Institute of Water Chemistry
TUM School of Natural Sciences
Technical University of Munich

Annual Report 2024

Institute of Water Chemistry &

Chair of Analytical Chemistry and Water Chemistry

INSTITUTE OF WATER CHEMISTRY

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Group photo of the Chair of Analytical Chemistry and Water Chemistry &

Institute of Water Chemistry (IWC) in Raitenhaslach in 2024

Content

Dear colleagues and friends,

the year 2024 has seen the conclusion of multiple successful projects and the acquisition of exciting new ones.

In the Raman & REM group the applicability of stimulated Raman scattering for the analysis of nanoplastics in flow has been demonstrated for the first time in collaboration with Vrije Universiteit Amsterdam. To support the development of reference materials for microplastics, homogeneity and stability was proven by the IWC's automated µ-Raman-based analysis in collaboration with the Joint Research Centre of the European Commission. Furthermore, a new project funded by the Bavarian Research Foundation – BayWater is started, where Raman & REM and Bioanalytics and Microanalytical Systems groups are involved. The goal of the entire project is to reduce water demand as well as costs and energy consumption in industrial production processes using modern membrane technologies and treatment methods.

In the Lasers and Particles group, the DetectRespi project was successfully finished together with our project partners. The system for a highly parallel detection of bacterial pathogens of respiratory diseases proved its value in first real-world tests. The biomolecular as well as the optical system are now finished. Also, the FluRam project, dealing with Raman spectroscopy as HPLC and flow-through sensor, has successfully been completed, and a follow-up project will start soon.

In the Isotope Laboratory several publications from the Targeted Environmental Analysis Group have highlighted the necessity of careful sample cleanup prior to dedicated isotope analysis. A quartz crystal microbalance was developed as innovative detector to guide such efforts. In parallel, the Environmental and Isotope Analysis Group provided labelled sulfamethoxazole in a worldwide concerted effort to study the fate of this antibiotic – and associated resistance - in field experiments on four different continents. Both groups spearheaded a community effort for a Nature Water review article that features the prospects of Compound-specific Isotope Analysis for Water Management.

Three new projects are being started in the Bioanalytics and Microanalytical Systems group. In the Bavarian Research Foundation-funded BayWater project, our task is to establish rapid methods for quantifying the reduction efficiency of advanced oxidation processes based on UV-LED activation of peroxodisulfate. This will be addressed for bacteria, viruses and micropollutants using microarray immunoassays, flow cytometry and qPCR. A completely new field of research is being started in the AIF-ZIM LiThermie project: a magnetic particle-based reactor will be established to enrich lithium from geothermal water in an environmentally friendly way. Finally, funding has been awarded within the Horizon Europe "UrbaQuantum" project to establish a monitoring system for pathogenic bacteria and viruses.

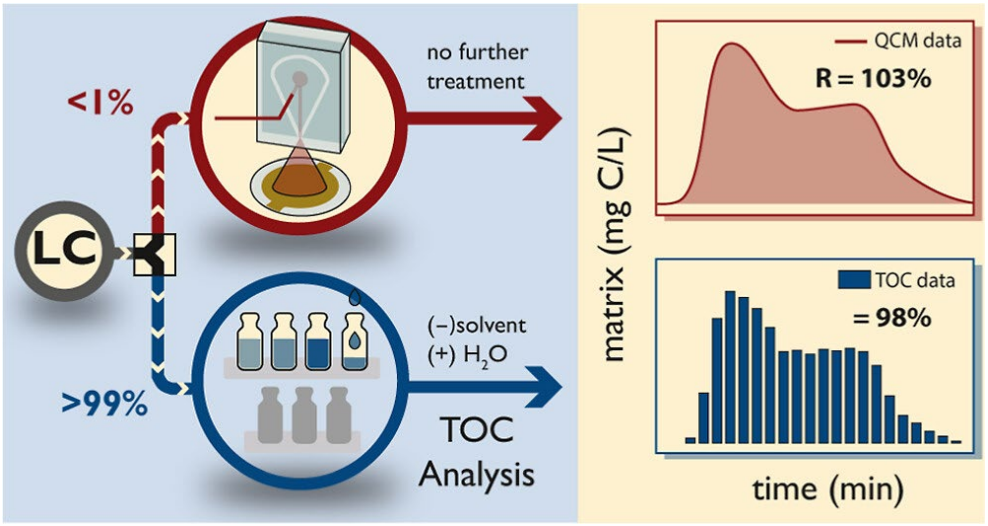
Like every year, my deep thank goes to members of our institute - Ph.D. students, technicians, secretaries, Postdocs and guest scientists – without whom this would not have been possible. And thanks to you, our friends, for your continued support. This year, I look forward to seeing you at our upcoming Alumni Day on July 4th 2025, and in our yearly meeting in fall, where we will have the opportunity again to discuss the latest developments in the water sector. I would be delighted if this would also be an opportunity to team up for common future research initiatives!

Kind regards, Martin Elsner

Quartz Crystal Microbalance as a Holistic Detector for Quantifying Organic Matrices during Liquid Chromatography: 1. Validation

Christopher Wabnitz | Group: Targeted Environmental Analytics

A Quartz Crystal Microbalance is brought forward as a holistic detector for quantifying organic matrices during liquid chromatography and, thereby, to guide sample clean-up prior to dedicated analysis.



A matrix in highly complex samples can cause adverse effects on the trace analysis of targeted organic compounds. A suitable separation of the target analyte(s) and matrix before the instrumental analysis is often a vital step for which chromatographic cleanup methods remain one of the most frequently used strategies, particularly high-performance liquid chromatography (HPLC). The lack of a simple real-time detection technique that can quantify the entirety of the matrix during this step, especially with gradient solvents, renders optimization of the cleanup challenging.

Here, we explored the possibilities and limitations of quartz crystal microbalance (QCM) dry-mass sensing for quantifying complex organic matrices during gradient HPLC. To this end, this work coupled a QCM and a microfluidic spray dryer with a commercial HPLC system using a flow splitter and developed a calibration and data processing strategy. The system was characterized in terms of detection and quantification limits, with LOD = 4.3−15 mg/L and LOQ = 16−52 mg/L, respectively, for different eluent compositions. Validation of natural organic matter in an environmental sample against offline total organic carbon analysis confirmed the approach's feasibility, with an absolute recovery of 103 ± 10%. Our findings suggest that QCM dry-mass sensing could serve as a valuable tool for analysts routinely employing HPLC cleanup methods, offering potential benefits across various analytical fields.

C. Wabnitz, A. Canavan, W. Chen, M. Reisbeck, R. Bakkour, *Anal. Chem.* **2024**, 96, 7429 − 7435, DOI 10.1021/acs.analchem.3c05440

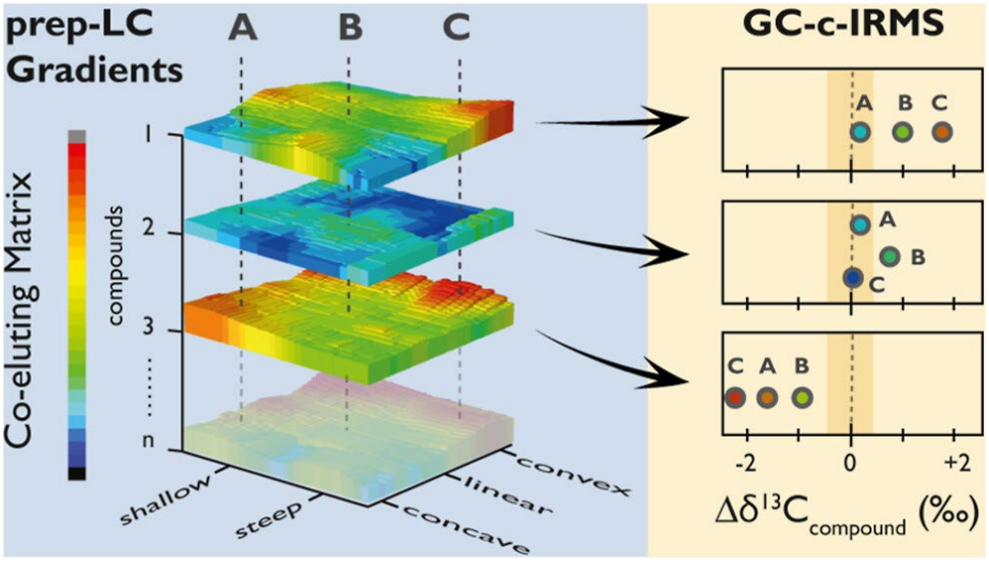
Funding
IWC-TUM

Cooperation
TUM School of Computation, Information and Technology, Heinz Nixdorf Chair of Biomedical Electronics, TUM

Quartz Crystal Microbalance for Quantifying Organic Matrices during Liquid Chromatography: 2. Cleanup for Isotope Analysis

Christopher Wabnitz | Group: Targeted Environmental Analytics

Dedicated sample cleanup by preparative HPLC was guided by a Quartz Crystal Microbalance as innovative holistic detector. The cleanup greatly improved the accuracy of subsequent isotope analysis, which would otherwise have been off by up to 2‰.



C. Wabnitz, W. Chen, M. Elsner, R. Bakkour, *Anal. Chem.* **2024**, 96, 7436 - 7443, DOI 10.1021/acs.analchem.3c05441

In carbon-compound-specific isotope analysis (carbon CSIA) of environmental micropollutants, purification of samples is often required to guarantee accurate measurements of a target compound. We have brought forward an innovative approach to couple a quartz crystal microbalance (QCM) with high-performance liquid chromatography (HPLC) for the online quantification of matrices during a gradient HPLC purification. This work investigates the benefit for isotope analysis of polar micropollutants typically present in environmental samples.

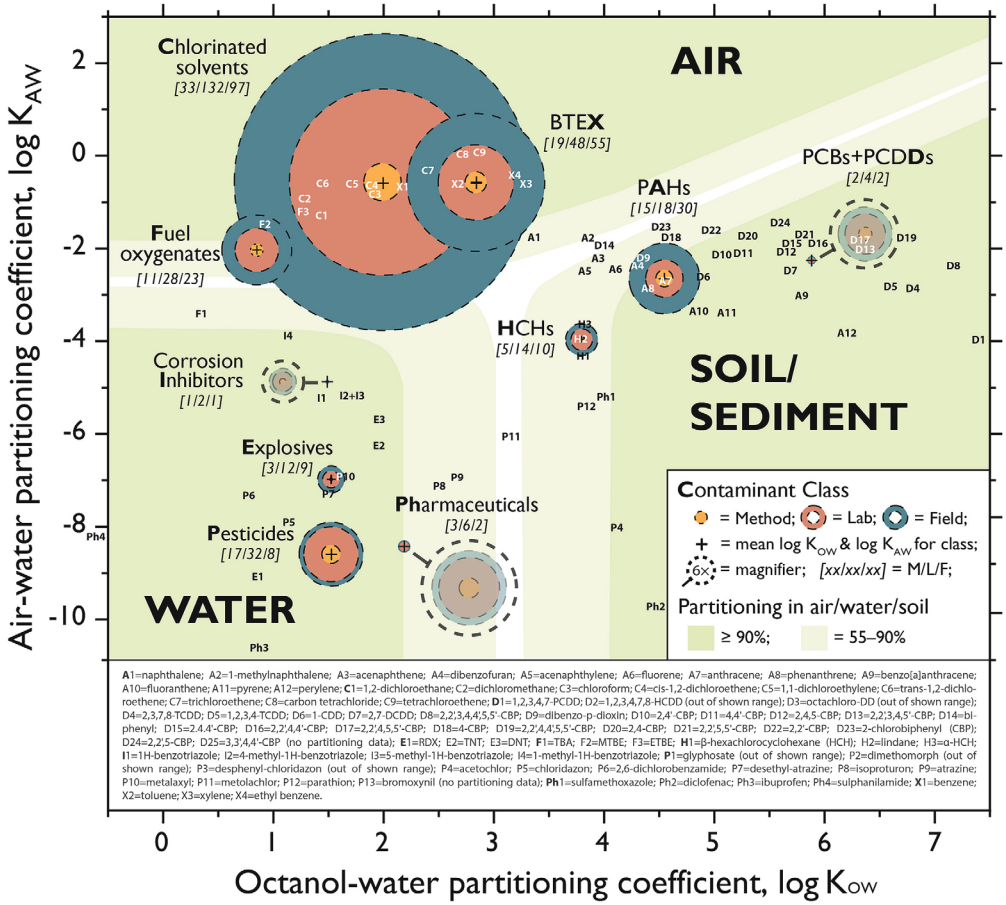
Here, we studied the impact of the natural organic matter (NOM) on the isotopic integrity of model analytes and the suitability of the NOM-to-analyte ratio as a proxy for the sample purity. We further investigated limitations and enhancement of HPLC purification using QCM on C_{18} and C_8 phases for single and multiple targets. Strong isotopic shifts of up to 3.3% toward the isotopic signature of NOM were observed for samples with an NOM-to-analyte ratio $\geqslant$10. Thanks to QCM, optimization of matrix removal of up to 99.8% of NOM was possible for late-eluting compounds. The efficiency of HPLC purification deteriorated when aiming for simultaneous purification of two or three compounds, leading to up to 2.5% less NOM removal. Our results suggest that one optimized HPLC purification can be achieved through systematic screening of 3 to 5 different gradients, thereby leading to a shift of the boundaries of accurate carbon CSIA by up to 2 orders of magnitude toward lower micropollutant concentrations.

Funding
IWC-TUM

Lack of selectivity in sample preparation – An achilles heel of Compound-specific Isotope Analysis for environmental micropollutants

Targeted Environmental Analytics Group

Compound-specific Isotope Analysis is particularly sensitive to background interferences. Considering current limitations, prospects are given on dedicated efforts to improved future sample cleanup.



The role of compound-specific isotope analysis (CSIA) in environmental research has been proven over the last few decades. Despite advances in analytical methods and instrumentation, the Figure above shows that applications of CSIA to low-concentration environmental contaminants, especially at the field scale, remain limited.

We argue that this limitation stems from underdeveloped sample preparation techniques, particularly the lack of required selectivity. Drawing from an extensive review of nearly 600 CSIA studies on contaminants, we (i) analyze methodologies' distribution and dedication to field studies, discussing their connection with the maturity of suitable sample preparation techniques. Additionally, we (ii) examine general trends in sorbent phase technologies, assessing their adequacy to meet CSIA's targeted nature and applicability to micropollutants. In advocating for a paradigm shift, we (iii) emphasize the need to adapt future CSIA development strategies in light of past and current innovations.

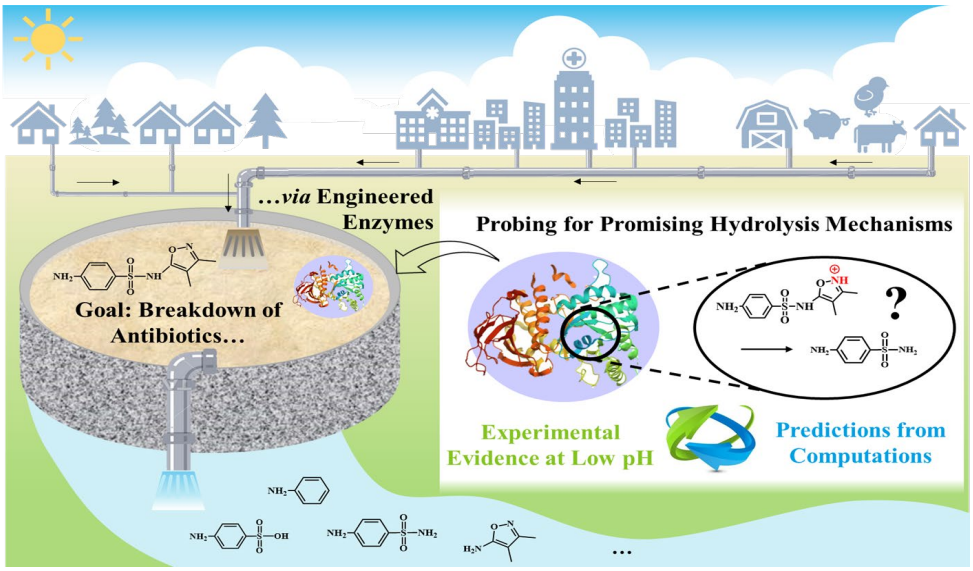
R. Bakkour, C. Wabnitz, D. Glöckler, *Trend. Anal. Chem.* **2024**, 180, 117908, DOI 10.1016/j.trac.2024.117908

Funding
IWC-TUM

Exploring Reaction Paths for Sulfonamide Hydrolysis: Insight from Experiments and Computations

Lihong Chai | Group: Environmental Chemistry and Isotope Analysis

A synergy of experiments and computations is explored to decipher possible hydrolysis mechanisms of sulfonamides. This insight is key to creating novel enzymes with specific functions to remove such antibiotics from water.



Sulfonamides (SAs) have been widely used as antibiotics in human and veterinary medicine. In the environment, they have been detected both in unchanged and in metabolized form as a result of incomplete biotransformation. Antibiotics have attracted particular attention because of their potential to give rise to bacterial antibiotic resistance. Much interest is, therefore, directed at their targeted elimination. While many studies have focused on detecting oxidative biodegradation through associated metabolite identification, only limited information is available on the possibility to break them down via hydrolysis. Therefore, our project probes for putative hydrolysis mechanisms of SAs based on experimental and computational evidence.

