Technical University of Munich
School of Natural Sciences
Department of Chemistry

Annual Report 2022

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 December 2022 at the CRC building, Department of Chemistry, School of Natural Sciences at the Technical University of Munich, Garching.

Content

Dear colleagues and friends,

characterizing immunity in pandemics, eliminating analytical interferences in isotope analysis, spearheading automated nanoparticle analysis, characterizing the chemistry of aerosols – also last year we had the opportunity to advance many exciting research projects at our institute.

In the project CoVrapid funded by the Bayerische Forschungsstiftung our Bioanalytics Group established the chemiluminescence microanalysis platform MCR R for human immunodiagnostic assay formats like antibody tests and surrogate neutralization assays. Through several publications and conference presentations we demonstrated the performance of the approach for CoV-SARS 2 thereby introducing a uniquely flexible medical research and diagnostic platform.

Isotope analysis of water pollutants can delineate sources and demonstrate their natural degradation, but is limited by organic background interferences. In the Targeted Environmental Analysis Group underlying drivers were characterized that make cyclodextrin-based based extraction materials so attractive for enrichment of organic analytes from water. We could show that these materials co-enrich much less organic matter compared to traditional solid phase extraction (SPE) sorbents lowering limits for compound-specific isotope analysis by almost an order of magnitude.

While microplastics has received much recent attention, the potential of smaller particles to penetrate biological membranes sparks even greater interest in nanoplastics. Adequate chemical characterization methods of organic nanoparticles, however, still await development. The Raman / SEM group has been very active in pushing Raman microspectroscopy (RM) to lower the limits of automated nondestructive chemical analysis of complex environmental and industrial samples. The development work of Christian Schwaferts earned him a PhD with summa cum laude, and for her work on automation Elisabeth von der Esch was awarded the doctorate price of the German Water Chemistry Society. Congratulations, Christian and Eli!

Even though our Lasers and Aerosols group is still waiting for their labs in Garching and, therefore, faces a very unsatisfactory situation, the project with the Bavarian Landesamt für Umwelt on the chemical characterization of aerosol nanoparticles is coming to a very successful end. Together with our partner LFU, we are able to present a new concept for a fast, high-throughput instrument for the chemical characterization of aerosol particles. As a follow-up to this project, we will try also to integrate a novel aerosol sampling system, which is less prone to artifact formation.

In the WIPANO project LegioRapid, finally, our Bioanalytics group could standardize protocols for cultivation-independent quantification of Legionella pneumophila in cooling towers. For the first time quantitative polymerase chain reaction (qPCR) and immunomagnetic separation were combined with flow cytometry and our LegioTyper system and shown to qualify for rapid monitoring of process water in the event of *Legionella pneumophila* contaminations. For quantification of *Legionella pneumophila* in bioaerosols, everything is now established in our laboratory: bioaerosol chamber, cooling tower models, sampling devices and novel rapid bioanalytical methods.

Not only science-wise last year has seen multiple highlights. After two years of the pandemics we were very grateful about the opportunity of so many joyful social events. In spring joined with our new neighbors from the Chair of Synthetic Biotechnology (Prof. Brück) to celebrate the inauguration of our new common office floor. After five years in transition, most of us finally moved into our final offices! In the beautiful surrounding of Raitenhaslach we had our first Institute retreat in late September. In October we took advantage of a wonderful sunny day to visit the limnological research station at the Osterseen, where I got a very nice birthday surprise – Thank You! A particular highlight was, finally the yearly meeting with the Friends from the Institute, where we discussed 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!

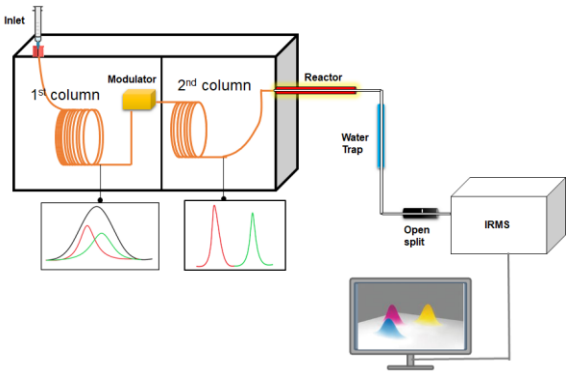
This, finally brings me to saying Thank You again – thanks to our students, technicians, secretaries and scientists for their dedication and invaluable contributions, and thanks to you, our friends, for your continued support!

Kind regards,

Miniature Combustion Reactors to Increase Sensitivity and Selectivity, and to Facilitate GCxGC for Compound-specific Isotope Analysis (CSIA)

Complete peak separation and enhanced sensitivity are two notorious challenges for sensitive CSIA. Comprehensive gas chromatography (GCxGC) could be a game-changer[1], but hinges on the development of robust miniature online combustion reactors.

State of the Art Online combustion tubes must offer sufficient oxidation capacity and catalytic surface area to accomplish complete analyte conversion to CO_2, while being narrow enough to preserve the sharp shape of analyte peaks when the continuous carrier stream carries them to an IRMS (isotope ratio mass spectrometer). The current step change when He carrier gas passes from narrow GC capillary columns (inner diameter, i.d.: 0.22–0.32 mm) to wide commercial combustion tubes (i.d.: 0.5 mm) generates substantial peak broadening.



GCxGC-C-IRMS system; the modulator releases the trapped and focused portion (slices) from the first column into the thinner second column to enable further separation.

Analytical Approach To tackle the challenge of enabling GCxG-C-IRMS on a routine basis, we consider three different designs: (i) A high-temperature combustion reactor made of a capillary column of which the wall is coated with a catalytic material. This design ensures miniaturization and provides a catalytic surface to enable oxidation of analytes. Yet it presently is of limited longevity, requires a high temperature and a trickling stream of oxygen within the carrier gas. (ii) A solid-electrolyte reactor, in which the combustion occurs via electrochemical oxidation. This design has the advantage that it eliminates the need to add a chemical oxidant, but it still needs to be tested and optimized for longevity and the potential for miniaturization. (iii) A low temperature catalytic combustion reactor. If successful, this makes it easier to integrate the conversion reactor into GCxGC instruments, and it allows for a wider range of materials. Yet, such a low temperature solution needs to be miniaturized and carefully tested for quantitative conversion of a range of target analytes.

Results We aim to explore the promise of the three designs - a wall-coated capillary (WCC) reactor, a solid-electrolyte reactor (SER), and a low-temperature reactor (LTR) - to pioneer robust solutions for miniaturized reactors that can facilitate routine GCxGC-C-IRMS.

Habib Al-Ghoul

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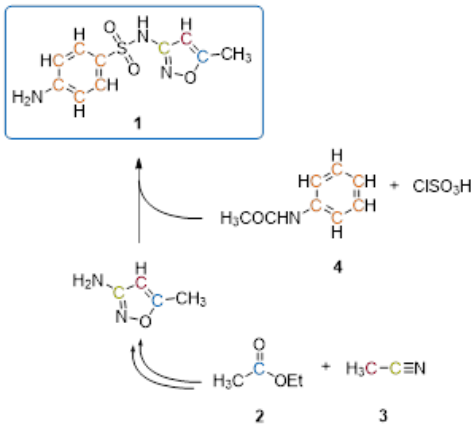
Funding
IWC

Development of the Synthesis of ^{13}C-Labeled Sulfamethoxazole from Suitable Precursor Substances

Synthesizing entirely or partially ^{13}C-labeled sulfamethoxazole enables a variety of experiments such as tracer experiments in the environment, degradation experiments to investigate position-specific isotope effects, and the calibration of ESI orbitrap MS for the determination of isotope ratios.



Synthesis scheme for potential position-specific ^{13}C-labels (colored) or entirely ^{13}C-labeled sulfamethoxazole (1) using labeled ethyl acetate (2), acetonitrile (3), and acetanilid (4).

State of the Art Experiments with entirely or partially ^{13}C-labeled compounds of environmental concern are rare due to the limited availability and high expenses of ^{13}C-labeled compounds. However, such compounds offer a variety of interesting experiments, including tracer experiments in the environment and degradation experiments in the lab to investigate position-specific isotope effects.

Analytical Approach The antimicrobial sulfamethoxazole (SMX) is used as a model compound because of its wide adoption in veterinary medicine to treat and prevent infectious diseases in intensive animal husbandry.

(i) To target a realistic environmental field experiment, fully ^{13}C-labeled SMX is warranted to deconvolute changes in concentrations caused by repetitive application or remobilization from those induced by degradation. This enables the distinction between previous contaminations with SMX and the introduced ^{13}C-labeled SMX. Furthermore, the isotopic label facilitates the identification of transformation products.

(ii) Compound-specific isotope analysis (CSIA) is a powerful tool to characterize degradation pathways through the measurement of isotope effects. CSIA offers the possibility of identifying putative degradation processes, such as biodegradation or photolysis, even without knowing the exact pathways and metabolites. However, it has not been possible to identify the changes in bonding contributing to these effects. Here, a possible approach relies on degradation experiments with ^{13}C-labels at different positions within the SMX molecule.

To tackle these challenges, the total synthesis of SMX is developed to obtain entirely or partially ^{13}C-labeled compounds.

Results The total synthesis of SMX can be achieved by the formation of the isoxazole moiety with ^{13}C-labeled versions of ethyl acetate (2) and acetonitrile (3), while the aromatic moiety can be synthesized from commercially available ^{13}C-labeled acetanilide. Different reaction conditions are being tested, and yields are being optimized.

Aoife Canavan

Funding
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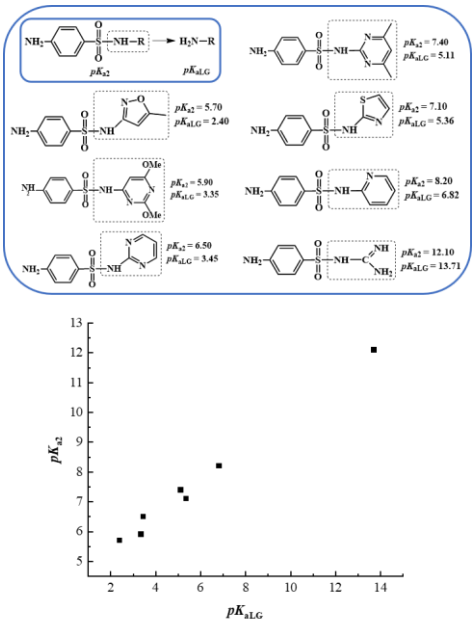
IAEA

Novel Enzymes for the Targeted Removal of Sulfonamides from Water

A synergetic combination of experiments and computations aims to lay the foundation for generating novel enzymes for targeted removal of sulfonamides from water, thereby competing with Darwinian evolution in much shorter time.

State of the Art Introduced as the earliest first-line antibiotics, sulfonamides (SAs) have been widely used in human and veterinary medicine. This leads to a release of large amounts into the environment, where they persist both in unchanged and in metabolized form as a result of incomplete biotransformation. They receive increased attention because of their potential to foster the development of antibiotic resistance[1]. For this reason, our project aims to create novel enzymes to effectuate targeted removal of SAs from water.



The relationship between pK_{a2} of the SAs and pK_{aLG} of leaving groups.

Analytical Approach Computational chemistry approaches based on quantum chemical calculations can be used to explore reactivities by characterizing detailed potential energy surfaces (PESs) and electronic properties of putative SA degradation reactions. Subsequent molecular docking can screen for promising enzymes from relevant databases to bind, and transform SAs, where MD simulation can be applied to estimate the stability of mutational scaffolds with targeted functions. In parallel, compound-specific isotope analysis (CSIA) will be performed to test computed underlying reaction mechanisms of SAs by experimentally measuring associated isotope fractionation.

Results In a first step, the reaction mechanism of SAs in aqueous hydrolysis was considered. Insight from literature[2] and our computational calculations suggest that the -SO_2-NH- group would have to be protonated to generate good leaving groups and to facilitate hydrolysis. A pronounced correlation between the pK_{a2} values of SAs and the pK_{aLG} values of leaving groups implies that any substituent effects in *R* that make H_2N-*R* a better leaving group, will also make the protonation of the -SO_2-NH-*R* group more difficult. This is a piece of key information for the design of putative catalytic enzyme scaffolds as a starting point for directed evolution.

Lihong Chai

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Cooperation

Dr Etienne Derat (Sorbonne Université)

Prof Lynn Kamerlin (Georgia Institute of Technology; Uppsala University)

Prof José Manuel Sanchez Ruiz (University of Granada)

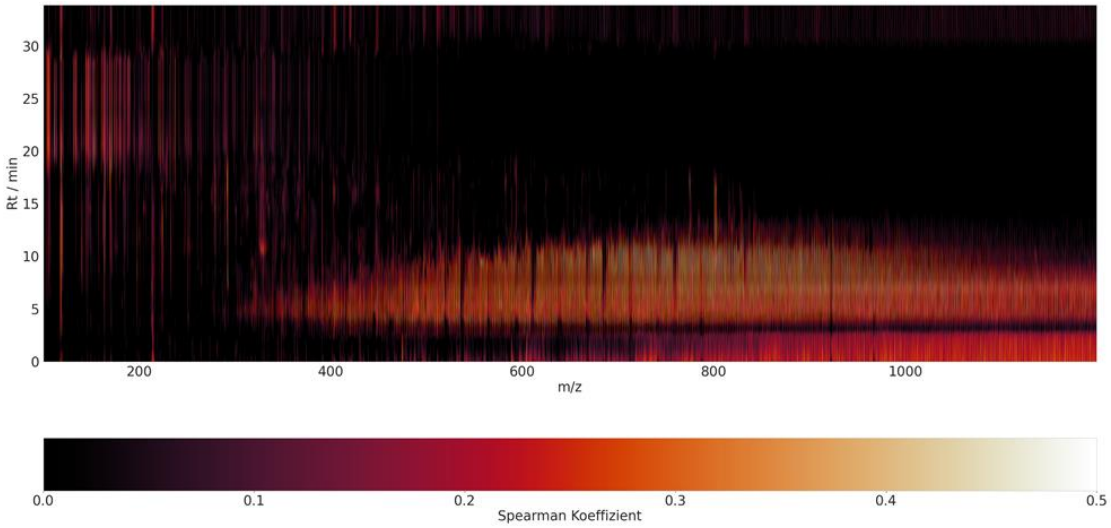
Mining for Microbiological Markers in Non-Target-Screening Data

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 contaminations.

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 give a result.

Analytical Approach We aim to identify markers of microbiological pollution within the NTS results. Since this data is acquired anyway, our approach would allow mining it as an early warning system for microbiological contamination.



Correlation between *Clostridium perfringens* and the intensities in the NTS measurements (N=387).

Surface water samples were analyzed for NTS via LC-MS, and for selected microbiological parameters with cultivation methods, by the Zweckverband Landeswasserversorgung. In a first step we reduced the data size by binning LC-MS data within small areas, and calculated the correlation between the LC-MS intensity of each area with microbiological parameters. The figure shows the result of such a correlation. In a next step we try to identify markers within the areas of the highest correlation and use them to create a prediction model for microbiological contamination.

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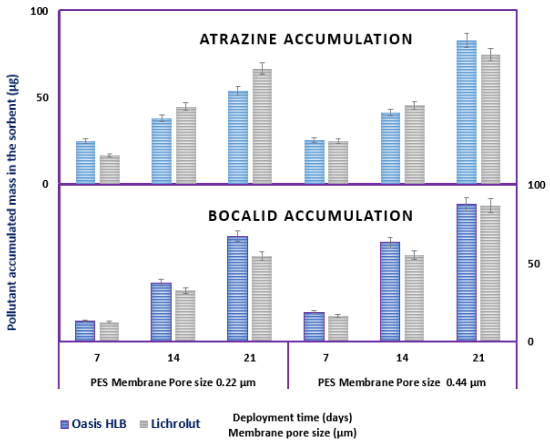
Cooperation
Zweckverband Wasserversorgung (LW), TZW, LRZ

Leonhard Prechtl

Development of refined POCIS-type passive samplers to increase the uptake kinetics of polar micropollutants

Polar Chemical Integrative Passive Samplers (POCIS) offer a promising approach to extract pollutants directly in the field, alleviating the need of transporting and handling large sample volumes for sensitive Compound-specific Isotope Analysis (CSIA).

