Institute of Hydrochemistry
Department of Chemistry
Technical University of Munich

Annual Report 2019

Institute of Hydrochemistry

Chair of Analytical Chemistry and Water Chemistry

Technical University Munich
Chair of Analytical Chemistry and Water Chemistry
Marchioninistraße 17
81377 München
Tel: +49 89 2180-78232
Fax: +49 89 2180-78255
www.hydrochemistry.tum.de

Members of the Institute of Water Chemistry (IWC) in December 2019

Contents

Dear friends and colleagues,

In days when we are minimizing physical contact, giving remote classes, and avoiding travels, it seems almost incredible that just about a year ago we were hosting the international ISOTOPES conference. In the beautiful scenery of Raitenhaslach the conference brought together leading scientists of analytical, theoretical and pure chemistry to discuss developments in enzymology, biogeochemistry and environmental sciences. The breadth of topics highlights the central role that isotope effects / isotope distributions play in almost all fields of natural and life science. At our institute we are pursuing this approach to improve instrumental analysis, to trace metabolites in organisms and to follow pollutants in the water cycle. A big THANK YOU to the organization team headed by Cornelia Popp, Christine Beese and Dr. Rani Bakkour from our IWC!

As another highlight from the institute, Dr. Natalia Ivleva was awarded the venia legendi (Habilitation) in appreciation of her work to advance Raman microspectroscopy (RM) for environmental analysis. Through her focus on biofilms, micro- and nanoplastic particles, and by including stable isotope labelling, her group is now setting out to quantify nanoplastics, and to target carbon flow and cell interactions in microbial communities down to the µm-scale or single-cell level. Congratulations, Natascha!

In parallel, the Haisch group has used Raman microscopy to fight the single most deadly infectious disease in the world - tuberculosis. In close cooperation with colleagues from LMU, analytical approaches were developed to identify activity and dormancy in Mycobacteria. In parallel, analytical tools were advanced to support cultivation and exploitation of algae biomass in cooperation with Prof. Thomas Brück from the Werner Siemens-Lehrstuhl for Synthetic Biotechnology. Finally, a more fundamental study of photoacoustics observed a new effect on colloidal nanoparticles which might be used in biosensing. Stay tuned - more is to come!

In the Bioanalytics group analytical development aimed at combating yet another deadly illness - the water-bourne legionnaires' disease. Within the BMBF project LegioTyper, the Seidel group developed microarray-based analysis to distinguish for the first time Legionella pneumophila serogroups in water of evaporative cooling systems and of urine.

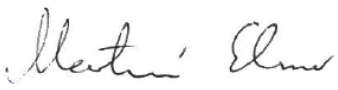
This is prime information to take decisions in outbreak management. In parallel, by transferring the manufacturing process from glass to plastic chips, we can now produce microarray chips in a much quicker and more economic way which offers entirely new opportunities for future projects. More will be told in next year's report!

Why are organic micropollutants (pesticides, pharmaceuticals) so persistent? – In an ERC Consolidator Grant project in the Isotope Group we discovered the relevance of mass transfer at low pollutant levels. Bioavailability limitation appears to be the trigger for physiological adaptation that puts a limit to biodegradation when concentrations become low. This "persistence by dilution" offers a new perspective on the recalcitrance of many pharmaceuticals and pesticides in the environment. Importantly, this understanding provides a much-needed starting point to search for innovative bioremediation approaches to target low level contaminations.

Organization-wise the year 2019 has seen the first stage of our move to Garching. As an advance party, the isotope group has moved out of the Helmholtz Zentrum and translocated into the chemistry building at Lichtenbergstr. 4. Since the construction work is still not fully finished, it will take some more time until the next stage can go on. In the meantime, as IWC we are having our home at two physical locations: the two final stops of the subway U6!

Finally, I cannot conclude this Editorial without thanking those who have made these results possible in challenging times: our Ph.D. students, technicians, secretaries, Postdocs and guest scientists. A big Thanks to all members of the institute for their work and dedication! And thank you to you - our friends - for your continued support!

Kind regards,

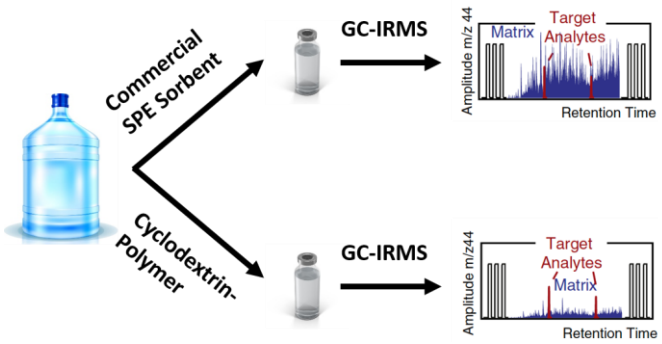


Martin Elsner

Selective Extraction of Pesticides from Surface Water for Carbon Isotope Analysis using Crosslinked Cyclodextrin Polymers

Application of compound-specific isotope analysis to field studies is limited due to low environmental concentrations of micropollutants. Crosslinked cyclodextrin polymers can contribute to significant improvements of sample preparation.

State of the Art Compound-specific isotope analysis (CSIA) has been demonstrated to be highly suitable for evaluating sources and transformation processes of micropollutants in laboratory experiments [1]. However, it remains a major challenge to transfer the method to the field-scale due to low environmental occurrence of micropollutants (sub-µg/L range). To this end, extraction of micropollutants from large volumes (>5 L) becomes inevitable to meet the low sensitivity of isotope-ratio mass spectrometry. Commercial sorbents employed for solid phase extraction (SPE) may process large volumes but lack selectivity to extract micropollutants without co-enrichment of concurrent dissolved organic matter (DOC).



Schematic illustration of the impact of selective extraction of target analytes with cyclodextrin polymers on carbon isotope analysis compared to commercial SPE sorbents.

Analytical Approach Recently, crosslinked cyclodextrin polymers (CyD-P) have been synthesized with high surface area (263 m^2/g) and fast kinetics [2]. In this work, we explore the feasibility of employing tailor-made CyD-Ps for selective extraction of pesticides from surface water for carbon isotope analysis in comparison to HLB-based commercial sorbents. To this end, CyD-Ps with different pocket sizes, namely α-, β- and γ-CyD-P were synthesized and used as SPE sorbents to extract a selection of 11 pesticides from surface water.

Results β-CyD-P showed highest mean recoveries (68.5%) followed by γ-CyD-P (67.7) and α-CyD-P (64.6%) compared to OASIS HLB, LiChrolut© EN and Supel™-Select HLB with 72.9%, 71.5% and 63.8%, respectively. DOC-to-analyte ratios illustrate that sorption onto α- and β-CyD-P is more selective than onto HLB-based sorbents (by factor 2-4 and 1.5, respectively). However, sorption of NOM of different molecular sizes (<1, 1-3, 3-10, >10 kDa) on CyD-Ps did not show selective preference for smaller fractions. Our findings illustrate that the CyD-Ps are promising sorbents for selective extraction of pesticides from surface water contributing thereby to significant improvements of sample preparation for carbon analysis of micropollutants.

David Glöckler, Christopher Wabnitz

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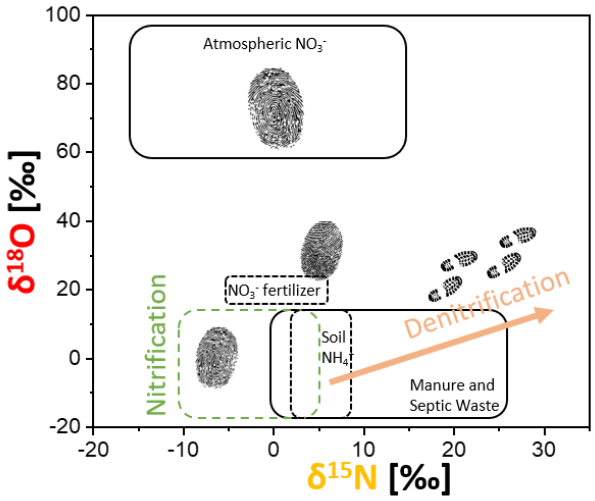
Funding
DFG – CRC 1253: CAMPOS

Cooperation
-

Development of Rapid and Sensitive Isotope Analysis of $\delta^{15}N$ and $\delta^{18}O$ to Decipher Sources and Turnover of Nitrate

Understanding processes governing natural attenuation of nitrate is of pivotal importance. A novel method for isotope analysis for nitrate enables process studies in high spatial and temporal resolution.



Typical values of $\delta^{15}N$ and $\delta^{18}O$ of nitrate derived or nitrified from various N sources. The arrow indicates typical expected slopes for data resulting from denitrification of nitrate.

State of the Art Nitrate is a notorious groundwater contaminant worldwide [1]. Elevated nitrate loads in rivers lead to eutrophication which, in turn, adversely affects the ecology of surface and marine waters. Consequently, determining nitrate sources in natural water systems and understanding processes effectuating its turnover and elimination are of pivotal importance. However, to decipher sources and turnover of nitrate on the landscape scale, concentration measurements alone cannot provide conclusive information since compound concentrations may also change due to dilution and sorption.

Analytical Approach Isotope ratios provide isotopic fingerprints of different sources and can give concentration-independent evidence of transformation since these ratios specifically change due to reactions of the compound (e.g. denitrification). However, time-consuming sample preparation of available analytical techniques for nitrate isotope analysis (e.g. microbial denitrifier method) still prevents isotope studies in high spatial and temporal resolution. Therefore, an available GC-IRMS method for rapid δ15N determination in nitrate by derivatization of benzene in acidic aqueous solution [2] was successfully established in our laboratory.

Results Calibration with international reference materials (USGS32, USGS34) and in-house working standards verified isotopic integrity throughout the derivatization process (slope of regression line approx. 1) enabling measurement and normalization of a wide range of $\delta^{15}N$ values (from -1.8±1.0‰ to +180.0±1.0‰). The method detection limit of 50 mg-NO_3^-/L will be further improved by pre-concentration of water samples. In order to apply dual element isotope analysis, the analytical protocol is modified to prevent oxygen isotope exchange with water, ensuring the integrity of $\delta^{18}O$ isotope values. The application of this method to field samples will contribute to identifying processes that control spatial and temporal patterns of nitrate reactivity.

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Dr. Marc Schwientek and Dr. Karsten Osenbrück – University of Tübingen

David Glöckler

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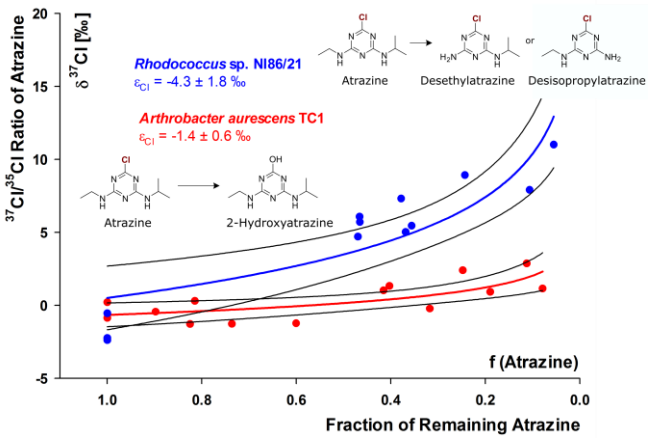
Compound-Specific Chlorine Isotope Fractionation in Biodegradation of Atrazine

This study determines for the first-time chlorine isotope effects during biodegradation of atrazine. Providing a better mechanistic understanding, this offers the basis to apply triple element (3D) isotope analysis in environmental assessments.

State of the Art Atrazine is a frequently detected groundwater contaminant. It can be microbially degraded by oxidative dealkylation or hydrolysis. In previous work[1-3], carbon and nitrogen isotope effects were found to reflect these different transformation pathways. However, chlorine isotope fractionation could be a particularly sensitive indicator of natural transformation since chlorine isotope effects are fully represented in the molecular average while carbon and nitrogen isotope effects are diluted by non-reacting atoms.



Chlorine isotope fractionation during microbial degradation of atrazine by *A. aurescens* TC1 (red) and *Rhodococcus* sp. NI86/21 (blue) and corresponding enrichment factors ε. (95 % confidence intervals are given as values and as black lines).

Analytical Approach In this study compound-specific isotope analysis was used to assess chlorine, carbon and nitrogen isotope effects during atrazine hydrolysis with *Arthrobacter aurescens* TC1 and oxidative dealkylation with *Rhodococcus* sp. NI86/21.

Results Carbon and nitrogen isotope fractionation was consistent with previous studies[1-3]. Furthermore, dual element isotope slopes of the different elements provided reliable indicators for the differentiation of the pathways. For hydrolysis chlorine isotope fractionation was rather small (ε_{Cl} = -1.4 ± 0.6 ‰) despite the fact that the chlorine is cleaved off. This indicates that C-Cl bond cleavage is not the rate-determining step. For oxidative dealkylation chlorine isotope fractionation was more pronounced (ε_{Cl} = -4.3 ± 1.8 ‰) even though the C-Cl bond is not cleaved. This indicates that non-covalent interactions between the enzyme complex and the chlorine cause significant chlorine isotope fractionation. This demonstrates the importance of constraining expected isotope effects of new elements in controlled laboratory experiments before using the approach in the field.

Christina Lihl, Benjamin Heckel

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Funding

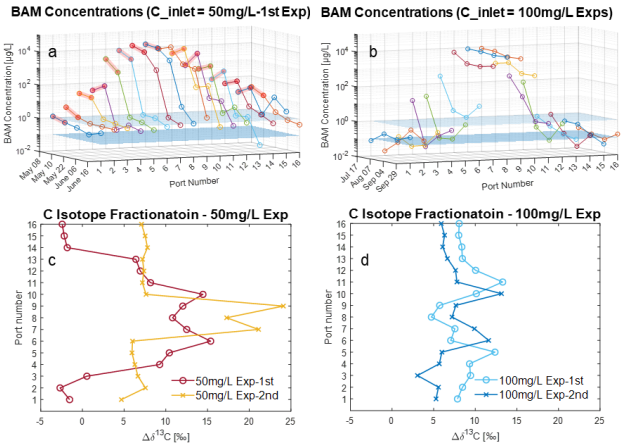
Swiss National Science Foundation, National Science Center in Poland

Cooperation

Ponsin V., Torrentó C., Hunkeler D., Grzybkowska A., Dybala-Defratyka A.

Exploring Mass Transfer Limitation in Organic Micropollutant Biodegradation - Combined Insight from Compound-Specific Isotope Analysis (CSIA) and Reactive Transport Modeling

We conducted quasi two-dimensional sediment tank experiments to investigate the bottleneck of biodegradation of 2,6 dichlorobenzamide in low concentration ranges by using compound-specific isotope analysis.



(a) 50mg/L and (b) 100 mg/L inlet concentration conditions. Results of $\delta^{13}C$ in both (c) 50mg/L experiment and (d) 100 mg/L experiments showed a turn-over of isotope fractionation with increasing distance from the central port 8 and decreasing concentrations.

State of the Art Many organic micropollutants persist in groundwater at low concentrations even though they are in principle (bio)degradable. Slow mass-transfer between degrading microbes and bulk-solution has been hypothesized to determine pollutant uptake into microbial cells (bioavailability limitation), thus limiting the overall turnover [1]. Recently, CSIA has been applied as a promising tool to probe for the onset of such bioavailability limitations at low pollutant concentrations[2]. Whether bioavailability limitations inhibit micropollutant biodegradation in groundwater sediments, however, has not yet been verified by direct observation.

Analytical Approach We conducted quasi two-dimensional sediment tank experiments to investigate the biodegradation of 2,6- dichlorobenzamide (BAM) and the magnitude of associated compound-specific isotope fractionation across mixing-controlled concentration gradients. A solution of BAM containing ^{13}C and ^{15}N at natural isotopic abundance was injected in the middle of the tank (inoculated with *Aminobacter* MSH1). An oxygen-rich medium was injected above and below the BAM solution, generating a steady-state plume of BAM and two fringes facilitating mixing of electron donor (BAM) and acceptor (O_2).

Results Our results show that isotope fractionation was highest at fringe locations, where O_2 and BAM were well mixed. As the concentration of BAM dropped further, measured isotope fractionation decreased with increasing distance from the center. We hypothesize that the drop is not attributable to the absence of further biodegradation, but that it can be explained by rate-limiting mass transfer of BAM into cells as BAM concentrations decrease.

Fengchao Sun

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Cooperation

Prof Olaf Cirpka
Prof. Christian Griebler
Dr. Martin Thullner

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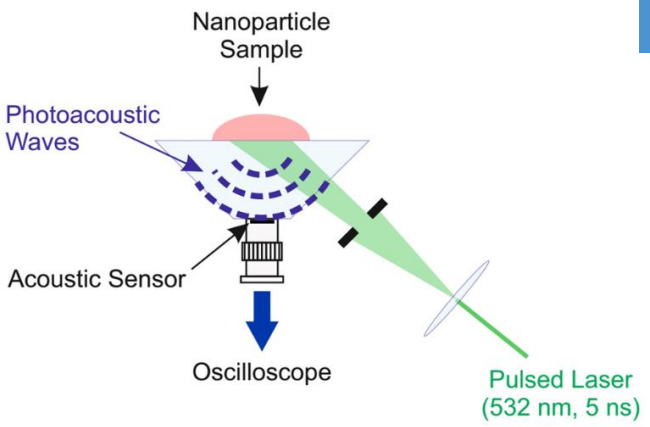
Photoacoustic heating of gold nanoparticles

Gold nanoparticles (GNPs) have been shown to offer many advantages in biomedical photoacoustic (PA) imaging, perhaps most notably as exogenous contrast agents. Although GNPs have been used in previous biomedical PA imaging studies, more in depth fundamental research can lead to new imaging methods.

State of the Art Biomedical photoacoustic (PA) imaging is an emerging noninvasive imaging modality that that combines spectroscopic contrast with high ultrasound resolution and penetration depth. The use of gold nanoparticles (GNPs) in PA imaging provides many advantages, such as improved contrast due to the high absorption coefficient of GNPs. While the use of GNPs in PA imaging is not new, little is known about the fundamental PA signal generation process from GNPs. Silica-coated GNPs are often used due to their increased stability, low toxicity, and improved functionalization possibilities.



Custom photoacoustic scanner for collecting signals from gold nanoparticle samples.

