UNIVERSITÄT
DUISBURG
ESSEN

Offen im Denken

2025

Jahresbericht

Annual Report

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Instrumental Analytical Chemistry

Dear friends and colleagues,

we are pleased to give you an overview of the IAC group activities of the previous year 2025. I start with our most precious Christmas present: Water research at the University of Duisburg-Essen will thrive. As one step forward to strengthen its position as a strategic research area of the university, just before Christmas we got the official endorsement for funding of the research building FutureWaterCampus, a journey that began already almost nine years ago. Realization surely will keep us busy in the coming years and we look forward to the synergies with the Active Sites research building that is currently been erected next door at the Thurmfeld near the university campus in Essen. Sadly though, in May 2025 we got the final evaluation of our excellence cluster proposal REASONS, "River Ecosystems in the Anthropocene – Sustainable Scientific Solutions", and despite the extremely positive evaluation by the reviewer panel, in the end our proposal was not selected for funding at this highly competitive stage of excellent project suggestions. We are nevertheless proud that our proposal was the first ever at UDE to reach the final stage. And we still believe in the novelty and relevance of our approach and are currently seeking ways to realize funding of the depicted ideas at smaller scale.

In our continued and newly started collaborative research projects RESIST and AMTEC-PRO, work has started, although in the latter case we realized how much time is needed in advance if you hire international students outside the EU. Therefore, we are very happy that Saima Asghar was able to finally join us early December. In addition, we are extremely happy that further new and continuation projects have been selected for funding by DFG. This includes the very favourably reviewed proposal of Maryam Vosough, which will continue to fund her work on advanced chemometric multi-block analysis of chemical and biological data in collaboration with Alexander Probst for the next three years. Equally well reviewed was the continuation proposal of Maik Jochmann in collaboration with the group of Stefan Haderlein in Tübingen that will further investigate the fate of aminopolyphosphonates and formation of glyphosate in technical water treatment processes. Finally, although starting only in 2026, our collaborative proposal with Stephan Barcikowski and Christoph Rehbock at UDE on the evaluation of Pulsed laser diffusion enhancement in liquids with the example of coffee

preparation received funding and will continue the preliminary work of Anna Ziefuß and Tina Friedenauer on that topic in a more systematic manner.

We participated actively in several conferences and meetings in 2025, foremost the organization of the 27th International Symposium on Advances in Extraction Technologies (ExTech 2025) in Mülheim an der Ruhr held under the auspices of the German Chemical Society (GDCh), Working Group Separation Science. Thanks to the excellent work of the entire IAC team this event was a great success valued very much by all participants. Thanks go also to all IAC members who splendidly presented our work at national and international conferences throughout the year. This includes the six Ph.D. students at IAC who successfully defended their theses. Furthermore, three Master and six Bachelor students finished their thesis at our department or external partner institutes with a home supervisor at IAC and contributed to our successful work.

Again, we successfully communicated our research results with 41 papers published in international peer-reviewed journals and books. Three of them appeared in a topical collection of Analytical and Bioanalytical Chemistry on "Computational mass spectrometry for exposomics in non target screening" that I guest-edited together with my colleagues Gerrit Renner and Saer Samanipour. And many stem from collaborative efforts with colleagues, for which I am very grateful. As usual, we continued our fruitful collaboration with Prof. Sina Dobaradaran who visited us twice for two-months stays, partially funded by the Alexander-von-Humboldt foundation, and we look forward to his next stay in Essen.

I thank my fabulous team for their excellent work at IAC and all partners from academia, industry, and funding agencies for their great support and fruitful collaborations. I hope you are interested in our IAC report and welcome very much feedback or collaboration interests for the future. I wish all of you the best and success in 2026, and I renew my hope for a more peaceful near future.

Torsten C. Schmidt

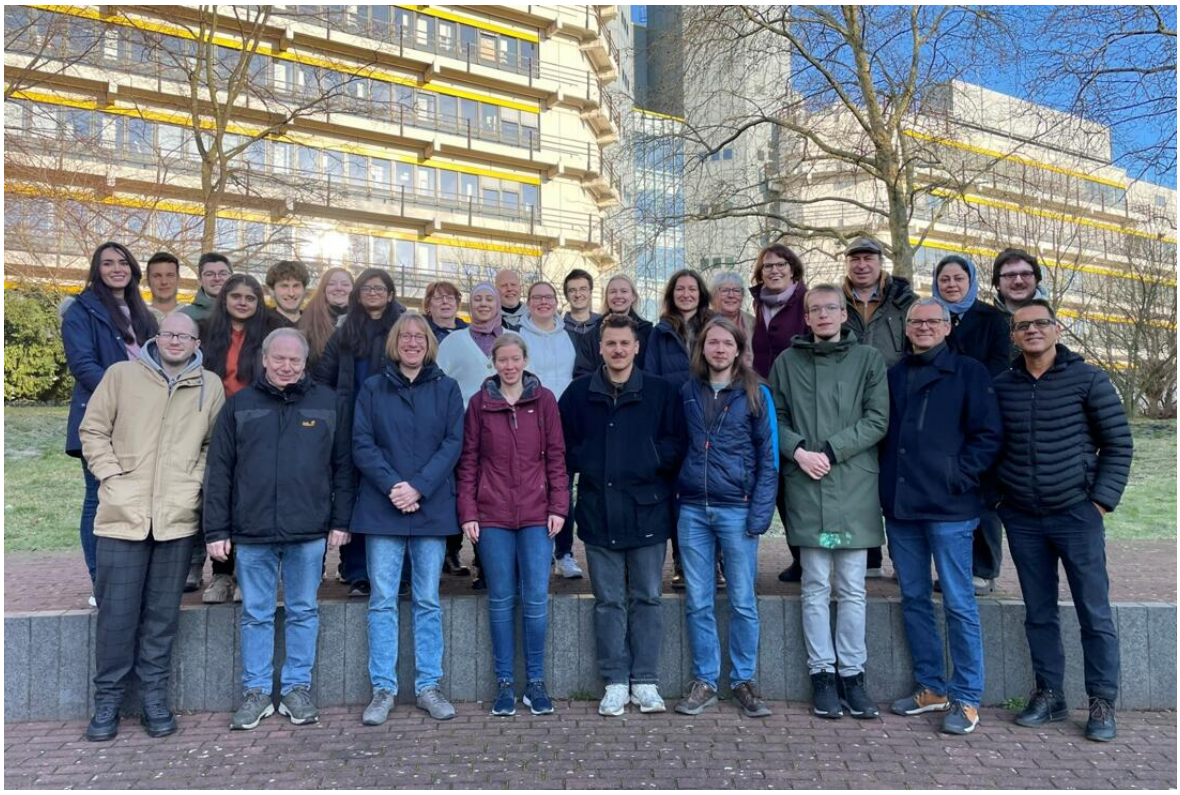

Figure 1: IAC Team 2025

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Staff

Head of Chair

Prof. Dr. Torsten C. Schmidt

Secretarial Office

Lydia Vaaßen

Regular Staff

Dr. Anam Asghar	Advanced Oxidation Processes
Dipl.-Ing. Simone Bettinger	Laboratory engineer, Instrument, and Lab Supervision
Dr. Maik Jochmann	Stable Isotope Analysis, Sample Preparation, and Gas Chromatography
Dr. Klaus Kerpen	2D-Fluorescence Spectroscopy, Advanced Oxidation Processes, Laser Commissioner, IT Administrator
Dipl.- Ing. Robert Knierim	Laboratory Equipment, Glassware, Support of guest scientists
Dr. Gerrit Renner	Analytical Data Science, Project Administration
Dr. Amir Salemi	Sampling & Sample preparation, Gas Chromatography
PD Dr. Ursula Telgheder	Ion Mobility Spectrometry, Analysis of PFAS - Sum parameter, Expert advice for course of studies, Radiation Protection Commissioner
Claudia Ullrich	Laboratory Assistant, Safety Officer

Apprentices

Davin Boras
Ayliz Colak

Research and Teaching Assistants

Fatemeh Afzalnia
Alina Hofrath
Daniel Höhn
Rajshree Jeewon
Robin Jung
Jan Niklas Oesterschlink
Thorben Sarnowski
Leonardo Solazzo
Matthias Stüwe

PhD Students (internal)

Saima Asghar	Probe compounds and method development for the analysis of reactive oxygen species in proton therapy
Felix Drees	Data Processing in Non-Target Screening
Annika Gruhlke	Investigation of Isotopic Fractionation and Transformation Products of Oxidative Degradation of Phosphonates via LC-IRMS and LC-HRMS
Isabel Halbhuber	Method development for determining the total fluorine parameter in PFAS analysis using spectroscopic and chromatographic methods
Daniel Höhn	Data processing of high-resolution mass spectrometry data for non-target screening
Michelle Hußock	Characterization of Nutrients, Pollutants, and Their Environmental Impacts in a Manure Recycling Process Using an Upflow Anaerobic Sludge Bed Reactor
Katharina Klein	Influence of organic matter on oxidative transformation processes
Shaista Khaliq	Diet-consumer interactions under variable stressor conditions as revealed by stable isotope studies of individual amino acids
Michael Leupold	Investigations of transformation reactions of antibiotics by photocatalysis in aqueous systems
Felix Niemann	Isotope fractionation associated with abiotic Imidacloprid degradation
Sarah P. Rockel	Development and evaluation of a 2D-LC-IRMS coupling for the use of conventional reversed-phase chromatography in component-specific stable isotope analysis

Duaà Tahboub	Studies on electrochemical treatment processes for the decomposition of Persist Organic Pollutants (POPs) in contaminated ground and surface water
Kaliyani Wickneswaran	Development & Optimization of GC-MS/MS and GC-IRMS methods for Fatty Acid Profiling & Food Webs

PhD Students (external)

Reyhaneh Armin	Non-target analysis of organic micropollutants in industrial wastewater
Indra Bartels	Analysis of suggested SARS-Cov-2 treatment pharmaceuticals in surface waters
Sandro Castronovo	Examination of micropollutant degradation in biological wastewater treatment: a proteomics approach
Joanna Flottmann	Analysis of highly polar trace substances in water with LC-HRMS(/MS)
Matin Funck	Development of a Sampling-Procedure allowing subsequent qualitative and quantitative Pyrolysis-GC/MS analysis for Subμ-Plastics in the Aquatic Environment
Annika Fechner	Development of an ion mobility spectrometry system with miniaturized thermodesorption and non-radioactive ion source for the detection of germs in food
Jana Hinz	Development and application of multidimensional GC-IMS methods for the analysis of volatile and semivolatile substances in safety and health research
Malte Hübschen	Automated sample preparation and gas chromatographic analysis in the field of food and consumer goods
Frank Jacobs	Development of an automated microextraction technique
Michelle Klein	Effect-directed analysis for monitoring and evaluation of surface and wastewater
Sara Schäfer	Oxidative transformation of organic compounds in ultrapure water by ozonation and UV photolysis
Hannah Schanzmann	Schnelle, nicht-invasive Identifikation nosokomialer Infektionen
Robert Schmidt	Correlation of spectrometric methods and digital sensor technology for evaluating the plant volatilome and its relevance to quality
Fabian Ude	Non-radioactive, energetically variable ionization unit for pollutant analysis in building materials based on FAIMS technology

Mike Wenzel	Determination of microplastics in soils and mosses
Modestus Wigger	Methoden der digitalen Sensorik von Lebensmitteln basierend auf der Ionenmobilitätsspektrometrie

Guest Scientists

Prof. Dr. Sina Dobaradaran

Long-term visiting scientist

Bushehr University of Medical Sciences, Iran

Long-term visiting scientist working on the analysis of environmental contaminants including microplastics, pharmaceuticals and emerging pollutants in marine and coastal ecosystems of the Persian Gulf region.

- A comprehensive study on environmental emissions of primary aromatic amines by cigarette butts and compare with unsmoked cigarette levels.
- Study of the kinetics of aromatic amines releases from cigarette butts into the water environments.
- Determining the acute toxicity of CBs leachates for aquatic organisms (my next project)

Prof. Dr. Maryam Vosough

Long-term visiting scientist

Chemistry and Chemical Engineering Research Center of Iran (CCERCI), Department of Clean Technologies, Chemometrics laboratory

Development of chemometrics-based approaches for Non-Target analysis of micropollutants in water environment using LC-HRMS/MS

High-resolution mass spectrometry generates huge datasets (“big analytical data”), making robust pre- and post-acquisition data treatment vital for reliable non-targeted analysis workflows. This is particularly critical in environmental applications, where trace organic micropollutants and their transformation products must be identified inside complex matrices and across a wider chemical space than in metabolomics. Chemometrics, integrating mathematical, statistical, and machine learning methods, can be systematically embedded across multiple stages of environmental non-targeted analysis to address these challenges.

Nuria Mauleon

ERASMUS Intern

CPIFP Corona de Aragón, Zaragoza, Spain

ERASMUS internship (April 07, 2025 - June 20, 2025) in Higher Level Vocational Education and Training in Laboratory Analysis and Quality Control. Preparation and analysis of samples using advanced laboratory techniques, including extraction of PAHs and PFAS sample preparation. Internship Tutor: Simone Bettinger

Guest Editorship: Computational Mass Spectrometry for Exposomics in Non-Target Screening

Figure 2: Cover of the special issue

In 2025, our working group acted as guest editors for the special issue "Computational Mass Spectrometry for Exposomics in Non-Target Screening" in Analytical and Bioanalytical Chemistry (Volume 417). This issue brought together leading contributions that advance computational approaches for managing the complexity of high-resolution mass spectrometry (HRMS) data in environmental and exposomics research. The special issue includes an editorial and a curated selection of research articles focused on algorithm development, chemometric evaluation, large-scale spectral library generation, and applied investigations in environmental and biological systems. A unifying theme is the integration of open-source software, reproducible workflows, and FAIR data principles into non-target screening (NTS). Several articles examine computational efficiency and robustness. For example, a newly developed region-of-interest (ROI) algorithm achieved significant data compression and enhanced peak detection in LC-HRMS datasets. Another study presented a stochastic parameter-optimization strategy for feature-detection algorithms, quantitatively demonstrating improved true-positive rates and reduced false discoveries in PFAS screening workflows. A comparative chemometric analysis showed that different processing strategies (feature-based versus ROI-based) can produce systematically different variance structures and prioritization outcomes in river water datasets, highlighting the importance of methodological transparency and multi-workflow validation.