State of the Art CSIA is a powerful tool to track the biodegradation of micropollutants in aquatic systems. The low occurrence of target compounds (i.e. ng/L range), combined with the limited sensitivity of gas chromatography hyphenated to isotope ratio mass spectrometers (GC-IRMS), makes water sampling challenging for CSIA. Recently, the observation that isotopic fractionation was absent during sampling with Oasis HLB-loaded POCIS demonstrated the promise for a successful combination with CSIA. [1] However, it is pivotal to increase the uptake kinetics of POCIS in order to rapidly collect a critical analyte mass for GC-IRMS analysis. Therefore, we are exploring the dependence of uptake kinetics on extracted masses of atrazine and boscalid in POCIS with i) different types of sorbents (Oasis HLB and LiChrolut EN) and ii) different membrane pore sizes (0.22 µm and 0.45 µm).



Uptake kinetics of Atrazine and Boscalid, in different sorbents and membrane pore sizes.

Analytical Approach POCIS were calibrated to monitor the concentrations of atrazine and boscalid in water under controlled laboratory conditions. Two series of experiments (main tank and control tank) were set up to evaluate the uptake kinetics. Experimental conditions were kept constant during the entire deployment time (Flow rate 13 cm/s, water pH 7 and pesticide concentration 20 µg/L). Analysis was performed using a Gas Chromatograph - Mass Spectrometer (GC-MS).

Results The pollutant characterization in extracts revealed that with higher membrane pore sizes pollutant uptake kinetics increased significantly (around 23%) for both model compounds. Specifically, the two redefined POCIS (a Oasis HLB sorbent and a LiChrolut sorbent, both enclosed by a PES membrane of 0.44 µm pore diameter) showed a rapid accumulation of the micropollutants. Both reached the critical mass for GC-IRMS analysis more rapidly compared to conventional POCIS, representing promising alternatives for a better performance in combination with CSIA.

Armela Tafa

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Funding

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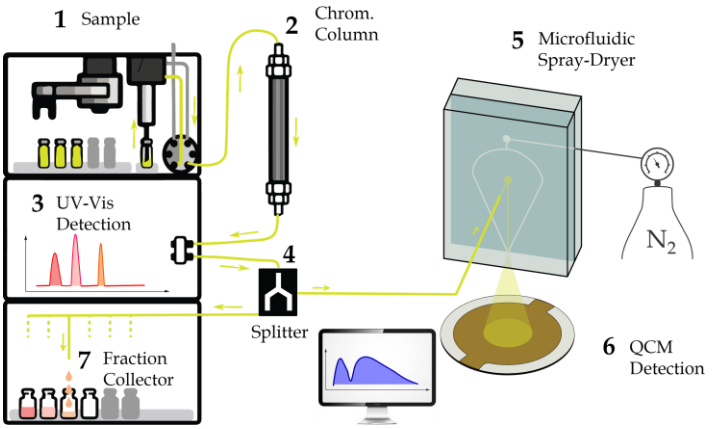
Online Natural Organic Matter Quantification by Dry Mass Sensing to Optimize Sample Treatment Protocols

We bring forward a quartz crystal microbalance and a microfluidic spray-dryer to monitor and quantify matrix compounds online via dry mass sensing. This lays the foundation for optimizing purification of organic extracts in liquid chromatography-based sample clean-up.



A flow splitter (4) was installed after the UV detection (3) and before a fraction collector (7). Using a split ratio of 200:1, the high flow (i.e., 99.5%) is collected (7) for later isotope analysis, whereas the low flow (i.e., 0.5%) is directed to a microfluidic spray-dryer (5) centered above the QCM detector (6).

State of the Art Compound-specific isotope analysis (CSIA) of complex environmental samples often necessitates extensive sample purification with the goal to separate small organic analytes (e.g., pesticides) from complex unresolved background (e.g., natural organic matter, NOM). An effective optimization of the purification is only possible if both the analyte and the matrix are monitored and quantified online. While there are methods at hand to monitor the analyte during clean-up procedures (e.g. UV-Vis in HPLC), online monitoring of total NOM in such samples remains challenging.

Analytical Approach In this work, we couple a quartz crystal microbalance (QCM) with an HPLC system using a microfluidic spray-dryer (see Figure) to monitor and quantify elution of NOM during a chromatographic purification process [1].

Results Validation measurements confirmed that QCM dry mass sensing accurately mimicked offline TOC analysis and demonstrated the ability of the system to quantify NOM in environmental extracts using different solvents and chromatographic conditions. For different methanol-water compositions, the limit of detection ranged between 3.8 and 7.8 mg/L, while the limit of quantification was between 13.7 and 26.8 mg/L. Gradient optimization screening was facilitated by our dry mass sensing approach and showed that NOM co-elution could be decreased by a factor of between 1.5 for early eluting analytes (e.g. 2,4-dichlorobenzamide) and up to 5 times for late eluting analytes (e.g. boscalid). Background measurements on GC-IRMS for these samples agreed with the observed decrease on the QCM – a 5-fold decrease in NOM co-elution led to a significant decrease of the baseline rise. Using the QCM it is possible to observe the amount of interfering mass and, therefore, to predict when the relative amount of complex unresolved mixtures to the analyte has a detrimental effect on isotope analysis.

Funding
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Cooperation
Zenon Toprakcioglu/
University of Cambridge

Christopher Wabnitz and Wei Chen

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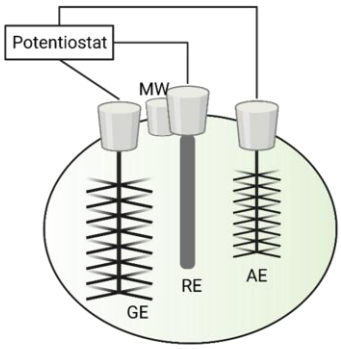
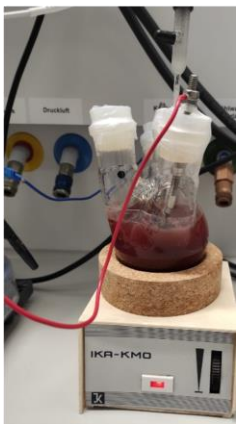
Exploring the role of bacteria in microbial biofilms to help harvest renewable energy in the beverage industry

***Rhodopseudomonas pentothenatexigens* was investigated as a possible exoelectrogenic bacterium and a putative key player from the biofilm of a microbial fuel cell inf beverage wastewater.**

State of the Art Harvesting renewable energy through microbial fuel cells (MFC) is promising in wastewater treatment processes. After hydrolysis and fermentation have been facilitated in the anaerobic process, intermediate products can be fed directly into the MFC. Here, their degradation can generate electrical energy increasing the degree of self-sufficiency of small and medium-sized companies in the field of wastewater treatment.





Testing *Rhodopseudomonas pentothenatexigens* for its exoelectrogenic power − Fed batch reactor with a three-electrode set-up (GE: counter electrode, RE: reference electrode, AE: working electrode, MW: medium exchange).

Analytical Approach *R. pentothenatexigens* could be enriched as a putative exoelectrogenic (electron-donating) bacterium and a possible key player from the biofilm of a MFC. It was subsequently tested in a fed batch reactor and a three-electrode set-up (counter and working carbon electrode, reference electrode Ag/AgCl), connected to a potentiostat. Experiments were conducted under exposure to light and under anoxic conditions at room temperature. Biofilm growth and the maximum current density were monitored over time using chronoamperometry. Raman microspectroscopy (RM) and scanning electron microscopy (SEM) were used for *in situ* 2D imaging to visualize the morphology, thickness, and chemical composition of the biofilm.

Results 2D RM imaging and SEM analyses visualized the biofilm development. The biofilm continuously covered the anode surface with a thickness of 3–7 µm and a homogeneous distribution of carotenoid signals. In the MFC batch mode, the measured current density reached a maximum of 0.320 A/m^2 over a period of 1000 hours. This compares favorably with reported current density ranges of exoelectrogens with synthetic medium as substrate between 0.340 A/m^2 for *Shewanella oneidensis* and 3.9 A/m^2 for *Geobacter sulphurreducens*.[1] Thus, the isolate does not only show a similar performance, but is also adapted to given environmental conditions and can thus proliferate by metabolizing organic matter and producing bioelectricity.

Irina Beer

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Cooperation

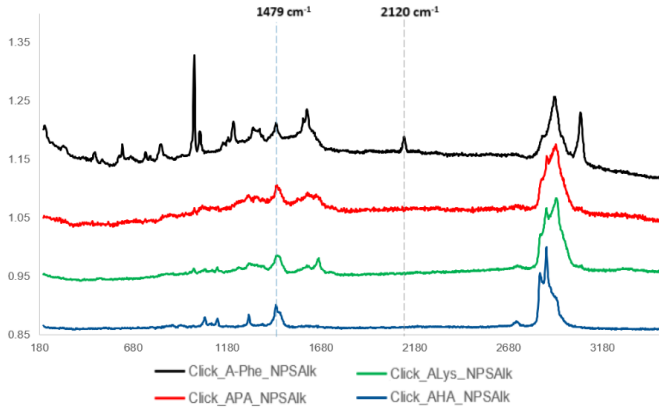
Dr. Karl Glas (Water System Engineering, Chair of Food Chemistry and Molecular Sensory Science, TUM School of Life Sciences Weihenstephan)

Synthesis and application of alkyne-modified silver nanoparticles

Silver nanoparticles (Ag NPs) were synthesized and functionalized with alkyne tags, characterized via Raman microspectroscopy (RM) and subsequently tested to capture azide compounds in a "click" reaction.

State of the Art Ag NPs are known to increase the Raman signal of different analytes and are widely used in surface-enhanced Raman scattering (SERS) studies. Alkyne-modified Ag NPs are suggested to be applicable for detection of active cells after capturing them *via* an azide-alkyne cycloaddition ("click" reaction).[1] The aim of this study was to synthesize alkyne-modified Ag NPs and to explore their ability to capture azide-compounds for SERS.

Analytical Approach Ag NPs were synthesized according to Leopold *et al.*,[2] reduced and modified with an alkyne-functionalized thiol *5-(1,2-dithiolan-3-yl)-N-(prop-2-ynyl)* according to Shi *et al.*[3] They were washed in *n*-Butanol and water. To test feasibility of subsequent "click" reactions 4-Azido-L-homoalanine, 6-Azido-L-lysine, 3-Azidopropionic acid and 4-Azido-L-Phenylalanine were investigated. Raman spectra were obtained before and after azide-alkyne cycloaddition.



Raman spectra of the products of the alkyne-azide coupling. A-Phe – 4-Azido-L-Phenylalanine, APA – 3-Azidopropionic acid, A-Lys – 6-Azido-L-lysine, AHA – 4-Azido-L-homoalanine.

Results Alkyne-modified Ag NPs were synthesized. Covalent binding of an alkyne-funtionalized dithiolane to Ag NPS was proven via RM based on the decrease of the S–S stretching mode of the dithiolane at 502 cm^{-1} and simultaneous formation of Ag–S bonds that persisted after 5–7 washing steps. RM also demonstrated azide-alkyne coupling as proof of the "click" reaction based on the disappearance of the alkyne peak at ~2120 cm^{-1} and appearance of triazole-related peaks at 1430–1480 cm^{-1}. We therefore bring forward alkyne-modified Ag NPs to capture active cells by click chemistry for subsequent SERS detection.

Oleksii Morgaienko

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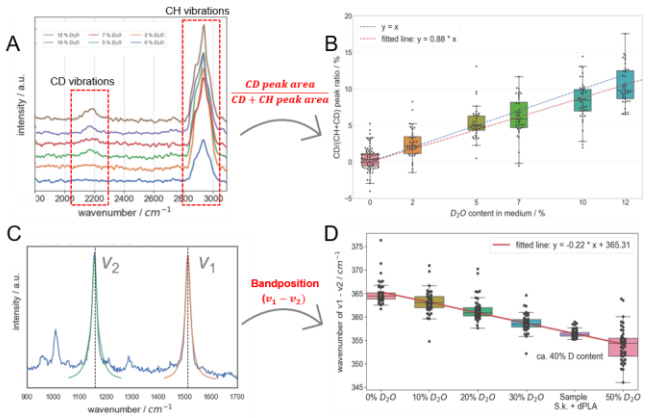
Funding
IWC-TUM

Potential of stable isotope Raman microspectroscopy for the analysis of biodegradation of microplastics

Stable isotope Raman microspectroscopy (SIRM) is used with the aim to track stable isotope labels from microplastic (MP) particles into microbial biomass. Biodegradation of deuterated polylactic acid (dPLA) by *Sphingomonas koreensis* is studied at the single-cell level.

State of the Art Indirect methods for the analysis of biodegradation of plastics focus either on measuring properties of the remaining polymer or on the monitoring of metabolites. The only direct confirmation so far has tracked ^{13}C-labels from polymer into microbial biomass with Nano Secondary Ion Mass Spectrometry (SIMS).[1] While NanoSIMS features very high spatical resolution, SIRM is attractive because of lower costs, simpler sample preparation and additional structural data on the single-cell level. Since heavier isotopes lead to red-shifted Raman bands, reference spectra of cells with different isotope contents can be used for quantification.[2]



Reference spectra of *S.k.* cells are shown to determine Raman features for the quantification of the D-content of the cells. (A+B) Peak areas of C-D and C-H vibrations in the mean spectra of ca. 30 *S.k.* cells incubated with different D_2O ratios can be linearly related to their D-content. (C+D) Alternatively, in the presence of carotenoids, the difference between the ν_1 and ν_2 vibrations also stands in linear correlation with the D-content of *S.k.* cells, labeled with D_2O.

Analytical Approach While ^{13}C-labeled polymers can help monitor carbon uptake by bacteria, these polymers are expensive and difficult to obtain. D-labeled polymers (e.g., dPLA) and reverse labeling were therefore tested as alternatives. Reverse labelling grows cells initially on L-lactate-$^{13}C_3$ before transfer into carbon free medium with PLA MP particles.

Results Different features in the Raman spectra of *S. koreensis* were selected to quantify their ^{13}C- or D-content. Deuteration of *S. koreensis* with D_2O leads to a C-D vibrations, which can be differentiated from other signals around 2200 cm^{-1}. The ratio of their peak area and the sum of the C-D and C-H vibrations can be used for quantification in the absence of carotenoids. The latter are pigments produced by *S. koreensis* which induce a resonance Raman effect. The band position of their ν_3-vibration (C=C str.) can also be used for quantification. Biodegradation experiments of dPLA showed ca. 40 % deuteration of *S. koreensis* after 4 months of incubation. Further control experiments regarding PLA hydrolysis etc. are in progress.

Kara Müller

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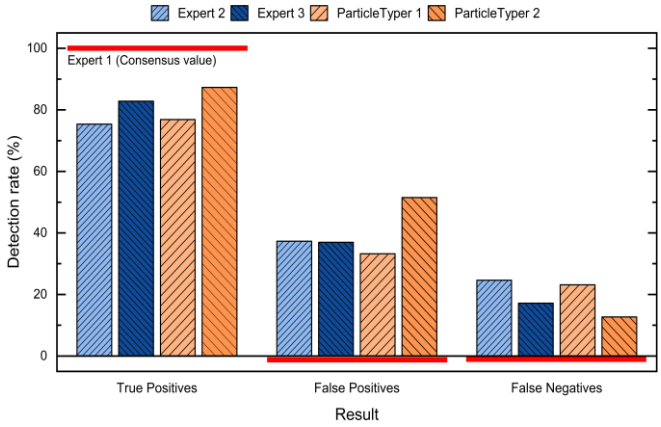
Cooperation

Jürgen Allgaier, FZ Jülich

Improved object detection for automated micro-Raman analysis as part of the software *TUM-ParticleTyper 2*

An improved version of *TUM-ParticleTyper* was developed that enables fully automated measurement and evaluation of microplastic particles deposited on a filter surface and within the entire relevant size range of 1 µm to 1 mm.



Comparison of particle detection rates by automated image segmentation (*TUM-ParticleTyper 1* and *2*) with recognition abilities of three experts (while expert 1 being set as consensus value).

State of the Art Particle numbers, shape and size distributions are relevant properties in the field of microplastic analysis which can be provided *via* recognition in dark-field images of particles deposited on a filter surface and subsequent Raman measurements for chemical identification. Automated recognition was enabled by *TUM-ParticleTyper*[1], yet only for particles > 10 µm.