Sulphamethoxazole, sulphisoxazole, sulphamethiazole, sulphathiazole, sulphapyridine, sulphadiazine, sulphadimidine and sulphadimethoxine were exposed to a range of pH conditions (2.0, 4.0, 6.0, 8.0, or 10.0) over three months. While most selected SAs were hydrolytically stable in buffer solutions at pH 4.0, 6.0, 8.0, and 10.0, five out of eight SAs (sulphisoxazole, sulphapyridine, sulphadiazine, sulphadimidine, and sulphadimethoxine) were degraded effectively at pH 2.0. In addition, hydrolytic metabolites, such as sulphanilic acid, sulphanilamide, aniline and some of the corresponding leaving groups were identified and quantified by HPLC-UV. We aim to identify further SA transformation products by analysis with Orbitrap high-resolution mass spectrometry (HRMS). In a complementary approach, isotope effects (e.g., $^{13}C/^{12}C$, $^{15}N/^{14}N$) in individual sulfonamide compounds are measured by gas chromatography - isotope ratio mass spectrometry (GC-IRMS). In combination with quantum chemical calculations, we aim to use this evidence to derive a mechanistic understanding as computational guidance for directed evolution of novel enzymes for curbing micropollutant contamination in drinking and waste water.

Funding
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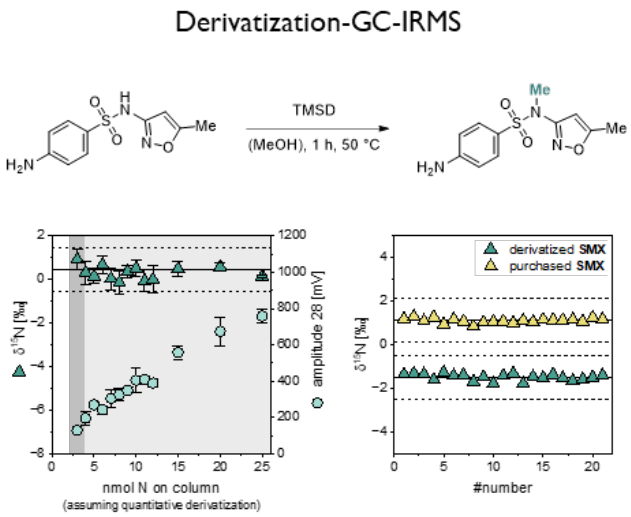
Cooperation
Prof. Dr. Etienne Derat (Sorbonne Université)

Isotope Analysis to Assess the Fate of Sulfamethoxazole

Aoife Canavan | Group: Environmental Chemistry and Isotope Analysis

A derivatization gas chromatography isotope ratio mass spectrometry (derivatization-GC-IRMS) method is developed to access nitrogen isotope values during degradation processes for further mechanistic insights.



The continuous introduction of micropollutants into the environment through livestock farming, agricultural practices, and wastewater treatment is a major concern. Among these pollutants are synthetic sulfonamide antibiotics such as sulfamethoxazole, which are not always fully degraded and pose a risk of fostering antimicrobial resistance. It is challenging to assess the origin and degradation of sulfonamides with conventional concentration measurements. Compound-specific stable isotope ratios ($^{13}C/^{12}C$ or $^{15}N/^{14}N$) can provide additional information because they can trace different sources of the same chemical by their different isotopic fingerprints and detect transformation in the environment based on the detection of associated isotope effects. This study introduces compound-specific isotope analysis of nitrogen-isotope ratios at natural abundances by derivatization-gas chromatography hyphenated with isotope ratio mass spectrometry (derivatization-GC-IRMS) as a new and more precise method for tracing the origin and degradation of sulfonamides. Here, sulfamethoxazole was used as a model compound to develop and optimize the derivatization conditions using (trimethylsilyl)diazomethane as a derivatization reagent. With the optimized conditions, accurate and reproducible $\delta^{15}N$ analysis of sulfamethoxazole by derivatization-GC-IRMS was achieved in two different laboratories with a limit for precise isotope analysis of 3 nmol N on column, corresponding to 0.253 µg non-derivatized SMX. Application of the method to four further sulfonamides, sulfadiazine, sulfadimethoxine, sulfadimidine, and sulfathiazole, shows the versatility of the developed method. Its benefit was demonstrated in a first application, highlighting the possibility of distinguishing sulfamethoxazole from different suppliers.

Q. Dou, A. Canavan, Y. Fu, L. Xiang, Y. Wang, X. Wang, X. Jiang, C. Dirr, F. Wang, M. Elsner, *Anal. Bioanal. Chem.* **2024**, 416, 4237–4247, DOI 10.1007/s00216-024-05361-2.

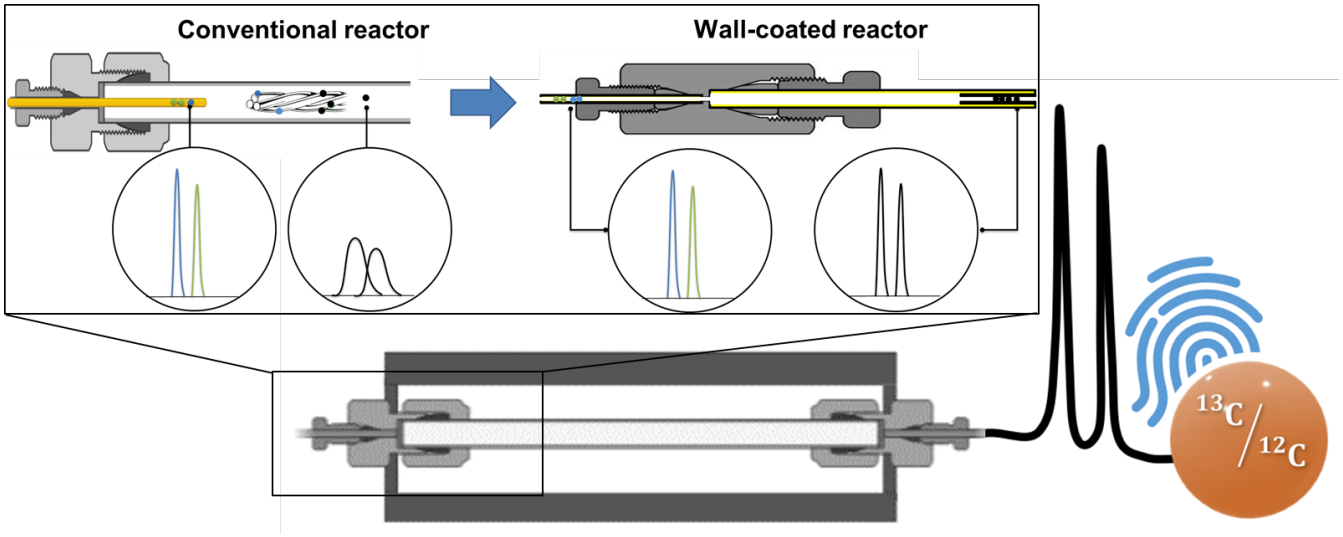
Funding
IAEA – CRP D1.50.22

Cooperation
IAEA

Optimizing Peak Resolution for Compound-specific Isotope Analysis (CSIA)

Habib Al-Ghoul | Group: Environmental Chemistry and Isotope Analysis

A wall-coated tube specifically designed for online combustion in GC-IRMS aims to minimize peak broadening and facilitate GCxGC-IRMS.



The online combustion of analytes between gas chromatography and isotope ratio mass spectrometry (GC-C-IRMS) has enabled compound-specific isotope analysis (CSIA) for various applications, such as assessment of environmental contaminants or doping in sports. However, CSIA is challenged by the need for complete peak separation and for best sensitivity.

Comprehensive gas chromatography could deliver a breakthrough, but hinges on the development of robust miniaturized online combustion tubes that offer sufficient oxidation capacity and catalytic surface area to accomplish complete analyte conversion to CO_2, while being narrow enough to preserve narrow analyte peak shapes within the continuous flow carrier stream. The current step change when He carrier gas passes from GC capillary columns (inner diameter, i.d.: 0.22–0.32 mm) to commercial combustion tubes (i.d.: 0.5 mm) generates substantial peak broadening. Even smaller GC capillaries are needed, however, to support GCxGC applications and to improve sensitivity by reducing flows and, therefore, minimizing losses in an open split before IRMS. Since commercial reactor tubes are not compatible with fast GC-C-IRMS and GCxGC-C-IRMS, efforts have been directed at developing alternative miniaturized reactor tubes.

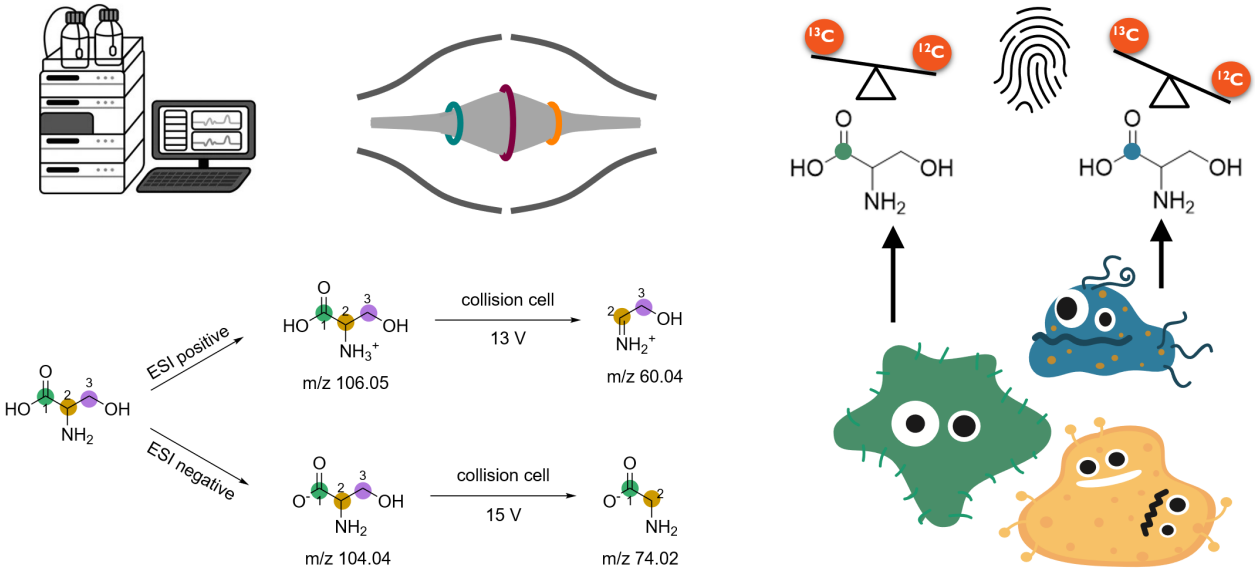
Funding
IWC-TUM

To pioneer the necessary dramatic reduction of reactor tube size, a Ni wall-coated catalytic microreactor is constructed by electroless plating. This approach has the benefit of simplicity, while allowing for the fabrication of narrow bore capillary reactors (inner diameter < 0.2 mm), which is not achievable with hand loading of metal wires. The weight of the coating is determined by ICP-MS, while the layer thickness is measured by SEM and EDX. An 18 cm long Ni layer is coated in the middle of a 30.5 cm long quartz (o.d. 1.5 mm, i.d. 0.32 mm) to fit the furnace hot zone. Precise and accurate data were obtained for caffeine, with an overall mean $\Delta\delta^{13}C$ of -0.16‰ and a standard deviation of ±0.12 ‰.

Position-specific isotope analysis of serine via Orbitrap mass spectrometry

Leonhard Prechtl | Group: Environmental Chemistry and Isotope Analysis

Position specific $^{13}C/^{12}C$ analysis at natural abundance in the amino acid serine is targeted by Orbitrap mass spectrometry. The goal is to monitor the metabolism and origin of legionella for which serine serves as nutrient.



Serine is a proteinogenic amino acid and an essential nutrient for the bacterium *Legionella pneumophila*, which relies on serine as its primary source of carbon and energy. Consequently, variations in the metabolism of *L. pneumophila* are expected to be reflected in the carbon isotope ratios of serine within its proteins.

Traditional methods for serine isotope ratio analysis have relied on bulk isotope analysis of pure serine using EA-IRMS, with position-specific analysis of the carboxy carbon achieved through ninhydrin reaction and subsequent CO_2 measurement. Comprehensive position-specific isotope analysis of serine has previously required extensive derivatization for GC-Orbitrap analysis.

We explored a novel method for position-specific isotope analysis of serine using ESI-Orbitrap, eliminating the need for derivatization. This method combines whole-molecule isotope ratio measurements with those obtained from various fragments generated in a collision cell, in both positive and negative ESI modes.

To support this method, we have prepared homogeneous position-specific carbon isotope standards for all carbon atoms in serine, resulting in eight distinct standards with varying $^{13}C/^{12}C$ isotope ratios. These standards enable precise calibration and referencing of serine isotope measurements on the Orbitrap mass spectrometer and facilitate inter-laboratory comparisons of measured isotope ratios.

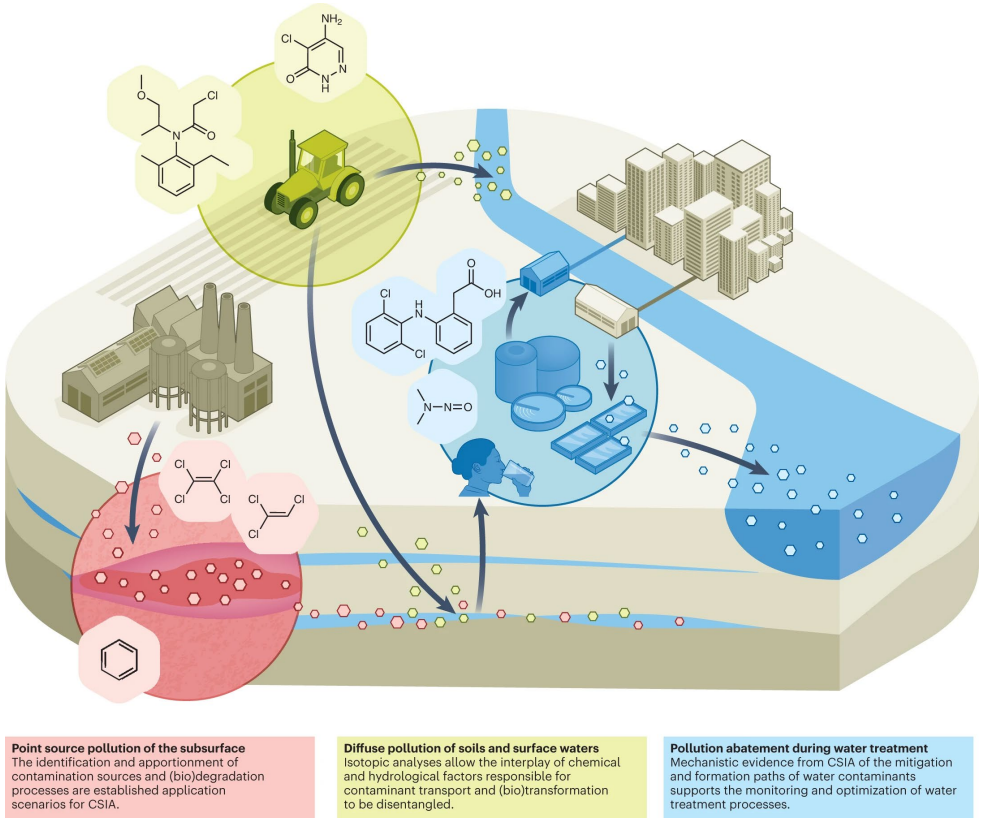
Funding
IWC-TUM

In the future it is our objective to conduct metabolic studies of *L. pneumophila* by monitoring the change of serine carbon isotope ratios without the need of expensive ^{13}C-labeled serine in the growth medium. This might also allow metabolic studies of *L. pneumophila* samples directly in environmental settings.

Compound-specific isotope analysis of organic contaminants to assess environmental fate and manage chemical pollution

Environmental Chemistry and Isotope Analysis / Targeted Environmental Analytics

Prototypical scenarios of water contamination from legacy pollutants at contaminated sites, agricultural use of pesticides, and abatement of pollutants in water treatment systems illustrate success stories of CSIA and ongoing developments for future applications.



T. B. Hofstetter, R. Bakkour, D. Buchner, H. Eisenmann, A. Fischer, M. Gehre, S. B. Haderlein, Patrick Höhener, D. Hunkeler, G. Imfeld, M. A. Jochmann, S. Kümmel, P. R. Martin, S. G. Pati, T. C. Schmidt, C. Vogt, M. Elsner, *Nature Water* **2024**, 2, 14–30, DOI 10.1038/s44221-023-00176-4.

The management and mitigation of chemical pollution are key elements of sustainable development initiatives that aim to provide safe and clean water. While environmental scientists are developing the capabilities to assess the fate, (eco)toxicity and risks of a plethora of synthetic chemicals comprehensively, notorious pollution scenarios and decontamination challenges call for targeted and case-specific evaluation of chemical hazards.

We review the utility and perspectives of compound-specific isotope analysis for obtaining an understanding of environmental processes that allows one to identify pollution sources, assess contaminant (bio) transformation and gain insights into reaction pathways. Three prototypical scenarios of water contamination, namely point-source pollution of groundwater at contaminated sites, diffuse pollution of soils and surface waters through pesticide use and the abatement of pharmaceuticals and disinfection by-products in water treatment systems, illustrate success stories of compound-specific isotope analysis and highlight current developments to address challenges for future applications.

