ASAC
AUSTRIAN SOCIETY OF ANALYTICAL CHEMISTRY

Young Analysts Forum 2026

TU Graz
Graz University of Technology

May 27 – 28, 2026

Graz University of Technology

BOOK OF ABSTRACTS

Oral Presentations

Session 1: Chromatography 1

Chair: Christian Klampfl

09:45 – 10:30	Keynote 1: The Story of MOSH and MOAH: A Journey from Analytical Challenges to Toxicological Relevance **Andrea Hochegger** *Graz University of Technology*
10:30 – 10:50	T01: Feature Based Molecular Networking Approach for Exploring the Chemical Profile and Quantification of polyphenols in Stevia rebaudiana, Bert.f using HR-LC-ESI-Orbitrap-MSn **Livhuwani Mafhala** *Constructor University Bremen*
10:50 – 11:10	T02: Chemical composition of modern alternative nicotine products available in Slovenia **Matjaž Rantaša** *University of Maribor*

K01

The Story of MOSH and MOAH: A Journey from Analytical Challenges to Toxicological Relevance

Andrea Hochegger[1], Aleksandra Gorska[2], Christian Kirchnawy[3], Giorgia Purcaro[2]

[1] *Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, 8010 Graz, Austria*

[2] *Analytical Chemistry Lab, Gembloux Agro-Bio Tech, University of Liège, 5030 Gembloux, Belgium*

[3] *Österreichisches Forschungsinstitut für Chemie und Technik, Franz-Grill-Straße 5 / Objekt 213, 1030 Vienna, Austria*

Mineral oil hydrocarbons, commonly divided into saturated (MOSH) and aromatic hydrocarbons (MOAH), are complex mixtures of hydrocarbons originating from crude mineral oil. They can contaminate food through ubiquitous sources, e.g. via the environment, during processing, but also from packaging materials. The potential mutagenicity and carcinogenicity of the MOAH fraction and the enrichment of MOSH in the human body were considered as a potential health threat by EFSA in 2012 [1]. Since then, MOSH/MOAH have emerged as highly discussed food contaminants, due to the significant challenges arising from their proper analysis in the complex matrix “food”, the lack of standardized methods and suitable reference materials, but also due to the lack of regulatory limits and the still unclear health effects.

This talk will provide an overview of the development of MOSH/MOAH analysis - from early quantification strategies to standardized methods and automated analysis workflows Considerable effort has gone into developing standardized, sensitive, reliable analysis approaches, which are based on the state-of-art analysis technique of online-coupled high-pressure liquid chromatography - gas chromatography with flame ionisation detection (HPLC-GC-FID).

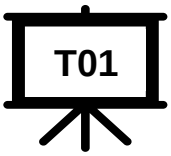
Furthermore, recent advances in the toxicological evaluation will be discussed. Current assessments indicate that MOSH are unlikely to pose a significant health risk at current exposure levels. In contrast, specific subgroups within MOAH - particularly those containing

higher numbers of aromatic rings - are still considered potentially genotoxic and carcinogenic, while for others the available data remain inconclusive [2]. This has shifted the focus towards determining the actual composition, rather than sum parameters: more advanced chromatographic techniques, such as comprehensive two-dimensional gas chromatography (GC×GC) gained importance, providing a much more detailed characterization of the highly complex mixtures, thereby exploring compositional diversity. Emerging approaches integrate chemical characterization with bioanalytical tools, linking composition to real toxicological relevance.

In summary, the challenge of “MOSH/MOAH analysis” underlines the role of modern, fit-for-purpose analytical methods enabling not only quantification but also a deeper, effect-oriented understanding of complex contaminant mixtures.

[1] https://doi.org/10.2903/j.efsa.2012.2704.

[2] https://doi.org/10.2903/j.efsa.2023.8215.



Feature Based Molecular Networking Approach for Exploring the Chemical Profile and Quantification of polyphenols in Stevia rebaudiana, Bert.f using HR-LC-ESI-Orbitrap-MSn

Livhuwani Mafhala, Heba Handoussaa, Sukhmanpreet Kaur, Anna Schneider, Aya Hesham, Noha Sherif, Salma El Shamy, and Nikolai Kuhnert

Constructor University Bremen, Campus Ring 1, 28759 Bremen, Germany
lmafhala@constructor.university

Stevia rebaudiana Bertoni (SR) is a high-value natural sweetener rich in bioactive diterpene glycosides and therapeutic metabolites. Despite the intensive research, its full metabolomic profile has not been revealed yet. In the current research tandem MS data obtained from UHPLC-ESI-Orbitrap- high-resolution mass spectrometry was utilized to generate feature-based molecular networking (FBMN) approach via in variable data-dependent acquisition (DDA) mode to qualitatively and quantitatively characterize SR chemical classes. Using three solid-to-solvent ratios (1%, 4%, and 8% w/v) of SR aqueous extracts. FBMN analysis through the Global Natural Products Social Molecular Networking (GNPS2) platform yielded 7956 nodes, 2903 Edges and 315 molecular families. Fourteen compounds, including three glycosides, five stevioside isomers, and six hydroxycinnamic acid derivatives, were annotated to regioisomeric levels for the first time. Targeted quantification of eight major metabolites related to the classes under the study depicted significant concentration-dependent variations. These findings provide valuable insights for phytochemical map of SR, clarifying the enclosed metabolites and their interconnected biosynthetic pathways.

[1] Ceunen, S.; Geuns, J. M. C. Steviol Glycosides: Chemical Diversity, Metabolism, and Function. J. Nat. Prod. 2013, 76 (6), 1201–1228. https://doi.org/10.1021/np400203b.

[2] Ferdous, J.; et al.: Therapeutic Effects of Natural Food Additives Steviol Glycosides From Stevia Rebaudiana: A Comprehensive Review With Mechanisms. Journal of Food Biochemistry 2025, 2025 (1), 7772203. https://doi.org/10.1155/jfbc/7772203.

[3] Peteliuk, V.; et al.: Natural Sweetener Stevia Rebaudiana: Functionalities, Health Benefits and Potential Risks. EXCLI Journal; 20; ISSN 1611-2156 2021. https://doi.org/10.17179/EXCLI2021-4211.

This work was supported by the Alexander von Humboldt foundation via the Georg Forster Research Fellowship for Experienced Researchers of the first author. Also, the authors would like to acknowledge the Deutsche Akademische Austauschdienst (DAAD) for funding researchers' mobility.

T02

Chemical composition of modern alternative nicotine products available in Slovenia

Matjaž Rantaša, Matjaž Finšgar

University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia
matjaz.rantasa@um.si

The use of modern alternative nicotine products has increased in recent years, evolving into a multi-billion global industry. The public perceives these products as safer alternatives to conventional smoking, which may be partially supported by some recent studies. However, they can still cause adverse health effects, that are not fully understood yet. Their use is particularly prevalent among the younger population. According to the National Institute of Public Health, almost 30% of Slovenian middle school students have used electronic cigarettes, 12% have used nicotine pouches (NPs), while 8% have used heated tobacco products, with these trends continuing to rise [1]. Despite existing regulations, which oversee the production and sale of such products, compliance is not always ensured, especially regarding the presence or concentration of certain compounds. Due to the rapid evolution of these products and the continuous introduction of new formulations, regular chemical analysis is essential to ensure regulatory compliance and consumer safety.

Various e-liquids, NPs and heatsticks available on the Slovenian market were analyzed for volatile flavouring compounds using gas chromatography. The number of identified compounds greatly exceeded the reported compounds on the labelling, with a total of 311 compounds in e-liquids, 163 compounds in NPs, and 25 compounds in heatsticks. Some of these compounds were potentially harmful to human health, while others should not be present at all. Nicotine content did not exceed regulatory limits in any of the samples, while in several cases it was lower than the values declared on the packaging. Elemental composition was determined using inductively coupled plasma mass spectrometry following acid digestion. Heatsticks contained, on average, 459.13 ± 48.03 µg of heavy metals per one unit of consumption, with lower concentrations determined in both NPs and e-liquids [2, 3]. As some products contain metallic components, which may leach heavy metals during use, their

surfaces were further evaluated using surface analysis techniques, i.e. X-ray photoelectron spectroscopy and time-of-flight secondary ion mass spectrometry, to assess surface changes which occur during use. Additionally, thermogravimetric analysis coupled with Fourier transform infrared spectroscopy was employed to investigate the thermal behavior of these products, to estimate the mass fractions of major components, and to identify the gaseous products released during thermal decomposition.

1) NIJZ. Uporaba novih tobačnih in nikotinskih izdelkov med mladimi v Sloveniji narašča. 11.9.2025]; Available from: https://nijz.si/zivljenjski-slog/tobacni-in-povezani-izdelki/uporaba-novih-tobacnih-in-nikotinskih-izdelkov-med-mladimi-v-sloveniji-narasca/.

2) Rantaša, M., D. Majer, and M. Finšgar, The analysis of e-liquids: A study on chemical diversity and metal content using gas chromatography-mass spectrometry and inductively coupled plasma-mass spectrometry. Journal of Separation Science, 2024. 47(17): p. 2400443.

3) Rantaša, M. and M. Finšgar, Flavourings, nicotine content, and elemental composition as indicators of regulatory compliance in nicotine pouches and heated tobacco products. Analyst, 2026.

The authors acknowledge the financial support of the Slovenian Research Agency (Grant No.: P2-0118, J2-50076, J7-50226, J2-50086, BI-TR/25-27-002 and GC-0007), and a young researcher fellowship for M.R. The project is co-financed by the Republic of Slovenia, the Ministry of Higher Education, Science and Innovation, and the European Union under the European Regional Development Fund.

Session 2: Chemical Sensors & Biosensors

Chair: Torsten Mayr

11:40 – 12:00	T03: Glucose and lactate optical biosensors for microfluidic cell culture monitoring **Iga Malicka** *Graz University of Technology*
12:00 – 12:20	T04: Integrated In-Line Optical Sensing of Electrochemical H_2O_2 Production in a Microfluidic Reactor **Desislava Yordanova Apostolova** *University of Ljubljana*
12:20 – 12:40	T05: Covalent Immobilisation of pH-Sensitive Azo Dyes on Cellulose Substrates for Colourimetric Response Studies **Iva Karneluti** *University of Zagreb*
12:40 – 13:00	T06: Luminescent Surface-Anchored Metal-Organic Frameworks as a Novel Material for Gas Sensing Applications **Theresa Mautz** *Graz University of Technology*

T03

Glucose and lactate optical biosensors for microfluidic cell culture monitoring

Iga Malicka[1*], Stefanie Fuchs[2], Alessia Moruzzi[3], Madalena Cipriano[3,4,5], Christiane Luley[6,7], Bernd Nidetzky[6,7], Peter Loskill[3,4,5] and Torsten Mayr[1]

[1] *Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry, Stremayrgasse 9, 8010 Graz, Austria*
**iga.malicka@tugraz.at*

[2] *PyroScience AT GmbH, Rechbauerstraße 4, 8010 Graz, Austria*

[3] *NMI, Markwiesenstraße 55, 72770 Reutlingen, Germany*

[4] *Eberhard Karls University Tübingen, Department for Microphysiological Systems, Institute of Biomedical Engineering, Waldhörnlestraße 22, 72072 Tübingen, Germany*

[5] *Eberhard Karls University Tübingen, 3R-Center for In vitro Models and Alternatives to Animal Testing, Waldhörnlestraße 22, 72072 Tübingen, Germany*

[6] *Graz University of Technology, Institute of Biotechnology and Biochemical Engineering, Petersgasse 12, 8010 Graz, Austria*

[7] *acib GmbH, Krenngasse 37, 8010 Graz, Austria*

Microphysiological systems allow to mimic human tissues and organs in laboratory conditions, serving as a useful tool in drug testing and analyzing the mechanisms of diseases. Monitoring glucose and lactate in those systems allows to obtain valuable information on the metabolic state of the cultured cells. The majority of available glucose and lactate biosensors are electrochemical [1]. The few reported optical sensors are based on luminescence oxygen-quenching after enzymatic oxidation of the analyte. Despite many advantages of these approaches, integration of those sensors into microphysiological systems still remains a challenge.

Hereby we present enzyme-based optical glucose [2] and lactate sensors that can be straightforwardly incorporated into microphysiological systems. The sensors consist of oxygen sensitive particles and a respective enzyme immobilized in a polymeric matrix. Additionally, a catalyst for the degradation of hydrogen peroxide is added to enhance the sensors' stability.

The sensors can be easily integrated into a desired system by spotting the formulation onto a chip-sealing tape or directly into the microfluidic chip. The spot size can be altered according to the width of the microfluidic channel. Additionally, the dynamic range of the sensors can be modified by implementing diffusion membranes of different porosities, allowing to adjust the sensors' properties to the needs of a specific cell culture system.

We evaluated the influence of different conditions (e.g. pH, temperature, flow rate) on the sensors' performance, along with the investigation of their stability. We measured glucose and lactate level in cell culture supernatant and effluent cell culture media, respectively. The results were compared to commercially available methods and confirmed the sensors' suitability for microphysiological systems.

[1] Fuchs, S. et al., ACS Biomater. Sci. Eng. 7 (2021) 2926 – 2948

[2] Fuchs, S. et al., Biosens Bioelectron. 237 (2023) 115491

This research has been supported by the Medical Research Council NC3Rs under the CRACK IT Challenge Program with the project number NC/C023204/01 (SensOoChip).

T04

Integrated In-Line Optical Sensing of Electrochemical H_2O_2 Production in a Microfluidic Reactor

Desislava Yordanova Apostolova[1]*, Maris Minna Mathew[1], Tomaž Gril[1], Miha Nosan[1], Torsten Mayr[2], Boštjan Genorio[1]

[1] *University of Ljubljana, Faculty of chemistry and chemical technology, Večna pot 113, 1000 Ljubljana, Slovenia*
**desislava.apostolova@fkkt.uni-lj.si*

[2] *Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Stremayrgasse 9/II, 8010 Graz, Austria*

Hydrogen peroxide (H_2O_2) is widely used in industry, but its conventional anthraquinone production is energy-intensive, relies on scarce platinum group metals, and requires transporting concentrated H_2O_2. Electrochemical synthesis on carbon electrocatalysts via the two-electron oxygen reduction reaction (ORR) offers a safer, more sustainable alternative.

A microfluidic electrochemical reactor with integrated in-line optical sensing for real-time H_2O_2 detection will be presented. The sensing system was implemented in two different configurations: a parallel-plate electrode design and a reactor with a gas diffusion electrode (GDE) in the cathodic half-cell. The optical sensor enabled non-invasive, in situ monitoring and demonstrated reliable performance up to 10 mM. Measurements were validated using an independent off-line electrochemical method, showing good agreement.

Electrochemical performance was evaluated using Chronoamperometry (CA) and Chronopotentiometry (CP), providing insight into the relationship between reactor design, operating conditions, and H_2O_2 generation. These results highlight the potential of combining microfluidic reactors with integrated optical sensing for efficient monitoring and optimization of electrochemical H_2O_2 production.

[1] Perry S. C., Nat. Rev. Chem. 3 (2019) 442-458

[2] Chen S., ACS Sustain. Chem. Eng., 6 (2018) 311-317

[3] Apostolova D. Y., Chem. Eng. J., 525 (2025) 170301

[4] Apostolova D. Y., Chem. Commun., (2026) DOI: 10.1039/d6cc01364c

The financial support from the Slovenian Research and Innovation Agency (ARIS) through grants P2-0423, P1-0447, J7-4636, J2-50086, J7-50227, J2-60044 and L2-3161, as well as the infrastructure programme I0-0022, is gratefully acknowledged.

