

UNIVERSITÄT
DUISBURG
ESSEN

Open-Minded



2022

**Jahresbericht
Annual Report**

Content

Instrumental Analytical Chemistry	2
Instrumental Analytical Chemistry Group Members (2022)	4
Head of Chair	5
Secretarial Office	5
Regular Staff	5
Apprentices	5
Research, Teaching, and Technical Assistants.....	5
Ph.D. Students	6
Internal	6
External.....	7
Internal Research Group: Oxidative Processes	8
Guest Scientists	9
Awards.....	12
Running Projects at IAC 2022	17
Theses completed in 2022.....	51
Ph.D. Thesis	51
Master Theses	58
Bachelor Theses.....	59
Publications	60
Invited Lectures	64
Conferences and Meetings.....	65
Teaching	67
Miscellaneous.....	68

Instrumental Analytical Chemistry



Dear friends and colleagues,

in 2022 the third year of the Covid-19 pandemic has passed that affected many more people in my group than in the years before, including me. And yet, we all know that other crises became more important in the past year, starting with the horrible war in Ukraine. Beyond the human tragedy, the subsequent jump in energy costs and interferences in supply chains affected our work at the university significantly. To round up, the University of Duisburg-Essen faced a heavy cyberattack early December that still keeps us busy. One could easily argue that this was a year we shall soon forget. Nevertheless, we kept up our successful work at IAC thanks to my fabulous team and we are pleased to give you an overview of our activities in 2022 with this annual report.

Teaching has been almost back to normal, at least until the cyberattack but I am confident that students will not face any difficulties due to this unforeseen event. We could also participate again in conferences and meetings in presence, including the successful 5th MWAS in Muelheim co-organized by IWW Water Centre, one of the few conference series held in presence without pandemic interruption. Some of our PhD students have been awarded for their poster presentations during these meetings (details see later) and I would like to congratulate them for these achievements. In addition, I was truly honored to have been awarded myself unexpectedly with the “Ruhr Award for Arts and Science” by my home town, the city of Muelheim, in December 2022. I see this award as a recognition of the whole group effort and the outstanding work of my team members over the past 16 years.


In terms of people at IAC we are happy to have found Simone Bettinger as successor for Gerd Fischer. Simone already integrated exceptionally well into our team and takes over more and more responsibilities for maintenance of our lab equipment. Dr. Anam Asghar decided to stay at IAC as junior research group leader for oxidative processes after her Humboldt fellowship ended early 2022. She has already established very successful collaborations with colleagues from the chemistry and engineering faculty active in CENIDE, including a full proposal for a profile building project linking water research at ZWU and material research at CENIDE.

Furthermore, Prof. Amir Salemi and Prof. Maryam Vosough settled in and are contributing to several research projects including the preparation of our Excellence cluster proposal with the amended title “River Ecosystems in the Anthropocene” that we have to submit in the first months of 2023. Further guest researchers included Anaëlle Mortagne-Coderch, a student intern for four months from Toulouse, and Dr. Ana Belen Martinez Piernas for a six-months postdoctoral stay from the University of Jaén. Finally, of course, Prof. Sina Dobaradaran visited us again two times and we are looking forward to his next stay in Essen still funded by the Alexander-von-Humboldt foundation.

In 2022, four PhD students at IAC successfully defended their theses and three more have already submitted with defense dates early 2023. Thanks mostly to the active PhD students and postdocs we have again been very successful in publishing in international journals with an all-time high number of 33 papers, most of which appeared in premier journals of the field.

As usual, at the end I would like to thank all group members and students again 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 2023 that above all hopefully will see peace again in Ukraine and surely an end at least of the pandemic Covid-19 situation with its last active restrictions.



Torsten C. Schmidt

Instrumental Analytical Chemistry Group Members (2022)



Contact: Instrumental Analytical Chemistry
Faculty of Chemistry
University Duisburg-Essen
Universitätsstr. 5
45141 Essen

Phone: +49 201 183-6772/6774
Fax: +49 201 183-6773
email: torsten.schmidt@uni-due.de

www.uni-due.de/iac

Head of Chair

Prof. Dr. Torsten C. Schmidt

Secretarial Office

Lydia Vaaßen

Regular Staff

Dr. Anam Asghar	Advanced Oxidation Processes
Simone Bettinger	Laboratory engineer, Instrument and Lab Supervision
Dr. Maik Jochmann (AOR)	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
PD Dr. Ursula Telgheder	Ion Mobility Spectrometry, 2D-Fluorescence Spectroscopy, Expert advice for course of studies, Radiation Protection Commissioner
Claudia Ullrich	Laboratory assistant, Safety officer

Apprentices

Maximilian Budweg (since July 2022)

Tom Hadler (until December 2022)

Research, Teaching, and Technical Assistants

Rukiyye Abis

Felix Drees

Sara Khani

Michael Leupold

Sarah Rockel

Kaliyani Wickneswaran

Isabell Halbhuber

Ph.D. Students

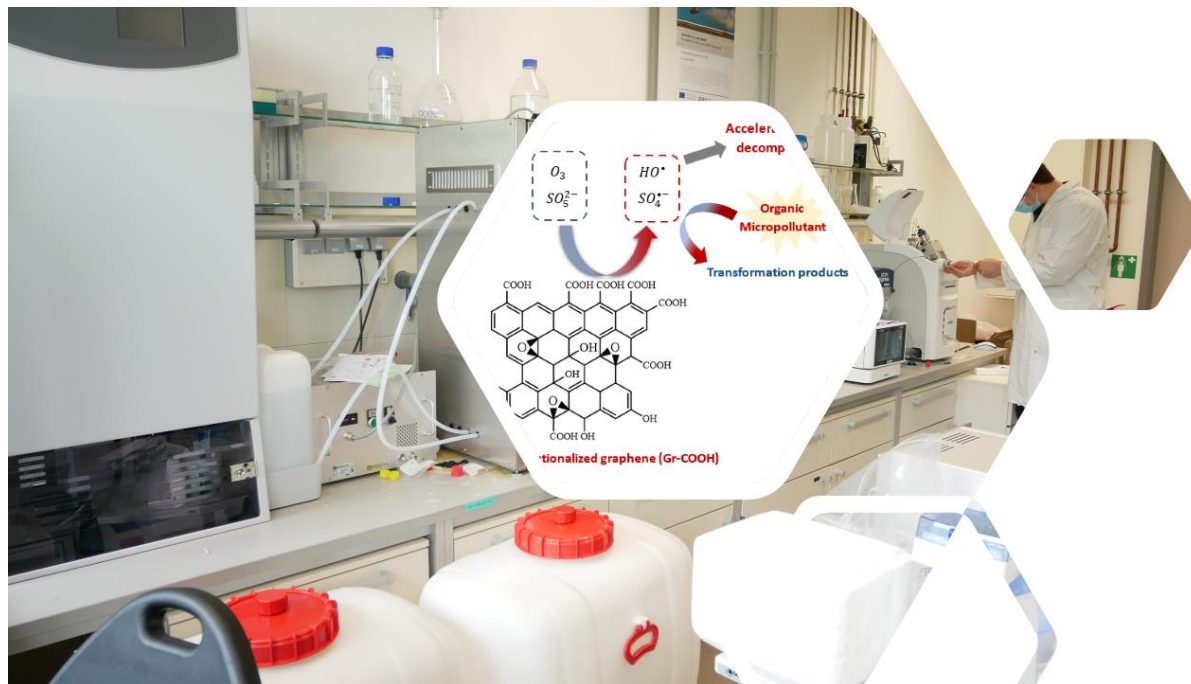
Internal

Mohammad Sajjad Abdighahroudi	Reactions of Chlorine Dioxide with Nitrogen-Containing Heterocycles
Felix Drees	Data Processing in Non-Target Screening
Tobias Hesse	The Potential of LC-IRMS: Carbon stable isotope analysis of amino acids in a host-parasite system and a proof-of-principle study for $\delta^{15}\text{N}$ measurements of nitrate
Lotta Hohrenk-Danzouma	Data processing strategies for LC-HRMS-based non-target analysis of organic micropollutants in aqueous matrices
Katharina Klein (Hupperich)	Influence of organic matter on oxidative transformation processes
Sasho Joksimoski	Novel coupling techniques for the determination of organic compounds in complex samples by ion mobility spectrometry
Shaista Khaliq	Diet-consumer interactions under variable stressor conditions as revealed by stable isotope studies of individual amino acids
Nerea Lorenzo Parodi	Aromatic amines as biomarkers in human urine: Analytical method development and epidemiological studies
Michael Leupold	Investigations of transformation reactions of antibiotics by photocatalysis in aqueous systems
Robert Marks	Coupling techniques in the field of isotope ratio mass spectrometry
Valentina Merkus	Characterization of transformation processes using high-resolution mass spectrometry
Xenia Mutke	Treatment of membrane concentrates by oxidative processes
Felix Niemann	Isotope fractionation associated with abiotic Imidacloprid degradation
Max Reuschenbach	Automated data processing and data analysis in high-resolution mass spectrometry
Jens Terhalle	Investigation of transformation reactions of phenolic compounds by oxidative processes in aqueous systems
Lucie Tintrop	Automated and miniaturized sample preparation in gas chromatographic analysis
Duaà Tahboub	Studies on electrochemical treatment processes for the decomposition of Persist Organic Pollutants (POPs) in contaminated ground and surface water

External

Reyhaneh Armin	Non-target analysis of organic micropollutants in industrial wastewater
Alexander Augustini	Chemical characterization of the ingredients of electronic cigarettes and the inhaled products.
Indra Bartels	Analysis of suggested SARS-Cov-2 treatment pharmaceuticals in surface waters
Nico Bätz	Effect-directed identification and reduction of diffuse immissions in rivers
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 Sub μ -Plastics in the Aquatic Environment
Annika Fechner	Kopplung eines miniaturisierten Thermodesorptionschips und einer μ -Plasma-Ionisierungsquelle zur Analyse flüssiger Proben mittels Ionenmobilitätsspektrometrie
Jana Hinz	Development and application of multidimensional GC-IMS methods for the analysis of volatile and semivolatile substances in safety and health research
Malte Hübchen	Automated sample preparation and gaschromatographic 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 waste water
Kjell Kochale	Automated hyphenation of effect-based and instrumental analysis
Susann Pristat	Development of procedure tests for hot and cold coils considering the optimization of transport logistics of slabs
Lars Reinders	Analytical monitoring of personalized drugs containing monoclonal antibodies: An alliance of patient and personnel safety
Sara Schäfer (Saß)	Oxidative transformation of organic compounds in ultrapure water by ozonation and UV photolysis
Hannah Schanzmann	Schnelle, nicht-invasive Identifikation nosokomialer Infektionen
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
Tobias Werres	Characterization of extra-column volumes in capillary high-performance liquid chromatography

Internal Research Group: Oxidative Processes by Dr. Anam Asghar



The Oxidative Processes Group at IAC explores the fundamental aspects of oxidative water/wastewater treatment processes. We combine knowledge from the fields of water science and analytical chemistry with expertise in the field of oxidative processes.

Within the broad field of oxidative processes and with a clear idea about the poor quality of surface water, non-pointed wastewater disposal, and inefficient treatment efficiencies of existing wastewater treatment plants, our group covers the following aspects:

- Understanding the fundamental mechanisms in oxidative water treatment processes (e.g., ozonation, ozonation/ HSO_5^- , photo-oxidation (UV and UV/ HSO_5^-)).
- Heterogenous photocatalysis over immobilized or suspended TiO_2 , catalytic ozonation and HSO_5^- Activation with transition metal oxides, transition metal-based perovskites, and undoped/doped carbonaceous catalyst. The major research interest is to elucidate the possible synergistic effects through the formation of different reactive oxygen species.
- Influence of water matrix components (inorganic compounds and natural organic matter)
- Reaction pathways in pollutant degradation and by-product formation.

Guest Scientists



Prof. Sina Dobaradaran

Long-term visiting scientist

Bushehr University of Medical Sciences, Iran

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 release from cigarette butts into the water environments

Determining the acute toxicity of CBs leachates for aquatic organisms (my next project)



Anaëlle Mortagne- Coderch

Student intern from the University of Toulouse, France
(May 02 to August 26, 2022)

Internship Tutors: Torsten C. Schmidt, Amir Salemi

Topic: Creation of a reusable vial of BSTFA automatize GC-MS analysis of on-fibre derivatization compounds



Dr. Ana Belén Martínez Piernas

Postdoc from the University of Jaén, Spain
(May 01 to October 31, 2022)

Funded by Ministerio De Universidades Programa “José Castillejo” Para Estancias De Movilidad en El Extranjero De Jóvenes Doctores

Topic: Application of nontarget screening by LC-HRMS and chemometric approaches for the evaluation of organic pollutants in complex environmental water: Influences of user-defined parameter settings for individual steps in NTS data processing workflows based on MzMine3.



Dr. Amir Salemi

Visiting Scientist

Development and Optimization of Automated Sample Preparation Coupled with GC-MS Analysis

Besides contributing to a few research studies focused on sample preparation and determination of organic micropollutants in water media, a gas-generating vial has been developed for online and automated derivatization of organic contaminants prior to GC analysis. The main aim of the current work is to develop, optimize and apply an automated SPME Arrow-GC-MS method for the determination of multiclass semivolatile organic contaminants in water media and screening of Ruhr River for their presence and variations.



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

One clear challenge with high-resolution mass spectrometric-based instruments is the generation of massive quantities of data (“big analytical data”) and their pre-processing and processing steps. So, developing post-acquisition data handling tools is increasingly critical for reliable non-targeted analysis workflows. In particular, this is the case for non-targeted environmental data, as the goal is to track and identify trace quantities of organic micropollutants and their transformation products in the presence of strong matrix effects and generally in a more extensive chemical space than metabolomics study. Chemometrics, a powerful interdisciplinary field that uses mathematical, statistical, and machine learning tools to analyze high-dimensional and complex chemical information, can be appropriately incorporated in different environmental non-targeted analysis workflow stages.

Based on previous studies in this area, the following research activities and collaborations were conducted in 2022:

- Co-supervision of Dr. Lotta Hohrenk-Danzouma’s Ph.D. thesis (Data processing strategies for LC-HRMS based non-target analysis of organic micropollutants in aqueous matrices)
- Principal Investigator: Developing multiway modeling methods for the simultaneous non-targeted analysis of fused HRMS data (in progress).
- Collaboration and co-supervision of Ph.D. theses of Felix Drees (Aqua-flow project and non-target screening investigations of industrial wastewater) and Reyhaneh Armin (Time series non-target screening of organic micropollutants in industrial wastewater), which are in progress.
- Developing an improved feature reduction method for non-targeted screening of multigroup wastewater samples (by Reza Lotfi, my Ph.D. student in CCERCI, as part of his Ph.D. thesis at CCERCI).
- Principal Investigator: Comparing some machine learning tools to prioritize features in simulated and metabolomics data (work is in progress).

Awards

Sarah Rockel



Kurita Water Science Award 2022, Kurita Europe GmbH

"Photolysis of Aminotris(methylenephosphonic acid) (ATMP) – Investigation of the influence of pH-dependent speciation on degradation mechanism and isotopic fractionation"

Faculty Award - Best Master's Degree in Water Science, University of Duisburg-Essen

Max Reuschenbach



Best Poster Award, MWAS 2022, 14th – 15th September 2022

"Data Quality Score Describes Non-Target Screening Features' Reliability"

Felix Drees



1st Feralco Water Award (Best Master Thesis), University of Duisburg-Essen

"Investigation of the degradation of polyphosphonates by compound-specific stable carbon isotope analysis coupled with high-resolution mass spectrometry: kinetic isotope effects and degradation products"

Faculty Award - Best Master's Degree in Water Science, University of Duisburg-Essen

Katharina Klein



Best Poster Award, MWAS 2022, 14th – 15th September 2022

"Influence of oxidation processes on optical properties of natural organic matter – Application of excitation-emission matrix fluorescence spectroscopy"

Christina Sommer



Young Scientist Award 2022 – Master Thesis, Centre for Water and Environmental Research (ZWU), 8th June 2022

"Determination and ecotoxicological evaluation of transformation products resulting from the ozonation of ibuprofen"

Robert Marks



Best Poster Award, ISC 2022, 18th – 22nd September 2022

"How to Couple LC-IRMS with HRMS – A Proof of Concept Study"

Ruhr Award for Arts and Science of the city of Mülheim awarded to Prof. Dr. Torsten C. Schmidt

With about 200 guests, the artist Alexander Voß and Prof. Schmidt celebrated in the customer hall of the Sparkasse at Berliner Platz in Mülheim an der Ruhr on 04.12.2022. Together with the artist, Prof. Schmidt received the Ruhr Award for his 15 years of research work at the IWW from Mayor Marc Buchholz. Torsten C. Schmidt developed methods that improve the degradation of pollutants during wastewater treatment to avoid further drinking water contamination.

The Cultural Committee of the City of Mülheim thus honors:

„seine Arbeit am Institut für Wasserforschung in Mülheim, die er wesentlich geprägt und damit zu einer Spitzenposition in Deutschland geführt hat. Seine Erfolge tragen zur weiteren Verbreitung und Festigung des hervorragenden Wissenschaftlichen Ruf Mülheims als Standort für Spitzenforschung bei.“
(Zitat WAZ 26.08.2022)

Translation:

[...] his work at the Institute for Water Research in Mülheim, which he has significantly shaped and thus led to a top position in Germany. His successes contribute to the further spread and consolidation of Mülheim's excellent scientific reputation as a location for cutting-edge research.



Prof. Torsten C. Schmidt

During the online Conference of the German Water Chemistry Society, Prof. Torsten C. Schmidt was awarded as honorary president of the society.



Running Projects at IAC 2022

NRW Graduate School Future Water: Global water research in the metropolitan region Ruhr (Future Water)

Involved staff: Lotta Hohrenk-Danzouma (IAC Ph.D. student), Dr. Vanessa Kramer and Anja Cargill (Coordinator), Prof. Dr. Torsten C. Schmidt (Speaker)

Partners: Prof. Dr. Bernd Sures, Prof. Dr.-Ing. André Niemann, Prof. Dr. Martin Denecke, Prof. Dr. Rainer Meckenstock, Prof. Dr. Jens Boenigk, Prof. Dr. Nicolai Dose (University of Duisburg-Essen), Prof. Dr. Marc Wichern (Ruhr-University Bochum), Dr. Jochen Türk, Michelle Klein (IUTA), Prof. Dr. Sigrid Schäfer (IU Internationale Hochschule GmbH), Prof. Dr. Mark Oelmann (HRW Mülheim), Dr. Steven Engler (Ruhr-University Bochum) and many mentors and collaborators from the water and wastewater sector

Funding: Ministry for Culture and Science of the State of North-Rhine Westphalia (NRW) through the joint project "Future Water: Global water research in the metropolitan region Ruhr."