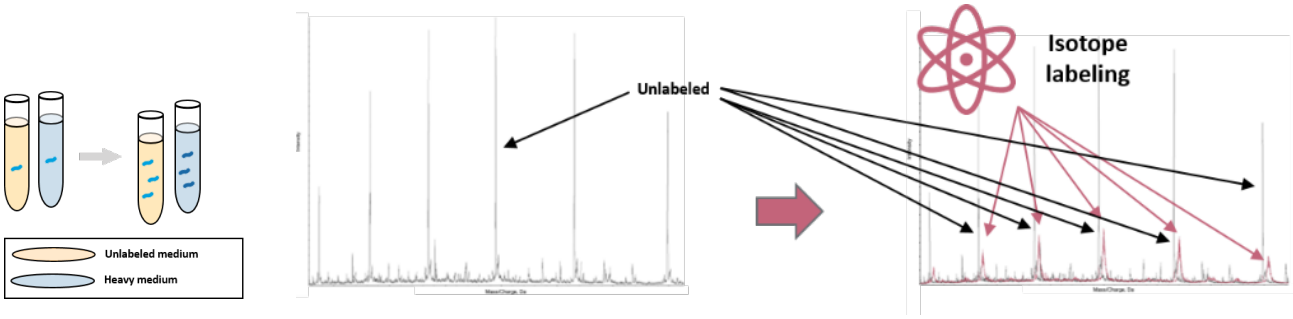
Funding
IWC-TUM

Cooperation
Expert Group on Environmental Isotopes, Water Chemistry Society, GDCh

A preclinical model for a new tuberculosis therapy based on mass spectrometry, isotopic labeling, and artificial intelligence

Anja Dollinger | Group: Lasers and Particles

Stable isotopic labeling of Mycobacteria, amongst them the bacterium causing tuberculosis, is used to track dynamic changes in protein synthesis and gain insights into metabolic mechanisms. This approach helps studying antibiotic effects and their impact on cellular metabolism, with LC-MS facilitating precise protein identification.



Each year, approximately 1.25 million people worldwide die because of tuberculosis (TB) [1]. Successful treatment of this disease requires the administration of at least four antibiotics over a period of 4-12 months. This is problematic because these therapies are costly, have many side effects, and lead to genetic and phenotypic resistances (dormancy; persister cells). There is a high need to shorten therapy and develop new treatment strategies ("End-TB-Strategy", WHO) [1], as well as to find new combinations of standard drugs and personalize the treatment. However, preclinical models that simulate the interaction between multiple agents are lacking.

To better understand how different drugs work, this project aims to develop advanced proteomic technologies by combining HPLC, mass spectrometry (Q-TOF), and self-learning algorithms. Stable isotopic labeling is used to quickly detect changes in mycobacterial metabolism by observing dynamic alterations in mature full-length proteins. The newly developed pipeline employs self-learning algorithms to track proteins across various charge states and modifications. Additionally, a workflow for analyzing LC-MS data and a reference database for intact mycobacterial proteins were created, enabling the comparison and detailed study of different samples, including the identification of secondary modifications. Stable isotopic labeling helps visualize protein synthesis rates and the impact of antibiotics on the bacteria.

References
[1] World Health Organization, Global tuberculosis report 2024, **2024**.

Funding
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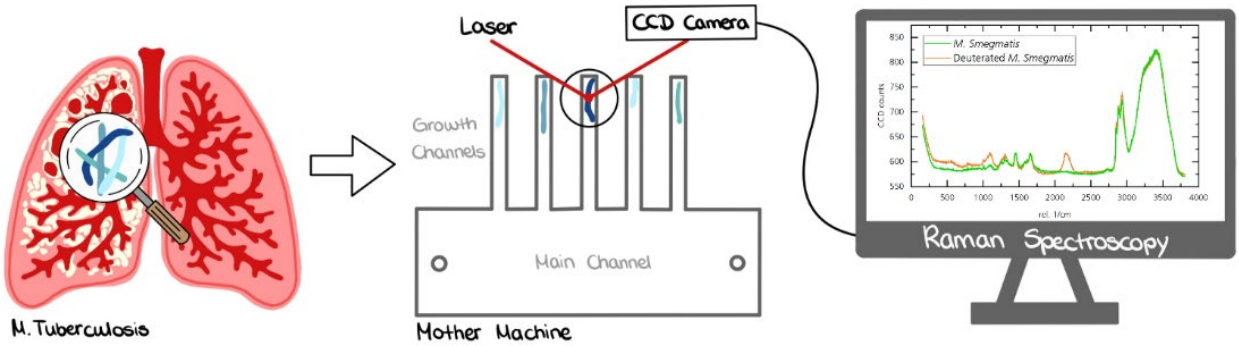
Cooperation
Ludwig-Maximilians-University of Munich

Helmholtz Center Munich German Research Center for Environmental Health

Vibrational spectroscopic methods for high-throughput investigations on individual bacteria

Ida Kalleder | Group: Lasers and Particles

The *mother machine* is a microfluidic system featuring a larger main channel and narrow dead-end side channels. A single bacterium, called mother cell, can be trapped in those growth channels and investigated over several generations in a non-fixed mode employing a combination of Raman spectroscopy and stable isotope labeling.



Tuberculosis (TB) is one of the deadliest infectious diseases worldwide. The treatment of TB is inherently difficult due to the ability of the bacteria to switch into a dormant state, in which the metabolism is shut down, and no antibiotics can affect the bacteria [1]. The search for new and more effective drug combinations and their effect on bacteria on a single-cell level is, therefore, of high interest.

To investigate the effect of toxins, e.g., antibiotics, on *Mycobacterium tuberculosis*, the model bacterium *Mycobacterium smegmatis* is introduced into the mother machine consisting of the broader main channel for nutrient supply and narrow (~2 µm) growth channels trapping single bacteria. The bacteria in the growth channels can be exposed to different drugs, followed by an incubation step with a medium containing 50% deuterated water at 37 °C for 16 h. The incorporation of the deuterated medium and, thus, the C-H/C-D exchange in single cells can be investigated using a Raman system.

The measurement results are displayed through false-color images, giving the ratio of deuterated and undeuterated components of the bacteria. By the deuterium content of the bacteria, the metabolism activity after toxin exposure can be evaluated, and differences between live and dead bacteria can be seen.

References
[1] Salina et al., Microorganisms **2022**, DOI 10.3390/microorganisms10122334
[2] Long et. al., Lab on a Chip **2013**, DOI 10.1039/C2LC41196B

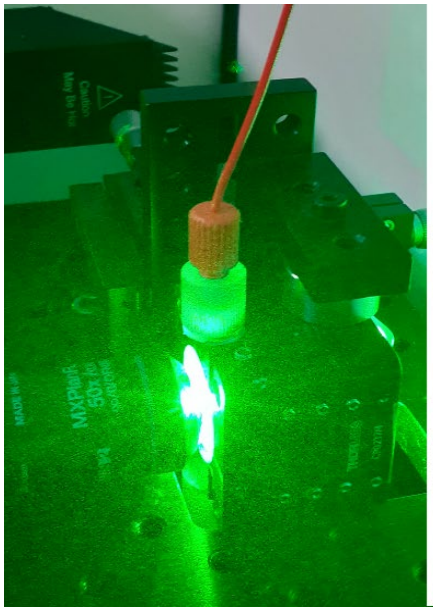
Funding
IWC-TUM

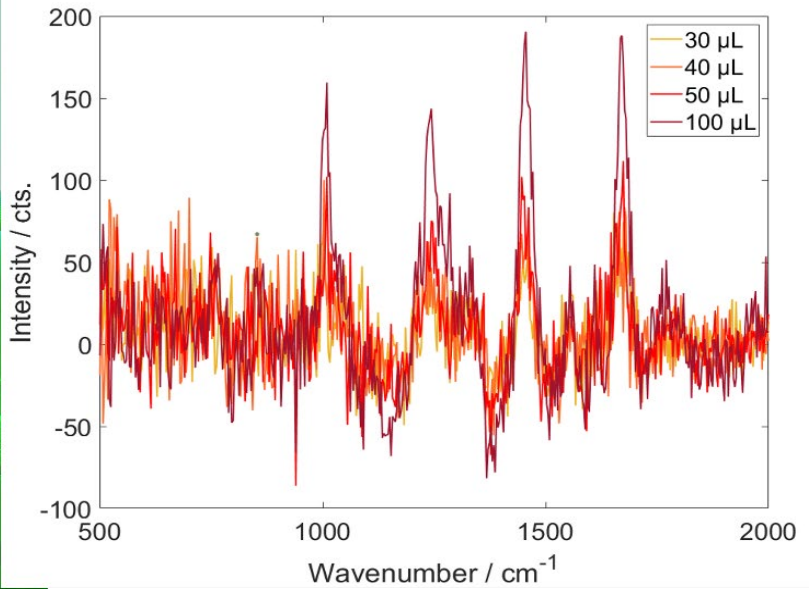
Fraunhofer ITMP-IIP

FluRam: A Raman-based HPLC detector

Lucas Hirschberger | Group: Laser and Particles

Raman spectroscopy is a selective analytical technique based on molecular vibration. We venture to employ this technique as a novel approach for HPLC detection.





High-performance liquid chromatography (HPLC) is a widely used analytical separation technique. Raman spectroscopy provides molecular characteristics, enabling non-destructive analysis of chemical composition and molecular structure. This project uses a high-power laser (532 nm; <1.5 W) and very specific optics to achieve a high signal intensity. The chromatographic separation can be accurately analyzed in real time, enabling the optimization of synthesis and purification processes. In the developed detector prototype, a quartz capillary is installed with standard HPLC connectors on both sides. Quartz glass is the optimal material as a window material because of its lower number of bands and its position in the spectrum. A measurement and evaluation scheme at various flow rates for different eluents is developed for coupling the detector to an HPLC system.

Using a size exclusion chromatography (SEC) column, we investigated the application of the detector system for the separation and structure analysis of various proteins, such as monoclonal antibodies (mAb). The transient background enhancement in the Raman spectrum due to the fluorescence properties of the analyte requires for dedicated chemometric data evaluation procedures. While the flow system is primarily designed for HPLC detection, it it can be employed for process analysis in chemistry and pharmacy.

Funding
AiF-ZIM

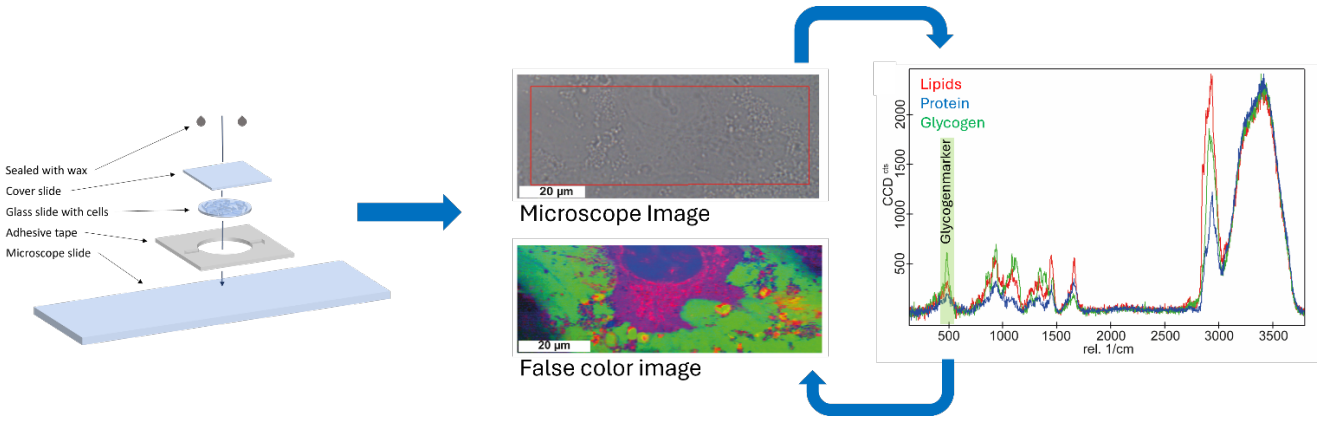
Cooperation

Soliton GmbH
Solectrix GmbH

Raman imaging of myoblasts for the label-free detection of cellular components

Eva Krois | Group: Laser and Particles

Raman imaging is used to gain further knowledge on *Pompe* disease on a single-cell level. The local distribution of proteins, lipids, and glycogen is investigated. Our findings may help to improve treatment of this rare muscle disease.



Pompe disease is a rare, inherited muscle disorder caused by a decreased or complete failing activity of lysosomal acid alpha-glucosidase (GAA). This enzyme is responsible for breaking glycogen into glycose. Thus, *Pompe* disease leads to an accumulation of glycogen in tissue, especially in cardiac and skeletal muscles. Patients who suffer from *Pompe* disease struggle with muscle weakness, breathing difficulties, later leading to wheelchair dependency, among others. This clinical picture results in a need for further investigation of *Pompe* disease [1].

Myoblasts are a precursor form of muscle tissue and, therefore, are of special interest regarding the topic. Through Raman imaging it is possible to investigate myoblasts non-destructive, label-free, non-fixated, on a single-cell level. The cells are placed in a custom-designed closed measurement chamber, ensuring a stable environment and a constant nutrient supply during the measurement. Results of the Raman imaging are depicted in false color images showing the three components that are of highest interest: proteins (blue; mainly found in the nucleus), lipids (red, found in lysosomes surrounding the nucleus), and glycogen (green; found in accumulations in the cytoplasm). Our work shows two main findings: First, already myoblasts, as a very early form of cell culture, show high accumulations of glycogen in cells affected by *Pompe* disease compared to control cells; second, the accumulations of glycogen in cells affected by *Pompe* disease can not only be found in lysosomes, as expected but in large planar areas in the cytoplasm. These findings can lead to a deeper insight into *Pompe* disease on a single-cell level and can contribute to a broader understanding of the disease.

Funding
IWC-TUM

Cooperation
Friedrich-Baur-Institute at the Department of Neurology, LMU, Munich

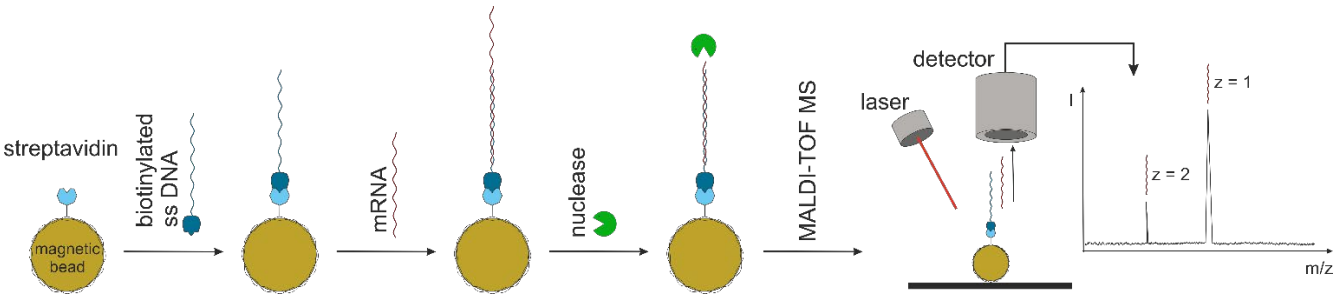
References

[1] Hintze, S. et al., *Int. J. Mol. Sci.* **2020**, 21, 2642; doi:10.3390/ijms21072642.

Monitoring system for bacterial nucleic acids

Susanne Dietrich | Group: Lasers and Particles

The bacterial nucleic acid metabolism is monitored via hybridization on magnetic particles and matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) readout.



Tuberculosis is amongst the most common causes of death from a single infectious agent worldwide. Mycobacteria can down-regulate their metabolism for extended periods, making them less susceptible to antibiotic treatment. The currently recommended treatment extends over four to six months, with drugs being rich in side effects. Investigating the regulatory mechanisms involved at a cellular level is essential to develop efficient therapies [1, 2]. However, an analytical method for determining the metabolic state of such bacteria is missing.

The first step in the gene expression process is transcription, where genetic information stored in DNA is transcribed in a messenger-RNA (mRNA). This mRNA fulfills the messenger function in protein biosynthesis (translation). Gene expression is regulated dynamically to react to changes in the activity state of the cell. By analyzing parameters such as the rate of formation, quantity, and composition of mRNA over time, the adaption of the metabolic activity of the cells can be understood and characterized.

Functionality and performance were tested successfully on magnetic beads coated with the complementary DNA as substrate. Analysis was performed by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) without a further elution step. The specificity was determined by hybridization of DNA oligonucleotides, which differ in up to six nucleobases in the middle of the strand. It turned out that one mutation leads to a significant signal reduction. Specificity is higher for mutations located in the middle of the target strand. Despite the use of single-strand specific nucleases, it was not yet possible to obtain blunt ends after the digestion of a single-stranded overhang, but either varying degrees of digested overhang or partly digested hybrids. The assay is now tested on extracted RNA from bacteria.

References

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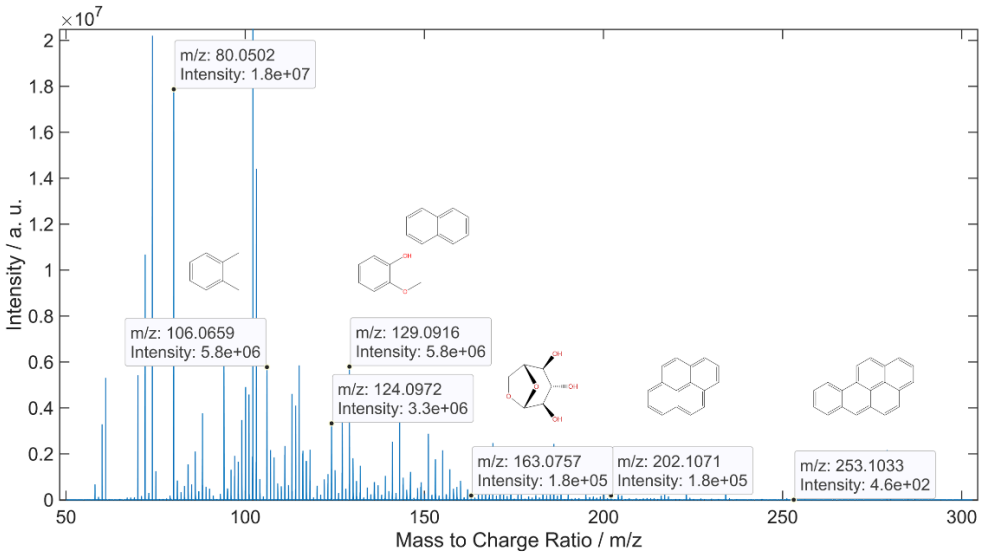
Cooperation
Institute of Infectious Diseases and Tropical Medicine, LMU

Chemical characterization of atmospheric particles by laser desorption MS

Felix Ludwig | Group: Lasers and Particles

Laser desorption (LD) mass spectrometry offers a new approach to fast qualitative analysis of particulate matter sampled from the atmosphere.