A key achievement is the creation of a large-scale in silico MS/MS spectral library based on the NORMAN Suspect List Exchange, which enables annotation of previously uncharacterized chemical space. This resource substantially expands annotation coverage in retrospective groundwater analyses and marks a significant advance toward scalable exposomics. In addition, applied studies identified 124 PFAS at an AFFF-contaminated field site, introduced new terminology for structured classification, and developed open metabolomics workflows in C. elegans that connect xenobiotic metabolism to neurodegenerative pathways. Collectively, the special issue reinforces the conceptual and technical foundations of computational mass spectrometry in exposomics. It emphasizes reproducibility, open data repositories such as Zenodo and GitHub, chemometric rigor, and algorithmic innovation. For our working group, this issue not only demonstrates leadership in the field but also provides a reference framework for future developments in automated, uncertainty-aware, and interoperable NTS pipelines.

Awards and Recognitions

Student Award Analytical Chemistry (GDCh)
Daniel Höhn
GDCh - Division of Analytical Chemistry
Awarded for the best analytical chemistry performance in the Master program Water Science.

Kurita Award
Daniel Höhn
Kurita Water and Environment Foundation
Awarded for his master thesis *qPattern: Development of a Quality-Focused, User-Independent and Automated Componentisation Strategy for Non-Target Screening with HPLC-HRMS.*

Award of the Faculty of Chemistry
Isabell Schelhorn
Faculty of Chemistry, University of Duisburg-Essen
Awarded for the best performance in the Master program Water Science.

Best Science Video at ExTech2025
Sarah Rockel
ExTech2025, Mülheim an der Ruhr
Awarded for the best scientific video in the context of the ExTech2025 conference.

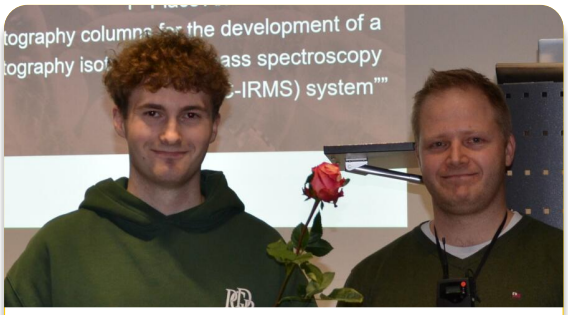
Young Scientist Award - Centre for Water and Environmental Research (ZWU) 2025

Dr. Robert G. H. Marks

ZWU, University of Duisburg-Essen

Awarded for his PhD thesis *"Liquid chromatography with simultaneous isotope ratio and high-resolution mass spectrometry detection: A powerful new tool for process investigation"*.

Link to thesis



Axel-Semrau Award

Matthias Stüwe

Axel Semrau GmbH & Co. KG

For his outstanding Bachelor thesis in 2025: *Characterization and application of thermo responsive liquid chromatography columns for the development of a testosterone measurement method in a two-dimensional liquid chromatography isotope ratio mass spectroscopy (2D-LC-IRMS) System.*

Early Career Editor - Separation and Purification Technology

Dr. Anam Asghar

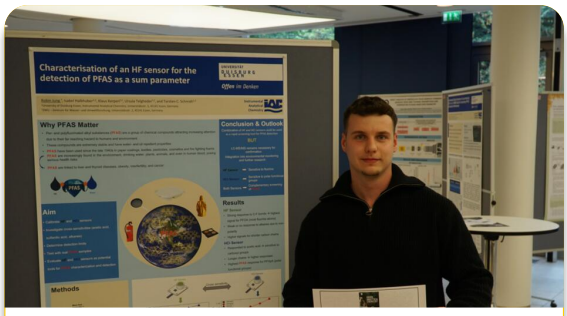
Elsevier - Separation and Purification Technology (IF 9.0)

Dr. Anam Asghar was appointed as a member of the Early Career Editorial Board of the journal *Separation and Purification Technology* (Impact Factor: 9.0) starting in February 2025. The appointment followed a competitive international selection process, in which nearly 1,000 applications were evaluated.

As part of this role, Dr. Asghar contributes to the peer-review process by reviewing scientific manuscripts, supports the editorial team through consultation activities, assists in the development of special issues when requested, and represents the journal within the scientific community through conference participation and professional outreach.

Further information: Editorial Board

3rd Feralco Award - Best Master Thesis
Isabell Schelhorn
Feralco / Water Science, University of Duisburg-Essen
Awarded for one of the best master theses in Water Science. The title of the work is: *Characterization of Encapsulated Plant Protection Products by High-Performance Liquid Chromatography*.



3rd Poster Award at ExTech2025
Robin Jung
ExTech2025, Mülheim an der Ruhr
Characterisation of an HF sensor for the detection of PFAS as a sum parameter.

Poster Award at ICNTS 2025
Daniel Höhn
ICNTS 2025, Erding
A Parameter-Free Algorithm for Feature Componentisation in Non-Target Screening.

Running Projects

Natural Water to Hydrogen

Understanding Active Sites' Dynamics for Sustainable Electrocatalytic Hydrogen Production Using Non-Purified Water Sources

Involved Staff: Dr. Anam Asghar, Prof. Dr. Torsten C. Schmidt
Partners: University of Duisburg-Essen (UDE)
Funding: UDE Research Profile "Natural Water to Hydrogen"

Figure 3: Natural Water to Hydrogen Logo

The "Natural Water to Hydrogen" research profile is an initiative undertaken by the University of Duisburg-Essen (UDE). Its primary goal aims to enhance the sustainability of hydrogen (H_2) production through water electrolysis. This is achieved by establishing a platform for gaining a fundamental understanding of the processes occurring at electrodes and membranes within aqueous environments. This understanding enabled us to determine the precise water-quality requirements for electrolysis, which can vary depending on the catalyst and membrane used. This has so far achieved via comprehensive efforts that draw upon expertise from the fields of water research, electrocatalysis, and membrane technology.

Within this system, IAC works closely with the involved research groups to assess the impact of water quality parameters on electrolyzer performance and on membrane and catalyst activity. A central focus is the standardization of analytical protocols for the quality analysis of alkaline electrolytes used in anion exchange membrane (AEM) electrolyzers, where reliable, reproducible measurements are particularly difficult due to high pH and elevated total dissolved solids. Standardized solution preparation procedures and optimized analytical methods were developed and systematically validated. Cation analysis using ICP-MS and ICP-OES achieved limits of detection of 0.09–0.97 µg/L and 0.02–0.05 mg/L, respectively, with recoveries of 90–105% following optimized dilution and interference-removal strategies.

Anion analysis by ion chromatography with conductivity detection reached detection limits of 0.05 mg/L and quantification limits of 5 mg/L, with recoveries ranging from 82–97%. Total organic carbon analysis, incorporating acidification to pH < 2, inorganic carbon removal, and high-temperature oxidation at 680 °C, yielded a limit of detection of 0.09 mg/L, a limit of quantification of 0.26 mg/L, and recoveries of approximately 95%. In addition, amine analysis using SPME-GC-MS enabled the sensitive and selective determination of trace amines in highly alkaline matrices. Overall, the recognized protocols demonstrated high robustness and repeatability and were successfully applied across multiple work packages, supporting membrane, catalyst, and electrode characterization, membrane stability analysis, and the identification of empirical trends within the project.

UV-Induced Photodegradation and Ozonation: Role of Natural Organic Matter

Involved Staff: Anam Asghar, Torsten C. Schmidt
Partners: –
Funding: Internal

UV-Induced Photodegradation

The photochemical degradation of organic micropollutants (OMPs) by UV-based processes is strongly influenced by the presence of natural organic matter (NOM) in water matrices. NOM is a heterogeneous mixture of compounds with diverse molecular weights and functional groups, which can both promote and inhibit photochemical transformation routes. In particular, NOM can absorb UV radiation, scavenge reactive intermediates, or alter the formation of photochemically produced reactive intermediates (PPRIs), thus affecting the efficiency of UV-driven treatment processes. This project examines the inhibitory role of NOM in UV-induced photodegradation, using atrazine as a model OMP. To systematically assess the influence of molecular size and functional moieties, tannic acid, gallic acid, catechin, and tryptophan were employed as NOM surrogates, representing phenolic, carboxylic, and amino functional groups. Their effects were compared with those of Suwannee River NOM as a reference material.

Photolysis experiments were carried out under regulated conditions, and constant concentrations of key PPRIs, including hydroxyl radicals, singlet oxygen, as well as triplet excited NOM states, were quantified using selective probe compounds. The results show that NOM induces a pronounced inhibition of atrazine photodegradation, with the inhibition increasing with NOM concentration. The dominant inhibition mechanism was identified as the inner filter effect, while phenolic and carboxylic moieties additionally acted as antioxidants by quenching excited triplet states and reactive intermediates. Overall, this project provides mechanistic insight into how NOM functional groups control photochemical transformation processes and stresses the importance of water matrix effects when applying UV-based advanced oxidation processes.

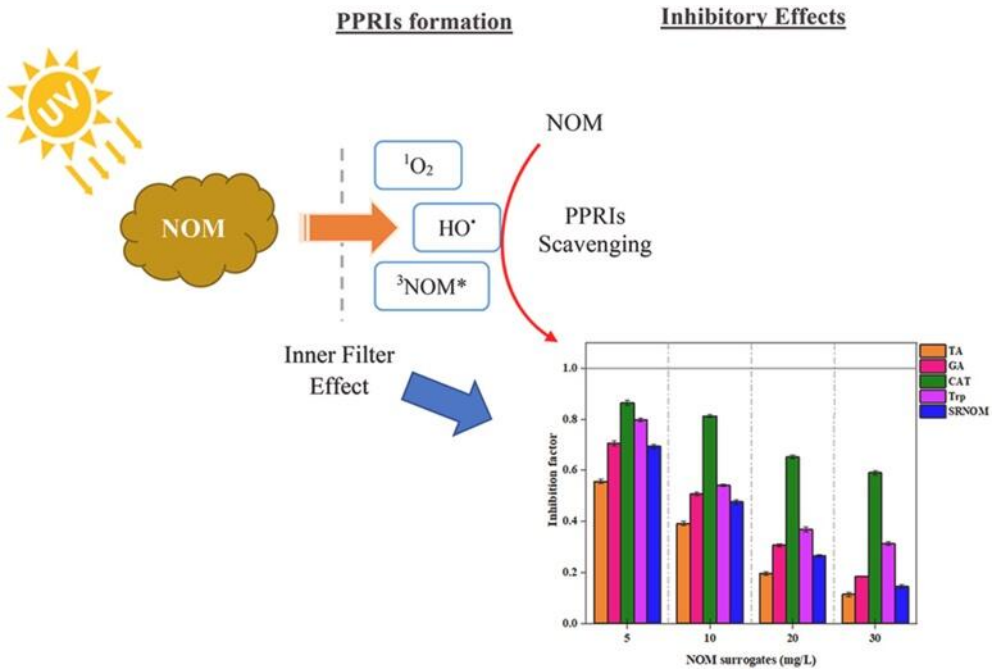


Figure 4: Effects of natural organic matter on the photodegradation of organic micropollutants, using atrazine as a probe compound.

Ozonation

Ozonation is widely applied for the removal of organic micropollutants (OMPs), but its effectiveness is strongly influenced by natural organic matter (NOM) present in water matrices. NOM can promote ozone decomposition and hydroxyl radical (HO•) formation, thereby enhancing the degradation of ozone-recalcitrant compounds, while simultaneously acting as a radical scavenger and increasing ozone demand at higher concentrations.

This project examines the twofold role of NOM in ozonation, centering on its ability to either stimulate or inhibit HO• formation and, consequently, the degradation of atrazine, a model OMP. NOM surrogates with distinct functional moieties, tannic acid, gallic acid, catechin, and tryptophan, were used to represent phenolic, carboxylic, and amine functionalities and compared with Suwannee River NOM. Batch ozonation experiments were performed under circumneutral conditions, and ozone exposure, hydroxyl radical exposure, and radical yields were quantified using established probe compounds and the R_{ct} concept. The results show that at low NOM concentrations, electron-rich functional groups, such as phenols and amines, enhance ozone decomposition and transiently elevate HO• concentrations, resulting in rapid atrazine degradation. In contrast, higher NOM concentrations exert inhibitory effects by increasing ozone consumption and enhancing the efficient scavenging of HO•, particularly by carboxylic-rich moieties.

This project advances mechanistic understanding of NOM-controlled radical chemistry in ozonation processes and provides important insights on optimizing ozone-based advanced oxidation processes in NOM-rich waters, particularly for treating ozone-resistant organic micropollutants.

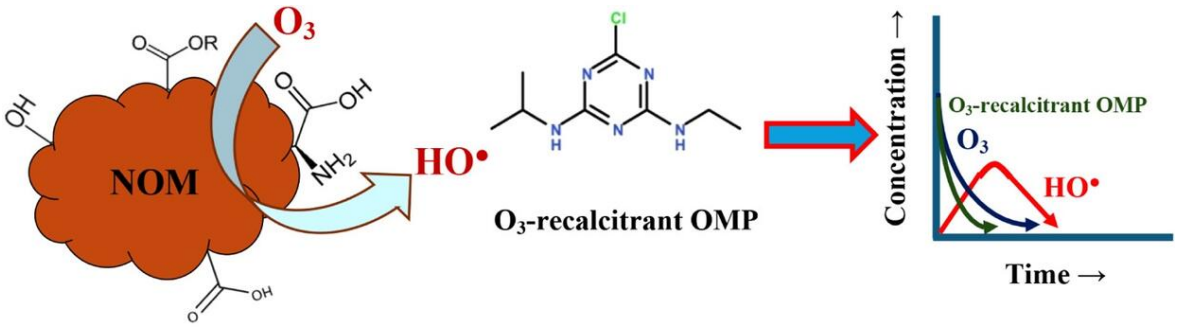


Figure 5: Dual role of natural organic matter as an inhibitor or stimulator of hydroxyl radical formation in the ozonation process.