The multiperspective of inter- and transdisciplinary approaches allows for conducting innovative and path-breaking research. Combining knowledge and methods across disciplines makes identifying hitherto unnoted research questions possible. Tackling questions from different and novel angles allows for finding answers that have not been conceived before. Furthermore, integrating practitioners into these processes can enhance the relevance of the research questions, the fit of the methods applied, the effectiveness of research processes, and the applicability and outreach of the results.

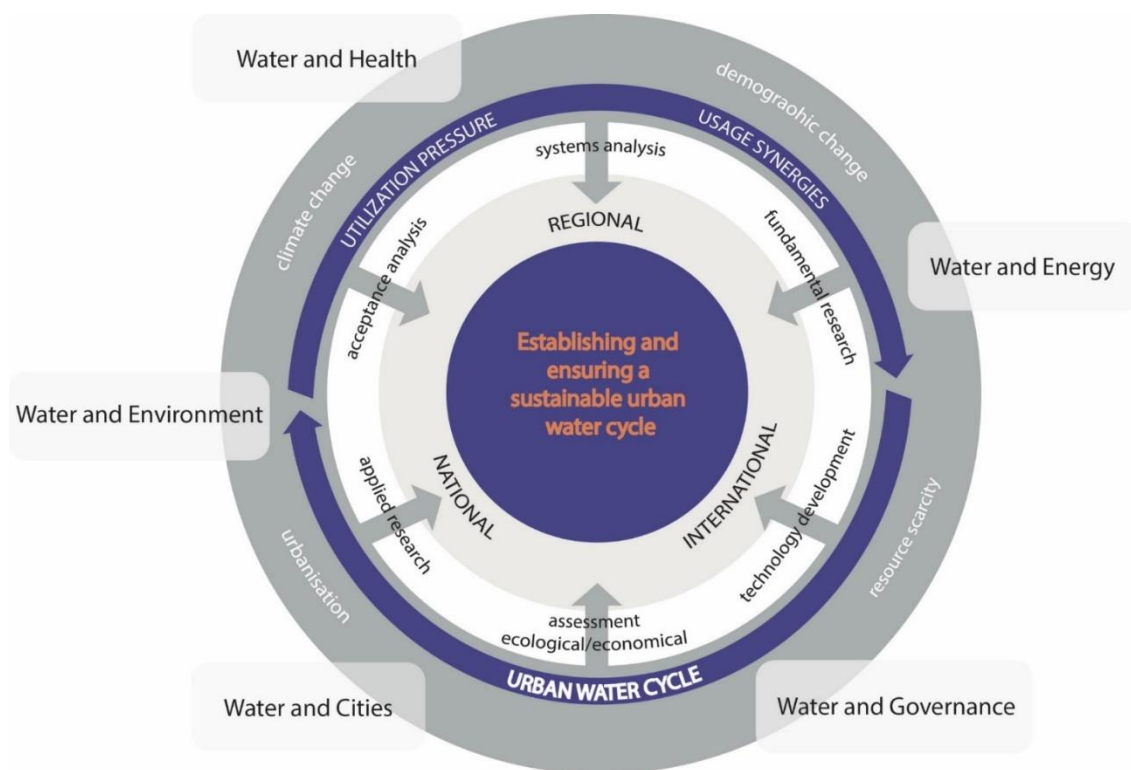
This approach is at the heart of the graduate school "Future Water," located in the Ruhr metropolitan area in Western Germany.

In 2014, various academic and applied institutes joined forces to develop strategies for sustainable water management with a particular focus on the urban water cycle. The following figure describes the many facets of that work. The wide array of disciplinary backgrounds represented in the graduate school made building bridges between the natural sciences, applied engineering, and social sciences possible and necessary. In Future Water, 12 Ph.D. students and a coordinator position are funded. In addition, the Centre for Water and Environmental Research (ZWU) at UDE coordinates the activities of Future Water. In 2019, a continuation of the graduate school in a second funding phase, 2019-2022, was granted. The funding ended in June 2022.

At IAC, one project (Lotta Hohrenk-Danzouma) focuses on analyzing micropollutants introduced by diffuse sources with non-target screening. Non-target screening is based on high-resolution mass spectrometry and can detect a broad range of analytes at low concentrations in one full scan measurement. It provides a complete overview of compounds present in a sample, enables the identification of formerly unknown contaminants, and reveals temporal or spatial trends.

Tiny streams can be affected by the diffusive introduction of pollutants like agricultural run-off due to smaller dilution ratios and peak exposures after heavy rainfalls. Passive samplers accumulate organic micropollutants over a specific period; more comprehensive monitoring is possible, and episodic pollution events are less likely to be missed than spot samples.

With non-target analysis approaches, huge datasets are recorded, and extensive data processing is necessary. Different chemometric tools can be further used for data mining and prioritizing relevant pollutants. The current project analyzed passive sampling extracts with an LC-HRMS-based non-target screening method and temporal- and spatial trends. The results were recently published in *Environmental Science and Technology* (doi.org/10.1021/acs.est.1c08014).



Inhibitory and/or stimulatory role of dissolved organic matter in advanced oxidative processes

Involved Staff: Dr. Anam Asghar, Dr. Klaus Kerpen, Dr. Torsten C. Schmidt

The degradation of organic micropollutants (OMPs) by advanced oxidation processes (AOPs) poses a significant challenge due to the complexity and diversity of water matrices. Water matrix constituents, particularly dissolved organic matter (DOM), impact their effectiveness. DOM is a complex mixture of heterogeneous compounds with a continuum of functional groups and molecular sizes. The reactivities and concentrations of such functional groups determine the extent of the NOM-oxidant interactions and, thus, simultaneously induce promoting and inhibiting effects. Therefore, during the application of AOPs, DOM can block light penetration, scavenge radicals/oxidants, and enhance the formation and reactivity of useful reactive oxidative species to eliminate OMPs and alter the transformation pathways. Therefore, the research needs to advance the structural and practical understanding of how DOM can be exploited to enhance the synergistic properties effects of DOM and improve the performance of oxidative processes.

To develop a comprehensive understanding of the multiple roles of DOM in the application of AOPs, it is necessary to look at the underlying mechanisms probably by choosing appropriate surrogates or model DOM/NOM model compounds of different sizes and functional groups and subsequently investigate their role in oxidative processes. Therefore, this project aims to pitch the idea of using different NOM/DOM model compounds having different molecular sizes and functional groups to understand the mechanisms governing synergistic and/or inhibitory properties of DOM in AOPs.

Characterization of transformation processes using high-resolution mass spectrometry

Involved staff: Valentina Merkus, Prof. Dr. Torsten C. Schmidt

Involved students: Michael Leupold, Sarah Rockel, Christina Sommer

Partners: Esther Smollich, Prof. Dr. Bernd Sures, Aquatic Ecology, University of Duisburg-Essen

Funding: Fonds der Chemischen Industrie (FCI)

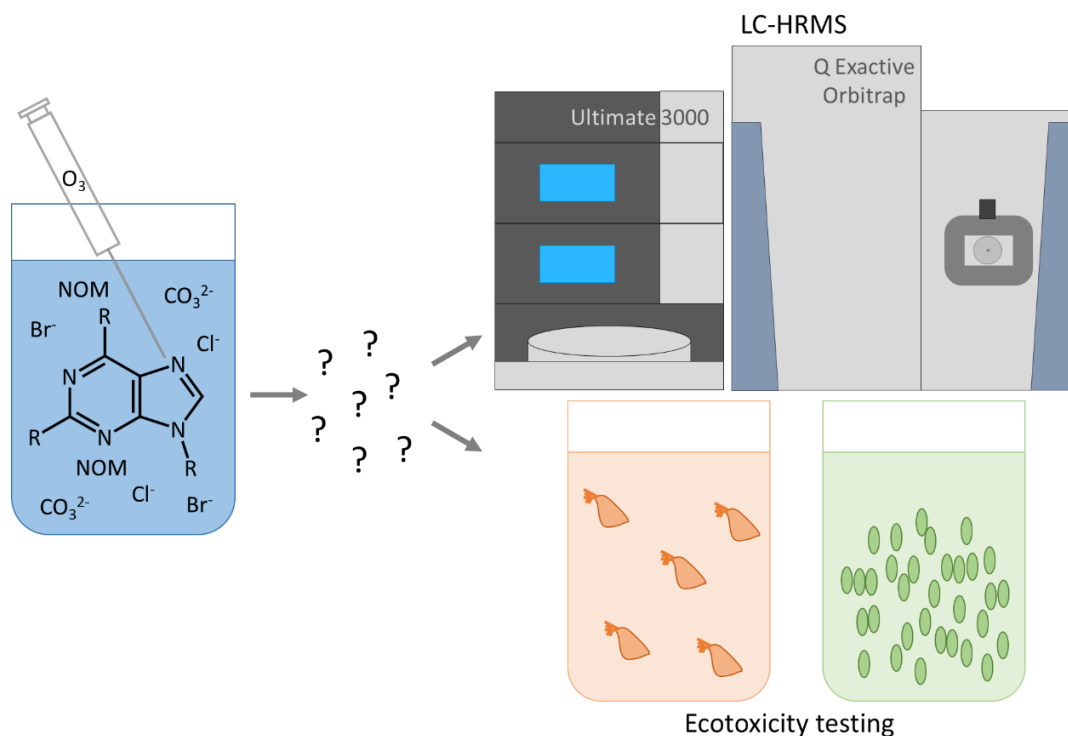


Figure 1: Ozonation of sample compounds in defined water matrices to unknown products (left) followed by transformation product identification by LC-HRMS (top right) and ecotoxicity testing (bottom right).

Oxidation processes are widely used in wastewater treatment to remove micropollutants, although there is still a lack of knowledge of the ongoing mechanisms. It is known that organic substances are transformed into reaction products. These transformation products may then reach the environment instead of the original pollutants. Here they may cause several negative impacts like ecotoxicological or endocrine effects. Hence, there is interest in identifying transformation products of widely spread contaminants and understanding their formation in various water matrices.

However, examinations are barely possible for all compounds due to the high number of detected pollutants in wastewater. Therefore, the ozonation of small, general structures and related, more complex structures, including environmentally relevant pollutants, is investigated in this project. Special attention is given to the influence of water-matrix components such as alkalinity, organic matter, and inorganic anions. This work aims to predict the ozonation of micropollutants on their general structure and dependence on the water matrix. Purine, its derivatives guanine and adenine, and the antiviral guanine derivatives acyclovir and penciclovir were chosen as model substances. The project includes examinations of their

ozonation like stoichiometry, reaction kinetics, quantification of target products, and identifying unknown transformation products using high-resolution mass spectrometry.

The first results of reaction kinetics and stoichiometry indicate different sites of ozone attack at the derivatives and show that the impact of hydroxyl radicals varies depending on the analytes and reaction conditions. Altogether, similarities in ozonation were not observed for the three basic structures but for guanine and its antiviral derivatives.

The second part of the project is the ecotoxicological examination of the ozonation of ibuprofen. First, ecotoxicity is studied by standardized tests such as acute toxicity testing on *Daphnia magna* and freshwater algae tests with *Desmodesmus subspicatus*. Simultaneously, transformation products are identified, and their formation and degradation, depending on the ozone dosage, are examined by high-resolution mass spectrometry. Parameters such as pH are changed to affect the formation of oxidation products and, therefore, the ozonated mixture's ecotoxicity. Statistical correlation of product formation and observed ecotoxic effects allows identifying potentially ecotoxic products. As a result, it was possible to detect six ozonation products that might be more toxic to green algae than ibuprofen. Moreover, results underline the importance of mixture toxicity in transformation processes.

Photocatalysis of the β -lactam antibiotic amoxicillin and clavulanic acid for the Prevention of the spread of antibiotic resistance

Kinetics, matrix effects, and transformation processes

Involved Staff: Michael Leupold, Dr. Anam Asghar, Prof. Dr. Torsten C. Schmidt

Partner: Prof. Dr. Barcikowski, Prof. Dr. Folker Meyer, Dr. Dr. Ricarda Schmidhausen

Funding: Internal

The research project aims to remove antibiotics and antibiotic resistance genes in hospital wastewater by photocatalysis to counteract the environment's global contamination and antibiotic agents' associated loss of efficacy. In urban areas, antibiotics and resistance genes enter the environment through wastewater because wastewater treatment plants are not optimized to remove pharmaceuticals or resistance genes. Resistance genes in the environment threaten human health, as they can travel from there back to the population (Westphal-Settele et al., 2018). If nothing is done, antibiotics will soon become ineffective in combating infectious diseases, which is predicted to lead to 10 million annual deaths worldwide by the middle of this century (O'Neill, 2016). One solution strategy is to treat wastewater using photocatalysis (Nosaka et al., 2017). Unfortunately, whether universal antibiotics and antibiotic-resistance genes can be removed in complex matrices is unclear. Nevertheless, photocatalysis is promising because, compared to other treatment methods, it can be expected to produce high yields of reactive oxygen species that can effectively degrade pharmaceuticals.

A photocatalytic reactor for testing photocatalytic materials was developed during the research project. Using the two beta-lactams, amoxicillin, and clavulanic acid, as examples, it will be shown how the presence of artificial matrices influences the kinetics and transformation product formation. In addition to the analytical methods of coupling liquid chromatography with high-resolution mass spectrometry, parameters relevant to degradation, such as dissolved organic carbon, pH, and dissolved oxygen, will be measured. A schematic overview of the reactor and the planned online and at-line measurements are attached to Figure 1. The knowledge gained will then be used halfway through the research project to study amoxicillin and clavulanic acid and their corresponding resistance genes in real hospital wastewater.

Furthermore, since many different antibiotics and corresponding resistance genes can be expected to be found in real hospital wastewater, a group of ten relevant antibiotics and their corresponding resistance genes will also be selected according to their relevance, quantified in real samples, and tested for photocatalytic degradability. The group should contain antibiotics from all important substance classes. Finally, the research data will be published in lectures, poster contributions, publications, and suitable databases.

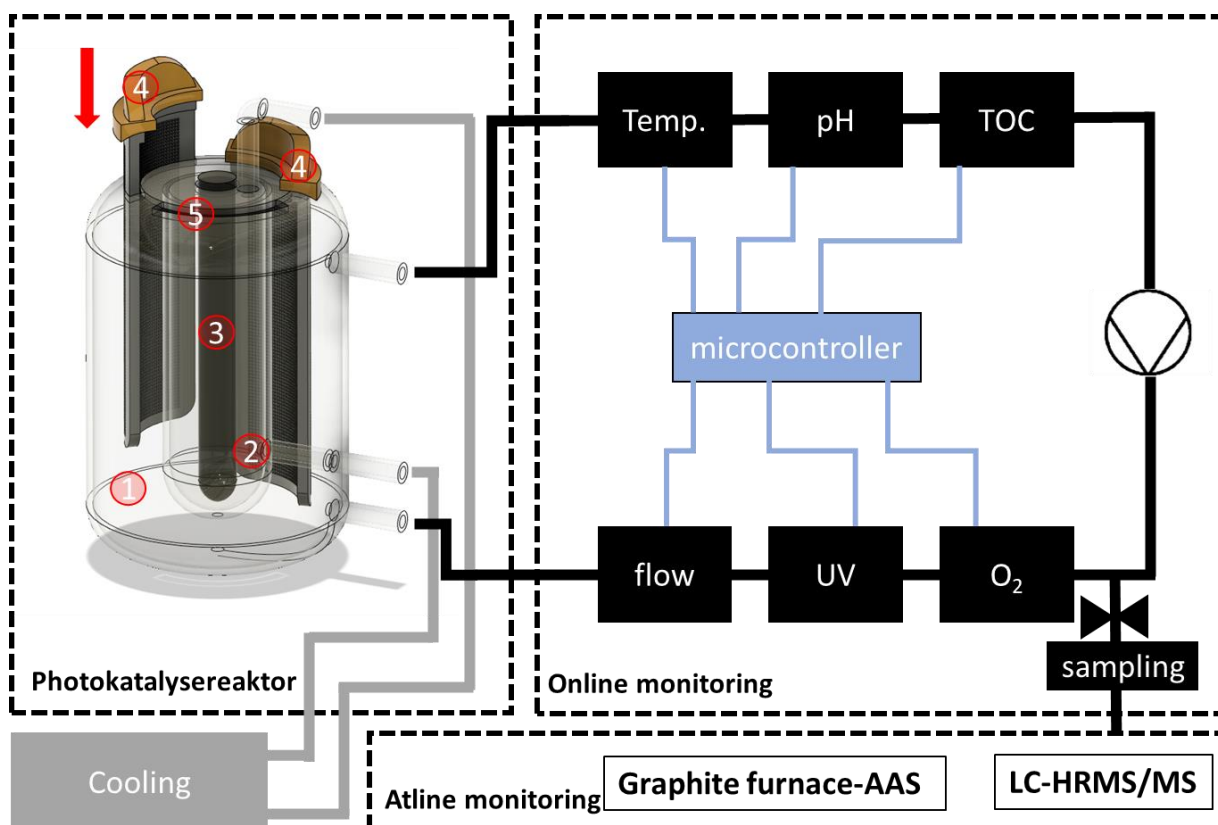


Figure 1 schematic overview of the reactor and planned online and at-line measurements. (1) reaction chamber, (2) cooling system, (3) low-pressure lamp, (4) immobilized photocatalyst on a module, (5) module slot.

Literature:

Nosaka, Y., & Nosaka, A. Y. (2017). Generation and Detection of Reactive Oxygen Species in Photocatalysis. *Chemical Reviews*, 117(17), 11302-11336.

<https://doi.org/10.1021/acs.chemrev.7b00161>

O'Neill, J. (2016). Tackling drug-resistant infections globally: final report and recommendations.

