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

Annual Report 2023

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 2023

Content

Dear colleagues and friends,

after our isotope ratio mass spectrometers had been for two years in the basement and one year in the ramp up, last year has seen our isotope lab finally fully functional again. Kudos to our technician Felix Antritter! These mass spectrometers for compound-specific isotope analysis enable us to measure minuscule differences in the natural abundance of stable carbon, nitrogen, hydrogen and chlorine isotopes. This allows deciphering different sources of chemically identical substances, and tracing their transformation in the environment. A particular highlight was last year's acquisition of an Orbitrap Exploris mass spectrometer. Its high mass resolution of 240 000 enables stable isotope analysis of several elements simultaneously and allows us to explore intramolecular isotope ratios in organic structures. Stay tuned for more to come in the next years!

Last year has seen the conclusion of excellent PhD theses. Julia Klüpfel completed her dissertation on the development of rapid automated chemiluminescence microarray immunoassays for SARS-CoV-2 serological assessments. Besides three publications, the outstanding scientific achievements in her doctoral thesis were honored with summa cum laude. David Glöckler graduated with distinction on his comprehensive work on the selectivity of cyclodextrin polymers as part of the Bakkour group's endeavor to enhance sensitivity in stable isotope analysis of aquatic micropollutants. His careful investigations into the role of polarity vs. cavity size to select for target analytes against background organic matter has earned him three publications in Analytical Chemistry and summa cum laude. Last but not least, Christian Schwaferts got the Doctoral Award 2023 from the Water Chemistry Society for his work on nanoplastics analysis. Congratulations to Julia, David and Christian, and to their advisors Michael, Rani and Natascha!

In the Laser and Particles group the FluRam project on online Raman spectroscopy is coming to a success. Under the guidance of Prof. Christoph Haisch, the new Raman system, which was developed together with our project partners, is now being applied for HPLC detection. Beyond that, the experience from this project is harvested together with different partners for Raman-based process monitoring in flow- and bioreactor experiments. Raman microscopy proved to be a precious tool also in a medical study together with the Friedrich Baur Institute (Klinikum der LMU-München) on rare muscular glycogen storage diseases. Findings from this collaboration are likely to directly influence treatment strategies.

In the Bioanalytics Group, the topic of pathogens and rapid tests continued to drive us to collect pathogen-containing bioaerosols from the air and to rapidly quantify them using our bioanalytical methods. Moreover, with our research work, we are on a good way to get acceptance that pathogens are an important pollutant for water quality testing. Thanks to our PhD students, we have advanced several third-party-funded research projects within the area of culture-independent determination of *Legionella pneumophila* in evaporative cooling systems. For the first time, we have successfully incorporated molecular biological and antibody-based rapid tests in a VDI guideline.

Achievements from our group leaders were also recognized on several occasions. A Human Frontier Science Program (HFSP) grant was awarded to Dr. Rani Bakkour with colleagues from the Max Planck Institute for their endeavour to uncover paleo diets from a deeper look into the isotopic composition of amino acids in tooth enamel. Dr. Natalia Ivleva was invited to the International Advisory Board of Analytical and Bioanalytical Chemistry and guest-edited a special issue (https://doi.org/10.1007/s00216-023-04747-y) on Advances in Chemical Analysis of Micro- and Nanoplastics A TUM News Release highlighted the Raman/REM group's most recent advances on Automated analysis of microplastics (https://www.ch.nat.tum.de/hydrochemistry/news-announcements/news-single-view/article/tum-news-release-automated-analysis-of-microplastics-1/).

As always, all of this would not have been possible without every member of our institute: Ph.D. students, technicians, secretaries, Postdocs and guest scientists. Thanks to all of you for your dedication and your invaluable contribution over the last year!

And, last but not least, thanks to you, our friends, for your continued support. I hope to see many of you at our upcoming Alumni Day on July 5th 2024, and on our yearly meeting in fall, where we will have the opportunity again to discuss the latest developments in the water sector and set the course for an even closer collaboration in the future. If you are an alumnus from our institute and have not yet joined the Friends' Association – now is the time!

Kind regards, Martin Elsner

Mining for Microbiological Markers in Non-Target-Screening Data

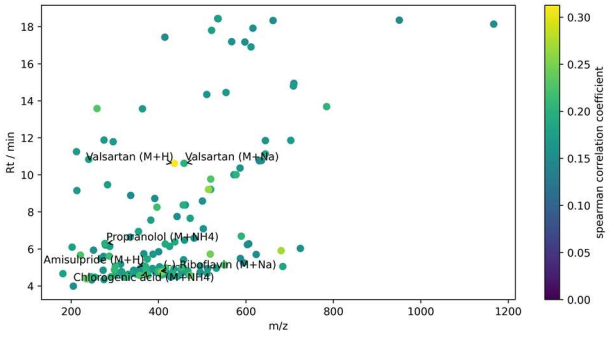
Non-target-screening (NTS) maps the mass spectra of unknown water-born organic compounds after liquid chromatographic separation (LC) to screen for emerging chemical pollutants in surface water. Our goal is to mine this data of unknown compounds also for potential markers of microbiological contaminants.

State of the Art In 2019 twenty-nine percent of the drinking water in Germany originated directly or indirectly from surface water. NTS with LC coupled to high resolution tandem mass spectrometry (LC-MS) is an innovative approach to screen for the occurrence of new organic pollutants in surface water. In comparison to conventional target monitoring, NTS is not limited to pre-selected analytes. In recent years it found increasing use for monitoring river water by water suppliers and agencies.

In contrast, for the routine microbiological analysis of surface water traditional cultivation-based methods are used. These methods are labor intensive, limit the targets to cultivable bacteria and take several days to provide a result.

Analytical Approach We aim to identify markers for microbiological pollution within the NTS results. Since this data is acquired anyways, our approach would allow mining it as an early warning system for microbiological contamination. River water samples were analyzed for NTS via LC-MS, and for the microbiological parameters with cultivation methods, by the Zweckverband Landeswasserversorgung. The NTS data were uploaded to the cloud processing platform developed within the K^{2}I project and processed online with enviMass.[1] We then correlated the features extracted with enviMass with the result of the microbiological measurements to identify substances indicating a high microbiological contamination of the sample.

Results We observed that valsartan shows a moderate correlation with the concentration of *E. coli* in the river water. Valsartan, an antihypertensive drug, is prevalent in municipal wastewater. Within a waste water treatment plant it is quickly degraded to valsartanic acid.[2] Consequently, its presence can serve as an indicator of wastewater discharge into the river, potentially contributing to the elevated levels of *E. coli*, a fecal bacterium.



Correlation between features extracted with Envimass from LC-MS NTS data and the colony count of *E. coli* in the same samples.

Leonhard Prechtl

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(1) enviMass version 3.5 LC-HRMS trend detection workflow - R package; Zenodo, 2019, DOI: 10.5281/zenodo.1213098

(2) Bayer, A.; Asner, R.; Schussler, W.; Kopf, W.; Weiss, K.; Sengl, M.; Letzel, M. Behavior of sartans (antihypertensive drugs) in wastewater treatment plants, their occurrence and risk for the aquatic environment. Environ. Sci. Pollut. Res. Int. 2014, 21 (18), 10830-10839. DOI: 10.1007/s11356-014-3060-z

Funding

BMBF – K2I

Cooperation

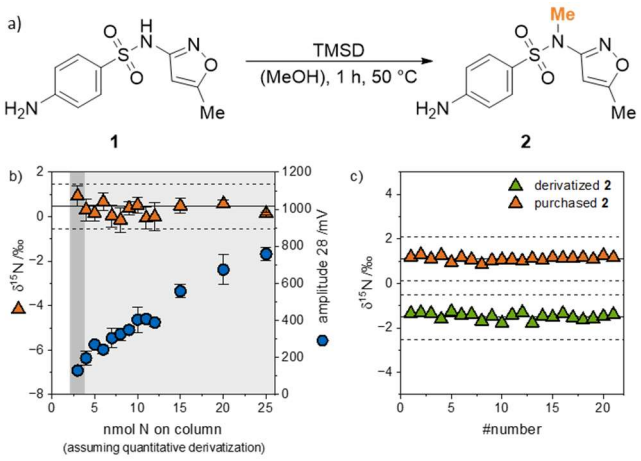
Zweckverband Landes-wasserversorgung BW

Leibniz-Rechenzentrum

Technologiezentrum Wasser

Development of a derivatization method to facilitate gas chromatography isotope ratio mass spectrometry for nitrogen isotope analysis of sulfamethoxazole

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.



Figures illustrating (a) the derivatization of sulfamethoxazole (**1**) to the methylated derivative (**2**); (b) the δ15N values of sulfamethoxazole and corresponding peak amplitudes to show the dependence of isotope values on applied analyte amount assuming quantitative derivatization; c) the δ15N values of derivatized sulfamethoxazole and authentic compound (**2**) compared to the respective EA-IRMS values (black lines).

State of the Art Compound-specific isotope analysis is a powerful tool for characterizing degradation pathways, including photolysis and biodegradation, through occurring isotopic effects. Current investigations into the degradation processes of sulfamethoxazole, an antimicrobial employed in animal husbandry, have used liquid chromatography hyphenated with isotope ratio mass spectrometry (LC-IRMS).[1] While valuable, the LC-IRMS technique is restricted, however, to determining carbon isotope values exclusively. Hence, there is a great current interest in exploring the isotopic effects of heteroatoms, particularly nitrogen.

Analytical Approach Here, a method for nitrogen isotope analysis of sulfamethoxazole is developed using derivatization-GC-IRMS. Sulfamethoxazole is methylated using trimethylsilyl diazomethane (see Figure).

ResultsThe derivatization of sulfamethoxazole (1) using trimethylsilyl diazomethane resulted in the desired methylated product (2). Prior to GC-IRMS analysis, the derivatization conditions, including reaction time and temperature, were optimized, achieving reproducible yields of up to 87%. The developed derivatization-GC-IRMS method for nitrogen isotope analysis of sulfamethoxazole shows a limit of 3 nmol N, assuming quantitative derivatization. Furthermore, no deviation from the elemental analyzer value was observed for both the derivatized and authentic standard, indicating no nitrogen isotope fractionation during the combustion and the derivatization procedure. The developed method has the potential to identify nitrogen isotope fractionation in degradation processes, aiding in understanding transformation pathways using dual-element isotope analysis.

Aoife Canavan

Funding

IAEA – CRP D1.50.22

Cooperation

IAEA

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

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 sulfonamides from water.

State of the Art Sulfonamides (SAs) have been widely used in human and veterinary medicine, and they have been released into the environment. There, 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 the development of antibiotic resistance. While many studies have focused on detecting oxidative biodegradation and associated metabolite detection, only limited information is available on the possibility to break them down via simple hydrolysis. Therefore, our project aims to decipher possible hydrolysis mechanisms of SAs by combining experimental and computational evidence.

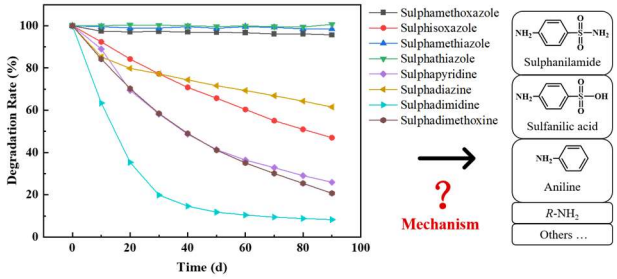


Figure 1. The degradation rate of sulfonamides over time and their detected metabolites at 60℃ in pH 2.0 buffer solution

Analytical Approach Hydrolysis experiments of 8 selected SAs were performed at pH 2.0, 4.0, 6.0, 8.0, or 10.0 buffer solutions over three months, with an initial concentration of 25 mg/L and at a temperature of 60 ℃. Experiments were conducted in triplicates and with controls. Reaction samples of each compound were taken every ten days and stored in a freezer at -20 ℃ before they were measured by HPLC-UV. In parallel, quantum chemical calculations were conducted to explore reactivities by characterizing detailed potential energy surfaces (PESs). All quantum chemical calculations were performed with the QRCA 4.2.1 program.

Results All selected SAs were found to be hydrolytically stable in buffer solutions at pH 4.0, 6.0, 8.0, and 10.0. When the pH was 2.0, in contrast, 5 out of 8 SAs (sulphisoxazole, sulphapyridine, sulphadiazine, sulphadimidine, and sulphadimethoxine) were degraded effectively, and their main products, such as sulphanilic acid, sulphanilamide, aniline and the corresponding leaving groups were identified by HPLC-UV (Figure 1). From computations, a significant difference in protonation energy was predicted at different positions inside the molecular structure of the selected SAs, and these predictions are being validated by NMR measurement. In combination with computed activation energies, this insight is instrumental in predicting possible sites of hydrolytic attack and subsequent hydrolysis.

Lihong Chai

Funding

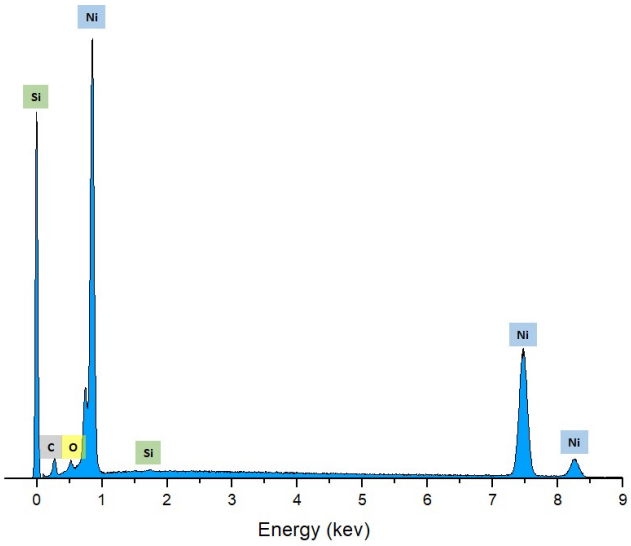
Chinese Scholarship Council, CSC

Cooperation

Prof. Dr Etienne Derat (Sorbonne Université)

A Ni-wall coated microreactor to Increase Sensitivity and Selectivity and to Facilitate GCxGC for Compound-specific Isotope Analysis (CSIA)

Complete peak separation and enhanced sensitivity are two prominent current challenges for sensitive CSIA. Comprehensive gas chromatography (GCxGC) could be a game-changer, but hinges on the development of robust miniature online combustion reactors.



The deposited layer on inner channel of the coated quartz tube investigated by EDX (energy dispersive X-ray fluorescence radiation).

State of the Art 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.

Analytical Approach 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. To pioneer the necessary dramatic reduction of reactor tube size, a Ni wall-coated catalytic microreactor is being constructed. This approach has the benefit of simplicity, while allowing for the fabrication of a capillary reactors with an inner diameter of 0.1 mm, which is not achievable with hand loading of metal wires. The coating is accomplished by flushing a Ni plating solution, consisting of 0.06M nickel (II) acetate and 0.5M hydrazine, at 88ºC for 10 minutes. The weight of the coating is determined by ICP-MS, while the layer thickness is measured by SEM and EDX..

Results A 17 cm long layer of nickel was coated in the center of a 30 cm long quartz tube (outer diameter 1.5 mm, inner diameter 0.32 mm). The EDX spectrum shows signals for silicon and oxygen caused by the quartz substrate and peaks for nickel, indicating the successful deposition of nickel. The average thickness of the layer measured was 12.6 µm ± 1.6 µm.

Funding
IWC

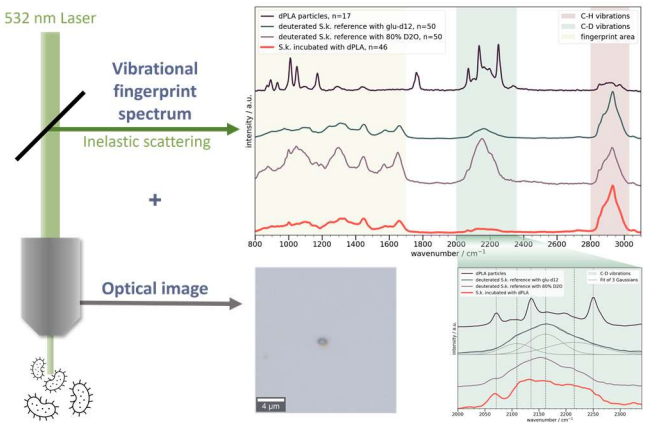
Habib Al-Ghoul

Cooperation

Stable isotope Raman microspectroscopy to trace deuterium from labeled (micro) plastic into environmental bacteria

Raman spectroscopy is used to study the microbial degradation of (micro) plastics. Quantitative data about the C-D vibrations of different biomolecules indicates D-lipids as a major metabolic product.