Isotopic Fractionation and Transformation Products of Oxidative Degradation of Aminopolyphosphonates via LC-IRMS/HRMS

Involved Staff: Annika Gruhlke, Dr. Maik Jochmann, Prof. Dr. Torsten C. Schmidt
Partners: Prof. Dr. Stefan Haderlein, Dr. Daniel Buchner, Jule Werner (Environmental Mineralogy & Chemistry group, University of Tübingen)
Funding: German Research Foundation (DFG), Project Grant 457490294

Aminopolyphosphonates (APPs) are strong chelating ligands and have therefore been used since the 1980s to purify reverse osmosis concentrates, in detergents, and in the paper and textile industries. However, the possible disadvantages of APP use, such as eutrophication of natural waters, remobilization of heavy metals, and the formation of toxic transformation products, are not sufficiently known. Therefore, the degradation by ozonation, persulfate, and percarbonate oxidation of three APPs, aminotris(methylphosphonic acid) (ATMP), ethylenediamine-tetra(methylenephosphonic acid) (EDTMP), and diethylenetriaminepenta-(methylenephosphonic acid) (DTPMP), will be investigated. To assess the influence of different reaction conditions, pH, temperature, and oxidizing agent concentration will be varied. In addition, quenchers will be used to investigate the influence of different reactive species on degradation and isotope fractionation. For this purpose, a coupling of liquid chromatography-isotope ratio mass spectrometry (LC-IRMS) and LC high-resolution mass spectrometry (HRMS) with a flow-through splitter after LC separation will be used. This method was successfully developed by *Marks et al.* for ATMP and its photolysis products. LC-IRMS, which measures the isotopic signature of carbon in the analytes, is used to gain insight into degradation pathways through analyzing isotopic fractionation in the products.

Of particular interest is (aminomethyl)phosphonic acid (AMPA), which is considered genotoxic. It is a transformation product of all APPs and glyphosate, so the origin of AMPA can be determined by LC-IRMS. Furthermore, it has been postulated that glyphosate itself is a transformation product of EDTMP and DTPMP, so that the coupling method can be used to identify glyphosate if it is formed. In addition, it can be used to distinguish between different degradation pathways and industrially produced glyphosate.

Extracellular Volatile Metabolome of Nosocomial Pathogens by TD-GC-MS and GC-IMS

Involved Staff: Hannah Schanzmann, PD Dr. Ursula Telgheder
Partners: Hamm-Lippstadt University of Applied Sciences, ION-GAS GmbH, Witten/Herdecke University with Helios University Hospital Wuppertal
Funding: Bundesministerium für Bildung und Forschung (BMBF), Grant No. 13GW0428C

Hospital-acquired infections, such as nosocomial pneumonia, are among the greatest challenges in inpatient care. They lead to increased mortality, longer stays, higher treatment costs, and thus a socioeconomic burden. Therefore, a rapid and reliable diagnosis is crucial for starting targeted antibiotic therapy. However, culture-based diagnostic procedures often take up to 48 hours to identify the causal pathogen. Hence, a technology enabling faster detection of specific pathogenic agents needs to be developed. The project presented here aims to identify pathogens based on their specific microbiological volatile organic compound (mVOC) profiles in exhaled air. To measure these mVOCs from bacterial reference cultures and human breath, a benchtop system consisting of a thermal desorption (TD) gas chromatograph with a mass spectrometer (MS) is established. In addition, an ion mobility spectrometer (IMS) was coupled as a second detector, with the MS and IMS sharing the same flow line via a flow splitter. Nearly identical retention times can be achieved within 30 minutes, with slight deviations of 0.06 to 0.24 minutes. This enables the identification of unknown compounds in the IMS chromatogram using unambiguous mass spectral identification. The coupling of TD-GC-MS-IMS has been built up for the first time.

To find specific mVOCs as a benchmark of selected known pathogens such as *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Streptococcus pneumonia*, *Legionella pneumophilia*, *Acinetobacter baumannii complex*, and *Escherichia coli* grown in vitro, the volatiles in the culture's headspace were extracted onto TD tubes using a self-made sampling chamber. The TD tubes were subsequently measured using the TD-GC-MS-IMS. Measurements of selected pathogens demonstrate the significant advantage of the new coupling: identifying unknowns in IMS measurements using a mass spectrometric database, as no IMS databases are currently available. Approximately 600 bacterial measurements were conducted to ensure comprehensive data collection, yielding 25 marker compounds. Among these, 21 were confirmed using MS and validated with reference standards. Additionally, mixed cultures of two or more selected pathogens were prepared, and the identified marker compounds were also detected.

To assess the system's efficacy in breath analysis, characteristic VOCs such as ethanol, isoprene, acetone, 2-propanol, and 1-propanol were successfully identified in exhaled air using the dual detector system, as evidenced by matching IMS and MS spectra. A proof-of-principle trial has already been conducted in the clinical setting. Breath profiles were measured in 11 patients with nosocomial pneumonia. The data analysis is still ongoing, and the volatile fingerprints obtained in these patient measurements will be compared with the results from the in vitro studies.

Probe Compounds and Method Development for the Analysis of Reactive Oxygen Species in Proton Therapy

Involved Staff: Saima Asghar, Anam Asghar, Anzehla Galstyan, Torsten C. Schmidt
External Advisor: Emine Gökçe (Sewa GmbH, Essen)
Partners: University of Duisburg-Essen, Technische Universität Dortmund, Universitätsklinikum Essen
Funding: German Research Foundation (DFG)

Reactive oxygen species (ROS) play a central role in DNA damage induced by proton therapy, especially when radiosensitizers are used. Indirect radiation effects mediated by ROS significantly contribute to the biological effectiveness of proton irradiation. However, the analytical investigation of ROS remains highly challenging due to their short lifetimes, low steady-state concentrations, and rapid temporal evolution during and after irradiation. This project began in October 2025 and aims to investigate ROS-driven mechanisms of DNA damage in proton therapy, with particular emphasis on sensitizer-enhanced effects. Reliable detection and quantification of ROS is further complicated in complex matrices, such as nanoparticle-containing systems, simulated brain fluid, and microgel-based environments. To surmount these limitations, suitable ROS probe compounds and compatible analytical methods will be tested and validated, enabling the characterization of ROS formation and decomposition pathways during proton irradiation.

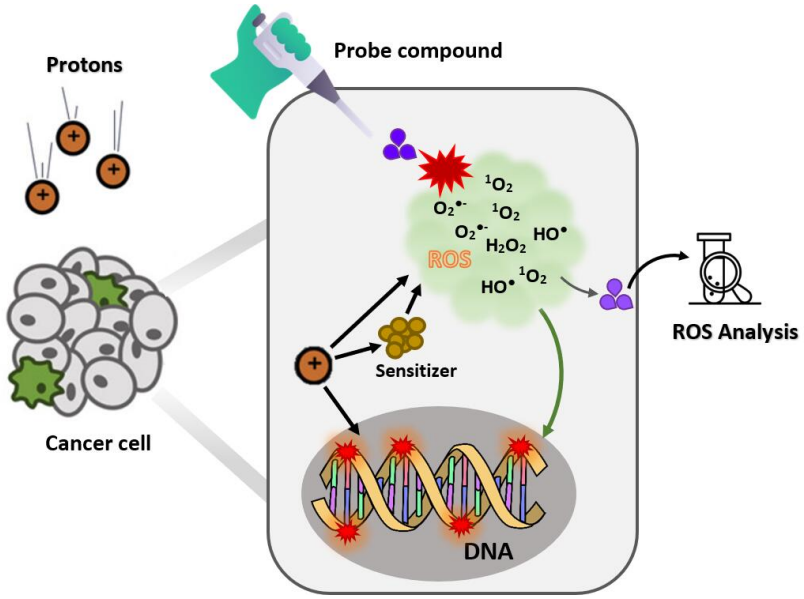


Figure 6: Schematic diagram of reactive oxygen species (ROS) in proton therapy.

Overall, the project aims to establish an improved analytical system for studying ROS-mediated processes in proton therapy and to support the formulation of advanced approaches for assessing radiation-induced oxidative mechanisms at the molecular level.

N-Nitrosamines in Workplace Air – NNOccSafe

Involved Staff: Jana Hinz, Prof. Michaela Wirtz, PD Dr. Ursula Telgheder
Partners: Bonn-Rhein-Sieg University of Applied Sciences
Funding: German Social Accident Insurance (DGUV)

The 2025 yearly report continues from the results presented in the previous account, further focusing on the developed thermal desorption-based GC-IMS methods for the analysis of nine nitrosamines in workplace air. In this reporting period, filter materials were tested regarding their ability to precipitate nitrosamine precursor substances, the potential of artefact formation on Tenax TA sample tubes was determined through the construction of a nitrous oxide test gas facility, and the methods were evaluated regarding its suitability for the determination of nitrosamines in workplace air according to the Technical Rules for Hazardous Substances (TRGS) 552 and 402 and the norm DIN EN ISO 22065.

While the analyte signals of NDMA and NDEA (absolute mass emitted by the calibration gas generator: 14.1 ng each, calculated from the set flows and the measured permeation rate) could be detected and identified readily for the reference measurements, no significant nitrosamine signals could be detected when the impinger (containing a 3% acid solution of ascorbic, amidosulfonic and phosphoric acid), ADS tube (Dräger, Lübeck, Germany), and molecular sieve filters were used. Using the acid-impregnated round filters or pure solid amidosulfonic acid, up to 96.7% of the detected nitrosamine analyte signals were lost. Based on these experiments, the use of pre-filters for air sampling of nitrosamines was deemed to be ineffective and highly prone to error. For this reason, filters were not used in subsequent measurements to check for artefact formation due to nitrogen oxides in the sampling volume.

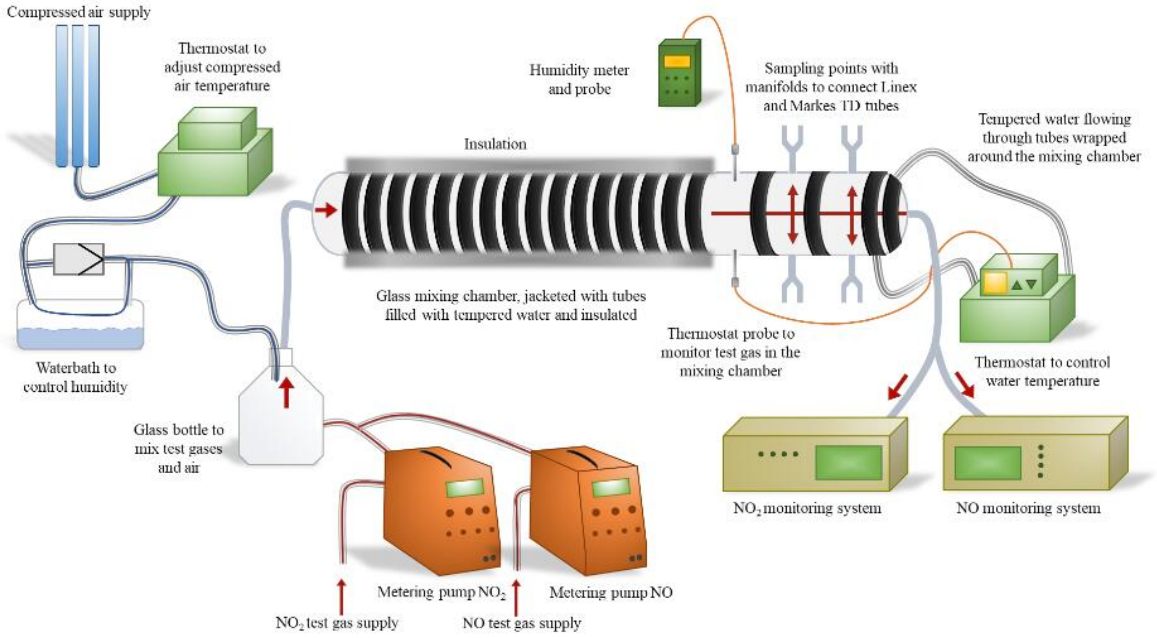


Figure 7: Schematic overview of the constructed test gas facility at the IFA laboratories.

N-nitrosation is regarded as the most common pathway of N–N-bond formation. Nitrosonium

ions (NO^+) from the nitrogen oxide-containing air generated in the constructed test gas facility (see Fig. 7) are subjected to a nucleophilic attack by an NH-containing compound, such as the secondary amines spiked onto the sample tubes, which are connected to the test gas facility and subjected to increasing NO_x concentrations. No artefact formation above the limit of quantification could be identified on the Markes sample tubes. The identified nitrosamine signals do not show an upward trend with increasing nitrogen oxide concentration, and in particular, no signal was detected at 4 ppm.

Since the carrier gas flow is split in the OPTIC-GC-DT-IMS measurement method, larger quantities of the precursor amines are spiked onto the Linex sample tubes. This, in turn, allows for a higher potential of artefact formation under the influence of NO_x-containing air, which is reflected in the results. The signals of the artificially formed nitrosamines could be clearly detected and quantified in the spectra. An approximate trend of the detected quantities with increasing nitrogen oxide concentration can also be observed. As a possible conclusion, the decisive factor in sampling using Tenax TA sorbent seems to be the presence of precursor nitrosatable amines, as the above-described investigations showed that the amount of secondary amines on the sample tube had a significantly greater influence than the nitrogen oxide concentration in the sampling volume on the formation of nitrosamine artefacts. If these can be classified as negligible by preliminary measurements, TD-based analysis for nitrosamines in the workplace air becomes possible, and the advantages of this IMS-based method can be harnessed. For one of the sampler types, the Markes Tenax TA sample tubes, a method categorisation of limited suitability for monitoring nitrosamine acceptance concentrations (0.075 µg/m³) according to the TRGS 402 could be concluded, based on the employed working range and the determined limits of detection and quantification.

Table 4: Table 1: Method validation parameters for nitrosamine analysis by TD-GC-FAIMS using Markes Tenax TA sample tubes.

TD-GC-FAIMS	LOD (ng)/(µg/m³)	LOQ (ng)/(µg/m³)	Rel. StD.	Working range (ng)/(µg/m³)	Suitability acc. to TRGS 402
NDMA	0.39 / 0.008	1.3 / 0.027	14%	1.3–4 / 0.027–0.085	LOQ ≤ AK, working range LOQ up to 2 AK
NMEA	0.30 / 0.006	0.93 / 0.020	11%	0.93–4 / 0.020–0.085	LOQ ≤ AK, working range LOQ up to 2 AK
NDEA	0.14 / 0.003	0.39 / 0.008	6%	0.39–4 / 0.008–0.085	LOQ ≤ 0.2 AK, working range LOQ up to 2 AK

TD-GC-FAIMS	LOD (ng)/(µg/m³)	LOQ (ng)/(µg/m³)	Rel. StD.	Working range (ng)/(µg/m³)	Suitability acc. to TRGS 402
ND-iso-PA	0.20 / 0.004	0.59 / 0.012	7%	0.59–4 / 0.012–0.085	LOQ ≤ 0.2 AK, working range LOQ up to 2 AK
ND-n-PA	0.15 / 0.003	0.45 / 0.009	7%	0.45–4 / 0.009–0.085	LOQ ≤ 0.2 AK, working range LOQ up to 2 AK

Sum Parameter for Organically Bound Fluorine: Thermal Conversion of PFAS to HF

Involved Staff: Isabel Halbhuber, Michael Leupold, Klaus Kerpen, Florian Uteschil, Robin Jung, Matthias Stüwe, Simone Bettinger, Ursula Telgheder
Partners: Cornelsen Umwelttechnologie GmbH
Funding: Federal Ministry for Economic Affairs and Climate Protection (BMWK) – Central Innovation Programme for SMEs (ZIM)

Perfluoroalkylated and polyfluoroalkylated substances (PFAS) are of great industrial interest due to their excellent water-, grease-, and dirt-repellent properties as well as their chemical and thermal stability. However, LC-MS/MS analysis can only detect a fraction of the numerous PFAS, leaving many compounds unaccounted for. Therefore, determining a sum parameter for total organic fluorine (TOF) is a promising alternative. A method that converts organic fluorine compounds to hydrogen fluoride (HF) followed by spectrometric detection offers a feasible approach. In the method presented here, PFAS are first enriched on a solid-phase material, then thermally converted quantitatively to HF, and finally detected spectroscopically. For enrichment, various solid-phase materials were evaluated, and the best-performing anion-exchange material achieved sorption rates above 95% for the selected PFAS. A thermo-module was developed to enable rapid thermal decomposition, reaching temperatures close to 1000 °C within seconds while remaining inert to HF. Combustion experiments showed that PFAS decomposition is strongly temperature-dependent, with complete conversion occurring reliably between 900 and 1000 °C.