T05

Covalent Immobilisation of pH-Sensitive Azo Dyes on Cellulose Substrates for Colourimetric Response Studies

Iva Karneluti[1]*, G. J. Mohr[2], D. Joshy[1], I. Perković[1], H. Yilmaz[1], I. M. Steinberg[1]

[1] *University of Zagreb Faculty of Chemical Engineering and Technology, General chemistry, Trg Marka Marulića 19, 10000 Zagreb, Croatia*
**izuvic@fkit.hr*

[2] *Joanneum Research Materials, Franz-Pichler-Straße 30, 8160 Weiz, Austria*
***Gerhard.Mohr@joanneum.at*

Wearable and non-invasive optical sensing platforms are increasingly being explored for real-time monitoring of physiologically relevant parameters. Among these, pH represents a fundamental parameter that can be monitored using simple and visually interpretable colourimetric systems. In this work, a cellulose-based material is functionalized by covalent immobilisation of a pH-sensitive azo dye using vinylsulfonyl chemistry [1-2]. The immobilisation is achieved via Michael addition between the reactive dye moiety and hydroxyl groups of the cellulose substrate, a commercially available face sheet mask. This procedure enables stable attachment of the dye molecules while preserving their optical response to the analyte of interest. The resulting material exhibits a reversible colourimetric response over the investigated pH range. A rapid response time of less than 2 minutes was observed, supporting its potential for near real-time monitoring. A distinct colour transition from blue through green to yellow-brown is observed with increasing pH, enabling straightforward visual interpretation. Unlike physically incorporated systems, the covalent linkage eliminates dye leaching, resulting in enhanced stability and repeatability of the optical response. Colourimetric evaluation was performed using CIELAB colour space analysis, with particular emphasis on monitoring the hue angle as a quantitative descriptor for tracking pH-induced colour changes. The combination of a biocompatible cellulose substrate and a covalently immobilised indicator dye results in a flexible and lightweight material with potential for integration into practical applications. This approach demonstrates that covalent immobilisation provides a stable and reproducible route for introducing pH-responsive functionality into cellulose-based materials.

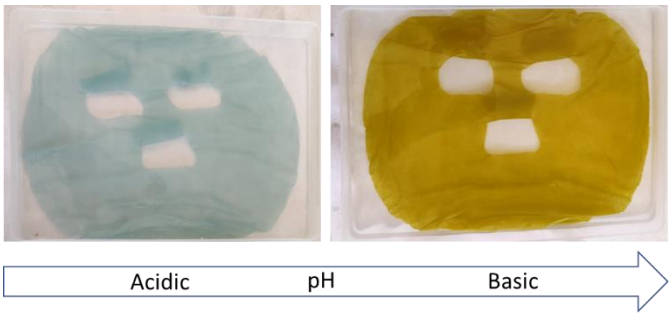


Figure 1. Cellulose-based covalently functionalized pH sensitive material in acidic and basic solution.

[1] Mohr G. J. et al., Anal. Bioanal. Chem. 392 (2008) 1411–1418

[2] Mohr G. J. et al., Mikrochim. Acta. 192 (2025) 405

This work is supported by the Croatian Science Foundation under the project WearSense HRZZ IP-2022-10-2595.

T06

Luminescent Surface-Anchored Metal-Organic Frameworks as a Novel Material for Gas Sensing Applications

Theresa K. Mautz[1*], Fabian Gasser[2], Fernando Warchomicka[3], Roland Resel[2], Christian Slugovc[4], Sergey M. Borisov[1]

[1] *Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria.*
**theresa.mautz@tugraz.at*

[2] *Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria*

[3] *Institute of Materials Science, Joining and Forming, Graz University of Technology, Kopernikusgasse 24 8010 Graz, Austria*

[4] *Institute for Chemistry and Technology of Materials, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria*

Over the past two decades, Metal-Organic-Frameworks (MOFs), three-dimensional porous networks consisting of organic linkers and metal nodes, have emerged as a new class of materials with a broad field of applications. Due to their exceptional stability under harsh conditions (high temperatures, pressure, or the presence of organic solvents), their high internal surface area and porosity, they represent an ideal platform for luminescence-based gas sensing applications, offering stable alternatives to commercial sensors for harsher environments. Pt(II)- and Pd(II)-Porphyrins – prominent indicators for optical sensing of oxygen – additionally contribute excellent organic building blocks for MOFs together with Zirconium-Oxo Clusters as metal nodes. These microcrystalline materials exhibit promising oxygen sensitivity in the gas phase,[1] but immobilization on a support material and the limited sensitivity in organic solvents remain issues. Porphyrin-based Surface-Anchored Metal Organic Frameworks (SURMOFs) may represent a notable improvement due to thin and stable MOF films that can be obtained directly on a solid, transparent substrate supports.

Herein, we report synthesis of SURMOFs, consisting of Pt(II)TCPP and Indium-Oxo-Clusters, on functionalized glass and flexible poly(ethylene terephthalate) supports, revealing room temperature phosphorescence in the red part of the electromagnetic spectrum. At 21 kPa oxygen in the gas phase ~ 50-fold quenching compared to nitrogen atmosphere is observed. In addition, we were able to demonstrate for the first time the luminescence and oxygen sensitivity of the SURMOFs in organic solvents, which enables them to be used as new optical sensors in these challenging conditions.

[1] T. Burger, M.V. Hernández, C. Carbonell, J. Rattenberger, H. Wiltsche, P. Falcaro, C. Slugovc, S.M. Borisov, ASC Appl. Nano Mater., 6 (1), 248-260 (2023).

This work was financially supported by the lead-project LP03 “Porous Materials at Work for Sustainability” at Graz University of Technology.

Session 3: Spectroscopy

Chair: Helmar Wiltsche

14:00 – 14:20	T07: Silicon: small element, big analytical challenge **Christina Mühlthaler** *Graz University of Technology*
14:20 – 14:40	T08: Combined optical and mass spectrometric analysis of single microparticles via in-line microscopy-SP ICP-MS **Bernhard Grüner** *University of Graz*
14:40 – 15:00	T09: Advancing UV Aging Studies of Immobilized Microplastics: Tracking the Photo-Oxidation-Behaviour at the Particle Level **Jakob Lauß** *University of Innsbruck*
15:00 – 15:20	T10: The Beauty and the Burden: Insights into Firework-derived Single Particles using ICP-TOFMS and AF4 **Manuel Candussi** *University of Graz*

T07

Silicon: small element, big analytical challenge

Christina Mühlthaler and Helmar Wiltsche

Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, 8010 Graz, Austria

Silicon is the second most abundant element on Earth and the backbone of modern technology semiconductors, solar cells, glass, ceramics, advanced alloys and biomaterials all rely on accurate Si quantification. Yet despite its ubiquity, silicon remains one of the most difficult elements to measure reliably in the analytical laboratory.

There are three intertwined problems that make Si quantification uniquely challenging. First, volatile losses: in acidic HF digestion, silicon is converted to SiF_4, a gas that sublimes at – 95.5 °C, and to H_2SiF_6, which decomposes back to SiF_4 above 110 °C so simply venting a hot vessel can release the analyte. Second, contamination: borosilicate glassware, mineral acids, polymer labware, lab air and even cosmetics constantly contribute Si to method blanks. Third, spectral interferences: the most abundant isotope, ^{28}Si, overlaps with $^{14}N_2^+$, $^{12}C^{16}O^+$ and $^{12}CH_4N^+$ in ICP-MS, requiring high-resolution or reaction-cell techniques for trace work.

The work on microwave-assisted digestion (Multiwave 5000 with SVT50 and HF100 rotors) provides the empirical heart of the talk. A spike of 200 mg L^{-1} silicon as H_2SiF_6 was digested in 5 mL HNO_3 + 1 mL HF with different organic matrices. With no carbon source recovery reached 96 %; with 0.4 g glycine, 88 %; with nicotinic acid, 58 %; with glucose, only 18 %. The matrix, not the chemistry, governed the loss: carbon-driven exothermic reactions raised vessel pressure prematurely, triggered venting at temperatures where the silicon fluorides were already volatile, and let analyte escape with the gases.

Three intuitive remedies cooling the vessel overnight before venting, reducing the HF volume and complexing free HF with boric acid each recovered only 10–20 % of the lost silicon. The decisive fix was a change of vessel: single-use, fully sealed HF100 cells (Rotor 16), which never vent during the run, consistently delivered spike recoveries above 93 % across every carbon-rich matrix tested. Combined with sub-boiled HNO_3, PFA labware, polished water,

validated blanks and matched certified reference materials, this protocol routinely achieves > 95 % recovery in the laboratory at relative standard deviations below 5 %.

The take-home: silicon is the element that gets away. Its accurate quantification depends less on the choice of detector than on the integrity of the digestion vessel and on validating every batch with blanks, spike recoveries and reference materials.

T08

Combined optical and mass spectrometric analysis of single microparticles via in-line microscopy-SP ICP-MS

Bernhard Grüner, Raphael Hauer, Matthias Elinkmann, Thomas Lockwood, Raquel Gonzalez de Vega, Christian Hill, Ulrich Hohenester, David Clases

University of Graz, Universitätsplatz 1/II, 8010 Graz, Austria
bernhard.gruener@uni-graz.at

Single particle inductively coupled plasma–mass spectrometry (SP ICP-MS) has become an increasingly powerful tool for particle characterization, providing information on number concentration, elemental composition, as well as mass and size distributions. More recently, micrometre-sized particles have gained attention. For instance, microplastics can be studied via their carbon content, while unicellular organisms are often analysed to investigate elemental accumulation. A critical parameter for accurate particle analysis is the transport efficiency, which describes the fraction of particles that successfully enter the plasma. While this parameter is typically assumed to be constant for small particles, this assumption breaks down for micrometre-sized particles, including cells. As a result, significant errors arise in the determination of number concentrations, as well as mass and size distributions. In this work, we demonstrate that particle transport efficiency decreases with increasing particle size. We further show how this size dependence distorts measured size distributions and hinders accurate quantification of particle number concentrations. This limitation constrains the applicability of SP ICP-MS for quantitative microscale analysis and highlights the need for correction strategies and models to account for this detection bias.

We present a novel approach for determining size-dependent transport efficiency by directly coupling an orthogonal in-line microscope to SP ICP-MS for particle counting and characterization. Using dynamic image analysis in a specially designed measurement cell, all particles are scanned before entering the ICP. This enables optical characterization of microparticles in terms of size and morphology, while allowing correlative analysis with SP ICP-MS data to retrospectively determine and correct for size-dependent transport efficiency.

Beyond transport efficiency, the integration of orthogonal in-line microscopy also enables the evaluation of particle shape, sedimentation, and agglomeration behaviour, providing complementary insights that are not accessible through SP ICP-MS alone.

T09

Advancing UV Aging Studies of Immobilized Microplastics: Tracking the Photo-Oxidation-Behaviour at the Particle Level

Jakob Lauß, Christoph Kappacher, Jovan Badzoka, Krzysztof B. Beć, Christian W. Huck

University of Innsbruck, Institute of Analytical Chemistry and Radiochemistry, Innrain 80, 6020 Innsbruck, Austria
jakob.lauss@uibk.ac.at

UV-induced aging alters the chemical structure of microplastics and complicates their spectroscopic identification. Simulating the photo-oxidation behaviour of microplastics with existing experimental approaches is often limited to bulk materials or static particle systems, restricting mechanistic insight and control over irradiation conditions.

Here, we present a particle-resolved approach to investigate UV-induced aging using FT-IR imaging. Individual microplastic particles are immobilized on an infrared-transparent potassium bromide (KBr) substrate, enabling time-resolved monitoring of the same particles over extended irradiation periods. This allows direct observation of spectral evolution without ensemble averaging and provides access to particle-specific degradation pathways with improved reproducibility.

In addition, a custom-built UV irradiation setup for suspension experiments is explored, enabling continuous stirring during exposure to improve homogeneity compared to static systems.

Advanced spectral analysis, supported by 2D-Correlation Spectroscopy facilitates band assignment and interpretation of overlapping features formed during photo-oxidation.

Overall, these approaches address key limitations of current UV aging studies and support more detailed investigation of microplastic degradation and its spectroscopic implications.

Funding: This research was partially funded by the Interreg Bayern-Österreich program through the project “MikAlp” (Project ID: BA0100116, co-financed by the European Union)

T10

The Beauty and the Burden: Insights into Firework-derived Single Particles using ICP-TOFMS and AF4

Manuel Candussi, Sara Escudero Cernuda, Thomas E. Lockwood, Benedikt Tschofenig, David Clases

University of Graz, Analytical Chemistry, Universitätsplatz 1/I, 8010 Graz, Austria
manuel.candussi@uni-graz.at

Fireworks represent an intense episodic source of fine particulate matter (PM2.5), yet the particle-resolved chemical composition and size remain insufficiently understood. In this study, single particle inductively coupled plasma time-of-flight mass spectrometry (SP ICP-TOFMS) combined with asymmetric flow field-flow fractionation (AF4) was used to investigate PM2.5 in Graz around New Year's Eve 2023. Despite a city-wide firework ban, single particle analysis revealed a pronounced and short-lived increase in characteristic pyrotechnic tracers on 1 January, particularly Bi, Ba, Sr, and Cu. Beyond these established tracers, significant increases were observed for particles containing potentially toxic elements such as Pb, V, and Cr, alongside Mg, Al, La, Ag, Ti, Ca, and Zn. This demonstrates that fireworks emissions are not limited to typical metals used for colouring, but introduce a wider spectrum of metal-containing particles, including elements of known toxicological concern. AF4 analysis showed that a substantial fraction of these particles occurs in the range of a few hundred nanometres, a size range associated with efficient inhalation and deep lung deposition. Together, these results demonstrate that episodic firework events generate chemically complex, metal-containing PM, emphasizing the importance of particle-resolved approaches for assessing inhalation exposure and potential health impacts.

Session 4: Chromatography 2

Chair: Barbara Siegmund

15:50 – 16:10	T11: The separation of bicyclic boronate based β-lactamase inhibitors under SFC conditions **Alina Spindler** *Johannes Kepler University Linz*
16:10 – 16:30	T12: Shedding light on the arsenic metabolism in higher fungi – an investigation into the arsenic metabolome of edible mushrooms **Lorenz Steiner** *University of Graz*
16:30 – 16:50	T13: Benchmarking LC–HRMS NTA Workflows for Robust Phenolic Marker Discovery in Wine Authentication **Santiago Souza Nava** *FFoQSI - BOKU University*

T11

The separation of bicyclic boronate based β-lactamase inhibitors under SFC conditions

Alina Spindler, Lucas Sternbauer, Markus Himmelsbach, Christian Klampfl

Johannes Kepler University Linz, Institute of Analytical and General Chemistry/ Department of Analytical Chemistry, Altenberger Straße 69, 4040 Linz, Austria
alina.spindler@thermofisher.com

β-lactamase inhibitors are a substance class currently receiving attention in the pharmaceutical industry. These substances are co-formulated with β-lactam antibiotics to treat infections caused by multidrug resistant gram-negative bacteria. The first developed inhibitors already achieved regulatory approvals by authorities; more recently discovered inhibitors such as bicyclic boronates with a broader inhibition range are currently under investigation in late-stage clinical phases. [1]

Hence, the objective was to study the chromatographic behavior of these bicyclic boronates under supercritical fluid conditions to facilitate research in pharmaceutical development and medicinal chemistry as well as to demonstrate the suitability of supercritical fluid chromatography (SFC) for pharmaceutical quality control.

We present a phase-appropriately validated SFC-UV method to analyze the new β-lactamase inhibitor QPX7728 [1] and its corresponding prodrug [2] as well as other structurally related analogues. Under the applied chromatographic conditions, challenging elution and separation problems initially encountered could be overcome, thereby enabling the analysis of chiral and achiral compounds within 12 minutes in a single run using only one column.

The research and resulting method demonstrate the benefits of SFC and its valuable contribution as an addition to well-established techniques from R&D to QC.

[1] Hecker S. J., et al.: J. Med. Chem. 63 (2020) 7491

[2] Reddy K. R., Parkinson J., Sabet M., Tarazi Z., Boyer S. H., Lomovskaya O., Griffith D. C., Hecker S. J., Dudley M. N., J. Med. Chem. 64 (2021) 17523

T12

Shedding light on the arsenic metabolism in higher fungi – an investigation into the arsenic metabolome of edible mushrooms

Lorenz Steiner, Julia Truschner, Andrea Raab, Jan Borovicka, Walter Gössler, Bassam Lajin

Karl-Franzens-Universiät Graz, Analytical Chemistry, Universitätsplatz 1/II, 8010 Graz, Austria
lorenz.steiner@uni-graz.at

Arsenic is ubiquitous in our environment, albeit its concentrations may greatly vary from one local to another. In the earth's crust, arsenic is predominantly encountered in its inorganic form, either as arsenate or arsenite, respectively, which is generally regarded as cytotoxic. Arsenate inside the cell contributes to the formation of reactive oxygen species contributing to oxidative stress, and mimics phosphate, potentially interfering with proper cell-function. Arsenite binds to thiol moieties in proteins, enzymes, and cofactors, inhibiting their function. Hence, a mechanism for the detoxification of inorganic arsenic had to be developed in all forms of life.