Analytical Approach To enable detection also of particles down to 1 µm, they are deposited on Au-coated PC membranes (0.8 µm pore size) and microscopically imaged. Before a method of binarisation (`cv2.adaptiveThreshold`) is applied, the original image is processed through several functions to facilitate accurate object detection. Results of both *ParticleTyper* versions in six different particle images were compared to analysis by three experts.

Results The new development *TUM-ParticleTyper 2* is designed to work in combination with a computerised Raman microspectroscopy system via desktop recognition. Compared to *TUM-ParticleTyper* (2020) additional methods (e. g., *random window sampling*)[2] enable the analysis of particles down to 1 µm. When compared to experts (268–321 objects overall) and the original *ParticleTyper* version which already provides acceptable results that lie between the one of two other experts, the result of *TUM-ParticleTyper 2* shows an improved detection rate (87% true positives). False positives at this stage are less relevant as subsequent Raman point measurements for material identification serve for verification. False positives are therefore acceptable as long as they occur to a moderate extent and thus do not slow down the analysis to a significant extent.

Oliver Jacob and Alejandro Ramírez-Piñeiro

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Funding

Bundesministerium für Bildung und Forschung, BMBF

Cooperation

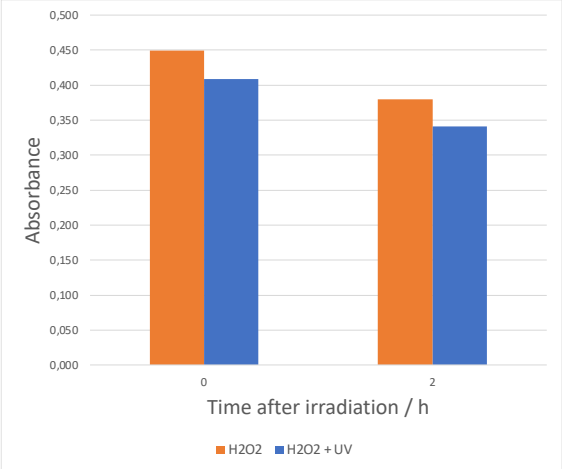
Dr. Aaron Beck, Prof. Eric Achterberg (GEOMAR, Kiel, Germany)

Developing a sample pretreatment for microplastic analysis of ocean samples by Raman microspectroscopy

Within the field of microplastic analysis, degradation of organic matrix in ocean water samples is important. For this purpose, treatment with H_2O_2 in combination with UV-C irradiation was tested.

State of the Art Raman microspectroscopy is often used to identify and quantify microplastic particles down to 1 µm in environmental samples.[1] However, obstacles may arise from the presence of organic matrix, which can hamper the success of the analysis, especially when focusing on the lowest size range (1 µm–50 µm diameter).

Analytical Approach Test samples were filtered on gold-coated polycarbonate membranes (pore size 0.8 µm). As pretreatment options, the efficiency of citric acid followed by KOH, Fenton's reaction (in each case after filtration), and H_2O_2 under irradiation with UV-C light (prior to filtration) were compared.



Absorbance (λ=500 nm) of algae extract suspension treated with H_2O_2 (orange) and H_2O_2 + UV light (blue). Absorbance was registered directly after irradiation and 2 hours after irradiation.

Results Without sample preparation, the presence of organic matrix hindered the identification of particles based on Raman spectra. We therefore focused on different methods for removal of the matrix. Blanks for treatment with citric acid and KOH revealed that citric acid represents a source of particulate contamination. Two different protocols of Fenton's reaction were applied.[2,3] In both cases difficulties arose from residues of iron precipitate so that too many particles were found on the filter. For this reason, the attention was focused on a strategy that employed as few reagents as possible. UV light is known to promote the formation of hydroxyl radicals in H_2O_2. To test its efficiency, algae extract was added to H_2O_2 (35% in H_2O) (1:20) and samples were irradiated by UV-C light (100–280 nm, 1 hour). For control samples no UV radiation was applied. Finally, absorbance at 500 nm was registered. Samples that were treated with UV light showed lower absorbance revealing that degradation of organic matrix was more efficient. Hence, this method represents a good starting point for further development and optimization of H_2O_2 treatment combined with UV light irradiation.

Annachiara Morganti and Oliver Jacob

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Erasmus+

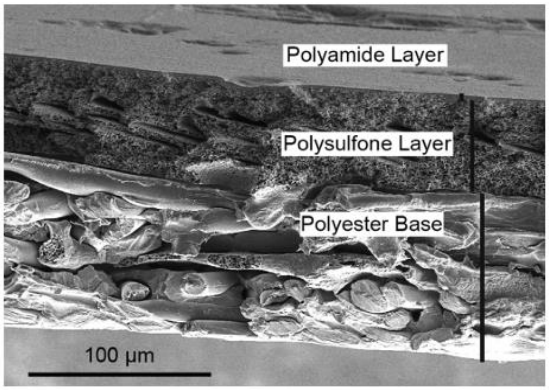
Bundesministerium für Bildung und Forschung, BMBF

Cooperation

Prof. Francesca Modugno (University of Pisa)

Analysis of micro- and nanoplastic particle removal from reverse osmosis membranes / systems

Raman microspectroscopy and scanning electron-spectroscopy are deployed to develop a tool for the analysis of reverse osmosis system damage. This way, morphological and chemical changes, including biofouling and the abrasion of plastic particles can be detected to evaluate different strategies for membrane clogging / damage.



Cross section view of a RO membrane showing the three different layers (1. Polyamide: ~ 100 nm; 2. Polysulfone: ~ 50 µm; 3. Polyester Base: ~ 120–150 µm)[2]

State of the Art Reverse osmosis (RO) is a ubiquitous water treatment method consisting of various process steps with a range of chlorine-based chemicals.[1] Since aging and disintegration of RO membranes result in performance decline, monitoring their performance and ensuring an ideal working environment is crucial.[2] Vibrational spectroscopy such as Raman microspectroscopy is widely pursued for representative non-destructive analysis of micro- and nanoplastics.[3]

Analytical Approach After soaking the membranes in various disinfectant solutions, morphological changes of RO membranes are monitored using SEM, while chemical membrane alterations are detected via Raman mapping. Analyte solutions from the RO system are aliquoted and then deposited on Au-coated filters (polycarbonate, 0.8 µm pore size). The particles are identified with the help of image analysis using *TUM-ParticleTyper*.[4]

Results Raman analysis of RO membranes using both red (785 nm) and green (532 nm) lasers revealed, as expected, a strong polysulfone signal. In contrast, the detection of the very thin polyamide cover layer (around 100 nm) turned out to be very challenging so that no reference Raman spectra of the polyamide layer could be obtained yet. Although some plastic particles from the suspended matter of RO system tests were identified as polyamide, due to missing reference spectra, only a tentative assignment is possible. Furthermore, it is difficult to distinguish them from contamination (e.g., skin particles), which show similar Raman signatures. Overall, plastic contamination of RO water samples was found to be low.

Marcel Klotz and Maximilian Huber

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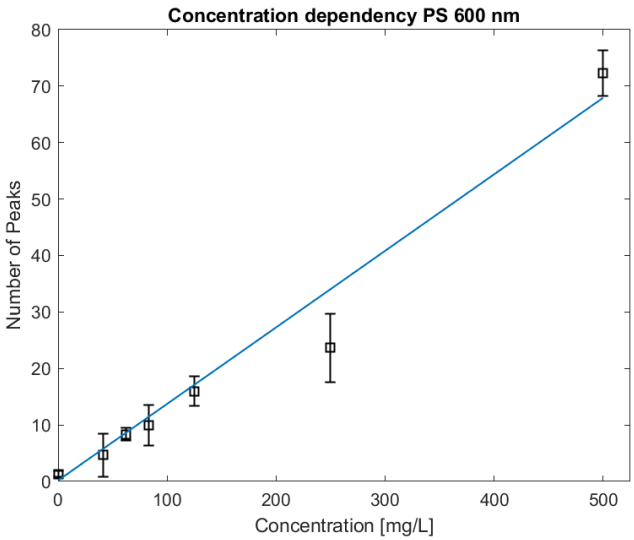
Cooperation
Dr. Karl Glas (TUM-AGW);
Dr. Florian Meier (Postnova Analytics GmbH);

Multi-parameter analysis of nanoplastics: stimulated Raman scattering for particle characterization and quantification

Stimulated Raman scattering was explored for online detection of nanoplastics in a flow-cell. In contrast to spontaneous Raman individual particles were observable. (Semi-)quantification, particle size estimation and chemical information, are, thus, accessible in only one measurement.

State of the Art To detect nanoplastics in real samples, limitations of current methods must be overcome such as the low sensitivity in online-coupled field-flow fractionation (FFF) – (spontaneous) Raman microspectroscopy[1]. It is therefore necessary to develop suitable preconcentration procedures and to lower the detection limit of current analytical techniques. To this end stimulated Raman scattering (SRS) holds great promise for fast microplastics analysis on a filter[2] or in flow-based systems.[3]



Correlation of the number of detected peaks per measurement with the injected concentration to obtain a calibration curve for 600 nm polystyrene (PS) beads using a linear weighted fit.

Analytical Approach The SRS setup described in [2] was tested for its potential application in flow-based systems (e.g., hyphenation with FFF). Therefore, different plastic particles of various sizes and shapes were injected into a custom-made flow cell. To enable detection not only in epi-mode, but also in transmission a new flow-cell with a polycarbonate bottom was designed.

Results The significantly improved time resolution (60.5 µs per data point versus 10 s) in combination with weaker 3D optical trapping allows for detection of individual particles down to 100 nm. This enables semi-quantification of nanoplastics. Furthermore, the shape of the peaks ranged from Gaussian-like over an exponentially decaying intensity to a constant signal intensity over a long time. This can be interpreted as different strengths of optical trapping. Signals from untrapped particles can be used to estimate particle size only from Raman data by the width of the peak since it is dependent on the flow rate and the particle diameter. Due to a higher number of scattering centers bigger particles also result in a higher average signal.

Maximilian Huber

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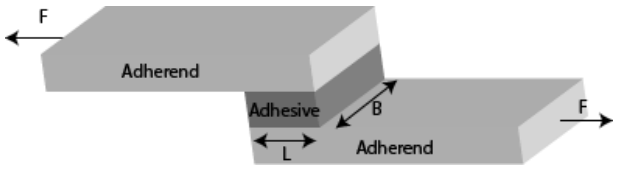
Dr. Karl Glas (TUM-AGW);

Dr. Florian Meier (Postnova Analytics GmbH);

Prof. Freek Ariese, Dr. Liron Zada (VU Amsterdam)

Development of non-destructive prediction models for the quality of adhesives

Industrially, the performance of adhesives is most commonly tested using the destructive lap-shear test which results in high costs. For this reason attempts are made to develop alternative approaches based on non-destructive spectroscopic methods to predict the results of the lap-shear test and, in turn, the performance of the adhesives.



Depiction of the industrially standard lap-shear test the results of which are hoped to be achieved non-destructively.

State of the Art Current analytical methods used to test the performance and strength of adhesives are limited. The most common and industrially accepted test is the lap-shear test, in which the two adherends are pulled in opposite directions until the adhesives give way. Even though this test provides reliable data, because of its destructive nature it also results in high costs and low sustainability. The aim of this project is, therefore, to clarify whether the results from the lap-shear test can be predicted using non-destructive, spectroscopic methods.

Analytical Approach To solve the problem of sample destruction, the goal is to track the polymerisation of the adhesive using Raman and Infrared spectroscopy. The polymerisation will be performed under varying environmental parameters such as temperature, humidity, etc. Afterwards, the lap-shear test will be performed, and the data will be combined in a multivariate fashion in order to find correlations between the spectra at different environmental parameters and the performance in the lap-shear test. From this data attempts will be made to develop prediction models for the adhesive performance, based solely on the spectroscopic data.

Results This project is at a very early stage. So far, the focus has been on optimising the parameters of the IR and Raman measurements and to overcome the interference caused by strong fluorescence of the adhesive in Raman spectra. Furthermore, possibilities were explored to solve the problem that the adhesive begins to melt at relatively low Laser energy inputs further complicating the measurement process. By analysing the adhesive with a 785 nm Raman laser, it was possible to acquire spectra in which all expected peaks could identified and assigned to the corresponding molecular vibrations of their functional groups. Further experiments are being undertaken to check the suitability of other available Raman lasers at 473 nm, 532 nm and 633 nm for the analysis of adhesives.

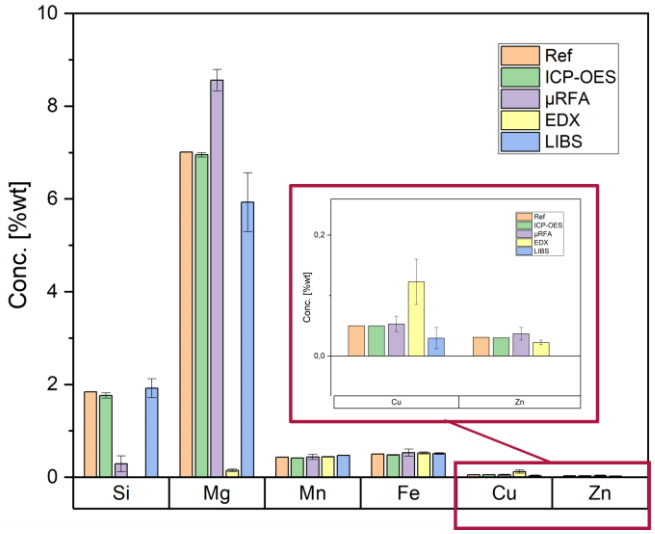
Alexander Thomas

Funding
BMW Group
Cooperation
Laser Technik Berlin (LTB)

Quantitative material characterization in metal particles – A comparative study

Analytical methods applicable to industrial particle characterization need to meet specific needs. Comparing the element quantification results of EDX, µ-XRF and LIBS, while considering corresponding (dis-) advantages, lays the foundation for a fact-based choice of the most suitable method.

State of the Art Energy-dispersive X-ray spectroscopy (EDX) and µ-X-ray fluorescence spectroscopy (µ-XRF) are well-established analysis methods that are widely used for particle characterization. Quantification algorithms for standardized analysis are typically provided by the manufacturers. In contrast, for LIBS as fairly new method in this context quantification models have been developed in house, especially for the use in particle characterization.[1] Comparing the methods is essential to identify the best-suited approach for specific characterization needs.



Visualization of quantification results of Si, Mg, Mn, Fe, Cu and Zn. Reference values (Ref, orange) have been taken from the certificate. For the other methods, the results of five particles are displayed.

Analytical Approach Four certified reference materials (CRM) for aluminum particles are used as samples. To characterize inhomogeneities in these materials, microstructure analysis is performed. Five particles of each CRM are analyzed individually by µ-XRF, EDX and LIBS in this order and evaluated using the standardized quantification models. The results are compared to the certified elemental composition as well as to ICP-OES measurements of the particles as internal reference.

Results The evaluation showed that the different methods gave a different performance for individual elements. X-ray based methods showed disadvantages for the quantification of Si and Mg, since the Al-matrix signal overlaps strongly with the analyte signals, while LIBS yielded more accurate results. Mn and Fe could be quantified with high accuracy with all studied methods. With the chosen measurement parameters, the analyzed sample volume was highest for EDX (~$8*10^5$ µm^3), followed by LIBS and µ-XRF with similar volumes (~$3*10^3$ µm^3). The analysis effort and time is similar for the used X-ray based methods (~5 min/measurement) while LIBS is significantly faster (~30 s/measurement).