State of the Art Biodegradation of plastics starts with the microbial colonization of the plastic surface, followed by the excretion of extracellular enzymes for depolymerization. The mono- and oligomers are then taken up by microbes and mineralized to CO_2 and water or used for biomass formation. ^{13}C labels allow the monitoring of $^{13}CO_2$ and its incorporation into biomass.[1] However, ^{13}C-labels are expensive and not available for most plastics.



Left: Scheme of Raman microspectroscopy measurements of single microbial cells. Right: Raman spectra of cells incubated with different deuterium sources (orange: dPLA, purple: D_2O, green: glucose-d_{12}) are compared to the pure dPLA spectrum (black). The C-D region of the Raman spectra (highlighted in green) allows to differentiate deuterated biomass from deuterated polymer.

Analytical Approach We use deuterated polylactic acid (dPLA) in combination with Raman microspectroscopy as an alternative approach. The spectroscopic method gives chemical information, which is essential to differentiate deuterium in the plastic from deuterated biomass. It also allows us to trace the label into different biomolecules (i.e., lipids, proteins, and DNA). This approach requires less experimental effort and costs compared to the previous ^{13}C-nanoSIMS approach and provides additional metabolic information (deuteration of lipids, proteins, and DNA).

Results After 3 weeks of incubation of *Sphingomonas koreensis* with dPLA, biomass spectra that show a new C-D band were discovered. Chemical information and comparisons to *S. koreensis* reference spectra, obtained with glucose-d_{12} and D_2O, allowed us to assign this band to deuterated biomass. However, it shows an increased ratio of D-lipids to D-proteins compared to both references. This is supported by the low phenylalanine deuteration and indicates a different metabolic pathway. An exchange of D from dPLA with the aqueous medium with subsequent uptake of D_2O by *S. koreenis* can thus be ruled out. Deuterium was further traced into microbial carotenoids with resonance Raman spectroscopy, which allows high-throughput applications.

Kara Müller

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Funding

German Research Foundation, DFG (Project IV 110/2-2)

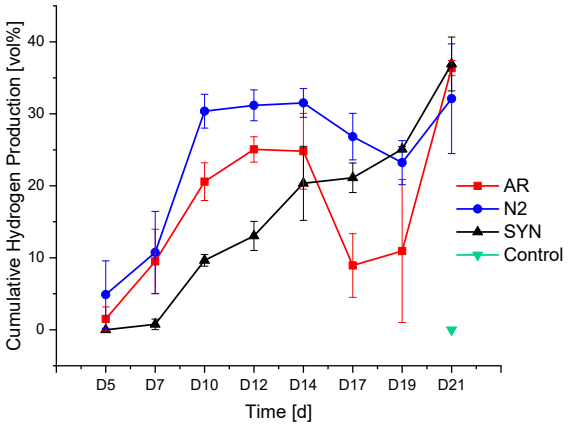
Cooperation

Jürgen Allgaier, FZ Jülich

Exploring the potential of bio-gas production by the bacterium *Rhodopseudomonas pentothenatexigens*

The bacterium *Rhodopseudomonas pentothenatexigens* shows bio-hydrogen production under anaerobic and Vis-IR-illumination.

State of the Art The project focuses on the optimization of wastewater treatments in the brewing industry by improving the anaerobic microbiological treatment of wastewater. The central element of this treatment is made up of exoelectroactive bacteria, which actively produce electricity and are also capable of producing biogases. The key objective is to couple a microbial fuel cell with air electrodes to exploit the entire hidden energy potential.



Cumulative hydrogen production over a period of 21 days. (AR: brewery wastewater sparged with argon, N_2: brewery wastewater sparged with nitrogen, SYN: synthetic medium sparged with nitrogen, Control: brewery wastewater without bacteria.

Analytical Approach Bacteria of the species *Rhodopseudomonas pentothenatexigens* (*R. pentothenatexigens*) were inoculated into brewery wastewater and into a synthetic medium (glutamic and malic acid) for comparison. Incubation was carried out anaerobically, under light conditions (ca. 400 nm – 750 nm) and at room temperature. Hydrogen production was observed over a period of 21 days. To determine hydrogen production, samples were taken at regular intervals. The measurement of hydrogen in the gas phase was carried out with a mass spectrometer (THERMO Star™, Gas Analysis System).

Results The bacterium *R. pentothenatexigens*, isolated and identified from brewery effluent, was used to understand the energy transfer during anaerobic, microbial metabolism of organic matter in wastewater. This bacterium is particularly suitable because it can survive and multiply in this type of wastewater and can naturally release electrons into the environment and thus produce electricity. To increase the efficiency of electricity production, the energy flow of the bacterial metabolism must be known. To reveal this, in addition to monitoring the electrons released, the analysis of the by-products, such as the production of bio-gases, must also be investigated. The experiment demonstrated the natural synthesis of hydrogen under the conditions that also apply in the microbial fuel cell. In addition, more hydrogen was produced in the brewing wastewater than in the synthetic medium, which once again demonstrates the exploitation of this species for real applications (see figure). It was also shown that the type of gassing plays a role in the well-being of the bacteria. More hydrogen was produced under nitrogen fumigation than under argon fumigation. The proliferation of the bacteria also mimicked this trend. To conclude, the results obtained from this experiment indicate that not all the energy produced is released as free electrons and thus the production of bio-gas in the form of hydrogen is another energy source that needs further investigations.

Irina Beer

Funding

Federal Ministry for Economic Affairs and Climate Action (Project 20789 N)

Cooperation

Prof. Dr. Thomas Hofmann, Dr. Karl Glas (TUM School of Life Sciences), Prof. Dr. Köhler (TUM School of Natural Sciences)

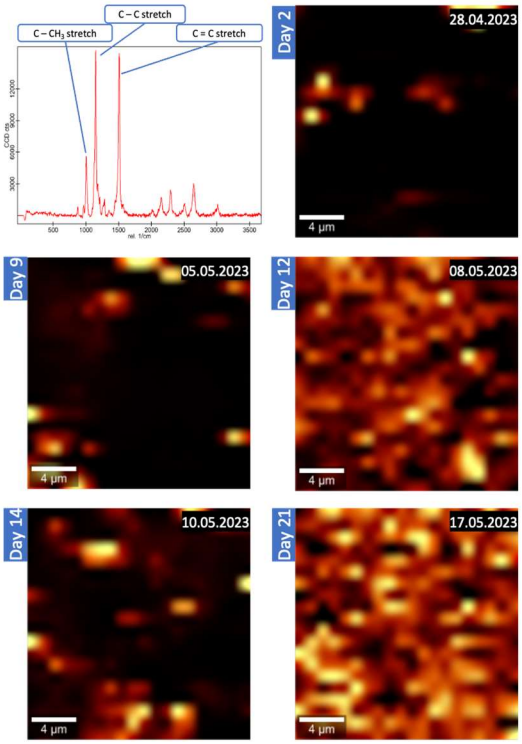
Development of an efficient microbial fuel cell and investigation of biofilm formation using Raman microspectroscopy

Raman microspectroscopy is used with the aim of investigating the biofilm formation of the bacterial species *Rhodopseudomonas pentothenatexigens* in microbial fuel cells (MFCs), in order to enhance the effectiveness of the MFCs as well as proving the exoelectrogenic activity of the investigated bacteria.

State of the Art The MFC research is mostly focused on a laboratory scale since the commercialization requires a cheap fabrication and stable performance with suitable MFC setups and the right bacteria. The bacterial species *Rhodopseudomonas pentothenatexigens* are known to produce bio-hydrogen, which has been first reported by *Phankhamla* et al. (2014).[1] Since the strain *R. palustris* of the genus *Rhodopseudomonas* is capable of producing both bio-hydrogen and electricity[2] while showing similarities to *R. pentothenatexigens* such as size, shape and color, the hypothesis of *R. pentothenatexigens* also being able to produce electricity formed.

Analytical Approach The biofilm formation of *R. pentothenatexigens* was investigated employing Raman microspectroscopy and making use of the produced carotenoids, which are well measurable due to the resonance Raman signals of these chromophores. Furthermore, the exoelectrogenic activity of the bacteria was examined using a potentiostat as well as a voltmeter.

Results The development of an MFC employing *R. pentothenatexigens* was successful and experiments indicating the exoelectrogenic activity of the species could be conducted. The biofilm formation of *R. pentothenatexigens* was furthermore investigated in a flow cell using Raman microspectroscopy and the general concept of biofilm formation investigation could be proven to work.



Resonance Raman spectrum of the carotenoids produced by *R. pentothenatexigens* and Raman mapping images recorded using the 63 × magnification water immersion objective for an area of 20 µm × 20 µm using a 532 nm laser with 1 mW at the sample and 1 s per measurement point for the MFC flow cell with brewery wastewater after the second inoculation.

Ida Keussen and Irina Beer

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Federal Ministry for Economic Affairs and Climate Action (Project 20789 N)

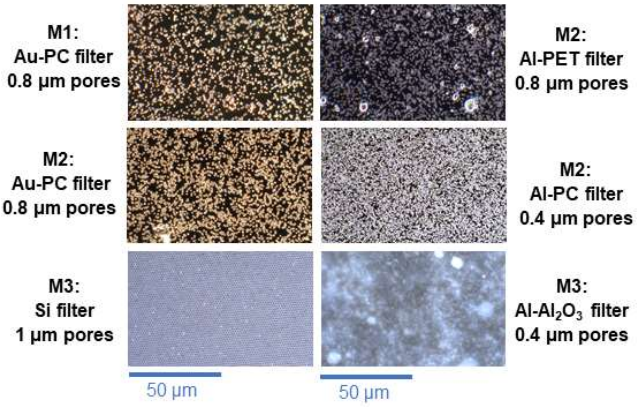
Cooperation

Dr. Karl Glas (TUM, Chair of Food Chemistry and Molecular Sensory Science)

Towards efficient automated Raman-micro spectroscopic analysis of small microplastics

Further development of a method for efficient analysis of microplastic particles and fibers in aqueous and food matrices. The aim is a reliable identification and quantification of small microplastics.

State of the Art Public concern is growing over the ingestion of microplastics through consumables like drinking water and milk, and its potential impact on human health. A reliable method for the automated analysis of microplastic particles down to 1 µm has already been developed by O. Jacob *et al.* with the *TUM-ParticleTyper 2*.[1] This software automates the image and spectrum acquisition and determines the particle sizes. To improve the spectrum quality, different filter types have been suggested.[2]



Optical microscope images depicting the surfaces of various filters acquired using dark field illumination at a magnification of 100×. The images were significantly brightened, given the reduced illumination necessary for processing with *TUM-ParticleTyper 2*. The labels M1-3 denote different manufacturers.

Analytical Approach Optimization of spectral quality is achievable through the adjustment of parameters such as laser power, integration time, and number of accumulations of spectra, but also with the selection of a filter substrate characterized by minimal or absent background interference within the regions corresponding to characteristic polymer bands. A variety of different, commercially available filters are tested for their ability to improve the Signal-to-Noise ratio of Raman spectra obtained from small particles.

Results So far six filters are in the progress of being evaluated for the usage in automated Raman microspectroscopy analysis with *TUM-ParticleTyper 2*. Aluminum-coated filters have shown promising low background interference regions corresponding to characteristic polymer bands. Although the obtained Si filter cannot be considered for the analysis of particles below 1 µm due to its pore size, it is of interest as these filters are chemically more stable than the Al-coated filters. The Al-coated filters demand increased attention during sample preparation, particularly regarding the pH levels of the sample during the filtration process. Further investigation is in progress.

Isabel Jüngling

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Funding
Nestlé S.A.

Cooperation
Nestlé S.A.

Is fragmentation of plastic waste leading to a measurable concentration of small microplastics in the open ocean?

Results for microplastic particles in open ocean water in the region of the North Atlantic Garbage Patch are presented.

State of the Art Gaining knowledge of particle numbers and size distributions of microplastics (MPs, synthetic polymer particles and fibers in the size range 1–1000 µm) in open ocean water can provide an indication for MP sedimentation as a sink for plastic waste in the environment. Of special importance is the statement about the quantity of small MPs (particle sizes 1–50 µm). At the Institute of Water Chemistry, *TUM-ParticleTyper 2* was developed for automated Raman microspectroscopy-based analysis of MPs at the entire size range.[1]

Station	depth / m	Plastic types *without PCV* Size class 1 – 50 µm
1	75	**1968**
22	80	140
36	75	**1191**
53	75	149
69	75	340
	300	*198*
	150	*166*
81	*75*	*310*
	50	*178*
	25	*0*
102	75	**1422**
		1876
field blanks		0
		449

Particle counts within the size class 1–50 µm, including common plastic types (without PC, PVC), according to the minimum particle diameter. Results above the LoD (~570 particles, determination based on 11 laboratory blanks) are in bold print.

Analytical Approach Ocean water samples (1 L each) were collected during the HOTMIC cruise SO279 (CTD device, FS SONNE, 2020). For sample preparation, a method known from wastewater treatment (photo-FENTON, H_2O_2 + UV-C irradiation (variant without Fe II catalyst)) was optimised and applied. Automated detection, Raman-based identification and quantification of MPs, as well as evaluation of results, were controlled through *TUM-ParticleTyper 2* (*random window sampling*[2] mode).

Results 11 laboratory blank samples were analysed and resulted in a limit of detection (LoD) of 570 particles (total count of plastic (PE, PP, PS, PET, PTFE, PMMA) particles). PVC was excluded from the results, as the Niskin bottles used aboard for sampling were made of this polymer. Furthermore, the results revealed a significant contamination from PVC for three samples and one field blank. Results, including recurrent plastic types only (PE, PP, PS, PET), were beneath the (adapted) LoD in all cases. For the future analysis of ocean water samples the sampling of higher volume can be recommended to improve the representativity of analysis. Improved sample preparation can increase the plastic-to-non-plastic ratio and, hence, improve the feasibility of analysis.

Oliver Jacob

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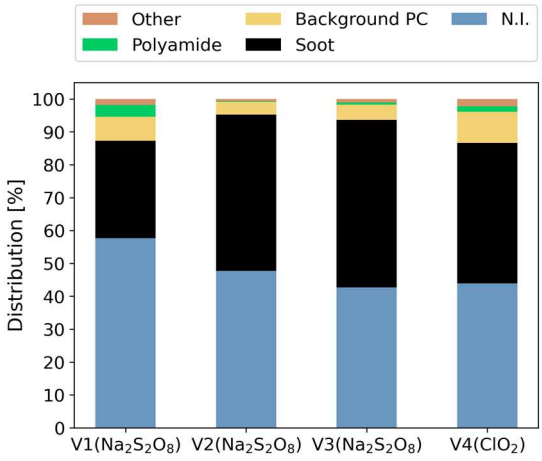
Cooperation

A. Beck, E. Achterberg (HOTMIC, GEOMAR, Kiel)

Investigation of adverse effects of disinfectants on polyamide membranes in reverse osmosis systems

Raman microspectroscopy, coupled with the in-house automation software *TUM-ParticleTyper 2*, is utilized to establish a methodology for assessing damage in reverse osmosis (RO) systems.



Particle type distribution in actual persulfate samples: V1-V2 at Reynolds number (Re) = 200, pressure (P) = 9 bar, transmembrane pressure (TMP) = 7.5 bar, and concentrations (C) of 8 and 10 g/L; V3 at Re = 50, P = 9 bar, TMP = 7.5 bar, and C = 10 g/L; and V4 involving chlorine dioxide at Re = 125, P = 5 bar, TMP = 5 bar, and C = 1 g/L. The distribution is displayed divided into the fractions of N.I. (non-identified), soot, filter background, polyamide, and other analyte particles.

State of the Art The water purification performance of RO systems diminishes due to the polyamide (PA) membrane's aging, disintegration, and fouling.[1] Identifying and applying optimal disinfection conditions is, therefore, crucial. Raman microspectroscopy demonstrates high suitability for non-destructive analysis of microplastics. Integrating this technique with automatic measurement software improves particle detection and overall efficiency, reducing analysis time and diminishing human bias, thereby enhancing result credibility.[2]

Analytical Approach Particles from various analyte disinfectant solutions are deposited onto filters within a laminar flow bench, followed by analysis via Raman microspectroscopy facilitated by the automation software *TUM-ParticleTyper 2*. A series of measurements involving variations in acquisition time and laser power was carried out beforehand and tested on representative aliquot and blank samples to determine an effective method for actual samples.

