UNIVERSITÄT
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Open-Minded

2021

Jahresbericht

Annual Report

Content

Instrumental Analytical Chemistry

Dear friends and colleagues,

Last year I expressed my hope to see a quick relief from the Corona pandemic in 2021. But, unfortunately, you all know that this did not occur, and nobody yet truly knows when we will be able to return to a more normal situation. Nevertheless, we at IAC have faced the challenges of this special time with confidence, and we are pleased to give you an overview of our activities in 2021 with this annual report.

Over the year, we have improved the quality of video-based meetings that, without dissent, have their advantages in some cases, particularly to replace long travels for short meetings. We also managed to improve digital formats in teaching further but welcomed a return to teaching in presence at least for a while this winter term as much as most students. Luckily, our practical courses could almost unaffectedly take place with the established hygiene and safety concepts. I have to thank again my fabulous team at IAC that helped me master all the additional challenges posed by the pandemic.
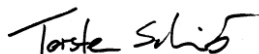
In 2021 almost all conferences and meetings had to be cancelled or transferred to mere online meetings. This is for sure no full replacement for exchanging ideas and developing networks among researchers. Beyond science, we are also social beings who need personal interactions, including a drink at the bar to chat over. Our virtual water chemistry conference in May 2021 was a success in terms of the number of participants and quality of presentations but still lacked exactly this most important personal exchange aspect of meetings. You can imagine that I had something else than an online conference in mind for the last water chemistry conference I chaired. For the next conferences, I wish my successor Thomas Ternes all the best. Of course, I will still be involved in the meetings and the water chemistry society in general, the more so since the board decided to elect me as honorary president. To stand next to my scientifically outstanding predecessors in the field, Martin Jekel and Fritz Frimmel is truly an honor for me.

2021 has again seen some major successes for the research profile area water research at UDE, most recently the selection of our network proposal "Water4Future – From Monitoring to Measures" for a full proposal to be submitted end of January and keeping some of us busy over Christmas vacation. Furthermore, our concept for an excellence cluster proposal, "Ecosystem Health" in 2023, has been approved by UDE and receives support in the running preparation phase, including the official establishment of a Water Graduate School at UDE. The CRC RESIST has successfully started in its initial year.

In terms of people at IAC, we first need to say farewell to Gerd Fischer, who retired end of January 2021. Due to the Corona situation, we did not even have the chance to celebrate on this occasion properly, but I wish to say thanks for the many years in which he was a cornerstone of the successful work and lately, particularly project administration at IAC. It was hard over the year to cope with the loss of his experience and knowledge, but in the end, we managed somehow with combined team efforts. In 2022 we will hopefully find a successor with new tasks, though, due to the growing need to maintain the lab infrastructure. Furthermore, finally, the hopefully long-term transfer of two previous guest scientists from Iran to UDE, Prof. Amir Salemi and Prof. Maryam Vosough (see below), took place, and we hope to continue our fruitful collaboration over the next years. Prof. Sina Dobaradaran, a regular guest scientist at UDE, received a fellowship by the Alexander-von-Humboldt foundation to continue his successful work on the environmental impacts of cigarette butts. 2021 has not seen as many Ph.D. students defending their thesis, but we will likely return to the 2020 record number in 2022 since many thesis works are almost finished and close to submission. As part of that finalizing step, many of the Ph.D. students successfully published their work, largely contributing to the final number of 21 papers (and seven more already accepted for 2022) in international journals, most of which appeared in premier journals of the field.

As usual, in 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. Finally, I wish all of you the best and success in 2022 and all of us the final relief from the Corona burden we all yearn for.

Torsten C. Schmidt

Instrumental Analytical Chemistry Group Members (2021)

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Head of Chair

Prof. Dr. Torsten C. Schmidt

Secretarial Office

Lydia Vaaßen

Regular Staff

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
Dipl.- Ing. Gerd Fischer (until 01/21)	Project Administration, IT Administration
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

Tasja Herrmann	Laboratory assistant

Research, Teaching, and Technical Assistants

Felix Drees

Simon Nikutta

Christina Sommer

Felix Niemann

Kaliyani Wickneswaran

Michelle Lüling

Ph.D. Students

Internal

Mohammad Sajjad Abdighahroudi	An investigation of Pharmaceutical and Personal Care Products (PPCPs) as potential precursors for Nitrogenous Disinfection Byproduct (N-DBPs)
Tobias Hesse	Liquid chromatographic methods for stable isotope analysis
Lotta Hohrenk-Danzouma	Suspect and non-target screening of diffuse immissions into aquatic systems
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
Seyed Mohammad Seyed Khademi	Direct immersion SPME Arrow – Corona discharge IMS for the determination of pesticides in water samples
Nerea Lorenzo Parodi	Aromatic amines as biomarkers in human urine: Analytical method development and epidemiological studies
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	Fraktionierung stabiler Isotope während der Photolyse von Imidacloprid
Max Reuschenbach	Automatisierte Datenprozessierung und -analyse in der hochauflösenden Massenspektrometrie
Nenad Stojanovic	Development and application of advanced stable isotope methods to study compound degradation at real field sites
Jens Terhalle	Transformation processes and Isotope effects in natural and technical aqueous systems
Lucie Tintrop	Probenvorbereitung und Mikroextraktionstechniken für wässrige Proben in der GC-MS
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 Analyse organischer Spurenstoffe in Industrieabwässern
Alexander Augustini	Chemical characterization of the ingredients of electronic cigarettes and the inhaled products.
Anastasia Barion (Günter)	Disk SPE-based sensitive determination of organochlorine pesticides and polybrominated diphenyl ethers in water
Indra Bartels	Untersuchung von Transformationsprodukten und –prozessen am Beispiel von virustatisch aktiven Pharmazeutika und analytischen und ökotoxikologischen Methoden
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
Matin Funck	Development of a Sampling-Procedure allowing subsequent qualitative and quantitative Pyrolysis-GC/MS analysis for Subµ-Plastics in the Aquatic Environment
Annika Fechner	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
Oliver Höcker	Characterisation of anaerobic processes in biogas generation using non-target screening
Frank Jacobs	Development of an automated microextraction technique
Sarah Klaes	Development and optimization of an electrochemical flow cell and coupling with the multi-elemental analysis
Michelle Klein	Effect-directed analysis for monitoring and evalutation 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
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	Microfluidic characterisation of high performance liquid chromatography systems with the main emphasis on the intrinsic efficiency

Guest Scientists

Prof. Sina Dobaradaran

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 the cigarette butts into the water environments

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

Dr. Anam Asghar

Postdoctoral Research Scientist

Alexander-von-Humboldt Georg Forster

Project Title: Oxidation of Micropollutants: Synergistic effects of ozone integrated peroxymonosulfate (PMS) oxidative processes

With the research expertise in oxidative processes, the main aim of this visit is to advance my research exposure further and investigate the fundamental mechanism of oxidative wastewater treatment processes. The first phase of this project focused on the yields of oxidants (i.e., hydroxyl and sulfate radicals) in ozone and ozone/peroxymonosulfate (PMS) processes. The synergetic effects of these oxidants were evaluated with the main focus on the targeted screening of transformation products formed from oxidative degradation of micropollutants (MPs) in a pure and mixed water matrix. In continuation to current research activities, this work, in its second phase, further intends to focus on the degradation of MPs and subsequent formation of transformation products in heterogeneous oxidative processes. In such processes, the experimental protocol demands similar challenges as that of homogenous processes, but the particular challenge would surely be the activity of the catalyst in the presence of a water matrix.

Prof. Maryam Vosough

Chemistry and Chemical Engineering
Research Center of Iran, Tehran, Iran

Visiting Scientist

Following initial studies and collaborations in "Development of chemometrics approaches in non-target screening (NTS) of micropollutants in surface and wastewater samples using LC-HRMS/MS", more challenging aspects of NTS are currently being investigated. The main aim of this study is the classification and prioritization of pollutants and their transformation products based on new discriminating environmentally-related criteria. In this regard, the factors connected to sampling times and matrix complexity are comprehensively evaluated.

Dr. Amir Salemi

Visiting Scientist

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

Besides contribution in a few research studies focused on sample preparation and determination of organic micropollutants in water media, a review article entitled *"Sample preparation for determination of water taste and odor compounds: A review "*was published in *Trends in Environmental Analytical Chemistry*. The main aim of the current work is to develop, optimize and apply a gas generating vial for automated online on-fiber derivatization of steroid hormones following their extraction from environmental water samples and prior to GC-MS analysis.

Awards

Gerrit Renner

Dissertation Award, Water Chemistry Society

Dies Academicus Dissertation Award, University of Duisburg-Essen

Dissertation Award, german Working Group for Analytical Spectroscopy

"Development of new spectroscopic and multivariate chemometric methods for the characterization of microplastics in the marine environment"

Shaista Khaliq

2nd Feralco Water Award (Best Master Graduates), University of Duisburg-Essen

"New Insights into the Nutrient Flow of a Host-Parasite System Revealed by Compound Specific Isotope Analysis of Glucose and Amino Acids"

Mischa Jütte

Mischa Jütte (rechts) wird der DVGW Studienpreis im Wasserfach durch Dr.-Ing Dirk Waider, Vizepräsident Wasser des DVGW überreicht. (Bild: © DVGW/ BILDSCHÖN) Abgedruckt in: Newsletter Institut IWAR, Ausgabe 2, Jahr 2021

DVGW Studienpreis (Best Master Thesis), Deutsche Verein des Gas- und Wasserfaches e.V.