In our research, we discovered two distinct trends in the metabolism of arsenic in higher fungi: Either arsenic is partially methylated, resulting in the biosynthesis of dimethylarsinic acid, methylarsonic acid, dimethylarsinoylacetic acid, and dimethylarsinoylethanol, retaining the As=O moiety and the +5 oxidation state. In other mushrooms, arsenic is methylated and reduced, leading to the biosynthesis of a large number of arsenic species, such as arsenobetaine, arsenocholine, etc., all containing an R–As$(CH_3)_3$ motif. In these compounds arsenic is present in the +3 oxidation state.

In our work, we further broadened our understanding of the arsenic metabolism in various edible mushrooms, including the commonly eaten penny bun (Boletus edulis) and cauliflower mushroom (Sparassis crispa), using liquid chromatography coupled with inductively coupled plasma tandem mass spectrometry and electrospray mass spectrometry.[1]

[1] Steiner, L., Raab, A., Lajin, B. et al. Anal Bioanal Chem (2025).

T13

Benchmarking LC–HRMS NTA Workflows for Robust Phenolic Marker Discovery in Wine Authentication

Santiago Souza Nava

FFoQSI - BOKU University, Institute of Analytical Chemistry, Dresdner Straße 107, 1200 Vienna, Austria
santisouza97@gmail.com

Non-targeted LC–HRMS is increasingly applied in food authenticity studies, yet molecular feature detection and marker discovery remain highly sensitive to software selection, parameterization, and matrix complexity. Here, we benchmarked and harmonized non-targeted analysis (NTA) workflows to enhance robustness in phenolic marker discovery for barrel-aged Grüner Veltliner wines, using a ground-truth approach to discriminate them from stainless-steel-aged wines. Wine samples and a phenolic standard mixture (QC-Std), covering key compound classes such as hydroxycinnamic acids, flavonols, and stilbenes, were analyzed using an Agilent 6550 Q-TOF LC–MS. QC-Std mixture was used as an external benchmarking reference to systematically evaluate NTA software performance and optimize critical parameters, including m/z tolerance, retention-time alignment, peak detection, deconvolution, and adduct grouping. Data was processed using MS-DIAL, MZmine, and XCMS, comparing default and QC-Std–optimized workflows. Samples, pooled wines (QC-Wine) with the QC-Std were used to assess precision in terms of area variance (CV<25%), RT (STD) and mass accuracy (STD) to retain robust features, while selected samples was acquired in data-dependent mode for validation of fragmentation spectra. A feature-based neural network approach has been developed to support pattern recognition and marker prioritization. Results show that software selection and parameter optimization strongly influence feature detection, with parameter tuning reducing false positive detection rate by up to 96% and improving reproducibility. Software algorithm-dependent differences were observed, particularly in adduct grouping and peak integration. Although only a limited fraction of features was consistently detected across all software tools, multivariate analysis enabled

clear discrimination between stainless-steel–aged and oak-aged wines. These resultsdemonstrate the importance of systematic benchmarking and provide a basis for standardized NTA workflows in food authenticity research.

[1] Bayen S., Trends Food Sci. Technol. 149 (2024) 104550

[2] Qin Z., Trends Food Sci. Technol. 143 (2024) 104298

[3] Mialon N., Food Chem. 398 (2023) 133856

[4] Zhong P., Compr. Rev. Food Sci. Food Saf. 21 (2022) 2445-2488

Session 5: Materials, Food and Environmental 1

Chair: David Clases

09:00 – 09:45	Keynote 2: Pesticide Residue Analysis in Food: Daily Business and Future Challenges **Leo Krammer** *Institut Dr. Wagner*
09:45 – 10:05	T14: Investigating mixing dynamics and water-sediment-interaction in rivers of the Brazilian Amazon with DGT passive sampling **Antonia Siebenbrunner** *Montanuniversität Leoben*
10:05 – 10:25	T15: Hidden Fluorine in Gasoline: Multi-Technique Detection of Fluorinated Species in Alkylation Streams **Viktoria Müller** *University of Graz*

Pesticide Residue Analysis in Food: Daily Business and Future Challenges

Leo Krammer

Institut Dr. Wagner Lebensmittelanalytik GmbH, Römerstraße 19, 8403 Lebring, Austria

Plant protection products (PPPs) are ubiquitously used in agriculture to benefit the health of plants, thereby ensuring access to sufficient and balanced food of appropriate quality. The active substances of PPPs can be divided into several subclasses of pesticides (e.g., herbicides, insecticides, etc.) and their usage can result in residues on or in the plants and soil and ultimately on the harvested crops. However, customers must expect their food to be safe and healthy, which is why a harmonized system for maximum residue levels (MRLs) of pesticides has been established in the European Union in 2005 based on good agricultural practice and the lowest consumer exposure necessary to protect vulnerable consumers. As plants and food of plant origin can be considered as very challenging matrices and control laboratories aim to cover as many analytes as possible (with their respective MRLs typically in the ppb range), control laboratories must rely on efficient workup strategies as well as highly sensitive and selective analytical methods, which need to be constantly improved to meet the ever-changing circumstances and requirements.

T14

Investigating mixing dynamics and water-sediment-interaction in rivers of the Brazilian Amazon with DGT passive sampling?

Antonia Siebenbrunner[1]*, Stefan Wagner[1], Amauri Antonio Menegário[2], Thomas Prohaska[1], José Lucas Martins Viana[2], Luiz Felipe Pompeu Prado Moreira[2], Melina Borges Teixeira Zanatta[2], Ézio Sargentini Junior[3], Johanna Irrgeher[1]

[1] Department General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700, Leoben, Austria
**antonia.siebenbrunner@unileoben.ac.at*

[2] Environmental Studies Center (CEA), São Paulo State University (UNESP), Avenida 24-A, 1515, 13506-900, Rio Claro, SP, Brazil

[3] Coordenação de Dinâmica Ambiental, Instituto Nacional de Pesquisas da Amazônia, 69083-000 Manaus, AM, Brazil

Rio Negro and Solimões are two Amazonian rivers with contrasting characteristics (e.g., pH, trace metal content) due to the vast geological differences of their drainage basins. Because complete mixing of these large rivers occurs only >100 km downstream from their confluence (Manaus, Brazil), the system exhibits complex mixing dynamics, presenting an ideal study area for testing passive sampling techniques. In this study, we employed time-integrated passive sampling using diffusive gradients in thin films (DGT) along with traditional snapshot grab sampling for subsequent (multi-collector) ICP-MS measurements of alkaline earth metal (Sr, Ba, Ca) concentrations and 87Sr/86Sr isotope ratios [1]. DGT and grab samples from the Rio Negro and Solimões confluence matched within uncertainty in terms of Sr, Ba, and Ca concentrations and 87Sr/86Sr ratios [cDGT/csoln = 1.04 ± 0.15, n = 33, corrected for ionic strength effects; Δ(87Sr/86Sr)DGT−grab = (−0.07 ± 0.43) ‰, n = 33]. In comparison to grab sampling, DGT provided 15-fold pre-concentrated, low-matrix samples, facilitating isotopic analysis. The distinct geological conditions resulted in remarkably diverse Sr isotope ratios [Δ(87Sr/86Sr)max−min = (42.22 ± 0.91) ‰], enabling isotope pattern deconvolution (IPD) for unveiling river end-member contributions and mixing dynamics. IPD revealed pronounced variability of the Rio Negro contribution to the mixture [(8.4 ± 0.4) % in the dry vs (43 ± 3) %

in the wet season, Rio Negro side of the confluence, 15 km downstream]. DGT devices applied to sediments sampled the diffusion-available (i.e., labile and therefore potentially bioavailable) Sr fraction, providing insights into sediment-water interactions not available from sediment digests. Sediment composition appeared to follow river water with a time lag, suggesting that the sediment acts as an (isotopic) sink between the dry and wet season.

[1] Wagner S., Anal. Chem. 2022, 94, 16, 6338–6346

The authors thank the Austrian Science Fund (FWF) and Slovenian Research and Innovation Agency (ARIS) [projects MURmap (FWF-Grant-DOI: 10.55776/I5491; ARIS-Grant-Number J1-3023; Webpage: https://www.murmap.at/en/) and DISCOVER (FWF-Grant-DOI: 10.55776/PIN8195924; ARIS-Grant-Number: J1-60008; Webpage: https://discover-drava.at/en], as well as the São Paulo Research Foundation (FAPESP) [grant number: 23/11694-5] for funding this research. Student and staff mobility was funded via the Erasmus+ program.

T15

Hidden Fluorine in Gasoline: Multi-Technique Detection of Fluorinated Species in Alkylation Streams

Viktoria Mueller, Markus Rotzinger, Zofia Kowalewska, Klaus Zangger, Joerg Feldmann

University of Graz, Universitätsplatz 1, 8010 Graz, Austria
viktoria.mueller@hutton.ac.uk

Fluorine-containing species in gasoline samples from different stages of the alkylation process were investigated using multiple analytical techniques, including combustion ion chromatography (CIC), inductively coupled plasma mass spectrometry (ICP-MS/MS), gas chromatography with atomic emission detection (GC-AED), high-resolution continuum source molecular absorption spectrometry (HR-CSMAS), gas chromatography–Orbitrap mass spectrometry (GC-Orbitrap), and ^{19}F nuclear magnetic resonance spectroscopy (^{19}F NMR). This work examines the potential presence of fluorinated compounds in gasoline associated with the alkylation process using complementary analytical techniques targeting both total and molecular fluorine.

Significant variability in fluorine concentrations was observed between samples and analytical methods. CIC measurements indicated total fluorine concentrations ranging from <10 to 321 mg F/L. Comparable trends were observed using HR-CSMAS and ICP-MS/MS. ^{19}F NMR confirmed the presence of several fluorine containing compounds, with the fluorine bound to secondary and/or tertiary carbon. GC-AED analysis further identified volatile fluorinated compounds, reaching up to 269 mg F/L in certain samples, GC–Orbitrap analysis provided high-resolution accurate mass data, allowing molecular formula assignment for the detected compounds.

Overall, the results demonstrate that fluorinated species can occur at various stages of the alkylation process and that combining bulk fluorine determination with molecular-specific techniques provides a more comprehensive understanding of fluorine distribution in refinery streams.

Session 6: Materials, Food and Environmental 2

Chair: David Clases

10:25 – 10:45	T16: When Sampling Skews Reality: Evaluation of High- and Low-Volume PM2.5 Sampling Biases in Atmospheric Per- and Polyfluoroalkyl Substances Quantification **Andreas Roth** *University of Graz*
10:45 – 11:05	T17: Volatile chemical products as precursors of urban new particle formation and air pollution **Markus Tischberger** *Technical University of Vienna*
11:05 – 11:25	T18: Is arsenic essential? **Helen Lord** *University of Graz*
11:25 – 11:45	T19: Sampling-Related Variability in ICP-MS Multi-Element Analysis of Urban Leaf Samples — Evidence from Kampala, Uganda **Paul Töppmann** *Montanuniversität Leoben*

T16

When Sampling Skews Reality: Evaluation of High- and Low-Volume PM2.5 Sampling Biases in Atmospheric Per- and Polyfluoroalkyl Substances Quantification

Andreas Roth, Viktoria Müller, Jörg Feldmann

University of Graz, Analytical Chemistry, TESLA, Universitätsplatz 1, 8010 Graz, Austria
andreas.roth@edu.uni-graz.at

Accurate atmospheric measurement of per- and polyfluoroalkyl substances (PFAS), a class of persistent fluorinated chemicals widely used in industrial and consumer products and known for their environmental mobility and potential health risks, is essential, yet current air-sampling approaches are inconsistent and prone to artefacts, limiting data comparability. Atmospheric measurements often utilize active air sampling without sorbent phases under the implicit assumption thatsampling rate does not influence measured concentrations.

Here, PM2.5 samples were collected simultaneously at two sites using high-volume (HV, 500 L min-1) and low-volume (LV, 38 L min-1) samplers. Filters underwent liquid extraction and targeted liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis for 43 target PFAS (legacy and emerging) quantification alongside elemental characterization using inductively coupled plasma mass spectrometry (ICP-MS). Significant discrepancies between sampling approaches were observed for PM2.5 and PFAS concentrations, indicating that normalization to sampled air volume is unsuitable, whereas elemental concentrations per g PM remained consistent

On average 10 (± 2) PFAS were detected per sample. Several PFAS differed significantly when normalized to the mass of PM. ΣPFAS and ΣPFCA and ΣPFSA were consistently elevated in LV relative to HV sampler filters by a factor of 3.5, 4 and 2.4 respectively while others showed no significant difference.

These results demonstrate substantial methodological biases in sorbent-free active PM2.5 sampling and highlight the need to reassess current approaches for accurate atmospheric PFAS quantification.

The authors gratefully acknowledge the financial support of the University of Graz (Austria). They also thank Dipl.-Ing. Benedikt Tschofenig and Dipl.-Ing. Karin Fröhlich, as well as the Departments for Air Pollution Control and Environmental Laboratory for providing the necessary samples and for their valuable support throughout the project.

T17

Volatile chemical products as precursors of urban new particle formation and air pollution

Markus Tischberger, Rulan Verma, Emese Papp, Marco Lair, Melanie Ellmauer, Hinrich Grothe, and Dominik Stolzenburg

TU Wien, Institute of Materials Chemistry/Research unit of Atmospheric Physical Chemistry, Getreidemarkt 9/165, 1060 Vienna, Austria
markus.tischberger@tuwien.ac.at

As combustion-related volatile organic compound (VOC) emissions continue to decline, volatile chemical products (VCPs) - including emissions from cleaning agents, personal care products, adhesives, coatings, sealants, and asphalt - are increasingly recognized as major contributors to urban VOC budgets [1,2]. While assessing their poorly constrained new particle formation (NPF) potential is essential for sustainable city development, it requires knowing the entire VCP volatility distribution [3].

Here, we demonstrate the capabilities of ultra-high-resolution multi-pressure chemical ionization Orbitrap mass spectrometry [4] in combination with a newly designed oxidation flow reactor (OFR) to investigate the complete oxidation chain of selected VCP emissions. Following evaporation, gas-phase sample molecules undergo oxidation by ozone and OH radicals within the OFR, where UVC LEDs replace the commonly used but environmentally detrimental mercury discharge lamps to power the atmospheric simulation. Newly formed particles are monitored with a differential mobility particle sizer (DMPS). Switching between ionization at low pressure (<1 mbar) with fluoranthene for VOC detection and atmospheric pressure with uronium [5] and nitrate for measuring moderately (MOMs) and highly oxygenated organic molecules (HOMs) enables the capture of a full volatility basis set (VBS).

We show that experiments across a variety of VCPs - including cleaning and personal care products, coatings, and bitumen - can be performed, demonstrating the versatility of our setup for studying the simulated atmospheric oxidation and NPF potential of these substances. Focusing on cleaning products, we identify substantial manufacturer specific variability, with

increasingly complex formulations and enhanced VOC co emissions leading to higher NPF potential.

These insights are critical for mitigating urban air pollution and transforming cities into healthier living spaces.

[1] B.C. McDonald et al., Science, 359 (2018) 760-764

[2] G.I. Gkatzelis et al., Environmental Science & Technology, 55 (2021) 188-199

[3] D. Stolzenburg, N. Sarnela, F. Bianchi et al., npj Clim Atmos Sci, 8 (2025) 75

[4] A. Shcherbinin et al., Analytical Chemistry, 96 (2024) 19926-19932

[5] A. Shcherbinin et al., Analytical Chemistry, 97 (2025) 21282-21290

This research was funded by the Vienna Science and Technology Fund (WWTF, project VRG22-003) and the Austrian Science Fund (FWF, project PAT8221324).

T18

Is arsenic essential?

