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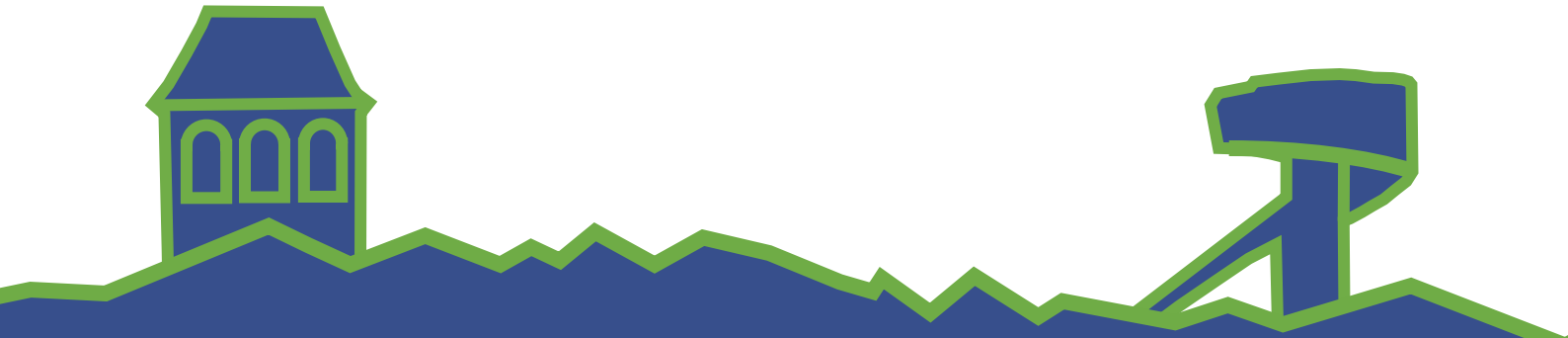
ASAC
AUSTRIAN SOCIETY OF ANALYTICAL CHEMISTRY

JUNG ANALYTIKER:INNEN FORUM 2025

Innsbruck 8.–9. Mai



Young Analysts Forum 2025

Abstract Booklet

BRUKER

FRONTIER LAB

YMC EUROPE GMBH

nu AMETEK

LACTAN Chemikalien und Laborgeräte Vertriebsgesellschaft m.b.H. & Co KG

Agilent

Analysis & Sensing | ASA | Chemistry Europe

SHIMADZU Excellence in Science

Metrohm

adsi Austrian Drug Screening Institute

SCS Swiss Chemical Society Division of Analytical Sciences

KNAUER

Program

Thursday

	Time	Talk	Title	Speaker
	9:30-9:45	Opening		Christian Huck & Christian Klampfl
Session 1: Bioanalysis	9:45-10:30	Plenary Talk 1	Bioanalytics from bench to bedside - how to create tomorrow's in vitro diagnostics	Klaus Weinberger
Session 1: Bioanalysis	10:30-10:45	Oral 1	Identification and label-based quantification of insecticidal crystal proteins of Bacillus thuringiensis by targeted high-resolution LC-MS/MS	Sara Schlachter
Session 1: Bioanalysis	10:45-11:00	Oral 2	Development and implementation of yeast-based reference materials for ion mobility-mass spectrometry	Valeria Mandatelli
Session 1: Bioanalysis	11:00-11:15	Oral 3	Tolterodine as a novel candidate for CYP3A4 activity assessment via metabolic volatiles to predict drug responses	Rebecca Hofer
		Coffee Break		
Session 2: Particles and Metals	11:45-12:00	Industry Talk 1	Identification and Quantification of Microplastics in environmental samples by Pyrolysis-GC/MS	Michael Soll (Frontier Lab)
Session 2: Particles and Metals	12:00-12:15	Oral 4	Tracing Metal Nanoparticle Accumulation in Edible Wild Mushrooms	Andrés Suárez Priede
Session 2: Particles and Metals	12:15-12:30	Oral 5	Investigation of Fluorine-based and Metal Particles Introduced to Food through Non-stick Cookware	Bernhard Grüner
Session 2: Particles and Metals	12:30-12:45	Oral 6	Detection and characterization of secondary micro- and nanoplastics after environmental aging using single particle ICP-MS and OF2i	Manuel Candussi
Session 2: Particles and Metals	12:45-13:00	Oral 7	Quantification of Precious Metals in Oxidic Matrices using Microdroplet-based LA-ICP-TOFMS	Tobias Schöberl
		Lunch @Uni Lounge		
Session 3: Chromatography	14:30-15:15	Plenary Talk 2	Identification and quantification of bio- and eco-toxicological markers by elemental mass spectrometry	Raquel Gonzalez De Vega
Session 3: Chromatography	15:15-15:30	Oral 8	Optimization of liquid chromatography high resolution mass spectrometry for investigation of PFOA and PFOS degradation ability by Pseudomonas strains	Ha Anh Thai
Session 3: Chromatography	15:30-15:45	Oral 9	Elution Revolution: Reversing Chiral Recognition by Swapping D- for L-Cellulose	Anna Florentina Lehrhofer
		Coffee Break		
	16:15-16:30	Industry Talk 2	Analytical Science in Technical Research and Development at Novartis Austria	Christian Kirchler (Novartis)
	16:30-17:00	ASAC Award	MobiLipid: A Tool for Enhancing CCS Quality Control of Ion Mobility–Mass Spectrometry Lipidomics by Internal Standardization	Felina Hildebrand
	17:00-18:00	Posters and Pints		
	19:30	Dinner @mariatheresia		

Friday

	Time	Talk	Title	Speaker
Session 4: Spectroscopy	9:00-9:15	Industry Talk 3	Ideal Stationary Phase and Hardware Combinations for Improved LC/MS Results	Robin Poller (YMC)
	9:15-9:30	Oral 10	Advancing in-situ monitoring of enzymatic reactions via mid-infrared spectroscopy using functionalized silica particles	Katharina Schütz
	9:30-9:45	Oral 11	Raman Spectroscopy for Real-Time Diatomic Trace Gas Detection	Severin Hager-Roiser
	9:45-10:00	Oral 12	Multi-Pathlength Mid-IR Spectroscopy for Optimal Absorbance	Lisa Riedlsperger
	10:00-10:15	Oral 13	The role of quantum chemical calculation in NIR spectral analysis	Justyna Grabska
	10:15-10:30	Oral 14	Label-Free Chemical Spectroscopy of Cancer Cells using O-PTIR	Nikolaus Hondl
		Coffee Break & Casual Poster Session		
Session 5: Materials, Food and Environmental	11:00-11:45	Plenary Talk 3	Mid-IR Laser Spectroscopy	Georg Ramer
	11:45-12:00	Oral 15	Sustainable Innovation Demands Advanced Analysis: Characterizing Paper-Grade Pulps for Next-Gen Fibers	Ivan Melikhov
	12:00-12:15	Oral 16	Chemical Tracing of a Previously Underexplored Off-Odour in Pork Using GC-MS, Sensory Analysis and Statistical Evaluation	Julian Bleicher
	12:15-12:30	Oral 17	Unravelling Photocatalytic Mechanisms in Organic Semiconductors with Time-Resolved Spectroscopy and Mass Spectrometry	Mariia Ferree
	12:30-12:45	Oral 18	LC-IM-HRMS and non-targeted analysis for advancing the investigation of phytosiderophore-metal complexes	Laura Zellner
	12:45-13:00	Closing & Prize Ceremony		Christian Huck & Christian Klampfl
	13:00	Snacks & Conclusion of the Event		

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Session 1:

Bioanalysis

Oral Presentation 1

Identification and label-based quantification of insecticidal crystal proteins of Bacillus thuringiensis by targeted high-resolution LC-MS/MS

Sara Schlachter, Stefano D'Amico, Beatrix Stessl, Martina Ludewig, Elisabeth Reiter, Irmengard Strnad, Evelyn Rampler

University of Vienna

Bacillus thuringiensis (Bt) belonging to Bacillus cereus group is frequently applied in in organic farming due to its ability to produce insecticidal crystal proteins. Products containing Bt are the most important biopesticides in control of insect pest due to their effectiveness, high specificity to the target organism and harmlessness to non-target organisms and environment. The insecticidal proteins produced by Bt can be divided into two classes, depending on whether they are formed in the parasporal inclusions at stationary growth phase (Cry and Cyt proteins) or in the vegetative growth phase (Vip and Sip proteins). The insecticidal proteins differ in their activity and target organism.
Biopesticides containing certain strains of the Bt subspecies spp. kurstaki, spp. aizawai, spp. israelensis and spp. tenebrionis are authorized in the EU and mainly used for vegetables and fruit production. A morphological differentiation between Bt and the foodborne pathogen B. cereus is not possible and not included in routine diagnostics. The incomplete diagnostics lead to products being categorised as unsafe and withdrawn from the market. The loss along the value chain is considerable and does not contribute to a sustainable production. For this reason, an improved and more efficient analysis is required.
The aim of this study is to develop a label-based quantitative targeted LC-MS/MS method for distinction of the different toxins, subspecies and strains of Bt based on specific marker peptides. Commercially available products were

used to characterize insecticidal proteins from the different subspecies; either, directly isolated from products, cultivated on agar plates or applied to various herbs according to the manufacturer's instructions. The proteins were extracted using 50 mM ammonium bicarbonate, pH 10.5, digested by trypsin and resulting peptides purified by SPE. Untargeted DDA and DIA measurement were performed to characterize the protein profile depending on the subspecies and identify specific marker peptides. The sample preparation was optimized in view of extraction solution and enrichment method.

Specific marker peptides could be identified for the three Bt subspecies spp. kurstaki, spp. aizawai and spp. israelensis. Specificity was proofed in silico by BLAST analysis. The Cry proteins, Cry4Aa, Cry4Ba and Cry11Aa, were identified as major insecticidal proteins produced by spp. israelensis. Cry1Ac, Cry2Aa and Cry2Ab, were assigned to the spp. kurstaki, whereas for spp. aizawai Cry1Ad, Cry1Ca and Cry1Da were specific. Cry1Aa and Cry1Ab were identified as major Cry proteins produced by both spp. kurstaki and spp. aizawai.

Based on these results a targeted PRM method was created containing totally 12 peptide sequences, of which four specific peptides were used for differentiation of the subspecies and four shared peptides with their corresponding heavy isotope labeled peptides for absolute quantification.

Oral Presentation 2

Development and implementation of yeast-based reference materials for ion mobility-mass spectrometry

Valeria Mandatelli, Brigitte Gasser, Stephan Hann, Tim Causon

BOKU University

Ion mobility-mass spectrometry (IM-MS) has become increasingly popular in recent years for research and industry purposes, especially in the fields of biotherapeutics, environment and food safety. Based on a rapid separation of ions with respect to the size-to-charge, IM-MS is typically performed between chromatographic separation and a time-of-flight mass analyzer, providing an arrival time distribution that allows derivation of a collision cross section (CCS), which depends on physical characteristics of the ion such as size, charge and conformation. While CCS can be derived for all ions measured in a sample, which makes it a valuable parameter for the identity confirmation of small molecules, standardization for analytical workflows has not yet been established. One potential solution to address this gap is to develop new reference materials suitable for typical bioanalytical applications, using IM-MS. The aim of the project is to develop reference materials based on yeast, developing their production and optimising the workflow to ensure the broadest analytical coverage and suitability for all major commercial IM-MS instruments. Starting from the strain CBS 7435 of Komagataella phaffii (also known as P. pastoris), an industrially relevant yeast that provides a high yield and biomass concentration, different materials will be developed for three key classes of compounds: metabolites, lipids and peptides. Depending on the biomolecule class of interest, different protocols are used for quenching and/or washing steps and for the extraction of the final material. All reference materials are being evaluated on a drift tube IM-MS (Agilent LC-DTIM-QTOFMS 6560)

that, in addition to having a strong link to fundamental IM theory, provides excellent repeatability and interlaboratory reproducibility precision.
In contrast to previous developments focused on pathway coverage, our focus is achieving suitable chemical space coverage with our materials to provide a benchmark for key fields of IM-MS applications (i.e., lipidomics, metabolomics, proteomics). The final materials are intended to be suitable for both positive and negative electrospray ionization, with a good stability and be delivered with a user-friendly means to report results versus certified values. This project is part of MobiliTraIN, an MSCA Doctoral Network, in which close collaboration between the different projects is expected, so the reference materials and workflows for implementing them will be tested and applied across diverse IM-MS instrumentation within the entire network.