"Oxidation of nitrogen-containing micropollutants with chlorine dioxide in surface water"
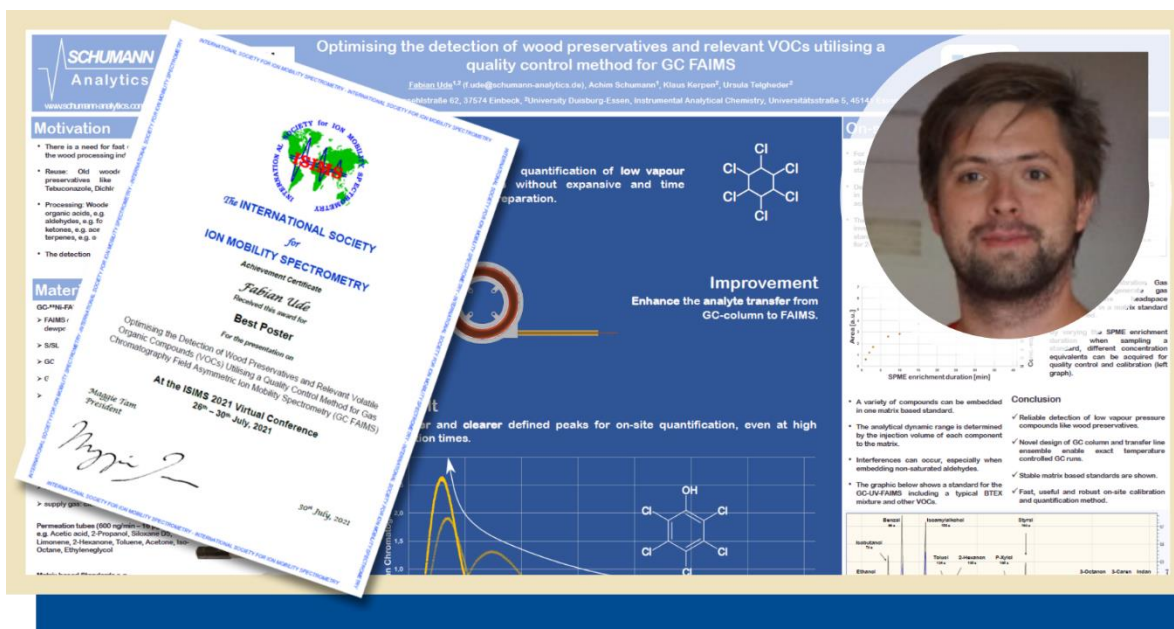
Julia Banholzer

1st Axel-Semrau Award (Best Bachelor Graduates), University of Duisburg-Essen

"Optimierung und Weiterentwicklung der Aufbereitungsmethode und des qPCR-Nachweises von Krankheitserregern/SARS-CoV-2 im Abwasser als Basis für ein Monitoring"

Fabian Ude

Best Poster Award, ISIMS 2021 Virtual Conference, 26th – 30th July, 2021

"Optimising the Detection of Wood Preservatives and Relevant Volatile Organic Compounds (VOCs) Utilising a Quality Control Method for Gas Chromatography Field Asymmetric Ion Mobility Spectrometry (GC FAIMS)"

IAC Image Movie

In 2021, we took a new step towards modern external communication and successfully produced an image film, which is available on the IAC website (www.uni-due.de/iac). The film gives an excellent overview of life in our working group. At this point, we would like to thank our IAC member Michelle Lüling again.
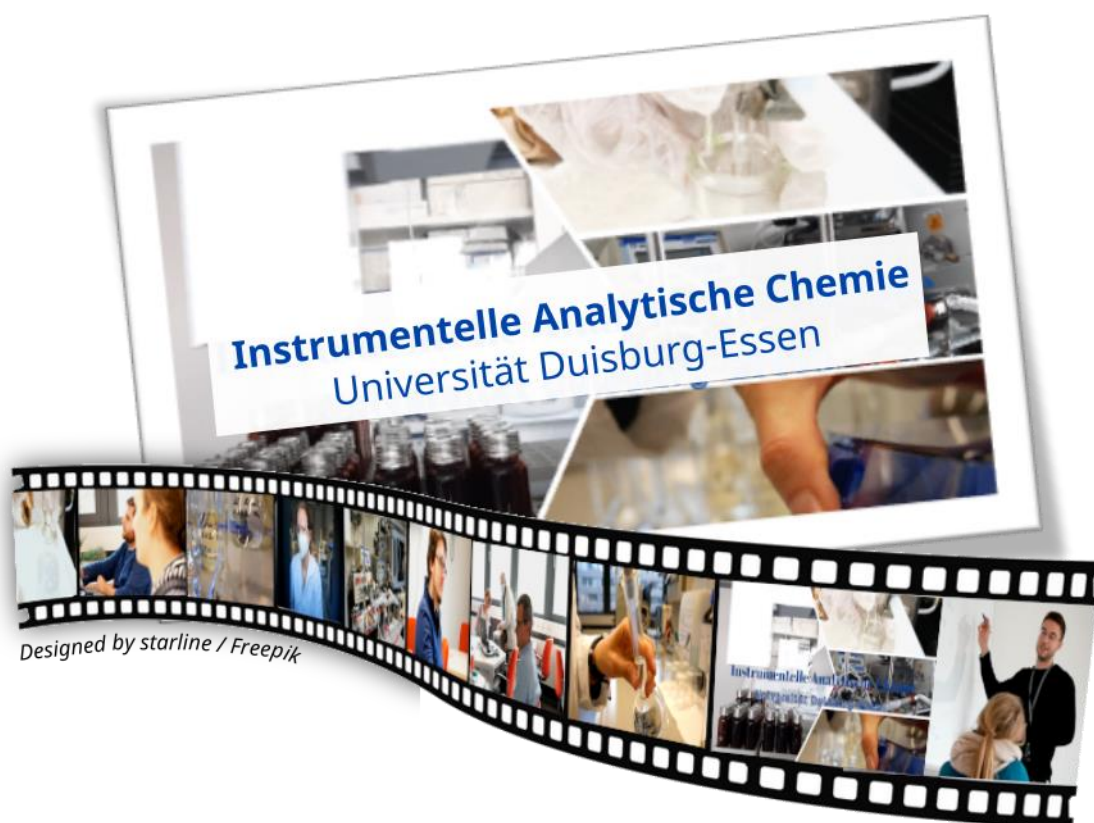
I joined the IAC in 2015, and over the years, she became dear to me. Since I also like to be active in an artistic way, I wanted to combine this with the workgroup. To that end, I created an image film that reflects the IAC's character and shows what we are currently working on. — Michelle Lüling

Running Projects at IAC 2021

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

Involved staff: Lotta Hohrenk-Danzouma (IAC PhD student), Claudia Freimuth (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, Nico Bätz (IUTA), Michelle Klein (IUTA), Prof. Dr. Sigrid Schäfer (EBZ Business School Bochum), Prof. Dr. Mark Oelmann (HRW Mülheim), Dr. Steven Engler (RUB) 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 conducting innovative and path-breaking research. Combining knowledge and methods across disciplines makes it possible to identify hitherto unnoted research questions. Tackling questions from different and novel angles allows finding answers that have not been conceived before. Furthermore, the integration of 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. Altogether, in Future Water, 12 Ph.D. students and a coordinator position are funded. In addition, the Centre does coordination for Water and Environmental Research (ZWU) at UDE. In 2019, a continuation of the graduate school in a second funding phase 2019-2022 was granted.

At IAC, one project (Lotta Hohrenk-Danzouma) focuses on analyzing micropollutants introduced by diffuse sources with nontarget screening. Nontarget 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 nontarget 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 analyzes passive sampling extracts with an LC-HRMS-based nontarget screening method and temporal- and spatial trends.
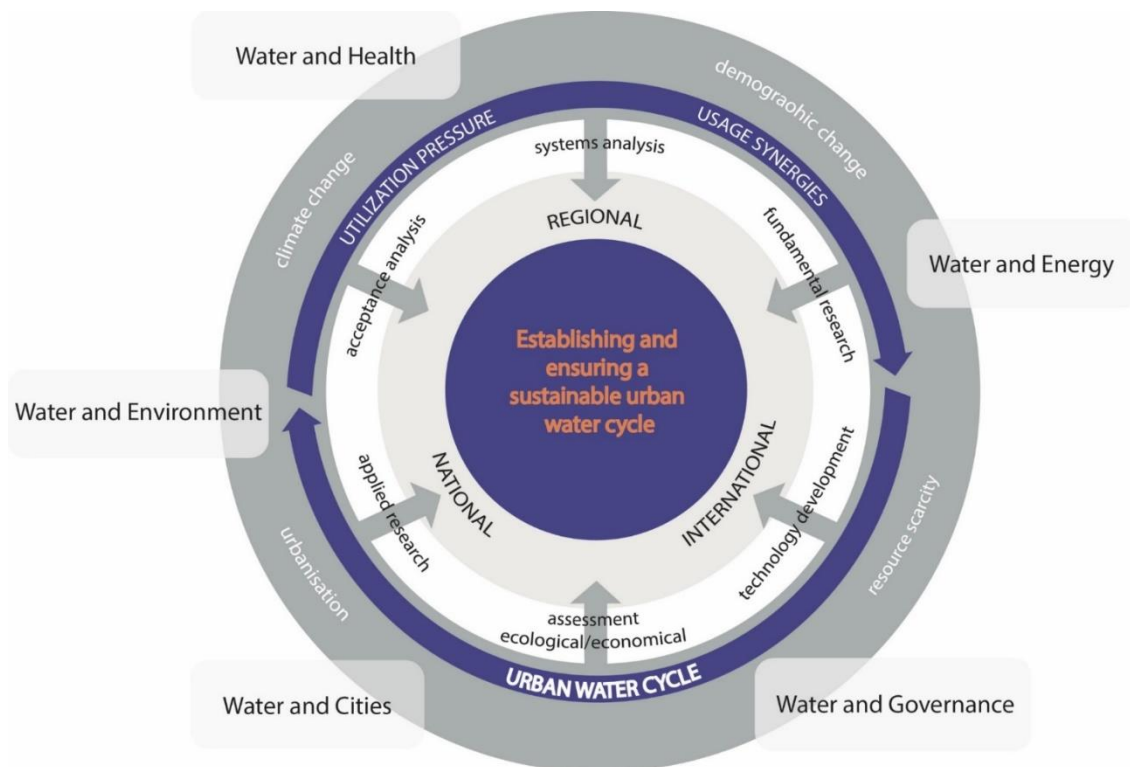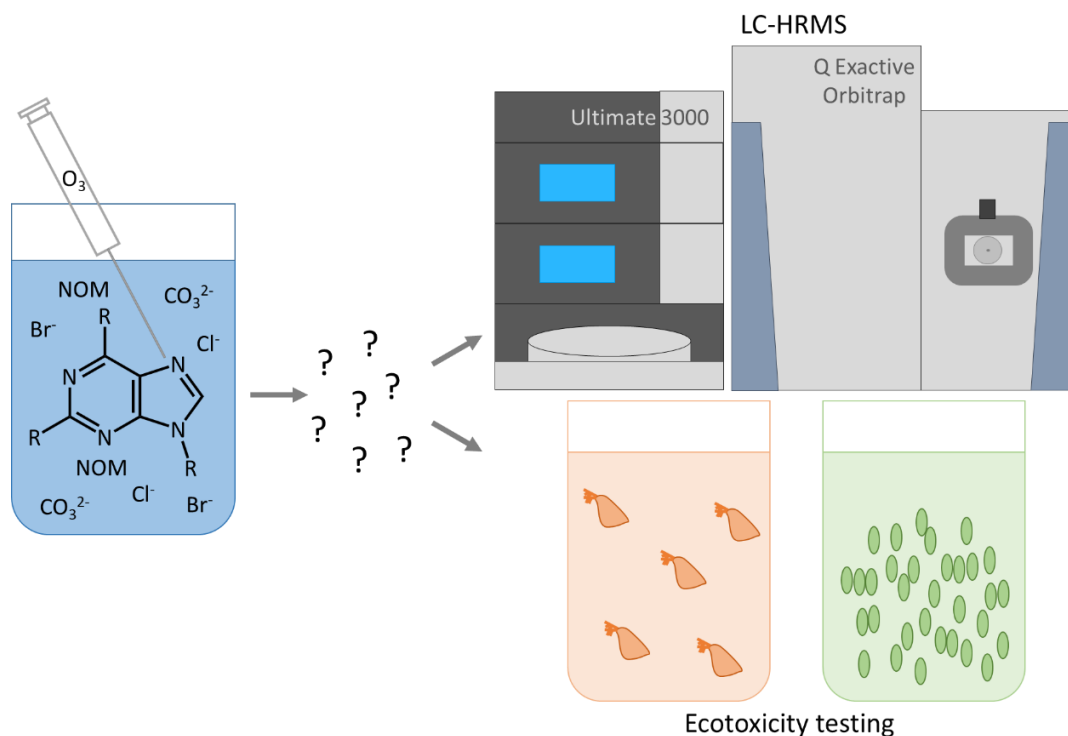
Characterization of transformation processes using high-resolution mass spectrometry