Aerosols in the environment have been known to affect the human health long-term. Increasingly, ultrafine particles (UFPs) with a diameter smaller than 100 nm have caught the attention of the research community, as they have a high retention in the lungs. Since the toxicity of these particles is highly dependent on their chemical composition, analytical methods for the qualitative and quantitative analysis are necessary [1]. The standard procedure centers around high performance liquid chromatography (HPLC) in combination with mass spectrometry, which necessitates laborious sample preparation and long measurement durations. This project focusses on the development and examination of routine-applicable methods to characterize the molecular composition of fine and ultrafine particles.

Since the qualitative analysis of particle collections sampled on aluminum prove to work, as shown in last years report, the next step lies in the optimization of the system. By integration of a closed-off laser cell and heated transfer tubing, the background signal was drastically reduced. A change in the sample substrate material to quartz led to an sample-independent LD, since we were able to heat the substrate with our IR-Laser irrespective of the sample quantity and material. This could be the decisive step towards quantitative LD-MS without internal standard and is the focus of our research in 2025.

Funding
IWC-TUM

References

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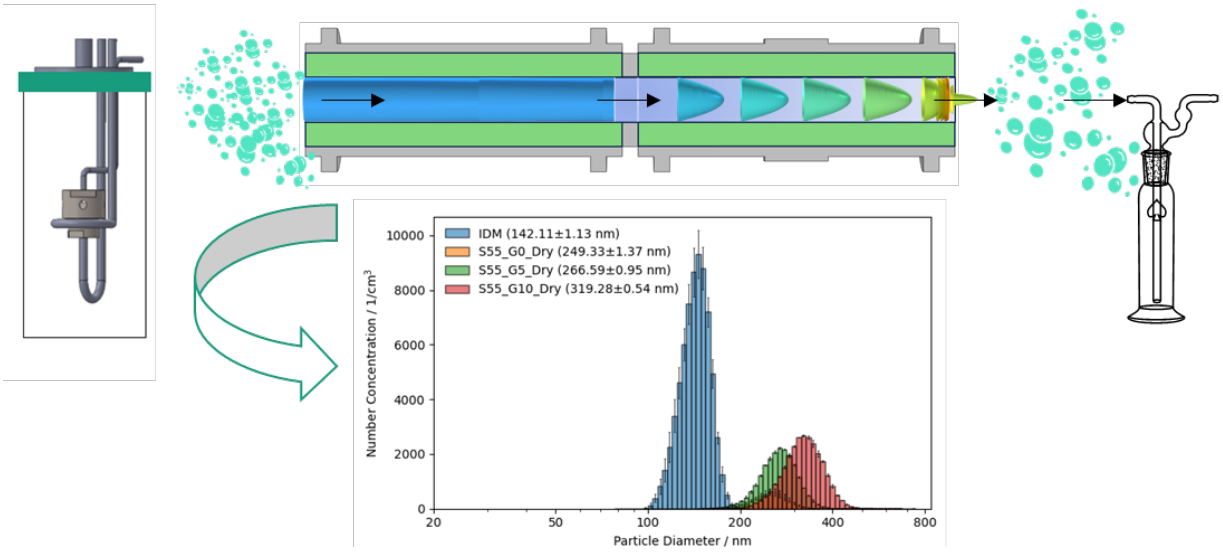
Generation and sampling of human respiration: viability preservation of airborne microorganisms

Nico Chrisam | Group: Laser and Particles

A laboratory setup for the analysis of human(-like) respiratory aerosol is developed to validate existing aerosol instrumentation and identify the effect of environmental changes on pathogen transmission and viability.



Inactivation is a common issue when analyzing bioaerosols. Microorganisms only propagate successfully under specific conditions of temperature, humidity, and pressure. Analytical instruments often alter these conditions, causing stress to the organisms resulting in a loss of viability and microbial activity. To thoroughly analyze the life cycle of airborne microorganisms from emission to deposition, it is crucial to minimize the impact of the analysis methods on the analyte [1].

Common methods for aerosol generation produce a high number of particles (10^5 - 10^7 cm^{-3}) but often compromise microbial viability due to repeated resuspension, high shear forces, or sudden changes in humidity. We developed a nebulization system based on Bubble-Burst, which mimics particle production in human respiration. To elevate the sampling efficiency of air-suspended viruses and bacteria, we propose the use of a growth tube in conjunction with an impinger. This system aims to minimize adverse conditions during sampling by condensing water at supersaturated conditions onto the droplets, thereby preventing desiccation and increasing the analyte's size.

References
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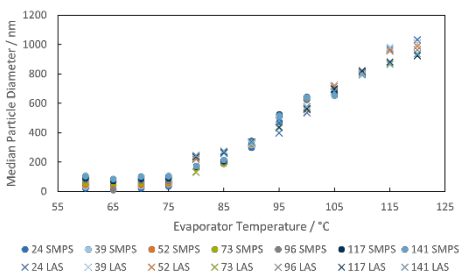
Funding
IWC-TUM

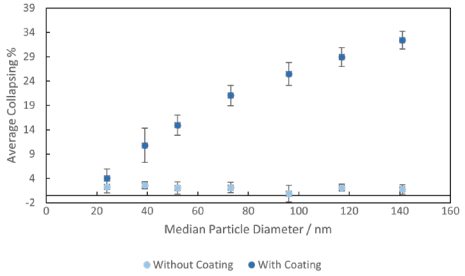
Cooperation
Fraunhofer ITMP

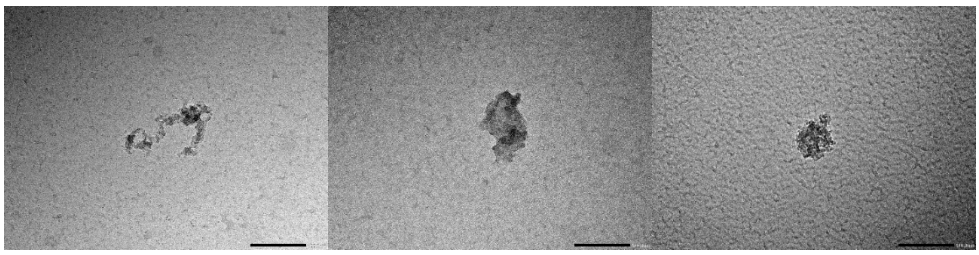
Size-Dependent Collapsing of Soot-Like Particles

Kevin Maier | Group: Laser and Particles

The collapse of soot-like particles after coating with 1-Hexadecanol and removal of the coating with a catalytic stripper was systematically investigated for different initial particle sizes.







The restructuring of soot particles is a known phenomenon influencing the morphology and optical properties of the particles. [1,2] In our work we investigated the effect of coating and coating-removal with a catalytic stripper.

For that, a monodisperse aerosol containing soot-like particles was produced with a spark discharge generator and differential electrical mobility classifier. This aerosol was generated with median electrical mobility diameters ranging from 24 to 141 nm. The particles were coated by mixing with 1-Hexadecanol vapor at elevated temperatures and subsequent cooling to room temperature leading to supersaturation and ultimately condensation. By varying the evaporator temperature to produce the coating vapor, the concentration could be varied. With a higher concentration of coating material, a thicker coating layer was reached as shown in the top left figure. With that particle diameters of up to 1 µm were obtained. The final diameter reached after coating was found to be independent of the initial particle diameter and only dependent on the coating vapor concentration. The coating was removed from the particles again by catalytic oxidation, which led to a collapse of the soot-like particles. This collapse depended on the initial particle size, with a reduction of the median electrodynamic diameter of up to 30 % for particles with an initial size of 141 nm as shown in the top right figure. Investigating the differences between the untreated (bottom left), the coated (bottom middle), and the coated and stripped particles (bottom right) with TEM, a restructuring of the formerly fractal soot-like particles towards collapsed particles was observable.

Funding
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References
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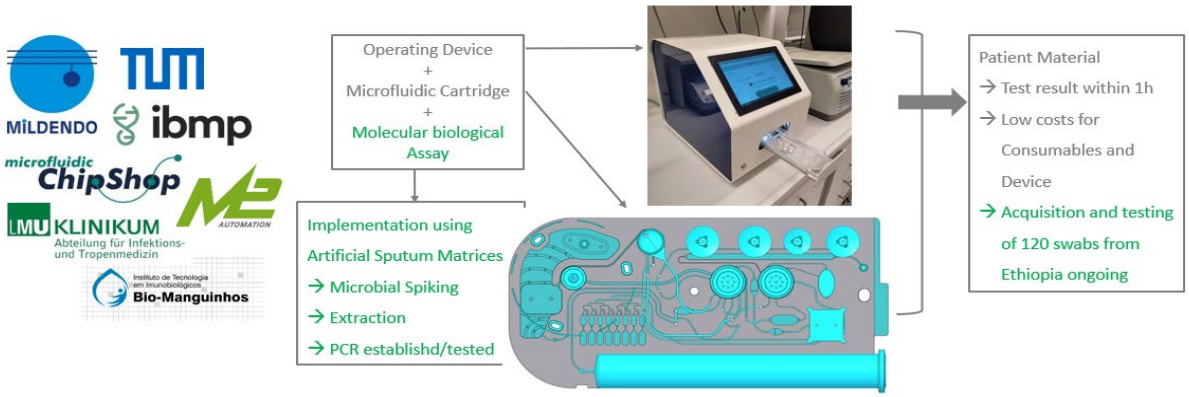
[2] Bambha et al. *Carbon* **2013**, DOI 10.1016/j.carbon.2013.04.070

Development of a molecular biological Lab-on-a-Chip-Platform for the highly parallel detection of bacterial pathogens of respiratory diseases

Amelie Hohensee, Eva Krois | Group: Laser and Particles

Realization of a molecular biological platform for the highly parallel detection of viral and bacterial pathogens of respiratory diseases. The main tasks were the establishment of the biochemical assays for the Lab-on-a-Chip platform regarding the bacterial and fungal respiratory panel, as well as the design and implementation of the optical readout system.



One of the main tasks is the design of specific primers and probes for the individual microorganisms of the respiratory panel. Real Time PCR, specifically the TaqMan System, serves to evaluate the designed primers and probes. The sensitivity, specificity, and the amplification efficiency of the PCRs are determined. The evaluation is followed by multiplexing experiments, which are essential for the final implementation of the cartridge. PCR-positive controls are established by cloning and support the work on primer evaluation and multiplexing. In a later process of the cartridge development, the designed probes are immobilized on a three-dimensional matrix on the DNA microarray. Fifteen of the final 16 primer pairs for eight organisms are designed and tested on sensitivity, specificity, and amplification efficiency by PCR. Specific hydrolysis probes are designed and tested in real-time PCRs. The functionality tests are performed on organism-specific genomic DNA, cloned positive controls, and nucleic acid extracts of respiratory patient samples. The first experiments on primer and probe multiplexing were performed, but the final results are still pending.

The fluorescence dye Cy5 is used to detect the DNA microarray afterward. Therefore, an optical readout system is set up. The unit includes a laser diode as an excitation source with a wavelength of 654 nm and a CMOS-sensor-based camera. In addition, a set of suitable filters and a dichroitic mirror are used to ensure optimal excitation, homogenous illumination, and a reliable readout with a sufficient signal-to-noise ratio. The system will be implemented into the device designed by the cooperation partner.

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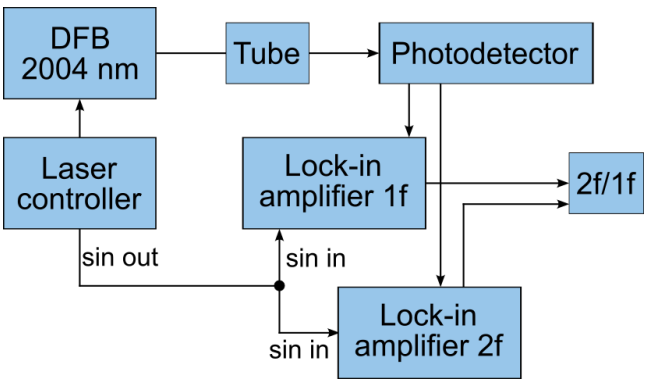
SEICOR: Ship Emission Inspection with Calibration-free Optical Remote Sensing

Ahmad Assarenayati, Quentin Ewinger | Group: Laser and Particles

An open-path Tunable Diode Laser Absorption System is developed to monitor gaseous and particulate emissions from ships passing through the light beam. Typical applications are harbor entrances, rivers, or channels.



Different gas emissions of combustion engines can be detected by UV-, vis- or IR optical absorption. Open-path absorption spectroscopy, where a light beam is sent through the volume of interest, and the transmitted light is detected, is suitable for distances of kilometers and more. In our case, a retroreflector on the opposite side of the ship, usually on the other side of the waterway, reflects the light back so that the light source and the detection can be placed at the same position. To reduce the signal-to-noise ratio, a distributed feedback (DFB) laser and a lock-in detector are employed. The laser and detection setup will be integrated into the Airyx telescope to be tested over a longer distance.

In parallel to the gas-phase detection, we also work on a setup for the detection of soot emissions from the ship. Soot absorbs light over a wide range in the UV and vis. The spectral behaviour in this range is described by the Ångström coefficient, which varies for different soot species and ages. Measurements at several wavelengths may be suitable to even distinguish soot from different origins.

Funding
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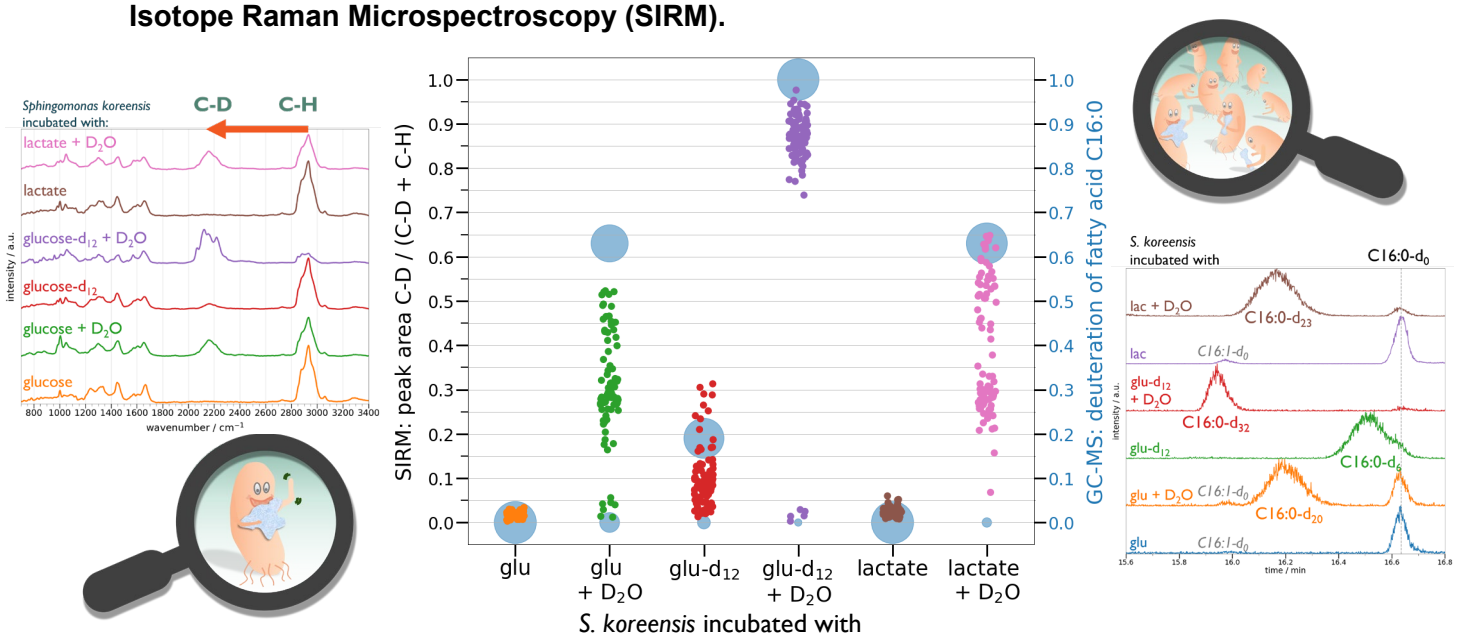
Comparison of Raman Microspectroscopy and Fatty Acid Methyl Ester (FAME)-GC-MS to Quantify Deuterium Incorporation in Bacteria

Kara Müller | Group: Raman & SEM

A Fatty Acid Methyl Ester Gas Chromatography-Mass Spectrometry (FAME-GC-MS) method was established to compare bulk microbial lipid deuteration to total cell deuteration of single cells measured by Stable Isotope Raman Microspectroscopy (SIRM).