Helen Lord, Fernando Mendoza, Joerg Feldmann, Viktoria Mueller

University of Graz, Universitätsplatz 3, 8010 Graz, Austria
helen.lord@uni-graz.at

Marine macroalgae, which live in arsenic-rich environments, are regularly exposed to oxidative stress. They can accumulate arsenic in high concentrations, and a linear correlation exists between concentrations of arsenolipids and reactive oxygen species (ROS). It is thought so far that the formation of arsenosugars and arsenolipids is purely a detoxification strategy, but these organic arsenic species could also serve a functional biological role. Analytical techniques (HPLC-ICP-MS and ESI-qTOF-MS), combined with proteomic and transcriptomic data, will determine whether these arsenic compounds actively contribute to cellular protection in the brown seaweed Fucus spiralis.

Using a two-way ANOVA test, concentrations of key arsenosugars (As-SO_3 and As-SO_4) in Fucus spiralis increase significantly with higher arsenic exposure and increase further in samples exposed to UV-induced oxidative stress compared to samples under normal light conditions. This suggests an adaptive response to the experimental conditions imposed in the present work. Considering arsenosugars are precursors to arsenolipids, this increase could indicate enhanced arsenolipid production, pointing towards a protective function of these compounds.

T19

Sampling-Related Variability in ICP-MS Multi-Element Analysis of Urban Leaf Samples — Evidence from Kampala, Uganda

Paul Töppmann[1*], Simone Trimmel[1], Doreen Mirembe[2], Johanna Irrgeher[1], Gabriel N. Kasozi[2], Thomas Prohaska[1]

[1] Department General, Analytical and Physical Chemistry, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700, Leoben, Austria
**paul.toeppmann@unileoben.ac.at*

[2] Makerere University, Department of Chemistry, Uganda

Urban air pollution caused by traffic-related particulate matter remains insufficiently characterised in many rapidly urbanising regions, especially in the Global South. Trace metals associated with vehicular emissions can accumulate in the environment, including on and within plant leaves. Therefore, biomonitoring using leaf samples is accomplished in this study for investigating urban air quality.

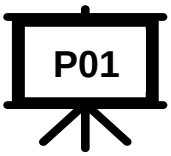
44 leaf samples from ten plant species were collected across seven districts in Kampala, Uganda, including both traffic-exposed and background locations. Mature and young leaves were sampled from the same plants at each site. Following drying and homogenisation, samples were digested using microwave-assisted acid digestion with nitric acid (HNO_3), hydrogen peroxide (H_2O_2) and tetrafluoroboric acid (HBF_4), and analysed for 48 elements using inductively coupled plasma tandem-mass spectrometry (ICP-MS/MS). Eight elements (Ba, Cr, Cu, Fe, Ni, Pb, Sb, and Zn) were finally selected for evaluation based on their relevance to traffic emissions and potential health risks.

Significantly higher mass fractions of Fe, Pb, and Sb were observed in mature leaves at traffic-exposed sites compared to immature leaves. Cu content differed significantly between plant species, with higher mass fractions measured in avocado and pitomba leaves compared to mango. No statistically significant differences were observed between districts or between traffic-exposed and background sites overall.

The observed variability suggests that the outcome is strongly influenced by sampling parameters rather than solely by environmental exposure. In particular, leaf maturity, plant species, and spatial distribution may affect the elemental contents and limit comparability between sites. These findings highlight that, while leaf-based biomonitoring can give detailed insights into urban air quality, sampling design is a critical determinant of data quality and interpretation.

This research was funded by the Austrian Science Fund FWF, grant number P 33099-N (DOI: https://doi.org/10.55776/P33099). Student mobility to Uganda was funded by the Erasmus KA171 programme.

Poster Presentations



Method Development for Arsenic Speciation and Routine Anion Measurements in Natural Freshwater and Mine Waste Waters

Matthias Rittberger[1]*, Donata Bandoniene[1], Stefan Wagner[1], Shaun T. Lancaster[1], Lukas Wolf[1], Frederik Dunkel[2], Phillip Gopon[2], Johanna Irrgeher[1]

[1] Montanuniversität Leoben, Department General, Analytical and Physical Chemistry, Franz-Josef-Strasse 18, 8700, Leoben, Austria
**matthias.rittberger@stud.unileoben.ac.at*

[2] Montanuniversität Leoben, Department Applied Geosciences and Geophysics, Peter Tunner-Straße 5/II, 8700, Leoben, Austria

In this project, a method for arsenic (As) speciation in natural waters was developed alongside routine anion measurements in river water samples from the Drava and Meža River, Slovenia. Common inorganic anions (F^-, Cl^-, NO_2^-, NO_3^-, Br^-, PO_4^{3-}, SO_4^{2-}) were assessed according to the United States Environmental Protection Agency (US EPA) Method 300.0 in 28 surface water samples, where F^-, Cl^-, NO_3^- and SO_4^{2-} were determined. None of the concentrations of the measured anions were passing limit or guideline values in drinking or natural water regulations set by the World Health Organization (WHO) or US EPA. Concentrations were comparable to literature values for natural waters.

Arsenic species (arsenite (AsIII) and arsenate (AsV)) were determined in water originating from mine waste in a historic mining district near Knittelfeld, Styria, where copper and gold were mined until the 19th century.

The toxicity, environmental mobility and accumulation of As is strongly dependent on its species. Therefore, it is necessary to identify the specific species and to retain the species during sampling, preparation and management. For stabilization, 50 mL of sample were filtered with a 0.45 µm syringe filter and stabilized with 0.5 mL of 0.125 mol L^{-1} EDTA. IC-ICP-MS was used for speciation using a Dionex ICS-6000 DC system with a Dionex Ionpac AS7 2x250 mm column coupled to an Agilent 7500 ICP-QMS.

The As speciation was successfully applied to 11 water samples. The As concentrations in most of the analyzed samples were high (> 10 ng mL^{-1}, WHO guideline value), with AsV being the predominant species. The highest As concentration was determined in an adit, where distinct variations in the AsV /AsIII ratios were detected, which indicates an oxidation of AsIII. Samples taken at the end of the adit had the highest total As concentration of 561 ng mL^{-1} with an AsV /AsIII ratio of 0.9. At the entrance the total As concentration was 465 ng mL^{-1} with an an AsV /AsIII ratio of 3.7.

P02

Development of an ICP-MS/MS Approach for Fluorine Analysis: Comparative Evaluation of the $[BaF]^+$ and $[SrF]^+$ Methods

Franziska Peer, Andrea Raab, Raquel Gonzalez de Vega, Jörg Feldmann

University of Graz, Analytical Chemistry/TESLA, Universitätsplatz 3, 8010 Graz, Austria
franziska.peer@edu.uni-graz.at

Fluorine is widely present in modern consumer and industrial products, including food packaging, pharmaceuticals, textiles, and firefighting foams, often in the form of per- and polyfluoroalkyl substances (PFAS).[1] While combustion ion chromatography (CIC) is an established technique for total fluorine determination, it is limited by long analysis times and species-dependent combustion efficiencies, highlighting the need for faster and more robust analytical approaches.[1]

Inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) offers a promising alternative through the formation of metal–fluoride adduct ions. Barium forms the $[^{138}Ba^{19}F]^+$ adduct due to its high bond dissociation energy for the $[Ba\text{-}F]^+$of 6.39 eV ($[Ba\text{-}O]^+$: 4.00 eV) and a relatively low second ionization potential (10 eV)[2], making it a preferred approach for fluorine analysis. Strontium is also capable of forming adducts, mainly $[^{88}Sr^{19}F]^+$; however, due to its slightly lower bond dissociation energy for $[Sr\text{-}F]^+$ (5.43 eV; in comparison $[SrO]^+$: 3.06 eV) and a higher second ionization potential of 11 eV, the resulting signal intensity is typically reduced compared to the $[BaF]^+$ method.[2]

Despite this limitation, the $[SrF]^+$ approach presents important advantages. In samples containing gadolinium, spectral interferences can compromise the $[BaF]^+$ method on the m/z 157, necessitating an alternative strategy. Additionally, the $[SrF]^+$ method appears to be less sensitive to matrix effects, offering improved robustness across diverse sample types. Coupled with the inherent benefits of ICP-MS/MS, including rapid analysis and multi-element capability, this makes $[SrF]^+$ a compelling complementary approach.

This study aims to critically evaluate the performance of the $[SrF]^+$ method for fluorine determination and to assess its potential as a reliable alternative in cases where the $[BaF]^+$ approach is limited.

[1] Al Zbedy, A.; Aro, R.; Akhdhar, A.; Müller, V.; Ebel, R.; Brownlow, A.; Norton, G. J.; Yeung, L. W. Y.; Feldmann, J. Comparison of CIC and HR GFMAS for the measurements of extractable organofluorines (EOF) in different biological tissues of pilot whales. Anal. Chim. Acta 2025, 1351, 343855.

[2] Jamari, N. L.A.; Behrens, A.; Raab, A.; Krupp, E. M.; Feldmann, J. Plasma processes to detect fluorine with ICPMS/MS as [M–F] + : an argument for building a negative mode ICPMS/MS. J. Anal. At. Spectrom. 2018, 33, 1304–1309.

This work is financially supported by Agilent.

P03

Influence of Ozone and UV Light on the Degradation of PFAS in aqueous solutions

Florian Taferner, Raquel Gonzalez de Vega, Jörg Feldmann, Viktoria Müller

University of Graz, Analytical Chemistry, Universitätsplatz 1, 8010 Graz, Austria
florian.taferner@edu.uni-graz.at

Per- and polyfluoroalkyl substances (PFAS) represent a large class of persistent synthetic chemicals widely used in industrial and consumer products due to their unique physicochemical properties. However, their extreme chemical stability and resistance to degradation have led to increasing environmental accumulation and growing concerns regarding potential ecological and human health impacts. Conventional wastewater treatment plants (WWTPs) are generally not capable of effectively removing PFAS, which promotes their continuous release into aquatic environments.

This study investigates the degradation and potential defluorination of selected PFAS compounds, with a focus on perfluorooctanoic acid (PFOA) and perfluorohexane sulfonate (PFHxS). Different advanced treatment approaches, including ozonation, UV irradiation, and a combined ozone–UV process, were evaluated under controlled laboratory conditions. The degradation behavior of the target compounds was monitored using LC-MS/MS, while fluoride release as an indicator of C–F bond cleavage was quantified using fluoride ion-selective electrodes (ISE) and combustion ion chromatography (CIC).

The results demonstrate varying removal efficiencies depending on the applied treatment method, with combined processes showing enhanced degradation compared to single treatments. The detection of released fluoride suggests partial defluorination of PFAS during advanced oxidation processes. Overall, the findings contribute to a better understanding of PFAS degradation pathways and support the development of improved treatment strategies for PFAS-contaminated water streams.

P04

Planarized Microfluidic Electrode Rails Enable Low-Retention Maxwell–Wagner–Sillars Impedance Detection of Gold Nanoparticles

Max Schimpf[1], Silvia Schobesberger[1], Guenther Hiebl[1], Antonio Torres[1], Tamas Novak[1], Peter Ertl[1], Heinz D. Wanzenboeck[2], and Martin Frauenlob[1]

[1] *TU Wien, Faculty of Technical Chemistry, Vienna, Austria*

[2] *TU Wien, Faculty of Solid State Electronics, Vienna, Austria*

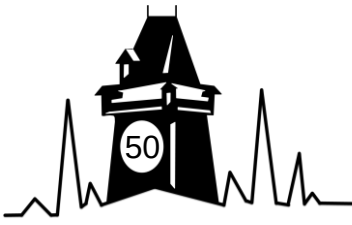
Impedance-based detection is a powerful analytical tool that allows for label-free characterization of size, concentration, and surface charge with high sensitivity. It is particularly valuable for applications such as quality control of nanomedicines, virology, and the analysis of biological markers like exosomes. However, particle retention within the sensing pore presents a major obstacle for repeated measurements by causing baseline drift and physical blockages. This fouling compromises data accuracy and reproducibility through cross-contamination and flow disruption, limiting sensor reusability.

Therefore, we report here on a planarized microfluidic electrode rails (MRs) that reduce the upstream metal step by >97% and lower passive nanoparticle retention by about threefold while preserving a strong gold-nanoparticle (AuNP) impedance peak under flow. The frequency-localized peak is consistent with Maxwell–Wagner–Sillars (MWS) interfacial polarization and provides a direct electrical signature of suspended AuNPs.

Matched IDE and MR devices were fabricated on borosilicate glass. MRs were formed by depositing a 300 nm PECVD Si_3N_4 leveling layer, back-etching the sensing openings, and sputtering Ti/Au rails over the planarized topography. Profilometry confirmed that the~4 µm sensing gap was preserved, while the upstream lead-to-substrate step was reduced from~0.34 µm to~0.004 µm (>97%). CFD simulations in 50 µm-high channels at 1 mm s-1 showed smoother wall-adjacent streamlines at the planarized transition, supporting the geometric rationale for reducing nonspecific accumulation.

We evaluated the architecture with retention and bulk-suspension impedance experiments. Fluorescent 100 nm bead load–flush assays quantified passive particle accumulation under repeated microfluidic handling. Separately, MR electrodes were challenged with 1.9 ×1011 AuNP mL-1 suspensions in 0.0005×PBS and compared with matched buffer baselines at 20, 50, and 100 mV excitation. Electrochemical impedance spectra were collected from 200 kHz to 100 Hz using an AD5940-based readout, and baseline-corrected spectra were analyzed for the dominant MWS magnitude peak within the nanoparticle-sensitive frequency band. MRs reduced passive bead retention by about threefold relative to conventional IDEs. In the bulk AuNP measurements, particle-containing solutions separated clearly from buffer in |Z|, and the baseline-corrected MWS peaks reached $\Delta|Z|/|Z0|$= 145–171% at 78–95 kHz across the tested excitation amplitudes.

These results show that planarized electrode rails can suppress geometry-driven retention while preserving a strong AuNP-specific impedance signature. The approach provides a compact route to nanoparticle-based microfluidic EIS in which electrode topography and MWS peak selection are treated as coupled design parameters.



P05

Printing Regimes and Their Influence on Potential Migrants in Food Contact Material

Lara Skef, Erich Leitner

Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Stremayrgasse 9/II, 8010 Graz, Austria
lara.skef@tugraz.at

The transition toward a circular and climate-neutral packaging economy, as outlined in the EU Green Deal and the Roadmap 2030, is accelerating the use of recycled materials and alternative printing technologies in food packaging [1]. A range of printing regimes is employed in food packaging, including flexographic, gravure, offset, digital, and UV-curing technologies. Each regime imposes specific requirements on ink formulation, curing or drying mechanisms, and substrate interactions. Consequently, the selected printing technology defines the chemical composition of the final material, which subsequently enters recycling loops and may contribute to cumulative contamination patterns [2].

Past contamination incidents already showed how distinct regimes give rise to different volatile and semi-volatile profile, migration pathways and health-relevant contaminants. The widespread occurrence of mineral oil hydrocarbons (MOSH/MOAH) in food has been largely associated with offset printing inks and recycled fibre-based materials [3]. In contrast, the migration of photoinitiator isopropyl thioxanthone (ITX) from UV-cured printed packaging into cereals in 2005 led to product recalls. These cases underline the necessity for advanced analytical strategies capable of addressing complex, printing regime-dependent migration patterns.

At the European level, the assessment of printing regime migrants lacks a harmonised regulation and remains based on the general requirements of Regulations (EC) No. 1935/2004 and (EC) No. 2023/2006, supplemented by national measures such as the Swiss Ordinance on materials and articles in contact with food and the German Printing Ink Ordinance becoming applicable in 2026.

This study focuses on paper-based materials, where gas-phase migration of volatile and semi-volatile compounds released from printed surfaces is a key migration mechanism. Using gas chromatography (GC), different sample preparation, separation, and detection strategies are compared to better understand and adress regime-dependent migration profiles and to support more targeted safety assessment of printed packaging.

[1] European Parliament and Council. Regulation (EU) 2025/40 of the European Parliament and of the Council of 19 December 2024 on packaging and packaging waste, amending Regulation (EU) 2019/1020 and Directive (EU) 2019/904, and repealing Directive 94/62/EC. Off J Eur Union. 2025 Jan 22;L40.

[2] Clemente I, Aznar M, Nerín C, Bosetti O. Migration from printing inks in multilayer food packaging materials by GC-MS analysis and pattern recognition with chemometrics. Food Addit Contam Part A Chem Anal Control Expo Risk Assess. 2016;33(4):703–714. doi:10.1080/19440049.2016.1155757.