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)

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 the 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 general examinations of their ozonation like stoichiometry, reaction kinetics, quantification of target products, and identifying unknown transformation products using high-resolution mass spectrometry. 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 guanine and its antiviral derivatives.

The second part of the project is the ecotoxicological examination of the ozonation of ibuprofen. Ecotoxicity is studied by standardized test systems such as acute toxicity testing on *Daphnia magna* and the freshwater algae test 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.

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

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 kt a^{-1} to 49 kt a^{-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 ng L^{-1} to low μg L^{-1} range but are predicted to increase due to increased production and usage (Armbruster et al., 2020). The quantitatively most important 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).
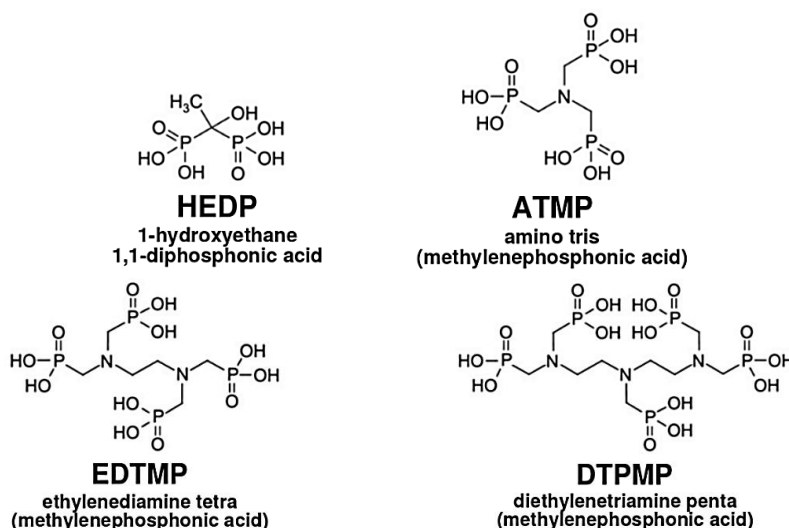
Polyphosphonic acid complexing agents widely used in Europe (adapted from Rott et al. (2018)). ATMP and EDTMP were selected as model compounds in the proposed research

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 altogether hamper the assessment of the environmental fate of APPs and the design of treatment strategies for 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. Anam Asghar, Dr. Klaus Kerpen, Prof. Dr. Torsten C. Schmidt,
Involved students: Kaliyani Wickneswaran, B. Sc
Partners: Dr. Vanessa Wirzberger, Prof. Dr. Holger Lutze, TU Darmstadt
Funding: DFG

It was shown that matrix components could affect the transformation product (TP) formation during oxidative processes. This was firstly observed in the transformation of dimethylsulfamide to the cancerogenic compound *N*-nitrosodimethylamine (NDMA), which required the presence of bromide. Yet, 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 one primary task in the current project.
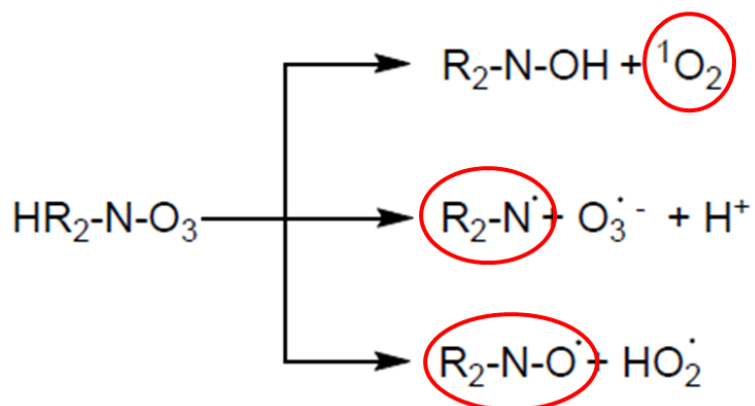

Figure 1: Possible reaction pathway of nitrogen-containing compounds and their reactive intermediates

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 will be studied.

Furthermore, the structural changes of NOM (Suwannee River and Upper Mississippi River) upon reactions with oxidants used in water treatment (O_3, ClO_2, and $SO_4^{\bullet-}$) is investigated using excitation-emission measurements/matrices (EEM), UV-Vis spectroscopy, NPOC measurements, and characterization of oxidation processes (yields of secondary oxidants such $\bullet OH$ or $HOCl$, exposures, and rate constants). Additionally, we want to find dependencies to replace labor-intensive and time-consuming measurements with quick and straightforward measurements using partial least square regression (see Figure 2).
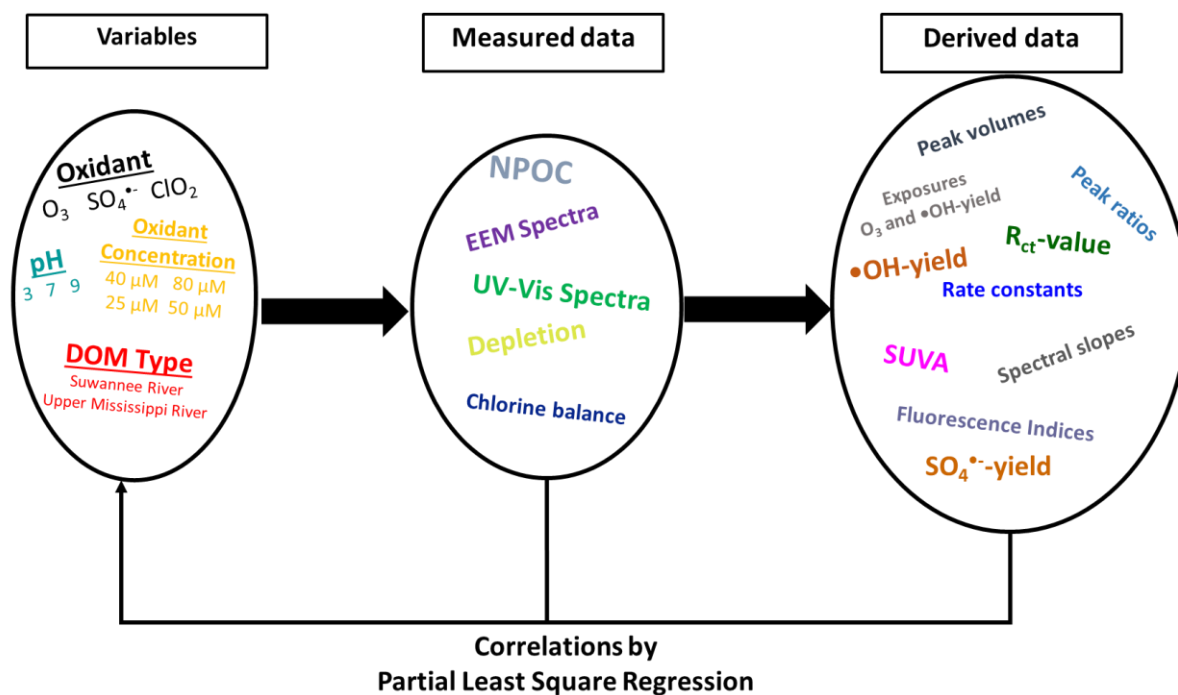

Figure 2: Variables, measured and derived data for investigating the structural changes of NOM via oxidation

Characterization of the metabolome of P. aeruginosa in biofilms as a lung infection model