Before coupling the thermo-module with the helium plasma, it was necessary to verify that fluorine emission lines can be observed under the chosen conditions. Hexafluoroisopropanol was used as a model substance and analyzed in the helium plasma. After injecting approximately 1 µL of the model substance, the helium emission line at 704 nm decreased, and two new emissions at 733 nm and 739 nm appeared, which can be attributed to fluorine lines. This

confirms that spectroscopic HF detection is feasible. Coupling the thermo-module with the helium plasma and using solid-phase enrichment is expected to lower the detection limits for total fluorine determination, with near-complete conversion of PFAS to HF occurring in the thermo-module rather than in the plasma.

Automated Fatty Acid Profiling in Biological Matrices (CRC Resist, A25)

Involved Staff: Kaliyani Wickneswaran, Prof. Dr. Torsten C. Schmidt
Partners: University of Duisburg-Essen, Ruhr-Universität Bochum, Kiel University, Leibniz Institute of Freshwater Ecology and Inland Fisheries (IGB) Berlin, Helmholtz Centre for Environmental Research, Helmholtz Centre for Ocean Research Kiel (GEOMAR)
Funding: German Research Foundation (DFG)

In 2025, Project A25 progressed from method development to the consolidation and validation of a reproducible, matrix-robust, and automation-compatible fatty-acid (FA) workflow based on GC–MS/MS, designed as a direct precursor for subsequent GC–IRMS/CSIA implementation. A central achievement was the successful establishment of an integrated extraction and derivatization strategy for heterogeneous biological samples. In contrast to aqueous FA workflows, complex biological matrices required controlled reaction kinetics, solvent-phase management, and matrix-tolerant automation to ensure stable yields and chromatographic performance. These challenges were addressed by developing a thermomorphically assisted one-pot workflow that enables stable FA derivatization with high repeatability under fully automated conditions (PAL-compatible sample preparation and measurement routine).

Method performance was validated in an ISO 12966-4 aligned framework and anchored using two certified reference materials (BCR-162R and NIST SRM 3275-1) to demonstrate quantitative reliability beyond a single reference system. Validation covered key analytical criteria, including repeatability (RSD/precision), linearity, LOQ determination, matrix spike/recovery, and concentration back-calculation to verify calibration performance and quantitative consistency under routine conditions. Across the validated scope, GC–MS/MS measurements showed stable retention times, reproducible response behaviour, and robust signal intensities, fulfilling prerequisites for quantitative trophic-marker analysis and matrix-diverse FA profiling. Beyond reference materials and the initial food matrices used for method verification, the workflow was successfully applied to the first ecological sample sets, including leaf litter and invertebrates, yielding consistent, interpretable FA signature patterns. This effectively provides an initial FA-signature baseline for upcoming applications in aquatic food-web studies.

Crucially, method development in 2025 explicitly accounted for downstream isotope analysis: derivatization chemistry and handling were selected to ensure compatibility with compound-specific isotope analysis (CSIA) and to minimize risks of analytical or isotopic bias. The consolidated, automation-ready FA workflow therefore forms the analytical basis to integrate QFASA-type FA profiling with GC–IRMS-based CSIA, establishing a direct bridge between

structural FA signatures and isotopic food-web reconstruction. Overall, Project A25 now provides a validated, scalable, and automation-ready FA methodology for biological matrices, directly supporting CRC RESIST objectives to quantify stressor-induced changes in aquatic food webs and to strengthen mechanistic ecosystem assessment.

Membrane Based Photocatalysis of Antibiotic Residues in Clinical Wastewater

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Partners: –
Funding: Zentrum für Wasser- und Umweltforschung, Stiftung Zukunft NRW

In the first part of the project, two reactor systems were designed and constructed to test and characterize immobilized photocatalytic materials. The focus was on photocatalysis for water applications, using the aminopenicillin amoxicillin as a model compound. Comprehensive online analytics for key water-chemical and optical parameters were implemented. These include lamp spectrum, dissolved oxygen, pH, and temperature, all of which are continuously monitored during photocatalytic degradation. In addition, the reaction solution can be purged with argon (inert gas) or oxygen to simulate oxic or anoxic conditions, as may occur in wastewater. To investigate the influence of photocatalysis without the superimposed effect of photolysis (degradation of contaminants by direct UV irradiation), various chemical UV cutoff filters such as potassium nitrite, potassium nitrate, and potassium hydrogen phthalate were evaluated. By using a suitable filter, photolytic processes can be suppressed. This is crucial for developing quantification methods for reactive oxygen species (ROS) in photocatalytic processes. Furthermore, this approach allows the influence of dissolved oxygen on the photocatalytic process to be investigated. The applicability of the reactor system was demonstrated using aminopenicillin, amoxicillin as an example. In this context, degradation rate constants for the photocatalytic degradation of amoxicillin at different pH values were successfully determined. Using the developed setups, amoxicillin could be degraded to less than 5% of its initial concentration, indicating complete degradation.

The photocatalytic material was immobilized on a polyether sulfone membrane in cooperation with the Department of Technical Chemistry of the University of Duisburg-Essen. It was successfully demonstrated in both reactor systems that the membranes are suitable for repeated use. In degradation experiments using a simulated environmental matrix, it was shown that the membranes can degrade amoxicillin even in the presence of natural organic matter, as typically found in wastewater. An analytical method was developed to identify possible transformation products of photocatalytic amoxicillin degradation. The method separates the substance mixture by liquid chromatography and detects compound-specific chemical characteristics using high-resolution mass spectrometry (Orbitrap MS), such as exact mass, which can be used for identification. Using the developed method, transformation products in the form of previously unknown features of amoxicillin were identified. These identifications

will contribute to evaluating their ecological relevance. To sample urban wastewater, with a particular focus on hospital effluents, an additional analytical method was developed. The method allows chromatographic separation of a panel of 23 antibiotics and their sensitive detection at nanogram-per-liter (ng/L) levels using liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS, triple quadrupole MS).

Using 24-hour composite samples collected at various sampling sites, several representatives of different antibiotic classes, including -lactams, macrolides, fluoroquinolones, and sulfonamides, were successfully detected by standard addition at low double-digit ng/L levels within a complex wastewater matrix. This demonstrates the robustness and sensitivity of the analytical approach for trace-level quantification in real-world samples. Furthermore, it was shown that the TiO_2 polyether sulfone-based photocatalytic membranes can reduce antibiotic residues even in a complex water matrix following targeted treatment, highlighting their potential for wastewater remediation.

Methods of Digital Food Sensing Based on Ion Mobility Spectrometry

Involved Staff: Modestus Wigger, Stefanie Sielemann, Ursula Telgheder
Partners: Hamm-Lippstadt University of Applied Sciences, Symrise AG
Funding: Hamm-Lippstadt University of Applied Sciences

Gas chromatography-ion mobility spectrometry (GC-IMS) has become a powerful tool for analyzing food aromas. Compared with conventional gas chromatography-mass spectrometry (GC-MS), GC-IMS offers high sensitivity for many aroma-active volatile compounds with lower acquisition and maintenance costs. Building on these advantages, this Ph.D. project explores further applications of GC-IMS in food sensing. Analyzing the volatile compounds in the kitchen herb oregano, which is produced by plants of *Origanum vulgare*, is one of these applications. First, the aroma profile of commercially available dried oregano and fresh leaves from different species of the genus *Origanum* is characterized. Due to the limited ability to identify these with GC-IMS, a GC-MS was also used. The GC-MS data allow identification tentatively via database comparison, and retention index-based assignment of peaks from both detectors enables identification in the GC-IMS. In addition, the results can be verified by targeted measurement of reference substances. Using these methods, a detailed comparison of the aroma profiles of six *Origanum* species is possible.

A second motivation is the risk of food fraud. Commercial oregano is usually sold dried and may be adulterated with non-oregano plant material, such as olive leaves. Therefore, a feasibility study is conducted to assess whether GC-IMS can support authenticity testing of oregano by detecting atypical volatiles. A third focus is the analysis of industrially extracted oregano essential oils. Headspace sampling is standard in GC-IMS but can bias analyte distributions. Another aspect is that the complex mixture of terpenoids forming the essential oil is liquid. Therefore, liquid injection is evaluated as an alternative technique, which has been used rarely in GC-IMS due to cross-sensitivities between common solvents and the IMS detector. By

selecting IMS-compatible solvents, it is demonstrated that liquid injection can be robustly coupled to GC-IMS. Using *Origanum vulgare* extracts as a model, this approach provides sensitive, rapid analysis while retaining the practical advantages of GC-IMS. Demonstrating the feasibility of liquid injection allows established GC-MS approaches and their routine extraction procedures to be applied to GC-IMS.

Characterization of Nutrients, Pollutants, and Environmental Impacts in a Manure Recycling Process

Involved Staff: Michelle Hußock, Gerrit Renner, Torsten C. Schmidt
Partners: Wetsus European Centre of Excellence for Sustainable Water Technology, Oosterhof Holman Milieutechniek B.V., Federatie Agricycling NL, 3N Kompetenzzentrum Niedersachsen Netzwerk Nachwachsende Rohstoffe und Bioökonomie e.V, Hochschule Osnabrück University of Applied Sciences, Maatschap Broekroelofs, B.E.S. GmbH & Co. KG, DLV Rundvee Advies B.V., Humus Guru GmbH
Funding: Interreg Germany-Netherlands, (co-)funded by the European Union

Each year, millions of tons of manure accumulate in Germany and the Netherlands. Manure is a valuable fertilizer due to its high content of essential plant nutrients. However, the nutrient composition is not ideal for the plant. As a result, plant health can potentially be impaired and soil degradation accelerated. Furthermore, excess nutrients can leach into groundwater and surface waters, contributing to contamination of drinking water and eutrophication. As part of the ReFarM project, an innovative Upflow Anaerobic Sludge Bed (UASB) reactor was designed to provide a sustainable solution for manure management. By recovering valuable nutrients, it facilitates the production of more efficient fertilizers and soil conditioners.

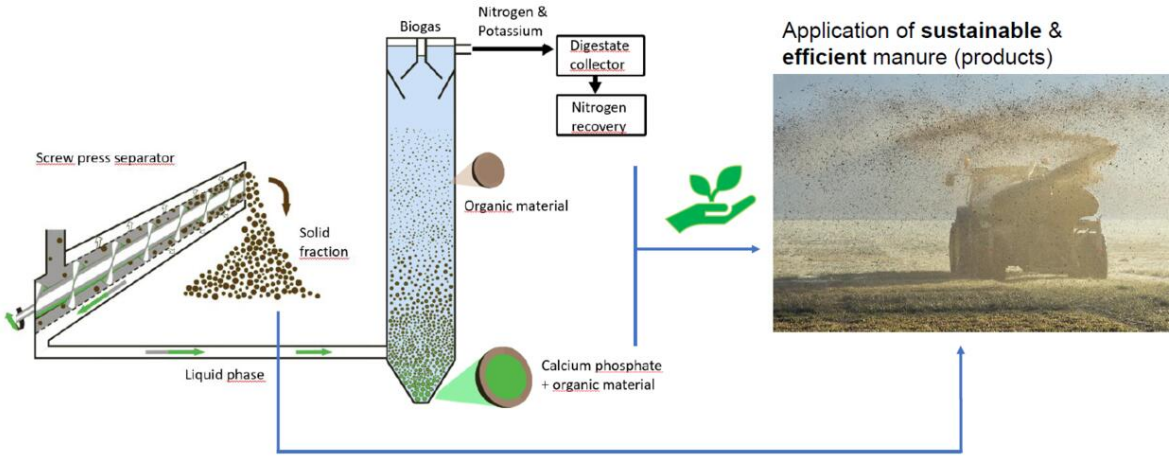

Figure 8: Schematic of the UASB reactor used in the manure recycling process.

Effectively improving soil health and reducing water pollution through manure recycling requires nutrient analysis, as well as the identification and characterization of potential pollutants. In this work, the focus is on the characterization of (heavy) metals and organic micropollutants.

The manure transformation process is analyzed for Ca, K, Mg, Zn, Cu, Ni, Pb, Cd, As, and Cr using ICP-OES and ICP-MS. To this end, sample preparation and analytical procedures are initially optimized by analyzing various manure samples. By collecting and analyzing samples at different time points and reactor heights, accumulation and transformation processes will be tracked and better understood.

Antibiotics are investigated as key organic micropollutants. Their typically low concentrations (in the low ng/L range), the complexity of the environmental matrix, and their diverse physico-chemical properties make sample preparation and determination particularly challenging. LC–MS/MS methods have already been successfully applied to analyze several veterinary antibiotics in manure. However, comparatively little attention has so far been given to their analysis by supercritical fluid chromatography (SFC). With its ability to separate compounds across a wide polarity range, SFC is a promising, potentially more environmentally friendly alternative. The goal of this project is to develop and optimize an SFC–MS/MS method for selected veterinary antibiotics used in livestock farming. In parallel, the LC separation of these compounds will be optimized to enable a direct comparison between the two chromatographic techniques. The optimized methods will provide a basis for application to manure samples and for evaluating solid-phase extraction (SPE)-based sample preparation strategies. Once antibiotic concentrations in manure have been determined, their influence on microorganisms in the reactor can subsequently be investigated.