Westphal-Settele, K., Konradi, S., Balzer, F., Schönfeld, J., & Schmithausen, R. (2018). Die Umwelt als Reservoir für Antibiotikaresistenzen. *Bundesgesundheitsblatt - Gesundheitsforschung - Gesundheitsschutz*, 61(5), 533-542. <https://doi.org/10.1007/s00103-018-2729-8>

Compound-specific stable isotope analysis of aminopolyphosphonate complexing agents to elucidate their sorption and transformation processes in environmental and technical systems

Involved staff: Robert Marks, Dr. Maik A. Jochmann

Involved students: Felix Drees, Sarah Rockel

Partners: Prof. Dr. Stefan B. Haderlein, Center for Applied Geoscience, Univ. Tübingen, Dr. Daniel Buchner, Center for Applied Geoscience, Univ. Tübingen

Funding: German Research Foundation (DFG) Project Grant 457490294

Phosphonates are strong metal complexing agents with growing commercial importance. The global consumption of phosphonates increased from 56 kt a⁻¹ in 1998 to 96 kt a⁻¹ in 2012 (and from 15 kta⁻¹ to 49 kta⁻¹ in Europe) (Rott et al., 2018). Since the 1980s, they have been used to replace the structurally similar aminopolycarboxylates (e.g., ethylenediaminetetraacetic acid, EDTA) and polyphosphates, which were partially phased out due to adverse environmental effects such as heavy metal remobilization from sediments and surface water eutrophication (Jarvie et al., 2006; Wu et al., 2003). Phosphonate concentrations in German rivers are currently in the ngL⁻¹ to low µgL⁻¹ range but are predicted to increase due to increased production and usage (Armbruster et al., 2020). The quantitatively most essential phosphonates are 1-hydroxyethane 1,1-diphosphonic acid (HEDP), 2-phosphonobutane 1,2,4-tricarboxylic acid (PBTC), amino tris-(methylenephosphonic acid) (ATMP), ethylenediamine tetra-(methylenephosphonic acid) (EDTMP) and diethylenetriamine penta-(methylenephosphonic acid) (DTPMP) (see Fig. 1). ATMP, EDTMP, and DTPMP are termed aminopolyphosphonates (APP).

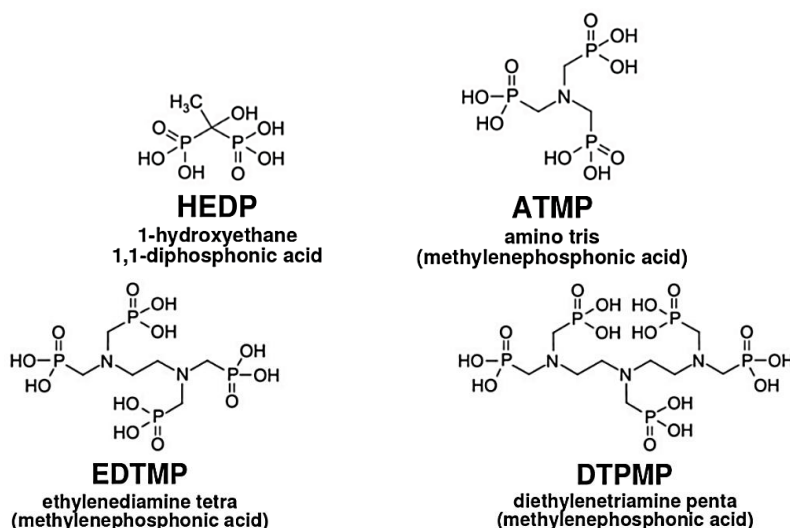


Figure 2: Polyphosphonic acid complexing agents are widely used in Europe (adapted from Rott et al. (2018)). ATMP and EDTMP were selected as model compounds in the proposed research

The current ability to assess the environmental fate of aminopolyphosphonates is poor, primarily due to the lack of knowledge about the significance of sorption and degradation processes for the overall removal of APPs from the aqueous phase. Furthermore, reaction mechanisms and pathways of AAP transformation reactions are not fully identified, hampering a prediction of the effects of crucial parameters (e.g., pH, cation concentrations, competing ligands) on the fate of APP in environmental and technical systems. Furthermore, as product analyses often comprised only orthophosphate and total phosphorous, the knowledge regarding transformation products is incomplete. These knowledge gaps hamper assessing the environmental fate of APPs and the design of treatment strategies for the efficient removal of APP in technical systems. Hence, a more detailed evaluation of the effects of decisive parameters (pH, complexing cations, degree of complexation, etc.) on sorption and transformation processes is needed. Therefore, we will conduct carefully designed experiments and will apply LC-CISA (liquid chromatography-isotope ratio mass spectrometry) in combination with LC-HRMS (LC-high resolution mass spectrometry) and other advanced analytical techniques and experimental procedures to identify and characterize the most significant attenuation processes and mechanisms of APPs as well as their major transformation products.

Effects of the water matrix on transformation product formation

Involved Staff: Katharina Klein, M. Sc., Dr. Vanessa Wirzberger, Dr. Anam Asghar, Kaliyani Wickneswaran, B. Sc, Dr. Gerrit Renner, Dr. Maryam Vosough, Dr. Klaus Kerpen, Prof. Dr. Torsten Schmidt, Prof. Dr. Holger Lutze (external, TU Darmstadt)

Funding: DFG

It was shown that matrix components could affect the transformation product (TP) formation during oxidative processes. This was first observed in the ozonating dimethylsulfamide to the cancerogenic compound *N*-nitrosodimethylamine (NDMA), which required the presence of bromide. However, such effects of the water matrix on transformation processes are hardly investigated. The present project deals with matrix effects on transformation processes governed by natural organic matter (NOM). In the reaction of *N*-containing pollutants, reactive intermediates such as aminyl radicals, nitroxide radicals, and singlet oxygen can be formed, and their reactions to final products (Figure 1) are hardly studied yet, which is one primary task in the current project.

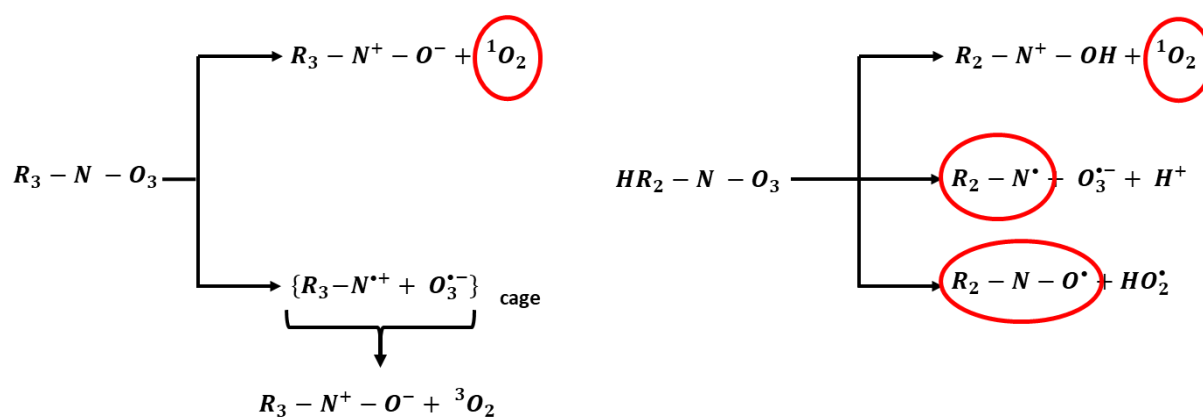


Figure 1: Possible reaction pathway of nitrogen-containing compounds and their reactive intermediates

Thereby kinetics of the reaction with aminyl radicals with simple model compounds representing reactive sites of pollutants will be investigated using laser flash photolysis coupled with time-resolved UV-Spectroscopy (ICCD Camera). Moreover, the formation of singlet oxygen was studied *via* luminescence measurement using a NIR-photomultiplier. Therefore, a reference reaction ($OCl^- + H_2O_2 \rightarrow Cl^- + H_2O + {}^1O_2$), known to yield singlet oxygen, was used to calibrate the system.

Furthermore, the changes in the optical properties of NOM (Suwannee River and Upper Mississippi River) upon reactions with oxidants used in water treatment (O_3 , ClO_2 , and $O_3 + PMS$) are investigated using excitation-emission measurements/matrices (EEM), UV-Vis spectroscopy, NPOC measurements (see Figure 2).

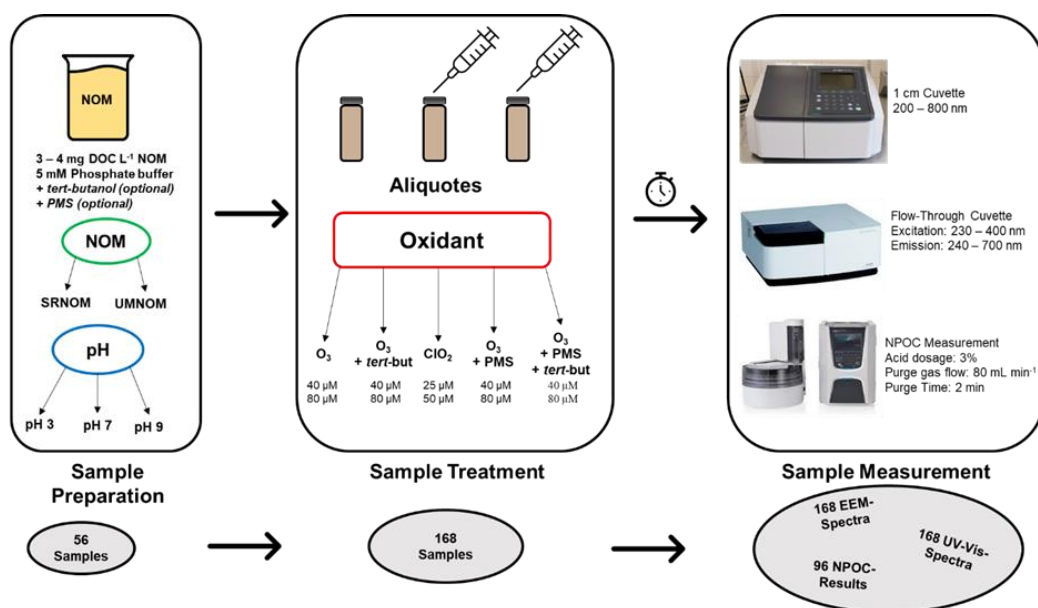


Figure 2: Variables, measured and derived data for investigating the structural changes of NOM via oxidation

Therefore, we used the multivariate approach parallel factor analysis (PARAFAC) to decompose the complex mixed EEM into different underlying components and additionally calculated the changes of SUVA, Peak Ratios, and absorption at 254 nm. To study the different effects caused by oxidant, NOM type, or pH value, we used the chemometric method ANOVA simultaneous component analysis (ASCA) (see Figure 3).

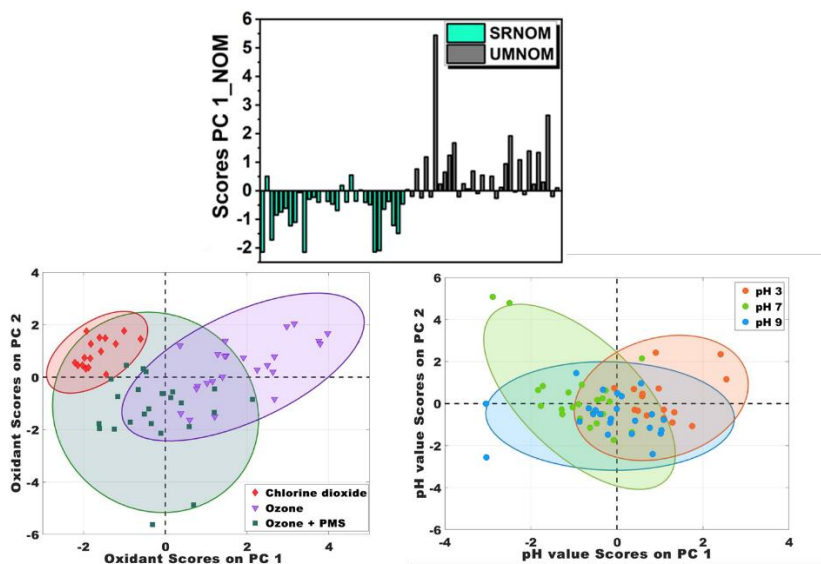


Figure 3: Scores of the ASCA model for O_3 , ClO_2 , and $O_3 + PMS$. Top: NOM Scores for PC 1_NOM. Left: Oxidant Scores for PC 1 and Oxidant Scores for PC 2. Right: pH value Scores for PC 1 and pH value Scores for PC 2. The corresponding ellipses show confidence with a 95% limit.

Global Young Faculty VII: AG: Applied Science Communication

Involved staff: Dr. Gerrit Renner

Partners: Dr. Christian Mainka, Dr. Valentina Nachtigall, Dr. Baoxiang Peng (Ruhr-University Bochum), Dr. Frédéric Etienne Kracht, Dr. Maximilian Krug, Dr. Fatih Özcan, Dr. Sven Reichenberger, (University of Duisburg-Essen), Dr. Sabrina Pospich (Max-Planck-Institute of Molecular Physiology), Dr. Daniel Siegmund (Fraunhofer Umsicht)

Funding: Stiftung Mercator

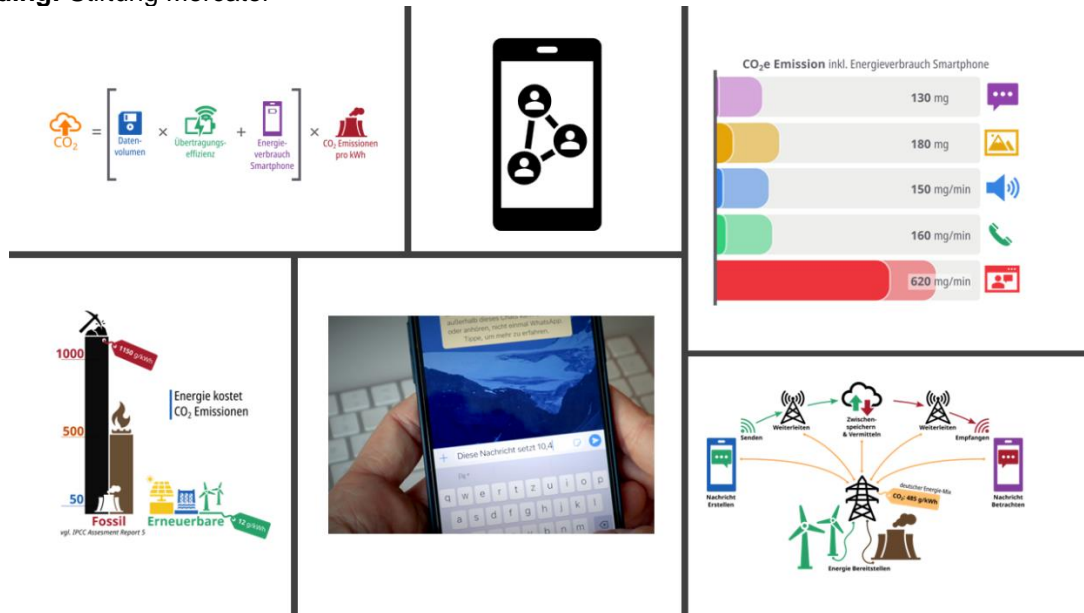


Figure 1: Materials used in an educational video that explains why using instant messenger services indirectly emits carbon dioxide equivalents. The video is part of a study investigating whether knowledge transfer affects knowledge transfer if the person transferring knowledge is perceived as an influencer or scientist.

Communicating scientific research results is an essential part of academic work. In science communication, researchers face the challenge of conveying their research activities, results, and implications to their peers or the general public in a targeted manner.

Central questions in this context could be: Why is my research relevant? Who could benefit from my research results? How can I reach my target audience? What do I need to pay attention to when communicating with a non-academic public?

In our interdisciplinary project, we are developing a framework from different perspectives – including chemistry, educational science, computer science, communication science, and physics – to improve science communication and support researchers in their communicative work. To do this, we analyze selected, target group-oriented formats to identify under which conditions communication intentions and effects of scientific messages can diverge. These analyses are based on our own experiences and those of active communicators in science and the public.

This project aims to identify evidence-based, target group-related success strategies for conducting successful and exceptionally efficient science communication. This should inform communicator scientists about future communication strategies and media.

AutoExtrakt – Development of a fully automated microextraction device and its application for the analysis of substances in complex matrices from food and environmental origin

Involved staff: Frank Jacobs, Dr. Klaus Kerpen, Prof. Dr. Amir Salemi, PD Dr. Ursula Telgheder

Partners: GERSTEL GmbH&Co.KG

Funding: Federal Ministry for Economic Affairs and Energy (BMWi)
by the Central Innovation Programme for SMEs (ZIM)

This project aims to develop a fully automated and efficient extraction technique that enables sensitively analysis of toxicologically relevant substances in environmental and food samples. The substances are to be reliably detected both qualitatively and quantitatively. The extraction technology to be developed will enable laboratories for environmental and food controls to sensitively detect and quantify residues of environmental pollutants or aromatic substances in an automated process.

A new sample preparation technique based on SBSE (Stir bar Sorptive extraction) is being developed. SBSE as a technique is limited by the manual labor necessary in the sample preparation process. The motivation for this project was to automate the complete sample preparation process by using an x/y/z-sampler. Because of the new form factor, the sample agitation was done in a revised vertical shaking unit (QuickMix), so the tray could be cooled and heated. A wash and drying station is implemented to clean and dry the sorbent after extraction. The loss of analytes is minimized by featuring a centrifuge for drying the sorbent. For complete automatization of the process, an online conditioning station is also being introduced.

The Setup of the System consists of an MPS Autosampler (GERSTEL GmbH&Co.KG, Mülheim, Germany) configured with a QuickMix, Wash/Drying-Station, Thermal Desorption Unit (TDU2) and Agilent 7890B GC with 5977B MS. A DoI approach was chosen for determining interdependency of parameters like sample extraction time, salt concentration and extraction temperature. The concentration range for calibration of 22 pesticides described in DIN 27108 was determined from low ng/L to 100 µg/L. Each measurement was performed in triplet as a minimum. In addition, blank measurements were done to ensure no carryover was present.