Biodegradable polymers are desired for many agricultural applications, where they are difficult to retrieve entirely after their use. While conventional techniques to analyze plastic biodegradation, such as monitoring CO_2 production, miss a direct link between the polymer and the degradation products, we established a stable isotope Raman microspectroscopy (SIRM) approach to trace deuterium from labeled plastics into microbial biomass.[1] Based on the vibrational fingerprint spectra, we observed deuterations of single microbial cells based on the red-shift of the C-H vibrations of lipids, proteins, and DNA into the Raman-silent region after degradation of perdeuterated deuterated polylactic acid (dPLA). Those C-D vibrations indicated a larger D-lipid to D-protein and D-DNA ratio compared to reference experiments with D_2O and glucose-d_{12}. These findings suggest that the depolymerization products of dPLA can be used as direct building blocks for lipids.

In a complementary approach, fatty acid deuteration of bulk samples can be quantified by derivatization to fatty acid methyl esters with subsequent analysis by gas chromatography-mass spectrometry (FAME-GC-MS). In a feasibility study we compare these complementary techniques for two different bacteria strains deuterated with different substrates (D_2O in combination with glucose or lactate and glucose-d_{12}). While SIRM provides information on the total deuteration of single cells and their lipid to protein and DNA ratios, FAME-GC-MS allows to separate deuterated from non-deuterated fatty acid methyl esters based on retention times and further identifies different isotopologues. The next step is using this approach to study the biodegradation of dPLA.

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Dr. Hanna Wacklin-Knecht (European Spallation Source, Lund University)

Dr. Jürgen Allgaier (FZ Jülich)

Maria Heiling (IAEA)

Reference
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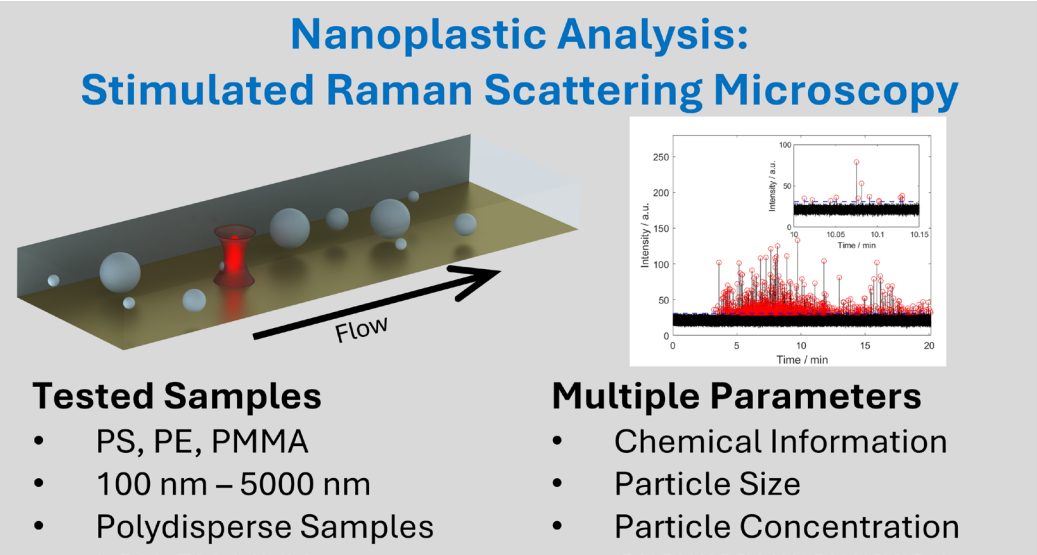
Multi-Parameter Analysis of Nanoplastics in Flow

Maximilian Huber | Group: Raman & SEM

Stimulated Raman Scattering can be used to derive chemical information, concentration and particle size at the individual particle level. Due to the significantly reduced integration time, it enables nanoplastics analysis in flow with high time resolution and sensitivity compared to spontaneous Raman.



M. J. Huber, L. Zada, N. P. Ivleva, F. Ariese, *Anal. Chem.* **2024**, 96, 22, 8949–8955, DOI 10.1021/acs.analchem.3c05881.

Here, we demonstrate the detection of nanoplastics (NPLs) in flow with Stimulated Raman Scattering (SRS) for the first time. NPLs (plastic particles <1000 nm) have recently been detected in different environmental samples and personal care products. However, their characterization is still an analytical challenge. Multiple parameters, including size, chemical composition and concentration (particle number and mass) need to be determined. In an earlier paper, online field flow fractionation (FFF)-Raman analysis with optical trapping was shown to be a promising tool for the detection of particles in this size range.[1] SRS which is based on the enhancement of a vibrational transition by the matching energy difference of two laser beams, would allow for much more sensitive detection and, hence, much shorter acquisition times compared to spontaneous Raman microspectroscopy (RM).[2] Here, we show the applicability of SRS for the flow-based analysis of individual, untrapped NPLs. It was possible to detect polyethylene (PE), polystyrene (PS) and poly(methyl methacrylate) (PMMA) beads with diameters of 100 – 5000 nm. The high time resolution of 60.5 µs allows us to detect individual signals per particle and to correlate the number of detected particles to the injected mass concentration. Furthermore, due to the high time resolution, optically trapped beads could be distinguished from untrapped beads by their peak shapes. The SRS wavenumber settings add chemical selectivity to the measurement. Whereas optical trapping is necessary for the flow-based detection of particles by spontaneous RM, the current study demonstrates that SRS can detect particles in a flow without trapping. Additionally, the mean particle size could be estimated using the mean width (duration) and intensity of the SRS signals.

Funding
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Cooperation
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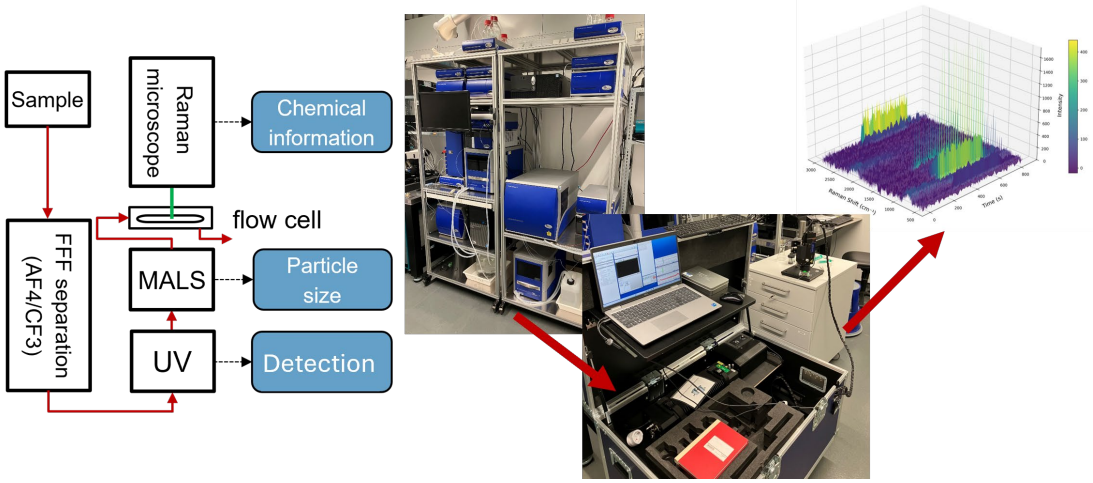
References
[1] Schwaferts et al., *Anal. Chem.* **2020**, doi.org/10.1021/acs.analchem.9b05336.
[2] Zada et al., *J. Raman Spectrosc.* **2018**, doi.org/10.1002/jrs.5367.

Towards an Efficient Online Raman Detector for Field Flow Fractionation

Maximilian Huber | Group: Raman & SEM

Online-coupled field flow fractionation (FFF)-confocal Raman microspectroscopy (RM) allows for a physicochemical characterization of nanoplastics. To get a step closer towards routine analysis, here, a more cost-efficient Raman detector was evaluated.



Increasing awareness of micro- and nanoplastic pollution in the environment is accompanied by growing interest in approaches for the comprehensive analysis of the associated particles. While several techniques are available that can provide concentration, size and material characterization for investigations in the microplastic range (1 µm – 1 mm), studies in the nanoplastic range (below 1 µm) remain challenging. One hybrid technique that shows great potential is the online combination of field flow fractionation (FFF, used for particle separation and size characterization via multi-angle light scattering (MALS)) and confocal Raman microspectroscopy (RM) enabled by optical trapping (OT).[2] This has been shown to deliver size-resolved chemical information on polydisperse samples, even in complex mixtures.[1] Due to the high cost of advanced Raman microscopes this combination is not always practical for routine analyses of nanoplastics. Therefore, a much more affordable mobile Raman microscope, the confocal alphaCART from Oxford Instruments WITec, was tested for its applicability. It could be shown that the OT and spectroscopic performance (signal-to-noise ratio (SNR) and spectral resolution) are comparable to an automated stand-alone Raman microscope, e.g. the Oxford Instruments WITec *alpha300 apyron*. The system was validated using 100 nm, 300 nm, and 500 nm polystyrene (PS) spheres and a polydisperse polyethylene (PE) sample. While the overall performance was very similar, instabilities in the manual z-stage created difficulties in obtaining reproducible measurements (as a shift in the focus point over time can vary the performance of the OT drastically). Furthermore, to allow for an automated online coupling with FFF, an automated laser shutter would be needed, to ensure that trapped particles are released periodically, and the separation is maintained over the whole time of elution. Overall, this cost-optimized and versatile confocal Raman system is a promising step toward bringing online-FFF-RM to routine analysis of various (plastic) particles in the nanometer range.

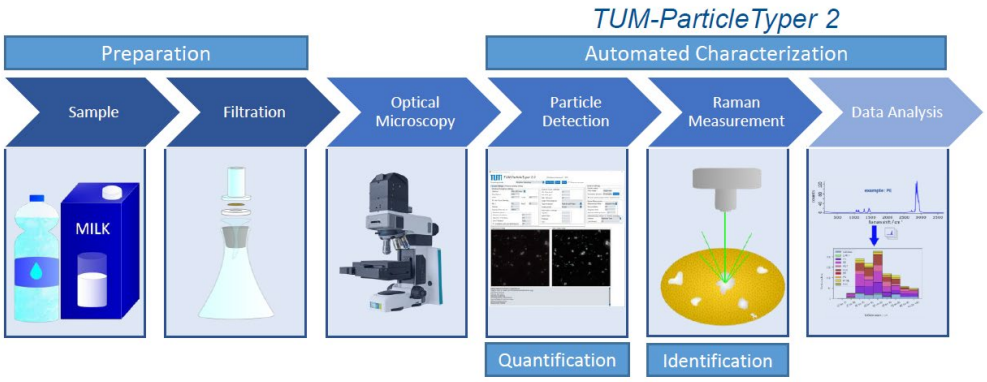
Funding
BMWK
Cooperation
Oxford Instruments WITec
Postnova Analytics GmbH

References
[1] Huber et al., *Anal. Bioanal. Chem.* **2023**, doi.org/10.1007/s00216-023-04689-5.
[2] Schwaferts et al., *Anal. Chem.* **2020**, doi.org/10.1021/acs.analchem.9b05336.

Representative and Reliable Analysis of Small Microplastic in Real Samples

Isabel Jüngling | Group: Raman & SEM

A Raman micro-spectroscopy-based method utilizing the *TUM-ParticleTyper 2* is developed to enhance the detection, quantification, and analysis of small microplastic content in real samples.



Precise detection and measurement of small microplastics in real-world samples are essential for assessing their potential effects on the environment and human health. Achieving representative and reliable analysis involves several steps, beginning with sample preparation. For mineral water, the primary investigated real sample, nitric acid is utilized to dissolve minerals, effectively reducing the overall particle count and minimizing measurement time. The selection of filter materials is another crucial factor, as it directly influences the accuracy of subsequent analyses. Filters, including aluminum-coated, gold-coated, and silicon filters, were systematically evaluated based on their optical and spectral properties, particularly their ability to minimize background interference during Raman microspectroscopy (RM) analysis. After filtration, the prepared filters are examined using optical microscopy, where a high visual contrast between plastic particles and the filter surface is essential for accurate particle size determination using our open-source software *TUM-ParticleTyper 2*.[1] Further optimization of RM settings was performed through systematic evaluations with reference plastic particles, ensuring reliable and reproducible measurements. Data acquisition and analysis are automated with *TUM-ParticleTyper 2*, allowing for efficient processing of particles ranging from 5 µm to 1000 µm through *FullSurface* scans. For particles in the size range 1 – 20 µm, *RandomWindowSampling* is employed, analyzing a subset of the filter surface with a higher magnification objective to improve detection sensitivity. This comprehensive approach ensures robust and efficient analysis of small microplastics, providing critical insights into their potential environmental and health impacts.

Funding
Nestlé S.A.

Cooperation
Nestlé S.A.

Reference
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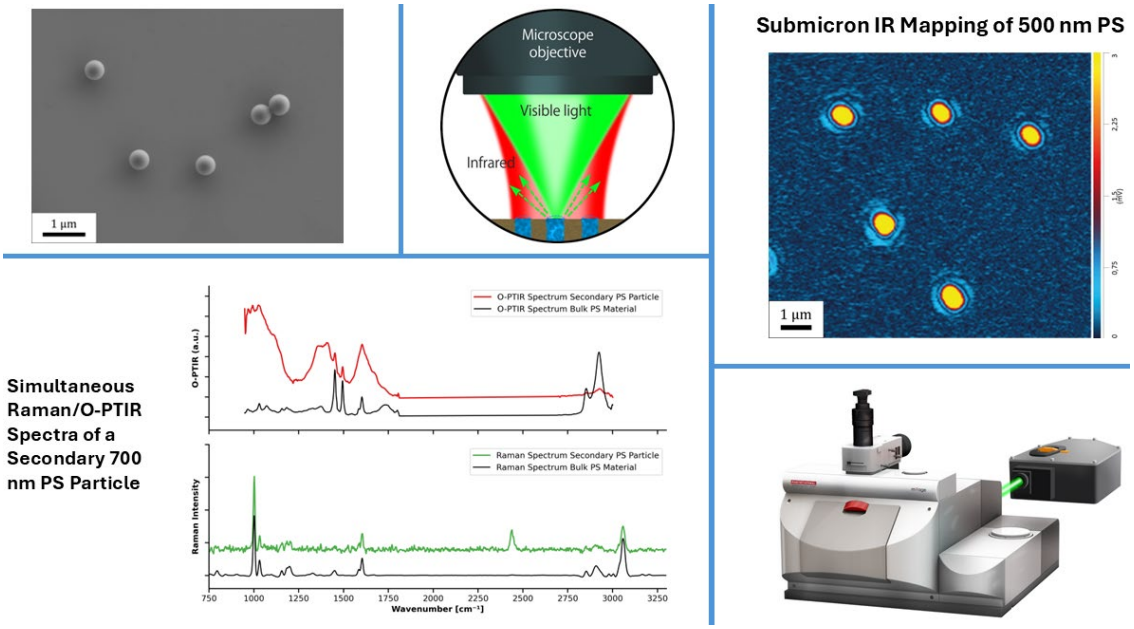
Advanced Nanoplastics Analysis using Optical-Photothermal Infrared Spectroscopy

Marcel Klotz | Group: Raman & SEM

Optical-Photothermal Infrared Spectroscopy enables sub-micron IR resolution with simultaneous Raman analysis, advancing the characterization of micro- and nanoplastics.



The middle top picture and the bottom right picture were obtained from the websites under https://www.photothermal.com/ on January 10, 2025.

The widespread presence of nanoplastics (plastic particles smaller than 1 µm) in the environment, including drinking water, has become a significant concern due to their ability to penetrate biological barriers and to carry toxic substances.[1] Traditional spectroscopic methods face challenges in their ability to characterize these particles, as conventional Infrared (IR) Spectroscopy can only analyze particles that are ~10 µm or larger due to diffraction limits. Although Raman Spectroscopy can characterize particles at sub-micron levels, it is limited by factors such as fluorescence interference and low signal intensity.[2] Our research showcases Optical-Photothermal Infrared Spectroscopy (O-PTIR) as an innovative solution that combines high-resolution sub-micron IR capabilities with simultaneous Raman Spectroscopy. Using O-PTIR, we successfully characterized secondary nanoplastic particles made of polyethylene terephthalate (PET) and polystyrene (PS) that are smaller than 1 µm, obtaining high-quality spectra. We further measured reference particles as small as 500 nm and 300 nm, demonstrating the method's exceptional performance. Sub-micron IR mapping enabled the simultaneous acquisition of spatial and chemical information from 500 nm PS beads, demonstrating the method's effectiveness for nanoscale analysis. The dual-mode capability of O-PTIR allows for the collection of both IR and Raman data, improving the accuracy of plastic particle identification and potentially uncovering insights into associated additives, such as coatings and dyes. These findings demonstrate the applicability of O-PTIR as a powerful tool for nanoplastic research, with significant potential for real-world applications, including testing drinking water samples and assessing environmental contamination. By overcoming the limitations of conventional methods, O-PTIR opens new pathways for comprehensive characterization of nanoplastics.

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[1] Magrì et al., *ACS Nano* **2018**, doi.org/10.1021/acsnano.8b01331.
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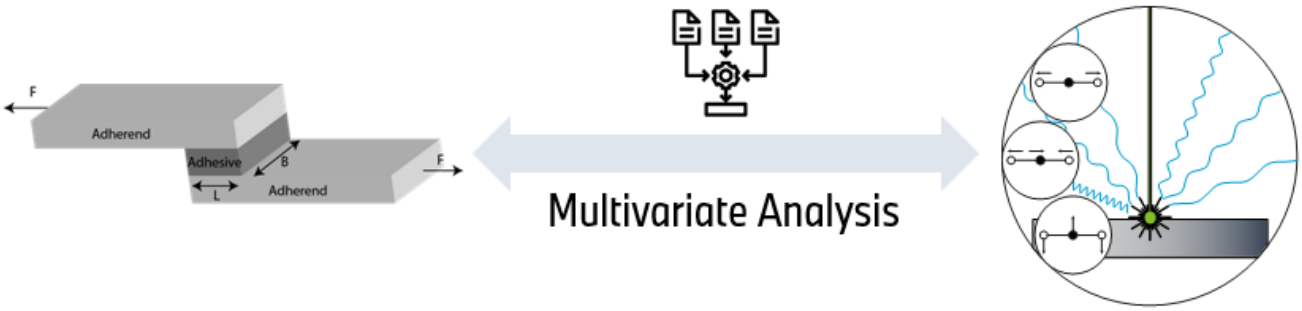
Cooperation
Dr. Miriam Unger
Photothermal Spectroscopy Corp.

