Vrije University Amsterdam, the Netherlands* Unravelling key bioactivity drivers in the environment-food-human continuum by High Throughput Effect-Directed Analysis
19:30	*Dinner*

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 Single Compounds to Complex Mixtures: Uncovering and Prioritizing Transformation Products in Natural and Engineered Systems
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 Asay
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	**Haizhou Liu,** *University of California, Riverside, USA* UV Direct Photolysis of PFAS Compounds: Degradation Mechanisms and Transformation Products
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 Broggini

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

11:50 – 12:10	**Frank Wania**, *University of Toronto Scarborough, Canada* 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	*Lunch*
14:00 – 16:00	**Workshops** Workshops programs are at the end of this document
Workshop D	**Status/Demonstration of NTS processing workflows** Organizers: Carolin Huber, *Eawag, CH*; Rick Helmus, *University of Amsterdam, NL*; Paolo Bonini, *oloBion*, *ES*
Workshop E	**Hazard predictions for NTS prioritisation** Organizers: Jonathan Martin, *Stockholm University, SE;* Christine Gallampois, *Umea University, SE*; Nikiforos Alygizakis, *Environmental Institute, SK*
Workshop F	**Analytical approaches to expand the NTS chemical space** Organizers: Andrea Brunner, *TNO, NL*; Nanna Hjort Vidkjær, *GEUS, DK*
16:00 – 16:30	*Coffee break*
16:30 – 18:00	Poster session – individual discussions

Plenary Lecture

Chair Susan Richardson

18:15 – 19:15	**Timo Niedermeyer**, *Freie Universität Berlin, Germany* Weighing in on Natural Products – Mass Spectrometry in Untargeted and Targeted Specialized Metabolomics
19:30	*Dinner*

Friday, 17 April, 2026

Oral Session 5: Applications

Chairs: Nicole Bandow, Emma Schymanski

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

Posters (alphabetical order)

1. **Liezel Mari Abaya**, *State University of New York at Buffalo, USA*
A Dual Similarity (Entropy + Cosine) Approach for High-Confidence Non-Targeted Analysis of Environmental Samples

2. **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

3. **Vittorio Albergamo**, *NYU Grossman School of Medicine, USA*
Integrating Non-Targeted Screening for Chemical Exposure Assessment in Humans and Consumer Products

4. **Isabelle André**, *ISCR - Rennes, France*
Monitoring the chemical quality of wastewater by combining passive integrative sampling and untargeted mass spectrometry analysis

5. **Nicole Bandow**, *Umweltbundesamt, Germany*
The Strategic Role of Ion Mobility–Enhanced Non-Target Screening in Future Chemical Regulation

6. **Nicole Bandow**, *Umweltbundesamt, Germany*
Advancing Non-Targeted Screening for Regulatory Applications: Insights from the European Partnership PARC

7. **Joseph Beaney**, *University of Bath, UK*
Establishing an Effect-Directed Analysis Workflow for Assessing Environmental Risks of Hazardous Chemicals and Their Mixtures

8. **Samia Boudah**, *L'Oréal R&I, France*
Advanced Characterization of Environmental Pollutant Metabolism in Human Skin

9. **Jolien Bridelance**, *Flemish Environment Agency (VMM), Belgium*
Graphical PowerBI report of screeningresults in Flanders

10. **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

11. **Teofana Chonova**, *Eawag, Switzerland*
Insights from the workshop Today and Tomorrow of Non-Target Screening Portals

12. **Konstantina Diamanti**, *National and Kapodistrian University of Athens, Greece*
Investigating the comparability of experimental CCS values across different instrumental platforms

13. **Jonas Dietrich**, *Wageningen University and Research, the Netherlands*
Spectral alerts for prioritizing contaminant class during nontarget screening

14. **Victoria Eriksson**, *Linköping University, Sweden*
Enhancing nontarget screening of wastewater micropollutants using ammonium fluoride additive and multi-fractionation solid-phase extraction

15. **Ben Faill**, *University of Bath, UK*
Transitioning from targeted analysis to high-resolution mass spectrometry for a comprehensive water-based epidemiology workflow

16. **Pablo Gago Ferrero**, *IDAEA-CSIC, Spain*
Nontarget HRMS profiling of the glioblastoma chemical exposome and its potential links to air pollution