Tolterodine as a novel candidate for CYP3A4 activity assessment via metabolic volatiles to predict drug responses

Valentina Stock[1], Rebecca Hofer[1], Franziska Lochmann[1], Vera Spanke[2], Klaus R. Liedl[2], Jakob Troppmair[3], Thierry Langer[4], Hubert Gstach[4], Christian Dank[4], Chris A. Mayhew[1], Sarah Kammerer[5], Veronika Ruzsanyi[1]

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[2] Department of General, Inorganic and Theoretical Chemistry, University of Innsbruck

[3] Daniel Swarovski Research Laboratory, Medical University of Innsbruck

[4] Department of Pharmaceutical Sciences, University of Vienna

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Cytochrome P450 (CYP) enzymes are essential for drug metabolism, influencing both therapeutic efficacy and adverse effects. Among them, CYP3A4 plays an important role in the metabolism of several drugs [1,2]. Traditional approaches to assess CYP activity, such as 13CO2 breath tests, are limited by the need for isotopically labelled substrates and the use of a non-specific volatile biomarker [3]. In this study we have investigated tolterodine as a substrate that once metabolised in the human body generates acetone as a potential biomarker for a non-invasive breath test specifically targeting CYP3A4 activity. CYP3A4 converts tolterodine to N-dealkylated tolterodine (non-volatile) and acetone (volatile). A novel headspace and liquid sampling setup was developed for metabolite quantification. Proton transfer reaction time-of-flight mass spectrometry and liquid chromatography-mass spectrometry were used to

detect and characterise volatile and non-volatile metabolites, respectively. The metabolism of tolterodine was investigated in vitro using CYP3A4-overexpressing HepG2 cell clones. In vitro metabolism of 100 µM tolterodine over 4 h by CYP3A4 resulted in 2.2 ± 0.3 µM of N-dealkylated tolterodine and 2.0 ± 0.6 nM of acetone. Tolterodine biotransformation showed TC50 values of 414 µM and 375 µM in HepG2-CYP3A4 and reference cells, respectively. Over 24 hours, acetone and N-dealkylated tolterodine levels showed a continuous increase in HepG2-CYP3A4 cells, whereas treatment with CYP3A4 inhibitors resulted in a significant reduction in metabolite formation. This study highlights tolterodine as a promising substrate for assessing CYP3A4 activity in HepG2 cells. Its biotransformation generates both a volatile and a non-volatile metabolite, which could serve as biomarkers of enzymatic activity. These findings contribute to the advancement of non-invasive breath tests using unlabelled precursors as a potential tool for individualised CYP enzyme activity monitoring and personalised drug therapy optimisation.

We acknowledge the FWF for funding the Project PREDICT (Project Number: P35312-B).

[1] Guengerich, F.P., (2008). Cytochrome P450 and chemical toxicology, Chemical research in toxicology, 21(1): p. 70-83.

[2] Pinto, N., Dolan, M.E., (2011). Clinically relevant genetic variations in drug metabolizing enzymes, Current drug metabolism, 12(5), 487-497.

[3] Leeder, J.S., Pearce, R.E., Gaedigk, A., Modak, A., Rosen, D.I (2008). Evaluation of a [13C]-dextromethorphan breath test to assess CYP2D6 phenotype. The Journal of Clinical Pharmacology, 48(9), 1041-1051.

Session 2:

Particles and Metals

Tracing Metal Nanoparticle Accumulation in Edible Wild Mushrooms

Andrés Suárez Priede, Hannes Gödde, Mario Corte-Rodríguez, Simone Bräuer, Jörg Bettmer

University of Oviedo & University of Graz

Metal nanoparticles (NPs) are a subject of growing interest in scientific research due to their unique properties and diverse applications. Their origin can be both natural (geogenic and biogenic) or synthetic. As these nanoparticles are increasingly incorporated into products and derivatives of human activity, their presence and accumulation in the environment is on the rise. Several studies have indicated that metal nanoparticles exhibit higher toxicity to organisms compared to similar concentrations of non-nanoparticulate metals [1].
While the absorption and accumulation of trace metals in soils by various organisms have been extensively studied, detailed research on the behaviour of metal nanoparticles in this context is still limited. Fungi, known for their ability to absorb and bioaccumulate metals, represent a particularly interesting group of organisms in this regard. Moreover, some studies have highlighted the ability of fungi, including the well-known mushrooms, to biogenically produce nanoparticles [2]. Given the importance of mushrooms in the human diet, it becomes essential to investigate the presence and bioaccumulation of metal nanoparticles in these organisms. This study employs four sets of samples from Boletus edulis and Boletus aereus from different locations, including samples from the growth soil, to attempt to study their ability to produce and/or absorb and accumulate metal nanoparticles present in the environment, as well as to characterize them.

Different analytical techniques are described to be optimal for this kind of studies. Among them, single particle analysis by inductively coupled plasma-mass spectrometry (SP-ICP-MS) has been already employed to characterize selenium nanoparticles in different mushroom species [2]. It was then applied in this work to address the presence and characteristics of metallic nanoparticles in the mentioned fungi samples, as well as in the corresponding soil samples. Additionally, high resolution transmission electron microscopy (HR-TEM) with energy-dispersive X-ray spectroscopy (EDX) was used as complementary technique to elucidate more data about the NP's size and composition.

[1] A. B. Sengul, E. Asmatulu, Environ. Chem. Lett. 2020, 18, 1659-1683.
[2] K. L. LeBlanc, T. Kumlung, A. Suárez-Priede, P. Kumkrong, T. Junvee, S. Deawtong, J. Bettmer, M. Montes-Bayón, Z. Mester, Anal. Bioanal. Chem. 2023, DOI: 10.1007/s00216-023-05031-9.

Investigation of Fluorine-based and Metal Particles Introduced to Food through Non-stick Cookware

Bernhard Grüner, Raquel Gonzalez de Vega, Lhiam Paton, Thebny Thaíse Moro, Etienne Skrzypek, Jörg Feldmann, David Clases

University of Graz

Nano- and microparticles present unique properties which make them interesting for usage in various industrial and consumer products. Particularly, the application of nanotechnology in food-related products is growing, such as the incorporation of nanomaterials into food contact materials (FCMs) used for cookware. Throughout their lifecycle, FCMs are frequently exposed to highly stressful conditions, including scraping and cleaning with abrasive pads. Thus, understanding the potential migration of nanoparticles from these materials into food is crucial for assessing their safety. In order to elucidate migration characteristics, the release of nano- and micro-sized particles in four different pan coatings under three typical consumer conditions was investigated. Scratching conditions were simulated by abrasion with a fork and steel wool, and the release of nano- and microparticles was assessed by single particle inductively coupled plasma-mass spectrometry (SP ICP-MS) measurements. As Teflon is widely used in nonstick cookware, the main objective of this study was to investigate the release of fluorine containing particles. Typically, the high ionization potential of F impedes ionization in the ICP ion source. To overcome this challenge, a solution of barium was introduced simultaneously with the sample to promote the generation and subsequent detection of [BaF]+ ions by ICP-tandem mass spectrometry (ICP-MS/MS). The release of the F-containing particles was found to occur independently of changes in temperature, food, coating or damage to the coating. Additionally, the release

of metal-based particles was analysed using SP ICP-MS with time-of-flight mass spectrometry (ToF-MS) detection (SP ICP-ToF-MS) using a non-target screening method. Results indicate that the release of metal NPs is influenced by coating type, damage to the coating, temperature and food. In most cases, particles containing Cr, Co, Ni and Pb, were released. Given the potential adverse health effects associated with increased exposure to such elements, this work provides a foundation for future monitoring campaigns to assess the migration of particulate contaminants from FCMs into food.

Oral Presentation 6

Detection and characterization of secondary micro- and nanoplastics after environmental aging using single particle ICP-MS and OF2i

Manuel Candussi, Svenja Seiffert, Patrizia Pfohl, Christian Neuper, Christian Hill, David Clases

University of Graz

Microplastics pose significant environmental concerns due to their widespread presence and potential impact on ecosystems and human health. These particles can result from degradation of larger plastic debris, accumulate in ecosystems and are challenging to analyse comprehensively. Two analytical techniques, single particle inductively coupled plasma-mass spectrometry (SP ICP-MS) and optofluidic force induction-Raman spectroscopy (OF2i-Raman) have recently been advanced to address persistent challenges in this field. ICP-MS, operating in single-particle mode, is an element-selective technique and can detect carbon in individual particles which allows to determine particle number concentration and size distribution. In OF2i, single particles are trapped in the liquid phase by a laser beam. By analysing the inelastically scattered light of each particle, molecular and species information can be obtained. In conjunction, these methods offer a novel multi-modal approach for studying micro- and nanoplastics (MNPs). In this work, both methods were developed, optimised and benchmarked using polystyrene reference particles. The main objective was to investigate the degradation and fragmentation of frequently used polymers such as polyamide-6, thermoplastic polyurethane, and low-density polyethylene under a UV-aging regime. Size detection limits of around 800 nm were achieved for aged samples for SP ICP-MS. OF2i-Raman successfully distinguished between three polymers in mixed samples and

identified polyamide-6 particles extracted from soil, suggesting its applicability to real-world matrices. The combination of SP ICP-MS and OF2i-Raman has demonstrated a vast potential to provide detailed insights into particle size- and number-based data, as well as the chemical properties of MNPs. This dual-method approach not only highlights the degradation behaviour of commonly used polymers but also represents a significant advancement in analytical techniques for the study of MNPs in environmental samples.

Quantification of Precious Metals in Oxidic Matrices using Microdroplet-based LA-ICP-TOFMS

T. Schöberl, M. Bachmann and D. Günther

ETH Zurich

Since its introduction, laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) has been applied across various fields, offering rapid analysis of different sample types. [1] Nonetheless, quantification can remain challenging due to matrix dependent interactions between laser and sample. [2] Therefore, reference materials (RMs) and internal standardization are required for quantitative analysis. Unfortunately, microanalytical RMs are limited in availability and may be unsuitable due to a narrow range of certified mass fractions of elements of interest. Thus, developing viable non-matrix-matched quantification methods remains an important goal. Although other solution-based calibration methods have been reported [3], microdroplet-based calibration presents a promising alternative.

This work represents a microdroplet-based quantification approach for precious metals in glass RMs using LA-ICP-TOFMS. Utilizing a similar dual sample introduction setup (see below) described previously [4], aerosols from droplet production and laser ablation were combined. Behaviour of droplets and laser aerosol in the plasma was compared, and suitable internal standards were evaluated. Proof of concept will be demonstrated for the quantification of Au, Ag, Pt, Pd, Re and Rh in NIST SRM 610. Key findings on droplet behaviour, non-matrix quantification capabilities and respective figures of merit will be presented.

[1] T., Van Acker; S., Theiner; E., Bolea-Fernandez; F., Vanhaecke; G., Koellensperger Nature Reviews Methods Primers, 2023, 3, 1-18

[2] B. J., Fryer; S. E., Jackson; H. P. Longerich The Canadian Mineralogist, 1995, 33, 303-312
[3] E.V., Cromwell; P., Arrowsmith Analytical Chemistry, 1995, 67, 131-138
[4] B., Ramkorun-Schmidt; S.A., Pergantis; D., Esteban-Fernandez; N., Jakubwoski; D. Günther Analytical Chemistry, 2015, 87, 8687-8694

Session 3:

Chromatography

Optimization of liquid chromatography high resolution mass spectrometry for investigation of PFOA and PFOS degradation ability by Pseudomonas strains

Ha Anh Thai, Felina Hildebrand, Teresa Steininger-Mairinger, Stefan Heinl, Reingard Grabherr, Stephan Hann

BOKU University

Per- and polyfluoroalkyl substances (PFAS) are fully (per-) or partially (poly-) fluorinated compounds containing a variable length of hydrophobic alkyl chains with different hydrophilic functional groups, such as carboxylate, sulphonamide, phosphonate, sulfonate or hydroxyl [1]. Since 1940, these "forever-chemicals" have been synthesized and utilized for various industrial and commercial products [2]. Due to environmental and health risks caused by PFAS [3-5], degradation and elimination methods for existing PFAS from different environmental compartments (e.g. water and soil) are essential. This project focuses on the bioremediation of perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) with bacteria, a method that has low initial costs, low equipment requirements, relies on natural processes and can be applied to contaminated environmental sites.

To achieve accurate quantification of PFOA and PFOS, a liquid chromatography high resolution mass spectrometry (LC-HRMS) method based on reversed-phase separation and detection on MS1 level was developed and validated. A major focus was placed on the optimization of the experimental setup of the biodegradation experiments as well as sample pretreatment and analysis in terms of contamination and adsorption of PFAS. It was observed that standards and samples should be prepared in at least 50% methanol in polypropylene vials as standards prepared in less methanol (8%) experienced a loss of PFAS

over time. This is also recommended by the Austrian standard EN 17892 for PFAS determination in drinking water [6]. To exclude contamination of samples, different labware used in the workflow was studied after incubation with methanol and medium. No contamination of PFOA and PFOS was observed in the tested labware materials. Furthermore, it was found that different MS optics (iFunnel QTOF versus TOF) contributed differently to the linearity of the calibration curves of the two analytes. It was observed that the transfer of ions through the ion funnel results in a quadratic fit of the calibration curve, ranging from 0.02 µg/L to 7 µg/L. This suggests a loss of PFAS in the lower concentration range, which might be due to increased fragmentation of the [M-H]- ion within the ion funnel of the QTOF at low concentrations, despite the application of settings obtained by fragile ion tuning. The calibration curve obtained by TOF measurement met the criteria for linearity.