Combination of Spectroscopic and Mechanical Testing of Adhesives for the Development of Prediction Models

Alexander Thomas | Group: Raman & SEM

In order to reduce the dependence on the destructive testing of adhesives and, therefore, increase the sustainability and speed of analysis, Fourier transformed Infrared (FTIR) spectroscopy is applied. Databases of destructive tests combined in a multivariate fashion with vibrational spectra of adhesives cured under a variety of environmental conditions are used to predict the mechanical properties of samples cured under unknown conditions.



Adhesives are of ever-growing importance in the industry, with applications ranging from construction to the automotive and aviation industry.[1] Therefore, the quality control of these adhesives is of utmost importance as they are greatly impacted by factors such as temperature and relative humidity (rH).[2] Most commonly, the quality of adhesives is tested via destructive methods, greatly reducing the sustainability and not allowing for inline quality control. Vibrational spectroscopy offers the opportunity to elevate these problems by fast and non-destructive measurements. Therefore, this project focusses on the development of prediction models for the quality of adhesives based on FTIR analysis. For this, adhesives were cured under a variety of different temperatures and relative humidities. The same samples were then measured via FTIR in order to create a first database of the spectral differences dependent on the curing conditions. The samples were then subjected to the destructive lap-shear test, to create a second database containing the differences in mechanical properties in dependence on the curing conditions. For future samples cured under unknown conditions, the spectra will be compared to the first database via partial least squares-discriminant analysis (PLS-DA). This should allow for the determination of the environmental factors present when the adhesive was cured. With this information, the mechanical properties of the sample will be inferred from the second database, and predictions of adhesive stability will be matched against destructive lap-shear tests. It is our goal to enable predictions in the future from FTIR analysis without the need for such destructive tests.

Funding
BMW Group

Cooperation
BMW Group

References
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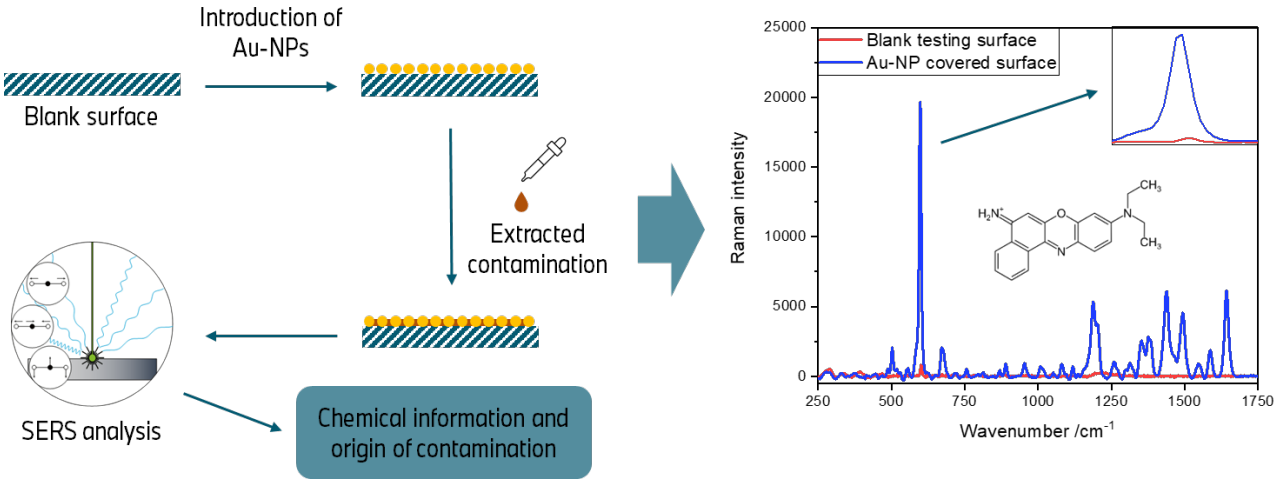
Analysis of (Organic) Filmic Contaminations via Surface-Enhanced Raman Scattering

Jannis Gehrlein | Group: Raman & SEM

Surface-enhanced Raman scattering (SERS) is used to analyze residue of organic compounds on metallic surfaces in the context of technical cleanliness of automotive parts.



Several production steps during the assembly of a car containing high-voltage components require utmost cleanliness of the involved parts. Here, the presence of (organic) filmic contaminations, e.g. residue of cooling lubricants, on the surfaces of the components can lead to severe quality problems. For example, faulty adhesive joints can result in defects in liquid-proof sealings.[1] Furthermore, flawed welded connections with the possible consequence of generation of metallic particles can arise.[2] As a result, a powerful analytical tool for the detection of filmic contaminations is necessary to obtain qualitative information of the disruptive substances and, therefore, to determine the origin of the contamination. Most commercially available methods either focus on the quantitative information without being able to give structural insight of the contamination (e.g. fluorescence spectroscopy) or are too complex to be used in a small-scale laboratory in production surroundings (e.g. gas chromatography-mass spectrometry). Here, the use of SERS is a promising approach to close this existing gap. In this project, gold nanoparticles (Au-NPs) are assembled on easily reproducible and low-priced testing surfaces. Subsequently, the extracted contamination from a workpiece is introduced onto the prepared surface and analyzed with Raman spectroscopy. After optimization of the Au-NP deposition parameters, it was possible to drastically increase the Raman signal intensity of the Raman-resonant dye Nile Blue A and, therefore, to lower the respective limit of detection. Further experiments will focus on transferring the achieved results to more realistic and complex contaminations in the context of production settings. Additionally, extensive characterization of the prepared surfaces will be performed to understand Au-NP assembly and ensure reproducibility of the preparation method.

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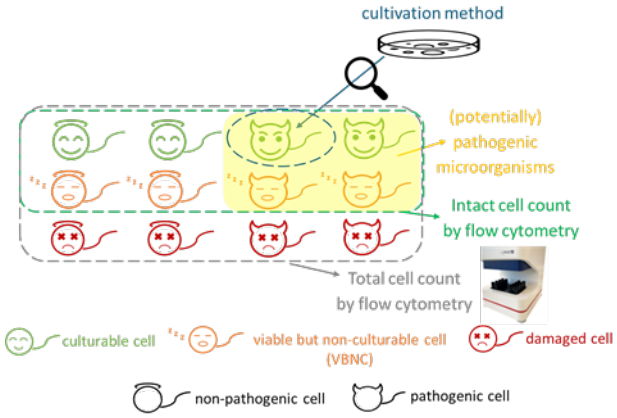
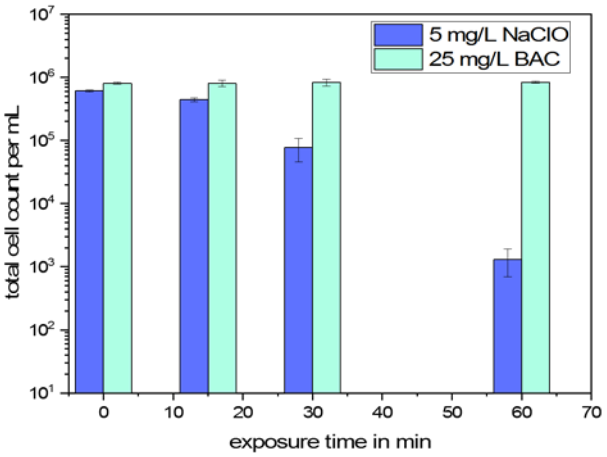
Rapid and effect-based analysis of biocides used in evaporative cooling systems by flow cytometry

Yiao Liang | Group: Bioanalytics and Microanalytical Systems

Total cell counting and intact cell counting by flow cytometry (FCM) were employed as rapid, cultivation-independent, and effect-based methods for analyzing DNA and cell membrane damage during biocide treatment.





Biocides, encompassing both oxidizing agents such as chlorine and non-oxidizing agents like quaternary ammonium compounds, are extensively employed to minimize the risk of *Legionella pneumophila* growth in evaporative cooling systems. Meanwhile, the minimization of biocide usage is required by sustainability and wastewater directives. Currently applied cultivation test methods to quantify biocide effects on *Legionella pneumophila* need long testing times and can cause risk underestimation due to the viable but non-culturable status induced by biocides. Moreover, the total microbial population, which is neglected by cultivation methods, is of great importance, as its uncontrolled growth can lead to the formation of biofilm, which inhibits heat transfer, causes biocorrosion, and is the habitat of *Legionella pneumophila*. In this work, we employed total cell counting (TCC) and intact cell counting (ICC) by flow cytometry (FCM) as rapid and cultivation-independent methods for effect-based biocide analysis. A cartridge-based flow cytometer was employed, which was developed explicitly for bacteria analysis [1]. Using TCC and ICC by FCM, we detected DNA and cell membrane damage during the treatment of the representative oxidizing biocide sodium hypochlorite and non-oxidizing biocide benzalkonium chloride. Based on TCC and ICC results, we could calculate an FCM-based survival rate to quantify biocide effects. In our experiments, the total removal of culturable *Legionella pneumophila* could be guaranteed if the FCM-based survival rate of all other remaining bacteria was under 50%. Furthermore, the FCM-survival rate has a significantly better correlation (R^2 = 0.9666) with the microbial growth after biocide treatment compared with the cultivation-based survival rate ($R^2 \leq 0.898$). As a result, TCC and ICC by FCM could be a good solution to minimize health-related risk while controlling microbial growth with minimized biocide usage.

Funding
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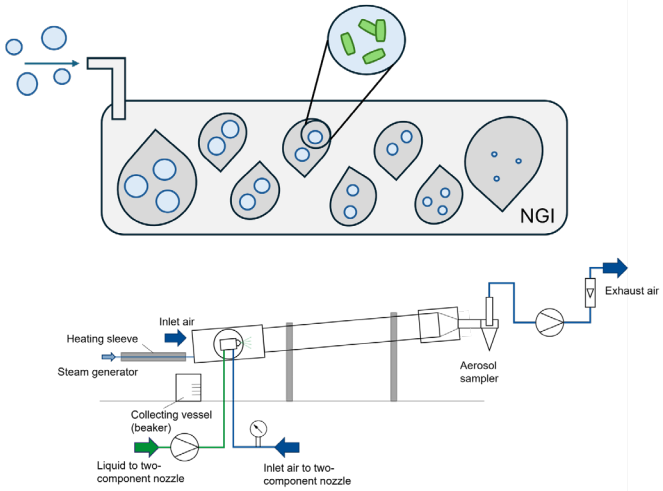
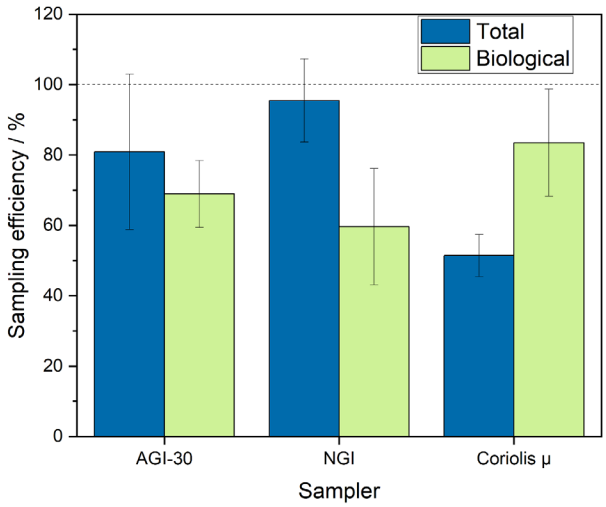
The Next Generation Impactor (NGI) - A new application for *L. pneumophila* in aerosols

Lena Heining | Group: Bioanalysis and Microanalytical Systems

The Next Generation Impactor (NGI) was evaluated for the sampling of airborne bioaerosols and the size-dependent separation of wet droplets containing *L. pneumophila*.





Bioaerosol generation, sampling, and cultivation-independent quantification of pathogenic bacteria play a crucial role in studying dose-response effects of *Legionella pneumophila*. Here, the Next Generation Impactor (NGI), initially created for pharmaceutical inhaling studies, was assessed for its potential to sample airborne bioaerosols and to separate size-dependent wet droplets by incrementally increasing the airflow speed. This stainless-steel sampler was shown in this study to be suitable for sampling prior to cultivation-independent analysis of pathogen-containing bioaerosols using washable cups. The applicability was studied by quantifying the total and intact cell count of *L. pneumophila* by flow cytometry after being dispersed into a droplet aerosol. Our results demonstrate a high total sampling efficiency of 95.5% ± 11.8% despite a lower biological sampling efficiency of 59.7% ± 16.5% for dry aerosols. However, by elevating the relative humidity (RH) to 100% in a liquid aerosolization unit, the biological sampling efficiency increased to over 90% for *L. pneumophila*. More than 50% of the cells were found in stage 1 using the liquid aerosolization unit. In comparison, 80% of the cells were sampled in stages 4-6 at 30% RH. While at 100% RH the droplet size mattered, at 30% RH it was the size distribution of dry particles - in this case *L. pneumophila* - which was relevant due to evaporation processes, thereby explaining the size differences. These findings indicate the potential of the NGI for further exploration and application in studying other aerosol-borne pathogens, especially concerning the size distribution of wet droplets, viability, or effect-based bioanalysis.

L. Heining, L. Welp, A. Hugo, M. Elsner, M. Seidel, *Journal of Aerosol Science.* **2024**, 183, 106460, https://doi.org/10.1016/j.jaerosci.2024.106460.

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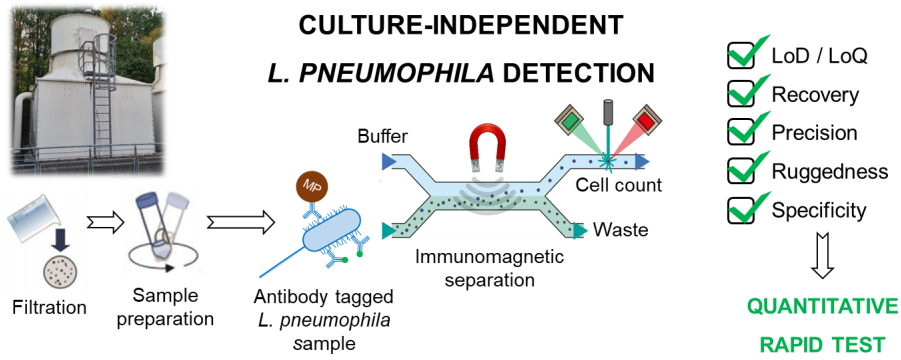
Culture-independent quantification of *Legionella pneumophila* in evaporative cooling systems using immunomagnetic separation coupled with flow cytometry

Philipp Streich | Group: Bioanalytics and Microanalytical Systems

To confirm the presence of *Legionella* spp. in evaporative cooling systems rapid screening methods are important. The combination of immunomagnetic separation with flow cytometry is developed as a quantitative rapid test to report the water quality of such systems and to determine the species *L. pneumophila* in parallel.



Legionella pneumophila, a pathogenic bacterium, is frequently detected in high concentrations within the process water of evaporative cooling systems (ECS). If dispersed into the environment through bioaerosols, it can lead to outbreaks with severe, often fatal consequences. The officially accepted detection method for *Legionella* spp. in water samples relies on cultivation, but is time-consuming and may underestimate the amount of viable *L. pneumophila*. Consequently, culture-independent methods are gaining more attention for their potential as rapid tests.

The cartridge-based immunomagnetic separation (IMS) coupled with flow cytometry (FCM) is a novel antibody-based, culture-independent approach for quantifying *L. pneumophila*. This technique employs a panel of antibodies targeting serogroups (Sg) 1-15. Here, the IMS-FCM method was evaluated and characterized as a quantitative rapid test using standard analytical procedures. Calibration experiments with viable, cryopreserved *L. pneumophila* standards yielded detection limits of 100, 105, and 88 viable cells per 100 mL for Sg 1, Sg 4, and Sg 6, respectively. Additionally, the practical applicability of IMS-FCM was demonstrated on real ECS samples and compared against cultivation results. While cultivation failed to detect any positive results, IMS-FCM revealed *L. pneumophila* concentrations ranging from 0 to 80,000 viable cells per 100 mL [1].

This study highlights IMS-FCM as an effective, quantitative, culture-independent rapid test for monitoring of viable *L. pneumophila*. Moreover, IMS-FCM offers adaptability for target-detection by developing specific antibodies or nanobodies against other bacteria. This flexibility allows the method to be applied in detecting additional pathogens, such as *Pseudomonas aeruginosa*, *Escherichia coli*, and *Enterococcus faecalis*, across various freshwater and engineered water systems.