Maria Lanzinger

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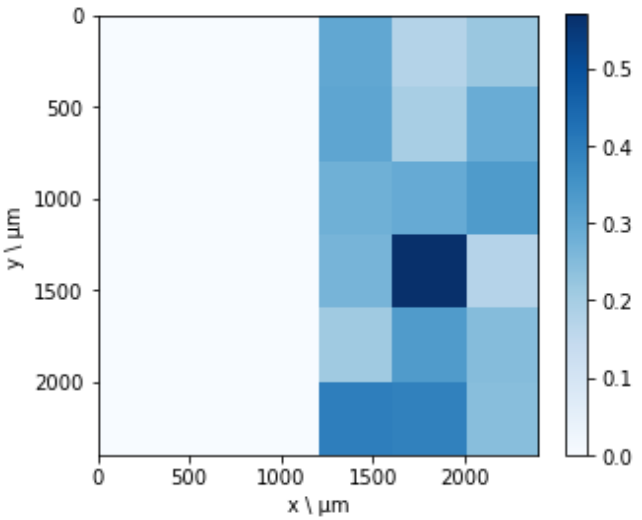
Funding
BMW Group
Cooperation
Laser Technik Berlin (LTB)

Method development for elemental analysis of metallic surfaces and subsequent chemical imaging using laser-induced breakdown spectroscopy (LIBS)

Knowledge of surface inhomogeneities and their respective elemental composition plays a crucial part in the analysis of solid samples. Here, fast chemical imaging of metallic alloys without complex sample preparation is approached by developing a method using LIBS.



False-color image of two adjacent Ni-plated steel samples. The sample on the right has an additional Si-coating on its surface, which could be detected using the proposed method. The intensities on the color bar are relative values of the chosen Si I emission line (288.16 nm) to the most suitable Ni I emission line (341.48 nm). Pixel size in the shown image is 400 × 400 µm.

State of the Art In the development of highly efficient and powerful battery cells technical cleanliness is of outmost importance. Even small metallic particles in the µm-range can result in the occurrence of a short circuit within the cell. Therefore, exact knowledge of metallic surfaces of cell material is a considerable benefit and can provide a powerful tool for the clarification of incidents related to the abrasion of pieces from the respective metallic surface. LIBS analysis has several benefits compared to other suitable techniques. In contrast to scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDX), measurements are performed under atmospheric pressure and depth scans, resulting in 3D images, are possible. In comparison to micro X-ray fluorescence spectroscopy (µ-XRF), LIBS has a higher sensitivity and does not face limitations in the analysis of lighter elements.

Analytical Approach In a first application, nickel-coated steel samples with silica surface treatment were investigated. Optimal LIBS parameters and pattern step sizes for nickel matrices were developed using a certified reference material (matrix: Ni >99 $\%_{wt}$) to maximize signal-to-noise ratio and spatial resolution without overlap of the resulting craters. The local element distribution of silica was estimated by setting the intensity of a non-disturbed Si emission line (288.16 nm) in ratio to the matrix signal (Ni I @ 341.48 nm). The results are visualized in a false-color image.

Results The preliminary results show that a clear distinction between treated and not-treated areas in terms of silica content is achievable. They also pave the path for further optimization of spatial resolution and lay the foundation for analysis of different matrices, analytes and a possible depth scan with multiple laser pulses (3D-imaging).

Funding
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Cooperation
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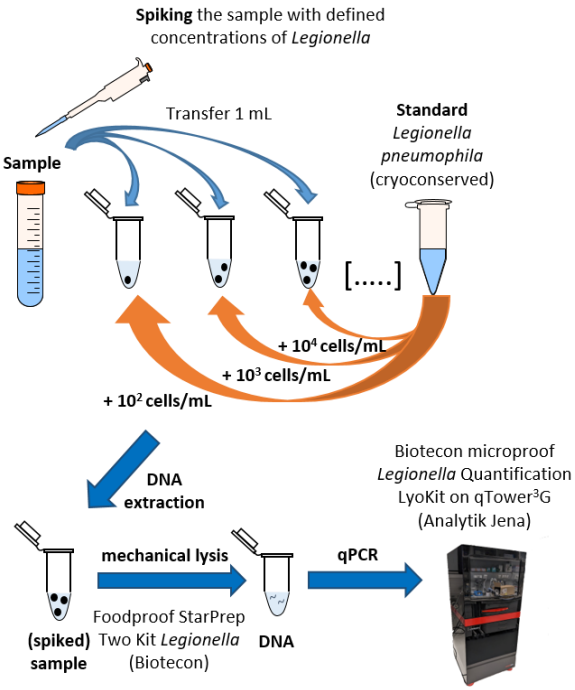
Jannis Gehrlein and Maria Lanzinger

Calibration strategy for qPCR to cope with complex matrices in agricultural air purification systems

To handle environmental samples with strong matrix effects, an improved calibration approach for qPCR was developed. This assay was used to quantitatively investigate the prevalence of *Legionella* in agricultural biofilter systems.

State of the Art qPCR is highly influenced by matrix effects. PCR inhibitors, influences on DNA-extraction yield or a high biodiversity of bacteria are challenges. Especially environmental samples can differ significantly depending on sampling side, time, weather conditions, transportation means and also between operators in the laboratory. Usually, a calibration with DNA standards is not suitable to account for these site-specific factors.



Analytical Approach To reduce the influence of matrix effects, a novel standard addition approach for qPCR systems was developed. By spiking the sample directly with a bacteria standard, influences that occur within different samples are reduced. Based on values from different spiking levels and with the help of an algorithm[1] the unspiked sample concentration is calculated using values of different spiking levels.

Results First, tests with a classical calibration approach using a calibration curve in mineral water or biofilter samples that showed negative results in the culture were performed. Air samples before and after passing the filter were analyzed as well as wash water from the filter. This approach showed highly unreliable results while analyzing real samples. Changing the calibration strategy to a standard addition method overcame the high matrix effects, quantitative results that were also correlating with the quantification of a culture approach could be generated. With this improved qPCR calibration method, it could be shown, that *Legionella* spp. and *Legionella pneumophila* are present in samples of the wash water and clean air of an agricultural biofilter, indicating a release of bacteria from the biofilter into the air. Further analysis will be performed to understand the prevalence in different agricultural filter systems as well as the influence of the season on the amount of Legionella. Additionally, the developed calibration strategy can be used for a various analytical approaches regarding complex matrices.

Marco Matt and Gerhard Schwaiger

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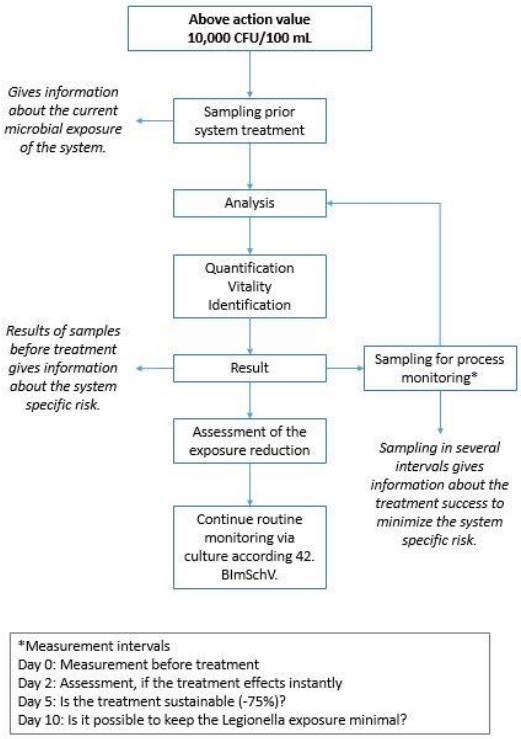
FKZ 28N-2-002-02
Cooperation
Thünen-Institut für Agrartechnologie

LegioRapid – Standardization of the analysis of Legionella in evaporative systems containing process water using culture-independent detection methods

The WIPANO project LegioRapid developed protocols for the detection of *Legionella spp.* and *L. pneumophila* in process water using culture-independent methods. In the future, these methods can be established in laboratories with *Legionella* expertise.



State of the Art According to the 42. BImSchV, the culture method is the gold standard to analyze the microbiological contamination of evaporative cooling systems. However, cultivation takes up to 10 days for the detection of *Legionella* spp. To establish new methods for routine analysis, protocols with a complete analytical strategy and a novel range of application were developed and published inside the VDI guideline 4250-2.

Analytical Approach The focus of the IWC in this project was the evaluation of antibody-based methods like the immunomagnetic separation (IMS) coupled with flow cytometry (FCM) as a quantitative assay and the LegioTyper for subtyping *L. pneumophila* serogroup 1. Both methods used frozen Legionella cryo standards. Their performance was tested across the whole analytical process, including enrichment *via* filtration, antibody incubation, measurement and data evaluation. Subsequently, real samples from different evaporative systems were investigated with these methods and results were verified against cultivation.

Results In Germany, the culture method is and will constitute a gold standard according to the 42. BImSchV. Within the VDI guideline 4250-2, however, culture independent methods like the IMS-FCM are foreseen when measures are to be monitored after an action value is exceeded - e.g. when the success of disinfection steps is to be controlled. Furthermore, the qualitative assessment of the hygienic statutes can be recorded within one day. Subsequent to this fast detection, complementary repeated cultivation measurements within one to two weeks are necessary to ultimately prove that a disinfection was successful and the system specific risk is eliminated. The implementation and establishment of culture-independent methods in form of the VDI guideline 4250-2 therefore enables the development of new ways of effective and hygiene-related water analysis and risk management to improve the 42. BImSchV in the future.

Philipp Streich

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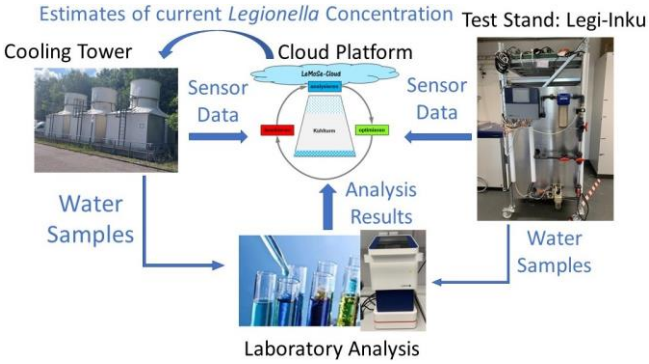
Cooperation

Bavarian Health and Food Safety Authority, Association of German Engineers e. V., GWK Präzisionstechnik GmbH, Institute of Medical Microbiology and Hygiene, Institute of Virology, Medical Faculty “C. G. Carus”, Technical University of Dresden.

Development of a sensor-based indirect monitoring system for *Legionella pneumophila* in cooling towers by online data processing

To minimize chemical and microbial emissions from cooling towers, the dose of chemical disinfectants should be regulated based on the concentration of *Legionella pneumophila*. However, direct detection methods are not applicable for continuous monitoring due to their long measurement durations and high costs. For such cases, a sensor-based monitoring system can provide an alternative solution.



Schematic development process of the monitoring system

State of the Art According to the guideline 42. BImSchV, a periodic addition of biocides in cooling towers is required to avoid growth of *Legionella pneumophila* which can cause severe pneumonia. Considering the lack of monitoring, the dose of biocides is usually excessive to guarantee a desired disinfection effect, leading to unnecessary water pollution. Among the currently applied detection methods for *Legionella*, culture methods have the disadvantage of long processing times. In comparison, PCR and antibody-based methods enable a rapid detection of *Legionella*, but they require expensive consumables. To fill the gap of continuous monitoring, a functional sensor-based monitoring system was to be established.

Analytical Approach The monitoring system consists of sensors for data collection, a cloud platform and database for data management, and a software for data processing. The physical and chemical conditions in cooling towers can be simulated using a test stand with the same monitoring system. Water samples from the test stand were analyzed on the newly developed flow cytometry, the rqmicro.COUNT, to determine the total cell counts and *Legionella* concentrations under various conditions. The turbidity and concentrations of trace elements were determined by water sample analysis. Based on the recorded data and analysis results, the correlation between sensor data and *Legionella* concentration is investigated using data mining techniques. The resultant model can be adapted and developed according to the analysis results of water samples from cooling towers.

Results The test stand was designed and set up in our Bio2 laboratory. After calibration, examination, and optimization steps, the equipment was tested for continuous operation. Sensor data from the test stand were successfully transferred per an IoT system and stored in our database for data processing. To prepare prior knowledge for modeling by machine learning, existing models to describe microbial survival and growth patterns were collected and selected.

Yiao Liang

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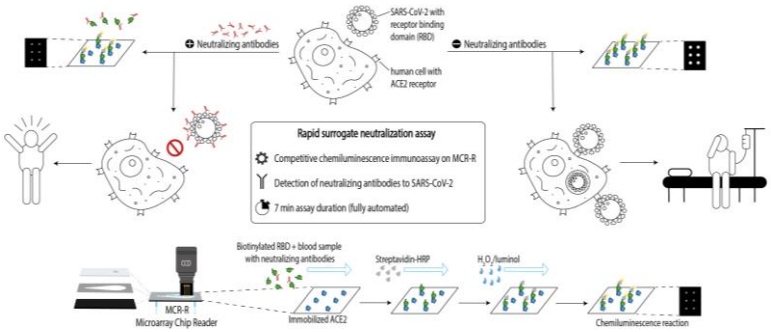
Cooperation
arteos GmbH
Keller & Bohacek GmbH & Co. KG (KEBO)

Development of a competitive chemiluminescence immunoassay for the automated detection of neutralizing SARS-CoV-2 antibodies



Schematic depiction of the measurement principle of a rapid surrogate SARS-CoV-2 neutralization assay.

Well-established SARS-CoV-2 rapid antibody tests cannot provide information about effective protective immunity and whether those antibodies truly prevent the cell entry of SARS-CoV-2. To gain this information, the neutralizing potential of SARS-CoV-2 antibodies needs to be determined. Therefore, a virus-free surrogate assay for the detection of SARS-CoV-2 antibodies has been developed on the microarray platform MCR-R.

State of the Art Rapid serological assays for the detection of neutralizing antibodies are important for determining the amount of antibodies formed after infection or vaccination and their neutralizing potential, preventing the cell entry of SARS-CoV-2. Besides active-virus neutralization assays, which require biosafety level 3 facilities, virus-free surrogate assays are currently used but take typically several hours until results are available.

Analytical Approach We developed a virus-free surrogate neutralization assay for the detection of neutralizing SARS-CoV-2 antibodies on the microarray platform MCR-R[1]. Therefore, the protein-receptor interaction between the viral receptor binding domain (RBD) and human angiotensin-converting enzyme 2 (ACE2) was determined to define suitable conditions for the inhibition of this binding in a competitive microarray immunoassay. This also marks the first time protein-protein measurements were realized on the MCR-R. For the neutralization assay, a serum sample was mixed with biotinylated RBD and injected into a microarray chip with immobilized ACE2.

Results The developed competitive binding inhibition assay was able to characterize a set of 80 samples correctly within 7 minutes per measurement. These results correspond to those obtained with a commercial surrogate neutralization assay and a time-intensive ELISA-based neutralization test. The developed competitive immunoassay could further be used to detect individuals with a high total IgG antibody titer, but only a low neutralizing titer, and to monitor the levels of neutralizing antibodies after vaccinations.

Sandra Paßreiter and Julia Klüpfel

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Funding

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Cooperation

Prof. Protzer, Institute of Virology

Prof. Knolle, Institute of Molecular Immunology

Prof. Hayden, Heinz-Nixdorf-Chair of Biomedical Electronics

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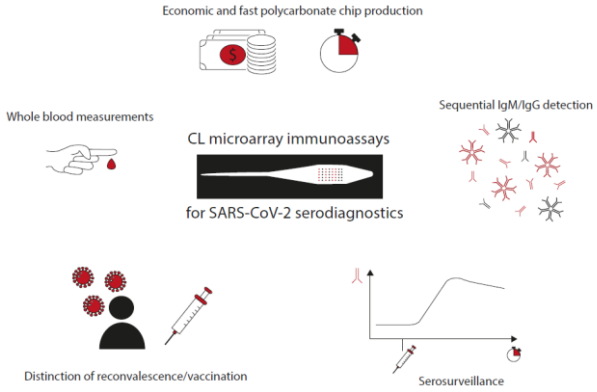
Optimization and extension of a SARS-CoV-2 antibody chemiluminescence microarray immunoassay (CL-MIA) for point-of-care (POC) applications

The COVID-19 pandemic has kept the world in suspense for almost three years. While it was hoped that vaccinations would pave the way back to normality, we are now facing breakthrough infections that often go unnoticed, making broad, cost-efficient serological monitoring with POC methods an important tool in the way out of the pandemic. Therefore, polycarbonate microarray chips have been developed and tested in a variety of POC applications.