Method development by Design of Experiments resulted in optimized parameters: 90 minutes of extraction time, 70°C, 30% of NaCl (w/w). With these parameters, the relative standard deviation between measurements was in the single digits for most investigated pesticides, with none rising above 40%. High standard deviation can be traced back to analytes being less compatible with sorbent material. Therefore, SA-SBSE (solvent-assisted-stir bar sorptive extraction)¹ could be helpful for those substances. First calibration results show good response in an extensive concentration range (1 - 1000 ng/L) for all analytes. Detection limits ranged from 2,93 ng/L to 187 ng/L, whereas LOQ ranged from 12.8 ng/L to 885 ng/L. These limits will be lower for calibrations in a more suitable range that fits the DIN 27108 specifications.

Investigation of Stable Isotope Fractionation during Abiotic Imidacloprid Degradation

Involved staff: Felix Niemann, Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt

Funding: Internal

Despite political efforts to ban neonicotinoids like Imidacloprid, it is still ubiquitously in surface waters worldwide. Originally designed as an insecticide for sucking pests, its toxic effects on non-target organisms like pollinators and aquatic organisms are particularly worrying. Moreover, in the environment, it can undergo physical and (bio-)chemical transformation processes that facilitate mineralization and potentially produce more hazardous substances than the starting substance. This raises the importance of characterizing the transformation processes, estimating their contribution, and identifying factors influencing them.

This study focuses on abiotic imidacloprid degradation, such as hydrolysis and photolysis, as they contribute significantly to its natural attenuation in water bodies. In laboratory experiments, influences like spectral distribution, dissolved oxygen content, pH value, and addition of photosensitizers and quenchers are being investigated. Mass-spectrometry and methods for their quantification shall identify the main transformation products. A sunlight simulator was set up and characterized to approach environmental conditions.

This study's novelty is compound-specific stable isotope analysis (CSIA) as a tool to identify characteristic isotope effects for individual transformation processes. This technique has been proven to grant valuable insights into reaction mechanisms. Developed methods could also potentially be used to trace point sources of Imidacloprid in surface waters and monitor its environmental fate.

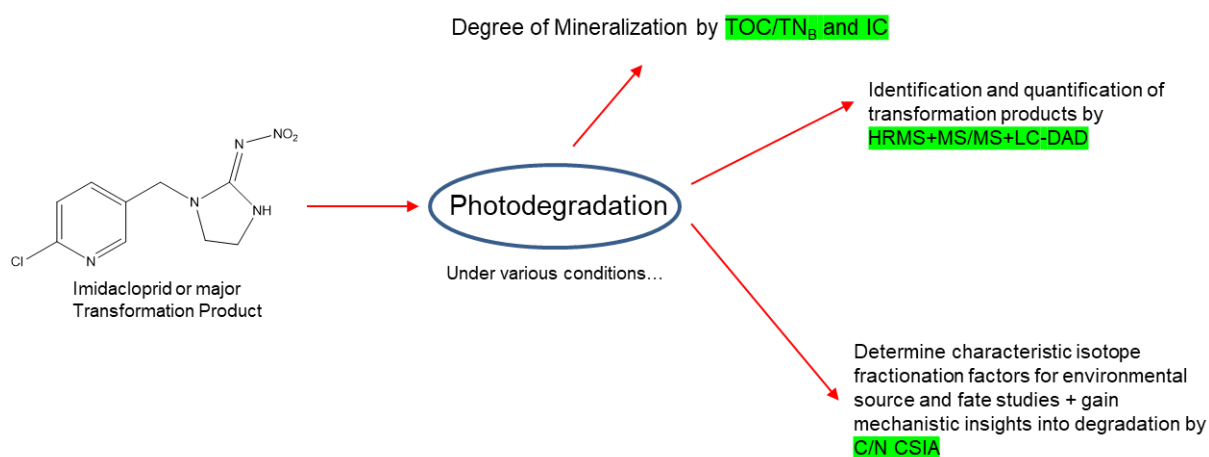


Figure 1: Flow chart of the project, including analytical methods utilized.

Polar compounds such as Imidacloprid are not directly analyzable by gas chromatography without derivatization. Therefore liquid chromatography coupled with a conversion interface and an isotope ratio mass spectrometer (LC-IRMS) was utilized for separation from its transformation products. The developed method uses only aqueous eluents, is robust, and could be tested successfully on real photolysis and hydrolysis samples.

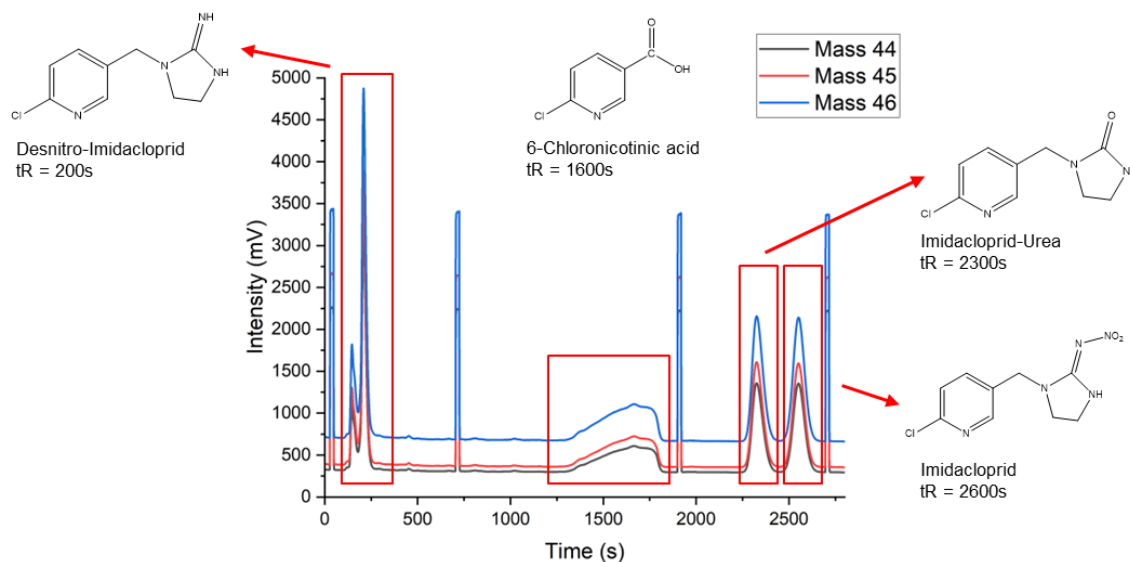


Figure 2: LC-IRMS separation of selected transformation products of Imidacloprid.

Insights into amino acid metabolism and incorporation by compound-specific carbon isotope analysis of three-spined sticklebacks

Involved staff: Tobias Hesse, Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt

Involved students: Shaista Khaliq

Funding: Internal

Interpretation of isotope data is of utmost importance in ecology to build sound models for studying animal diets, migration patterns, and physiology. However, our understanding of isotope fractionation and incorporation is still limited, as we do not know how much information about the metabolic history of consumers is reflected in the isotope signatures of individual compounds. We, therefore, measured the $\delta^{13}\text{C}$ values of individual amino acids in a controlled feeding experiment from muscle and liver tissue of three-spined sticklebacks (*Gasterosteus aculeatus*).

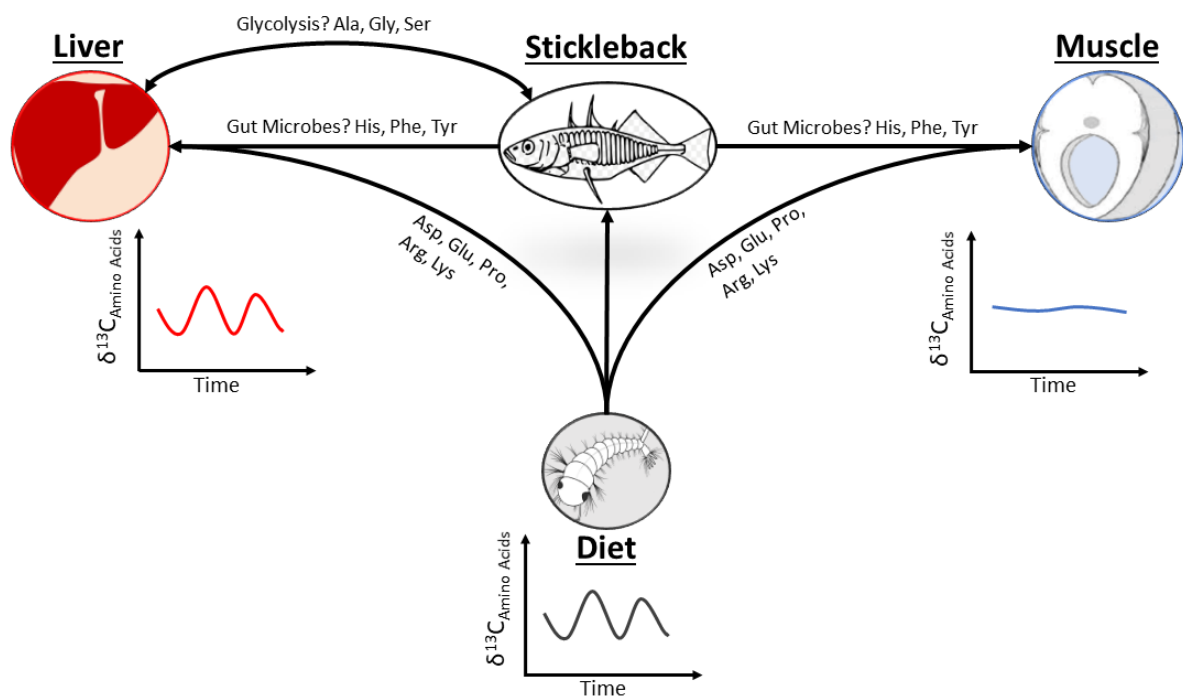


Figure 1: The isotopic composition of amino acids in the liver responds quickly to a shifting carbon isotope signature in diets. Some amino acids (Asp, Glu, Pro, Arg, Lys) are directly routed from the diet into liver and muscle tissue, while others (His, Phe, Tyr) seem to have at least some contribution from sources like gut microbes. Carbon isotope fractionation of Ala, Gly, and Ser in the liver might reflect constant cycling and conversion of nutrients.

The carbon isotope signatures of amino acids in the liver responded quickly to small shifts of only ~1 to 2 ‰ in dietary isotope compositions, indicating the liver's fast nutrient turnover and role as a regulatory organ. In contrast, the isotope signature in muscle tissue remained constant over time. No carbon isotope fractionation between diet and fish tissues was observed for the non-essential amino acids asparagine, glutamine, and proline, as well as the essential amino acids arginine, lysine, and threonine in both liver and muscle tissue, supporting the idea of direct nutrient routing as opposed to *de novo* synthesis on a protein-rich diet. Minor differences were observed for the glycolytic amino acids alanine, glycine, and serine in the liver, indicating that metabolic processes such as glycolysis or gluconeogenesis can be tracked by carbon isotope signatures of their main substitutes. Our results further show an unusually high isotope fractionation of histidine, which could stem from a low abundance of histidine in diets to match the demand of the fish consumer or from the enzymatic conversion of histidine to histamine. We demonstrate that compound-specific isotope analysis has great potential to investigate the central metabolic pathways of organisms and suggest further investigations using isotopically enriched materials to facilitate the correct interpretation of field data.

Isotope-labeling *in situ* derivatization and HS-SPME arrow GC-MS/MS for simultaneous determination of fatty acids and fatty acid methyl esters in water

Involved staff: Lucie K. Tintrop, Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt

Funding: Internal

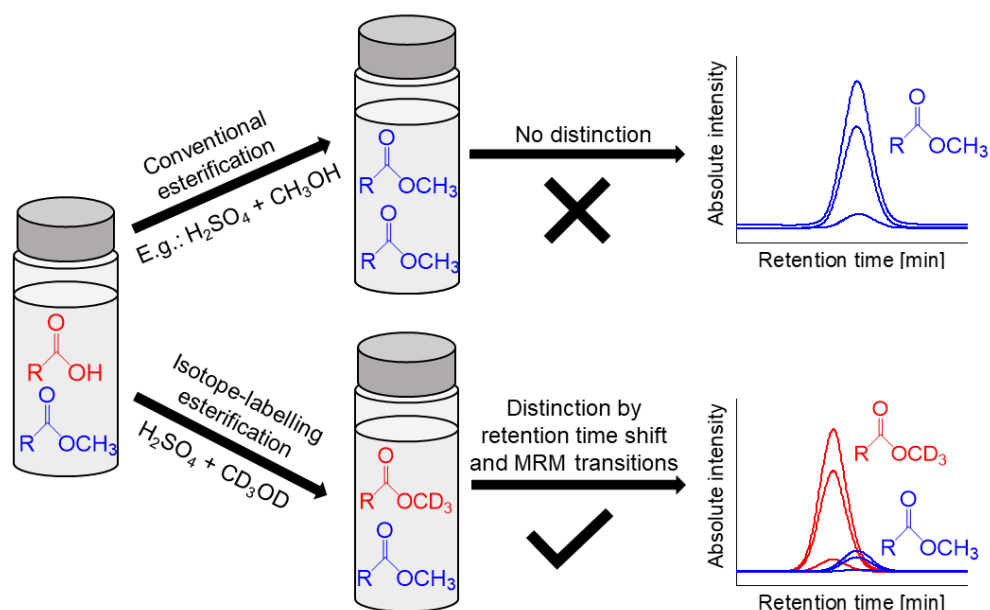


Figure 1: Principle and advantages of isotope-labeling methyl esterification compared to conventional methyl esterification for fatty acid derivatization.

Fatty acids (FAs) and fatty acid methyl esters (FAMES) are relevant substances in the food industry, microbiology, water analysis, and biodiesel production and are analyzed for quality or process control. FAs and FAMES are related and often appear together, as they can easily be transferred into each other. For some application fields, detecting FAs and FAMES in one GC run simultaneously is helpful. However, conventional derivatization methods for FAs are based on methyl esterification, in which the FAs are transformed into FAMES. The FAMES originating from methyl esterification and the FAMES naturally occurring in the sample cannot be distinguished using methyl esterification methods. An alternative derivatization approach is needed, which is fast, applicable to aqueous samples, and makes it possible to simultaneously detect FAs and FAMES in the same samples.

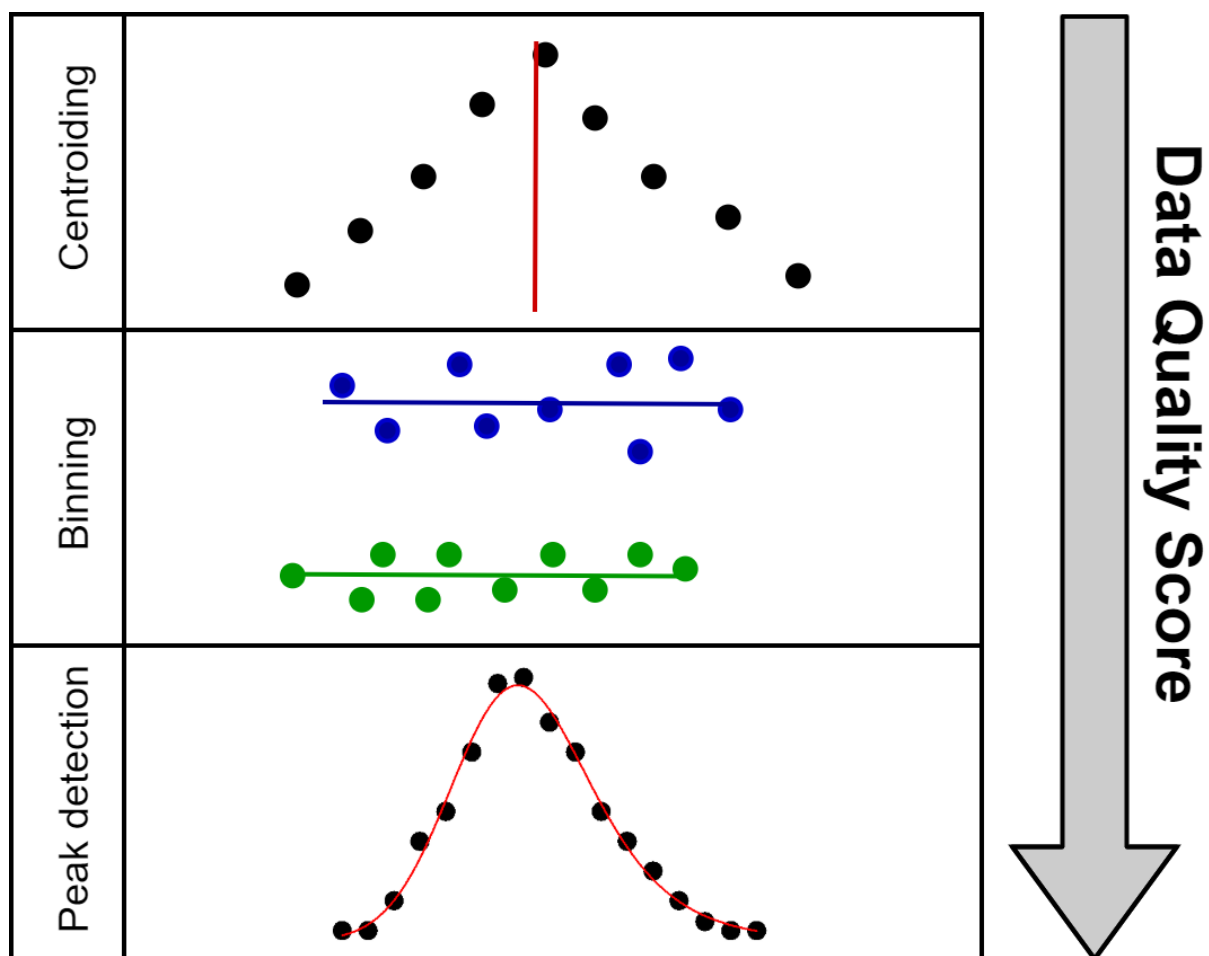
During this study, it was achieved to analyze homologous FAs and FAMES simultaneously in one GC run for the first time. A fully automated method was developed, which enabled the determination of 48 FAs and FAMES in aqueous samples by *in-situ* FA esterification followed by solvent-free headspace solid-phase microextraction arrow (SPME arrow). FAs are derivatized before analysis by isotope-labeling esterification with deuterated methanol (CD₃OD) to achieve a mass shift of +3 m/z compared to natural FAMES.