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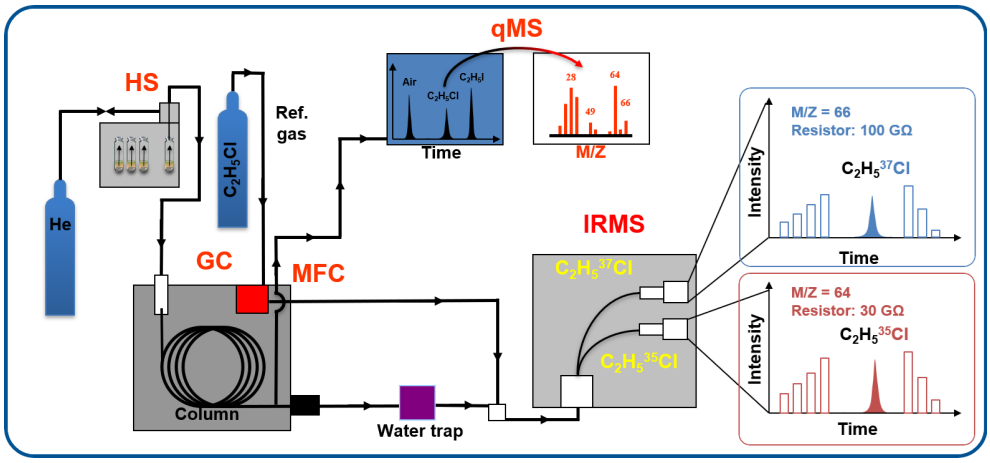
Determination of chlorine stable isotope ratios in aqueous samples by area-corrected continuous flow IRMS (ACCF-IRMS)

Andreas Auernhammer | Group: Bioanalytics and Microanalytical Systems

An area-corrected headspace-gas chromatography-continuous flow-isotope ratio mass spectrometry (AC-HS-GC-CF-IRMS) method is developed to enable the analysis of isotope ratios in chloride for reconstructing the evolution of saline waters.



The differentiation between the two stable isotopes of chlorine ^{35}Cl and ^{37}Cl represents a powerful analytical tool and enables the reconstruction of the evolution of saline waters. The isotopic signatures provide precise insights into the origin and fate of dissolved chloride, as well as the transport pathways of water. Previously, environmental chlorine isotope ratios have been measured after conversion to chloromethane with Dual Inlet Isotope Ratio Mass Spectrometry.[1] To avoid highly toxic iodomethane as reagent, phosphoric acid and ethanol can be used to measure chloroethane isotope ratios via purge and trap gas chromatography-continuous flow-isotope ratio mass spectrometry[2].

We developed a novel sample preparation and measurement technique and preserved the simplicity of the chloromethane protocol while taking advantage of the less toxic chloroethane preparation. In our approach, the formation of chloroethane occurs in a single step by reacting crystallized chloride with iodoethane in a sealed headspace vial, from which a gas sample is then directly injected into the HS-GC-CF-IRMS. Measurements were performed with a Finnigan-MAT Delta-S, equipped with a CNOS/MEMCO collector system (6-cup version) set to the masses m/z = 64 for $C_2H_5{}^{35}Cl$ and m/z = 66 for $C_2H_5{}^{37}Cl$.

The precision of our new method was assessed using the standard material ISL-354 yielding a $\delta^{37}Cl_{ISL\text{-}354}$ value of +0,05 ± 0,04 ‰ for n = 15. This standard deviation is significantly smaller compared to previously reported precision of ± 0,09 ‰[2] (n = 12) and ± 0,07 ‰[1] (n = 12). No memory effects were observed during the measurement of six different isotope standards ranging from -0,55 ‰ to +1,84 ‰. Moreover, the reaction and measurement accuracy was maintained after adding various ions. This demonstrates that the determination of chlorine isotope ratios via chloroethane using HS-GC-CF-IRMS offers distinct advantages in terms of handling, occupational safety and the quality of the measurement results compared to previous studies.

Funding
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Cooperation
Hydroisotop GmbH

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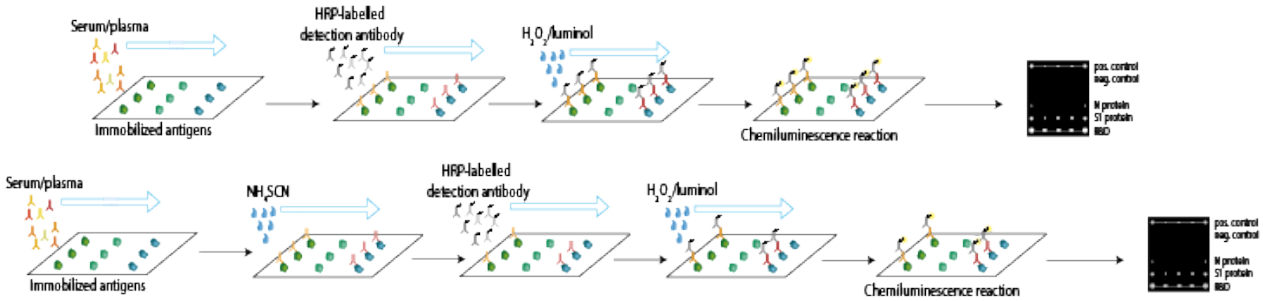
A Rapid Automated Immunoassay for the Detection of SARS-CoV-2 Antibodies

Sandra Paßreiter | Group: Bioanalytical and Microanalytical Systems

After showing the power of flow-based chemiluminescence microarray immunoassays for rapid identification of SARS-CoV-2 antibodies and their neutralization capacity, the next challenge is to establish an avidity IgG test on the same microarray analysis platform.



The next challenge is establishing an avidity IgG test on the same microarray analysis platform after showing the power of flow-based chemiluminescence microarray immunoassays for rapidly identifying SARS-CoV-2 antibodies and their neutralization capacity.[1] The amount of neutralizing antibodies and their avidity plays a crucial role in the protection from infection against SARS-CoV-2. In this context, avidity is the binding strength between an antibody and its epitope. The receptor-binding domain (RBD) of the antigen SARS-CoV-2 S1 and angiotensin-converting enzyme-2 (ACE2) is expected to bind with high affinity. Still, an incomplete avidity maturation can lead to a decline in the serological response. A standard method to determine avidity is to examine the stability of the antibody-antigen complex in the presence of chaotropic agents (e.g. urea, NH_4SCN). Commercially available tests are based on line blot immunoassays or ELISA approaches and can take up to several hours before results are available.[2,3]

To overcome these drawbacks, we want to present a rapid stopped-flow chemiluminescence (CL) microarray immunoassay to detect the avidity of SARS-CoV-2 IgG antibodies on the microarray platform MCR-R. The measurement procedure consists of two subsequent measurements, whereby the antibody-antigen complex is incubated with ammonium thiocyanate (NH_4SCN) during the second measurement (Fig. 1). We developed a rapid test to determine SARS-CoV-2 IgG avidity in human blood samples. The microarray immunoassay was able to characterize blood samples from 18 individuals over the course of 4 visits within 26 minutes per measurement. These first results compare favourably with those of two commercially available assays.

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TUM - Institute of Virology
TUM – Institute of Molecular Immunology

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Wang, Y.; Zeng, R.; Tian, S.; Chen, S.; Bi, Z.; Tang, D.; Knopp, D., Bimetallic single-atom nanozyme-based electrochemical-photothermal dual-function portable immunoassay with smartphone imaging. Analytical Chemistry 2024, 96(33), 13663-13671. DOI.org/10.1021/acs.analchem.4c02606.

Wu, D.; Wei, Q.; You, Z.; Gao, Y.; Knopp, D.; Tang, D., Miniature dual-channel electrochemical 3D-printed sensing platform for enzyme-free screening of L-lactic acid in foodstuffs accompanying pH recognition. Food Chemistry 2025, 465, 142188. DOI: 10.1016/j.foodchem.2024.142188.

Further publications

Adu-Gyamfi, J.J.; Heng, L.K.; Ivleva, N., Elsner, M.; Müller, K.; Vlasimsky, M.; Wang, F., Nuclear and isotopic techniques to assess the fate and impacts of plastic pollution on soil ecosystems and the environment. Rome, FAO, 2024. DOI: 10.4060/cc9677en.

Huber, M.J.; Ivleva, N.P., Stimulated Raman scattering for the analysis of nanoplastics. Wiley Analytical Science 2024.

Jacob, O.; Ivleva, N.P., Automatisierte Partikel-Quantifizierung. Wiley Analytical Science 2024.

Conference Presentations

Oral Presentations

Canavan, A.; Elsner, M. Going position-specific: challenges in referencing, 2024, Orbitrap Isotope Applications Workshop, Garching, Germany.

Elsner, M.; Canavan, A.; Dou, Q.; Wang, F.; Adu-Gyamfi, J.; Kheng Heng, L. Synthesis and isotope analysis of labelled antibiotics and their metabolites to trace spread and natural degradation in an agricultural field experiment, 2024, Second Research Coordination Meeting of the CRP D15022, “Isotopic Techniques to Assess the Fate of Antimicrobials and Implications for Antimicrobial Resistance in Agricultural Systems”, Vienna, Austria.

Huber, M.J.; Booth, A. M.; Beer, I.; Bianchi, I.; Drexel, R.; Geiss, O.; Mehn, D.; Meier, F.; Molska, A.; Parot, J.; Sørensen, L.; Vella, G.; Prina-Mello, A.; Vogel, R.; Caputo, F.; Ivleva, N.P. Inter-comparison of different fractionation and batch methods for the physicochemical characterization and quantification of nanoplastics, 2024, 23rd International Symposium on Field- and Flow-based Separations (iSFFF2024), Nantes, France.

Ivleva, N.P.; Müller, K.; Elsner, M. Stable isotope Raman microspectroscopy as novel approach for analysis of microbial degradation of microplastics, 2024, 11th International Symposium on Isotopomers, Tokyo, Japan.

Ivleva, N.P.; Müller, K.; Elsner, M. Applicability of stable isotope Raman microspectroscopy for analysis of microbial degradation of microplastics, 2024, SciX 2024, Raleigh, USA.

Ivleva, N.P.; Jacob, O.; Stefaniak, E.A.; Seghers, J.; La Spina, R.; Schirinzi, G.F.; Chatzipanagis, K.; Held, A.; Emteborg, H.; Koeber, R.; Elsner, M. Automated µ-Raman-based analysis of a candidate microplastics’ reference material, 2024, SciX 2024, Raleigh, USA.

Ivleva, N.P.; Müller, K.; Elsner, M. Stable isotope Raman microspectroscopy: applicability for analysis of microbial degradation of microplastics, 2024, XXVIII International Conference on Raman Spectroscopy (ICORS), Rome, Italy.

Müller, K.; Elsner, M.; Ivleva, N.P. Deuterium labels to study biodegradation of plastics with Raman spectroscopy, 2024, EGU General Assembly 2024, Vienna, Austria.

Seidel, M.; Agrawal, S.; Nocker, A.; Ho, J.; Schreiber, C.; Wurzbacher, C.; Zacharias, N. Anwendungsfelder für moderne bioanalytische Methoden zur Bestimmung von Pathogenen im Bereich Wasser, 2024, Wasser 2024, Limburg, Germany.

Seidel, M.; Agrawal, S.; Nocker, A.; Ho, J.; Schreiber, C.; Wurzbacher, C.; Zacharias, N. Moderne Analysemethoden für Pathogene im (Ab-)Wasser. 2024, 1. Schönberger Umwelttag, Schönberg, Germany.

Seidel, M. Aktuelle Entwicklungen: Alternative Untersuchungsmethoden zum Nachweis von Legionellen - Immunologische Nachweismethoden. 2024, 8. VDI-Fachkonferenz "Legionellen aus Rückkühlanlagen", Würzburg, Germany.

Poster Presentations

Al-Ghoul, H.; Elsner, M. Wall-coated Ni/NiO microreactors to facilitate GCxGC-C-IRMS, 2024, ISI 2024, Tokio, Japan.

Auernhammer, A.; Seidel, M. A precise and less hazardous method to determine chlorine stable isotope composition in aqueous samples, 2024, 11th International Symposium on Isotopomers, Tokio, Japan.

Canavan, A.; Elsner, M. Reference materials for position-specific isotope analysis of sulfamethoxazole by ESI-Orbitrap, 2024, 43rd Meeting of the German Association for Stable Isotope Research, Darmstadt, Germany.

Canavan, A.; Elsner, M. Nitrogen stable isotope analysis of five sulfonamides by derivatization-gas chromatography isotope ratio mass spectrometry, 2024, Gordon Research Conference: Environmental Science: Water, Holderness, USA.

Canavan, A.; Elsner, M. ^{15}N-isotope analysis of sulfonamides by derivatization-gas chromatography-isotope ratio mass spectrometry, 2024, Jahrestagung der Wasserchemischen Gesellschaft, Limburg an der Lahn, Germany.

Canavan, A.; Elsner, M. Nitrogen stable isotope analysis of five sulfonamides by derivatization-gas chromatography isotope ratio mass spectrometry, 2024, Analytica, Munich, Germany.

Chai, L.; Derat, E.; Elsner, M. Exploring reaction paths for sulfonamide hydrolysis: insight from experiments and computations, 2024, ASI, Darmstadt, Germany.

Huber, M.J.; Graewert, M.A.; Mühlbauer, M.; Drexel, R.; Meier, F.; Ivleva, N.P. Asymmetrical-flow field-flow fractionation hyphenated with small angle x-ray scattering: characterising the particle morphology and interactions of nanoplastics and inorganic nanoparticles, 2024, Analytica, Munich, Germany.

Huber, M.J.; Ivleva, N.P. Investigating (hetero-)agglomeration of nanoplastics using particle tracking analysis, 2024, SETAC, Sevilla, Spain.

Huber, M.J.; Wabnitz, C.; Bakkour, R.; Elsner, M.; Ivleva, N.P. Nanoplastic quantification via quartz crystal microbalance: an approach for coupling with FFF, 2024, 23rd International Symposium on Field- and Flow-based Separations (iSFFF2024), Nantes, France.

Huber, M.J.; Klotz, M.; Rupp, U.; Kreissl, S.; Boehmler, M.; Ivleva, N.P. Towards an efficient online Raman detector for field flow fractionation, 2024, SciX 2024, Raleigh (NC), USA.

Huber, M.J.; Dehne, H.; Klüpfel, J.; Ivleva, N.P. Particle tracking analysis & Raman spectroscopy for the characterization of LNP formulations, 2024, SciX 2024, Raleigh (NC), USA.

Jüngling, I.S.; Elsner, M.; Ivleva, N.P. Comparison of filters for the analysis of microplastics with Raman microspectroscopy, 2024, Wasser 2024, Limburg, Germany.

Jüngling, I.S.; Jacob, O.; Ramírez-Piñero, A.; Elsner, M.; Ivleva, N.P. Automated quantitative analysis of microplastic down to 1 µm by Raman microspectroscopy: TUM-ParticleTyper 2, 2024, Analytica, Munich, Germany.

Liang, Y.; Seidel, M. Digital networking of (bio-)analytical techniques and sensors to avoid *Legionella* in cooling systems, 2024, Analytica, Munich, Germany.

Liang, Y.; Heining, L.; Seidel, M. Cartridge-based flow cytometry for the analysis of total cell count to examine biocide efficiency in process water. 2024, Jahrestagung der Wasserchemischen Gesellschaft, Limburg an der Lahn, Germany.

Müller, K.; Elsner, M.; Ivleva, N.P. Stable isotope Raman microspectroscopy to analyze biodegradation of deuterated microplastics, 2024, Analytica, Munich, Germany.

Müller, K.; Elsner, M.; Ivleva, N. Stable isotope Raman microspectroscopy to analyze biodegradation of deuterated microplastics, 2024, Gordon Research Conference: Environmental Science: Water, Holderness, USA.

Müller, K.; Huber, C.; Eisenreich, W.; Elsner, M.; Ivleva, N.P. Comparison of stable isotope Raman microspectroscopy with fatty acid methyl ester (FAME)-GC-MS to analyze fatty acid deuteration in bacteria, 2024, ISI 2024, Tokyo, Japan.

Klotz, M.; Huber, M.; Elsner, M.; Ivleva, N.P. Investigating adverse effects of disinfectants on polyamide membranes via Raman techniques, 2024, Wasser 2024, Limburg, Germany.

Klotz, M.; Unger, M.; Kansiz, M.; Ivleva, N.P. Towards the analysis of nanoplastics with optical-photothermal infrared spectroscopy, 2024, ICORS 2024, Rome, Italy.

Paßreiter, S.; A rapid automated immunoassay for the detection of SARS-CoV-2 antibody avidity, 2024, Analytica, Munich, Germany.

Prechtl, L.; Seidel, M.; Elsner, M. Rapidly degrading drugs as markers for microbiological contamination in surface water, 2024, Analytica, Munich, Germany.

Prechtl, L.; Elsner, M. Position-specific isotope analysis of carbon in serine using ESI-Orbitrap, 2024, M.ASI 2024 Jahrestagung der Arbeitsgemeinschaft Stabile Isotope e.V., Darmstadt, Germany.

Prechtl, L.; Eisenreich, W.; Seidel, M.; Elsner, M. Position-specific isotope analysis of carbon in serine using ESI-Orbitrap, 2024, The 11th International Symposium on Isotopomers (ISI), Tokyo, Japan.

Invited Lectures

Canavan, A.; Huyen, N.X.; Thi, N.V.; Hu, H.-W.; He, J.; Borges Regitano, J.; Bezuidenhout, C.C.; Heiling, M.; Dou, Q.; Wang, F.; Elsner, M.; Heng, L.K.; Adu-Gyamfi, J.; Zaman, M. Using isotopic techniques to assess the fate of AMR in agricultural systems, 2024, Fighting Antimicrobial Resistance (AMR) in Food and Agriculture Using Nuclear and Related Technologies (side event from the 68th IAEA General Conference), Vienna, Austria.

Ivleva, N.P.; Jacob, O.; Stefaniak, E.A.; Seghers, J.; La Spina, R.; Schirinzi, G.F.; Chatzipanagis, K.; Held, A.; Emteborg, H.; Koeber, R.; Elsner, M. Towards a reference material for microplastics' number concentration – case study of PET in water using Raman microspectroscopy, 2024, PlasticTrace/COST Priority Stakeholder Workshop, Landsberg am Lech, Germany.