Analytical Approach We investigate experimentally the PA signal generated in different colloidal suspensions of GNPs using our in-house custom-built PA scanner. Our experimental results explore dependencies of the PA signal on particle shape, size, coating, and excitation fluence. We compare our experimental results to theoretical predictions from our own developed theoretical model.

Results Our theoretical model predicts that the presence of a silica coating should decrease the PA signal from a GNP. Our experimental results are consistent with this prediction and are important for understanding photoacoustic images from applications using silica-coated GNPs. We also discovered that the addition of a silica coating can quench the nonlinear signal generation from large diameter GNPs (>100 nm). This phenomena has potential to be exploited for biochemical sensing.

Genny Pang

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Funding

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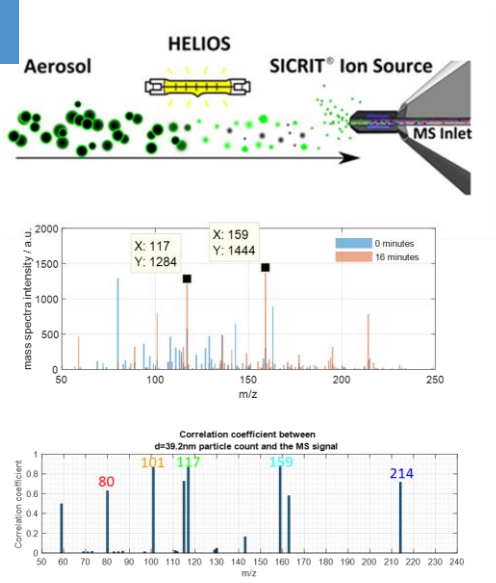
Cooperation

Institut für Physik Martin-Luther-Universität Halle-Wittenberg. Univ. Grenoble Alpes CNRS LIPhy

Down to Ten – Characterization of Combustion Engine Exhaust Particles in the Size Range from 10 to 23 nm

Nanoparticles emitted from combustion engines are considered a significant health issue. While current legislation limits number of particles larger than 23 nm emitted from vehicles, knowledge about even smaller particles is sparse.



Operation principle of our HELIOS/SICRIT/Mass Spectrometry system and example results from field measurements

State of the Art Current legislation on exhaust particle emission limits the emitted particulate solely on physical properties. However, in order to assess the impact of exhaust particles on potential health, air quality and climate, an understanding of their chemical nature is crucial. DownToTen seeks to develop reliable and robust methodologies to enhance the regulatory approach in the assessment of particle number emissions in the sub 23 nm region (down to at least 10 nm), focusing on state-of-the-art automotive powertrains with direct injection gasoline engines, but also diesel engines, under real-world operation conditions. One focus of the DownToTen project is the development of analytical methods for the detection and characterization of such particles.

Analytical Approach We apply the combination of a novel infrared-radiation-based evaporation system (HELIOS) with a new, highly efficient atmospheric ionization source (SICRIT) connected to a mass spectrometer in our in-house developed measurement system for online chemical aerosol characterization of exhaust gases. We validated our measurement system in the laboratory against standard reference aerosol instrumentation. Subsequently, our measurement system was used during a DownToTen measurement campaign at the Laboratory of Applied Thermodynamics, Aristotle University of Thessaloniki on a Volkswagen Up vehicle combined with reference measurements from an engine exhaust particle sizer spectrometer.

Results Our results of various laboratory-generated aerosols show excellent agreement with reference measurements with commercial aerosol mass spectrometers and other reference instrumentation measuring total organic mass of particulates. From our field measurements, correlation of mass spectra and particle size distribution identifies larger particles (~40 nm) as aromatic compounds (soot precursors) forming during the cycle, and smaller particles (<10 nm) as unburned fuel forming immediately after cycle start.

Genny Pang

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Cooperation

Aristotle University of Thessaloniki, AVL List GmbH, Ricardo UK Ltd, Tampere University of Technology, Graz University of Technology, Joint Research Center, Centro Ricerche FIAT

References

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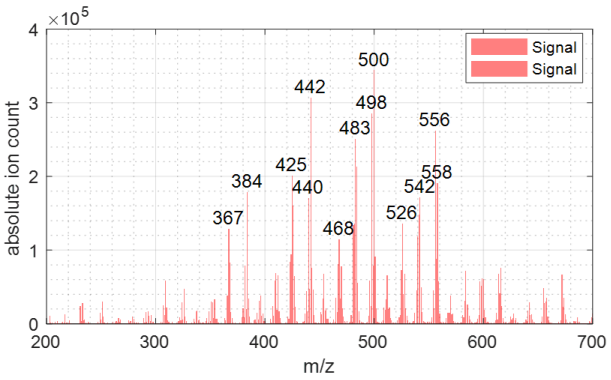
Sub-Zero-Emissions Diesel Engine

The much-debated gaseous and particulate emissions from combustion engines can be reduced significantly by the use of novel fuels. However, it has to be ensured that this approach does not result in the emission of other contaminants

State of the Art Particulate and NOx emissions are under critical discussion, banning of diesel-powered vehicles from cities is imminent. Fuels, which burn without the emission of soot, are an attractive alternative, since without the need for complex particle removing systems, the optimization of the whole engine and aftertreatment system towards low gaseous emissions is possible. One highly promising candidate for a soot-free alternative for Diesel fuels is Oxymethylenether (OME), which also has the potential of CO2 neutrality, as it can be produced completely from regenerative sources. We are aiming for a combustion engine that does not emit any contaminants based on the use of OME. This highly ambitious aim requires an extensive non-target screening for potential new contaminants.



Representative mass spectrum of the exhaust from a test motor operated with OME.

Analytical Approach To investigate the products of OME combustion, we apply our in-house developed aerosol characterization system based on a newly invented atmospheric ionization source (SICRIT) combined with a special infrared-based evaporation system (HELIOS) coupled with an ion-trap mass spectrometer. Initial laboratory experiments have investigated the mass spectra from different blends of pure OME and also OME burned on a catalytic burner. For future experiments, a heated flow reactor for investigating the products of reaction of OME on a diesel oxidation catalyst is in the process of being built for controlled tests in our laboratory. Field tests have used our HELIOS/SICRIT/Mass spectrometer system coupled with a particle counter system to analyze the exhaust gas from test engines at the TUM Chair of Internal Combustion Engines. Further tests are planned for a complete engine at MAN Truck & Bus.

Results The mass spectra measured with our HELIOS/SICRIT/Mass spectrometer system indicate that there are unidentified components with high molecular mass in the exhaust of the test motor operated with OME. A comparison of the data with analogous measurement under diesel operation are needed to determine whether the particle count is reduced and whether the same species are formed under OME operation.

Genny Pang

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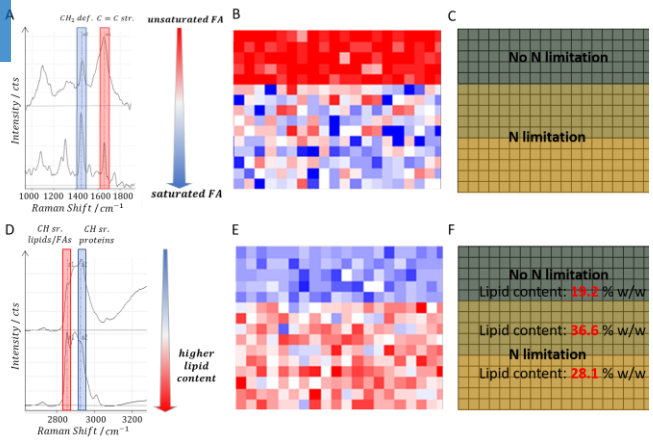
TUM Chair of Internal Combustion Engines, MAN Truck & Bus AG, Continental Emitec GmbH, ASG Analytik-Service-Gesellschaft mbH

Lipid monitoring in single algal cells for optimized biokerosene production

To determine the fittest cells and the most suitable parameters for optimal lipid production, a fast, non-destructive monitoring method was developed based on the information extracted from the spectral fingerprint of single cells.



(A, D) Raman bands used to determine relative content of saturated and unsaturated fatty acids as well as lipid content. (B, E) Image-based representation of lipid content (E) and unsaturated vs. saturated fatty acids (B). Each pixel corresponds to a Raman spectrum representing a single cell. (C, F) Description of data matrix structure shown in panels B, E. Algae cultivated under N repletion are colored in dark-green while algae cultivated under N depleted conditions are colored in lighter green tones. The result of reference analytics in panel F are in good agreement with the results of the Raman-based approach.

State of the Art For efficient biofuel production, the amount of lipids produced in single algal cells needs to be improved by process parameter optimization and/or by introducing mutations e.g. by exposure to neutron radiation. State-of-the-art analytics for the determination of total lipid content is based on calorimetric detection such as the sulfo-phospho vanillin assay. This assay, however, is limited to unsaturated lipids, requires ≈ 30 min of total analysis time, and is a destructive analysis method. (1)

Analytical Approach Single algal cells (Ø ≈ 1 µm) were investigated in microfluidic channels by means of Raman spectroscopy followed by a data evaluation step to determine relative amounts of saturated and unsaturated fatty acids as well as overall lipid content.

Results A Raman-based quality control step was introduced to pre-select the mutants that exhibit high lipid content on a single cell level for subsequent cultivation. First results based on off-line measurements indicate that the complex spectral fingerprint can be employed for differentiation between mutants with and without increased lipid production. Furthermore, the effect of different cultivation parameters on lipid content in wildtype cells was determined and verified by reference analytics. Building on these experiments, the first iteration of a flow cell design was realized that allows the investigation of single cells for Raman-based, real-time cell sorting such that the microorganisms are still viable and ready to be employed for highly efficient biofuel production.

Karin Wieland, Torben Schädler[1,2], David Bauer, Thomas Brück[2,3], Dirk Weuster-Botz[1,2], Christoph Haisch

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1 TUM, Institute of Biochemical Engineering, Garching, Germany

2 TUM-AlgaeTec Center, Taufkirchen, Germany

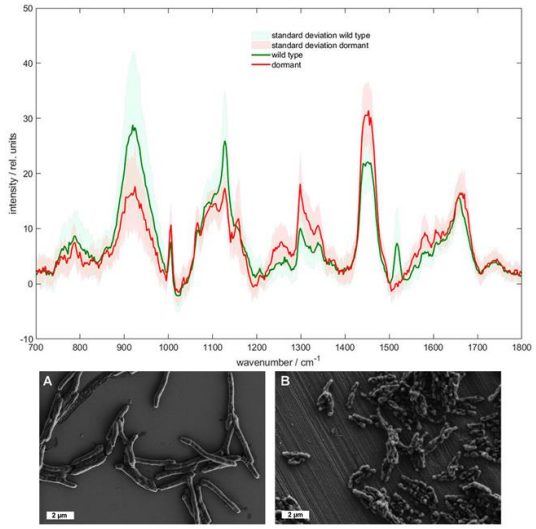
3 TUM, Werner Siemens-Chair of Synthetic Biotechnology, Garching, Germany

Application of Raman Spectroscopy for the Identification of the Dormant Growth State of *Mycobacterium Smegmatis*

Mycobacteria are known to reach a metabolic state called dormant or persistent, in which treatment is hampered due to lowered metabolic activity. Still analytical methods to identify this status need to be established. Single cell Raman spectroscopy in combination with MALDI-TOF-MS and chemometric approaches like cluster analysis are promising tools.

State of the Art Mycobacteria, known especially because of the pathogenic *M. tuberculosis* form an own family of bacteria. They have slow growth rates and are difficult to treat. One reason is their ability to reach a dormant called state. Here antibiotic treatment shows reduced effect and is therefore very time intensive. To understand and further study the behavior and treatment of Mycobacteria, it is of major interest to identify this special metabolic state. A typical method would be ATP measurements or cultivation based investigation of the growth rates. Since it is time intensive more efficient and instrument based methods are of great need.

Analytical Approach *Mycobacterium smegmatis*, which is non-pathogenic and with a doubling time of 3 hours easier to handle, is the typical laboratory test species of mycobacteria. It was brought to the dormant state according to a known protocol and the bacteria were then examined in comparison to the wild type via Raman spectroscopy, electron microscopy, MALDI-TOF-MS and ATP measurements.



Top: Averaged Raman spectra of wild type (green) and dormant (red) *M.smegmatis* Bottom: SEM images of wild type (A) and dormant (B) *M. smegmatis*.

Results While all other analytical methods afford time consuming sample preparation and are destructive, Raman spectroscopy allows for non-destructive single cell analysis. The Raman spectra (see figure) of the different cells were evaluated using cluster analysis. Thus the presence of subpopulations of the two investigated metabolic states could be shown. However, for a second line of evidence and a high throughput method MALDI-TOF-MS is the perfect counterpart and inevitable for an entire analysis.

David Bauer, Anna-Cathrine Neumann-Cip

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Cooperation
PD Dr. Wieser A. &
Dr. Neumann-Cip, A. C.,
Max von Pettenkofer
Institute, LMU, München

Fast Antibiotic Susceptibility Testing by Raman Spectroscopic Monitoring of Deuterium Uptake. Towards Clinical Applicability

Raman spectroscopy is the method of choice to monitor the metabolic deuterium uptake in microorganisms due to the development of a new Raman band.[1] It is the CD stretching vibration which evolves in the else empty region of the Raman spectrum. Thus, it allows for fast viability testing of cells and microorganisms. In this project, its applicability as fast antibiotic Susceptibility Test is critically studied and optimized towards a clinical application.

State of the Art Most established antibiotic susceptibility tests (AST) rely on optical detection of growth inhibition in presence of the drug. Hence, it takes several duplication cycles and a minimum time of 8 - 16 hours to obtain a reliable result by a disc diffusion based E-test, a gold standard for AST. Faster methods are urgently needed to tackle the spread of antibiotic resistant bacteria, one of the most threatening global health risks.

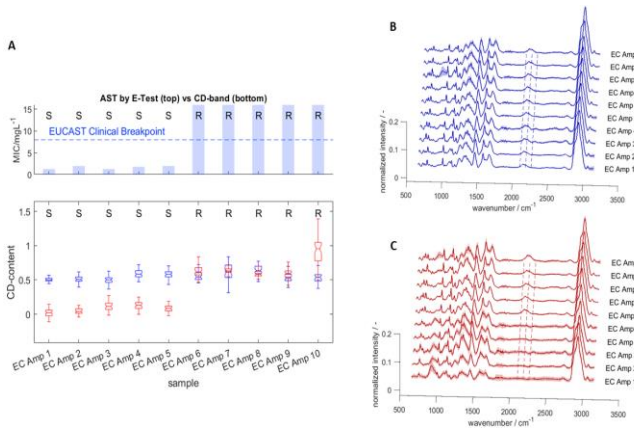

Figure A depicts the AST results of clinical isolates, tested with state of the art E-test (upper graph) and our developed Test (bottom graph). B and C show the regarding Raman spectra of the control culture and the antibiotic treated bacteria respectively.

Analytical Approach Raman spectra of bacteria represent an information of their overall molecular composition. In combination with the growth in heavy water (D_2O), the Raman spectra can be used to monitor metabolic activity. The incorporation of deuterium by the microorganisms leads to the appearance of the CD stretching vibration band (see Figures B and C). To allow for a reliable and fast measurement, a preparation of a highly concentrated bulk sample of bacteria was developed, allowing for the semi-automated recording of Raman-spectra of multiple bacteria at once.

Results After the development of a standard protocol for both gram-positive and Gram-negative bacteria, using four typical antibiotics with the reference bacteria *E. coli* ATCC 9637 and *E. faecalis* ATCC 29212, it was found that a preincubation with antibiotic but without addition of D_2O is critical to prevent the incorporation of deuterium. The protocol was then applied on 52 clinical isolates and successful classification of susceptible and resistant bacteria was obtained after down to 3.5 hours. The figure depicts a typical result of our test in comparison with the E-test and confirms the good agreement.

David Bauer

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DFG

Cooperation

Prof. Stief, Urologische Klinik der LMU München;

PD Dr. Wieser, Max von Pettenkofer-Institut, LMU

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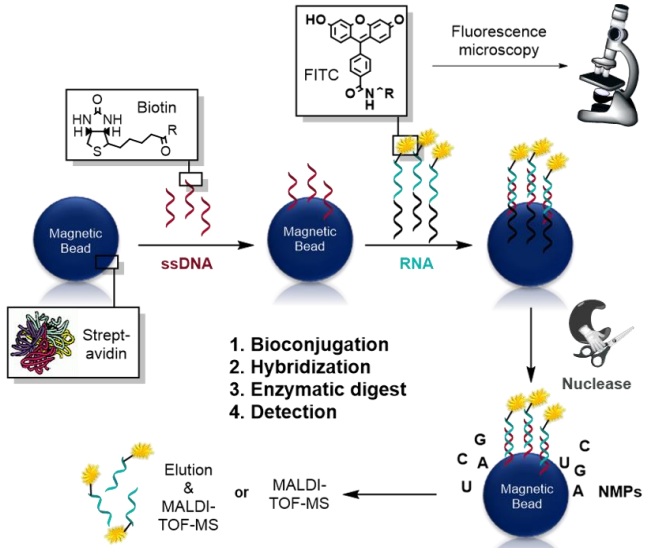
Detection of mycobacterial nucleic acids by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS)

A magnetic bead-based assay for the sequence-specific isolation of mycobacterial DNA and RNA is developed with a view to investigate gene expression.

State of the Art Nucleic acids are fundamental components of bacterial cells. DNA sequences code for certain protein determinants, mRNA mediates the expression. The detection of specific DNA sequences or their transcripts can provide deep insights into the regulation of different pathways. Therefore, strategies for the sequence-specific isolation of nucleic acids are indispensable[1].

Analytical Approach A biotinylated single-strand bait oligonucleotide, 16 to 20 bases in length, is coupled to a streptavidin coated magnetic bead in order to specifically isolate DNA or mRNA strands from mycobacterial cells by hybridization. Extensions are removed by a specific nuclease leaving behind the conjugated hybrid. MALDI-TOF MS analysis enables a fast detection of the isolated oligonucleotides.



Schematic illustration of the analytical approach using magnetic separation techniques.