Involved staff: Timo Köhler (AAC), PD Dr. Ursula Telgheder
Partners: Prof. Dr. Oliver Schmitz, Applied Analytical Chemistry, University of Duisburg – Essen, Dr. Jost Wingender, Environmental microbiology and biotechnology, University of Duisburg – Essen
Funding: German Research Foundation (DFG)
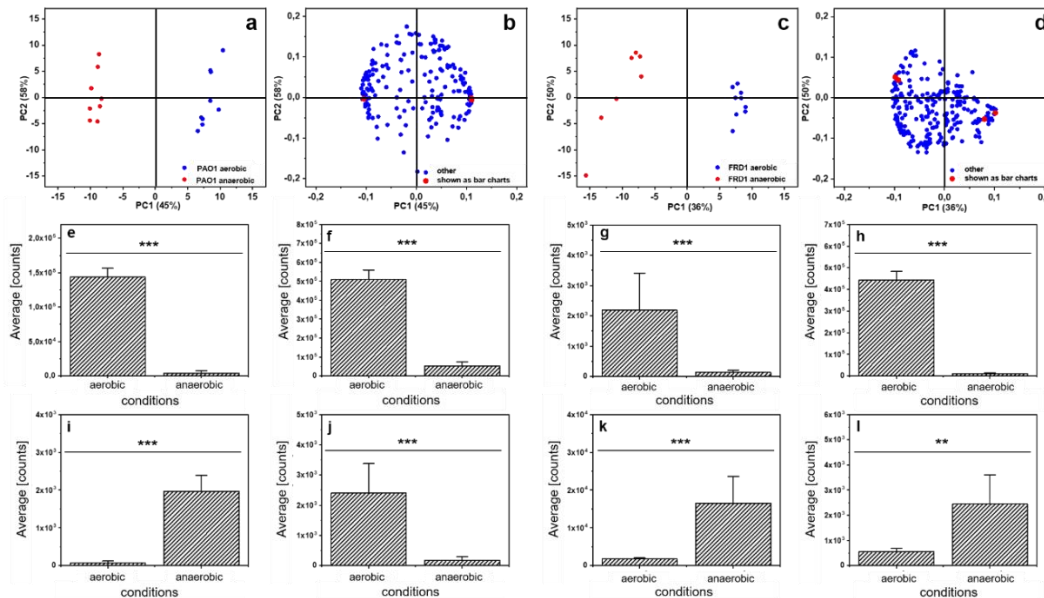
Graphic representation of the evaluation for the differentiation of cultivation conditions (aerobic (blue) vs. anaerobic (red) for the bacterial strains P. aeruginosa FRD1 and P. aeruginosa PAO1 using PCA and t-Test. The results of the PCA are shown as scores (a: PAO1; c: FRD1) and loadings plots (b: PAO1; d: FRD1). The peak intensities of selected VOCs shown in the bar charts correspond to the mean values from eight biological replicates. The standard deviation of the mean value is shown as an error bar. The substances (peak intensities are shown in the bar charts) e: 1-tetradecene (PAO1), f: 3-aminoquinoline (PAO1), g: dimethyl disulfide (FRD1), h: 2-aminoacetophenone (FRD1), i: 2,5-hexadione (PAO1), j: dimethyl disulfide (PAO1), k: benzaldehyde (FRD1), l: 2-hexanone (FRD1). The stars above symbolise the confidence level, where *** represents a p-value of 0.001, **0.01 and * 0.05 (n = 8).

Cystic fibrosis (CF) is an autosomal recessive hereditary disease that leads to the production of thickened mucus in the lungs, favoring polymicrobial infections, such as chronic lung infections with the opportunistic bacterial pathogen *Pseudomonas aeruginosa*.

A biofilm model combined with an adapted sampling and analysis method (Koehler et al. 2020) was applied to in vitro studies on different variables influencing the composition of the extracellular volatile metabolome of *P. aeruginosa*. A significant influence on the metabolome could be demonstrated for the culture medium and the atmosphere during cultivation (aerobic or anaerobic). Furthermore, a significant effect of the selected mucoid phenotype of the bacterium on the molecular level could be observed. Based on the results, a solid culture medium was developed to simulate the nutrient conditions in the lungs of a CF patient.

The extracellular volatile metabolome of bacterial strains *P. aeruginosa* ATCC10145, PAO1, and FRD1 was characterized under CF-like conditions in the in vitro biofilm model. In this study, bacterial strain-dependent metabolites were identified. Moreover, when *P. aeruginosa* PAO1 and FRD1 clinical isolates were compared, peaks of 36 metabolites showed significant variations in intensities. When the clinical isolates were compared with the reference strain, 28 metabolites (*P. aeruginosa* PAO1) and 70 metabolites (*P. aeruginosa* FRD1) were determined whose peaks showed significant deviation (p >95%) in intensity. Furthermore, the bacterial strains could be differentiated through two principal components.

Applied science communication – Kommunikation schafft Wissen, Wissen schafft Kommunikation

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

Designed by Macrovector / Freepik

Communicating the results of scientific research is an essential part of academic work. A prime example of the limitations and challenges of science communication is provided by the heated public debates about recent research findings on the SARS-COV-2 virus. Researchers are regularly challenged to communicate their research activities in science communication, resulting in complex issues appropriate for the target group, professional colleagues, and an interested or even the general public.

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 group? What should I pay attention to when addressing a non-academic public?

Aim of the Project

Our interdisciplinary project develops a framework to improve science communication and support researchers in their communicative work. To this end, we analyze selected, target group-oriented formats under which communication intentions and effects of scientific messages can diverge. The cornerstone of these analyses is our own experience and active colleagues communicating in science and the public. To this end, we consider diverse disciplinary fields (including chemistry, computer science, communication science, pedagogy, and physics) and different research aspects (e.g., basic research, applied research, industrial research, methodological research, etc.).

This project aims to identify evidence-based, target-group-related success strategies for successful and, above all, efficient science communication. Our work should enable communicating scientists to make informed decisions about specific communication strategies and media in the future.

Investigation of stable isotope fractionation during photolysis of Imidacloprid and its transformation products

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

Despite some political efforts to ban neonicotinoids like Imidacloprid, it is still found 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, it can undergo physical and (bio-)chemical transformation processes that facilitate mineralization in the environment and potentially produce substances more hazardous than the starting substance. This raises the importance of characterizing the transformation processes, estimating their contribution, and identifying factors influencing them.

The focus of this study lies on photolysis as it contributes to the natural attenuation of Imidacloprid exposed to sunlight. In laboratory experiments, influences like spectral distribution, pH-value, photosensitizers, and quenchers shall be investigated. Main transformation products shall be identified by mass-spectrometry and methods for their quantification implemented. The novelty of this study will be the use of compound-specific stable isotope analysis as a tool to identify isotope effects for individual transformation products. This technique has 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.
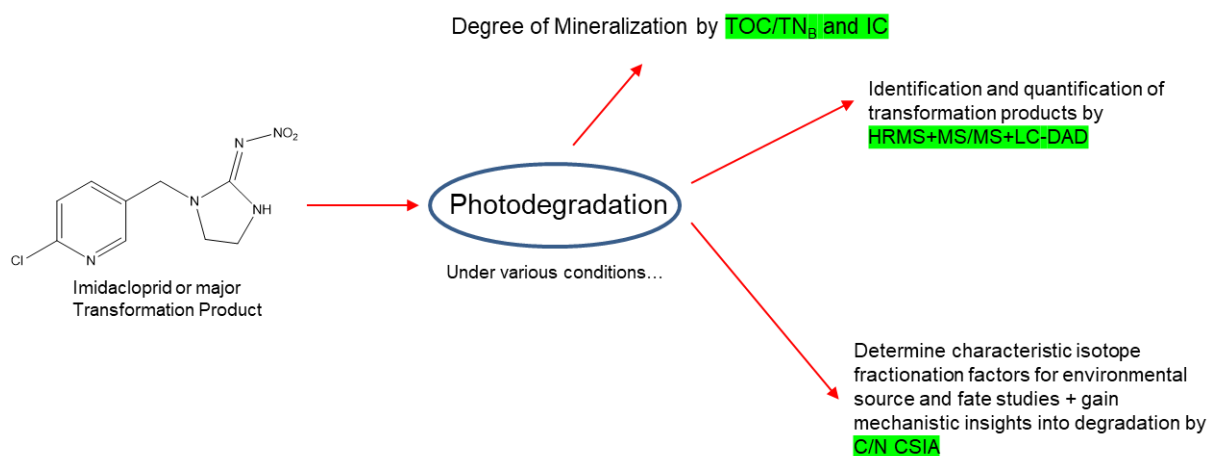

Figure 1: Flow chart of the project, including analytical methods planned to be utilized.

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

Involved staff: Sasho Joskimoski, Dr. Klaus Kerpen, Prof. Dr. Amir Salemi, PD Dr. Ursula Telgheder
Partners: Frank Jacobs, 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 the sensitive 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.

The basis of this automation is SBSE (stir bar sorptive extraction). By automating sample preparation, the advantages of SBSE are to be largely retained, while sample throughput and thus efficiency is to be increased even further. Automating the analytical methods allows further spreading the technique, as the manual effort has deterred potential customers. Matrix-dependent sample preparation is usually carried out manually. Due to a large number of samples, automated processing is advantageous. Through automation, the analytics can be carried out continuously if the configuration of the autosampler and the method have been adapted to the matrix.

The modules developed in the project were tested in trials with a pesticide standard solution to check the analytical and technical parameters for long-term stability and performance. This consisted of 22 pesticides taken from DIN27108 with different chemical properties to represent a broader range of analytical characteristics.

The analytes were purchased as pure substances, and the stock standard solutions were prepared at 1mg/mL concentrations. These individual standards were then freshly mixed and diluted to prepare working standard solutions with concentrations between 0.01µg/L and 100 µg/L. The feasibility of the extraction procedure at different concentrations was first investigated using a preliminary calibration series. Almost linear correlations between analyte concentration and signal area were found (coefficient of determination R^2>0.96). The results also showed that no carryover could be detected between the runs.

A response surface methodology was implemented to study the most relevant extraction parameters and find the optimum extraction conditions in the next step. Extraction time (10 - 120 min), extraction temperature (30 - 80 $^{\circ}$C), and salting-out effect (added NaCl, 0 - 30%) were the main factors that were optimized using a central composite design. The results showed that the extraction temperature and added salt positively affected the peak area (in fact, the geometric mean of the peak area of the individual analytes, as the primary response) 70 ^{0}C and 30% of were the optimum values. As Figure 1 shows, extraction time also showed a positive effect on extraction efficiency, but despite other parameters, since the equilibrium was not observed, it was decided to perform additional experiments to determine the equilibrium (maximum efficiency).