Data Processing of High-Resolution Mass Spectrometry Data for Non-Target Screening

Involved Staff: Daniel Höhn, Gerrit Renner, Torsten C. Schmidt
Partners: –
Funding: Internal

In 2025, we continued developing our software library for data processing in non-target screening, qAlgorithms (available here: https://github.com/odea-project/qAlgorithms). qAlgorithms is a data processing utility that aims to provide fully automated evaluation and quality assurance of complex LC-HRMS data. The algorithms in qAlgorithms are rooted in well-established statistical tests and use standard linear regression as their primary problem-solving strategy. This allows us to be fully deterministic without requiring the user to supply and optimise algorithm parameters, which is a time-consuming and error-prone process even for domain experts. While this design allows users to treat processing as a “black box”, we always supply additional layers of data. For the user, it is thus possible to treat the output features as the commonly found *m/z* – RT – intensity triplet or to consider more precise descriptors. These are summarised in the data quality score, a number between zero and one, that is (roughly) equivalent to the commonly used R^2. For in-depth details, the outcomes of all processing steps are preserved within the output, and every feature can be traced back to the profile points that produced it.

Our efforts were in part directed towards ensuring program correctness and eliminating a large number of logic errors that would have falsified any produced results. Furthermore, we can enhance the computational performance of qAlgorithms to reduce processing times. Performance measures proved useful for spotting subtle programming errors and highlighted properties of the data system that we can utilise as descriptive statistics for our peak model. This focus on quality descriptors and complete automation sets our work apart in the relatively crowded field of peak-detection algorithms for chromatography. Additional advancements are the conceptual development of a full parameter-free componentisation strategy using our peak model. The design uses a novel clustering method in which the distance between two features is defined as the shape similarity of their profiles. This similarity can be obtained for two or more signals simultaneously without scaling the data using linear regression. After obtaining all pairwise distances, individual features can be merged into components. Finally, a goodness-of-fit is calculated to describe the components' similarity to the original set of features. We hope that these progressions will prove useful to the scientific community at large and, especially, to the joint CogniFlow project involving Ricardo Cunha, which is set to begin in Q1 2026.

Latent spaces in non-target screening: a two-dimensional anomaly index to identify hotspots in river longitudinal studies

Involved Staff: Felix Drees, Dr. Gerrit Renner, Prof. Torsten C. Schmidt
Partners: –
Funding: Internal

Non-target screening (NTS) employing high-resolution mass spectrometry (LC-HRMS) has become a central instrument for characterizing complex environmental samples. In contrast to traditional approaches that monitor a predefined list of target compounds, NTS captures thousands of signals (features) that together form a high-dimensional chemical fingerprint [1]. This fingerprint is increasingly used in monitoring rivers and wastewater systems to track changes in water quality, detect unknown dischargers or process disturbances, and flag samples of concern, even when the underlying compounds have not yet been identified [2]. To interpret and visualize such complex fingerprints, unsupervised dimensionality compression methods such as principal component analysis (PCA), Uniform Manifold Approximation and Projection (UMAP), or autoencoder-based neural networks can be applied. The resulting score plots define latent spaces in which sample clusters, gradients, and outliers are immediately apparent [3, 4]. Samples that lie far from a reference cluster are intuitively considered unusual and prioritized for more detailed chemical or ecotoxicological follow-up. However, these latent spaces are not objective, immutable coordinate systems. They emerge from a series of modeling decisions, including feature selection, preprocessing, algorithm choice, hyperparameter selection, training set composition, and initialization, that introduce model variability. Furthermore, the type of variation matters: changes may occur within existing patterns of features or through the appearance of entirely new signals. This elicits questions

about how stable and comparable latent spaces really are, and how different forms of change along a river system can be captured more explicitly [5].

In our experimental study, river water was sampled quarterly at thirteen sites along the River Ruhr, with upstream stations serving as chemical references. Samples were analyzed by LC-HRMS (SCIEX TripleTOF 6600) on a Zorbax Eclipse XDB-C18 column (100 x 6.6 mm, 40 C) using a 40-minute water/acetonitrile gradient (0.1% formic acid, 100 uL injection). Feature extraction plus alignment were performed in EnviMass (v4.5). Latent spaces were constructed from upstream samples using PCA and parametric UMAP. For each downstream sample, we calculated the latent-space distance to the reference cluster, as well as a novel-feature factor representing the number and cumulative intensity of features absent or below a threshold in the reference. Together, these metrics define a two-dimensional anomaly space. Simulated data sets were additionally used to probe the behavior of this anomaly index under regulated perturbations, including feature removal, batch shifts, and the introduction of new peaks. We propose a conceptual framework that separates two dimensions of anomaly in NTS data: latent-space distance and the emergence of new features. Samples near the river source form a consistent reference cluster in PCA/UMAP space; for each downstream sample, the latent-space distance reflects distortion of the established chemical fingerprint, while the novel-feature factor quantifies contributions from newly emerging signals. The structure of this two-dimensional anomaly space is illustrated in Fig. 9.

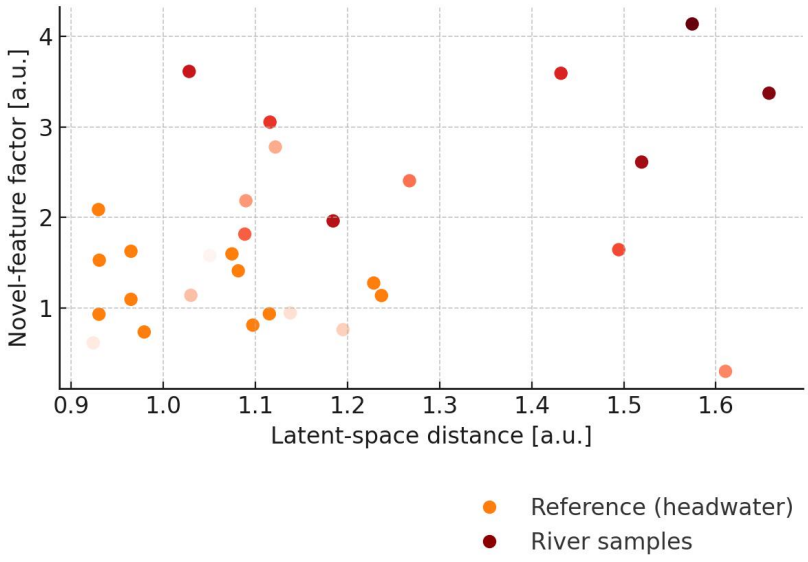

Figure 9: Simulated anomaly index for a longitudinal river study. Orange points show samples taken near the source of the river; red points show downstream river samples in the space of latent-space distance (x) and novel-feature factor (y). The red color gradient from light to dark indicates increasing distance from the river source. Three colored boxes highlight the anomaly types (a-c).

Within this space, three archetypal cases can be distinguished: (a) high distance but few new features, representing shifted but known fingerprints; (b) many new features at moderate distance; and (c) samples extreme in both dimensions. Simulated case studies indicate that although PCA, parametric UMAP, and autoencoder-based latent spaces vary regarding ro-

bustness, the dual-indicator concept is method-independent. Applied to river longitudinal data, this approach identifies sections with pronounced fingerprint shifts or the strong emergence of new features as potential hotspots, which can then be selected for targeted chemical identification or ecotoxicological testing. Overall, this approach treats score plots not simply as qualitative visualizations, but as quantifiable, model-dependent latent spaces whose stability and informational content can be explicitly examined. The combination of latent-space distance and the novel-feature factor offers a new perspective on anomaly detection in NTS and delivers a robust framework for sample prioritization based on chemical fingerprints.

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2D-LC-IRMS Coupling for Compound-Specific Stable Isotope Analysis

Involved Staff: Sarah P. Rockel, Matthias Stüwe, Leonardo Solazzo, Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt
Funding: German Research Foundation (DFG), Project Grant 537343248

Compound-specific stable isotope analysis (CSIA) by liquid chromatography coupled to isotope ratio mass spectrometry (LC-IRMS) enables the determination of stable carbon isotope signatures of non-volatile and thermally labile compounds without derivatization. The technique is useful for pharmaceutical authentication, anti-doping analysis, and forensic investigations. However, LC-IRMS is restricted to fully aqueous mobile phases because the wet-chemical oxidation interface converts all oxidizable carbon to CO2. The use of organic eluents would introduce additional carbon and compromise isotope ratio accuracy. As a result, conventional reversed-phase LC methods relying on organic solvent gradients cannot be directly applied, significantly limiting chromatographic flexibility and complicating method development. To overcome these limitations, temperature-responsive liquid chromatography

(TRLC) was implemented as a novel separation concept for LC-IRMS. TRLC stationary phases based on poly(N-isopropylacrylamide) (PNIPAAm) exhibit a reversible change in hydrophobicity depending on temperature. Below the lowest critical solution temperature (LCST), the polymer is in a hydrophilic, expanded state, whereas increasing temperature induces a transition to a hydrophobic, collapsed conformation. This temperature-dependent change in retention behaviour enables selective modulation of analyte retention under strictly aqueous conditions without altering the mobile phase composition (see Fig. 10). The approach, therefore, provides an alternative strategy for gradient-like selectivity control that is fully compatible with LC-IRMS requirements.

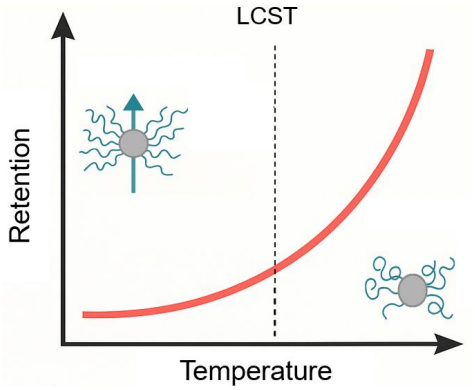


Figure 10: Temperature-controlled retention mechanism of a PNIPAAm-based TRLC column showing polymer expansion below and collapse above the lowest critical solution temperature (LCST), resulting in increased retention at higher temperatures.

Within this project, TRLC was coupled to LC-IRMS for the first time and systematically evaluated for compound-specific carbon isotope analysis. Steroids, particularly testosterone and structurally related compounds, were selected as model analytes. The developed system demonstrated stable ^{13}C measurements under both isothermal and temperature-gradient conditions, with reproducibility within the accepted precision limits of LC-IRMS. Importantly, no isotopic bias was observed as a result of temperature modulation of the stationary phase. In one-dimensional TRLC-IRMS, several steroid standards were successfully separated in a fully aqueous mobile phase. The application of temperature gradients improved peak shapes and detection limits compared to purely isothermal operation. The method was applied to a commercial testosterone gel formulation, enabling accurate isotope ratio determination without interference from matrix components.

To further extend the analytical capabilities, TRLC was integrated into a two-dimensional LC-IRMS configuration. A reversed-phase separation using organic solvents was applied in the first dimension to enhance selectivity and remove matrix. Target analytes were transferred via heart-cut modulation to a second, aqueous TRLC dimension prior to oxidation. This setup enabled the resolution of structurally similar steroids, such as testosterone and epitestosterone, which could not be separated in a single aqueous dimension. In addition, complex oil-based pharmaceutical preparations containing testosterone esters were successfully analysed, demonstrating the robustness of the approach for challenging sample matrices. Overall,

this work establishes temperature-responsive liquid chromatography as a powerful extension of the LC-IRMS methodology. By enabling temperature-controlled retention modulation under fully aqueous conditions and facilitating integration into two-dimensional systems, TRLC significantly expands the applicability of compound-specific isotope analysis. The developed approach opens new perspectives for pharmaceutical authenticity testing, anti-doping applications, and the investigation of complex forensic and environmental samples.

Cogniflow: Intelligent data-driven software tool for monitoring wastewater quality using machine learning

Involved Staff: Daniel Höhn, Gerrit Renner, Torsten C. Schmidt
Partners: Ricardo Cunha (IUTA e.V.)
Funding: Internal/ zukunftsfähige und nachhaltige Abwasserbeseitigung in Nordrhein-Westfalen (ZunA-NRW)

This project introduces a semantically structured, reproducible framework for computational workflows in analytical chemistry, addressing the increasing demand for transparent, machine-interpretable, and policy-controlled data-processing environments in laboratories that rely on complex digital pipelines. The framework integrates a pipeline execution engine, a semantic description layer based on JSON-LD and SHACL, a structured data storage backend known as the Data Hive, and a formalized governance layer that documents architectural decisions and constraints. Collectively, these components establish a robust, controlled, and traceable infrastructure for analytical data evaluation. Modern analytical chemistry generates vast volumes of heterogeneous data, especially in fields like high-resolution mass spectrometry, process analytics, and sensor-based monitoring. Evaluating this data usually requires multi-step computing workflows combining signal processing, transformation, aggregation, and persistence. In many laboratories, these workflows develop organically and often lack a formal structure to ensure repeatability and long-term traceability. Parameter changes are frequently undocumented, storage strategies are inconsistent, and workflow configurations are difficult to validate before execution. This project addresses these problems by introducing an explicitly defined pipeline model that separates semantic definition, execution logic, and data persistence.