The deuterated methyl group results in a so-called chromatographic isotope effect and, thus, a slightly shorter retention time ($\Delta RT = 0.03$ min). Additionally, the deuterated methyl group leads to specific transitions by using GC-MS/MS operating in multiple reaction monitoring mode, which was used to identify the derivatives. Utilizing these features of the developed method makes the distinction between FAs and FAMEs straightforward. Esterification parameters (time, temperature, content of deuterated methanol, pH) were optimized by Design of Experiment to be 20 min, 50 °C, 4 v/v% CD₃OD, and pH 2.1. The method was validated and showed good recoveries and method detection limits. FAs and FAMEs could be detected in aqueous samples from surface water, wastewater treatment plant outlet, and bioreactors at different conditions.

Development of a Data Quality Score for the Processing of Non-Target-Screening Data generated by HPLC-HRMS

Involved staff: Max Reuschenbach, Dr. Gerrit Renner, Prof. Dr. Torsten C. Schmidt

Funding: Friedrich-Ebert-Stiftung e.V., Internal



Data generated by Non-Target Screening (NTS) with HPLC-HRMS is extensive and complex. Manual data processing of NTS is not feasible due to its complexity, so automated processing scripts such as feature detection algorithms are used instead. Generally speaking, there are many software solutions available for feature detection available. The different algorithms, however, possess different modes of action and, thus, are hardly comparable in their results. Furthermore, the established algorithms cannot estimate the influence of fluctuating data quality on the processing result. However, this quality is a valuable metric as it automatically allows us to filter out potential false-positive entries from the feature lists. Thus, this project analyzes the specific NTS processing steps, develops concepts to estimate data quality in the individual steps with a Data Quality Score (DQS), and combines the individual DQS values into a combined score. Furthermore, to reduce the influence of non-optimized user parameters in feature detection, we aim to develop parameter-free processing algorithms.

In the first work package, we dealt with the centroiding of HRMS profile data. This step reduces peaks in profile-mode mass spectra to their centroids possessing the peak's position and area. Information about asymmetry or high noise amplitudes of peaks is not retained during the processing step, conventionally, even though it is valuable to detect isotopic fine structures or non-resolved isobaric analytes. We developed a regression-based procedure applying error propagation rules to estimate the centroid's quality (DQSc). Low DQSc centroids show lower mass accuracy and precision over consecutive MS scans and, thus, are considered less reliable for feature detection. Using DQSc, we can now conserve the central profile information previously lost for further processing steps. The code of the centroiding algorithm is available as an open-source published in the journal *Analytical and Bioanalytical Chemistry* (DOI: 10.1007/s00216-022-04224-y).

The second work package was the construction of extracted ion chromatograms (EICs) from multiple consecutive HRMS scans (also called binning). Binning ions from the same ion family are grouped, and only their representative m/z value (e.g., mean) is retained. Only the chromatographic profile in the EIC is relevant for this group of ions. We developed a binning routine free of user-input parameters based on order statistics to extract EICs from Centroid data quickly and efficiently. As a core element, we perform a statistical test on whether a group of ions is drawn from one identical population. If that is not true, the bin must be split further. We applied this procedure in a highly dynamic algorithm, and the whole dataset was grouped into bins constructing EICs. To analyze data quality, we followed a concept from cluster analysis, the silhouette criterion. This criterion assigns bins a high DQSb if the m/z dispersion within a bin is small compared to the distance to neighboring bins.

In the future third work package peaks in the EICs will be detected, characterized, and their data quality analyzed. Further, the DQS from all three previous processing steps will be combined so that the user can easily access the reliability of obtained features.

Studies on electrochemical treatment processes for the decomposition of Persistent Organic Pollutants (POPs) in contaminated ground and surface water

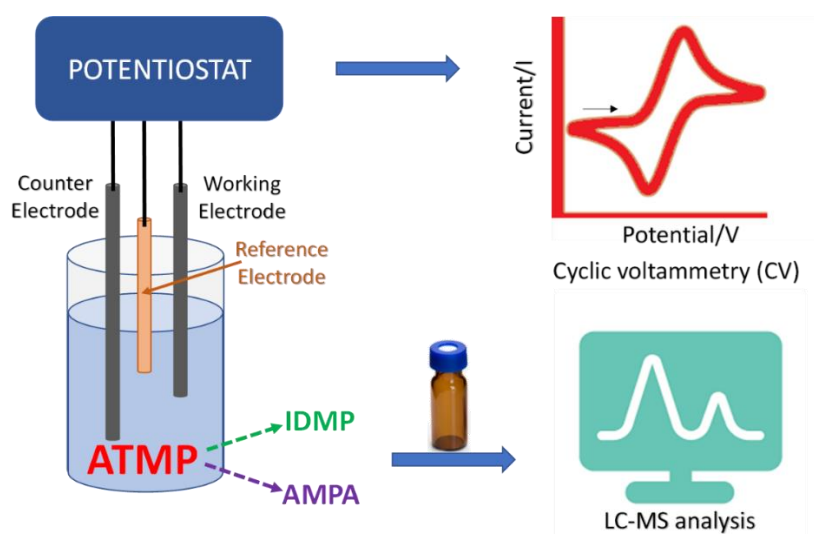
Involved staff: Dua'a M.F. Tahboub, PD Dr. Ursula Telgheder

Funding: The German Academic Exchange Service (DAAD)

The presence of persistent organic pollutants in water is a severe environmental problem affecting human health and the ecological system. Perfluorinated compounds (PFC) and phosphonates are persistent, non-biodegradable compounds and release into surface water and groundwater in large quantities. These harmful compounds' degradation, removal, and detection are significant challenges in analytical and environmental chemistry. The primary purpose of this research project is to develop and optimize an electrochemical degradation (ED) method for water pollutants (PFCs and phosphonates) using cyclic voltammetry (CV) prior to LC-MS analytical determination.

In order to investigate the ED technique, Aminotris(methylenephosphonic acid) (ATMP) is considered a model substance for phosphonates degradation. However, the degradation of ATMP in the aquatic system generates intermediate products such as (IDMP) iminodi(methylene)phosphonate and (AMPA) aminotris(methylenephosphonic acid). Therefore, AMPA is a hazardous and toxic compound.

In this study, it is essential to set the electrochemical cell, optimize the proper electrolyte solution, select and characterize the working electrode and measure the oxidation potential of the water pollutant (i.e., ATMP). Accordingly, degradation experiments are carried out in water media without supporting electrolytes (SE) and are to be compared to a SE-containing electrolyte. Pristine graphite electrode (GRE), glassy carbon (GCE) electrode and boron-doped diamond electrode (BDD) are to be employed as working electrodes vs. (Ag/AgCl 3M KCl) as a reference electrode, individually, for CV experiments without any modification step or added chemicals. Furthermore, performing a long-term CV experiment to achieve complete ATMP degradation before LC-MS determination of the degraded compounds along the measured time.



Membrane processes in drinking water supply (KonTriSol)

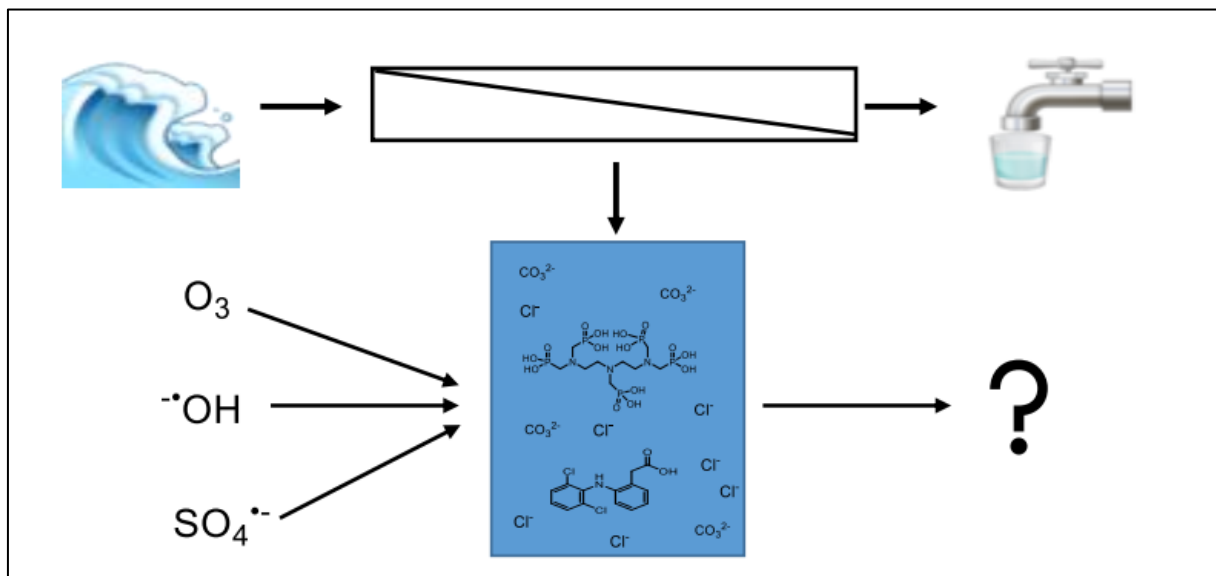
Part: Membrane concentrate treatment with oxidative processes

Involved staff: Xenia Mutke, Prof. Dr. Holger V. Lutze (TU Darmstadt), Prof. Dr. Torsten C. Schmidt

Involved students: Kittitouch Tavichaiyuth, Felix Drees, Orkan Akin, Philipp Swiderski

Partners: IWW Water Centre, TZW, University Frankfurt, Technical University Berlin, Technical University Hamburg, Cornelsen Umwelttechnologie, Delta Umwelt-Technik, Lagotec, Lanxess, Solenis, Funding: Federal Ministry of Education and Research (BMBF)

The project KonTriSol deals with determining the technical, legal, and economic feasibility of nanofiltration (NF) and reverse osmosis (RO) processes. In drinking water treatment systems, NF and RO membrane technologies enable the reduction of water hardness, inorganic water constituents, natural organic substances, and anthropogenic substances. The resulting concentrates contain a high concentration of these substances and antiscalants added during treatment. The direct disposal of these concentrates into the environment could be hazardous to aquatic organisms and thus increase the micropollutant contamination of water bodies.



The IAC project part aims to investigate the potential of different oxidative processes for the treatment of membrane process concentrates. Therefore, in the first phase of this project, various oxidants (i.e., ozone, hydroxyl radicals, and sulfate radicals) were applied to evaluate the degradation of targeted antiscalants. Later, the effect of natural organic matter (NOM) and other radical scavengers was also considered. Finally, the second phase of this project evaluated the degradation efficiencies of antiscalants and trace organic pollutants using simulated and real water concentrates.

Diet-consumer interactions under variable stressor conditions as revealed by stable isotope studies of individual amino acids (A13: CRC RESIST)

Involved staff: Shaista Khaliq, Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt

Partners: University of Duisburg-Essen, Ruhr-Universität Bochum, Leibniz Institute of Freshwater Ecology and Inland Fisheries, University of Cologne, Kiel University, University of Koblenz-Landau and Helmholtz Centre for Environmental Research

Funding: German research foundation (DFG)

The analysis of food webs allows for detailed conclusions on diet-consumer interactions and the origin of resources in ecosystems. Food webs derived from compound-specific stable isotope analysis (CSIA) of amino acids (AAs) can be used to unravel species' niches and trophic links between species under conditions of multiple stressors increase and release, thus allowing closer insight into ecosystem structures and functions characterizing response to degradation and recovery. Simplifying food webs with fewer trophic levels is particularly expected under stress conditions that should be reflected in $\delta^{15}\text{N}$ of trophic and source AAs. In addition, $\delta^{13}\text{C}$ analysis of essential and non-essential AAs will reveal changes in food sources due to ecological degradation and during recovery. Below is a schematic illustration of the relationship between AAs for estimating trophic levels.

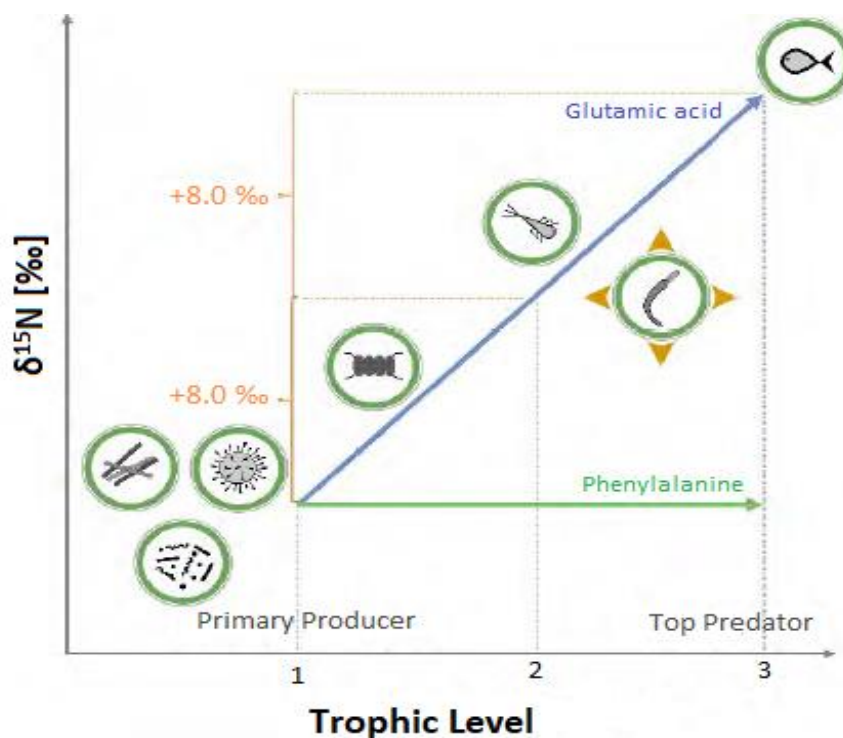


Figure 1: Schematic illustration of the relationship between source AA (phenylalanine: Phe) and trophic AA (glutamic acid: Glu) according to their nitrogen isotope composition to estimate trophic levels of organisms from primary producers to top predators.

In this project, three specific hypotheses (SH) will be used to test the central hypothesis MH2 and MH3 of RESIST by doing CSIA of AAs of samples (macroinvertebrate, fish, and parasite) using GC-C-IRMS. These hypotheses are: (i) Hydro morphological stressors will mainly change the isotope values of higher organisms' non-essential and trophic amino acids. At the same time, stressors affecting water quality will also impact isotope values of essential and source amino acids and reflect changes in the community composition of primary producers (SH A13-1). (ii) Complex food webs can only recover if various food sources have been re-established (SH A13-2). (iii) Heteroxenous parasites indicate the complexity of aquatic food webs, as revealed by CSIA under recovery conditions, while monoxenous parasites can also thrive on degraded sites (SH A13-3). In this regard, Work package (WP) 1 focuses on sampling, measurement, and data evaluation for the historical samples from 2012-2020 (macroinvertebrate) and the yearly field samples (macroinvertebrate, fish, and parasite). WP2 will focus on testing SH A13-1 by analyzing isotope data from fish, invertebrates, and parasite samples from the field sampling program on chosen degraded, recovered, and near-natural sites in the Emscher/Boye catchment. Moreover, in WP3, we will construct food webs based on the trophic positions (TPs) of organisms in a combined effort with other projects of RESIST. The following equation can calculate TPs of organisms.

$$TP_{Glu/Phe} = (\delta^{15}N_{Glu} - \delta^{15}N_{Phe} - 3.4) / 7.6 + 1$$

Non-Target Screening and Ecotoxicological Evaluation of Industrial Wastewater

Involved staff: Felix Drees, Prof. Dr. Maryam Vosough, Prof. Dr. Torsten C. Schmidt

Involved students: Janina Marie Pytlik (Bachelor Thesis)

Partners: Jörg Gisselmann (Head of Environmental Operations, Evonik Industries AG, Marl), Nazmun Nahar, Esther Smollich, Prof. Dr. Bernd Sures (Aquatic Ecology, University of Duisburg-Essen)

Industrial production and processing sites are potential environmental emission sources for organic (micro)pollutants. In particular, process and wastewaters, which are discharged into adjacent watercourses, play a central role since complex and dynamic compositions of chemical components characterize them.

In this context, a non-target screening combined with ecotoxicological investigations can provide essential information to improve on-site water treatment and protect the environment. Those with the greatest ecotoxicological potential can be prioritized and eventually identified from many components. In addition, transformation products unknowingly emerging from chemical processes happening in the water sewer system and water treatment processes can be identified.

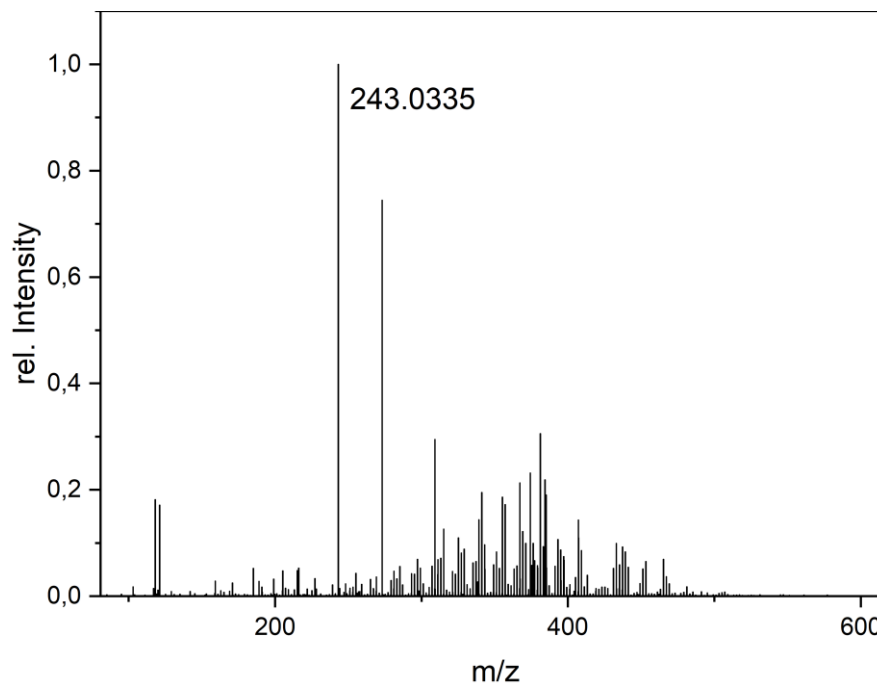


Figure 1: Exemplary mass spectrum resolved by MCR-ALS. It shows the relative intensities of all included regions of interest (m/z).