Results The 3 mW and 0.5 s measurement mode was selected for optimal efficiency and accuracy. Laboratory blanks indicated minimal analyte particle levels, primarily TiO_2 and cellulosic material. The particle distribution in the aliquots, exemplary given for the two aliquots of the actual sample V3, showed consistent concentrations of PA (0.68% and 0.58% of all identified particles), confirming the method's accuracy. PA and other analyte particle fractions varied significantly among actual samples, with no clear correlation between measurement parameters and particle distribution. The results showed higher PA content for V1 than V2 at 3.63% compared to 0.22%, despite a lower disinfectant concentration under elsewise constant parameters (8 g/L vs. 10 g/L of $Na_2S_2O_8$). A direct result comparison, however, is challenging due to the limited number of analyzed samples.

Marcel Klotz and Maximilian Huber

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AiF-ZIM (KK 5022305CR0)

Cooperation

Dr. Karl Glas (TUM, Chair of Food Chemistry and Molecular Sensory Science);

Dr. Fritz Küke (Dr. Küke GmbH)

References

(1) Antony, A.; Branch, A.; Leslie, G.; Le-Clech, P. Impact of membrane ageing on reverse osmosis performance – Implications on validation protocol. J. Membrane Sci. 2016, 520, 37–44. DOI: 10.1016/j.memsci.2016.07.036.

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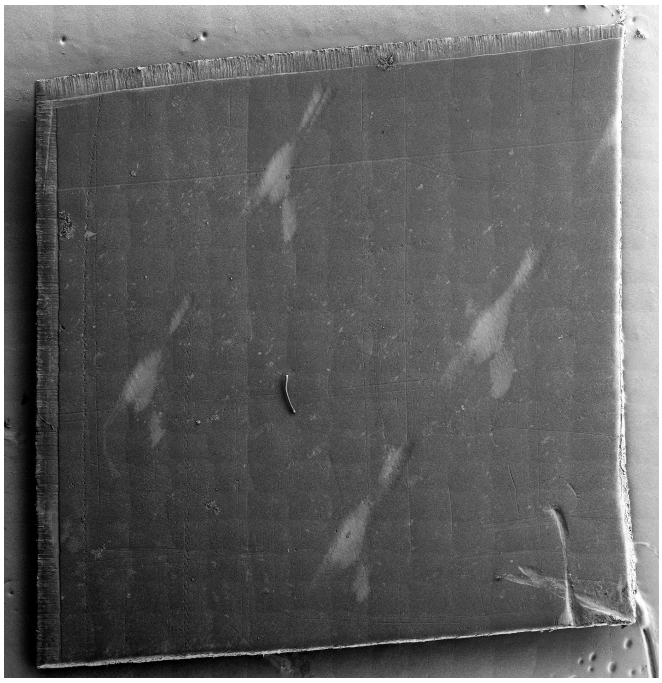
Automated SEM analysis of reverse osmosis membrane damage for Methylene Blue test validation

Reverse osmosis (RO) membrane damage was analyzed using automated scanning electron microscopy (SEM) mapping. The results can be compared to breakthrough areas in Methylene Blue (MB) tests to assess the membrane damage.

State of the Art One of the routinely most used methods to assess RO membrane damage is SEM. It can provide information on the surface morphology of the membrane and its changes under various conditions including scaling and fouling.[1] However, this technique is mostly used to visualize only a very small fraction of the total membrane surface and thus might not yield representative results. To address this shortcoming a MB-based test[2] was refined by our project partners (TUM, Group Glas). To validate this test, large areas must be compared between the MB test and SEM images. This necessitates automated SEM image acquisition.



Stitched image of an automated SEM mapping of an RO membrane (5 mm × 5 mm).

Analytical Approach 5 mm × 5 mm cuts of RO membranes treated with various disinfectants (provided by the Dr. Küke GmbH) were sputtered with an Au/Pd-alloy to increase conductivity for prolonged measurements. Utilizing a special script automated SEM mapping was performed using a secondary electron detector on a Zeiss Sigma 300VP at 1 kV to further reduce charging of the sample. The images were stitched automatically and compared to the results from previously performed MB tests (TUM, Group Glas).

Results The script to perform the automated SEM mapping was optimized to minimize sample charging and to improve image acquisition rate while maintaining good image quality. Besides some larger particles, the imprints of the feed spacer mesh are clearly visible. The large-scale analysis of RO membranes allows for a validation of the MB test results. Both methods are in good agreement with each other. However, the cause of some membrane damages, especially sharp breakthrough defects, remains unclear.

Maximilian Huber

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Funding

AiF-ZIM (KK 5022305CR0)

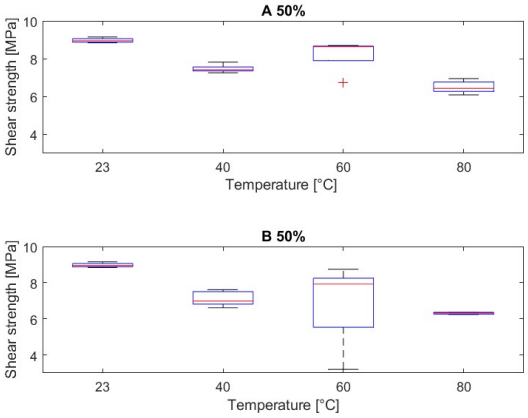
Cooperation

Dr. Karl Glas (TUM, Chair of Food Chemistry and Molecular Sensory Science);

Dr. Fritz Küke (Dr. Küke GmbH)

Analysis of adhesive performance depending on the conditions during curing and mechanical testing

A polyurethane adhesive is cured and tested under varying temperatures and relative humidities (rH). The failure force, mode and fracture image are recorded. The testing conditions greatly impacting the performance of the adhesive, with the curing conditions resulting in a smaller impact.



Lap shear test results for Groups **A** and **B** for 50% rH. Reduction in strength with increasing temperature and similar curves for both sample groups visible.

State of the Art The performance of adhesives is strongly influenced by their curing and testing conditions. Higher levels of humidity during the curing process can result in side-reactions occurring, and higher temperatures may lead to higher levels of crosslinking, causing the physical properties of the polymers to change. Alongside this, the testing conditions can also greatly impact the performance of adhesives.[1]

Analytical Approach The performance of the adhesives was tested using the single lap joint (SLJ) shear test. The samples were prepared in accordance with ISO 4587:2003 with 5 samples tested for each experiment. The chosen parameters were 23 °C, 40 °C, 60 °C and 80 °C, with the rH set at 25%, 50% or 75%. The samples were split into three categories. They were either cured at norm conditions (23 °C, 50%) then tested at the chosen conditions (A), cured and tested at the chosen conditions (B) or cured at the chosen conditions and then tested under norm conditions (C).

Results According to the received data, the testing conditions have a very large impact on the overall performance for the chosen adhesive. When increasing the test temperature to 80 °C the amount of force the adhesive can withstand reduces by over 33%. For groups A and B we found very similar results, indicating that the influence of the testing conditions is far greater than the influence of the curing condition. Increasing the relative humidity also decreases the amount of force the adhesive can withstand, up until around 60 °C, when the high temperature predominates and the forces recorded at 25%, 50% and 75% begin to align more closely. The impact of the curing conditions is smaller, not exceeding 15% of the maximum force, however, the de-/increase in force visible in group C is also observable when comparing groups A and B.

Alexander Thomas

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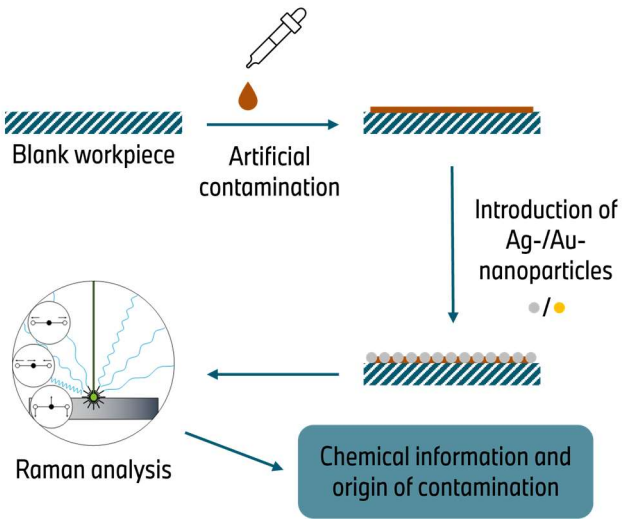
Funding
BMW AG

Cooperation
BMW AG

Analysis of (organic) filmic impurities on metallic surfaces via surface enhanced Raman scattering (SERS)

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.

State of the Art With the accelerated growth of e-mobility and the related transition from combustion engines to high-voltage battery packs, the requirements of technical cleanliness have strongly gained importance. Metallic particles stemming from welding processes represent one of the most hazardous issues. The generation of these particles is promoted by the presence of thin organic films on the workpieces, mostly lubricants.[1] To analyze these films, a powerful analytical technique is required. While the widely used method of fluorescence measurements only yields limited information about the chemical composition of the analyte, more sophisticated methods like secondary ion mass spectrometry or X-ray photoelectron spectroscopy require the presence of expensive and industrially uncommon instruments.



Approach of the SERS test experiments. Samples are artificially contaminated with Raman active compounds and nanoparticles are subsequently introduced onto the surface. The SERS effect is expected to enhance the spectroscopic signal of the analytes and, as a result, concentrations and film thicknesses below the detection limit of conventional Raman spectroscopy shall be analyzed.

Analytical Approach Analysis of organic films is approached *via* SERS. The aim is partial coating of contaminated surfaces with Ag- or Au-nanoparticles and subsequent examination with Raman microspectroscopy. Raman signals of analytes in direct proximity to the metal particles can be enhanced by several orders of magnitude due to localized surface plasmon resonances. As a result, it is expected to obtain signals of the contaminant for concentrations that are considerably lower than the detection limit for conventional Raman spectroscopy.

Results Different parameters for nanoparticle coatings were applied on glass and Al-surfaces which are currently examined for their structural properties. Spectroscopic results of these samples with Raman active test compounds are performed in the next step to optimize the choice of nanoparticle material and laser wavelength.

Jannis Gehrlein

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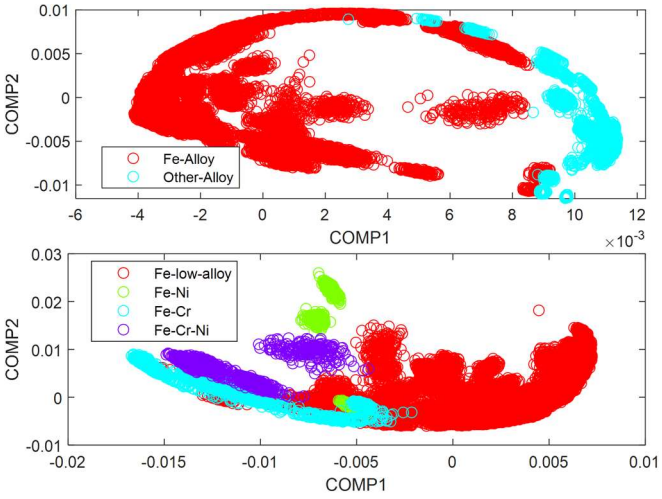
Funding
BMW Group

Cooperation
BMW Group

Decreasing Fe-alloy matrix effects by pre-classification in quantitative LIBS analysis

To tackle the large impact of matrix effects typical for Fe-alloys in LIBS analysis, data processing steps are implemented. This way, adequately accurate results for quantitative LIBS of Fe-alloys are generated.



2D visualization of 2-step multi-dimensional PLS-DA classification of the Fe-alloy training data. First a rough classification (top) in "Fe-alloy" and "Other Alloy" is performed. In the fine classification (bottom) the samples from class "Fe-alloy" are further divided. The calibrations are developed accordingly to the here defined classes.

State of the Art LIBS is gaining relevance in industrial analysis due to its short measurement time, easy application and high sensitivity. However, the method is strongly impacted by matrix effects, that change the linear correlation of analyte concentration and signal output.[1] Especially for complex matrixes, like Fe-alloys, that can consist of various alloy elements in a wide concentration range, this behavior decreases analysis accuracy. By optimizing measurement and evaluation parameters, the accuracy of element quantification vis LIBS can be increased.

Analytical Approach Using the signal-to-noise-ratio, LIBS measurement parameters can be optimized for the analysis of Fe-alloys. These parameters are used to collect a large training and validation set of certified reference materials (CRMs) and evaluated using multivariate data analysis. By including spectral regions instead of single signals into the evaluation, we expect decreased impact of matrix effects and increased accuracy. As the change in matrix composition is larger for Fe-alloys compared to e.g., aluminum alloys, 2-step pre-classification is included into the evaluation to pre-filter for similar CRMs.

Results For the evaluated training data, a 2-step PLS-DA classification before quantification yielded the best results, by first rough filtering followed by fine filtering different matrices. As the resulting classes are close to each other in composition, the overlap hampered accurate classification. To decrease the danger of large inaccuracies in quantification due to misclassification, the concentration regions used for calibration were chosen in such a way, that they overlap. This way, the adequately accurate results were achieved in validation.

Maria Lanzinger

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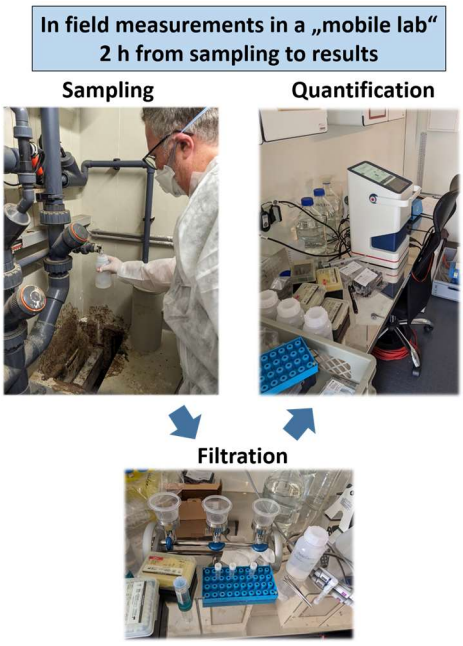
Funding
BMW AG

Cooperation
LTB Lasertechnik Berlin

Cultivation-independent methods identify the source for *Legionella pneumophila* in agricultural exhaust air purification systems

Agricultural exhaust air purification systems (APS) are used for the reduction of ammonia and odor in pig farms. *Legionella pneumophila* that are emitted as bioaerosols could be a health risk. A field study was conducted using a mobile flow cytometer for rapid quantification of *Legionella pneumophila* in process water, clean air, barn air, and fresh water supply to identify the source for growth of *Legionella pneumophila*.

State of the Art APS are widely used in pig fattening farms. Pilot studies[1] have already shown that *Legionella*, an airborne human pathogen could be present in these systems. However, the source of contamination was not found and culture methods gave negative results due to overgrowing caused by the microbiome. Therefore, culture-independent methods such as the novel standard addition qPCR[2] or antibody-based methods were explored to gain reliable results in this complex environmental matrix.



Workflow of in-field measurements with the IMS-FCM.

Analytical Approach For the field study, antibody-based flow cytometry with immunomagnetic separation (IMS-FCM) was explored as a mobile detection system. Additionally, as an orthogonal method to confirm the in-field results in the laboratory, the standard addition method for qPCR[2] was advanced to overcome the matrix effects in APS samples that influences classical qPCR approaches.

Results In wash water of three different APS, monitored over 1 year, qPCR and IMS-FCM confirm a high prevalence of 10^4 – 10^5 *Legionella*/mL. While air that was sampled directly after the barn showed no *Legionella*, filtered air that was released from the APS showed 10^2 – 10^4 *Legionella*/m^3. This indicates a carryover of *Legionella* from the wash water to the released air. In-field measurements finally proved that the fresh water used for the APS was a source of *Legionella*, suggesting the need of pretreatment to prevent the prevalence of *Legionella* in the APS in the future.