State of the Art Over the last three years, more than 6.7 mio. people died from infection with SARS-CoV-2. As even vaccines do not necessarily protect from infection, serosurveillance is crucial to gain deeper insights into the mechanisms of immunity. Typical antibody tests have the drawbacks that they are time-consuming and laborious. Additionally, most tests cannot distinguish vaccinated and convalescent individuals, making it impossible to detect vaccination breakthroughs.



Possible point-of-care applications for the SARS-CoV-2 antibody CL-MIA.

Analytical Approach We optimized the previously developed CoVRapid CL-MIA[1] for the use of polycarbonate (PC) microarray chips to reduce chip cost, production time, assay time and required sample amount. Different SARS-CoV-2 antigens were covalently immobilized on the chip to enable an indirect non-competitive microarray immunoassay on the novel platform MCR-R.[2] For different POC applications serological information was obtained in minutes without the need of specialized laboratories or extensive manual steps.

Results The CL-MIA on PC microarray chips achieved a reduction of production time, costs, and sample amount by approx. 90% and of assay time by 50%. Additionally, a diagnostic sensitivity and specificity of 100% was obtained. In terms of POC applications, the use of whole blood was proven possible, as well as the sequential measurement of IgM and IgG, the distinction of vaccinated and convalescent individuals and the concentration-dependent progress measurement of antibody titer after vaccination. Therefore, this CL-MIA is a valuable and versatile tool in SARS-CoV-2 serosurveillance, to help find a way out of current and future pandemics.

Julia Klüpfel and Sandra Paßreiter

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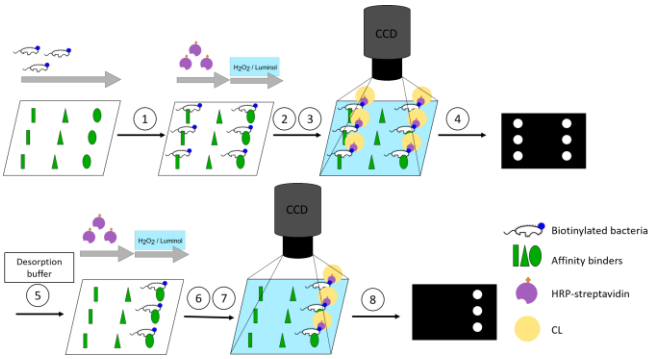
Prof. Protzer, Institute of Virology
Prof. Knolle, Institute of Molecular Immunology
Prof. Hayden, Heinz-Nixdorf-Chair of Biomedical Electronics
GWK Präzisionstechnik GmbH
ISAR Bioscience GmbH

Flow-based chemiluminescence microarrays as screening platform for affinity binders to capture and elute bacteria

For fast affinity ligand screening, a flow-based chemiluminescence microarray platform was established. Different ligands and elution buffers were tested for *Escherichia coli* and *Enterococcus faecalis*.



Concept of the screening assay. (1): Capture of the biotinylated bacteria through the affinity binders depending on the affinity. (2): Binding of the HRP-labelled streptavidin. (3): CL reaction. (4): Image acquisition. (5): Desorption of bacteria by desorption buffer depending on reversing of affinity. (6): Binding of the HRP-streptavidin. (7): CL reaction. (8): Image acquisition.

State of the Art The affinity between affinity binders like antibiotics, proteins or antibodies and bacteria can be utilized for their capture and subsequent elution by competitive desorption through salt, proteins or pH changes. To find new affinity binders and optimize suitable elution conditions a flow-based chemiluminescence (CL) microarray screening assay was developed.

Analytical Approach The screening assay was established on the MCR-R (Microarray Chip Reader – Research), with polycarbonate chips which were coated with succinylated Jeffamine® ED-2003. Affinity ligands were immobilized before the flow-through microarray was assembled. Subsequently biotinylated bacteria were incubated in stopped-flow mode on the chip. After blocking the surface with casein, horseradish peroxidase - labeled streptavidin (SA-HRP) was added to attach to the biotin, catalyze a CL reaction of luminol and hydrogen peroxide and, thereby, label the captured bacteria. The signal was recorded by a CCD camera. Subsequently, elution was performed by flushing the chip with an elution buffer and the chip was measured again, starting from the SA-HRP step, to explore how well the bacteria desorbed.

Results The assay was performed with biotinylated *E. coli* and *E. faecalis*, which are gram-negative and gram-positive bacteria, respectively. The affinity ligands tested were Polymyxin B (PmB), Concanavalin A, lysozyme, polyclonal antibodies against *E. coli* and against *Enterococci*. Two different elution modes were tested, with and without incubation. The respective dedicated antibodies were found to capture both *E. coli* and *E. faecalis* strongest, followed by PmB. Whereas *E. coli* was best eluted from the antibody with 100 mM glycine at pH 2.5 without incubation, no suitable condition was identified for *E. faecalis*. In contrast, when captured by PmB, both bacteria were conveniently eluted by 100 mM methyl-α-D-manno-pyranoside solution with incubation. This shows the power of the platform to systematically screen for optimized affinity ligands and elution buffers.

Julia Neumair

Funding

International Graduate School of Science and Engineering (IGSSE), TUM

Cooperation

Prof. Burgkart, MRI, TUM

References

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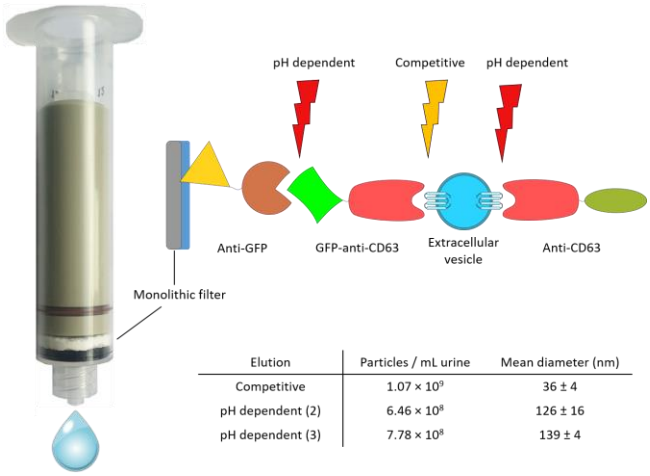
Nanobody-functionalized monolithic filters for the enrichment of extracellular vesicles from urine

Extracellular vesicles (EVs) are of great interest because they carry a lot of information like biomarkers for diseases. For their enrichment from urine we bring forward monolithic filters coated with nanobodies specific for cell surface-associated proteins.

State of the Art Extracellular vesicles are secreted by cells mostly for intercellular signaling. Consequently, they carry information like biomarkers for diseases. They appear abundant in body fluids, but need to be enriched before analysis. Cell surface-associated proteins like tetraspanin CD63 offer the opportunity for immuno-based enrichment. Here, monolithic immuno-filtration is promising to process larger sample volumes,[1] while nanobodies – i.e., single domain antibodies, more precisely the variable part of a heavy chain-only antibody – has preferable physicochemical qualities.



Elution	Particles / mL urine	Mean diameter (nm)
Competitive	1.07×10^9	36 ± 4
pH dependent (2)	6.46×10^8	126 ± 16
pH dependent (3)	7.78×10^8	139 ± 4

Filtration module for monolithic immuno-filtration with schematic illustration of capture and elution of extracellular vesicles from monolithic filter using nanobodies. The table shows the particles found in the elution fractions for competitive (one fraction) and pH dependent elution (2 fractions).

Analytical Approach In-house produced macroporous monolithic filters were first functionalized with an anti-GFP nanobody. After blocking, green fluorescent protein (GFP)-labelled anti-CD63 nanobodies were bound. Urine samples diluted with Tris•HCl were circulated over the modified filters to facilitate binding of the extracellular vesicles. Competitive elution from the filters was performed using a second anti-CD63 nanobody construct. Afterwards elution through a pH change using glycine at pH 2.5 followed.

Results SEM analysis of the monoliths confirmed pore sizes of 22.4 ± 8.8 µm. Spectroscopic measurements revealed immobilization of 180 ± 1 µg of GFP-anti-CD63, which corresponds to 97.9 ± 0.8 % of the used amount. It was possible to bind and elute extracellular vesicles using anti-CD63 nanobodies bound to monolithic filters. Competitive elution mostly eluted small vesicles with a diameter below 100 nm, while pH dependent elution yielded particles above 100 nm. SDS-PAGE showed pH dependent elution of GFP-anti-CD63, which can enhance the elution of vesicles. We could show that monolithic immuno-filtration can be used for the enrichment of EVs from urine. This will allow for a non-invasive screening of patient samples for biomarkers, e.g. for cancer.

Julia Neumair

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Funding

International Graduate School of Science and Engineering (IGSSE), TUM

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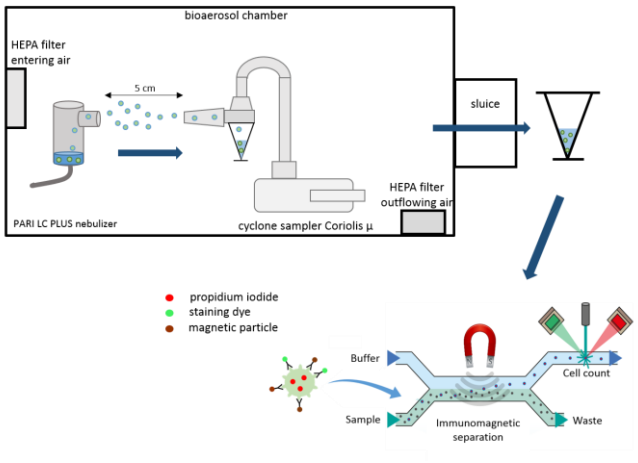
Prof. Ario de Marco, Laboratory for Environmental and Life Science, University of Nova Gorica, Slovenia

Development of sampling and analytical strategies for *Legionella pneumophila* in aerosols

Inhaled aerosols of cooling systems, which are contaminated with *Legionella pneumophila,* can cause a severe case of pneumonia. For adequate monitoring of such microbial contamination it is important to have suitable strategies for sampling and analysis.



Schematic workflow for experiments with bioaerosols: generation of aerosols with *L. pneumophila* in aerosol chamber with Pari LC Plus Nebulizer, sampling with cyclone sampler (Coriolis µ) and subsequent performing of Immunomagnetic separation (IMS) coupled with flow cytometry (FCM) for quantification of cell concentrations.

State of the Art *Legionella* outbreaks have occurred repeatedly in cooling towers in recent years.[1] So far, the 42. BImSchV only regulates the monitoring of *Legionella pneumophila* concentrations in water, but not in aerosols. In addition, the correlation between the concentration in water and in air has not been fully investigated yet. This is the reason why it is important to continue with research on this topic. The problem with the analysis of *L. pneumophila* is that it can enter a viable-but-not-culturable (VBNC) state. To avoid underestimation and long analysis time through cultivation, it is necessary to develop culture-independent methods.

Analytical Approach All experiments with bioaerosols were performed in a bioaerosol chamber[1] to exclude any risk of exposure. Magnetic particles and a green staining dye, which are coupled to anti-*L. pneumophila* Sg 1 antibodies, were used for immunomagnetic separation (IMS) and flow cytometry (FCM). With IMS, the matrix was removed and only bacteria cells were detected with flow cytometry (FCM) by measuring green and red fluorescence. Through further addition of a red staining dye, a distribution between intact and damaged cells is possible.

Results With the immuno-based IMS-FCM a rapid quantification of *L. pneumophila* Sg 1 is possible. In combination with the aerosol sampler Coriolis µ a recovery of 63.7 ± 34.1% for Total *Legionella* Count (TLC) and of 63.0 ± 13.5% for Intact *Legionella* in aerosols was obtained, respectively. This indicates a high biological sampling efficiency with Coriolis µ as there is no decrease of recovery for intact cells after sampling. In addition, the determined LODs of 4.0 x 10^3 cells mL^{-1} (TLC) and 5.8 x 10^3 (ILC) cells mL^{-1} are comparable to those received by qPCR and cultivation.

Lena Heining

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Funding
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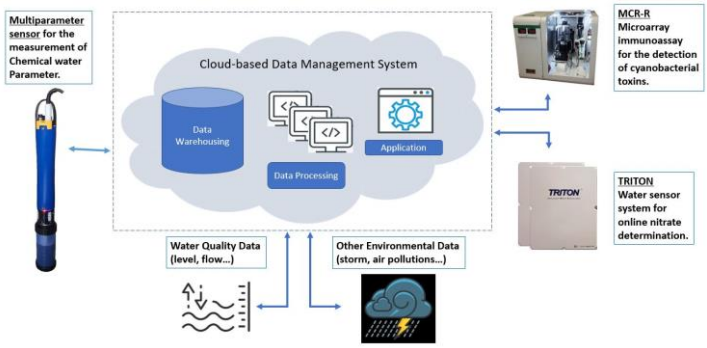
Cooperation
Institut für Energie- und Umwelttechnik, Duisburg

Cloud-based early warning system for algae monitoring in surface water

Eutrophication of water bodies together with climate change promote algal blooms, which pose a significant health risk to humans and animals due to formation of highly toxic cyanotoxins. It is therefore important to monitor endangered waters and to detect algal blooms at an early stage.

State of the Art The European Bathing Water Directive § 8 requires appropriate monitoring of surface waters if their profile indicates a possible mass proliferation of cyanobacteria.[1] Currently, hazard assessment is based on experience, visual inspections of water bodies and discrete sampling. Despite these efforts, the production of microcystins often go undetected until accidents occur. Thus, it is favorable to establish an early warning system in lakes which serve for recreation.



Schematic representation of an early warning system for algal blooms.

Analytical Approach For the development of a cloud-based early warning system, it is important to combine sensors for water chemistry parameter and immunanalytical systems for automated microcystin quantification. All data should be stored in one online database. For this purpose, different measurement principles are combined: The TRITON water sensor system, for continuous nitrate determinations in surface water, the Microarray Chip Reader – Research (MCR-R), for the immunanalytical quantification of cyanobacterial toxins such as Microcystin-LR and a multiparameter sensor, for the continuous monitoring of water chemical parameters such as pH, turbidity, conductivity, temperature and oxygen saturation.

Results Long-term field measurements were carried out with the multiparameter sensor at the small lake Brombach, Bavaria. In this way, data on the temporal changes of the water chemical target parameters were collected. Furthermore, in cooperation with the Werner Siemens Chair of Synthetic Biotechnology (Prof. Brück), a photobioreactor was put into operation to simulate algal blooms and to investigate the relationship between algal growth, toxin formation, nutrient concentrations, water chemistry parameters and other stress factors. These data will be used to develop a prediction model that forms the basis for a sensor-based early warning system for algae monitoring in surface waters.

Andreas Auernhammer

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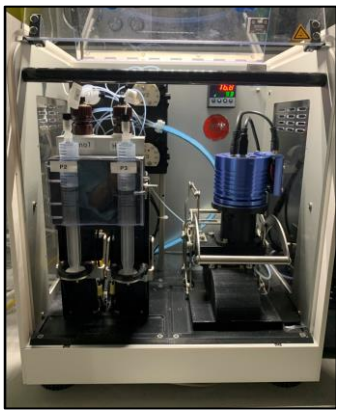
Flow-based chemiluminescence sandwich microarray-immunoassay (CL-SMIA) for the quantification of protein biomarkers from nasal secretions

Airway allergies and bacterial or viral infections are prevalent in the whole world. While their pathophysiologic processes differ largely, their symptoms often look the same. Analyzing protein biomarkers in nasal secretion would be a non-invasive method able to differentiate between allergy or infection. Therefore, a rapid multiparameter immunoassay is needed which is able to quantify multiple protein biomarker in parallel.



CL-SMIA for protein biomarker on the MCR R.

State of the Art It is presently difficult to differentiate between allergy and infection without performing clinical tests. However, these diagnostic tests can be expensive, time-consuming, and sometimes invasive. A rapid diagnosis is therefore important for precise treatment and medication. One way to achieve this is by analyzing protein biomarkers from nasal secretions that play a role in the pathophysiology of either precondition.

Analytical Approach The aim of the study was the establishment of a rapid flow-based chemiluminescence sandwich microarray-immunoassay (CL-SMIA) for the quantification of protein biomarkers (cytokine or chemokine CCL26, IFN-β, IL-24, IL-29, IL-37, OSF-2, and SCGB1A1). The CL-SMIA was compared with the commercial analysis platform Meso Scale Discovery (MSD) U-plex and a conventional sandwich enzyme-linked immunosorbent assay (ELISA) on microtiter plates.