[3] European Food Safety Authority (EFSA). Scientific opinion on mineral oil hydrocarbons in food (MOSH/MOAH). EFSA J. 2012;10(6):2704. doi:10.2903/j.efsa.2012.2704

Biochemical characterisation of cellulase adsorption to cotton and polyester

Lukas Gruber, Paul Haager, Felice Quartinello, Judith Rudolf-Scholik, Birgit Herbinger, Christian B. Schimper

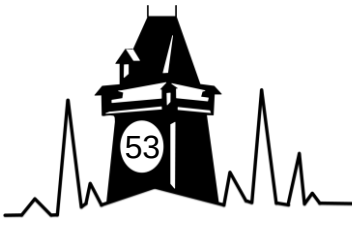
Josef Ressel Centre ReSTex, Fachhochschule Wiener Neustadt, Biotech Campus Tulln, Konrad Lorenzstrasse 10, 3430 Tulln, Austria
207487@fhwn.ac.at

The characterization of enzymatic processes on different substrates is essential for the development of efficient recycling strategies for textile waste. In particular, cotton–polyester blends pose a significant challenge, requiring selective approaches for component separation (Gritsch et al., 2023).

Within the Restex project, cellulases are investigated for their ability to degrade the cellulose fraction of textile fibers (Egan et al., 2025). The focus of this study lies on the analytical quantification of enzyme behavior under defined conditions. Special attention is given to the interaction between enzymes and different solid substrates.

A key analytical component of this work is the observation of enzyme adsorption behaviour, using photometric measurements with a microplate reader (Tecan Infinite M Plex). The Bradford assay is applied to quantify changes in protein concentration (Bradford, 1976). The study focuses on how the enzymatic concentration in solution varies by substrate and temperature. Cellulase formulations for different applications are examined to evaluate potential differences in their behavior.

First results indicate that adsorption of cellulases to cotton-based substrates occurs rapidly after substrate addition, whereas no measurable adsorption is observed in case of polyester fibers. The data further suggests that temperature strongly influences the adsorption behavior, with effects only within the active temperature range of the enzymes. Evidence is gained for monitoring adsorption and desorption processes, but due to the variability in the data, no definitive evidence for these mechanisms can be concluded at this stage.



Gritsch, S.M. et al. (2023) “Closing the cycle: Enzymatic recovery of high purity glucose and polyester from textile blends,” Resources, Conservation and Recycling, 188, p. 106701.

Egan, J. et al. (2025) “Diving into commercial cellulase formulations for circular polyester/cotton separation through targeted depolymerization of cotton,” Frontiers in Bioengineering and Biotechnology, 13, p. 1632772.

Bradford Marion, M. (1976) “A Rapid and Sensitive Method for the Quantitation of Microgram Quantities of Protein Utilizing the Principle of Protein-Dye Binding,” Analytical Biochemistry, 72, p. 248-254.

This work was conducted at the Josef Ressel Centre “Recovery Strategies of Textiles”, which is funded by the Christian Doppler Research Association on behalf of the Austrian Federal Ministry of Economy, Energy, and Tourism and the National Foundation for Research, Technology, and Development.

P07

Characterization of patient-derived leukocytes using machine learning-assisted Surface-Enhanced Raman Spectroscopy

Jasmin Antony[1]*, David Lilek[1,2], Selma Ljubijankic[3], Christoph Wiesner[3], Raphael Rossmanith[1], Klaus Geissler[4], Birgit Herbinger[1], Katerina Prohaska[1]

[1] *Biotech Campus Tulln, University of Applied Sciences Wiener Neustadt, Tulln, Austria*
**122397@fhwn.ac.at*

[2] *Department of Chemistry and Physics of Materials, Paris Lodron University Salzburg, Salzburg, Austria*

[3] *IMC Krems University of Applied Sciences, Krems, Austria*

[4] *Faculty of Medicine, Sigmund Freud University, Vienna, Austria*

Surface-Enhanced Raman Spectroscopy (SERS) is a powerful vibrational spectroscopic technique for the identification and characterization of biological materials. The primary objective of this study was to evaluate the potential of SERS to differentiate between monocytes from healthy anonymous blood donors (controls) and those derived from patients diagnosed with Chronic Myelomonocytic Leukaemia (CMML) prior to treatment [1,2].

To address this research question, a Raman Microscopy approach with a 785 nm laser was developed and applied using in-house established SERS substrates. The solid substrates used are APTES-functionalized surfaces coated with 40 nm gold nanoparticles and were characterized by scanning electron microscopy (SEM) and UV/Vis analysis to increase reproducibility [3].

For classification, spectra from six healthy donors were combined and compared with spectra from individual CMML patients, each displaying distinct mutation profiles. To assess classification performance, multiple supervised machine learning strategies were applied, including linear discriminant analysis (LDA) with prior dimensionality reduction, logistic regression, support vector machines with L1 and L2 regularization, and tree-based methods. Evaluation metrics included the area under the receiver operating characteristic curve (AUC), the p-values achieved by the McNemar test, as well as confusion matrices. For validation purposes, nested cross-validation was applied [4,5].

The logistic regression 1 model provided the best possible signal assignment to differentiate between control and patient, demonstrating that SERS combined with machine learning strategies enables differentiation between healthy and CMML-derived monocytes, highlighting the potential of SERS as a promising analytical tool for diagnostics of hematologic malignancies. Future studies should aim to harmonize the number of spectra obtained from control (n = 1020) and patient (n = 315) to improve statistical robustness.

[1] Geissler K., Jäger E., Barna A., Gurbisz M., Marschon R., Graf T., Nösslinger T., Pfeilstöcker M., Machherndl-Spandl S., Stauder R., Zebisch A., Sill H., Öhler L., Kusec R., Hoermann G., & Valent P. (2022). Multistep pathogenesis of chronic myelomonocytic leukemia in patients. European journal of haematology, 109(1), 50–57.

[2] Lilek D., Mayr A., Grossinger C., Rechthaler J., Steininger L., Zimmermann D., Gamsjaeger S., Wilts B. D., Musso M., Wiesner C., Grünfelder A., Herbinger B., Prohaska K. (2025). Potential of SERS and proteomics for biomarker detection in cancer cells. Analytical and Bioanalytical Chemistry.

[3] Mayr A., Grossinger C., Rechthaler J., Draxler M., Steininger L., Zimmermann D., Gamsjaeger S., Lilek D., Grünfelder A., Herbinger B., Prohaska K. (2025). Integrating Surface-enhanced Raman Spectroscopy and Proteomic Profiling for Biomarker Validation in Hodgkin Lymphoma Cells. ANAKON 2025. Leipzig, Germany.

[4] Zimmermann D., Lilek D., Posch N., Hermann D-R., Pytel N., Herbinger B., Prohaska K. (2023). Classification of single cells by Raman spectroscopy and machine learning: comparison of common algorithms. Scientific Computing. Graz, Austria.

[5] Lilek D., Zimmermann D., Steininger L., Musso M., Wilts B., Gamsjaeger S., Herbinger B., Prohaska K. (2025). Machine Learning of Raman Spectroscopic Data: Comparison of Different Validation Strategies. Journal of Raman Spectroscopy.

The authors gratefully acknowledge financial support of RTI-strategy Lower Austria 2027 in the project GLF21-1-019, “Reproducible label-free surface-enhanced Raman spectroscopy, SERS, for Diagnostics of Melanoma (Ra-Dia-M)”.

P08

Cell History Effects on Fluoride Release and Electrolyte Degradation during Low-Temperature LIB Recycling

Tina Carola Spirk*, Walter Gössler

[1] *University of Graz, Universitätsplatz 3, 8010 Graz, Austria*

[2] *ProtectLiB GmbH, Schubertstraße 6a, 8010 Graz, Austria*

**tina.spirk@protectlib.at*

The thermo-mechanical approach for lithium-ion battery recycling applied at ProtectLiB integrates a low-temperature step to remove volatile, potentially flammable electrolyte components before mechanical separation of black mass, separator, housing, and current collectors. Although mild conditions (less than 100 °C, moderate vacuum) are applied $LiPF_6$ and carbonates are partly degraded, generating hydrogen fluoride (HF), fluorophosphates, and organic products including formic and acetic acid [1,2]. Cycling temperature alters electrolyte decomposition and cell stability [3], yet the effect of cell history on fluoride release during low-temperature recycling has not been quantified.

Cylindrical cells were aged under immersion-cooled conditions in minimodules built and cycled at Virtual Vehicle and compared to non-cycled reference cells. After recycling at the ProtectLiB research plant, recovered electrolyte and alkaline washing solution (capturing volatiles from thermal treatment) were analysed by different methods.

Recovered electrolyte consisted mainly of dimethyl carbonate, methyl acetate, acetic acid, formic acid, and further $LiPF_6$ hydrolysis products. Free fluoride was approximately twice as high in the electrolyte from the less-cycled, thermally more uniformly aged module; the same trend was observed in the corresponding washing solution. Reversed-phase chromatography of the recovered electrolyte from both aged modules resulted in two additional signals which could not be detected in the uncycled reference cells. These degradation products in the electrolyte are currently under further investigation.

Covering the broad range of compounds and degradation products in recovered electrolyte and washing solution required a complementary set of analytical techniques. Further work should extend this workflow by coupling established separation and detection methods, such as IC-ICPMS/MS, to enable the speciation and quantification of fluorine- and phosphorus-containing degradation products.

[1] Kraft V. et al., RSC Adv. 5 (2015) 80150;

[2] Weber W. et al., J. Chromatogr. A 1394 (2015) 128; [3] Börner M. et al., J. Power Sources 342 (2017) 382

P09

Printed Hydrogel-Based Sensing Platforms on Textile Substrates for Dual pH and Urea Detection

Ivana Perković[1], Iva Karneluti[1], Deepak Joshy[1], Hüma Yilmaz[1], Gerhard J. Mohr[2], Ivana Murković Steinberg[1]

[1] *University of Zagreb, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb*
iperkovic@fkit.unizg.hr

[2] *Joanneum Research Materials, Franz-Pichler-Straße 30, 8160 Weiz, Austria*

The growing interest in wearable technologies and non-invasive chemical monitoring has stimulated the development of flexible and biocompatible colourimetric sensing platforms capable of real-time detection of physiologically relevant analytes. Among these, pH-responsive hydrogel systems integrated onto textile substrates represent a promising approach due to their simplicity, visual interpretability, and compatibility with low-cost materials. In this work, cellulose-derived and synthetic textile substrates, namely cotton and polyester fabrics, are functionalized with printed hydrogel layers containing a pH-sensitive indicator dye. The hydrogel formulations are prepared using a commercially available hydrogel matrix (D4 Hydromed), a mixed ethanol–water solvent system (EtOH:H_2O = 9:1), and the pH-sensitive dye GJM 534 (pKa ≈ 7.35). Deposition is performed using a modified DIW-based printing system, enabling controlled and reproducible patterning directly onto textile surfaces. Two sensing systems are investigated: hydrogels containing only the pH-sensitive dye, and hydrogels incorporating both the dye and the enzyme urease. The pH responsiveness of the printed materials is evaluated using Britton–Robinson buffer solutions over a broad pH range, while enzyme-functionalized systems are additionally exposed to urea solutions of varying concentrations. The sensing mechanism is based on urease-catalysed hydrolysis of urea, generating ammonium and hydroxide ions that induce a local increase in pH and consequently a colourimetric response of the indicator dye. By comparing the responses of enzyme-free and enzyme-containing hydrogel systems, the contribution of enzymatic activity to the overall sensor behaviour can be distinguished. In parallel, an alternative approach involving covalent

immobilization of the pH-sensitive dye onto cellulose substrates prior to hydrogel deposition is explored in order to improve dye retention and long-term stability. The resulting textile-integrated sensing systems exhibit reversible and visually distinguishable colour changes, demonstrating their potential for wearable and non-invasive monitoring of pH and urea levels.

[1] G. J. Mohr et al., Mikrochim. Acta 192 (2025) 405

[2] Kuswandi et al., BioImpacts 12(1) (2022) 43–50

[3] P. Xi et al., Talanta (2023) 124507

[4] N. Promphet et al., Sens. Actuators B Chem. (2020) 128549

[5] Soft Matter 21 (2025) 2268

This work is supported by the Croatian Science Foundation under the project WearSense HrZZ IP-2022-10-2595.

P10

AI-Driven Analysis of Abiotic Stress Responses in Soybean Using LC–MS/MS-Based Proteomics and Raman Spectroscopy

Katrin Herbst[1]*, Judith Rudolf-Scholik[1], David Lilek[1,2], Fabio Zaccharini[1], Barbara Korbei[3], Birgit Herbinger[1], Justyna Rechthaler[1]

[1] *Biotech Campus Tulln, University of Applied Sciences Wiener Neustadt, Konrad-Lorenz-Strasse 10, 3430 Tulln, Austria*
**121037@fhwn.ac.at*

[2] *Department of Chemistry and Physics of Materials, Paris Lodron University Salzburg, Salzburg, Austria*

[3] *Institute for Molecular Plant Biology, BOKU University*

Climate change increasingly exposes crops to abiotic stress conditions such as drought and flooding, significantly impacting agricultural productivity. Soybean (Glycine max), as a major global crop, is particularly sensitive to these stress factors, necessitating a deeper understanding of the underlying molecular responses.

In this study, we investigate stress-induced alterations in the soybean leaves. A dual approach was applied: bottom-up LC-MS/MS-based proteomics to identify stress-responsive proteins and Raman spectroscopy as non-destructive method to detect biochemical changes. Proteomic analyses were performed using a Sciex ZenoTOF 7600 system and for Raman spectroscopy a 1064 nm fibre-based Raman system was used. Stressed, non-stressed, and recovering plants are compared to capture dynamic proteomic changes associated with stress exposure and recovery. To ensure robust and reproducible protein identification, different extraction protocols were systematically evaluated. A Tris-HCl-based buffer supplemented with SDS and β-mercaptoethanol yielded the highest protein recovery and reproducibility.

In parallel, Raman spectroscopy was applied as a non-destructive approach to detect biochemical changes associated with stress prior to the appearance of visible symptoms. After establishing a measurement method, machine learning approaches were applied. Although the spectra showed low fluorescence and enabled effective baseline correction, spectral noise remained, which was reduced through preprocessing techniques. High spectral quality, which

was automatically evaluated based on the number and intensity of the detected peaks, was reached. Correlating spectral features with proteomic data could provide a comprehensive understanding of stress-induced molecular alterations and enable the identification of early stress markers.

Overall, this combined strategy contributes to the development of biomarker-based approaches for early stress detection and advances analytical frameworks for studying plant responses to abiotic stress.

[1] Altangerela, N. et al. PNAS. 114(13) (2017) 3393 - 3396.

[2] Butler, H. J. et al. Analytical Methods. 7(10 (2015) 4059-4070

[3] Doelllinger, J. et al. Molecular & Cellular Proteomics. 19 (2020) 209-222.

[4] Duong, V.-A. & Lee, H. International Journal of Molecular Sciences. 24 (2023) 5350.

[5] Dupree, E.J. et al. Proteomes. 8 (2023) 14.

[6] Jiang, Y et al. ACS Measurement Science Au. 4(4) (2024) 338–417.

The authors gratefully acknowledge the scientific support from BOKU University and BioOmics

P11

Identification of sulfur compounds in reaction aroma – comparison of two different systems based on comprehensive GC×GC

David Asen, Erich Leitner

Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry, Stremayrgasse 9/II, 8010 Graz, Austria
d.asen@tugraz.at

According to EU regulation (EC) No 1334/2008, thermal process flavorings are defined as compounds derived from heating mixtures of ingredients with a goal of generating characteristic aroma compounds through controlled thermal reactions [1]. These reactions commonly include reducing sugars and amino compounds. These reaction aromas are widely used in the food industry to recreate desirable cooked, roasted, or savory notes, which are closely linked to consumer acceptance and overall sensory appeal of food products. Among the key precursors are sulfur-containing compounds such as cysteine and thiamine, playing a crucial role due to their ability to form highly potent odorants [2].

In general, volatile sulfur compounds (VSCs) are known for extremely low odor thresholds and dramatic influence on the sensory profile of foods. They are present in a wide range of thermally processed foods such as meat, coffee, baked goods, and vegetables. This chemically diverse class includes thiols, disulfides, polysulfides, and sulfur-containing heterocycles, formed mostly through Maillard-type reactions and Strecker degradation pathways. However, analysis of VSCs remains challenging due to their instability, low concentrations, and possible co-elution issues with other volatile compounds [3].