After finding the equilibration time and deciding on the practically optimum values of the set of parameters, establishing the calibration function, calculating the analytical performance characteristics, and analyzing real samples will be the next steps in method development.
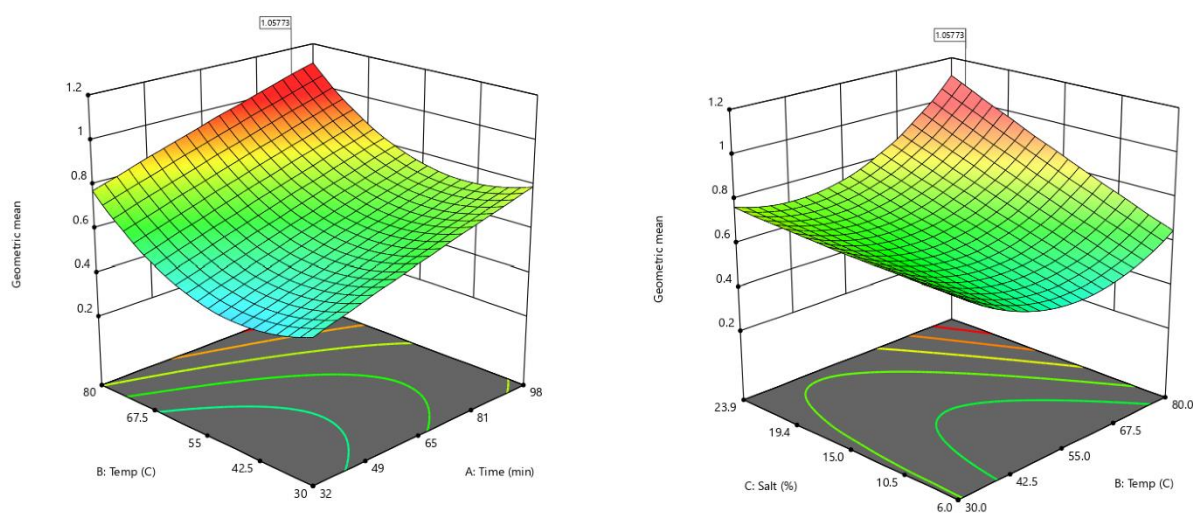

Figure 1. Response surfaces demonstrating effects and interactions of the main factors

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 δ13C values of individual amino acids in a controlled feeding experiment from muscle and liver tissue of three-spined sticklebacks (*Gasterosteus aculeatus*).
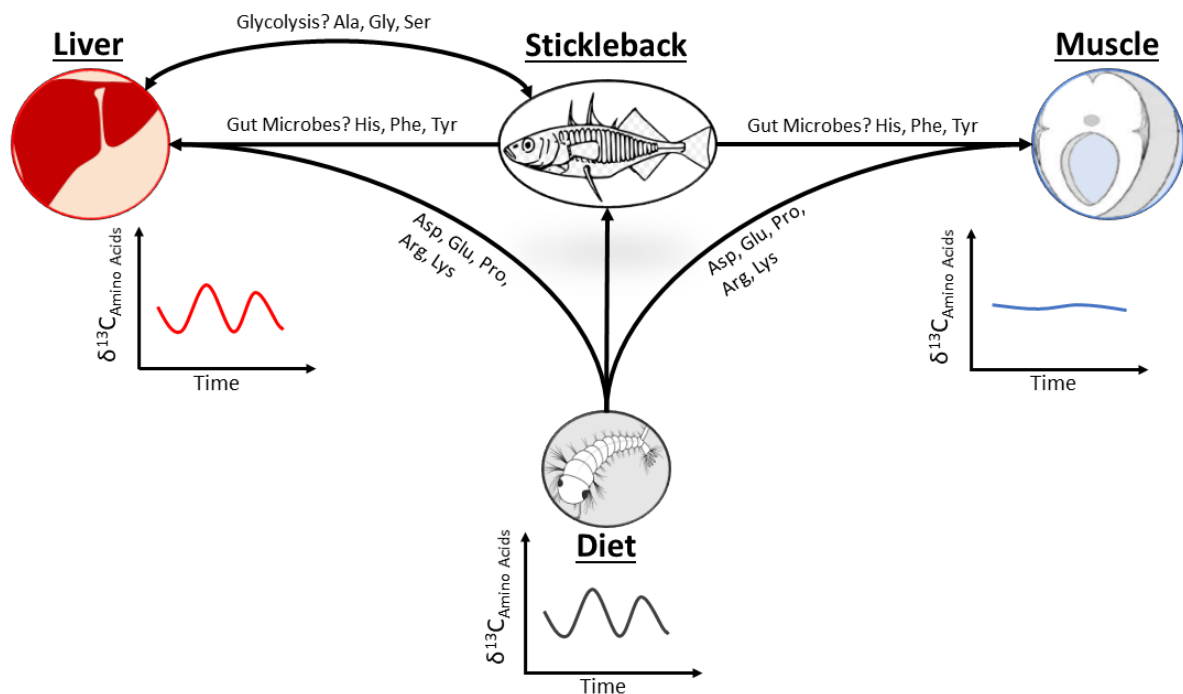

The isotopic composition of amino acids in the liver responds quickly to a shifting carbon isotope signature in diets. Some amino acids (Asp, Glu, Pro, Arg, Lys) are directly routed from the diet into liver and muscle tissue, while others (His, Phe, Tyr) seem to have at least some contribution from sources 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 even 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.

Optimization and automation of a rapid and selective analysis of fatty acid methyl esters from aqueous samples by headspace SPME arrow extraction followed by GC-MS/MS analysis

Involved staff: Lucie K. Tintrop, Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt
Funding: Internal
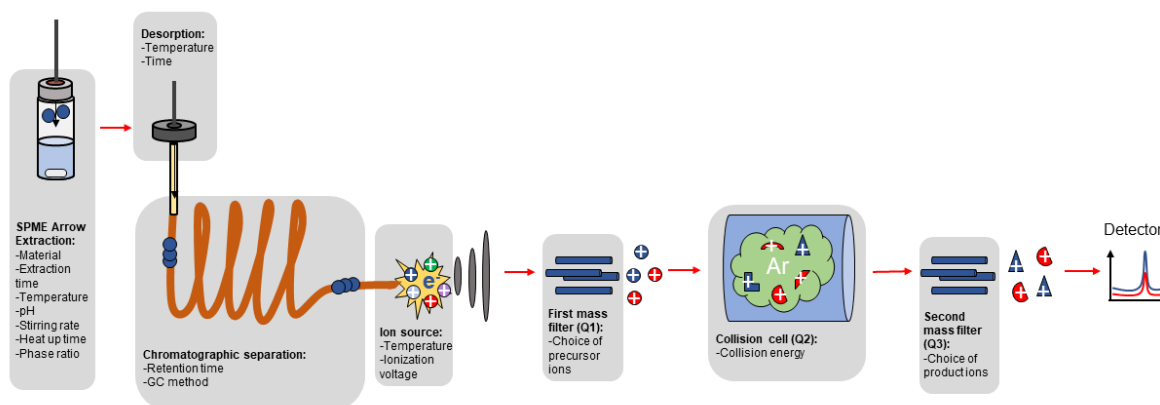
Optimization workflow and parameters for the SPME arrow extraction followed by GC-MS/MS analysis of FAMEs from aqueous samples.

Fatty acid methyl esters (FAMEs) are relevant in various application fields, mainly dealing with biological and industrial processes, whereas their analysis serves for monitoring reasons. Some of these application fields require the analysis of FAMEs from aqueous samples, but the methods for this are still limited as extraction is needed. Due to the increasing interest in green, sustainable analytical methods, extensive solvent consumption for liquid-liquid extraction and solid-phase extraction have lost practicality. Thus, extraction procedures were miniaturized, leading to the invention of microextraction methods. The solid-phase microextraction (SPME) is entirely solvent-free and applicable for direct analyte extraction from aqueous samples. The further development to the SPME arrow rectified mechanical stability and the size of the sorption phase resulting in enhanced sensitivity.

This study developed a fully automated and thoroughly optimized sample preparation method to determine FAMEs in aqueous samples. These requirements make the SPME arrow the optimal extraction method for this study.

The automation was done with the help of a PAL RTC autosampler and included pH adjustment, standard addition, sample movement to modules, SPME arrow extraction, cleaning, and injection. In addition, the extraction parameters such as temperature, time, material, and cleaning were optimized regarding response increase in sample preparation. Furthermore, as an analytical method for the FAMEs, a GC-MS/MS MRM method was developed, using molecular ions and specific EI fragments as precursor ions. And finally, ion source parameters (temperature, ionization voltage) and the collision energy were optimized.

The results obtained in this study demonstrate that the combination of the SPME arrow extraction and the GC-MS/MS MRM method enables using the benefits of both optimally. Due to detailed optimization of multiple parameters and an overlapping schedule of the autosampler method, the overall method was able to analyze 24 FAMEs directly from aqueous samples in a time of 44 min per sample. Validation of the method showed linearity for almost all FAMEs over two orders of magnitude, reasonable limits of detection of 3-1870 ng/L, and a recovery of 69-127 %. Extraction efficiencies were in the range of 13-59 %, which is comparable to standard efficiencies for SPME arrow extractions. In addition, this green sample preparation approach has a wide range of applicability to different sample types due to the headspace extraction and the resulting lower influence of the sample matrix.

Development of a Data Quality Score for the Processing of Non-Target-Screening Data generated by HPLC-HRMS
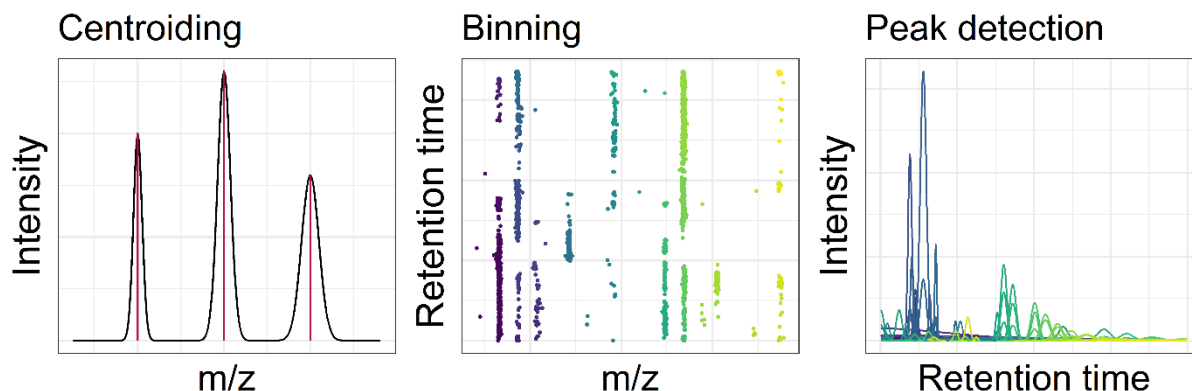
Figure 2: Overview of the subsequent steps in data processing of HPLC-HRMS data for non-target screening. First the profile mass spectra are centroided, the centroids are then binned into mass traces, which are then analyzed regarding chromatographic peaks.