Results For successful implementation of the separation technique, synthetic oligonucleotides were used for demonstration. Utilization of fluorescence dyes coupled to the oligonucleotides allows monitoring every single step by fluorescence microscopy. One single mutation in the complementary base sequence leads to failure, illustrating the system's high specificity. Mass spectrometric analysis of the hybrid attached to the magnetic bead surface results in the detection of only the hybridized strand, whereas an elution at high temperature enables measurement of both the single strand masses. With nucleases, 3' and 5' extensions of initially 16 bases respectively are expected to be digested generating hybrid double strands with blunt ends. Up to date, additional masses can be detected which correspond to the complementary strands with still one up to six bases left.

Jessica Beyerl, Dr. Anna-Cathrine Neumann-Cip, PD Dr. Andreas Wieser
(Division of Infectious Diseases and Tropical Medicine, University Hospital, LMU Munich)

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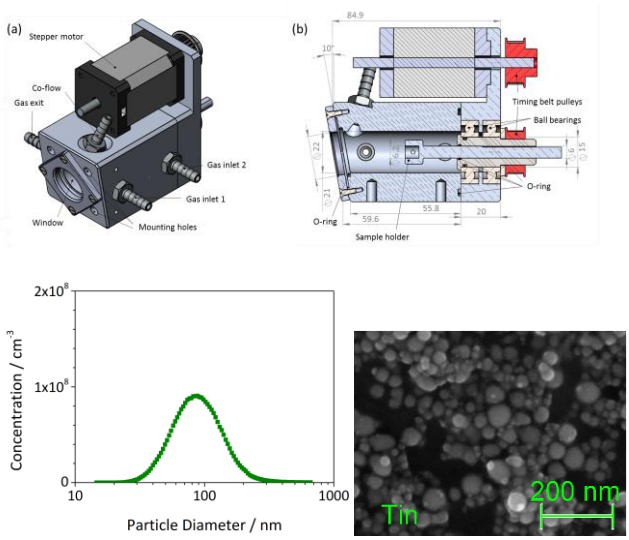
Division of Infectious Diseases and Tropical Medicine
University Hospital
LMU Munich

Cooperation
Max-von-Pettenkofer Institute LMU

Laser-ablation for the Generation of Aerosol Nanoparticles

Aerosols, defined as a suspension of small solid or liquid particles in gas, are ubiquitous in the environment, notably as air pollutants. We develop an aerosol generation device based on laser ablation by a nanosecond pulsed Nd:YAG laser and perform a systematic study of the effect of ablation parameters on aerosol formation from different metals and graphite.

State of the Art Aerosols, defined as a suspension of small solid or liquid particles in gas, are ubiquitous in the environment, notably as air pollutants. Study of aerosols is also important in many other branches of science, including chemical engineering, meteorology, nanoscience, and medicine, to name a few. In aerosol science, there is a demand for a reliable method for the generation of reference aerosols with specified size and concentration properties. Reference aerosols with a well-defined size and concentration profile are required for laboratory simulation of atmospheric environment for air pollution research.



Top: Ablation chamber for the generation of aerosol nanoparticles. Bottom left: size distribution of laser-generated Sn particles, right: SEM image of the same ensemble.

Analytical Approach Aerosols were generated via pulsed laser ablation in a custom-designed ablation chamber (see Figure). The bulk material sample to be ablated in cylindrical form is held in the airtight ablation chamber by a rotating shaft, which is driven by a stepper motor. The gas is pumped through the cell, with a gas flow oriented directly onto the ablation spot. The generated aerosol is characterized by various techniques.

Results The effect of laser parameters (irradiance, repetition rate) and ablation chamber parameters (gas flow rate, rotational speed) on the aerosol properties were investigated, and conditions were determined where the aerosol particle size and concentration were influenced. More agglomeration of primary particles to form larger aerosol particles was found to occur in condition of high concentration. We investigated the effect of dilution gas on the aerosols generated and found certain metals are prone to reacting with oxygen when the aerosols are ablated in synthetic air, and graphite is oxidized to CO when the ablation occurs in the presence of oxygen.

Funding
IWC-TUM

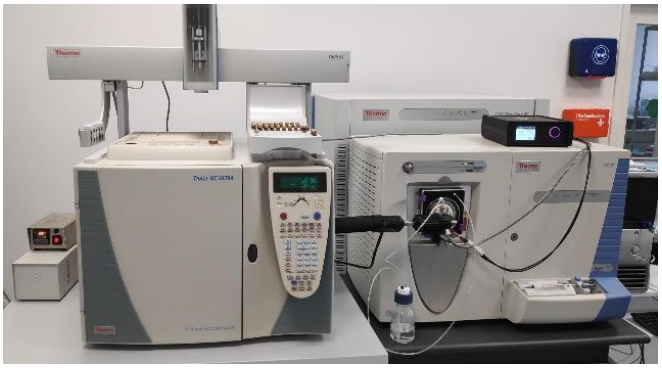
Matthias Bauer, Christoph Haisch

SICRIT – A novel soft ionization technique for the GC-HRMS measurement of alkanes

SICRIT allows for the soft ionization of alkanes via characteristic oxidized species with the generic formula M-(2n-1H)+mO. The molecular mass of different alkane isomers can be directly determined from these species. In combination with GC, this leads to detailed information about complex alkane mixtures like crude oil or diesel.

State of the Art Complex alkane mixtures comprise hundreds of different compounds and up to millions of alkane isomers. Current methods for the analysis of alkane mixtures are usually based on GC-FID, GC-EI-MS or FI-MS. For EI, strong fragmentation and absence of the molecular ion make the distinction between alkanes with different chain lengths impossible. Therefore, in many cases only *n*-alkanes are quantified, leading to up to 95% of unresolved complex mixture.[1] FI is a soft ionization technique producing molecular ions, but suffers from low reproducibility, low sensitivity and high costs.

Analytical Approach SICRIT is a soft ionization technique based on a dielectric barrier discharge (DBDI), that allows for the ionization of a broad analyte range. It can be coupled to any LC-MS system and different separation techniques such as LC, GC, or SPME. In combination with GC and a high resolution MS, the determination of individual sum formulas in complex mixtures is possible without complete separation by GC.



Coupling of GC to a high resolution orbitrap MS via GC-/SPME module and the SICRIT ionization source allowing completely automated measurements.

Results SICRIT ionizes alkanes with little fragmentation, forming characteristic oxidized species **M-(2n-1H)+mO** which allow for the determination of the original molecular mass. An ionization mechanism via hydride abstraction and subsequent oxidation with water could be proposed based on isotope labeling experiments. The pattern of oxidized species distinguishes alkanes from other oxygen containing analytes with the same sum formula. LODs in the low ppb-range can be achieved. The system can be used to determine the mass distribution of alkanes in complex hydrocarbon mixtures such as diesel. The measured results are in good agreement with state-of-the-art GC-EI-MS measurements. The simultaneous measurement of various other components such as (alkylated-)PAHs is also possible.

Markus Weber, Jan Wolf

Funding
Plasmion GmbH

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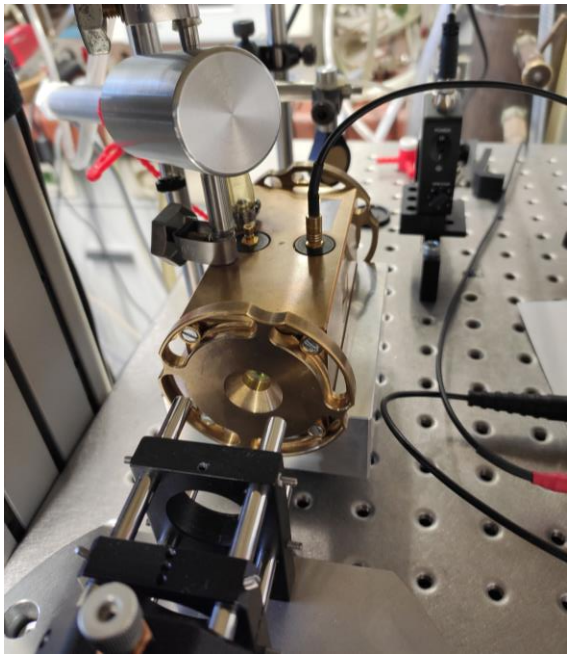
Fundamentals of Aerosol Photoacoustic Spectroscopy

The quantitative measurement of light absorption by aerosol is critically important in the field of atmospheric aerosols, because light-aerosol interaction modify the local and global atmospheric energy balance and plays a significant role in the warming of the atmosphere. Aerosol Photoacoustic Spectroscopy (PAS) represents a promising technique. An innovative photoacustic system calibrated against particles, instead versus known gaseous samples, is currently developed and tested.

State of the Art PAS has been shown to be capable of accurately measuring aerosol ab-sorption after calibrating the photoacoustic instrument against a known gas-eous standard. As result, the technique is routinely applied for studying concentrations of aerosols and for exhaust gas analysis. The aim of our study is a fundamental understanding of the complete PAS signal generation on particles. The main idea is to exploit a combination of single particle, particle ensemble, and theoretical PA studies, addressing the two main issues in the field; i.e. the particle size dependence of the PA response and light absorp-tion under high relative humidity conditions.



Experimental setup for ensemble photoacoustic spectroscopy: resonator cell 4kHz and infrared QCL.

Analytical Approach An IR quantum cascade laser (QCL) with wavelength 9.47µm is used as light source. In the PA cell, the PA signal as well as the optical transmission are measured with high precision. During the measurements, the relative humidity and temperature are monitored continuously at the sample inlet of the PA cell.

Results A large series of measurements is performed under variation of humidity and temperature on a sample of methanol in vapor state. That was chosen in order to test and calibrate the system, since methanol strongly absorbs in the optical range of the laser. Results are compared to PA measurements with droplets of Thetraetylene glycol (TEG) for studying the PA signal generation in small-sized spherical particles.

Emilio Ambra

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Cooperation
ETH Zurich

Determination of unfolding and aggregation mechanisms of protein therapeutics

The secondary and tertiary structure of protein therapeutics is characterized via Raman spectroscopy to identify and study the mechanisms of denaturation pathways.

State of the Art The protein's conformation and aggregation behavior can be examined with various analytical methods like nano differential canning fluorimetry (nDSF), circular dichroism (CD) or light scattering methods. A common approach is to incubate the protein of interest with different amounts of a denaturant and monitor the changes in secondary and tertiary structure over time.

Analytical Approach The molecular vibrations are studied by Raman spectroscopy to understand the conformational stability of protein therapeutics. The secondary structure is characterized by the position and shape of the Amide I band at around 1650 wavenumbers, which is affected by the protein-specific composition of α-helices, β-sheets and random coils. D_2O was used as solvent to avoid spectral interference with water in the Amide I region of the protein. [1]

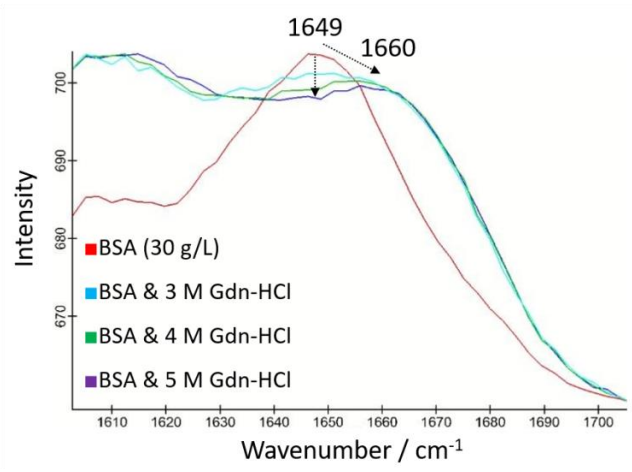

Figure 1: Raman spectra of BSA (30 mg mL^{-1}) with different amounts of Guanidine-Hydrochloride (3 M, 4 M & 5 M). Data points represent the mean of 42 single spectra, which were acquired with a 532 nm laser at a laser power of 40 mW, integration time of 10x5 seconds. Denaturation of BSA leads to a decrease and shift of the Amide I region to higher wavenumbers.

Results Bovine Serum Albumin (BSA) was used as a model protein due to its large proportion of α-helices. The maximum intensity of the Amide I band of BSA is detected at 1649 cm^{-1} (Figure 1). The addition of the denaturant leads to a two level alteration of the Amide I band which is observed by the intensity decrease of the band at 1649 cm^{-1} and a shift of the Amide I band to higher wavenumber regions.

Christian Haase

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Funding

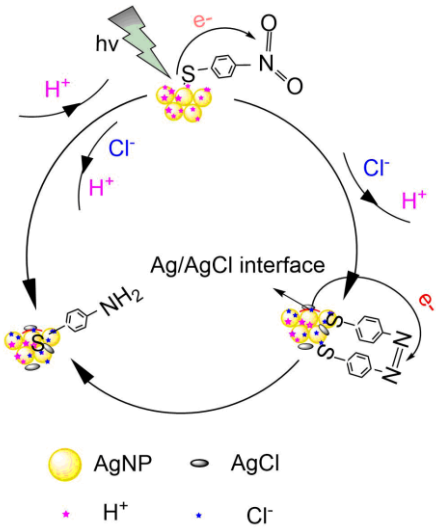
Ludwig Maximilian University of Munich, Department of Pharmacy, Pharmaceutical Technology and Biopharmaceutics

Cooperation

Prof. Dr. Wolfgang Frieß, Ludwig Maximilian University of Munich

Kinetic and Mechanistic Investigation of the Photocatalyzed Reduction of 4-Nitrothiophenol Observed on a Silver Plasmonic Film via Surface-Enhanced Raman Scattering

A simple method was developed to prepare low-cost silver plasmonic film for SERS (surface-enhanced Raman microscopy) detection of 4-nitrothiophenol (4-NTP) photocatalytic reduction. The reduction of 4-NTP to 4-aminothiophenol (4-ATP) was carried out under carefully controlled reaction conditions in order to uncover the molecular pathways on plasmonic Ag surface.



The reaction route of the photocatalyzed reduction of 4-NTP to 4-ATP in presence of H^+ and Cl^-.

State of the Art Based on the high local chemical sensitivity, SERS is proved to be an ideal technique for studying chemical reactions. Moreover, it is applicable for the investigation of photocatalytic reaction due to its inherent presence of photons.

Analytical Approach Firstly, the solid silver film was prepared basing on the silver nanoparticle self-assembly at the liquid-liquid interface. The photoreduction was performed on the film in the presence of different conditions and monitored by SERS. Thus, different reaction intermediates can be identified by their unique SERS bands. Then, the reaction mechanism was simulated with MATLAB.

Results We were able to systematically control the concentration of positive and negative ions in the reaction environment and observe the selective surface reduction of 4-NTP with SERS under different conditions. Through time-resolved SERS measurements, we obtained concentration time histories of the reactants, intermediates, and products of the 4-NTP to 4-ATP reduction, and used these measurements to propose a reaction mechanism for the process and determine individual reaction rate constants. Finally, by interpreting the relationship between Cl^--concentration and reaction pathway, we confirmed that hot-electron generated by the decay of excited surface plasmons of AgNPs can only induce the reduction of 4-NTP to DMAB. The factors that influence the reaction pathway and the hot-electron utilized in the depletion of DMAB to 4-ATP were figured out.

Li Qiu

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Cooperation

Genny A. Pang, Guangchao Zheng, et.al.

References

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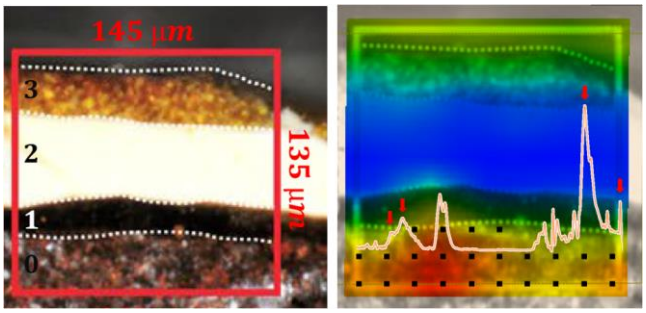
"The Return of the Hunters" by Jean Dunand – A multi-analytical study on the use of Vietnamese lacquer as painting medium

Cross-sections of Jean Dunand's 8-piece wall panel "The Return of the Hunters" were investigated by means of THM-GC/MS, UV/Vis microscopy, SEM-EDX and µATR-FTIR spectroscopic mapping to form a comprehensive image of the painting's elemental and chemical composition. (1)

State of the Art The investigation of the different layers a painting is composed of is crucial for developing an appropriate and meaningful conservation-restoration strategy. It was known that the investigated wall panel was subject to previous modifications; therefore, our investigations were crucial to preserve all original layers during the restoration campaign.



(Left) Optical microscopy image of cross-sectioned sample with the µATR-FTIR mapped aera of 134x145 µm² indicated by the red box. The different layers of this cross-section are marked with the numerals 0-3. (Right) False-color PC1 score image of the mapped aera with the averaged spectral profile of the positions marked in black squares representing layer 0 which mainly consists of gypsum. Typical gypsum bands in the corresponding IR spectrum are highlighted by red arrows.

Analytical Approach Elemental and chemical information are equally important; hence, a great variety of analytical methods was required for a comprehensive screening. THM-GC/MS was employed for determining the lacquer type. UV and visible light, and SEM-EDX were used for investigating the lacquer paint stratigraphy to detect inorganic components. µ-ATR-FTIR spectroscopic mapping was employed to investigate the spatial distribution of the lacquer in the painting's cross-section as well as its additives detected with THM–GC/ MS.

Results Multivariate analysis of µATR-FTIR mapping allowed to get a detailed picture on the spatial distribution of different components along the cross-section of the wall panel. Dunand's favorite "Laque arrachée" technique which used Vietnamese lacquer mixed with linseed oil, pine resin, and quartz to form the black layer 1 on top of a ground layer (gypsum with red iron particles as coloring material; layer 0) was determined. The pale-yellow layer 2 contains Vietnamese lacquer mixed with linseed oil and pine resin, titanium white and bone white pigments. The lacquer layer was composed of Vietnamese lacquer mixed with linseed oil, pine resin and shellac (layer 3). Additionally, Dunand used both of gold and copper metals for different finishing color effects to the paint surface.