In this study, two comprehensive two-dimensional gas chromatography (GC×GC) systems were evaluated for their performance in analyzing reaction aroma. For that purpose, a model reaction mixture with thiamine as a precursor was employed. A cryogenic modulation GC×GC coupled with time-of-flight mass spectrometer (TOFMS) was compared to a flow-modulated GC×GC system coupled with both TOFMS and sulfur chemiluminescence detector (SCD). The comparative results highlight the strengths of each approach and demonstrate the

benefits of combining advanced chromatographic separation with element-specific detection for sulfur containing compounds characterization.

[1] European Parliament and Council of the European Union, Off. J. Eur. Union L 354 (2008) 34–50.

[2] Fontes V. M. de S., Galvão M. de S., Carvalho L. M. de, Guedes F. L. do N., Lima M. dos S., Bezerra T. K. A., Madruga M. S., Food Chem. 445 (2024) 138398.

[3] Skef L., Asen D., Panto S., Erich L., Anal. Bioanal. Chem. (2026), Accepted for Review.

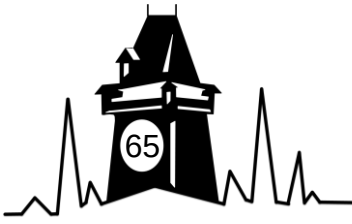
It’s raining PFAS? Temporal trends of PFAS in rainwater samples using LC-ESI-MS/MS and CIC

Lili Anna Boros, Viktoria Müller, Julian Rüdiger, Jörg Feldmann

Analytical Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria
lili.boros@student.tugraz.at

Per- and polyfluoroalkyl substances (PFAS) are ubiquitous environmental contaminants that undergo atmospheric deposition and bioaccumulate within the food web, posing severe risks to human health. While current research heavily relies on targeted analysis, this approach overlooks a massive fraction of unidentified organofluorines in the atmosphere. To bridge this gap, this study focuses on quantifying targeted PFAS compounds while simultaneously investigating the presence of unknown fluorinated compounds in rainwater samples from the Schmücke weather station. Monthly pooled samples over the course of six months were prepared using solid phase extraction and analysed for targeted analysis using LC-ESI-MS/MS and for extractable organic fluorine using CIC to assess fluorine mass balance. In correlation with meteorological data, results will show temporal variations across seasons and identify trends in the atmospheric transport and deposition of PFAS. Various distributions of short and long chain PFAS are expected due to their difference in volatility and solubility.

Ultimately, this research aims to provide vital occurrence data, which is essential to developing effective environmental monitoring and mitigation strategies.



P13

Ratiometric pH Sensing with Dually Emissive Umbelliferone Dyes

Matthias Schwar, Sergey M. Borisov

Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry, Stremayrgasse 9/II, 8010 Graz, Austria
matthias.schwar@tugraz.at

Sensing and imaging of pH values is of highest importance in research, diagnostics and industry. Within optical methods, analyzing fluorescence intensity is a practical approach, which generally does not require sophisticated or expensive setups. However, some disadvantages, including dependency of the sensor signal on the intensity of the light source, indicator concentration, and alignment of the optical components must be considered. These limitations are addressed in ratiometric systems, which are commonly realized by adding an additional analyte-insensitive emitter into the polymeric host material of the sensor. However, utilization of a single dually-emitting dye is preferred as it simplifies sensor preparation in various formats, e.g. nano- or microparticles and also avoids issues due to potential stability differences of indicator and reference.

To expand the library of these generally rare dyes, we investigated 7-hydroxycoumarin derivatives (umbelliferones) reported decades ago by O.S. Wolfbeis and co-workers.[1] Despite exhibiting attractive spectral properties and pH response, the reported dyes were poorly suitable for the preparation of robust optical pH sensors due to their hydrophilic character and associated leaching out of the hydrogel sensor matrix. In order to mitigate this characteristic, we introduced hydrophobic alkyl chains into the dye structure, serving as an “anchor” and enhancing retainment. Notably, these modifications did not adversely affect the photophysical and sensing properties.

The dyes feature well-separated fluorescence bands of the respective neutral and deprotonated form and high brightness. Immobilized in hydrogel, they are suitable for pH measurements around pH 6.5, utilizing the fluorescence emission ratio. Fine-tuning of their apparent pK_a-value is possible by adjusting the dye concentration in the sensor matrix via

manipulation of the FRET efficiency from the protonated to the deprotonated form or by selection of the hydrogel host polymer.

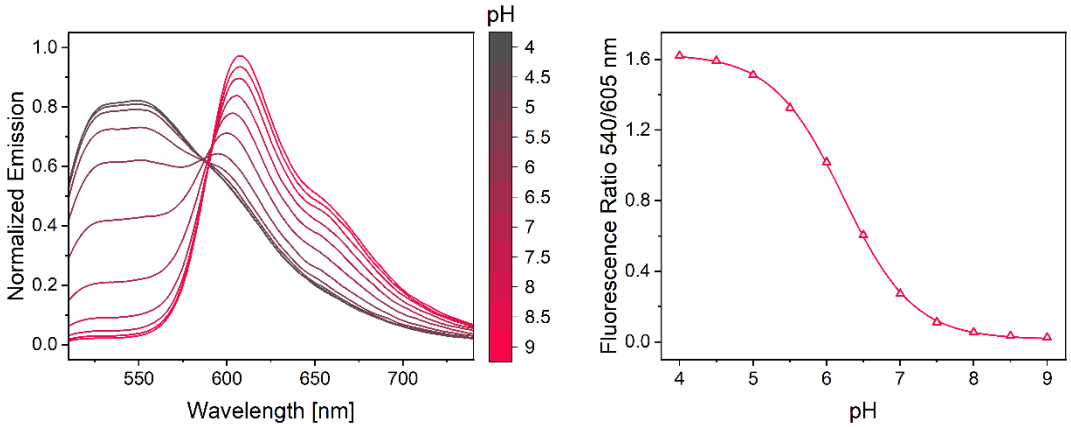


Figure 1: pH dependent emission spectra of the new dye “bBCeU” in Hydrogel D4 (λex 493 nm), the corresponding calibration curve of the fluorescence ratio and respective dye structure.

[1] O. Wolfbeis, E. Koller, P. Hoghmuth, Bull. Chem. Soc. Jpn. 58. 731-734 (1985).

P14

Influencing factors in protein determination using the Bradford assay for the measurement of cellulases in the context of textile recycling

Paul Haager, Lukas Gruber, Felice Quartinello, Agnes Grünfelder, Birgit Herbinger, Christian B. Schimper

Josef Ressel Centre ReSTex, Fachhochschule Wiener Neustadt, Biotech Campus Tulln, Konrad Lorenzstrasse 10, 3430 Tulln, Austria
205737@fhwn.ac.at

Textile recycling technologies have gained increasingly importance in the European Union. A substantial portion of textiles is composed of cotton–polyester blends, whose separation and recycling remain technically challenging (Gritsch et al., 2023).

Within the Josef Ressel Centre ReSTex, biochemical methods are explored as a promising approach to recycle these blended textile materials. In particular, cellulases are employed to selectively degrade the cellulose fraction, thereby enabling the separation of cotton and polyester components (Egan et al., 2025). The aim of this study is to establish a reliable and validated method to determine the binding behaviour of cellulase formulations towards cellulosic substrates.

Monitoring the distribution, adsorption, and stability of cellulases in solution and on cellulose surfaces is achieved by determination of the protein content in the solution by the Bradford assay. It is a photometric technique which allows sensitive and efficient detection at a wavelength of 595 nm (Bradford, 1976).

We report an optimized method and the determination of influencing factors like pipetting variability, matrix effects, time dependencies and the influence of the temperature.

Gritsch, S.M. et al. (2023) “Closing the cycle: Enzymatic recovery of high purity glucose and polyester from textile blends,” Resources, Conservation and Recycling, 188, p. 106701.

Egan, J. et al. (2025) “Diving into commercial cellulase formulations for circular polyester/cotton separation through targeted depolymerization of cotton,” Frontiers in Bioengineering and Biotechnology, 13, p. 1632772.

Bradford Marion, M. (1976) “A Rapid and Sensitive Method for the Quantitation of Microgram Quantities of Protein Utilizing the Principle of Protein-Dye Binding,” Analytical Biochemistry, 72, p. 248-254. [5] Quartinello, F., Vecchiato, S., Weinberger, S., Kremenser, K., Skopek, L., Pellis, A., & Guebitz, G. M. (2018). Highly Selective Enzymatic Recovery of Building Blocks from Wool-Cotton-Polyester Textile Waste Blends. Polymers, 10(10), 1107.

This work was conducted at the Josef Ressel Centre “Recovery Strategies of Textiles”, which is funded by the Christian Doppler Research Association on behalf of the Austrian Federal Ministry of Economy, Energy, and Tourism and the National Foundation for Research, Technology, and Development.

P15

Aerosol Characterisation for Single Particle Analysis

Paul Michael Stüger, David Clases, Matthias Elinkmann, Thomas Lockwood, Anton Nrecaj

University of Graz, Institute of Chemistry, Universitätsplatz 1, 8010 Graz, Austria
paul.stueger@uni-graz.at

SP ICP-MS has been used mainly to characterise nanoparticles, however, it can also be extended to target microparticles such as cells. In this context, particle transport efficiency becomes a critical parameter, which is, unlike for nanoparticles, not a constant at the micro scale and varies dynamically with particle size and the underlying droplet–particle interactions.

While nanoparticles are typically incorporated within aerosol droplets and follow their transport pathways, microparticles and cells can approach or exceed the size of the droplets themselves, which raises the question of how the particles are transported and how they interact with the aerosol if they exceed its size. In order to enable quantitative analyses within the microscale, transport efficiency and drift effects need to be understood to calibrate size and mass in SP ICP-MS accurately.

One access to understand aerosol dynamics is using a DIA and a DIF device to evaluate size distributions and alterations within the presence of sample-based microparticles. The first device is a dynamic image analyser, that uses frequent illumination of a camera to capture images of the aerosol based on which the size distribution amongst other parameters is determined. The second device is a laser diffraction particle size analyser, which uses size-dependent laser diffraction of the aerosol or particles to calculate their size distribution. Both instruments are modified from their original use (solid matter analysis) into prototypes, that allow the direct measurement of primary, secondary and tertiary aerosol produced by nebulisers.

In a sequential approach starting with analysing pure water at various positions in the mist, fundamental processes in aerosol generation are inquired including size and velocity dependence with varying gas flows and sample flows. Furthermore, more media/surfactants

are tested to understand specific parameters including for example surface tension. For the analysis of microplastics an aerosol dryer is added to record particles free of water or solvents.

The results show a strong distance dependence from the nebuliser tip for the size and velocity of the aerosol and also increasing sizes with higher gas/ sample flows. It can be shown that common solvents like methanol or acetonitrile decrease the average droplet size. Specific mechanisms like the Kelvin-Helmholtz break up and the formation of primary (directly at the tip) and secondary aerosol could be identified as well. Velocity measurements prior and after the spray chamber show no relevant size dependent differences between the droplets. The method has also proven to be able to characterise microplastics in different sizes with live images.

The results are intended to provide a better understanding of the exact transport and flow processes in nebulisers and spray chambers in order to ensure reliable analysis of microparticles including cells by ICP-MS.

P16

Comparative evaluation of enantioselective LC-MS/MS workflows for the quantification of D- and L-2-hydroxyglutarate in finger sweat

Michael Wolf, Vincent Sunder-Plassmann, Daniel Wasinger, Gregor Hahn, Markus Raderer, Andrea Bileck, Samuel Meier-Menches, Matthias Preusser, Christopher Gerner

University of Vienna, Faculty of Chemistry/Department of Analytical Chemistry/AG Gerner, Waehringer Straße 38, 1090 Vienna, Austria
michael.wolf@univie.ac.at

D-2-hydroxyglutarate (2-HG) is a critical oncometabolite for monitoring IDH-mutated cancers. Analyzing 2-HG in finger sweat offers a promising non-invasive approach for longitudinal monitoring, but the low sample amounts and enantiomeric nature of 2-HG present significant analytical challenges. This study systematically compared three literature-based chromatographic workflows to establish a robust LC-MS/MS method: (1) chiral LC using a Chiralpak QN-AX column [1], (2) derivatization with TSPC [2], and (3) derivatization with DATAN [3], followed by RP-UHPLC-MS/MS.

Chiral LC failed to achieve a reliable enantiomeric separation. TSPC derivatization showed limited chromatographic resolution (Rs = 1.8, FWHM-based), and the procedure proved unsuitable for routine use due to the high reactivity and poor stability of the TSPC reagent. In contrast, DATAN derivatization provided reproducible diastereomer formation with chromatographic baseline separation (Rs = 2.5). During MS optimization, significant in-source fragmentation of the DATAN-2-HG derivative was identified. This phenomenon was leveraged to develop a pseudo-MS3 approach by monitoring a specific in-source fragment via PRM. This strategy significantly increased the signal-to-noise ratio compared to the direct detection of the DATAN-2-HG precursor, effectively filtering out matrix-derived interferences.

The DATAN-based method was partially validated, showing a linear range of 10–320 ng/mL ($R^2 > 0.999$) and an LOQ of 10 ng/mL for both D- and L-2-HG. At 40 ng/mL, recovery was 102.1% and 100.2%, accuracy 96.6% and 93.8%, method precision 3.6% and 4.0%, and workflow precision 2.4% and 4.7% for D- and L-2-HG, respectively. This method is currently

applied to clinical samples to evaluate the suitability of finger sweat as a diagnostic matrix for monitoring patients treated with IDH-inhibitors.

[1] Calderón C., J. Chromatogr. A. 1467 (2026) 239

[2] Cheng QY., Sci. Rep. 5 (2015) 15217

[3] Struys EA., Clin. Chem. 50 (2004) 1391

P17

Determination of Phosphorus Purity from the Thermochemical Treatment of Sewage Sludge Ash: The Challenges of Scaling Up

Sydney Simbürger, Sara Widhalm, Johanna Irrgeher, Thomas Prohaska, Christoph Gatschlhofer, Zlatko Raonic, Shaun T. Lancaster

Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Franz-Josef-Strasse 18, 8700 Leoben, Austria
sydney.simbuerger@stud.unileoben.ac.at

Phosphorus is a critical raw material used as a precursor to produce products that play a fundamental role in our society, especially as fertilizers. Secure and reliable supply chains are crucial for Europe and the circular economy is becoming more essential to address global stability issues. In Austria it is projected that as much as 60% of imported phosphorus needs can be covered through recycling. Within the PHOBOS project, a pyrometallurgical process is being developed to enable industrial-scale recovery of white phosphorus (P_4) from sewage sludge ash and sewage sludge charcoal as input materials. Impurities in such production of P_4 arise due to possible formation of red phosphorus during the process, as well as carry-over of other elements from the input material composition. This poster focuses on designing and testing an analytical concept safely capable of assessing the purity of P_4 of sample sizes up to 1 kg. While methods exist for P_4 analysis, the community lacks methods that can be scaled up to industry-level process requirements while ensuring safe handling.

In the analytical approach, an organic extraction approach using carbon disulphide (CS_2) is proposed to separate P_4 from the potential impurities. X-ray fluorescence analysis of a sewage sludge ash input material identified Al, Ca, Fe, and S as potential metal impurities. The quantity of P_4 can then be determined gravimetrically following distillation, and the other impurities can be determined by inductively coupled plasma mass spectrometry (ICP-MS). Experiments using red phosphorus spiked with these target metals during the organic extraction procedure, followed by ICP-MS analysis, obtain a mass balance of each target impurity to understand transport pathways during the P_4 extraction procedure. The first stages of the project involve designing the analytical approach in the absence of P_4 to assess the recovery of the impurities and to ensure safe handling under an oxygen-free environment.

This project (PHOBOS) has been carried out within the framework of the Austrian Research Promotion Agency (FFG) Raw Materials 2024 program and was funded by the Federal Government.