Finally, the optimized method was applied to different Pseudomonas strains with potential PFAS degradation capability as well as to purified enzymes (haloalkane dehalogenase, decarboxylase), which were shown to be involved in PFAS degradation in a previous study [7]. Both the Pseudomonas strains and the enzymes were incubated with PFOA and PFOS separately to investigate their PFAS degradation capability. PFOA and PFOS were quantified by external calibration with internal standardization (13C8PFOA and 13C8PFOS). Preliminary results revealed a low degree of biodegradation by some of the selected strains and enzymes, indicating that the degradation conditions need further optimization, mainly in terms of temperature and incubation time.

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Elution Revolution: Reversing Chiral Recognition by Swapping D- for L-Cellulose

Lehrhofer, A. F., Bacher, M., Melikhov, I., Sulaeva, I., Kohout, M., Potthast, A., Rosenau, T., Hettegger, H.

BOKU University

Chirality is a fundamental feature involved in most biological processes. While it can be rather readily observed on the molecular level, chirality transfer and thus enantioselective interactions on the macroscopic level are not similarly well understood. In this work, we did not only exploit the inherent chirality of cellulose and utilized its derivatives for the separation of small enantiomeric molecules by high-performance liquid chromatography (HPLC), but also used synthetic L-cellulose (instead of the natural D-glucose-based polysaccharide) to create the enantiomeric counterpart (= the molecular mirror image) of conventional chiral selectors based on natural cellulose. By employing phenyl-carbamate derivatives of this synthetic quasi-enantiomer of cellulose, we confirmed for the first time the inversion of the elution order of chiral analytes when exchanging D- for L-cellulose. The synthetic chiral stationary phases based on either D- and L-glucopyranose repeating units, were evaluated regarding their enantioseparation behavior and compared to their aliquot derived from the natural biopolymer using a set of representative test analytes. In this way, structure-property relationships and molecular interactions upon enantioseparation were derived. Using equimolar mixtures of L- and D-cellulose derivatives as the chiral stationary phase, we further demonstrated complete cancellation of the chiral separation. These findings contribute to the fundamental understanding of the overall separation mechanism of cellulose-based chiral selectors on both molecular and supramolecular levels. Our results

emphasize the importance of the hierarchical chirality of these chiral stationary phases.

ASAC Award

MobiLipid: A Tool for Enhancing CCS Quality Control of Ion Mobility–Mass Spectrometry Lipidomics by Internal Standardization

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Ion mobility-mass spectrometry (IM-MS) is a strong tool for LC-based lipidomics as it offers an additional separation dimension as well as an IM-derived collision cross section (CCS). The CCS value of an ion is a conditional property that can increase identification confidence. However, most IM-MS instruments rely on an external CCS calibration based on a standardized set of calibrants to derive CCS values. As these calibrants are not matched to the analytes of interest, chemical dissimilarities between analytes and CCS calibrants can pose a challenge during CCS calibration and introduce an unknow bias in the derived CCS values. Drift tube (DT) IM-MS is the only technology, which remains a direct link to the primary experimental method to derive CCS values.

In this work, MobiLipid, a R markdown-based tool for CCS quality control of IM-MS lipidomics workflows by internal standardization, was introduced. The tool is based on internal standardization with uniformly (U)13C-labeled lipids derived from an U13C-labeled yeast extract. To enable CCS quality control by

internal standardization, a DTCCSN2 library for U13C-labaled yeast lipids containing 377 DTCCSN2 values was established using a LC-DTIM-MS workflow. Based on the established library values, the tool allows for an automated calculation and compensation of CCSN2 biases introduced due to external CCS calibration. CCSN2 biases can be corrected for across 10 lipid classes without additional external measurements requiring only three U13C-labeled lipids per lipid class-adduct combination.
Finally, the CCS quality control workflow was demonstrated for trapped IM (TIM)-MS. An unlabeled lipid yeast extract was spiked with U13C-labeled lipids and measured by LC-TIM-MS. After deriving TIMCCSN2 values, MobiLipid automatically calculates the CCSN2 bias between derived TIMCCSN2 values and DTCCSN2 library values for U13C-labeled lipids. The mean absolute biases of the herein LC-TIM-MS dataset were 0.78% and 0.33% in positive and negative ionization mode, respectively. The integrated CCS correction led to a reduction of the mean absolute CCSN2 bias for 10 lipid classes in both ionization polarities to approximately 0%.

Session 4:

Spectroscopy

Advancing in-situ monitoring of enzymatic reactions via mid-infrared spectroscopy using functionalized silica particles

Katharina Schütz, Adea Loxha, Felix Frank, Bernhard Lendl

TU Wien

The integration of enzyme-based biosensors into analytical chemistry has significantly improved the selectivity of specific analyte detection. When combined with mid-infrared (mid-IR) spectroscopy, these biosensors enable the monitoring of reaction progress by utilizing the characteristic fingerprint region of the target analyte. To achieve this, bioactive substances such as enzymes can be immobilized on small carriers like silica particles and glass beads. They then catalyze reactions whose specific signature can be probed by mid-IR spectroscopy. Within a transmission-based measurement set-up, this approach facilitates the effective implementation of biosensors in the mid-IR region.

In this study, we aimed to enhance the real-time monitoring of enzymatic reactions with a specific focus on examining aminolysis using Fourier-transform infrared (FTIR) spectroscopy. For that, a protocol for functionalizing silica particles was established, enabling the immobilization of various lipase enzymes. These modified particles were then packed into a small column, which was subsequently incorporated into a transmission configuration. Samples containing different concentrations of a model fatty acid methyl ester (FAME) dissolved in heptane were prepared and circulated through the set-up, first through the packed column, then through the transmission cell. An amine was added to the solution, which resulted in an enzymatic reaction that could be monitored in real-time. Using FTIR spectroscopy, this approach allowed the successful detection of enzymatic reactions at concentrations as low as 20–40 ppm.

Based on these findings, the next step will focus on capturing the particles directly in the transmission cell, thereby making the column obsolete. This advancement will support the miniaturization of the system and improve sensitivity, bringing the system closer to a compact, portable device for in-situ reaction monitoring using infrared spectroscopy.

Oral Presentation 11

Raman Spectroscopy for Real-Time Diatomic Trace Gas Detection

Severin Hager-Roiser, Robert Zimmerleiter, Paul Gattinger, Ivan Zorin, Markus Brandstetter

Research Center for Non Destructive Testing GmbH

Since its experimental discovery in 1928 by Raman and Krishnan, Raman scattering has been utilized for a multitude of different measurement applications, including non-destructive measurement of gases.
While infrared absorption is more frequently employed for optical gas measurements due to the typically higher molecular cross section, certain molecules are infrared-inactive while being Raman-active at the same time. This is the case e.g. for homonuclear, diatomic gases like N2 and O2. Furthermore, only one single-wavelength laser is needed in Raman spectroscopy to detect any Raman-active substance, which allows measurement of complex gas mixtures with only a single monochromatic laser source.
However, when measuring gases, the low cross section of Raman scattering in combination with the low molecule density in the gas phase becomes a main challenge. To overcome this issue, various Raman enhancement techniques have been developed.
In this contribution, we start with the fundamental mechanisms behind Raman scattering and describe the most common enhancement techniques. These include Fiber-Enhanced Raman Spectroscopy (FERS) and Cavity Enhanced Raman Spectroscopy (CERS), where the laser beam is reflected many times to increase the Raman signal.
Furthermore, a non-resonant CERS setup with >40 laser reflections for real-time gas-quality monitoring and trace detection of diatomic gases is presented.

This measurement setup allows for gas measurements with short response times and detection limits below 100 ppm for infrared-inactive diatomic gases without cross-sensitivity.

Oral Presentation 12

Multi-Pathlength Mid-IR Spectroscopy for Optimal Absorbance

Lisa Riedlsperger, Alicja Dabrowska, Bernhard Lendl

TU Wien

Mid-infrared spectroscopy is a well-established method for analysing proteins and peptides, as it tempts with its rapid, label-free and highly selective analysis. The protein spectrum, with its characteristic amid I (1600 – 1700 cm-1) and amide II (1500 – 1600 cm-1) bands, provides valuable information on both the secondary structure as well as the concentration of proteins. However, transmission measurements of aqueous solutions are challenging due to the high background absorbance of the water matrix, which leads to reduced sensitivity or even complete signal saturation.
Here, we report a novel setup that integrates a tunable quantum cascade laser (EC-QCL), a wedge-shaped transmission flow cell, and a pyroelectric array detector. This configuration enables the simultaneous measurement of liquid samples across multiple optical pathlengths, allowing for the analysis over a wide range of concentrations while remaining within the dynamic range of the detector. To determine the optimal pathlength at each wavenumber, we introduce the pathlength-to-noise ratio (PNR) as a new performance metric. PNR accounts for the influence of variable pathlengths on the detectability of a substance while ensuring low noise levels. We demonstrate the advantages of this multi-pathlength approach by measuring aqueous solutions of bovine serum albumin (BSA) and beta-lactoglobulin (bLG). While this work serves as a successful proof-of-concept, several challenges remain. The potential for future refinements will be discussed in detail.

Oral Presentation 13

The role of quantum chemical calculation in NIR spectral analysis

Justyna Grabska, Krzysztof B. Beć, Christian W. Huck

University of Innsbruck

Near-infrared (NIR) spectroscopy is a well-established analytical technique known for its rapid, non-destructive nature and suitability for both laboratory and in-field applications. The growing availability of miniaturized, portable NIR spectrometers has further expanded the possibilities for on-site analysis. However, the complex nature of NIR spectra—characterized by broad, overlapping overtone and combination bands—often hampers straightforward spectral interpretation, especially in the context of structural discrimination and compound identification. In addition, the limited spectral range of handheld devices can compromise the reliability and sensitivity of analytical predictions. Quantum chemical calculations provide a powerful complementary tool for addressing these challenges. With the use of theoretical NIR spectra, these methods allow for a deeper understanding of the spectral features associated with specific molecular structures. They offer critical insights into the origin and behavior of absorption bands, enabling more informed selection of relevant wavenumber regions in calibration models. This is particularly valuable when dealing with structurally similar compounds or when experimental reference data are limited or difficult to obtain. We demonstrate how quantum chemical simulations can help in the development and optimization of NIR analytical models. These approaches offer a better understanding of the fundamental interactions underlying NIR spectra and support the design of more accurate, robust, and transferable calibration strategies.

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Label-Free Chemical Spectroscopy of Cancer Cells using O-PTIR

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Cancer is a major global public health issue and one of the most frequent causes of death around the world, with both incidence and mortality rates rapidly increasing. [1] Early detection and intervention significantly improve treatment outcomes, making the early identification of metastasis crucial for determining the most effective treatment. [2] Offering label-free chemical analysis, FTIR spectroscopy has been successfully used to identify cancer marker bands in cell and tissue samples [4,5]. However, applications in water demand a different approach due to the broad IR absorption band of water. Relying on the refractive index contrast between the sample and its environment, Optical Photothermal Infrared (O-PTIR) spectroscopy is considered a promising alternative to traditional chemical-staining-based pathology methods. [3] Our custom O-PTIR setup, was specifically designed to study cancer cells in aqueous media. In addition to the acquisition of spectra in several milliliters of water and the identification of biomarker bands, our system also allows us to perform chemical imaging based on these marker bands. By combining our findings with classification models, we can distinguish between healthy, cancerous and metastasizing cells. Moreover, we are able to analyze the chemical composition of individual cells. Additionally, we are collaborating with our partners in the Tumor-LN-oC project to build a lab-on-a-chip system which enables us to monitor the metastasis of cancer cells. Here, we present a basic overview of O-PTIR spectroscopy and imaging, comparing it to

conventional FTIR spectroscopy. Furthermore, we present our supervised learning approach towards differentiating between cancerous and healthy cells, comparing spectra obtained through conventional FTIR microscopy with those acquired using our custom O-PTIR instrument.