Non-target screening (NTS) allows detecting organic micropollutants without reference substances. For this purpose, the diverse substances from the real samples are first separated by high-performance liquid chromatography (HPLC) and then detected by high-resolution mass spectrometry (HRMS). However, the generated data must be processed with automated processing scripts due to the complex structure.

Many different processing scripts and software are available, both open-source and proprietary. The output results of the processing scripts are stored in a feature list that compactly aggregates the information about the sample content. However, different workflows show significantly different output results in their feature lists even when processing the same data file. Further, a high number of false-positive features are produced. Therefore, this project sets in: To improve the traceability in the generation of the feature lists by developing a Data Quality Score (DQS). The DQS estimates the reliability in the generation of an entry in the feature list, and therefore, helps to identify false-positive features. As presented in figure 1, all steps of HPLC-HRMS processing are considered: Centroiding of high-resolution profile mass spectra, binning of centroids into mass traces, and the subsequent peak detection in the chromatographic domain with a peak fit. As in each step, the data is aggregated. Each step has an associated DQS that will be combined to a total DQS that describes the overall reliability of that feature.

The DQS will be attached to the usual information contained in the feature list (retention time, m/z, intensity). This can either prioritize features based on a DQS threshold or better detect potential false positives. Further, the DQS can be applied as weighting factors in comparative analysis between samples of different origins. Thus, the DQS offers a significant benefit compared to conventional data processing routines.

## 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.
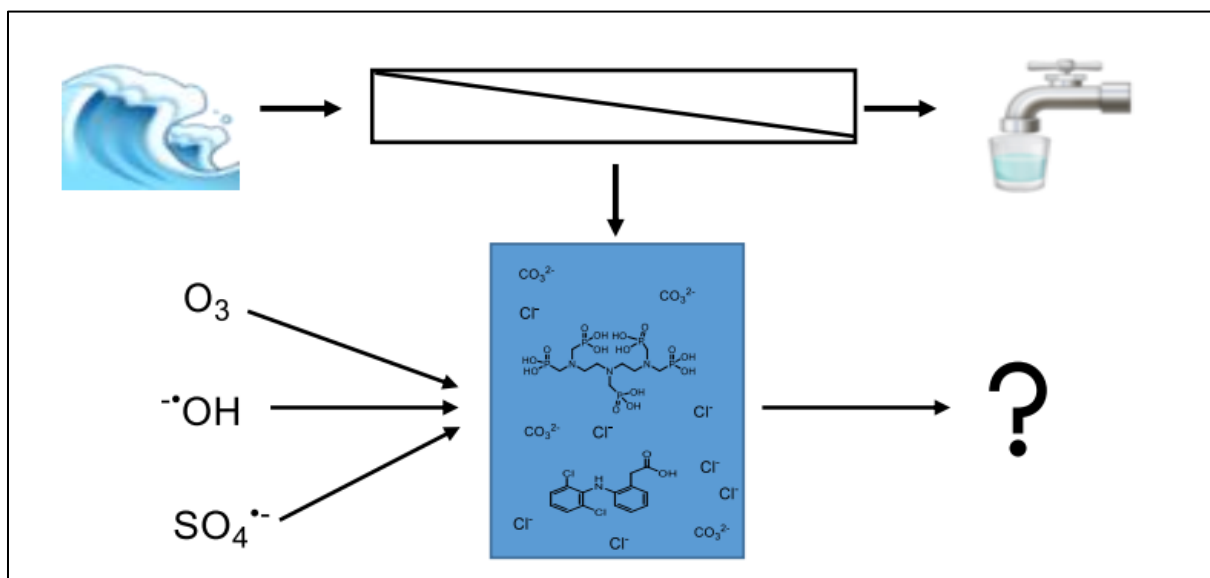
The IAC project part aims to investigate the potential of different oxidative processes for the treatment of membrane process concentrates. Therefore, in the first phase of this project, various oxidants (i.e., ozone, hydroxyl radicals, and sulfate radicals) were applied to evaluate the degradation of 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

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. Simplification of food webs with fewer trophic levels is expected under stress conditions that should be reflected in $\delta15N$ of trophic and source AAs. In addition, $\delta13C$ analysis of essential and non-essential AAs will reveal changes in food sources due to ecological degradation and during recovery.
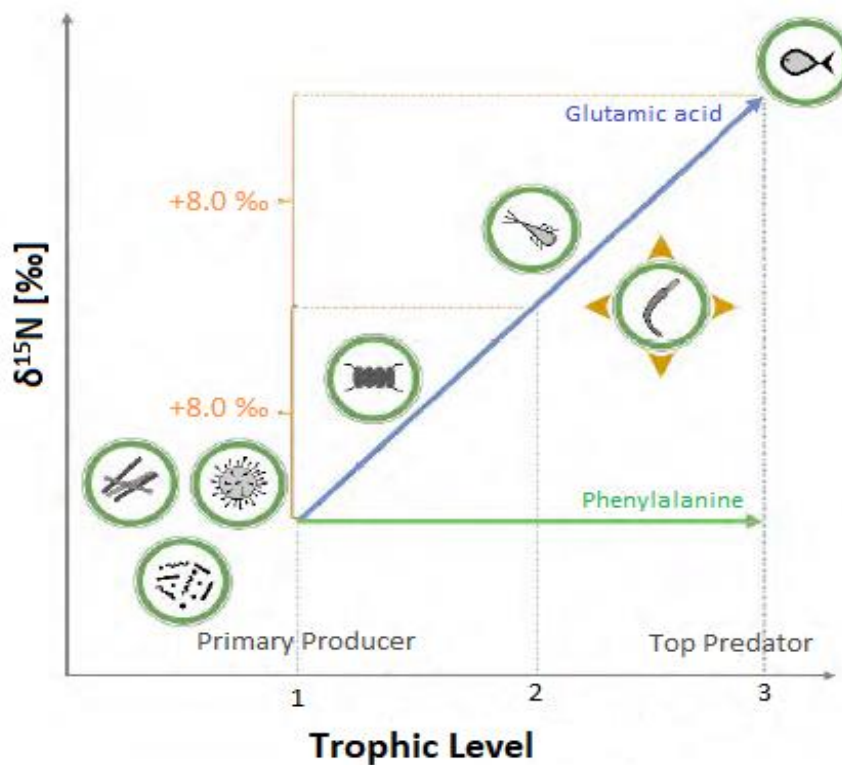
Schematic illustration of the relationship between source AA (phenylalanine: Phe) and trophic AA (glutamic acid: Glu) according to their nitrogen isotope composition to estimate organisms' trophic levels from primary producers top predators.

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) Hydromorphological stressors will mainly change the isotope values of non-essential and trophic amino acids in higher organisms. 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 strive 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, invertebrate, and parasite samples from the field sampling program on chosen degraded, recovered, and near-natural sites in the Emscher/Boye catchment. And in WP3, we will construct food webs based on trophic positions (TPs) of organisms in a combined effort with other projects of RESIST. The following equation can calculate the TPs of organisms.

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

Multi-Ion - Non-radioactive, energetically variable ionization unit for fast and selective pollutant analysis in building materials based on FAIMS technology

Involved staff: Sasho Joskimoski, Dr. Klaus Kerpen, Fabian Ude, Robert Marks, PD Dr. Ursula Telgheder
Involved students: Dionisio Tzimis
Partners: Schumann Analytics GmbH
Funding: Federal Ministry for Economic Affairs and Energy (BMWi) by the Central Innovation Programme for SMEs (ZIM)

A system for analyzing pollutant emissions from wood and other building materials was developed within this project. The analytical system has a sensitive ionization unit and does not have any regulatory requirements (radiation protection) for operation. The project has developed two ion mobility spectrometers with detectable chemical ionization. An X-ray tube is used, which is operated so that no radiation protection requirements apply and yet photons and reactant ions are available for efficient and flexible ionization. This combines the advantages of chemical ionization with those of non-radioactive sources. The energy of the X-rays can be varied in a range of 0 -5 keV.