P18

From Superfood to Safety: Acrylamide, HMF, and Furan Formation in Roasted Lupin-Based Foods

Medina Cehic, Barbara Siegmund

Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry, Stremayrgasse 9/II, 8010 Graz, Austria
medina.cehic@tugraz.at

Lupin has recently been named the “Superfood of the Year 2026” by the Biovision Foundation [1], highlighting its potential as a sustainable and regionally available ingredient in plant-based foods. Due to its favorable agronomic properties and nutritional profile, lupin is increasingly used in a variety of food applications, including roasted products. However, thermal processing not only contributes to desirable flavor development but also leads to the formation of neo-formed contaminants (NFCs), such as acrylamide (AA), 5-hydroxymethylfurfural (HMF), as well as furan and its derivatives, which are of toxicological concern.

These thermal-process contaminants primarily arise from the Maillard reaction, but – as for furan derivatives – also from the degradation of ascorbic acid, carbohydrates, and amino acids, as well as from lipid oxidation, particularly from polyunsaturated fatty acids (PUFAs) as precursors. Acrylamide is classified as probably carcinogenic to humans and is subject to benchmark levels, whereas furan is considered possibly carcinogenic, and structurally related alkylfurans are also regarded as compounds of toxicological concern that require further evaluation by regulatory authorities. This discrepancy highlights the need for a comprehensive understanding of NFC formation in emerging plant-based foods.

The present contribution focuses on the formation of key NFCs during thermal processing of lupin based foods and their analytical determination. A deeper understanding of these mechanisms is essential for developing targeted mitigation strategies that reduce contaminant levels while maintaining desirable sensory properties of lupin-based foods.

[1] Biovision – Stiftung für ökologische Entwicklung (2026). Superfood des Jahres 2026.

Development of optical spectrometric methods to characterise single particles

Sabrina Hörmann

Universität Graz, 8010 Graz, Austria

Pharmaceutical formulations require reliable characterisation due to the heavy influence of particle size, morphology, identity and aggregation on product quality and performance. Although there are various approaches available for particle characterisation, none are fit to determine all particle properties, while showing several other limitations for practical use. The usage of non-aqueous media for pharmaceutical formulation is also becoming more widespread, posing a problem for analytical measurements of particles in these, as the most established approaches are developed solely for applications in aqueous systems. Therefore, a multimodal approach combining Raman spectroscopy, in-line microscopy, and spICP-MS will be developed to obtain the desired information on the particles.

The Raman Spectroscopy method will be developed and optimized using polystyrene and later applied on the pharmaceutical formulation. In this technique an optical trap, where a laser aligned to the sample stream captures particles in a measurement cell, is used. The resulting scattering patterns are used for the identification of particles and contaminants. A novel approach investigated in the workflow of this work will examine whether the Raman signal can be used to determine particle size. For in-line microscopy, particles flowing through a measurement cell are illuminated by backlight and their shadow images are processed to determine size, shape, and agglomeration. Single particle ICP-MS is included to determine protein particle through the sulphur detection. As proteins intrinsically contain sulfur through amino acids, it can serve as a label-free elemental marker and gives information about the protein amount in the sample.

The results should prove that the combined approach is feasible as a practical and efficient strategy for assessing particle size, identity, shape, and agglomeration in non-aqueous systems. By integrating these techniques, we hope that the findings contribute to the development of more reliable analytical workflows for particle characterisation of pharmaceutical formulations in non-aqueous media.

P20

Exploiting the heavy atom effect: A Se-functionalized Zn(II) Schiff base as a TADF-based temperature sensor

Lukas Sommerauer, Lisa Eiber, Sergey M. Borisov

Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry, Stremayrgasse 9/II, 8010 Graz, Austria
lukas.sommerauer03@gmail.com

Temperature is a fundamental parameter in chemical, physical, and biological systems. While contact-based sensors are ubiquitous, they often fail in applications requiring high spatial resolution or measurements within sealed environments. [1] Luminescent temperature sensors address these limitations by enabling contactless measurements through physical barriers. Among the available read-out methods, decay lifetime is attractive, as it is an intrinsic molecular property. [1] Dyes exhibiting thermally activated delayed fluorescence (TADF) are particularly promising, [2] as reverse intersystem crossing (RISC) - the thermally driven repopulation of the singlet state - accelerates with temperature, shortening the observed lifetime. [3] Classical TADF emitters, however, display lifetimes of tens of microseconds to milliseconds [2] and show cross-sensitivity towards oxygen. Shortening lifetimes by reducing the singlet–triplet energy gap (ΔEST) has been explored, but ΔEST must be tuned carefully - small enough to allow RISC, yet large enough to retain thermal sensitivity. [4] Spin–orbit coupling (SOC) provides a quantum mechanical mechanism for the otherwise spin-forbidden singlet–triplet transitions and is greatly strengthened by heavy atoms. [5] Selenium has been shown to enhance SOC and promote RISC in chalcogen-bearing lumiphores. [6] We therefore designed a Zn(II) Schiff base bearing phenylseleno-substituted carbazole donors, in an attempt to strengthen SOC while the Zn(II) coordination simultaneously locks the donor–acceptor geometry into a twisted conformation, spatially separating the HOMO and LUMO and lowering ΔEST. [4] Embedded in a polystyrene matrix, the dye exhibits a temperature sensitivity of 2.5 %/K and a lifetime of 2.9 ms at room temperature - comparable to related Zn(II) Schiff bases without selenium, suggesting that phenylseleno substitution at the donor does not measurably accelerate RISC in this complex.

[1] Wang X., Wolfbeis O.S., Meier R.J., Chem. Soc. Rev. 42 (2013) 7834.

[2] Steinegger A., Borisov S.M., ACS Omega 5 (2020) 7729.

[3] Valeur B., Berberan-Santos M.N., Molecular Fluorescence: Principles and Applications, 2nd ed., Wiley-VCH, Weinheim, 2012, p. 60

[4] Im Y., Kim M., Cho Y.J., Seo J.-A., Yook K.S., Lee J.Y., Chem. Mater. 29 (2017) 1946.

[5] Dos Santos J.M., Hall D., Basumatary B., Bryden M., Chen D., Choudhary P., et al., Chem. Rev. 124 (2024) 13736, pp. 13743–13744

[6] Riebe S., Wölper C., Balszuweit J., Hayduk M., Gutierrez Suburu M.E., Strassert C.A., et al., ChemPhotoChem 4 (2020) 398.

PFAS accumulation and trophic transfer in invertebrates from a semi-urban area

Marianna Elisabetta Pace, Viktoria Müller, Jörg Feldmann

Analytical Chemistry, University of Graz, Universitätsplatz 3, 8010 Graz, Austria
mariannaelisabetta.pace@studenti.unipr.it

Per- and polyfluoroalkyl substances (PFAS) are persistent and toxic contaminants, with documented effects on organisms and human health.

Since only a limited number of studies have investigated PFAS accumulation in arthropods, this study aims to assess the presence of PFAS in 20 invertebrate samples collected at Lustbühel, a semi-urban area near Graz, to understand PFAS biomagnification across different trophic levels.

A fluorine mass balance approach was applied to assess PFAS through target analysis (TA), extractable organic fluorine (EOF), and total fluorine (TF) in invertebrate samples using LC-MS/MS and combustion ion chromatography (CIC).

Differences in fluorine content are expected among species according to their feeding strategies (herbivores, omnivores, and carnivores). Carnivores are expected to show the highest organofluorine content, reflecting biomagnification across trophic levels. Variations in PFAS accumulation among prey species may further highlight the role of arthropods as bioindicators and the relevance of this study for ecological risk assessment.

P22

Minimally Invasive Sampling for Elemental and Isotopic Analysis of Historical Metal Artefacts: The Medieval Rupertus Cross from Bischofshofen, Austria

Zoya Ayesha Raza[1]*, Stefan Wagner[1], Reinhard Gratz[2], Eva Hody[3], Elisabeth Krebs[4], Robert Linke[5], Elisabeth Sobieczky[6], Simone Trimmel[1], Thomas Prohaska[1], Johanna Irrgeher[1]

[1] *Montanuniversität Leoben, Department General, Analytical and Physical Chemistry, Franz-Josef-Strasse 18, 8700 Leoben, Austria*
**zoya.raza@unileoben.ac.at*

[2] *Dommuseum Salzburg, DomQuartier Salzburg, 5020 Salzburg, Austria*

[3] *Bundesdenkmalamt, Landeskonservatorat für Salzburg, 5020 Salzburg, Austria*

[4] *Metallrestaurierung Krebs, 1040 Wien, Austria*

[5] *Bundesdenkmalamt, Referat Naturwissenschaftliches Labor, 1030 Wien, Austria*

[6] *IMAREAL, Institut für Realienkunde, Universität Salzburg, 3500 Krems, Austria*

In this study, a minimally invasive sampling strategy for thin layers of historic copper on the early medieval clerical artifact, the Rupertus Cross (8th century), on loan from the parish church of Bischofshofen to the Dommuseum Salzburg, was developed, enabling subsequent elemental analysis and Cu and Pb isotope ratio measurements for authentication and provenance determination.

The cross (h=158,8 cm, w=96,6 cm, d=3.67 cm) is made from poplar wood. It is covered on its front and sides with fire-gilded copper sheets 0.34-0.5 mm thick. The origin of the metal used for the cross's revetments remains unknown. Because of the material's fragility, and in accordance with preservation requirements, a minimally invasive sampling strategy was developed. Different sample types from the metal cover (front and side sheets, nails, etc.) were sampled using metal-free, low-lint wipes (about 1.0 x 1.0 cm) soaked in diluted HNO_3 for < 1 min.

Elemental contents were recovered by leaching the wipes for 48 h in diluted HNO_3 and subsequent measurements by ICP-MS. To account for heterogeneity, replicate analyses were performed where possible. individual wipe leaching solutions yielded total Pb amounts of 0.01 – 10 µg (within sample type RSD ~20 – 130%) and total Cu amounts 10 – 600 µg (within sample type RSD ~2 – 95%), providing sufficient analyte for isotope ratio analysis by MC-ICP-MS but revealing substantial heterogeneity in elemental abundances and elemental ratios, which limits the utility of elemental fingerprints. Cu isotope ratios were inconclusive due to large variability (δ65Cu/63Cu up to 2 ‰).

Pb isotope ratios showed a spread in δ208Pb/206Pb of ~10 ‰ across sample types, but promising within-sample homogeneity (~0.1–1.5 ‰) with measurement uncertainty <0.5 ‰. Pb isotopic signatures aid association, authenticity, and provenance, while the minimally invasive technique yields high-quality, cost-effective results for archaeometallurgy and heritage science.

Figure: © Dommuseum Salzburg/J. Kral

This work was created within a research project of the Austrian Competence Centre for Feed and Food Quality, Safety and Innovation FFoQSI. The COMET competence centre FFoQSI is funded by the Austrian federal ministries BMIMI, BMWET and the Austrian provinces Lower Austria, Upper Austria and Vienna within the scope of COMET - Competence Centers for Excellent Technologies. The programme COMET is managed by the Austrian Research Promotion Agency FFG.

Santiago Souza Nava1, Zora Jandric1, Stephan Hann1,2

1 FFoQSI GmbH – Austrian Competence Centre for Feed and Food Quality, Safety & Innovation, Head Office: Technopark 1D, 3430 Tulln, Austria

2 BOKU University, Institute of Analytical Chemistry, Department of Natural Sciences and Sustainable Resources, Muthgasse 18, 1190 Vienna, Austria

P23

Arsenic Speciation Analysis in Mushrooms: Current Challenges and how to address them

Julia Truschner, Lorenz Steiner, Andrea Raab, Jan Borovicka, Walter Goessler, Bassam Lajin

University of Graz, Institute of Chemistry/Analytical Chemistry, Universitätsplatz 1, 8010 Graz, Austria
julia.truschner@uni-graz.at

Over the course of at least a billion years, the fungal kingdom has evolved into a highly diverse group comprising more than two million species [1]. Many fungal fruiting bodies are capable of accumulating arsenic in various chemical forms, typically dominated by a single prevailing arsenic species, most commonly methylarsonic acid (MA), dimethylarsinic acid (DMA), arsenobetaine (AB), or inorganic arsenic species such as As(III) and As(V) [2,3].

Based on their arsenic speciation profiles, mushrooms can be classified into “cationic” and “anionic” types. Most “cationic” type mushrooms are typically dominated by arsenobetaine (AB) and other cationic arsenic species. However, in certain species, including for example Sparassis and Boletus, AB is only present in small amounts or is entirely absent, while a broad distribution of other cationic arsenic species is observed. Nevertheless, in all “cationic” type mushrooms low concentrations of anionic arsenic species, including MA, DMA, dimethylarsinoylacetic acid (DMAA) and inorganic arsenic, are present. In contrast, “anionic” type mushrooms contain either exclusively anionic arsenic species or exhibit a predominantly anionic arsenic profile with negligible contributions from cationic arsenic species. Consequently, fungal species exhibit consistent arsenic speciation profiles. This intrinsic diversity implicates significant analytical challenges, particularly with respect to the chromatographic separation and comprehensive detection of all arsenic species within these complex biological matrices.

In this work, we investigate the analytical challenges associated with the chromatographic separation and determination of diverse arsenic species across different mushrooms. Using optimized analytical methodologies based on molecular- and element-selective detection in

combination with systematically varied chromatographic conditions, we evaluate strategies that enable the separation of newly identified arsenic compounds from already known arsenic species. Furthermore, we discuss the differences of cationic arsenic species versus anionic arsenic species profiles of several mushrooms with particular focus on their similarities and differences.

[1] Case NT, Gurr SJ, Fisher MC, Blehert DS, Boone C, Casadevall A, Chowdhary A, Cuomo CA, Currie CR, Denning DW, Ene IV, Fritz-Laylin LK, Gerstein AC, Gow NAR, Gusa A, Iliev ID, James TY, Jin H, Kahmann R, Klein BS, Kronstad JW, Ost KS, Peay KG, Shapiro RS, Sheppard DC, Shlezinger N, Stajich JE, Stukenbrock EH, Taylor JW, Wright GD, Cowen LE, Heitman J, Segre JA, Nature. 638 (2025) 49

[2] Steiner L, Raab A, Lajin B, Borovička J, Truschner J, Goessler W, Anal. Bioanal. Chem. (2025)

[3] Braeuer S, Goessler W, Anal. Chim. Acta. 1073 (2019) 1

P24

The Impact of Dyes on Textile Recycling

Anna Rechberger, Jeannie Egan, Felice Quartinello, Birgit Herbinger, Christian Schimper

Josef Ressel Centre ReSTex, FH Wiener Neustadt, Campus Tulln, Konrad-Lorenz-Straße 10, 3430 Tulln an der Donau, Austria
206412@fhwn.ac.at

Less than 20% of the annually approx. 90 million tonnes of textile waste are being recycled [1], [2]. One major challenge during textile recycling is coloured fabric. Until now, research focused on developing separation techniques for recycling, rather than on how colours affect these processes. One difficulty of recycling dyed fabrics arises from the diversity of dye classes and their binding mechanisms to the fibres.

This work focuses on how a biochemical separation route for cotton/polyester textiles is affected by two dye classes: direct dyes and reactive dyes. Direct dyes adhere to cellulose via secondary bonding mechanisms (Van-der-Waals, hydrogen bonds, dipole bonds) and have large, planar structures [3]. The second dye class, reactive dyes, form covalent bonds with cellulose [4].

The biochemical reaction involves enzymatic hydrolysis of cotton into glucose but leaves the PET fibres untouched [5]. The reaction will be gravimetrically quantified by weight loss of the fabric. Furthermore, since the selected dyes will only colour the cotton part, the remaining fabric will appear lighter and thus it can be analysed by chroma metric methods. This contribution will report how selected representatives of these two dye classes influence the hydrolysis behaviour of cellulases during biochemical separation of cotton-polyester blended textiles.

[1] T. Brydges et al., “Textile Recycling-Positive Change or Toxic Truth?,” Procedia CIRP, vol. 135, pp. 374–378, 2025, doi: 10.1016/j.procir.2024.12.053.

[2] “Unsustainable fashion and textiles in focus for International Day of Zero Waste 2025.” Accessed: Apr. 13, 2026. [Online]. Available: https://www.unep.org/news-and-stories/press-release/unsustainable-fashion-and-textiles-focus-international-day-zero

[3] R. M. Christie, Colour chemistry. Royal Society of Chemistry, 2015.

[4] M. Clark, Handbook of textile and industrial dyeing. Volume 1: Principles, processes and types of dyes. Woodhead Pub., 2011.