Gerhard Schwaiger and Marco Matt

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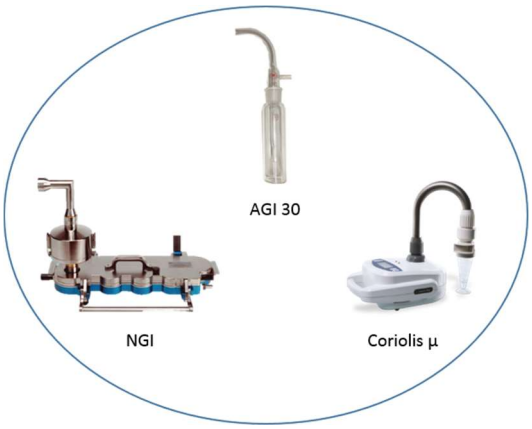
Federal Ministry of Food and Agriculture - BMEL
FKZ 28N-2-002-02

Cooperation
Thuenen-Institute for Agricultural Technology

Next-generation-impactor (NGI) as a new sampling system for *Legionella pneumophila* in aerosols

For the first time, a NGI was applied for sampling of bioaerosols. As this sampler consists of 8 different stages, study of droplet size distribution was possible. This enables new research opportunities for bioaerosols.

State of the Art For the analysis of *Legionella pneumophila* in aerosols of cooling towers a suitable sampling strategy is needed. A high physical but especially a high biological sampling efficiency, which describes the survival of bacteria after the collection, is desired. So far, only studies were performed regarding other samplers or with culture-dependent methods.[1, 2] The Next-generation-impactor (NGI) consists of 8 stages with different cut-off parameters, so a size distribution can be achieved.



All three applied aerosol samplers with three different physical principles. The Next-Generation-Impactor (NGI) with impaction on a dry surface, the All-Glass-Impinger 30 (AGI-30) with impingement in a liquid and the Coriolis® µ with sampling in a liquid through a vortex.

Analytical Approach Aerosols containing *L. pneumophila* were generated with the PARI LC PLUS nebulizer. These aerosols were then collected with the aerosol samplers, respectively, and concentrations of total and living cells were obtained by flow cytometry. For the NGI a reproducible method was established to wash cells from the sampling surface into a liquid. With the measured concentrations, the survival of bacteria cells can be determined. All samples were also quantified by cultivation on BCYE plates.

Results Differences in biological sampling efficiencies were found by comparing the three samplers. Hereby, the lowest survival can be seen with the NGI at 59.0 ± 16.5%, while with the wet samplers, higher values were obtained with 69.0 ± 9.5% for the AGI-30 and 83.5 ± 15.3% for the Coriolis® µ. This can be explained through the different sampling techniques. With the NGI, cells are collected on a dry surface, which can lead to drought stress for the cells. The results by cultivation indicate similar conclusions, as lower recoveries (NGI: 0.009 ± 0.007%; AGI-30: 34.1 ± 29.8%; Coriolis® µ: 37.9 ± 2.2%) were obtained than by flow cytometry. This demonstrates that *Legionella* cells switch to the VBNC state through sampling stress, especially with the NGI. These results show the necessity of culture-independent methods.

Lena Heining

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Funding

AIF (LegioAir)

FKZ: IGF-2147N/2

Cooperation

Institut für Umwelt & Energie, Technik & Analytik e.V. (IUTA)

Trickling biofilm chamber for effect-based analysis of biocides in biofilms containing *Legionella pneumophila*

Biocides can perform differently for cells in biofilms than in water. Therefore, we developed a suitable system to imitate the biofilm growth in evaporative cooling systems. To this end, experiments with real process water and naturally growing biofilm were conducted.

State of the Art *L. pneumophila* can grow in biofilms in cooling systems, which cannot be detected by water sampling. Therefore, it is important to get directly information regarding the growth of *Legionella* in biofilms. This is especially important when biocides are applied as it is stated that biofilms can shield *Legionella* from disinfectants.[1]

Analytical Approach The trickling biofilm chamber was developed together with IUTA within the project LegioAir to enable experiments regarding biofilm growth with *L. pneumophila*. In comparison to other biofilm chambers, water is not flowing through the chamber, but it is sprayed on the glass slides to form a biofilm mimicking a trickling biofilter. In addition, the efficiency of biocides on cells in a biofilm can be investigated.

Structure of the biofilm chamber located in the aerosol chamber in the Bio2 laboratory.

Results The trickling biofilm chamber was built out of glass, in which water circulates from the reservoir on the bottom to the top, where it is nebulized with a two-component nozzle. The nebulized water then settles back into the reservoir. In the reservoir and under the nozzle slides for biofilm growth were installed. With this, a biofilm growth in process water and in nebulized water can be realized. Different materials can be used to recreate those applied in real evaporative cooling systems. Parameters like temperature of the water were monitored, which can be customized. Also, pH value and conductivity were recorded. First tests showed an even growth of biofilm on glass slides within repeating experiments using deionized water that contained naturally occurring microorganisms. In addition, *Legionella* cells were also found in the biofilm. In further experiments, real process water will be used, and the efficiency of biocides will be investigated.

Lena Heining

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Funding

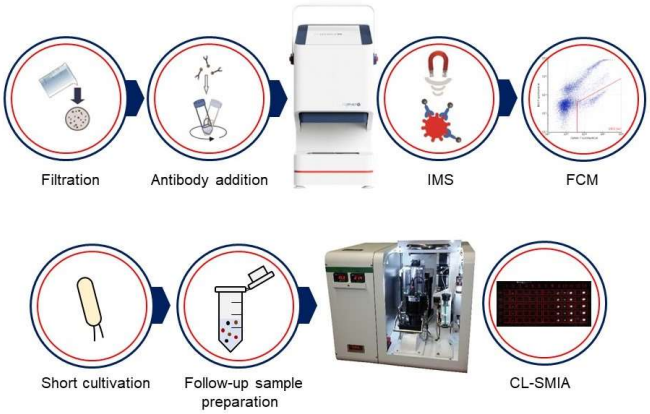
AIF: LegioAir
FKZ: IGF-2147N/2

Cooperation

Institut für Umwelt & Energie, Technik & Analytik e.V. (IUTA)

Rapid quantification and subsequent subtyping of *Legionella pneumophila*

Immunomagnetic separation (IMS) coupled with flow cytometry (FCM) is used for rapid culture-independent quantification of *Legionella pneumophila*, while the chemiluminescence sandwich microarray immunoassay (CL-SMIA) can subtype *L. pneumophila* serogroup 1 after short cultivation of samples prepared by IMS-FCM. The combination of both methods is important to quickly assess the environmental health risk of evaporative cooling systems.



Schematic workflow of the combination of the IMS-FCM method with the CL-SMIA. 100 mL water sample is prepared via filtration and antibody addition for the IMS-FCM. The quantitative result is given in a fluorescence plot. Afterwards, the viable cells are cultivated and spiked as a follow-up sample. The CL-SMIA is performed on the LegioTyper recording CL-images with subtype specific microarray pattern.

State of the Art According to the 42. BImSchV, cultivation is the gold standard to analyze the microbiological exposure of evaporative cooling systems. To establish new and rapid methods for routine analysis and for controlling the efficiency of disinfection measures, culture-independent methods are receiving increased interest. Furthermore, assays are required that can assess the environmental health risk by serogroup subtyping after exceeding the 42. BImSchV.

Analytical Approach Water samples spiked with *L. pneumophila* subtype Philadelphia in a concentration range of 10^2-10^5 cells/100 mL were measured using IMS-FCM and the corresponding waste fractions were stroke on BCYE-plates. After 4 d of incubation at 37 °C single colonies were collected and resuspended in 1 mL water. The concentration was adjusted to 10^7 cells/mL and used directly as a follow-up sample for the LegioTyper, which successfully performed CL-SMIA for subtyping.

Results The proof-of-concept approach showed that the *Legionella* cells were cultivatable after IMS-FCM. Therefore, subtyping can be performed after cultivation. Two different process water samples were analyzed. The IMS-FCM quantified *L. pneumophila* concentrations above 1,000 and 200,000 cells/100 mL. Further, subtyping were possible, leading to the result that the systems were contaminated with non-serogroup 1. With this approach, it was demonstrated that the genus *L. pneumophila* was present in the system, but it did not belong to serogroup 1, which is responsible for more than 90% of hospital-related cases of Legionnaires' disease.

Philipp Streich

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Cooperation

GWK Präzisionstechnik GmbH, Institute of Medical Microbiology and Virology, Technical University of Dresden

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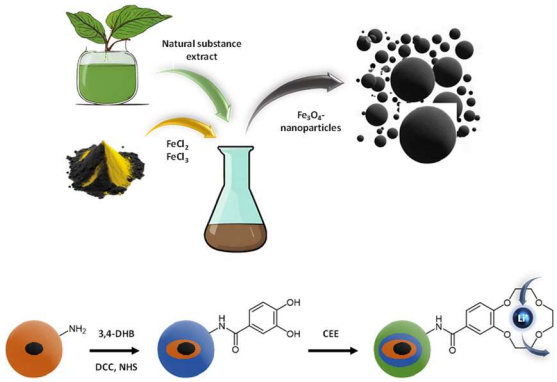
(1) Streich P., Redwitz J., Walser-Reichenbach S., Herr C.E.W., Elsner M., Seidel M., Culture-Independent Quantification of Legionella pneumophila in Evaporative Cooling Systems Using Immunomagnetic Separation Coupled with Flow Cytometry. Appl. Microbiol. 2024, 4, 284-296. DOI: 10.3390/applmicrobiol4010019.

Green chemistry approach: crone ether functionalized superparamagnetic iron oxide nanoparticles for resource recovery.

Superparamagnetic iron oxide nanoparticles (SPIONs) can be used to enrich lithium or rare earths from environmental sources if they are functionalized with crone ether as scavenger molecules. SPION-based resource recovery produces no waste of organic solvents and needs a minimum of energy.



Scheme of the green synthesis approach of Fe_3O_4-NP and its functionalization with APTES, DHB and DCC.

State of the Art Methods for extracting resources from water are based, for example, on precipitation, ion exchange, lithium manganese oxide sieves or solvent extraction. Drawbacks include filter body blockage, contamination of processed water, large-scale waste of organic solvents, or high energy consumption.[1] Using SPIONs for resource extraction eliminates most of these disadvantages. To date, SPIONs have primarily been employed in the field of biomedicine. In water chemistry, however, their applications have been rather limited, with the exception of selective phosphate removal from wastewater. The utilization of SPIONs for the extraction of raw materials from natural sources represents a novel approach.

Approach SPIONs are synthesized via coprecipitation, where simultaneous precipitation of iron(II) and iron(III) salts in a basic solution results in the formation of Fe_3O_4 nanoparticles. The surface modification strategy includes silanization with (3-aminopropyl)triethoxysilane (APTES), coupling of 3,4-dihydroxybenzoic acid (3,4-DHB) using dicyclohexylcarbodiimide (DCC) and N-hydroxysuccinimide (NHS), followed by ring closure with 1,2-bis-(2-chloroethoxy)-ethane (CEE), resulting in the formation of the crown ether.

Outlook The generated nanoparticles will be used to extract lithium and other valuable metals such as rare earths from seawater and geothermal water. In order to make the synthesis and functionalization of the SPIONs more sustainable and resource-efficient, a green synthesis approach will be pursued. This involves replacing toxic and harmful chemicals with natural substance extracts and in-situ surface functionalization, which significantly reduces chemical and energy consumption.[2]

Andreas Auernhammer

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IWC,

Hydroisotop GmbH (Schweitenkirchen, Germany)

Cooperation

Hydroisotop GmbH (Schweitenkirchen, Germany)

Effect-based analysis of microorganisms: cultivation-independent evaluation of biocides by flow cytometry

Flow cytometry (FCM) is a powerful cultivation-independent method for characterizing microorganisms at a single-cell level. We employed FCM to evaluate the effects of different biocides on the pathogen *Legionella pneumophila* (*Lp*) and the whole microbial community in process water (PW) for a rapid, comprehensive assessment.

State of the Art The biocide efficiency is usually evaluated based on the effectiveness against one target microorganism determined by cultivation-based methods. However, cultivation-based methods cannot detect viable but non-culturable (VBNC) bacteria, which can be the majority of viable bacteria under stress conditions like biocide treatments. Moreover, the growth of many pathogens like *Lp* is highly correlated with composition of the microbial community in which they are present. Assessment of the target pathogen in the VBNC state and other microorganisms in the microbiological system should therefore be included in the evaluation of biocide efficiency to assess regrowth potential after biocide dosing. In this work, we employed a cartridge-based FCM, which enables wash-free and on-site measurements and can avoid cross-contamination between samples.[1,2]

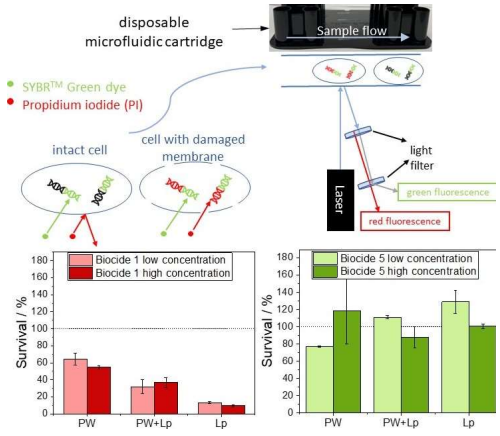

Figure 1: Detection principle of the FCM and representative results.

Analytical Approach We used the cartridge-based FCM to analyze total cell count (TCC) and intact cell count (ICC, incl. VBNC) in PW. First, we characterized the FCM using self-prepared PW with naturally occurring microorganisms. Afterward, we employed the FCM to evaluate the disinfection effects of 6 different biocides on naturally occurring microorganisms in PW, *Lp* in sterile filtered PW, and on *Lp* in non-filtered PW. The survival after biocide was determined using the equation: survival= $(ICC/TCC)_{after}/(ICC/TCC)_{before}$.

Results As shown in Figure 1, while with Biocide 1 (2,2-Dibromo-2-cyanoacetamide) a reduction of up to 90% was detected, Biocide 5 (Isothiazolinone) showed no remarkable effect on intact cells. In contrast, cultivation methods determined no colonies on yeast extract agar or BCYE agar, showing no difference between the two biocides. Therefore, both biocides inactivate *Lp* and other microorganisms present in process water, but only Biocide 1 damages the cells, especially on *Lp*.

Yiao Liang, Lena Heining

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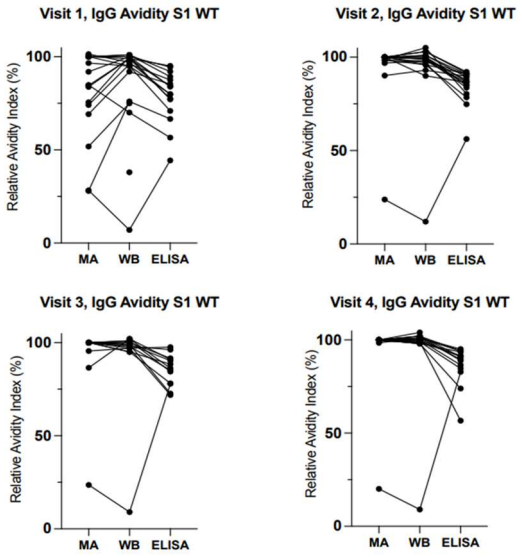
Funding
IWC

Rapid avidity test for SARS-CoV-2 antibodies by flow-based chemiluminescence microarray immunoassay

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

State of the Art It is not only the amount of neutralizing antibodies, but also their avidity, which plays a crucial role in the protection from infection against SARS-CoV-2.[1] In this context, avidity is defined as the strength of binding between an antibody and its epitope. It is expected that the receptor-binding domain of the antigen SARS-CoV-2 S1 and angiotensin-converting enzyme-2 (ACE2) binds with high affinity, but that an incomplete avidity maturation can lead to a decline of the serological response.[1,2]

A common 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 either based on line plot immunoassays or ELISA approaches and take several hours before results are available.[1,2]



Comparison of first results for SARS-CoV-2 S1 wt with ELISA and line assay from Mikrogen shows promising results (MA = Microarray, WB = Line assay). Results for ELISA/Line assay and diagrams: Annika Willmann, Institute of Virology), TUM

Analytical Approach We developed a stopped-flow chemiluminescence (CL) microarray immunoassay for the detection of 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. The IgG avidity was expressed as avidity index (AI) using the formula:
AI = (CL NH_4SCN-treated sera) / (CL of NH_4SCN-untreated sera) × 100%.

Results The developed avidity assay was able to characterize blood samples from 18 individuals over the course of 4 visits within 26 minutes per measurement. These first results correspond to those obtained with a commercial line immunoassay from Mikrogen and a time-intensive ELISA from Virion/Serion. Further optimization and other development steps are still in progress.