Valentina Pintus[1], Anthony J. Baragona[2], Karin Wieland, Michael Schilling[3], Silvia Miklin-Kniefacz[4], Christoph Haisch & Manfred Schreiner[1]

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Academy of Fine Arts, Vienna

TUM – IWC

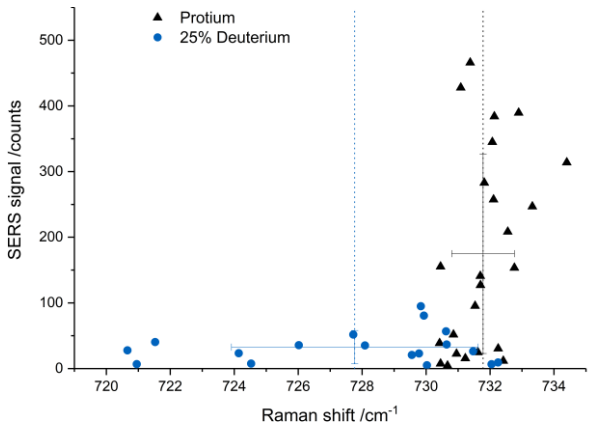
Cooperation

1 Institute of Science and Technology in Art, Academy of Fine Arts Vienna, Austria. 2 Institute of Art and Technology, Department of Conservation Science, University of Applied Arts, Vienna, Austria. 3 Getty Conservation Institute, Los Angeles, CA, USA. 4 Atelier Bernardgasse, 4/1, Vienna, Austria

Stable isotope Raman microspectroscopy for nondestructive analysis of microorganisms and biofilms at the single-cell level

Detection and characterization of microorganisms is essential for both environmental studies and clinical diagnostics. An emerging technique for nondestructive analysis of microorganisms and biofilms at single-cell resolution is stable isotope Raman microspectroscopy.

State of the Art Stable isotope-based analytical methods gain increasing relevance in different scientific fields. Although mass spectrometry-based (MS) methods enable sensitive analysis of bulk samples (e.g., isotope ratio mass spectrometry, IRMS) or provide a spatial resolution down to 50 nm (e.g., nanoscale secondary ion mass spectrometry, NanoSIMS), these methods are destructive and require time-consuming sample preparation. Here, a combination of Raman microspectroscopy (RM) with the stable isotope approach – stable isotope Raman microspectroscopy (SIRM) – can extend the capabilities of the well-established techniques with a nondestructive, quantitative and spatially-resolved analysis.



SERS signal at around 733 cm^{-1} of *E. coli* with and without 25% D_2O addition, plotted against Raman shift.[1]

Analytical Approach SIRM provides characteristic fingerprint spectra of samples with the spatial resolution of a confocal optical microscope, containing information about stable isotope-labeled substances and the amount of a label (based on red shift of bands of the labeled substances). Simultaneously, the spectra deliver information on the chemical composition and structure of samples. Furthermore, this method requires no or limited sample preparation, and can be performed *in situ* and *in vivo* without spectral interference of water.

Results We demonstrated that SIRM in combination with surface-enhanced Raman scattering (SERS) can be successfully applied for the analysis of carbon metabolism / flow and the microbial cell activity (Figure)[1], and tested this method for the analysis of the degradation of environmental pollutants. The goal of our follow-up study is to develop and evaluate a SIRM-based method for quantitative and nondestructive 2D & 3D analysis of biofilms involved in the biodegradation of a most prominent emerging pollutant in the aquatic environment – microplastic (MP).

Ruben Weiss, Natalia P. Ivleva

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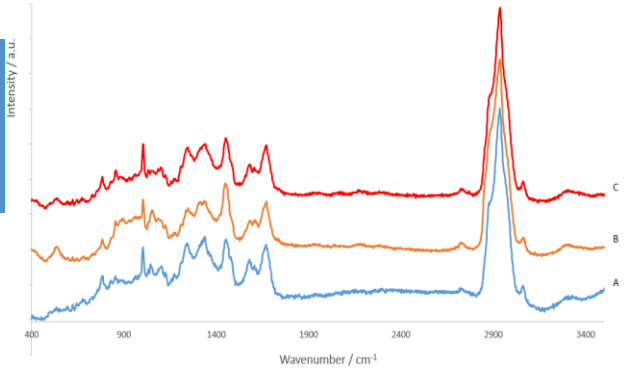
Cooperation

Prof. Dr. Michael Wagner, University of Vienna, Division of Microbial Ecology, Austria

Raman microspectroscopy analysis of the atrazine biodegraders under different physiological conditions

Atrazine biodegrader *Arthrobacter aurescens* TC1 was grown and incubated under different physiological conditions. Raman microspectroscopy analysis is applied for determination specific features of bacteria grown on the different substrates.



Average Raman spectra of *Arthrobacter aurescens* TC1. A) Control, n=17. B) Incubated with atrazine, n=18. C) Incubated with atrazine+lactate-NO_3, n=18.

State of the Art Nowadays, the micropollutants such as atrazine are still observed in the environment.[1] Therefore, identification and characterization of active microorganisms responsible for degrading organic pollutants is challenging. Mostly, classical screening (e.g., gene sequencing, gene fingerprinting) describes which bacteria present in a studied sample but does not disclose who is really metabolically active and growing. Therefore, efficient analytical approach for characterization of the active cells of micropollutant biodegraders is on demand.

Analytical Approach Raman microspectroscopy (RM) can deliver sensitive, minimally invasive and a rapid tool with a simple sample preparation. RM is approach capable for efficient characterization of microorganisms on the single cell level.[2] Coupling with bioorthogonal non-canonical amino acid tagging (BONCAT) and proteomics analysis can reveal specific chemical features of the atrazine biodegraders.

Retentostat, fed-batch and batch systems are used to grow microorganisms with change of physiological substrates input. Incorporation of artificial amino acid analogues into newly synthesized proteins and further proteomics analysis along with RM allow to disclose metabolic changes in the biodegraders' cells. Isolation of the newly synthesized proteins is based on azide-alkyne click-chemistry reaction.

Results Atrazine biodegraders were grown in the presence of atrazine and/or lactate+nitrate substrates. Proteins which incorporated azidohomoalanine were extracted from the bacterial biomass and specifically bound to dibenzocyclooctyne beads for the proteomics analysis. RM revealed minor changes in bacterial cells upon different physiological conditions.

Oleksii Morgaienko

Funding
IWC-TUM

Cooperation
Helmholtz Zentrum München,
California Institute of Technology

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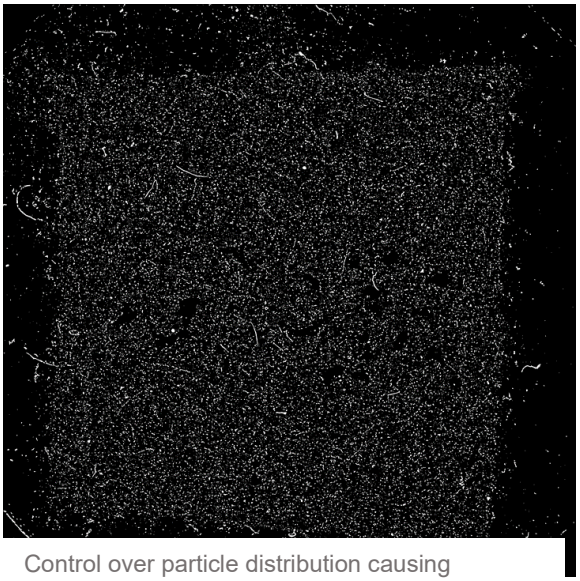
Validation of an automated microplastic particle analysis routine

Abstract: A statistically sound analysis of microplastics requires the measurement of thousands of individual particles from each sample. Therefore, automation is key to enable such an analysis in a reasonable amount of time, but the procedure also needs to be validated properly.

State of the Art. Microplastic (MP) particles (plastic fragments 1 µm – 1 mm) can already be characterized through automated Raman microspectroscopy (RM).[1] But is this analysis quantitative, in the entire size range?

Analytical Approach.

For validation three different stages of the analysis were evaluated individually. 1) Validation, that particles are quantitatively deposited on filter, through comparison of different filtration methods. 2) Validation of the image-based particle detection and morphological characterization for RM, scanning electron microcopy and fluorescence microscopy. 3) Validation of the single point measurement approach through comparison of Raman mapping vs. Raman single point analysis at the particle centers determined through image analysis.



Control over particle distribution causing particles to deposit within the desired (square) area, to alleviate the clinging of particles the glass walls of the filtration device inhibiting quantitative transferal.

Results.

So far, it is possible to control the distribution of the particles on the filter (Figure) and to, therefore, allow for a quantitative transfer from sample to filter without wall effects. For our image recognition software *TUM-ParticleTyper* we determined the size limit for a quantitative analysis to be tied to the image resolution. With our setup we can quantify particles, spheres and fibers as small as 10 µm on a filter surface of 256 mm^2 (20× magnification) with RM. The comparison of Raman mapping vs. single point analysis in similar time frames provided evidence that a single point measured at the center of a particle is representative for the particle, as the requirement that both measurements be equally swift only allows for very short integration times during mapping. This led to very weak signals, even when using reference materials. For the evaluation of the overall process round robin tests were successfully conducted. However, the comparison between different groups remain to be assessed by the respective organizing institutions.

Elisabeth von der Esch, Alexander J. Kohles, Oliver Jacob, Philipp M. Anger

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Bayerische Forschungsstiftung

Bundesministerium für Bildung und Forschung

IWC-TUM

Cooperation

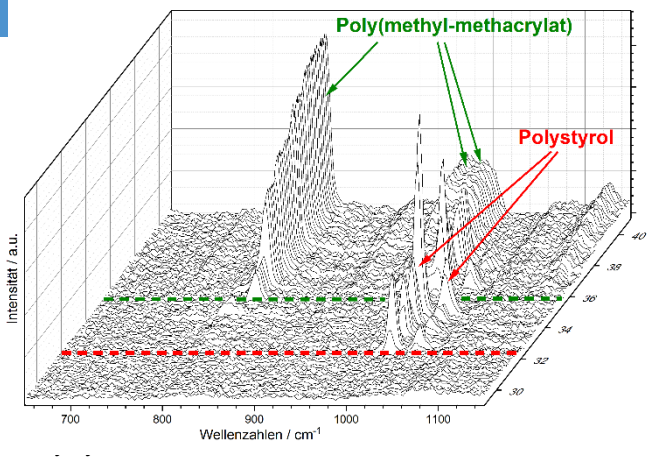
Mikropartikel in der aquatischen Umwelt und in Lebensmitteln (MiPAq)

Mikroplastik im Wasserkreislauf (MiWa)

On-line coupling of field flow fractionation and Raman Microspectroscopy

Abstract: Raman Microspectroscopy has been coupled to field flow fractionation for comprehensive analysis of subµ (plastic) particles. The multi-detector setup provides particle separation, physical characterization along with chemical identification.

State of the Art. Environmental microplastic (MP) is analyzed either spectroscopically or by gas-chromatography-mass-spectrometry. These established methods, however, have size limitations in the range of 1 µm – 10 µm or weight limits in the low µg range. And state of the art techniques for nanoparticle characterization does not provide chemical information for synthetic polymers. Thus, there is a methodological gap for the chemically identification of plastic particles in the subµ range.



Poly(methylmethacrylate) 500 nm at minute 36. Both can be identified by their specific vibrational bands.

Analytical Approach. Raman microspectroscopy (RM) is able to unambiguously identify plastic particles by their fingerprint spectra and is, further, unaffected by water in the sample. Field flow fractionation (FFF) is a particle separation technique that works for particles in the whole nanometer range by applying a separation force on the eluting suspension. Subsequent detectors (UV, multi angle light scattering, MALS) produce physical information on the particle fractions, like particle size. A laser-optical focusing-based flow cell enables the on-line coupling of RM to FFF and thereby gives vibrational spectroscopic information on the eluting particles.

Results. The on-line coupling was realized for asymmetric flow field-flow fractionation and centrifugal field-flow fractionation for separation by different principles and gives size and chemical information on each particle system (see Figure). This was enabled by a flow cell that uses laser-optical focusing of the particles in the Raman laser to circumvent the sensitivity limitation of many Raman flow cells. It has been shown that particles within the size range of 200 nm – 5 µm and concentrations of around 1 mg/L can be analyzed. It has been further shown that a distinction between different polymers and from inorganic particles is possible. Thus, we present a method that has the potential for the analysis of environmental subµ plastic particles and produce identification and size.

Christian Schwaferts

Reference

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Funding

Bundesministerium für Bildung und Forschung

IWC-TUM

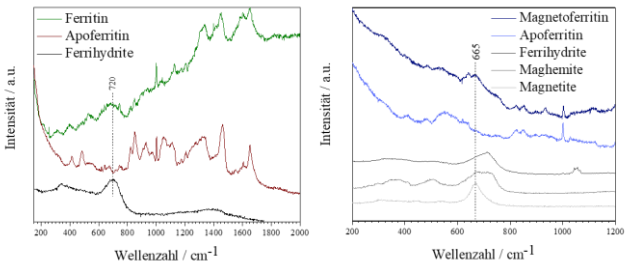
Cooperation

Innovative Analysemethoden für Submikroplastik (SubµTrack)

Non-invasive characterization of Ferritin and Magnetoferritin by Raman Microspectroscopy

Ferritin and magnetoferritin have been considered as bio-based nanoparticles for various biological and medical applications. Their properties differ in their chemical composition and structure of the iron core. Raman microspectroscopy has been proven to be a suitable tool for a non-invasive characterization of the iron core.

State of the Art Ferritin is a universal intracellular iron storage protein composed of a spherical protein shell with an outer and inner diameter of 12 nm and 8 nm, respectively, and an iron core located inside the cavity. The cavity of this protein acts like a reaction chamber for natural formation and storage of nano-sized particles via biomineralization.[1] Knowledge on the chemical composition and structure of the iron core is highly warranted in the fields of nano technologies as well as biomolecules and medicine.



Left: Raman spectrum of ferritin, corresponding apoferritin which is the protein shell without the iron core, and the reference ferrihydrite.
Right: Raman spectrum of magntoferritin, its corresponding apoferritin and the references ferrihydrite, maghemite and magnetite.

Analytical Approach We show that Raman microspectroscopy (RM) is a suitable approach for a non-destructive analysis of proteins containing such nano-sized iron oxides. Our approach pillared on (i) synthesis of suitable reference materials, i.e. ferrihydrite, maghemite and magnetite nanoparticles; (ii) optimization of parameters for Raman spectroscopic analysis; (iii) comparison of Raman spectra from ferritin with apoferritin and our reference minerals; (iv) validation of Raman analysis by Mössbauer spectroscopy and X-ray diffraction as two independent complementary approaches.

Results Our results reveal that the iron core of natural ferritin and magnetoferritin is composed of the iron(III)hydroxide ferrihydrite ($Fe_2O_3 \cdot 0.5\ H_2O$) and iron oxide magnetite (Fe_3O_4), respectively.[2] Subsequently, ferritin and magnetoferritin were incorporated into lysosomes, testing the feasibility of the Raman microspectroscopy to analyze the iron core in more complex media. However, most likely due to the low iron compounds/biological matrix ratio, an optimization of the Raman set up is still required.

Carolin Hartmann

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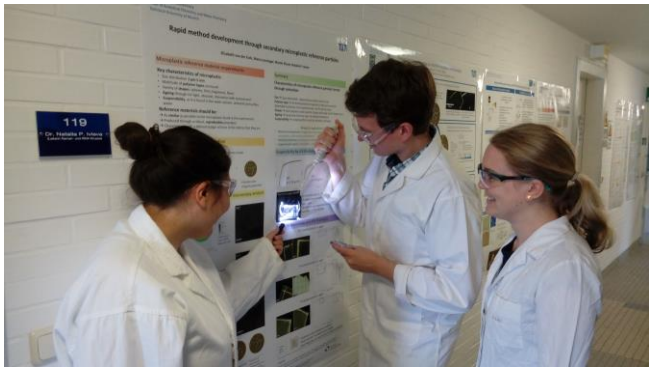
Funding
International Graduate School of science and Engineering, IGSSE.

Cooperation
Prof. Dr. G. Westmeyer, Susanne Pettinger,
TUM School of Medicine/ Klinikum Rechts der Isar

Characterization of chemical and morphological changes in microplastics during bacterial colonization/degradation at environmentally relevant conditions

Biodegradable plastics replace traditional plastics in several fields most predominantly in agriculture as biodegradable mulch films. However, biodegradable microplastic particles are only rarely found in environmental samples and using Raman micro-spectroscopy, we want to shed some light on possible reasons.



Sample collection for bacterial isolate identification and microplastic characterization using Raman micro-spectroscopy (reenactment).

State of the Art Microplastic characterization on the single particle level is often done by Raman microspectroscopy, which allows the morphological characterization as well as the chemical identification of the polymer. The assignment of the chemical identity is done via database matching. This leads to the questions: “What happens when microplastic is colonized and/or degraded by bacteria? Can the spectra still be identified by correlation to pristine database spectra?

Analytical Approach Bacteria isolated from a microplastic suspension were incubated at conditions close to those found in the environment (25 °C, shaking) in microplastic suspension (using aged polylactic acid (PLA) particles in ultrapure water) and the growth of the bacteria was monitored. Changes in particle composition and morphology were analyzed via Raman microspectroscopy and scanning electron microscopy (SEM) analysis at different time points during the three-week experiment.

Results The isolated bacteria grew under the chosen conditions (confirmed by culture using agar plates) and Raman spectra of the microplastic particles taken over the course of the experiment showed changes in band positions and relative intensities. These changes correspond to possible biofilm formation and bacterial degradation of microplastic particles. By SEM analysis, single microplastic particles and bacteria were visualized and changes in the morphology could be observed. Further data evaluation is currently in progress and additional experiments to further elucidate the changes in Raman spectra are planned. It was shown for the first time that pristine biodegradable plastic differs in morphology and Raman spectra compared to microbially aged microplastic particles.

Funding

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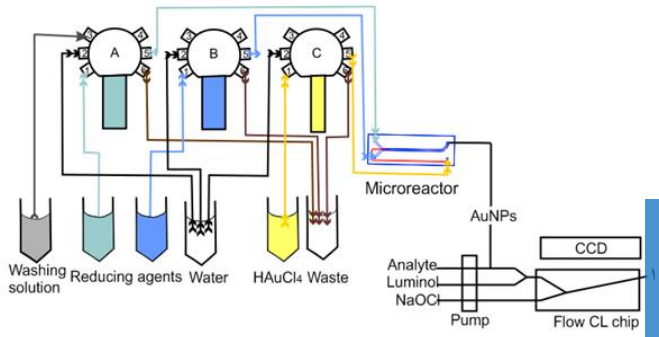
IWC-TUM

Elisabeth von der Esch, Lisa Göpfert, Christian Schwaferts

Synthesis of gold nanoparticles in a 3D flow-based microreactor and their application in analytics

Gold nanoparticles was synthesized in a 3D microfluidic device without fouling. This approach allows rapid, easy, low cost and automated synthesis of the gold colloidal which can coupled online with chemiluminescence measurement systems.