Results Sandwich ELISAs with commercial antibodies for the biomarkers CCL26, IFN-β, IL-24, IL-29, IL-37, OSF-2 and SCGB1A1 were evaluated by calibration studies. The CL-SMIA was established for IFN-β and was compared with sandwich ELISA and MSD U-plex assay by calibration. The performance for each immunoassay platform was nearly equal achieving limit of detections of 5.34 pg/mL, 5.7 pg/mL, and 1.96 pg/mL, respectively. Recoveries using nasal secretion samples spiked with IFN-β were rather low (54 - 84 % and 17 - 23 % for sandwich ELISA and CL-SMIA, respectively).

Comparison of these three methods showed that the CL-SMIA is the most rapid method with results for each measurement after 1 h and 15 min. Additionally, in a multiplex approach it is also the most cost-effective assay. This study provides a first approach for the possible quantification of protein biomarkers in nasal secretion using a semi-automated and flow-based CL-SMIA. A full automation of the CL-SMIA is expected to enhance the assay performance.

Marie Kröger and Julia Neumair

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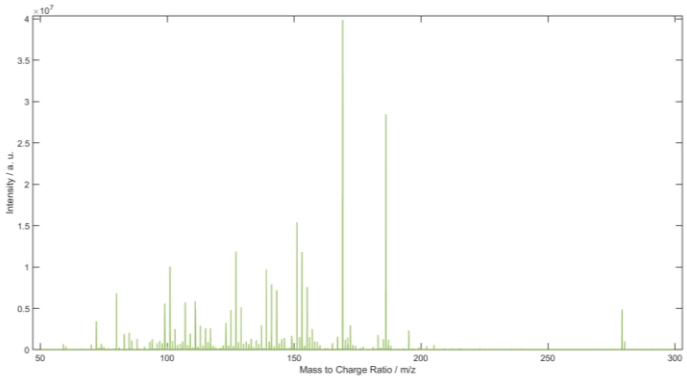
Zentrum für Allergie- und Umweltforschung (ZAUM)

Laser Desorption of Ultrafine Environmental Particles

Ultrafine particles (UFPs) have been proven to negatively affect human health. This necessitates a reliable method for day-to-day qualitative analysis.

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 options for offline measurements.[1] Since off-line sampling strategies offer a cost-efficient solution for the monitoring of environmental aerosols, the goal of this project is the development and evaluation of new methods to analyze off-line sampled ultrafine particles with mass spectrometry.



Mass spectrum of a laser desorbed impactor collection with a mean aerodynamic diameter of 95 nm.

Analytical Approach Atmospheric particles were collected with an electrical low-pressure impactor (ELPI) on aluminum substrates. Based on a development of last year, a CO_2-laser was effectively employed for localized desorption of semi-volatile compounds from the collected particles. Subsequently, the generated vaporized compounds were ionized via a SICRIT ion source from Plasmion – the start-up founded by alumnus J.-C. Wolf – and subsequently analyzed with an Orbitrap Exactive mass spectrometer. To test the viability of this setup for routine analysis, samples were collected daily for 23h, and measured on the same day, over two separate weeks. The high sensitivity of the SICRIT-MS setup allows performing the analysis on only a quarter of the impactor plate surface, thus allowing further analyses of the collected samples with Raman spectroscopy, SEM/EDX, and HPLC-fluorescence spectroscopy to complement and validate the acquired data.

Results Our system for the laser desorption of ultrafine particles in combination with highly sensitive dielectric barrier discharge ionization (DBDI) mass spectrometry allowed for measurements of environmental samples within minutes of sample collection, a vast improvement compared to time-consuming extraction procedures and long HPLC methods. With this, a range of tracers of woodburning and combustion of fossil fuels, as well as markers for natural aerosols were observed. Additionally, the localized desorption enabled the measurement of aliquots and thereby the addition of further analytical methods.

Felix Ludwig and Nico Chrisam

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Funding

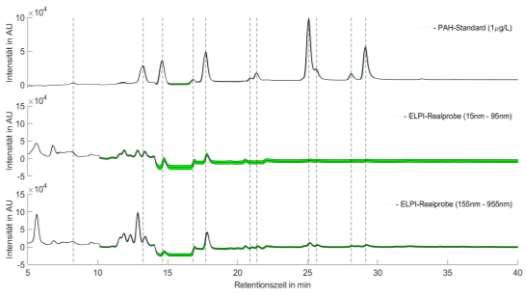
Bayerisches Landesamt für Umwelt (LfU)

Cooperation

Bayerisches Landesamt für Umwelt (LfU)

Development of an HPLC Method for the Targeted Analysis of Polycyclic Aromatic Hydrocarbons in Environmental Samples.

Air pollution is a major health concern for Europeans and fine particulate matter is associated with 238.000 premature deaths in 2020.[1] As the chemical composition of anthropogenic aerosols can be very diverse, the development of methods for the specific identification and quantification of these compounds is a necessity to employ appropriate guideline values.



Comparison of a Fluorescence chromatogram of a PAH-Standard-Mixture with the chromatograms of an anthropogenic sample.

State of the Art. The analysis and identification of organic compounds by HPLC (high-performance liquid chromatography) allow the separation of complicated substance mixtures or samples with strong matrix influence.[2] Fluorescence detectors in particular are very sensitive when it comes to polycyclic aromatic hydrocarbons (PAH), as the characteristic emission wavelengths of these compounds can be specifically incorporated into the method development enabling a more precise separation.[3]

Analytical Approach Atmospheric particles were collected with an electrical low-pressure impactor (ELPI) on aluminum substrates. Afterward, the soluble organic compounds were extracted for 24h using Soxhlet extraction. Standard solutions of 15 different PAHs as well as mixtures of these were prepared. UV-absorption and fluorescence-emission spectra were recorded using an Aqualog® 1000 (HORIBA Europe GmbH, Oberursel, Deutschland), and led to a 50-minute bi-gradient method at 35°C. The method starts at 70% Methanol, thus focusing primarily on nonpolar substances and aromatic compounds.

Results. The established HPLC-Method enables the separation of the complex mixture into a total of 12 signals, allowing the unambiguous differentiation of nine PAHs. The remaining six PAHs could each be separated into pairs. The analysis of the anthropogenic aerosol sample showed that the compounds anthracene, fluoranthene, and pyrene had the highest concentration while the compounds chrysene to benzo(ghi)perylene appeared only in traces. To verify these results, mass spectroscopic measurements are foreseen.

Nico Chrisam

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Funding

Bayerisches Landesamt für Umwelt (LfU)

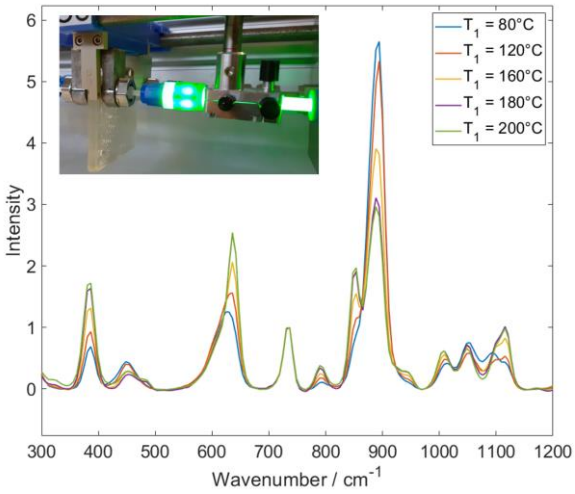
Cooperation

Bayerisches Landesamt für Umwelt (LfU)

In-Line Raman Spectroscopy for Microflow Systems

For continuous reaction monitoring, in-line Raman spectroscopy is applied using a modified Raman probe adapter. The approach has been successfully used to monitor reaction products in acid catalytic esterification of alcohols and nitration of aromatic substrates in microflow reactors.

State of the Art Continuous microflow reactors are an emerging technology that offers several advantages over conventional batch synthesis methods, such as enhanced mixing efficiency, easier temperature control, and increased user safety. To take advantage of flow reactors, in-line Raman spectroscopy is a fast alternative to offline analysis methods. It provides no sample preparation and real-time process understanding, allowing in-process corrections and integration with advanced process control strategies. Based on the spectral fingerprint and sophisticated data analysis, different parameters, such as reactant consumption, product formation, and variations in reaction conditions, can be analyzed simultaneously.[1]



Graph: Raman spectra of reaction mixture during acid catalyzed esterification of acetic acid to ethyl acetate depending on different reaction temperature. Inlet: Raman probe adapter fixed behind microflow reactor plate.

Analytical Approach For in-line Raman spectroscopy (CW laser, 532 nm), a developed aluminum adapter was attached directly to the PFA (perfluoroalkoxy alkanes,) tubing downstream of the microflow reactor plates (Corning® Advanced-Flow™ Reactors). The focus of the Raman laser lies inside the process flow. The intensities of the signal bands of the PFA tube were used for the normalization of the Raman spectra during data analysis. The spectra were processed by MATLAB (R2021b) to monitor the temporal evolution of educts and product concentrations.

Results The developed Raman probe adapter enables in-line Raman spectroscopy in a continuous flow reactor system for real-time process monitoring and analysis. For the practical implementation of in-line Raman spectroscopy in microflow systems, the acid catalytic esterification of acetic acid with ethanol and the nitration of guanidinium carbonate to nitroguanidine (NQ) were characterized as model reactions. Because monitoring of the reactants and nitro compounds was feasible with the in-line Raman spectroscopy setup in a continuous flow, the influences of various reaction parameters, such as reaction temperature, total flow rate, and stoichiometry of the reactants, on product formation were studied. The intensities of prominent bands of the substances were selected for the calibration to determine yields.

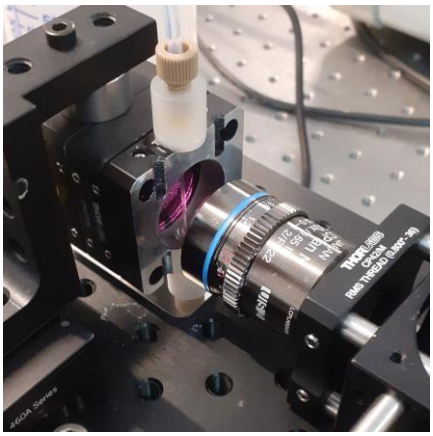
Lucas Hirschberger

Funding
IWC
Cooperation
Department of Chemistry, Energetic Materials Research, LMU

FluRam – Development of a Raman-Based HPLC Detector

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

State of the Art While high-performance liquid chromatography (HPLC) is a common analytical separation method, commercial solutions for inline hyphenation with vibrational spectroscopy do not exist. Here Raman spectroscopy can provide vibrational spectra to inform about the chemical composition and molecular structure of a sample in a non-destructive way. In contrast to infrared spectroscopy, it has the advantage that water, a common eluent in HPLC methods, does not produce interfering signals. Previous approaches for the hyphenation of Raman and HPLC were based on the use of SERS (surface-enhanced Raman spectroscopy) substrates to increase analyte signals. Instead of SERS, in this project, powerful lasers with a line focus are used. This setup has been found to enable Raman analysis of chromatographic separation in real time, holding promise to aid in the optimization of syntheses and purification processes.



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

Analytical Approach For the development of a capillary flow cell, different types of design were tested using a Raman setup (λ = 532 nm) to determine suitable flow cell shapes and window materials. 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 being used. To spearhead spectral processing, different method approaches such as baseline correction, normalization, derivations, and signal smoothing are tested.

Results In the developed detector prototype, a quartz capillary ($Ø_{inner}$ 0.5 mm, $Ø_{outer}$ 1 mm) was installed in the flow system using connections for HPLC connectors on both sides. Quartz glass proved optimal as a window material because of its low number of interfering bands and their convenient location in the spectrum. A linear capillary shape was found to be best suited for the sensor prototype. With the linear shape, the lowest amount of turbulence and mixing of the fluid occurred at the interface of the capillaries with the cell. As a result, time-resolved measurements were found to be possible with the entire setup. For further development, the use of the detector in process analytics for the detection of various substances in microfluidic systems is planned.

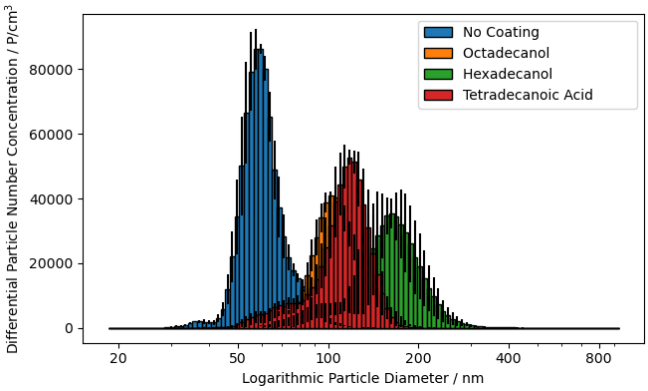
Lucas Hirschberger

Funding
AiF-ZIM
Cooperation
Soliton GmbH
Solectrix GmbH

AeroCal – Production of Calibration Aerosol Particles

To control the increasingly stringent legal thresholds of aerosol particle emissions, reliable, simple-to-use aerosol generators are required for calibration purposes. We propose a novel system for a precise generation of soot-like calibration aerosol particles.

State of the Art For the approval of new automotive types to the European market, manufacturers must meet emission regulations with a maximum particle emission of $6 \cdot 10^{11}$ particles per kilometer. To accurately monitor compliance with these regulations, the measuring instruments should regularly be calibrated with a soot-like test aerosol.[1] Currently, a few aerosol generators can provide such an aerosol, but to obtain a monodisperse test aerosol with a defined concentration, expert users and extensive equipment are required. Hence, in this project, an easy-to-use calibration aerosol generator, based on the redispersion of pre-produced standard particles, shall be developed.



Differential Particle Number Concentration over the Logarithmic Particle Diameter of Spark-Discharge-Generated Soot, Coated with Different Substances.

Analytical Approach As a first step in the development of the aerosol generator, the coating, and collection of standard particles were tested. For these experiments, a monodisperse, soot-like aerosol was generated using a spark discharge generator and a differential electrical mobility classifier. This test aerosol was modified by coating it with various organic substances (Octadecanol, Hexadecanol, and Tetradecanoic Acid). The particle size distribution was then measured with a differential mobility particle sizer and the particles were deposited on sample substrates for SEM and TEM analysis by electrostatic precipitation. Larger amounts of particles were collected by electrostatic precipitation, impinging, and filtration.

Results By coating the particles with organic substances, the median particle diameter could be increased from 60 to up to 250 nm. The coating thickness is influenced by the concentration ratio of the coating substance vapor and the soot aerosol. Of the three tested substances, coating with hexadecanol yielded the thickest coating layer, as shown in the adjacent figure. Tetradecanoic acid is prone to homogenous nucleation at higher concentrations. A suitable device for the efficient collection of larger particle amounts is yet to be found.

Kevin Maier

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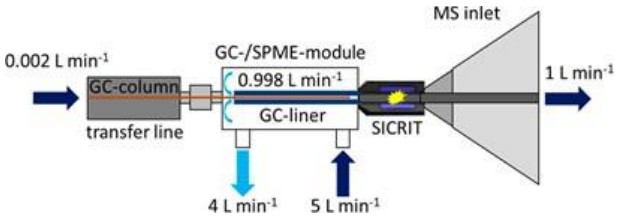
Funding
AiF-ZIM
Cooperation
ParteQ GmbH
Finke Elektronik GmbH

Optimization of GC-SICRIT-HRMS and LC-SICRIT-HRMS for the Detection of Nitrosamines

SICRIT is a versatile ionization technique that can be used for direct measurements or for coupling with gas (GC) and liquid chromatography (LC). It softly ionizes a wide variety of compound classes, ranging from non-polar components like alkanes and polycyclic aromatic hydrocarbons (PAHs) to highly polar amines, nitrosamines, and nitro compounds. Because of the elevated interest in sensitive detection methods by the pharmaceutical industry, nitrosamines were chosen as target analytes to compare the performance of different coupling techniques,

State of the Art Nitrosamines are highly cancerogenic compounds found in food, beverages, consumer goods, and drugs.[1] After the detection of nitrosamines in angiotensin receptor blocker drugs and following recalls a high demand for sensitive detection methods exists.