Sandra Paßreiter

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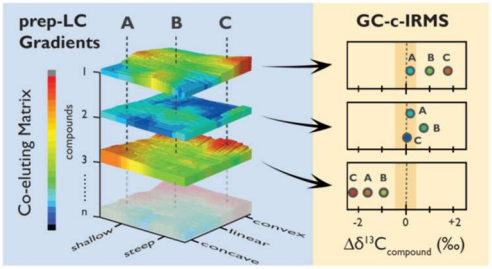
Prof. Protzer, Institute of Virology, TUM
Prof. Knolle, Institute of Molecular Immunology, TUM
ISAR Bioscience GmbH

Optimizing Liquid Chromatography Prior to Isotope Analysis Using Online Matrix Quantification

Matrix removal during liquid chromatography is optimized using a quartz crystal microbalance for online matrix quantification. The benefit for isotope analysis of polar micropollutants is further investigated.



Illustrative depiction of liquid chromatographic separation of n compounds (1, 2, 3, ...n) at different gradients (A, B, & C) and consequent impact on $\delta^{13}C$ of the corresponding compound using GC-IRMS. Co-eluting matrix was quantified using QCM.

State of the Art Compound-specific isotope analysis (CSIA) using gas chromatography isotope ratio mass spectrometry (GC-IRMS) of environmental pollutants often requires sufficient purification of extracted samples. Often, high-performance liquid chromatography (HPLC) is used for this purpose.[1] The respective HPLC purification can, however, only be optimized efficiently if both the target analyte and the matrix natural organic matter (NOM) are monitored online during the chromatographic run.

Analytical Approach In this work, a quartz crystal microbalance (QCM) was coupled with an HPLC using a flow-splitter and a spray-dryer to online monitor NOM during the HPLC purification and thus quantify the co-eluting matrix throughout the chromatographic run (see heatmap in Fig). Furthermore, the impact of NOM on the isotopic integrity of model analytes during GC-IRMS analysis was investigated.

Results We found a direct correlation between the mass of NOM injected and the background intensity measured on GC-IRMS (m/z 44, $R^2 > 0.999$). The matrix background can have a significant influence on the measured isotope values: While the $\delta^{13}C$ value of desethylatrazin (DEA) (29.4±0.5‰) was not shifted, the $\delta^{13}C$ value of caffeine (CAF) (-1.2±0.5‰) was shifted up to -3.3±0.8‰ towards the isotopic signature of NOM (-27±1‰) for samples with a NOM/analyte ratio ≥10. This shows that the measured $\delta^{13}C$ values are not compound specific but rather a bulk measurement of analyte and matrix. To remove the matrix before the GC-IRMS measurement, HPLC purification optimized using QCM proved successful with a NOM removal of up to 99.8% for late-eluting compounds. For simultaneous purification of two or three compounds, including early, middle, and late eluting compounds, the efficiency decreases with up to 2.5% less NOM removal during the HPLC purification. Screening 3 to 5 gradients, including linear, concave, and convex ones, was sufficient to achieve maximal NOM removal. This shows that the QCM is a valuable additional detector for HPLC purification prior to CSIA.

Christopher Wabnitz

Funding
IWC-TUM

Cooperation
Dr. Mathias Reisbeck, TUM

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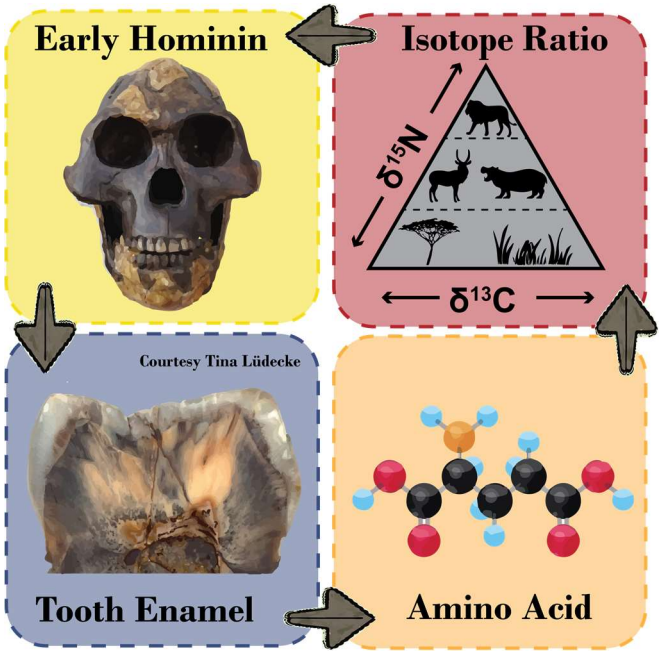
Purification of amino acids from ancient tooth enamel to enable high resolution isotope measurements

Position-specific isotope analysis for amino acids preserved in fossilized tooth enamel can reveal paleodiet of early hominins who lived few million years ago.

State of the Art The importance of plant versus animal nutrition and how this might relate to the increase in brain size for our ancestors is an unresolved question in human evolution. To this end, stable isotope analysis in biomarkers found in fossils offers valuable information. Moreover, paleoanthropologists have recently discovered that amino acids (AAs) can be preserved in tooth enamel over million years. Combined with recent analytical advances in stable isotope instrumentations achieved through high resolution mass spectrometry, this can unravel the paleo diet for early hominins. Yet, the minute amounts of AAs found in tooth enamel pose an analytical challenge for isotope analysis. Therefore, analytical methodologies that provide selective separation of AAs from complex teeth extracts are warranted.[1]



The workflow shows roughly how to identify the paleodiet of early hominins. Based on the $\delta^{15}N$ value of amino acids, extracted from fossil tooth enamel, conclusions can be derived whether our ancestors consumed meat or enjoyed a plant-based diet.

Analytical Approach In this work, we explore the use of urea monomers a promising building block for a polymer to separate amino acids. While the association constants of different amino acids with urea monomers are promisingly high (K_a = 5.1*10^3 L/mol for alanine, = 23*10^3 L/mol for phenylalanine and = 54.8*10^3 L/mol for tryptophan)[2], an approach for immobilizing them onto a high-surface polymer is still needed. To this end, we will produce crosslinked cyclodextrin polymers using tetrafluoroterephthalonitrile (TFN) as crosllinker following two strategies, namely, β-cyclodextrin derivative of urea as a building block and post-synthesis derivatization of TFN β-cyclodextrin polymer to introduce the urea functional group. The generated polymers will then be assessed in HPLC columns with the aim of being able to separate the amino acids precisely with a controlled pH gradient.

Andrea Weiß

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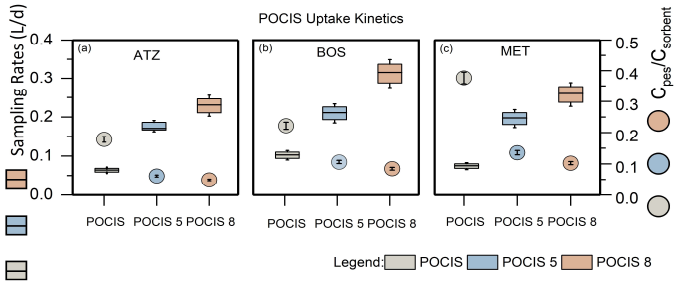
Mainz, Boulder

Enhancing CSIA Potential through Redesigned POCIS: Improving Sensitivity and Uptake Kinetics

Increasing PES membrane pore size shows a significant increase in sampling rates (R_s) of Atrazine (ATZ), S-metolachlor (MET), and Boscalid (BOS).



R_s for ATZ, BOS, and MET for the commercial (i.e., POCIS) and redesigned passive samplers (POCIS 5 & POCIS I) shown using the box plots, while the lag phase values ($C_{PES}/C_{sorbent}$) are shown in circles.

State of the Art Compound-specific isotope analysis (CSIA) is pivotal in tracing micropollutant biodegradation like pesticides. However, due to the latter typical low concentrations (ng/L range) and CSIA sensitivity limitations, sampling water poses significant challenges. Active sampling of large water volumes is required to supply adequate amounts for accurate isotope analysis. While passive sampling (POCIS, in particular) can mitigate the sample volume burdens with no isotopic fractionation, an increase in the sampling rates of PICIS is crucial to achieve the critical mass for CSIA within reasonable durations. Therefore, changes in R_s of ATZ, MET, and BOS were investigated when the membrane pore size increases from 0.1 μm (conventional) to 8 μm (redesigned).

Analytical Approach POCIS was calibrated in two controlled lab settings (main and control tank) to monitor ATZ, BOS, and MET concentrations in water and assess their uptake kinetics. Consistent conditions prevailed throughout deployment (stirring speed of 1500 rpm, pH of 7, C = 0.12 mg/L). Concentrations were measured via gas chromatography mass spectrophotometry (GC/MS) and isotope measurements using a gas chromatography combustion isotope ratio mass spectrometry (GC/C/IRMS).

Results Increasing the membrane pore size from 0.1 to 8 μm progressively increases the R_s for all three analytes (see Fig) by factors of 3.6±0.2, 3.5±0.1, and 3.0±0.1 for ATZ, MET, and BOS, respectively. Enlargement of the membrane pores resulted in diminished lag phases (see Fig), signifying the absence of any delay in the transfer of analytes from water to the sorbent. According to Fick's Law, R_s and deployment time are inversely proportional, meaning that the increase in uptake kinetics shortens the deployment time by the same factors and reduces the entire sample preparation time. Lastly, the accumulated mass in the passive samplers surpassed the GC/C/IRMS critical mass, enabling $\delta^{13}C$ and $\delta^{15}N$ measurements with no isotopic fractionation within typical uncertainties of ±0.5 ‰ and ±1 ‰ for δ^{13} C and $\delta^{15}N$, respectively. We conclude that the redesigned POCIS (PES 8μm) shows greater suitability to combine with CSIA compared to the conventional one.

Funding
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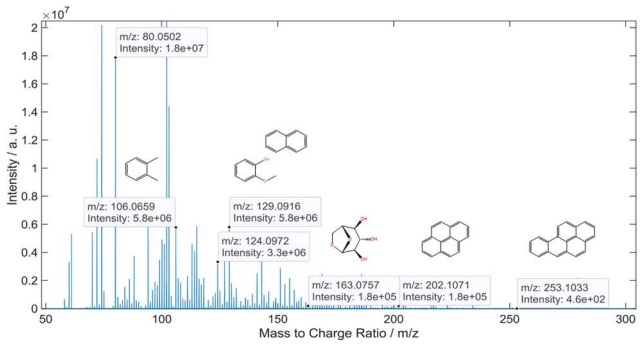
Armela Tafa

Chemical characterization of ultrafine particles by laser desorption mass spectrometry

Ultrafine particles (UFPs) attract increasing public attention due to their adverse health effects. These effects depend on size, shape, and chemical composition. We propose a new robust and simple-to-use approach for the chemical analysis of sampled particles.

State of the Art A wide range of methods for the chemical analysis of atmospheric particles has been developed in the last decades, yet there is a distinct lack of simple-to-use, high-throughput options for offline measurements. This project aims to develop and evaluate new methods to analyze offline sampled ultrafine particles with mass spectrometry.

Analytical Approach Atmospheric particles were collected with a Dekati Low-Pressure Impactor (DELPI), which, compared to the ELPI used up to now, does not charge the collected particles by corona discharge ionization. Thus, chemical artifact formation of organic substances on the surface, our primary analyte for source apportionment, is prevented. Although our earlier experiments with CO_2-laser desorption of the semi-volatile compounds from the collected particles proved effective, we developed a closed desorption cell to reduce background signals from volatile solvents in the lab environment. The vaporized compounds are then introduced to ionization via a SICRIT ion source from Plasmion GmbH, the start-up IWC alumnus J.-C. Wolf founded, and subsequently analyzed with an Orbitrap Exactive mass spectrometer. Currently, we are working on innovative data processing procedures for mass spectrometry, enabling the classification of environmental sample data. Additionally, we are further testing Raman spectroscopy as an orthogonal analysis method, yielding additional information on inorganic compounds and various soot species.



Exemplary mass spectrum from an impaction sample (D50 95 nm, 24h sampling), measured with LD-SICRIT-MS.

Results Our system for the laser desorption of ultrafine particles in combination with highly sensitive DBDI mass spectrometry allows for measurements of environmental samples after only minutes of aerosol collection. The data evaluation and fusion with the Raman data collected on the same samples could lead to a versatile, fast analytical method for in-depth chemical analysis of particles.

Felix Ludwig

Funding

Bayerisches Landesamt für Umwelt (LfU)

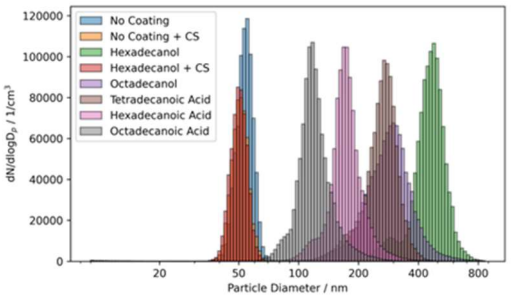
Cooperation

Bayerisches Landesamt für Umwelt (LfU)

AeroCal – calibration aerosol generator

Like any analytical instrument, aerosol counting instruments should be calibrated regularly. Also, for studies on aerosol processes, a defined aerosol is required. Instruments for assessing vehicle exhaust emissions pose a particular challenge, as an aerosol similar to the emitted soot is needed. We are developing a device to produce such aerosol by controlled redispersion of pre-produced particles.

State of the Art. Condensation Particle Counters and other instruments for aerosol measurements should be calibrated regularly with well-defined aerosol. Currently, complex combinations of different instruments are required. At first, raw aerosol is produced, e.g. in a burner, after which conditioning is necessary. Then, the desired particle size is selected by electrical mobility classification, and a defined concentration is set by dilution. A reference instrument is then needed to verify the produced concentrations.



Particle size distribution of spark discharge generated soot after coating with different substances, plus after catalytic stripping.

Analytical Approach For our system, well-characterized soot particles are collected and embedded into a matrix. For the application, they are redispersed in a specially developed device. We produce calibration aerosol by a spark discharge generator and an electrical mobility classifier. After being coated with different substances, the particles are deposited into a storage device. After redispersion, the coating is removed by a catalytic stripper, thus restoring the original size distribution. Additionally, we assess the physical properties of particles produced by our project partner, ParteQ GmbH, transmission electron microscopy (TEM). We compared powder samples and samples from diffusional deposition directly on TEM-grids.

Results. The median particle diameter of the produced soot particles could be increased from 54 nm (w/o coating) to 448 nm (hexadecanol coating), indicating complete encapsulation of the particles. Removing the coating substance with a catalytic stripper yielded a median particle size of 50 nm, slightly below the original particle size. A comparison of non-coated particles after catalytic stripping and particles after coating and stripping showed a minute difference of 1.3 nm. We will repeat these experiments with thermal treatment before the coating process. After that, the device for redispersion of the particles from a container will be optimized. For the soot samples from our project partner, the primary particle diameters were easily accessible for both, powder and grid samples. However, the different sampling techniques lead to different results regarding the amount of coating and agglomerate size. In future experiments, other sampling methods should be employed to obtain a representative measurement of the agglomerate size.

Kevin Maier

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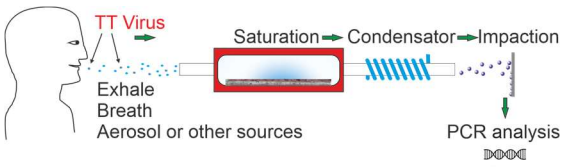
Cooperation
ParteQ GmbH
Finke Elektronik GmbH

VirusImpact: biochemistry

The goal of this project is the development of a model virus system for studies on viruses in Breath Air Aerosol (BAA). For this aim, a novel sampling device will be constructed, and collected virions will be detected via PCR and qPCR.

State of the Art It is well-known that numerous infectious diseases are spread via droplets or aerosols in the air. Yet, there is a significant lack of reliable data on the dispersion, aging, and deposition of BAA-carrying viruses. The main reason for this shortcoming is the limited comparability of the numerous studies in the field, which is caused by the fact that these studies are carried out with a wide range of different particle systems. The release process by the human respiratory tract, which is responsible for the distribution of viruses in various (size) fractions and number densities inside BAA articles, is not accessible by these systems. However, the release conditions are responsible for the further fate of the particles, such as drying, aging, and sedimentation, but also for the infectivity of the enclosed viruses. These effects can only be assessed by clinical tests with patients (e.g. influenza or COVID-19 patients), implicating significant health risks and a considerable health burden for the patient.