Huber, M.J.; Ivleva, N.P.; Centrifugal FFF hyphenated with Raman: size-resolved chemical analysis of nanoplastics, 2024, Analytical Solutions, Ede, Netherlands.

Ivleva, N.P. Analysis of micro- and nanoplastics by Raman-based methods, 2024, 7th International Microplastics Symposium, Seoul, Korea.

Ivleva, N.P. Towards reliable and representative analysis of small microplastics and nanoplastics, 2024, Columbia University, Department of Chemistry, Group of Prof. Wei Min, New York City, USA.

Ivleva, N.P. Micro/nanoplastics – what progress has been made in the analytical sciences? 2024, 16th International Akademie Fresenius Conference "Contaminations and Residuals in Food", Düsseldorf, Germany.

Colloquium for Analytical Chemistry and Water Chemistry Guest Lecture

Prof. Maria Emanuela Minunni, Chair of Analytical Chemistry, Dipartimento di Farmacia, Università degli Studi di Pisa, *"Affinity Sensing: Trends and Challenges"* (25.01.2024)

Dr. habil. Karolina Nowack, Technical Biogeochemistry, Helmholtz Centre for Environmental Research – UFZ, "*New solutions for 'hidden' origin of soil-bound contaminant residues and surface runoff management"* (17.06.2024)

Ass. Prof. Dr. Michael Zumstein, Division of Environmental Geosciences (EDGE), Centre for Microbiology and Environmental Systems Science, University of Vienna, Austria, "*Peptidases in Wastewater and their Potential to Break Down Anthropogenic Chemicals"* (18.11.2024)

Organization of Conferences and Conference Sessions

Session "Tracking Anthropogenic Emissions: Environmental Analysis of Elements, Organic Trace Chemicals and Isotopes (GDCh)", Analytica, Munich, Germany, 09.04.-12.04.2024.

Session "Sensors in Environmental Practice" (GDCh - WChG)", Analytica, Munich, Germany, 09.04.-12.04.2024.

Jahrestagung der Wasserchemischen Gesellschaft, Limburg an der Lahn, Germany, 06.05.-08.05.2024.

Scientific Committees & Memberships

Elsner, M., Young Academy of Europe, YAE (Member)

Elsner, M., Wasserchemische Gesellschaft, Fachgruppe der GDCh (Vice President)

Elsner, M., Environmental Science & Technology (Member of the Editorial Advisory Board)

Elsner, M., ACS ES&T Water (Member of the Editorial Advisory Board)

Elsner, M., Journal of Isotopes in Environmental and Health Studies (Member of the Editorial Advisory Board)

Elsner, M., Evaluation Panel Member of the Swiss National Science Foundation

Elsner, M., Bayer. Fachausschuss für Kurorte, Erholungsorte & Heilbrunnen Member

Elsner, M., Dean of Studies, Faculty of Chemistry, Technical University of Munich

Elsner, M., TUM Water Cluster, Speaker, Technical University of Munich

Ivleva, N. P, Member of ISO/TC 147/SC 2/JWG 1 "Joint ISO/TC 147/SC 2 - ISO/TC 61/SC 14 WG: Plastics (including microplastics) in waters and related matrices" (DIN Expert)

Ivleva, N. P, Member of ISO/TC 61/SC 14 "Plastics and Environment" / WG 4 „Microplastics“ (DIN Expert)

Ivleva, N. P, Member of DIN-Normenausschuss NA 054-01-06 AA „Kunststoffe und Umweltaspekte“

Ivleva, N. P, Member of NA 057 DIN-Normenausschuss „Lebensmittel und landwirtschaftliche Produkte“, NA 057-08-05 AA Arbeitsausschuss „Bestimmung von Mikroplastik in Lebensmitteln“

Ivleva, N. P, Member of the Expert Committee at the Wasserchemische Gesellschaft: “Kunststoffe in der aquatischen Umwelt”

Seidel, M., Member of the Scientific Committees at the European BioSensor Symposium

Seidel, M., Member of the working group „Messen und Bewerten von Legionellen“ (NA 134-03-07-09 UA) bei der Kommission Reinhaltung der Luft im VDI und DIN

Seidel, M., Member of the working group „Bioaerosole und biologische Agenzien – Luftgetragene Mikroorganismen und Viren“ (NA 134-03-07-04 UA) bei der Kommission Reinhaltung der Luft im VDI und DIN

Seidel, M. Member of the Deutschen Expertenrates für Umwelttechnologie und Infrastruktur

Seidel, M., Member of the working group CEN/TC 264/WG 28 “Microorganisms in ambient air” (NA 134-03-07-03-01 AK)

Seidel, M. Chairman of the expert committee at the Wasserchemische Gesellschaft: Pathogens and antibiotic resistant bacteria in the water cycle

Theses

PhD Theses

Melina Grasmeier: Biosensor-based monitoring of TNF antagonists and anti-drug antibodies in inflammatory bowel disease

Christopher Wabnitz: Novel strategies to guide sample preparation for compound-specific isotope analysis

Ruben Weiß: Raman-Mikrospektroskopie und oberflächenverstärkte Raman-Streuung für die zerstörungsfreie, dreidimensionale Analyse von Mikroorganismen und Biofilmen

M.Sc. Theses

Nico Chrisam: Development of a sampling system for the analysis of viruses in breath air aerosol

Kristina Krahulikova: Palladium-based microreactors for complete oxidation of volatile organic compounds (VOCs)

Anna Marini: Studying the monolith adsorption filtration of e. coli cells in mineral and wastewater by flow cytometry

B.Sc. Theses

Leon Aschenbrenner: Generation, coating and collapsing of calibration aerosols

Otto Teuscher: Comparison of extraction methods to assess nitrogen stable isotope analysis of sulfamethoxazole during degradation processes

Diego Timmermanns: An analysis of the uptake kinetics of polar organic chemical integrative samplers with a cyclodextrin-tetrafluoroterephtalonitril-polymer as sorbent and an 8µm pore size / investigating the efficiency and selectivity of novel sorbent materials for POCIS in aquatic environments

Alžbeta Tonyková: Analysis of micro- and nanoplastics: particle debris from reverse osmosis membranes and preconcentration of nanoplastics

Friederike Wiskandt: Kulturunabhängige und effektbasierte Analyse der Auswirkungen von Bioziden auf Legionella pneumophila in Prozesswasser

Teaching

Winter Semester

Analytische Chemie I, Instrumentelle Analytik

240242322 Geo-Umwelt LMU (B.Sc. Geo.) M. Elsner

Chemische Analytik II - Organische Spurenanalytik für Geowissenschaftler

820486258 Geo-Umwelt LMU (B.Sc. Geo.) M. Elsner

Wasserchemie 1

820005191 Geo-Umwelt LMU (B.Sc. Geo.) M. Elsner

Angewandte Wasserchemie

0000005206 Chemistry (M.Sc. Hydrogeo.) M. Elsner, R. Bakkour

Chemische Analytik II – Organische Spurenanalytik für Geowissenschaftler

820486258Geo-Umwelt LMU (BSc Geo.) M. Elsner

Current Research in the Instrumental Analysis of Trace Components 1 (Lab course)

0000001973 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Current Research in the Instrumental Analysis of Trace Components 1 (Lecture)

0000002469 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Environmental Chemistry

0000001972 Chemistry (MSc Env. Eng.) M. Elsner, R. Bakkour

Fortgeschrittene analytische Verfahren

0000004763 Chemistry (BSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar

240037914 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Spurenanalytik für Biochemiker

0000005683 Biochemistry (BSc) M. Seidel, N. P. Ivleva

Instrumentelle Methoden der Anorganischen Chemie

(CH3000b) 0000002336 (MSc Chem.) M. Elsner, N. P. Ivleva

Lab Rotation Analytical Chemistry 1 (CH3124)

0000002910 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Lab Rotation Analytical Chemistry 2 (CH3125)

0000002932 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Seminar Institut für Wasserchemie

0000004167 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Summer Semester

Automatisierung und Visualisierung von Laborprozessen und Daten

0000004577 Chemistry (M.Sc. Chem.) M. Elsner, N. P. Ivleva

Biochemische Analytik

0000001651 Weihenstephan (B.Sc. Bio.) M. Seidel

Biochemische und molekularbiologische Verfahren in der Umweltanalytik II – Enzymatische Verfahren, DNA Sonden

820032502 M. Seidel

Spurenanalytik für Studierende der Biochemie

0000005683 Garching (B.Sc. Biochem.) M. Seidel, N.P. Ivleva

Case Studies in Analytical and Environmental Chemistry

0000002532 Chemistry (M.Sc. Chem.) M. Elsner, R. Bakkour

Aerosole: Bedeutung, Vorkommen und deren Charakterisierung

0000005602 Chemistry C. Haisch, R. Nießner

Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar

240037914 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Instrumentelle Methoden der Anorganischen Chemie (CH3000b)

0000002336 (M.Sc. Chem.) M. Elsner, N. P. Ivleva

Lab Rotation Analytical Chemistry 1 (CH3124)

0000002910 Chemistry (M.Sc. Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Lab Rotation Analytical Chemistry 2 (CH3125)

0000002932 Chemistry (M.Sc. Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Physikalisch-chemische Aerosolcharakterisierung

0500003556 Chemistry C. Haisch

Physikalisch-chemische Aerosolcharakterisierung Blockpraktikum

0500001944 Chemistry C. Haisch

Praktikum Umweltmesstechnik

820176417 Chemistry C. Haisch

Seminar Institut für Wasserchemie

0500003454 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

GIST TUM-Asia

Biochemical Process Engineering

Chemical Engineering (B.Sc.) M. Seidel

Staff

Chair Holder and Institute Director

Univ.-Prof. Dr. Martin Elsner

Group Leader and Senior Scientists

Dr. Rani Bakkour

Appl.-Prof. Dr. Christoph Haisch

PD Dr. Natalia Ivleva

PD Dr. Michael Seidel

Technical & Administrative Staff

Felix Antritter

Christine Beese

Christine Benning

Susanne Mahler

Cornelia Popp

Dorothea Skottke

PhD Students

M.Sc. Chem. Habib Al-Ghoul

M.Sc. Chem. Aoife Cavan

M.Sc. Chem. Lucas Hirschberger

M.Sc. Chem. Maximilian Huber

M.Sc. Chem. Oliver Jacob

M.Sc. Chem. Isabel Jüngling

M.Sc. Chem. Sophia Kienast

M.Sc. Chem. Marcel Klotz

M.Sc. Chem.-Ing. Yiao Liang

M.Sc. Chem. Felix Ludwig

M.Sc. Chem. Kevin Maier

M.Sc. Chem. Kara Müller

M.Sc. Chem. Sandra Paßreiter

M.Sc. Chem. Carmen Pedri

M.Sc. Chem. Leonard Prechtl

M.Sc. Chem. Armela Tafa

M.Sc. Chem. Christopher Wabnitz

External PhD Students

M.Sc. Chem. Andreas Auernhammer

M.Sc. Chem. Simona Balherr

M.Sc. Chem. Irina Beer

M.Sc. Chem. Lihong Chai

M.Sc. Chem. Nico Chrisam

M.Sc. Chem. Susanne Dietrich

M.Sc. Chem. Anja Dollinger

M.Sc. Chem. Jannis Gehrlein (BMW AG)

M.Sc. Chem. Melina Grasmeier

M.Sc. Chem. Lena Heining

M.Sc. Chem. Amelie Hohensee

M.Sc. Chem. Oliver Jacob

M.Sc. Chem. Ida Kalleder

M.Sc. Chem. Eva Krois

M.Sc. Chem. Maria Lanzinger (BMW AG)

M.Sc. Chem. Julia Neumair

M.Sc. Chem.-Ing. Helge Oesinghaus (AG Glas, TUM)

M.Sc. Chem. Janine-Melanie Potreck

M.Sc. Biochem. Gerhard Schwaiger

M.Sc. Chem. Philipp Streich

M.Sc. Chem. Alexander Thomas (BMW AG)

M.Sc. Chem. Markus Weber (Plasmion GmbH)

Master Students

B.Sc. Chem. Anna Hofmeir

B.Sc. Chem. Nico Chrisam

B.Sc. Chem. Kristina Krahulikova

External Master Students

B.Sc. Env. Eng. Shuyan Peng

B.Sc. Chem. I-Shan Chiang

Bachelor Students

Alžbeta Tonyková

Leon Aschenbrenner

Otto Teuscher

Diego Timmermanns

Friederike Wiskandt

Guests

Dr. Susanna Oswald

Dr. Anna-Cathrine Neumann-Cip

Student Assistants

Barbara Matic

Vivien Okwieka

Anna Dobmeier

Equipment

Aerosol Research

1 Aerosol chamber (1 m^3)

1 Aerosol flow tube (10 L)

1 Ozone analyzer (UV absorption)

1 NO/NO_2 analyzer (Chemiluminescence)

1 Aerodynamic particle sizers (0.5–25 µm)

1 Laser Aerosol Spectrometer (size range 90 nm–7.5 µm)

1 Berner impactor (9 stages, 50 nm–16 µm)

1 Electrical low-pressure impactor (12 stages, 30 nm–10 µm)

2 Low-volume filter samplers (PM 10, PM2.5)

1 High-volume filter sampler (PM 2.5)

3 Differential mobility particle sizer systems (10–1000 nm)

2 Diffusion batteries (5–300 nm)

5 Condensation nucleus counters

3 Electrostatic classifiers (10–1000 nm)

2 Spark-discharge soot aerosol generators (polydisperse ultrafine carbon aerosol)

1 Berglund-Liu aerosol generator (monodisperse aerosols, 0.8–50 µm)

1 Floating bed aerosol generator (powder dispersion)

1 Rotating brush aerosol generator (powder dispersion)

1 Tube furnace

1 AVL Micro Soot Sensor with dilution unit

2 FT/IR gas analyzers

Microarray Technology

1 Chemiluminescence Microarray Reader, MCR 3, GWK Präzisionstechnik GmbH

3 Chemiluminescence Microarray Reader, MCR R, GWK Präzisionstechnik GmbH

1 Ink-Jet Microdispenser, SciFlexarrayer S1, Scienion

2 Contact Microarrayer, BioOdyssee Caligrapher, BioRad

2 Cutting Plotter, Graphtec CE6000–40

Microbiology

1 Flow Cytometer, CyFlow Cube 6, Sysmex Partec GmbH

1 Bead Beater Homogenizer, MP Biomedicals

1 Water Microbiology Colilert-18 and Quanti-Tray 2000, IDEXX

2 Clean Benches

1 Bioaerosol Chamber

2 Microbiological Incubator, Binder

1 Temperature Controlled Shaking Incubator

1 Autoclave, Certoclav

1 Autoclave, SHP Steriltechnik

1 Cyclone Impinger Coriolis µ, Bertin

1 Munich Microorganism Concentrator, MMC 3

1 Monolithic Affinity Filtration Unit

Further equipment for bioanalytics

1 Cooled Centrifuge, Universal 320R, Hettich

1 Climatic Chamber, Binder

4 Drying Cabinets, Memmert

1 Washer Disinfector, DS 500 Lab, International Steel CO.SPA

1 Photometric ELISA Reader, Biotek

1 96-channel Washer, Biotek

1 Turbidometer, WTW GmbH

1 Nanophotometer, Implen GmbH

1 -80 °C Freezer

Standard Lab Equipment

1 Lyophilizer, Alpha 1-4 LSC, Christ

1 Ultrapure Water System, Direct-Q 3 UV, Millipore

1 Centrifuge, Eppendorf 5804 R

2 Fluorescence Spectrometer LS 50, Perkin Elmer

1 UV-Vis Spectrometer, Perkin Elmer

Chromatography, Mass Spectrometry and Particle Separation

2 GC-IRMS (Isotope Ratio Mass Spectrometer) Instruments

1 LC-IRMS

1 GC-MS

1 Orbitrap-based benchtop MS, Exactive/HCD-System, Thermo Fischer

1 MS, Thermo Fisher LTQ

2 Concentrators for dynamic headspace analysis

2 HPLC, UV/VIS array detector, programmable fluorescence detector

1 Ion Chromatograph, Dionex

1 LC system, ECONO

1 Preparative HPLC

Elemental Analysis

1 Flame-Photometer, BWB Technologies

1 ICP-MS, Perkin -Elmer Nexion 350D

Laser

2 He/Ne-laser

5 Nd-YAG -laser, pulsed

1 Nd-YAG Laser 2 W cw, 532 nm narrow band

3 Nd-YAG-laser, cw

Several diode lasers (600–1670 nm; up to 2 W CW)

Several Quantum Cascade Laser systems

3 Optical parameter oscillator (410 nm–2.1 µm)

Optoelectronics/Spectrometer

3 Echelle spectrometer

1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700

1 Fluorescence spectrometer, Perkin Elmer LS-50

1 Fluorescence spectrometer, Shimadzu RF 6000

1 UV/VIS spectrometer, analytic jena Specord 250 plus

1 UV/VIS spectrometer, analytic jena Spekol 1500

4 Digital storage oscilloscopes (400 MHz, 500 MHz)

1 Wavemeter

Microscopy

2 Laser Raman microscope, WITec *alpha300R* (532/633 nm)

1 Laser Raman microscope, WITec *apyron* (532/785 nm)

1 Laser Raman microscope, Horiba LabRam HR (532/633/785 nm)

1 Temperature controlled stage (-196 °C – 600 °C, Linkam THMS 600)

1 SEM/EDX system, Zeiss Gemini

Sum Parameters

2 Coulostat for C quantification, Coulomat 702

1 DOC analyser, UNOR 6 N

1 TOC analyser, Shimadzu TOC-L