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Session 5:

Materials, Food an Environmental

Oral Presentation 15

Sustainable Innovation Demands Advanced Analysis: Characterizing Paper-Grade Pulps for Next-Gen Fibers

Ivan Melikhov, Irina Sulaeva, Mirjana Kostić, Markus Bacher, Sonja Schiehser, Thomas Rosenau, Antje Potthast

BOKU University

Molar mass distribution (MMD) analysis of cellulosic materials plays a crucial role in both academic research and industrial development, particularly in the context of sustainable man-made cellulosic fiber production. However, achieving full dissolution of cellulosic samples — an essential prerequisite for reliable MMD analysis— remains a significant challenge. Despite decades of research, the dissolution of cellulose continues to be a complex and often debated topic. Understanding the underlying reasons affecting cellulose dissolution is important for advancing analytical techniques and industrial processes.

In this study, we first investigated the effect of DMSO activation on the dissolution of cellulose samples for subsequent SEC analysis in the DMAc/LiCl solvent system. Our findings revealed that while DMSO activation enhances cellulose dissolution by decreasing the crystallinity index of samples, it also contributes to the partial removal of hemicellulose components — raising concerns for samples with high hemicellulose content, such as paper-grade pulp.

Given the increasing interest in paper-grade pulp as a cost-effective and environmentally friendly alternative to dissolving pulp for use in the production of man-made cellulosic fibers, it is essential to develop analytical methods capable of accurately characterizing these complex feedstocks — for example, by checking polymer degradation, evaluating spinnability, and ensuring fiber

quality. To address their limited solubility, we optimized the DMSO activation protocol to retain hemicellulose fractions while maintaining its positive effect on overall sample dissolution. This refined method enables accurate MMD analysis of hemicellulose-rich pulp samples in their original state, offering a valuable tool for evaluating sustainable raw materials in next-generation fiber production.

Chemical Tracing of a Previously Underexplored Off-Odour in Pork Using GC-MS, Sensory Analysis and Statistical Evaluation.

Mag. med. vet. Julian Bleicher; Kathrine H. Bak, PhD.; Univ-Prof. Dr. med. vet. Karin Schwaiger

FFoQSI GmbH

The sensory evaluation of the odour and flavour profiles of pork is a crucial factor in ensuring a level of meat quality that meets consumer expectations. In recent years, a previously underexplored off-odour has been increasingly detected during such assessments, which has also been reflected in a growing number of consumer complaints. To investigate this phenomenon, a project was initiated in which over 300 pork samples were evaluated with a specific focus on this off-odour and analysed using gas chromatography-mass spectrometry (GC-MS) to identify potentially relevant volatile compounds that might be associated with the sensory intensity of the off-odour. In addition, further product-specific parameters such as husbandry conditions, weight at slaughter, pH at classification and the sex of the animals were collected and examined in a multivariate statistical analysis. The aim of this project is to identify the chemical basis of this off-odour and to explore its statistical relationship with other influencing factors. The results of this project provide new insights that may contribute to a more objective assessment of meat quality and to the chemical characterisation of this previously little-considered sensory phenomenon.

Unravelling Photocatalytic Mechanisms in Organic Semiconductors with Time-Resolved Spectroscopy and Mass Spectrometry

Mariia Ferree, Jan Kosco, Nisreen Alshehri, Lingyun Zhao, Catherine S. P. De Castro, Christopher E. Petoukhoff, Iain McCulloch, Martin Heeney and Frédéric Laquai

Ludwig Maximilian University of Munich, Chemistry department

Significant advancements in organic semiconductors in recent years have demonstrated their high potential for use in organic photovoltaics, photocatalysis, and other energy conversion systems. [1] At the same time, time-resolved spectroscopic techniques, such as transient absorption (TA) and time-resolved photoluminescence (TRPL), are essential tools for investigating the dynamics of charge/energy transfer in these materials. [2] By monitoring spectral evolution over time, TA provides information about the generation, recombination, and transfer of charge carriers; while TRPL gives insights into the dynamics of excitons. Together, these techniques broaden our understanding of exciton generation, recombination and energy/charge transfer in optoelectronic and photocatalytic systems, which is crucial for their further development.

In our work, we rationalise observed photocatalytic activity and selectivity of organic and hybrid photocatalysts by combining time-resolved and quasi-steady state spectroscopic techniques with gas chromatography-mass spectrometry (GC-MS) product characterisation. As an example, we studied organic bulk heterojunction nanoparticles (NPs) consisting of polymer electron donors (PM6, PCE10) and small molecule acceptors (PCBM, Y6, ITIC), functionalised with metal cocatalysts (Ag or Au), for photocatalytic CO_2

conversion into CO and CH_4. [3] The reaction products and their origin were identified and quantified using a home-built setup integrated with GC-MS. Additionally, we employed TRPL, TA, and photoinduced absorption spectroscopies to assess the charge carrier generation efficiency and transfer from the organic semiconductors to metal cocatalysts and the charge accumulation at the metallic surface reaction sites.

In this talk, I would like to highlight the effectiveness of mass spectrometry in mitigating false positive results when performing CO_2 conversion using complex organics-based photocatalysts. I also aim to demonstrate how the listed analytical approaches enable a deeper understanding of the underlying mechanisms of photocatalytic reactions and provide critical insights into the design of more efficient photocatalysts.

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LC-IM-HRMS and non-targeted analysis for advancing the investigation of phytosiderophore-metal complexes

Laura Zellner[1], Sangeeta Kumari[2], Andreea Spiridon[3], Eva Oburger[3], Tim Causon[4], Christian Klampfl[1], Stephan Hann[4]

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Phytosiderophores (PS) are root exudates released by graminaceous plants that play a crucial role in the acquisition of micronutrients, particularly iron. Upon release into the rhizosphere, PS can also complex other transition metals present in the soil environment, potentially influencing their availability and uptake. Understanding micronutrient acquisition mediated by PS requires investigating their interactions and competition with transition metals at the root-soil interface. However, the characterization of intact PS-metal (PS-Me) complexes remains analytically challenging.

To address this challenge, we developed ion mobility-mass spectrometry (IM-MS) and liquid chromatography-high-resolution mass spectrometry (LC-HRMS) methods for the detailed characterization of PS-Me complexes. A mixed-mode stationary phase (reversed-phase + anion exchange) enabled the separation of nine PS-Me species, namely deoxymugineic acid (DMA), mugineic acid (MA), and 3''-epi-hydroxydeoxymugineic acid (epi-HMA) complexed with Fe(III), Cu(II), and Ni(II), respectively, while also retaining the free ligands. Utilizing PS-Me and PS standards, the method allowed for the quantification of

all investigated PS-Me complexes in soil extracts via external calibration and facilitated competitive complexation studies.
To expand our detection coverage of PS-Me complexes beyond those initially targeted, a software tool called Metalpicker for post-processing of LC-HRMS files was developed. By leveraging the distinctive isotopic distribution of transition metals, a tentative identification of potential features was done. These features were further investigated using targeted analysis. Validation using the samples processed with standard software demonstrated its accuracy, yielding comparable results and confirming its reliability for non-targeted metal complex analysis and quantification.
To further enhance the selectivity of our PS-Me analysis workflow, we determined collision cross-section (CCS) values for the investigated PS-Me complexes as well as the free ligands. An interlaboratory study between BOKU and JKU demonstrated the robustness of these measurements, with low relative standard deviations (≤0.15%), highlighting the reproducibility of DT-IMS measurements.
Overall, this work establishes an analytical framework for studying PS-mediated metal acquisition. The combination of advanced LC-HRMS and IM-MS methodologies enables accurate characterization and quantification of PS-Me complexes. Additionally, the newly developed Metalpicker software proves to be a promising tool for untargeted analysis of metal complexes, allowing the detection of previously unrecognized PS-Me species. These advancements enhance our understanding of metal interactions in the rhizosphere and provide valuable insights for future research on plant nutrition and soil chemistry.

Posters

Poster Presentation 1

Detection and characterization of secondary micro- and nanoplastics after environmental aging using single particle ICP-MS and OF2i

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University of Graz

Microplastics pose significant environmental concerns due to their widespread presence and potential impact on ecosystems and human health. These particles can result from degradation of larger plastic debris, accumulate in ecosystems and are challenging to analyse comprehensively. Two analytical techniques, single particle inductively coupled plasma-mass spectrometry (SP ICP-MS) and optofluidic force induction-Raman spectroscopy (OF2i-Raman) have recently been advanced to address persistent challenges in this field. ICP-MS, operating in single-particle mode, is an element-selective technique and can detect carbon in individual particles which allows to determine particle number concentration and size distribution. In OF2i, single particles are trapped in the liquid phase by a laser beam. By analysing the inelastically scattered light of each particle, molecular and species information can be obtained. In conjunction, these methods offer a novel multi-modal approach for studying micro- and nanoplastics (MNPs). In this work, both methods were developed, optimised and benchmarked using polystyrene reference particles. The main objective was to investigate the degradation and fragmentation of frequently used polymers such as polyamide-6, thermoplastic polyurethane, and low-density polyethylene under a UV-aging regime. Size detection limits of around 800 nm were achieved for aged samples for SP ICP-MS. OF2i-Raman successfully distinguished between three polymers in mixed samples and

identified polyamide-6 particles extracted from soil, suggesting its applicability to real-world matrices. The combination of SP ICP-MS and OF2i-Raman has demonstrated a vast potential to provide detailed insights into particle size- and number-based data, as well as the chemical properties of MNPs. This dual-method approach not only highlights the degradation behaviour of commonly used polymers but also represents a significant advancement in analytical techniques for the study of MNPs in environmental samples.

Poster Presentation 2

GS/MS analysis of Jasminum sambac (L) Aiton leaves extracted biomolecules based on change in solvents polarity

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The term jasmine comes from the Arabic word Yasmin, which means "gift from God." Jasmine oil is one of the primary aromatherapy substances used to induce a sense of well-being and mental relaxation. The differences in the composites structures of Jasminum sambac undergo to harvest time (day and time), geographic origin, genetic variability, abiotic (climate/weather, soil, etc.), and biotic limitations (herbivores, parasites, etc.). Additionally, Jasminum sambac leaves are a significant source of polyphenol compounds. The objectives of this study are to investigate the qualitative and quantitative variation in bioactive compounds extracted from J. sambac leaves using solvents of increasing polarity (e.g., water, and ethanol) and to identification bioactive structures of Iraqi J. sambac leaves which harvested near Tigris river. Fresh Jasminum sambac (L.) Aiton leaves were collected from a flower nursery near the Tigris River in Baghdad and taxonomically identified at the Department of Biology, University of Basrah, Iraq. The leaves were washed with tap and deionized water, shade-dried at room temperature for several days, then ground into a fine powder and stored at 7°C. For aqueous extraction, many grams of leaf powder were mixed with distilled water, stirred for 2 hours, filtered under vacuum, concentrated using a rotary evaporator, and dried. For ethanolic extraction, the same procedure was followed using absolute ethanol and concentration with final drying using oven dryer.

The compounds extracted from aqueous extraction include the variety of oxygenated organic molecules such aldehydes, ketones, esters, and furans, along with few sulfur containing and aromatic derivatives in small to medium molecular weight associated with leaves of plant based. The ethanolic extract contains primarily fatty acids and their esters (e.g., palmitic, oleic, stearic acid), along with alcohols (e.g., phytol, elaidolinoleyl alcohol) and minor amounts of aromatic and furan derivatives.

The aqueous extraction (likely more polar solvent) yielded mainly low molecular weight, polar compounds such as furfural, benzaldehyde, and hydroxyl compounds. In contrast, the ethanolic extract, being less polar, extracted mainly non-polar and semi-polar fatty acids, esters, and alcohols. The ethanolic extract showed peaks with longer retention times, indicating extraction of less volatile, non-polar compounds, while the polar extract showed mostly shorter retention times. Using both polar and less polar solvents provides a broader phytochemical profile of Jasminum sambac, capturing both hydrophilic and lipophilic bioactive molecules.

Poster Presentation 3

A comparison of GC/AED and GC/MS for the determination of fluorobenzoic acids in water samples using TMSH derivatization and fabric phase sorptive extraction

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TU Wien

In this study, a fabric phase sorptive extraction (FPSE) protocol combined with gas chromatography was developed to monitor the concentrations of fluorobenzoic acids (FBAs) in water samples. FBAs are widely used as tracers in petrochemical exploration due to their stability and ease of detection, making them useful for evaluating environmental safety and preventing potential ecological harm [1]. Because FBAs typically occur at trace levels, a preconcentration step is essential. For this purpose, FPSE was employed as a green sample preparation technique that uses sol-gel coated fabric substrates as extraction devices, offering several benefits in bioanalysis [2]. Since FBAs are acidic, they need to be derivatized to make them more volatile and stable for GC analysis. For this, we used trimethylsulfonium hydroxide (TMSH) as the methylating agent at 75°C for 1 hour. TMSH was chosen because it is a safe, stable, one-step reagent that produces fewer byproducts compared to other agents. A comparative study was carried out between two analytical techniques for FBAs determination: gas chromatography coupled with atomic emission detection (GC/AED) and gas chromatography-mass spectrometry (GC/MS). GC/MS demonstrated superior sensitivity and selectivity for the quantification of FBAs and was finally selected as the preferred method for validation.