The adaptation of the ionization unit to an existing FAIMS system was successfully implemented. Equally successful was implementing a new technical setup of a drift-time ion mobility spectrometer using the ionization unit as an alternative to the FAIMS system. As a result, two new measurement systems are available. Thus, it is possible to perform a comprehensive analysis of building materials (e.g., wood) concerning common pollutants such as pentachlorophenol (PCP) and lindane (HCH) within about 50 minutes. In addition, all relevant VOCs (volatile organic compounds) are detected qualitatively and can be determined quantitatively with sufficient accuracy (see figure below).
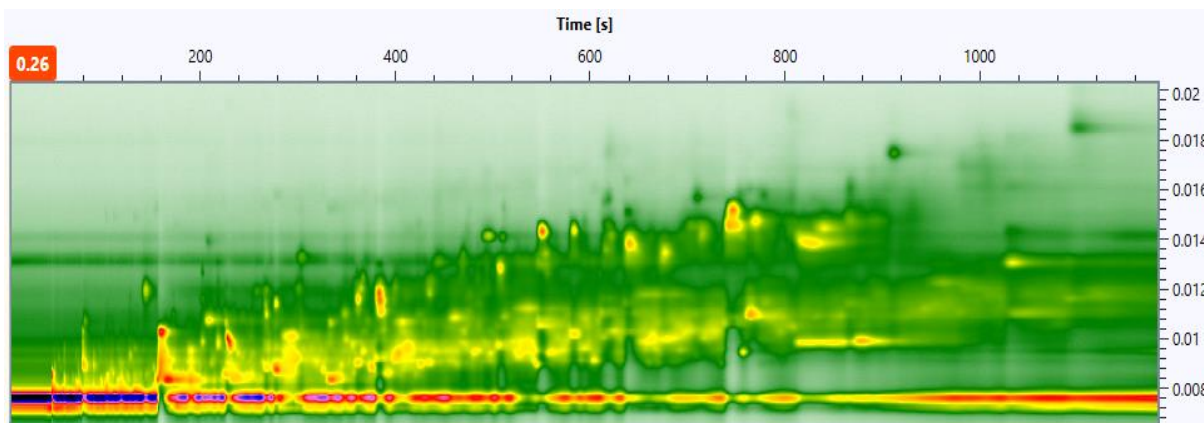
GC-DTIMS contour plot of typical VOCs of a wood sample (positive measurement mode)

Theses completed in 2021

Ph.D. Theses

Seyed Mohammad Seyed Khademi

"Direct Immersion-Solid Phase Microextraction Arrow-Corona Discharge Ion Mobility Spectrometry for Determination of Pesticides in Environmental Samples"

Summary

Application of Ion Mobility Spectrometry (IMS) in analytical chemistry as a fast, sensitive low-cost, and simple technique for the determination of explosives, pharmaceuticals and, environmental samples such as surface water has been introduced in the last three decades. However, the implementation of IMS to analyze pesticides in real water samples is under challenge due to the interfering of water clusters during detection, the complexity of surface water matrix, and trace amounts of pesticides that existed in real water samples. On the other hand, a fast and straightforward technique (analysis time < 1 min) is required to detect contaminants discharged into the drinking water sources.

In the presented thesis, direct immersion-solid phase microextraction Arrow coupled with a drift tube IMS (DT-IMS) was investigated to overcome the limitation of this analytical instrument in the determination of pesticide contaminants in real water samples. The extraction optimization procedure of SPME Arrow was performed using a modified IMS injection port compatible with the Arrow device. The optimization of the SPME Arrow procedure was performed by using GC-Mass spectrometry.

The theoretical study of ionization of the target pesticides dichlorovos, cybutryne, terbutryn, and quinoxyfen in the positive mode of corona discharge ionization source of the IMS was investigated using density functional theory and B3LYP method as well as Gaussian09® software. With the help of computational chemistry, assigning the peak in the IMS spectrum was possible for the selected pesticides.

The detection limits were calculated to 13-124 µg L^{-1}, RSD from 5.2-7.5%; average recoveries ranged from 88-107% to detect the selected pesticides in surface water by SPME Arrow – DT-IMS. In conclusion, the SPME-Arrow as a simple sample preparation method coupled with the DT-IMS can be introduced as a low-time consuming, inexpensive, and simple method for determining selected pesticides at concentration levels of µg L^{-1} in surface water.

Master Theses

Christina Sommer

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

Felix Niemann

"Development of an LC-IRMS System for Stable Nitrogen Isotope Analysis"

Shaista Khaliq

"New Insights into the Nutrient Flow of a Host-Parasite System Revealed by Compound Specific Isotope Analysis of Glucose and Amino Acids"

Insa Naendrup

"Referenzgasgemisch zur Kalibration von MCC-IMS-basierten Messgeräten"

Samuel Thebingbuß

"Design-of-experiments as a tool for the method optimization of gas chromatographic analysis"

Master Theses

Bachelor Theses

Orkan Akin

"Untersuchung des Abbaus von Benzotriazolen durch UV-erzeugte Sulfatradikale"

Willi Eßer

"Diskriminierungsfreie Aufkonzentrierung von Wasserproben mittels der Mikrowellentechnik. Bestimmung der Effektivität dieses Verfahrens am Beispiel ausgewählter organischer Spurenstoffe"

David Kniesel

„Insight Into the Formaton of Hydroxyl and Sulfate Radicals in Ozone/PMS Systems: An Application of Heterogeneous Catalysts"

Alina Manz

"Einfluss der Prozessierung auf die Datenauswertung im Bereich der Non-Target Analyse mittels HPLC-HRMS"

Damian Schomers

"Elimination of iodinated x-ray contrast media on textile adsorbers"

Kaliyani Wickneswaran

„Die Untersuchung vom Einfluss der Ozonierung auf Natural Organic Matter mit Excitation-Emission-Matrizes"

Publications

Peer-reviewed Journals

1. W. Kaziur-Cegla, L. Wykowski, M. A. Jochmann, K. Molt, A.Bruchmann, T. C. Schmidt:
In-tube dynamic extraction a green solventless alternative for a sensitive headspace analysis of volatile organic compounds in olive oils
Adv. Sample Prep. **1** (2021), 100002
DOI: 10.1016/j.sampre.2021.100002

2. S. K. Zahraei, A. Salemi, T. C. Schmidt:
Sample preparation for determination of water taste and odor compounds: A review
Trends Environ. Anal. Chem. **32** (2021), e00149
DOI: 10.1016/j.teac.2021.e00149

3. L. M. H. Reinders, M. D. Klassen, T. Teutenberg, M. Jaeger, T. C. Schmidt:
Development of a multidimensional online method for the characterisation and quantification of monoclonal antibodies using immobilized flow-through enzyme reactors
Anal. Bioanal. Chem. **413** (2021), 7119–7128
DOI: 10.1007/s00216-021-03683-z

4. O. Höcker, D. Flottmann, T. C. Schmidt, C. Neusüß:
Non-Targeted LC-MS and CE-MS for Biomarker Discovery in Bioreactors: Influence of Separation, Mass Spectrometry and Data Processing Tools
Sci. Tot. Environ. **798** (2021), 149012
DOI: 10.1016/j.scitotenv.2021.149012

5. R. Akhbarizadeh, S. Dobaradaran, G. Parhizgar, T. C. Schmidt, R. Mallaki:
Potentially toxic elements leachates from cigarette butts into different types of water: A threat for aquatic environments and ecosystems?
Environ. Res. **202** (2021) 111706
DOI: 10.1016/j.envres.2021.111706

6. M. Funck, M. M.S. Al-Azzawi, A. Yildirim, O. Knoop, T. C. Schmidt, J. E. Drewes, J. Tuerk:
Release of microplastic particles to the aquatic environment via wastewater treatment plants: The impact of sand filters as tertiary treatment
Chem. Eng. J. **426** (2021) 130933
DOI: 10.1016/j.cej.2021.130933

7. M. S. Abdighahroudi, M. Jütte, K. Hupperich, X. A. M. Mutke, T. C. Schmidt, H. V. Lutze:
Mechanisms and byproduct formation in the application of chlorine dioxide
Compr. Anal. Chem. **92** (2021), 51-83
DOI: 10.1016/bs.coac.2021.01.003

8. L. M. H. Reinders, M. D. Klassen, C. vom Eyser, T. Teutenberg, M. Jaeger, T. C. Schmidt, J. Tuerk:
Quality control of cytostatic drug preparations - Comparison of workflow and performance of Raman/UV and high performance liquid chromatography coupled with diode array detection (HPLC-DAD)
Anal. Bioanal. Chem. **413** (2021), 2587-2596
DOI: 10.1007/s00216-021-03223-9

9. F. Lutz, N. Lorenzo Parodi, T. C. Schmidt, J. Niemeyer:
Heteroternary Cucurbit[8]uril Complexes as Supramolecular Scaffolds for Self-assembled Bifunctional Photoredoxcatalysts
Chem. Comm. 57 (2021), 2887-2890
DOI: 10.1039/d0cc08025j

10. S. Angel, F. Schneider, S. Apazeller, W. Kaziur-Cegla, T. C. Schmidt, C. Schulz, H. Wiggers:
Spray-flame synthesis of LaMO3 (M = Mn, Fe, Co) perovskite nanomaterials: Effect of spray droplet size and esterification on particle size distribution
Proc. Combust. Inst. **38** (2021), 1279-1287
DOI: 10.1016/j.proci.2020.07.116

11. E. Dopp, H. Pannekens, A. Gottschlich, G. Schertzinger, L. Gehrmann, M. Kasper-Sonnenberg, J. Richard, M. Joswig, T. Grummt, T. C. Schmidt, M. Wilhelm, J. Tuerk:
Effect-based evaluation of ozone treatment for removal of micropollutants and their transformation products in waste water
J. Toxicol. Environ. Health A **84** (2021), 418-439
DOI: 10.1080/15287394.2021.1881854

12. S. Begall, R. Nappe, L. Hohrenk, T. C. Schmidt, H. Burda, A. Sahm, K. Szafranski, P. Dammann, Y. Henning:
Life expectancy, family constellation, and stress in giant mole-rats (*Fukomys mechowii*)
Philos. Transact. B **376** (2021), 20200207
DOI: 10.1098/rstb.2020-0207

13. F. Soleimani, R. Akhbarizadeh, S. Dobaradaran, T. C. Schmidt, M. Marzband, R. BasirianJahromi:
Environmental fate of cigarette butts and their toxicity in aquatic organisms: A comprehensive systematic review
Environ. Res. **195** (2021), 110881
DOI: 10.1016/j.envres.2021.110881

14. M. Hammad, P. Fortugno, S. Hardt, C. Kim, S. Salamon, T. C. Schmidt, H. Wende, C. Schulz, H. Wiggers:
Large-scale synthesis of iron oxide/graphene hybrid materials as highly efficient photo-Fenton catalyst for water remediation
Environ. Technol. Innov. **21** (2021), 101239
DOI: 10.1016/j.eti.2020.101239

15. N. Baetz, L. Rothe, V. Wirzberger, B. Sures, T. C. Schmidt, J. Tuerk:
High-Performance Thin-Layer Chromatography in Combination with a Yeast-Based Multi-Effect Bioassay to Determine Endocrine Effects in Environmental Samples
Anal. Bioanal. Chem. **413** (2021), 1321-1335
DOI: 10.1007/s00216-020-03095-5

16. J. C. Vivas Muñoz, C. K. Feld, S. Hilt, A. Manfrin, M. Nachev, D. Köster, M. A. Jochmann, T. C. Schmidt, B. Sures, A. Ziková, K. Knopf:
Eye fluke infection changes diet composition in juvenile European perch (Perca fluviatilis)
Sci. Rep. **11** (2021), 3440
DOI: 10.1038/s41598-021-81568-y