At the heart of the system is a pipeline engine that executes workflows described in a structured, machine-readable format. Each pipeline is defined using a semantic layer based on JSON-LD, enabling workflow structures to be represented as graphs of typed entities. SHACL constraints enforce the validity of these descriptions, ensuring that pipeline configurations adhere to a formally defined schema before execution. Invocation files specify which pipeline to execute and how entry points are configured; these are fully validatable and designed to remain semantically expressive while simplifying the authoring process. The execution engine interprets the validated graph and deterministically resolves configuration overrides, guaranteeing that runtime behavior is reproducible and auditable. The Data Hive serves as

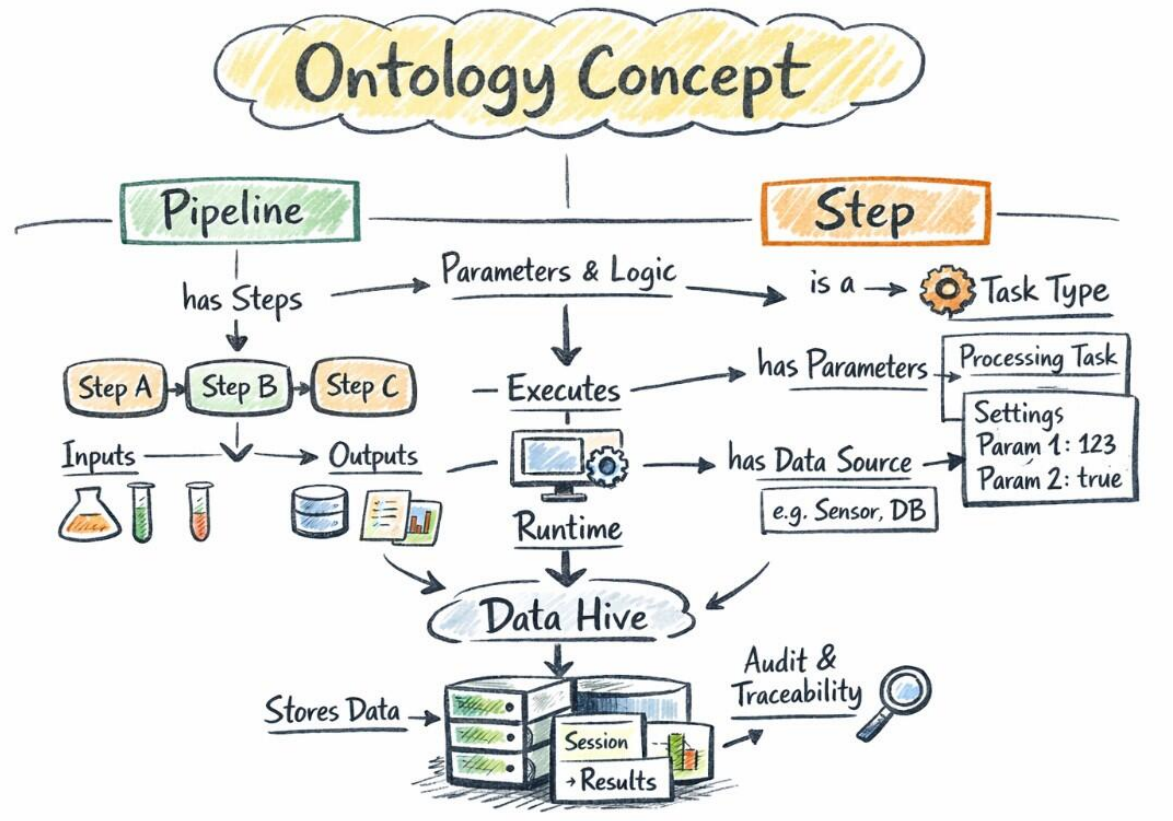


Figure 11: Conceptual overview of the Cogniflow framework for semantically structured and reproducible analytical workflows.

the system's structured storage layer for pipeline outputs and is built around a single-writer principle to ensure controlled persistence. Data writing occurs through a dedicated native component that acts as a gatekeeper, preventing uncontrolled access to storage. Each pipeline run is associated with a session and produces a manifest recording metadata such as pipeline identifier, run identifier, session identifier, storage mode, schema fingerprint, and physical table locations. This manifest-based approach ensures that every result can be traced precisely back to its calculative context.

The storage model adapts automatically to varying data regimes. When a small number of runs generate large tables, results are stored in a partitioned-by-run mode that keeps datasets clearly separated. Conversely, in scenarios where many runs produce very small tables, such as sensor monitoring with thousands of micro-batches, the system switches to a session-compacted mode, consolidating results to avoid proliferating small Parquet files. This reduces metadata overhead and improves query performance. The adaptive storage policy is formally specified and enforced, demonstrating that performance factors are integral to the architectural design rather than an afterthought.

In addition to execution and storage, the project stresses governance and architectural transparency. A dedicated structure maintains architecture decision records and formal specifications, ensuring that structural requirements, storage policies, and design principles are thoroughly documented and auditable. Tasks that alter core behavior are described with

explicit validation criteria. This approach supports long-term maintainability and is consistent with the scientific imperative for traceable methodological decisions, enabling controlled system evolution and avoiding unintended architectural drift. From the analytical chemistry perspective, the framework delivers a foundation for reproducible digital workflows in data-intensive environments. It supports structured algorithm integration, explicit parameter control, and formally validated execution. By uniting semantic workflow modeling, policy-controlled data storage, and deterministic runtime behavior, the system establishes an infrastructure tailored to the requirements of contemporary laboratory data science. It is particularly suited to applications such as non-target screening, advanced chromatographic data processing, and automated monitoring systems, where traceability, scalability, and procedural strictness are essential.

To summarize, the project delivers a formally structured computational framework integrating semantic description, controlled execution, adaptive storage, and documented governance. It marks a step toward a somewhat more transparent and reproducible digital laboratory environment, where analytical data processing is not only automated but also explicitly defined, validated, and auditable.

Pipe Reactor System for PFAS Remediation (TOFfloc)

Involved Staff: Dr. Klaus Kerpen, Simone Bettinger, PD Dr. Ursula Telgheder
Partners: Cornelsen Umwelttechnologie GmbH
Funding: Federal Ministry for Economic Affairs and Climate Protection (BMWK) – Central Innovation Programme for SMEs (ZIM)

PFAS are a group of anthropogenic substances that have been detected worldwide in the aquatic environment, wildlife, and humans over the past decade. PFAS are characterized by two main properties: their high thermal stability and their remarkable chemical stability, both of which are attributable to the carbon–fluorine bonds throughout the molecule. However, these exceptional properties also make them highly persistent in the environment and largely resistant to degradation, leading to their ubiquitous presence worldwide and, due to their toxic properties, posing a risk to both human health and the environment. The analysis of PFAS is associated with many challenges, on the one hand due to the large number of unknown compounds, and on the other hand due to the lack of standards and robust analytical methods for their quantification using conventional methods for specific compounds.

The aim of the research project was to develop a pipe reactor system controlled by on-site PFAS analysis, enabling the rapid and effective treatment of PFAS-containing wastewater, such as wastewater generated during the cleaning of firefighting foam tanks in fire service vehicles and stationary fire suppression systems, using the PerfluorAd process. The analytical method to be developed is based on the determination of total organic fluorine (TOF). This parameter is then used to control the dosing of the specific precipitating agent PerfluorAd into the pipe reactor system. During the course of the project, it became apparent that other

sectors, such as soil washing operations and landfills, also have a strong interest in a rapid analytical method for estimating PFAS concentrations. For this reason, the project objective was adapted to enable the analytical system to operate as a standalone module, allowing it to be offered to the market independently of PerfluorAd.

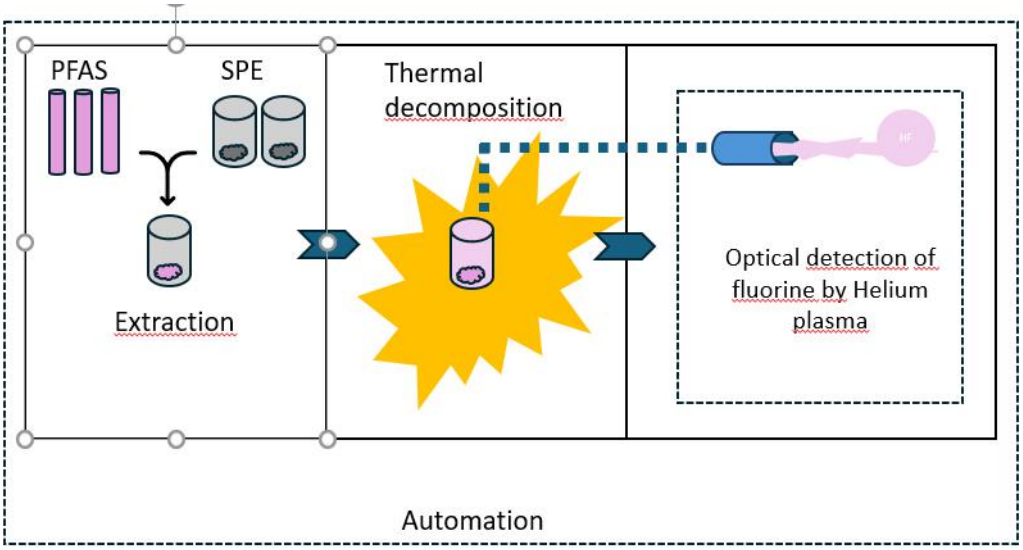


Figure 12: Schematic structure of the analytical system for the determination of total organic fluorine (TOF)

Regenerable Adsorber for PFAS Removal in Contaminated Water (FluorSorb)

Involved Staff: Isabel Halbhuber, Dr. Klaus Kerpen, Simone Bettinger, PD Dr. Ursula Telgheder
Partners: InstrAction GmbH
Funding: Federal Ministry for Economic Affairs and Climate Protection (BMWK) – Central Innovation Programme for SMEs (ZIM)

The project aims to develop a regenerable adsorbent capable of successfully removing PFAS from water. The makeup and structure of the adsorbent are intended to ensure near-complete removal of both PFAS and their replacement compounds. A key aspect of the analytical work is the development of a solid-phase extraction (SPE)-based enrichment method that enables the concentration and detection of short-chain PFAS at ultra-trace levels. Within this enrichment procedure, inorganic fluoride is quantitatively separated from organic fluorine compounds (PFAS) prior to analysis. Suitable solid phases were selected for analyte enrichment, and the experimental parameters, including the eluent type and volume, sample volume, enrichment, and extraction time, were determined. As shown in Fig. 13, high adsorption efficiencies were observed for the materials HR_XA (100 ± 3%) and HR_XAW (101 ± 5%) across all water types and for all analyzed PFAS. Deviations were observed only for PFOS in pond water, which can be attributed to issues with the SPE procedure and the analytical method. The material ND 067_1 showed lower PFBA efficiency in tap water (54%), whereas ND 064_2 exhibited

reduced efficiencies for both PFBA and PFPeA in tap water (9% and 63%) and in pond water (39% and 90%). The lower adsorption efficiency of PFBA, a short-chain PFAS, is due to the greater hydrophobicity of the functional groups in the ND materials compared to those in the CHROMABOND HR resins.

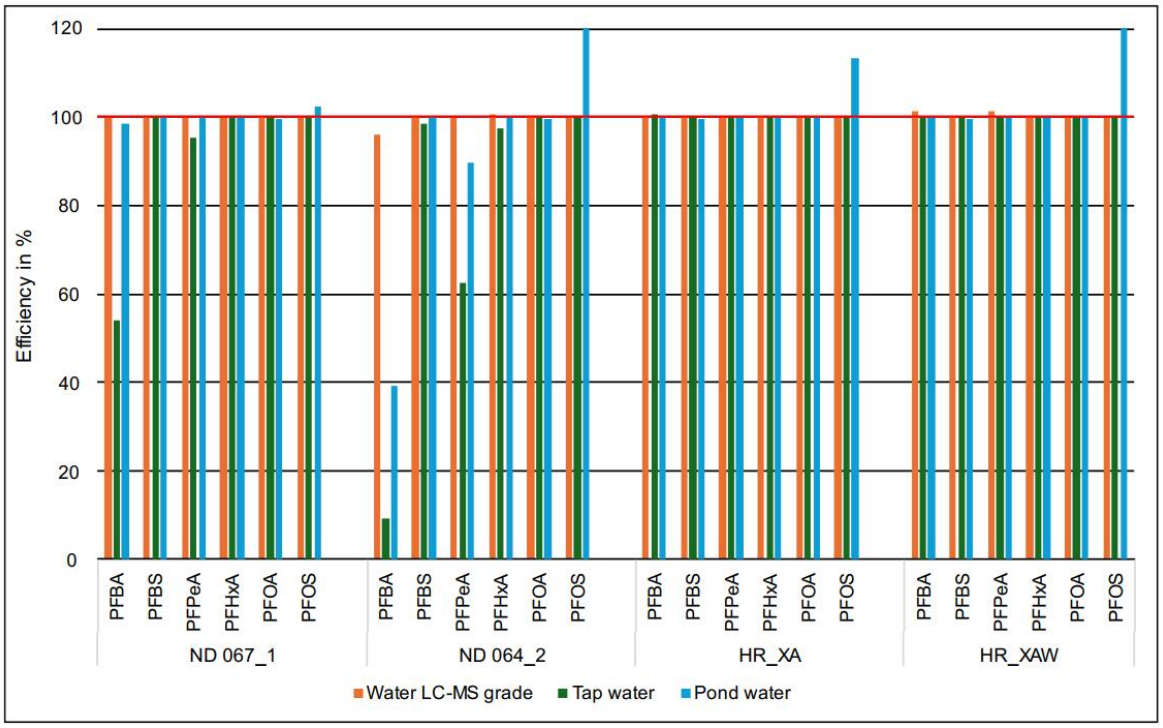


Figure 13: Comparison of the adsorption efficiency of different water matrices on various materials. A PFAS mixture with a concentration of 2000 ng L-1 of PFBA, PFBS, PFPeA, PFHxA, PFOA, and PFOS was used to determine the adsorption efficiency of different materials from various matrices using UPLC-MS/MS. The materials used were ND 067_1 and ND 064_2 from InstrAction, as well as HR_XA and HR_XAW from Macherey-Nagel.

To characterize the PFAS adsorber and its starting materials using various analytical techniques, Raman spectra were recorded, and TOF-MS analyses were performed on the PVA polymer solution, the coated PFAS adsorbers, and the uncoated silica gel supports. Furthermore, a method for the direct analysis of the developed adsorber materials was designed. Using a mass spectrometer (ionization: ESI) from Advion equipped with a PlateExpress sample introduction system, solid adsorber material could be analyzed directly.

Theses Completed in 2025

Doctoral Theses

Mike Wenzel

03 February 2025

Development of sustainable sample preparation methods for microplastic analysis

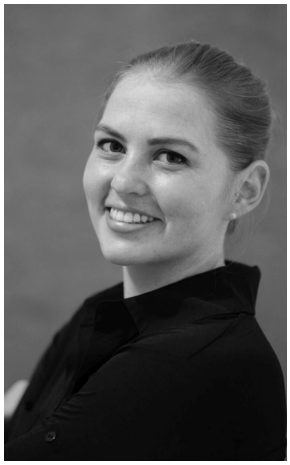
The pollution of the environment by microplastics is a topic of great concern, as they are found in all environmental compartments, while the ecotoxicological consequences and impacts on human health remain unpredictable. Therefore, assessing the fate of microplastics in the environment utilizing instrumental analytical techniques is a significant part of microplastics research. In this context, reducing the mostly dominant matrix is required to minimize interferences during analysis. However, due to the lack of standardization in microplastic research, several sample preparation methods with variable protocols have been developed, significantly hampering inter-study comparisons. Most of these methods still utilize ecotoxicologically harmful chemicals. However, these chemicals can and should generally be avoided in analytical chemistry workflows to comply with the principles of green analytical chemistry (GAC).