Poster Presentation 4

Development and implementation of an on-line MS process sensor for emission monitoring along the polymer recycling chain

M. Annerl, K. Wieland, C. Burgstaller, K. Wutz, M. Weber, J.-C. Wolf, C. Haisch, E. Rosenberg

TU Wien

Considerable effort has been directed to improve sustainability and efficiency in mechanical polymer recycling. However, the recycled material often does not provide the properties for functionally equivalent reuse. A crucial issue is the unpleasant odor emanating from the recycled material, attributed to the emission of volatile organic compounds (VOCs). These VOCs can pose health and environmental risks. Potential sources can be traced back to the polymer's original use (e.g., food contact) or additives/contaminants (e.g., other polymers, dyes, stabilizers), which were originally added to the polymer or are present in the waste stream due to limitations of the preceding sorting and washing process.

This study aims to identify the specific VOCs emitted or formed due to mechanical and thermal stress during the extrusion process of virgin and post-consumer polymers. For this purpose, we are using online ambient ionization mass spectrometry (AIMS) with the novel soft ionization source "SICRIT". AIMS offers several advantages over traditional methods for detecting VOCs, such as gas chromatography-mass spectrometry (GC-MS), including reduced analysis time and the ability to analyze complex mixtures without necessarily requiring prior separation. By implementing this online technique in the degassing zone

of an extruder, we hope to gain a better understanding of the VOC formation and their prevention along the polymer recycling chain.

To lay a solid foundation for our research, a thorough characterization of four virgin materials (PP, PS, PA6, and PET) using a benchtop GC-MS with a custom-made, fully automized sample preparation has been performed. In this initial phase essential reference data was collected to accurately identify VOCs emitted from these materials. Building upon these findings, polypropylene (PP) has been studied in more detail, introducing different foreign polymer contaminants (PS, PA6, and PET) or stabilizers (Irganox 1010/B225FF) to investigate their impact on the emission pattern.

In this preliminary study, defined polymer blends were prepared by either mixing milled virgin materials or extrusion. The polymer reference blends were weighed into headspace vials and sealed. Afterwards they were melted in a custom-built heating tray and a defined volume of the gas phase was sampled for GC-MS analysis. The collected data were processed in two ways: (1) The VOCs in the total ion chromatogram (TIC) were identified via spectral matching and Kovats retention index; (2) The m/z sum spectrum of certain MS scans was used to train PLS models for the quantification of individual contaminants.

The GC-MS analysis results reveal a linear correlation between the weight percentage of certain polymer contaminants (<5wt%) and specific m/z ratios in the m/z sum spectra. Future work will focus on more complex polymer blends and the employment of the SICRIT ionization source coupled with a time-of-flight mass spectrometer (TOF-MS) to demonstrate the real-time capability of this setup.

Evaluation of different sample preparation techniques and derivatization reactions for the determination of nonsteroidal anti-inflammatory drugs in water samples using gas chromatography

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Pharmacologically active substances used to treat various illnesses can enter aquatic environments through effluents from wastewater treatment plants. Nonsteroidal anti-inflammatory drugs (NSAIDs) are commonly detected in water samples and their presence raises environmental and health concerns [1]. The aim of this study was to examine different sample preparation techniques and derivatization reactions in order to determine four NSAIDs, including ibuprofen, naproxen, diclofenac, and ketoprofen, in water samples using gas chromatography-mass spectrometry (GC-MS). Due to the low concentration levels of NSAIDs in water samples, sample preparation techniques play an important role, in order to preconcentrate the analytes and remove interferences from the sample matrix. In recent years, there has been growing interest in environmentally friendly techniques that use fewer solvents and produce less waste compared to classical techniques. Different sample preparation techniques were studied, such as fabric phase sorptive extraction (FPSE), magnet-integrated fabric phase sorptive extraction (MI-FPSE), and capsule phase microextraction (CPME) and different sol-gel materials were examined to find the most effective extraction technique. Accordingly, the main parameters that affect the microextraction procedure (i.e., the sample volume, the adsorption time, the stirring rate, the salt addition and acid addition, the elution time, the eluent, and the elution solvent) were studied.

NSAIDs are non-volatile and thermally unstable, and this makes them less suitable for direct GC analysis. To overcome this, derivatization is often required to transform the carboxylic acid group to ester derivative and thus increase their volatility [2]. Different derivatization reactions were examined in order to find the optimum derivatization agent, including N,O-bis(trimethylsilyl)trifluoroacetamide (BSTFA), trimethylsulfonium hydroxide (TMSH), methyl chloroformate, ethyl chloroformate, butyl chloroformate, and isobutyl chloroformate. The derivatization conditions of the optimum reaction (i.e., the reaction time, the reaction temperature, and the volume of the reagent) were investigated. The optimum combination for the GC-MS determination of NSAIDs from water samples included MI-FPSE of the analytes followed by BSTFA derivatization.

The research work was supported by the Bodossaki Foundation under the Scholarship Programme for Visiting Research Scientists.

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Poster Presentation 6

Development of a QuEcheERS method to analyze PFAS in vegetables with HPLC-QQQ MS/MS

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Due to the upcoming critics on the "forever chemicals" poly- and perfluoroalkyl substances (PFAS) the occurrence in vegetable samples is examined. PFAS are a variety of compounds that have an alkyl chain with at least one fully fluorinated carbon. They are stable, very persistent in the environment and widely spread due to the wide number of scopes of applications. The thermal and chemical stability is used in different industrial fields as well as everyday products, but these properties could also lead to bioaccumulation in plants, humans and animals. Exposure to PFAS can happen through different routes like inhalation of air and dust, intake of food and drinks, and dermal adsorption. Some PFAS are classified as toxic like perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA). Known effects of PFAS on health are decreased fertility, developmental effects in children, increased risk of cancer and many more.

In this study, 23 PFAS including different carbonic acids, sulfonic acids, sulfonamides and ethers were analyzed in various vegetable samples. Therefore, a QuEchERS (quick, easy, cheap, efficient, rugged, safe) extraction method was developed by testing different salts, solvents and solid-phase extraction adsorbents on tomato matrices. The final procedure includes a salt mixture and charcoal, which transfer the PFAS into the acetonitrile organic solvent. The optimized method shows a recovery of 80-130% for 18 of 23 analytes. The concentrated sample is then measured by high performance liquid chromatography coupled with a triple quadrupole mass spectrometer (HPLC-QQQ MS/MS) with optimized fragmentation voltage, collision energies,

and proper selection of the qualifier and quantifier ion. For the chromatographic part a C18 column with an additional delay column was chosen.
The tomato samples had especially high amounts of PFOA, which is 11 ng per kilogram of tomatoes. Also, low amounts of PFOS and perfluorohexanoic acid (PFHxA) were found, 0.25 ng/kg and 2.14 ng/kg, respectively.

Screening of various pre-treatments for enhancing cotton removal from cotton/PET blends

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Textile production has increased from 23.9 million metric tons (MMT) in 1975 to 111 MMT in 2019, resulting in an increase in waste and pollution, contributing about 10% to global carbon emissions. Only 25% of textile waste is recycled or reused, while the rest ends up in landfills or is incinerated. About 60% of the total textile waste consists of cotton and polyester (PET) blends [1]. The ReSTex project (Josef Ressel Centre for Recovery Strategies for Textiles) addresses this challenge by focusing on the enzymatic separation of these blended fabrics. By application of cellulase, cotton is hydrolysed into glucose, while PET can be recovered. However, the supramolecular structure of cellulose limits the enzymatic process [2]. To overcome this limitation, pre-treatments are required to partially open the cellulose matrix and facilitate improved enzyme attachment.

This study targets the effect of two pre-treatment methods: i) NaOH at different concentrations (1-6M)—which are commonly known for pre-treatment—, and ii) ionic liquid solvents (ILS), which are promising solvents as they modify the structure of cellulose with minimal environmental impact [2]. Cellulose removal is quantified via monitoring of reducing sugars and glucose concentration (by neocuproine method and HPLC respectively). Additionally, FT-IR and weight loss are used to determine cotton degradation, while SEM delivers images of the surface morphology of the remaining fibres. Preliminary results on 50/50% PET/cotton textiles reveal that treatment with NaOH significantly improves

cellulose degradation, and peaks at a weight loss of up to 44% at 4M, compared to 17% for conventional hydrolysis. The effect stabilises at higher concentrations of NaOH. These data are confirmed by reducing sugars and FT-IR analysis. SEM reveals that the PET fibres remain intact at 4M, suggesting a good recovery potential of the material. The preliminary results on this contribution highlight the importance of pre-treatment in cellulose degradation. Research will continue with ILS to develop more data for sustainable textile recycling solutions.

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Mass Spectrometry-Based Investigations into the Mechanism of Action of Novel Platinum Complexes as Potential Anticancer Agents

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Cisplatin (DDP) and oxaliplatin (OxPt) are widely used anticancer drugs known for their DNA-binding properties. However, their clinical efficacy is often hindered by dose-limiting side effects and the development of resistance. This underscores the need for novel chemotherapeutics with enhanced selectivity and reduced toxicity. To address this, we targeted molecular structures selectively present in cancer cells. In this context, two novel platinum complexes, $[Pt(Butene\text{-}ASA)Cl_3]^-$ (1) and [Pt(L-Ala)(Butene-ASA)Cl] (2), were synthesized as potential cyclooxygenase inhibitors and evaluated for their anticancer properties.

High-resolution electrospray ionization mass spectrometry (HR-ESI-MS) combined with LC-MS techniques was employed to investigate whether these new complexes share the same mechanism of action as cisplatin and oxaliplatin. Additionally, a top-down approach was implemented to identify the specific interaction sites between the platinum-based agents and model biomolecules.

The binding interactions between a model oligonucleotide and the platinum complexes were analyzed in both positive and negative ionization modes. The results confirmed the strong affinity of cisplatin for DNA and the fast kinetics of the reaction, with the oligonucleotide being completely platinated after just 3 hours. Conversely, significantly fewer interactions were observed when the same oligonucleotide was incubated with complex 2. Furthermore, both

complexes were tested for their ability to bind model peptides and proteins, where complexes 1 and 2 exhibited a greater number of adduct formations compared to DDP and OxPt. Finally, a competitive LC-MS assay was developed to examine the binding preferences of complex 2 for different proteins featuring the same potential interaction sites in different microenvironments.
The use of mild ionization conditions, in combination with a top-down approach and LC-MS competitive assays, enabled the characterization of distinct reactivity profiles for complexes 1 and 2 compared to DDP and OxPt. These findings open new avenues for the development of platinum-based anticancer drugs with potentially improved efficacy and tolerability.
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Poster Presentation 9

Optical Photothermal Infrared Spectroscopy for Sub-Micron Analysis of Intricate Biological Structures

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Infrared spectroscopy provides a unique spectral fingerprint of the sample under investigation by probing its vibrational molecular transitions. Recent technological developments, such as optical photothermal infrared spectroscopy (OPTIR), have overcome limitations of conventional infrared techniques, thus making it an increasingly valuable analytical tool in the biochemical and medical field. OPTIR is a microscopic technique that breaks the infrared diffraction limit which is in the range of 5-10 µm and achieves sub-micron spatial resolution (500nm nominal resolution). At the same spectral artifacts well known from conventional reflection spectroscopy are minimized. These advancements enable the study of complex biological samples such as cells, tissue sections, etc. It can further provide real-time insights into biochemical processes without altering the sample. OPTIR allowed us to measure and characterize micro- and nanoplastics in biological samples, such as particle-fed macrophages. We could detect the intake of nanoparticles by macrophages, highlighting the potential of OPTIR spectroscopy in studying cellular interactions with environmental contaminants. This approach could be further applied to investigate cellular responses and microplastics contamination, contributing to a deeper understanding of cellular mechanisms and their implications for human health.