17. T. Werres, T. C. Schmidt, T. Teutenberg:
The influence of injection volume on efficiency of microbore liquid chromatography columns for gradient and isocratic elution
J. Chromatogr. A **1641** (2021), 461965
DOI: 0.1016/j.chroma.2021.461965

18. V. Wirzberger, M. Klein, M. Woermann, H. V. Lutze*, B. Sures, T. C. Schmidt*:
Matrix composition during ozonation of N-containing substances may influence the acute toxicity towards Daphnia magna
Sci. Tot. Environ. **765** (2021), 142727
DOI: 10.1016/j.scitotenv.2020.142727

19. S. Dobaradaran, T. C. Schmidt, W. Kaziur-Cegla, M. A. Jochmann:
BTEX compounds leachates from cigarette butts into water environment: A primary study
Environ. Pollut. **269** (2021), 116185
DOI: 10.1016/j.envpol.2020.116185

20. R. L. Khatoonabadi, M. Vosough, L. L. Hohrenk, T. C. Schmidt:
Employing complementary multivariate methods for a designed nontarget LC-HRMS
screening of a wastewater-influenced river
Microchem. J. **160** (2021), 105641
DOI: 10.1016/j.microc.2020.105641

21. T. Perl, N. Kunze-Szikszay, A. Braeuer, M. Quintel, T. Roy, K. Kerpen, U. Telgheder:
Aluminium release and fluid warming: provocational setting and devices at risk
BMC Anesthesiology **21** (2021), 163
DOI: 0.1186/s12871-021-01378-7

22. R.G.H. Marks, K. Kerpen, D. Diesing, U. Telgheder:
Electrochemical degradation of perfluorooctanoic acid in aqueous solution by boron-doped
diamond electrodes under pulsed voltage conditions
Journal of Electroanalytical Chemistry **895** (2021), 115415
DOI: 10.1016/j.jelechem.2021.115415

23. A.L.R.M. Augustini, S. Sielemann, U. Telgheder:
Strategy for the identification of flavor compounds in e-liquids by correlating the analysis of
GCxIMS and GC-MS
Talanta **230** (2021), 122318
DOI: 10.1016/j.talanta.2021.122318

24. S.M.S. Khademi, A. Salemi, M. Jochmann, S. Joksimoski, U. Telgheder:
Development and comparison of direct immersion solid phase micro extraction Arrow-GC-MS
for the determination of selected pesticides in water
Microchemical Journal **164** (2021), 106006
DOI: 10.1016/j.microc.2021.106006

25. S. Klaes, T. Lostak, E. Pappert, K. Kerpen, U. Telgheder:
Characterization of hot-dip coated steel by coupling of a flow cell with ICP-OES
Talanta **224** (2021), 121783
DOI: 10.1016/j.talanta.2020.121783

Other Publications

1. L. Hohrenk-Danzouma, G. Renner:
Auf Spurensuche: Non-Target-Screening in der Wasseranalytik
Faszination Chemie (27-10-2021)
https://faszinationchemie.de/wissen-und-fakten/news/auf-spurensuche-non-target-screening-in-der-wasseranalytik/

2. L. Hohrenk-Danzouma, G. Renner:
Non-Target-Screening in der Wasseranalytik
Analytik News (25-11-2021)
https://analytik.news/fachartikel/2021/53.html

3. G. Renner:
Von Mikro bis Nano
Mitteilungsblatt der Fachgruppe Analytische Chemie **3** (2021), 24-26
ISSN: 0939-0065

Conferences and Meetings

Organization

Annual Meeting of the Water Chemistry Society, online, the 10th of May to 12, 2021

(for more details, check http://www. www.gdch.de/wasser2021)

Due to the COVID-19 pandemic, the 2020 Annual Meeting of the Water Chemistry Society, unfortunately, had to be canceled. Therefore, we are all the more pleased that it could take place one year later, at least in an online format. For the last time, Torsten Schmidt and his team were allowed to organize the conference. However, the annual meeting was on a different scale than the years before.

With the online platform used, there was the possibility to show many elementary parts of the traditional annual conference. Moreover, thanks to the versatile technical offer, the lectures could be followed live or streamed afterward. Therefore, there was no need to miss out on the discussions at the posters, and the participants could visit booths in the trade exhibition and exchange technical information there.

The special topic "Havel catchment area – water body-rich and water-poor" of the conference on Tuesday afternoon was chosen due to the extreme events of the last years and their impact on water quantity and quality. The regular awards were given this time for two years:

Willy-Hager-Award 2020:

David B. Miklos, Linde GmbH Engineering Division: "Enhanced Removal of Trace Organic Chemicals from Wastewater Treatment Plant Effluents Using UV-Based Advanced Oxidation Processes"

Ph.D. Award 2020:

Fabian Fischer, Eberhard Karls Universität Tübingen: "Bioavailability of organic micropollutants in cell-based bioassays"

Award of the Water Chemistry Society 2020:

Arne Wick, Bundesanstalt für Gewässerkunde (BfG): "Tracking down the microbial degradation of organic trace substances-From the identification of degradation pathways to the isolation of active enzyme fractions."

Willy-Hager-Award 2021:

Benedikt M. Aumeier, RWTH Aachen University: "The hydrothermal solution for decentralized drinking water treatment."

Ph.D. Award 2021:

Peter Carl, Bundesanstalt für Materialforschung und -prüfung (BAM): „Particle-based multianalyte fluorescence immunoassays for environmental analysisand biotechnology"

Ph.D. Award 2021:

Gerrit Renner, University of Duisburg – Essen (IAC): "Development of new spectroscopic and multivariate chemometric methods for the characterization of microplastics in the marine environment."

Award of the Water Chemistry Society 2021:

Thorsten Hüffer, University of Vienna: "Interactions of microplastics with xenobiotics in the aquatic environment-Influence of particle aging on sorption and desorption."

Invited Lectures

Ursula Telgheder:

„Ionenmobilitätsspektrometrie in der Umweltanalytik"

8. IMS Anwendertreffen in Potsdam (virtuell), 17.-19.03.2021

Torsten C. Schmidt:

"Water analysis using target, suspect, non-target analysis: What can we do with all the data?"

4th International and 23rd National Conference on Environmental Health (virtual), 02.-04.03.2021

Anam Asghar, Torsten C. Schmidt:

"Is Catalytic Ozonation a Suitable Approach to Treat Wastewater?"

5th International and 24th National Conference on Environmental Health (virtual), 14.-16.12.2021

Institute Colloquium

(in cooperation with the research group of Prof. Oliver Schmitz)
Dr. Joachim Weiss, ThermoFisher Scientific

"Mixed-mode liquid chromatography – An exciting development in separation science"

November 21, 2021

Teaching

At IAC, we teach mainly in the Bachelor and Master program "Water Science," a unique science-based curriculum focusing 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" (provided in the faculty of biology) and "Management and Technology of Water and Wastewater – MTW3" (offered in the faculty of engineering).

Summer term

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

- Lecture "Water – The Lecture" (B.Sc. Water Science, in German)

- Virtual Excursion to Wastewater Treatment Plant Duisburg-Kaßlerfeld (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, 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)

- Excursion to the Drinking Water Treatment Plant incl. Ultrafiltration, Roetgen (M.Sc. Water Science, in English)

Miscellaneous

Gerd's Farewell

At the end of January 2021, we had to say goodbye to Gerd Fischer, who entered a well-deserved retirement. Since 1978, he initially worked in the Department of Applied Chemistry (at that time still Gesamthochschule Duisburg), then moved to Instrumental Analytical Chemistry under Prof. Dr. Alfred Golloch. Even after the takeover of Prof. Dr. Torsten C. Schmidt as head of the IAC in 2006, Gerd Fischer remained loyal to the IAC. Whether it was about expert information and support in the IT area, national and international symposia organization, or efficient handling of administrative matters in the processing of third-party funding projects, he was always a competent contact person. We wish you, Gerd, all the best for your new phase of life true to the motto:
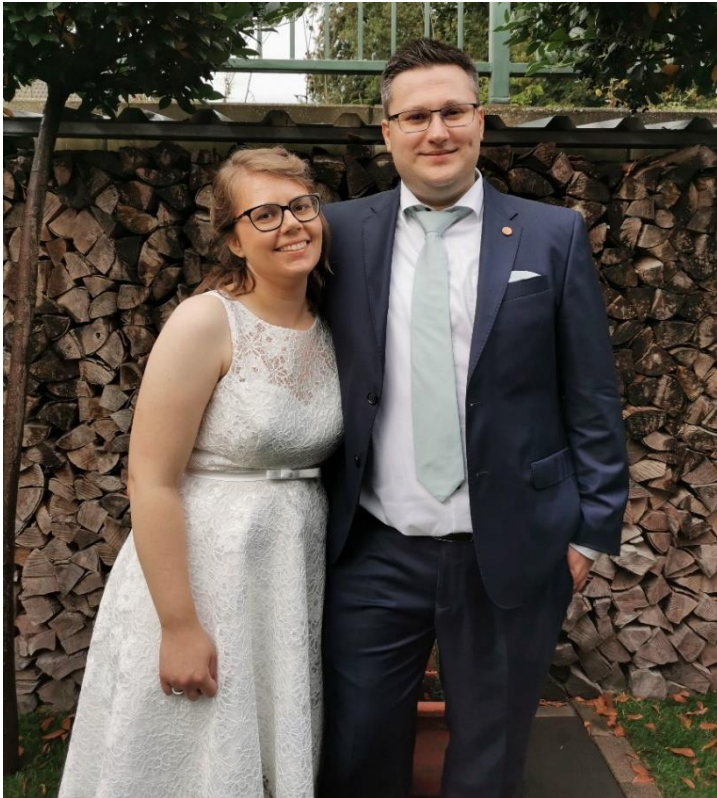
Claudia's Anniversary

On the 21st of January in 2021, Claudia Ullrich celebrated her 40th anniversary. Congratulations! We are looking forward to the next years!

Births

Richard Mutke,
29.11.2021

Wedding

Katharina Klein
with Husband Sascha

10.09.2021

Felix Drees
with Wife Romina and Son Benett

02.10.2021