Schema of planned TT virus detection approach.

Analytical Approach This project aims to establish the TT virus (TTV) as a non-infectious, universal model virus system for studies on viruses in BAA. Depending on the world region, between 10 and more than 90% of all adults carry this virus, which is considered not to cause any adverse health effects. The TT virus is contained in the respiratory tract and thus also in BAA, so it will be used as a model organism in this project. For that purpose, a novel sampling device, comprising a water condensation chamber and an impinger, will be constructed to sample viruses contained in BAA with high efficiency. Collected TTV will be detected and analyzed by biomolecular methods such as PCR and qPCR, which are optimized for the expected low amounts of virions.

Results One major challenge on the biomolecular part of this project is the need to detect all TT virus subtypes. The qPCR assay developed here is based on a consensus sequence of numerous well-defined TTV variants and can detect most naturally occurring TTV subtypes. The determination of the limit of detection for this assay is currently in progress.

Florian Opperer

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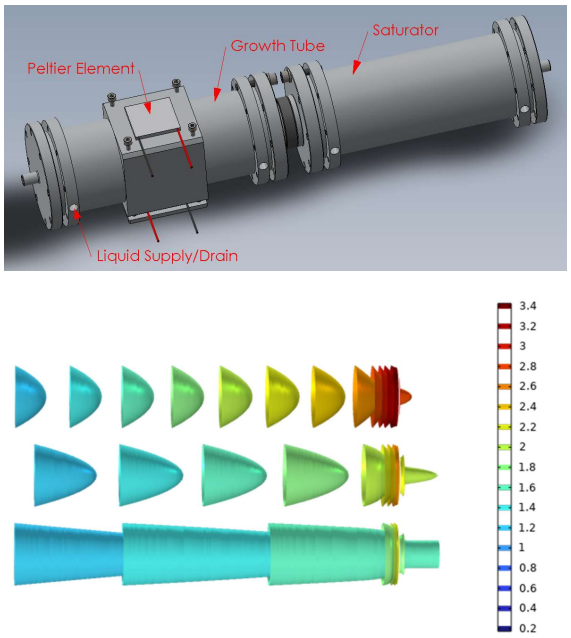
Deutsche Forschungsgemeinschaft (DFG)
Cooperation
Max von Pettenkofer Institut

VirusImpact: condensation-based aerosol sampling

Common sampling methods for breath air aerosol have difficulties sampling viable viral particles from the air because of their size and fragility under high flow conditions. Hence, we constructed a condensation-based aerosol sampler.

State of the Art There is no standardized, efficient, and fast way of collecting viruses contained in breath air aerosol (BAA). To this day, methods for sampling viruses and bacteria reveal inconclusive information about the amount and infectivity of these particles because viruses are not only small, with diameters in the nanometer range, but also very fragile. As viral concentrations in BAA can be very low, collection methods must be specifically designed to sample a sufficient air volume without damaging the analyte.



CAD-Visualization of the growth unit including all relevant components (top) and simulated isosurface of the humidity saturation inside the unit at 1, 2, and 10 L·min^{-1} flow rate (bottom).

Analytical Approach In this work, different methods for sampling viral and bacterial particles have been investigated, and their efficiency in sampling bioaerosols is discussed. Based on these findings, a high throughput sampling device for the immediate analysis of the sample after collection without additional treatment will be constructed. Different types of condensation devices have been developed. We performed a series of finite element simulations, and built the optimized device. A series of measurements allows us to characterize the sampling device and determine its efficiency compared to the established methodologies.

Results

We tested the system primarily on sodium chloride particles and observed saturation of the sample flow for all flow rated at a temperature of 55 °C. Combined with a Peltier cooling element, resulting in temperature differences above 30 °C, a supersaturation of more than 700 % is expected.

We found that any standard instrumentation for aerosol characterization, which all require sheath flow or dilution with dry gas, leads to a very fast re-drying of condensation-grown particles. Thus, the instrumental characterization of the newly developed condensation device is impaired by these measurements. Hence, we will adapt our instruments for these measurements.

Nico Chrisam

Funding

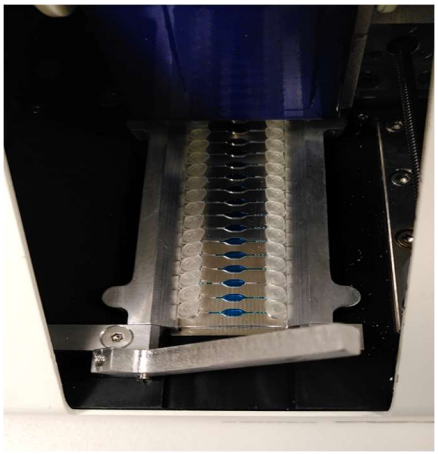
Deutsche Forschungsgemeinschaft (DFG)

DetectRespi

Development of a bio-molecular lab-on-a-chip platform for the highly parallel detection of bacterial and fungal pathogens generating respiratory diseases. The molecular biological basis of this platform is a multiplex PCR coupled to a DNA microarray.

State of the Art Currently, there are a few point-of-care (PoC) diagnostic systems that work based on molecular biology. The disadvantages of these systems are often low multiplexing grades and high costs regarding the consumables and the operating devices. In addition, manual intervention and the need for different sample matrices make using these platforms inconvenient.

Analytical Approach The development of the molecular biological assay of the lab-on-a-chip platform is performed by the Division of Infectious Diseases and Tropical Medicine (LMU KUM). The main task is the design of specific primers and probes for the individual microorganisms of the pathogen panel. Real-time PCR, specifically the TaqMan System, evaluates the designed primers and probes. Within this frame, the sensitivity and specificity checks of the primers are executed, followed by multiplexing experiments. Later in cartridge development, the probes are immobilized on a three-dimensional matrix on the DNA microarray. The cloning of PCR-positive controls supports primer evaluation and multiplexing work. One main task of TUM is the design and realization of the optical readout unit for the DNA microarray. The readout of the array will be done by fluorescence labeling the PCR products using Cy5. Construction of the unit includes the choice of the best-suited camera module, the integration, and the illumination tasks to allow for optimal excitation and readout. Thus, glass slides spotted with different concentrations of Cy5 and in different geometries are used for experimentation.



Primer Evaluation by Real-Time PCR using 16 chamber PCR chips and the ChipGenie edition TSO from the company Microfluidic ChipShop.

Results Eleven of the final 16 primer pairs for seven organisms are designed and tested on functionality by Real-time PCR. Further primers are designed and have to be evaluated using organism-specific DNA. First, duplexing experiments were performed and showed improvable results. The following working step is to assess PCRs with patient samples or artificial patient material. Regarding the optical readout of the DNA microarray, experiments with known Cy5 concentrations as a starting point were successfully carried out using a system consisting of a CCD camera, a set of lenses, and an excitation source with a wavelength of 645 nm. This setup is currently further optimized to fit the technical requirements of the future device.

Eva Krois, Amelie Hohensee

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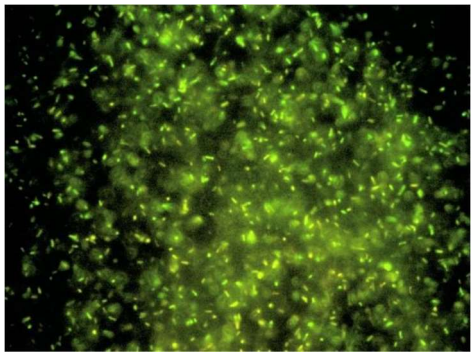
Cooperation
Mildendo mbH, M2 Automation, Tropeninstitut KUM, IBMP, Biomanguinhos

Non-targeted toxicological testing based on bacterial viability decline

We investigated the influence of different substances on the behavior of GFP-labeled *E. coli* cultures as non-targeted toxicological markers. Growth and fluorescence were tested as potential indicators for environmental contamination.

State of the Art In an era of rapidly evolving chemical innovation, globalization, and consumerism, humans and the environment are being exposed to hazardous chemicals more frequently than ever. This increase in toxin exposure necessitates the early identification of dangerous substances. Toxicity assays are conducted either in a targeted or non-targeted manner. Targeted assays specifically test the toxicity of one given substance, whereas non-targeted assays provide insight into the toxicity of a wide range of chemicals without predefined targets. An example of such a non-targeted in vitro assay is the internationally standardized luminescent bacteria test (DIN EN ISO 11348-1-3), used in the EU chemical legislation for the assessment of aquatic toxicity.



E.coli culture expressing GFP on a microscope slide viewed under a fluorescence microscope with a 63x oil immersion lens.

Analytical Approach In this study, the feasibility of using recombinantly expressed fluorescent proteins as a biotoxicity marker is investigated, with intended application in a non-targeted in vitro toxicity assay. For this purpose, an *E. coli* Top10 culture inducibly expressing mCherry was subjected to a series of controlled experiments. The fluorescence intensity and optical density of a liquid culture over time, following exposure to various toxins, were monitored using an imager. We employed an Odyssey M imager (Model 3340) of LI-COR Biosciences for the readout.

Results This instrument reveals optical density parallel to fluorescence intensity with high spatial resolution. However, the optical density proved inconsistent and unreliable, necessitating a different measurement method in the future. More promisingly, the fluorescence trends provided valuable insights into the response of FP expression to the various cytotoxins. Due to the lack of reliable absorption data, which would reveal bacteria density, we could not establish a quantitative correlation between fluorescence signal and cytotoxicity. Our findings suggest that recombinantly expressed proteins could hold promise as sensitive and dynamic indicators for assessing cellular responses to various toxicants, offering potential application in a non-targeted in vitro toxicity assay.

Mark Dresel, Amelie Hohensee, Florian Opperer

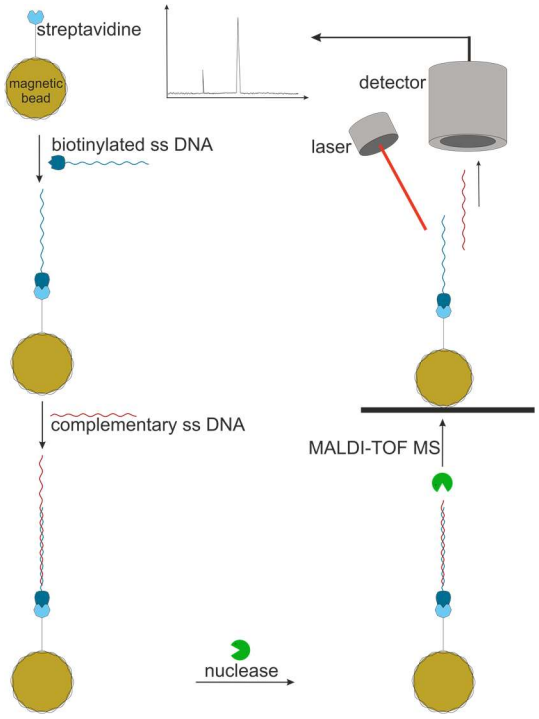
Funding
IWC
Cooperation
Division of Infectious Diseases and Tropical Medicine, LMU Klinikum

Chip-based monitoring system for bacterial nucleic acids by MALDI-TOF MS readout

We develop a chip-based monitoring system for bacterial nucleic acids by MALDI-TOF MS readout. Intended applications are investigations on mycobacteria and other microorganisms, for instance under the influence of novel antibiotics.

State of the Art One of the most common causes of death from a single infectious agent worldwide is tuberculosis, which is an infectious disease that can be transmitted through the air. 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. To develop efficient therapies, investigating the regulatory mechanisms involved at a cellular level is important.[1, 2] There is a high need to develop new treatment strategies and shorten therapy ("End-TB-Strategy", WHO).[1] However, an analytical method for determining the metabolic state of such bacteria is missing.

Analytical Approach In order to specifically isolate DNA or mRNA strands from mycobacterial cells by hybridization, a complementary biotinylated single-strand oligonucleotide is coupled to a streptavidin-coated magnetic bead. Extensions are removed by a single-strand-specific nuclease, leaving behind the conjugated hybrid. *Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry* (MALDI-TOF MS) analysis enables fast detection of the isolated oligonucleotides without further elution.



Schematic illustration of the workflow to isolate DNA by hybridization using magnetic separation techniques.

Results Functionality and performance were tested successfully on magnetic beads coated with the complementary DNA as substrate. 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 using single-strand specific nucleases, it was not yet possible to obtain blunt ends after the digestion of a single-stranded overhang, but instead varying degrees of digested overhang or partly digested hybrids. To enable high-throughput screening and multiplex analysis, the assay is now transferred to a chip-based format compatible with MALDI-TOF MS measurement.

Susanne Dietrich

Funding

Fraunhofer Institute for Translational Medicine and Pharmacology ITMP, Immunology, Infection and Pandemic Research, Munich, Germany

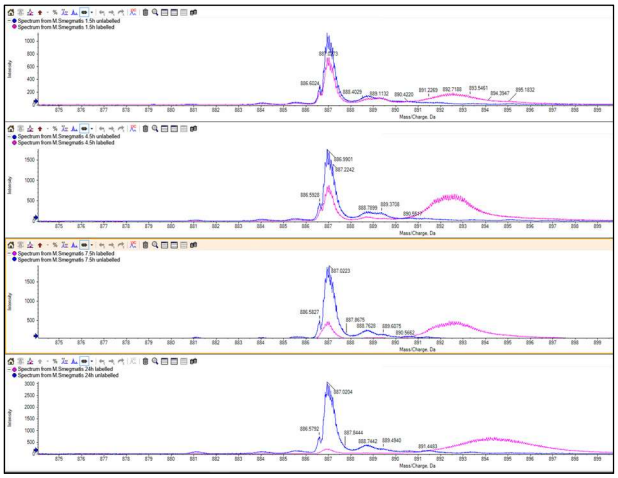
Cooperation

Division of Infectious Diseases and Tropical Medicine, LMU Klinikum

DynamicKit

Development of a preclinical model for a new tuberculosis therapy based on mass spectrometry, isotopic labeling, and artificial intelligence-based data evaluation.

State of the Art Each year, approximately 1.3 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 based on new treatment strategies ("End-TB-Strategy", WHO)[1], but also to constantly find new combinations of standard drugs and to focus on personalized medicine. However, this is difficult because preclinical models that simulate the interaction between multiple agents are lacking.



Mass spectra of a labeled vs unlabeled peak of a mycobacterial protein at different time points (blue: unlabeled; pink: labeled; from above to below: 1.5h, 4.5h, 7.5h, 24h).

Analytical Approach To better understand the mode of action of different drugs, this project aims to develop novel proteomic technologies combining mass spectrometry (Q-TOF) and self-learning algorithms. Viable and dormant mycobacterial cultures are confronted with antibiotics of various drug classes and target structures. New LC-MS and LC-MS/MS methods for analyzing mature full-length proteins are established using dynamic labeling with stable isotopes to rapidly detect changes in mycobacterial metabolism.

Results In general, protein extraction of mycobacterial mature proteins is challenging since their stable cell wall is rich in lipids. Our dedicated protocol allows us to quantify up to 300 and identify 1,000 mycobacterial proteins. Our newly developed pipeline uses self-learning algorithms to track the proteins in different charge states and modifications. Furthermore, a workflow for the analysis of LC-MS data and a reference database for intact proteins of mycobacteria was developed, enabling the comparison and quantification of different samples and the determination of secondary modifications of intact proteins. Stable isotopic labeling made it possible to illustrate the protein formation rate and visualize the effect of antibiotics on the bacterium.

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Cooperation

LMU: KUM, Dep. of Biology, Chair of Medical Microbiology and Hospital Epidemiology, Max von Pettenkofer Inst., Helmholtz Center Munich for Environmental Health; TUM, Dep. of Mathematics

Anja Dollinger

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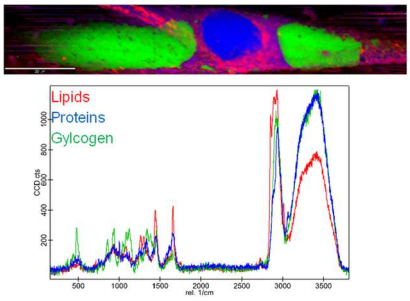
Raman imaging of myoblasts for the label-free detection of cellular components

To gain further knowledge on Pompe disease on a single-cell level, we employ Raman imaging to study the distribution of proteins, lipids, and glycogen within myoblasts.