State of the Art Gold nanoparticles exhibit unique size and shape dependent physical and chemical properties which make AuNPs an attractive material in multifunctional applications especially in electrochemical and bioanalytical systems [1]. The synthesis of gold nanoparticles is well known, however it was shown, that microfluidic reactors are able to synthesize gold nanoparticles with narrower size distributions and faster reaction rates compared to conventional batch synthesis [2]. Moreover, the synthesis process could be controlled in-line by methods like single particle ICP-MS.



Scheme of online synthesis and measurement system

Analytical Approach In this project, we report an automated tape based microfluidic device for the continuous flow synthesis of gold nanoparticles (AuNPs). Our choice was to obtain colloidal crystals by a simple one-phase reaction in which gold (III) is reduced and stabilized by glucose. The synthesized gold nanoparticles were used as catalyst for luminol-NaOCl chemiluminescence system. The synthesis setup was directly coupled with a CCD camera. Therefore, online synthesis and measurement were achieved in a microfluidic system.

Results In this work, an automated taped based three-dimension (3D) flow-focused fluidic microreactor was used to synthesize AuNPs through a single-phase reaction without fouling in room temperature. This method was cheap, simple, rapid, and low cost without using heating or UV light. After optimizing parameters of synthesis, the chemiluminescence signal were enhanced hundreds times. Therefore, the gold nanoparticles can act as catalyst for flow-based homogeneous chemiluminescense assay. It is the first time for online synthesis and directly coupled with chemiluminescence measurement. For further application, with help of aptamer, some antibiotics will be detected online.

Yanwei Wang

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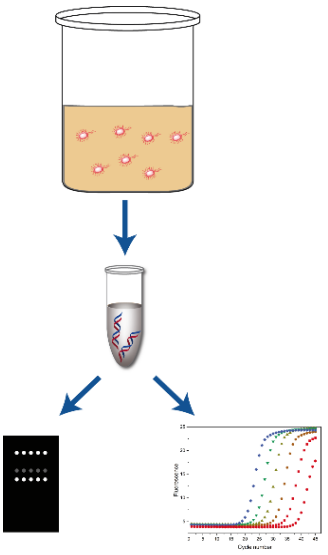
(2) Wagner, J.; Kohler, J. M., Continuous synthesis of gold nanoparticles in a microreactor. Nano Lett ***2005,*** *5 (4), 685-91.*

Funding
China Scholarship Council

DNA microarray for antibiotic resistance gene *bla*$_{CTX-M}$

Treatment of bacterial infections is a growing challenge due to antibiotic resistant bacteria. These bacteria are also present in environmental waters and monitoring of these is critical to gather information about the spread and occurrence of resistance, for example by detecting the resistance gene *bla*$_{CTX-M}$.



Overview of experimental setup. Bacterial DNA is extracted and analyzed using two different methods.

State of the Art Antibiotic resistance genes (ARGs) are the genes that are responsible for resistances in bacteria. To detect these, various molecular biological methods can be used such as the current gold standard (quantitative) polymerase chain reaction (qPCR). Another possibility is the use of isothermal nucleic acid amplification tests that apply a different technique allowing in-field measurements in the future due to their isothermal incubation in contrast to thermal cycling for qPCR measurements.

Analytical Approach The DNA microarray uses the heterogeneous asymmetric recombinase polymerase amplification (haRPA)[1,2] for DNA amplification on each spot and chemiluminescence detection, which takes only 40 min at 39 °C. The assay for the detection of the ARG *bla*$_{CTX-M}$ cluster 1 was compared to the standard qPCR method by analyzing DNA extracts from *Escherichia coli* and *Klebsiella pneumoniae* carrying the respective ARGs.

Results Comparing the haRPA assay for *bla*$_{CTX-M}$ cluster 1 with the qPCR assay showed a higher limit of detection for the haRPA assay. However, the newly developed assay is sensitive enough to be used as a screening tool and due to its spatial resolution on the chip surface multiplex measurements of different ARGs or species-specific genes are possible.

Lisa Göpfert

References

(1) Kunze, A.; Dilcher, M.; Abd El Wahed, A.; Hufert, F.; Niessner, R.; Seidel, M., On-chip isothermal nucleic acid amplification on flow-based chemiluminescence microarray analysis platform for the detection of viruses and bacteria. Anal. Chem. 2015, 88, (1), 898–905.

(2) Kober, C.; Niessner, R.; Seidel, M., Quantification of viable and non-viable Legionella spp. by heterogeneous asymmetric recombinase polymerase amplification (haRPA) on a flow-based chemiluminescence microarray. Biosens. Bioelectron. 2018, 100, 49–55.

Funding

BMBF (Project METAWATER; (FKZ: WU1346A), JPI Water Project)

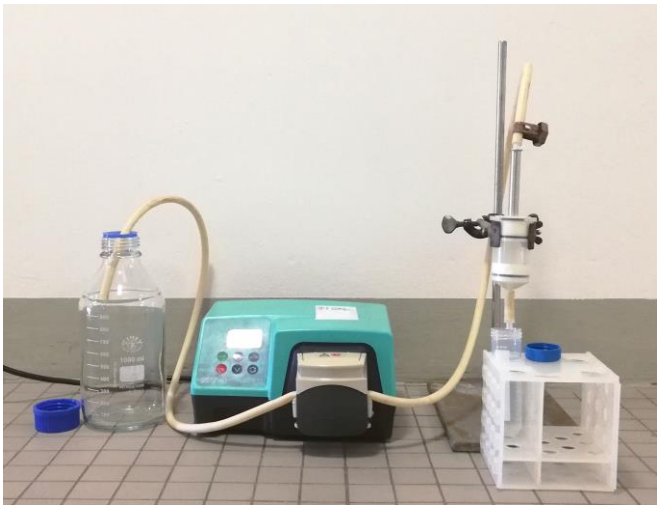
Cooperation

Bayerisches Landesamt für Gesundheit und Lebens-mittelsicherheit (LGL)

Culture-independent detection of *Pseudomonas aeruginosa* in tap water

Contamination of tap water with *Pseudomonas aeruginosa* can cause severe health effects in humans. Hence, rapid and reliable methods for the detection of even low numbers of bacteria in tap water are needed. A promising method is the combination of monolithic adsorption filtration (MAF filtration) and quantitative polymerase chain reaction (qPCR), allowing for the concentration and quantitative analysis of *P. aeruginosa* in tap water.

State of the Art The presence of the multiresistant, pathogenic bacteria *P. aeruginosa* in water installations poses a severe threat to human health. To date, the standard method for the detection of *P. aeruginosa* is cell culture, which has a number of disadvantages such as a long incubation time and difficulties due to the formation of biofilms. Culture-independent methods are often sensitivity-limited, as very low numbers of bacteria have to be detected.



MAF filtration setup used for the concentration of *P. aeruginosa* from tap water samples.

Analytical Approach To achieve the concentration of *P. aeruginosa* from tap water samples, MAF filtration was used. This in-house developed method is based on electrostatic interactions between a monolith surface and bacteria.[1,2] The filter functionalization as well as the sample pH value, filtration volume, and elution buffer were optimized to allow for a subsequent quantitative detection by qPCR after an additional concentration step using centrifugal ultrafiltration (cUF). For the detection, primers as well as a qPCR method were developed.

Results We could show for the first time that *P. aeruginosa* can be adsorbed on MAF-OH at pH 3 and eluted with beef extract buffer containing glycine (pH 9.5) with a recovery of 67 ± 1 % for 5 L-water samples. The combination of rapid enrichment by MAF and cUF and subsequent qPCR for the detection of *P. aeruginosa* in tap water has achieved a concentration factor of more than 2200, enabling the analysis of samples containing cell numbers as low as 100 CFU mL^{-1}. Future work will aim on further decreasing the limit of detection of the method.

Lisa Göpfert, Julia Klüpfel

Funding
IWC-TUM

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(1) Wunderlich, A., Torggler, C., Elsässer, D., Lück, C., Niessner, R., Seidel, M., Rapid quantification method for Legionella pneumophila in surface water, Anal. Bioanal Chem. 2016, 408, 2203 – 2213.
(2) Peskoller, C., Niessner, R., Seidel, M., Development of an epoxy-based monolith used for the affinity capturing of Escherichia coli bacteria, J. Chrom. A. 2009, 1216, 3794 – 801.

LegioTyper: Culture-independent detection system for the rapid risk assessment of *Legionella pneumophila* outbreaks

Legionella outbreaks are often caused by bioaerosols that originate from technical facilities such as cooling towers, evaporative recooling systems and hot water systems and lead to severe infections in humans. The detection of an outbreak source with culture-based methods is very time-consuming, calling for the development of faster detection methods.

Legionella pneumophila analysis platform LegioTyper.

State of the Art *Legionella*, especially *L. pneumophila* Serogroup 1, pose a threat to human health as is evident in increasing numbers of legionellosis cases. Hence, outbreaks have to be detected and contained rapidly, but the gold standard for detection, cell culture, takes ten days and only detects culturable *Legionella* spp. This shows the necessity of rapid, culture-independent serotyping methods for *L. pneumophila*.

Analytical Approach To allow a direct analysis of *L. pneumophila* in different sample types without the necessity of cultivation, a chemiluminescence sandwich microarray immunoassay (CL-SMIA) was developed.[1] To optimize the microarray chip manufacturing, a polycarbonate chip was used.[2] The serotyping of all *L. pneumophila* Sg 1 subgroups is done using a panel of ten sensitive capture antibodies. These antibodies bind selectively to the LPS structure of the distinct *Legionella* Sg 1 subgroups.

Results The microarray-based immunoassay platform LegioTyper, derived from the Munich Chip Reader 3 (MCR3), was developed and tested with various sample types. It was shown the first time that a serotyping of *L. pneumophila* Sg 1 subgroups directly from environmental samples as well as from urine is possible. Analysis can be done cost-effectively and within 34 min, allowing to rapidly narrow down the number of possible *Legionella* outbreak sources. Subsequent genotyping methods can then be focused on the most probable sources, facilitating a quick containment of outbreaks.

Catharina Kober

References

(1) Wunderlich, A.; Torggler, C.; Elsaesser, D.; Lück, C.; Niessner, R.; Seidel, M., Rapid quantification method for Legionella pneumophila in surface water. Anal. Bioanal. Chem. 2016, 408(9), 2203-2213.

(2) J. Bemetz, C. Kober, V. Meyer, R. Niessner, M. Seidel (2019) Succinylated Jeffamine ED-2003 coated polycarbonate chips for low-cost analytical microarrays. Anal. Bioanal. Chem. 2019, 411, 1943-1955.

Funding

BMBF (FKZ: 13N13698)

Cooperation

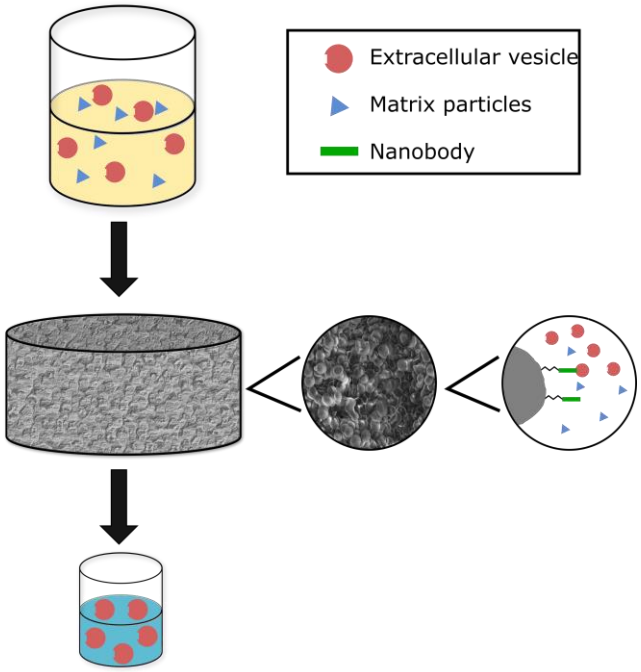
Occupational and Environmental Health, Epidemiology, Bavarian Health and Food Safety Authority, Institute of Medical Microbiology and Hygiene, Institute of Virology, Medical Faculty “C. G. Carus”, Technical University of Dresden GWK Präzisionstechnik GmbH

Enrichment and detection of extracellular vesicles in urine via monolithic immunofiltration using nanobodies

Extracellular vesicles carry a lot of information of their cell of origin, like RNA, proteins, or biomarkers. Because of this, they bear a high importance for medicinal diagnostics. However, a low concentration in human body fluids requires prior enrichment.

State of the Art Extracellular vesicles are vesicles, which are secreted by cells mostly for intracellular signaling. Hence, they carry a lot of information and even biomarkers for diseases like Alzheimer's disease or cancer. Proteins, which are secreted on their outside, allow nanobodies to attach. Nanobodies are similar to single domain antibodies, more precisely the variable part of a heavy chain-only antibody.

Analytical Approach For the enrichment of extracellular vesicles, an immunofiltration is used with in-house produced, epoxy-based monoliths as filters and nanobodies as immune receptor. In order to detect the extracellular vesicles on the monolith, a colourimetric reaction is used. Therefore, a second, horseradish peroxidase-labelled nanobody is used. A colour reaction takes place with 3,3',5,5'-tetramethylbenzidin and hydrogen peroxide. Small fractions were collected and the absorption (450 nm) was measured. Elution was done with glycine buffer (pH 2.2).



Scheme for the monolithic immunofiltration of extracellular vesicles using nanobodies as catcher.

Results Enrichment and detection of extracellular vesicles in processed urine was successful. In order to distinguish between unspecific binding and real binding of the vesicles, the slopes of the colour reaction were analyzed. Unspecific binding leads to a very fast and strong increase of the absorption, whereas the presence of the vesicles leads to a slower increase. In addition, a concentration dependency was observed. Elution with glycine was partially successful. The vesicles seem to denaturize, as only proteins of the inside the vesicles could be found, but no proteins from the outside.

Julia Neumair, Jorge Guojardo

Funding

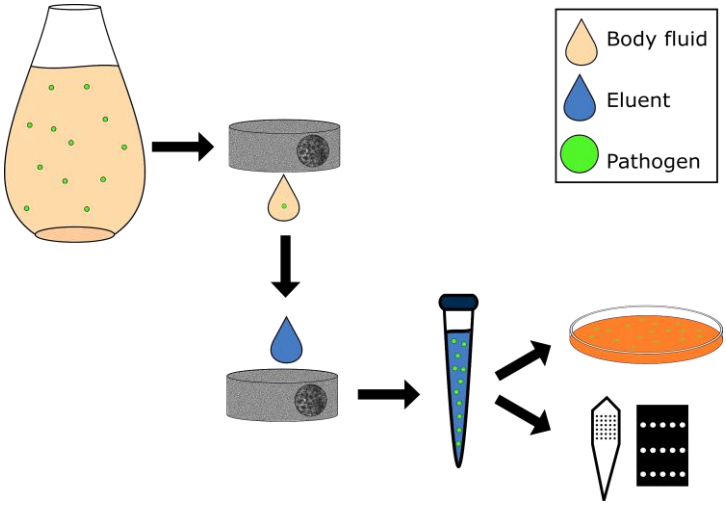
International Graduate School of Science and Engineering (IGSSE), TUM

Cooperation

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

Rapid enrichment for early and highly sensitive pathogen detection in human body fluids with monolithic affinity filtration

Infected body fluids are in most cases severe and highly lethal, when left untreated or with wrong or belated treatment. The low concentration of pathogens inside the fluid can lead to an extended identification time. Using monolithic affinity filtration and later a DNA-based detection method, we want to decrease the detection time and consequently the time until treatment.



Workflow for enrichment and detection of bacteria and fungi in human body fluid using monolithic affinity filtration. The infected body fluid gets filtrated using a monolithic affinity filter. After elution with a suitable eluent, detection with both culture and a DNA-based method take place.

State of the Art The pathogens, which cause human body fluid infections, are mainly Gram-negative and Gram-positive bacteria, like *Escherichia coli* and *Enterococcus faecalis*, but also in rare cases fungi, like *Candida*. Culture-based detection methods, the current gold standard, are stretched to their limit, as the concentration of the pathogens inside the fluid is very low.

Analytical Approach The two crucial parts for monolithic affinity filtration are the monolith itself and suitable affinity ligands. The monolith is produced in-house via self-polymerization of an epoxy-resin and has pores with a size of 22 µm[1]. As affinity ligands, antibiotics and antifungals will be investigated. For this, our project partners use a 2D fluorescence-based system (DANI) to study the adsorption and desorption behavior between the ligands and pathogens. We developed suitable array disks for this system.

Results We achieved to produce disks for the 2D system in a fast and easy way. A 0.25 mm polycarbonate plate was cut into object slide-sized chips and on each nine disks with a diameter of 10 mm were carved. After modifying the nine disks at once, they can easily be taken out and used for DANI measurements. For surface modification, Jeffamine ED-2003, a diamono-PEG/PPG triblock copolymer, was used. Dimethyl suberimidate was tested as an alternative homobifunctional cross-linker. As test-model both biocytin and an anti-streptavidin horseradish peroxidase antibody were used. We could show that this linker is suitable for our surface chemistry.

Julia Neumair

Funding

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

Cooperation

Experimental Orthopedics, Klinikum Rechts der Isar (TUM)

Klinik und Poliklinik II, Klinikum Rechts der Isar (TUM)

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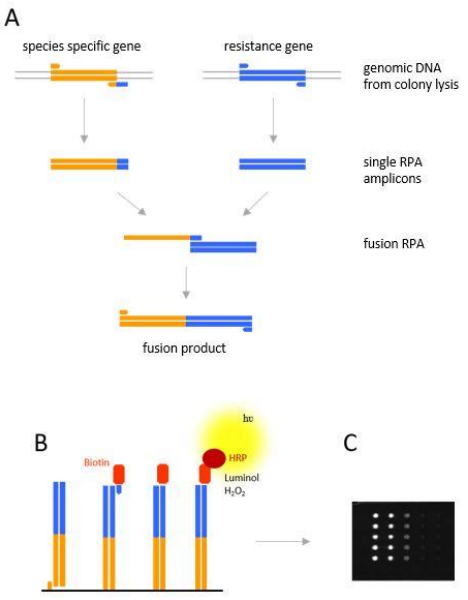
(1) Peskoller, C.; Niessner, R.; Seidel, M., Development of an epoxy-based monolith used for the affinity capturing of Escherichia coli bacteria, Journal of Chromotography A. 2009, 1216 (18), 3794 – 3801.