Despite the growing importance of GAC, its principles are not yet well integrated into microplastics research. Therefore, this thesis primarily focuses on developing sustainable (matrix-reducing) sample preparation methods for microplastic analysis. An optimized version of the hydrophobicity-water/air-based enrichment cell for microplastics, called µSEP, is presented and characterized. The advantage of µSEP is its greenness by design, as it relies on the hydrophobic adhesion of microplastics to air bubbles within a water-filled separation column. This means only water and air are required. This thesis presents two new sample preparation methods for µSEP to extend its usefulness to microplastics in soils and atmospherically deposited microplastics in moss. The new methods are suitable for analysis using thermal extraction-desorption gas chromatography-mass spectrometry (TED-GC-MS) and Raman microspectroscopy (µRaman) to provide a wide range of information on microplastics in the environment, including mass concentration, polymer type, particle number, size, and shape.

Regarding soils, TED-GC-MS analysis showed that µSEP provides suitable, robust recoveries. Within a sample preparation time of 60 min, average recoveries of 77% ± 11% for PET, 42% ±

11% for PS, and 65% ± 12% for PP were determined. Moreover, µRaman analysis shows that a high separation effectiveness can be achieved. Additionally, the AGREEprep metric provides evidence that µSEP is beneficial in GAC compared to commonly used sample preparation methods. Regarding moss, the developed method, named µPEEL (microplastics extraction through exfoliation), includes exfoliation of microplastics from the moss surface, a sieving step, and µSEP. The application of µPEEL produces robust and appropriate recoveries, a high separation effectiveness, and meets the requirements of GAC. Furthermore, matrix effects, such as retention time shifts in pyrolysis products, can be minimized when µPEEL is applied before TED-GC-MS analysis. Subsequently, µPEEL was applied to environmental moss samples to investigate whether moss could serve as a biomonitoring system for atmospherically deposited microplastics. Synergies between TED-GC-MS and µRaman results were observed, with the same polymer types (PET, PP, PE) identified in both. The results show that moss may be a suitable biomonitoring system, as the determined polymer masses, particle numbers, and diversity could be linked to the distance and type of potential microplastic emission sources.

Additionally, this work conducted a review of the existing literature concerning recognized matrix effects and established strategies for their mitigation, focusing on thermoanalytical methods such as TED-GC-MS or py-GC/MS. Already established matrix-effect alleviation strategies were critically discussed, and an analytical workflow was proposed to mitigate a wide range of matrix effects. The combination of matrix reduction, thermochemolysis, and standard addition seems to be a suitable approach. Further, it can be observed that the use of chemicals during sample preparation can induce matrix effects. In conclusion, this thesis demonstrates that the principles of GAC can be applied to microplastic research and that their implementation can additionally enhance the accuracy of analysis.



Michelle Klein

10 June 2025

Analysis of Endocrine Disrupting Compounds and their Effects in Aquatic Environments

The substances that drive progress and improve our quality of life also pose unintended risks to both human health and ecosystems, necessitating careful assessment and management. Aquatic environments, among the most biodiverse and vital ecosystems on earth, provide essential ecological services and sustain countless species. Protecting these environments requires interdisciplinary collaboration across environmental sciences, such as toxicology and chemistry, to address the direct and indirect consequences of anthropogenic pollution. To enhance water quality, particularly amid growing environmental challenges, it is crucial to bridge the gap between chemical analyses and effect-based methods (EBMs). One category of emerging contaminants is endocrine-disrupting chemicals (EDCs), which can exert harmful effects even at concentrations below 1 ng/L. They are pollutants that interfere with organisms' hormonal systems, potentially causing adverse health effects. This thesis aims to apply effective methodologies for monitoring EDC in freshwater, with a focus on their occurrence,

biological impact, and the sustainability of their analysis. Sample preparation is crucial in these concentration ranges, with solid-phase extraction (SPE) being the most common method. Micropollutant concentrations in unenriched samples may be insufficient for detection, particularly in water samples with reduced contamination load. Although concentrations may fall below detection limits, biological activity may still be present, necessitating sample enrichment for reliable analysis. However, enrichment can introduce masking effects due to high chemical loads, obscuring the endpoints of interest. Furthermore, standardized procedures for these processes are still lacking. EBM targeting EDCs primarily uses receptor-mediated bioassays to assess specific toxicity pathways. This study demonstrated the efficacy of applying various *Arxula* yeast-based bioassays in detecting endocrine activity (estrogen, androgen, and progestogen) in aquatic samples. While surface water (SW) samples exhibited higher effect concentrations due to direct pollution sources like wastewater treatment plants, groundwater (GW) samples showed a dominance of inhibitory effects.

Estrogens were among the first group of chemicals to raise awareness of EDC exposure in the environment. Chemical analyses such as GC-MS/MS and LC-MS/MS have demonstrated the ability to detect all estrogens of interest. The validated chemical methods, now included in the new ISO 13646:2025 standard, demonstrated strong performance with acceptable repeatability and reproducibility. A crucial cleanup step using silica gel cartridges was required to accurately detect all target estrogens; without it, compounds such as EE2 remained undetected. GC-MS/MS achieved a 0.4 pg/L detection limit for the critical EE2 (EQS: 35 pg/L) with a 10,000-fold enrichment. In times of resource scarcity, environmental pollution, and climate change, evaluating analyses for sustainability provides insights into potential improvements. The application of software tools for green analytical chemistry (GAC) and white analytical chemistry (WAC) helps to assess sustainability aspects of different methods. While GAC focuses on environmental burden and safety, WAC also considers additional factors, such as performance and efficiency. Advancements in in-situ SPE and process miniaturization can significantly enhance the sustainability of EDC analysis. Automation, particularly in EBM, holds substantial potential to improve efficiency and reduce manual intervention in complex workflows. Additionally, effect-directed analysis (EDA) offers both green and analytical advantages by reducing the number of samples requiring extensive chemical characterization.

Shaista Khaliq

23 October 2025

Amino Acid Isotope Analysis in Aquatic Ecosystems: Method Development, Host–Parasite Dynamics, and Food Web Applications

This Ph.D. thesis explores compound-specific isotope analysis of amino acids (CSIA-AA) as a tool for studying nutrient cycling, trophic interactions, and metabolic processes in aquatic ecosystems. Focusing on fish, parasites, and macroinvertebrates, the research utilizes established CSIA-AA techniques to enhance accuracy and reliability in ecological studies. It also addresses technical and methodological challenges, proposing suitable solutions wherever possible. The study optimizes sample preparation, derivatization,

and instrument performance to ensure precise isotope measurements. Modifications to chromatographic conditions, instrumental parameters, and appropriate isotopic corrections enable the adaptation of CSIA-AA methods to the specific needs of ecological applications.

A significant focus is applying CSIA-AA to host–parasite systems, specifically the three-spined stickleback (*Gasterosteus aculeatus*) and its parasite, *Schistocephalus solidus*. The study examines nitrogen isotope patterns to track nutrient assimilation. Findings indicate that parasites acquire nutrients passively from their hosts, with minimal differences in trophic position between the parasites and their hosts. Specific amino acids, such as alanine and glycine, exhibit distinct fractionation patterns associated with metabolic processes, including gluconeogenesis and immune responses. The thesis extends CSIA-AA to freshwater food webs, studying *Gammarus* populations over multiple years. Carbon and nitrogen isotope analysis reveals that microbial and algal sources play a significant role in energy flow, and *Gammarus* primarily functions as a primary consumer. These findings highlight the significance of detrital food webs and offer insights into the factors that influence nutrient cycling in freshwater ecosystems. This research enhances the application of CSIA-AA in ecological studies by refining analytical methods for investigating nutrient flows, energy transfers, and trophic interactions. The findings contribute to isotope ecology by enhancing our understanding of nutrient dynamics and food web stability in freshwater environments. This work lays the foundation for further applications of CSIA-AA in ecological research and biogeochemical investigations.

Fabian Ude

28 October 2025

Gas chromatography drift tube ion mobility spectrometry with non-radioactive ionization for on-site pollutant analysis in building materials

This study describes the development of a gas chromatography–drift tube ion mobility spectrometer (GC-DTIMS) and the associated analytical methods for the qualitative and quantitative detection of wood preservatives in wood-based materials. The substances considered include pentachlorophenol (PCP), lindane, and dichloro-diphenyltrichloroethane (DDT). The system employs a photon source that generates photons with sufficient energy to produce reactant ions in ambient air, enabling chemical ionization at atmospheric pressure. A specially designed transfer element guides the eluting compounds from the column into the drift tube using a carrier gas stream. To maintain compactness and portability, the components are housed in a benchtop case and feature three custom-designed circuit boards for high voltage supply, ion gate operation, and ion source control. A programmable logic controller (PLC) manages system coordination and interfaces with a computer via OPC UA. Data acquisition and evaluation are handled by two independently developed C#-based software applications.

The analytical application was the quantitative determination of PCP in wood chips and wood flour, using solid-phase microextraction (SPME). The method achieves a detection limit of 0.1 mg kg-1 for PCP in wood flour, fulfilling the requirements of the German Waste Wood

Ordinance without the use of solvents or derivatization reagents, and offers a shorter analysis time than conventional techniques. A further application involves the non-destructive, qualitative identification of wood preservatives in cultural heritage objects, where prior treatment is often unknown. This method provides a basis for safer handling and display in museums and collections.

Reyhaneh Armin

24 November 2025

Method Development and Data Processing Strategies for the Non-Target Screening of Industrial Wastewater

Ongoing industrial growth and technological progress have contributed to the release of various substances into the environment, including heavy metals, inorganic compounds, and polar or non-polar organic pollutants. Therefore, the proper treatment and monitoring of industrial wastewater is essential for mitigating environmental pollution and safeguarding public health. Wastewater treatment plants (WWTPs) play a vital role in reducing the environmental impact of industrial effluents. However, their efficiency may often be challenged by the presence of unknown and emerging pollutants. During routine monitoring, this category of pollutants remains unaccounted for, as traditional approaches focus primarily on sum parameters or target compounds. This thesis investigated the application of non-target screening (NTS) via liquid chromatography-high-resolution mass spectrometry (LC-HRMS) in combination with novel data analysis techniques for improved industrial wastewater monitoring, enabling the detection of both known and unknown contaminants.

The thesis initially focused on the first step of NTS data analysis, feature extraction. Various open-source and commercial feature-extraction software tools, namely MarkerView, MZmine3, OpenMS, SIRIUS, and XCMS, were evaluated for their performance in time-trend analyses and in identifying patterns within an industrial wastewater matrix. This comprehensive comparison incorporated several techniques, including Spearman's rank correlation and other multivariate statistical approaches, such as principal component analysis (PCA) and sparse principal component analysis (SPCA), which is applied here to NTS data for the first time. Despite optimized parameters, the results showed notable differences in feature recall rates, with the software under- and overestimating the number of detected features due to its underlying mathematical framework. XCMS, OpenMS, and MZmine3 demonstrated better harmony in their outputs. The study also concluded that using at least two peak detection tools can reduce the number of false negatives and improve the robustness of marker detection in complex longitudinal datasets.

Building on this foundation, a direct application was realized through the development of a prioritization tool tailored for monitoring the wastewater system of a chemical industrial park, with the goal of protecting the WWTP and preventing potential contaminant releases. Developed in MATLAB, this tool enables simultaneous spatial and temporal prioritization of

features detected in the WWTP influent. The first module allows the creation of wastewater feature fingerprints of localized wastewater sources. The second module prioritizes temporal features in consecutive influent samples based on their intensity trends. A 7-day study of the WWTP's influent following the creation of fingerprints for 36 plants revealed that although the majority of the features could be traced to their source, a percentage of the features were not accounted for, due to various reasons, such as in-sewer transformations. By combining these feature-prioritization techniques, the tool enables early detection of pollution sources and fluctuations in wastewater composition. Another major contribution of this study was the development of an extended LC-HRMS workflow for detecting highly polar compounds, which are often overlooked by conventional reversed-phase chromatography. A zwitterionic hydrophilic interaction liquid chromatography (ZIC-HILIC) method was optimized and validated for industrial wastewater analysis, significantly enhancing the detection of polar contaminants. The results demonstrated that incorporating ZIC-HILIC into routine NTS workflows increased the range of detectable substances, providing a more comprehensive overview of wastewater composition.

Annika Fechner

27 November 2025

Development of an ion mobility spectrometry system with miniaturized thermodesorption and non-radioactive ion source for the detection of germs in food

Ion mobility spectrometry (IMS) is a fast and sensitive analytical technology with strong potential in food safety, but conventional systems rely on radioactive ionization and are limited to gaseous samples. This work presents the development of a miniaturized, non-radioactive IMS system for direct analysis of liquid samples with a focus on microbial contamination. The Flexible microTube Plasma (FμTP) source enabled stable operation in both positive and, for the first time with this type of source, negative ion mode. A functional negative reactant ion peak was identified, improving the detection efficiency for analytes such as propofol and demonstrating robust negative ionization without external dopants. The FμTP was further integrated into a commercial IMS instrument using a 3D-printed ionization chamber made from cycloolefin copolymer, which allowed precise positioning, stable electrical contact, and full software integration. Test measurements confirmed reproducible ionization and detection of volatile analytes down to 2.04 µg/L (2-decanone, $R^2 = 0.96$).

A thermal desorption chip (TDC) was developed for automated liquid sample introduction, combining preconcentration, controlled desorption, and humidity compensation. Quantitative calibration yielded linear responses ($R^2 = 0.998$), detection limits down to 0.076 µg/mL, and recoveries up to 98.3%. Compared to headspace sampling, the TDC provided up to 2.7-fold higher signals, enabled detection of dimer species, and increased intensities by a factor of 12 with preconcentrated volumes up to 0.5 mL. It also maintained stable signals across the humidity range, with only minor reductions between 20% and 28% relative humidity, whereas conventional coupling suffered near-complete loss at 100% relative humidity. In a

realistic application, characteristic volatile organic compound profiles of inoculated poultry samples were detected and reliably distinguished from controls using multivariate analysis. This system demonstrates a rapid, portable, and robust approach to microbial detection in food processing, combining novel negative ion chemistry, advanced sample introduction, and commercial-level integration, and represents a significant step beyond conventional IMS designs toward practical application in food safety monitoring.