On-line implementation of Raman-spectroscopy for real-time monitoring in the pulp and paper industry

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The recovery of chemicals after the extraction of cellulose from wood in the pulp and paper industry is a crucial step toward circular process flows, offering both environmental and economic benefits. The main component of the "cooking liquor" used in the extraction process is $Mg(HSO_3)_2$. After cooking, the residual material is concentrated and burned. SO_2 is subsequently recovered from the hot exhaust gas using a cascade of Venturi scrubbers. Through repeated interactions between the gas and a fresh $Mg(OH)_2$ suspension, the magnesium bisulfite cooking liquor is formed in a two-step reaction process.
The variable input streams as faced in the bio-based industry in combination with harsh conditions (temperatures above 60°C, pH range 4-7, high ionic strength) and the complex interactions between the gas and liquid phases lead to the unwanted formation of insoluble salts, ultimately resulting in clogged pipes and unscheduled downtimes.
A key step in improving recovery efficiency is a deeper understanding of the chemical interactions occurring in the Venturi scrubbers. Raman spectroscopy is employed as a non-destructive, in-situ process monitoring tool. Utilizing multivariate regression models, the spectral data are translated into critical

process-relevant parameters. Continuous real-time monitoring of variables such as free SO_2, total SO_2, MgSO3, and sulfate based on the Raman spectroscopic fingerprint enables precise process control of the interactions between the flue gas containing SO_2 and the $Mg(OH)_2$ slurry. By developing and optimizing a multivariate regression model based on several hundred at-line and on-line reference spectra, we can predict multiple target variables. We also demonstrate a test-wise, on-line implementation of our sensor directly on site at the chemical recovery plant. Our approach allows for the determination of critical process parameters within seconds. Changes in the chemical system can therefore be detected and corrected at an early stage, preventing undesired precipitations and reducing long downtimes and the loss of valuable chemicals.

Development of a Fluorophilic Ion-Exchange Material with Dual Binding Mechanism for Solid-Phase Extraction of PFAS

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that have prompted regulatory authorities worldwide to establish stringent limits in drinking water, groundwater, and surface water. These regulations have created significant challenges for PFAS detection, driving the urgent need for reliable and selective solid-phase extraction (SPE) materials for PFAS analysis.

To address this need, we developed highly crosslinked copolymers composed of 3-(1H,1H,2H,2H-perfluorooctyl)-1-vinylimidazolium chloride as a comonomer with ethylene dimethacrylate at various molar ratios. Designed for ionic fluorosurfactants, these copolymers exhibit a dual binding mechanism that synergistically combines fluorophilic interactions and electrostatic attraction, enhancing both selectivity and binding efficiency.

We evaluated the adsorption behavior and recovery of short- and long-chain PFAS acids, comparing the results with those of commercial SPE cartridges.

Characterization revealed that a monomer-to-crosslinker ratio of 2:1 achieved the highest porosity and ion-exchange capacity (412.7 ± 22 μeq g^{-1}). Recovery experiments consistently demonstrated high PFAS recoveries (98.8%–121.6%), while enrichment studies using effluent wastewater confirmed the material's robustness in complex environmental matrices (recoveries: 90.8%–99.2%).
These findings highlight the potential of this innovative polyelectrolyte as a selective, regenerable, and efficient alternative to conventional SPE materials, positioning it as a superior candidate for PFAS enrichment, detection, and environmental remediation applications.

Fight Fire with Fire: Side-Chain Perfluorinated Polyvinylimidazolium for Selective and Reversable PFAS Adsorption

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants, posing significant risks to human health and ecosystems. Conventional remediation technologies such as activated carbon and ion exchange resins are often ineffective for short-chain PFAS removal. In this study, a novel side-chain perfluorinated polyvinylimidazolium-based polymer (FP) was synthesized and evaluated for selective and reversible adsorption of PFAS. Characterization techniques, including SEM, EDS, IR spectroscopy, and BET analysis, confirmed the morphology, elemental composition, and surface properties of the polymer. Adsorption experiments were conducted for perfluorooctanoic acid (PFOA), hexafluoropropylene oxide dimer acid (GenX), and perfluorobutanoic acid (PFBA) in both single- and multi-component systems, and compared against a commercial powdered activated carbon

(PAC). The FP exhibited superior adsorption capacities, particularly for short-chain PFAS, and favorable kinetics modeled by pseudo-second-order equations. Competitive adsorption studies and tests in real wastewater matrices demonstrated the polymer's selectivity and robustness. Furthermore, regeneration studies confirmed that PFAS could be efficiently desorbed using a mild regeneration solution, enabling multiple reuse cycles without significant loss of capacity. These results suggest that side-chain perfluorinated polyvinylimidazolium materials are promising candidates for efficient and sustainable PFAS remediation strategies.

From Waste to Value: Analytical Characterization of Recycled Plastics

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TU Graz

The transition towards a more circular economy for plastics has become an increasingly important topic in the European Union. Ambitious goals were set, which include that by 2030, 55% of all plastic packaging waste must be recycled, and that a minimum content of post-consumer recycled (PCR) plastic is mandatory for PET- as well as non-PET packaging.[1] This also includes contact-sensitive applications such as food packaging. To reach these targets, Regulation (EU) 2022/1616 was established, which encourages the development of new recycling processes (novel technologies), especially for polymers other than PET. Since the products resulting from novel technologies can enter the market before the process is fully evaluated by the European Food Safety Authority (EFSA), strict monitoring and regular safety reports are required. This includes providing detailed data on potential contaminants in both the input materials and the recycled product to ensure they meet the safety standards for food contact materials set out in regulations (EC) No 1935/2004 and (EU) No 10/2011.[2] However, currently there is no standardized method or unified approach available for generating the required analytical data.

Therefore, aim of this work is to characterize different post-consumer recycled plastics, focusing on polyolefins (HDPE, LDPE, PP). To achieve this, a combination of sample preparation techniques is applied, including solid-phase microextraction (SPME), solvent extraction, and migration testing. Both targeted and untargeted analytical approaches are used, primarily based on gas chromatography (GC-FID, GC-MS, GC×GC-ToFMS) as well as liquid

chromatography. In addition, a genotoxic screening of the materials is performed. The resulting data will contribute to the development of a comprehensive database, which will serve as a foundation for an automated assessment strategy for PCR plastics.

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Interactions between Perfluorinated Alkylated Substances (PFAS) and Microplastics (MPs): Findings from an Extensive Investigation

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Per- and polyfluoroalkyl substances (PFAS) and microplastics (MPs) are widespread, persistent environmental contaminants posing significant ecological and health risks. This study explores interactions be tween these two contaminants using liquid chromatography-tandem mass spectrometry (LC-MS/MS), examining 18 synthetic polymers and eight different PFAS. Experimental results at concentrations of 100 µg L^{-1} revealed near-complete adsorption (up to 8 mg/g polymer) by polyamide (PA) polymers, influenced significantly by polymer type, functional groups (especially amide groups), PFAS polarity, and envi ronmental pH conditions. Computational modeling employing global optimization (MACE-OFF23 neural network potential) followed by reoptimization at the GFN2-xTB/GBSA level confirmed the experi mental findings, showing notably stronger interactions for polyamide compared to polyethylene. This highlights polyamide as a potential candidate for PFAS remediation and underscores the need for further studies under realistic environmental conditions.

Simulating the Environmental Weathering and Photo-oxidation of Polypropylene and Polyethylene terephthalate

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Microplastics (MP), tiny particles of less than 5 mm in diameter, are a major environmental pollutant and an increasing global concern. Several potential negative health effects have been reported as a result of MP exposure and intake. Consequently, the accurate detection and quantification of MP particles in the environment, along with the determination of their polymer type (e.g., PE, PP, PS, PET, …), are critical. Infrared (IR) Imaging has emerged as a leading method for this purpose, offering both information on the MP particle count as well as the polymer type, while providing spatial resolution of the studied sample. The polymer type is determined through the correlation score of the acquired spectra of a sample with pre-recorded reference spectra of common polymer types. However, environmental degradation, particularly UV irradiation, alters the chemical structure and IR spectra of MPs, complicating this correlation matching. Therefore, understanding the degradation behavior and the spectral changes under the influence of UV light is of great interest. This study investigates the effects of UV irradiation on the IR spectra of PE, PP, PS and PET MP particles with a diameter of roughly 100µm. MP particles were immobilized in a rigid matrix, and spectra were recorded at defined time intervals. 2D Correlation Spectroscopy revealed distinct spectral changes, demonstrating its effectiveness for UV degradation studies.

Poster Presentation 16

Determination of transport efficiency in laser ablation single particle inductively coupled plasma mass spectrometry for soft tissue analysis

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Recent studies have demonstrated the applicability of the "single particle" mode in laser ablation - inductively coupled plasma - mass spectrometry to map and size particles simultaneously. The transport efficiency (TE) is an important parameter in this configuration and affects the detection of individual nanoparticles, reliability of nanoparticle characterization, and related applications. This study introduces a novel method for the precise determination of TE, based on counting upconversion nanoparticles from gels characterized by fluorescent microscopy. The method was found to be most suitable for the 2940 nm laser ablation system, achieving virtually quantitative nanoparticle desorption, with TE primarily governed by ablation cell design and aerosol transport efficiency. With the 213 nm laser, attention had to be paid to incomplete desorption and possible nanoparticle redeposition at low laser fluences to avoid variability in TE measurements. Finally, use of the 193 nm laser induced nanoparticle disintegration, resulting in elevated baseline noise and lower sensitivity, which prevented the use of this approach for the determination of TE. This study highlights the versatility of the proposed method, while also identifying its limitations in terms of wavelength and fluence.

Mass Spectrometry Imaging of Bacteria in Colorectal Carcinoma-Derived Spheroids

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Masaryk University

Mass spectrometry is a powerful analytical tool for characterizing molecular changes in biological systems, including cancer and microbial interactions. In colorectal cancer, the gut microbiome plays a crucial role in tumor progression. For our study, we selected Bacteroides fragilis, a common Gram-negative anaerobic bacterial species known for its association with inflammation and metabolic disruptions in colorectal cancer. Traditional matrix-assisted laser desorption/ionization (MALDI) mass spectrometry identifies bacteria based on unique protein patterns, however it requires the isolation of bacteria from biological material followed by cultivation. This approach cannot be applied to mass spectrometry imaging (MSI) and also it can be particularly challenging for anaerobic organisms. For our experiments, we worked with spheroids, which are three-dimensional cell cultures that can mimic tissues and microtumors. They support the viability of anaerobic bacteria in laboratory conditions and offer a platform for the development of MALDI MSI for the detection of bacteria in tissues. In our study, we applied MALDI MSI to visualize lipid distributions in spheroids derived from HCT116 and HT29 colorectal carcinoma cell lines cultivated with Bacteroides fragilis strains. We aim to detect bacterial-specific lipids as alternative biomarkers of bacterial presence and identify bacteria-induced lipidome alterations of carcinoma cell lines. This approach can deepen our understanding of host-microbe interactions at the molecular level and the role of bacteria in cancer progression, and also holds the potential for

identifying bacteria species based on their lipid profiles directly from clinical tissues.

We gratefully acknowledge the financial support of the Czech Science Foundation (project no. 24-10924S) and the Ministry of Education, Youth and Sports (project EXCELES LX22NPO5102).

Optimizing Lipid Nanoparticles for Efficient and Safe Drug Delivery: The Impact of Particle Size on Transfection Efficiency and Cytotoxicity

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Emerging global health challenges—such as pandemics, cancer, and genetic disorders—demand innovative therapeutic approaches for rapid and targeted treatment. Lipid nanoparticles (LNPs) have become an important tool for the delivery of nucleic acids and other therapeutic agents, playing a key role in the development of mRNA-based vaccines. These nanoparticles offer protection from degradation and enable targeted transport to cells, making them a possible solution for gene therapy and other applications. [1]
However, despite their success, the optimization of LNP formulations remains a challenge. Achieving the right balance between maximizing transfection efficiency and minimizing cytotoxicity and immunogenicity is essential for their safe and effective use. One of the most important factors influencing the biological performance of LNPs is their particle size. [2] Particle size not only affects the pharmacokinetics and biodistribution of LNPs in vivo, but also their cellular uptake, intracellular trafficking, transfection efficiency, and cytotoxicity. Smaller LNPs typically exhibit improved tissue penetration and faster cellular uptake, while larger particles offer more efficient cargo encapsulation or facilitate endosomal escape. However, a comprehensive understanding of how particle size influences these parameters remains underexplored. [3]
This study investigates the impact of LNP size on cellular uptake, transfection efficiency, and cytotoxicity using human liver (Hep-G2) and lung (A549) cell

lines, representing two primary organs exposed to circulating nanoparticles. [4] We compared three different LNP sizes to evaluate their effects on cell viability and proliferation. The research integrates cell viability assays (CCK-8, RealtimeGlo) and fluorescence microscopy to analyze cellular responses and optimize LNP design for improved biocompatibility.

To gain a deeper understanding of LNP behavior during cellular uptake and gene delivery, three types of LNPs will be used. A lipophilic dye will be incorporated to stain the LNP membrane, enabling us to monitor interactions between the LNPs and the cell membrane during the initial uptake process. Additionally, a fluorescent dye encapsulated within the LNPs will allow tracking of their internalization and endosomal escape. Another batch of LNPs will carry mRNA encoding for green fluorescent protein (eGFP), which will enable the evaluation of successful transfection through the expression of fluorescence in the target cells. This combination of markers will provide a comprehensive approach to studying LNP behavior at various stages of cellular uptake and gene delivery.