A microarray for the fast identification of antibiotic resistance genes in pathogens via molecular fusion

The detection of antibiotic-resistant bacteria in the environment is a big challenge for modern society. Numbers of these pathogens in important matrices such as water or food are rising and therefore reliable methods for their identification are needed.

State of the Art In order to enable accurate risk assessment regarding antibiotic-resistant bacteria, two types of information are needed. Is the bacterial species pathogenic and which resistance does it carry? Mostly, molecular biological methods only look for the latter, namely the resistance gene. Sometimes, the species is also identified by analysis of specific genes or culture methods. Especially for analyzing potential danger to human health and to monitor the development, both aspects are needed. In this project we aim to combine both questions in a single step.



Workflow for the generation of fusion products (A) and their detection (B,C).

Analytical Approach The aim of this work is the generation and detection of DNA fusion-products carrying an antibiotic resistance- and a species-specific gene at the same time. For the generation of these fusion products, an isothermal recombinase polymerase amplification (RPA) is used to amplify the antibiotic resistance gene and species-specific gene. Afterwards, both gene amplicons are fused together to a single strand using an additional RPA. The fusion-product is detected on a chemiluminescence based microarray chip[1] by a further RPA amplification directly on the chip surface.

Results As a proof of principle, we were able to show the generation of *E. coli* and *K. pneumoniae* fusion-products. These fusion-products from *E. coli carrying* CTX-M resistance genes could be detected on DNA microarray chips.

Katharina Sollweck, Philipp Streich

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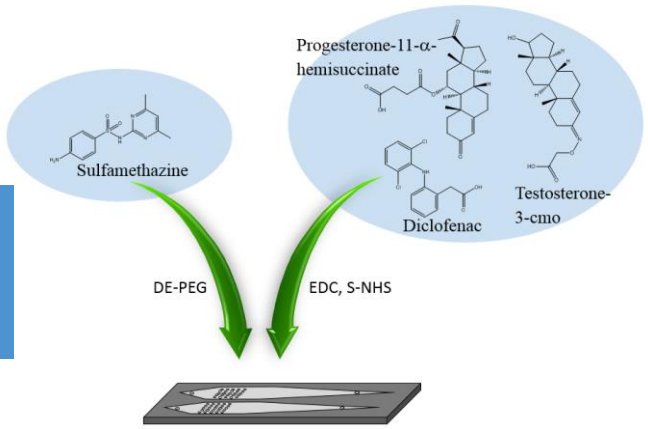
(1) Kunze, A.; Dilcher, D.; Abd El Wahed, A.; Hufert, F.; Niessner, R.; Seidel, M., On-chip isothermal nucleic acid amplification on flow-based chemiluminescence microarray analysis platform for the detection of viruses and bacteria. Anal. Chem. 2015, 88, 898–905.

Funding
IGGSE

Cooperation

A regenerable immuno-chip enabling simultaneous detection of chemically diverse small molecules in a single detection step.

By now it is possible to simultaneously detect 13 different antibiotics in complex matrices like milk and surface water with the MCR 3, an automated microarray chip reader, developed at the IWC. But not only the identification of antibiotics is important, there are several other contaminants which need to be monitored. The former immobilization strategy was to use epoxy-activated Jeffamine ED-2003 glass chips for all antibiotics.[1] In this project we aim to develop a strategy for directed immobilization of diverse small molecules depending on their functional groups.



Schematic immobilization strategy for analytes with different reactive groups on the same surface using different crosslinking strategies.

State of the Art Multiplexing the analysis of diverse molecules is a difficult task. Especially if the size and chemical properties vary a lot. Usually, mass spectrometry measurements are performed to tackle this problem. Immunoassays show a great advantage due to their lower cost and ease of performance.

Analytical Approach In this project, the used platform is a fully automated chemiluminescence-based microarray chip reader (MCR3). The chosen analytes are diclofenac, progesterone, testosterone and sulfamethazine. Having different reactive groups, different crosslinking strategies to the chip surface are being used. The glass surface of the microarray is modified to expose amino groups of a polyether amine. The amino-group of sulfamethazine is immobilized using an intermediate layer of poly(ethylene glycol)diglycidyl ether while the other analytes are immobilized by sulfo-NHS and EDC as crosslinkers between the amine group on the surface and the carboxy-group of the analytes. The compounds are detected via HRP-labelled antibodies creating chemiluminescence.

Results We could show the successful immobilization of the mentioned analytes while using the methods described above.

Katharina Sollweck, Andreas Auernhammer, Fabio di Nardo

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Funding

IWC-funding

Cooperation

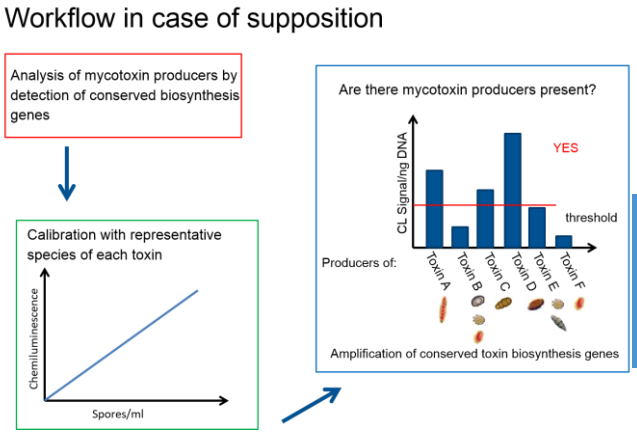
Fabio di Nardo, Turin

A chemiluminescence-based microarray chip for the detection of mycotoxin producers in indoor air

In industrialized countries, a big part of people‘s lifes is spent indoors. Indoor mold as a cause for allergies and infections is long known but hardly dealt with. Also, the fact that indoor molds can produce very harmful mycotoxins is largely undervalued. Mycotoxins are small volatile secondary metabolites produced by fungi which can cause disease and even death in humans. Little is known about the quantity and occurrence of these in indoor scenarios. We are aiming to develop a molecular, rapid and reliable technique for the detection of mycotoxin producers.

State of the Art To date the most commonly used methods to test for fungal contamination in indoor air are culture-based or microscopy methods which are relatively inaccurate. They often estimate wrong numbers due to spores aggregating or not being culturable. Also, these methods mostly do not give information about possible mycotoxin production.

Analytical Approach The aim of this work is to provide a fast and reliable molecular biological method to specifically detect mycotoxin producers amongst indoor air contaminants. For this, an isothermal recombinase polymerase amplification assay[1] on a microarray chip is being developed. In case of supposed fungal contamination, this DNA-based Chip can be used to identify toxin producers. A mycotoxin biosynthesis gene is amplified on the chip surface where the amplicon can directly be detected via chemiluminescence. In the future, many different genes are planned to be detected.



Overview of the DNA-based method for the quantification of mycotoxin producers in indoor air. First, the system must be calibrated by spore numbers for a representative mycotoxin producer and the respective gene. For every gene, this needs to be repeated. In the end, an overview over the potential risk of mycotoxin production or presence can be generated.

Results As a proof of principle, we were able to amplify a zearalenone biosynthesis gene from *Fusarium culmorum* on the DNA-chip. This amplification was successfully calibrated in a spore-dependent manner.

Katharina Sollweck, Gerhard Schwaiger

References
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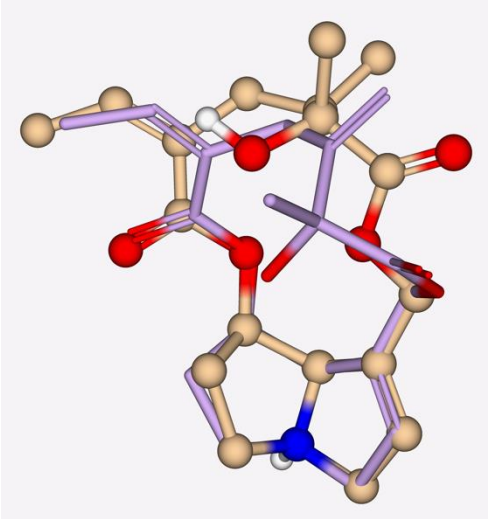
Funding
AIF-ZIM

Cooperation
Domatec GmbH

Development of an immunological screening method for the determination of toxicologically relevant pyrrolizidine alkaloids in herbal tea and related matrices

Structurally diverse and ubiquitous toxicologically relevant pyrrolizidine alkaloids (PAs) have gained increasing interest due to their occurrence in a wide range of plant-based food and feed sources. Food industry is requested to keep PA concentrations at a minimum as legal regulations are expected to be implemented prospectively. Therefore, a screening method is requested for cost- and time-effective monitor-ing of unprocessed plant resources. In this context, bioanalytical methods based on immunological detection of the alkaloids are most suitable.



Alignment of seneciphylline (purple, reference structure) and senecionine with retronecine as basic structure; N = blue, O = red, H = white.

State of the Art PAs are naturally occurring alkaloids. They are suspected to occur in more than 6000 plant species as a defence mechanism against herbivores. Worldwide more than 660 PAs including corresponding N-oxides (PANOs) can be identi-fied. In particular the 1, 2-unsaturated PAs are metabolized to highly reactive pyrrole esters, which form harmful DNA- and protein adducts. Therefore, their occurrence in human food sources (e.g. herbal tea) is undesired. The aim of this project is to develop and validate an immunological screening method for the determination of toxicologically relevant PAs, in particular retronecine-based alkaloids.

Analytical Approach Based on the necine base retronecine, suitable hapten-protein conjugates were synthesized and used for the generation of a monoclonal antibodies (mab). After screening, the most suitable monoclonal antibody was extensively characterized and used for the immunoassay development.

Results For the first time, a highly sensitive (ppb-range) indirect competitive ELISA for retronecine was developed. Further, cross-reactivity testing showed high binding affinity for complete retronecine-PAs but not for heliotridine- and otonecine-based compounds. The elucidation of the antigenic determinant (epitope) was performed by molecular modelling techniques. Possible matrix interferences were investigat-ed. Numerous plant-based extracts with/without preliminary sample preparation (SPE) were analysed, and results validated using LC-MS. Finally, first experi-ments focused on synthesis of molecularly imprinted polymers (MIPs) for higher selective SPE and preparation of a cost-effective lateral flow assay (dipstick) for rapid on-site analysis revealed promising results.

Katharina Zirngibl, Dietmar Knop

Funding

FEI – Research Association of the German Food industry (AiF 19010N)

Cooperation

Prof. Gareis & Dr. Gottschalk, Chair of Food Safety, Veterinary Faculty, Ludwig-Maximilians-University (LMU)

ISOTOPES 2019
The Cross-Disciplinary Conference on Stable Isotope Sciences

Organizing and hosting the biannual international conference ISOTOPES 2019 in July made the year 2019, as well as the historical venue in Raitenhsaslch, memorable for us.

With a long tradition of 20 years of bringing together scientists from vast range of disciplines interested in stable-isotope research, we continued this tradition in the 11th Isotopes conference to cover diverse topics spanning from computational and organic chemistry, enzymology, analytical chemistry, to environmental sciences and pollutant dynamics.

(Front Left to Right)

(Front Row) Florian Einsiedl, Reinhard Niessner, Mathew J. Vetticatt, Sam Hay, Nigel Scrutton, Harald Hertle, Gerhard Zinsberger, Katherine H. Freeman, Vicent Moliner, Thomas B. Hofstetter, Martin Elsner, Rani Bakkour, Torsten C. Schmidt, Gérlad Remaud, Steven D. Schwartz, Daniel O'Leary, Ian Williams

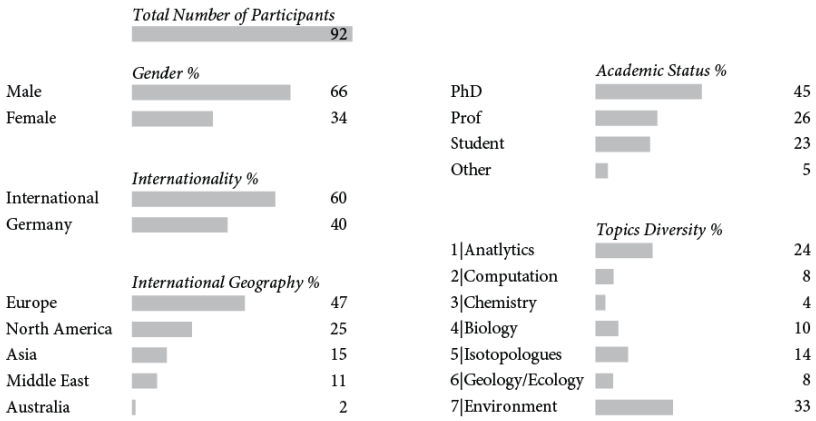
(Middle Row) Min Zhu, Steffen Kümmel, Jing Wei, Elizabeth Phillips, Agnieszka Dybala-Defratyka, Faina Gelman, Aileen Melsbach, Christina Lihl, John Glancy, Jeremy Zimmermann, Joachim Mohn, Andreas Hilkert, Roland A. Werner, Hilary Stuart-Williams, Andrew J. Bennet, Christine Beese, Andrea Watzinger, Natalia Ivleva, Natalia Malina, Oleksii Morgaienko, Charlotte E. Bopp, Mehdi Gharasoo, Nadav Knossow, Almog Gafni, Julian Renpenning, Martin Jiskra, Michaela Löffler, Ivonne Nijenhuis, Ann Sullivan Ojeda

(Back Row) Anja Wunderlich, Tetyana Gilevska, Thomasz Kuder, Fengchao Sun, Caroline Poyntner, Gabriel Sigmund, Marco Farren-Dai, Samantha Hardman, Kristýna Kantnerová, Joanna Rupacher, Renaat van Geel, Daniel Buchner, Jurgen Schleucher, Tobias Hesse, Thomas Piper, Youping Zhou, Cornelia Popp, Sarah Willach, Jens Terhalle, Deb Jaisi, Christian Ostertag-Henning, David Glöckler, Matthias Gehre, Simon Leitner, Philip Martin, Christopher Wabnitz, Johannes Büsing, Stefan Haderlein

Photo of the conferees taken on July 9th ,2019 in front of the building TUM Science & Study Center Raitenhaslach

The scientific background of the participants reflected the cross-disciplinary nature of the conference. *Advances in Analytics* represented 22/92 (24%), *Computation & Theory* 7/92 (8%), *Isotope Effects in Chemistry* 4/92 (4%), *Isotope Effects in Biology and Enzymology* 9/92 (10%), *Isotopologues* 13/92 (14%), *Earth/Planetary Sciences, Biogeochemistry and Ecology* 7/92 (7%), and *Environmental and Water Chemistry/Microbiology* 30/92 (33%). Also, the international share of the participants was significant at the conference (55/92, 60%), whereas participants from German institutions comprised the rest (37/92, 40%). Excluding Germany, the international representation was mostly European (26/55, 47%), followed by North

American (14/55, 25%), Asian (8/92, 15%), Middle Eastern (6/55, 11%), and Australian (1/55, 2%).



Participants distribution of gender, internationality, geography, academic status and topic diversity

What stands out in retrospective is, on the one hand, the breadth of topics covered, which is a telling indication of the central role that isotope effects/isotope distributions are playing in almost all fields of natural and life science. On the other hand, the continuous refinement of theoretical understanding and the enabling role of instrumental advances reflect the maturity of a discipline that no longer is a stand-alone scientific community, but has blended into multiple areas of applied research. We are proud to have attracted it for the first time to Germany and look forward to the next meetings in the upcoming years.

Martin Elsner, Rani Bakkour

HABILITATION Dr. Natalia P. Ivleva
Raman Microspectroscopy for Environmental Analysis

"Everything in life is vibration", Dr. Ivleva proudly quotes Albert Einstein to express her passion for Raman microspectroscopy.

Dr. Natalia P. Ivleva

(R. Bakkour) Congratulations on your success Natascha. Would you tell us the essence of your work habilitation?
(N. P. Ivleva) Thank you Rani. In my habilitation work, I present new application fields for Raman microspectroscopy (RM) along with thorough discussions on the feasibility and limitations of the methods with the focus on the analysis of soot, microplastic and nanoplastic particles as well as microorganisms and biofilms.

(R. Bakkour) What is the advantage of Raman Microspectroscopy (RM) for such environmental applications?
(N. P. Ivleva) RM has been shown to be an efficient technique for the characterization of the nanostructure of combustion aerosol particles, and, therefore it is well suited for the prediction of the structure-related reactivity of e.g., (bio)diesel soot samples. Take another anthropogenic pollutants like microplastics and nanoplastics, they have been found in the environment and food, but the degree of contamination remains uncertain. Beside identification power we can achieve with RM, automated RM-based analysis can in fact enable us to reliably quantify those plastic particles down to 1 µm and even below.

(R. Bakkour) Besides microplastic and particles, your work developed more environmental applications, right?
(N. P. Ivleva) Yes, indeed. RM and surface-enhanced Raman scattering in combination with the stable isotope approach are shown to be an emerging tool for the nondestructive 2D & 3D characterization of the molecular and isotopic composition of microorganisms on the single-cell level, which can enable *in situ* investigations of ecophysiology and metabolic functions of microbial communities.

(R. Bakkour) We all know that you have a lively working group we admire you for leading. I'm certain you would like to say something to them.
(N. P. Ivleva) For sure, I would like to thank Prof. Dr. Reinhard Niessner, former director of IWC, who helped me to find the right way in analytical and environmental chemistry. I warmly thank also Prof. Dr. Marin Elsner who gave me an opportunity to continue my research at the institute and to further build up my Raman and SEM group. I also would like to thank IWC group leaders – PD Dr. Michael Seidel, PD Dr. Thomas Baumann and Prof. Dr. Christoph Haisch for their support. In particular, I want to thank current and former member of my group – Philipp M. Anger, Elisabeth von der Esch, Oleksii Morgaienko, Christian Schwaferts, Ruben Weiss, Dr. Carolin Hartmann, Dr. Patrick Kubryk, Dr. Alexandra Wiesheu as well as former PhD students of Aerosol and Laser groups. They helped me enormously in realizing my ideas and projects, and in developing new research topics in very positive and inspiring atmosphere.