Master Theses

Mahsa Estejab	Standardizing Analytical Protocols for the determination of Metal Impurities in Alkaline Electrolytes: Comparing GF-AAS, ICP-MS, and ICP-OES Techniques
Daniel Höhn	qPattern: Development of a Quality-Focused, User-Independent and Automated Componentisation Strategy for Non-Target Screening with HPLC-HRMS
Sara Khani	Non-Target LC-HRMS Screening of Wastewater Influent: Data Processing Approaches for Pattern Recognition and Biomarker Prioritization

Bachelor Theses

Robin Jung	Charakterisierung eines HF-Sensors für die Detektion von PFAS als Summenparameter
Philipp Klein	Investigation of Oxidative Degradation of Aminopolyphosphonates by Sodium Persulfate via Liquid Chromatography-Isotope Ratio Mass Spectrometry/High Resolution Mass Spectrometry
Paul Jasper Mielke	Optimierung der Anreicherung von Per- und Polyfluorierten Alkylsubstanzen (PFAS) mittels Festphasenextraktion (SPE)
Nadja Reich	Untersuchung verschiedener Photokatalysatoren in Gegenwart einer artifiziellen Wassermatrix am Beispiel des Aminopenicillins Amoxicillin
Thorben Sarnowski	Assessment of supercritical fluid chromatography for the separation of selected veterinary antibiotics
Matthias Stüwe	Characterization and application of thermo responsive liquid chromatography columns for the development of a testosterone measurement method in a two-dimensional liquid chromatography isotope ratio mass spectroscopy (2D-LC-IRMS) system

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Invited Lectures and Outreach

Invited Lectures

Greening sample preparation in the analysis of organic compounds and microplastic
T. C. Schmidt, M. Wenzel, L. K. Tintrop, A. Salemi, W. Engewald, G. Renner, J. Schram, M. A. Jochmann, J. Tuerk
9th International Conference on Environmental Health, Shahid Beheshti University of Medical Sciences, Tehran
December 16, 2025 (online)

From source to tap: The future of water monitoring using liquid chromatography high-resolution mass spectrometry
T. C. Schmidt, R. Armin, F. Drees, J. Flottmann, V. Hinnenkamp, Lotta Hohrenk-Danzouma, M. Reuschenbach, G. Renner, M. Vosough
International Symposium on Environmental Monitoring of Chemicals of Emerging Concern, Copenhagen
March 26, 2025

Greening sample preparation in the analysis of organic pollutants and microplastic
T. C. Schmidt, M. Wenzel, L. K. Tintrop, A. Salemi, W. Engewald, G. Renner, J. Schram, M. A. Jochmann, J. Tuerk
ANAKON 2025, Leipzig
March 11, 2025

Data treatment processes for large and diverse analytical data sets
G. Renner, R. Cunha
International Symposium on High Performance Liquid Phase Separations and Related Techniques (HPLC 2025), Bruges
June 15, 2025

Modulare Datenverarbeitungspipelines: Automatisierung und Standardisierung analytischer Messdaten
G. Renner
Langenauer Wasserforum 2025, Langenau
November 17, 2025

Outreach

S.U.N.I. – SommerUni in Natur- & Ingenieurwissenschaften

18. August 2025: "Der Blick ins Wasser"

Figure 14: S.U.N.I. visiting our laboratories

S.U.N.I. is a unique platform for young people to support their study choice orientation in the natural and engineering sciences. By attending impressive experiments and presentations, the participants have the opportunity to experience the university's everyday life in special events and get to know the fields of work in science and technology in order to receive support for their study and career development process. The event "A glance at the water" includes sampling procedure at a small lake with subsequent analysis and water treatment of the samples in the lab. The participants learn fundamental strategies of chemical analysis and treatment techniques.

Figure 15: Sampling at the lake

Trial Course of Studies (Probestudium Chemie)

13. Januar 2026: "Water Science – Zur Struktur des Wassermoleküls und den Folgen"

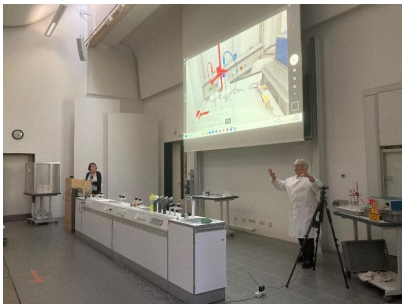

Figure 16: Experimental lecture

In addition to the early studies, pupils from upper classes have the opportunity to gain in-depth insights into the study areas of natural sciences, engineering and (economic) computer science, to speak with teachers, to explore the facilities of the University of Duisburg-Essen. Within the program of the Faculty of Chemistry, Claudia Ullrich, Dr. Klaus Kerpen, Simone Bettinger and Dr. Ursula Telgheder presented an experimental lecture about the special properties of water. At first glance, the water molecule has a very simple structure. And yet it is something very special. Physicochemical: water is different as all structurally related compounds. That's why life, as we know it, makes it possible. Meaning: Water is involved in all biological and very many non-biological processes in our environment. It is an ideal solvent for many components, therefore the chemistry of and in aqueous systems is particularly diverse. The lecture went on from the special properties of water to water purification illustrated with simple experiments.

Conferences and Meetings

27th International Symposium on Advances in Extraction Technologies

ExTech 2025 in Mülheim an der Ruhr

The 27th International Symposium on Advances in Extraction Technologies (ExTech 2025) took place from 8 to 11 September 2025 in Mülheim an der Ruhr. Organized under the GDCh Division of Separation Science, the conference addressed recent advances in sampling and sample preparation for analytical chemistry. Microplastics analysis, PFAS, and sustainable ("green") approaches formed the main theme. Founded in 1999 by Janusz Pawliszyn, the ExTech rotates annually across the globe. In 2025, it returned to Germany for the first time in over twenty years. The Stadthalle Mülheim served as an ideal venue. Situated on the River Ruhr and well connected to public transport, it offered spacious facilities for lectures, poster sessions, an industrial exhibition, and short courses under one roof. Continuous catering, a riverside terrace, and an adjacent park encouraged informal exchange during breaks. Participants widely praised the atmosphere and functionality of the location.

Around 160 experts from more than 20 countries attended, including 86 doctoral degree holders. Roughly half traveled from abroad. Notably, about one quarter came from industry, a remarkable share for a scientific conference that greatly enhanced practice-oriented discussions. Early-career researchers were well represented, too: approximately 35 doctoral candidates and students used the conference to present their results, gain first-hand experience, and build professional networks.

Scientific Program

The program offered substantial breadth: four short courses, three plenary lectures, 13 keynote talks, 40 contributed presentations, and 73 posters. On the afternoon of 10 September, an interactive panel discussion titled "Green (Analytical) Chemistry: Between Vision and Reality" complemented the sessions. Chaired by Prof. Elia Psillakis (Technical University of Crete), who leads the EuChemS-DAC Sample Preparation Study Group, the panel invited the audience to critically examine both the aspirations and realities of sustainable analytical chemistry. Ten leading instrument and technology manufacturers presented their latest developments in an accompanying exhibition. All sponsors and partners, especially the DFG and the Fonds

der Chemischen Industrie (FCI), were gratefully acknowledged during the opening ceremony. Media partners, including Analytical and Bioanalytical Chemistry, Analytica Chimica Acta, Green Analytical Chemistry, and Advances within Sample Preparation, contributed to the conference's visibility. The organizers also announced a virtual special issue featuring outstanding contributions on microplastics, PFAS, and green sample preparation.

The three plenary lectures formed the scientific highlights of each conference day. Prof. Dr. Janusz Pawliszyn (University of Waterloo, Canada), founder and honorary chair of the ExTech series, opened with "Microextraction Technologies with Sky Limit Opportunities." He showed how an extensive understanding of physicochemical fundamentals can yield innovative extraction technologies, highlighting advances in solid-phase microextraction (SPME) and its applications in forensic, environmental, and clinical analysis. Prof. Dr. Nicole Pamme (Stockholm University, Sweden) presented "Environmental Analysis and Clinical Diagnostics in Resource-Limited Settings." Her microfluidic lab-on-a-chip systems enable on-site analysis that can be operated even by minimally trained personnel. Through case studies in medical diagnostics and environmental monitoring, she illustrated the potential of distributed approaches to expand data collection across geographic and temporal dimensions. Prof. Dr. Elia Psillakis (Technical University of Crete, Greece) delivered the third plenary on "Shaping a Sustainable Future for Analytical Chemistry." She argued that improvements in analytical chemistry frequently remain incremental and isolated, and called for a systemic shift toward truly sustainable laboratory practices. Drawing on the three pillars of sustainability, i.e., environmental, social, and economic, she urged the community to pursue transformative rather than merely stepwise solutions.

Keynote Lectures and Thematic Breadth

The keynote lectures reflected the community's current research priorities throughout a wide spectrum. Each session began with an invited expert providing a comprehensive overview of the topic. Dr. Emanuela Gionfriddo (University at Buffalo, USA) introduced high-throughput microextraction techniques for efficiently separating small molecules from complex matrices. Prof. Leon Barron (Imperial College London, UK) addressed the miniaturization of passive sampling systems for large-scale monitoring of organic trace contaminants. In the environmental proteomics session, Prof. Damià Barceló (IDAEA-CSIC, Spain) presented a method combining sample fractionation with MALDI-TOF mass spectrometry to detect proteins in wastewater as biomarkers. This approach possesses notable promise for wastewater-based epidemiology. The microplastics sessions also brought compelling contributions. Dr. Thorsten Hüffer (University of Vienna) examined the analytical challenges posed by the complexity of plastic particles and additives in environmental samples. Prof. Maria Llompart (University of Santiago de Compostela, Spain) introduced sample preparation strategies targeting pollutants released from tire-based microplastics.

In the PFAS session, Dr. Satoshi Endo (NIES, Japan) presented experimental and modeling approaches to better characterize the partitioning and sorption behavior of these persistent

contaminants. His novel method of thermally converting PFAS to hydrogen fluoride for quantitative sum-parameter determination attracted particular attention. Prof. Verónica Pino (Universidad de La Laguna, Spain) demonstrated that metal–organic frameworks (MOFs) are promising sorbents for microextraction, combining large surface areas, tunable pore sizes, and strong chemical stability. Prof. Giorgia Purcaro (University of Liège, Belgium) demonstrated that optimized sample preparation, combined with comprehensive two-dimensional gas chromatography (GC×GC), can substantially increase analytical detail for complex samples. Prof. Elena Stashenko (Universidad Industrial de Santander, Colombia) concluded the keynote program with "The Social Role of Sample Preparation." Her lecture brought out the societal dimensions of analytical methods in means concerning their influence on data quality, accessibility, and ecological footprint.

Poster Sessions and Awards

The poster program comprised 73 contributions across the following categories: Automation & Robotics, Bioanalysis, Environmental Analysis, Food Analysis, Green Analytical Chemistry, and New Materials & Technologies. The well-attended sessions provided early-career researchers with valuable opportunities to interact with international experts. Awards recognized the strongest contributions: Jennifer Mabel Luna Díaz (University of the Balearic Islands, Spain) received first prize for a sustainable ultrasound-assisted extraction method for parabens in water samples. Anna Thu Hoai Nguyen (University of Copenhagen, Denmark) earned second place for developing a novel microfluidic chip for electromembrane extraction. Two third prizes went to Jorge Pasán (Universidad de La Laguna, Spain) and Robin Jung (University of Duisburg-Essen). All awardees received certificates and monetary prizes sponsored by scientific journals.

Science Video Challenge

For the first time, ExTech featured a Science Video Challenge. Early-career researchers submitted short, self-produced videos presenting their research. The best entries were screened on 10 September, and the audience voted on the winners. Sarah Rockel (University of Duisburg-Essen) won first prize, followed by Jelle Verdonck (KU Leuven, Belgium) and Indra Bartels (Niederrhein University of Applied Sciences). The format was enthusiastically received, promoting both imagination and science communication. It is expected to inspire comparable initiatives at future conferences.

Social Program

Outside the scientific sessions, ExTech 2025 offered a varied social program with plentiful opportunities for personal exchange. On Tuesday evening, GERSTEL hosted participants at its company premises. Guided tours offered a behind-the-scenes look at the production facilities, while a food truck served street food in a relaxed setting. The evening proved a memorable highlight of the conference week. The networking dinner on Wednesday evening

was held at the Stadthalle's integrated restaurant. Over an excellent meal, participants took part in stimulating conversations across disciplines and career stages, deepening contacts made during the day and establishing new ones. The photo booth, available throughout the conference, became a particular crowd favorite. Participants used it enthusiastically, creating light-hearted moments and lasting mementos of the time shared in Mülheim.

Conclusion

ExTech 2025 furthered the field of extraction science and strengthened international, interdisciplinary networks. Participants praised the combination of high-caliber lectures, practice-oriented discussions, and strong involvement of early-career researchers. The thematic range, from fundamental methodology through environmental and food analysis to clinical applications, yielded valuable cross-disciplinary insights. Dedicated formats for young scientists, including short courses, embedded young-scientist sessions, and poster and video awards, were widely used and contributed to early-career development. The active dialogue between academia and industry should accelerate technology adoption and stimulate collaborative research. Hosting ExTech in the Ruhr region additionally reinforced Germany's international visibility as a research hub in extraction science. We gratefully acknowledge the DFG for its generous financial support, without which this conference would not have been possible at this scale.

Teaching

Teaching

At IAC, we are involved in teaching mainly in the Bachelor and Master program "Water Science," which is a unique science-based curriculum with a focus on chemistry, analytics, and microbiology (see details at https://www.uni-due.de/water-science/). All courses are also optional for students in the Bachelor and Master program "Chemistry." Some are also offered as elective courses for chemistry students studying towards a teacher's degree and for students of the related Master programs "Environmental Toxicology" (offered in the faculty of biology) and "Management and Technology of Water and Wastewater – MTW3" (offered in the faculty of engineering).

Summer term

- Lecture "Water – The Lecture" (B.Sc. Water Science, in German)
- Lecture and Tutorial "Oxidative Processes" (M.Sc. Water Science, in English)
- Lecture and Tutorial "Stable Isotope Analysis" (M.Sc. Water Science, in English)
- Laboratory Practical "Stable Isotope Analysis" (M.Sc. Water Science, in English)
- Lecture and Tutorial "Quality Management" (M.Sc. Water Science, in English)
- Laboratory Practical "Environmental Analytics" (M.Sc. Environmental Toxicology, in English)

Winter term

- Lecture and Tutorial "Water Analysis" (B.Sc. Water Science, in German)
- Laboratory Practical "Analytical Chemistry" (B.Sc. Water Science and Chemistry, in German)
- Laboratory Practical "Water Chemistry and Analysis" (B.Sc. Water Science, in German)
- Lecture and Tutorial "Water Chemistry" (M.Sc. Water Science and Environmental Toxicology, in English)
- Lecture, Tutorial, and Seminar "Chemometrics and Statistics" (M.Sc. Water Science and Environmental Toxicology, in English)
- Lecture "Sample Preparation in Analytical Chemistry" (M.Sc. Water Science, in English)
- Individual Practical Projects "Analytical Chemistry" (M.Sc. Water Science, in English)