The findings of this study will contribute to the development of safer and more effective LNP-based drug delivery systems, ultimately advancing clinical applications of these promising therapeutic agents.

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From Migration to Prohibition: New European Regulation for Bisphenols in Food Contact Materials

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Bisphenols are a group of industrially significant compounds widely used in the manufacture of plastics and resins. Their applications range from food packaging, tableware, and reusable water bottles to non-food uses such as epoxy-based paints and printing inks.1 Over time, their versatility has also resulted in unintended migration into materials like paper and board used in food contact materials (FCMs), raising concerns reflected in the EU's 2030 roadmap for a toxic-free circular economy. Among the various bisphenols, bisphenol A (BPA) is by far the most extensively studied, owing to its weak estrogenic activity and classification as an endocrine-disrupting chemical (EDC).2

Under Commission Regulation (EU) No 10/2011, the use of bisphenols in plastic FCMs was already subject to specific migration limits (SMLs) of 0.05 mg/kg for both BPA and bisphenol S (BPS). However, evidences linking BPA to potential adverse health effects has led to increasingly stringent regulatory measures:

- In 2023, the European Food Safety Authority (EFSA) revised its safety assessment, reducing the tolerable daily intake (TDI) by a factor of 20,000—from 4 µg/kg to just 0.2 ng/kg body weight per day.3
- This re-evaluation led to the adoption of Regulation (EU) 2024/3190, which prohibits the intentionally use of BPA and its salts in specified FCMs and articles, further extending the prohibition to other bisphenols with similar

endocrine-disrupting properties, while setting a "not detected" criterion for SMLs, with an analytical detection limit of 1 µg/kg of packaging material

- Additionally, new testing requirements are set that BPA residuals must be verified using extraction methods, while migration tests must align with EU Regulation 10/2011 parameters

While these regulatory changes represent a significant advance in consumer health protection, they present considerable analytical challenges. The newly imposed detection thresholds are several orders of magnitude lower than previous limits, making many existing validated methods insufficiently sensitive. Therefore, the demand for ultra-sensitive, highly selective analytical techniques is high and growing.

Gas chromatography after derivatization is already widely employed for the analysis of bisphenols across various matrices.5 In response, this study aims to develop a highly sensitive and selective GC-MS/MS method for the simultaneous determination and quantification of 10 selected bisphenols in FCMs to ensure reaching the desired detection limits and compliance with regulatory limits.

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Targeted Analysis of 1000 Analytes Using UPLC-Orbitrap-HRMS: Method Transfer and Optimization Strategies

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In the era of digital transformation, the integration of big data into food safety enables trend monitoring, risk prediction, and rapid response to emerging contaminants. High-resolution mass spectrometry (HRMS), particularly Orbitrap-based systems, supports this shift by allowing simultaneous targeted quantification and non-targeted screening within a single run—creating opportunities for retrospective data mining even from routine workflows.
While HRMS offers high mass accuracy and full-scan capability, its adoption in quantitative routine settings is limited by the lack of harmonized validation guidelines. Our currently validated method employs a triple-quadrupole LC-MS/MS system operating in single polarity mode (2 × 20-minute runtime), using two fragment ions per precursor and acquiring 12–15 data points per peak. In contrast, literature suggests that HRMS methods used for

quantification purposes often rely on a single adduct, with 6–9 data points per peak being sufficient.

To evaluate the performance of Orbitrap HRMS while maintaining required identification criteria, we transferred our method to a UHPLC-Orbitrap IQ-X platform, aiming to retain existing chromatographic conditions and, ideally, implement fast polarity switching (FPS).

To date, over 400 fungal metabolites have been analyzed using Orbitrap acquisition only, with FPS. However, Orbitrap acquisition with FPS was found to be suboptimal for quantification due to a low number of data points per peak (3–6). To overcome this, we leveraged the full capabilities of the Orbitrap Tribrid system and opted for two separate polarity measurements per sample.

The Orbitrap mass analyzer was used for full-scan acquisition, preserving the ability for retrospective data mining. Additionally, Ion Trap MS^2 scans were incorporated to meet identification criteria (fragmentation pattern), and Ion Trap tSIM (targeted Selected Ion Monitoring) scans were added to improve quantification performance.

This dual-detector setup preserved the advantages of Orbitrap full-scan data for retrospective analysis while enhancing quantification reliability through Ion Trap SIM and MS^2 scans. Method compliance with key validation parameters—mass accuracy, ion selection, identification level, and peak point density—was assessed. Dynamic range and linearity were evaluated, and LOQ/LOD determination is planned in the future.

This study underscores the critical considerations in transferring high-throughput LC-MS/MS workflows to Orbitrap Tribrid platforms, aiming to demonstrate that Orbitrap Tribrid instruments could effectively support the dual goals of robust quantification and future-ready data mining even within routine targeted analysis.

Poster Presentation 21

Microplastic Detection in Blood and Urine: A Comparative Study of Sample Preparation Methods using LDIR

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Microplastics have recently been detected in human biological samples, raising concerns about potential health effects, although conclusive evidence is still missing. To address the resulting need for reliable analytical frameworks, the master's thesis develops and evaluates sample preparation methods for microplastic detection in blood and urine.

A step-by-step approach is adopted, beginning with an in-depth review of legal and ethical frameworks for working with biological samples, followed by protocols for contamination-free sampling, transport, and storage. For blood samples, oxidative, alkaline, and enzymatic digestion methods are tested; for urine, direct filtration, alkaline, and oxidative digestion are compared. After microplastic/matrix separation the particles will be analysed using Laser Direct Infrared spectroscopy (LDIR, Agilent Technologies), allowing for the chemical identity as well as size of natural occurring and spiked particles. The performance of each method is evaluated with respect to digestion efficiency, matrix compatibility and potential contamination.

This study aims to identify robust routine preparation protocols suitable for complex biological matrices and to contribute toward methodological standardization in microplastic research. By combining regulatory, ethical, and analytical considerations, this work lays the foundation for high-quality, reproducible data and supports future harmonisation and monitoring efforts regarding human exposure to microplastics.

Cellular Uptake and Distribution of Nickel Ions: When Strength Becomes a Weakness in Joint Replacements

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Joint replacements are commonly made from alloys containing nickel, titanium, and other elements, each contributing essential properties to the final material. Nickel, in particular, enhances mechanical strength, durability, and corrosion resistance. However, despite these advantages, nickel is not considered an ideal component due to its potential adverse effects on the human body. Mechanical wear and minor surface damage of the implant can lead to the release of nickel ions, as well as nano – and microparticles of nickel and other elements, into the surrounding tissues and even into the bloodstream. Nickel ions pose a significant risk due to their cytotoxic effects on cells, which can be particularly harmful to tissues in patients with nickel allergies. In severe cases, this can lead to tissue degradation around the implant. Understanding the mechanisms of nickel penetration and cellular uptake is therefore crucial.[1,2] To investigate this, we designed an experiment to study the effects of nickel on different cell

cultures. The behavior of nickel was analyzed over time and in relation to its concentration. Using Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS), we examined the intracellular distribution of nickel after uptake and quantified its presence in different cellular compartments.

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Development of a mid-infrared based quality assurance method for hydrogen peroxide containing water decontamination concentrates

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Many hydrogen peroxide based products in pharmaceutical, medical and cosmetic industries are still predominantly quantified using wet chemical methods. These typically involve redox titrations with potassium permanganate or sodium thiosulfate. To reduce the amount of chemicals in quality control and further promote sustainability, an innovative analytical model has been developed. This model enables the rapid determination of hydrogen peroxide concentration in water decontamination products using ATR-MIR spectroscopy in combination with the PLSR methodology. 52 batches of three commercially available water decontamination products containing 1.41-2.35 % hydrogen peroxide were used for method development. PLSR (partial least squares regression) models showed excellent prediction accuracy.

Cadmium Accumulation in Organ Tissues After Inhalation of Cadmium-Based Nanoparticles

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Cadmium and its toxic effects are a very current issue at this time, as poisoning by this element can cause serious health problems or even death. Cadmium is transported through the bloodstream and is found in a wide range of tissues. Thus, long-termed exposure to cadmium can lead to cancer and adverse effects on organ systems (skeletal, reproductive, cardiovascular, etc.). [1] The distribution of cadmium and other biogenic elements was studied in the organs of mice - lungs, livers and kidneys. For the inhalation experiment, mice were divided into 3 groups. The first group was continuously exposed to CdO NPs for 11 weeks. The second group was exposed to CdO NPs for 11 weeks and then inhaled clean air for 5 weeks to determine whether the CdO NPs were permanently deposited in the tissues. In the third group (the control group), mice were exposed to the same conditions at each time point but breathed only clean air. After each exposure period, the mice were sacrificed and the organs were dry frozen, placed in agar medium, and cut into 20 µm thin cryosections. Samples were analyzed by laser ablation combined with inductively coupled plasma mass spectrometry (LA-ICP-MS) using a Nd:YAG laser.

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Poster Presentation 25

Mid-Infrared Spectroscopy for Qualitative and Quantitative Wheat Protein Analysis

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Wheat is among the top three crops cultivated by humankind and contributes to about 19% of the daily protein intake per capita worldwide.1 Studying wheat protein is therefore crucial for human nutrition, the food industry, in allergy and intolerance research, as well as in environmental and agronomic research. Mid-infrared spectroscopy (MIR) combined with attenuated total reflection (ATR) is a straightforward technique to assess biological material among other types of samples.2 However, its application for food analysis is still scarce. In this study, we employed ATR-MIR to study the Osborne protein fractions of 60 Austrian wheat samples across four sampling sites in a qualitative and quantitative manner. We could show that ATR-MIR can be used to study the secondary structure of each protein fraction and to find regional differences of the wheat samples through principal component analysis (PCA). Furthermore, the protein content of each fraction was quantified using the amide II band and significantly ($p < 0.001$) differences between the sampling sites were found. This shows that quantitative and qualitative protein analysis by using ATR-MIR might be used to study the effects of different environment on wheat proteins.

In conclusion, the results of this study provide a solid evidence base for the application of ATR-MIR in wheat protein analysis.

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Poster Presentation 26

Exploring sol-gel Carbowax 20M coated foams as microextraction platforms for the monitoring of multi-class pesticides in fruit juice samples

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To ensure food safety and fair practice in international trade form fruit juices, it is imperative to develop reliable and sensitive analytical methods for the monitoring of pesticides. In this study, a simple and efficient foam-in-syringe solid-phase extraction (FIS-SPE) method was developed as a front-end to high performance liquid chromatography-diode array detection (HPLC-DAD) for the monitoring of multi-class pesticides. For this purpose, so-gel Carbowax 20M coated foams were fabricated, characterized, and evaluated as microextraction platforms. The main steps that concerned the performance of the FIS-SPE procedure were optimized. Accordingly, the proposed method was validated in terms of sensitivity, linearity, accuracy, precision, and selectivity. The greenness of the method and its practicality were also assessed using appropriate metric tools. Under optimum conditions, the relative recoveries were 84.8-117.6 % and the RSDs were better than 12% for intra-day and inter-day studies. The limits of detection (LODs) were 0.8 – 1.5 ng mL-1 and the limits of quantification were 2.5 – 5.0 ng mL-1. As a proof-of-concept, the proposed method was used for the analysis of different commercially available fruit juice samples.

Introduction of a Novel Biosensor for Nanoscale Analysis of Immunoglobulin G Antibodies via AFM-IR

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Understanding and controlling antibody stability is crucial in biopharmaceutical development, as protein misfolding, denaturation, and aggregation - caused by stress factors such as temperature changes, pH variations, mechanical stress, or light exposure – can compromise the antibody's biological functionality.(1,2) These structural changes may lead to a loss of therapeutic efficacy or even trigger immune responses in patients.(2) This study investigates the potential of atomic force microscopy coupled to infrared spectroscopy (AFM-IR)(3) for nanoscale characterization of immunoglobulin G (IgG) antibodies in both their native and denatured states, captured by a biosensor, thus providing high-resolution chemical and structural insights into this model protein system. The introduction of a biosensor offers distinct selectivity for analysing the targeted antibodies, but the AFM-IR system requires a homogeneous sensor surface with a thin layer of covalently anchored selective capture proteins for IgG that absorb minimally in the targeted infrared regions, all while functioning under ambient conditions.

A novel biosensor design is introduced, utilizing direct surface functionalization of silicon substrates with covalently immobilized antibody-capturing proteins. These proteins exhibit high yet reversible selective affinity for the Fc region of IgG(4), allowing for straightforward biosensor regeneration through pH variation, which enhances the biosensor's applicability. The system's early-stage success is demonstrated by silicon substrate functionalization with (3-Aminopropyl)triethoxysilane (APTES) and glutaraldehyde (GA), verified through AFM scans and water contact angle analysis of the surfaces. Ongoing research

is focused on model protein binding tests, with particular emphasis on optimizing antibody-capturing protein G immobilization strategies.
By integrating a reversible biosensor design for AFM-IR analysis, this work introduces a novel approach for studying native and denatured antibodies at the nanoscale. This approach holds the potential for enhancing quality control in biopharmaceutical production by enabling the development of inline sensors for antibody stability testing during bioprocessing.