17. **Christine Gallampois**, *Umeå University, Sweden*
Identification of chemicals in Baltic Sea sediments prioritized from non-target screening by Machine Learning-based toxicity prediction

18. **Fanshu Geng**, *Cornell University, USA*
Integrating suspect and nontarget screening to elucidate biotransformation products and pathways of polyfluoroalkyl substances

19. **Rick Helmus**, *University of Amsterdam, the Netherlands*
patRoon 3.0: Enhanced non-target analysis workflows with ion mobility separation and other major improvements

20. **Nina Hermes**, *Bundesanstalt für Gewässerkunde, Germany*
A time series analysis approach to evaluate non-target screening data for the prioritization of discontinuously discharged compounds

21. **Daniel Höhn**, *Universität Duisburg-Essen, Germany*
Fully Automated Feature Detection Workflow for Non-Target Screening with HPLC-HRMS

22. **Joelle Houriet**, *Swiss Federal Institut for Metrology (METAS), Switzerland*
Multilaboratory Untargeted Mass Spectrometry Metabolomics Collaboration to Identify Bottlenecks and Comprehensively Annotate A Single Dataset

23. **Heewon Jang**, *Changwon National University, South Korea*
Characterizing Pharmaceuticals and Their Transformation Products under Anoxic and Aerobic Conditions: A Non-Target Screening Approach

24. **Susana Kimura**, *University of Calgary, Canada*
From Micropollutant to DBP Driver: The Unexpected Reactivity of 1-Chlorobenzotriazole in Water Disinfection

25. **Christoph Kornpointner**, *Environment Agency Austria, Austria*
Non-Target Screening based Clustering Analysis of Chemical Fingerprints in Austrian Surface Waters

26. **Christoph Kornpointner**, *Environment Agency Austria, Austria*
Non-target screening of surface water samples from Austrian rivers and lakes

27. **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

28. **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)

29. **Aina Lara**, *oloBion, Spain*
Anchoring Retention-Time Prediction for Environmental Non-Target Screening Using a Standard Metabolite Library

30. **Theodora Lee**, *National Environment Agency Singapore, Singapore*
From Detection to Decision: A Non-Targeted Analysis Framework for Prioritising Contaminants in Urban Waterways.

31. **Thomas Letzel**, *Analytisches Forschungsinstitut für Non-Target Screening GmbH, Germany*
Non-Target Screening in (chemical) process monitoring and (retrospective) data handling concepts

32. **Martin Loos**, *enviBee GmbH, Switzerland*
Machine learning for the non-targeted detection of industrial micropollutants

33. **Maria Margalef**, *Vrije Universiteit Amsterdamj, 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 Untargeted DNA Adductomics Workflow Using Astral HRMS: Integrating MS^2 and Neutral Loss Analysis

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

Workshops programs

Workshop A: Structure elucidation

Chairs: Kai Dührkop, Bright Giant, DE; Lee Ferguson, Duke University, US; Viktoriia Turkina, University of Amsterdam, NL

This workshop brings together both developers and users of non-target analysis (NTA) workflows to discuss current challenges and advances in annotation and structural elucidation. The session aims to create an open discussion where participants can exchange experiences and identify key challenges and prospects in structural elucidation within NTA workflows.

Part 1: Short presentations
A series of talks (7–15 minutes each) with different aspects of structural elucidation:

- **Kai Dührkop (15 min)** – Overview of structure elucidation and new approaches, including structure elucidation with SIRIUS
- **Frederic Béen (7–10 min)** – Annotation of transformation products (TPs), including CCS and molecular networking approaches
- **Rick Helmus (10 min)** – Algorithmic perspectives on annotation using patRoon, including challenges and implementation insights
- **Viktoriia Turkina (7–10 min)** – Informative use of databases for compound identification
- **Jonas Dietrich (7–10 min)** – General perspectives on annotation, including common pitfalls and hidden challenges
- **Joëlle Houriet (7–10 min)** – Interlaboratory comparison of annotation workflows and reproducibility

Part 2: Interactive discussion
The second part will be fully dedicated to discussion with key topics :

- Reliability and comparability of annotation workflows
- Challenges from both algorithmic and experimental perspectives
- Hidden pitfalls in structural elucidation
- Opportunities for improving transparency, reproducibility, and confidence in NTA results