State of the Art Pompe disease is a rare, inherited glycogen storage disorder. It is caused by a decreased activity of lysosomal acid alpha-glucosidase (GAA), which leads to glycogen accumulation in body tissue, mainly in cardiac and skeletal muscles. Patients with Pompe disease suffer e.g. from muscle weakness, breathing difficulties, or wheelchair dependency. The current treatment is an enzyme replacement therapy with limited clinical efficacy.[1,2,3]

Analytical Approach Myoblasts, a precursor form of muscle tissue, are measured via Raman spectroscopy. We place non-fixated primary muscle cell cultures into a closed measuring chamber. The sample is then measured by a Raman system using a 532 nm excitation laser and a 63× oil immersion objective. The skeletal Raman modes of carbohydrates differentiate regions of high and low glycogen content within cells. Different cell lines of patients diagnosed with Pompe disease and control cell lines are measured.



False color image of a Myoblast affected by Pompe disease (top); Overlay of the spectra of the main components of the taken Raman image (bottom). The color code for both is as follows: red: lipids, blue: proteins, green: glycogen.

Results False color images of pre-processed data are created. They allow differentiating between lipids, proteins, and glycogen as the main components within a cell. Primary cells of patients diagnosed with Pompe disease show a highly increased amount of glycogen compared to control cell lines. The glycogen accumulations are primarily distributed in the cytoplasm, thereby surrounding lysosomes and nuclei. In contrast, control cell lines show only low or no glycogen contents within cells. These results are in good agreement with biological assays as well as PAS staining of samples of the same cell lines. We plan to further investigate tissue sections affected by Pompe disease and enzyme-treated myoblasts regarding the respective amount and distribution of glycogen.

Eva Krois

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Funding

IWC

Cooperation

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

FluRam –Raman-based HPLC-detection

A novel type of HPLC detection system is developed based on Raman spectroscopy. For this purpose, we designed a capillary flow cell. The experiments were performed using a dedicated flow system as well as a commercial HPLC system.

State of the Art. High-performance liquid chromatography (HPLC) is a standard analytical separation method. Up to now, there are no commercial analytical solutions for separation using inline vibrational spectroscopy techniques. Raman spectroscopy provides specific information about the chemical composition and structure of a sample in a non-destructive way. Compared to infrared spectroscopy, water, a common eluent in HPLC methods, does not produce interfering signals. Previous approaches for coupling Raman and HPLC were based on SERS (surface-enhanced Raman spectroscopy) applications to enhance analyte signals. Instead of SERS, this project uses powerful line-focused lasers to obtain the analytical signal at low concentrations. The setup has been found to enable Raman analysis of chromatographic separation in real time, holding promise to aid in optimizing syntheses and purification processes. The device provides real-time Raman analysis of chromatographic separations to improve synthesis and purification.

The newly developed flow cell with HPLC connections, integrated into the optical setup of Soliton GmbH with a point focus.

Analytical Approach The novel flow cell is integrated into the sensor system. The setup is tested in a dedicated flow system using different flow rates and analyte concentrations for optimization. For the development of a measurement and evaluation procedure for automated detection and quantification of test analytes in different eluents, the software MatLab (R2021) is used. Currently, we test various spectral processing techniques, such as baseline correction, normalization, derivatives, and signal smoothing.

Results. In the developed detector prototype, a linear quartz capillary ($Ø_{inner}$ 0.5 mm, $Ø_{outer}$ 1.0 mm) was installed in the flow system using connections for HPLC connectors on both sides. With the linear shape, the fluid's lowest amount of turbulence and mixing occurred at the interface of the capillaries with the cell. A wavelength of 532 nm and a power of 1.5 W were chosen as excitation wavelength and laser power. As a result, time-resolved measurements were found to be possible with the entire setup. The detector allows measuring and controlling gradients with different eluents over time. For further development, the use of the sensor in process analytics for detecting various substances in microfluidic systems is planned.

Lucas Hirschberger

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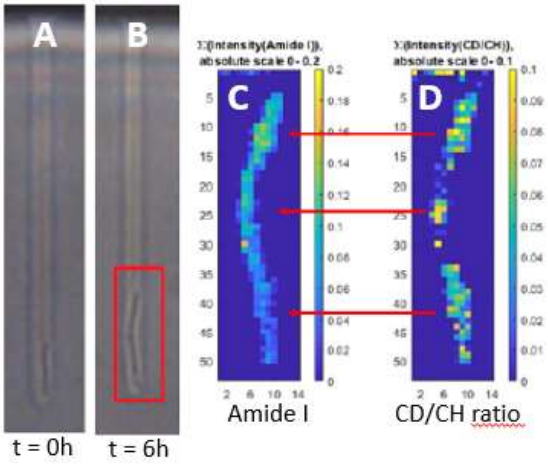
Cooperation
Soliton GmbH
Solectrix GmbH

Tracking mycobacteria with a mother machine cultivation system and Raman microscopy

***Mycobacterium tuberculosis*, the causative agent of tuberculosis (TB), develops a wide range of phenotypes during infection, resulting in distinct subpopulations with different antibiotic susceptibility. To date, the lack of single-cell techniques allowing us to assess the mycobacterial metabolism and heterogeneous viability over time limits the appropriate investigation of their survival strategy.**

State of the Art *Wang et al*. designed the mother machine, a microfluidic lab-on-a-chip tool that allows single-cell trapping at the dead-ends of parallelized growth channels.[1] The device enables observing bacterial daughter cells over several dividing cycles under precisely controlled growth conditions. Raman spectroscopy offers a rapid and non-destructive technique to determine the chemical composition of living bacteria on a single-cell level. With Raman spectroscopy, it is possible to track the ability of bacteria to incorporate deuterium from a heavy water (D_2O) source, which can discriminate between metabolically active and inactive organisms.



D_2O incorporation of a trapped *M. smegmatis* cell. A) and B) Microscopically visualized bacterial growth in a 6 h timeframe. C) Intensity distribution of the amide reference band after a large area scan (red box). D) Intensity distribution of the CD/CH ratio after the same large area scan (red box).

Analytical Approach This project aims to combine these techniques and adapt them to the characterization of mycobacteria over time. In cooperation with the research group of PD Dr. Andreas Wieser (Division of Infectious Diseases and Tropical Medicine, LMU Munich) and the group of Prof. Dr. Rädler (Faculty of Physics, LMU Munich), a mother machine device was constructed via PDMS microfabrication allowing to trap the model organism *Mycobacterium smegmatis* inside its 2 µm wide channels.

Results We were able to improve the loading efficiency of the microfluidic device. Stable isotope labeling of the trapped cells is achieved by substituting 50% of the water with D_2O in the growth medium. Thus, we confirmed the viability of the trapped bacteria and the overall the device's function. Cell division could be observed. While the Raman parameters were optimized, sample destruction by Raman measurement remains a significant challenge.

Jessica Beyerl, Eva Krois

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Funding

Verein zur Förderung von Wissenschaft und Forschung (WiFoMed), LMU Munich

Cooperation

Division of Infectious Diseases and Tropical Medicine, LMU Klinikum

Faculty of Physics, LMU Munich

SEICOR

The acronym stands for *Ship Emission Inspection with Calibration-free Optical Remote Sensing* and describes a new and cost-effective way to measure ship emissions across a river or harbor inlet via open-path light absorption.

State of the Art The project partner Airyx produces an open-path optical absorption device with an ultraviolet and visible light source to detect NO_2 and SO_2 over a distance of up to several kilometers. What is missing up to now is the CO_2 concentration, which will allow us to correlate other concentrations, such as NO_2 and SO_2, to the respective fuel consumption. To fill this gap, an infrared system is developed to analyze CO_2 and later other gases with infrared absorption bands like NO.

Analytical Approach At first, a wavelength has to be determined where the desired gas absorbs while other gases do not absorb, and, technically very relevant, cost-effective optical components can be employed, which are also suitable for the UV and vis spectral range. The latter is required to integrate the new IR system into the existing UV-vis system. A test stand provides a fixed optical path length of 2 m with a precisely tunable CO_2 concentration. The laser diode emits light into the tube, and a detector on the other side measures the transmission. A line-sweep distributed feedback (DFB) laser with a lock-in detector is used to reduce the signal-to-noise ratio. Frequency modulation over an absorption band of CO_2 results in a signal modulation with double the frequency. Multiplying and averaging over time drastically reduces the noise. Later, the laser and detection setup will be integrated into the Airyx telescope to be tested over a longer distance.

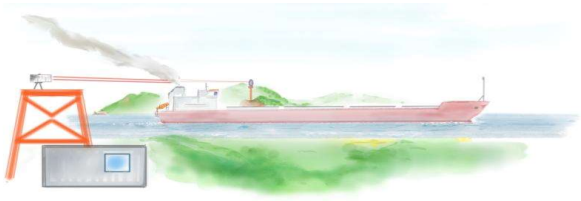

Illustration of the SEICOR project idea by C. Haisch.

Results Based on HITRAN simulations and transmission measurements of various optical components, a 2004 nm, 6 mW DFB laser was purchased. We designed a gas absorption test tube and performed first experiments with a different digital lock-in amplifier in a simplified setup with a DFB laser and different modulation schemas. The lock-in was able to detect the signal buried under noise.

Alexia Kotlarov

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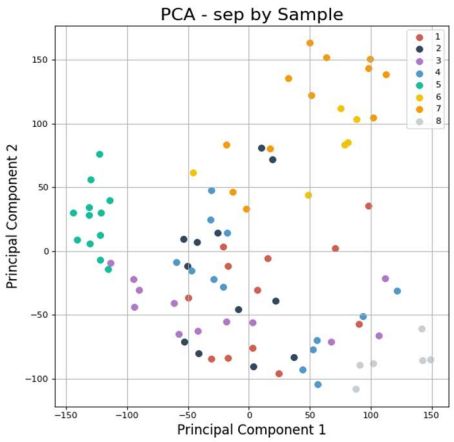
Ministry for Economic Affairs
and Climate Action
Cooperation
Airyx GmbH
HORIBA Europa
Universität Bremen

Direct thermal desorption mass spectrometry of fingerprints

Direct mass spectrometry (MS) is a powerful technique for fast and sensitive chemical analysis in forensics. The project aimed to develop a method for detecting various drugs and identifying persons through the analysis of fingerprints.

State of the Art Mass spectrometry is traditionally used in combination with chromatographic separation for optimal analytic performance. However, in recent years, ambient ionization techniques have been developed, allowing for direct analysis of samples without sample preparation or chromatography. One of those techniques is SICRIT, a soft plasma ionization based on a dielectric barrier discharge.[1] A primary application area for ambient MS is fast and reliable identification of forensic samples like drugs or explosives.[2]

Analytical Approach In this project, a thermal desorption device was designed for the direct desorption of fingerprints from glass cover slides into a high-resolution Orbitrap-MS equipped with the SICRIT ion source. Samples consisted of fingerprints spiked with drugs (fentanyl, heroin, cocaine). In addition, the fingerprints of eight different persons should be distinguished based on their lipid profiles by a machine learning algorithm.



Principal component analysis (PCA) of spectra generated by direct thermal desorption SICRIT-MS of fingerprints from 8 different persons.

Results Heroin, cocaine, and fentanyl could be detected in the fingerprints at low pg levels, which is sufficient for identification, even with only minor contact with illicit drugs. In preliminary tests, various non-polar and polar lipids were softly ionized with the thermal desorption SICRIT setup. In the fingerprints, primarily triglycerides, diglycerides, and cholesterol esters were found. A machine learning pipeline was constructed to distinguish the fingerprints of eight persons collected over multiple days based on their characteristic lipid profiles. The best results were achieved through a Random Forest classifier applied with a truncated SVD for dimensionality reduction. The resulting accuracy for the identification was >96 %. Triglycerides were the most significant features, followed by diglycerides and cholesterol esters. Volatile compounds were less characteristic for different persons due to substantial day-to-day variations.

Ciara Conway, Markus Weber

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Funding
Plasmion GmbH

SICRIT- high-resolution mass spectrometry (HRMS) for exposomic-metabolomic research through direct respiratory analysis

We developed a system for direct mass spectrometric analysis of breath. Biomarkers and metabolites can be identified through soft ionization HRMS, allowing for the determination of elemental compositions of individual analytes.

State of the Art Metabolomics is the intersection of biology and chemistry, where the main focus is on metabolic pathways, often including thousands of compounds. Typically, studies require invasively collected samples such as blood or tissue, and analysis is performed through time-consuming chromatography coupled to MS. Breath analysis, particularly direct breath analysis, through ambient MS, provides a non-invasive, real-time alternative to conventional methods.[1] For this application, a broad coverage of ionizable compounds from non-polar to polar is required.

Setup for direct breath measurement via SICRIT-Orbitrap-MS.

Analytical Approach Exhaled breath was diluted and collected with a heated transfer tube to avoid condensation. The breath was directly transferred to an Orbitrap-MS equipped with a SICRIT ion source. This plasma-based ionization technology allows us to determine the elemental composition of hundreds of compounds during a single exhale. The setup was applied to investigate the metabolism of pharmaceutically active compounds in an asthma inhaler.

Results The two main active components of the asthma inhaler (*Relvar*) are Vilanterol and fluticasone furoate. Both components could be soft-ionized as protonated molecules. In addition, shortly after inhalation of the asthma medication, metabolites of these compounds (in particular fluticasone) could also be measured. Besides monitoring medication, metabolite profiles of different persons were compared, where various compounds including amino acids, lipids, and hormones could be identified.

Ciara Conway, Markus Weber

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Plasmion GmbH

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Tiedje, J.M.; Fu, Y.; Mei, Z.; Schäffer, A.; Dou, Q.; Amelung, W.; Elsner, M.; Adu-Gyamfi, J.; Heng, L.; Virta, M.; Jiang, X.; Smidt, H.; Topp, E.; Wang,F. Antibiotic resistance genes in food production systems support One Health opinions. Current Opinion in Environmental Science & Health 2023, 34, 100492. DOI: 10.1016/j.coesh.2023.100492.

Wang, Y.; Xiang, L.; Amelung, W.; Elsner, M.; Gan, J.; Kueppers, S.; Christian, L.; Jiang, X.; Adu-Gyamfi, J.; Heng, L.; Ok, Y. S.; Ivleva, N. P.; Luo, Y.; Barceló, D.; Schäffer, A.; Wang, F. Micro- and nanoplastics in soil ecosystems: Analytical methods, fate, and effects. TrAC Trends in Analytical Chemistry 2023, 169, 117309. DOI: 10.1016/j.trac.2023.117309.

Weber, M.; Wolf, J. C.; Haisch, C. Effect of Dopants and Gas-Phase Composition on Ionization Behavior and Efficiency in Dielectric Barrier Discharge Ionization. Journal of the American Society of Mass Spectrometry 2023, *34* (4), 538-549. DOI: 10.1021/jasms.2c00279.

Weng, J.; Müller, K.; Morgaienko, O.; Elsner, M.; Ivleva, N. P. Multi-element stable isotope Raman microspectroscopy of bacterial carotenoids unravels rare signal shift patterns and single-cell phenotypic heterogeneity. Analyst 2023, 148 (1), 128-136. DOI: 10.1039/D2AN01603F.

Conference Presentations

Oral Presentations

Beer, I.; Brunschweiger, S.; Glas, K.; Elsner, M.; Ivleva, N. P. Using imaging techniques for a deeper understanding of electricity production in microbial biofilms growing on brewery waste, ANAKON 2023, 11.–14.04.2023, Vienna, Austria.

Elsner, M.; Sun, F.; Kundu, K.; Ehrl B.; Gharasoo M.; Marozava, S.; Mellage, A.; Merl-Pham,J.; Peters, J.; Wang, Z.; Bakkour, R.; Melsbach, A.; Cao, X.; Zimmermann, R.; Griebler C.; Thullner, M.; Cirpka, O.; Isotope Factionation Reveals Limitations and Microbial

Regulation of Pollutant Biodegradation at Low Concentrations, Goldschmidt 2023, 09.07-14.07, 2023, Lyon, France.

Haisch, C. Novel approach for high-throughput, simple-to-use chemical characterization of environmental aerosol particles, European Aerosol Science Conference 2023, 02.-08.09.2023, Malaga, Spain.

Huber, M.; Zada, L.; Ariese, F.; Ivleva, N. P. Stimulated Raman Scattering: A new approach to detect nanoplastics in flow, SciX2023, 08.–13.10.2023, Sparks-Nevada, USA.

Huber, M.; Ivleva, N. P. Stimulated Raman Scattering: A new approach to detect nanoplastics in flow, ANAKON 2023, 11.–14.04.2023, Vienna, Austria.