[5] J. Egan, S. Wang, J. Shen, O. Baars, G. Moxley, and S. Salmon, “Enzymatic textile fiber separation for sustainable waste processing,” Resources, Environment and Sustainability, vol. 13, Sep. 2023, doi: 10.1016/j.resenv.2023.100118.

Recycled Plastics and Food Safety: Insights from Analytical Characterization

Elise Hecht[1], Florian Wagner-Hackl[1], Erich Leitner[1], Barbara Siegmund[1], Christian Kirchnawy[2], Natascha Matausch[2], Andrea Hochegger[1]

[1] *Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, 8010 Graz, Austria*

hecht@tugraz.at

[2] *Austrian Research and Testing Institute, Franz-Grill-Straße 5, 1030 Wien, Austria*

The increasing incorporation of post-consumer recycled (PCR) plastics into packaging is a key element of the European Union's circular economy strategy. According to Regulation (EU) 2025/40, a minimum recycling content of 10% is mandatory by 2030 for non-PET packaging in contact-sensitive applications such as food packaging [1].

In contrast to PET, the current availability and quality of recycled polyolefins suitable for food-contact is insufficient to meet these targets. This problem is addressed in Regulation 2022/1616, which establishes a regulatory framework for recycled plastic materials intended for food contact. Under this framework, products produced by new recycling technologies may be placed on the market prior to a final authorization by the European Food Safety Authority (EFSA), under the condition that a comprehensive safety documentation is provided. This includes contaminant characterization in input and output materials, assessment of decontamination efficiencies and initial batch-to-batch monitoring of contamination levels. Moreover, compliance of the materials with Regulations (EC) 1935/2004 and (EU) 10/2011 has to be ensured [2]. Due to the lack of harmonized analytical methods, the generation of this data remains challenging.

This work addresses these regulatory requirements by systematically characterizing PCR polyolefins, including HDPE, LDPE and PP. Solid-phase microextraction, solvent-based extraction and migration experiments are coupled with advanced chromatographic techniques, including GC-FID, GC-MS, GC-ECD, GC×GC-ToFMS, as well as LC-MS/MS.

This approach enables both targeted quantification and non-targeted screening of a broad range of substance classes. In parallel, a genotoxicity screening using the Ames MPF test is performed, with particular emphasis on identifying correlations between positive genotoxic responses and specific substance classes detected in the materials. Additionally, human sensory evaluation of the samples is conducted to investigate the formation of off-odours throughout the recycling process.

The generated data support the development of a centralized contaminant database for post-consumer recycled plastics. This forms the basis for an automated, risk-based evaluation concept that aims to support regulatory decision-making and the safe implementation of novel recycling technologies.

[1] https://eur-lex.europa.eu/eli/reg/2025/40/oj/eng

[2] https://eur-lex.europa.eu/eli/reg/2022/1616/oj/eng

P26

Screening of cellulase formulations and pretreatments for enzymatic separation of polyester/cotton blended textiles

Martina Demuth, Felice Quartinello, Melina Sophie Zirbs, Agnes Grünfelder, Judith Rudolf-Scholik, Birgit Herbinger, Christian B. Schimper

Fachhochschule Wiener Neustadt, Biotech Campus Tulln, Josef Ressel Centre ReSTex, Konrad Lorenzstrasse 10, 3430 Tulln, Austria
martina.demuth@students.boku.ac.at

Textile recycling and circular manufacturing are urgent priorities since an estimated amount of 12,6 million tonnes of textile waste are generated worldwide each year. Furthermore, the textile industry accounts for 10% of global carbon emissions, driven mainly by the production and incineration of petrochemical-derived fibres, making it the fifth largest greenhouse gas emitter [1, 2]. Most of the produced materials are mixed textiles, especially polyester/cotton blends, which are hardly recyclable [3, 4]. Biochemical methods using cellulases are a promising route to separate and valorise these blends [5].

Building on previous research from the Josef Ressel Centre Recovery Strategies for Textiles (ReSTex) project [6], this work develops and optimises robust and scalable strategies for biochemical recycling of polyester/cotton textile blends. The targeted outcome is the recovery of high-purity PET suitable for fibre spinning and reintegration into textile production, alongside valorisation of the cotton fraction via hydrolysis to either cellulose fibres of sufficient length for regenerated fibre production or glucose as a fermentable substrate for bioethanol.

In this work four commercial cellulase formulations are evaluated in combination with alkali pretreatments using NaOH of varying concentrations upon suitability for this process. Additionally, the lengths of fibres released during hydrolysis are measured and compared. Analytical methods include photometric assays, gravimetric measurements, FT-IR, SEM, HPLC, and optical microscopy.

Outcomes show that cotton removal depends on both enzyme formulation and NaOH concentration. Pretreatments increase degradation with increasing NaOH concentration (from

15% up to 85% cotton mass reduction). It was found that cellulase formulations enriched with endoglucanases are less responsive to alkali swelling pretreatments. Overall, the effectiveness of the enzyme formulations depends on their composition and intended use case.

[1] Directive (EU) 2025/1892 of the European Parliament and of the Council of 10 September 2025 Amending Directive 2008/98/EC on Waste, EP, CONSIL (2025).

[2] Juanga-Labayen, J. P., Labayen, I. V., & Yuan, Q. (2022). A Review on Textile Recycling Practices and Challenges. Textiles, 2(1), 174–188.

[3] Mihalyi, S., Sykacek, E., Campano, C., Hernández-Herreros, N., Rodríguez, A., Mautner, A., Prieto, M. A., Quartinello, F., & Guebitz, G. M. (2024). Bio-upcycling of viscose/polyamide textile blends waste to biopolymers and fibers. Resources, Conservation and Recycling, 208, 107712.

[4] Gritsch, S. M., Mihalyi, S., Bartl, A., Ipsmiller, W., Jenull-Halver, U., Putz, R. F., Quartinello, F., & Guebitz, G. M. (2023). Closing the cycle: Enzymatic recovery of high purity glucose and polyester from textile blends. Resources, Conservation and Recycling, 188, 106701.

[5] Quartinello, F., Vecchiato, S., Weinberger, S., Kremenser, K., Skopek, L., Pellis, A., & Guebitz, G. M. (2018). Highly Selective Enzymatic Recovery of Building Blocks from Wool-Cotton-Polyester Textile Waste Blends. Polymers, 10(10), 1107.

[6] https://www.fhwn.ac.at/en/research/josef-ressel-centre-restex

The authors declare that financial support was received for the research of this work. The financial support by the Austrian Federal Ministry of Economy, Energy and Tourism, the National Foundation for Research, Technology and Development and the Christian Doppler Research Association is gratefully acknowledged.

P27

Towards mycotoxin detection in an industrial setting using near-infrared spectroscopy

Aikaterini Kouseri, Rudolf Krska, Stephan Freitag

BOKU University, Department of Agrobiotechnology, IFA-Tulln, Institute of Bioanalytics and Agro Metabolomics, Heiligenstädter Straße 81-87/1/9, 1190 Vienna, Austria
aikaterini.kouseri@boku.ac.at

Mycotoxins are toxic secondary metabolites produced by fungi that frequently contaminate cereal crops like maize, posing significant risks to food safety and public health. Their presence is therefore strictly regulated and requires extensive monitoring. A range of analytical techniques, including chromatographic methods such as liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS), as well as immunoassays, are widely used for mycotoxin analysis [1]. However, they are associated with high costs, labor-intensive workflows, and long analysis times [1], highlighting the need for rapid, more sustainable alternatives.

Infrared spectroscopy (IRS) offers a promising solution for rapid mycotoxin screening, since it enables fast, non-destructive and reagent-free analysis [2]. Nevertheless, IRS does not detect mycotoxins directly, as they are typically present at trace levels and their spectral signatures are masked by dominant matrix components [1]. Instead, it enables indirect detection by capturing chemical and physical changes in the sample matrix caused by fungal infection [1]. Consequently, contamination must be predicted by correlating spectral features with mycotoxin concentrations determined by reference methods, using chemometric models. Despite this potential, the reported model performance metrics are often insufficient for routine and industrial applicability [2].

In the present work, we aim to investigate the potential of near-IRS combined with chemometrics for the screening and quantification of regulated mycotoxins in maize. Emphasis is placed on evaluating the influence of LC-MS/MS reference method uncertainty on model performance, as well as on developing robust calibration models using real-world

samples collected in an industrial setting. Both classification and quantitative prediction approaches will be explored, supported by internal and external validation strategies. The expected outcome of this work is a better understanding of IR-based mycotoxin analysis and the factors affecting model robustness, as well as the development of models with practical industrial applicability. Overall, the project supports the development of faster, cost-effective and sustainable tools for routine mycotoxin analysis.

[1] Freitag S., Sulyok M., Logan N., Elliott C.T., Krska R., Compr. Rev. Food Sci. Food Saf. 21 (2022) 5199–5224.

[2] Freitag S., Mycotoxins: Screening Confirmatory Anal. (2025).

P28

Assessment of PFAS in Atmospheric Deposition Using Low-Volume Filter Sampling

Eleftheria Motso, Victoria Müller, Jörg Feldmann

Analytical Chemistry, University of Graz, Universitätsplatz 3, 8010 Graz, Austria
eleftheriamotso@gmail.com

Per- and Polyfluoroakyl substances (PFAS) are of increasing environmental concern due to their persistence, long range transport potential, and adverse effects on ecosystems and human health. This study investigates the occurrence of PFAS in atmospheric dry deposition collected over 12 months at seven monitoring stations in Germany using Low-Volume filter sampling.

Particulate matter (PM10) samples were analyzed using complementary analytical strategies: targeted analysis (TA) by LC-MS/MS and extractable organic fluorine (EOF) determination by Combustion Ion Chromatography (CIC). This combined approach enables quantification of known PFAS compounds while also capturing unidentified organofluorine substances.

Results show temporal variation in PFAS concentrations and reveal a substantial fraction of unidentified fluorinated compounds through EOF analysis, highlighting the complexity of atmospheric PFAS contamination. The findings emphasize the importance of integrated analytical approaches for comprehensive characterization of PFAS in atmospheric particulate matter.

P29

Multi-Resonance Emitters as Self-Referenced Optical Temperature Sensors

Lisa Eiber, Andreas Russegger, Sergey M. Borisov

Graz, University of Technology, Institute for Analytical Chemistry and Food Chemistry, Stremayrgasse 9/III, 8010 Graz, Austria
eiber@tugraz.az

Multi-Resonance Emitters (MREs) have gained significant attention as new emitters for OLED applications.[1] Those emitters have outstanding properties like strong absorption, high quantum yields approaching 100% and sharp emission bands of both, (thermally activated delayed) fluorescence (TADF) and phosphorescence.[2] These properties also make MREs promising for intensity-based, self-referenced ratiometric temperature measurements. The major drawback, however, is the large share of prompt fluorescence, which accounts for less usable signal and loss of sensitivity.

In this work we optimized MREs for ratiometric temperature sensing at ambient and physiological conditions. This was achieved by altering the donor moieties to increase the singlet-triplet energy gap and shift the phosphorescence to TADF transition from low temperatures to the more relevant range. Further, heavy atoms such as selenium and gold were implemented into the structure to enhance the intersystem crossing and thus reduce the share of prompt fluorescence as well as the luminescence lifetimes.

The resulting dyes show excellent separation of TADF and phosphorescence emission bands, high quantum yields and very little prompt fluorescence. Some dyes prove to be exceptionally sensitive to temperature changes in the physiological range, qualifying them for applications in live cells. Additionally, emission bands typically fall into the green (TADF) and yellow-orange (phosphorescence) range which enables readout through simple RGB-cameras.

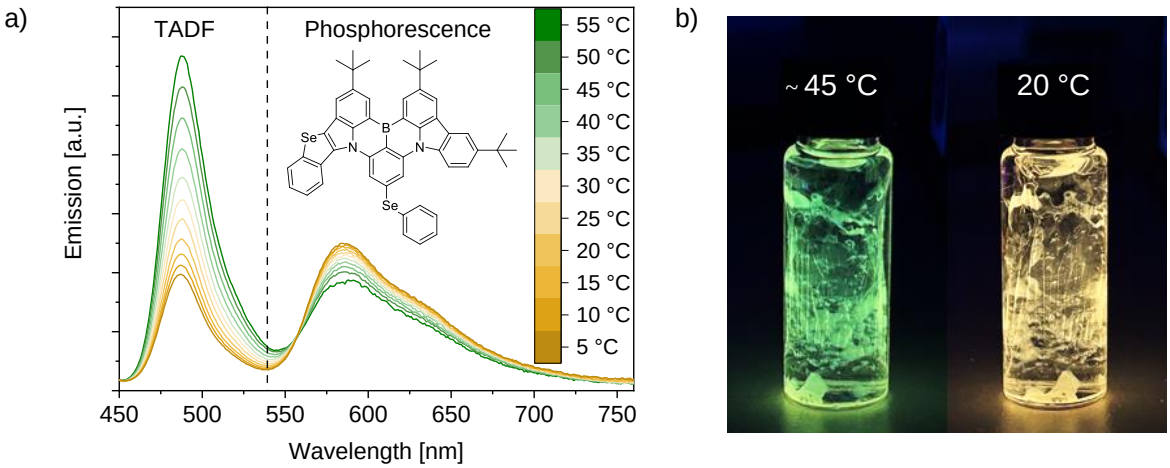


Figure 1. a) TADF- and phosphorescence emission of a Se-MRE at different temperatures, measured in a polystyrene matrix and anoxic conditions. b) Photographic image of the emission of an Au-MRE at different temperatures in a polystyrene matrix at air.

[1] X. Wu, S. Ni, C.-H. Wang, W. Zhu, P.-T. Chou, *Chem. Rev.*, 125, 14 (2025), 6685–6752.

[2] S. Cai, et al., *Angew. Chem. Int. Ed.*, 61 (2022).

P30

Combining NIR and Raman spectroscopy by machine learning tools for the characterisation of cotton-polyester blended textiles

Leon Otto Gasteiger[1], David Lilek[1,2*], Jean Marie Egan[1,3], Birgit Herbinger[1], Christian B. Schimper[1]**

[1]Josef Ressel Centre ReSTex, Fachhochschule Wiener Neustadt, Biotech Campus Tulln, Konrad-Lorenz-Straße 10, 3430 Tulln, Austria
[*]david.lilek@fhwn.ac.at
[**]christian.schimper@fhwn.ac.at

[2] Department of Chemistry and Physics of Materials, Paris Lodron University Salzburg, Jakob-Haringer Straße 2a, 5020 Salzburg, Austria

[3] BOKU University, Department of Chemistry, Institute of Chemistry of Renewable Resources, Tulln, Austria

The use of spectroscopy in the textile industry promotes rapid and effective textile sorting processes and enables automation. Most commonly MIR and NIR detection systems are used. In combination with machine learning, optical spectroscopy can be applied in both process control and sorting in textile waste lines. Previously, we described the detection limits of different NIR sensor systems and the use of different data processing tools for their interpretation [1,2].

This work focuses on the characterisation of the same set of cotton-polyester blended textiles, as described earlier [1,2] with a Raman microscope using 532nm and 785nm lasers. To mitigate fluorescence effects originating from the samples, additionally a fibre-coupled system with a 1064nm laser was employed. The Raman spectra measured with this laser exhibited a flatter baseline and sharper peaks in comparison to spectra measured on the same samples with a 785nm laser or a 532nm laser. Data analysis by PCA and t-SNE allowed a clear differentiation of the spectra according to cotton content. Since NIR spectroscopy shows an overarching water peak in wet samples and is negatively influenced by dark colours, we coupled the 1064nm Raman spectra with NIR spectra to evaluate whether Raman spectroscopy can overcome limitations of NIR spectroscopy [3]. Additionally, we analysed the

trade-off between measurement speed and spectrum quality to determine an optimal balance between these two. This is particularly important for real-world industrial applications, where optimized speed and efficiency have significant economic implications.

[1] Yayla S. S., Lilek D. M., Herbinger B., Schimper C. B., ASAC Junganalytiker:innen Forum (2024).

[2] Lilek D., Yayla S. S., Stipanovic H., Fink T.-K., Egan J., Herbinger B., Tischberger-Aldrian A., Schimper C. B., Appl. Sci. 16 (2026) 3242.

[3] ScienceDirect Topics, Raman Spectroscopy - an overview (2026).