Workshop B: Harmonization & NTS portals

Chairs: Nicole Bandow, UBA, DE; Nina Hermens, BFG, DE; Yasuyuki Zushi, AIST, JP

Introduction to workshop (5 min)

1.) 4 presentations for input (5 min each +5 min in total for comprehension questions
   - Teofana Chonova: Towards harmonized NTS portals in Europe: current landscape and future directions
   - Nicole Bandow: Harmonization and quality Assurance of NTS in PARC
   - Tomasz Letzel: Challenges in Harmonization of NTS pipelines, data workflows and data storage for retrospective handling
   - Lapo Renai: Chemical space-aware curation of suspect lists: measurability harmonizing suspect screening

2.) Discussion (60 including short wrap up at the end from the chairs

Workshop C: Bioanalytical Approaches linked to NTS

Chairs: Pablo Gago-Ferrero, IDAEA-CSIC, ES; Vittorio Albergamo, New York University, US

1. Overall Concept

Nontarget and suspect screening with hyphenated high-resolution mass spectrometry have become core tools for bioanalytical approaches connecting complex mixtures of exogenous chemicals to biological responses. This workshop will use concrete case studies to walk through that continuum:

- High-throughput LC/GC-based exposome profiling
- Biomimetic chromatography to capture specific vs. nonspecific chemical–biological interactions
- Effect-directed analysis (EDA) linked to machine-learning prioritization
- Machine-learning tools to predict bioactivity directly from HRMS data

A series of presentations (~10 min) will highlight complementary bioanalytical strategies, followed by a moderated discussion on how these tools can be combined in practice and what methodological advances are most urgently needed.

2. Proposed Structure

2.1 Introduction and Goals

Introduction: why bioanalytical approaches are essential for making nontarget screening biologically meaningful, and how the selected case studies fit together along the external–internal exposure continuum.

2.2 Short Presentations / Demonstrations

Theme A – Screening Strategies

1. **Comprehensive Exposome Profiling**
    - **Speaker:** Catherine Mullins (Emory University)
    - **Focus:** Demonstration of a high-throughput LC-HRMS exposome platform for large human cohorts, including QA/QC strategy and how the framework can be adapted to other NTS laboratories.

2. **Biomimetic Chromatography to Bridge Hydrophobicity and Bioaccumulation**
    - **Speaker:** Carrie McDonough (Carnegie Mellon University)
    - **Focus:** Quantify specific and nonspecific interactions of PFAS; correlation of biomimetic retention with traditional RPLC and application to prioritize features with high bioaccumulation potential.

Theme B – Effect-Directed and ML-Enabled Prioritization

3. **EDA, Machine-Learning Prioritization, and De Novo Annotation**
    - **Speaker:** Frank Menger (Stockholm University)
    - **Focus:** Integration of AhR reporter assays with LC-HRMS-based NTS and machine-learning tools (MS2Tox, MS2Quant, SIRIUS/CSI:FingerID/MSNovelist)

4. **MLinvitroTox for Large-Scale In-Silico Bioactivity Prediction**
    - **Speaker:** Léna Aisch (Eawag)
    - **Focus:** Demonstration of MLinvitroTox, a machine-learning model that predicts bioactivity across 490 in-vitro assays from molecular fingerprints

3. Structured Discussion (~60 minutes)
Moderated by the chairs. Participants will be encouraged to describe their own challenges and to discuss how the presented tools could be adapted or integrated into their workflows.

Workshop D: Status/Demonstration of NTS processing workflows

Chairs: Carolin Huber, Eawag, CH; Rick Helmus, University of Amsterdam, NL; Paolo Bonini, oloBion, ES

14:00- 14:10 Introduction

14:15-14:20 Martin Loos (enviBee) “LC-HRMS/MS Spectral Search System Enabling Compound Identification with Higher Confidence”

14:25-14:30 Rick Helmus (Amsterdam University) “patRoon 3.0: Enhanced non-target analysis workflows with ion mobility separation and other major improvements”

14:35-14:40 Alessandro Spadaro (Thermo Fisher) “Enhancements in untargeted Screening with HRMS”

14:45-14:50 Paolo Bonini (oloBion) “Strategies for in silico MSMS prediction”