Click here to access Dr. Ivleva's habilitation thesis.

Natalia P. Ivleva, Rani Bakkour

Alumni day – Institute of Hydrochemistry and Isotope Group at IGÖ

June the 26th marks the day of the first alumni day held under the auspices of Prof. Martin Elsner. It was therefore also the first joint alumni day of the institute of hydrochemistry and the isotope group from the IGÖ.

The day started early afternoon with a session of alumni sharing their career path with the current PhD students and the IWC staff. The session was started by an encouraging talk about early career obstacles by Gerhard Pappert who is working as an independent Science Writer. Followed by Jan Wolf who told us about his way from the scientific laboratory to successfully founding his own company, named Plasmion. After a short break Kerstin Krause from Sandoz gave valuable insights to various positions at a globally operating pharma company. The session was completed by Rüdiger Düsing who focused on the impressive cutting edge technology he is working on at Zeiss. The effort of the speakers was acknowledged by a

Alumni of the institute of hydrochemistry and the isotope group at the IGÖ together with the current members of the Insitute of hydrochemistry and the isotope group.

plethora of questions directly after their talk and continued at the latter part of the event. All of the speakers were also awarded with a special IWC version of a famous board game, customized to “Das verrückte IWC” by Sebastian Wiesemann, Elisabeth von der Esch and countless helping hands.

After the career insights all of the alumni met at the meadows in front of the IWC building for a joint dinner and cold drinks. A short tour through the building gave the opportunity to share all the good memories about the lively time working in science which brings us altogether.

We were impressed about the number of alumni who are still interested in the institute and even more impressed (but not surprised) about the helpfulness of the people working at the IWC including the permanent staff and the current Post Doc, PhD and master students.

Philipp M. Anger, David Bauer, Jessica Beyerl

Publications

Peer-Reviewed Journals

Anger, P. M.*; Prechtl, L.*; Elsner, M.; Niessner, R.; Ivleva, N. P., Implementation of an open source algorithm for particle recognition and morphological characterisation for microplastic analysis by means of Raman microspectroscopy. *Analytical Methods* 2019**,** *11*, (27), 3483-3489. *Shared 1st authorship.
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Conference Contributions

Oral Presentations

Elsner, M. Bestimmung von Umweltverschmutzungen in Wasserschutzgebieten durch Isotopenanalyse. *DVGW-Wassertreff Hof- Regionale Leitveranstaltung Trinkwassergewinnung und Qualitätsmanagement für Mitteldeutschland und Bayern*, 22.-23.5.2019, Hof, Germany

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Ivleva, N. P. Anwendbarkeit der Raman-Mikrospektroskopie in der Wasseranalytik. 13. Weihenstephaner Seminar für Wassertechnologie, 12.-13.09.2019, Freising, Deutschland

Ivleva, N. P. Raman microspectroscopy for environmental analysis. *Division of Geological and Planetary Sciences*, *California Institute of Technology (Caltech)*, 20.09.2019, Pasadena CA, USA

Ivleva, N. P. Raman microspectroscopy for identification and quantification of microplastics: Applicability and limitations, state-of-the-art of analytical methods for reliable detection of micro- and nanoplastics. European Commission. *Joint Research Centre EU*, 13.-14.5.2019, Ispra, Italy

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Schwaferts, Sogne, Drexel, Meier, Klein, Niessner, Elsner, Ivleva 2019. Kopplung von Asymmetrischer Fluss-Feldflussfraktionierung und Raman-Mikrospektroskopie für die Analyse von Submikrometer-Plastik. *ANAKON 2019*, 25.-29. März 2019, Münster, Deutschland.

Sollweck, K.; Seidel, M., Mikroarray-basierte Messmethoden zur schnellen Identifizierung von Schimmelpilzen und deren Mykotoxine aus Innenraumluft. *ANAKON*, 25.-28.3.2019, Münster, Germany.

Sun, F.; Melsbach, A.; Wang, Z.; Bakkour, R.; Gharasoo, M.; Mellage, A.; Griebler, C.; Thullner, M.; Cirpka, O.S.; Elsner, M. Exploring mass transfer limitation in organic micropollutant biodegradation: Combined insight from compound-specific isotope analysis (CSIA) and reactive transport modelling. *AGU Fall Meeting 2019*, 9.12. - 13.12. 2019, San Francisco, USA

Sun, F.; Melsbach, A.; Wang, Z.; Gharasoo, M.; Griebler, C.; Thullner, M.; Cirpka, O.S.; Elsner, M. Bioavailability as bottleneck for biodegradation of organic micro pollutants in groundwater? – Evidence from compound-specific isotope analysis in two-dimensional tank experiment. *EGU General Assembly 2019*. 7.4.-12.4.2019, Wien, Austria

von der Esch, E.; Anger, P. M. Baumann, T.; Nießner, R.; Elsner, M.; Ivleva N. P. 2019. Raman-Mikrospektroskopie für die Einzelpartikel-Analyse von Mikroplastik. *ANAKON 2019*. 25.-29. März 2019, Münster, Deutschland

von der Esch, E.; Anger, P. M.; Baumann, T.; Nießner, R.; Elsner, M.; Ivleva N. P. 2019. Raman microspectroscopy as a tool for microplastic particle analysis. *EGU General Assembly 2019*. 7.-12. April 2019, Vienna, Austria

Poster Presentations

Ehrl, B.; Kundu, K.; Marozava, S.; Gharasoo, M.; Mogusu, E. O.; Kim, K.; Hofstetter, H; Pedersen, J.; Elsner, M.; Membrane permeability: an overlooked bottleneck for micropollutant degradation at low concentrations?. *TransCon 2019.* 29.4-3.5.2019 in Monte Veritá, Ascona, Switzerland

Gafni, A.; Lihl, C.; Elsner, M.; Ronen, Z. Gleman, F.; Bernstein, A.; Carbon and nitrogen isotope fractionation along degradation of the nitrile herbicide Bromoxynil. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

Glöckler, D.; Bakkour, R.; Wabnitz, C.; Sigmund, G.; Seidel, M.; Elsner, M.; Graphen-modifizierte Polymermonolithe für die Extraktion von Mikroschadstoffen aus großen Probenvolumina für die substanzspezifische Isotopenanalytik, *Wasser* 2019. 27.-29. Mai 2019, Erfurt, Deutschland. **Posterpreis 2. Platz**

Glöckler, D.; Bakkour, R.; Wabnitz, C.; Sigmund, G.; Seidel, M.; Elsner, M.; Graphene-modified polymer monoliths for high throughput extraction of micropollutants for compound-specific isotope analysis. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany. **Poster Prize 4th Place**

Glöckler, D.; Elsner, M.; Compound-specific stable isotope analysis (CSIA) to detect pollutant degradation in groundwater. *DVGW-Wassertreff Hof- Regionale Leitveranstaltung Trinkwassergewinnung und Qualitätsmanagement für Mitteldeutschland und Bayern*, 22.-23.5.2019 in Hof

Göpfert, L.; Elsner, M.; Seidel, M., Kulturunabhängige Detektion von antibiotikaresistenten bakteriellen Pathogenen aus Oberflächenwasser. Tagung Wasser 2019, 27.-29.5.2019, Erfurt, Germany

Heller, S. ; Neumair, J.; Sollweck, K.; Papanakli, L., Würstle, S., Obermeier, A., Burgkart, R., Seidel, M., Schmid, R., Elsner, M., Schneider, J., Rapid enrichment for pathogen detection in human body fluids by monolithic affinity filtration. *IGSSE Forum*, 24.-26.6.2019, Raithenhaslach, Germany

Kober, C.; Lück, C.; Zamfir, M.; Herr, C.; Seidel, M. Rapid detection of *Legionella pneumophila* as a screening tool for an improved outbreak management. 20. HRWM, 15.-20.9.2019, Vienna, Austria

Kundu, K.; Ehrl, B. N.; Gharasoo, M.; Marozava, S.; Merl-Pham, J.; Griebler, C.; Elsner, M.; Defining lower limits of biodegradation: Isotope fractionation in chemostat reveals rate-limiting mass transfer triggering physiological adaptation. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

Lihl, C,; Douglas, L. M.; Franke, F.; Perez de Mora, A.; Meyer, A. H.; Daubmeier, M.; Edwards, E. A.; Nijenhuis, I.; Sherwood Lollar, B.; Elsner, M.; Mechanistic dichotomy in bacterial trichloroethene dechlorination revealed by carbon and chlorine isotope effects. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

Lihl, C.; Repenning, J.; Schürner, H.; Daubmeier, M.; Heckel, B.; Melsbach, A.; Gehre, M.; Elsner, M.; Synthesis and characterization of a calibration standard for stable chlorine isotope analysis. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany. **Poster Prize 2nd Place**

Melsbach, A.; Elsner, M.; Instrumental modifications of a gas chromatograph-isotope ratio mass spectrometer towards sensitive and accurate carbon isotope analysis of micropollutants. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

Melsbach, A.; Torrentó, C.; Ponsin, V.; Lachat, L.; Prasuhn, V.; Hofstetter, T. B.; Hunkeler, D.; Elsner, M.; $^{13}C/^{12}C$ and $^{15}N/^{14}N$ isotope analysis of desphenylchloridazon to investigate its environmental fate in a systematic field study. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

Morgaienko, O.; Marozava, S.; Klein, P.; Schwaferts, C.; Elsner, M.; Ivleva, N. P., Combining of BONCAT (bioorthogonal noncanonical amino acid tagging) and SERS (surface enhanced Raman scattering) for characterization of bacteria degrading organic pollutants. *ANAKON 2019*, 24.-28.03.2019, Münster, Germany

Morgaienko, O.; Marozava, S.; Klein, P.; Schwaferts, C.; Elsner, M.; Ivleva, N. P., Coupling of BONCAT (bioorthogonal noncanonical amino acid tagging) and SERS (surface enhanced Raman scattering) for characterization of active cells. *Isotopes 2019*, 07.-10.07.2019, Reitenhaslach, Germany

Neumair, J.; Heller, S.; Sollweck, K.; Papanakli, L.; Würstle, S.; Obermeier, A.; Schmid, R.; Schneider, J.; Elsner, M.; Seidel, M., Rapid enrichment for pathogen detection in human body fluids by monolithic affinity filtration (REP-MAF). *AC@TUM*, 25.-26.07.2019, Burghausen, Germany

Schwaferts, C.; Niessner, R.; Elsner, M.; Ivleva, N. P. Detection and identification of submicrometer plastic particles using Raman microspectroscopy and scanning electron microscopy. *ANAKON 2019*. 25.-29. März 2019 in Münster. **Poster Prize 1st Place**

Schwaferts, Niessner, Elsner, Ivleva, 2019. Detektion und Identifizierung von Subµ-Plastikpartikeln mit Raman-Mikrospektroskopie. *Wasser 2019*. 27.-29. Mai 2019, Erfurt, Deutschland

Sollweck, K.; Schwaiger, G.; Elsner, M., Seidel, M.; A chemiluminescence based microarray detection system for mycotoxin producers in indoor air. VDI/BAuA Expert Forum, Bioaerosols: From measurement to assessment, 27.-28.11.2019, Berlin, Germany

Sollweck, K.; Schwaiger, G.; Shimaj, E.; Streich, P.; Elsner, M.; Seidel, M.; Chemiluminescence based microarray detection systems for environmental contaminants. *AC@TUM*, 25.-26.7.2019, Raithenhaslach, Germany

Sun, F.; Melsbach, A.; Wang, Z.; Bakkour, R.; Gharasoo, M.; Mellag, A.; Griebler, C.; Thullner, M.; Cirpka, O. A.; Elsner, M.; Bioavailability as bottleneck for biodegradation of organic micro-pollutants in groundwater? – Evidence from compound-specific isotope analysis in two-dimensional tank experiment. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

von der Esch, E.; Anger, P. M.; Baumann, T.; Niessner, R.; Elsner, M.; Ivleva, N. P. 2019. Raman microspectroscopy as a tool for microplastic particle analysis. *EGU General Assembly 2019*, 7.-12. April 2019, Vienna, Austria. **Outstanding Student Poster and PICO (OSPP) Award winner**

von der Esch, E.; Lanzinger, M.; Elsner, M. Ivleva, N. P. 2019 Herstellung von sekundärem Mikroplastik zur Methodenentwicklung. *Wasser 2019*, 27.-29. Mai 2019, Erfurt, Germany

Wabnitz, C.; Bakkour, R.; Glöckler, D.; Elsner, M.; Selective extraction of pesticides from surface water using crosslinked cyclodextrin polymers. *ISOTOPES 2019*, July 7 – 12, 2019, Raitenhaslach, Germany.

Invited Lectures

Elsner, M.: Exploring transformation pathways and limits of biodegradation by stable isotope fractionation. *8th Late Summer Workshop of the Water Chemistry Society,* 22.-25.9.2019, Haltern, Germany (Plenary Talk)

Elsner, M.; Compound-specific isotope analysis (CSIA): Perspectives to study reaction mechanisms in complex systems. *Isranalytica.* 21.-24.1.2019, Tel Aviv, Israel (Plenary Talk)

Elsner, M.; Heckel, B.; Lihl, C.; Mehlsbach, A.; Sun, F.; Ehrl, B.; Gharasoo, M.; Marozava, S.; Kundu, K.; Ivleva, N.; Bakkour, R.; Reaktive Spione in chemischen Substanzen: Stabilsotopen als Schlüsselanalyten zur Prozessaufklärung in komplexen Systemen. *ANAKON.* 25.-28.3.2019, Münster, Germany (Plenary Talk)

Elsner, M.; Heckel, B.; Lihl, C.; Melsbach, A.; Sun, F.; Ehrl, B.; Gharasoo, M.; Marozava, S.; Kundu, K.; Ivleva, N.; Bakkour, R.; Reactive tracers in chemical substances: Analysis of stable isotopes to elucidate processes in complex systems. *Seminar of the Joint Mass Spectrometry Centre*, Universität Rostock, 7.5.2019, Rostock, Deutschland

Haisch, C.: A QCL-based photoacoustic sensor for online monitoring of N_2O emissions of wastewater treatment plants. *SCIX 2019*, 13.-18.08.2019, Palm Springs, California, USA

Haisch, C.; Bauer, D.; Qui, L.; Magistro, G.; Stief, C.; Wieser, A.: "Deuterium uptake as Raman-based antibiotic susceptibility test in a clinical scenario"

Ivleva, N. P. Applicability of Raman microspectroscopy for environmental analysis. *University Tübingen*, 5.6.2019, Tübingen Deutschland

Ivleva, N. P. Applicability of Raman microspectroscopy for environmental analysis. *Institute of Biogeochemistry and Pollutant Dynamics, Swiss Federal Institute of Technology (ETH) Zurich*, 29.10.2019, Zürich, Switzerland

Ivleva, N. P. Raman microspectroscopy in analytical chemistry. *Universitäres Zentrum für Gesundheitswissenschaften am Klinikum Augsburg - UNIKA-T*, 7.6.2019, Augsburg, Deutschland

Kober, C.; Gründel, A.; Bemetz, J.; Petzold, M.; Sollweck, K.; Zamfir, M.; Heese, C.; Herr, C.; Lück, C.; Niessner, R.; Seidel, M., Legionellenschnelltest: Stand der Forschung. *TÜV Süd*, 17.9.2019, München, Germany

Niessner, R. Modern spectroscopy as a tool for aerosol characterization, University of Vienna, *Summer School Basic Aerosol Science, Aerosol Physics & Environmental Physics*, 4.7.2019, Vienna, Austria

Niessner, R. Particles – A challenge (not only) for analysts, University of Gothenburg, Dept. of Chemistry, 16.5.2019, Gothenburg, Sweden

Niessner, R. Täglich nervt der Grenzwert! Dieselabgase messen, aber richtig, *TELI-Jour-fix/Internationaler Presse Club München*, 26.2.2019, Munich, Germany

Seidel, M., Automated bioanalytical methods to control water treatment and aquatic environments. *University of Stuttgart*, 14.5.2019, Stuttgart, Germany

Seidel, M., Microarray-based methods for cultivation-independent detection of pathogenic bacteria and viruses. *Heinz-Nixdorf-Lectures at TranslaTUM*, 5.2.2019, München, Germany

Seidel, M., Schnellnachweis von Pathogenen im Wasser. *DVGW-Wassertreff Hof*, 23.5.2019, Hof, Germany

Scientific Committees, Memberships, and Consulting

Bakkour, R.

ISOTOPES 2019, The Cross-Disciplinary Conference on Stable Isotope Sciences
July 7 – 12, 2019, Raitenhaslach, Germany
(Co-organizer, Scientific Advisory Board Member, & Session Convenor *Advances in Analytics*)

International Atomic Energy Agency - Training workshop on isotope techniques in ecological, food, and environmental research
29-30 January, 2019, Ljublijana, Slovenia
(Trainer)

Elsner, M.

die Junge Akademie der Europäischen Wissenschaften
(Member)

ISOTOPES 2019, The Cross-Disciplinary Conference on Stable Isotope Sciences
July 7 – 12, 2019, Raitenhaslach, Germany
(Organizer)

Journal of Isotopes in Environmental and Health Studies
(Editorial Member)

Wasserchemische Gesellschaft, Fachgruppe der GDCh
(Board Member)

Haisch, C.

Condensed Matter Physics laboratory at the Ecole Polytechnique
29 Oct 2019, Paris, France
(PhD Thesis Committee Member)

SCIX 2019
13.-18. Oct 2019, Palm Springs, California, USA
(Session Convener)

Ivleva, N. P.

DIN-Normenausschuss NA 054-01-06 AA „Kunststoffe und Umweltaspekte“
(Expert)

ISO/TC 61/SC 14 "Plastics and Environment" / WG 4 „Microplastics“
(Expert)

Niessner, R.

DECHEMA (Society for Chemical Engineering and Biotechnology), ProcessNet-AMA-Fachgruppe Mess- und Sensortechnik,
Frankfurt, Germany
(Appointed Member)

European Research Council
Brussel (EU)
(Appointed Panel Member)

German Federal Institute for Risk Assessment (BfR), Standing Commission on Safety of consumer products
Berlin, Germany
(Appointed Member)

Journals of Analytical Sciences, Analytical & Bioanalytical Chemistry, Fresenius Environmental Bulletin, International Journal of Environmental Analytical Chemistry, Talanta, Toxicological & Environmental Chemistry
(Advisory Board Member)

Seidel, M.