Ivleva, N. P.; Jacob, O.; Ramírez-Piñero, A.; Elsner, M. TUM-ParticleTyper 2: Automated quantitative analysis of (microplastic) particles and fibers down to 1 µm by Raman microspectroscopy, SciX2023, 08.–13.10.2023, Sparks-Nevada, USA.

Ivleva, N. P.; Müller, K.; Elsner, M. On the Potential of Stable Isotope Raman Microspectroscopy for Analysis of Microbial Degradation of Microplastics, SciX2023, 08.–13.10.2023, Sparks-Nevada, USA.

Ivleva, N. P.; Jacob, O.; Ramírez-Piñero, A.; Elsner, M. Automated quantitative analysis of (microplastic) particles and fibers down to 1 µm by Raman microspectroscopy, International Conference on Advanced Vibrational Spectroscopy (ICAVS12), 27.08–01.09.2023, Kraków, Poland.

Müller, K.; Elsner, M.; Ivleva, N. P. On the Potential of Analysing Biodegradability of Microplastics with Stable Isotope Raman Microspectroscopy, SETAC Europe 33rd Annual Meeting, 30.04.–04.05.2023, Dublin, Ireland.

Müller, K.; Elsner, M.; Ivleva, N. P. Stabilisotopenansatz für die direkte Analyse der Bioabbaubarkeit von Mikroplastik mittels Raman-Mikrospektroskopie, Wasser 2023, 15.–17.05.2023, Augsburg, Germany.

Seidel, M. Moderne Analysemethoden für Pathogene im Kontext Abwasser. 11. Kitzbüheler Wassersymposium, 8.-9.11.2023, Kitzbühel, Austria.

Seidel, M. Rapid hygienic assessment for mobile water supply systems. 3rd International Symposium ,,Mobile Water Supply on Operations", Munster, Germany, 11 - 13 September 2023.

Poster Presentations

Al-Ghoul, H.; Elsner, M. Miniature Combustion Reactors to Increase Sensitivity and Selectivity, and to Facilitate GCxGC for Compound-specific Isotope Analysis (CSIA), *ANAKON 2023*, 11.04-14.04.2023, Vienna, Austria.

Al-Ghoul, H.; Elsner, M. Miniature Combustion Reactor to Facilitate GCxGC-C-IRMS, *German Association for Stable Isotope Research Meeting 2023 (GASIR 2023)*, 27.09-29.09.2023, Bayreuth, Germany.

Auernhammer, A.; Ertl, S.; Seidel, M. Algae toxin monitoring in surface water combined with microarray- and isotope analysis of trace substances, *ANAKON 2023*, 11.04-14.04, 2023, Vienna, Austria.

Beer, I.; Brunschweiger, S.; Glas, K.; Elsner, M.; Ivleva, N. P. Die Rolle von Mischbiofilmen in der Aufbereitung von Abwasser im Getränkesektor, *Wasser 2023*, 15.–17.05.2023, Augsburg, Germany.

Canavan, A.; Elsner, M. 15N-Isotope Analysis of Sulfamethoxazole by Derivatization-Gas Chromatography-Isotope Ratio Mass Spectrometry, *German Association for Stable Isotope Research Meeting 2023 (GASIR 2023)*, 27.09-19.09.2023, Bayreuth, Germany.

Glöckler, D.; Wabnitz, C.; Harir, M.; Schmitt-Kopplin, P.; Elsner, M.; Bakkour, R. Universal vs. selective sorbents for targeted isotope analysis of aquatic contaminants, *ANAKON* 2023, 11.04-14.04, 2023, Vienna, Austria.

Heining, L.; Welp, L.; Hugo, A.; Elsner, M.; Seidel, M. Combination of immunomagnetic separation with flow cytometry for the detection of *Legionella pneumophila* in aerosols, *ANAKON 2023*, 11.04-14.04, 2023, Vienna, Austria.

Heining, L.; Welp, L.; Hugo, A.; Elsner, M.; Seidel, M. Combination of the cyclone sampler Coriolis® µ with different quantitative analytical methods for the detection of *Legionella pneumophila* in aerosols, *European Aerosol Conference 2023*, 03.09-08.09, 2023, Málaga, Spain.

Huber, M.; Zada, L.; Ariese, F.; Elsner, M.; Ivleva, N. P. Multi-Parameter Analysis of Nanoplastics: Taking Advantage of High Time Resolution Enabled by Stimulated Raman Scattering, *SETAC Europe 33rd Annual Meeting*, 30.04.–04.05.2023, Dublin, Ireland.

Huber, M.; Zada, L.; Ariese, F.; Elsner, M.; Ivleva, N.P. Stimulierte Raman-Streuung zur zeitlich hoch aufgelösten online-Detektion von Nanoplastik, *Wasser 2023*, 15.–17.05.2023, Augsburg, Germany.

Jacob, O.; Ramírez-Piñero, A.; Elsner, M.; Ivleva, N. P. How precisely can we analyse very small microplastic particles? *SETAC2023*, 30.04.–04.05.2023, Dublin, Ireland.

Jacob, O.; Ramírez-Piñero, A.; Elsner, M.; Ivleva, N. P. Mit welcher Präzision können kleine Mikroplastikpartikel analysiert werden?, *Wasser* 2023, 15.–17.05.2023, Augsburg.

Lanzinger, M.; Kaufmann, S.; Schuster, M.; Ivleva, N. P. Comparative Study of EDX, µXRF and LIBS for Element Quantification in Metallic Particles, *ANAKON 2023*, 11.04-14.04, Vienna, Austria.

Liang, Y.; Heining, L.; Seidel, M. Elsner, M.; Seidel, M. Cartridge-based flow cytometry for the determination of total count of bacteria in process water, *ANAKON 2023*, 11.04-14.04, 2023, Vienna, Austria.

Lihong, C.; Etienne, D.; Elsner, M. Novel Enzymes for the Targeted Removal of Sulfonamides from Water, *Wasser 2023*, 15.05.-17.05.2023, Augsburg, Germany.

Müller, K.; Elsner, M.; Ivleva, N. P. On the Potential of Stable Isotope Raman Microspectroscopy for Analyzing Microbial Degradation of Microplastics, *Anakon 2023*, 11.04.-14.04.2023, Vienna, Austria.

Neubauer, C.; Bakkour, R.; Lüdecke, T. Uncovering the real paleo diet: Novel isotope analytics of amino acids from fossil hominin teeth, *22nd HFSP Awardees Meeting*, 6.12-08.12.2023, Cape Town, South Africa.

Schwaiger, G.; Bromann, S.; Clauss, M.; Seidel, M. Culture independent, standard addition based qPCR method for quantification of *Legionella* in complex agricultural matrix, *ANAKON 2023*, 11.04-14.04, 2023, Vienna, Austria.

Seidel, M.; Schwaiger, G.; Streich, P.; Heining, L.; Elsner, M. Rapid Qantification of pathogens in water. *Gordon Research Conference: Urbanization, Water and Food Security*, 16.-21.7.2023, Lucca, Italy.

Streich, P., Seidel, M. Antibody-based rapid detection and subtyping methods for analysis of *L. pneumophila* in process water, *ANAKON 2023*, 11.04.-14.04.2023, Vienna, Austria.

Streich, P., Seidel, M. Kulturunabhängige, Antikörper-basierte Messtechniken zur schnellen Überwachung von *Legionella pneumophila* in Prozesswässern, *Wasser 2023*, 15.05.-17.05.2023, Augsburg, Germany.

Tafa, A.; Elsner, M.; Bakkour, R. Redesign of passive samplers increase sensitivity of compound-specific isotope analysis, *Goldschmidt 2023*, 09.07-14.07, 2023, Lyon, France.

Thomas, A.; Kaufmann, S.; Huber, D.; Ivleva, N.P. Developement of prediction models for the quality of adhesives using FTIR and Raman spectroscopy, *ANAKON 2023*, 11.04- 14.04, Vienna, Austria.

Prechtl, L.; Bader, T.; Winzenbacher R.; Seidel M.; Elsner, M. Exploring microbiological markers in non-target screening data, *Wasser 2023*, 15.05.-17.05.2023, Augsburg, Germany.

Prechtl, L.; Seidel M.; Elsner, M. The search for markers for microbiological contamination in surface water, *International Conference on Non-Target Screening 2023*, 16.10.-19.10.2023, Erding, Germany.

Wabnitz, C.; Canavan, A.; Chen, W.; Toprakcioglu, Z.; Elsner, M.; Bakkour, R. Online-Detektion natürlicher organischer Stoffe zur Optimierung der Probenvorbereitung für substanzspezifische Isotopenanalyse, *Wasser 202*3, 15.05.-17.05.2023, Augsburg, Germany.

Wabnitz, C; Chen, W.; Elsner, M.; Bakkour, R. Online matrix monitoring using QCM dry mass sensing for sample preparation optimization, *ANAKON 2023*, 11.04-14.04, 2023, Vienna, Austria.

Invited Lectures

Elsner, M.; Sun, F.; Kundu, K.; Ehrl B.; Gharasoo M.; Marozava, S.; Mellage, A.; Merl-Pham,J.; Peters, J.; Wang, Z.; Bakkour, R.; Melsbach, A.; Cao, X.; Zimmermann, R.; Griebler C.; Thullner, M.; Cirpka, O.; Isotope Factionation Reveals Limitations and Microbial Regulation of Pollutant Biodegradation at Low Concentrations (Keynote Lecture), German Association for Stable Isotope Research Meeting 2023 (GASIR 2023), 27.09-19.09.2023, Bayreuth, Germany.

Elsner, M.; Canavan, A.; Wang, F.; Adu-Gyamfi, J.; Kheng Heng, L.; Compound-Specific Isotope Analysis (CSIA) to Trace Sources and Transformation of Pharmaceuticals in the Environment (Keynote Lecture), 4th International Conference on Risk Assessment of Pharmaceuticals in the Environment (ICRAPHE), 09.10-10.10.2023, Barcelona, Spain.

Huber, M.; Zada, L.; Ariese, F.; Ivleva, N.P. Analysis of nanoplastics in flow with spontaneous and stimulated Raman scattering techniques, Foresight Workshop on Future Laser-Based Technologies, 24–26.07.2023, Riga, Latvia.

Ivleva, N. P. Raman microspectroscopy for analysis of (plastic) microparticles: Applicability and limitations, 19th Confocal Raman Imaging Symposium, September 25.–27.09.2023, Ulm, Germany.

Ivleva, N. P. Raman microspectroscopy for analysis of micro- and nanoplastics (Keynote Lecture), ANAKON 2023, 11–14.04.2023, Vienna, Austria.

Colloquium for Analytical Chemistry and Water Chemistry Guest Lecture

Prof. Dr. Stephen Schrettl, TUM, Professorship of Functional Materials for Food Packaging, *“Responsive Polymer Films through Supramolecular Assembly”* (16.01.2023)

Dr.-Ing. Martina Gastl, TUM, Weihenstephan Research Centre for Brewing and Food Quality, *„Das Forschungszentrum Weihenstephan BLQ stellt sich vor"* (23.01.2023)

Prof. Dr. Corinna Dawid, TUM, Professorship of Functional Phytometabolomics, *"Promoting human health and well-being through sustainable agri-food systems by means of phytometabolomics approaches"* (20.06.2023)

Prof. Dr. Wenwang-Zhon, Department of Chemistry, University of California-Riverside, CA 92521 USA, *"Advancing Analysis of Biological Complexes and Vesicles using Open-Channel Separation"* (26.06.2023)

Prof. Dr.-Ing. Michael Zavrel, TUM Campus Straubing, Professorship of Bioprocess Engineering, *"Development of Bioprocesses based on Agricultural Residues"* (17.07.2023)

Dr. Thomas Hofstetter, Eawag/Environmental Chemistry, *"Using structure-function relationships to assess the evolving biodegradation potential of contaminant degrading enzymes"* (08.11.2023)

Dr. Hans-Christian Müller, Independent consultant in the chemical industry, *"Why Does Industry Need Analytics? What Do You Need To Be A Good Analyst?"* (08.12.2023)

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

Haisch, C. Organizing Committee of CLEO Europe (Conference on Lasers and Electro-Optics), 26 – 30 June 2023, Munich

Ivleva, N. P, Analytical Bioanalytical Chemistry, Springer (Member of International Advisory Board)

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

M.Sc Geo. David Glöckler: Tailor-made Sorbents to Enhance Sensitivity in Stable Isotope Analysis of Aquatic Micropollutants: Comprehensive Investigations on the Selectivity of Cyclodextrin Polymers.

MSc. Julia Theresa Klüpfel: Development of Rapid Automated Chemiluminescence Microarray Immunoassays for SARS-CoV-2 Serological Assessments.

M.Sc. Theses

Claudia Bari: Optimization and characterization of microarray chips using the amino density estimation by colorimetric assay.

B.Sc. Nico Crisam: Development of a sampling system for the analysis of viruses in breath air aerosol.

B.Sc. Xue Lui: Investigating the physiological dynamics of *Mycobacterium smegmatis* using microfluidics and Raman Spectroscopy.

B.Sc. Chem. Jannis Gehrlein: Method Development for Chemical Imaging of Silicatized Nickel Surfaces Using Laser-Induced Breakdown Spectroscopy (LIBS).

B.Sc. Chem. Ida Keussen: Development of an Efficient Microbial Fuel Cell and Investigation of Biofilm Formation using Raman Microspectroscopy.

B.Sc. Chem. Marcel Klotz: Investigating Adverse Effects of Disinfectants on Polyamide Membranes in Reverse Osmosis Systems using Raman-based Approaches.

B.Sc. Li Yicheng: Optimization of the pre-germination of *Bacillus* probiotics for aquaculture application.

B.Sc. Theses

Mark Dresel: Illuminating cellular toxicity: Recombinant fluorescent proteins as non-targeted toxicological markers for viability decline of modified *E. coli*-cultures.

Talee Barghouti: Development of a Colony-Based Approach for Subtyping *Legionella pneumophila* Serogroup 1 Using CL-SMIA.

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. Bakour

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. Bakour

Fortgeschrittene analytische Verfahren

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

Hydrochemisches Praktikum

820678299 Hydrology (MSc) N. P. Ivleva

Hydrochemisches Praktikum für Geologen

0000003397 Hydrology (MSc Geo.) N. P. Ivleva

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. Bakour

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

Apl.-Prof. Dr. Christoph Haisch

PD Dr. Natalia Ivleva

PD Dr. Michael Seidel

Post Docs

Dr. Florian Opperer

Technical & Administrative Staff

Felix Antritter

Christine Beese

Christine Benning

Susanne Mahler

Marco Matt, Dipl.-Ing

Cornelia Popp

Sonja Rottler, Dipl.-Ing. (FH)

PhD Students

M.Sc. Chem. Andreas Auernhammer

M.Sc. Chem. Susanne Dietrich

M.Sc. Geo. David Glöckler

M.Sc Chem. Lena Heining

M.Sc. Chem. Lucas Hirschberger

M.Sc. Chem. Maximilian Huber

M.Sc. Chem. Oliver Jacob

M.Sc. Chem. Isabel Jüngling

M.Sc. Chem. Marcel Klotz

M.Sc. Chem. Julia Klüpfel

M.Sc. Chem. Eva Krois

M.Sc. Chem-Ing. Yiao Liang

M.Sc. Chem. Felix Ludwig

M.Sc. Chem. Alexia Kotlarov

M.Sc. Chem. Kevin Maier

M.Sc. Chem. Kara Müller

M.Sc. Chem. Julia Neumair

M.Sc. Chem. Sandra Paßreiter

M.Sc. Biochem. Gerhard Schwaiger

M.Sc. Chem. Philipp Streich

M.Sc. Chem. Armela Tafa

M.Sc. Chem. Andrea Weiss

M.Sc. Chem. Christopher Wabnitz

External PhD Students

M.Sc. Chem. Jessica Beyerl (LMU KUM)

M.Sc. Chem. Ciara Conway (Plasmion GmbH)

M.Sc. Chem. Anja Dollinger (LMU KUM)

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

M.Sc. Chem. Amelie Hohensee (LMU KUM)

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

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

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

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

Master Students

B.Sc. Chem. Nico Chrisam

B.Sc. Chem. Xue Lui

External Master Students

B.Sc. Chem. Annachiara Morganti

B.Sc. Chem.-Ing. Li Yicheng

Bachelor Students

Talee Barghouti

Alžbeta Tonyková

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

1 Orbitrap Exploris 240

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