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Poster Presentation 28

The Mechanism of Interaction of G-Quadruplexes With the Plant Alkaloid Fagaronine

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Fagaronine is a plant alkaloid from the group of benzophenanthridine alkaloids, which is commonly found in the roots of the Fagara zanthoxyloïdes plant. Several benzo[c]phenanthridine alkaloids have already been shown to have a stabilizing effect on non-canonical structures, in particular on G-quadruplexes, which are secondary DNA structures occurring on guanine-rich sequences, especially at the ends of telomeres. Increasing the stabilization of these structures can inhibit DNA replication or transcription, which can result in a significant reduction in cell division.

Since the stabilizing effects of fagaronine on G-quadruplex structures have already been demonstrated, I am focusing this work on a more detailed study of the interaction mechanism to better understand the alkaloid's stabilizing influence. A series of experiments, including NMR spectroscopy, have been carried out with three types of G-quadruplexes (parallel, antiparallel, hybrid).

Chemical and Physical Characterization of Ship Emissions

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Emissions from ships represent a significant source of aerosol release into the atmosphere. Consequently, the detailed characterization of ship-borne emissions is essential for evaluating their environmental fate and potential impacts on human health. Ship exhaust plumes are characterized by elevated concentrations of both gaseous and particulate pollutants, including carbon monoxide (CO), nitrogen oxides (NO_x), polycyclic aromatic hydrocarbons (PAHs), and organosulfur compounds. During atmospheric transport, these aerosols undergo chemical transformation processes, commonly referred to as "aging," which involve complex multiphase chemical reactions.

In the present study, we perform a novel comparison between emissions measured from a controlled engine test bench and those observed in situ under real-world conditions at sea. Within the framework of the project ULTRHAS (ULtrafine Particles from TRansportation – Health Assessment of Sources), both fresh and laboratory-aged exhaust from a localized single-cylinder, four-stroke marine engine were investigated. Laboratory aging was simulated using a photochemical emission aging flow tube reactor (PEAR), designed to emulate atmospheric processing over a period equivalent to one to ten days. This process resulted in the degradation of primary incomplete combustion products, such as PAHs, and the concurrent formation of oxygenated compounds.

To contextualize the laboratory findings within real-world environmental exposure scenarios, the complementary project PlumeBaSe (Tracing of Ship Plumes and Impact to Seawater) was initiated. This initiative focuses on

investigating the transport and transformation of ship-emitted aerosols within the Baltic Sea region. A series of coordinated measurement campaigns were conducted, utilizing shipborne, airborne (airship-based), and land-based platforms to quantify the physicochemical characteristics of ship plumes, including particle number concentration and size distribution. Furthermore, particulate matter samples were collected for subsequent analysis of semi-volatile organic compounds using direct thermal desorption comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOF-MS).

With the combined top-down and bottom-up approach, a comprehensive chemical and physical characterization of ship emissions and their fate in the environment is facilitated.

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A novel extraction method for Prymnesium parvum from whole culture

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Introduction: Harmful algal blooms (HABs) can cause massive fish kills, especially when toxic microalgae like Prymnesium parvum are involved. This species produces prymnesins (PRMs) in either A-, B-, and C-type variants, with A-type being the most toxic. In summer 2022, a P. parvum bloom in the Oder River led to the death of around 1000 tons of fish, snails, mussels and other small animals. High salinity, temperature, and low water levels likely triggered the bloom. Unlike other toxic algae, P. parvum retains PRMs in its biomass, making toxin release mechanisms unclear. Common extraction methods include solid-liquid (SLE) and liquid-liquid extraction (LLE), but both suffer from PRM losses. Solid-phase extraction (SPE) offers cleaner samples but lower yields. This study aimed to optimize PRM extraction by combining advantages of all three methods, resulting in a more efficient and scalable approach for natural and lab samples.

Materials and methods: As no commercial standards are available, the methods were optimized in such a way that intra-batch comparisons were conducted, and no absolute quantification took place. Samples were measured on an ultrahigh-performance liquid chromatography 1290 Infinity System (Agilent, KA, USA) coupled to a QTRAP® 6500+ (Sciex, MA, USA) mass spectrometer with an electrospray ionization source in positive mode. Fragmentation was performed with collision-induced dissociation and corresponding transitions were selected based on the findings in Binzer et al. (2019). The A-type P. parvum strain UTEX-2797 was used as the primary model, with additional analyses on the B-type strain ODER1 and C-type strain RCC-7010. PRMs were extracted using SLE, LLE, and SPE. A novel hybrid SLE-SPE protocol was developed to enhance extraction efficiency and sample purity. PRM stability assessments, additive effects, and extraction yield across growth phases were quantified to refine the protocol for downstream applications.
Results and discussion: This study aimed to develop an MRM method for all three PRM types and to optimize PRM extraction by evaluating existing protocols and developing a novel method integrating multiple techniques.
A multiple reaction monitoring (MRM) method was developed to enable targeted PRM analysis. Due to the large molecular size of PRMs and their high chlorine content, low-resolution settings were chosen over unit resolution to optimize detection sensitivity.
Sonication was tested as a potential strategy to release PRMs into the culture medium for easier extraction. However, due to PRM instability in the medium and incomplete toxin release, this approach was ineffective. SPE was identified as the most efficient method, offering advantages in desalination, purification, and reduced processing time. Losses of up to 27% were observed in conventional SLE and LLE due to evaporation and reconstitution steps. Optimizing SPE conditions led to the development of a protocol using 50% MeOH in whole culture, improving PRM yield across all toxin types. The method enhanced PRM interaction with the sorbent while preventing cartridge clogging, likely due to facilitated cell lysis.
A comparison between MeOH and EtOH in SPE demonstrated that while MeOH remained superior, 40% EtOH yielded results comparable to LLE, offering a

greener alternative. Extraction efficiency remained stable across different growth phases, though PRM loss was observed after freeze-thaw cycles. The new SPE method provided higher robustness, reduced solvent consumption, and improved sample purity compared to conventional approaches.

From Black Liquor to Lignin Insights: Harnessing SEC for Precise Quantification and Molar Mass Measurement

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Lignin is a complex and heterogeneous natural aromatic polymer. In pulp and paper mills, it is extracted from plant biomass through various chemical processes, resulting in an annual production of up to 70 million tons of lignin as a by-product. Despite this large quantity, most of the technical lignin is currently only used as on-site biofuel.

Industrial pulping involves harsh conditions designed to efficiently remove lignin from biomass by degrading or chemically modifying it. Consequently, technical lignins differ significantly from their native forms in terms of size, bonding patterns, composition, and functional groups. After pulping, lignin is dissolved in the cooking liquor along with hemicelluloses, degradation products, and cooking chemicals, with quantities varying based on the feedstock and pulping conditions. To quantify and analyze the lignin in the liquor, time-consuming isolation steps such as acidic/CO2 precipitation and/or ultrafiltration are required, posing a major bottleneck in lignin analysis.

We recently introduced a method for direct quantification and simultaneous determination of the molar mass distribution (MMD) of lignin in kraft black liquor.1 This technique involves the direct injection of diluted black liquors into an aqueous SEC-UV system, enabling fast and reliable lignin characterization. In this study, we expanded the applicability of our method to other pulping liquors, including spent sulfite and alkaline (wheat straw) liquors. Additionally, we enhanced the molar mass characterization by comparing different calibration standards, such as polystyrene sulfonate and polysaccharide standards, and correcting the conventional calibration with multi-angle laser light scattering (MALLS).

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Behaviour of Fluorinated Pharmaceuticals and Pesticides in Wastewater and Surface Water

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Fluorinated pesticides and pharmaceuticals have gained a significant market share in the agrochemical sector [1] and the pharmaceutical industry [2]. Between 18% and 25% of pharmaceuticals approved since 1991 [3], and approximately 70% of registered pesticides since 2015, are estimated to contain at least one fluorine atom [1]. While their use is very beneficial due to their biological and chemical properties [1,2], several studies have highlighted the environmental concerns, such as bioaccumulation, toxicity or developmental abnormalities in fish embryos associated with these fluorinated substances [1–3].

In our previous studies, storage and the associated potential degradation of fluorinated pesticides and pharmaceuticals were investigated in more detail in order to ensure reliable and accurate analysis of these molecules in environmental samples. Now the study focuses on the degradation behaviour of the same compounds under ozonation—a promising method for wastewater treatment—using a laboratory setup. The objective is to analyse both the degradation of the target compounds and the formation of any resulting metabolites or unexpected by-products. The results are intended to provide a better understanding for the handling of standards and environmental samples under varying conditions as well as their behaviour under ozone treatment, which is intended as an additional wastewater treatment step for organofluorine compounds.

To facilitate this process, an ozone reactor was built and integrated into a laboratory experimental setup, allowing for the treatment of analytes with

ozone while preventing any release of ozone into the atmosphere. During the experiments, an O_2/O_3 gas mixture was bubbled through aqueous solutions of the target substances inside the reactor for a duration of 30 minutes. Samples were collected every 5 minutes through a septum, enabling continuous sampling without interrupting the ongoing experiment. To determine the progress of degradation, the samples are analysed using LC-ESI-MS/MS. A non-target analysis using LC-ESI-HRMS is performed to identify potential metabolites.

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Poster Presentation 33

Discrimination of Coffea arabica cultivars: Multispectral near-infrared and UV-Vis spectroscopy supported by non-linear chemometrics

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Coffee is one of the most widely consumed beverages in the world owing to its cultural significance and beneficial effects on health. Coffea Arabica (Arabica) is considered the most valued coffee species, and makes up the majority of the worldwide production. This study evaluated the feasibility of a multispectral approach to perform rapid discrimination of shelf-ready coffee beans of the most significant Arabica cultivars Typica and Bourbon, their natural crossing, and their important cultivars. Spectral analysis was performed by a benchtop FT-NIR (1,000–2,500 nm), benchtop UV-Vis (200–1,000 nm), and a handheld spectrometer operating on a broad Vis-NIR (350–2,500 nm) region. The spectral analysis was hyphenated with multivariate data-analytical approaches including various linear, non-linear, as well as Artificial Neural Network (ANN) classification techniques and Two-Dimensional Correlation Spectroscopy (2D-COS). Additionally, low-level- (LLDF) and mid-level- (MLDF) data fusion approaches and variable selection (VS) were performed on the collected spectral data sets. Synchronous 2D-COS analysis enabled a detailed comparison of the UV, Vis and NIR spectral regions. The study successfully shows that even closely related Arabica cultivars, are discriminable from each other by NIR and UV-Vis spectroscopy, including on-site capable handheld spectrometers. Non-linear and ANN classifiers provided reliable (95%) authentication results. The performance of the benchtop NIR spectrometer outperformed the handheld NIR-Vis and UV-Vis spectrometer in classification

accuracy. Furthermore, LLDF in combination with VS turned out to be a potent tool to further refine the performance in authentication of coffee cultivars.

(Toxic) secondary metabolites of plants and filamentous fungi in food as potential contributors to the onset of psychosis

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Plants and fungi produce a wide range of secondary metabolites, which play a role in defense and protection against environmental stressors. While some of these compounds, like alkaloids, are known to be toxic, little is known about their combined effects on human health, especially in relation to psychosis. Psychosis is a mental disorder characterized by delusions, hallucinations, negative symptoms, and disorganized behavior. It has traditionally been explained through genetic and environmental factors, however, the role of nutritional factors, particularly exposure to natural toxins, is an underexplored area. Recent evidence suggests that fungal metabolites, such as mycotoxins, can disrupt tryptophan metabolism, alter serotonin pathways, and contribute to oxidative stress and immune dysregulation - all mechanisms implicated in psychiatric vulnerability. The recently started cooperation project between

FFoQSI - Austrian Competence Centre for Feed and Food Quality, Safety and Innovation and the Department of Psychiatry of the Hospital Tulln, aims to extend and optimize the existing Liquid Chromatography - Mass Spectrometry (LC-MS/MS) method developed at BOKU University, for simultaneous detection and quantification of hundreds of plant and fungal secondary metabolites, including serotonin and mycotoxin-related compounds in food and urine samples of psychotic patients. We hypothesize that secondary metabolites will be present at elevated levels in the food consumed by patients prior to the onset of psychotic symptoms, and that increased concentrations of serotonin and toxic metabolites will be detectable in their urine. This project will provide new insights into how everyday nutritional and environmental exposures might contribute to the development of psychosis, potentially opening new pathways for early detection, prevention, and intervention strategies.