Schematic drawing of the GC-SICRIT-MS coupling. Compounds are separated via GC and enter the ionization source one at a time, while the atmosphere is controlled by an overflow of reactant gas.

Analytical Approach Nitrosamines have been measured via LC as well as GC coupled to high-resolution mass spectrometers via the SICRIT ionization source. The influence of various parameters on ionization was investigated: flow rate and composition of the mobile phase for LC or helium versus nitrogen as carrier gas for GC as well as different reactant gases.

Results Sensitivities for analysis of nitrosamines were found to be similar to conventional atmospheric pressure chemical ionization (APCI) when hyphenated to LC. Overall, the sensitivity decreases with increasing flow rates likely due to the competing ionization of solvent and analytes. However, SICRIT causes less fragmentation compared to APCI, while offering the possibility to better measure apolar compounds compared to electrospray ionization (ESI).

In comparison to studies described in the literature using GC with electron impact ionization (GC-EI-MS), no loss in sensitivity was observed when using the SICRIT source. This can be explained by the large dilution (>1:100) of the carrier gas with reactant gas present in the SICRIT setup. Here, the ionization is mostly determined by the choice of reactant gas. Humidified nitrogen and dry nitrogen both lead to similar LODs between 0.2 and 3 pg on column. Humid nitrogen generally causes less fragmentation than dry nitrogen and is therefore the preferred reactant gas for analytes with relatively high proton affinity.

Markus Weber

Funding
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IWC
Cooperation
Plasmion GmbH

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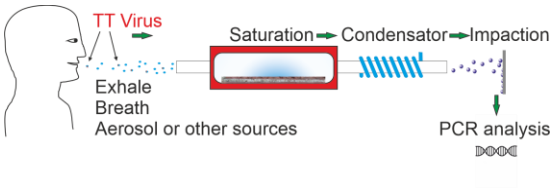
VirusImpact

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 fact 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, 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 as well as a considerable health burden for the patient.



Schematic of planned sampling device, comprising a water condensation chamber and an impinger.

Analytical Approach 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 as well as a considerable health burden for the patient.

Florian Opperer and Nico Chrisam

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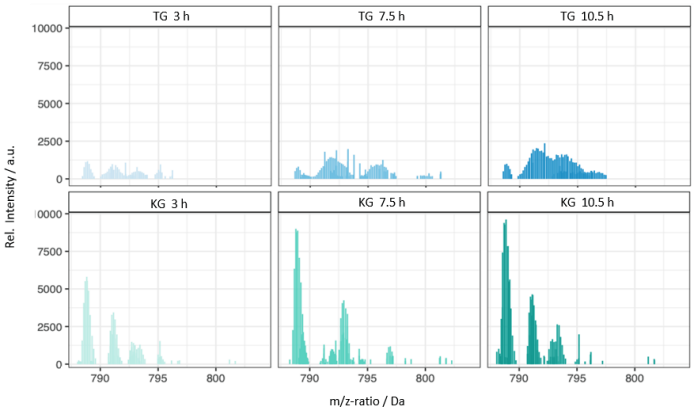
Cooperation

Max von Pettenkofer Institut

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 1.4 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 not only problematic because the therapies are costly and have many side effects, but they also lead to genetic and phenotypic resistances among the bacteria (dormancy; persister cells). Thus, there is a high need to shorten therapy and develop new treatment strategies ("End-TB-Strategy", WHO).[1] Also, new combinations of standard drugs and a focus on personalized medicine are required. However, this is difficult because preclinical models that simulate the interaction between multiple agents are lacking.



Mass spectra of isotope-labeled (first row, “TG”) and isotope-unlabeled (second row, “KG”) mycobacterial proteins at different time points (left: 3 h, middle: 7.5 h, right: 10.5 h).

Analytical Approach For a better understanding of 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 as well as dormant mycobacterial cultures are confronted with antibiotics of various drug classes and target structures. New LC-MS and LC-MS/MS methods for the analysis of 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 to identify about 1,000 mycobacterial proteins. With our newly developed pipeline using self-learning algorithms, we can 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 were developed, enabling the comparison and quantification of different samples as well as the determination of secondary modifications of intact proteins. Stable isotopic labeling made it possible to illustrate the rate of protein formation as well as the visualization of 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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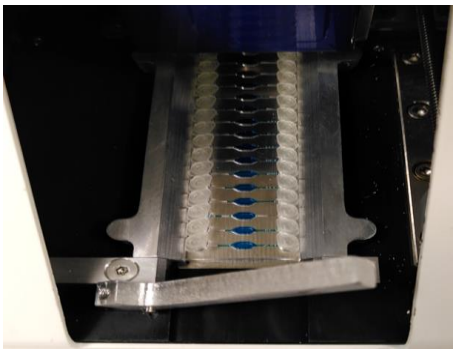
DetectRespi

This project develops a molecular biological Lab-on-a-Chip-Platform for the highly parallel detection of viral and bacterial pathogens of 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 as well as the operating devices. In addition, manual intervention and the need for different sample matrices make the use of these platforms inconvenient.



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

Analytical Approach The biochemical assays for the Lab-on-a-Chip platform are developed 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 panel. Real-Time PCR, specifically the TaqMan System, serves for evaluation of the designed primers and probes. Within this frame, the sensitivity and specificity checks of the primers are executed, followed by multiplexing experiments. In a later process of cartridge development, the probes are immobilized on a three-dimensional matrix on the DNA microarray. The cloning of PCR-positive controls supports the work on primer evaluation and multiplexing. It enables the calculation of the exact amount of plasmid copies in one microliter of sample. The main task of the TUM is the design and realization of the optical read-out unit for the DNA microarray. The evaluation of the array will be done by fluorescence labeling of the PCR products using Cy5. Optimization of the unit design includes the choice of the best-suited camera module, the integration as well as the illumination tasks to allow for an optimal excitation and read-out. Thus, glass slides spotted with different concentrations of Cy5 and in different geometries are used for experimentation.

Results Eleven of the final 16 primer pairs for seven organisms are designed and tested on functionality by PCR and agarose gel electrophoresis. In combination with their probes, 6 real-time PCRs are set up. Further primers are designed and have to be evaluated using organism-specific DNA and two final positive controls are to be cloned. Multiplexing of primers and the evaluation of the primers in combination with patient samples are the next working steps. 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 optimized to fit the technical requirements of the future device.

Amelie Hohensee and Eva Krois

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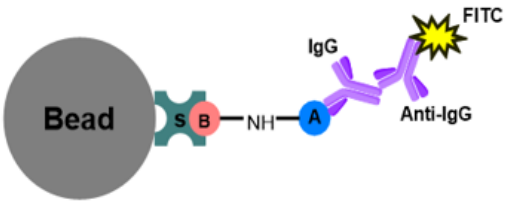
Avidity-based approach for the subclass- and variant-specific detection of anti-SARS-CoV-2 IgG, IgA, and IgM by flow cytometry

We developed a methodology to detect simultaneously IgG, IgM, and IgA against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) nucleocapsid (N-) and spike (S-) protein in human serum by flow cytometry. Avidity determination enables us to distinguish between variant-specific immune responses.

State of the Art In epidemiological research highly specific serologic screening techniques are essential for the indirect recognition of infections, evaluating the vaccine efficacy, and understanding the immune response.

Analytical Approach Biotinylated wild-type SARS-CoV-2 N- or S-antigen molecules were attached to the functional streptavidin surface of magnetic beads. During incubation with human plasma samples, present anti-N or anti-S antibodies were captured by the immobilized affinity ligands. To distinguish between IgG, IgM, and IgA subclasses, different fluorophore secondary antibodies were used. The immune complex was purified by magnetic separation from the sample matrix. The detection was carried out by means of a BD Accuri C6 Plus flow cytometer. The use of different magnetic bead sizes for N- and S-antigen coating allows the measurement of anti-N- and anti-S-antibodies simultaneously. In parallel, we determined the SARS-CoV-2 variant that triggered the specific immune response in the sample. For this purpose, we measured the avidity by the degree of release of antibody bound to its antigen by defined treatment with a chaotropic agent. This assay is based on the slightly modified fit between the variable regions of anti-SARS-CoV-2 variant antibodies and the wild-type epitope.



Structure of the immune complex attached to the functional magnetic bead for the IgG subclass-specific detection of anti-SARS-CoV-2 antibodies by flow cytometry.

Results For high titer plasma our method allowed for both serologic analysis, as well as a reliable assessment of the virus variant that caused the respective immune response. Sample preparation and measurement parameters are now optimized to increase sensitivity.

Jessica Beyerl

Funding

Forschungszentrum Jülich GmbH, Jülich University Hospital of the LMU Munich

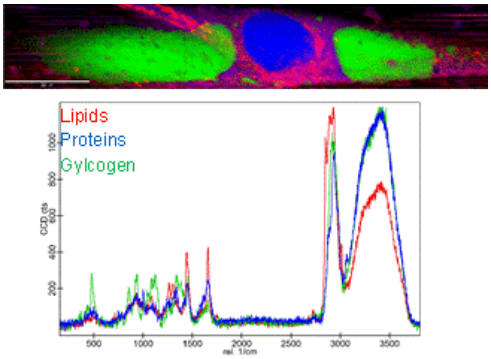
Cooperation

Roche Diagnostics GmbH Penzberg

Raman Imaging of Myoblasts

Raman Imaging is used as a non-invasive method for the label-free detection of lipids, proteins, and glycogen within Myoblasts. The project aims to gain further knowledge on Pompe disease on a single-cell level.

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 from e.g. muscle weakness, breathing difficulties, or wheelchair dependency. The current treatment (an enzyme replacement therapy) is limited regarding clinical efficacy.[1,2,3]



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.

Analytical Approach In this project, Myoblasts, as a precursor form of muscle cells, are studied. Non-fixated primary muscle cell cultures are placed in a closed measuring chamber. The sample is measured by a Raman system using a 532 nm excitation laser and a 63× oil immersion objective. After pre-processing of the data, the regions of high and low glycogen content within cells are differentiated by the skeletal modes of carbohydrates.

Results Different cell lines of patients diagnosed with Pompe disease as well as control cell lines were measured to study and compare the accumulation of glycogen in single cells. False color images were created out of the collected data. Through these, it is possible to display the lateral distribution of a pre-defined number of main component spectra in a given Raman image. They allow differentiating between lipids, proteins, and glycogen as main components within single cells. Measurements show a clear difference in the amount of glycogen between cells affected by Pompe disease and control cell lines. Primary cells of patients diagnosed with Pompe disease show a highly increased amount of glycogen. The glycogen accumulations are mostly distributed in the cytoplasm, thereby surrounding lysosomes and nuclei. On the contrary, control cell lines show only low or no glycogen contents within cells. The results will be compared to classical biochemical assays in the next step.

Eva Krois

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Funding

IWC

Cooperation

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

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Poster Presentations

Auernhammer, Andreas.; Hu,, C.D., Seidel, M., Multiparametersensor-basiertes intelligentes Frühwarnsystem für das Algenmonitoring im Oberflächenwasser. *Dresdner Sensor Symposium*, 05.-07.12.2022, Dresden, Deutschland.

Beer, I.; Brunschweiger, S.; Glas, K.; Elsner, M.; Ivleva, N.P.; Characterisation of anodic biofilms from microbial fuel cells based on imaging techniques*. Biofilms10, Ecology meets Technology*, 09-11.05.2022, Leipzig, Germany.

Beer, I.; Brunschweiger, S.; Glas, K.; Elsner, M.; Ivleva, N.P.; Characterization of Biofilms from Microbial Fuel Cells with Raman- and Scanning Electron Microscopy-based Techniques. *SETAC Europe 32nd Annual Meeting*, 15.-19.05.2022, Copenhagen, Denmark.

Beer, I.; Brunschweiger, S.; Glas, K.; Elsner, M.; Ivleva, N.P.; Charakterisierung von Biofilmen aus mikrobiellen Brennstoffzellen mittels Raman-Mikrospektroskopie. *Wasser 2022*, 23.-25.05.2022 (online).

Beer, I.; Brunschweiger, S.; Glas, K.; Elsner, M.; Ivleva, N.P.; Imaging Techniques for Chemical and Morphological Characterization of Biofilms. *Analytica Conference*, 21.-24.06.2022, Munich, Germany.

Canavan, A., Elsner, M., Position-Specific Isotope Analysis using 13C-Labels on Sulfamethoxazole. *Analytica Conference 2022*, 21.-24.06.2022, Munich.

Canavan, A., Elsner, M., Position-Specific Isotope Analysis using 13C-Labels on Sulfamethoxazole. *ISI Isotopes*, 29.05.-03.06.2022, Zürich.

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., Limitations and Microbial Regulation of Pollutant Biodegradation at Low Concentrations. *Gordon Research Conference on Environmental Sciences: Water*, 19.-24.06.2022, Holderness, NH, USA.

Glöckler, D., Wabnitz, C., Harir, M., Schmitt-Kopplin, P., Elsner, M., Bakkour, R., Cyclodextrin-Polymere als selektives Festphasenmaterial für sensitive substanzspezifische Kohlenstoffisotopenanalytik von Mikroschadstoffen. *Wasser 2022*, 23. - 25.05.2022, Virtual Conference.

Glöckler, D., Harir, M., Schmitt-Kopplin, P., Elsner, M., Bakkour, R., Selective Extraction by Cyclodextrin Polymers: New Perspectives for Compound-specific Isotope Analysis of Micropollutants. *Gordon Research Conference on Environmental Sciences: Water*, 19. 24.06.2022, Holderness, NH, USA.

Glöckler, D., Harir, M., Schmitt-Kopplin, P., Elsner, M., Bakkour, R., Universal vs. Selective Sorbents for: Targeted Isotope Analysis of Aquatic Contaminants. *ISI Isotopes*, 29.05.-03.06.2022, Zürich.

Heining; L.; Seidel, M.; Microarray platform for sero- and subtyping of *Legionella pneumophila* in aerosols. *Analytica Conference*, 21.-24.06.2022, Munich, Germany.

Heining; L.; Seidel, M.; Entwicklung von Sammel- und Analysestrategien für Legionella pneumophila in Aerosolen aus kontaminiertem Wasser in Verdunstungskühlanlagen. *Wasser 2022*, 23.-25.05.2022 (online).

Huber, M.; Beer, I.; Caputo, F.; Parot, J.; Sogne, V.; Meier, F.; Elsner, M.; Ivleva, N. P.; Towards the analysis of real samples using online-coupled field-flow fractionation-

Raman microspectroscopy: importance of suitable reference materials. *SETAC Europe 32nd Annual Meeting*, 15.-19.05.2022, Copenhagen, Denmark.

Huber, M.; Beer, I.; Sogne, V.; Meier, F.; Elsner, M.; Ivleva, N. P.; Online coupling of field-flow fractionation and Raman microspectroscopy: Towards the analysis of environmental samples. *Wasser 2022*, 23.-25.05.2022 (online).

Huber, M.; Beer, I.; Caputo, F.; Parot, J.; Sogne, V.; Meier, F.; Elsner, M.; Ivleva, N. P.; Further development of field-flow fractionation-Raman coupling: importance of suitable reference materials. *Analytica Conference*, 21.-24.06.2022, Munich, Germany.

Huber, M.; Zada, L.; Ariese, F.; Ivleva, N. P., Online-Coupled FFF-Raman Microspectroscopy: Taking advantage of faster acquisition times enabled by stimulated Raman scattering. *22nd International Symposium on Field- and Flow-Based Separations*, 11.-14.09.2022, Riverside, USA.

Jacob, O.; Ramírez-Piñeiro, A.; Elsner, M.; Ivleva, N. P.; Reliable object detection as a prerequisite for a sound analysis of small microplastic particles. *Wasser 2022*, 23.-25.05.2022 (online).

Jacob, O.; Ramírez-Piñeiro, A.; Elsner, M.; Ivleva, N. P.; Advanced image recognition as requirement for a valid analysis of very small (1—10 µm) microplastic particles. *SETAC Europe 32nd Annual Meeting*, 15.-19.05.2022, Copenhagen, Denmark.

Jacob, O.; Ramírez-Piñeiro, A.; Elsner, M.; Ivleva, N. P.; Methods of image processing for the analysis of microplastic particles down to 1 µm. *Analytica Conference*, 21.-24.06.2022, Munich, Germany.