For non-target analysis, water samples are analyzed by liquid chromatography coupled with high-resolution mass spectrometry. Subsequently, the generated raw data is first filtered following the regions of interest approach and then resolved by multivariate curve resolution alternating least-squares (MCR-ALS) modeling, which provides information on mass spectra (Figure 1), quantities, and chromatographic profiles (Figure 2) of each chemical component. Tentative identification is then made by comparison with different chemistry databases.

Regarding ecotoxicological evaluation, standardized acute and non-specific toxicity tests systems based on *Daphnia magna* (planktonic crustacean), *Desmodesmus subspicatus* (green algae), and *Aliivibrio fischeri* (bacteria) are applied.

The project is realized in cooperation with Evonik Industries AG, represented by Mr. Jörg Gisselmann, at the chemical park in Marl. As one of the largest production sites in Europe, it is a prime example of complex wastewater flows and their environmental challenges. With exciting scientific questions arising from data processing, we hope to support Evonik in its corporate sustainability strategy.

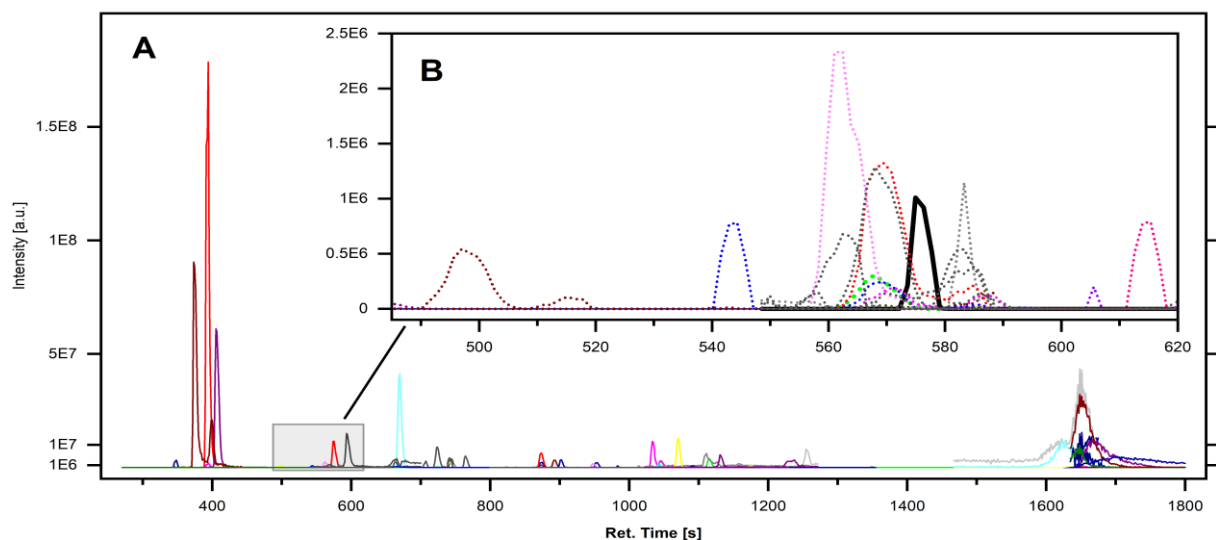


Figure 2: Chromatographic profiles resolved by MCR-ALS of an exemplary sample. Panel A shows the total chromatogram, whereby panel B focuses on a highly condensed chromatographic part. Axes show signal intensities in dependence on retention time.

Innovative water technologies of the FutureWaterCampus (InnoWat-FWC) – Photocatalysis section

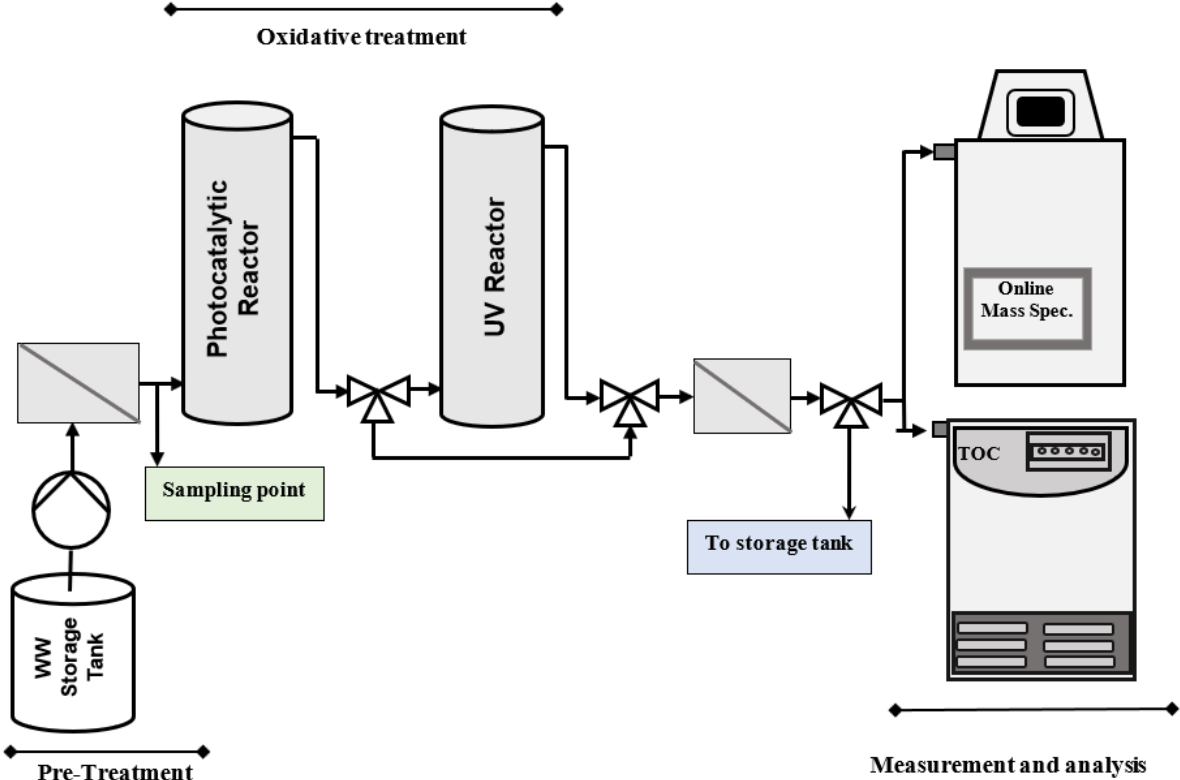
Involved staff: Felix Niemann, Dr. Klaus Kerpen, Dr. Anam Asghar, Dr. Torsten C. Schmidt

Funding: Europäischer Fonds für regionale Entwicklung (EFRE)

To promote innovation, research and support the establishment and expansion of research infrastructures and competence centers, InnoWat-FWC" was secured via the "Research Infrastructures NRW" competition and the European Regional Development Fund (ERDF). In this project, the participants in the ZWU network are jointly working to develop innovative water technologies for sustainable treatment and management of water and wastewater. The other research objectives include the development of integrated procedures, processes, and technologies in the field of algae, membrane, and photocatalysis for water management with far-reaching areas of application.

In the IAC department, the project investigates photocatalytic-based advanced oxidation processes for the degradation of recalcitrant organic micropollutants in ambient environments, i.e., in the presence of inorganic and organic water matrices. Photocatalytic-based processes have attention due to high yields of reactive oxygen species (ROS), thereby ensuring the complete mineralization of organic micropollutants (OMPs).

This project will be completed in collaboration with cooperative partners within the ZWU network. At the IAC, a modular, fully continuous photocatalytic water treatment train is developed (Scheme 1). Central elements of the water treatment train include i) flow-through photoreactor, ii) membrane systems for separating suspended solids and catalyst nanoparticles from the water phase, and iii) online water quality measurement technologies, i.e., TOC analyzer and mass spectrometer. The modular photocatalytic treatment train setup was built in the project's first phase. Preliminary tests will be planned to optimize process conditions for the modular wastewater treatment train. Photocatalyst materials will be obtained from our collaboration partner at UDE Duisburg and tested for photocatalytic degradation of micropollutants in ambient environments.



Scheme of the pilot plant treating wastewater effluent with online monitoring.

Development of a method for the analysis of the extracellular volatile metabolome of nosocomial pathogens by thermal desorption 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

Funding: Bundesministerium für Bildung und Forschung, Grant No. 13GW0428C

Nosocomial pneumonia is the most common cause of death among hospital-acquired infections. Therefore, a rapid and reliable diagnostic 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 for the targeted detection of nosocomial infections needs to be developed. The project aims to identify pathogens based on their specific microbiological volatile organic compound (mVOC) profiles in exhaled air. Therefore, a mobile ion mobility spectrometer in combination with a gas chromatographic pre-separation unit (GC-IMS) was set up and had to be validated to measure these mVOCs from the human breath directly at the patient's bedside.

The headspace of bacterial reference cultures grown on plates (*Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Streptococcus pneumoniae*, *Legionella pneumophila*, *Acinetobacter baumannii* complex, and *Escherichia coli*) is measured using the mobile GC-IMS to determine specific mVOC profiles and marker compounds. Furthermore, as the sampling chamber contains an incubator, freshly inoculated agar plates can be measured continuously during their growth phase.

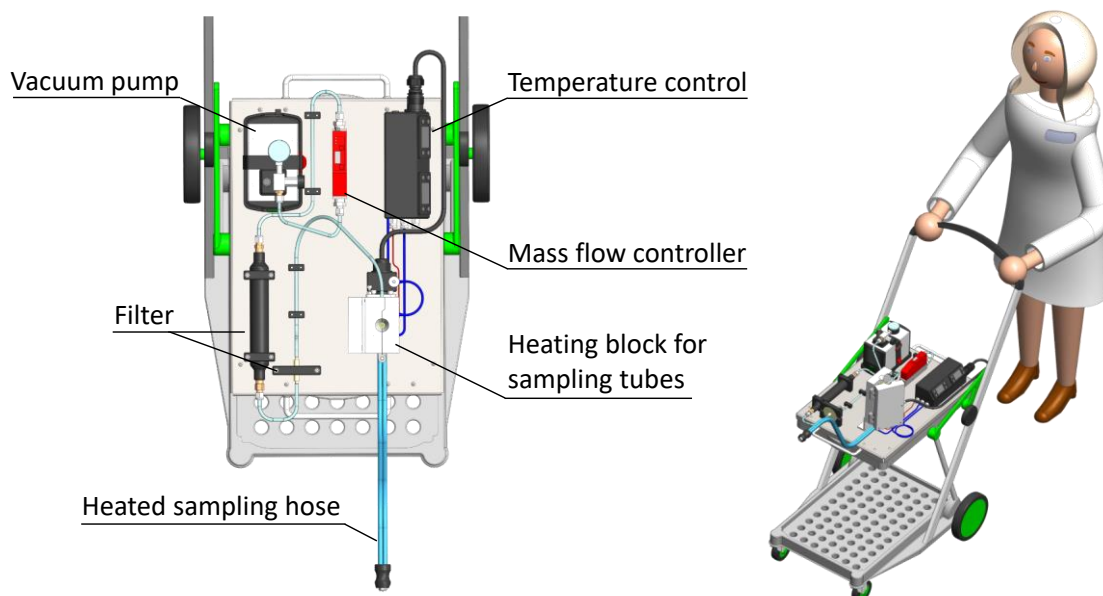


Figure 1: Mobile solution for sampling microbial volatile organic compounds on sampling tubes for thermal desorption. On the left, the individual components are named. The mobile solution is in its entirety on the right.

Since identifying the individual mVOCs is essential to infer the specific metabolism of the pathogens, a thermal desorption gas chromatograph coupled to a mass spectrometer (TD-GC-MS) is established for validation. For parallel detection of the mVOCs, an IMS was introduced as a second detector in the same flow line using a flow splitter. Such a TD-GC-MS-IMS system has been built for the first time. In addition, a mobile and heatable solution was developed to ensure reproducible sampling for applying mVOCs on sampling tubes (see Fig. 1).

Initial measurements of selected bacterial strains demonstrate that especially the high detection power of the IMS enables the sensitive detection of pathogen-specific VOC patterns. Individual mVOCs can be identified using MS and an established IMS database of more than 30 relevant substances. For example, Indole can be found in *Escherichia coli*, a product of its tryptophan metabolism. Furthermore, it could be shown that specific mVOCs can be detected already after six hours of incubation. The next step will be performing a proof of principle trial in the clinical setting.

Non-radioactive ionization for spectrometry and spectroscopy

Involved staff: Annika Fechner, PD Dr. Ursula Telgheder

Partners: Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V.

Ion mobility spectrometry (IMS) is used in analytics to detect volatile organic compounds (VOCs). One major step in analyzing samples using IMS is sample ionization. As radioactive ionization sources are the benchmark in commercialized IMS, developing a non-radioactive alternative is relevant. The Flexible Microtube Plasma (F μ TP) is evaluated as a possible alternative. Initially developed by the Miniaturisation working group at ISAS e.V., this highly miniaturized ionization source might be the perfect candidate for coupling with the compact structure of an IMS. The use of the F μ TP as an ionization source for the IMS has already been successfully realized under laboratory conditions. In this project, the coupling of the F μ TP and a commercial IMS is validated and optimized. So far, the setup of the coupling is already adapted. For this purpose, components of the commercial IMS were redesigned and manufactured using 3D-Printing. After those adaptations, the F μ TP could be successfully connected to the IMS. The developed F μ TP-IMS shows excellent ionization efficiency.

Furthermore, the coupling of the F μ TP and the commercial IMS was optimized for long-term stability and is currently validated. Additionally, the F μ TP should replace the standard ionization source in commercial Gas Chromatography-IMS (GC-IMS). For this purpose, components of the GC-IMS were already redesigned and manufactured by 3D-Printing, too. Presently, the adaption and function of the GC-F μ TP-IMS coupling are developed.

The developed couplings will be optimized to analyze different biologically relevant samples, e.g., the abattoir's signal molecules of bacteria and germs. A thermal desorption chip (TDC) will be used for a liquid sample application. The TDC was individually developed for the enrichment and controllable release of complex sample mixtures. In addition, it offers a miniaturized form of pre-separation and sample evaporation for the IMS through adjustable temperature programs. It has already been shown that it has excellent potential for directly measuring liquid sample mixtures using IMS.

Furthermore, the TDC is in an ongoing optimization for tasks in F μ TP-IMS. By means, it will be optimized and characterized, especially regarding an increased sensitivity for different substance classes and the use of the smallest analyte concentrations in complex samples. Here, the first results prove an increased method sensitivity for multiple substances. Current adaptations include an efficient cleaning system to increase the TDC's lifetime and an automated sample application to simplify the TDC-F μ TP-IMS approach.

Development of a new method for the determination of N-nitrosamines in the air at the workplace in the context of occupational safety - NNOccSafe

Involved staff: Jana Hinz, PD Dr. Ursula Telgheder

Partners: Bonn-Rhein-Sieg University of Applied Sciences

Funding: German Social Accident Insurance (DGUV)

Within the framework of a doctoral thesis, research regarding the selective and sensitive analysis of nine different N-nitrosamines relevant to occupational safety in Germany is being carried out as defined in the "NNOccSafe Project", funded by the German Social Accident Insurance (DGUV). The work aims to develop a method based on the coupling of gas chromatography (GC) and ion mobility spectrometry (IMS) that supersedes the current state of the art for nitrosamine analysis regarding sensitivity, selectivity, economy, and ease of operation. Furthermore, the research aims to form the basis for an on-site or mobile technique for analyzing volatile nitrosamines in the relevant industries.

In 2022, the work was largely affected by the aftermath of the flooding in Rheinbach in July 2021. Nonetheless, some of the research goals for that year could be achieved. The focus was on developing three different analysis methods on the three IMS instruments available for the research: a GC-drift tube IMS with a tritium ion source, a GC-drift tube IMS with an X-ray ion source, and a GC-field asymmetric IMS equipped with a ^{63}Ni ion source. These three systems are coupled to different sample preparation techniques, for which methods were also developed.

Another aim was the generation of calibration gas standards for the different nitrosamines to facilitate the enrichment of the analytes from the gas phase onto sorbent-packed (thermal desorption, TD) tubes. This task was performed using a calibration gas generator system based on the principle of permeation of the analyte molecules through a permeable material like polyethylene into a gas stream.

The results show that it is possible to detect, separate and identify nine nitrosamines relevant to occupational safety in approximately 10 minutes on each of the different analysis systems using the developed GC-IMS methods. Furthermore, it became clear that the drift tube IMS facilitates a much more selective analysis, as each nitrosamine shows distinct and characteristic drift times for the ions it produces. In contrast, the compensation voltages measured in the field asymmetric IMS for the nitrosamines were more comparable.

Within the framework of two BSc and one MSc theses, the sample preparation techniques solid phase microextraction (SPME), liquid injection, large volume injection (LVI), TD, headspace (HS), and in-tube extraction (ITEX) were or are being evaluated regarding highest enrichment factor/best sensitivity and compared among each other. The results of the MSc practical work are given in Figure 1, comparing instrument detection limits (IDLs) as the mean of all nine nitrosamines, between techniques, with TD and LVI recording the lowest IDLs for specific analytes.