Expert Committee at the Wasserchmische Gesellschaft - Pathogens and Antibiotic Resistant Bacteria in the Water Cycle
Since November 2019, Germany
(Chairman)

Awards

Reinhard Niessner: Clemens – Winkler-Medal, German Chemical Society, Analytical Division, University of Münster, 25.3.2019

Theses

Habilitation

Dr. Natalia Ivleva; Raman Microspectroscopy for Environmental Analysis, October 2019

PhD Theses

MSc Chem. Aileen Melsbach,: Sensitive Isotope Analysis of Micropollutants in Complex Sample Matrices

MSc Chem.-Ing. Jonas Bemetz: Folienbasierter Mikroreaktor für die NMR-relaxometrische online-Charakterisierung magnetischer Nanopartikel und flussbasierte Mikroarrays

Exam. Lebensm. Chem. Carolin Hartmann: Zerstörungsfreie Analyse des Eisenkerns von Ferritin und Magnetoferritin mittels Raman-Mikrospektroskopie

MSc Biochem. Stefanie Mak: Incorporation of Platelet Glycoprotein Receptors into Lipid Bilayer Nanodiscs for the Detection of Autoantibodies in Autoimmune Thrombocytopenia

M.Sc. Theses

Merlin Junk, BSc Chem.: Bestimmung des Einflusses der Alterung auf die Detektierbarkeit von Mikroplastik mittels Raman Mikrospektroskopie, Oktober 2018 - May 2019

Oliver Jacob, BSc Chem.: Automatisierte Detektion von Mikroplastik in Kläranlagen, since Novmeber 2019

BSc Elisabeth Ackermann: Combination of Monolithic Adsorption Filtration with Antibody- and DNA-based Microarray Methods for the Detection of *Legionella pneumophila* in Tap Water

BSc Matthias Bauer: Laser Ablation for Aerosol Generation

BSc Jorge Guajardo: Development of Detection Method of Extracellular Vesicles from Urine by Monolithic Adsorption Filtration and Recombinant Nanobodies

BSc Michael Hofmann: Analysis of Transformation Products after the Ozonation of Trace Organic Compounds

BSc Merlin Junk: Influence of Humic Substances on Detectabilitiy of Microplastics via Raman Microspectroscopy

BSc Julia Klüpfel: Quantification of *Pseudomonas aeruginosa* in Tap Water Samples after Concentration by Monolithic Adsorption Filtration

BSc Leonhard Prechtl: Development of an Effect Orientated Analytical Method by Coupling of a Neurotoxicity Assay with LC-MS

BSc Gerhard Schwaiger: Detection of Mycotoxin Producers in Indoor Air Via a Microarray-assisted Amplification

BSc Yasmin Selic: Raman-Investigations of Protein Expression by Bacteria

BSc Elmedina Shimaj: New Strategies for Bioanalytical Quantification of Diclofenac

BSc Daniel Toller: Investigating Dehalogenation of Chlorinated Ethanes with Vitamin B12 and Inorganic Degradants using Compound-Specific-Isotope-Analysis

BSc Andreas Vohburger: Application of a Novel Mass Spectrometry System for Exhaust Gas Analysis

BSc Christopher Wabnitz: Selective Extraction of Pesticides from Surface Water for Carbon Isotope Analysis using Crosslinked Cyclodextrin Polymers

BSc Markus Weber: Laser-induced Breakdown Spectroscopy (LIBS) for the Analysis of Aerosols

B.Sc. Theses

Jin Rui Leong: Testing for Specificity of Primer Sets for the Detection of Mycotoxin Producers on Heterogeneous Asymmetric Recombinase Polymerase Amplification

Yu Rui Leu: Synthesis of Stable Gold Nanoparticles Using Microreactor

Constance Ong: Monitoring of Total Bacteria Count in a Sandfilter Surface Water Model

Hendrik Pfaadt: Crosslinked Cyclodextrins for Pesticide Enrichment from Water - from Synthesis to Evaluation

Anton Podolov: Optimierung von Substanzspezifischer Stabilisotopenanalytik – Charakterisierung der Verbrennung von organischen Substanzen in einem miniaturisierten Nickel-Platin Reaktor

Institute Colloquia

Prof. Dr. Johann Plank, Department of Chemistry, Technical University of Munich: Bauchemie – spannende Chemie zu Zement, Polymeren und Nanomaterialien (18.01.2019)

Dr. Michael Sander, Department of Environmental Systems Science, Institute of Biogeochemistry and Pollutant Dynamics, ETH Zürich: Biodegradation of Synthetic Polymers in Agricultural Soils: Insights Gained from Using Carbon Stable Isotope Labelled Polyesters (25.01.2019)

Prof. Dr. Michael Krautblatter, Department of Civil, Geo and Environmental Engineering, Technical University of Munich: Monitoring, Analysis and Early Warning of Landslides (11.03.2020)

Prof. Dr. Antje Bäumner, Institute of Analytical Chemistry, University of Regensburg: Functional Nanomaterials and (Electro) Chemiluminescent Approaches for Highly Sensitive Detection in Miniaturized Biosensors (17.05.2019)

Prof. Dr. Qingzhi Zhu, School of Marine and Atmospheric Sciences, Stony Brook University of New York: Light Shed on the Dark Side of Sediment - Fine Scale Biogeochemical Heterogeneities and Processes in Benthic Communities Revealed by Planar Optodes (05.08.2019)

Teaching

GIST TUM-Asia

Industrial Chemistry (M.Sc.)

Bioengineering & Bioprocessing; Seidel

Chemical Engineering (B.Sc.)

Biochemical Process Engineering; Seidel

TUM

Chemistry (B.Sc./M.Sc.)

Hydrogeological, Hydrochemical and Environmental Analysis Seminar (Hydrogeologisches, Hydrochemisches und Umweltanalytisches Seminar); Elsner, Baumann, Haisch, Knopp.

Graduate Course in Analytical Chemistry: Lecture in Organic Trace Analysis-Physical and Chemical Separation Methods (Nebenfach Analytische Chemie: Vorlesung Organische Spurenanalytik-Physikalisch-chemische Trennmethoden); Elsner, Seidel, Haisch, Ivleva, Bakkour.

Graduate Course in Analytical Chemistry: Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Kurpraktikum Organische Spurenanalytik); Elsner, Seidel, Haisch, Ivleva, Bakkour

Graduate Course in Analytical Chemistry: Research Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Forschungspraktikum Organische Spurenanalytik); Elsner, Seidel, Haisch, Ivleva, Bakkour

Trace Analysis Techniques (Spurenanalytische Techniken); Elsner, Seidel, Haisch

Environmental Organic Chemistry: Elsner, Bakkour

Biosciences (B.Sc./M.Sc.)

Analytical Chemistry – Separation Techniques, Chemical and Biochemical Sensors (Analytische Chemie – Trenntechniken, chemische und biochemische Sensoren); Knopp

Geosciences (B.Sc./M.Sc.)

Analytical Chemistry I: Instrumental Analysis for Geoscientists (Analytische Chemie I: Instrumentelle Analytik für Geowissenschaftler); Elsner

Analytical Chemistry II – Organic Trace Analysis for Geoscientists (Chemische Analytik II – Organische Spurenanalytik für Geowissenschaftler); Elsner

Contaminant Hydrogeology (Transport von Schadstoffen im Grundwasser); Baumann

Remediation Design (Erkundung und Sanierung von Grundwasser-schadensfällen); Baumann

Technical Hydrogeology (Technische Hydrogeologie); Baumann

Fluidflow in Porous Media Lab (Hydrogelogisches Laborpraktikum); Baumann, Haisch

Hydrogeochemical Modelling (Hydrogelogische Modelierung II); Baumann

Hydrogeological Field Lab (Hydrogeologische Feldmethoden); Baumann

Hydrogeological Mapping (Hydrogeologische Kartierung); Baumann

Hydrogeological and Hydrochemical Field Trips (Hydrogeologische und Hydrochemische Exkursion); Baumann

Water Chemistry I (Wasserchemie I); Elsner

Water Chemistry II – Hydrocolloids, Micellar Systems and Photochemical Transformations (Wasserchemie II – Hydrokolloide, micellare Systeme und photochemische Umsetzung); Elsner

Hydrochemical Lab (Hydrochemisches Praktikum); Haisch, Baumann

Equipment

Hydrogeology

Two pilot scale tanks with flow lengths of up to 10 m allow transport experiments in a controlled environment while preserving almost natural conditions. Apart from studies on the transport behaviour of contaminants and colloids, these facilities are used for testing sensor prototypes and serve as a test bed for numerical models

Großhadern Unsaturated Zone field laboratory (10 m deep)

1 Analytical Autoclave, Büchi Midiclave

Dioxin Laboratory

3 High security labs with locks, separate activated carbon filter and high-performance particle filter systems

Aerosol Research

1 Aerosol chamber (1 m3)

1 Aerosol flow tube (10 L)

1 Ozone analyzer (UV absorption)

1 NO/NO_2

analyser (Chemiluminescence)

2 Aerodynamic particle sizers (0.5-25 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)

2 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 Cyclone Impinger (Coriolis µ, Berlin)

1 Micro soot sensor with dilution unit

Bioseparation

1 Crossflow-ultrafiltration unit (6 m^2 hollow fibre module, Inge-AG)

1 Munich Microorganism Concentrator (MMC 3)

1 Monolithic Affinity Filtration Unit

Microarray Technology

2 Chemiluminescence Microarray Reader (Immunomat, IWC)

4 Chemiluminescence Microarray Reader (MCR 3, GWK GmbH)

1 Ink-Jet Microdispenser (SciFlexarrayer 31, scienion)

2 Contact Microarrayer (BioOdyssee Caligrapher, BioRad)

1 Cutting Plotter (Graphtec CE6000-40)

Microbiology

1 Flow Cytometer (Cell Lab Quanta SC, Beckman Coulter)

1 Flow Cytometer (CyFlow Cube 6, Sysmex Partec GmbH)

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

3 Clean benches

1 Microbiological Incubator (BD 53, Binder)

1 Autoclave (Century 2100, Prestige Medical)

1 Autoclave (SHP Steriltechnik)

1 Bio-2-Aerosol Chamber

Standard Lab Equipment

1 Lyophilizer (Alpha 1-4 LSC, Christ)

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

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

1 Refrigerated Centrifuge (Universal 320R, Hettich)

1 Centrifuge (Eppendorf 5804 R)

1 Climatic chamber (Memmert HCP 108)

2 Fluorescence reader systems, time-resolving

3 Photometric reader systems

1 384-channel washer, Biotek

1 Turbidometer (WTW GmbH)

1 Nanophotometer (Implen GmbH)

Chromatography and Particle Separation

3 GCs with FID, NPD, ECD, TEA, and AED

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

1 GC/MS, VG Autospec

1 GC/MS, Shimadzu

1 Portable Micro-GC, MITEC

1 Asymmetrical Field-flow-fractionation system, Postnova

2 Concentrators for dynamic headspace analysis

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

1 Capillary electrophoresis system

1 Ion chromatograph, Dionex 4500 i

1 Ion chromatograph, Dionex BioLC (Photodiode Array Detector, Electrochemical Detector)

1 Ion chromatograph, Metrohm 881

1 LC system, ECONO

1 Preparative HPLC

1 Zetaphoremeter, SEPHY

Elemental Analysis

1 TXRF, Atomika EXTRA II a

1 Flame-Photometer, Eppendorf ELEX 6361

2 AAS systems with flame atomization, electrothermal atomization, hydrid system, Perkin-Elmer PE 3300, ELAN 4100

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

1 CO_2-laser

3 Dye-laser (tunable with frequency doubler)

5 N_2-laser

8 Diode-lasers (600-1670 nm; up to 2 W CW)

1 Laser diode array with 10 diodes (0.8 µm-1.8 µm)

1 Laser diode with external resonator

2 Optical parameter oscillator (410 nm-2.1 µm)

Optoelectronics/Spectrometer

1 Rowland spectrometer

2 Echelle spectrometer

1 ICCD spectrometer system

1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700

1 Fluorescence spectrometer, Perkin Elmer LS-50

1 Fluorescence spectrometer, Shimadzu RF 540

1 UV/VIS spectrometer, Beckman DU 650

1 UV/VIS spectrometer, analytic jena Specord 250 plus

1 UV/VIS spectrometer, analytic jena Spekol 1500

2 Boxcar integrator

4 Digital storage oscilloscopes (400 MHz, 500 MHz)

3 optical multichannel analysators with monochromators, time-resolving

1 Wavemeter

SEM/Microscopy

1 SEM/EDX system, Zeiss Gemini

1 Polarisation microscope for phase analysis

1 Fluorescence microscope

1 Image analysis software for anutomated image processing

1 Inert gas glovebox

1 Laminar flow box

Raman-Microscopy

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

1 Laser Raman microscope, Renishaw 2000 (514/633/785 nm)

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

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

Sum Parameters

2 Coulostat for C quantification, Coulomat 702

1 DOC analyser, UNOR 6 N

1 TOC analyser, Shimadzu TOC-L

1 AOX/TOX, Sigma

Staff 2019

Director of Institute and Chair

Univ.-Prof. Dr. Martin Elsner

Senior Researchers

Dr. Rani Bakkour
PD Dr. Thomas Baumann (-3/19), external (Fakultät BGU) (4/19-)
Prof. Dr. Christoph Haisch
Dr. habil. Natalia P. Ivleva
PD Dr. Michael Seidel

Post Docs

Dr. Benjamin Heckel
Dr. Genny Pang
Dr. Klemens Thaler (-5/19)
Dr. Martina Ueckert (-12/19)
Dr. Noemi Utry (-12/19)
Dr. Karin Wieland (5/19-)

Technical & Administrative Staff

Birgit Apel
Christine Beese
Roland Hoppe
Joachim Langer (-6/2019)
Susanne Mahler
Cornelia Popp
Hatice Poyraz
Christine Benning
Sebastian Wiesemann

PhD Students

MSc Phys. Emilio Ambra
MSc Chem. Philipp Anger (-8/19)
MSc Chem. David Bauer
MSc Lemi. Irina Beer (12/19-)
MSc Chem. Elisabeth von der Esch
MSc Umwelt-Ing. Lorenza Gilardi (-2/19)
MSc Geo. David Glöckler
MSc Umweltchem. Lisa Göpfert
Exam. Lebensm. Chem. Carolin Hartmann (-1/19)
MSc Geol. Bernhard Köhl
Dipl.-Phys. Peter Menzenbach
MSc Chem. Verena Meyer (-4/19)
Dipl.-Biochem. Oleksii Morgaienko
MSc Chem. Julia Neumair (2/19-)
MSc Chem. Li Qiu
MSc Bio. Christina Lihl (3/19-)
MSc Tox. Aileen Melsbach (3/19-)

MSc Chem. Christian Schwaferts
MSc Biol. Katharina Sollweck
MSc Hydrogeol. Fengchao Sun (8/19-)
MSc Chem. Yanwei Wang
MSc Chem. Ruben Weiß (-2/19)
MSc MBT Katharina Zirngibl

External PhD Students

MSc Chem. Franziska Adler (Stadtwerke München) (3/19-)
MSc Chem. Jessica Beyerl (LMU-Tropeninstitut) (11/18-)
MSc Chem. Matthias Edelmann (TUM, Lebensmittelchem. u. molekulare Sensorik)
MSc Chem. Melina Grasmeier (Klinikum rechts der Isar) (7/19-)
MSc Tox. Anne Landmesser (ABF GmbH München)
MSc Bio. Christina Lihl (Helmholtz Zentrum München) (-2/19)
MSc Biochem. Stefanie Mak (Klinikum rechts der Isar) (-10/19)
MSc Tox. Aileen Melsbach (Helmholtz Zentrum München) (-2/19)
MSc Chem. Janine Potreck (Klinikum rechts der Isar) (2/18-)
MSc Geol. Marina Spona-Friedl (Helmholtz Zentrum München)
MSc Hydrogeol. Fengchao Sun (Helmholtz Zentrum München) (-7/19)
MSc Chem. Markus Weber (Plasmion GmbH Augsburg) (4/19-)
MSc Leb.Chem. Johannes Zwickenpflug (ABF GmbH Planegg) (5/19-10/19)

Master Students

BSc Biochem. Elisabeth Ackermann (-5/19)
BSc Chem. Andreas Auernhammer (10/19-)
BSc Chem. Matthias Bauer (-5/19)
BSc Chem. Carolin Feyerabend (Lehrstuhl Siedlungswasserwirtschaft) (8/19-)
BSc Ind. Chem. Jorge Adrian Guajardo (TUM Asia) (-4/19)
BSc Chem. Ing. Michael Hofmann (1/19-12/19)
BSc Chem. Oliver Jacob (11/19-)
BSc Chem. Merlin Junk (-4/19)
BSc Chem. Julia Klüpfel (4/19-9/19)
BSc Chem. Leonhard Prechtl (4/19-10/19)
BSc Biochem. Gerhard Schwaiger (6/19-12/19)
BSc Chem. Yasmin Selic (3/19-8/19)
BSc Pharm. Elmedina Shimaj (Erasmus) (-8/19)
BSc Chem. Philipp Streich (10/19-)
BSc Daniel Toller (-2/19)
BSc Chem. Andreas Vohburger (4/19-9/19)
BSc Chem. Christopher Wabnitz (4/19-9/19)

Bachelor Students

Nur Atiqah Binte Bedin (12/19-)
Ju Rui Leu (-2/19)
Henrdrik Pfaadt (-3/19)
Anton Podolhov (8/19-11/19)
Constance Ong (1/19-4/19)

Guests

BSc Valerie Hecht (Fakultät BGU) (5/19-12/19)

Dr. Fabio di Nardo (DAAD) (10/19-)
BSc Ayesha Navaid (Fakultät BGU) (4/19-11/19)
Dr. Genny Pang (-5/19)
BSc Sophia Rupp (Fakultät BGU) (4/19-6/19)
Dr. Jan-Christoph Wolf (Plasmion GmbH)
Dr. Klaus Wutz (Plasmion GmbH)

Student Assistants

Ayesha Navaid Anwar (-3/19)
Beatriz von der Esch (10/19-)
Alexander Kohles