15:55-15:00 Jens Jacobsen (Waters) “tbd”

15:05-15:10 Joelle Houriet (METAS) “How Low Can You Go? Selecting Intensity Thresholds for Untargeted Metabolomics Data Preprocessing”

15:15-15:20 Jean-Pierre Lebroton (Sciex) “tbd”

15:20-15:45 Plenary discussion

15:50-16:00 Conclusion and Wrap up

Workshop E: Hazard predictions for NTS prioritisation

Chairs: Jonathan Martin, Stockholm University, SE; Christine Gallampois, Umea University, SE; Nikiforos Alygizakis, Environmental Institute, SK

Input of 10 minutes of

1. Jeong-Eun. Pusan National University, Korea. “Prioritization of monitoring compounds from SNTS identified organic micropollutants in contaminated groundwater using a machine learning optimized toxpi model.’
2. Emma Palm. University of Luxembourg, Luxembourg. “Non-target analysis of PMT compounds and transformation products in drinking water in and around Luxembourg.”
3. Kurisu Futoshi. University of Tokyo, Japan. "Screening non-target and suspect compounds in treated wastewater and surface water using ecotoxicity and concentration estimates."
4. Theodora Lee. National Environment Agency, Singapore. “From detection to decision: a non-targeted analysis framework for prioritizing contaminants in urban waterways.”
5. Christine Gallampois, Umeå University, Sweden. “Machine Learning to prioritise the identification of the most active features in the Aliivibrio fischeri assay.”
6. Pablo Gago Ferrero. IDAEA, Spain. “From air to brain: NTS-based prioritisation of neurotoxic pollutants in glioblastoma using BBB and AChE predictions.”

Moderated discussion by Jonathan and Nikiforos with the speakers and the audience

Workshop F: Analytical approaches to expand the NTS chemical space

Chairs: Andrea Brunner, TNO, NL; Nanna Hjort Vidkjær, GEUS, DK

Participants will collaboratively generate:

1. A community-identified map of bottlenecks limiting chemical-space coverage
2. A prioritized overview of analytical strategies that effectively expand NTS chemical space
3. An "action agenda" summarizing needs, opportunities, and next steps for the NTS community

1. Workshop introduction – Andrea and Nanna (5 min)

- Brief intro + workshop outcomes

2. Presentation: Chemical Space Overview – Lapo Renai, University of Amsterdam (10 min)
Focus: The interface between virtual contaminant space and measurable LC–ESI–HRMS space, with emphasis on designing analytical methods and compound panels that maximize the breadth, diversity, and characterization of the overlapping region.

3. Joint Exercise: "Brainstorming Chemical Space Coverage" (15 min)

Participants add sticky notes addressing:
A) Key factors influencing chemical-space coverage
B) Best analytical approaches to maximize chemical-space coverage
C) What is missing for further expansion of chemical space—tools, techniques, or community efforts needed.

4. Short 5-min Presentations

4.1. Victoria Eriksson, Linköping University
Focus: Reducing matrix effects by optimizing sample preparation by SPE and increasing ionization efficiency in HRMS analysis using mobile phase additives

4.2. Catherine Mullins, Gangarosa Department of Environmental, Rollins School of Public Health, Emory University
Focus: Automated sample preparation; HILIC vs RP; positive/negative ionization

4.3. Racchana Ramamurthy, McGill University
Focus: Beyond LC-HRMS—LC vs GC, complementary analytical techniques to enhance coverage of PFAS chemical space (pyrolysis-GC-MS, hydrolysis assays, TOP assays, 19F NMR).

4.4. Michael Mohr, Landeswasserversorgung
Focus: DDA, DIA, intelligent acquisition; online continuous measurement vs composite/spot sampling.

5. Group Discussions (25 min discussion + 15 min round-up)

Participants split into groups of 5-6 people. Each group discusses the three themes introduced in the exercise:

A) Key factors affecting chemical-space coverage (→ community map of bottlenecks)
B) Best analytical approaches to maximize coverage (→ prioritized overview)
C) Missing tools, techniques, community needs (→ action agenda)

Groups use the collective input from the brainstorming exercise as a starting point.
Round-up: each group presents their poster (~2 min/group)

6. Round-up – Andrea and Nanna (15min)