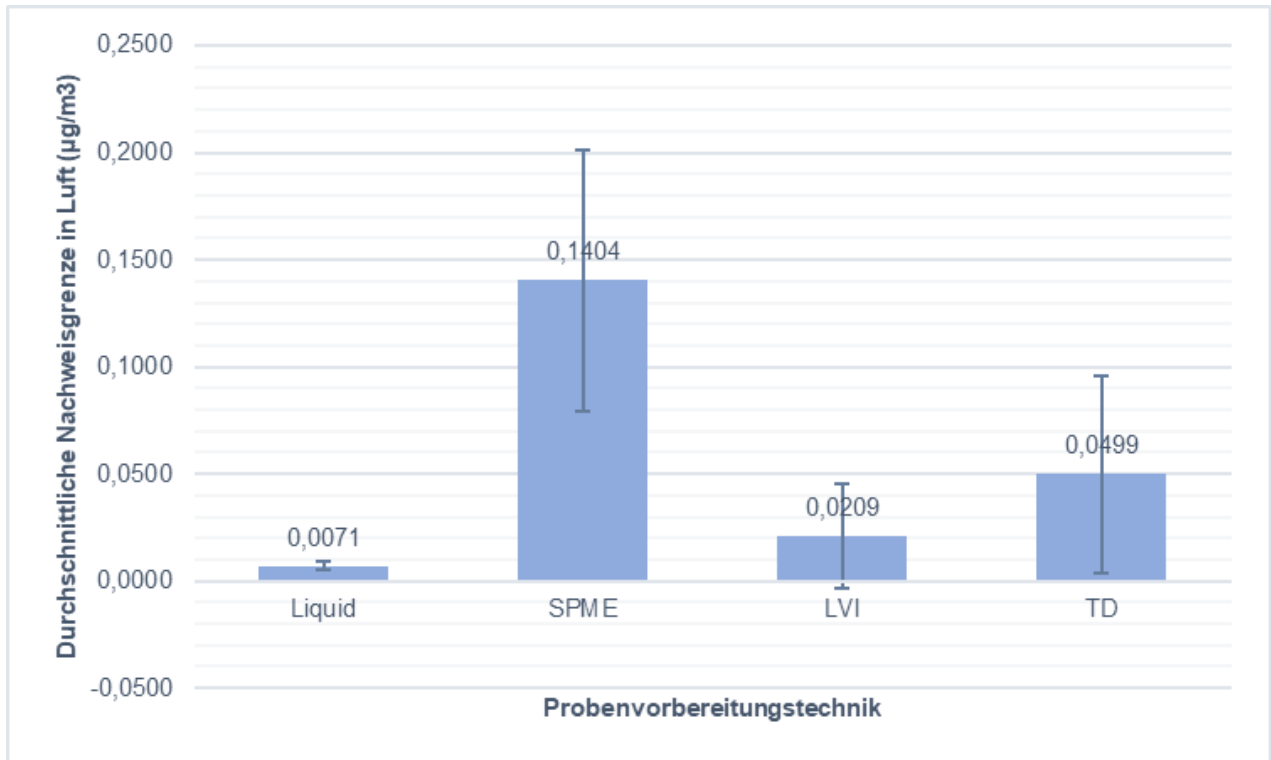


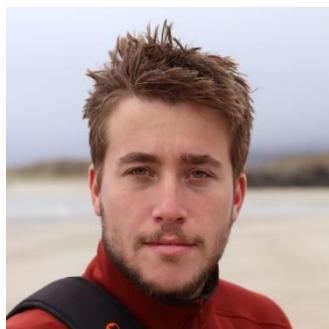
Figure 1: Comparison of four sample preparation techniques (liquid injection, solid phase microextraction, large volume injection, and thermal desorption) in terms of instrument detection limit, given as nitrosamine concentration in air, at a sample volume of 400 L (and an elution volume of 2 mL).

Gas standards of the nitrosamines NDMA, NMEA, NPIP, and NDBA were generated for approximately two months, resulting in stable permeation rates and gas concentrations in the $\mu\text{g}/\text{m}^3$ range, with NDBA showing the strongest permeation. These values were achieved at a temperature in the permeation chamber of 35 °C at a total gas flow of 1.25 L/min.

Current goals for the upcoming research include determining the limits of detection and quantification for the headspace and ITEX sample preparation methods to compare them to the other evaluated techniques. The TD technique must be further developed, and different sorbents must be compared to avoid the formation of nitrosamine artifacts. Sampling techniques must be implemented, and the most suitable method for analyzing nitrosamines in air at the workplace must be determined to begin with the validation procedure. The aim is to complete these steps within the current year, 2023.

Theses completed in 2022

Ph.D. Thesis



21.01.2022

Oliver Höcker

"Nanoflow Interfacing for High Sensitivity CE-MS Coupling: Technical Development for Trace Analysis and Non-Targeted Metabolomics"

Summary

Capillary electrophoresis coupled with mass spectrometry (CE-MS) is a powerful technique in many fields of analytical chemistry, especially for separating charged molecules. However, the widespread standard sheath liquid interface lacks sensitivity which is why many studies and inventions have attempted improvement. Based upon two novel principles, a porous tip interface and a nanoflow sheath liquid interface were developed to systematically study their performance compared to the standard sheath liquid interface. Both nanoflow interfaces showed similar improvements in the sensitivity of 13 to 114 times over the standard interface for organic acids, peptides, and monoclonal antibodies. Furthermore, the nanoflow sheath liquid interface demonstrated higher versatility and easier manufacturing than the sheathless porous tip approach in these experiments. Therefore, it was chosen for further technical improvement and application for trace analysis of drinking water and non-targeted metabolomics analysis.

The characterization of its electrical current flows and resistances disproved the misconception that electroosmosis is the main driving force for the sheath liquid flow, as found in the literature. Improvements in handling and robustness were achieved by introducing a second capillary into the emitter for sheath liquid supply with a switching function for both capillaries. The resulting valve mechanism enabled a conditioning mode and separation mode. By this means, not only emitter lifetime and usability were strongly improved, but also unique functions added, such as a divert to waste function for exclusion of MS interfering matrix components, online preconditioning with MS incompatible cleaning/coating agents, and the potential of online capillary isoelectric focusing with MS detection (CIEF-MS). This two-capillary nanoflow sheath liquid interface prototype was then applied for enrichment-free trace analysis and quantification of anionic micropollutants in drinking water. A CE-Orbitrap method with nanoflow interfacing was developed to quantify halogenated acetic acids down to the ng/L range, which is required to meet the strict WHO Guidelines for Drinking Water Quality.

Seven drinking water samples from various production plants in Germany were analyzed. The quantitative results (0.1 to 6.2 µg/L) were verified by a validated liquid chromatography-MS

(LC-MS) method, which emphasizes the strength of CE-MS as an alternative technique for analyzing highly polar and ionic compounds in water. A subsequent suspect screening indicated the presence of halogenated methane sulfonic acids, which were identified and quantified by standard compounds (0.2 to 2.6 $\mu\text{g/L}$). Reviewing the data, a screening revealed around 20 additional anionic suspects, such as sweeteners, organic sulfonates, sulfates, and inorganic ions, which shows the perspective for non-targeted analysis and discovery of contaminants. Non-targeted screening can be used as an exploratory tool in many fields of application. In this context, a workflow for discovering metabolites by LC- and CE-MS in bioreactors was implemented. Substrate samples of biogas plants for methane production were analyzed to uncover the differences in metabolite concentration in varying process conditions.

This work evaluated the influence of different separation techniques, mass spectrometer instruments, and data processing software on the outcome of a non-targeted analysis. The samples were separated by both capillary zone electrophoresis (CZE), and reversed-phase LC (RPLC) coupled to time-of-flight (TOF) and Orbitrap mass spectrometers. The non-targeted data were processed with mzMine and XCMS, and the resulting features were prioritized by partial least square regression (PLSR), which enabled the distinction between high and low gas yield reactor conditions with ranking by Variable Importance in Projection (VIP). As expected, RPLC-MS and CZE-MS delivered complementary information but also a good correlation between 10% of the commonly detected features regarding fold change and importance for the PLSR model. Unexpectedly, big differences between data sets were observed between TOF and Orbitrap (<50% common features), which suggest a significant influence on the discovery of biomarkers if different MS instrumentation is used. Between MZmine and XCMS, significant differences in the total number of features were found (<57% common features), despite having a good overlap for features that were prioritized by the VIP ranking (up to 95% common features). This indicates a comparable performance for finding true positive features but highlights the drawbacks of automated data processing tools, which generate high numbers of false positive features. This work underlined the high complexity of non-targeted workflows, and it was clearly shown that different approaches and slight variations could strongly impact the outcome.

Overall, next-generation nanoflow electrospray interfaces for CE-MS coupling offer a strong potential to establish new fields of application by combining its strength for separating ionic compounds with high-sensitivity detection. However, automation, affordable instrument parts, and broad instrument compatibility are essential to stimulate broader CE-MS use further. Hopefully, this thesis supports CE-MS as a technique on its way to becoming a more widely accepted technique next to chromatography.

Ph.D. Thesis



15.06.2022

Jens Terhalle

"Investigation of transformation reactions of phenolic compounds by oxidative processes in aqueous systems"

Summary

Ozone (O_3) and chlorine dioxide (ClO_2) have been used as a disinfectant for a long time, and their use in trace organic compound abatement in water treatment has recently been suggested. Phenolic moieties in trace organic compounds (TrOCs) and dissolved organic matter are the main reaction sites for both oxidative agents. The mechanistic understanding of phenolic compound transformation may help to predict oxidant depletion, secondary oxidant, and transformation products (TPs) formation. Therefore, the reaction of phenolic compounds with ClO_2 and O_3 was investigated. A new concept for the indirect determination of hypochlorous acid (HOCl) in the reaction of phenol with ClO_2 by 2- and 4-bromophenol was developed. The reaction formed $62 \pm 4 \%$ chlorite and $42 \pm 3 \%$ HOCl per ClO_2 consumed. Adding ClO_2 to real wastewater ($5 \times 10^{-5} \text{ M } ClO_2$) resulted in the transformation of 40 % atenolol and 47 % metoprolol (TrOCs), while the selective HOCl scavenger, glycine, largely diminished their transformation. This indicates that the reaction with HOCl transformed both compounds (e.g., $k(\text{atenolol} + \text{HOCl}) = 3.5 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$), formed in reactions of ClO_2 with the wastewater matrix.

During the investigation of the ozonation of phenolic compounds, the amount of O_3 to degrade one mole of compound (stoichiometric ratio) increased with increasing pH for phenol, 4-methyl phenol, and 4-methoxy phenol. On the other hand, in the case of 4-chlorophenol, the stoichiometric ratio of O_3 decreased with increasing pH, which was explained by the formation of organic TPs. However, the increase in the stoichiometric ratio of O_3 in the case of phenol and activated phenols could be explained by the formation of highly reactive superoxide, which strongly contributes to O_3 depletion.

The results of the reverse order dosage experiments contradict previous studies suggesting that formed organic products are responsible for enhanced O_3 amount. In the additional investigation by compound-specific stable isotope analysis (CSIA), a dependence of the reaction rate constant to carbon isotope fractionation was observed. The fractionation strongly depends on the phenol speciation. With decreasing pH values and reaction rates $< 10^5 \text{ M}^{-1} \text{ s}^{-1}$, the isotope enrichment factor ϵ increases (ϵ is between -5.2 and -1.0 ‰).

For faster reactions ($>10^5 \text{ M}^{-1} \text{ s}^{-1}$), the carbon isotope enrichment was not significant anymore (ϵ is between -1.0 and 0 ‰). Based on these data, we propose correlating isotope enrichment factors with kinetic data for aromatic compounds. In conclusion, this work confirmed the postulated mechanism of ClO_2 with phenol and found an influence of HOCl on compound transformation. Additionally, the high stoichiometry of O_3 in the reaction with phenol could not be explained. However, prior assumptions could be refuted, and new starting points (e.g., investigation of superoxide) could be found. Finally, the correlation of isotope enrichment factors with reaction rate constants supported the use of CSIA in investigating oxidative reactions. This thesis shows fundamental aspects for further studies of compounds with other functional groups in ClO_2 application and for using CSIA in oxidation reactions.

Ph.D. Thesis



13.09.2022

Sarah Maria Klaes

"Development of an analytical method for the examination of steel sheet using flow-cell ICP-OES in the context of laboratory digitisation"

Summary

The focus of this dissertation is developing a new method for analyzing hot-dip galvanized steel sheets, which enables complete automation of the analysis. One focus of this work was the development of a flow cell using a 3D printing process that allows the continuous detachment of the coating with diluted HCl acid.

The coupling of the flow cell with ICP-OES and the method development of the analysis procedure followed this. First, it was essential to find interference-free analysis lines for the elements to be investigated that cover the required calibration range with the corresponding determination limit.

The coupling of ICP-OES and flow cell with subsequent validation for the investigation of Z and ZM material has shown that reproducible coating mass and composition results can be determined with the method. In addition, the continuous detachment with parallel measurement of the resting potential and transient ICP-OES measurement allows a deeper insight into the coating structure than the wet-chemical method. In the quantitative evaluation, determining the Fe content above the limit of quantification as a criterion for automatic evaluation posed a problem, as detachment of the base material occurred with an increasing Fe content. This could be prevented by using methenamine as an inhibitor so that the

evaluation of the Fe content was also possible automatically over the determination limit. Due to this, the analysis procedure was optimized with the help of methenamine as an inhibitor so that the detachment of the base material was prevented and an automated evaluation of all coating components could be implemented. In addition, it was shown that using the inhibitor can shorten the measurement time. Comparing the results from the FC-ICP-OES method with the results of the reference measurements from the wet chemical detachments and the GD-OES measurements could confirm the correctness of the measurement results. Thus, the validation results of the FC-ICP-OES and the wet-chemical overlay investigation resulted in a recovery rate of 99 % for the overlaying mass of Z material and a recovery rate of 98 % for the overlaying mass of ZM material. When comparing the FC-ICP-OES results with the determined layer thicknesses of the GD-OES measurement, a recovery rate of 103 % for the layer thickness of the Z material and a recovery rate of 102 % for the layer thickness of the ZM material was obtained.

The final automation was realized with a cobot. For this purpose, the manual FC-ICP-OES method was first divided into individual steps to design the sequences in a workspace for the cobot so that the cobot can carry them out. In this way, it is possible to realize an automated analysis procedure for examining hot-dip galvanized steel sheets and use it in routine analysis.

Ph.D. Thesis



17.11.2022

Lotta Hohrenk-Danzouma

"Data processing strategies for LC-HRMS based non-target analysis of organic micropollutants in aqueous matrices"

Summary

Many organic micropollutants (OMPs) are introduced into the aquatic environment and raise concerns due to their potential impact on ecosystems and human health. The high sensitivity and selectivity of liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) enable to screen a broad range of OMPs at trace concentrations without restriction on predefined analytes. Thus, LC-HRMS-based non-target screening (NTS) approaches are increasingly crucial in water analysis as they provide the potential to identify formerly unknown compounds and obtain a more comprehensive overview of pollution loads. However, with NTS, large amounts of data are recorded within each measurement, making sophisticated data processing strategies necessary. The first task of a data processing workflow is a reliable extraction of analyte signals, so-called features, from raw data. After this step, complex

datasets with thousands of features are obtained. Subsequently, it is essential to reduce and prioritize features that are relevant to the studied research question. This thesis addresses several aspects of data processing strategies, focusing on feature extraction and feature prioritization steps based on multivariate chemometric methods.

Nevertheless, high-quality measurement data are essential for the following data processing. A generic qualitative screening method was developed for an LC-HRMS analytical system. The sensitivity and selectivity to detect a broad range of OMPs at environmentally relevant concentrations and the stability of peak areas and retention times, enabling the comparison of several samples, were confirmed. On this basis, the importance of the feature extraction step was emphasized by first identifying weaknesses in the consistency of results obtained from different programs and presenting an alternative chemometric-based approach.

The comparability of feature extraction with four commonly used open-source and commercial software tools was investigated by examining the overlap of feature lists obtained from processing the same raw data set with MZmine2, enviMass, Compound Discoverer, and XCMS online. Results show a low coherence between different processing tools, as the features overlap between all four programs was around 10%, and for each software, between 40% and 55% of features did not match with any other program. The deviating implementation of filtering steps, such as replicate- and blank filters, was identified as one source of observed discrepancies. This comparison showed the need for higher robustness of data processing tools, a better understanding of algorithms, and the influence of different parameter settings for each approach. Even though a general standardization of feature extraction is not feasible, a higher awareness of the impact of this step and a transparent and detailed reporting of the entire data processing workflow was encouraged with this work.

In addition, an alternative chemometric feature extraction procedure based on regions of interest (ROI) and multivariate curve resolution alternating least squares (MCR-ALS) was employed on an NTS dataset of water samples for the first time. This approach circumvents several error-prone processing steps as there is no need for chromatographic alignment or grouping of multiple features of the same analyte. The approach was employed on samples with different complexity, including a target data set of spiked drinking water samples and an NTS dataset obtained from different steps of a waste-water treatment plant and upstream of the receiving river. For all samples, chromatographic peaks and the corresponding mass spectra of OMPs were fully resolved in the presence of highly co-eluting irrelevant and interfering peaks. In the next step, features discriminating between several sample classes of the NTS data set were prioritized based on several multivariate and univariate chemometric methods. By that, from 101 resolved features (MCR-ALS components), 24 were selected and tentatively identified.

Subsequently, the benefits of feature prioritization based on complementary unsupervised and supervised pattern recognition methods were further examined. A comprehensive

chemometric-based data processing workflow was employed on a dataset influenced by seasonal and spatial trends to reveal hidden data patterns and to find a subset of discriminating features between samples. Samples were obtained from a passive sampler monitoring campaign of three small streams and one major river over four sampling periods. After employing unsupervised explorative chemometric tools to obtain a general overview of samples, ANOVA simultaneous component analysis (ASCA) was used to disentangle the influence of spatial and seasonal effects and their interaction. A target and non-target dataset were compared and showed a dominant influence of different sampling locations and individual temporal pollution patterns for each river. With the limited target analytes, general seasonal pollution patterns were apparent, but NTS data provide a more holistic view of site-specific pollutant loads. With a complementary partial least squares-discriminant analysis (PLS-DA) and a Volcano-based prioritization strategy, 223 sites and 45 season-specific features were selected and tentatively identified.

Overall, this thesis demonstrates that data processing is crucial in NTS to obtain meaningful results for comprehensive environmental monitoring. Furthermore, for feature extraction and prioritization, the remaining challenges and the capabilities of implementing advanced multivariate chemometric tools to exploit the potential of NTS fully were highlighted.

Master Theses

Carmen Maria Babel nee Samol

“Electrochemical processes of anions on carbon electrodes in aqueous solutions”

Martin Brüßler

"Formation of N-Nitrosamines during ozonation and removal by biological post-treatment"
(at IUTA, Host supervisor: Dr. Jochen Türk)

Felix Drees

“Investigation of the degradation of polyphosphonates by compound-specific stable carbon isotope analysis coupled with high-resolution mass spectrometry: kinetic isotope effects and degradation products”

Katharina Hellmann

“Development of a TED-GC-MS method for the extension of moss monitoring by the parameter microplastic for the determination of atmospheric deposition”

Michael Leupold

"Influence of water matrix components on the ozonation of purines, archetypes of nitrogen-containing pollutants"

Sarah Rockel

“Photolysis of Aminotris(methylenephosphonic acid) (ATMP) - Investigation of the influence of pH-dependent speciation on degradation mechanism and isotopic fractionation”

Rafael Rosner

„Automatisierte Peakdetektion und -charakterisierung für verschiedene hochauflösende Massenspektrometersysteme“

Philipp Swiderski

“The degradation of micropollutants by ozone in reverse osmosis concentrates.”