Lanzinger, M. ; Huber, D.; Kaufmann St.; Schuster M.; Ivleva, N. P., Application of quantitative Laser-Induced Breakdown Spectroscopy in Technical Cleanliness. *Analytica Conference*, 21.-23.06.2022, Munich, Germany.

Lihong, C., Elsner, M., Etienne, D., Metabolic Mechanism of Sulfonamide Cleavage: A Combined Computational and Experimental Study on Sulfamethoxazole. *Analytica Conference*, 21.-24.06.2022, Munich.

Neumair, J.; Seidel, M.; Flow-based screening assay for the investigation of affinity binders for bacteria. *Analytica Conference*, 21.-24.06.2022, Munich, Germany.

Müller, K.; Elsner, M.; Ivleva, N.P.; Exploring the potential of Raman microspectroscopy for the analysis of microbial degradation of microplastics. *SETAC Europe 32nd Annual Meeting*, 15.-19.05.2022, Copenhagen, Denmark.

Müller, K.; Weng, J.; Elsner, M.; Ivleva, N.P.; Potential of stable isotope Raman microspectroscopy for the analysis of biodegradation of microplastics. *Wasser 2022*, 23.-25.05.2022 (online). **Poster Prize 3rd Place.**

Müller, K.; Weng, J.; Elsner, M. Ivleva, N.P.; Applicability of a reverse stable isotope labeling approach to show biodegradation of microplastics on a single-cell level. *10th International Symposium on Isotopomers and 12th Isotopes Conference,* 30.05.-02.06.2022, Dübendorf, Switzerland.

Müller, K.; Weng, J.; Elsner, M.; Ivleva, N.P.; Potential of a direct and reverse D- and ^{13}C-labelling approach for the analysis of microbial degradation of microplastics. *Analytica Conference*, 21.-24.06.2022, Munich, Germany.

Müller, K.; Elsner, M.; Ivleva, N.P.; Applicability of stable isotope Raman microspectroscopy for the analysis of biodegradation of microplastics. *International symposium on Managing*

land and Water for Climate-smart Agriculture, 25.-29.07.2022, Vienna, Austria. **Poster Prize 1st Place.**

Schwaiger, G, Seidel, M. Quantification of Legionella spp. by a heterogeneous isothermal nucleic acid amplication test. *Analytica Conference*, 21.-23.06.2022, München, Deutschland.

Schwaiger, G, Seidel, M. Etablierung einer standardisierten Gesamtmethode zur molekularbiologischen Quantifizierung von Legionellen in warmwasserführenden Anlagen, *Wasser 2022*, 23.-25.05.2022 (online).

Tafa, A., Elsner, M., Bakkour. R., Suitability of passive sampling for compound-specific isotope analysis of micropollutants in aquatic environments. *Analytica Conference*, 21.-24.06.2022, Munich.

Tafa, A., Elsner, M., Bakkour. R., Suitability of passive sampling for compound-specific isotope analysis of micropollutants in aquatic environments. *ISI Isotopes*, 29.05.-03.06.2022, Zürich.

Wabnitz, C., Canavan, A., Wei, C., Toprakcioglu, Z., Elsner, M., Bakkour, R., Online monitoring of natural organic matter using dry mass sensing for optimizing CSIA sample preparation. *Analytica Conference*, 21.-24.06.2022, Munich.

Wabnitz, C., Canavan, A., Wei, C., Toprakcioglu, Z., Elsner, M., Bakkour, R., Coupling a quartz crystal microbalance with liquid chromatography for online NOM monitoring. *ISI Isotopes*, 29.05.-03.06.2022, Zürich.

Invited Lectures

Ivleva, N. P., Applicability of Raman Microspectroscopy for Environmental Analysis. *University of Ulm*, *GDCh Lectures*, 15.12.2022, Ulm, Germany

Ivleva, N. P., Raman Microspectroscopy for Environmental Analysis. *University of Innsbruck*, *CMBI Lecture Series*, 14.11.2022, Innsbruck, Austria

Ivleva, N. P., Hyphenation of Field-Flow Fractionation and Raman Microspectroscopy for Size-resolved Analysis of Nanoplastics (Keynote Lecture). *22nd International Symposium on Field- and Flow-Based Separations*, 11-14.09.2022, Riverside, CA, USA

Ivleva, N. P., Chemical Analysis of Nanoplastics: Challenges, Advanced Methods and Perspectives. *Analytica Conference 2022*, 21.-23.06.2022, Munich, Germany

Ivleva, N. P., Bunsen-Kirchhoff Award Lecture: Raman Microspectroscopy for Environmental Analysis. *Analytica Conference 2022*, 21.-23.06.2022, Munich, Germany

Seidel, M. Analytics and sensor technology in urban water systems. *Seminarreihe am IWAS der Universität Stuttgart*, 4.7.2022, Stuttgart, Deutschland.

Seidel, M. Molekularbiologische Methoden zum schnellen Nachweis von Pathogenen im Wasserkreislauf. *5. Mühlheimer Wasseranalytisches Seminar*, 14.9.-15.9.2022, Mühlheim, Deutschland.

Seidel, M. Schnelle Nachweismethoden für Pathogene und antibiotikaresistente Bakterien im Kontext Abwasser, *10. Kitzbüheler Wassersymposium*, 21.-22.9.22, Kitzbühel, Österreich.

Colloquium for Analytical Chemistry and Water Chemistry Guest Lecture

Prof. Jonas Bergquist, Uppsala University, Sweden, Analytical Chemistry and Neurochemistry at the Department of Chemistry - BMC: Deep diving into the complex nature of (brain) water in search of markers of disturbance - technologies that connect limnology to neurology (06.07.2022).

Prof. Dr. Andrea Erhardt, University of Kentucky, Kentucky Stable Isotope Geochemistry Laboratory (KSIGL): Using sulfate and methane isotopes to track the causes and extent of elevated methane concentrations in the groundwater of Eastern Kentucky (14.11.2022).

Scientific Committees & Memberships

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

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

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

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

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

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

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

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

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

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

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

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

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

Exhibition

Exhibitor with the topic “Expert Laboratory Legionella” (Philipp Streich) and “Digital early warning system for algae blooms” (Andreas Auernhammer) at the booth of Bayern Innovative at IFAT 2022, Munich.

Theses

PhD Theses

MSc Chem. Christian Schwaferts: Characterization and Identification of Micro- and Nanoplastic by Raman Microspectroscopy, Scanning Electron Microscopy, Field-Flow Fractionation and Chemometrics.

M.Sc. Theses

BSc Wei Chen: The Application of Online Matrix Monitoring During HPLC Purification Using Dry Mass Sensing on a Quartz Crystal Microbalance.

BSc Jonas Flechtner: Authentication of Monovarietal Extra Virgin Olive Oils by Fluorescence, UV-VIS, FTIR, and Raman Spectroscopy with Chemometric Methods.

BSc Charlotte Heinritz: Detection of Biotin by Specific Streptavidin-Biotin Interaction Based on Luminescent Lanthanide-Nanoparticles.

BSc Marie Kröger: Establishment of a Flow-Based CL-SMIA for the Quantification of Protein Biomarkers from Nasal Secretions in Comparison with Sandwich ELISA.

BSc Zoe Liestmann: Development of an Electrochemiluminescence Immunoassay for Selected Pathogens in Wastewater.

BSc Anton Podolhov: Carbon Isotope Analysis of Glyphosate and AMPA after Molecularly-Imprinted Solid-Phase Extraction.

BSc Alexander Thomas: Production of Metal Alloy Reference Particles and Analysis of Their Size, Morphology and Elemental Composition.

B.Sc. Theses

Fabian Gallo: Influence of Free Lipopolysaccharides of Legionella Pneumophila on a Chemiluminescence Sandwich Microarray Imunoassay (CL-SMIA).

Sonja Rahm: Assessment of a Quantification Method for Glyphosate and AMPA on Gas Chromatography-Mass Spectrometry Using Derisatization: Limitations and Implications for Implementation.

Katharina Speer: Analytical and Experimental Comparison of a Silicon Dioxide Chromatography Process against Established State of the Art Procedures.

Carl Witthöft: Investigating biological degradation of transformation products after oxidative treatment of benzoic acid by ozone/hydrogen peroxide and UV/peroxide.

Teaching

Winter Semester 2020/2021

Analytische Chemie I, Instrumentelle Analytik

240242322 Geo-Umwelt LMU (BSc Geo.) M. Elsner

Chemische Analytik II - Organische Spurenanalytik für Geowissenschaftler

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

Wasserchemie 1

820005191 Geo-Umwelt LMU (BSc Geo.) M. Elsner

Angewandte Wasserchemie

0000005206 Chemistry (MSc 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 (Practica)

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) R. Bakour, C. Haisch

Hydrochemisches Praktikum für Geologen

0000003397 Hydrology (MSc Geo.) R. Bakour, C. Haisch

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 2021

Automatisierung und Visualisierung von Laborprozessen und Daten

0000004577 Chemistry (MSc Chem.) M. Elsner, N. P. Ivleva, E. v. d. Esch

Biochemische Analytik

0000001651 Weihenstephan (BSc 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 (BSc Biochem.) M. Seidel, N.P. Ivleva

Case Studies in Analytical and Environmental Chemistry

0000002532 Chemistry (MSc 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 (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

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

Post Docs

Dr. Aileen Melsbach
Dr. Florian Opperer

Technical & Administrative Staff

Felix Antritter
Christine Beese
Christine Benning
Roland Hoppe
Susanne Mahler
Marco Matt, Dipl.-Ing
Cornelia Popp
Sonja Rottler, Dipl.-Ing. (FH)
Sebastian Wiesemann

PhD Students

MSc Chem. Habib Al-Ghoul
MSc Phys. Emilio Ambra
MSc Chem. Andreas Auernhammer
MSc Leb. Chem. Irina Beer
MSc Chem. Aoife Canavan
MSc Environ. Sci. Lihong Chai
MSc Geo. David Glöckler
MSc Chem. Lena Heining
MSc Chem. Lucas Hirschberger
MSc Chem. Maximilian Huber
MSc Chem. Oliver Jacob
MSc Chem. Julia Klüpfel
MSc Chem. Eva Krois
MSc Chem.-Ing. Yiao Liang
MSc Chem. Felix Ludwig
MSc Chem. Kevin Maier
Dipl.-Biochem. Oleksii Morgaienko
MSc Chem. Kara Müller
MSc Chem. Julia Neumair
MSc Chem. Sandra Paßreiter
MSc Chem. Leonhard Prechtl
MSc Chem. Christian Schwaferts
MSc Biochem. Gerhard Schwaiger
MSc Chem. Philipp Streich
MSc Chem. Armela Tafa
MSc Chem. Christopher Wabnitz

External PhD Students

MSc Chem. Franziska Adler (Stadtwerke München)
MSc Chem. Jessica Beyerl (LMU-Tropeninstitut)
MSc Chem. Leopold Daum (TUM, Heinz-Nixdorf-Lehrstuhl für Biomedizinische Elektronik)
MSc Leb. Chem. Anja Dollinger
MSc Chem. Melina Grasmeier (Klinikum rechts der Isar)

MSc Chem. Amelie Hohensee (LMU-Tropeninstitut)
MSc Chem. Maria Lanzinger (BMW)
MSc Chem.-Ing. Helge Oesinghaus
MSc Chem. Alexander Thomas
MSc Chem. Markus Weber (Plasmion GmbH, Augsburg)

Master Students

BSc Chem. Marcel Klotz
BSc Chem. Wei Chen
BSc BWL-Chem. Jonas Flechtner
BSc Nutrition/Biomed. Marie Kröger
BSc Chem. Anton Podolhov

External Master Students

BSc Biotechn. Claudia Bari
BSc Chem. Jannis Gehrlein
BSc Chem. Charlotte Heinritz
BSc Chem. Zoe Liestmann
BSc Chem. Annachiara Morganti
BSc Chem. Alexander Thomas

Bachelor Students

Fabian Gallo
Sonja Rahm
Katharina Speer
Carl Witthöft

Guests

Dr. Jamila Boudaden (Fraunhofer Institut EMFT München)
Dr. Dusan Hemzal (Masaryk University, Brünn)
Prof. Dr. Andrea Erhardt (University of Kentucky-USA)
MSc med. Corinna Winkler (Klinikum rechts der Isar)
Dr. med. Silvia Würstle (Klinikum rechts der Isar)

Student Assistants

Wei Chen
Nico Chrisam
Tobias Forner
Charlotte Heinritz
Marie Kröger
Nina Weidlein

Equipment

Aerosol Research

1 Aerosol chamber (1 m^3)

1 Aerosol flow tube (10 L)

1 Ozone analyzer (UV absorption)

1 NO/NO_2 analyzer (Chemiluminescence)

1 Aerodynamic particle sizers (0.5–25 µm)

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

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

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

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

1 High-volume filter sampler (PM 2.5)

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

2 Diffusion batteries (5–300 nm)

5 Condensation nucleus counters

3 Electrostatic classifiers (10–1000 nm)

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

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

1 Floating bed aerosol generator (powder dispersion)

1 Rotating brush aerosol generator (powder dispersion)

1 Tube furnace

1 AVL Micro Soot Sensor with dilution unit

2 FT/IR gas analyzers

Microarray Technology

1 Chemiluminescence Microarray Reader, MCR 3, GWK Präzisionstechnik GmbH

3 Chemiluminescence Microarray Reader, MCR R, GWK Präzisionstechnik GmbH

1 Ink-Jet Microdispenser, SciFlexarrayer S1, Scienion

2 Contact Microarrayer, BioOdyssee Caligrapher, BioRad

2 Cutting Plotter, Graphtec CE6000–40

Microbiology

1 Flow Cytometer, CyFlow Cube 6, Sysmex Partec GmbH

1 Bead Beater Homogenizer, MP Biomedicals

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

2 Clean Benches

1 Bioaerosol Chamber

2 Microbiological Incubator, Binder

1 Temperature Controlled Shaking Incubator

1 Autoclave, Certoclav

1 Autoclave, SHP Steriltechnik

1 Cyclone Impinger Coriolis µ, Bertin

1 Munich Microorganism Concentrator, MMC 3

1 Monolithic Affinity Filtration Unit

Further equipment for bioanalytics

1 Cooled Centrifuge, Universal 320R, Hettich

1 Climatic Chamber, Binder

4 Drying Cabinets, Memmert

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

1 Photometric ELISA Reader, Biotek

1 96-channel Washer, Biotek

1 Turbidometer, WTW GmbH

1 Nanophotometer, Implen GmbH

1 -80 °C Freezer

Standard Lab Equipment

1 Lyophilizer, Alpha 1-4 LSC, Christ

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

1 Centrifuge, Eppendorf 5804 R

2 Fluorescence Spectrometer LS 50, Perkin Elmer

1 UV-Vis Spectrometer, Perkin Elmer

Chromatography, Mass Spectrometry and Particle Separation

2 GC-IRMS (Isotope Ratio Mass Spectrometer) Instruments

1 LC-IRMS

1 GC-MS

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

1 MS, Thermo Fisher LTQ

2 Concentrators for dynamic headspace analysis

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

1 Ion Chromatograph, Dionex

1 LC system, ECONO

1 Preparative HPLC

Elemental Analysis

1 Flame-Photometer, BWB Technologies

1 ICP-MS, Perkin -Elmer Nexion 350D

Laser

2 He/Ne-laser

5 Nd-YAG -laser, pulsed

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

3 Nd-YAG-laser, cw

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

Several Quantum Cascade Laser systems

3 Optical parameter oscillator (410 nm–2.1 µm)

Optoelectronics/Spectrometer

3 Echelle spectrometer

1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700

1 Fluorescence spectrometer, Perkin Elmer LS-50

1 Fluorescence spectrometer, Shimadzu RF 6000

1 UV/VIS spectrometer, analytic jena Specord 250 plus

1 UV/VIS spectrometer, analytic jena Spekol 1500

4 Digital storage oscilloscopes (400 MHz, 500 MHz)

1 Wavemeter

Microscopy

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

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

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

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

1 SEM/EDX system, Zeiss Gemini

Sum Parameters

2 Coulostat for C quantification, Coulomat 702

1 DOC analyser, UNOR 6 N

1 TOC analyser, Shimadzu TOC-L