Christian Seuken

“Temporal dynamics of Microplastics $\geq 10 \mu\text{m}$ in the effluent of a wastewater treatment plant”
(at TZW Karlsruhe, Host supervisor: Dr. Nicole Zumbülte)

Bachelor Theses

Gözde Ergun

„Analytische Charakterisierung von Wasserkreisläufen nach Einsatz von Kalkprodukten bei der Papierherstellung“

Daniel Höhn

„Postprozessierung und komparative Analyse von Featurelisten generiert durch Non-Target-Screening mittels HPLC-HRMS“

Björn Lang

„Etablierung eines Interfaces zwischen der instrumentellen und der wirkungsbezogenen Analytik“

(at IUTA, Host supervisor: Dr. Thorsten Teutenberg)

Jana Lieske-Overgrand

„Optimierung einer in situ-Derivatisierung mit deuteriertem Methanol und GC-MS/MS Methode zur Analyse von Fettsäuren aus wässrigen Proben“

Anke Schulz

„Untersuchung der Reaktionskinetik von Aminylradikalen mittels Laserblitzlichtphotolyse“

Publications

1. A. Mohammadi, S. Dobaradaran, T. C. Schmidt, M. Malakootian, J. Spitz: Emerging contaminants migration from pipes used in drinking water distribution systems: a review of the scientific literature
Environ. Sci. Pollut. Res. **29** (2022), 75134-75160
DOI: 10.1007/s11356-022-23085-7
2. M. Wenzel, B. Fischer, G. Renner, J. Schoettl, C. Wolf, J. Schram, T. C. Schmidt, J. Tuerk: Efficient and sustainable microplastics analysis for environmental samples using flotation for sample pre-treatment
Green Anal. Chem. **3** (2022), 100044
DOI: 10.1016/j.greeac.2022.100044
3. G. Sieber, B. Freudenberg, L. Netzel, T. C. Schmidt, F. Brandenstein: The Premise of Interdisciplinarity and Its Actual Absence—A Bibliometric Analysis of Publications on Heavy Rainfall
Water **14** (2022), 3001
DOI: 10.3390/w14193001
4. L. M. H. Reinders, D. Noelle, M. D. Klassen, M. Jaeger, T. C. Schmidt, J. Tuerk, T. Teutenberg: Development and validation of a method for airborne monoclonal antibodies to quantify workplace exposure
J. Pharm. Biomed. Anal. **221** (2022), 112046
DOI: 10.1016/j.jpba.2022.115046
5. M. S. Abdighahroudi, X. A. M. Mutke, M. Jütte, K. Klein, T. C. Schmidt, H. V. Lutze: Reaction of Chlorine Dioxide with Saturated Nitrogen-Containing Heterocycles and Comparison with the Micropollutant Behavior in a Real Water Matrix
Environ. Sci. Technol. **56** (2022), 11589–11601
DOI: 10.1021/acs.est.1c08381
6. L. M. H. Reinders, M. D. Klassen, T. Teutenberg, M. Jaeger, T. C. Schmidt: Comparison of originator and biosimilar monoclonal antibodies using HRMS, Fc affinity chromatography and 2D-HPLC
Anal. Bioanal. Chem. **414** (2022), 6761–6769
DOI: 10.1007/s00216-022-04236-8
7. M. Reuschenbach, L. L. Hohrenk-Danzouma, T. C. Schmidt, G. Renner: Development of a Scoring Parameter to Characterize Data Quality of Centroids in High-Resolution Mass Spectra
Anal. Bioanal. Chem. **414** (2022), 6635–6645
DOI: 10.1007/s00216-022-04224-y
8. L. K. Tintrop, M. A. Jochmann, T. Beesley, M. Küppers, R. Brunstermann, T. C. Schmidt: Optimization and automation of rapid and selective analysis of fatty acid methyl esters from aqueous samples by headspace SPME arrow extraction followed by GC-MS/MS analysis
Anal. Bioanal. Chem. **414** (2022), 6473–6483
DOI: 10.1007/s00216-022-04204-2
9. T. Werres, T. C. Schmidt, T. Teutenberg: Peak broadening caused by using different micro liquid chromatography detectors
Anal. Bioanal. Chem. **414** (2022), 6107–6114
DOI: 10.1007/s00216-022-04170-9

10. V. I. Merkus, C. Sommer, E. Smollich, B. Sures, T. C. Schmidt*:
Acute ecotoxicological effects on daphnids and green algae caused by the ozonation of ibuprofen
Sci. Tot. Environ. **847** (2022), 157611
DOI: 10.1016/j.scitotenv.2022.157611
11. T. Hesse, M. Nachev, S. Khaliq, M. A. Jochmann, F. Franke, J. P. Scharsack, J. Kurtz, B. Sures, T. C. Schmidt:
Insights into amino acid fractionation and incorporation by compound-specific carbon isotope analysis of three-spined sticklebacks
Sci. Rep. **12** (2022), 11690
DOI: 10.1038/s41598-022-15704-7
12. N. Baetz, T. C. Schmidt, J. Tuerk:
High-Performance Thin-Layer Chromatography in Combination with an Acetylcholinesterase Inhibition Bioassay with Pre-Oxidation of Organothiophosphates to Determine Neurotoxic Effects in Storm-, Waste-, and Surface water
Anal. Bioanal. Chem. **414** (2022), 4167–4178
DOI: 10.1007/s00216-022-04068-6
13. W. Kaziur-Cegla, M. A. Jochmann, K. Molt, A. Bruchmann, T. C. Schmidt:
In-tube dynamic extraction for analysis of volatile organic compounds in honey samples
Food Chem.: X **14** (2022), 100337
DOI: 10.1016/j.fochx.2022.100337
14. L. L. Hohrenk-Danzouma, M. Vosough*, V. I. Merkus, F. Drees T. C. Schmidt*:
Non-target analysis and chemometric evaluation of a passive sampler monitoring of small streams
Environ. Sci. Technol. **56** (2022), 5466-5477
DOI: 10.1021/acs.est.1c08014
15. M. S. M. Al-Azzawi, M. Funck; M. Kunaschk, E. von der Esch, O. Jacob, K. P. Freier, T. C. Schmidt, M. Elsner, N. P. Ivleva, J. Tuerk, O. Knoop, J. E. Drewes:
Microplastic sampling from wastewater treatment plant effluents: Best-practices and synergies between thermoanalytical and spectroscopic analysis
Water Res. **219** (2022), 118549
DOI: 10.1016/j.watres.2022.118549
16. S. Dobaradaran, X. A. M. Mutke, T. C. Schmid, P. Swiderski, G. E. De-la-Torre, M. A. Jochmann: Aromatic amines contents of cigarette butts: Fresh and aged cigarette butts vs unsmoked cigarette
Chemosphere **301** (2022), 134735
DOI: 10.1016/j.chemosphere.2022.134735
17. C. Thoben, T. Werres, I. Henning, P. R. Simon, S. Zimmermann, T. C. Schmidt, T. Teutenberg: Towards a miniaturized on-site nano-high performance liquid chromatography electrospray ionization ion mobility spectrometer with online enrichment
Green Anal. Chem. **1** (2022) 100011
DOI: 10.1016/j.greeac.2022.100011
18. A. R. Ziefuß, T. Hupfeld, S. W. Meckelmann, M. Meyer, O. J. Schmitz, W. Kaziur-Cegla, L. K. Tintrop, T. C. Schmidt, B. Gökce, S. Barcikowski:
Ultrafast cold-brewing of coffee by picosecond-pulsed laser extraction
npj Science of Food **19** (2022), 1-9
DOI: 10.1038/s41538-022-00134-6

19. G. Sigmund, H. P. H. Arp, B. M. Aumeier, T. D. Bucheli, B. Chefetz, W. Chen, S. T. J. Droge, S. Endo, B. I. Escher, S. E. Hale, T. Hofmann, J. Pignatello, T. Reemtsma, T. C. Schmidt, C. D. Schönsee, M. Scheringer:
Sorption and Mobility of Charged Organic Compounds: How to Confront and Overcome Limitations in Their Assessment
Environ. Sci. Technol. **56** (2022), 4702-4710
DOI: 10.1021/acs.est.2c00570
20. S. H. Schäfer, K. van Dyk, J. Warmer, T. C. Schmidt, P. Kaul:
A new sensor-based setup for the measurement of total organic carbon in ultrapure water systems
Sensors **22** (2022), 2004
DOI: 10.3390/s22052004
21. C. Kim, T. C. Schmidt, H. V. Lutze:
Oxidation of bromide by heat-activated persulfate – Effects of temperature and the organic matter surrogate phenol on kinetics and stoichiometry
Chem. Eng. J. (2022), 133533
DOI: 10.1016/j.cej.2021.133533
22. R. G. H. Marks, M. A. Jochmann*, W. A. Brand, T. C. Schmidt*:
How to Couple LC-IRMS with HRMS - A Proof-of-Concept Study
Anal. Chem. **94** (2022), 2981–2987
DOI: 10.1021/acs.analchem.1c05226
23. A. Asghar, H. V. Lutze, J. Tuerk, T. C. Schmidt:
Influence of Water Matrix on the Degradation of Organic Micropollutants by Ozone based Processes: A Review on Oxidant Scavenging Mechanism
J. Hazard. Mat. **429** (2022), 128189
DOI: 10.1016/j.jhazmat.2021.128189
24. V. Hinnenkamp, P. Balsaa, T. C. Schmidt*:
Target, suspect and non-target screening analysis from wastewater treatment plant effluents to drinking water by using collision cross section values as additional identification criterion
Anal. Bioanal. Chem. **414** (2022), 425–438
DOI: 10.1007/s00216-021-03263-1
25. T. Bornemann, P. Adam, V. Turzynski, P. A. Figueroa-Gonzalez, J. Rahlff, U. Schreiber, D. Koester, T. C. Schmidt, R. Schunk, B. Krauthausen, A. Probst:
Genetic diversity in terrestrial subsurface ecosystems impacted by geological degassing
Nature Comm. **13** (2022), 284-294
26. V. Wirzberger, V. I. Merkus, M. Klein, L. L. Hohrenk-Danzouma, H. V. Lutze, T. C. Schmidt*:
Bromide strongly influences the formation of reaction products during the ozonation of diclofenac, metoprolol and isoproturon
Sci. Tot. Environ. **815** (2022), 152427
DOI: 10.1016/j.scitotenv.2021.152427
27. J. Terhalle, S. E. Nikutta, D. L. Krzeczesa, H. V. Lutze*, M. A. Jochmann, T. C. Schmidt*:
Linking reaction rate constants and isotope fractionation of ozonation reactions using phenols as probes
Water Res. **210** (2022), 117931
DOI: 10.1016/j.watres.2021.117931

28. F. Soleimani, S. Dobaradaran, G. E. De-la-Torre, T. C. Schmidt, R. Saeedi:
Content of toxic components of cigarette, cigarette smoke vs cigarette butts: A
comprehensive systematic review
Sci. Tot. Environ. **813** (2022), 152667
DOI: 10.1016/j.scitotenv.2021.152667
29. M. Hammad, B. Alkan, A. K. Al-kamal, C. Kim, D. Klippert, T. C. Schmidt, C. W. M. Kay,
H. Wiggers: Enhanced heterogeneous activation of peroxymonosulfate by Ruddlesden-
Popper-type $\text{La}_2\text{CoO}_4+\delta$ nanoparticles for bisphenol A degradation
Chem. Eng. J. **429** (2022), 131447
DOI: 10.1016/j.cej.2021.131447
30. T. Koehler, J. Wingender, M. Lueling, S. Meckelmann, U. Telgheder, O. Schmitz:
Characterization of the extracellular volatile metabolome of *Pseudomonas aeruginosa*
applying an in vitro biofilm model under cystic fibrosis-like conditions
Frontiers in Bioscience-Landmark **27(5)** (2022), 156
DOI:10.31083/j.fbl2705156
31. S. Joksimoski, K. Kerpen, U. Telgheder:
Atmospheric pressure photoionization - High-field asymmetric ion mobility spectrometry
(APPI-FAIMS) studies for on-site monitoring of aromatic volatile organic compounds
(VOCs) in groundwater
Talanta **247** (2022), 123555
DOI:10.1016/j.talanta.2022.123555
32. A. L. R. M. Augustini, S. Sielemann, U. Telgheder:
Quantitation of Flavor Compounds in Refill Solutions for Electronic Cigarettes Using HS-
GCxIMS and Internal Standards
Molecules **27** (2022), 8067
DOI:10.3390/molecules27228067
33. P. R. Martin, D. Buchner, M. A. Jochmann, M. Elsner, S. B. Haderlein:
Two Pathways Compete in the Mn(II)-Catalyzed Oxidation of Aminotris(methylene
Phosphonate (ATMP)
Environ. Sci. Technol. **56** (2022), 4091-4100
DOI: 10.1021/acs.est.1c06407

Invited Lectures

T. C. Schmidt, L. Hohrenk-Danzouma, V. I. Merkus, F. Drees, M. Vosough:

Comprehensive Analysis of Organic Micropollutants in Water combining Passive Sampling, Non-Target Screening, and Advanced Chemometrics

virtual@6th International and 25th National Conference on Environmental Health, Ahvaz, December 22, 2022 (invited)

T. C. Schmidt, L. K. Tintrop, T. Werres, C. Thoben, S. Zimmermann, T. Teutenberg, M. A. Jochmann, A. Salemi:

Greening Sample Preparation by Miniaturization and Automation: Examples from GC and LC Analysis

XXIV International Symposium on Advances in Extraction Technologies (XXIV-ExTech) and the XV National Meeting of Analytical and Environmental Chemistry (XV-EQAA,) Iquique, Chile, October 19, 2022 (Plenary Lecture)

T. C. Schmidt, L. K. Tintrop, N. Lorenzo-Parodi, W. Kaziur-Cegla, N. Stojanović, A. Salemi, M. A. Jochmann:

Solventless Microextraction Techniques for Water Analysis

2nd European Sample Preparation e-Conference, March 14, 2022 (invited)

Conferences and Meetings

5. Mülheimer Wasseranalytisches Seminar (MWAS 2022)



The 5th Mülheimer Wasseranalytisches Seminar (MWAS 2022) was a highly successful event that brought together a diverse group of professionals involved in water analysis. The IWW organized the seminar and received support from IAC, who was part of the organization team.

Over 200 participants representing various backgrounds, including academic researchers, industry professionals, water suppliers, and measurement instrument manufacturers, attended the event. The attendees were treated to a series of excellent and exciting talks and posters that sparked lively discussions.

Kjell Kochale represented the IAC (external Ph.D. at IUTA) and gave a talk on Solutions for Laboratory Automation. IAC members also presented several scientific posters, two of which were awarded poster prizes (to Katharina Klein and Max Reuschenbach). Congratulations once again to both of them for their achievements.

In addition to the engaging talks and posters, the event also provided an excellent opportunity for networking and exchanging ideas with other professionals in the field. Overall, the 5th MWAS was a well-organized and successful event enjoyed by all who attended.

Looking forward to the next MWAS, we are already excited to meet in Mülheim and continue the discussions and exchange of ideas in the field of water analysis.

Ruhr-Rhein-Main Meeting at BfG (Koblenz)

2022-12-19 – 2022-12-20

The annual Ruhr-Rhein-Main (RRM) meeting was a resounding success, with research friends from the Technical University Darmstadt (AK Prof. Holger Lutze), the Bundesanstalt für Gewässerkunde (AK Prof. Thomas Ternes), and IUTA (AK Jochen Türk / Thorsten Teutenberg) in attendance. The meeting took place in Koblenz and brought together a diverse range of research topics, all of which fit under the umbrella of water chemistry and analytics.



The talks were of a high standard, with lively discussions afterward, and topics ranged from non-target screening to microplastics to oxidation processes, providing valuable insight and opportunities for collaboration. The groups' exchange of ideas and knowledge was the highlight of the meeting, and everyone was eager to learn more about each other's work.

On the evening before the meeting began, we took a trip to the Koblenz Christmas market, adding a touch of festive spirit to the occasion.

We at IAC are already looking forward to the next meeting in 2023, which will take place in Darmstadt. We are excited to continue the dialogue, exchange ideas and collaborate on new projects to drive the water analytics field forward. The annual meetings provide a platform for our researchers to come together, share their latest findings, and work together to find solutions to the most pressing challenges.

Talks:

- Non-Target Screening Vs. Human Factor: Challenges of Comparing Data
- Normal, Oder? – NTS zur Ermittlung nicht-kontinuierlicher, ungewöhnlicher und spezifischer Einleitung in die Oder
- Entwicklung einer NTS Methode zur Detektion von apolaren Substanzen in Schwebstoffen
- Overarching concept and framework of streamFind: Flexible data analysis and workflow designer to identify chemicals in the water cycle
- Quantification of polyvinyl chloride microplastic via pressurized liquid extraction and combustion ion chromatography
- Reaction of chlorine dioxide with phenolic compounds – Intrinsic formation of free chlorine
- Determination of Singlet Oxygen via photoluminescence
- Bromatbildung bei der Ozonung und Untersuchung alternativer Ozoneintragsysteme unter Berücksichtigung der Spurenstoffelimination
- Fate of biocide runoff from building materials: ecological risks and on-site treatment options
- Mechanistische Studien über die Inhibierung der Biofilmbildung mittels CeO₂-Nanokristallen als Haloperoxidase-Analoga

Teaching

At IAC, we are involved in teaching mostly 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). Unfortunately, excursions could still not be offered due to ongoing Corona restrictions, but we hope to be able to organize them again in 2023.

Summer term

Lecture and Tutorial "Water Chemistry" (*B.Sc. Water Science, in German*)

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*)

Individual Practical Projects "Analytical Chemistry" (*M.Sc. Water Science, in English*)

Miscellaneous



Noémie Schulte was born on March 29, 2022.



Naeem
On May 11, 2022, the Hohenk-Danzouma family had an offspring.